Full wwPDB EM Validation Report ⓘ

Sep 19, 2026 – 11:38 AM JST

PDB ID	:	9IOT / pdb_00009iot
EMDB ID	:	EMD-60747
Title	:	Cryo-EM structure of Escherichia coli hibernating ribosome with RNase I mutant
Authors	:	Tanzawa, T.; Minami, A.; Yoshida, H.; Kato, T.; Ogawa, T.
Deposited on	:	2024-07-09
Resolution	:	2.70 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:

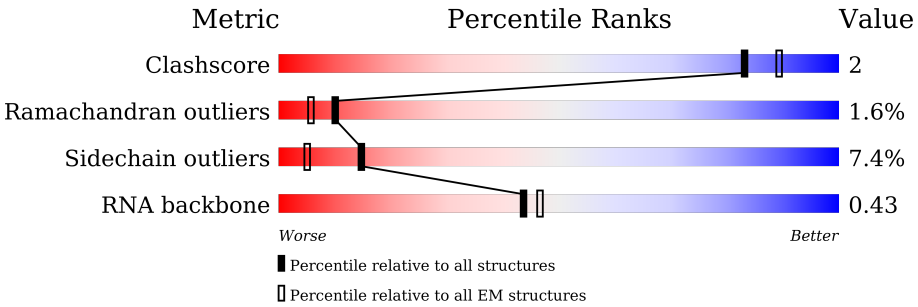
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	: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

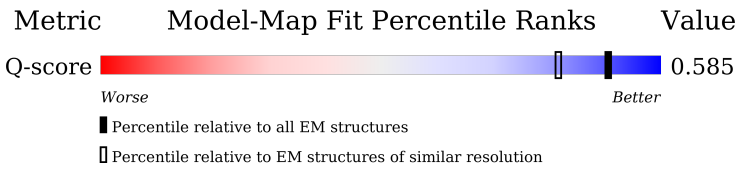
1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	0	63	17% 76% 19%
2	1	59	5% 95%
3	3	57	5% 79% 11% 7%

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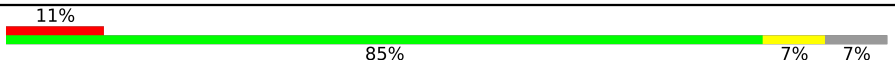
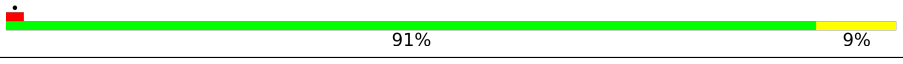
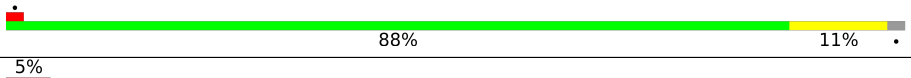
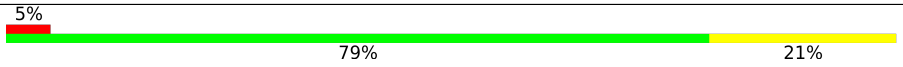
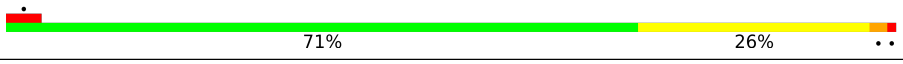
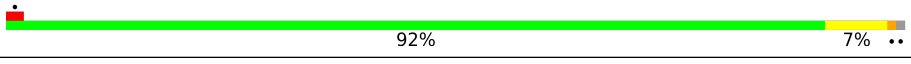
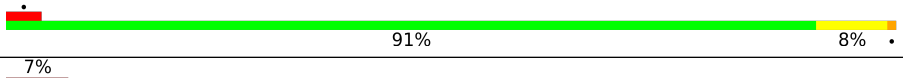
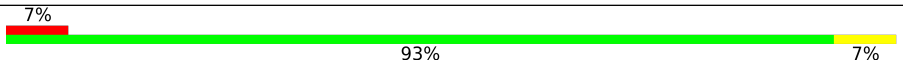
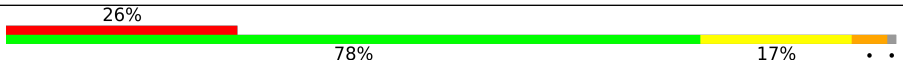
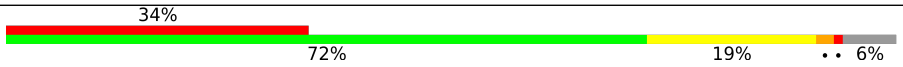
Mol	Chain	Length	Quality of chain
4	4	55	
5	5	46	
6	6	65	
7	7	38	
8	B	120	
9	D	273	
10	E	209	
11	F	201	
12	G	179	
13	H	177	
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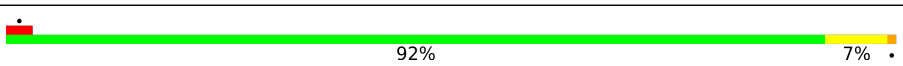
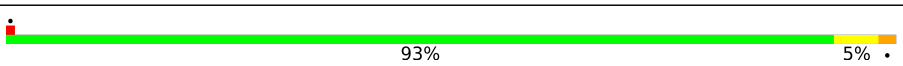
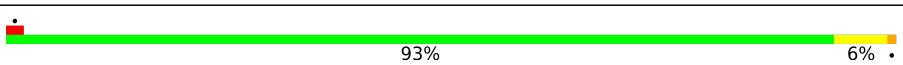
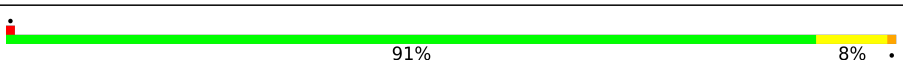
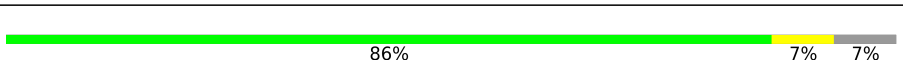
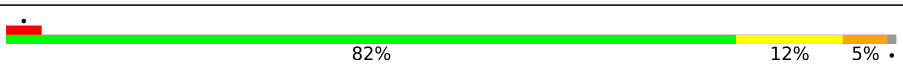
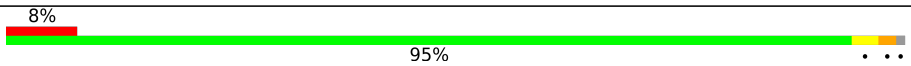
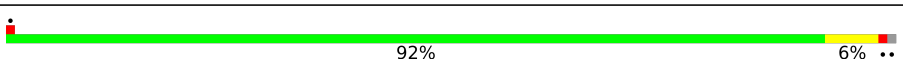
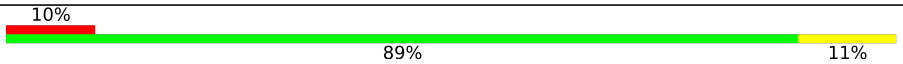
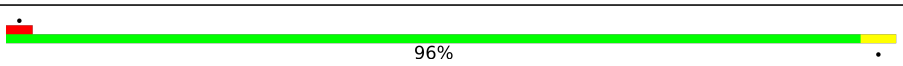
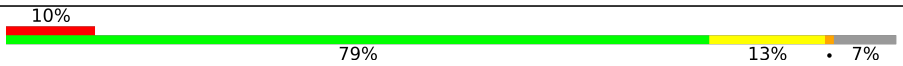
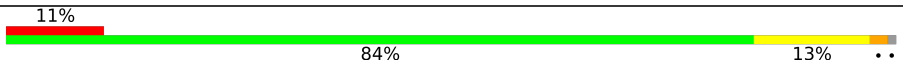
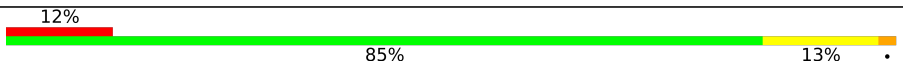
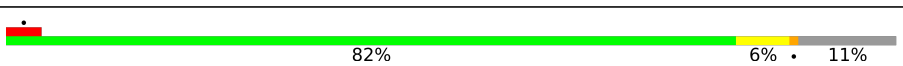
15	L	142	
16	M	123	
17	N	144	
18	O	136	
19	P	127	
20	Q	117	
21	R	115	
22	S	118	
23	T	103	
24	U	110	
25	V	100	
26	W	103	
27	X	94	
28	Y	85	

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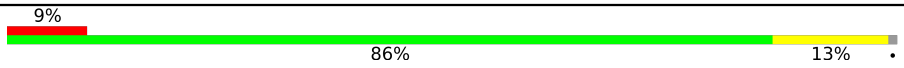
Mol	Chain	Length	Quality of chain
29	Z	78	
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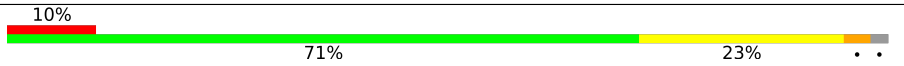
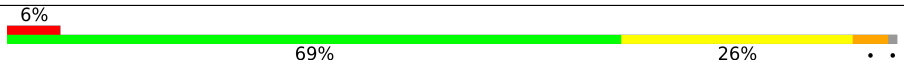
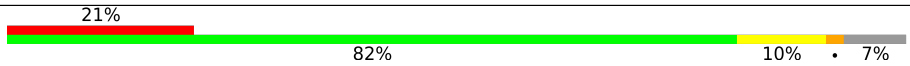
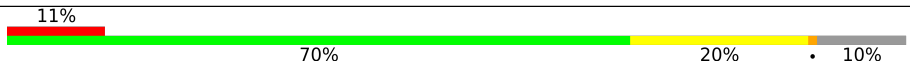
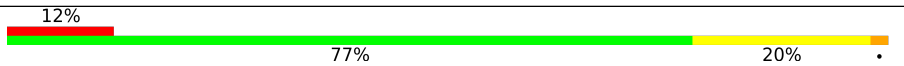
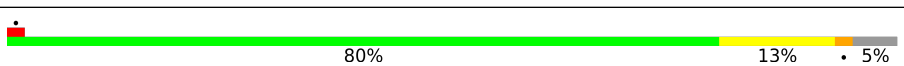
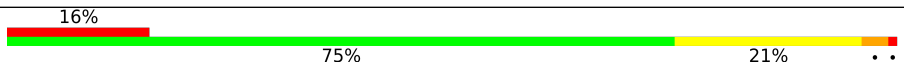
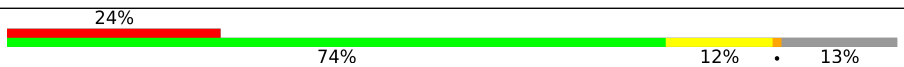
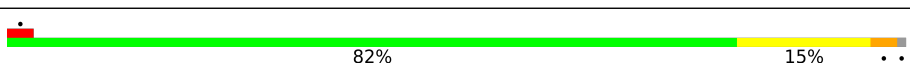
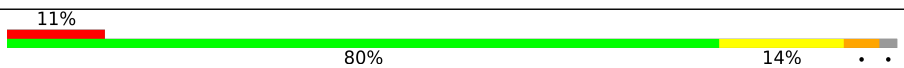
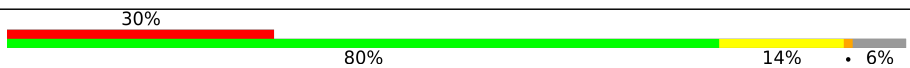
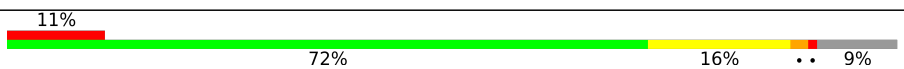
31	A	2904	
32	a	1542	
33	b	241	
34	c	233	
35	d	206	
36	e	167	
37	f	102	
38	g	179	
39	h	130	
40	i	130	
41	j	103	
42	k	129	
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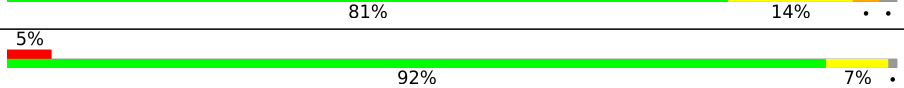
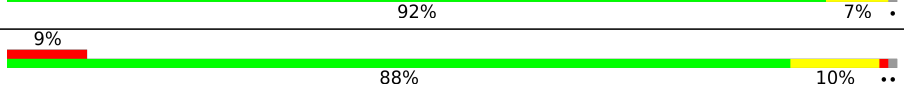
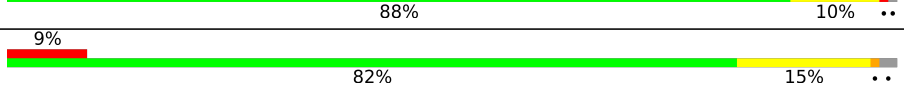
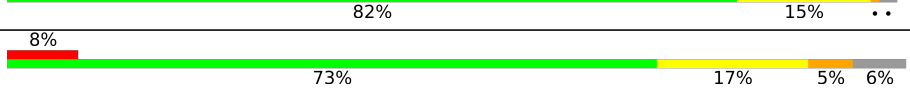
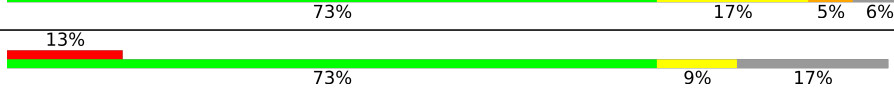
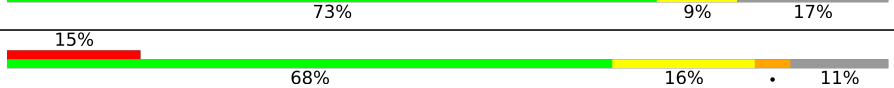
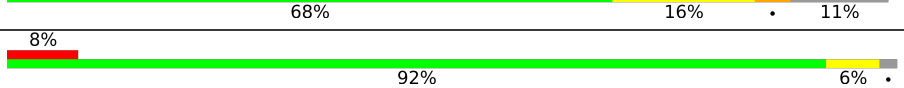
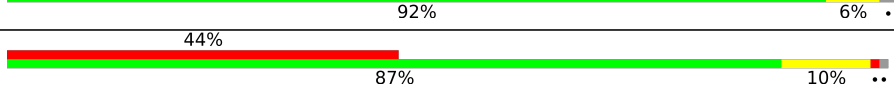
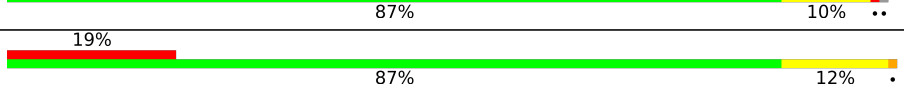
45	n	101	
46	o	89	
47	p	82	
48	q	84	
49	r	75	
50	s	92	
51	t	87	
52	u	71	
53	v	95	

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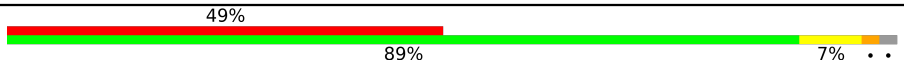
Mol	Chain	Length	Quality of chain
54	y	55	
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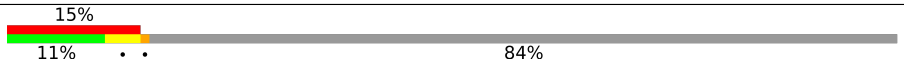
56	8	557	

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 143360 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 protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	61	495	305	97	92	1	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	58	449	281	87	79	2	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	55	434	263	92	78	1	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	4	51	410	263	75	72	0	0

- Molecule 5 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	46	377	228	90	57	2	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	64	504	323	105	74	2	0	0

- Molecule 7 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	120	Total	C	N	O	P	0	0
			2572	1145	470	837	120		

- Molecule 9 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	271	Total	C	N	O	S	0	0
			2075	1286	423	359	7		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	209	Total	C	N	O	S	0	0
			1556	975	288	290	3		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	201	Total	C	N	O	S	0	0
			1536	966	280	285	5		

- Molecule 12 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	177	Total	C	N	O	S	0	0
			1385	888	239	252	6		

- Molecule 13 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	166	Total	C	N	O	S	0	0
			1226	774	224	226	2		

- Molecule 14 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 15 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	142	Total	C	N	O	S	0	0
			1119	710	208	197	4		

- Molecule 16 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	123	Total	C	N	O	S	0	0
			939	590	179	164	6		

- Molecule 17 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	144	Total	C	N	O	S	0	0
			1045	650	207	186	2		

- Molecule 18 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	136	Total	C	N	O	S	0	0
			1070	684	205	175	6		

- Molecule 19 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	118	Total	C	N	O	S	0	0
			939	585	194	155	5		

- Molecule 20 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Q	116	Total	C	N	O	0	0
			873	538	175	160		

- Molecule 21 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	114	Total	C	N	O	S	0	0
			913	573	178	161	1		

- Molecule 22 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	S	117	Total	C	N	O	0	0
			944	603	192	149		

- Molecule 23 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	103	Total	C	N	O	S	0	0
			812	514	153	143	2		

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	110	Total	C	N	O	S	0	0
			850	529	163	155	3		

- Molecule 25 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	102	Total	C	N	O	0	0
			769	486	144	139		

- Molecule 27 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	94	Total	C	N	O	S	0	0
			746	474	136	134	2		

- Molecule 28 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 29 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 30 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2	67	Total	C	N	O	S	0	0
			504	313	95	90	6		

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A	2841	Total	C	N	O	P	0	0
			61011	27223	11229	19718	2841		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1534	Total	C	N	O	P	0	0
			32925	14692	6038	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	224	Total	C	N	O	S	0	0
			1527	972	283	267	5		

- Molecule 34 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	210	Total	C	N	O	S	0	0
			1636	1037	309	286	4		

- Molecule 35 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	205	Total	C	N	O	S	0	0
			1619	1012	307	296	4		

- Molecule 36 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	158	Total	C	N	O	S	0	0
			1129	702	216	205	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	102	Total	C	N	O	S	0	0
			770	491	138	137	4		

- Molecule 38 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	155	Total	C	N	O	S	1	0
			1183	742	233	204	4		

- Molecule 39 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	129	Total	C	N	O	S	0	0
			966	612	169	179	6		

- Molecule 40 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	127	Total	C	N	O	S	0	0
			955	594	194	166	1		

- Molecule 41 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	j	97	Total	C	N	O	0	0
			668	423	130	115		

- Molecule 42 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	117	Total	C	N	O	S	0	0
			853	527	167	156	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 43 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	122	Total	C	N	O	S	0	0
			933	576	189	163	5		

- Molecule 44 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	116	Total	C	N	O	S	0	0
			845	527	171	145	2		

- Molecule 45 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	100	Total	C	N	O	S	0	0
			794	493	163	135	3		

- Molecule 46 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	88	Total	C	N	O	S	0	0
			696	430	140	125	1		

- Molecule 47 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	80	Total	C	N	O	S	0	0
			617	388	124	104	1		

- Molecule 48 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	79	Total	C	N	O	S	0	0
			630	400	116	111	3		

- Molecule 49 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	r	62	Total	C	N	O	0	0
			481	304	90	87		

- Molecule 50 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	82	Total	C	N	O	S	0	0
			639	410	123	105	1		

- Molecule 51 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	85	Total	C	N	O	S	0	0
			652	403	135	111	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	70	Total	C	N	O	S	0	0
			521	329	111	80	1		

- Molecule 53 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	95	Total	C	N	O	S	0	0
			722	458	129	134	1		

- Molecule 54 is a protein called Ribosome modulation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	54	Total	C	N	O	S	0	0
			440	269	91	76	4		

- Molecule 55 is a protein called Ribonuclease I.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	245	Total	C	N	O	S	6	0
			1852	1169	326	345	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	55	PHE	HIS	engineered mutation	UNP P21338
z	133	PHE	HIS	engineered mutation	UNP P21338

- Molecule 56 is a protein called Small ribosomal subunit protein bS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	90	Total	C	N	O	S	0	0
			696	437	121	135	3		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Mg	0
			1	1	
57	B	6	Total	Mg	0
			6	6	
57	D	2	Total	Mg	0
			2	2	
57	E	1	Total	Mg	0
			1	1	
57	O	1	Total	Mg	0
			1	1	
57	A	337	Total	Mg	0
			337	337	
57	a	127	Total	Mg	0
			127	127	

- Molecule 58 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
58	z	1	Total	Ca	0
			1	1	

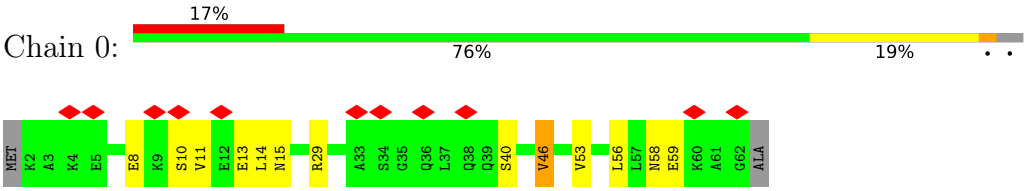
- Molecule 59 is water.

Mol	Chain	Residues	Atoms	AltConf
59	N	1	Total O 1 1	0
59	Y	1	Total O 1 1	0
59	A	25	Total O 25 25	0
59	a	5	Total O 5 5	0

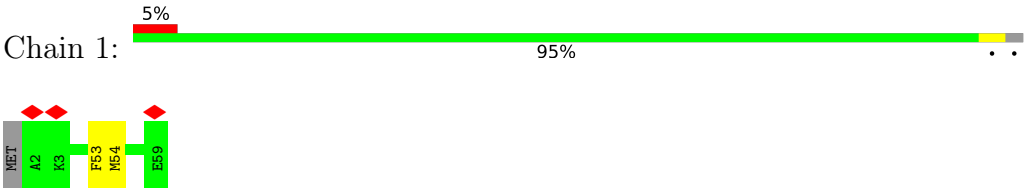
3 Residue-property plots (i)

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

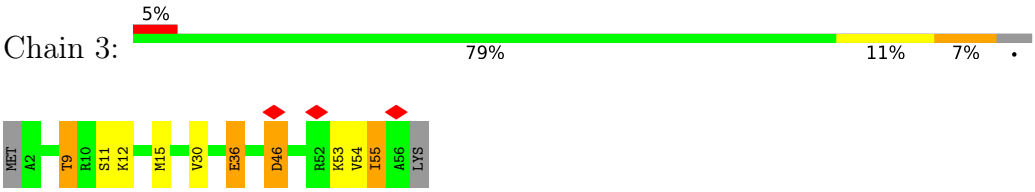
• Molecule 1: Large ribosomal subunit protein uL29



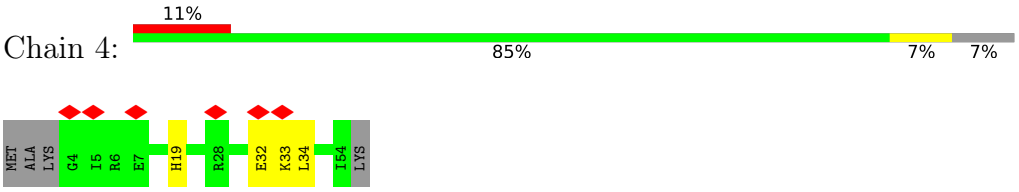
• Molecule 2: Large ribosomal subunit protein uL30



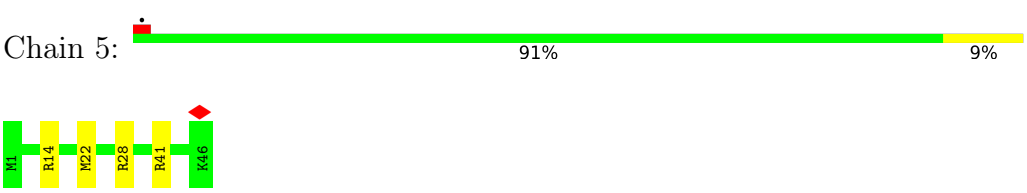
• Molecule 3: Large ribosomal subunit protein bL32



• Molecule 4: Large ribosomal subunit protein bL33



• Molecule 5: 50S ribosomal protein L34



• Molecule 6: Large ribosomal subunit protein bL35

Chain 6:

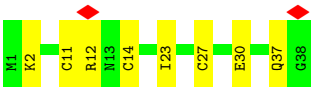




• Molecule 7: 50S ribosomal protein L36

Chain 7:

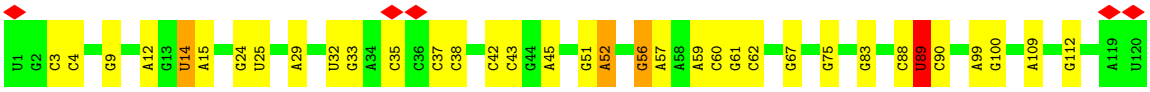




• Molecule 8: 5S rRNA

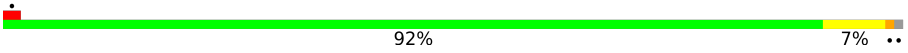
Chain B:





• Molecule 9: Large ribosomal subunit protein uL2

Chain D:

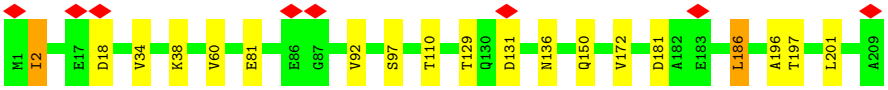




• Molecule 10: 50S ribosomal protein L3

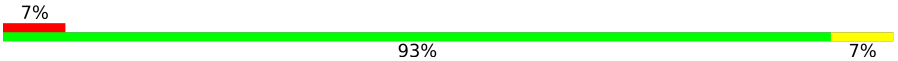
Chain E:

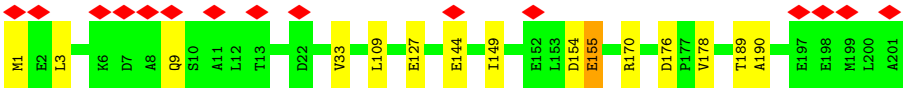




• Molecule 11: 50S ribosomal protein L4

Chain F:

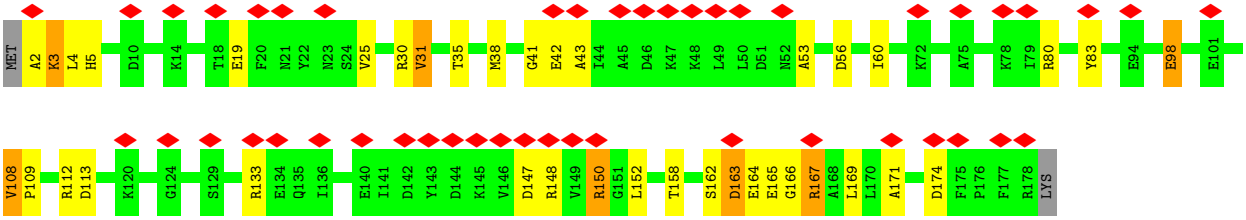




• Molecule 12: Large ribosomal subunit protein uL5

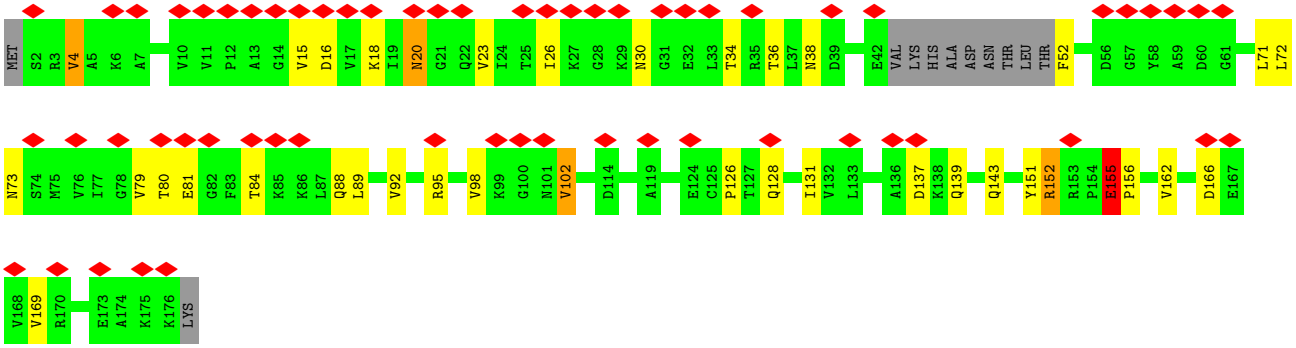
Chain G:



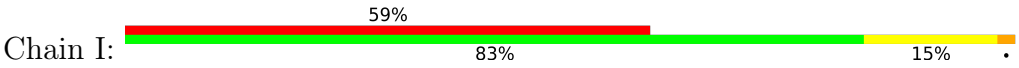


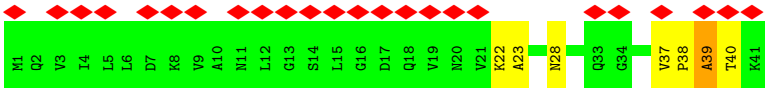
• Molecule 13: Large ribosomal subunit protein uL6





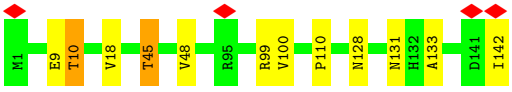
• Molecule 14: Large ribosomal subunit protein bL9





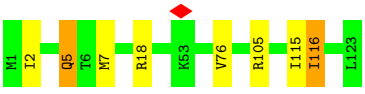
• Molecule 15: 50S ribosomal protein L13



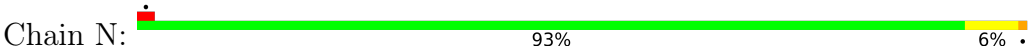


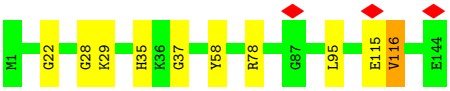
• Molecule 16: 50S ribosomal protein L14





• Molecule 17: Large ribosomal subunit protein uL15

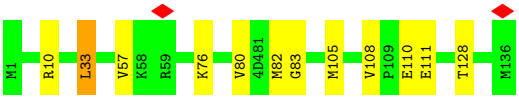




• Molecule 18: Large ribosomal subunit protein uL16

Chain O:

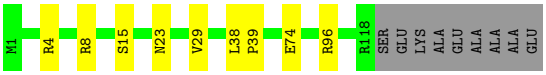




• Molecule 19: Large ribosomal subunit protein bL17

Chain P:

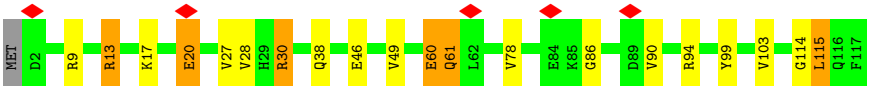




• Molecule 20: Large ribosomal subunit protein uL18

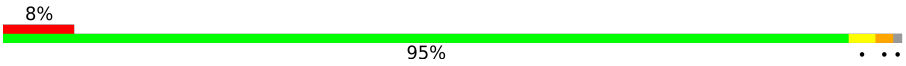
Chain Q:

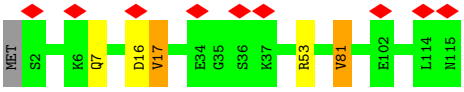




• Molecule 21: Large ribosomal subunit protein bL19

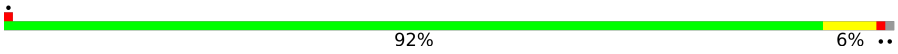
Chain R:

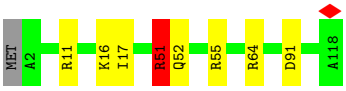




• Molecule 22: Large ribosomal subunit protein bL20

Chain S:

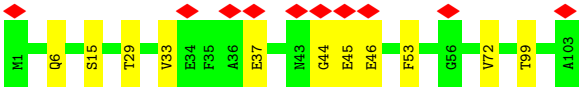




• Molecule 23: 50S ribosomal protein L21

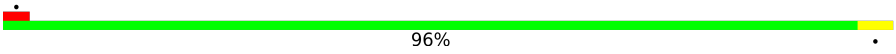
Chain T:

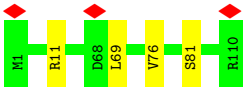




• Molecule 24: 50S ribosomal protein L22

Chain U:

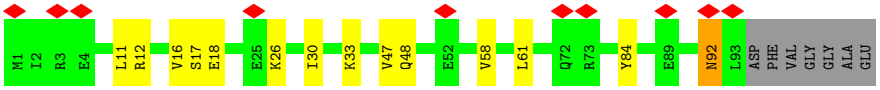




• Molecule 25: Large ribosomal subunit protein uL23

Chain V:

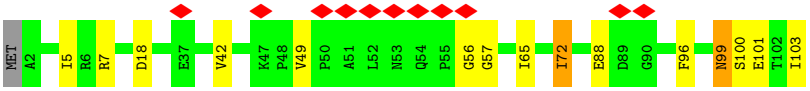




• Molecule 26: Large ribosomal subunit protein uL24

Chain W:

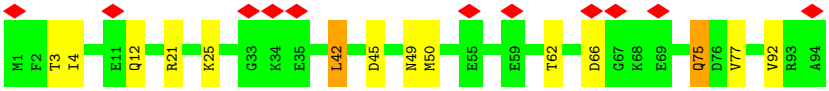




• Molecule 27: 50S ribosomal protein L25

Chain X:

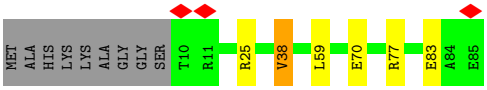




• Molecule 28: Large ribosomal subunit protein bL27

Chain Y:

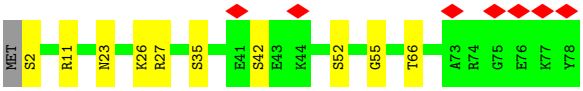




• Molecule 29: Large ribosomal subunit protein bL28

Chain Z:

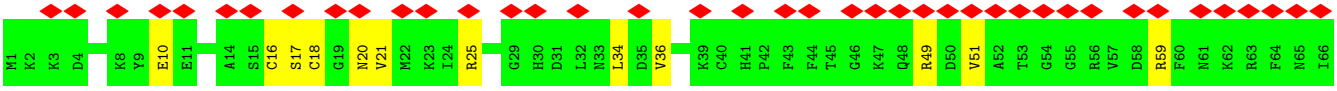




• Molecule 30: Large ribosomal subunit protein bL31

Chain 2:



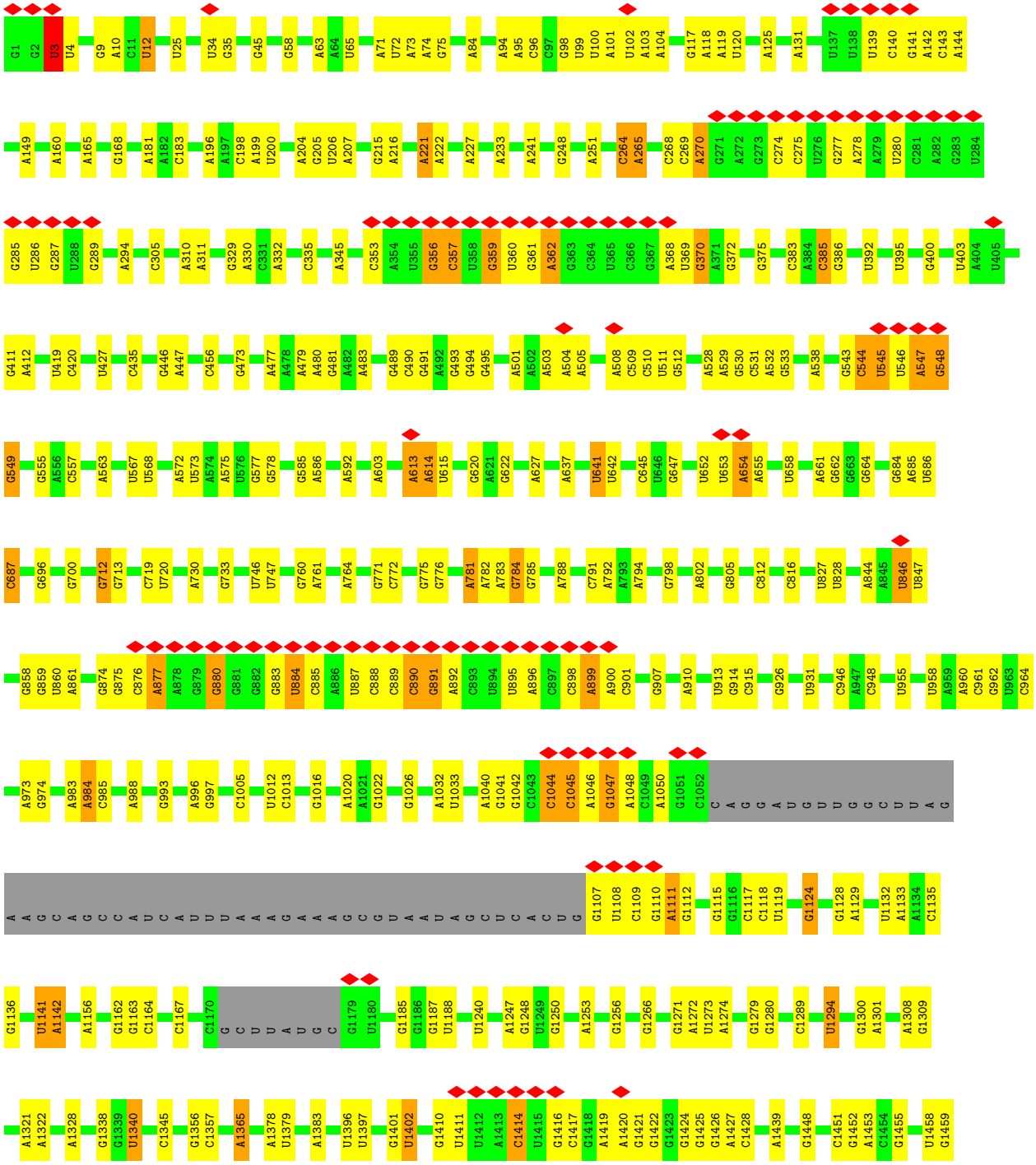


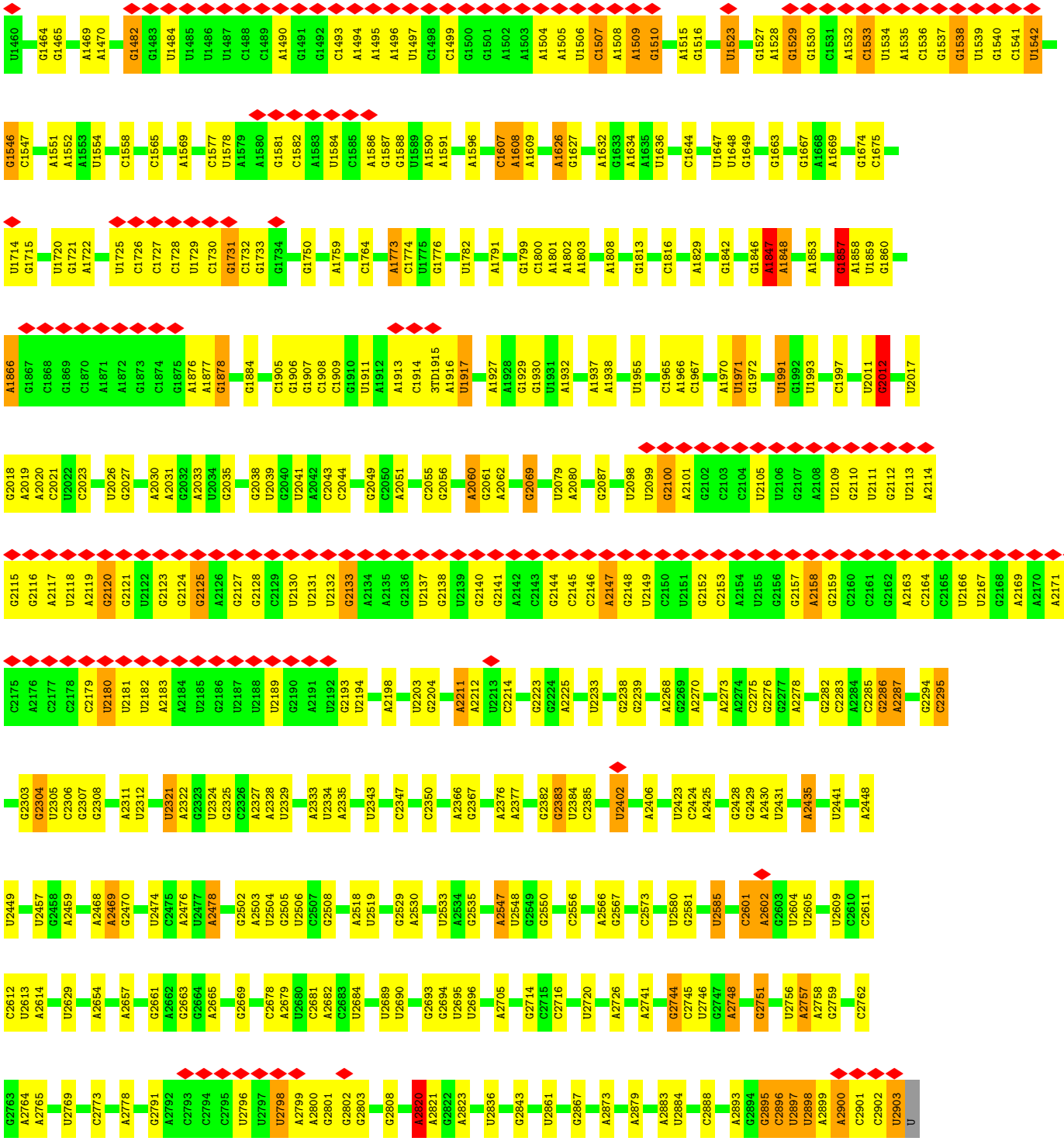


• Molecule 31: 23S rRNA

Chain A:



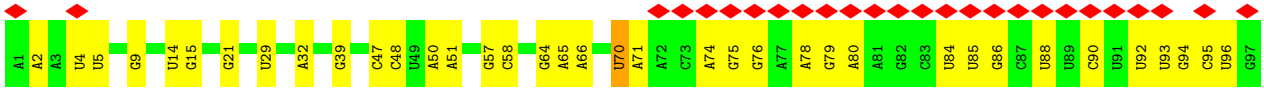


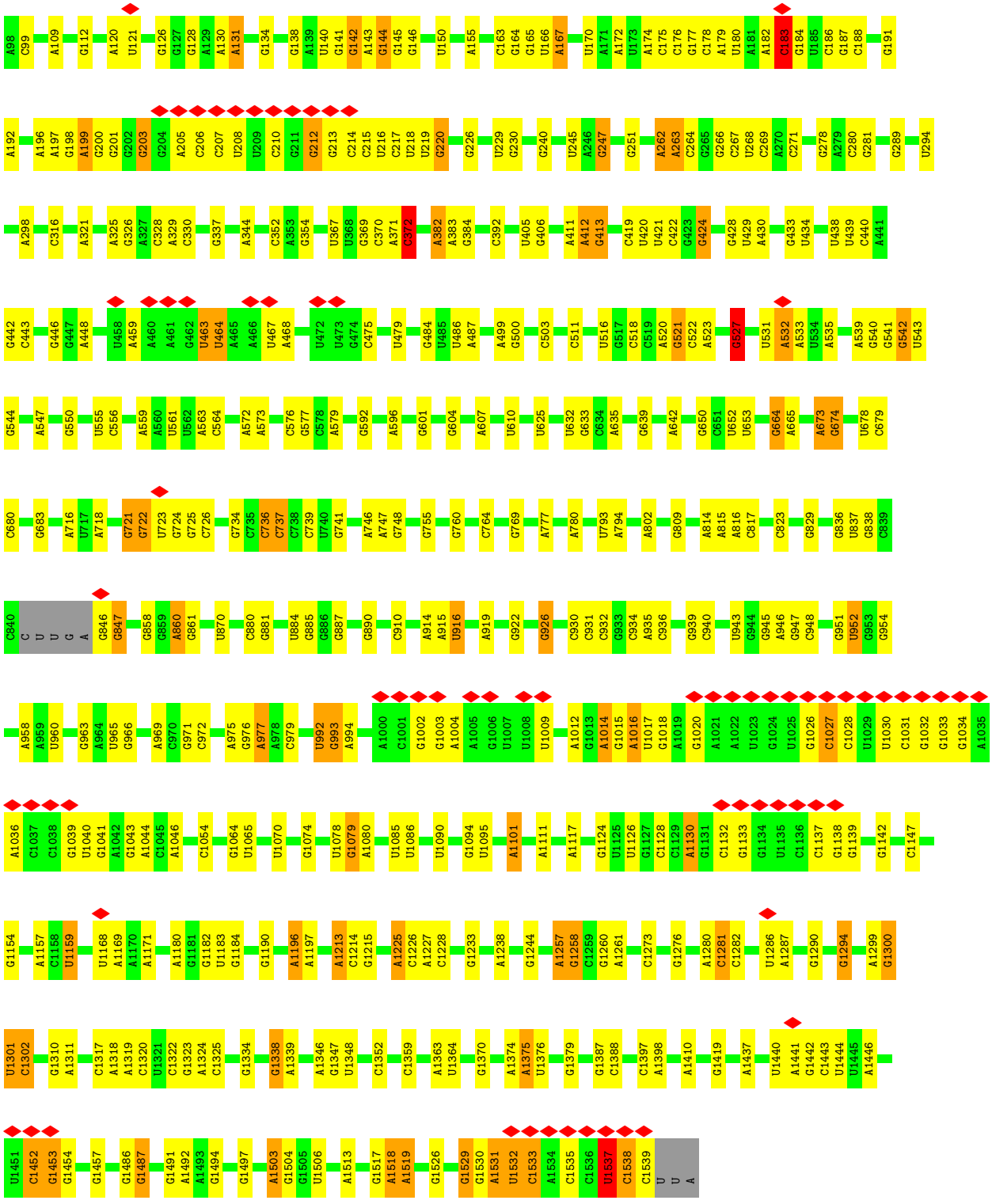


• Molecule 32: 16S rRNA

Chain a:



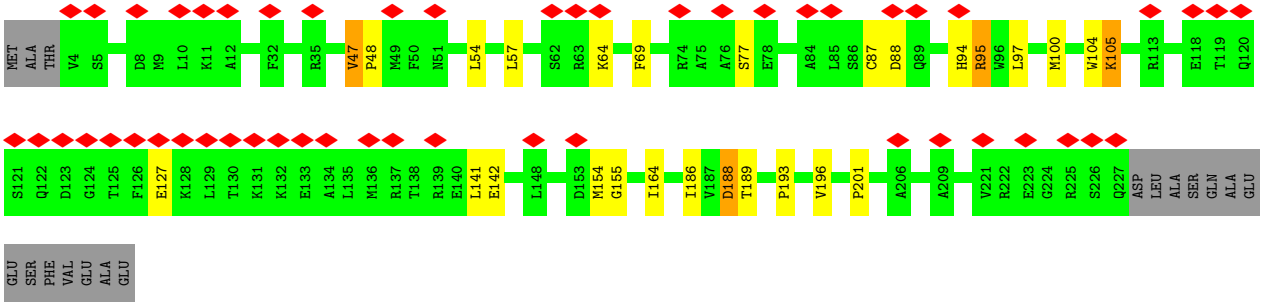




• Molecule 33: Small ribosomal subunit protein uS2

Chain b:

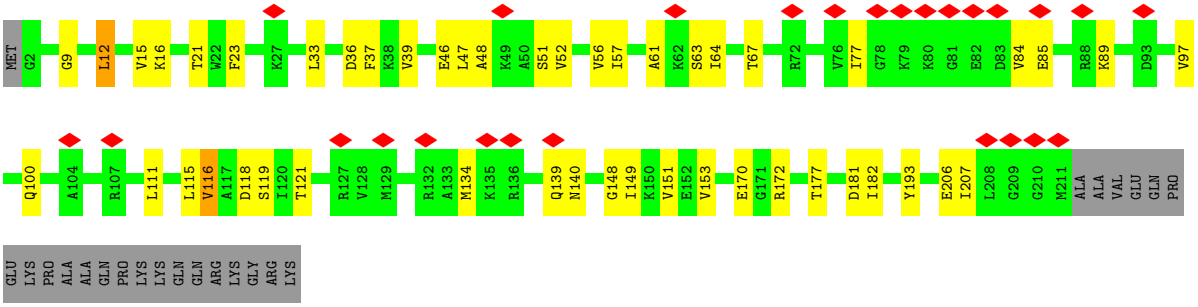




• Molecule 34: Small ribosomal subunit protein uS3

Chain c:

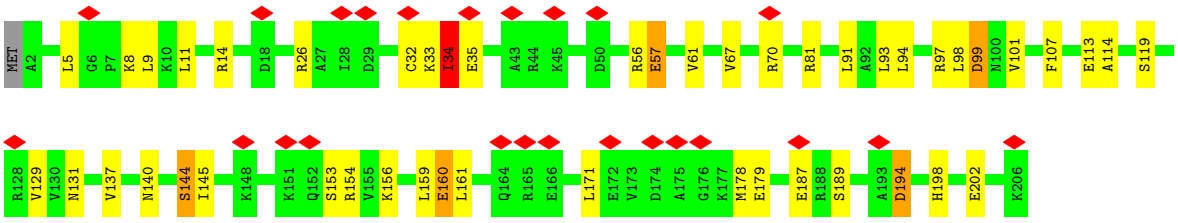




• Molecule 35: Small ribosomal subunit protein uS4

Chain d:

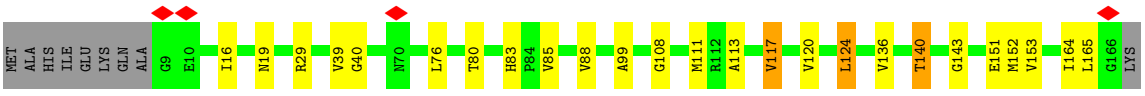




• Molecule 36: Small ribosomal subunit protein uS5

Chain e:

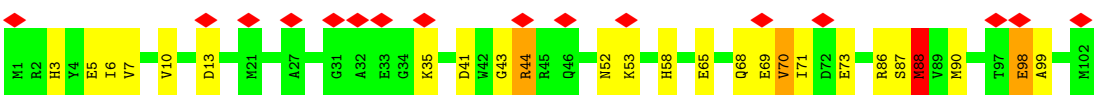




• Molecule 37: Small ribosomal subunit protein bS6, fully modified isoform

Chain f:

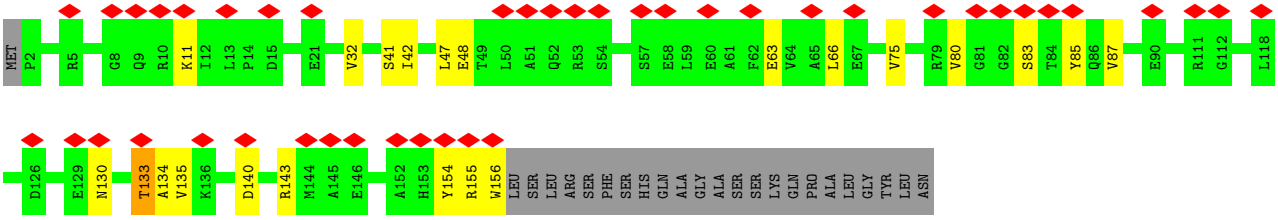




• Molecule 38: Small ribosomal subunit protein uS7

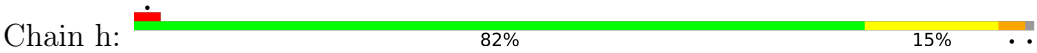
Chain g:

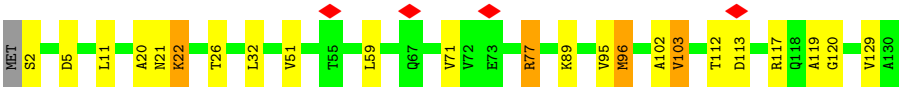




• Molecule 39: Small ribosomal subunit protein uS8

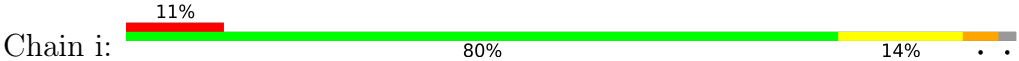
Chain h:

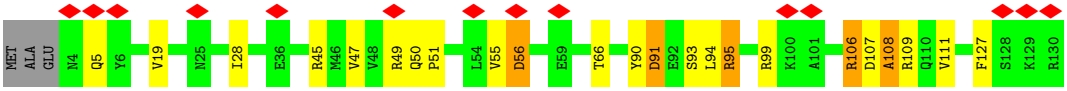




• Molecule 40: Small ribosomal subunit protein uS9

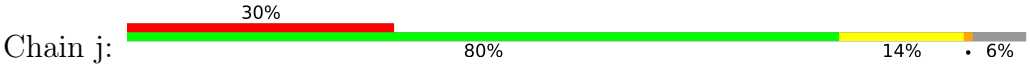
Chain i:





• Molecule 41: Small ribosomal subunit protein uS10

Chain j:

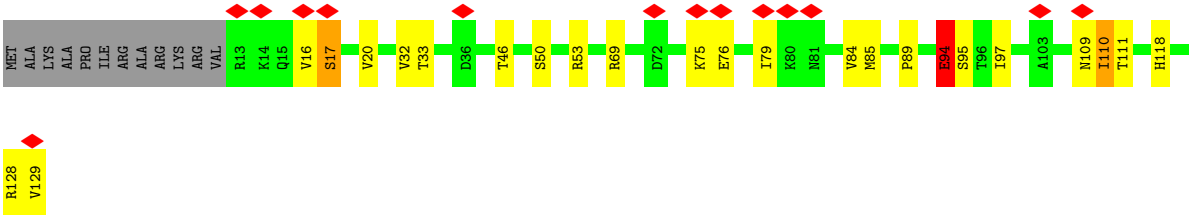




• Molecule 42: Small ribosomal subunit protein uS11

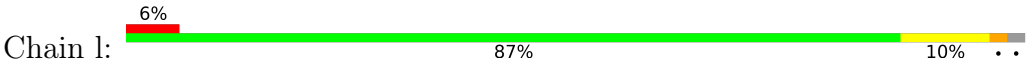
Chain k:

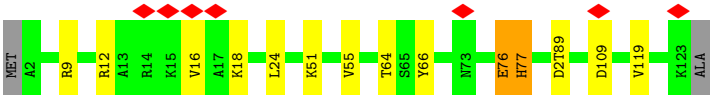




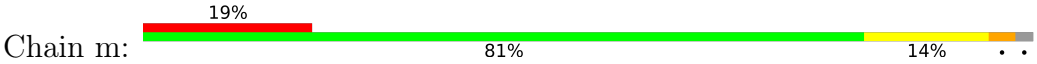
• Molecule 43: Small ribosomal subunit protein uS12

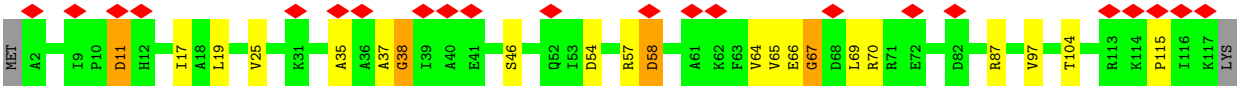
Chain l:



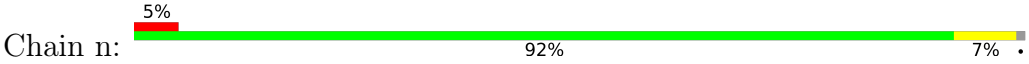


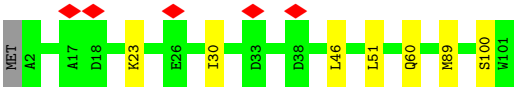
• Molecule 44: Small ribosomal subunit protein uS13



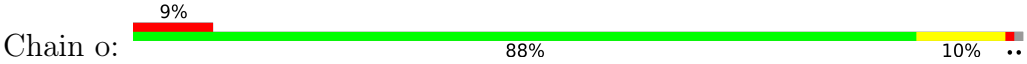


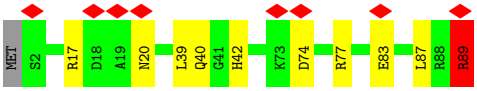
• Molecule 45: Small ribosomal subunit protein uS14



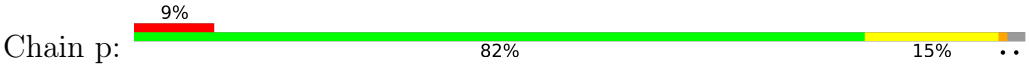


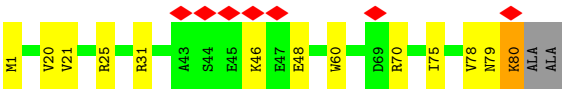
• Molecule 46: Small ribosomal subunit protein uS15





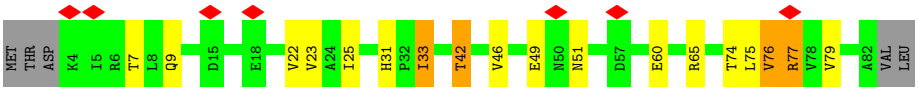
• Molecule 47: Small ribosomal subunit protein bS16





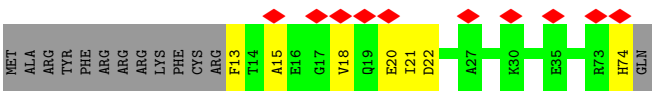
• Molecule 48: Small ribosomal subunit protein uS17





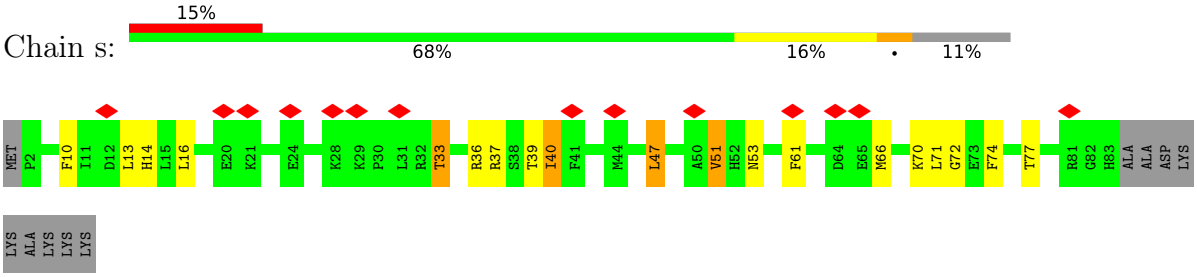
• Molecule 49: Small ribosomal subunit protein bS18





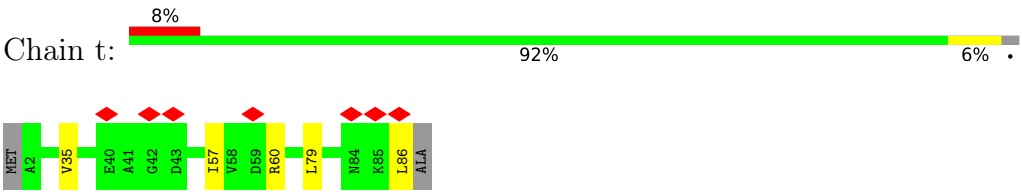
• Molecule 50: Small ribosomal subunit protein uS19

Chain s:



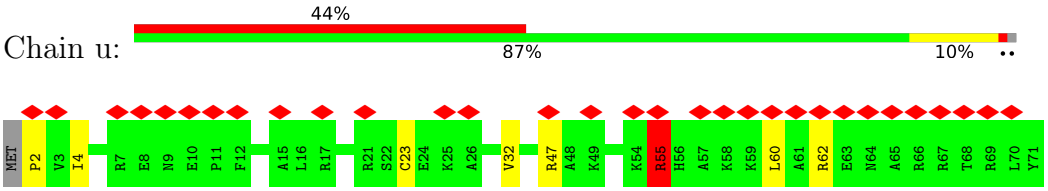
• Molecule 51: Small ribosomal subunit protein bS20

Chain t:



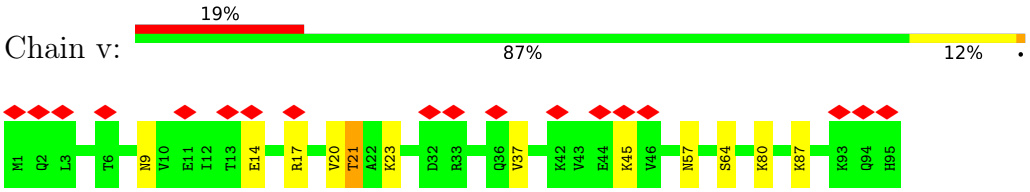
• Molecule 52: 30S ribosomal protein S21

Chain u:



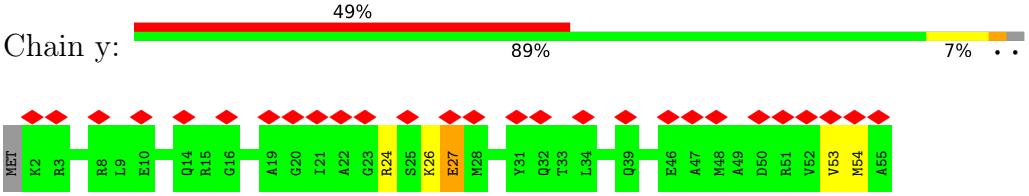
• Molecule 53: Ribosome hibernation promoting factor

Chain v:



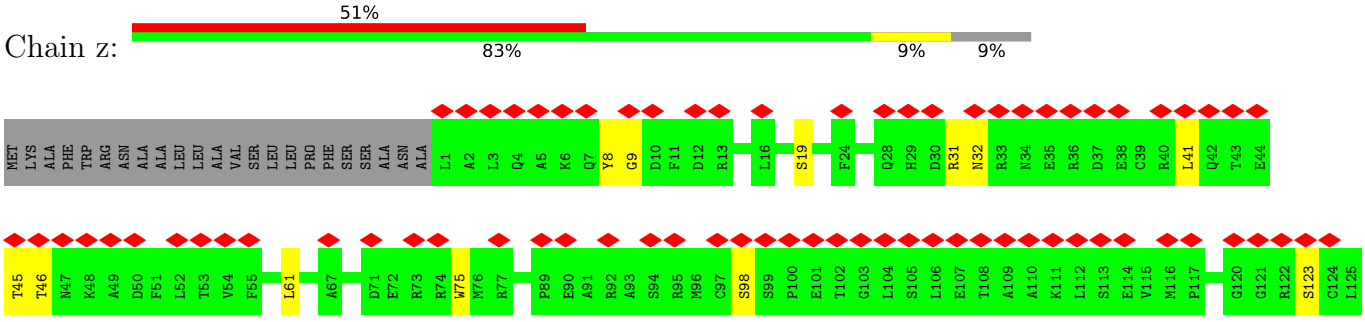
• Molecule 54: Ribosome modulation factor

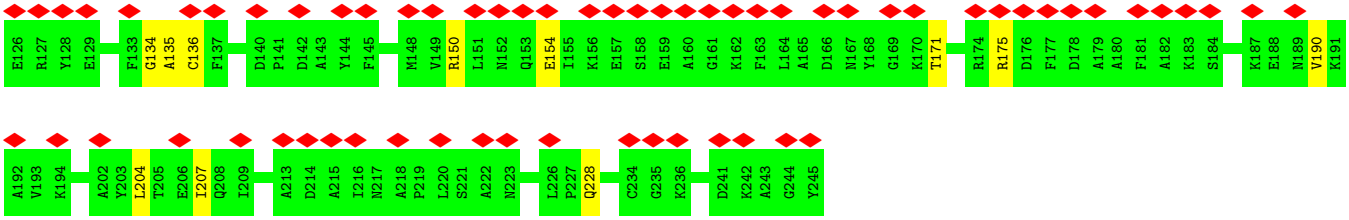
Chain y:



• Molecule 55: Ribonuclease I

Chain z:

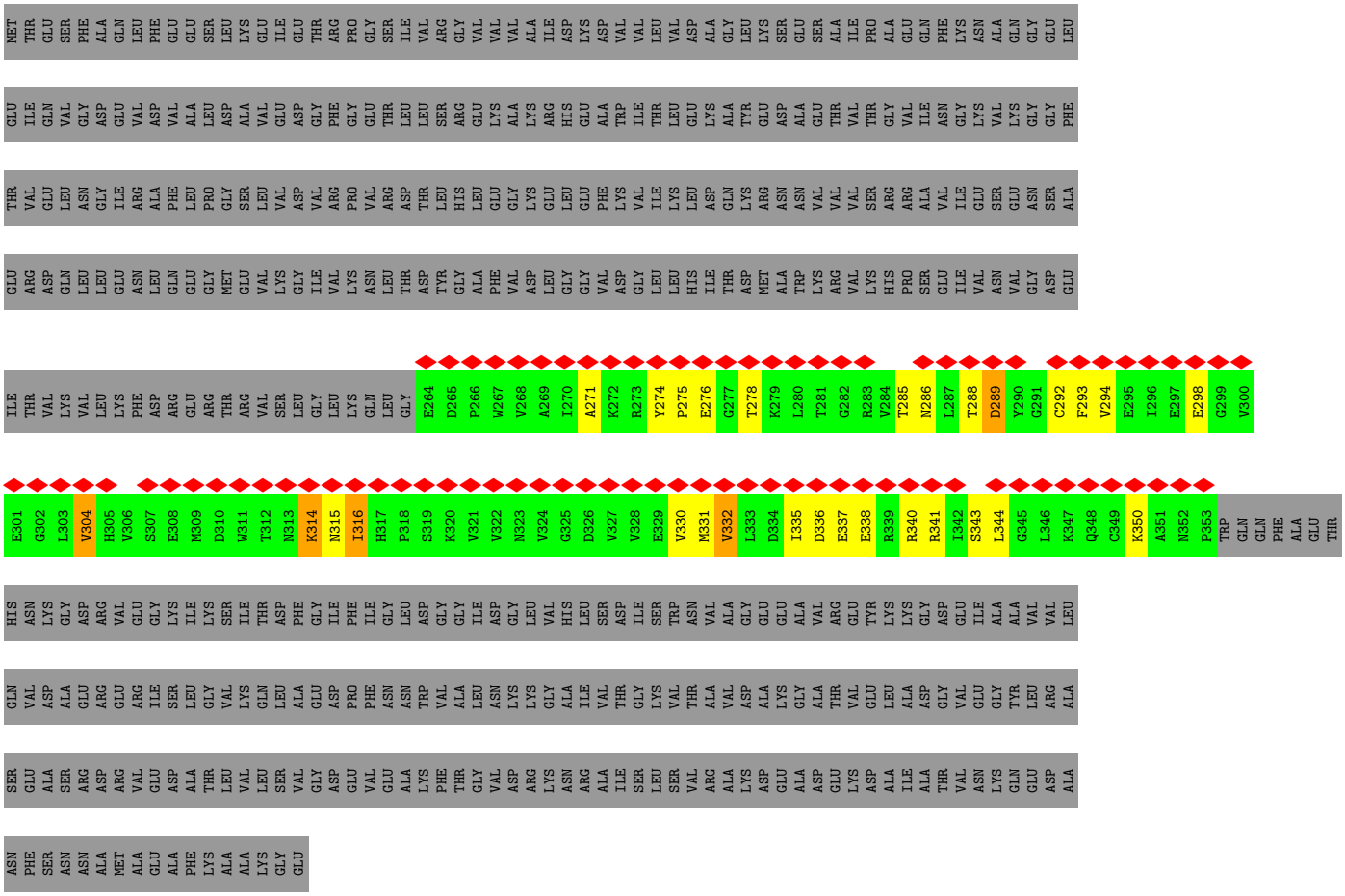




• Molecule 56: Small ribosomal subunit protein bS1

Chain 8:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50955	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.297	Depositor
Minimum map value	-1.544	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.120	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	487.2, 487.2, 487.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.218, 1.218, 1.218	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.49	0/496	1.14	2/660 (0.3%)
2	1	0.53	0/453	0.93	0/605
3	3	0.56	0/440	1.01	1/588 (0.2%)
4	4	0.57	0/417	0.98	0/557
5	5	0.56	0/380	1.03	0/498
6	6	0.55	0/513	0.97	0/676
7	7	0.50	0/303	0.88	0/397
8	B	0.59	0/2876	0.90	5/4483 (0.1%)
9	D	0.57	0/2114	0.97	0/2842
10	E	0.55	1/1566 (0.1%)	0.93	0/2107
11	F	0.50	0/1555	0.95	0/2092
12	G	0.53	0/1409	1.01	1/1896 (0.1%)
13	H	0.56	0/1244	1.02	1/1685 (0.1%)
14	I	0.66	0/306	0.98	0/413
15	L	0.49	0/1142	0.94	0/1539
16	M	0.54	0/948	0.92	1/1270 (0.1%)
17	N	0.66	2/1054 (0.2%)	0.99	1/1403 (0.1%)
18	O	0.53	0/1076	0.92	0/1436
19	P	0.53	0/952	0.94	0/1272
20	Q	0.56	0/883	1.01	0/1188
21	R	0.53	0/925	0.89	1/1238 (0.1%)
22	S	0.59	1/957 (0.1%)	1.04	0/1274
23	T	0.53	0/825	0.88	0/1102
24	U	0.56	0/857	0.91	0/1149
25	V	0.53	0/744	1.01	0/994
26	W	0.55	0/777	0.99	0/1038
27	X	0.51	0/759	0.98	0/1018
28	Y	0.55	0/589	0.96	0/779
29	Z	0.54	0/635	0.93	0/848
30	2	0.59	0/514	0.98	0/690
31	A	0.60	2/67756 (0.0%)	0.90	99/105698 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	a	0.59	2/36585 (0.0%)	0.90	45/57065 (0.1%)
33	b	0.56	0/1555	1.01	2/2123 (0.1%)
34	c	0.54	0/1663	0.98	2/2241 (0.1%)
35	d	0.51	0/1641	1.08	2/2200 (0.1%)
36	e	0.56	0/1142	0.99	0/1541
37	f	0.56	0/789	1.05	2/1077 (0.2%)
38	g	0.55	0/1202	0.99	0/1622
39	h	0.53	0/976	1.01	0/1309
40	i	0.56	0/967	1.00	0/1295
41	j	0.57	0/677	0.95	0/926
42	k	0.56	0/860	0.96	0/1162
43	l	0.53	0/936	0.91	0/1260
44	m	0.59	0/854	1.07	0/1149
45	n	0.53	0/806	1.03	0/1075
46	o	1.02	4/704 (0.6%)	1.07	1/944 (0.1%)
47	p	0.73	2/627 (0.3%)	1.02	1/846 (0.1%)
48	q	0.54	0/639	1.04	0/859
49	r	0.56	0/488	0.99	0/659
50	s	0.56	0/656	0.97	0/887
51	t	0.51	0/658	1.05	0/875
52	u	0.66	1/529 (0.2%)	1.07	0/712
53	v	0.49	0/732	0.94	0/990
54	y	0.58	0/447	0.99	0/594
55	z	0.60	0/1928	0.98	0/2611
56	8	0.67	0/707	1.04	0/960
All	All	0.59	15/154233 (0.0%)	0.92	167/230417 (0.1%)

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
3	3	0	1
5	5	0	2
9	D	0	1
11	F	0	1
12	G	0	2
17	N	0	2
18	O	0	1
19	P	0	1
20	Q	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	S	0	1
24	U	0	1
28	Y	0	2
29	Z	0	2
33	b	0	1
35	d	0	3
36	e	0	1
37	f	0	1
41	j	0	1
42	k	0	2
43	l	0	1
45	n	0	1
52	u	0	1
53	v	0	1
54	y	0	1
All	All	0	35

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	o	89	ARG	CB-CG	15.38	1.98	1.52
46	o	89	ARG	CA-C	8.82	1.71	1.52
46	o	89	ARG	CA-CB	8.61	1.70	1.53
46	o	89	ARG	CZ-NH1	8.52	1.44	1.32
47	p	80	LYS	C-O	8.15	1.39	1.23
47	p	80	LYS	CB-CG	7.89	1.76	1.52
17	N	37	GLY	N-CA	7.63	1.50	1.44
22	S	51	ARG	CZ-NH1	7.43	1.43	1.32
17	N	22	GLY	C-O	6.50	1.30	1.24
10	E	97	SER	CB-OG	5.70	1.53	1.42
31	A	578	G	O5'-C5'	5.46	1.50	1.42
52	u	55	ARG	CD-NE	5.37	1.53	1.46
32	a	527	G7M	O3'-P	5.18	1.61	1.56
32	a	1027	C	O5'-C5'	5.03	1.50	1.42
31	A	2069	G7M	O3'-P	5.00	1.61	1.56

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	652	U	O3'-P-O5'	-8.92	90.63	104.00
32	a	1375	A	O3'-P-O5'	-8.82	90.77	104.00
32	a	1347	G	O3'-P-O5'	-8.81	90.79	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	1378	A	O3'-P-O5'	-8.64	91.04	104.00
31	A	2367	G	O3'-P-O5'	-8.60	91.10	104.00
33	b	47	VAL	N-CA-CB	8.33	116.95	110.45
31	A	1905	C	O3'-P-O5'	-8.13	91.80	104.00
31	A	2468	A	O3'-P-O5'	-8.13	91.81	104.00
31	A	1565	C	O3'-P-O5'	-8.06	91.90	104.00
32	a	183	C	C2'-C3'-O3'	7.99	121.49	109.50
31	A	874	G	O3'-P-O5'	-7.98	92.03	104.00
31	A	1878	G	O3'-P-O5'	-7.91	92.14	104.00
32	a	1375	A	C2'-C3'-O3'	-7.86	101.91	113.70
31	A	2011	U	O3'-P-O5'	-7.85	92.23	104.00
31	A	1356	G	O3'-P-O5'	-7.78	92.33	104.00
31	A	2897	U	O3'-P-O5'	-7.71	92.44	104.00
31	A	1773	A	O3'-P-O5'	-7.69	92.46	104.00
47	p	80	LYS	CA-C-O	-7.60	107.88	120.80
32	a	931	C	O3'-P-O5'	-7.49	92.76	104.00
31	A	241	A	O3'-P-O5'	-7.44	92.83	104.00
32	a	21	G	O3'-P-O5'	-7.37	92.95	104.00
31	A	1857	G	O3'-P-O5'	-7.29	93.06	104.00
31	A	2611	C	O3'-P-O5'	-7.29	93.06	104.00
31	A	641	U	O3'-P-O5'	-7.29	93.06	104.00
32	a	541	G	O3'-P-O5'	-7.28	93.09	104.00
31	A	2366	A	O3'-P-O5'	-7.13	93.30	104.00
32	a	1529	G	O3'-P-O5'	-7.11	93.34	104.00
31	A	567	U	O3'-P-O5'	-7.10	93.35	104.00
31	A	652	U	O3'-P-O5'	-6.87	93.69	104.00
31	A	94	A	O3'-P-O5'	-6.85	93.73	104.00
32	a	1537	U	C2'-C3'-O3'	6.83	119.75	109.50
31	A	1847	A	O3'-P-O5'	-6.77	93.85	104.00
32	a	561	U	O3'-P-O5'	-6.75	93.87	104.00
31	A	1546	G	O3'-P-O5'	-6.73	93.90	104.00
32	a	1375	A	C4'-C3'-O3'	6.73	123.09	113.00
31	A	1328	A	O3'-P-O5'	-6.68	93.98	104.00
32	a	664	G	O3'-P-O5'	-6.66	94.01	104.00
31	A	206	U	O3'-P-O5'	-6.65	94.03	104.00
31	A	791	C	O3'-P-O5'	-6.65	94.03	104.00
32	a	1457	G	O3'-P-O5'	-6.61	94.08	104.00
37	f	73	GLU	CB-CA-C	-6.57	99.84	110.74
32	a	1078	U	O3'-P-O5'	-6.48	94.28	104.00
32	a	1437	A	O3'-P-O5'	-6.47	94.30	104.00
32	a	736	C	O3'-P-O5'	-6.45	94.33	104.00
32	a	126	G	O3'-P-O5'	-6.43	94.35	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	930	C	O3'-P-O5'	-6.42	94.37	104.00
31	A	528	A	O3'-P-O5'	-6.39	94.42	104.00
31	A	529	A	O3'-P-O5'	-6.37	94.45	104.00
31	A	2614	A	O3'-P-O5'	-6.37	94.45	104.00
31	A	2051	A	O3'-P-O5'	-6.35	94.48	104.00
32	a	725	G	O3'-P-O5'	-6.32	94.52	104.00
32	a	746	A	O3'-P-O5'	-6.26	94.61	104.00
32	a	809	G	O3'-P-O5'	-6.24	94.63	104.00
32	a	1387	G	C2'-C3'-O3'	6.20	123.00	113.70
31	A	2716	C	O3'-P-O5'	-6.17	94.74	104.00
31	A	846	U	O3'-P-O5'	-6.15	94.78	104.00
31	A	2367	G	C4'-C3'-O3'	-6.12	103.82	113.00
31	A	1971	U	O3'-P-O5'	-6.09	94.86	104.00
1	0	59	GLU	N-CA-CB	6.08	118.89	110.07
32	a	1352	C	O3'-P-O5'	-6.08	94.88	104.00
31	A	1596	A	O3'-P-O5'	-6.07	94.89	104.00
31	A	2519	U	O3'-P-O5'	-6.06	94.90	104.00
31	A	2896	C	O3'-P-O5'	-6.06	94.91	104.00
31	A	2745	C	C4'-C3'-O3'	-6.05	103.92	113.00
31	A	73	A	O3'-P-O5'	-6.04	94.93	104.00
31	A	2469	A	O3'-P-O5'	-6.04	94.94	104.00
31	A	2026	U	O3'-P-O5'	-5.97	95.04	104.00
31	A	204	A	O3'-P-O5'	-5.97	95.05	104.00
31	A	227	A	O3'-P-O5'	-5.96	95.06	104.00
32	a	176	C	O3'-P-O5'	-5.95	95.08	104.00
31	A	1308	A	O3'-P-O5'	-5.88	95.18	104.00
31	A	2384	U	C4'-C3'-O3'	5.87	118.20	109.40
32	a	716	A	O3'-P-O5'	-5.87	95.20	104.00
31	A	2895	G	C4'-C3'-C2'	-5.86	96.74	102.60
31	A	781	A	O3'-P-O5'	-5.86	95.21	104.00
32	a	652	U	C2'-C3'-O3'	5.86	118.29	109.50
32	a	523	A	O3'-P-O5'	-5.86	95.22	104.00
13	H	155	GLU	CB-CA-C	5.85	120.04	109.45
32	a	601	G	O3'-P-O5'	-5.84	95.23	104.00
31	A	2764	A	O3'-P-O5'	-5.81	95.28	104.00
31	A	2879	A	O3'-P-O5'	-5.81	95.28	104.00
31	A	512	G	O3'-P-O5'	-5.79	95.31	104.00
32	a	1190	G	O3'-P-O5'	-5.78	95.33	104.00
31	A	395	U	C4'-C3'-O3'	5.77	118.06	109.40
35	d	194	ASP	CB-CA-C	5.76	120.29	111.02
31	A	2808	G	O3'-P-O5'	-5.70	95.45	104.00
17	N	116	VAL	N-CA-CB	5.68	118.40	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	494	G	O3'-P-O5'	-5.67	95.49	104.00
31	A	385	C	O3'-P-O5'	-5.66	95.52	104.00
34	c	181	ASP	CA-CB-CG	5.65	118.25	112.60
31	A	1848	A	O3'-P-O5'	-5.63	95.55	104.00
31	A	2867	G	O3'-P-O5'	-5.63	95.55	104.00
8	B	57	A	O3'-P-O5'	-5.60	95.60	104.00
31	A	1552	A	O3'-P-O5'	-5.59	95.61	104.00
31	A	555	G	O3'-P-O5'	-5.58	95.63	104.00
31	A	2423	U	O3'-P-O5'	-5.58	95.62	104.00
31	A	2820	A	C2'-C3'-O3'	5.57	117.85	109.50
32	a	70	U	O3'-P-O5'	-5.57	95.65	104.00
31	A	1464	G	O3'-P-O5'	-5.55	95.67	104.00
31	A	2745	C	C2'-C3'-O3'	5.54	122.02	113.70
32	a	678	U	O3'-P-O5'	-5.53	95.71	104.00
31	A	926	G	O3'-P-O5'	-5.49	95.77	104.00
31	A	771	G	O3'-P-O5'	-5.47	95.80	104.00
32	a	542	G	O3'-P-O5'	-5.46	95.81	104.00
32	a	1387	G	C3'-C2'-C1'	-5.43	95.87	101.30
32	a	1387	G	C4'-C3'-C2'	-5.41	97.19	102.60
31	A	2343	U	C4'-C3'-O3'	-5.40	104.90	113.00
21	R	81	VAL	N-CA-CB	5.40	116.95	110.31
31	A	2060	A	O3'-P-O5'	-5.39	95.91	104.00
31	A	1162	G	O3'-P-O5'	-5.39	95.92	104.00
31	A	1117	C	O3'-P-O5'	-5.38	95.93	104.00
31	A	1185	G	O3'-P-O5'	-5.38	95.93	104.00
31	A	1274	A	O3'-P-O5'	-5.38	95.94	104.00
31	A	661	A	O3'-P-O5'	-5.37	95.95	104.00
33	b	188	ASP	CA-CB-CG	5.36	117.96	112.60
31	A	198	C	O3'-P-O5'	-5.35	95.98	104.00
8	B	83	G	O3'-P-O5'	-5.34	95.99	104.00
32	a	4	U	C2'-C3'-O3'	5.34	121.71	113.70
3	3	36	GLU	CB-CA-C	5.33	119.16	109.83
31	A	2049	G	O3'-P-O5'	-5.32	96.02	104.00
31	A	2321	U	C4'-C3'-O3'	-5.31	105.03	113.00
31	A	761	A	O3'-P-O5'	-5.30	96.05	104.00
31	A	2435	A	O3'-P-O5'	-5.28	96.08	104.00
32	a	1079	G	C4'-C3'-O3'	-5.28	105.08	113.00
31	A	577	G	O3'-P-O5'	-5.28	96.09	104.00
32	a	1359	C	O3'-P-O5'	-5.27	96.09	104.00
31	A	1909	C	O3'-P-O5'	-5.26	96.11	104.00
31	A	1448	G	O3'-P-O5'	-5.25	96.12	104.00
32	a	780	A	O3'-P-O5'	-5.25	96.12	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	1504	G	O3'-P-O5'	-5.23	96.15	104.00
8	B	14	U	O3'-P-O5'	-5.23	96.16	104.00
32	a	216	U	O3'-P-O5'	-5.23	96.16	104.00
31	A	95	A	O3'-P-O5'	-5.23	96.16	104.00
31	A	2684	U	O3'-P-O5'	-5.21	96.18	104.00
31	A	45	G	O3'-P-O5'	-5.21	96.18	104.00
31	A	875	G	O3'-P-O5'	-5.21	96.19	104.00
31	A	784	G	C2'-C3'-O3'	-5.20	105.89	113.70
31	A	72	U	O3'-P-O5'	-5.19	96.21	104.00
31	A	1044	C	C4'-C3'-C2'	-5.19	97.41	102.60
35	d	194	ASP	CA-CB-CG	5.18	117.78	112.60
46	o	89	ARG	CA-C-O	-5.18	111.99	120.80
31	A	2585	U	O3'-P-O5'	-5.18	96.24	104.00
31	A	1016	G	O3'-P-O5'	-5.17	96.25	104.00
34	c	116	VAL	N-CA-CB	5.16	117.55	110.54
31	A	3	U	C2'-C3'-O3'	5.15	121.42	113.70
16	M	5	GLN	N-CA-CB	5.14	119.18	110.49
31	A	1469	A	O3'-P-O5'	-5.14	96.28	104.00
31	A	1507	C	O3'-P-O5'	-5.14	96.29	104.00
1	0	46	VAL	N-CA-CB	5.13	117.52	110.54
31	A	1663	G	O3'-P-O5'	-5.13	96.31	104.00
31	A	2012	G	O3'-P-O5'	-5.12	96.33	104.00
12	G	31	VAL	N-CA-CB	5.10	116.28	110.72
8	B	3	C	O3'-P-O5'	-5.07	96.39	104.00
8	B	89	U	C3'-C2'-C1'	-5.07	96.43	101.50
31	A	493	G	O3'-P-O5'	-5.06	96.41	104.00
31	A	2285	C	O3'-P-O5'	-5.06	96.42	104.00
32	a	870	U	O3'-P-O5'	-5.05	96.42	104.00
32	a	1154	G	O3'-P-O5'	-5.05	96.42	104.00
37	f	70	VAL	N-CA-CB	5.05	117.03	110.57
32	a	167	A	O3'-P-O5'	-5.04	96.43	104.00
31	A	2383	G	O3'-P-O5'	-5.04	96.44	104.00
31	A	988	A	O3'-P-O5'	-5.04	96.44	104.00
31	A	2018	G	O3'-P-O5'	-5.03	96.45	104.00
31	A	844	A	O3'-P-O5'	-5.03	96.46	104.00
31	A	510	C	O3'-P-O5'	-5.02	96.47	104.00
32	a	372	C	O3'-P-O5'	-5.02	96.47	104.00
31	A	495	G	O3'-P-O5'	-5.00	96.50	104.00

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	46	ASP	Peptide
5	5	14	ARG	Sidechain
5	5	41	ARG	Sidechain
9	D	203	ARG	Sidechain
11	F	170	ARG	Sidechain
12	G	150	ARG	Sidechain
12	G	60	ILE	Peptide
17	N	28	GLY	Peptide
17	N	35	HIS	Peptide
18	O	10	ARG	Sidechain
19	P	8	ARG	Sidechain
20	Q	13	ARG	Sidechain
20	Q	30	ARG	Sidechain
20	Q	61	GLN	Peptide
20	Q	94	ARG	Sidechain
22	S	51	ARG	Sidechain
24	U	11	ARG	Sidechain
28	Y	25	ARG	Sidechain
28	Y	77	ARG	Sidechain
29	Z	27	ARG	Sidechain
29	Z	42	SER	Peptide
33	b	193	PRO	Peptide
35	d	144	SER	Peptide
35	d	70	ARG	Sidechain
35	d	81	ARG	Sidechain
36	e	29	ARG	Sidechain
37	f	86	ARG	Sidechain
41	j	9	ARG	Sidechain
42	k	69	ARG	Sidechain
42	k	79	ILE	Peptide
43	l	12	ARG	Sidechain
45	n	51	LEU	Peptide
52	u	55	ARG	Sidechain
53	v	14	GLU	Peptide
54	y	24	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	495	0	526	3	0
2	1	449	0	488	1	0
3	3	434	0	445	5	0
4	4	410	0	431	1	0
5	5	377	0	418	1	0
6	6	504	0	572	2	0
7	7	302	0	343	5	0
8	B	2572	0	1301	9	0
9	D	2075	0	2144	7	0
10	E	1556	0	1605	4	0
11	F	1536	0	1594	3	0
12	G	1385	0	1402	19	0
13	H	1226	0	1258	9	0
14	I	303	0	327	3	0
15	L	1119	0	1144	5	0
16	M	939	0	1014	2	0
17	N	1045	0	1121	1	0
18	O	1070	0	1150	4	0
19	P	939	0	989	3	0
20	Q	873	0	877	6	0
21	R	913	0	958	2	0
22	S	944	0	1017	4	0
23	T	812	0	835	2	0
24	U	850	0	911	0	0
25	V	738	0	807	6	0
26	W	769	0	812	4	0
27	X	746	0	762	7	0
28	Y	582	0	599	1	0
29	Z	625	0	652	4	0
30	2	504	0	483	5	0
31	A	61011	0	30710	162	0
32	a	32925	0	16593	143	0
33	b	1527	0	1353	8	0
34	c	1636	0	1709	16	0
35	d	1619	0	1659	15	0
36	e	1129	0	1149	9	0
37	f	770	0	717	8	0
38	g	1183	0	1176	9	0
39	h	966	0	1012	11	0
40	i	955	0	938	16	0
41	j	668	0	612	4	0
42	k	853	0	838	11	0
43	l	933	0	968	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	m	845	0	867	8	0
45	n	794	0	827	1	0
46	o	696	0	706	6	0
47	p	617	0	619	5	0
48	q	630	0	657	5	0
49	r	481	0	486	2	0
50	s	639	0	645	12	0
51	t	652	0	688	1	0
52	u	521	0	512	0	0
53	v	722	0	704	3	0
54	y	440	0	434	2	0
55	z	1852	0	1738	9	0
56	8	696	0	677	13	0
57	3	1	0	0	0	0
57	A	337	0	0	0	0
57	B	6	0	0	0	0
57	D	2	0	0	0	0
57	E	1	0	0	0	0
57	O	1	0	0	0	0
57	a	127	0	0	0	0
58	z	1	0	0	0	0
59	A	25	0	0	0	0
59	N	1	0	0	0	0
59	Y	1	0	0	0	0
59	a	5	0	0	0	0
All	All	143360	0	95979	558	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 (558) 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)
47:p:80:LYS:CG	47:p:80:LYS:CB	1.76	1.63
46:o:89:ARG:CG	46:o:89:ARG:CB	1.98	1.38
56:8:286:ASN:O	56:8:292:CYS:O	1.96	0.83
12:G:56:ASP:OD2	12:G:150:ARG:NH1	2.16	0.78
31:A:1857:G:O2'	31:A:1884:G:N2	2.18	0.76
31:A:12:U:H2'	31:A:12:U:O2	1.87	0.74
32:a:1537:U:O2'	32:a:1538:C:OP2	2.07	0.73
32:a:203:G:N2	32:a:215:C:C2	2.58	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:372:G:O2'	31:A:400:G:O6	2.08	0.68
29:Z:2:SER:O	31:A:1365:A:OP2	2.12	0.68
47:p:80:LYS:CG	47:p:80:LYS:CA	2.72	0.67
31:A:1421:G:N2	31:A:1495:A:N1	2.42	0.66
33:b:104:TRP:O	33:b:105:LYS:C	2.39	0.65
47:p:80:LYS:CB	47:p:80:LYS:CD	2.73	0.65
31:A:270:A:C8	31:A:370:G:C2	2.85	0.64
31:A:84:A:N1	31:A:98:G:O2'	2.30	0.63
32:a:945:G:C2	32:a:946:A:C8	2.86	0.63
32:a:823:C:HO2'	39:h:2:SER:N	1.96	0.63
31:A:568:U:H1'	31:A:2030:6MZ:H9C1	1.81	0.63
31:A:1509:A:H1'	31:A:1510:G:C8	2.33	0.63
31:A:544:C:O2'	31:A:545:U:C2	2.50	0.62
31:A:885:C:N3	31:A:891:G:O6	2.32	0.62
50:s:70:LYS:O	50:s:71:LEU:C	2.43	0.61
32:a:1518:MA6:H103	32:a:1519:MA6:H102	1.83	0.61
31:A:2402:U:H2'	31:A:2402:U:O2	1.99	0.61
33:b:47:VAL:HG23	33:b:48:PRO:HD3	1.83	0.61
1:0:29:ARG:NH1	25:V:11:LEU:O	2.34	0.60
32:a:721:G:H4'	32:a:722:G:O4'	2.01	0.60
12:G:2:ALA:O	12:G:3:LYS:C	2.44	0.60
30:2:10:GLU:O	30:2:25:ARG:HA	2.01	0.60
32:a:201:G:C2	32:a:217:C:O2	2.55	0.60
26:W:99:ASN:O	26:W:101:GLU:N	2.35	0.60
12:G:41:GLY:C	12:G:43:ALA:H	2.10	0.60
42:k:94:GLU:CD	42:k:95:SER:H	2.10	0.59
32:a:539:A:H2'	32:a:540:G:C8	2.36	0.59
30:2:16:CYS:SG	30:2:17:SER:N	2.75	0.59
32:a:1397:C:H2'	32:a:1397:C:O2	2.02	0.59
38:g:140:ASP:OD1	38:g:143:ARG:NH2	2.36	0.59
21:R:53:ARG:NH2	31:A:2720:U:OP1	2.36	0.58
31:A:1731:G:C2	31:A:1733:G:C5	2.90	0.58
19:P:23:ASN:ND2	31:A:1294:U:O2'	2.36	0.58
56:8:314:LYS:O	56:8:316:ILE:N	2.35	0.58
54:y:26:LYS:O	54:y:27:GLU:HG2	2.04	0.58
32:a:405:U:H5	32:a:499:A:N7	2.02	0.58
12:G:166:GLY:O	12:G:169:LEU:N	2.36	0.58
39:h:20:ALA:O	39:h:21:ASN:HB2	2.04	0.57
16:M:115:ILE:O	16:M:116:ILE:C	2.46	0.57
32:a:1503:A:C4	32:a:1531:A:C2	2.93	0.57
13:H:26:ILE:HG22	13:H:79:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1528:A:H2'	31:A:1529:G:O4'	2.03	0.57
15:L:128:ASN:OD1	15:L:128:ASN:O	2.21	0.57
31:A:547:A:N3	31:A:548:G:C6	2.73	0.57
31:A:1020:A:N1	31:A:1141:U:O2'	2.36	0.56
37:f:43:GLY:HA2	37:f:58:HIS:CD2	2.39	0.56
20:Q:114:GLY:O	20:Q:115:LEU:C	2.47	0.56
37:f:98:GLU:OE2	37:f:99:ALA:N	2.38	0.56
31:A:12:U:O2	31:A:12:U:C2'	2.53	0.56
31:A:356:G:C6	31:A:357:C:O2	2.58	0.56
40:i:50:GLN:N	40:i:51:PRO:HD2	2.20	0.56
50:s:66:MET:HG2	50:s:74:PHE:CZ	2.41	0.56
31:A:1523:U:O2	31:A:1523:U:O4'	2.23	0.55
32:a:247:G:C5	32:a:278:G:C2	2.94	0.55
31:A:720:U:O2	31:A:720:U:O5'	2.23	0.55
31:A:1529:G:C6	31:A:1530:G:C5	2.95	0.55
32:a:910:C:OP2	43:l:18:LYS:NZ	2.40	0.55
31:A:2294:G:C2'	31:A:2295:C:O5'	2.55	0.55
33:b:94:HIS:O	33:b:95:ARG:C	2.50	0.55
44:m:66:GLU:O	44:m:67:GLY:C	2.50	0.55
32:a:1257:A:H4'	32:a:1258:G:O5'	2.08	0.54
31:A:613:A:C6	31:A:614:A:C5	2.95	0.54
13:H:137:ASP:OD1	13:H:139:GLN:N	2.39	0.54
43:l:76:GLU:O	43:l:77:HIS:HB2	2.06	0.54
12:G:80:ARG:CB	12:G:83:TYR:CZ	2.91	0.54
12:G:98:GLU:OE2	30:2:25:ARG:NE	2.37	0.54
18:O:57:VAL:HG11	18:O:105:MET:HE1	1.90	0.54
7:7:2:LYS:NZ	31:A:2478:A:OP2	2.37	0.54
12:G:41:GLY:O	12:G:43:ALA:N	2.40	0.54
31:A:548:G:H2'	31:A:549:G:C4	2.42	0.54
32:a:846:G:O2'	32:a:847:G:C8	2.61	0.54
40:i:94:LEU:O	40:i:95:ARG:C	2.51	0.54
56:8:332:VAL:O	56:8:343:SER:O	2.25	0.54
42:k:46:THR:O	42:k:50:SER:OG	2.12	0.53
32:a:1133:G:C2	32:a:1142:G:C2	2.96	0.53
36:e:136:VAL:O	36:e:140:THR:HG23	2.08	0.53
38:g:155:ARG:O	38:g:156[B]:TRP:C	2.47	0.53
40:i:107:ASP:O	40:i:108:ALA:HB3	2.08	0.53
31:A:2802:G:C2	31:A:2803:G:C8	2.97	0.53
35:d:107:PHE:CG	35:d:145:ILE:HD11	2.43	0.53
31:A:1876:A:H2'	31:A:1877:A:O4'	2.08	0.53
31:A:368:A:H2'	31:A:369:U:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1581:G:C5	31:A:1582:C:C5	2.97	0.53
35:d:113:GLU:O	35:d:114:ALA:C	2.52	0.53
42:k:109:ASN:OD1	42:k:110:ILE:N	2.42	0.53
32:a:880:C:OP1	43:l:9:ARG:NH1	2.41	0.53
32:a:1397:C:O2	32:a:1397:C:C2'	2.56	0.53
20:Q:17:LYS:O	20:Q:20:GLU:HG3	2.10	0.52
32:a:1015:G:C6	32:a:1016:A:C6	2.98	0.52
32:a:247:G:C5	32:a:278:G:N2	2.78	0.52
34:c:12:LEU:O	34:c:16:LYS:O	2.28	0.52
39:h:102:ALA:O	39:h:103:VAL:C	2.53	0.52
25:V:61:LEU:HD12	25:V:61:LEU:C	2.35	0.52
25:V:84:TYR:OH	31:A:1340:U:OP1	2.24	0.52
9:D:257:THR:CG2	31:A:1803:A:O3'	2.57	0.52
54:y:26:LYS:O	54:y:27:GLU:CG	2.57	0.52
32:a:521:G:OP2	43:l:51:LYS:NZ	2.43	0.51
40:i:55:VAL:O	40:i:56:ASP:C	2.53	0.51
50:s:13:LEU:O	50:s:14:HIS:C	2.53	0.51
32:a:1310:G:OP2	44:m:87:ARG:NH2	2.43	0.51
44:m:37:ALA:O	44:m:38:GLY:C	2.53	0.51
32:a:1531:A:C6	32:a:1532:U:C2	2.99	0.51
31:A:1586:A:N7	31:A:1587:G:C5	2.78	0.51
32:a:144:G:N2	32:a:179:A:H1'	2.26	0.51
32:a:172:A:C5	32:a:174:A:C8	2.98	0.51
32:a:174:A:C6	32:a:175:C:C5	2.97	0.51
32:a:1531:A:N1	32:a:1532:U:C2	2.78	0.51
12:G:171:ALA:O	12:G:174:ASP:N	2.42	0.51
31:A:1050:A:C2	31:A:2751:G:C4	2.97	0.51
31:A:1731:G:N1	31:A:1733:G:C6	2.78	0.51
31:A:1866:A:C2	31:A:1876:A:C4	2.99	0.51
32:a:1323:G:H2'	32:a:1324:A:C8	2.45	0.51
8:B:29:A:C2	8:B:56:G:C2	2.99	0.51
9:D:217:ARG:NH2	31:A:781:A:OP1	2.42	0.51
31:A:544:C:H4'	31:A:545:U:C4	2.45	0.51
39:h:89:LYS:HD3	39:h:120:GLY:HA2	1.92	0.51
12:G:41:GLY:C	12:G:43:ALA:N	2.68	0.51
31:A:1530:G:N2	31:A:1542:U:O2	2.44	0.50
12:G:2:ALA:O	12:G:5:HIS:N	2.44	0.50
31:A:1727:C:H2'	31:A:1728:C:O4'	2.11	0.50
32:a:1126:U:C2	32:a:1281:C:C5	3.00	0.50
32:a:1159:U:C2	32:a:1182:G:C2	3.00	0.50
32:a:1324:A:H2'	32:a:1325:C:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1531:A:C6	32:a:1532:U:N3	2.79	0.50
40:i:127:PHE:CG	40:i:127:PHE:O	2.64	0.50
56:8:275:PRO:O	56:8:278:THR:OG1	2.24	0.50
32:a:174:A:C2	32:a:175:C:C6	3.00	0.50
39:h:5:ASP:OD1	39:h:77:ARG:NH1	2.45	0.50
31:A:1533:C:O2'	31:A:1538:G:N2	2.45	0.50
32:a:1117:A:O3'	40:i:106:ARG:HD2	2.11	0.50
38:g:47:LEU:O	38:g:48:GLU:C	2.55	0.50
31:A:1587:G:C4	31:A:1588:G:C8	3.00	0.49
32:a:463:U:H2'	32:a:464:U:C6	2.47	0.49
27:X:75:GLN:HA	27:X:75:GLN:OE1	2.11	0.49
31:A:1410:G:C6	31:A:1411:U:C4	3.01	0.49
31:A:1607:C:H4'	31:A:1608:A:O5'	2.12	0.49
32:a:448:A:C4	32:a:487:A:C2	3.00	0.49
32:a:247:G:C6	32:a:278:G:C2	3.00	0.49
15:L:99:ARG:O	15:L:100:VAL:C	2.56	0.49
35:d:98:LEU:O	35:d:99:ASP:C	2.55	0.49
32:a:736:C:H2'	32:a:737:C:C6	2.48	0.49
42:k:128:ARG:O	42:k:129:VAL:CB	2.59	0.49
31:A:2601:C:H4'	31:A:2602:A:N6	2.27	0.49
32:a:1128:C:O2'	32:a:1147:C:N3	2.40	0.49
44:m:11:ASP:O	44:m:46:SER:HB2	2.12	0.49
21:R:16:ASP:O	21:R:17:VAL:C	2.55	0.49
31:A:1540:G:C6	31:A:1541:C:C4	3.01	0.49
7:7:14:CYS:SG	7:7:27:CYS:SG	3.10	0.49
15:L:45:THR:OG1	22:S:64:ARG:NH2	2.46	0.49
25:V:12:ARG:HB2	25:V:33:LYS:O	2.13	0.49
32:a:1213:A:C8	32:a:1215:G:C6	3.01	0.49
39:h:21:ASN:O	39:h:22:LYS:C	2.56	0.49
55:z:134:GLY:O	55:z:135:ALA:C	2.56	0.49
50:s:61:PHE:O	50:s:66:MET:HE1	2.13	0.48
31:A:1626:A:HO2'	31:A:1627:G:P	2.37	0.48
32:a:1111:A:N1	34:c:177:THR:OG1	2.39	0.48
32:a:1538:C:N4	56:8:341:ARG:HB2	2.29	0.48
12:G:162:SER:O	12:G:165:GLU:N	2.46	0.48
32:a:664:G:H22	32:a:741:G:H1	1.61	0.48
32:a:1302:C:C5	44:m:17:ILE:HG13	2.48	0.48
50:s:10:PHE:O	50:s:39:THR:HG22	2.13	0.48
31:A:948:C:H1'	31:A:984:A:C8	2.49	0.48
31:A:2799:A:C6	31:A:2801:G:C5	3.02	0.48
34:c:206:GLU:C	34:c:207:ILE:HD12	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:58:TYR:OH	31:A:251:A:OP1	2.22	0.48
31:A:1494:A:C2	31:A:1495:A:C4	3.01	0.48
29:Z:26:LYS:NZ	31:A:205:G:O6	2.46	0.48
32:a:881:G:P	43:l:9:ARG:HH22	2.37	0.48
31:A:1540:G:C6	31:A:1541:C:C5	3.02	0.48
36:e:85:VAL:HG21	36:e:143:GLY:O	2.13	0.48
13:H:143:GLN:HE22	31:A:2744:G:H21	1.60	0.48
31:A:1846:G:C6	31:A:1847:A:C6	3.02	0.48
32:a:134:G:O6	47:p:25:ARG:NH1	2.47	0.48
3:3:11:SER:O	3:3:15:MET:HG3	2.13	0.48
31:A:1590:A:C2	31:A:1591:A:C4	3.02	0.48
32:a:109:A:C6	32:a:326:G:C6	3.02	0.48
32:a:1257:A:N3	32:a:1257:A:H2'	2.29	0.48
37:f:43:GLY:O	37:f:44:ARG:C	2.57	0.48
12:G:166:GLY:O	12:G:167:ARG:C	2.57	0.48
31:A:221:A:N1	31:A:265:A:O2'	2.46	0.48
31:A:620:G:N3	31:A:620:G:H5'	2.29	0.48
34:c:23:PHE:CD1	34:c:23:PHE:C	2.92	0.48
53:v:17:ARG:O	53:v:21:THR:OG1	2.32	0.48
15:L:9:GLU:C	15:L:10:THR:HG1	2.22	0.47
32:a:1002:G:C6	32:a:1003:G:C5	3.02	0.47
35:d:34:ILE:HD12	35:d:35:GLU:H	1.79	0.47
44:m:66:GLU:O	44:m:69:LEU:N	2.47	0.47
9:D:178:SER:OG	31:A:1799:G:N7	2.46	0.47
31:A:2547:A:H2'	31:A:2548:U:C6	2.48	0.47
32:a:191:G:C6	32:a:192:A:C5	3.02	0.47
32:a:382:A:C2	32:a:383:A:C4	3.02	0.47
29:Z:52:SER:O	29:Z:55:GLY:N	2.47	0.47
31:A:1540:G:N1	31:A:1541:C:C4	2.82	0.47
32:a:915:A:H2'	32:a:916:U:O5'	2.13	0.47
32:a:1225:A:H2'	32:a:1225:A:N3	2.29	0.47
31:A:143:C:H2'	31:A:144:A:C8	2.49	0.47
32:a:1538:C:OP2	56:8:341:ARG:NH2	2.48	0.47
34:c:47:LEU:O	34:c:48:ALA:C	2.58	0.47
35:d:33:LYS:O	35:d:34:ILE:C	2.58	0.47
31:A:1141:U:H4'	31:A:1142:A:O4'	2.15	0.47
32:a:330:C:O2	32:a:330:C:O4'	2.29	0.47
32:a:1486:G:H2'	32:a:1487:G:O4'	2.13	0.47
40:i:91:ASP:C	40:i:93:SER:H	2.22	0.47
31:A:887:U:O2'	31:A:889:C:OP2	2.23	0.47
31:A:2120:G:C2	31:A:2121:G:N7	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:212:G:N2	32:a:213:G:H1'	2.30	0.47
33:b:141:LEU:O	33:b:142:GLU:C	2.58	0.47
47:p:79:ASN:O	47:p:80:LYS:HD2	2.15	0.47
55:z:150:ARG:NH1	55:z:154:GLU:OE1	2.47	0.47
15:L:9:GLU:C	15:L:10:THR:OG1	2.58	0.47
31:A:294:A:C5	31:A:345:A:C2	3.02	0.47
11:F:154:ASP:O	11:F:155:GLU:C	2.58	0.47
31:A:1420:A:C2	31:A:2211:A:O4'	2.68	0.47
31:A:2898:U:O2	31:A:2898:U:H2'	2.15	0.47
14:I:38:PRO:O	14:I:39:ALA:C	2.57	0.47
16:M:18:ARG:HG3	16:M:18:ARG:HH11	1.80	0.47
31:A:2902:C:N4	31:A:2903:U:O2	2.48	0.46
32:a:145:G:C2	32:a:178:C:N3	2.83	0.46
35:d:94:LEU:O	35:d:97:ARG:HG2	2.15	0.46
56:8:274:TYR:HA	56:8:335:ILE:HD12	1.96	0.46
31:A:712:G:O6	31:A:719:C:N3	2.47	0.46
31:A:1907:G:C6	31:A:1908:C:C4	3.04	0.46
31:A:2294:G:H2'	31:A:2295:C:O5'	2.15	0.46
12:G:162:SER:O	12:G:163:ASP:C	2.58	0.46
31:A:544:C:C4	31:A:548:G:O6	2.69	0.46
32:a:218:U:H2'	32:a:219:U:O4'	2.15	0.46
32:a:1012:A:C2	32:a:1018:G:C2	3.03	0.46
13:H:20:ASN:OD1	13:H:20:ASN:N	2.47	0.46
13:H:72:LEU:O	13:H:73:ASN:C	2.59	0.46
31:A:278:A:N6	31:A:362:A:N7	2.63	0.46
31:A:543:G:C6	31:A:544:C:C2	3.04	0.46
31:A:684:G:C2	31:A:794:A:C2	3.04	0.46
48:q:31:HIS:CE1	48:q:33:ILE:HD12	2.51	0.46
6:6:27:ALA:O	6:6:28:ASN:HB2	2.14	0.46
7:7:37:GLN:HG3	31:A:1124:G:O2'	2.16	0.46
23:T:44:GLY:O	23:T:46:GLU:N	2.48	0.46
31:A:1482:G:HO2'	31:A:1509:A:H2	1.61	0.46
32:a:165:G:N2	32:a:166:U:C2	2.84	0.46
20:Q:13:ARG:NH1	31:A:2334:U:O2'	2.48	0.46
56:8:304:VAL:HA	56:8:344:LEU:O	2.16	0.46
18:O:76:LYS:NZ	18:O:83:GLY:O	2.48	0.46
20:Q:60:GLU:OE1	20:Q:61:GLN:N	2.49	0.46
32:a:187:G:N2	32:a:191:G:C5	2.84	0.46
49:r:20:GLU:O	49:r:21:ILE:C	2.58	0.46
13:H:151:TYR:O	13:H:152:ARG:C	2.58	0.46
32:a:213:G:C5	32:a:214:C:C5	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:673:A:H2'	32:a:674:G:C8	2.51	0.46
37:f:68:GLN:O	37:f:71:ILE:HG22	2.15	0.46
38:g:154:TYR:O	38:g:156[A]:TRP:CE2	2.69	0.46
26:W:96:PHE:CE2	26:W:103:ILE:HG22	2.51	0.46
31:A:1425:G:H2'	31:A:1426:G:C8	2.51	0.46
32:a:178:C:OP2	51:t:60:ARG:NH2	2.49	0.46
32:a:1157:A:C6	32:a:1180:A:C5	3.04	0.46
32:a:1002:G:C6	32:a:1003:G:C6	3.05	0.45
56:8:271:ALA:HA	56:8:274:TYR:HB2	1.97	0.45
12:G:38:MET:SD	12:G:53:ALA:HB1	2.56	0.45
29:Z:23:ASN:ND2	31:A:2079:U:O2'	2.49	0.45
31:A:285:G:C2	31:A:286:U:C2	3.05	0.45
1:0:8:GLU:OE1	1:0:8:GLU:N	2.45	0.45
3:3:54:VAL:HG23	3:3:55:ILE:HG23	1.98	0.45
14:I:38:PRO:O	14:I:40:THR:N	2.49	0.45
31:A:2303:G:C6	31:A:2304:G:C5	3.04	0.45
32:a:1074:G:O2'	32:a:1101:A:N1	2.49	0.45
32:a:1532:U:O4	32:a:1533:C:C4	2.69	0.45
7:7:23:ILE:HD13	31:A:1032:A:H1'	1.98	0.45
32:a:200:G:C2	32:a:201:G:C5	3.04	0.45
40:i:127:PHE:O	40:i:127:PHE:CD1	2.70	0.45
12:G:147:ASP:OD1	12:G:148:ARG:N	2.50	0.45
31:A:3:U:O4	31:A:2900:A:N1	2.50	0.45
9:D:254:GLY:O	9:D:255:LYS:C	2.60	0.45
31:A:1401:G:C2'	31:A:1402:U:O5'	2.65	0.45
36:e:40:GLY:HA3	36:e:117:VAL:HG13	1.98	0.45
13:H:80:THR:OG1	13:H:81:GLU:OE1	2.22	0.45
27:X:45:ASP:O	27:X:49:ASN:ND2	2.50	0.45
32:a:179:A:C4	32:a:180:U:C6	3.04	0.45
34:c:36:ASP:O	34:c:37:PHE:C	2.60	0.45
41:j:11:LYS:HA	41:j:70:HIS:O	2.17	0.45
10:E:38:LYS:HE3	10:E:81:GLU:OE2	2.17	0.44
13:H:155:GLU:C	13:H:155:GLU:OE1	2.61	0.44
18:O:33:LEU:HD22	18:O:128:THR:HB	2.00	0.44
31:A:2120:G:N2	31:A:2121:G:N7	2.65	0.44
32:a:1213:A:C8	32:a:1215:G:C5	3.05	0.44
36:e:83:HIS:CD2	39:h:96:MET:HE3	2.52	0.44
40:i:108:ALA:O	40:i:109:ARG:C	2.60	0.44
46:o:74:ASP:OD2	46:o:77:ARG:HD3	2.16	0.44
9:D:36:LYS:NZ	9:D:38:SER:OG	2.50	0.44
27:X:75:GLN:OE1	27:X:75:GLN:CA	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:142:G:C6	32:a:143:A:C5	3.05	0.44
32:a:433:G:C5	32:a:434:U:C5	3.05	0.44
32:a:1452:C:H1'	32:a:1453:G:C2	2.52	0.44
38:g:63:GLU:CD	38:g:63:GLU:C	2.85	0.44
42:k:75:LYS:O	42:k:76:GLU:C	2.59	0.44
32:a:1039:G:N2	32:a:1040:U:C2	2.86	0.44
50:s:33:THR:HG23	50:s:51:VAL:HA	1.99	0.44
26:W:7:ARG:NH2	31:A:99:U:O2	2.51	0.44
27:X:42:LEU:N	27:X:42:LEU:HD23	2.32	0.44
31:A:880:G:C2	31:A:898:C:C2	3.05	0.44
32:a:1503:A:C5	32:a:1531:A:C2	3.06	0.44
46:o:89:ARG:CG	46:o:89:ARG:CA	2.93	0.44
31:A:712:G:N3	31:A:712:G:O4'	2.50	0.44
31:A:1527:G:N2	31:A:1546:G:C6	2.86	0.44
32:a:64:G:C8	32:a:99:C:N4	2.86	0.44
25:V:47:VAL:O	25:V:48:GLN:C	2.59	0.44
31:A:2147:A:N7	31:A:2148:G:H1'	2.32	0.44
32:a:134:G:H1'	32:a:325:A:C5	2.53	0.44
32:a:145:G:N2	32:a:146:G:C4	2.85	0.44
32:a:174:A:C5	32:a:175:C:C5	3.05	0.44
32:a:198:G:C5	32:a:220:G:C2	3.06	0.44
8:B:89:U:C6	31:A:958:U:H2'	2.53	0.44
18:O:82:MET:HE2	31:A:960:A:H61	1.83	0.44
32:a:1453:G:H2'	32:a:1454:G:O4'	2.18	0.44
9:D:199:GLU:O	9:D:200:HIS:C	2.61	0.44
11:F:189:THR:O	11:F:190:ALA:C	2.60	0.44
26:W:57:GLY:N	31:A:483:A:O2'	2.49	0.44
31:A:720:U:O2	31:A:720:U:O4'	2.34	0.44
31:A:877:A:C5	31:A:899:A:C2	3.05	0.44
32:a:294:U:OP1	32:a:610:U:O2'	2.23	0.44
32:a:555:U:H2'	32:a:556:C:C6	2.53	0.44
35:d:119:SER:O	35:d:131:ASN:OD1	2.35	0.44
39:h:11:LEU:C	39:h:11:LEU:HD12	2.42	0.44
49:r:13:PHE:C	49:r:15:ALA:H	2.26	0.44
6:6:23:LYS:HA	6:6:48:ALA:O	2.18	0.44
8:B:59:A:H2'	8:B:60:C:O4'	2.18	0.44
23:T:37:GLU:HB3	23:T:53:PHE:CE1	2.53	0.44
32:a:946:A:H2'	32:a:947:G:C8	2.53	0.44
32:a:1299:A:C5	32:a:1301:U:C2	3.05	0.44
32:a:1410:A:C2	32:a:1491:G:C2	3.06	0.44
35:d:8:LYS:O	35:d:11:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:f:3:HIS:CE1	37:f:65:GLU:OE1	2.71	0.43
46:o:20:ASN:OD1	46:o:20:ASN:N	2.51	0.43
10:E:129:THR:OG1	31:A:1997:C:OP2	2.30	0.43
20:Q:60:GLU:OE1	20:Q:61:GLN:NE2	2.51	0.43
31:A:332:A:C2	31:A:335:C:C5	3.06	0.43
32:a:1318:A:H1'	50:s:37:ARG:HD3	2.00	0.43
40:i:91:ASP:C	40:i:93:SER:N	2.76	0.43
32:a:186:C:N4	32:a:187:G:C6	2.86	0.43
32:a:262:A:C6	32:a:263:A:C6	3.06	0.43
32:a:1244:G:C4	32:a:1294:G:N2	2.85	0.43
40:i:49:ARG:C	40:i:51:PRO:HD2	2.43	0.43
50:s:47:LEU:HD23	50:s:47:LEU:N	2.33	0.43
56:8:336:ASP:O	56:8:337:GLU:C	2.61	0.43
3:3:12:LYS:HD3	3:3:15:MET:HE2	2.01	0.43
31:A:2585:U:O2	31:A:2585:U:O4'	2.34	0.43
32:a:1374:A:C4	32:a:1375:A:C8	3.06	0.43
48:q:76:VAL:HG12	48:q:77:ARG:N	2.33	0.43
50:s:16:LEU:C	50:s:16:LEU:HD13	2.43	0.43
50:s:40:ILE:HG21	50:s:66:MET:O	2.18	0.43
31:A:543:G:C2	31:A:544:C:H1'	2.53	0.43
31:A:687:C:N3	31:A:788:A:H5'	2.33	0.43
31:A:2038:G:H2'	31:A:2039:U:O4'	2.18	0.43
31:A:2098:U:H2'	31:A:2099:U:O4'	2.19	0.43
34:c:21:THR:O	34:c:21:THR:OG1	2.34	0.43
31:A:1725:U:N3	31:A:1726:C:C4	2.87	0.43
32:a:860:A:H2'	32:a:861:G:O4'	2.18	0.43
31:A:547:A:H4'	31:A:548:G:N9	2.34	0.43
32:a:183:C:O2	32:a:183:C:O4'	2.36	0.43
37:f:69:GLU:OE1	37:f:69:GLU:N	2.49	0.43
8:B:24:G:N7	8:B:56:G:H2'	2.34	0.43
31:A:270:A:N6	31:A:369:U:O2'	2.51	0.43
31:A:1667:G:O2'	31:A:1991:U:O4	2.25	0.43
31:A:2286:G:N3	31:A:2286:G:H2'	2.34	0.43
31:A:2402:U:O2	31:A:2402:U:C2'	2.67	0.43
31:A:2694:G:H2'	31:A:2695:U:O4'	2.18	0.43
32:a:522:C:OP2	43:l:66:TYR:OH	2.34	0.43
32:a:816:A:OP1	32:a:1526:G:O2'	2.30	0.43
36:e:99:ALA:HB2	36:e:124:LEU:HD22	2.00	0.43
44:m:54:ASP:O	44:m:57:ARG:N	2.52	0.43
10:E:181:ASP:HB2	10:E:186:LEU:HB2	2.01	0.43
12:G:108:VAL:N	12:G:109:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:915:A:C2'	32:a:916:U:O5'	2.67	0.43
32:a:1130:A:O2'	40:i:5:GLN:NE2	2.52	0.43
32:a:1338:G:C6	32:a:1339:A:C6	3.07	0.43
35:d:9:LEU:HD13	35:d:32:CYS:HB3	2.00	0.43
31:A:1426:G:O5'	31:A:1426:G:H8	2.01	0.43
32:a:179:A:C5	32:a:180:U:C5	3.07	0.43
32:a:1276:G:N3	32:a:1282:C:O2'	2.44	0.43
40:i:50:GLN:N	40:i:51:PRO:CD	2.82	0.43
7:7:11:CYS:SG	7:7:27:CYS:SG	3.16	0.42
22:S:51:ARG:HD3	31:A:1156:A:C5	2.53	0.42
31:A:613:A:N6	31:A:614:A:C6	2.87	0.42
32:a:442:G:C6	32:a:443:C:C4	3.07	0.42
38:g:41:SER:OG	38:g:42:ILE:N	2.52	0.42
44:m:54:ASP:O	44:m:58:ASP:OD1	2.36	0.42
31:A:1721:G:O2'	31:A:1722:A:H8	2.02	0.42
31:A:2120:G:N2	31:A:2121:G:O6	2.52	0.42
42:k:16:VAL:O	42:k:17:SER:OG	2.27	0.42
42:k:84:VAL:HG11	42:k:97:ILE:HG13	2.00	0.42
27:X:21:ARG:HA	27:X:25:LYS:O	2.19	0.42
31:A:1050:A:C2	31:A:2751:G:C5	3.07	0.42
31:A:1853:A:N1	31:A:2087:G:H1'	2.34	0.42
31:A:2125:G:O2'	31:A:2174:C:N4	2.52	0.42
31:A:2678:C:H2'	31:A:2679:A:O4'	2.19	0.42
32:a:412:A:O2'	32:a:413:G:P	2.77	0.42
39:h:113:ASP:OD1	39:h:117:ARG:NH2	2.52	0.42
42:k:94:GLU:O	42:k:97:ILE:N	2.52	0.42
8:B:75:G:H5"	27:X:12:GLN:OE1	2.20	0.42
13:H:16:ASP:OD1	13:H:18:LYS:NZ	2.53	0.42
22:S:52:GLN:HA	22:S:55:ARG:HG3	2.00	0.42
31:A:883:G:C6	31:A:884:U:C4	3.08	0.42
31:A:1266:G:O2'	31:A:2012:G:O6	2.28	0.42
31:A:1859:U:H2'	31:A:1860:G:O4'	2.20	0.42
31:A:2601:C:H4'	31:A:2602:A:C6	2.54	0.42
32:a:371:A:H2'	32:a:372:C:O4'	2.19	0.42
32:a:992:U:H4'	32:a:993:G:O5'	2.20	0.42
46:o:39:LEU:O	46:o:40:GLN:C	2.62	0.42
2:1:53:PHE:CE2	2:1:54:MET:HG3	2.54	0.42
9:D:29:PRO:HG2	9:D:34:LEU:HD21	2.01	0.42
31:A:2376:A:H2'	31:A:2377:A:O4'	2.20	0.42
32:a:543:U:OP1	35:d:14:ARG:HD3	2.20	0.42
32:a:1453:G:C2	32:a:1454:G:C8	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:f:41:ASP:C	37:f:41:ASP:OD1	2.62	0.42
41:j:37:ARG:O	41:j:38:GLY:O	2.37	0.42
31:A:700:G:O2'	31:A:1632:A:N3	2.52	0.42
32:a:199:A:C2	32:a:219:U:O2	2.73	0.42
32:a:420:U:O2	32:a:424:G:C2	2.73	0.42
32:a:532:A:N1	34:c:193:TYR:CE1	2.88	0.42
32:a:947:G:C6	32:a:948:C:N3	2.87	0.42
36:e:151:GLU:H	36:e:151:GLU:CD	2.25	0.42
40:i:107:ASP:O	40:i:108:ALA:CB	2.67	0.42
8:B:32:U:C2	8:B:51:G:N2	2.88	0.42
32:a:1443:C:H2'	32:a:1444:U:O4'	2.19	0.42
34:c:148:GLY:HA3	34:c:172:ARG:O	2.19	0.42
35:d:57:GLU:OE2	35:d:57:GLU:O	2.37	0.42
31:A:1866:A:N1	31:A:1876:A:C8	2.87	0.42
32:a:229:U:H2'	32:a:230:G:O4'	2.19	0.42
32:a:604:G:C2	32:a:635:A:C2	3.07	0.42
48:q:49:GLU:C	48:q:51:ASN:H	2.27	0.42
31:A:1045:C:C2	31:A:1047:G:C2	3.08	0.42
32:a:75:G:H2'	32:a:76:G:O4'	2.20	0.42
32:a:155:A:C2	32:a:167:A:C2	3.08	0.42
32:a:527:G7M:O2'	32:a:535:A:N1	2.47	0.42
32:a:1086:U:H6	32:a:1086:U:O5'	2.02	0.42
42:k:16:VAL:O	42:k:17:SER:CB	2.68	0.42
56:8:288:THR:O	56:8:289:ASP:CG	2.63	0.42
12:G:80:ARG:CB	12:G:83:TYR:OH	2.68	0.42
14:I:22:LYS:O	14:I:23:ALA:C	2.62	0.42
31:A:1414:C:O2	31:A:1414:C:H2'	2.20	0.42
31:A:2133:G:O2'	31:A:2158:A:N3	2.50	0.42
32:a:146:G:C2	32:a:177:G:N7	2.87	0.42
32:a:203:G:C2	32:a:215:C:N3	2.88	0.42
32:a:769:G:H4'	32:a:1513:A:H4'	2.02	0.42
33:b:164:ILE:O	33:b:186:ILE:HB	2.20	0.42
55:z:204:LEU:HD21	55:z:207:ILE:HD11	2.01	0.42
19:P:38:LEU:N	19:P:39:PRO:HD2	2.35	0.41
31:A:889:C:N4	31:A:890:C:N4	2.68	0.41
31:A:1420:A:C8	31:A:2211:A:C6	3.08	0.41
31:A:1532:A:C6	31:A:1540:G:C2	3.08	0.41
31:A:1731:G:C2	31:A:1733:G:C6	3.08	0.41
31:A:2286:G:H4'	31:A:2287:A:O5'	2.19	0.41
34:c:9:GLY:HA3	45:n:89:MET:HE3	2.02	0.41
34:c:85:GLU:CD	34:c:85:GLU:C	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:e:83:HIS:CG	39:h:96:MET:HE3	2.54	0.41
38:g:80:VAL:HG21	38:g:85:TYR:CD2	2.55	0.41
41:j:92:LEU:HD13	41:j:93:ALA:N	2.35	0.41
22:S:91:ASP:C	22:S:91:ASP:OD1	2.63	0.41
31:A:2657:A:C2	31:A:2665:A:C4	3.08	0.41
38:g:63:GLU:O	38:g:66:LEU:N	2.54	0.41
31:A:264:C:O2	31:A:264:C:O4'	2.37	0.41
32:a:405:U:O2	32:a:405:U:O4'	2.37	0.41
33:b:188:ASP:OD1	33:b:189:THR:N	2.51	0.41
35:d:160:GLU:OE2	35:d:161:LEU:N	2.53	0.41
39:h:96:MET:HE2	39:h:96:MET:HB3	1.94	0.41
56:8:288:THR:O	56:8:289:ASP:CB	2.69	0.41
56:8:338:GLU:C	56:8:340:ARG:H	2.29	0.41
25:V:16:VAL:O	25:V:17:SER:HB3	2.19	0.41
31:A:359:G:C6	31:A:360:U:C2	3.09	0.41
31:A:1720:U:H2'	31:A:1721:G:O4'	2.20	0.41
35:d:198:HIS:O	35:d:202:GLU:HG2	2.20	0.41
12:G:164:GLU:C	12:G:164:GLU:CD	2.88	0.41
30:2:59:ARG:NH1	32:a:1311:A:OP1	2.53	0.41
32:a:264:C:O3'	48:q:65:ARG:NH1	2.52	0.41
8:B:61:G:C6	8:B:62:C:C4	3.08	0.41
11:F:127:GLU:OE1	11:F:127:GLU:N	2.50	0.41
27:X:4:ILE:CG2	27:X:50:MET:SD	3.08	0.41
31:A:1581:G:C6	31:A:1582:C:C4	3.08	0.41
31:A:2100:G:C6	31:A:2101:A:C5	3.08	0.41
31:A:2328:A:H2'	31:A:2329:U:C6	2.55	0.41
32:a:140:U:H2'	32:a:141:G:O4'	2.20	0.41
32:a:150:U:C4	32:a:170:U:C4	3.08	0.41
32:a:951:G:C2'	32:a:952:U:O5'	2.69	0.41
4:4:32:GLU:O	4:4:33:LYS:C	2.63	0.41
5:5:22:MET:HE2	5:5:28:ARG:HG2	2.03	0.41
31:A:1048:A:C8	31:A:1111:A:N6	2.88	0.41
31:A:1877:A:H2'	31:A:1878:G:O4'	2.21	0.41
32:a:131:A:O2'	32:a:262:A:N3	2.49	0.41
40:i:90:TYR:C	40:i:91:ASP:OD1	2.64	0.41
41:j:92:LEU:O	41:j:93:ALA:C	2.64	0.41
30:2:18:CYS:C	30:2:20:ASN:H	2.29	0.41
31:A:356:G:C6	31:A:357:C:C2	3.09	0.41
32:a:268:U:H2'	32:a:269:C:C6	2.56	0.41
32:a:1040:U:C2	32:a:1041:G:C8	3.08	0.41
36:e:16:ILE:CD1	36:e:113:ALA:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:o:39:LEU:O	46:o:42:HIS:N	2.54	0.41
53:v:64:SER:O	53:v:80:LYS:NZ	2.53	0.41
3:3:9:THR:HG21	31:A:2021:C:OP1	2.21	0.41
28:Y:38:VAL:HG23	28:Y:59:LEU:HB2	2.03	0.41
31:A:544:C:O2'	31:A:545:U:O2	2.38	0.41
31:A:1916:A:H2'	31:A:1917:PSU:O4'	2.21	0.41
31:A:2180:U:O4	31:A:2183:A:N6	2.48	0.41
31:A:2796:U:C4	31:A:2798:U:C4	3.09	0.41
32:a:413:G:O2'	32:a:428:G:N2	2.54	0.41
32:a:718:A:C4	42:k:118:HIS:CD2	3.09	0.41
32:a:1043:G:C6	32:a:1044:A:C6	3.08	0.41
32:a:1323:G:C6	32:a:1324:A:C6	3.09	0.41
33:b:97:LEU:HD12	33:b:97:LEU:O	2.21	0.41
34:c:89:LYS:C	34:c:89:LYS:HD3	2.46	0.41
34:c:118:ASP:O	34:c:119:SER:C	2.64	0.41
35:d:153:SER:O	35:d:154:ARG:C	2.62	0.41
3:3:46:ASP:O	3:3:53:LYS:NZ	2.55	0.41
31:A:964:C:O2'	31:A:2273:A:N3	2.52	0.41
31:A:2802:G:N2	31:A:2803:G:C4	2.89	0.41
32:a:1180:A:P	40:i:99:ARG:HH22	2.44	0.41
34:c:77:ILE:HA	34:c:84:VAL:HG23	2.03	0.41
34:c:134:MET:SD	34:c:153:VAL:HG12	2.60	0.41
34:c:139:GLN:O	34:c:140:ASN:C	2.64	0.41
38:g:133:THR:O	38:g:134:ALA:C	2.64	0.41
8:B:32:U:H2'	8:B:33:G:H8	1.86	0.40
31:A:356:G:C5	31:A:357:C:C2	3.09	0.40
42:k:94:GLU:OE1	42:k:95:SER:N	2.54	0.40
50:s:53:ASN:OD1	50:s:53:ASN:C	2.63	0.40
55:z:61:LEU:HD13	55:z:75:TRP:HB2	2.03	0.40
10:E:196:ALA:O	10:E:197:THR:C	2.64	0.40
12:G:2:ALA:O	12:G:4:LEU:N	2.54	0.40
31:A:2602:A:H2'	31:A:2602:A:N3	2.36	0.40
31:A:2758:A:C2	31:A:2759:G:H1'	2.57	0.40
32:a:203:G:N2	32:a:215:C:O2	2.52	0.40
32:a:1014:A:H2'	32:a:1015:G:O4'	2.21	0.40
36:e:164:ILE:O	36:e:165:LEU:C	2.65	0.40
37:f:88:MET:HG2	37:f:90:MET:HE2	2.02	0.40
55:z:45:THR:OG1	55:z:46:THR:N	2.54	0.40
1:0:11:VAL:O	1:0:15:ASN:HB2	2.20	0.40
19:P:4:ARG:HD2	31:A:2820:A:C8	2.56	0.40
31:A:1422:G:H1'	31:A:1496:A:N1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:926:G:C6	53:v:87:LYS:HG3	2.57	0.40
33:b:154:MET:O	33:b:155:GLY:C	2.65	0.40
8:B:51:G:C6	8:B:52:A:C6	3.09	0.40
20:Q:9:ARG:NH2	31:A:2295:C:OP2	2.54	0.40
31:A:2748:A:C2	31:A:2757:A:C5	3.09	0.40
32:a:1054:C:C2	32:a:1196:A:N7	2.89	0.40
32:a:1300:G:C6	32:a:1334:G:C5	3.10	0.40
50:s:36:ARG:NH2	50:s:72:GLY:O	2.55	0.40
31:A:654:A:N3	31:A:654:A:H2'	2.36	0.40
31:A:891:G:C6	31:A:892:A:C5	3.09	0.40
32:a:544:G:OP1	35:d:56:ARG:NH2	2.45	0.40
32:a:977:A:O2'	32:a:979:C:OP2	2.30	0.40
48:q:25:ILE:HB	48:q:42:THR:HG23	2.04	0.40
55:z:31:ARG:C	55:z:32:ASN:CG	2.89	0.40
55:z:228:GLN:O	55:z:228:GLN:NE2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	59/63 (94%)	58 (98%)	1 (2%)	0	100 100
2	1	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
3	3	53/57 (93%)	51 (96%)	2 (4%)	0	100 100
4	4	49/55 (89%)	45 (92%)	3 (6%)	1 (2%)	6 16
5	5	44/46 (96%)	42 (96%)	2 (4%)	0	100 100
6	6	62/65 (95%)	59 (95%)	3 (5%)	0	100 100
7	7	36/38 (95%)	35 (97%)	0	1 (3%)	4 9
9	D	269/273 (98%)	253 (94%)	12 (4%)	4 (2%)	8 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	E	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	24 48
11	F	199/201 (99%)	184 (92%)	12 (6%)	3 (2%)	8 22
12	G	175/179 (98%)	149 (85%)	20 (11%)	6 (3%)	3 7
13	H	162/177 (92%)	134 (83%)	22 (14%)	6 (4%)	2 6
14	I	39/41 (95%)	35 (90%)	3 (8%)	1 (3%)	4 11
15	L	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5 15
16	M	121/123 (98%)	113 (93%)	6 (5%)	2 (2%)	7 19
17	N	142/144 (99%)	135 (95%)	6 (4%)	1 (1%)	18 41
18	O	133/136 (98%)	125 (94%)	8 (6%)	0	100 100
19	P	116/127 (91%)	109 (94%)	7 (6%)	0	100 100
20	Q	114/117 (97%)	102 (90%)	9 (8%)	3 (3%)	4 11
21	R	112/115 (97%)	104 (93%)	7 (6%)	1 (1%)	14 35
22	S	115/118 (98%)	112 (97%)	3 (3%)	0	100 100
23	T	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	12 32
24	U	108/110 (98%)	107 (99%)	1 (1%)	0	100 100
25	V	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	5 14
26	W	100/103 (97%)	88 (88%)	8 (8%)	4 (4%)	2 5
27	X	92/94 (98%)	83 (90%)	9 (10%)	0	100 100
28	Y	74/85 (87%)	71 (96%)	3 (4%)	0	100 100
29	Z	75/78 (96%)	71 (95%)	4 (5%)	0	100 100
30	2	65/67 (97%)	51 (78%)	11 (17%)	3 (5%)	2 4
33	b	222/241 (92%)	184 (83%)	32 (14%)	6 (3%)	4 10
34	c	208/233 (89%)	184 (88%)	21 (10%)	3 (1%)	9 23
35	d	203/206 (98%)	177 (87%)	24 (12%)	2 (1%)	12 32
36	e	156/167 (93%)	146 (94%)	9 (6%)	1 (1%)	21 44
37	f	100/102 (98%)	83 (83%)	13 (13%)	4 (4%)	2 5
38	g	153/179 (86%)	131 (86%)	21 (14%)	1 (1%)	18 41
39	h	127/130 (98%)	110 (87%)	14 (11%)	3 (2%)	4 12
40	i	125/130 (96%)	110 (88%)	12 (10%)	3 (2%)	4 12
41	j	95/103 (92%)	81 (85%)	10 (10%)	4 (4%)	2 4
42	k	113/129 (88%)	95 (84%)	16 (14%)	2 (2%)	6 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
43	l	119/124 (96%)	113 (95%)	4 (3%)	2 (2%)	7 19
44	m	114/118 (97%)	102 (90%)	8 (7%)	4 (4%)	3 6
45	n	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
46	o	86/89 (97%)	74 (86%)	11 (13%)	1 (1%)	10 27
47	p	78/82 (95%)	69 (88%)	6 (8%)	3 (4%)	2 5
48	q	77/84 (92%)	64 (83%)	13 (17%)	0	100 100
49	r	60/75 (80%)	51 (85%)	9 (15%)	0	100 100
50	s	80/92 (87%)	64 (80%)	16 (20%)	0	100 100
51	t	83/87 (95%)	79 (95%)	4 (5%)	0	100 100
52	u	68/71 (96%)	61 (90%)	7 (10%)	0	100 100
53	v	93/95 (98%)	82 (88%)	9 (10%)	2 (2%)	5 14
54	y	52/55 (94%)	48 (92%)	2 (4%)	2 (4%)	2 5
55	z	249/268 (93%)	216 (87%)	30 (12%)	3 (1%)	10 27
56	8	88/557 (16%)	65 (74%)	17 (19%)	6 (7%)	1 1
All	All	5955/6743 (88%)	5353 (90%)	507 (8%)	95 (2%)	10 20

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	G	3	LYS
12	G	42	GLU
12	G	163	ASP
14	I	39	ALA
15	L	133	ALA
26	W	99	ASN
37	f	5	GLU
39	h	22	LYS
39	h	103	VAL
41	j	57	VAL
44	m	67	GLY
56	8	289	ASP
56	8	350	LYS
11	F	9	GLN
11	F	155	GLU
13	H	4	VAL
13	H	152	ARG
16	M	5	GLN

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Mol	Chain	Res	Type
17	N	29	LYS
20	Q	99	TYR
20	Q	115	LEU
33	b	87	CYS
34	c	61	ALA
34	c	64	ILE
36	e	108	GLY
37	f	44	ARG
40	i	56	ASP
40	i	95	ARG
40	i	108	ALA
41	j	38	GLY
44	m	38	GLY
12	G	112	ARG
15	L	10	THR
21	R	7	GLN
26	W	100	SER
33	b	88	ASP
33	b	95	ARG
33	b	127	GLU
35	d	189	SER
41	j	31	ARG
42	k	17	SER
44	m	35	ALA
47	p	48	GLU
56	8	304	VAL
4	4	19	HIS
11	F	144	GLU
13	H	102	VAL
13	H	156	PRO
30	2	51	VAL
34	c	51	SER
37	f	88	MET
38	g	130	ASN
39	h	119	ALA
42	k	94	GLU
53	v	45	LYS
54	y	27	GLU
55	z	8	TYR
56	8	315	ASN
56	8	316	ILE
7	7	12	ARG

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Mol	Chain	Res	Type
9	D	155	ALA
9	D	200	HIS
12	G	113	ASP
20	Q	86	GLY
23	T	45	GLU
25	V	26	LYS
26	W	56	GLY
30	2	49	ARG
35	d	34	ILE
37	f	7	VAL
43	l	77	HIS
43	l	109	ASP
46	o	17	ARG
47	p	46	LYS
53	v	9	ASN
55	z	41	LEU
56	8	293	PHE
12	G	167	ARG
15	L	110	PRO
16	M	116	ILE
25	V	92	ASN
33	b	105	LYS
33	b	201	PRO
47	p	31	ARG
30	2	36	VAL
9	D	148	PRO
10	E	2	ILE
13	H	92	VAL
13	H	126	PRO
44	m	115	PRO
55	z	9	GLY
26	W	72	ILE
41	j	33	GLY
54	y	53	VAL
9	D	113	GLY

5.3.2 Protein sidechains (i)

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
1	0	54/55 (98%)	46 (85%)	8 (15%)	3 8
2	1	48/49 (98%)	48 (100%)	0	100 100
3	3	46/48 (96%)	42 (91%)	4 (9%)	9 24
4	4	44/49 (90%)	43 (98%)	1 (2%)	44 73
5	5	38/38 (100%)	38 (100%)	0	100 100
6	6	51/52 (98%)	48 (94%)	3 (6%)	18 42
7	7	34/34 (100%)	33 (97%)	1 (3%)	37 67
9	D	212/218 (97%)	204 (96%)	8 (4%)	29 58
10	E	160/163 (98%)	149 (93%)	11 (7%)	14 34
11	F	161/165 (98%)	154 (96%)	7 (4%)	26 54
12	G	142/150 (95%)	132 (93%)	10 (7%)	14 34
13	H	124/138 (90%)	102 (82%)	22 (18%)	2 5
14	I	32/32 (100%)	30 (94%)	2 (6%)	16 39
15	L	113/116 (97%)	108 (96%)	5 (4%)	25 53
16	M	102/104 (98%)	98 (96%)	4 (4%)	28 57
17	N	101/103 (98%)	97 (96%)	4 (4%)	28 56
18	O	107/108 (99%)	102 (95%)	5 (5%)	23 51
19	P	95/103 (92%)	91 (96%)	4 (4%)	26 55
20	Q	81/87 (93%)	70 (86%)	11 (14%)	3 9
21	R	98/100 (98%)	96 (98%)	2 (2%)	48 76
22	S	88/90 (98%)	85 (97%)	3 (3%)	32 62
23	T	83/84 (99%)	77 (93%)	6 (7%)	13 32
24	U	92/93 (99%)	89 (97%)	3 (3%)	33 63
25	V	80/84 (95%)	76 (95%)	4 (5%)	22 48
26	W	80/84 (95%)	73 (91%)	7 (9%)	9 23
27	X	76/78 (97%)	69 (91%)	7 (9%)	8 22
28	Y	58/63 (92%)	55 (95%)	3 (5%)	21 47
29	Z	67/68 (98%)	64 (96%)	3 (4%)	24 52
30	2	53/60 (88%)	51 (96%)	2 (4%)	29 58
33	b	118/199 (59%)	111 (94%)	7 (6%)	18 42
34	c	168/190 (88%)	148 (88%)	20 (12%)	5 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	d	167/173 (96%)	145 (87%)	22 (13%)	4 10
36	e	111/126 (88%)	99 (89%)	12 (11%)	6 16
37	f	73/89 (82%)	63 (86%)	10 (14%)	3 9
38	g	112/147 (76%)	105 (94%)	7 (6%)	16 39
39	h	100/105 (95%)	90 (90%)	10 (10%)	7 19
40	i	87/107 (81%)	79 (91%)	8 (9%)	8 22
41	j	53/90 (59%)	48 (91%)	5 (9%)	8 21
42	k	82/98 (84%)	73 (89%)	9 (11%)	6 15
43	l	98/103 (95%)	92 (94%)	6 (6%)	17 40
44	m	79/96 (82%)	70 (89%)	9 (11%)	5 14
45	n	80/84 (95%)	75 (94%)	5 (6%)	16 39
46	o	72/77 (94%)	69 (96%)	3 (4%)	26 55
47	p	59/65 (91%)	52 (88%)	7 (12%)	5 13
48	q	70/78 (90%)	57 (81%)	13 (19%)	1 4
49	r	47/65 (72%)	44 (94%)	3 (6%)	16 38
50	s	66/79 (84%)	61 (92%)	5 (8%)	12 30
51	t	62/66 (94%)	58 (94%)	4 (6%)	15 37
52	u	43/61 (70%)	35 (81%)	8 (19%)	1 4
53	v	71/81 (88%)	66 (93%)	5 (7%)	14 34
54	y	42/44 (96%)	41 (98%)	1 (2%)	43 72
55	z	181/215 (84%)	176 (97%)	5 (3%)	38 68
56	8	75/461 (16%)	67 (89%)	8 (11%)	6 16
All	All	4636/5515 (84%)	4294 (93%)	342 (7%)	15 32

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	SER
1	0	13	GLU
1	0	14	LEU
1	0	40	SER
1	0	46	VAL
1	0	53	VAL
1	0	56	LEU

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Mol	Chain	Res	Type
1	0	58	ASN
3	3	9	THR
3	3	30	VAL
3	3	36	GLU
3	3	55	ILE
4	4	34	LEU
6	6	6	THR
6	6	44	LEU
6	6	55	LEU
7	7	30	GLU
9	D	34	LEU
9	D	38	SER
9	D	51	THR
9	D	65	VAL
9	D	129	THR
9	D	165	VAL
9	D	242	LYS
9	D	253	LYS
10	E	2	ILE
10	E	18	ASP
10	E	34	VAL
10	E	60	VAL
10	E	92	VAL
10	E	110	THR
10	E	131	ASP
10	E	136	ASN
10	E	172	VAL
10	E	186	LEU
10	E	201	LEU
11	F	1	MET
11	F	3	LEU
11	F	33	VAL
11	F	109	LEU
11	F	149	ILE
11	F	176	ASP
11	F	178	VAL
12	G	19	GLU
12	G	25	VAL
12	G	30	ARG
12	G	31	VAL
12	G	35	THR
12	G	98	GLU

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Mol	Chain	Res	Type
12	G	108	VAL
12	G	133	ARG
12	G	152	LEU
12	G	158	THR
13	H	4	VAL
13	H	15	VAL
13	H	20	ASN
13	H	23	VAL
13	H	30	ASN
13	H	34	THR
13	H	36	THR
13	H	38	ASN
13	H	52	PHE
13	H	71	LEU
13	H	84	THR
13	H	88	GLN
13	H	89	LEU
13	H	95	ARG
13	H	98	VAL
13	H	102	VAL
13	H	128	GLN
13	H	131	ILE
13	H	155	GLU
13	H	162	VAL
13	H	166	ASP
13	H	169	VAL
14	I	28	ASN
14	I	37	VAL
15	L	18	VAL
15	L	45	THR
15	L	48	VAL
15	L	131	ASN
15	L	142	ILE
16	M	2	ILE
16	M	7	MET
16	M	76	VAL
16	M	105	ARG
17	N	78	ARG
17	N	95	LEU
17	N	115	GLU
17	N	116	VAL
18	O	33	LEU

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Mol	Chain	Res	Type
18	O	80	VAL
18	O	108	VAL
18	O	110	GLU
18	O	111	GLU
19	P	15	SER
19	P	29	VAL
19	P	74	GLU
19	P	96	ARG
20	Q	20	GLU
20	Q	27	VAL
20	Q	28	VAL
20	Q	30	ARG
20	Q	38	GLN
20	Q	46	GLU
20	Q	49	VAL
20	Q	60	GLU
20	Q	78	VAL
20	Q	90	VAL
20	Q	103	VAL
21	R	17	VAL
21	R	81	VAL
22	S	11	ARG
22	S	16	LYS
22	S	17	ILE
23	T	6	GLN
23	T	15	SER
23	T	29	THR
23	T	33	VAL
23	T	72	VAL
23	T	99	THR
24	U	69	LEU
24	U	76	VAL
24	U	81	SER
25	V	18	GLU
25	V	30	ILE
25	V	58	VAL
25	V	92	ASN
26	W	5	ILE
26	W	18	ASP
26	W	42	VAL
26	W	49	VAL
26	W	65	ILE

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Mol	Chain	Res	Type
26	W	72	ILE
26	W	88	GLU
27	X	3	THR
27	X	42	LEU
27	X	62	THR
27	X	66	ASP
27	X	75	GLN
27	X	77	VAL
27	X	92	VAL
28	Y	38	VAL
28	Y	70	GLU
28	Y	83	GLU
29	Z	11	ARG
29	Z	35	SER
29	Z	66	THR
30	2	21	VAL
30	2	34	LEU
33	b	54	LEU
33	b	57	LEU
33	b	64	LYS
33	b	69	PHE
33	b	77	SER
33	b	100	MET
33	b	196	VAL
34	c	12	LEU
34	c	15	VAL
34	c	33	LEU
34	c	39	VAL
34	c	46	GLU
34	c	52	VAL
34	c	56	VAL
34	c	57	ILE
34	c	63	SER
34	c	67	THR
34	c	97	VAL
34	c	100	GLN
34	c	111	LEU
34	c	115	LEU
34	c	116	VAL
34	c	121	THR
34	c	149	ILE
34	c	151	VAL

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Mol	Chain	Res	Type
34	c	170	GLU
34	c	182	ILE
35	d	5	LEU
35	d	26	ARG
35	d	34	ILE
35	d	57	GLU
35	d	61	VAL
35	d	67	VAL
35	d	91	LEU
35	d	93	LEU
35	d	99	ASP
35	d	101	VAL
35	d	129	VAL
35	d	137	VAL
35	d	140	ASN
35	d	144	SER
35	d	156	LYS
35	d	159	LEU
35	d	160	GLU
35	d	171	LEU
35	d	178	MET
35	d	179	GLU
35	d	187	GLU
35	d	194	ASP
36	e	19	ASN
36	e	39	VAL
36	e	76	LEU
36	e	80	THR
36	e	88	VAL
36	e	111	MET
36	e	117	VAL
36	e	120	VAL
36	e	124	LEU
36	e	140	THR
36	e	152	MET
36	e	153	VAL
37	f	6	ILE
37	f	10	VAL
37	f	13	ASP
37	f	35	LYS
37	f	52	ASN
37	f	53	LYS

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Mol	Chain	Res	Type
37	f	70	VAL
37	f	87	SER
37	f	88	MET
37	f	98	GLU
38	g	11	LYS
38	g	32	VAL
38	g	75	VAL
38	g	83	SER
38	g	87	VAL
38	g	133	THR
38	g	135	VAL
39	h	26	THR
39	h	32	LEU
39	h	51	VAL
39	h	59	LEU
39	h	71	VAL
39	h	77	ARG
39	h	95	VAL
39	h	96	MET
39	h	112	THR
39	h	129	VAL
40	i	19	VAL
40	i	28	ILE
40	i	45	ARG
40	i	47	VAL
40	i	66	THR
40	i	91	ASP
40	i	106	ARG
40	i	111	VAL
41	j	6	ILE
41	j	8	ILE
41	j	44	THR
41	j	90	LEU
41	j	98	VAL
42	k	20	VAL
42	k	32	VAL
42	k	33	THR
42	k	53	ARG
42	k	85	MET
42	k	89	PRO
42	k	94	GLU
42	k	110	ILE

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Mol	Chain	Res	Type
42	k	111	THR
43	l	16	VAL
43	l	24	LEU
43	l	55	VAL
43	l	64	THR
43	l	76	GLU
43	l	119	VAL
44	m	11	ASP
44	m	19	LEU
44	m	25	VAL
44	m	58	ASP
44	m	64	VAL
44	m	65	VAL
44	m	70	ARG
44	m	97	VAL
44	m	104	THR
45	n	23	LYS
45	n	30	ILE
45	n	46	LEU
45	n	60	GLN
45	n	100	SER
46	o	83	GLU
46	o	87	LEU
46	o	89	ARG
47	p	1	MET
47	p	20	VAL
47	p	21	VAL
47	p	60	TRP
47	p	70	ARG
47	p	75	ILE
47	p	78	VAL
48	q	7	THR
48	q	9	GLN
48	q	22	VAL
48	q	23	VAL
48	q	33	ILE
48	q	42	THR
48	q	46	VAL
48	q	60	GLU
48	q	74	THR
48	q	75	LEU
48	q	76	VAL

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Mol	Chain	Res	Type
48	q	77	ARG
48	q	79	VAL
49	r	18	VAL
49	r	22	ASP
49	r	74	HIS
50	s	33	THR
50	s	40	ILE
50	s	47	LEU
50	s	51	VAL
50	s	77	THR
51	t	35	VAL
51	t	57	ILE
51	t	79	LEU
51	t	86	LEU
52	u	2	PRO
52	u	4	ILE
52	u	23	CYS
52	u	32	VAL
52	u	47	ARG
52	u	55	ARG
52	u	60	LEU
52	u	62	ARG
53	v	20	VAL
53	v	21	THR
53	v	23	LYS
53	v	37	VAL
53	v	57	ASN
54	y	54	MET
55	z	19	SER
55	z	136	CYS
55	z	171	THR
55	z	175	ARG
55	z	190	VAL
56	8	276	GLU
56	8	285	THR
56	8	294	VAL
56	8	298	GLU
56	8	314	LYS
56	8	330	VAL
56	8	331	MET
56	8	332	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81)

such sidechains are listed below:

Mol	Chain	Res	Type
1	0	38	GLN
1	0	45	GLN
7	7	37	GLN
9	D	60	GLN
9	D	90	ASN
9	D	134	ASN
10	E	67	HIS
10	E	126	ASN
10	E	136	ASN
10	E	148	GLN
11	F	29	HIS
11	F	90	GLN
11	F	115	GLN
12	G	63	GLN
12	G	81	GLN
13	H	143	GLN
14	I	28	ASN
15	L	40	HIS
15	L	58	ASN
15	L	128	ASN
16	M	5	GLN
17	N	54	GLN
18	O	45	GLN
18	O	60	GLN
19	P	23	ASN
19	P	73	ASN
20	Q	61	GLN
21	R	52	ASN
21	R	56	HIS
22	S	20	GLN
23	T	6	GLN
24	U	7	HIS
25	V	28	ASN
27	X	87	GLN
28	Y	46	HIS
28	Y	50	ASN
29	Z	23	ASN
29	Z	36	HIS
33	b	177	ASN
33	b	178	ASN
34	c	3	GLN
34	c	25	ASN

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Mol	Chain	Res	Type
35	d	36	GLN
35	d	59	GLN
35	d	89	ASN
35	d	131	ASN
35	d	164	GLN
36	e	89	HIS
36	e	135	ASN
37	f	3	HIS
37	f	37	HIS
37	f	52	ASN
37	f	63	ASN
38	g	68	ASN
38	g	86	GLN
38	g	148	ASN
39	h	16	ASN
40	i	5	GLN
40	i	110	GLN
41	j	99	GLN
42	k	28	ASN
42	k	40	ASN
43	l	5	ASN
43	l	77	HIS
43	l	96	HIS
44	m	8	ASN
45	n	60	GLN
46	o	28	GLN
46	o	35	GLN
46	o	46	HIS
46	o	51	HIS
47	p	9	HIS
48	q	31	HIS
49	r	54	GLN
50	s	69	HIS
50	s	83	HIS
53	v	36	GLN
54	y	36	GLN
55	z	32	ASN
55	z	152	ASN
55	z	228	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	A	2839/2904 (97%)	546 (19%)	71 (2%)
32	a	1532/1542 (99%)	305 (19%)	0
8	B	119/120 (99%)	21 (17%)	3 (2%)
All	All	4490/4566 (98%)	872 (19%)	74 (1%)

All (872) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	B	4	C
8	B	9	G
8	B	14	U
8	B	15	A
8	B	25	U
8	B	35	C
8	B	37	C
8	B	38	C
8	B	42	C
8	B	43	C
8	B	45	A
8	B	52	A
8	B	56	G
8	B	67	G
8	B	88	C
8	B	89	U
8	B	90	C
8	B	99	A
8	B	100	G
8	B	109	A
8	B	112	G
31	A	3	U
31	A	4	U
31	A	9	G
31	A	10	A
31	A	12	U
31	A	25	U
31	A	34	U
31	A	35	G
31	A	58	G
31	A	63	A
31	A	65	U
31	A	71	A
31	A	74	A
31	A	75	G

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Mol	Chain	Res	Type
31	A	96	C
31	A	100	U
31	A	101	A
31	A	103	A
31	A	104	A
31	A	117	G
31	A	118	A
31	A	119	A
31	A	120	U
31	A	125	A
31	A	131	A
31	A	139	U
31	A	140	C
31	A	141	G
31	A	142	A
31	A	149	A
31	A	160	A
31	A	165	A
31	A	168	G
31	A	181	A
31	A	196	A
31	A	199	A
31	A	200	U
31	A	207	A
31	A	215	G
31	A	216	A
31	A	221	A
31	A	222	A
31	A	233	A
31	A	248	G
31	A	264	C
31	A	265	A
31	A	268	C
31	A	269	C
31	A	270	A
31	A	274	C
31	A	275	C
31	A	277	G
31	A	280	U
31	A	287	G
31	A	289	G
31	A	305	C

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Mol	Chain	Res	Type
31	A	310	A
31	A	311	A
31	A	329	G
31	A	330	A
31	A	353	C
31	A	356	G
31	A	357	C
31	A	359	G
31	A	361	G
31	A	362	A
31	A	370	G
31	A	375	G
31	A	383	C
31	A	385	C
31	A	386	G
31	A	392	U
31	A	403	U
31	A	411	G
31	A	412	A
31	A	419	U
31	A	420	C
31	A	427	U
31	A	435	C
31	A	447	A
31	A	456	C
31	A	473	G
31	A	477	A
31	A	479	A
31	A	480	A
31	A	481	G
31	A	489	G
31	A	490	C
31	A	491	G
31	A	501	A
31	A	503	A
31	A	504	A
31	A	505	A
31	A	508	A
31	A	509	C
31	A	511	U
31	A	530	G
31	A	531	C

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Mol	Chain	Res	Type
31	A	532	A
31	A	533	G
31	A	538	A
31	A	544	C
31	A	545	U
31	A	546	U
31	A	547	A
31	A	548	G
31	A	549	G
31	A	557	C
31	A	563	A
31	A	572	A
31	A	573	U
31	A	575	A
31	A	585	G
31	A	586	A
31	A	592	A
31	A	603	A
31	A	613	A
31	A	614	A
31	A	615	U
31	A	622	G
31	A	627	A
31	A	637	A
31	A	642	U
31	A	645	C
31	A	647	G
31	A	653	U
31	A	654	A
31	A	655	A
31	A	658	U
31	A	662	G
31	A	664	G
31	A	685	A
31	A	686	U
31	A	687	C
31	A	696	G
31	A	712	G
31	A	713	G
31	A	730	A
31	A	747	5MU
31	A	760	G

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Mol	Chain	Res	Type
31	A	764	A
31	A	772	C
31	A	775	G
31	A	776	G
31	A	782	A
31	A	783	A
31	A	784	G
31	A	785	G
31	A	792	A
31	A	798	G
31	A	802	A
31	A	805	G
31	A	812	C
31	A	816	C
31	A	827	U
31	A	828	U
31	A	846	U
31	A	847	U
31	A	858	G
31	A	859	G
31	A	860	U
31	A	861	A
31	A	876	C
31	A	877	A
31	A	880	G
31	A	888	C
31	A	890	C
31	A	891	G
31	A	895	U
31	A	896	A
31	A	900	A
31	A	901	C
31	A	907	G
31	A	910	A
31	A	913	U
31	A	914	G
31	A	915	C
31	A	931	U
31	A	946	C
31	A	961	C
31	A	962	G
31	A	974	G

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Mol	Chain	Res	Type
31	A	983	A
31	A	984	A
31	A	985	C
31	A	996	A
31	A	997	G
31	A	1005	C
31	A	1012	U
31	A	1013	C
31	A	1022	G
31	A	1026	G
31	A	1033	U
31	A	1040	A
31	A	1041	G
31	A	1042	G
31	A	1045	C
31	A	1046	A
31	A	1047	G
31	A	1108	U
31	A	1109	C
31	A	1110	G
31	A	1111	A
31	A	1112	G
31	A	1115	G
31	A	1118	C
31	A	1119	U
31	A	1128	G
31	A	1129	A
31	A	1132	U
31	A	1133	A
31	A	1135	C
31	A	1136	G
31	A	1141	U
31	A	1142	A
31	A	1163	G
31	A	1164	C
31	A	1167	C
31	A	1187	G
31	A	1188	U
31	A	1240	U
31	A	1247	A
31	A	1248	G
31	A	1250	G

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Mol	Chain	Res	Type
31	A	1253	A
31	A	1256	G
31	A	1271	G
31	A	1272	A
31	A	1273	U
31	A	1279	G
31	A	1280	G
31	A	1289	C
31	A	1294	U
31	A	1300	G
31	A	1301	A
31	A	1309	G
31	A	1321	A
31	A	1322	A
31	A	1338	G
31	A	1340	U
31	A	1345	C
31	A	1357	C
31	A	1365	A
31	A	1379	U
31	A	1383	A
31	A	1396	U
31	A	1397	U
31	A	1402	U
31	A	1414	C
31	A	1416	G
31	A	1417	C
31	A	1424	G
31	A	1427	A
31	A	1428	C
31	A	1439	A
31	A	1451	C
31	A	1452	G
31	A	1453	A
31	A	1455	G
31	A	1458	U
31	A	1459	G
31	A	1465	G
31	A	1470	A
31	A	1482	G
31	A	1484	U
31	A	1490	A

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Mol	Chain	Res	Type
31	A	1493	C
31	A	1497	U
31	A	1499	C
31	A	1504	A
31	A	1505	A
31	A	1506	U
31	A	1507	C
31	A	1508	A
31	A	1509	A
31	A	1510	G
31	A	1515	A
31	A	1516	G
31	A	1523	U
31	A	1529	G
31	A	1533	C
31	A	1534	U
31	A	1535	A
31	A	1536	C
31	A	1537	G
31	A	1538	G
31	A	1539	U
31	A	1542	U
31	A	1547	C
31	A	1551	A
31	A	1554	U
31	A	1558	C
31	A	1569	A
31	A	1577	C
31	A	1578	U
31	A	1584	U
31	A	1607	C
31	A	1608	A
31	A	1609	A
31	A	1634	A
31	A	1636	U
31	A	1644	C
31	A	1647	U
31	A	1648	U
31	A	1649	G
31	A	1669	A
31	A	1674	G
31	A	1675	C

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Mol	Chain	Res	Type
31	A	1714	U
31	A	1715	G
31	A	1729	U
31	A	1730	C
31	A	1731	G
31	A	1732	C
31	A	1750	G
31	A	1759	A
31	A	1764	C
31	A	1773	A
31	A	1774	C
31	A	1776	G
31	A	1782	U
31	A	1791	A
31	A	1800	C
31	A	1801	A
31	A	1802	A
31	A	1808	A
31	A	1813	G
31	A	1816	C
31	A	1829	A
31	A	1842	G
31	A	1847	A
31	A	1848	A
31	A	1857	G
31	A	1858	A
31	A	1866	A
31	A	1906	G
31	A	1913	A
31	A	1914	C
31	A	1927	A
31	A	1929	G
31	A	1930	G
31	A	1932	A
31	A	1937	A
31	A	1938	A
31	A	1955	U
31	A	1965	C
31	A	1966	A
31	A	1967	C
31	A	1970	A
31	A	1971	U

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Mol	Chain	Res	Type
31	A	1972	G
31	A	1991	U
31	A	1993	U
31	A	2012	G
31	A	2017	U
31	A	2019	A
31	A	2020	A
31	A	2023	C
31	A	2027	G
31	A	2031	A
31	A	2033	A
31	A	2041	U
31	A	2043	C
31	A	2044	C
31	A	2055	C
31	A	2056	G
31	A	2060	A
31	A	2061	G
31	A	2062	A
31	A	2069	G7M
31	A	2080	A
31	A	2100	G
31	A	2105	U
31	A	2109	U
31	A	2110	G
31	A	2111	U
31	A	2112	G
31	A	2113	U
31	A	2114	A
31	A	2115	G
31	A	2116	G
31	A	2117	A
31	A	2118	U
31	A	2119	A
31	A	2120	G
31	A	2123	G
31	A	2124	G
31	A	2125	G
31	A	2127	G
31	A	2128	G
31	A	2130	U
31	A	2131	U

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Mol	Chain	Res	Type
31	A	2132	U
31	A	2133	G
31	A	2137	U
31	A	2138	G
31	A	2140	G
31	A	2141	G
31	A	2144	G
31	A	2145	C
31	A	2146	C
31	A	2147	A
31	A	2149	U
31	A	2152	G
31	A	2153	C
31	A	2157	G
31	A	2158	A
31	A	2159	G
31	A	2164	C
31	A	2166	U
31	A	2167	U
31	A	2169	A
31	A	2171	A
31	A	2172	U
31	A	2173	A
31	A	2179	C
31	A	2180	U
31	A	2181	U
31	A	2182	U
31	A	2189	U
31	A	2193	G
31	A	2194	U
31	A	2198	A
31	A	2203	U
31	A	2204	G
31	A	2211	A
31	A	2212	A
31	A	2214	C
31	A	2223	G
31	A	2225	A
31	A	2233	U
31	A	2238	G
31	A	2239	G
31	A	2268	A

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Mol	Chain	Res	Type
31	A	2270	A
31	A	2275	C
31	A	2276	G
31	A	2278	A
31	A	2282	G
31	A	2283	C
31	A	2286	G
31	A	2287	A
31	A	2295	C
31	A	2304	G
31	A	2305	U
31	A	2306	C
31	A	2307	G
31	A	2308	G
31	A	2311	A
31	A	2312	U
31	A	2321	U
31	A	2322	A
31	A	2324	U
31	A	2325	G
31	A	2327	A
31	A	2333	A
31	A	2335	A
31	A	2347	C
31	A	2350	C
31	A	2382	G
31	A	2383	G
31	A	2385	C
31	A	2402	U
31	A	2406	A
31	A	2424	C
31	A	2425	A
31	A	2428	G
31	A	2429	G
31	A	2430	A
31	A	2431	U
31	A	2435	A
31	A	2441	U
31	A	2448	A
31	A	2459	A
31	A	2469	A
31	A	2470	G

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Mol	Chain	Res	Type
31	A	2474	U
31	A	2476	A
31	A	2478	A
31	A	2502	G
31	A	2505	G
31	A	2506	U
31	A	2508	G
31	A	2518	A
31	A	2529	G
31	A	2530	A
31	A	2533	U
31	A	2535	G
31	A	2547	A
31	A	2550	G
31	A	2556	C
31	A	2566	A
31	A	2567	G
31	A	2573	C
31	A	2601	C
31	A	2602	A
31	A	2609	U
31	A	2612	C
31	A	2613	U
31	A	2629	U
31	A	2654	A
31	A	2661	G
31	A	2663	G
31	A	2669	G
31	A	2681	C
31	A	2682	A
31	A	2689	U
31	A	2690	U
31	A	2693	G
31	A	2696	U
31	A	2705	A
31	A	2714	G
31	A	2726	A
31	A	2741	A
31	A	2744	G
31	A	2746	U
31	A	2748	A
31	A	2751	G

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Mol	Chain	Res	Type
31	A	2756	U
31	A	2757	A
31	A	2762	C
31	A	2765	A
31	A	2769	U
31	A	2773	C
31	A	2778	A
31	A	2791	G
31	A	2798	U
31	A	2800	A
31	A	2820	A
31	A	2821	A
31	A	2823	A
31	A	2836	U
31	A	2843	G
31	A	2861	U
31	A	2883	A
31	A	2884	U
31	A	2888	C
31	A	2893	A
31	A	2895	G
31	A	2896	C
31	A	2897	U
31	A	2898	U
31	A	2899	A
31	A	2900	A
31	A	2901	C
31	A	2903	U
32	a	2	A
32	a	5	U
32	a	9	G
32	a	14	U
32	a	15	G
32	a	29	U
32	a	32	A
32	a	39	G
32	a	47	C
32	a	48	C
32	a	50	A
32	a	51	A
32	a	57	G
32	a	58	C

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Mol	Chain	Res	Type
32	a	65	A
32	a	66	A
32	a	70	U
32	a	71	A
32	a	74	A
32	a	78	A
32	a	79	G
32	a	80	A
32	a	84	U
32	a	85	U
32	a	86	G
32	a	88	U
32	a	90	C
32	a	92	U
32	a	93	U
32	a	94	G
32	a	95	C
32	a	96	U
32	a	112	G
32	a	120	A
32	a	121	U
32	a	128	G
32	a	130	A
32	a	131	A
32	a	138	G
32	a	142	G
32	a	144	G
32	a	163	C
32	a	164	G
32	a	182	A
32	a	183	C
32	a	184	G
32	a	188	C
32	a	196	A
32	a	197	A
32	a	199	A
32	a	203	G
32	a	205	A
32	a	206	C
32	a	207	C
32	a	208	U
32	a	210	C

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Mol	Chain	Res	Type
32	a	212	G
32	a	220	G
32	a	226	G
32	a	240	G
32	a	245	U
32	a	247	G
32	a	251	G
32	a	262	A
32	a	263	A
32	a	266	G
32	a	267	C
32	a	271	C
32	a	280	C
32	a	281	G
32	a	289	G
32	a	298	A
32	a	316	C
32	a	321	A
32	a	328	C
32	a	329	A
32	a	337	G
32	a	344	A
32	a	352	C
32	a	354	G
32	a	367	U
32	a	369	G
32	a	370	C
32	a	372	C
32	a	382	A
32	a	384	G
32	a	392	C
32	a	406	G
32	a	411	A
32	a	412	A
32	a	413	G
32	a	419	C
32	a	421	U
32	a	422	C
32	a	424	G
32	a	429	U
32	a	430	A
32	a	438	U

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Mol	Chain	Res	Type
32	a	439	U
32	a	440	C
32	a	446	G
32	a	459	A
32	a	463	U
32	a	464	U
32	a	467	U
32	a	468	A
32	a	475	C
32	a	479	U
32	a	484	G
32	a	486	U
32	a	500	G
32	a	503	C
32	a	511	C
32	a	518	C
32	a	520	A
32	a	521	G
32	a	527	G7M
32	a	531	U
32	a	532	A
32	a	533	A
32	a	542	G
32	a	547	A
32	a	550	G
32	a	559	A
32	a	563	A
32	a	564	C
32	a	572	A
32	a	573	A
32	a	576	C
32	a	577	G
32	a	579	A
32	a	592	G
32	a	596	A
32	a	607	A
32	a	625	U
32	a	632	U
32	a	633	G
32	a	639	G
32	a	642	A
32	a	650	G

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Mol	Chain	Res	Type
32	a	653	U
32	a	665	A
32	a	673	A
32	a	674	G
32	a	679	C
32	a	680	C
32	a	683	G
32	a	721	G
32	a	722	G
32	a	723	U
32	a	724	G
32	a	726	C
32	a	734	G
32	a	737	C
32	a	739	C
32	a	747	A
32	a	748	G
32	a	755	G
32	a	760	G
32	a	764	C
32	a	777	A
32	a	793	U
32	a	794	A
32	a	802	A
32	a	814	A
32	a	815	A
32	a	817	C
32	a	829	G
32	a	836	G
32	a	837	U
32	a	838	G
32	a	847	G
32	a	858	G
32	a	860	A
32	a	884	U
32	a	885	G
32	a	887	G
32	a	890	G
32	a	914	A
32	a	916	U
32	a	919	A
32	a	922	G

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Mol	Chain	Res	Type
32	a	926	G
32	a	932	C
32	a	934	C
32	a	935	A
32	a	936	C
32	a	939	G
32	a	940	C
32	a	943	U
32	a	952	U
32	a	954	G
32	a	958	A
32	a	960	U
32	a	963	G
32	a	965	U
32	a	966	2MG
32	a	969	A
32	a	971	G
32	a	972	C
32	a	975	A
32	a	976	G
32	a	977	A
32	a	992	U
32	a	993	G
32	a	994	A
32	a	1004	A
32	a	1009	U
32	a	1014	A
32	a	1016	A
32	a	1017	U
32	a	1020	G
32	a	1026	G
32	a	1027	C
32	a	1028	C
32	a	1030	U
32	a	1031	C
32	a	1032	G
32	a	1033	G
32	a	1034	G
32	a	1036	A
32	a	1046	A
32	a	1064	G
32	a	1065	U

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Mol	Chain	Res	Type
32	a	1070	U
32	a	1079	G
32	a	1080	A
32	a	1085	U
32	a	1090	U
32	a	1094	G
32	a	1095	U
32	a	1101	A
32	a	1124	G
32	a	1130	A
32	a	1132	C
32	a	1137	C
32	a	1138	G
32	a	1139	G
32	a	1159	U
32	a	1168	U
32	a	1169	A
32	a	1171	A
32	a	1183	U
32	a	1184	G
32	a	1196	A
32	a	1197	A
32	a	1213	A
32	a	1214	C
32	a	1225	A
32	a	1226	C
32	a	1227	A
32	a	1228	C
32	a	1233	G
32	a	1238	A
32	a	1257	A
32	a	1258	G
32	a	1260	G
32	a	1261	A
32	a	1273	C
32	a	1280	A
32	a	1281	C
32	a	1286	U
32	a	1287	A
32	a	1290	G
32	a	1294	G
32	a	1300	G

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Mol	Chain	Res	Type
32	a	1301	U
32	a	1302	C
32	a	1317	C
32	a	1319	A
32	a	1320	C
32	a	1322	C
32	a	1338	G
32	a	1346	A
32	a	1348	U
32	a	1363	A
32	a	1364	U
32	a	1370	G
32	a	1376	U
32	a	1379	G
32	a	1388	C
32	a	1398	A
32	a	1419	G
32	a	1440	U
32	a	1441	A
32	a	1442	G
32	a	1446	A
32	a	1452	C
32	a	1453	G
32	a	1487	G
32	a	1492	A
32	a	1494	G
32	a	1497	G
32	a	1503	A
32	a	1506	U
32	a	1517	G
32	a	1529	G
32	a	1530	G
32	a	1531	A
32	a	1532	U
32	a	1533	C
32	a	1535	C
32	a	1537	U
32	a	1538	C
32	a	1539	C

All (74) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	B	12	A
8	B	14	U
8	B	88	C
31	A	3	U
31	A	4	U
31	A	102	U
31	A	183	C
31	A	196	A
31	A	199	A
31	A	264	C
31	A	310	A
31	A	446	G
31	A	503	A
31	A	532	A
31	A	545	U
31	A	547	A
31	A	641	U
31	A	654	A
31	A	685	A
31	A	733	G
31	A	784	G
31	A	827	U
31	A	846	U
31	A	884	U
31	A	895	U
31	A	899	A
31	A	961	C
31	A	973	A
31	A	984	A
31	A	993	G
31	A	1044	C
31	A	1046	A
31	A	1107	G
31	A	1124	G
31	A	1128	G
31	A	1133	A
31	A	1141	U
31	A	1142	A
31	A	1187	G
31	A	1396	U
31	A	1416	G
31	A	1419	A
31	A	1451	C

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Mol	Chain	Res	Type
31	A	1458	U
31	A	1497	U
31	A	1507	C
31	A	1509	A
31	A	1523	U
31	A	1533	C
31	A	1536	C
31	A	1608	A
31	A	1626	A
31	A	1647	U
31	A	1857	G
31	A	2035	G
31	A	2144	G
31	A	2157	G
31	A	2163	A
31	A	2193	G
31	A	2275	C
31	A	2282	G
31	A	2308	G
31	A	2311	A
31	A	2324	U
31	A	2430	A
31	A	2518	A
31	A	2529	G
31	A	2581	G
31	A	2681	C
31	A	2751	G
31	A	2756	U
31	A	2820	A
31	A	2873	A
31	A	2895	G

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

39 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	$\#\|Z\|>2$
31	PSU	A	955	31	18,21,22	0.94	1 (5%)	22,30,33	0.61	0
18	4D4	O	81	18	9,11,12	0.53	0	8,13,15	0.81	0
31	PSU	A	1911	31	18,21,22	0.90	1 (5%)	22,30,33	0.74	1 (4%)
31	H2U	A	2449	31	18,21,22	0.74	1 (5%)	21,30,33	0.81	1 (4%)
31	OMU	A	2552	31	19,22,23	0.32	0	26,31,34	0.46	0
43	D2T	l	89	43	7,9,10	1.02	0	6,11,13	1.76	3 (50%)
32	2MG	a	1207	32	23,26,27	0.39	0	32,38,41	0.46	0
31	OMC	A	2498	31,57	19,22,23	0.32	0	26,31,34	0.54	0
31	PSU	A	2580	31	18,21,22	0.91	1 (5%)	22,30,33	0.84	1 (4%)
31	PSU	A	2605	31	18,21,22	0.87	1 (5%)	22,30,33	0.79	0
31	G7M	A	2069	31	23,26,27	0.65	1 (4%)	35,39,42	0.63	0
32	MA6	a	1518	32	23,26,27	0.25	0	34,38,41	0.66	1 (2%)
31	3TD	A	1915	31	18,22,23	1.05	1 (5%)	22,32,35	0.77	0
32	5MC	a	967	32	18,22,23	0.33	0	26,32,35	0.56	0
31	PSU	A	746	31,57	18,21,22	0.93	1 (5%)	22,30,33	0.63	0
32	2MG	a	1516	32	23,26,27	0.36	0	32,38,41	0.56	0
32	G7M	a	527	32	23,26,27	0.79	1 (4%)	35,39,42	0.68	1 (2%)
31	OMG	A	2251	31	23,26,27	0.34	0	33,38,41	0.41	0
10	MEQ	E	150	10	8,9,10	0.45	0	5,10,12	1.48	1 (20%)
31	2MG	A	1835	31	23,26,27	0.32	0	32,38,41	0.49	0
31	PSU	A	1917	31	18,21,22	0.93	1 (5%)	22,30,33	0.63	0
31	6MZ	A	2030	31	22,25,26	0.43	0	30,36,39	0.67	0
31	PSU	A	2604	31	18,21,22	0.98	1 (5%)	22,30,33	0.92	1 (4%)
31	6MZ	A	1618	31	22,25,26	0.29	0	30,36,39	0.52	0
31	PSU	A	2504	31	18,21,22	0.88	1 (5%)	22,30,33	0.85	1 (4%)
32	2MG	a	966	32	23,26,27	0.42	0	32,38,41	0.34	0
31	5MC	A	1962	31	18,22,23	0.36	0	26,32,35	0.48	0
31	5MU	A	1939	31	19,22,23	0.31	0	28,32,35	0.40	0
31	1MG	A	745	31	22,26,27	0.53	0	33,39,42	0.51	0
32	PSU	a	516	32	18,21,22	0.89	1 (5%)	22,30,33	0.64	0
32	4OC	a	1402	32	20,23,24	0.41	0	26,32,35	0.56	0
32	MA6	a	1519	32	23,26,27	0.26	0	34,38,41	0.75	1 (2%)
32	5MC	a	1407	32	18,22,23	0.31	0	26,32,35	0.61	0
32	UR3	a	1498	32	19,22,23	0.32	0	26,32,35	0.73	0
31	PSU	A	2457	31	18,21,22	0.89	1 (5%)	22,30,33	0.69	0
42	IAS	k	119	42	6,7,8	0.86	0	6,8,10	0.96	0
31	5MU	A	747	31	19,22,23	0.31	0	28,32,35	0.33	0
31	2MA	A	2503	31,57	22,25,26	0.92	1 (4%)	33,37,40	1.14	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	2MG	A	2445	31	23,26,27	0.39	0	32,38,41	0.41	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
31	PSU	A	955	31	-	0/7/25/26	0/2/2/2
18	4D4	O	81	18	-	1/11/12/14	-
31	PSU	A	1911	31	-	0/7/25/26	0/2/2/2
31	H2U	A	2449	31	-	0/7/38/39	0/2/2/2
31	OMU	A	2552	31	-	1/9/27/28	0/2/2/2
43	D2T	l	89	43	-	1/7/12/14	-
32	2MG	a	1207	32	-	0/9/27/28	0/3/3/3
31	OMC	A	2498	31,57	-	0/9/27/28	0/2/2/2
31	PSU	A	2580	31	-	0/7/25/26	0/2/2/2
31	PSU	A	2605	31	-	0/7/25/26	0/2/2/2
31	G7M	A	2069	31	-	2/7/25/26	0/3/3/3
32	MA6	a	1518	32	-	0/11/29/30	0/3/3/3
31	3TD	A	1915	31	-	1/7/25/26	0/2/2/2
32	5MC	a	967	32	-	0/7/25/26	0/2/2/2
31	PSU	A	746	31,57	-	1/7/25/26	0/2/2/2
32	2MG	a	1516	32	-	0/9/27/28	0/3/3/3
32	G7M	a	527	32	-	2/7/25/26	0/3/3/3
31	OMG	A	2251	31	-	0/9/27/28	0/3/3/3
10	MEQ	E	150	10	-	2/8/9/11	-
31	2MG	A	1835	31	-	0/9/27/28	0/3/3/3
31	PSU	A	1917	31	-	0/7/25/26	0/2/2/2
31	6MZ	A	2030	31	-	1/9/27/28	0/3/3/3
31	PSU	A	2604	31	-	0/7/25/26	0/2/2/2
31	6MZ	A	1618	31	-	0/9/27/28	0/3/3/3
31	PSU	A	2504	31	-	0/7/25/26	0/2/2/2
32	2MG	a	966	32	-	2/9/27/28	0/3/3/3
31	5MC	A	1962	31	-	0/7/25/26	0/2/2/2
31	5MU	A	1939	31	-	0/7/25/26	0/2/2/2
31	1MG	A	745	31	-	0/7/25/26	0/3/3/3
32	PSU	a	516	32	-	0/7/25/26	0/2/2/2
32	4OC	a	1402	32	-	1/9/29/30	0/2/2/2
32	MA6	a	1519	32	-	1/11/29/30	0/3/3/3
32	5MC	a	1407	32	-	1/7/25/26	0/2/2/2
32	UR3	a	1498	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	A	2457	31	-	0/7/25/26	0/2/2/2
42	IAS	k	119	42	-	0/7/7/8	-
31	5MU	A	747	31	-	0/7/25/26	0/2/2/2
31	2MA	A	2503	31,57	-	1/7/25/26	0/3/3/3
31	2MG	A	2445	31	-	2/9/27/28	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	1915	3TD	C6-C5	3.76	1.39	1.35
31	A	2604	PSU	C6-C5	3.69	1.39	1.35
31	A	746	PSU	C6-C5	3.62	1.39	1.35
31	A	1917	PSU	C6-C5	3.59	1.39	1.35
31	A	955	PSU	C6-C5	3.58	1.39	1.35
32	a	516	PSU	C6-C5	3.51	1.39	1.35
31	A	2457	PSU	C6-C5	3.45	1.39	1.35
31	A	1911	PSU	C6-C5	3.44	1.39	1.35
31	A	2580	PSU	C6-C5	3.36	1.39	1.35
31	A	2504	PSU	C6-C5	3.31	1.39	1.35
31	A	2605	PSU	C6-C5	3.17	1.39	1.35
32	a	527	G7M	C8-N7	2.98	1.38	1.33
31	A	2503	2MA	C6-N6	-2.42	1.28	1.34
31	A	2449	H2U	C2-N3	-2.19	1.34	1.38
31	A	2069	G7M	C8-N7	2.05	1.36	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	2503	2MA	C5-C4-N3	-3.15	123.65	127.19
31	A	2503	2MA	CM2-C2-N1	3.10	121.99	117.15
32	a	1519	MA6	C2-N1-C6	2.90	118.60	111.75
32	a	1518	MA6	C2-N1-C6	2.85	118.48	111.75
31	A	2580	PSU	C3'-C2'-C1'	2.77	104.86	101.64
10	E	150	MEQ	CB-CG-CD	2.46	118.53	113.04
43	l	89	D2T	OD1-CG-CB	-2.23	117.77	122.44
31	A	2449	H2U	N3-C2-N1	2.15	118.92	116.65
43	l	89	D2T	CB-CA-N	2.14	113.66	109.10
31	A	2604	PSU	C2'-C3'-C4'	-2.10	98.56	102.64
31	A	1911	PSU	C2'-C3'-C4'	-2.09	98.58	102.64
31	A	2504	PSU	C2'-C3'-C4'	-2.08	98.60	102.64
32	a	527	G7M	N9-C8-N7	-2.07	107.08	112.21
43	l	89	D2T	O-C-CA	-2.06	119.37	124.78

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	a	527	G7M	O4'-C4'-C5'-O5'
32	a	527	G7M	C3'-C4'-C5'-O5'
32	a	966	2MG	O4'-C4'-C5'-O5'
32	a	966	2MG	C3'-C4'-C5'-O5'
10	E	150	MEQ	OE1-CD-CG-CB
10	E	150	MEQ	NE2-CD-CG-CB
31	A	2445	2MG	C3'-C4'-C5'-O5'
32	a	1519	MA6	O4'-C4'-C5'-O5'
31	A	2069	G7M	C4'-C5'-O5'-P
31	A	2030	6MZ	O4'-C4'-C5'-O5'
31	A	2503	2MA	O4'-C4'-C5'-O5'
31	A	2552	OMU	C3'-C2'-O2'-CM2
32	a	1407	5MC	O4'-C4'-C5'-O5'
31	A	1915	3TD	O4'-C4'-C5'-O5'
31	A	2445	2MG	O4'-C4'-C5'-O5'
43	l	89	D2T	CG-CB-SB-CB1
31	A	746	PSU	O4'-C1'-C5-C6
32	a	1402	4OC	O4'-C4'-C5'-O5'
31	A	2069	G7M	O4'-C4'-C5'-O5'
18	O	81	4D4	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	a	1518	MA6	1	0
32	a	527	G7M	1	0
31	A	1917	PSU	1	0
31	A	2030	6MZ	1	0
32	a	1519	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 476 ligands modelled in this entry, 476 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

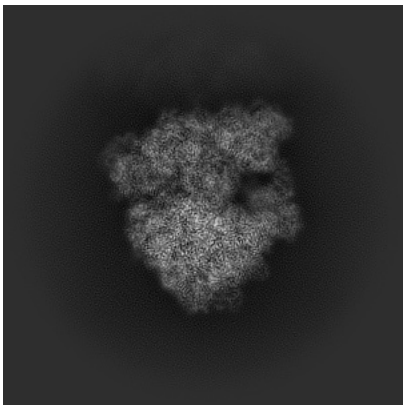
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60747. These allow visual inspection of the internal detail of the map and identification of artifacts.

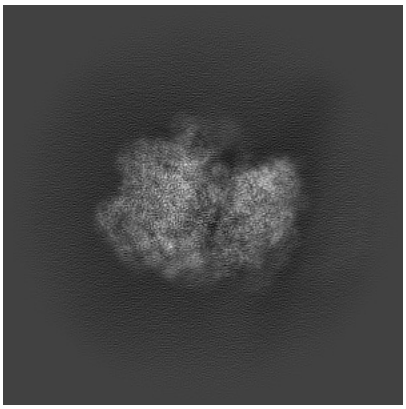
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

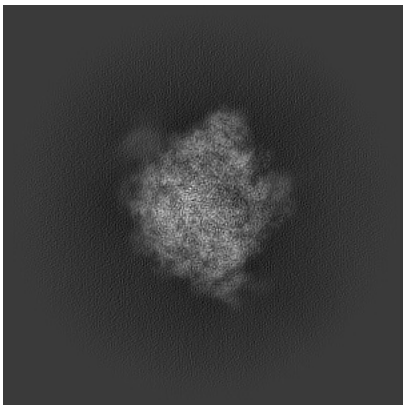
6.1.1 Primary map



X

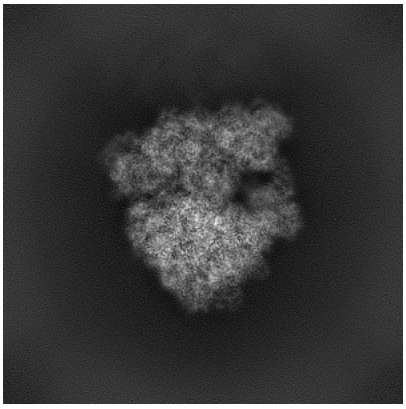


Y

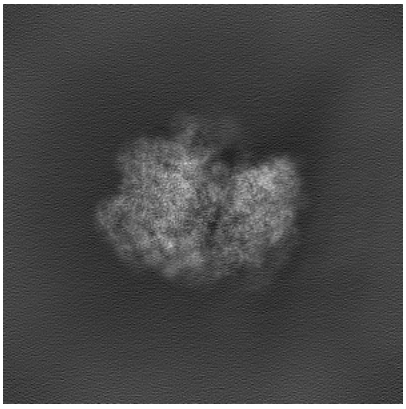


Z

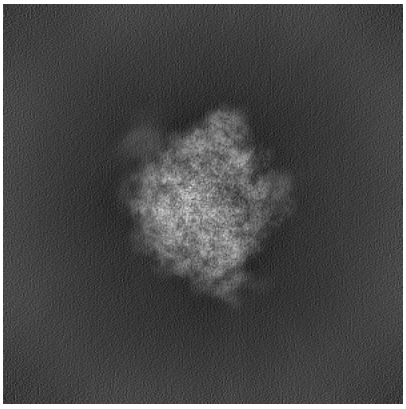
6.1.2 Raw map



X



Y

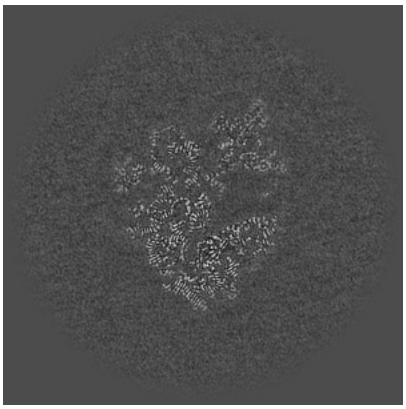


Z

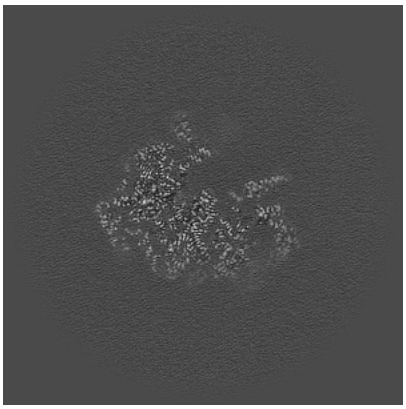
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

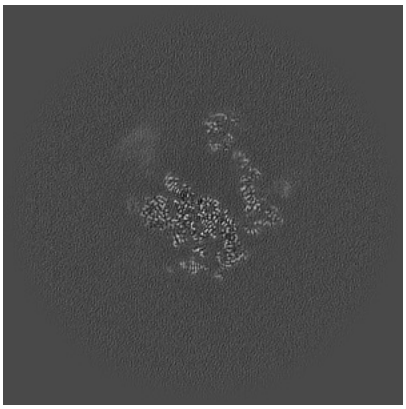
6.2.1 Primary map



X Index: 200

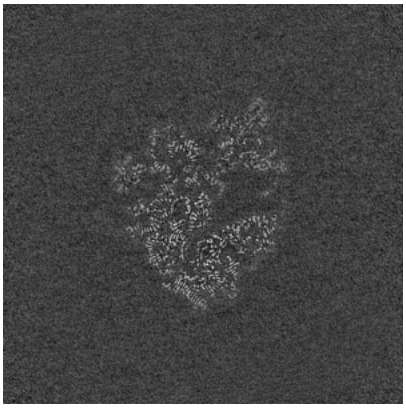


Y Index: 200

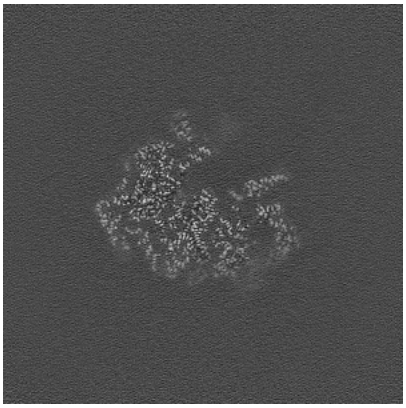


Z Index: 200

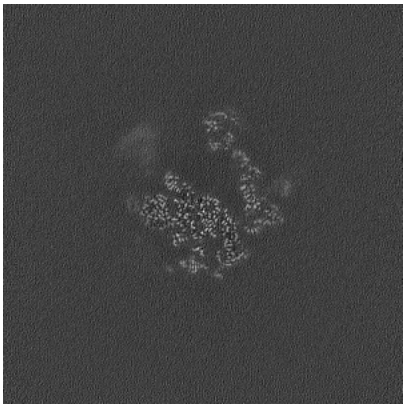
6.2.2 Raw map



X Index: 200



Y Index: 200

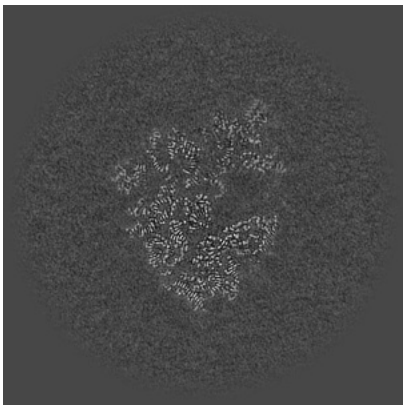


Z Index: 200

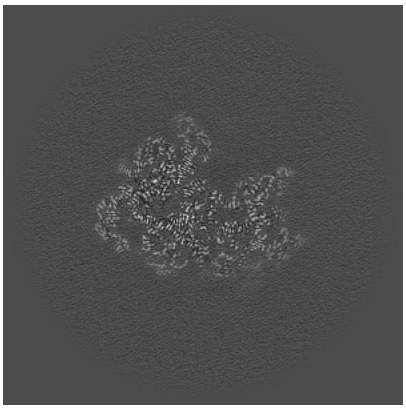
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

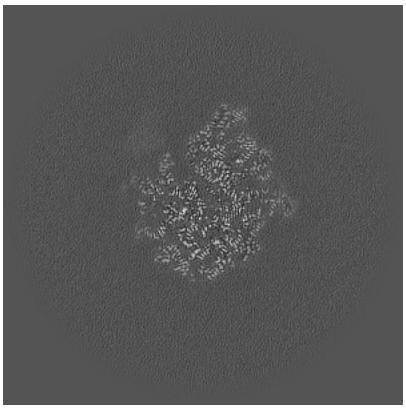
6.3.1 Primary map



X Index: 199

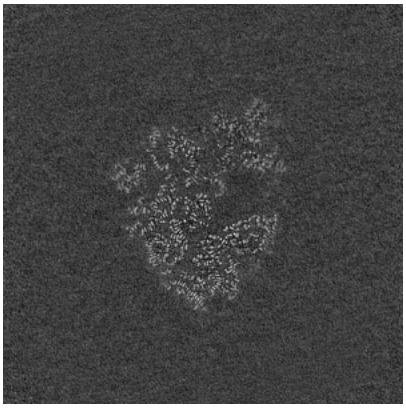


Y Index: 193

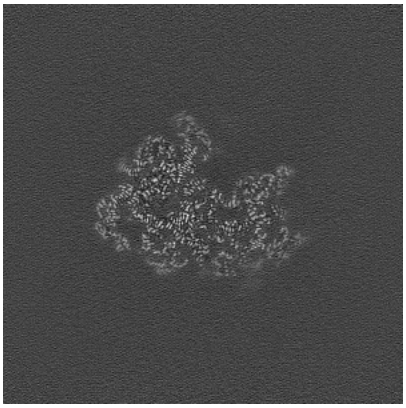


Z Index: 179

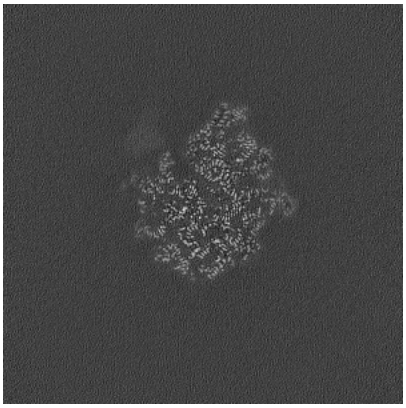
6.3.2 Raw map



X Index: 199



Y Index: 193

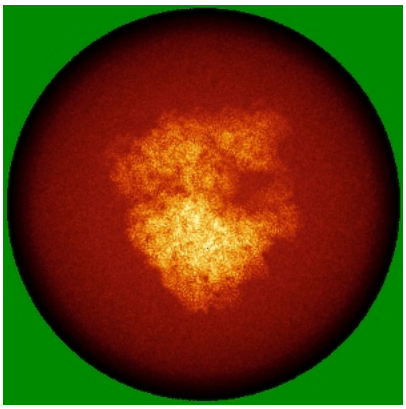


Z Index: 179

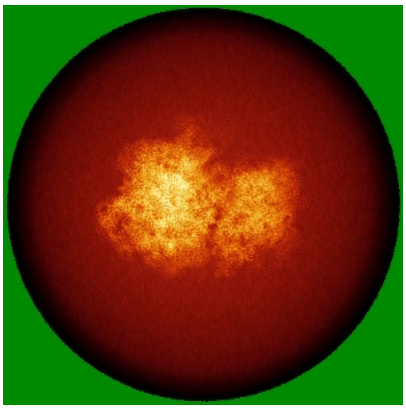
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

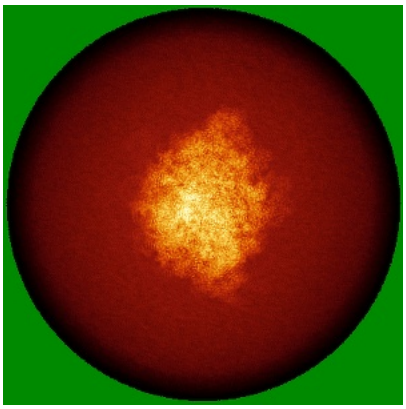
6.4.1 Primary map



X

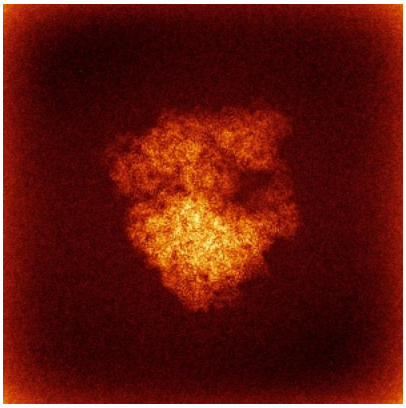


Y

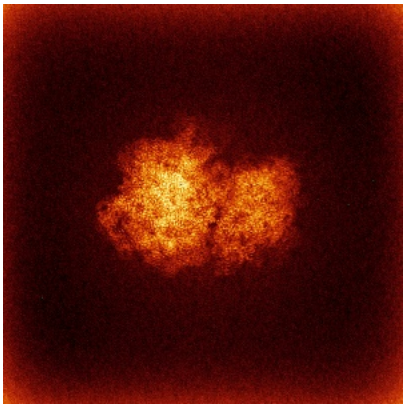


Z

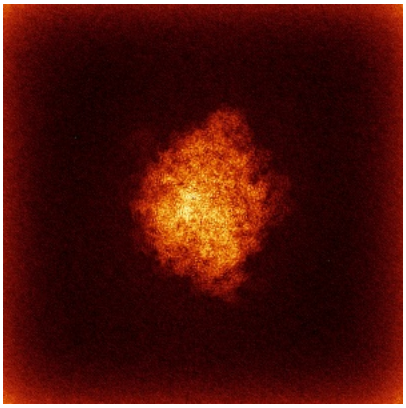
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

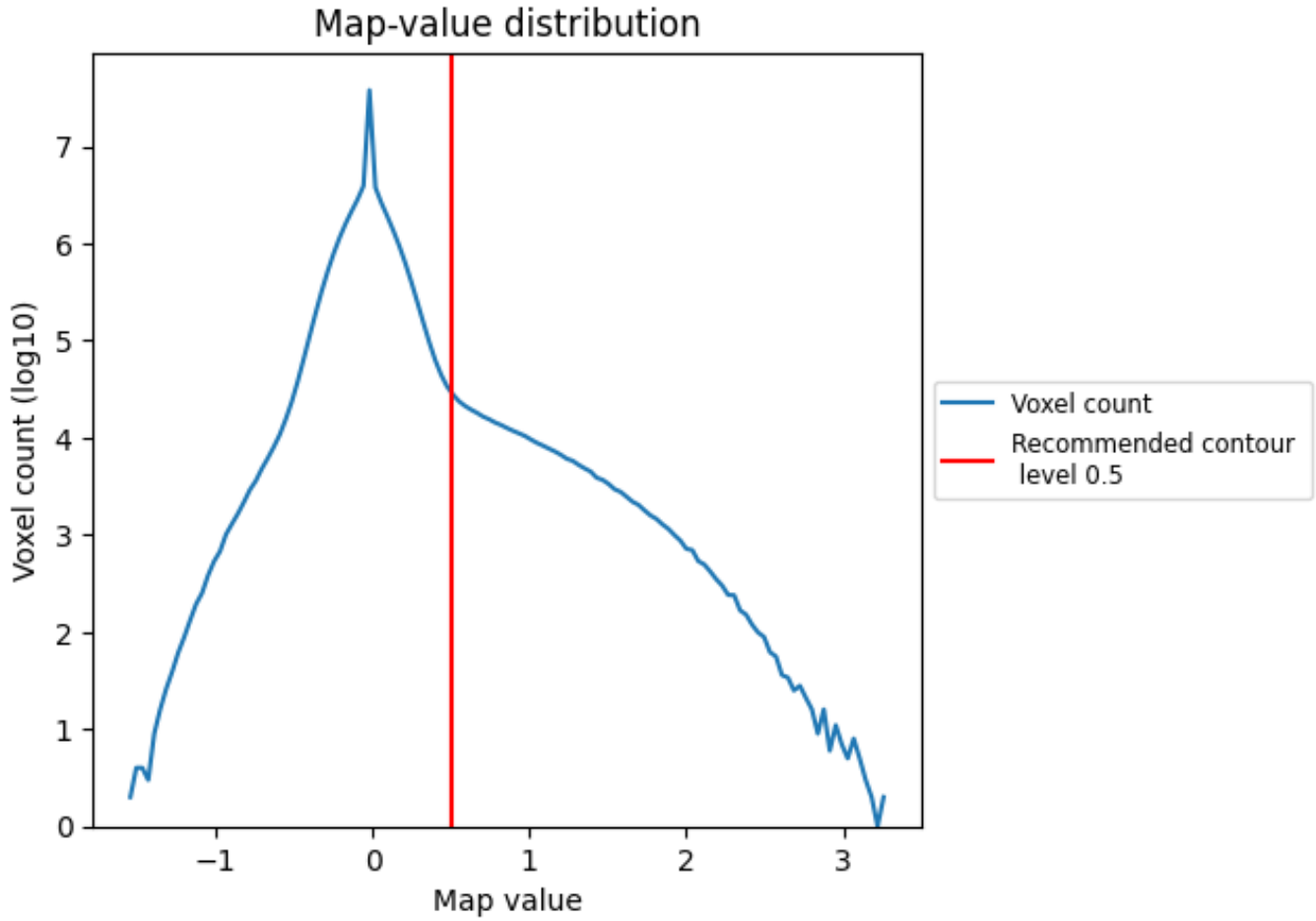
6.6 Mask visualisation (i)

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

7 Map analysis

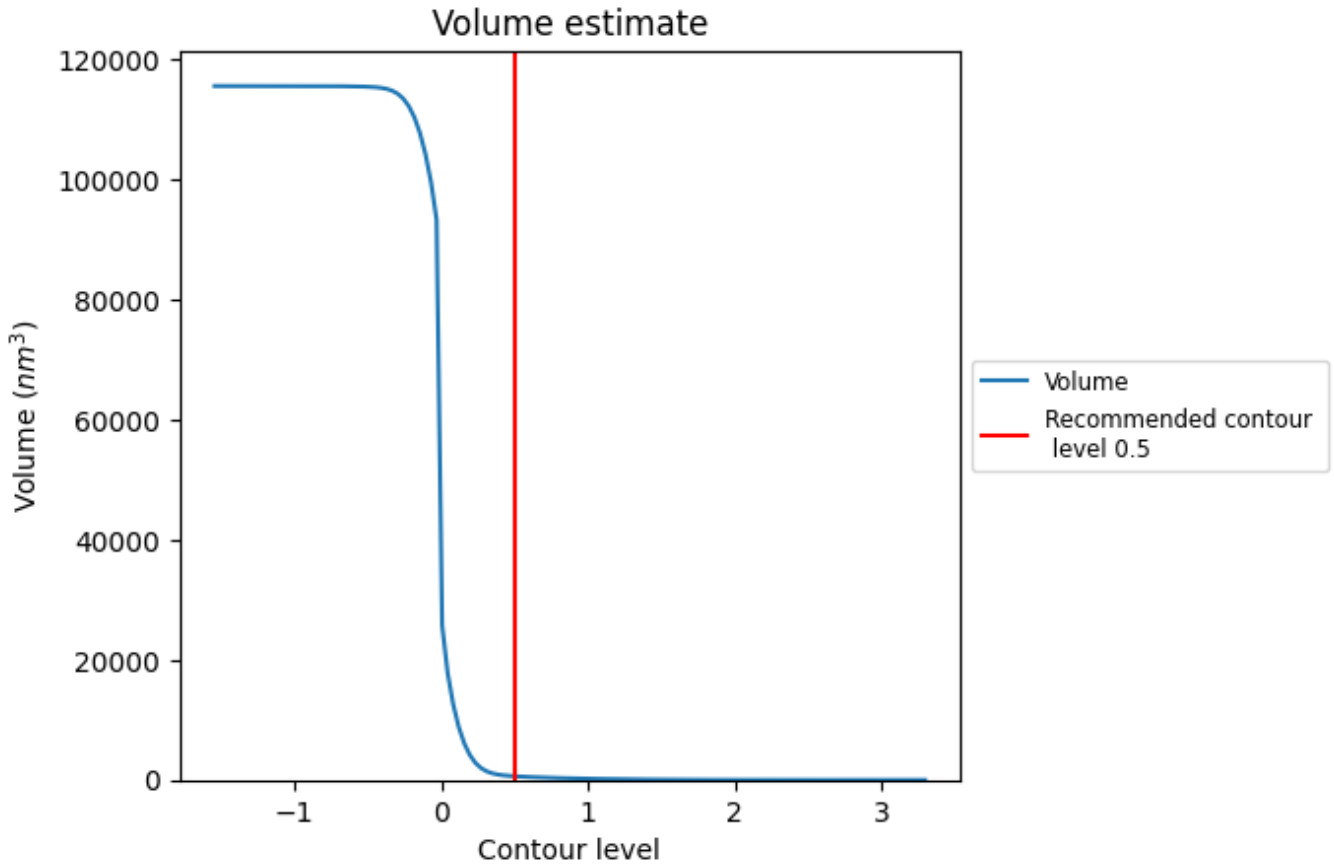
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

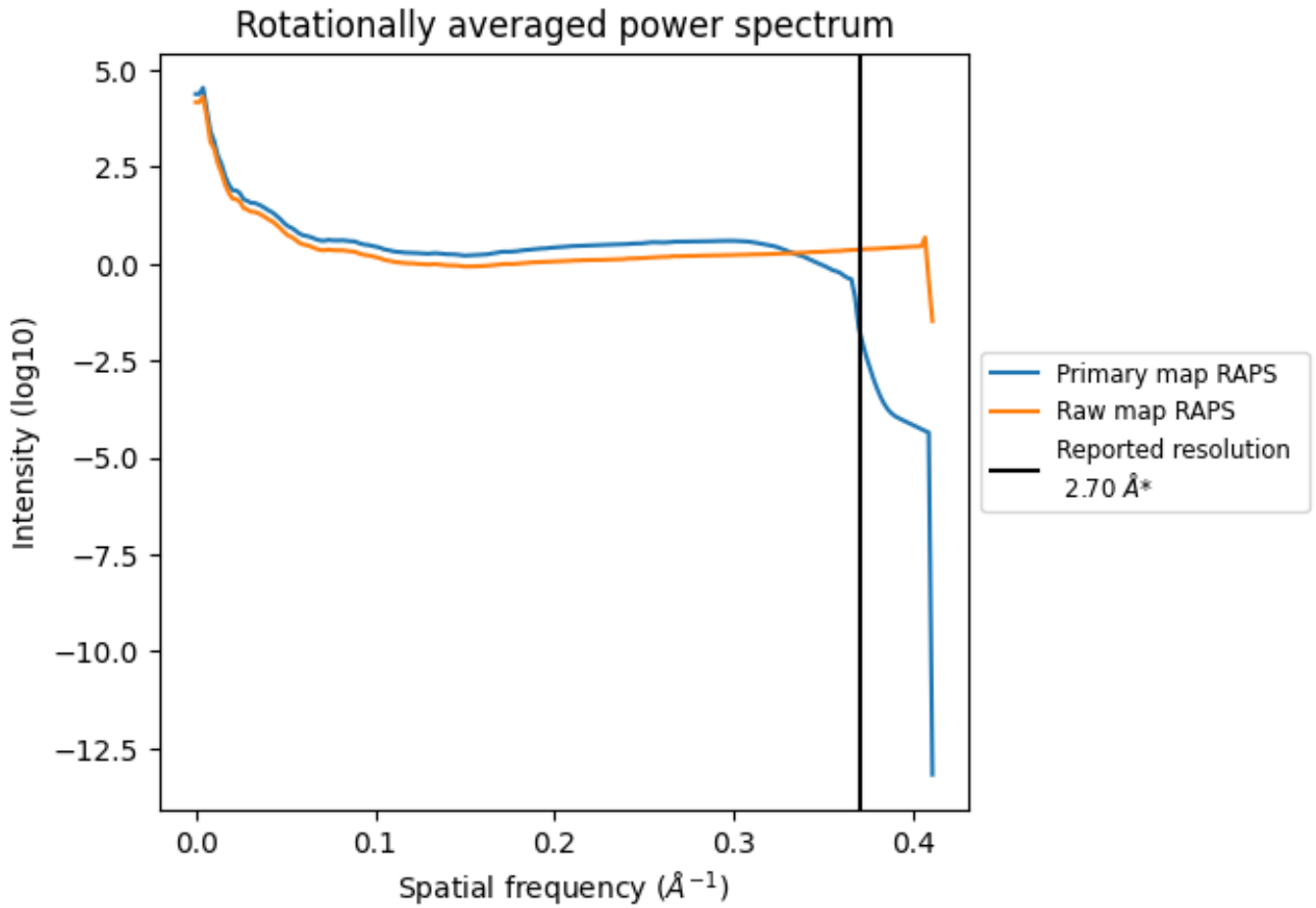
7.2 Volume estimate



The volume at the recommended contour level is 613 nm^3; this corresponds to an approximate mass of 554 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)

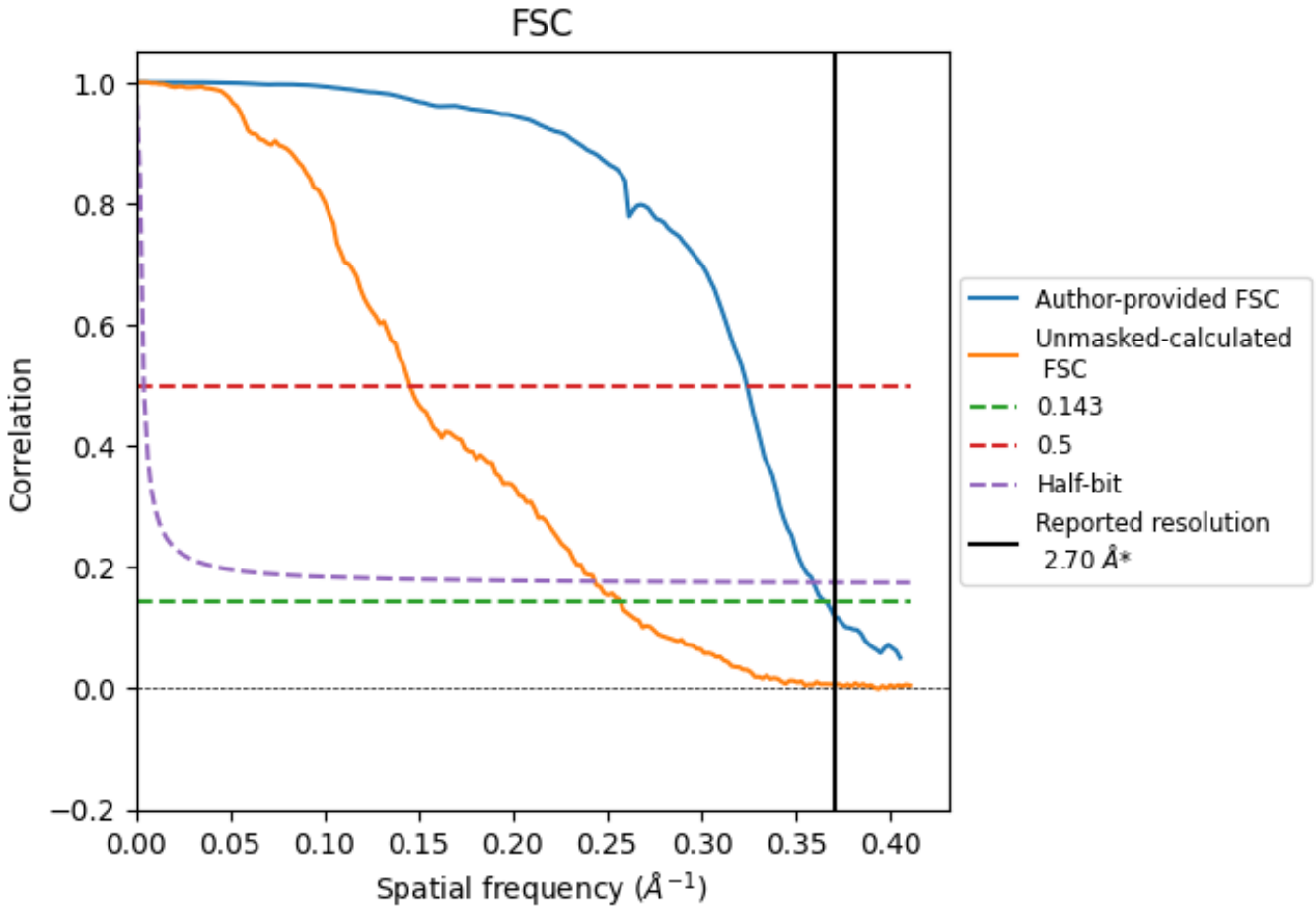


*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

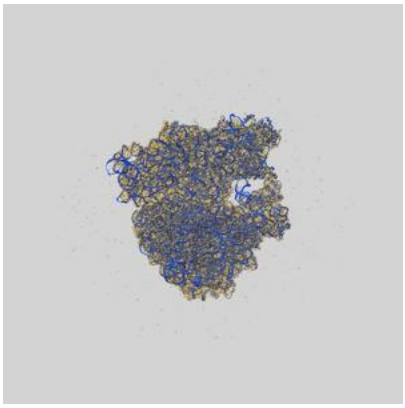
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.73	3.09	2.78
Unmasked-calculated*	3.89	6.88	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 2.7 by more than 10 %

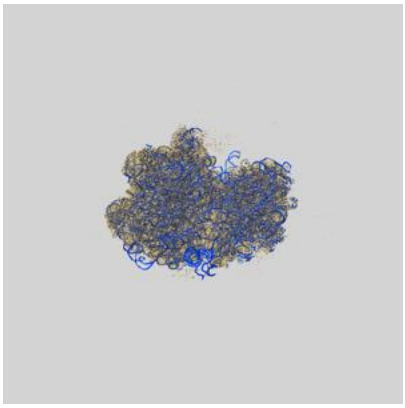
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60747 and PDB model 9IOT. Per-residue inclusion information can be found in section 3 on page 16.

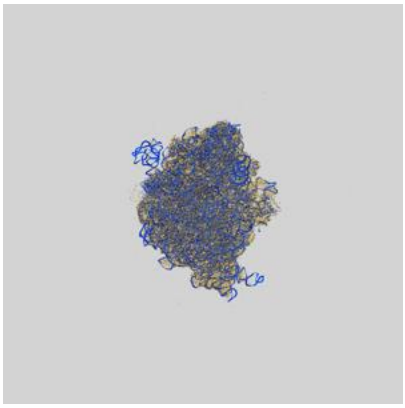
9.1 Map-model overlay



X



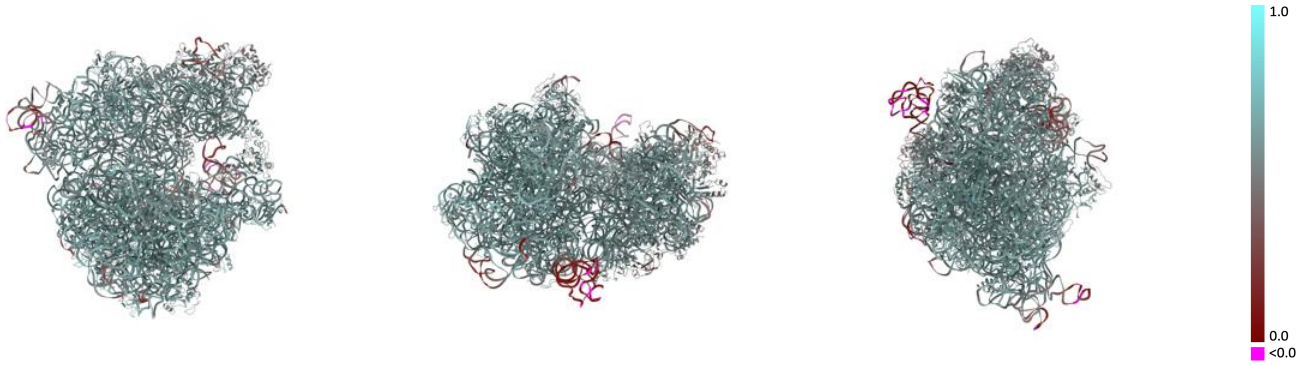
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

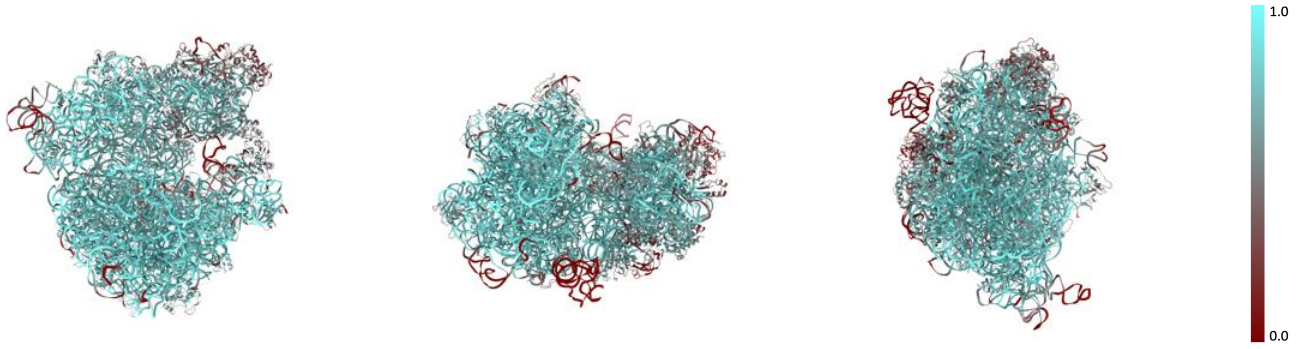
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

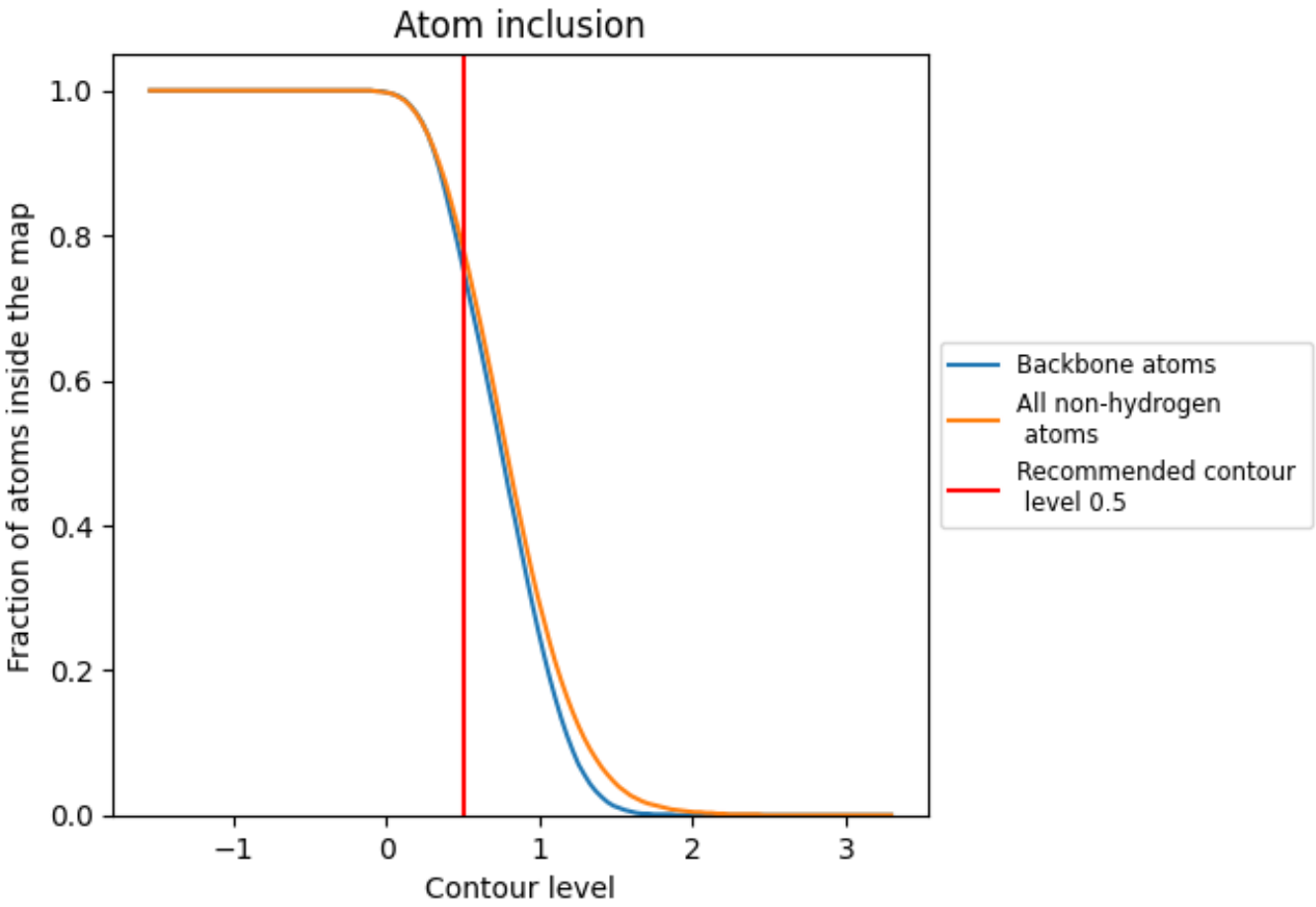
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 78% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.5850
0	0.6460	0.5730
1	0.7530	0.6060
2	0.3780	0.5070
3	0.8110	0.6240
4	0.7110	0.5940
5	0.8620	0.6370
6	0.8700	0.6340
7	0.7500	0.5980
8	0.0950	0.4070
A	0.8430	0.5870
B	0.8320	0.5870
D	0.8170	0.6260
E	0.7880	0.6180
F	0.7500	0.6050
G	0.5290	0.5350
H	0.5200	0.5310
I	0.3670	0.5370
L	0.7980	0.6130
M	0.7830	0.6170
N	0.8120	0.6220
O	0.7800	0.6190
P	0.8580	0.6270
Q	0.7250	0.5890
R	0.7650	0.6160
S	0.8520	0.6250
T	0.7680	0.6110
U	0.8100	0.6210
V	0.6760	0.5790
W	0.7000	0.5830
X	0.6800	0.5850
Y	0.7900	0.6170
Z	0.7550	0.6140
a	0.8250	0.5830
b	0.6040	0.5550



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Chain	Atom inclusion	Q-score
c	0.6580	0.5730
d	0.6680	0.5810
e	0.7610	0.6020
f	0.6030	0.5560
g	0.5340	0.5550
h	0.7440	0.6020
i	0.6440	0.5660
j	0.6060	0.5500
k	0.6680	0.5730
l	0.7230	0.6060
m	0.5840	0.5670
n	0.6970	0.5900
o	0.6970	0.5880
p	0.7530	0.5950
q	0.6440	0.5720
r	0.6640	0.5670
s	0.5890	0.5530
t	0.6860	0.5750
u	0.4650	0.5310
v	0.5760	0.5860
y	0.4600	0.5740
z	0.3780	0.5000