Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 10:29 AM EDT

PDB ID	:	8CVM / pdb_00008cvm
EMDB ID	:	EMD-27009
Title	:	Cutibacterium acnes 50S ribosomal subunit with P-site tRNA and Sarecycline bound in the local refined map
Authors	:	Lomakin, I.B.; Devarkar, S.C.; Bunick, C.G.
Deposited on	:	2022-05-18
Resolution	:	2.66 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:

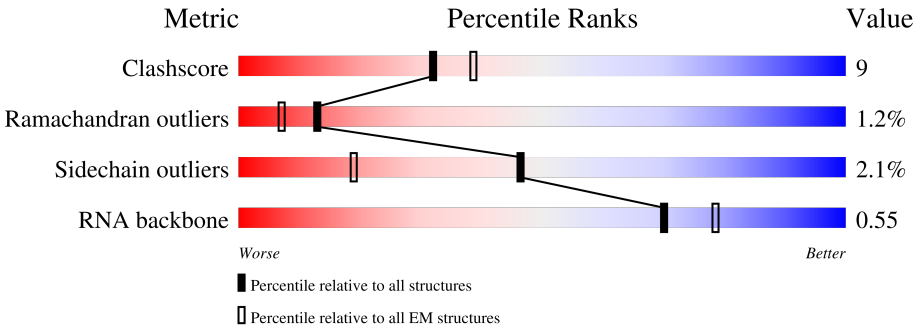
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

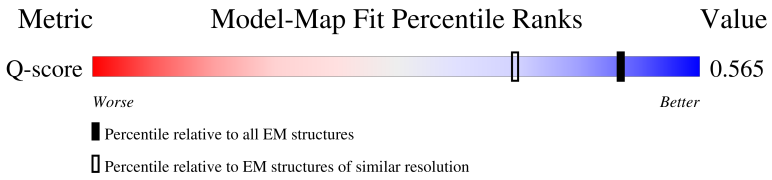
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.66 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.





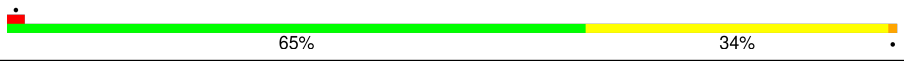
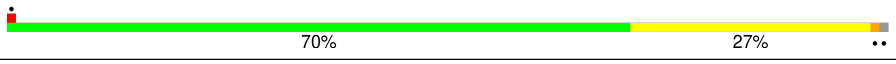
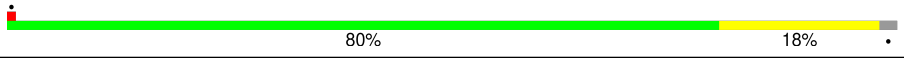
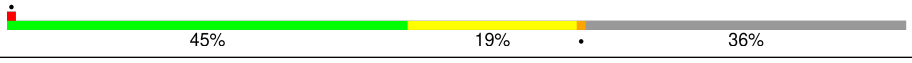
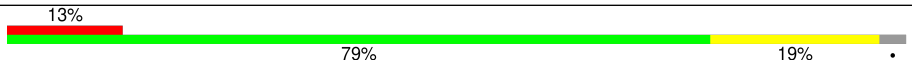
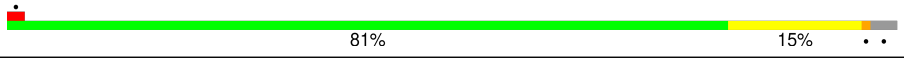
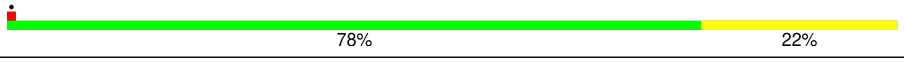
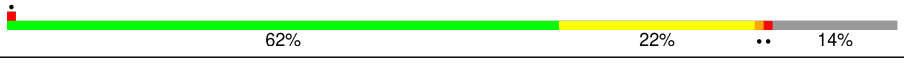
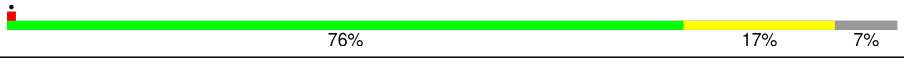
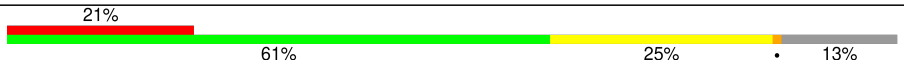
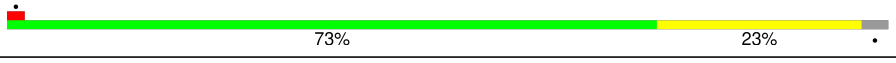
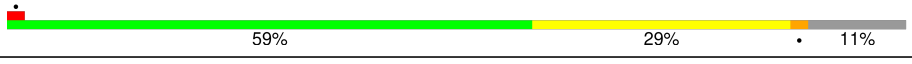
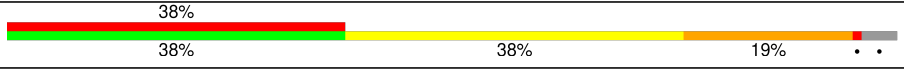
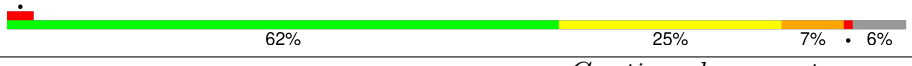
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9119 (2.16 - 3.16)

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	c	278	81% 17%
2	d	223	72% 23%
3	e	301	47% 22% 30%

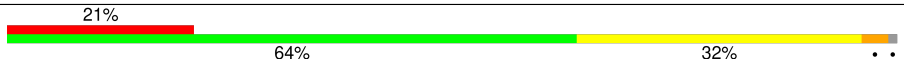
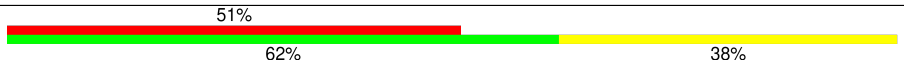
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Mol	Chain	Length	Quality of chain
4	f	210	
5	g	180	
6	i	147	
7	j	122	
8	k	146	
9	l	139	
10	m	187	
11	n	127	
12	o	117	
13	p	123	
14	q	102	
15	r	153	
16	s	102	
17	t	122	
18	u	205	
19	v	89	
20	w	61	
21	x	77	
22	y	60	
23	z	63	
24	0	56	
25	1	44	
26	2	68	
27	4	69	
28	a	3086	

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Mol	Chain	Length	Quality of chain
29	b	120	
30	V	24	
31	C	77	
32	3	37	

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 93049 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	c	274	2091	1289	425	372	5	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	d	214	1586	984	304	291	7	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	e	210	1577	979	301	295	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	f	203	1623	1025	299	290	9	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	g	177	1376	867	250	258	1	0	0

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	i	146	1139	718	213	205	3	0	0

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	122	Total	C	N	O	S	0	0
			946	596	177	169	4		

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	144	Total	C	N	O	S	0	0
			1072	675	196	199	2		

- Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	136	Total	C	N	O	S	0	0
			1082	685	210	181	6		

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	120	Total	C	N	O	S	0	0
			936	583	188	163	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	102	ILE	ASN	conflict	UNP A0A085AZY3

- Molecule 11 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	126	Total	C	N	O	S	0	0
			952	583	190	176	3		

- Molecule 12 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	o	114	Total	C	N	O	S	0	0
			896	559	174	162	1		

- Molecule 13 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	p	119	Total	C	N	O	S	0	0
			958	589	196	171	2		

- Molecule 14 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	102	Total	C	N	O	S	0	0
			778	487	140	150	1		

- Molecule 15 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	132	Total	C	N	O	S	0	0
			1017	624	204	182	7		

- Molecule 16 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	95	Total	C	N	O	S	0	0
			751	474	138	138	1		

- Molecule 17 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	t	107	Total	C	N	O	S	0	0
			833	516	163	153	1		

- Molecule 18 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	u	179	Total	C	N	O	S	0	0
			1376	865	240	268	3		

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	v	78	Total	C	N	O	0	0
			591	355	127	109		

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	60	Total	C	N	O	S	0	0
			474	290	102	77	5		

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	x	69	Total	C	N	O	0	0
			564	348	108	108		

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	y	58	Total	C	N	O	S	0	0
			467	290	91	83	3		

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	z	62	Total	C	N	O	S	0	0
			477	287	102	83	5		

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	0	50	Total	C	N	O	S	0	0
			423	253	91	73	6		

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	44	Total	C	N	O	S	0	0
			362	213	91	56	2		

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	67	Total	C	N	O	S	0	0
			513	315	110	87	1		

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	66	Total	C	N	O	S	0	0
			512	313	97	97	5		

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2903	Total	C	N	O	P	6	0
			62531	27850	11406	20366	2909		

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	120	Total	C	N	O	P	0	0
			2567	1145	466	836	120		

- Molecule 30 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	V	23	Total	C	N	O	0	0
			183	106	50	27		

- Molecule 31 is a RNA chain called Initiator fMet RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	C	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	3	37	Total	C	N	O	S	0	0
			302	184	66	47	5		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	c	3	Total	Mg	0
			3	3	
33	d	1	Total	Mg	0
			1	1	
33	k	2	Total	Mg	0
			2	2	

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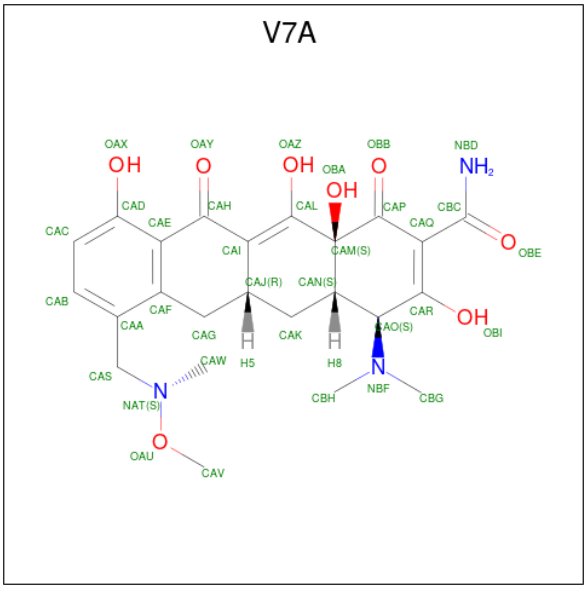
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Mol	Chain	Residues	Atoms	AltConf
33	1	1	Total Mg 1 1	0
33	a	294	Total Mg 294 294	0
33	b	2	Total Mg 2 2	0
33	C	2	Total Mg 2 2	0

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
34	w	1	Total Zn 1 1	0
34	z	1	Total Zn 1 1	0
34	0	1	Total Zn 1 1	0
34	4	1	Total Zn 1 1	0

- Molecule 35 is Sarecycline (CCD ID: V7A) (formula: $C_{24}H_{29}N_3O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
35	a	1	Total C N O 35 24 3 8	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	d	1	Total O 1 1	0
36	s	1	Total O 1 1	0
36	a	120	Total O 120 120	0
36	b	3	Total O 3 3	0

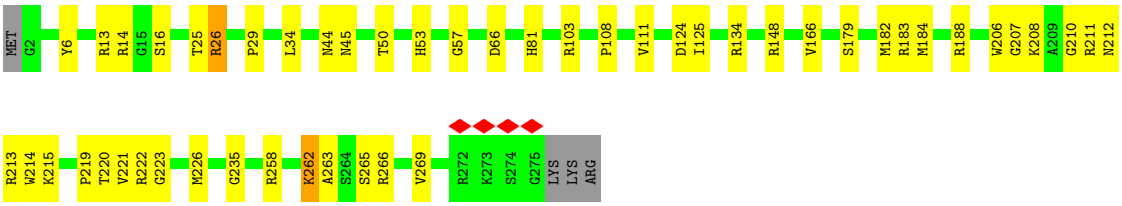
3 Residue-property plots (i)

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: 50S ribosomal protein L2

Chain c:

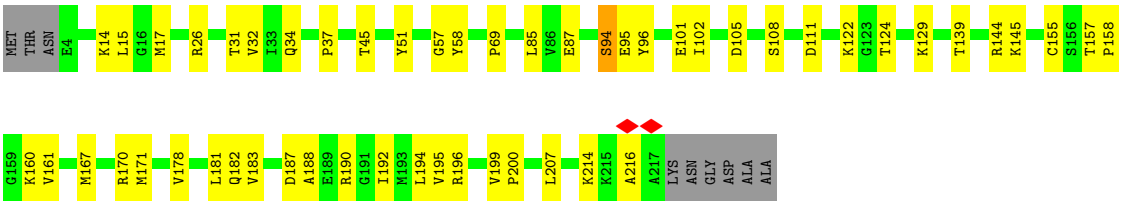




• Molecule 2: 50S ribosomal protein L3

Chain d:

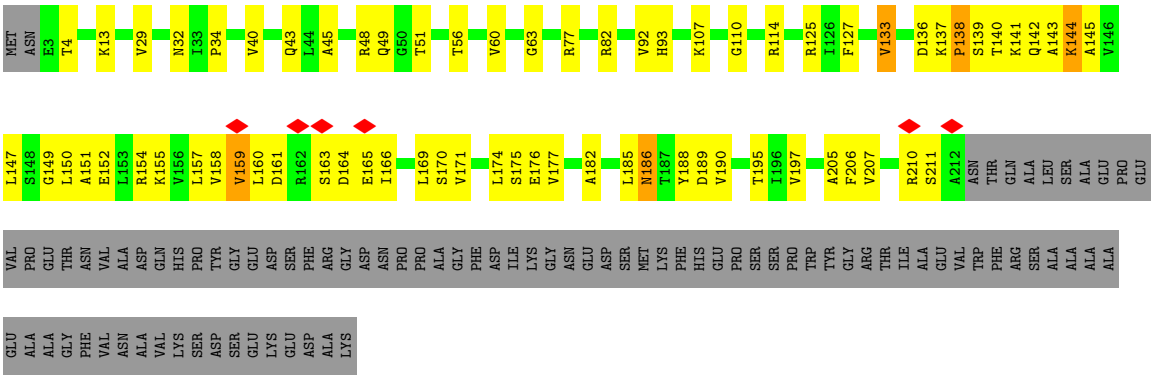




• Molecule 3: 50S ribosomal protein L4

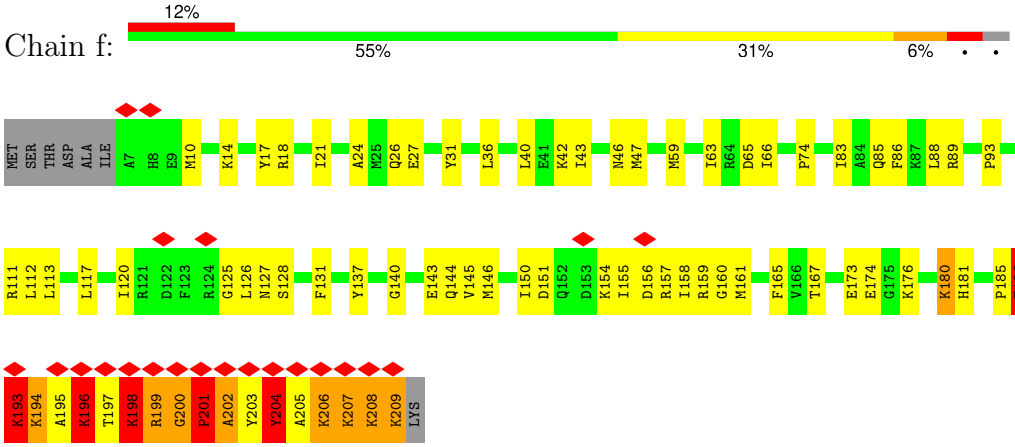
Chain e:





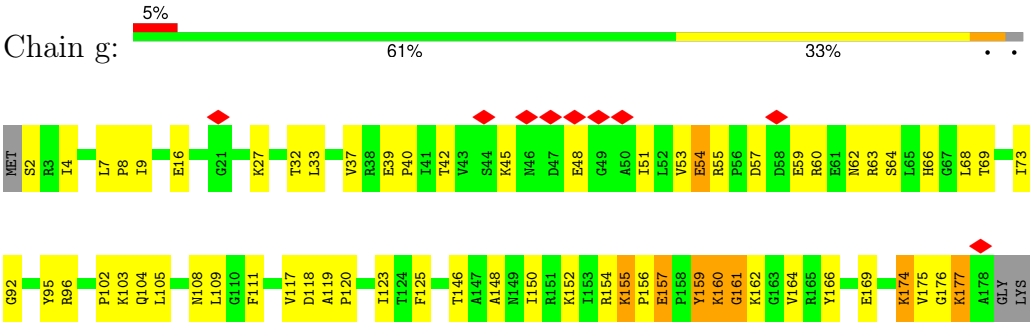
• Molecule 4: 50S ribosomal protein L5

Chain f:



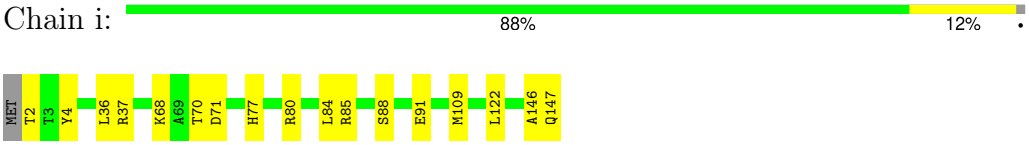
• Molecule 5: 50S ribosomal protein L6

Chain g:



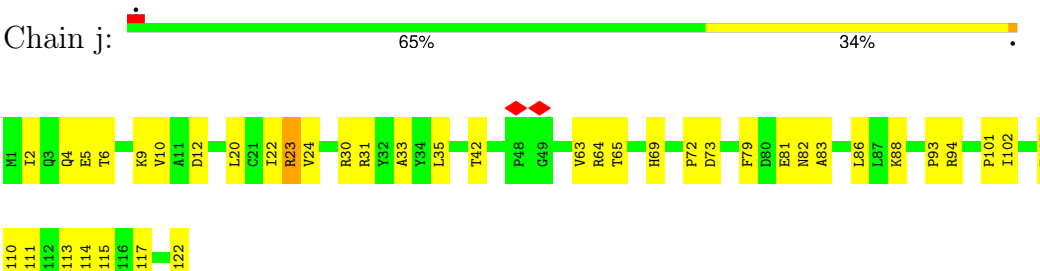
• Molecule 6: 50S ribosomal protein L13

Chain i:



• Molecule 7: 50S ribosomal protein L14

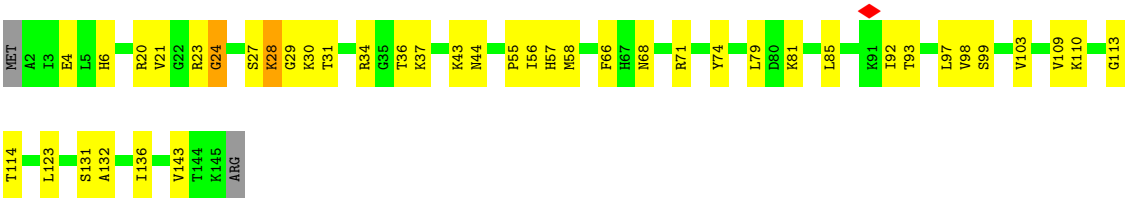
Chain j:



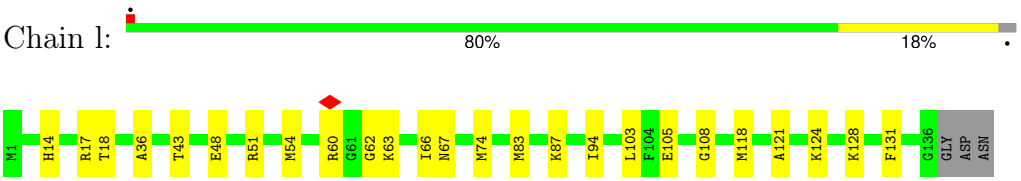
• Molecule 8: 50S ribosomal protein L15

Chain k:

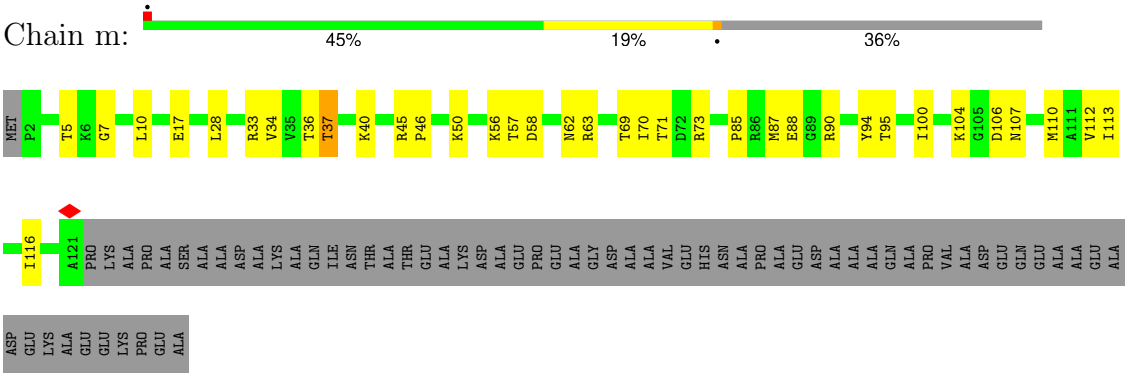




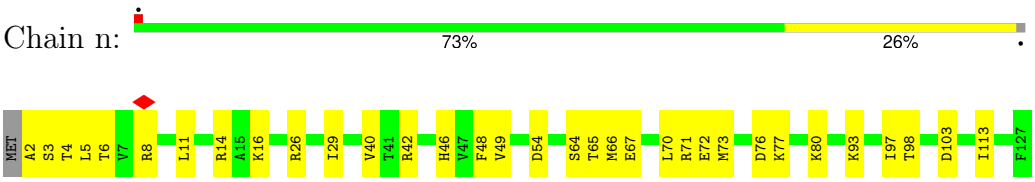
• Molecule 9: 50S ribosomal protein L16



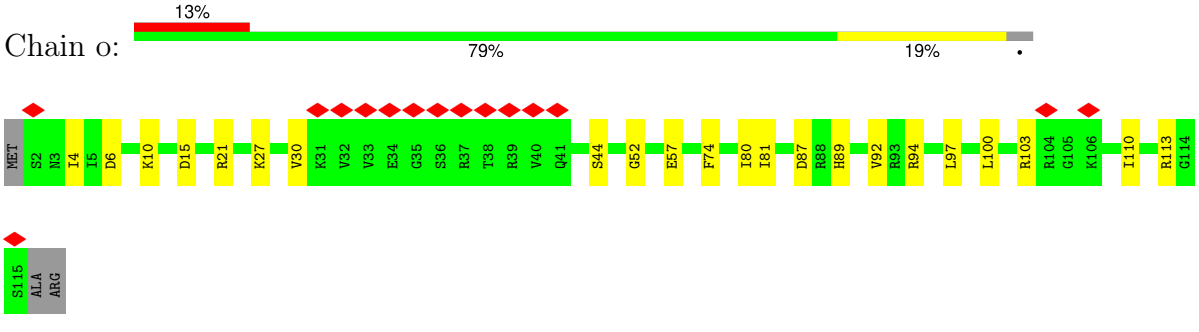
• Molecule 10: 50S ribosomal protein L17



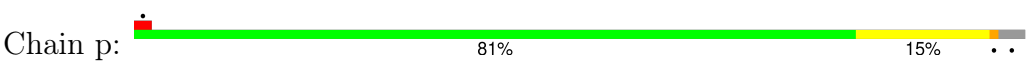
• Molecule 11: 50S ribosomal protein L18

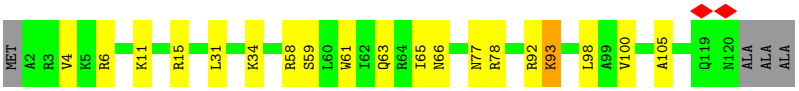


• Molecule 12: 50S ribosomal protein L19



• Molecule 13: 50S ribosomal protein L20

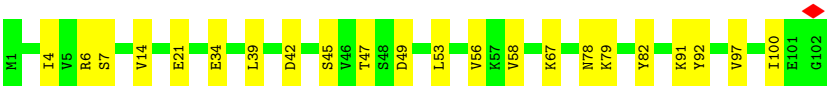




• Molecule 14: 50S ribosomal protein L21

Chain q:

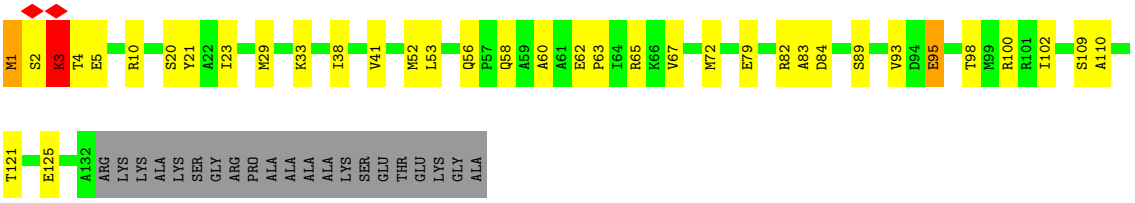




• Molecule 15: 50S ribosomal protein L22

Chain r:

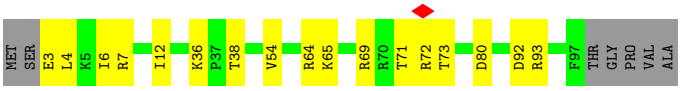




• Molecule 16: 50S ribosomal protein L23

Chain s:

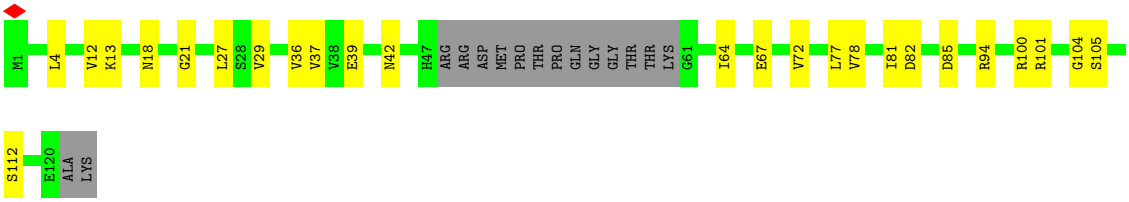




• Molecule 17: 50S ribosomal protein L24

Chain t:

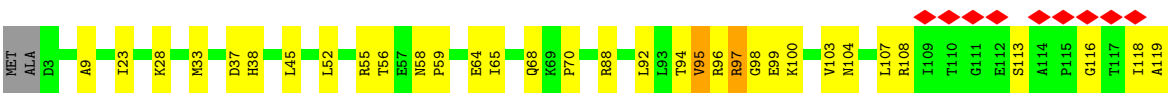


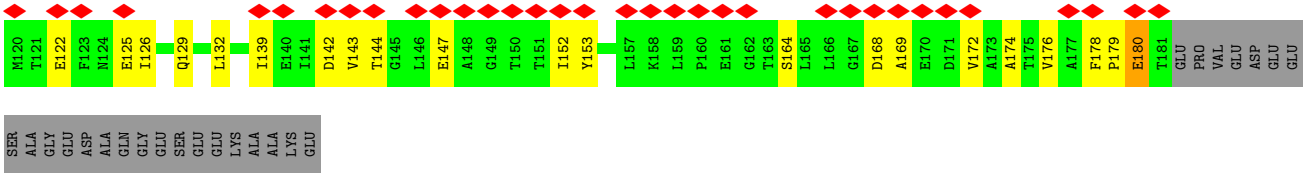


• Molecule 18: 50S ribosomal protein L25

Chain u:



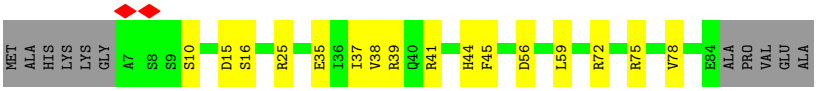




• Molecule 19: 50S ribosomal protein L27

Chain v:

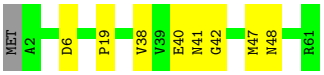




• Molecule 20: 50S ribosomal protein L28

Chain w:

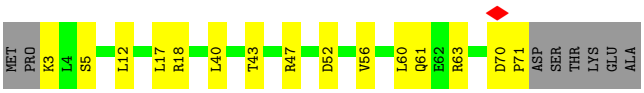




• Molecule 21: 50S ribosomal protein L29

Chain x:

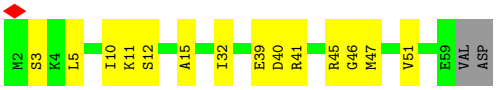




• Molecule 22: 50S ribosomal protein L30

Chain y:





• Molecule 23: 50S ribosomal protein L32

Chain z:

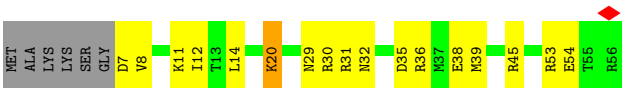




• Molecule 24: 50S ribosomal protein L33

Chain 0:

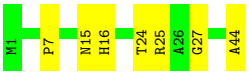




• Molecule 25: 50S ribosomal protein L34

Chain 1:

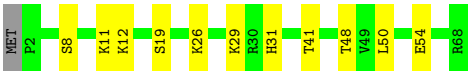




• Molecule 26: 50S ribosomal protein L35

Chain 2:

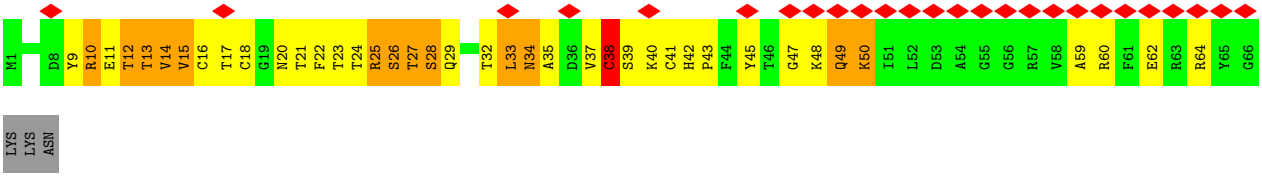




• Molecule 27: 50S ribosomal protein L31

Chain 4:

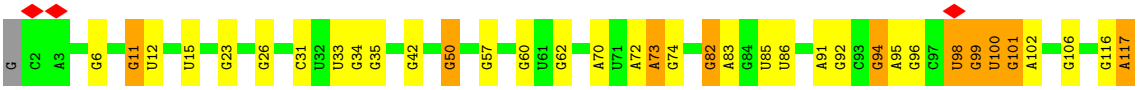


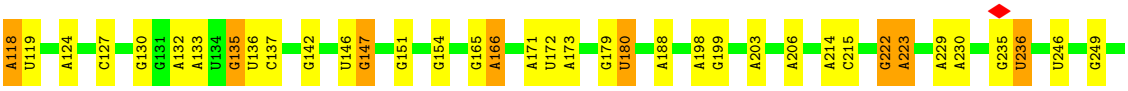


• Molecule 28: 23S ribosomal RNA

Chain a:

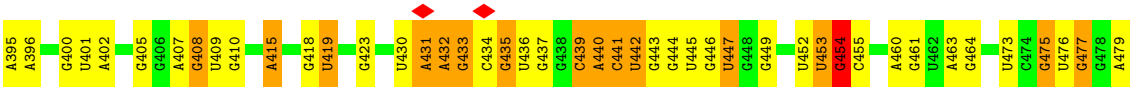




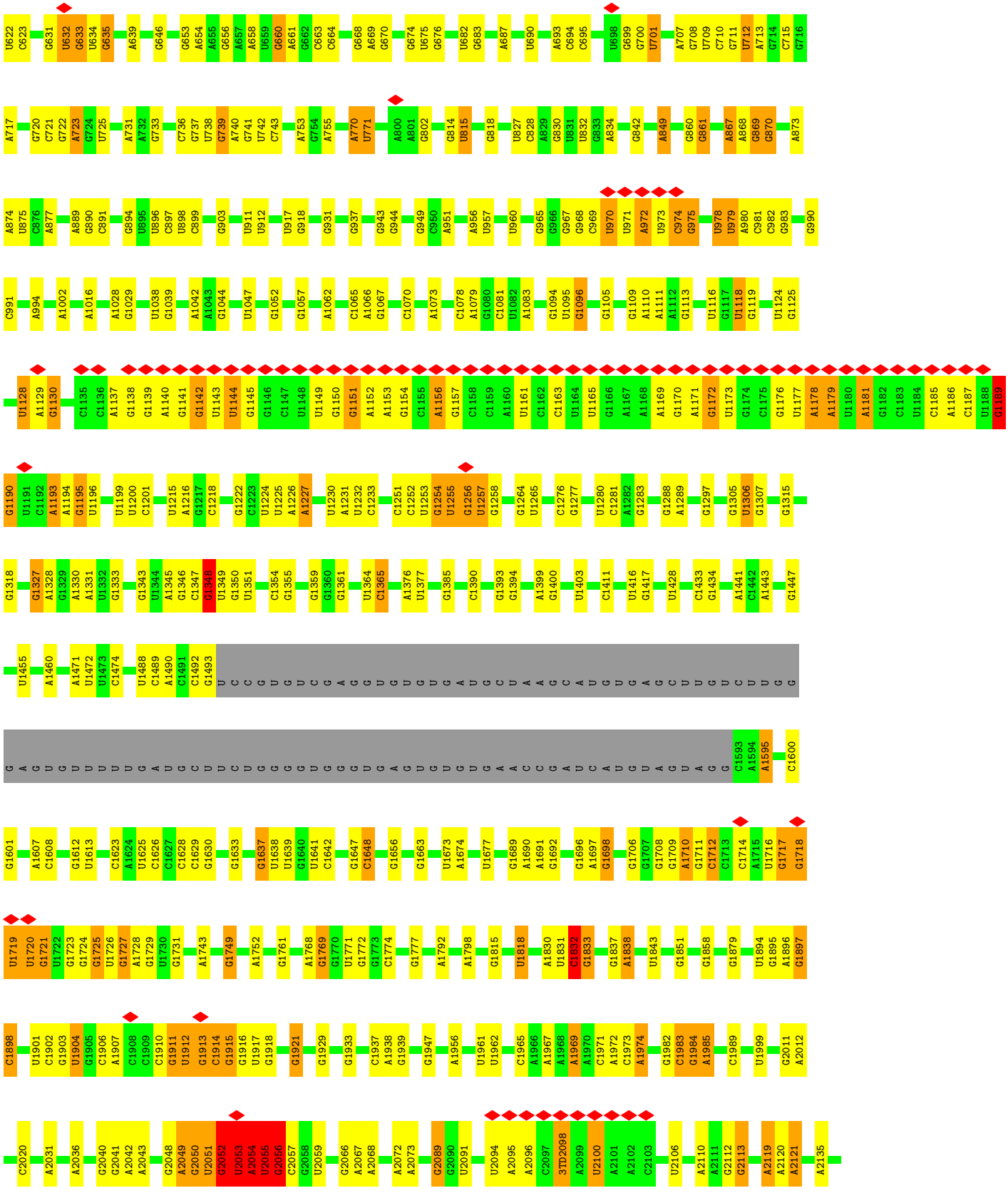


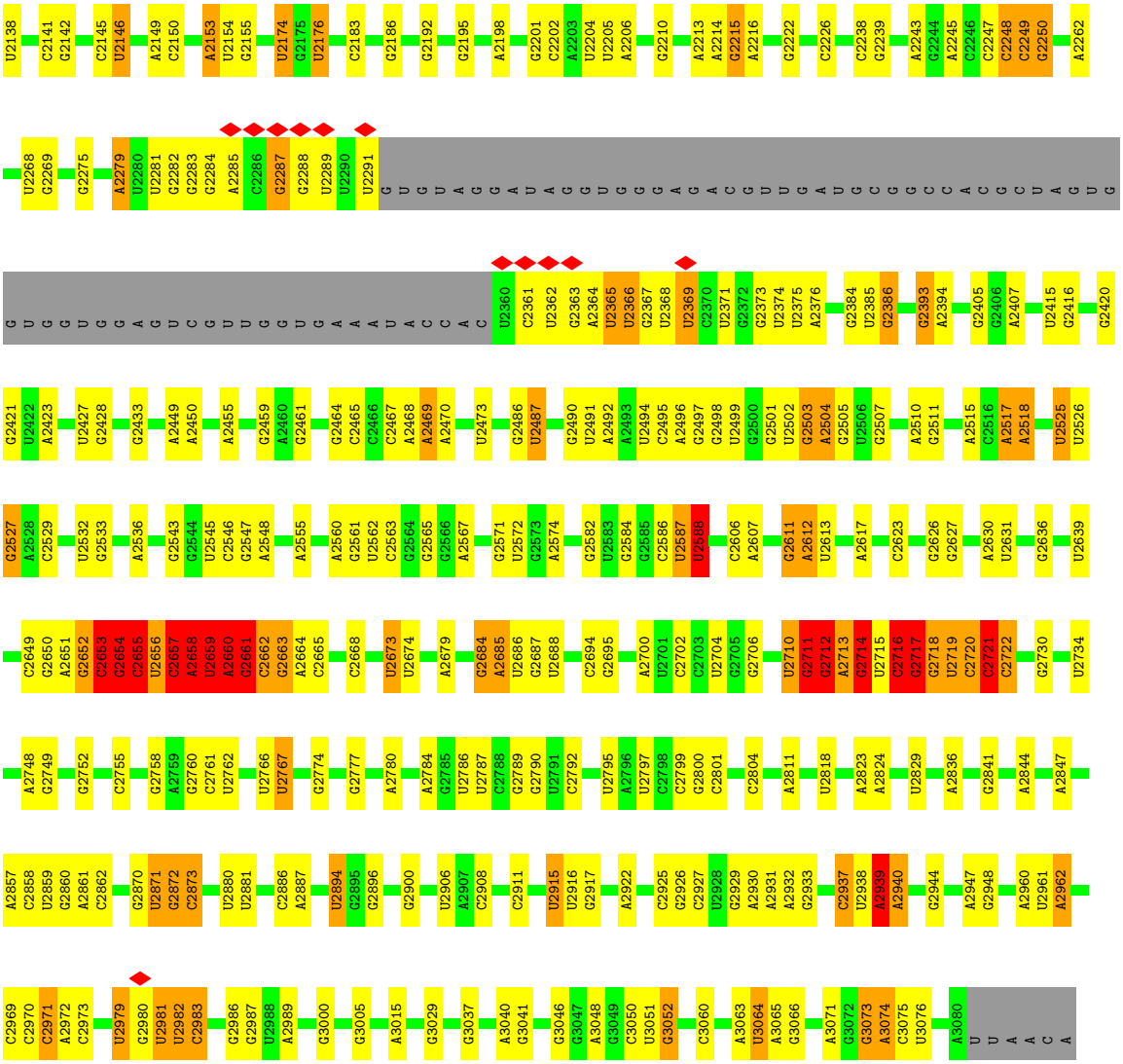








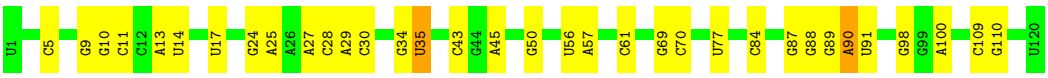




• Molecule 29: 5S ribosomal RNA

Chain b:

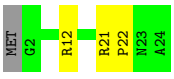




• Molecule 30: 50S ribosomal protein bL37

Chain V:

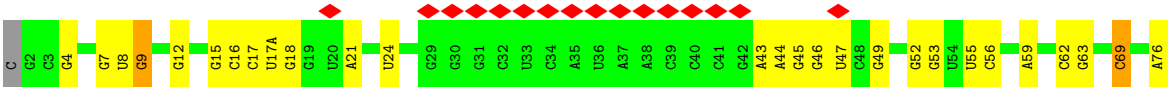




• Molecule 31: Initiator fMet RNA

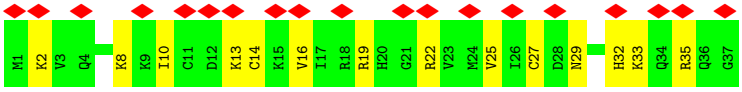
Chain C:





• Molecule 32: 50S ribosomal protein L36





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30.56	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.651	Depositor
Minimum map value	-0.589	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	363.12, 363.12, 363.12	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	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: V7A, OMU, 2MA, H2U, 3TD, 2MG, 5MU, 5MC, OMG, ZN, PSU, 4SU, OMC, MG

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	c	0.23	0/2132	0.38	0/2871
2	d	0.32	0/1611	0.46	0/2172
3	e	0.35	0/1600	0.61	0/2165
4	f	0.39	0/1652	0.58	1/2210 (0.0%)
5	g	0.34	0/1398	0.53	0/1884
6	i	0.24	0/1164	0.30	0/1574
7	j	0.25	0/957	0.41	0/1282
8	k	0.33	0/1090	0.59	1/1465 (0.1%)
9	l	0.23	0/1108	0.31	0/1488
10	m	0.24	0/949	0.39	0/1277
11	n	0.17	0/959	0.32	0/1281
12	o	0.19	0/909	0.30	0/1216
13	p	0.23	0/969	0.31	0/1292
14	q	0.22	0/785	0.38	0/1050
15	r	0.31	0/1028	0.42	0/1379
16	s	0.22	0/759	0.34	0/1022
17	t	0.17	0/840	0.33	0/1123
18	u	0.24	0/1396	0.42	0/1896
19	v	0.25	0/598	0.35	0/800
20	w	0.24	0/483	0.32	0/648
21	x	0.18	0/567	0.31	0/759
22	y	0.21	0/471	0.32	0/627
23	z	0.28	0/487	0.37	0/654
24	0	0.40	0/429	0.63	0/569
25	1	0.22	0/365	0.26	0/478
26	2	0.23	0/519	0.35	0/682
27	4	0.73	0/521	1.07	2/700 (0.3%)
28	a	0.26	1/69579 (0.0%)	0.35	73/108567 (0.1%)
29	b	0.19	0/2871	0.19	0/4475
30	V	0.23	0/184	0.32	0/236
31	C	0.14	0/1725	0.17	0/2689
32	3	0.18	0/305	0.31	0/401

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.27	1/100410 (0.0%)	0.37	77/150932 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	445	U	C1'-N1	5.90	1.57	1.48

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	1349	U	P-O3'-C3'	-9.86	105.41	120.20
28	a	315	G	P-O3'-C3'	-9.85	105.42	120.20
28	a	2661	G	P-O3'-C3'	-9.50	105.95	120.20
28	a	2653	C	P-O3'-C3'	-9.34	106.19	120.20
28	a	2940	A	P-O3'-C3'	-9.18	106.43	120.20
28	a	660	G	P-O3'-C3'	-8.94	106.79	120.20
28	a	2052	G	P-O3'-C3'	-8.51	107.44	120.20
28	a	2250	G	P-O3'-C3'	-8.48	107.48	120.20
28	a	440	A	P-O3'-C3'	-8.40	107.60	120.20
28	a	454	G	P-O3'-C3'	-8.38	107.62	120.20
28	a	452	U	P-O3'-C3'	-8.34	107.69	120.20
28	a	314	U	P-O3'-C3'	-8.30	107.75	120.20
28	a	2249	C	P-O3'-C3'	-8.27	107.79	120.20
28	a	2715	U	P-O3'-C3'	-8.22	107.88	120.20
28	a	2652	G	P-O3'-C3'	-8.16	107.96	120.20
28	a	1118	U	P-O3'-C3'	-8.04	108.14	120.20
28	a	2657	C	P-O3'-C3'	-8.03	108.15	120.20
28	a	2051	U	P-O3'-C3'	-8.03	108.16	120.20
28	a	2050	G	P-O3'-C3'	-7.93	108.30	120.20
28	a	2937	C	P-O3'-C3'	7.90	132.05	120.20
28	a	2939	A	P-O3'-C3'	-7.89	108.36	120.20
28	a	2654	G	P-O3'-C3'	-7.81	108.49	120.20
28	a	712	U	P-O3'-C3'	-7.75	108.58	120.20
28	a	2588	U	P-O3'-C3'	-7.74	108.59	120.20
28	a	1189	G	P-O3'-C3'	-7.64	108.75	120.20
28	a	2714	G	P-O3'-C3'	-7.61	108.78	120.20
28	a	990	G	P-O3'-C3'	-7.56	108.86	120.20
28	a	2718	G	P-O3'-C3'	-7.55	108.87	120.20
28	a	2053	U	P-O3'-C3'	-7.54	108.89	120.20
28	a	911	U	P-O3'-C3'	-7.46	109.01	120.20
28	a	2659	U	P-O3'-C3'	-7.45	109.02	120.20
28	a	2248	C	P-O3'-C3'	-7.30	109.25	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2719	U	P-O3'-C3'	-7.27	109.30	120.20
28	a	2887	A	P-O3'-C3'	-7.25	109.32	120.20
28	a	2662	C	P-O3'-C3'	-7.22	109.36	120.20
28	a	2655	C	P-O3'-C3'	-7.20	109.40	120.20
28	a	2721	C	P-O3'-C3'	-7.16	109.46	120.20
28	a	711	G	P-O3'-C3'	-7.10	109.55	120.20
28	a	2886	C	P-O3'-C3'	-7.00	109.71	120.20
28	a	2894	U	P-O3'-C3'	-6.98	109.74	120.20
28	a	304	G	P-O3'-C3'	-6.96	109.75	120.20
28	a	2153	A	P-O3'-C3'	-6.92	109.83	120.20
28	a	2525	U	P-O3'-C3'	-6.91	109.83	120.20
28	a	2711	G	P-O3'-C3'	-6.89	109.86	120.20
28	a	2055	U	P-O3'-C3'	-6.88	109.88	120.20
28	a	442	U	P-O3'-C3'	-6.83	109.96	120.20
28	a	1637	G	P-O3'-C3'	-6.81	109.98	120.20
28	a	1832	C	P-O3'-C3'	-6.79	110.02	120.20
28	a	2651	A	P-O3'-C3'	-6.78	110.04	120.20
28	a	441	C	P-O3'-C3'	-6.76	110.05	120.20
28	a	2658	A	P-O3'-C3'	-6.75	110.08	120.20
28	a	2660	A	P-O3'-C3'	-6.70	110.15	120.20
28	a	2054	A	P-O3'-C3'	-6.64	110.24	120.20
28	a	303	G	P-O3'-C3'	-6.61	110.28	120.20
28	a	2056	G	P-O3'-C3'	-6.59	110.31	120.20
27	4	39	SER	N-CA-C	-6.30	105.24	113.12
28	a	272	A	P-O3'-C3'	-6.30	110.75	120.20
28	a	2587	U	P-O3'-C3'	-6.30	110.75	120.20
28	a	2712	G	P-O3'-C3'	-6.27	110.80	120.20
27	4	38	CYS	CB-CA-C	-6.11	100.04	114.16
28	a	1348	G	P-O3'-C3'	-6.09	111.06	120.20
28	a	2612	A	P-O3'-C3'	-6.09	111.07	120.20
28	a	2710	U	P-O3'-C3'	-6.07	111.09	120.20
28	a	271	G	C2'-C3'-O3'	6.04	122.76	113.70
28	a	2049	A	P-O3'-C3'	-5.97	111.25	120.20
28	a	2717	G	P-O3'-C3'	-5.88	111.39	120.20
28	a	1638	U	P-O3'-C3'	-5.77	111.55	120.20
28	a	1833	G	P-O3'-C3'	-5.69	111.67	120.20
28	a	1187	C	P-O3'-C3'	-5.59	111.82	120.20
28	a	738	U	P-O3'-C3'	-5.55	111.87	120.20
28	a	439	C	P-O3'-C3'	-5.48	111.98	120.20
28	a	302	A	P-O3'-C3'	-5.45	112.03	120.20
8	k	24	GLY	CA-C-O	-5.43	118.40	122.37
28	a	272	A	C1'-O4'-C4'	-5.24	104.66	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	271	G	C4'-C3'-C2'	-5.22	97.38	102.60
4	f	201	PRO	N-CA-CB	-5.16	97.83	103.25
28	a	2716	C	P-O3'-C3'	-5.08	112.58	120.20

There are no chirality outliers.

There are no planarity outliers.

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	c	2091	0	2150	45	0
2	d	1586	0	1634	39	0
3	e	1577	0	1619	60	0
4	f	1623	0	1665	110	0
5	g	1376	0	1421	60	0
6	i	1139	0	1163	13	0
7	j	946	0	1011	32	0
8	k	1072	0	1106	32	0
9	l	1082	0	1117	19	0
10	m	936	0	997	25	0
11	n	952	0	995	21	0
12	o	896	0	928	16	0
13	p	958	0	986	19	0
14	q	778	0	824	15	0
15	r	1017	0	1070	28	0
16	s	751	0	803	11	0
17	t	833	0	883	15	0
18	u	1376	0	1397	35	0
19	v	591	0	581	10	0
20	w	474	0	487	4	0
21	x	564	0	582	11	0
22	y	467	0	504	11	0
23	z	477	0	479	16	0
24	0	423	0	429	17	0
25	1	362	0	387	5	0
26	2	513	0	565	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	4	512	0	497	43	0
28	a	62531	0	31359	616	0
29	b	2567	0	1297	21	0
30	V	183	0	202	4	0
31	C	1625	0	829	13	0
32	3	302	0	333	12	0
33	1	1	0	0	0	0
33	C	2	0	0	0	0
33	a	294	0	0	0	0
33	b	2	0	0	0	0
33	c	3	0	0	0	0
33	d	1	0	0	0	0
33	k	2	0	0	0	0
34	0	1	0	0	0	0
34	4	1	0	0	0	0
34	w	1	0	0	0	0
34	z	1	0	0	0	0
35	a	35	0	0	1	0
36	a	120	0	0	4	0
36	b	3	0	0	0	0
36	d	1	0	0	0	0
36	s	1	0	0	0	0
All	All	93049	0	60300	1215	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 9.

All (1215) 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)
3:e:142:GLN:HE21	3:e:174:LEU:HD21	1.14	1.10
27:4:38:CYS:SG	27:4:41:CYS:HB2	1.83	1.10
4:f:127:ASN:HA	4:f:192:PRO:HB3	1.42	0.98
27:4:16:CYS:HA	27:4:35:ALA:HB3	1.51	0.92
4:f:180:LYS:HA	4:f:186:PHE:HZ	1.34	0.91
24:0:8:VAL:HA	24:0:30:ARG:HH21	1.35	0.88
3:e:160:LEU:HB3	3:e:164:ASP:HB2	1.54	0.88
27:4:49:GLN:O	27:4:50:LYS:HB2	1.72	0.87
16:s:69:ARG:HH21	28:a:1411:C:H5”	1.38	0.87
4:f:43:ILE:HG12	4:f:105:MET:HG3	1.56	0.85
28:a:1912:U:H5’	28:a:1914:C:H5’	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:127:ASN:ND2	4:f:196:LYS:HB2	1.92	0.84
28:a:367:A:H61	28:a:444:G:H21	1.26	0.84
4:f:21:ILE:HD12	4:f:181:HIS:HB3	1.60	0.83
28:a:2654:G:H3'	28:a:2657:C:H42	1.44	0.82
8:k:20:ARG:NH2	28:a:1327:G:N7	2.26	0.82
28:a:669:A:H62	28:a:1328:A:H2	1.27	0.82
28:a:1831:U:H5'	28:a:1832:C:H5'	1.62	0.81
3:e:138:PRO:HG2	3:e:141:LYS:HB2	1.62	0.81
12:o:94:ARG:HH21	28:a:1937:C:H5	1.29	0.81
4:f:197:THR:O	4:f:201:PRO:HD2	1.82	0.80
28:a:2706:G:H22	28:a:2721:C:H5	1.29	0.80
8:k:36:THR:HG22	8:k:37:LYS:HG2	1.64	0.79
3:e:142:GLN:HG3	3:e:171:VAL:HG12	1.65	0.79
28:a:3073:G:H4'	28:a:3074:A:H5'	1.64	0.79
28:a:2053:U:H3'	28:a:2054:A:H8	1.46	0.79
1:c:262:LYS:HG3	1:c:263:ALA:H	1.47	0.78
28:a:1281:C:H5	28:a:1318:G:H1	1.31	0.78
4:f:180:LYS:HA	4:f:186:PHE:CZ	2.19	0.78
28:a:2053:U:H3'	28:a:2054:A:C8	2.19	0.77
3:e:142:GLN:NE2	3:e:174:LEU:HD21	1.97	0.77
4:f:195:ALA:O	4:f:199:ARG:HG3	1.84	0.77
28:a:2279:A:H61	28:a:2374:U:H3	1.32	0.77
28:a:302:A:H3'	28:a:303:G:H8	1.51	0.76
28:a:332:U:H3	28:a:449:G:H1	1.34	0.76
9:l:63:LYS:HG3	18:u:180:GLU:HG2	1.67	0.76
4:f:190:ASP:O	4:f:191:ASP:C	2.29	0.75
11:n:2:ALA:N	29:b:9:G:N7	2.34	0.75
3:e:152:GLU:HB3	3:e:176:GLU:HG3	1.66	0.75
28:a:142:G:H22	28:a:147:G:H22	1.33	0.75
1:c:222:ARG:NH1	28:a:1972:A:OP2	2.20	0.74
8:k:43:LYS:NZ	28:a:889:A:OP1	2.21	0.74
27:4:11:GLU:HA	27:4:25:ARG:HA	1.69	0.74
28:a:1716:U:O2'	28:a:1721:G:N2	2.21	0.74
10:m:10:LEU:HB2	10:m:17:GLU:HG3	1.70	0.74
28:a:970:U:H3	28:a:975:G:H1	1.35	0.74
28:a:1698:G:H1	28:a:1915:G:H22	1.35	0.74
28:a:1904:U:H5	28:a:1921:G:H21	1.32	0.73
28:a:85:U:H3	28:a:95:A:H61	1.36	0.73
4:f:180:LYS:CA	4:f:186:PHE:HZ	2.00	0.73
6:i:85:ARG:NH1	28:a:2823:A:OP1	2.21	0.73
13:p:31:LEU:HD22	28:a:664:C:H5'	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1623:C:H5	28:a:1731:G:H1	1.36	0.73
28:a:60:G:H22	28:a:92:G:H1	1.37	0.72
5:g:9:ILE:HB	5:g:51:ILE:HB	1.70	0.72
5:g:104:GLN:NE2	5:g:118:ASP:OD1	2.21	0.72
3:e:133:VAL:HA	3:e:141:LYS:HE2	1.71	0.72
27:4:47:GLY:HA2	27:4:50:LYS:NZ	2.05	0.72
28:a:360:A:H2	28:a:444:G:H22	1.35	0.71
28:a:2052:G:H21	28:a:2055:U:H5	1.37	0.70
27:4:18:CYS:HB2	27:4:41:CYS:SG	2.31	0.70
28:a:82:G:N2	28:a:102:A:OP2	2.23	0.70
18:u:52:LEU:HD22	18:u:55:ARG:HH12	1.57	0.70
28:a:2284:G:H1	28:a:2369:U:H3	1.38	0.70
2:d:178:VAL:HG12	2:d:181:LEU:HD11	1.72	0.70
5:g:177:LYS:N	28:a:2713:A:H5'	2.06	0.70
8:k:55:PRO:HG2	8:k:58:MET:HG3	1.74	0.70
28:a:2584:G:OP2	28:a:2584:G:N2	2.25	0.70
1:c:53:HIS:CE1	1:c:220:THR:HA	2.27	0.69
23:z:53:PRO:HD2	23:z:56:ASP:HB2	1.73	0.69
28:a:106:G:H4'	28:a:379:A:H5"	1.74	0.69
5:g:37:VAL:HG13	5:g:69:THR:HG21	1.74	0.69
28:a:86:U:H3	28:a:94:G:H1	1.40	0.69
18:u:64:GLU:HG3	18:u:70:PRO:HB3	1.74	0.69
4:f:143:GLU:OE2	4:f:145:VAL:HG12	1.93	0.69
28:a:6:G:H1	28:a:3076:U:H3	1.38	0.69
28:a:2042:A:H61	28:a:2066:G:H1	1.40	0.69
11:n:76:ASP:OD1	11:n:77:LYS:N	2.25	0.68
10:m:37:THR:HA	10:m:110:MET:HA	1.74	0.68
4:f:46:ASN:ND2	28:a:2495:C:O4'	2.26	0.68
8:k:114:THR:HB	28:a:723:A:H5"	1.76	0.68
28:a:712:U:H4'	28:a:739:G:N7	2.09	0.68
3:e:77:ARG:NH1	28:a:2627:2MG:OP1	2.24	0.68
3:e:158:VAL:O	3:e:160:LEU:N	2.24	0.68
10:m:33:ARG:NH2	23:z:60:VAL:O	2.27	0.68
28:a:2706:G:H1	28:a:2721:C:H41	1.42	0.68
28:a:372:U:H3	28:a:439:C:H42	1.40	0.68
4:f:204:TYR:HD2	4:f:205:ALA:N	1.91	0.67
28:a:2684:G:H5"	28:a:2685:2MA:H5"	1.75	0.67
28:a:2673:U:H5'	28:a:2752:G:H5"	1.76	0.67
18:u:107:LEU:O	18:u:108:ARG:NH1	2.28	0.67
28:a:2870:G:O2'	28:a:2872:G:N2	2.28	0.67
29:b:87:G:H21	29:b:90:A:H2	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:206:LYS:HE2	4:f:208:LYS:HB3	1.75	0.67
28:a:1490:A:H2	28:a:1772:G:H22	1.41	0.67
2:d:182:GLN:OE1	2:d:196:ARG:NH1	2.20	0.67
13:p:92:ARG:NH2	28:a:1081:C:OP2	2.28	0.67
4:f:107:GLU:OE2	27:4:25:ARG:HG3	1.94	0.67
14:q:67:LYS:HG2	14:q:91:LYS:HG3	1.76	0.66
5:g:2:SER:OG	5:g:66:HIS:ND1	2.27	0.66
7:j:10:VAL:HG12	7:j:12:ASP:H	1.59	0.66
4:f:125:GLY:HA2	4:f:185:PRO:HB2	1.77	0.66
4:f:190:ASP:O	4:f:192:PRO:N	2.29	0.66
25:1:24:THR:HG23	25:1:27:GLY:H	1.59	0.66
10:m:87:MET:HE3	10:m:94:TYR:HB3	1.78	0.66
5:g:152:LYS:NZ	28:a:2925:C:O2	2.29	0.65
18:u:178:PHE:HB3	18:u:179:PRO:HD2	1.79	0.65
8:k:103:VAL:HG21	8:k:109:VAL:HG13	1.79	0.65
28:a:379:A:O2'	28:a:380:G:O4'	2.14	0.65
1:c:66:ASP:OD1	1:c:103:ARG:NH1	2.30	0.65
28:a:1143:U:H4'	28:a:1144:U:H5'	1.78	0.65
8:k:24:GLY:O	8:k:29:GLY:HA3	1.96	0.65
27:4:45:TYR:C	27:4:47:GLY:H	2.05	0.65
28:a:2766:U:H2'	28:a:2767:U:H2'	1.77	0.65
7:j:107:ARG:HD3	7:j:115:VAL:HG11	1.77	0.65
4:f:201:PRO:HA	4:f:204:TYR:CD1	2.32	0.65
3:e:43:GLN:HG3	28:a:701:U:H1'	1.79	0.65
4:f:101:ARG:NH1	29:b:43:C:O2	2.30	0.65
28:a:552:G:N2	28:a:555:A:OP2	2.28	0.65
2:d:51:TYR:HH	28:a:2818:U:HO2'	1.45	0.64
22:y:5:LEU:HD11	22:y:45:ARG:HD2	1.79	0.64
28:a:85:U:O2	28:a:96:G:N2	2.31	0.64
28:a:1600:C:O2'	28:a:2393:G:N1	2.30	0.64
8:k:99:SER:HA	8:k:103:VAL:HG12	1.79	0.64
28:a:3037:G:N2	28:a:3040:A:OP2	2.26	0.64
11:n:42:ARG:HB2	11:n:113:ILE:HD11	1.80	0.64
27:4:47:GLY:HA2	27:4:50:LYS:HZ2	1.63	0.64
28:a:1698:G:H22	28:a:1915:G:N2	1.94	0.64
5:g:92:GLY:HA3	5:g:162:LYS:HG2	1.79	0.63
10:m:107:ASN:O	10:m:107:ASN:ND2	2.31	0.63
27:4:9:TYR:HD1	27:4:27:THR:HG23	1.64	0.63
28:a:2287:G:H1	28:a:2366:U:H3	1.47	0.63
3:e:43:GLN:HE22	3:e:186:ASN:HB2	1.64	0.63
4:f:203:TYR:O	4:f:205:ALA:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:154:ARG:HB2	3:e:177:VAL:HG22	1.81	0.63
11:n:46:HIS:ND1	11:n:65:THR:OG1	2.28	0.63
28:a:1139:G:H22	28:a:1185:C:H3'	1.63	0.63
28:a:127:C:C4	28:a:127:C:C2	2.87	0.63
22:y:3:SER:H	22:y:40:ASP:HB2	1.63	0.62
5:g:166:TYR:HB2	5:g:169:GLU:HB2	1.80	0.62
8:k:21:VAL:HG13	8:k:28:LYS:HB3	1.81	0.62
28:a:1962:U:OP2	28:a:1967:A:N6	2.23	0.62
9:l:124:LYS:NZ	28:a:2665:C:N3	2.46	0.62
25:1:15:ASN:ND2	28:a:770:A:OP1	2.32	0.62
28:a:1974:A:N6	28:a:2011:G:O2'	2.32	0.62
4:f:127:ASN:HA	4:f:192:PRO:CB	2.25	0.62
19:v:38:VAL:HG12	19:v:59:LEU:HB2	1.80	0.62
23:z:45:CYS:HB3	23:z:48:CYS:SG	2.39	0.62
4:f:208:LYS:O	4:f:208:LYS:HG2	2.00	0.62
9:l:128:LYS:NZ	28:a:1113:G:OP2	2.33	0.62
28:a:2721:C:H3'	28:a:2722:C:H5"	1.80	0.62
4:f:199:ARG:HB2	4:f:203:TYR:CE1	2.34	0.62
12:o:103:ARG:NH2	28:a:1937:C:O3'	2.33	0.62
28:a:50:G:O2'	28:a:117:A:N6	2.33	0.62
28:a:2049:A:C5	28:a:2050:G:H1'	2.35	0.62
28:a:289:U:HO2'	28:a:306:G:HO2'	1.47	0.61
5:g:103:LYS:HB3	5:g:119:ALA:HB3	1.83	0.61
3:e:127:PHE:HB2	3:e:197:VAL:HG12	1.83	0.61
4:f:200:GLY:HA2	4:f:203:TYR:CE2	2.36	0.61
21:x:17:LEU:HB3	21:x:60:LEU:HD21	1.81	0.61
24:0:45:ARG:NH2	28:a:2582:G:O2'	2.33	0.61
28:a:373:G:H22	28:a:437:G:H1	1.49	0.61
4:f:144:GLN:HG2	4:f:159:ARG:HG3	1.83	0.61
28:a:1255:U:O3'	28:a:1256:G:N2	2.34	0.61
28:a:2042:A:N6	28:a:2066:G:H1	1.99	0.61
4:f:187:LYS:O	4:f:187:LYS:HG2	1.99	0.61
28:a:350:A:H2'	28:a:351:G:H8	1.65	0.61
4:f:156:ASP:OD1	4:f:157:ARG:N	2.31	0.60
4:f:190:ASP:C	4:f:194:LYS:HB2	2.26	0.60
8:k:34:ARG:HD2	28:a:670:G:H1	1.66	0.60
28:a:358:C:H41	28:a:446:G:H21	1.48	0.60
1:c:166:VAL:HG21	1:c:182:MET:HE1	1.83	0.60
2:d:170:ARG:NH1	28:a:3005:G:O6	2.34	0.60
3:e:143:ALA:O	3:e:147:LEU:HD23	2.02	0.60
28:a:2872:G:H8	28:a:3052:G:C8	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:198:A:H2'	28:a:199:G:C8	2.36	0.60
5:g:53:VAL:O	5:g:66:HIS:NE2	2.30	0.60
4:f:197:THR:O	4:f:201:PRO:CD	2.49	0.60
15:r:3:LYS:HA	15:r:3:LYS:HZ2	1.65	0.60
25:1:7:PRO:HB2	28:a:1385:G:H4'	1.83	0.60
28:a:302:A:H3'	28:a:303:G:C8	2.33	0.60
1:c:25:THR:O	1:c:26:ARG:HB2	2.01	0.59
17:t:100:ARG:NH2	28:a:100:U:O4'	2.35	0.59
27:4:16:CYS:CA	27:4:35:ALA:HB3	2.30	0.59
15:r:1:MET:HE1	28:a:1288:G:H2'	1.83	0.59
5:g:109:LEU:HB3	5:g:154:ARG:HD2	1.84	0.59
8:k:81:LYS:HG3	8:k:85:LEU:HD13	1.84	0.59
17:t:13:LYS:HE2	17:t:21:GLY:HA2	1.84	0.59
8:k:68:ASN:HB3	8:k:71:ARG:HB2	1.84	0.59
21:x:47:ARG:NH2	28:a:73:A:OP1	2.32	0.59
27:4:16:CYS:O	27:4:16:CYS:SG	2.61	0.59
3:e:142:GLN:OE1	3:e:170:SER:HB3	2.02	0.59
5:g:95:TYR:HE2	5:g:162:LYS:HB3	1.66	0.59
28:a:83:A:H62	28:a:101:G:H8	1.49	0.59
6:i:147:GLN:HG3	13:p:78:ARG:HG3	1.84	0.59
28:a:2925:C:OP1	32:3:33:LYS:NZ	2.30	0.59
27:4:45:TYR:C	27:4:47:GLY:N	2.57	0.59
28:a:443:G:O5'	28:a:443:G:H8	1.86	0.59
28:a:279:A:N7	28:a:319:G:N2	2.51	0.58
28:a:480:A:H1'	28:a:500:G:O4'	2.03	0.58
28:a:1447:G:N7	36:a:3412:HOH:O	2.32	0.58
13:p:58:ARG:NH2	13:p:92:ARG:HH21	2.00	0.58
17:t:12:VAL:HG12	17:t:77:LEU:HD23	1.84	0.58
28:a:2052:G:H3'	28:a:2053:U:C5'	2.33	0.58
4:f:204:TYR:C	4:f:204:TYR:CD2	2.80	0.58
16:s:36:LYS:NZ	16:s:38:THR:OG1	2.36	0.58
28:a:1709:G:N2	28:a:1729:G:O6	2.35	0.58
3:e:32:ASN:OD1	3:e:34:PRO:HD2	2.03	0.58
4:f:195:ALA:HA	4:f:198:LYS:HE3	1.83	0.58
5:g:102:PRO:O	5:g:125:PHE:N	2.33	0.58
15:r:56:GLN:HE21	23:z:25:THR:H	1.51	0.58
28:a:2291:U:O2'	28:a:2362:U:O4	2.21	0.58
4:f:140:GLY:HA3	28:a:2487:U:H5"	1.86	0.58
3:e:133:VAL:HG11	3:e:137:LYS:HA	1.85	0.58
17:t:81:ILE:HG13	17:t:82:ASP:H	1.69	0.58
28:a:631:G:O2'	28:a:633:G:O4'	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:712:U:H4'	28:a:739:G:C8	2.38	0.58
31:C:4:G:H1	31:C:69:C:H42	1.50	0.58
28:a:2711:G:H2'	28:a:2712:G:C8	2.38	0.58
2:d:57:GLY:HA2	2:d:85:LEU:HD23	1.84	0.58
4:f:204:TYR:HD2	4:f:204:TYR:C	2.12	0.57
9:l:87:LYS:NZ	28:a:1039:G:OP2	2.37	0.57
15:r:38:ILE:HG13	15:r:93:VAL:HG23	1.86	0.57
18:u:126:ILE:HD11	18:u:139:ILE:HG21	1.86	0.57
28:a:2720:C:H41	32:3:2:LYS:HE3	1.67	0.57
1:c:57:GLY:HA2	1:c:214:TRP:HA	1.85	0.57
10:m:87:MET:HE1	10:m:116:ILE:HB	1.85	0.57
28:a:306:G:H4'	28:a:307:U:O5'	2.04	0.57
4:f:186:PHE:O	4:f:188:ALA:N	2.38	0.57
12:o:27:LYS:NZ	12:o:87:ASP:OD1	2.37	0.57
28:a:442:U:H3'	28:a:443:G:C8	2.39	0.57
28:a:461:G:N2	28:a:490:A:OP2	2.34	0.57
28:a:2052:G:N1	28:a:2054:A:H5"	2.19	0.57
28:a:2841:G:N2	28:a:2844:A:OP2	2.38	0.57
9:l:54:MET:HG3	9:l:121:ALA:HB2	1.85	0.57
3:e:142:GLN:HE21	3:e:174:LEU:CD2	2.04	0.57
28:a:1253:U:H2'	28:a:1254:G:C8	2.39	0.57
28:a:2145:5MC:H4'	28:a:2146:U:OP1	2.03	0.57
24:0:36:ARG:NH2	24:0:53:ARG:HE	2.03	0.57
28:a:2040:G:N2	28:a:2067:A:O2'	2.28	0.57
3:e:139:SER:HA	3:e:142:GLN:HE22	1.70	0.57
5:g:16:GLU:HB2	5:g:27:LYS:HB2	1.86	0.57
28:a:1289:A:N3	28:a:1315:G:O2'	2.37	0.57
11:n:65:THR:HA	11:n:70:LEU:HD22	1.87	0.56
28:a:357:G:N2	28:a:446:G:O6	2.37	0.56
4:f:201:PRO:HA	4:f:204:TYR:CE1	2.40	0.56
4:f:196:LYS:O	4:f:197:THR:C	2.48	0.56
5:g:59:GLU:HG2	5:g:62:ASN:HB2	1.86	0.56
8:k:30:LYS:HD3	8:k:31:THR:HG23	1.87	0.56
8:k:109:VAL:HG12	8:k:109:VAL:O	2.05	0.56
10:m:36:THR:O	10:m:37:THR:HG22	2.06	0.56
11:n:48:PHE:HD1	11:n:64:SER:HB3	1.69	0.56
14:q:82:TYR:CE1	28:a:1264:G:H5"	2.41	0.56
27:4:22:PHE:CG	27:4:23:THR:N	2.73	0.56
28:a:392:G:N1	28:a:395:A:OP2	2.34	0.56
2:d:87:GLU:OE2	28:a:2818:U:H4'	2.06	0.56
18:u:104:ASN:HB3	18:u:125:GLU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:967:G:H1	28:a:978:U:H3	1.53	0.56
4:f:46:ASN:OD1	4:f:47:MET:N	2.38	0.56
4:f:128:SER:O	4:f:176:LYS:NZ	2.39	0.56
5:g:57:ASP:HB3	5:g:62:ASN:OD1	2.05	0.56
19:v:25:ARG:NE	19:v:35:GLU:OE1	2.38	0.56
28:a:1698:G:H22	28:a:1915:G:H22	1.51	0.56
4:f:207:LYS:C	4:f:209:LYS:H	2.14	0.56
28:a:974:C:H3'	28:a:975:G:H8	1.71	0.56
28:a:949:G:H21	28:a:951:A:H62	1.54	0.56
3:e:150:LEU:O	3:e:154:ARG:NH1	2.39	0.56
6:i:68:LYS:NZ	28:a:1224:U:OP2	2.38	0.56
9:l:43:THR:HG22	9:l:94:ILE:HG22	1.87	0.56
23:z:61:VAL:HG12	23:z:63:ALA:H	1.69	0.56
28:a:1139:G:N2	28:a:1186:A:OP2	2.35	0.56
14:q:14:VAL:HB	14:q:97:VAL:HG21	1.87	0.55
31:C:7:G:O2'	31:C:49:G:OP2	2.21	0.55
28:a:430:U:H4'	28:a:431:A:H8	1.70	0.55
28:a:1489:C:H2'	28:a:1490:A:C8	2.41	0.55
28:a:2710:U:C3'	28:a:2711:G:H4'	2.36	0.55
3:e:139:SER:HA	3:e:142:GLN:OE1	2.07	0.55
18:u:95:VAL:HB	18:u:132:LEU:HD21	1.89	0.55
27:4:47:GLY:CA	27:4:50:LYS:NZ	2.69	0.55
28:a:179:G:N2	28:a:180:U:O4	2.37	0.55
28:a:1151:G:O2'	28:a:1179:A:O2'	2.25	0.55
28:a:2971:C:H1'	28:a:3071:A:H2	1.71	0.55
28:a:1727:G:H2'	28:a:1728:A:C8	2.42	0.55
28:a:2713:A:C2	28:a:2714:G:H1'	2.42	0.55
4:f:113:LEU:HD13	4:f:117:LEU:HD21	1.88	0.55
28:a:433:G:H2'	28:a:435:G:O4'	2.07	0.55
28:a:1912:U:H3'	28:a:1913:G:H3'	1.88	0.55
28:a:2052:G:N2	28:a:2055:U:H5	2.03	0.55
27:4:13:THR:O	27:4:32:THR:HA	2.07	0.55
28:a:379:A:N6	28:a:431:A:N7	2.54	0.55
28:a:631:G:O2'	28:a:633:G:OP1	2.23	0.55
28:a:1140:A:N6	28:a:1170:G:OP2	2.40	0.55
28:a:2872:G:O2'	28:a:2873:C:H6	1.90	0.55
6:i:80:ARG:HD2	28:a:2824:A:H5"	1.89	0.55
28:a:1130:G:H21	28:a:1194:A:H62	1.54	0.55
28:a:2706:G:N2	28:a:2721:C:H5	2.01	0.55
28:a:2872:G:O2'	28:a:2873:C:O5'	2.21	0.55
15:r:38:ILE:HA	15:r:41:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:96:ARG:O	18:u:97:ARG:C	2.49	0.55
16:s:72:ARG:O	16:s:73:THR:OG1	2.18	0.55
18:u:113:SER:HB2	18:u:147:GLU:HG3	1.88	0.55
26:2:8:SER:HA	26:2:11:LYS:HE2	1.89	0.55
28:a:2660:A:H3'	28:a:2661:G:H8	1.71	0.55
28:a:2979:U:OP1	28:a:2982:U:N3	2.40	0.55
4:f:17:TYR:HA	4:f:21:ILE:HG12	1.88	0.54
4:f:26:GLN:O	4:f:26:GLN:NE2	2.40	0.54
4:f:43:ILE:HD12	4:f:165:PHE:CD1	2.42	0.54
28:a:60:G:H22	28:a:92:G:H22	1.56	0.54
4:f:186:PHE:C	4:f:188:ALA:H	2.15	0.54
15:r:62:GLU:OE1	15:r:65:ARG:NH1	2.37	0.54
28:a:1169:A:O2'	28:a:1186:A:N1	2.36	0.54
1:c:266:ARG:NH2	28:a:2405:G:O5'	2.40	0.54
5:g:59:GLU:O	5:g:63:ARG:NE	2.35	0.54
10:m:69:THR:HG22	10:m:70:ILE:H	1.72	0.54
28:a:2658:A:H3'	28:a:2659:U:C6	2.43	0.54
10:m:69:THR:O	10:m:71:THR:N	2.40	0.54
18:u:23:ILE:HG23	18:u:28:LYS:HB2	1.90	0.54
19:v:75:ARG:NH2	28:a:2515:A:OP1	2.30	0.54
28:a:1647:G:H5"	28:a:1648:C:H5'	1.88	0.54
10:m:90:ARG:NH1	28:a:3060:C:O3'	2.41	0.54
11:n:4:THR:O	11:n:6:THR:N	2.40	0.54
27:4:18:CYS:SG	27:4:41:CYS:HB2	2.48	0.54
28:a:490:A:H2'	28:a:491:A:C8	2.42	0.54
28:a:1111:A:N3	28:a:2668:C:O2'	2.34	0.54
12:o:21:ARG:NH1	28:a:3029:G:O6	2.38	0.54
27:4:10:ARG:HH22	27:4:26:SER:C	2.16	0.54
28:a:454:G:C2	28:a:455:C:H1'	2.43	0.54
28:a:2718:G:HO2'	28:a:2719:U:H6	1.53	0.54
28:a:2777:G:N2	28:a:2780:A:OP2	2.33	0.54
2:d:129:LYS:NZ	28:a:2906:U:OP1	2.40	0.54
7:j:22:ILE:HD11	7:j:42:THR:HB	1.90	0.54
28:a:818:G:N7	36:a:3414:HOH:O	2.33	0.54
28:a:1628:C:O2'	28:a:1727:G:N3	2.31	0.54
28:a:2711:G:H2'	28:a:2712:G:N9	2.23	0.54
28:a:372:U:H2'	28:a:373:G:H8	1.73	0.54
1:c:108:PRO:HD2	1:c:111:VAL:HG21	1.89	0.54
10:m:58:ASP:OD2	10:m:63:ARG:NH1	2.41	0.54
12:o:74:PHE:HB3	12:o:81:ILE:HD11	1.89	0.54
28:a:565:G:N1	28:a:568:A:OP2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:y:10:ILE:HG13	22:y:11:LYS:HG2	1.89	0.53
27:4:41:CYS:SG	27:4:41:CYS:O	2.65	0.53
28:a:715:C:O2	28:a:725:U:O2'	2.25	0.53
3:e:125:ARG:HH22	3:e:150:LEU:HD22	1.73	0.53
10:m:34:VAL:HG23	28:a:1354:C:O3'	2.09	0.53
28:a:2938:U:H4'	28:a:2939:A:OP1	2.09	0.53
3:e:182:ALA:HB1	3:e:206:PHE:HB2	1.90	0.53
28:a:453:U:H4'	28:a:454:G:OP1	2.08	0.53
32:3:14:CYS:SG	32:3:27:CYS:SG	3.04	0.53
4:f:143:GLU:HG2	4:f:158:ILE:HG23	1.91	0.53
28:a:2020:C:O2'	28:a:2110:A:N3	2.34	0.53
28:a:2051:U:H3'	28:a:2052:G:H8	1.73	0.53
28:a:2658:A:H3'	28:a:2659:U:H6	1.73	0.53
18:u:65:ILE:HB	18:u:68:GLN:HB2	1.91	0.53
18:u:88:ARG:HH21	29:b:77:U:H5"	1.72	0.53
28:a:318:G:OP1	28:a:366:A:N6	2.42	0.53
28:a:1070:C:O2'	28:a:1083:A:N3	2.40	0.53
8:k:131:SER:OG	28:a:723:A:OP1	2.25	0.53
28:a:50:G:O2'	28:a:118:A:N6	2.42	0.53
28:a:971:U:H2'	28:a:972:A:C8	2.44	0.53
4:f:127:ASN:HD21	4:f:196:LYS:HB2	1.70	0.53
10:m:57:THR:HG23	10:m:62:ASN:ND2	2.24	0.53
27:4:43:PRO:HB3	27:4:48:LYS:O	2.09	0.53
28:a:439:C:H2'	28:a:440:A:H8	1.74	0.53
28:a:709:U:H2'	28:a:710:C:C6	2.44	0.53
28:a:1151:G:HO2'	28:a:1179:A:HO2'	1.56	0.53
3:e:49:GLN:HG2	3:e:51:THR:HG23	1.90	0.53
27:4:18:CYS:CB	27:4:41:CYS:SG	2.96	0.53
2:d:15:LEU:HD11	2:d:34:GLN:HB2	1.91	0.52
3:e:154:ARG:NH1	3:e:195:THR:OG1	2.42	0.52
4:f:200:GLY:O	4:f:201:PRO:C	2.51	0.52
8:k:56:ILE:HG13	8:k:57:HIS:N	2.25	0.52
28:a:418:G:O2'	28:a:419:U:OP1	2.25	0.52
28:a:1917:U:H2'	28:a:1918:G:C8	2.44	0.52
9:l:48:GLU:OE2	9:l:51:ARG:NH2	2.35	0.52
28:a:246:U:O2'	28:a:708:G:O2'	2.23	0.52
28:a:442:U:H2'	28:a:443:G:O4'	2.09	0.52
28:a:477:G:O2'	28:a:479:A:OP2	2.26	0.52
28:a:669:A:N1	28:a:894:G:O2'	2.37	0.52
28:a:2649:C:OP1	32:3:8:LYS:NZ	2.40	0.52
5:g:39:GLU:HG3	5:g:40:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:119:ALA:HB2	5:g:125:PHE:CE2	2.45	0.52
11:n:3:SER:O	29:b:11:C:N4	2.34	0.52
12:o:100:LEU:HD11	12:o:110:ILE:HD11	1.91	0.52
16:s:54:VAL:HG13	16:s:92:ASP:HB3	1.91	0.52
28:a:142:G:H21	28:a:147:G:H1	1.57	0.52
28:a:375:G:C2	28:a:376:U:H1'	2.44	0.52
7:j:108:GLU:HB2	7:j:110:LYS:NZ	2.24	0.52
9:l:62:GLY:O	18:u:180:GLU:HB2	2.09	0.52
28:a:660:G:H2'	28:a:661:A:C8	2.45	0.52
1:c:184:MET:HE3	1:c:266:ARG:HA	1.92	0.52
5:g:96:ARG:HG2	5:g:108:ASN:HB2	1.91	0.52
24:0:38:GLU:OE2	24:0:53:ARG:NH1	2.37	0.52
28:a:130:G:H22	28:a:154:G:H1	1.57	0.52
28:a:2288:G:H22	28:a:2365:U:H3	1.57	0.52
28:a:2704:U:O2'	28:a:2829:U:OP1	2.20	0.52
28:a:1647:G:H4'	28:a:1729:G:H21	1.74	0.52
4:f:85:GLN:HE21	28:a:2492:A:H2	1.57	0.52
5:g:109:LEU:HD13	5:g:154:ARG:CB	2.39	0.52
5:g:177:LYS:HG3	28:a:2713:A:C8	2.44	0.52
14:q:58:VAL:HG22	14:q:100:ILE:HG23	1.91	0.52
28:a:374:C:H42	28:a:436:U:H3	1.57	0.52
28:a:2248:C:H2'	28:a:2249:C:C6	2.45	0.52
28:a:2961:U:H5"	28:a:2962:A:H2'	1.92	0.52
2:d:94:SER:C	2:d:96:TYR:H	2.17	0.52
4:f:47:MET:HE3	4:f:66:ILE:HD12	1.91	0.52
27:4:13:THR:HA	27:4:23:THR:HA	1.92	0.52
28:a:1130:G:N1	28:a:1193:A:N7	2.58	0.52
28:a:868:A:H8	28:a:1961:U:HO2'	1.58	0.52
28:a:2938:U:H1'	28:a:2939:A:H5"	1.92	0.52
1:c:223:GLY:HA2	1:c:226:MET:SD	2.50	0.52
2:d:122:LYS:HG3	2:d:171:MET:HE3	1.91	0.52
4:f:145:VAL:HA	4:f:150:ILE:HD11	1.92	0.52
18:u:116:GLY:O	18:u:179:PRO:HD3	2.09	0.52
28:a:60:G:N2	28:a:92:G:H1	2.04	0.52
28:a:532:A:H8	28:a:1277:G:H21	1.57	0.52
1:c:44:ASN:ND2	28:a:1989:C:O2	2.43	0.51
27:4:38:CYS:O	27:4:42:HIS:HB2	2.10	0.51
1:c:258:ARG:NH1	28:a:1982:G:OP1	2.37	0.51
18:u:172:VAL:HG11	28:a:960:U:H4'	1.93	0.51
27:4:14:VAL:O	27:4:21:THR:HA	2.11	0.51
28:a:98:U:OP2	28:a:100:U:O2'	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:155:LYS:HG2	5:g:156:PRO:HD2	1.92	0.51
6:i:88:SER:OG	6:i:91:GLU:HG3	2.10	0.51
8:k:34:ARG:HH11	28:a:670:G:H1	1.58	0.51
1:c:25:THR:O	1:c:81:HIS:ND1	2.42	0.51
28:a:142:G:N2	28:a:147:G:H22	2.07	0.51
28:a:130:G:N2	28:a:154:G:H22	2.09	0.51
3:e:159:VAL:O	3:e:161:ASP:N	2.44	0.51
28:a:286:G:N7	28:a:313:G:N2	2.59	0.51
28:a:917:U:H2'	28:a:918:G:C8	2.46	0.51
21:x:17:LEU:HD22	21:x:56:VAL:HG13	1.92	0.51
28:a:374:C:H2'	28:a:375:G:C8	2.45	0.51
28:a:392:G:H21	28:a:415:A:H62	1.58	0.51
28:a:869:G:H5'	28:a:870:G:OP1	2.11	0.51
28:a:2915:U:H2'	28:a:2916:U:C6	2.46	0.51
31:C:52:G:H2'	31:C:53:G:H8	1.75	0.51
17:t:101:ARG:NH1	17:t:105:SER:OG	2.38	0.51
28:a:2040:G:H22	28:a:2067:A:HO2'	1.53	0.51
28:a:2284:G:H22	28:a:2369:U:H3	1.59	0.51
28:a:2503:G:O2'	28:a:2504:A:OP1	2.21	0.51
12:o:30:VAL:HG13	12:o:80:ILE:HD12	1.93	0.50
28:a:2048:G:N1	28:a:2059:U:OP2	2.34	0.50
28:a:2503:G:HO2'	28:a:2504:A:P	2.33	0.50
28:a:2721:C:H5'	28:a:2722:C:OP2	2.11	0.50
24:0:36:ARG:NH1	24:0:54:GLU:O	2.45	0.50
27:4:43:PRO:HG3	27:4:48:LYS:NZ	2.26	0.50
28:a:653:G:H2'	28:a:2213:A:N7	2.25	0.50
15:r:4:THR:O	15:r:5:GLU:C	2.54	0.50
28:a:1489:C:H2'	28:a:1490:A:H8	1.76	0.50
1:c:6:TYR:CG	1:c:13:ARG:HD2	2.47	0.50
15:r:102:ILE:HG23	15:r:110:ALA:HB1	1.92	0.50
28:a:60:G:H1	28:a:92:G:H1	1.60	0.50
28:a:303:G:H2'	28:a:304:G:C8	2.46	0.50
7:j:63:VAL:HG22	7:j:106:LEU:HD21	1.94	0.50
14:q:4:ILE:HB	14:q:39:LEU:HB3	1.94	0.50
15:r:82:ARG:NH1	15:r:84:ASP:OD1	2.45	0.50
28:a:1896:A:N6	28:a:1929:G:O2'	2.44	0.50
5:g:92:GLY:CA	5:g:162:LYS:HG2	2.40	0.50
28:a:1656:G:O2'	28:a:1696:G:N1	2.40	0.50
1:c:222:ARG:NH2	28:a:1971:C:OP1	2.44	0.50
3:e:149:GLY:O	3:e:150:LEU:HB2	2.12	0.50
24:0:30:ARG:HH22	24:0:31:ARG:NH2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:130:G:H22	28:a:154:G:H22	1.60	0.50
28:a:660:G:O2'	28:a:1331:A:OP1	2.30	0.50
3:e:160:LEU:HD23	3:e:163:SER:H	1.76	0.50
21:x:52:ASP:O	21:x:56:VAL:HG23	2.12	0.50
28:a:286:G:N2	28:a:287:U:O4'	2.45	0.50
28:a:1399:A:N6	28:a:1400:G:O6	2.45	0.50
3:e:29:VAL:HG21	3:e:114:ARG:HB3	1.94	0.50
28:a:2119:A:OP2	28:a:2145:5MC:N4	2.44	0.50
2:d:144:ARG:NH1	28:a:830:G:OP2	2.43	0.49
4:f:207:LYS:C	4:f:209:LYS:N	2.69	0.49
7:j:64:ARG:O	7:j:82:ASN:HA	2.12	0.49
10:m:56:LYS:NZ	10:m:90:ARG:O	2.45	0.49
18:u:58:ASN:ND2	18:u:103:VAL:HB	2.27	0.49
28:a:350:A:H2'	28:a:351:G:C8	2.45	0.49
28:a:2050:G:H2'	28:a:2051:U:O4'	2.12	0.49
28:a:2527:G:N3	28:a:2563:C:H2'	2.27	0.49
4:f:126:LEU:HD23	4:f:185:PRO:HG2	1.93	0.49
5:g:109:LEU:HD13	5:g:154:ARG:HB3	1.94	0.49
7:j:35:LEU:HD21	7:j:65:THR:H	1.77	0.49
16:s:3:GLU:HG2	28:a:151:G:H4'	1.93	0.49
20:w:38:VAL:HG21	20:w:47:MET:SD	2.52	0.49
28:a:338:U:O2'	28:a:339:U:O5'	2.29	0.49
28:a:2655:C:H2'	28:a:2655:C:O2	2.12	0.49
28:a:2970:C:O2'	28:a:2989:A:N3	2.41	0.49
1:c:16:SER:HB3	1:c:207:GLY:HA3	1.94	0.49
3:e:142:GLN:O	3:e:143:ALA:C	2.55	0.49
4:f:10:MET:HG2	4:f:14:LYS:HD3	1.95	0.49
8:k:58:MET:CE	28:a:257:G:H4'	2.42	0.49
23:z:14:ARG:HB3	28:a:15:U:H5"	1.94	0.49
28:a:742:U:H2'	28:a:743:C:C6	2.48	0.49
28:a:2183:C:O2'	28:a:2871:U:OP2	2.29	0.49
28:a:2720:C:N4	32:3:2:LYS:HE3	2.26	0.49
5:g:111:PHE:HE1	5:g:154:ARG:HH21	1.59	0.49
7:j:23:ARG:NH2	28:a:2730:G:H1'	2.27	0.49
16:s:4:LEU:HD22	21:x:61:GLN:HB2	1.95	0.49
28:a:254:G:OP2	28:a:256:C:N4	2.44	0.49
28:a:1095:U:H5'	28:a:1096:G:H5"	1.95	0.49
4:f:65:ASP:OD2	4:f:159:ARG:NH1	2.43	0.49
8:k:43:LYS:HG3	8:k:44:ASN:H	1.76	0.49
15:r:1:MET:CE	28:a:1288:G:H2'	2.43	0.49
22:y:3:SER:OG	22:y:40:ASP:OD1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1364:U:H5”	28:a:1365:C:OP2	2.12	0.49
28:a:2720:C:C5	32:3:2:LYS:HG2	2.48	0.49
28:a:2929:G:O6	28:a:2937:C:H5”	2.12	0.49
5:g:60:ARG:CZ	28:a:1118:U:H5”	2.42	0.49
7:j:12:ASP:OD2	7:j:86:LEU:N	2.42	0.49
28:a:2106:U:OP1	31:C:24:U:O2’	2.25	0.49
28:a:2660:A:H3’	28:a:2661:G:C8	2.46	0.49
29:b:5:C:OP1	29:b:61:C:O2’	2.29	0.49
1:c:134:ARG:HH21	1:c:188:ARG:HG3	1.77	0.49
2:d:190:ARG:HG3	2:d:192:ILE:HG12	1.94	0.49
12:o:89:HIS:HB3	12:o:113:ARG:HE	1.78	0.49
17:t:42:ASN:O	17:t:67:GLU:HA	2.11	0.49
25:1:16:HIS:HB2	25:1:44:ALA:HB3	1.93	0.49
28:a:235:G:H4’	28:a:236:U:C6	2.48	0.49
28:a:373:G:H2’	28:a:373:G:N3	2.27	0.49
28:a:1910:C:H4’	28:a:1911:G:C5	2.47	0.49
15:r:72:MET:HE2	15:r:83:ALA:HB1	1.95	0.49
23:z:53:PRO:HB3	28:a:3065:A:H5’	1.94	0.49
28:a:891:C:O2	28:a:2626:G:O2’	2.30	0.49
28:a:2586:C:N4	28:a:2587:U:O4	2.46	0.49
28:a:2859:U:H2’	28:a:2860:G:C8	2.48	0.49
28:a:2894:U:OP1	28:a:2896:G:H4’	2.13	0.49
28:a:2971:C:H1’	28:a:3071:A:C2	2.48	0.49
28:a:3046:G:C2	28:a:3048:A:H1’	2.48	0.49
28:a:1065:C:N3	30:V:21:ARG:NH2	2.60	0.49
28:a:1815:G:N2	28:a:1818:U:OP2	2.34	0.49
32:3:16:VAL:HG22	32:3:25:VAL:HG22	1.95	0.49
5:g:117:VAL:HG11	5:g:150:ILE:HD11	1.95	0.48
7:j:2:ILE:HB	7:j:33:ALA:HB3	1.94	0.48
18:u:9:ALA:HB2	18:u:45:LEU:HD23	1.95	0.48
28:a:433:G:H5’	28:a:435:G:O5’	2.11	0.48
28:a:1199:U:H2’	28:a:1200:U:C6	2.48	0.48
5:g:78:ILE:HA	5:g:81:THR:HG22	1.95	0.48
10:m:36:THR:O	10:m:40:LYS:HB2	2.13	0.48
28:a:171:A:H2’	28:a:172:U:C6	2.48	0.48
28:a:1933:G:O2’	28:a:3040:A:N1	2.42	0.48
2:d:200:PRO:HA	28:a:2862:C:H5’	1.94	0.48
3:e:140:THR:O	3:e:144:LYS:HG2	2.13	0.48
8:k:79:LEU:HG	8:k:113:GLY:HA2	1.94	0.48
15:r:3:LYS:HD3	15:r:4:THR:HG23	1.93	0.48
16:s:64:ARG:NH2	28:a:1416:U:OP2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:337:G:H22	28:a:355:U:H2'	1.78	0.48
28:a:1708:G:H22	28:a:1729:G:H1	1.60	0.48
28:a:2149:A:N3	28:a:2774:G:O2'	2.43	0.48
3:e:43:GLN:NE2	3:e:186:ASN:HB2	2.27	0.48
18:u:153:TYR:HA	18:u:172:VAL:HA	1.95	0.48
28:a:943:G:N3	28:a:2450:A:H2'	2.28	0.48
28:a:2986:G:H2'	28:a:2987:G:C8	2.48	0.48
5:g:159:TYR:HE1	28:a:2713:A:O3'	1.96	0.48
16:s:69:ARG:NH1	16:s:71:THR:HG22	2.27	0.48
27:4:11:GLU:CD	27:4:12:THR:H	2.22	0.48
28:a:130:G:H22	28:a:154:G:N2	2.11	0.48
28:a:614:G:OP1	28:a:615:C:OP1	2.31	0.48
28:a:974:C:H3'	28:a:975:G:C8	2.49	0.48
28:a:1393:G:H2'	28:a:1394:G:H8	1.78	0.48
28:a:1901:U:H2'	28:a:1902:C:C6	2.49	0.48
2:d:31:THR:HG21	2:d:199:VAL:HG22	1.94	0.48
3:e:139:SER:HA	3:e:142:GLN:NE2	2.28	0.48
3:e:139:SER:CA	3:e:142:GLN:HE22	2.26	0.48
5:g:95:TYR:CE2	5:g:162:LYS:HB3	2.46	0.48
9:l:18:THR:HG22	29:b:91:U:H5'	1.95	0.48
10:m:104:LYS:NZ	28:a:1361:G:O2'	2.34	0.48
27:4:43:PRO:HA	27:4:48:LYS:HB3	1.96	0.48
1:c:226:MET:HE2	28:a:867:A:N1	2.29	0.48
4:f:83:ILE:HG22	4:f:86:PHE:H	1.79	0.48
28:a:252:G:N2	28:a:473:U:O2'	2.33	0.48
28:a:2042:A:N6	28:a:2066:G:H22	2.11	0.48
28:a:2872:G:H8	28:a:3052:G:H8	1.59	0.48
28:a:2880:U:H2'	28:a:2881:U:C6	2.48	0.48
9:l:118:MET:HG3	9:l:131:PHE:CD1	2.49	0.48
11:n:40:VAL:HG13	11:n:49:VAL:HG22	1.95	0.48
13:p:58:ARG:HH22	13:p:92:ARG:HH21	1.61	0.48
17:t:94:ARG:NH1	17:t:112:SER:OG	2.37	0.48
28:a:135:G:H2'	28:a:136:U:C6	2.49	0.48
1:c:148:ARG:NH2	28:a:2386:G:H5'	2.28	0.48
4:f:207:LYS:HZ3	28:a:965:G:H4'	1.78	0.48
5:g:4:ILE:HG12	28:a:2933:G:H4'	1.94	0.48
14:q:91:LYS:H	14:q:91:LYS:HD2	1.79	0.48
28:a:618:G:O2'	28:a:620:C:C5	2.66	0.48
28:a:2533:G:H2'	28:a:2547:G:H22	1.79	0.48
30:V:21:ARG:HG3	30:V:22:PRO:HD2	1.96	0.48
3:e:114:ARG:HH21	3:e:210:ARG:HG2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:j:113:ARG:NH2	7:j:117:LEU:HD21	2.29	0.48
14:q:47:THR:HG22	14:q:53:LEU:HD22	1.96	0.48
28:a:358:C:H41	28:a:446:G:N2	2.11	0.48
28:a:1047:U:O2'	28:a:2455:A:N3	2.39	0.48
32:3:10:ILE:HB	32:3:32:HIS:CD2	2.49	0.48
2:d:187:ASP:OD2	2:d:190:ARG:HG2	2.14	0.47
4:f:199:ARG:HG3	4:f:199:ARG:H	1.52	0.47
17:t:27:LEU:HD21	17:t:39:GLU:HB3	1.96	0.47
21:x:40:LEU:HD21	21:x:43:THR:HA	1.96	0.47
28:a:50:G:H1'	28:a:117:A:H61	1.79	0.47
28:a:1156:A:O2'	28:a:2656:U:O3'	2.32	0.47
28:a:1612:G:H2'	28:a:1613:U:C6	2.48	0.47
28:a:1897:G:H1'	28:a:1898:C:H5'	1.96	0.47
31:C:52:G:H2'	31:C:53:G:C8	2.49	0.47
1:c:208:LYS:HD3	1:c:211:ARG:HG3	1.96	0.47
9:l:60:ARG:HD3	9:l:60:ARG:H	1.79	0.47
28:a:2215:G:OP1	28:a:2636:G:O2'	2.20	0.47
28:a:2510:A:H2'	28:a:2511:G:C8	2.49	0.47
2:d:94:SER:C	2:d:96:TYR:N	2.70	0.47
2:d:158:PRO:O	2:d:160:LYS:N	2.46	0.47
4:f:63:ILE:HD12	4:f:74:PRO:HG2	1.96	0.47
5:g:109:LEU:HD22	5:g:154:ARG:HD2	1.96	0.47
12:o:92:VAL:HG11	12:o:97:LEU:HD11	1.96	0.47
15:r:20:SER:OG	15:r:21:TYR:N	2.47	0.47
15:r:109:SER:O	28:a:1798:A:N6	2.40	0.47
28:a:116:G:OP2	28:a:118:A:O2'	2.26	0.47
28:a:603:A:HO2'	28:a:663:C:HO2'	1.62	0.47
13:p:92:ARG:O	13:p:93:LYS:HB2	2.14	0.47
23:z:57:ARG:HA	23:z:57:ARG:HD2	1.38	0.47
28:a:271:G:O2'	28:a:272:A:H5"	2.12	0.47
28:a:1488:U:H2'	28:a:1489:C:C6	2.50	0.47
28:a:1710:A:N6	28:a:1711:G:O6	2.47	0.47
28:a:1716:U:HO2'	28:a:1721:G:N2	2.12	0.47
28:a:2291:U:H1'	28:a:2361:C:H42	1.80	0.47
1:c:219:PRO:HG3	28:a:849:A:H2	1.79	0.47
8:k:123:LEU:HB2	8:k:143:VAL:HG12	1.96	0.47
28:a:2375:U:H2'	28:a:2376:A:C8	2.50	0.47
28:a:2714:G:H8	28:a:2714:G:O5'	1.96	0.47
28:a:2836:A:N1	28:a:2847:A:H5"	2.30	0.47
4:f:113:LEU:HA	4:f:117:LEU:HD21	1.96	0.47
4:f:120:ILE:HD11	4:f:146:MET:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:191:ASP:HB3	4:f:192:PRO:CD	2.44	0.47
26:2:12:LYS:NZ	28:a:254:G:O6	2.44	0.47
27:4:37:VAL:HG11	27:4:42:HIS:HD2	1.78	0.47
28:a:588:G:N1	28:a:591:A:OP2	2.47	0.47
28:a:1851:G:O2'	28:a:2174:U:O4	2.27	0.47
1:c:124:ASP:OD1	1:c:125:ILE:N	2.48	0.47
2:d:15:LEU:HD13	12:o:4:ILE:HG21	1.95	0.47
4:f:194:LYS:O	4:f:195:ALA:C	2.58	0.47
9:l:51:ARG:HG3	9:l:66:ILE:HD11	1.97	0.47
12:o:27:LYS:HG2	12:o:44:SER:OG	2.14	0.47
15:r:29:MET:HE1	15:r:60:ALA:HA	1.96	0.47
18:u:37:ASP:OD2	18:u:37:ASP:N	2.48	0.47
23:z:6:ARG:NH1	28:a:2202:C:H41	2.12	0.47
28:a:1343:G:O2'	28:a:2195:G:O6	2.23	0.47
28:a:2525:U:H2'	28:a:2526:U:C6	2.50	0.47
28:a:2588:U:OP2	28:a:2588:U:H2'	2.15	0.47
28:a:2986:G:H2'	28:a:2987:G:H8	1.79	0.47
31:C:43:A:H2'	31:C:44:A:C8	2.50	0.47
31:C:62:C:H2'	31:C:63:G:H8	1.80	0.47
3:e:107:LYS:NZ	28:a:690:U:OP2	2.42	0.47
4:f:207:LYS:NZ	28:a:965:G:H4'	2.30	0.47
5:g:45:LYS:HB3	5:g:48:GLU:HA	1.97	0.47
28:a:314:U:H3'	28:a:315:G:H8	1.80	0.47
28:a:2517:A:O2'	28:a:2518:A:OP1	2.32	0.47
4:f:193:LYS:O	4:f:196:LYS:HB3	2.15	0.47
5:g:59:GLU:HG3	5:g:62:ASN:H	1.79	0.47
17:t:81:ILE:HG13	17:t:82:ASP:N	2.30	0.47
28:a:834:A:H4'	28:a:1348:G:N3	2.29	0.47
3:e:63:GLY:HA3	3:e:82:ARG:HG2	1.97	0.47
28:a:252:G:O2'	28:a:473:U:O2	2.21	0.47
28:a:376:U:H2'	28:a:377:G:C8	2.50	0.47
28:a:433:G:OP2	28:a:433:G:N2	2.25	0.47
28:a:898:U:H2'	28:a:899:C:C6	2.50	0.47
28:a:1433:C:H2'	28:a:1434:G:O4'	2.14	0.47
28:a:2141:C:H2'	28:a:2142:G:C8	2.50	0.47
10:m:5:THR:O	10:m:7:GLY:N	2.47	0.46
10:m:28:LEU:HD13	10:m:34:VAL:HG12	1.97	0.46
15:r:3:LYS:HB3	15:r:4:THR:H	1.49	0.46
22:y:40:ASP:OD2	22:y:45:ARG:NH1	2.47	0.46
28:a:57:G:O2'	28:a:72:A:N1	2.45	0.46
28:a:254:G:H4'	28:a:475:G:C5	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:53:HIS:HE1	1:c:220:THR:HA	1.76	0.46
2:d:94:SER:O	2:d:96:TYR:N	2.48	0.46
4:f:189:LYS:HD2	4:f:190:ASP:H	1.79	0.46
4:f:207:LYS:HG3	28:a:965:G:O5'	2.15	0.46
8:k:23:ARG:HA	28:a:896:U:H2'	1.97	0.46
11:n:67:GLU:O	11:n:71:ARG:HG2	2.15	0.46
17:t:4:LEU:HD23	17:t:72:VAL:HG21	1.96	0.46
21:x:40:LEU:O	21:x:40:LEU:HD23	2.16	0.46
28:a:433:G:H5"	28:a:433:G:N3	2.29	0.46
28:a:1062:A:H2'	28:a:1065:C:H42	1.79	0.46
28:a:1716:U:HO2'	28:a:1721:G:H22	1.60	0.46
28:a:1771:U:H2'	28:a:1772:G:C8	2.50	0.46
4:f:59:MET:O	4:f:63:ILE:HG12	2.15	0.46
22:y:41:ARG:O	22:y:45:ARG:HG2	2.16	0.46
28:a:279:A:H5'	28:a:280:C:OP2	2.15	0.46
28:a:2415:U:H2'	28:a:2416:G:C8	2.50	0.46
3:e:13:LYS:HD2	3:e:13:LYS:HA	1.75	0.46
6:i:77:HIS:HD2	6:i:84:LEU:HD13	1.79	0.46
28:a:2938:U:OP2	32:3:19:ARG:NE	2.44	0.46
4:f:144:GLN:NE2	4:f:155:ILE:HG21	2.30	0.46
4:f:207:LYS:HE2	28:a:965:G:H4'	1.97	0.46
6:i:2:THR:HG23	28:a:1078:C:H42	1.79	0.46
7:j:31:ARG:HH12	28:a:2857:A:H5"	1.81	0.46
13:p:6:ARG:NH1	28:a:668:G:N7	2.60	0.46
27:4:15:VAL:HG22	27:4:17:THR:H	1.80	0.46
2:d:124:THR:O	28:a:1838:A:O2'	2.31	0.46
2:d:167:MET:HE1	28:a:2801:C:O2	2.16	0.46
7:j:22:ILE:HG23	28:a:2135:A:C2	2.51	0.46
18:u:97:ARG:O	18:u:132:LEU:HD22	2.15	0.46
28:a:1969:A:H1'	28:a:2121:A:N6	2.31	0.46
5:g:33:LEU:HD12	5:g:76:MET:HB2	1.97	0.46
5:g:150:ILE:HG22	5:g:164:VAL:HG11	1.96	0.46
24:0:12:ILE:HB	24:0:54:GLU:HG3	1.97	0.46
28:a:165:G:HO2'	28:a:166:A:P	2.38	0.46
28:a:305:U:O2'	28:a:307:U:H1'	2.16	0.46
28:a:1002:A:H5"	29:b:98:G:O2'	2.16	0.46
1:c:206:TRP:O	1:c:211:ARG:HD3	2.15	0.46
2:d:96:TYR:HE2	2:d:102:ILE:HD11	1.79	0.46
3:e:175:SER:HB3	28:a:408:G:O2'	2.15	0.46
7:j:64:ARG:HA	7:j:79:PHE:CD1	2.50	0.46
23:z:55:GLY:O	23:z:56:ASP:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1492:C:H2'	28:a:1493:G:C8	2.51	0.46
28:a:2072:A:H2'	28:a:2073:A:C8	2.51	0.46
28:a:2433:OMG:H1'	28:a:2433:OMG:HM23	1.70	0.46
28:a:2496:A:H2'	28:a:2497:G:C8	2.51	0.46
3:e:155:LYS:HZ1	3:e:189:ASP:C	2.24	0.46
8:k:98:VAL:HG21	8:k:109:VAL:HG11	1.98	0.46
28:a:2052:G:H2'	28:a:2055:U:O4	2.16	0.46
3:e:137:LYS:HE3	3:e:169:LEU:CD1	2.46	0.46
7:j:9:LYS:NZ	7:j:81:GLU:HB2	2.31	0.46
15:r:23:ILE:HG12	15:r:121:THR:HG23	1.97	0.46
15:r:62:GLU:HB3	15:r:63:PRO:HD3	1.98	0.46
28:a:2051:U:C4	28:a:2052:G:C5	3.03	0.46
2:d:69:PRO:HG3	28:a:2969:C:H1'	1.96	0.45
24:0:29:ASN:C	24:0:31:ARG:H	2.23	0.45
28:a:60:G:N2	28:a:92:G:H22	2.13	0.45
28:a:1171:A:H5"	28:a:1172:G:H5'	1.98	0.45
28:a:1354:C:H2'	28:a:1355:G:C8	2.51	0.45
4:f:201:PRO:O	4:f:202:ALA:C	2.59	0.45
7:j:64:ARG:HB2	7:j:83:ALA:HB3	1.98	0.45
7:j:93:PRO:HG3	7:j:114:ILE:HG13	1.97	0.45
13:p:4:VAL:HG22	28:a:1276:C:H1'	1.97	0.45
15:r:10:ARG:NH2	15:r:79:GLU:OE2	2.49	0.45
16:s:65:LYS:HA	16:s:80:ASP:OD2	2.17	0.45
28:a:26:G:N2	28:a:600:G:H1'	2.31	0.45
28:a:35:G:N3	28:a:539:G:O2'	2.49	0.45
28:a:1081:C:N4	36:a:3413:HOH:O	2.49	0.45
1:c:211:ARG:HG2	1:c:214:TRP:CZ2	2.51	0.45
5:g:42:THR:OG1	5:g:54:GLU:HG2	2.16	0.45
24:0:29:ASN:HD21	28:a:2467:C:P	2.38	0.45
28:a:491:A:H2'	28:a:492:U:O4'	2.16	0.45
3:e:185:LEU:O	3:e:186:ASN:ND2	2.49	0.45
8:k:58:MET:HE2	28:a:257:G:H4'	1.98	0.45
13:p:92:ARG:HH22	28:a:1081:C:P	2.39	0.45
16:s:6:ILE:HD11	21:x:18:ARG:HG2	1.97	0.45
28:a:439:C:H2'	28:a:440:A:C8	2.50	0.45
28:a:682:U:H2'	28:a:683:G:C8	2.52	0.45
3:e:40:VAL:HG13	3:e:188:TYR:HD1	1.81	0.45
3:e:137:LYS:O	3:e:137:LYS:HG3	2.17	0.45
13:p:66:ASN:ND2	28:a:1094:G:OP2	2.42	0.45
14:q:21:GLU:OE2	14:q:92:TYR:HB2	2.17	0.45
18:u:52:LEU:HD22	18:u:55:ARG:NH1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:y:47:MET:O	22:y:51:VAL:HG22	2.17	0.45
27:4:20:ASN:HB3	27:4:40:LYS:HZ1	1.81	0.45
28:a:432:A:O5'	28:a:433:G:N2	2.49	0.45
28:a:634:U:O2'	28:a:635:G:H8	1.98	0.45
28:a:1347:C:H5"	28:a:1348:G:H5'	1.98	0.45
4:f:151:ASP:OD2	4:f:154:LYS:HB3	2.16	0.45
4:f:186:PHE:C	4:f:186:PHE:CD2	2.94	0.45
4:f:192:PRO:O	4:f:193:LYS:C	2.60	0.45
23:z:8:MET:HE3	23:z:8:MET:HB2	1.84	0.45
24:0:7:ASP:OD1	24:0:7:ASP:N	2.49	0.45
26:2:19:SER:OG	28:a:737:G:OP1	2.29	0.45
28:a:2052:G:H1	28:a:2054:A:H5"	1.82	0.45
28:a:2282:G:H1	28:a:2371:U:H3	1.65	0.45
2:d:37:PRO:HB3	2:d:101:GLU:OE2	2.16	0.45
4:f:191:ASP:CB	4:f:192:PRO:CD	2.95	0.45
5:g:95:TYR:HA	5:g:108:ASN:O	2.16	0.45
5:g:105:LEU:HG	5:g:125:PHE:CD2	2.52	0.45
10:m:46:PRO:O	10:m:50:LYS:HG2	2.16	0.45
28:a:310:C:H2'	28:a:311:A:C8	2.51	0.45
28:a:2247:C:H2'	28:a:2248:C:C6	2.51	0.45
1:c:262:LYS:HG3	1:c:263:ALA:N	2.24	0.45
5:g:176:GLY:HA3	28:a:2713:A:C5'	2.47	0.45
11:n:93:LYS:NZ	11:n:98:THR:HA	2.31	0.45
18:u:143:VAL:HG11	18:u:176:VAL:HG11	1.98	0.45
24:0:11:LYS:HE2	24:0:11:LYS:HB2	1.79	0.45
28:a:828:C:O2'	28:a:1843:U:OP1	2.30	0.45
28:a:1230:U:H2'	28:a:1231:A:C8	2.52	0.45
28:a:2495:C:H2'	28:a:2496:A:H8	1.82	0.45
4:f:180:LYS:NZ	4:f:186:PHE:HE2	2.15	0.45
7:j:73:ASP:OD2	12:o:80:ILE:HD13	2.17	0.45
10:m:69:THR:HG22	10:m:70:ILE:N	2.32	0.45
10:m:106:ASP:OD2	28:a:1833:G:O2'	2.30	0.45
28:a:2141:C:H2'	28:a:2142:G:H8	1.81	0.45
28:a:2706:G:H1	28:a:2721:C:N4	2.10	0.45
29:b:14:U:OP2	29:b:70:C:O2'	2.35	0.45
4:f:198:LYS:HE3	4:f:198:LYS:HB3	1.62	0.45
5:g:148:ALA:HB2	28:a:2927:C:H5'	1.99	0.45
7:j:24:VAL:HG12	7:j:30:ARG:HD3	1.98	0.45
15:r:1:MET:HB3	15:r:1:MET:HE3	1.72	0.45
19:v:41:ARG:HH21	19:v:56:ASP:HB2	1.82	0.45
25:1:25:ARG:NH1	28:a:1443:A:O3'	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:26:LYS:HD3	26:2:48:THR:HB	1.98	0.45
28:a:1984:G:H3'	28:a:1985:A:H5'	1.98	0.45
28:a:2656:U:H3'	28:a:2657:C:C6	2.52	0.45
3:e:136:ASP:OD1	3:e:137:LYS:N	2.44	0.44
7:j:63:VAL:HG11	7:j:102:ILE:HG23	1.99	0.44
9:l:14:HIS:CD2	9:l:74:MET:HE1	2.52	0.44
11:n:14:ARG:HD3	29:b:30:C:OP1	2.17	0.44
17:t:29:VAL:HG13	17:t:36:VAL:HG12	1.99	0.44
23:z:39:HIS:ND1	23:z:40:LEU:O	2.48	0.44
28:a:277:A:OP2	28:a:320:G:N2	2.45	0.44
28:a:373:G:H22	28:a:437:G:H22	1.65	0.44
28:a:1359:G:O2'	28:a:1361:G:N7	2.44	0.44
28:a:1698:G:H1	28:a:1915:G:N2	2.09	0.44
4:f:190:ASP:HB3	4:f:194:LYS:HG2	1.98	0.44
11:n:8:ARG:NH1	29:b:17:U:OP2	2.49	0.44
14:q:42:ASP:HB3	14:q:45:SER:OG	2.17	0.44
15:r:52:MET:SD	23:z:24:ALA:HB1	2.57	0.44
17:t:78:VAL:HG21	17:t:85:ASP:HB3	1.99	0.44
28:a:214:A:H2'	28:a:215:C:O4'	2.17	0.44
28:a:753:A:H2'	28:a:755:A:H62	1.82	0.44
28:a:1137:A:N6	28:a:1189:G:C6	2.86	0.44
28:a:2091:U:O2'	31:C:12:G:H5"	2.17	0.44
28:a:2650:G:C2	28:a:2663:G:N3	2.85	0.44
1:c:213:ARG:HD2	1:c:213:ARG:HA	1.73	0.44
2:d:108:SER:OG	2:d:111:ASP:OD2	2.28	0.44
2:d:183:VAL:HG22	2:d:195:VAL:HG22	1.99	0.44
5:g:157:GLU:CD	5:g:160:LYS:H	2.24	0.44
24:0:35:ASP:OD1	24:0:35:ASP:N	2.47	0.44
27:4:20:ASN:ND2	27:4:38:CYS:SG	2.78	0.44
28:a:2710:U:C2	28:a:2711:G:H1'	2.52	0.44
3:e:157:LEU:HD12	3:e:182:ALA:HA	1.99	0.44
3:e:159:VAL:HG21	3:e:205:ALA:CB	2.47	0.44
5:g:45:LYS:HE3	5:g:48:GLU:HA	1.98	0.44
6:i:4:TYR:CG	13:p:100:VAL:HG11	2.52	0.44
7:j:105:GLU:OE2	7:j:105:GLU:N	2.45	0.44
12:o:6:ASP:O	12:o:10:LYS:HG2	2.17	0.44
12:o:15:ASP:OD1	12:o:15:ASP:N	2.46	0.44
18:u:152:ILE:HB	18:u:174:ALA:HB3	2.00	0.44
26:2:12:LYS:NZ	28:a:256:C:O2	2.40	0.44
28:a:1698:G:N2	28:a:1915:G:H22	2.14	0.44
28:a:2095:A:H62	28:a:2100:PSU:HN3	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2871:U:H5”	28:a:2872:G:H21	1.82	0.44
2:d:155:CYS:C	2:d:157:THR:N	2.75	0.44
4:f:180:LYS:HZ2	4:f:186:PHE:HE2	1.65	0.44
4:f:207:LYS:CE	28:a:965:G:H4’	2.47	0.44
7:j:2:ILE:HD12	7:j:6:THR:HG21	1.99	0.44
8:k:4:GLU:OE1	8:k:6:HIS:NE2	2.42	0.44
9:l:108:GLY:HA3	18:u:118:ILE:HG21	1.99	0.44
10:m:28:LEU:HD13	10:m:113:ILE:HG23	1.99	0.44
22:y:46:GLY:HA3	28:a:937:G:H5’	2.00	0.44
28:a:314:U:H3’	28:a:315:G:C8	2.52	0.44
28:a:373:G:N2	28:a:437:G:H1	2.13	0.44
28:a:631:G:H4’	28:a:632:U:H3’	1.99	0.44
28:a:861:G:N2	28:a:2423:A:OP1	2.51	0.44
28:a:1124:U:H2’	28:a:1125:G:H8	1.82	0.44
28:a:2449:A:H5”	28:a:2450:A:H5’	1.98	0.44
28:a:2718:G:O2’	28:a:2719:U:C6	2.70	0.44
5:g:32:THR:O	5:g:33:LEU:HD23	2.17	0.44
5:g:68:LEU:HD21	28:a:2940:A:C4	2.53	0.44
9:l:17:ARG:HD2	29:b:90:A:O2’	2.18	0.44
15:r:33:LYS:NZ	28:a:2195:G:N7	2.56	0.44
27:4:15:VAL:O	27:4:34:ASN:HA	2.17	0.44
28:a:304:G:H2’	28:a:305:U:C4	2.52	0.44
28:a:461:G:O2’	28:a:489:G:O6	2.30	0.44
28:a:1128:U:O2	28:a:1130:G:N1	2.51	0.44
28:a:2872:G:O2’	28:a:2873:C:P	2.75	0.44
29:b:28:C:H2’	29:b:29:A:O4’	2.17	0.44
4:f:89:ARG:NH1	31:C:56:C:N3	2.66	0.44
4:f:131:PHE:CE2	4:f:137:TYR:HB2	2.52	0.44
4:f:193:LYS:HE2	4:f:193:LYS:HB2	1.45	0.44
4:f:194:LYS:HD2	4:f:194:LYS:HA	1.50	0.44
24:0:32:ASN:N	24:0:32:ASN:HD22	2.16	0.44
28:a:1493:G:H1’	28:a:1769:G:N1	2.33	0.44
28:a:2051:U:H3	28:a:2056:G:H1	1.64	0.44
28:a:2245[A]:A:C6	35:a:3101:V7A:OBE	2.71	0.44
28:a:2718:G:O2’	28:a:2719:U:H6	2.00	0.44
1:c:221:VAL:HG21	28:a:867:A:N7	2.33	0.44
3:e:207:VAL:O	3:e:211:SER:HB3	2.17	0.44
4:f:40:LEU:HA	4:f:167:THR:HG22	2.00	0.44
14:q:79:LYS:HE3	28:a:654:A:O2’	2.17	0.44
15:r:63:PRO:O	15:r:67:VAL:HG23	2.18	0.44
28:a:547:G:O2’	28:a:558:G:O6	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:j:88:LYS:HG2	7:j:94:ARG:HG2	1.99	0.44
13:p:65:ILE:CD1	13:p:92:ARG:HG3	2.48	0.44
15:r:95:GLU:O	28:a:23:G:O2'	2.31	0.44
22:y:39:GLU:N	22:y:39:GLU:OE1	2.50	0.44
28:a:172:U:H2'	28:a:173:A:C8	2.53	0.44
28:a:430:U:H4'	28:a:431:A:C8	2.51	0.44
28:a:827:U:H2'	28:a:828:C:C6	2.53	0.44
28:a:2758:G:O2'	28:a:2761:C:OP2	2.27	0.44
31:C:15:G:H2'	31:C:59:A:N1	2.33	0.44
2:d:158:PRO:HB2	2:d:160:LYS:HG2	2.00	0.43
2:d:214:LYS:O	2:d:216:ALA:N	2.49	0.43
9:l:118:MET:HG3	9:l:131:PHE:HD1	1.82	0.43
28:a:581:G:H2'	28:a:582:G:O4'	2.18	0.43
28:a:2655:C:H5'	28:a:2657:C:N4	2.32	0.43
11:n:73:MET:HE1	11:n:80:LYS:HA	2.00	0.43
17:t:18:ASN:ND2	28:a:394:G:H5'	2.33	0.43
18:u:178:PHE:HB3	18:u:179:PRO:CD	2.48	0.43
20:w:40:GLU:O	20:w:42:GLY:N	2.52	0.43
28:a:405:G:H4'	28:a:407:A:C8	2.53	0.43
28:a:693:A:H2'	28:a:694:C:O4'	2.18	0.43
28:a:1723:G:H2'	28:a:1724:G:C8	2.54	0.43
28:a:1910:C:H2'	28:a:1912:U:C2	2.53	0.43
8:k:6:HIS:HB3	28:a:1280:U:O2	2.19	0.43
9:l:67:ASN:OD1	9:l:105:GLU:HG3	2.18	0.43
11:n:66:MET:HE2	29:b:27:A:H4'	1.99	0.43
14:q:53:LEU:HA	14:q:56:VAL:HG12	2.01	0.43
28:a:314:U:O2	28:a:314:U:H2'	2.18	0.43
28:a:430:U:H5"	28:a:431:A:H5'	1.99	0.43
28:a:454:G:H2'	28:a:455:C:O4'	2.18	0.43
28:a:1110:A:N3	36:a:3416:HOH:O	2.37	0.43
28:a:1137:A:H2'	28:a:1138:G:H8	1.83	0.43
28:a:1493:G:H5'	28:a:1595:A:H4'	1.99	0.43
28:a:2284:G:H2'	28:a:2285:A:H8	1.84	0.43
4:f:24:ALA:O	4:f:27:GLU:HG3	2.18	0.43
4:f:112:LEU:HD23	4:f:117:LEU:HD22	2.00	0.43
6:i:70:THR:HG23	6:i:71:ASP:OD2	2.19	0.43
28:a:344:U:O2	28:a:347:C:N4	2.51	0.43
28:a:400:G:H2'	28:a:401:U:O4'	2.18	0.43
28:a:409:U:H2'	28:a:410:G:O4'	2.18	0.43
31:C:4:G:H1	31:C:69:C:N4	2.16	0.43
9:l:83:MET:HE3	9:l:83:MET:HB3	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:m:100:ILE:HD11	10:m:112:VAL:HG12	1.99	0.43
17:t:27:LEU:N	17:t:37:VAL:O	2.47	0.43
28:a:2486:G:H22	28:a:2494:U:H3	1.67	0.43
2:d:57:GLY:O	2:d:58:TYR:HB3	2.18	0.43
3:e:56:THR:O	3:e:60:VAL:HG23	2.18	0.43
4:f:59:MET:HE3	4:f:93:PRO:HB2	2.01	0.43
4:f:196:LYS:HA	4:f:196:LYS:HD2	1.75	0.43
22:y:12:SER:HB2	22:y:32:ILE:HD11	2.00	0.43
24:0:20:LYS:N	24:0:20:LYS:HD2	2.34	0.43
28:a:302:A:C8	28:a:303:G:C8	3.07	0.43
28:a:373:G:H1	28:a:437:G:H1	1.66	0.43
28:a:1393:G:H2'	28:a:1394:G:C8	2.53	0.43
28:a:2036:A:N1	28:a:2269:G:H1'	2.34	0.43
4:f:161:MET:HB3	4:f:161:MET:HE2	1.82	0.43
5:g:161:GLY:O	5:g:162:LYS:C	2.62	0.43
28:a:130:G:H1	28:a:154:G:H1	1.67	0.43
28:a:373:G:N2	28:a:437:G:H22	2.16	0.43
28:a:1903:G:H2'	28:a:1904:U:C5	2.54	0.43
28:a:1972:A:H2'	28:a:1973:C:O4'	2.18	0.43
4:f:201:PRO:O	4:f:204:TYR:CD2	2.71	0.43
7:j:20:LEU:HB3	7:j:42:THR:HG22	2.00	0.43
18:u:97:ARG:HA	18:u:97:ARG:HD3	1.78	0.43
28:a:359:C:H2'	28:a:360:A:H8	1.83	0.43
28:a:771:U:H2'	28:a:873:A:N1	2.34	0.43
28:a:2722:C:O2'	28:a:2922:A:N3	2.44	0.43
1:c:179:SER:OG	28:a:1982:G:N7	2.43	0.43
2:d:105:ASP:HB3	2:d:188:ALA:HB2	2.00	0.43
5:g:73:ILE:HD13	5:g:76:MET:HE3	2.01	0.43
5:g:174:LYS:HD2	5:g:174:LYS:HA	1.33	0.43
7:j:64:ARG:NE	7:j:81:GLU:OE2	2.31	0.43
11:n:29:ILE:HG21	11:n:103:ASP:HB2	1.99	0.43
15:r:98:THR:HG23	15:r:100:ARG:HH12	1.84	0.43
28:a:314:U:C3'	28:a:315:G:H8	2.32	0.43
28:a:2606:C:O2	28:a:2611:G:O2'	2.35	0.43
28:a:2694:C:H2'	28:a:2695:G:O4'	2.19	0.43
28:a:2716:C:C4	28:a:2717:G:C8	3.07	0.43
28:a:2720:C:H4'	28:a:2721:C:OP2	2.17	0.43
31:C:9:G:N3	31:C:45:G:H2'	2.34	0.43
4:f:192:PRO:C	4:f:194:LYS:N	2.77	0.43
8:k:56:ILE:HG13	8:k:57:HIS:H	1.83	0.43
18:u:38:HIS:NE2	18:u:94:THR:HG21	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:0:29:ASN:O	24:0:31:ARG:N	2.48	0.43
27:4:59:ALA:HA	27:4:62:GLU:OE2	2.19	0.43
28:a:249:G:O2'	28:a:261:G:O6	2.27	0.43
29:b:13:A:N1	29:b:69:G:O2'	2.40	0.43
1:c:29:PRO:HG2	1:c:34:LEU:HD11	2.01	0.42
3:e:110:GLY:O	3:e:114:ARG:HD3	2.19	0.42
5:g:156:PRO:HD3	5:g:164:VAL:O	2.19	0.42
6:i:146:ALA:O	6:i:147:GLN:HG2	2.19	0.42
7:j:4:GLN:HG2	7:j:5:GLU:HG2	2.01	0.42
14:q:34:GLU:N	14:q:34:GLU:OE1	2.52	0.42
28:a:2051:U:H2'	28:a:2052:G:O4'	2.19	0.42
28:a:2571:G:H5"	28:a:2572:U:O4'	2.18	0.42
2:d:32:VAL:HG22	2:d:194:LEU:HD22	2.01	0.42
3:e:155:LYS:HZ1	3:e:190:VAL:N	2.17	0.42
6:i:37:ARG:HD2	6:i:109:MET:HG3	2.01	0.42
7:j:64:ARG:HD3	7:j:101:PRO:HG2	2.01	0.42
8:k:74:TYR:CD1	8:k:110:LYS:HB2	2.55	0.42
28:a:2050:G:H3'	28:a:2051:U:H6	1.84	0.42
28:a:2089:G:OP2	28:a:2113:G:H5'	2.19	0.42
1:c:14:ARG:NH2	28:a:1879:G:N7	2.60	0.42
4:f:111:ARG:HD3	27:4:26:SER:OG	2.19	0.42
13:p:58:ARG:HA	13:p:61:TRP:CE3	2.54	0.42
18:u:122:GLU:HG3	18:u:172:VAL:HG23	2.01	0.42
28:a:311:A:O2'	28:a:312:U:OP1	2.29	0.42
28:a:1894:U:H2'	28:a:1895:G:O4'	2.19	0.42
28:a:2042:A:O5'	28:a:2042:A:H8	2.02	0.42
1:c:226:MET:HG2	28:a:867:A:C2	2.54	0.42
5:g:120:PRO:HD2	5:g:123:ILE:HB	2.01	0.42
9:l:36:ALA:HB2	9:l:103:LEU:HD11	2.00	0.42
13:p:77:ASN:OD1	13:p:78:ARG:N	2.51	0.42
21:x:70:ASP:HA	21:x:71:PRO:HD2	1.91	0.42
22:y:15:ALA:HA	28:a:1052:G:O3'	2.20	0.42
28:a:903:G:N1	28:a:1265:U:OP2	2.34	0.42
28:a:1222:G:O2'	28:a:1227:A:N1	2.48	0.42
28:a:2861:A:H2'	28:a:2862:C:O4'	2.20	0.42
28:a:2870:G:O2'	28:a:2872:G:C2	2.72	0.42
4:f:160:GLY:HA3	28:a:2487:U:C2	2.54	0.42
7:j:108:GLU:HB2	7:j:110:LYS:HZ2	1.83	0.42
27:4:59:ALA:HA	27:4:62:GLU:CD	2.44	0.42
28:a:1142:G:N2	28:a:1163:C:O2	2.52	0.42
28:a:1906:C:H2'	28:a:1907:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2653:C:H2'	28:a:2654:G:O4'	2.19	0.42
28:a:2658:A:N3	28:a:2658:A:H2'	2.35	0.42
4:f:107:GLU:OE2	27:4:25:ARG:NH1	2.52	0.42
19:v:39:ARG:NH2	28:a:2545:U:O2'	2.52	0.42
24:0:14:LEU:HD21	24:0:39:MET:SD	2.59	0.42
26:2:50:LEU:HD23	26:2:54:GLU:HB3	2.01	0.42
28:a:1257:U:H2'	28:a:1258:G:O4'	2.20	0.42
28:a:1719:U:O2'	28:a:1720:U:OP1	2.29	0.42
13:p:98:LEU:HD22	13:p:105:ALA:HB3	2.02	0.42
27:4:60:ARG:O	27:4:64:ARG:HG2	2.19	0.42
28:a:98:U:H5'	28:a:99:G:O4'	2.20	0.42
28:a:2533:G:H1'	28:a:2548:A:N6	2.34	0.42
32:3:22:ARG:HD3	32:3:35:ARG:HD3	2.00	0.42
13:p:59:SER:O	13:p:63:GLN:HG3	2.20	0.42
14:q:78:ASN:OD1	14:q:78:ASN:N	2.53	0.42
15:r:53:LEU:HB2	15:r:65:ARG:HG3	2.02	0.42
28:a:335:U:H1'	28:a:447:U:C4	2.55	0.42
28:a:603:A:H1'	28:a:664:C:H1'	2.01	0.42
28:a:2473:U:OP1	28:a:2562:U:O2'	2.33	0.42
28:a:2546:C:H2'	28:a:2547:G:O4'	2.20	0.42
1:c:212:ASN:HA	1:c:215:LYS:HB2	2.02	0.42
4:f:198:LYS:O	4:f:199:ARG:C	2.62	0.42
5:g:176:GLY:HA3	28:a:2713:A:H5"	2.02	0.42
19:v:10:SER:OG	28:a:2459:G:OP2	2.26	0.42
19:v:37:ILE:HG21	19:v:78:VAL:HG11	2.02	0.42
23:z:35:CYS:SG	23:z:48:CYS:HB3	2.60	0.42
28:a:359:C:H2'	28:a:360:A:C8	2.55	0.42
28:a:814:G:H5'	28:a:815:U:H5"	2.02	0.42
28:a:1176:G:O2'	28:a:1181:A:N6	2.48	0.42
28:a:1492:C:H2'	28:a:1493:G:N7	2.34	0.42
31:C:62:C:H2'	31:C:63:G:C8	2.55	0.42
1:c:25:THR:O	1:c:25:THR:OG1	2.27	0.42
1:c:44:ASN:OD1	1:c:45:ASN:N	2.51	0.42
11:n:97:ILE:C	11:n:98:THR:HG1	2.28	0.42
15:r:89:SER:HB2	15:r:125:GLU:HG3	2.02	0.42
27:4:33:LEU:HD12	27:4:33:LEU:HA	1.77	0.42
28:a:982:C:H2'	28:a:983:G:O4'	2.19	0.42
28:a:2654:G:H2'	28:a:2660:A:H62	1.84	0.42
28:a:2870:G:O2'	28:a:2872:G:N1	2.52	0.42
1:c:183:ARG:NH2	28:a:1983:C:OP2	2.53	0.41
1:c:212:ASN:OD1	28:a:1974:A:H5"	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:214:TRP:CD1	28:a:1749:G:O4'	2.73	0.41
1:c:265:SER:OG	1:c:266:ARG:NH1	2.44	0.41
4:f:186:PHE:C	4:f:186:PHE:HD2	2.28	0.41
6:i:36:LEU:HD11	6:i:122:LEU:HB2	2.01	0.41
11:n:11:LEU:O	11:n:16:LYS:HE3	2.19	0.41
28:a:258:A:C5	28:a:259:G:H1'	2.55	0.41
28:a:868:A:H8	28:a:1961:U:O2'	2.02	0.41
28:a:1200:U:H2'	28:a:1201:C:C6	2.55	0.41
28:a:2718:G:O2'	28:a:2719:U:H5"	2.20	0.41
28:a:2872:G:HO2'	28:a:2873:C:P	2.43	0.41
28:a:2937:C:O2'	28:a:2938:U:H2'	2.20	0.41
1:c:182:MET:HB2	1:c:269:VAL:HG12	2.01	0.41
2:d:26:ARG:HE	7:j:72:PRO:HB3	1.84	0.41
3:e:144:LYS:O	3:e:145:ALA:C	2.63	0.41
10:m:85:PRO:O	10:m:88:GLU:HG2	2.20	0.41
12:o:52:GLY:HA2	12:o:57:GLU:HG2	2.02	0.41
18:u:168:ASP:OD1	18:u:169:ALA:N	2.53	0.41
27:4:9:TYR:CD1	27:4:27:THR:HG23	2.48	0.41
27:4:49:GLN:HG3	27:4:50:LYS:N	2.35	0.41
28:a:309:G:N3	28:a:310:C:H5	2.18	0.41
28:a:2050:G:H3'	28:a:2051:U:C6	2.54	0.41
28:a:2982:U:OP2	28:a:2983:C:N4	2.53	0.41
2:d:17:MET:HE1	28:a:2862:C:O2'	2.20	0.41
7:j:110:LYS:HG3	7:j:111:PHE:H	1.85	0.41
18:u:33:MET:HA	18:u:92:LEU:O	2.20	0.41
28:a:263:A:H2'	28:a:264:A:C8	2.54	0.41
28:a:315:G:C6	28:a:316:C:C4	3.08	0.41
28:a:2042:A:H2'	28:a:2043:A:O4'	2.21	0.41
28:a:2525:U:O3'	28:a:2555:A:H4'	2.20	0.41
4:f:127:ASN:HD21	4:f:196:LYS:CB	2.33	0.41
5:g:55:ARG:HB2	5:g:62:ASN:HB3	2.01	0.41
15:r:58:GLN:NE2	28:a:2192:G:OP1	2.54	0.41
19:v:72:ARG:NH2	29:b:10:G:H5"	2.35	0.41
20:w:6:ASP:OD1	20:w:48:ASN:N	2.53	0.41
20:w:19:PRO:HG2	28:a:2262:A:H4'	2.03	0.41
23:z:3:VAL:HG23	28:a:2198:A:C2	2.55	0.41
1:c:44:ASN:HB2	1:c:50:THR:HG23	2.01	0.41
4:f:31:TYR:OH	4:f:174:GLU:OE1	2.25	0.41
5:g:109:LEU:HD13	5:g:154:ARG:HB2	2.01	0.41
5:g:155:LYS:NZ	5:g:155:LYS:HB3	2.36	0.41
14:q:49:ASP:O	14:q:53:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:119:ALA:HA	18:u:176:VAL:HG12	2.03	0.41
28:a:631:G:H5'	28:a:632:U:C5	2.56	0.41
28:a:1194:A:N3	28:a:1195:G:H1'	2.34	0.41
28:a:2248:C:H2'	28:a:2249:C:H6	1.84	0.41
3:e:159:VAL:HA	3:e:182:ALA:H	1.85	0.41
3:e:165:GLU:HB3	3:e:169:LEU:HD12	2.01	0.41
5:g:9:ILE:O	5:g:51:ILE:N	2.53	0.41
7:j:31:ARG:HH22	28:a:2858:C:P	2.43	0.41
16:s:7:ARG:HH21	16:s:12:ILE:HG13	1.86	0.41
28:a:311:A:H2'	28:a:312:U:C6	2.55	0.41
28:a:443:G:H8	28:a:443:G:P	2.44	0.41
28:a:956:A:H2'	28:a:957:U:C6	2.56	0.41
28:a:1711:G:O6	28:a:1725:G:H2'	2.21	0.41
28:a:2504:A:H2'	28:a:2505:G:O4'	2.21	0.41
28:a:2711:G:H3'	28:a:2712:G:C5'	2.51	0.41
2:d:14:LYS:HB2	2:d:207:LEU:HD11	2.02	0.41
28:a:277:A:OP2	28:a:320:G:N1	2.49	0.41
28:a:418:G:HO2'	28:a:419:U:P	2.41	0.41
28:a:1345:A:H2'	28:a:1346:G:O4'	2.21	0.41
28:a:1364:U:C4	28:a:1403:U:H1'	2.56	0.41
28:a:1417:G:C2	28:a:1474:C:H4'	2.55	0.41
28:a:2205:U:O2'	28:a:2799:C:H5'	2.20	0.41
28:a:2268:U:H2'	28:a:2269:G:C8	2.55	0.41
28:a:2560:A:C5	28:a:2561:G:H1'	2.55	0.41
28:a:2720:C:H5"	28:a:2720:C:O2	2.21	0.41
28:a:2720:C:H3'	28:a:2721:C:O2	2.21	0.41
29:b:88:G:H2'	29:b:89:G:O4'	2.21	0.41
32:3:29:ASN:HB3	32:3:32:HIS:ND1	2.35	0.41
1:c:210:GLY:HA2	28:a:849:A:H5'	2.02	0.41
2:d:17:MET:HG2	2:d:31:THR:HA	2.03	0.41
3:e:139:SER:HA	3:e:142:GLN:CD	2.46	0.41
4:f:47:MET:HE3	4:f:66:ILE:HB	2.02	0.41
4:f:83:ILE:HB	4:f:88:LEU:HD21	2.02	0.41
4:f:192:PRO:O	4:f:194:LYS:N	2.54	0.41
5:g:64:SER:HB3	28:a:2939:A:C2	2.55	0.41
8:k:93:THR:HA	8:k:97:LEU:HD12	2.02	0.41
18:u:129:GLN:N	18:u:164:SER:O	2.51	0.41
18:u:142:ASP:OD1	18:u:144:THR:OG1	2.24	0.41
28:a:694:C:H2'	28:a:695:C:H6	1.85	0.41
28:a:1067:G:H2'	30:V:22:PRO:HG3	2.03	0.41
28:a:2872:G:O2'	28:a:2873:C:C6	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:213:ARG:NH1	28:a:849:A:N3	2.64	0.41
2:d:139:THR:OG1	28:a:2176:U:H4'	2.21	0.41
2:d:161:VAL:HG21	28:a:2800:G:H21	1.86	0.41
4:f:14:LYS:HE3	4:f:18:ARG:HE	1.86	0.41
4:f:42:LYS:O	4:f:43:ILE:HD13	2.20	0.41
4:f:128:SER:HB3	4:f:176:LYS:NZ	2.36	0.41
6:i:4:TYR:CD2	13:p:100:VAL:HG11	2.55	0.41
7:j:69:HIS:ND1	7:j:105:GLU:OE1	2.54	0.41
10:m:45:ARG:HG3	10:m:95:THR:OG1	2.20	0.41
12:o:103:ARG:HH22	28:a:1938:A:P	2.44	0.41
14:q:6:ARG:HG2	14:q:7:SER:N	2.35	0.41
19:v:15:ASP:OD1	19:v:16:SER:N	2.52	0.41
19:v:44:HIS:HD2	19:v:45:PHE:CE2	2.39	0.41
26:2:29:LYS:HD2	26:2:41:THR:HG23	2.02	0.41
27:4:13:THR:HB	27:4:23:THR:HG22	2.02	0.41
28:a:142:G:N2	28:a:147:G:H1	2.17	0.41
28:a:222:G:H4'	28:a:223:A:H4'	2.03	0.41
28:a:332:U:H2'	28:a:333:U:O4'	2.21	0.41
28:a:405:G:H4'	28:a:407:A:N7	2.36	0.41
28:a:721:C:H2'	28:a:722:G:O4'	2.21	0.41
28:a:771:U:H6	28:a:873:A:N1	2.18	0.41
28:a:949:G:H21	28:a:951:A:N6	2.16	0.41
28:a:1232:U:H2'	28:a:1233:C:C6	2.55	0.41
28:a:1629:C:H5'	28:a:1727:G:H1'	2.02	0.41
28:a:2469:A:O2'	28:a:2470:A:H3'	2.21	0.41
28:a:2655:C:H5"	28:a:2656:U:H5	1.86	0.41
28:a:2656:U:C4	28:a:2657:C:C2	3.09	0.41
28:a:2931:A:N1	28:a:2932:A:N6	2.69	0.41
28:a:3050:C:H2'	28:a:3051:U:O4'	2.21	0.41
4:f:36:LEU:HA	4:f:36:LEU:HD23	1.87	0.41
4:f:192:PRO:HB2	4:f:193:LYS:H	1.54	0.41
5:g:7:LEU:HA	5:g:8:PRO:HD3	1.95	0.41
21:x:3:LYS:HA	21:x:3:LYS:HD3	1.84	0.41
21:x:12:LEU:O	21:x:63:ARG:NH2	2.51	0.41
23:z:53:PRO:HD3	28:a:3064:U:O2'	2.21	0.41
27:4:20:ASN:HB3	27:4:40:LYS:NZ	2.36	0.41
28:a:431:A:H2'	28:a:432:A:O4'	2.21	0.41
28:a:715:C:H5"	28:a:736:C:O2'	2.22	0.41
28:a:1151:G:H21	28:a:1178:A:H2'	1.86	0.41
28:a:1717:G:O2'	28:a:1718:G:O4'	2.36	0.41
28:a:2281:U:H1'	28:a:2373:G:N2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2661:G:H2'	28:a:2662:C:O4'	2.21	0.41
28:a:2938:U:OP2	32:3:19:ARG:NH2	2.52	0.41
29:b:89:G:OP1	30:V:12:ARG:NH2	2.49	0.41
8:k:66:PHE:H	28:a:717:A:HO2'	1.67	0.40
28:a:272:A:O2'	28:a:273:G:H4'	2.20	0.40
28:a:463:A:C2	28:a:464:G:H1'	2.56	0.40
28:a:483:U:H2'	28:a:484:C:C6	2.55	0.40
28:a:2291:U:H5'	28:a:2363:G:N2	2.37	0.40
28:a:2427:U:H5"	28:a:2428:G:H5'	2.03	0.40
3:e:92:VAL:HG12	3:e:93:HIS:CG	2.56	0.40
8:k:92:ILE:HG23	8:k:92:ILE:O	2.21	0.40
11:n:72:GLU:OE1	11:n:72:GLU:N	2.53	0.40
13:p:11:LYS:O	13:p:15:ARG:HG3	2.21	0.40
28:a:343:C:H2'	28:a:344:U:C6	2.56	0.40
28:a:441:C:H2'	28:a:442:U:C6	2.56	0.40
28:a:978:U:H3'	28:a:979:U:O4'	2.22	0.40
28:a:1130:G:H21	28:a:1194:A:N6	2.18	0.40
28:a:2498:G:H2'	28:a:2499:U:O4'	2.21	0.40
28:a:2789:G:H2'	28:a:2790:G:O4'	2.20	0.40
28:a:2804:C:O2'	28:a:3005:G:N7	2.53	0.40
2:d:145:LYS:NZ	28:a:2760:G:OP2	2.53	0.40
3:e:93:HIS:CD2	28:a:670:G:H5'	2.56	0.40
3:e:137:LYS:HB3	3:e:166:ILE:HG23	2.03	0.40
8:k:132:ALA:O	8:k:136:ILE:HG13	2.20	0.40
11:n:76:ASP:OD2	29:b:50:G:H5"	2.20	0.40
17:t:100:ARG:HH11	17:t:104:GLY:HA2	1.87	0.40
28:a:622:U:H2'	28:a:623:C:C6	2.55	0.40
28:a:1189:G:C6	28:a:1190:G:C5	3.09	0.40
28:a:1712:C:H42	28:a:1724:G:H1	1.67	0.40
28:a:2662:C:N4	28:a:2663:G:C6	2.89	0.40
28:a:2980:G:H2'	28:a:2981:U:C2	2.57	0.40
29:b:88:G:H8	29:b:88:G:OP1	2.03	0.40
1:c:235:GLY:HA3	28:a:2780:A:H5"	2.03	0.40
3:e:45:ALA:O	3:e:48:ARG:HB2	2.21	0.40
4:f:173:GLU:HG2	4:f:174:GLU:N	2.35	0.40
4:f:194:LYS:C	4:f:196:LYS:N	2.78	0.40
5:g:146:THR:O	5:g:150:ILE:HG12	2.22	0.40
11:n:26:ARG:NH2	11:n:54:ASP:OD1	2.55	0.40
18:u:56:THR:HG23	18:u:59:PRO:HG3	2.03	0.40
28:a:11:G:O6	28:a:613:U:H2'	2.21	0.40
28:a:146:U:HO2'	28:a:147:G:P	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1251:C:H2'	28:a:1252:C:C6	2.57	0.40
28:a:2722:C:H5"	28:a:2722:C:H6	1.86	0.40
3:e:4:THR:HG22	3:e:4:THR:O	2.22	0.40
4:f:17:TYR:HA	4:f:21:ILE:CG1	2.52	0.40
4:f:126:LEU:O	4:f:186:PHE:CB	2.69	0.40
5:g:2:SER:OG	5:g:55:ARG:NH1	2.55	0.40
13:p:34:LYS:HE3	28:a:2201:G:O2'	2.21	0.40
24:0:39:MET:HE1	28:a:2468:A:N6	2.35	0.40
26:2:31:HIS:NE2	28:a:2574:A:OP2	2.49	0.40
27:4:42:HIS:HA	27:4:43:PRO:HD3	1.95	0.40
28:a:285:U:O2	28:a:313:G:N2	2.55	0.40
28:a:291:U:H5"	28:a:308:U:C5	2.56	0.40
28:a:1305:G:O3'	28:a:1306:U:H3'	2.21	0.40
28:a:2792[B]:C:H6	28:a:2792[B]:C:H2'	1.74	0.40
29:b:34:G:O2'	29:b:35:U:P	2.80	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	c	272/278 (98%)	254 (93%)	16 (6%)	2 (1%)	18 30
2	d	212/223 (95%)	198 (93%)	13 (6%)	1 (0%)	24 39
3	e	208/301 (69%)	185 (89%)	18 (9%)	5 (2%)	4 7
4	f	201/210 (96%)	168 (84%)	19 (10%)	14 (7%)	1 0
5	g	175/180 (97%)	162 (93%)	12 (7%)	1 (1%)	21 34
6	i	144/147 (98%)	139 (96%)	5 (4%)	0	100 100
7	j	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
8	k	142/146 (97%)	120 (84%)	22 (16%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
10	m	118/187 (63%)	112 (95%)	5 (4%)	1 (1%)	16	27
11	n	124/127 (98%)	120 (97%)	3 (2%)	1 (1%)	16	27
12	o	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
13	p	117/123 (95%)	109 (93%)	7 (6%)	1 (1%)	14	24
14	q	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
15	r	130/153 (85%)	123 (95%)	6 (5%)	1 (1%)	16	27
16	s	93/102 (91%)	87 (94%)	5 (5%)	1 (1%)	11	19
17	t	103/122 (84%)	99 (96%)	3 (3%)	1 (1%)	12	20
18	u	177/205 (86%)	168 (95%)	7 (4%)	2 (1%)	11	19
19	v	76/89 (85%)	73 (96%)	3 (4%)	0	100	100
20	w	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	12
21	x	67/77 (87%)	62 (92%)	4 (6%)	1 (2%)	8	13
22	y	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
23	z	60/63 (95%)	55 (92%)	3 (5%)	2 (3%)	3	4
24	0	48/56 (86%)	42 (88%)	6 (12%)	0	100	100
25	1	42/44 (96%)	42 (100%)	0	0	100	100
26	2	65/68 (96%)	65 (100%)	0	0	100	100
27	4	64/69 (93%)	50 (78%)	11 (17%)	3 (5%)	2	2
30	V	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
32	3	35/37 (95%)	35 (100%)	0	0	100	100
All	All	3274/3632 (90%)	3048 (93%)	188 (6%)	38 (1%)	13	17

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	c	26	ARG
3	e	151	ALA
3	e	159	VAL
3	e	186	ASN
4	f	188	ALA
4	f	189	LYS
4	f	190	ASP
4	f	191	ASP
4	f	192	PRO

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Mol	Chain	Res	Type
4	f	204	TYR
13	p	93	LYS
27	4	49	GLN
27	4	50	LYS
3	e	133	VAL
4	f	186	PHE
4	f	187	LYS
4	f	193	LYS
4	f	196	LYS
4	f	198	LYS
4	f	200	GLY
11	n	5	LEU
15	r	3	LYS
18	u	97	ARG
20	w	41	ASN
23	z	56	ASP
4	f	202	ALA
27	4	28	SER
16	s	93	ARG
1	c	262	LYS
3	e	138	PRO
10	m	37	THR
2	d	95	GLU
17	t	64	ILE
18	u	98	GLY
21	x	5	SER
4	f	201	PRO
5	g	161	GLY
23	z	55	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	c	216/220 (98%)	216 (100%)	0	100 100
2	d	166/172 (96%)	164 (99%)	2 (1%)	63 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	e	165/237 (70%)	164 (99%)	1 (1%)	78 88
4	f	169/175 (97%)	153 (90%)	16 (10%)	8 13
5	g	150/152 (99%)	142 (95%)	8 (5%)	20 35
6	i	118/120 (98%)	118 (100%)	0	100 100
7	j	101/101 (100%)	99 (98%)	2 (2%)	48 69
8	k	111/113 (98%)	109 (98%)	2 (2%)	51 72
9	l	108/110 (98%)	108 (100%)	0	100 100
10	m	100/142 (70%)	99 (99%)	1 (1%)	68 81
11	n	95/96 (99%)	95 (100%)	0	100 100
12	o	97/99 (98%)	97 (100%)	0	100 100
13	p	98/99 (99%)	98 (100%)	0	100 100
14	q	84/84 (100%)	84 (100%)	0	100 100
15	r	105/118 (89%)	101 (96%)	4 (4%)	29 49
16	s	84/89 (94%)	84 (100%)	0	100 100
17	t	91/103 (88%)	91 (100%)	0	100 100
18	u	149/168 (89%)	145 (97%)	4 (3%)	39 61
19	v	60/67 (90%)	60 (100%)	0	100 100
20	w	52/53 (98%)	52 (100%)	0	100 100
21	x	61/68 (90%)	61 (100%)	0	100 100
22	y	53/55 (96%)	53 (100%)	0	100 100
23	z	51/52 (98%)	50 (98%)	1 (2%)	48 69
24	0	47/51 (92%)	46 (98%)	1 (2%)	47 69
25	1	36/36 (100%)	36 (100%)	0	100 100
26	2	54/55 (98%)	54 (100%)	0	100 100
27	4	56/59 (95%)	42 (75%)	14 (25%)	0 0
30	V	16/17 (94%)	16 (100%)	0	100 100
32	3	35/35 (100%)	34 (97%)	1 (3%)	37 58
All	All	2728/2946 (93%)	2671 (98%)	57 (2%)	46 69

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	d	45	THR

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Mol	Chain	Res	Type
2	d	94	SER
3	e	144	LYS
4	f	180	LYS
4	f	186	PHE
4	f	187	LYS
4	f	189	LYS
4	f	190	ASP
4	f	193	LYS
4	f	194	LYS
4	f	196	LYS
4	f	198	LYS
4	f	199	ARG
4	f	201	PRO
4	f	204	TYR
4	f	206	LYS
4	f	207	LYS
4	f	208	LYS
4	f	209	LYS
5	g	54	GLU
5	g	155	LYS
5	g	157	GLU
5	g	159	TYR
5	g	160	LYS
5	g	174	LYS
5	g	175	VAL
5	g	177	LYS
7	j	23	ARG
7	j	122	ILE
8	k	27	SER
8	k	28	LYS
10	m	73	ARG
15	r	1	MET
15	r	2	SER
15	r	3	LYS
15	r	95	GLU
18	u	95	VAL
18	u	99	GLU
18	u	100	LYS
18	u	180	GLU
23	z	57	ARG
24	0	20	LYS
27	4	10	ARG

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Mol	Chain	Res	Type
27	4	12	THR
27	4	13	THR
27	4	14	VAL
27	4	15	VAL
27	4	24	THR
27	4	25	ARG
27	4	26	SER
27	4	27	THR
27	4	28	SER
27	4	29	GLN
27	4	33	LEU
27	4	34	ASN
27	4	38	CYS
32	3	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	135	ASN
2	d	25	ASN
2	d	55	GLN
3	e	93	HIS
3	e	142	GLN
5	g	22	GLN
6	i	47	HIS
6	i	118	GLN
8	k	75	GLN
11	n	110	HIS
12	o	41	GLN
12	o	56	GLN
13	p	81	ASN
13	p	119	GLN
24	0	29	ASN
27	4	34	ASN
32	3	20	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	a	2886/3086 (93%)	485 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	b	117/120 (97%)	11 (9%)	0
31	C	75/77 (97%)	10 (13%)	1 (1%)
All	All	3078/3283 (93%)	506 (16%)	1 (0%)

All (506) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	a	11	G
28	a	12	U
28	a	31	C
28	a	33	U
28	a	34	G
28	a	42	G
28	a	50	G
28	a	62	G
28	a	70	A
28	a	73	A
28	a	74	G
28	a	82	G
28	a	91	A
28	a	94	G
28	a	98	U
28	a	99	G
28	a	100	U
28	a	101	G
28	a	117	A
28	a	118	A
28	a	119	U
28	a	124	A
28	a	132	A
28	a	133	A
28	a	135	G
28	a	137	C
28	a	147	G
28	a	166	A
28	a	180	U
28	a	188	A
28	a	203	A
28	a	206	A
28	a	222	G
28	a	223	A
28	a	229	A

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Mol	Chain	Res	Type
28	a	230	A
28	a	236	U
28	a	255	G
28	a	272	A
28	a	273	G
28	a	279	A
28	a	283	U
28	a	284	G
28	a	285	U
28	a	286	G
28	a	287	U
28	a	288	G
28	a	289	U
28	a	290	G
28	a	304	G
28	a	305	U
28	a	307	U
28	a	309	G
28	a	310	C
28	a	311	A
28	a	312	U
28	a	313	G
28	a	314	U
28	a	316	C
28	a	318	G
28	a	321	U
28	a	322	U
28	a	324	U
28	a	325	G
28	a	332	U
28	a	335	U
28	a	336	G
28	a	337	G
28	a	338	U
28	a	339	U
28	a	340	C
28	a	341	U
28	a	342	G
28	a	345	G
28	a	346	C
28	a	347	C
28	a	348	G

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Mol	Chain	Res	Type
28	a	353	A
28	a	354	U
28	a	355	U
28	a	356	G
28	a	358	C
28	a	359	C
28	a	360	A
28	a	366	A
28	a	367	A
28	a	369	U
28	a	370	G
28	a	373	G
28	a	379	A
28	a	380	G
28	a	385	A
28	a	386	G
28	a	387	C
28	a	393	G
28	a	396	A
28	a	402	A
28	a	408	G
28	a	415	A
28	a	419	U
28	a	423	G
28	a	431	A
28	a	432	A
28	a	433	G
28	a	434	C
28	a	435	G
28	a	447	U
28	a	453	U
28	a	454	G
28	a	460	A
28	a	475	G
28	a	476	U
28	a	477	G
28	a	480	A
28	a	494	U
28	a	500	G
28	a	501	A
28	a	532	A
28	a	533	C

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Mol	Chain	Res	Type
28	a	544	U
28	a	545	G
28	a	546	A
28	a	570	G
28	a	592	G
28	a	593	A
28	a	596	U
28	a	618	G
28	a	619	C
28	a	620	C
28	a	621	G
28	a	632	U
28	a	633	G
28	a	635	G
28	a	639	A
28	a	646	G
28	a	656	G
28	a	658	A
28	a	674	G
28	a	675	U
28	a	676	G
28	a	687	A
28	a	699	G
28	a	700	G
28	a	701	U
28	a	707	A
28	a	713	A
28	a	720	G
28	a	723	A
28	a	731	A
28	a	733	G
28	a	739	G
28	a	740	A
28	a	741	G
28	a	770	A
28	a	771	U
28	a	802	G
28	a	815	U
28	a	832	U
28	a	842	G
28	a	849	A
28	a	860	G

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Mol	Chain	Res	Type
28	a	861	G
28	a	867	A
28	a	869	G
28	a	870	G
28	a	874	A
28	a	875	U
28	a	877	A
28	a	890	G
28	a	897	C
28	a	912	U
28	a	931	G
28	a	944	G
28	a	968	G
28	a	969	C
28	a	970	U
28	a	972	A
28	a	973	U
28	a	974	C
28	a	975	G
28	a	978	U
28	a	979	U
28	a	980	A
28	a	981	C
28	a	991	C
28	a	994	A
28	a	1016	A
28	a	1028	A
28	a	1029	G
28	a	1042	A
28	a	1044	G
28	a	1057	G
28	a	1066	A
28	a	1073	A
28	a	1079	A
28	a	1096	G
28	a	1105	G
28	a	1109	G
28	a	1116	U
28	a	1119	G
28	a	1128	U
28	a	1129	A
28	a	1130	G

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Mol	Chain	Res	Type
28	a	1141	G
28	a	1142	G
28	a	1144	U
28	a	1145	G
28	a	1149	U
28	a	1150	G
28	a	1151	G
28	a	1152	A
28	a	1153	A
28	a	1154	G
28	a	1156	A
28	a	1157	G
28	a	1161	U
28	a	1165	U
28	a	1172	G
28	a	1173	U
28	a	1177	U
28	a	1178	A
28	a	1179	A
28	a	1181	A
28	a	1189	G
28	a	1190	G
28	a	1193	A
28	a	1195	G
28	a	1196	U
28	a	1215	U
28	a	1216	A
28	a	1218	C
28	a	1225	U
28	a	1226	A
28	a	1227	A
28	a	1254	G
28	a	1255	U
28	a	1256	G
28	a	1257	U
28	a	1283	G
28	a	1297	G
28	a	1306	U
28	a	1307	G
28	a	1327	G
28	a	1330	A
28	a	1333	G

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Mol	Chain	Res	Type
28	a	1348	G
28	a	1350	G
28	a	1351	U
28	a	1365	C
28	a	1376	A
28	a	1377	U
28	a	1390	C
28	a	1428	U
28	a	1441	A
28	a	1455	U
28	a	1460	A
28	a	1471	A
28	a	1472	U
28	a	1595	A
28	a	1601	G
28	a	1607	A
28	a	1608	C
28	a	1625	U
28	a	1626	C
28	a	1630	G
28	a	1633	G
28	a	1637	G
28	a	1639	U
28	a	1641	U
28	a	1642	C
28	a	1648	C
28	a	1663	G
28	a	1673	U
28	a	1674	A
28	a	1677	U
28	a	1689	G
28	a	1690	A
28	a	1691	A
28	a	1692	G
28	a	1697	A
28	a	1698	G
28	a	1706	G
28	a	1710	A
28	a	1712	C
28	a	1714	C
28	a	1717	G
28	a	1718	G

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Mol	Chain	Res	Type
28	a	1719	U
28	a	1720	U
28	a	1721	G
28	a	1725	G
28	a	1726	U
28	a	1727	G
28	a	1743	A
28	a	1749	G
28	a	1752	A
28	a	1761	G
28	a	1768	A
28	a	1769	G
28	a	1774	C
28	a	1777	G
28	a	1792	A
28	a	1818	U
28	a	1830	A
28	a	1832	C
28	a	1837	G
28	a	1838	A
28	a	1858	G
28	a	1897	G
28	a	1898	C
28	a	1904	U
28	a	1911	G
28	a	1912	U
28	a	1913	G
28	a	1914	C
28	a	1915	G
28	a	1916	G
28	a	1921	G
28	a	1939	G
28	a	1947	G
28	a	1956	A
28	a	1965	C
28	a	1969	A
28	a	1974	A
28	a	1983	C
28	a	1984	G
28	a	1985	A
28	a	1999	U
28	a	2012	A

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Mol	Chain	Res	Type
28	a	2031	A
28	a	2041	G
28	a	2052	G
28	a	2053	U
28	a	2054	A
28	a	2055	U
28	a	2056	G
28	a	2057	C
28	a	2068	A
28	a	2089	G
28	a	2096	A
28	a	2098	3TD
28	a	2112	G
28	a	2113	G
28	a	2119	A
28	a	2120	A
28	a	2121	A
28	a	2138	U
28	a	2146	U
28	a	2150	C
28	a	2153	A
28	a	2154	U
28	a	2155	G
28	a	2174	U
28	a	2176	U
28	a	2186	G
28	a	2204	U
28	a	2206	A
28	a	2210	G
28	a	2214	A
28	a	2215	G
28	a	2216	A
28	a	2222	G
28	a	2226	C
28	a	2238	C
28	a	2239	G
28	a	2243	A
28	a	2250	G
28	a	2275	G
28	a	2279	A
28	a	2283	G
28	a	2287	G

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Mol	Chain	Res	Type
28	a	2289	U
28	a	2364	A
28	a	2365	U
28	a	2366	U
28	a	2367	G
28	a	2368	U
28	a	2369	U
28	a	2384	G
28	a	2385	U
28	a	2386	G
28	a	2393	G
28	a	2394	A
28	a	2407	A
28	a	2420	G
28	a	2421	G
28	a	2461	G
28	a	2464	G
28	a	2465	C
28	a	2469	A
28	a	2487	U
28	a	2490	G
28	a	2491	U
28	a	2501	G
28	a	2502	U
28	a	2503	G
28	a	2504	A
28	a	2507	G
28	a	2517	A
28	a	2518	A
28	a	2527	G
28	a	2529	C
28	a	2532	U
28	a	2536	A
28	a	2543	G
28	a	2565	G
28	a	2567	A
28	a	2588	U
28	a	2607	A
28	a	2611	G
28	a	2612	A
28	a	2613	U
28	a	2617	A

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Mol	Chain	Res	Type
28	a	2623	C
28	a	2630	A
28	a	2652	G
28	a	2653	C
28	a	2654	G
28	a	2655	C
28	a	2656	U
28	a	2657	C
28	a	2658	A
28	a	2659	U
28	a	2660	A
28	a	2661	G
28	a	2663	G
28	a	2664	A
28	a	2673	U
28	a	2674	U
28	a	2679	A
28	a	2684	G
28	a	2687	G
28	a	2688	U
28	a	2700	A
28	a	2702	C
28	a	2711	G
28	a	2712	G
28	a	2713	A
28	a	2714	G
28	a	2716	C
28	a	2717	G
28	a	2720	C
28	a	2721	C
28	a	2722	C
28	a	2748	A
28	a	2749	G
28	a	2755	C
28	a	2767	U
28	a	2784	A
28	a	2795	U
28	a	2797	U
28	a	2811	A
28	a	2871	U
28	a	2872	G
28	a	2873	C

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Mol	Chain	Res	Type
28	a	2900	G
28	a	2908	C
28	a	2911	C
28	a	2915	U
28	a	2917	G
28	a	2926	G
28	a	2930	A
28	a	2939	A
28	a	2944	G
28	a	2947	A
28	a	2948	G
28	a	2960	A
28	a	2962	A
28	a	2971	C
28	a	2972	A
28	a	2973	C
28	a	2979	U
28	a	2981	U
28	a	2982	U
28	a	2983	C
28	a	3000	G
28	a	3015	A
28	a	3041	G
28	a	3052	G
28	a	3063	A
28	a	3064	U
28	a	3066	G
28	a	3073	G
28	a	3074	A
28	a	3075	C
29	b	24	G
29	b	25	A
29	b	35	U
29	b	45	A
29	b	56	U
29	b	57	A
29	b	84	C
29	b	90	A
29	b	100	A
29	b	109	C
29	b	110	G
31	C	9	G

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Mol	Chain	Res	Type
31	C	16	C
31	C	17	C
31	C	17(A)	U
31	C	18	G
31	C	21	A
31	C	46	G
31	C	47	U
31	C	69	C
31	C	76	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	C	17(A)	U

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

22 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	$\#\|Z\| > 2$
28	5MU	a	2122	28	19,22,23	0.47	0	27,32,35	0.47	0
28	H2U	a	2631	28	18,21,22	0.48	0	19,30,33	1.08	1 (5%)
28	PSU	a	1038	28	18,21,22	1.03	1 (5%)	21,30,33	2.01	3 (14%)
28	PSU	a	2787	28	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
28	3TD	a	2098	28	19,22,23	4.27	6 (31%)	23,32,35	1.81	4 (17%)
28	PSU	a	2094	28	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
28	2MG	a	2018	28	23,26,27	0.47	0	33,38,41	0.55	0
31	PSU	C	55	31	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
28	OMG	a	2433	28,31	23,26,27	0.55	0	32,38,41	0.47	0
28	5MC	a	2145	28	19,22,23	0.58	0	26,32,35	0.70	0
28	PSU	a	2686	28	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
31	4SU	C	8	31	18,21,22	3.80	7 (38%)	25,30,33	2.30	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	OMU	a	2734	28	19,22,23	2.91	7 (36%)	25,31,34	1.85	5 (20%)
28	2MG	a	2627	28	23,26,27	0.52	0	33,38,41	0.47	0
28	PSU	a	2762	28	18,21,22	1.11	2 (11%)	21,30,33	1.96	5 (23%)
28	PSU	a	2786	28	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
31	5MC	C	32	31	19,22,23	0.49	0	26,32,35	0.61	0
31	5MU	C	54	31	19,22,23	0.38	0	27,32,35	0.62	0
28	PSU	a	2100	28	18,21,22	1.13	1 (5%)	21,30,33	1.88	4 (19%)
28	OMC	a	2680	28,33	19,22,23	0.62	0	25,31,34	0.74	0
28	2MA	a	2685	28,33	22,25,26	3.60	8 (36%)	32,37,40	2.05	9 (28%)
28	PSU	a	2639	28	18,21,22	1.08	2 (11%)	21,30,33	2.02	5 (23%)

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
28	5MU	a	2122	28	-	0/7/25/26	0/2/2/2
28	H2U	a	2631	28	-	0/7/38/39	0/2/2/2
28	PSU	a	1038	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2787	28	-	0/7/25/26	0/2/2/2
28	3TD	a	2098	28	-	2/7/25/26	0/2/2/2
28	PSU	a	2094	28	-	0/7/25/26	0/2/2/2
28	2MG	a	2018	28	-	0/9/27/28	0/3/3/3
31	PSU	C	55	31	-	0/7/25/26	0/2/2/2
28	OMG	a	2433	28,31	-	1/9/27/28	0/3/3/3
28	5MC	a	2145	28	-	1/7/25/26	0/2/2/2
28	PSU	a	2686	28	-	0/7/25/26	0/2/2/2
31	4SU	C	8	31	-	0/7/25/26	0/2/2/2
28	OMU	a	2734	28	-	0/9/27/28	0/2/2/2
28	2MG	a	2627	28	-	1/9/27/28	0/3/3/3
28	PSU	a	2762	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2786	28	-	0/7/25/26	0/2/2/2
31	5MC	C	32	31	-	0/7/25/26	0/2/2/2
31	5MU	C	54	31	-	0/7/25/26	0/2/2/2
28	PSU	a	2100	28	-	0/7/25/26	0/2/2/2
28	OMC	a	2680	28,33	-	0/9/27/28	0/2/2/2
28	2MA	a	2685	28,33	-	3/7/25/26	0/3/3/3
28	PSU	a	2639	28	-	0/7/25/26	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2098	3TD	C6-C5	13.12	1.49	1.35
28	a	2685	2MA	C4-N3	10.71	1.48	1.34
28	a	2098	3TD	C2-N1	9.47	1.48	1.37
31	C	8	4SU	C2-N3	7.39	1.50	1.38
31	C	8	4SU	C2-N1	7.23	1.49	1.38
31	C	8	4SU	C4-N3	7.04	1.44	1.37
28	a	2734	OMU	C2-N1	6.90	1.49	1.38
28	a	2685	2MA	C2-N3	6.89	1.45	1.34
28	a	2685	2MA	C2-N1	6.86	1.45	1.34
28	a	2734	OMU	C2-N3	6.60	1.49	1.38
31	C	8	4SU	C5-C4	6.15	1.49	1.42
28	a	2098	3TD	C6-N1	6.14	1.46	1.36
28	a	2734	OMU	C6-C5	5.79	1.48	1.35
31	C	8	4SU	C6-C5	5.61	1.48	1.35
31	C	8	4SU	C4-S4	-4.83	1.60	1.68
28	a	2098	3TD	C2-N3	4.77	1.48	1.38
28	a	2685	2MA	C5-C6	4.66	1.54	1.41
28	a	2685	2MA	C6-N1	4.53	1.41	1.35
31	C	55	PSU	C6-C5	3.79	1.39	1.35
28	a	2100	PSU	C6-C5	3.76	1.39	1.35
28	a	2094	PSU	C6-C5	3.68	1.39	1.35
28	a	2734	OMU	C4-N3	3.47	1.44	1.38
28	a	2685	2MA	C6-N6	-3.43	1.25	1.34
28	a	2686	PSU	C6-C5	3.43	1.39	1.35
28	a	2762	PSU	C6-C5	3.33	1.39	1.35
28	a	2786	PSU	C6-C5	3.30	1.38	1.35
28	a	2787	PSU	C6-C5	3.24	1.38	1.35
28	a	1038	PSU	C6-C5	3.17	1.38	1.35
28	a	2639	PSU	C6-C5	3.11	1.38	1.35
28	a	2098	3TD	C4-N3	2.98	1.46	1.40
28	a	2734	OMU	O2-C2	-2.84	1.18	1.23
28	a	2685	2MA	C5-N7	-2.79	1.34	1.39
28	a	2734	OMU	O4-C4	-2.77	1.19	1.24
31	C	8	4SU	C6-N1	2.74	1.44	1.38
28	a	2685	2MA	C8-N7	2.71	1.36	1.31
28	a	2098	3TD	O4-C4	-2.20	1.18	1.23
28	a	2762	PSU	C4-C5	-2.09	1.38	1.44
28	a	2734	OMU	C5-C4	2.06	1.48	1.43
28	a	2639	PSU	C4-C5	-2.01	1.38	1.44

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	8	4SU	C4-N3-C2	-7.91	119.73	127.31
28	a	2685	2MA	C5-C4-N3	-6.40	120.44	127.18
28	a	2734	OMU	C4-N3-C2	-5.81	119.40	126.61
28	a	2098	3TD	N1-C2-N3	5.73	120.30	116.13
28	a	1038	PSU	C4-N3-C2	-5.51	118.78	126.37
31	C	8	4SU	C5-C4-N3	5.39	119.76	114.75
28	a	2639	PSU	N1-C2-N3	5.09	120.53	115.17
28	a	2786	PSU	C4-N3-C2	-5.05	119.41	126.37
28	a	2787	PSU	C4-N3-C2	-5.02	119.46	126.37
28	a	1038	PSU	N1-C2-N3	4.98	120.42	115.17
28	a	2762	PSU	C4-N3-C2	-4.96	119.53	126.37
28	a	2639	PSU	C4-N3-C2	-4.89	119.64	126.37
28	a	2786	PSU	N1-C2-N3	4.88	120.31	115.17
28	a	2686	PSU	C4-N3-C2	-4.87	119.66	126.37
28	a	2686	PSU	N1-C2-N3	4.85	120.28	115.17
28	a	2094	PSU	C4-N3-C2	-4.83	119.72	126.37
28	a	2762	PSU	N1-C2-N3	4.82	120.25	115.17
31	C	55	PSU	C4-N3-C2	-4.82	119.73	126.37
28	a	2094	PSU	N1-C2-N3	4.79	120.22	115.17
28	a	2100	PSU	C4-N3-C2	-4.78	119.78	126.37
28	a	2787	PSU	N1-C2-N3	4.77	120.20	115.17
31	C	55	PSU	N1-C2-N3	4.74	120.17	115.17
28	a	2100	PSU	N1-C2-N3	4.70	120.12	115.17
28	a	2685	2MA	N9-C8-N7	-4.38	107.72	113.94
28	a	2098	3TD	C4-N3-C2	-4.15	120.22	124.61
28	a	2734	OMU	N3-C2-N1	3.87	119.93	114.89
31	C	8	4SU	C5-C4-S4	-3.86	119.90	124.31
31	C	8	4SU	N3-C2-N1	3.81	119.85	114.89
28	a	2734	OMU	C5-C4-N3	3.77	120.08	114.80
28	a	2685	2MA	N3-C4-N9	3.64	131.61	126.99
28	a	2631	H2U	C5-C4-N3	-3.41	113.06	116.69
28	a	2685	2MA	N3-C2-N1	-3.32	119.92	125.77
28	a	2734	OMU	O4-C4-C5	-2.98	120.02	125.16
28	a	2639	PSU	O2-C2-N1	-2.91	119.78	122.79
28	a	2685	2MA	C5-N7-C8	2.90	108.00	103.45
28	a	2686	PSU	O2-C2-N1	-2.84	119.86	122.79
28	a	2094	PSU	O2-C2-N1	-2.79	119.91	122.79
31	C	55	PSU	O2-C2-N1	-2.77	119.93	122.79
28	a	2639	PSU	C6-N1-C2	-2.67	120.21	122.69
28	a	2762	PSU	O2-C2-N1	-2.67	120.04	122.79
28	a	2786	PSU	O2-C2-N1	-2.61	120.10	122.79
28	a	2100	PSU	O2-C2-N1	-2.60	120.10	122.79
28	a	2639	PSU	C6-C5-C4	2.57	119.91	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	2685	2MA	C4-N9-C8	2.49	108.35	105.74
28	a	2787	PSU	O2-C2-N1	-2.46	120.25	122.79
28	a	2686	PSU	C6-N1-C2	-2.43	120.43	122.69
28	a	2094	PSU	C6-N1-C2	-2.42	120.45	122.69
28	a	2098	3TD	C6-C5-C4	2.41	119.81	118.19
28	a	1038	PSU	O2-C2-N1	-2.36	120.35	122.79
28	a	2762	PSU	C6-N1-C2	-2.35	120.51	122.69
28	a	2786	PSU	C6-C5-C4	2.33	119.75	118.17
31	C	55	PSU	C6-N1-C2	-2.33	120.53	122.69
28	a	2762	PSU	C6-C5-C4	2.31	119.73	118.17
28	a	2685	2MA	C4-C5-N7	-2.28	107.97	110.58
28	a	2786	PSU	C6-N1-C2	-2.24	120.61	122.69
28	a	2685	2MA	N6-C6-N1	2.23	120.04	117.03
28	a	2100	PSU	C6-N1-C2	-2.22	120.63	122.69
28	a	2734	OMU	O2-C2-N1	-2.20	119.93	122.80
28	a	2787	PSU	C6-N1-C2	-2.16	120.69	122.69
28	a	2094	PSU	C6-C5-C4	2.15	119.62	118.17
31	C	8	4SU	O2-C2-N1	-2.11	120.05	122.80
31	C	55	PSU	C6-C5-C4	2.10	119.59	118.17
28	a	2098	3TD	C1'-C5-C4	2.08	120.77	117.61
28	a	2685	2MA	CM2-C2-N1	2.08	120.23	117.13

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	a	2098	3TD	O4'-C4'-C5'-O5'
28	a	2433	OMG	C1'-C2'-O2'-CM2
28	a	2098	3TD	C3'-C4'-C5'-O5'
28	a	2685	2MA	O4'-C4'-C5'-O5'
28	a	2685	2MA	C3'-C4'-C5'-O5'
28	a	2627	2MG	C3'-C4'-C5'-O5'
28	a	2685	2MA	O4'-C1'-N9-C8
28	a	2145	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	2433	OMG	1	0
28	a	2145	5MC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	2627	2MG	1	0
28	a	2100	PSU	1	0
28	a	2685	2MA	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 310 ligands modelled in this entry, 309 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
35	V7A	a	3101	-	37,38,38	1.05	2 (5%)	43,60,60	0.89	2 (4%)

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
35	V7A	a	3101	-	-	8/13/72/72	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a	3101	V7A	CBC-NBD	4.99	1.47	1.33
35	a	3101	V7A	OAY-CAH	2.24	1.27	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	a	3101	V7A	CAM-CAP-CAQ	2.46	119.65	115.75
35	a	3101	V7A	CAP-CAM-CAL	2.09	112.33	109.88

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	a	3101	V7A	CAN-CAO-NBF-CBH
35	a	3101	V7A	CAP-CAQ-CBC-OBE
35	a	3101	V7A	CAR-CAQ-CBC-NBD
35	a	3101	V7A	CAR-CAQ-CBC-OBE
35	a	3101	V7A	CAA-CAS-NAT-CAW
35	a	3101	V7A	CAA-CAS-NAT-OAU
35	a	3101	V7A	CAW-NAT-OAU-CAV
35	a	3101	V7A	CAP-CAQ-CBC-NBD

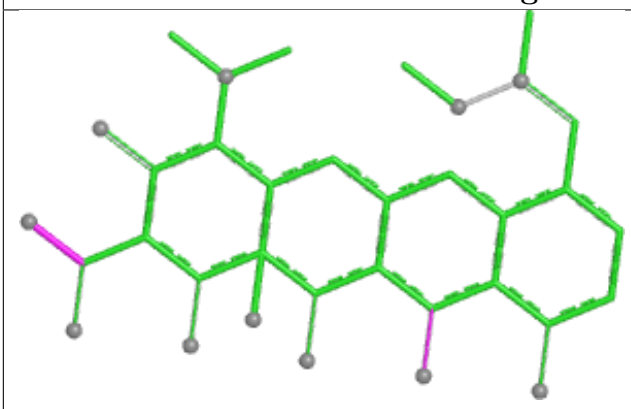
There are no ring outliers.

1 monomer is involved in 1 short contact:

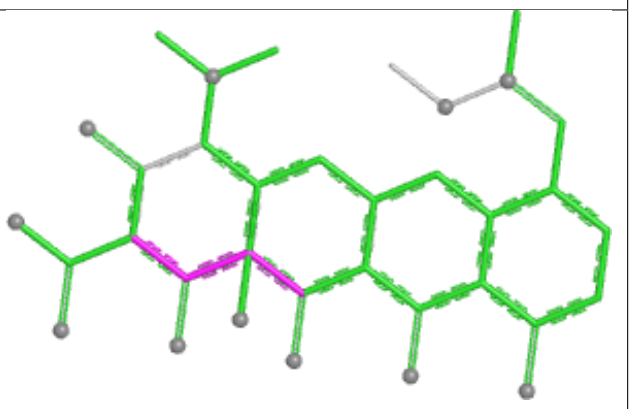
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	a	3101	V7A	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

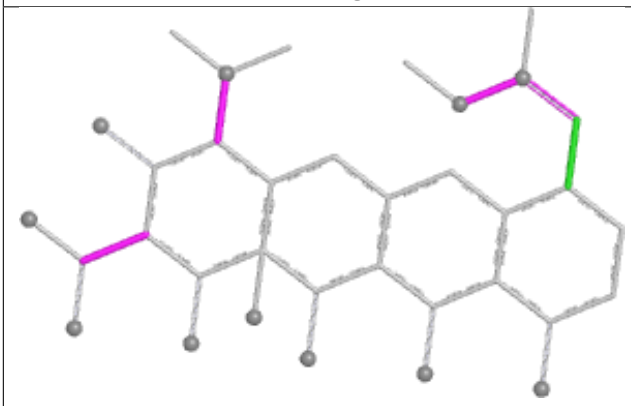
Ligand V7A a 3101



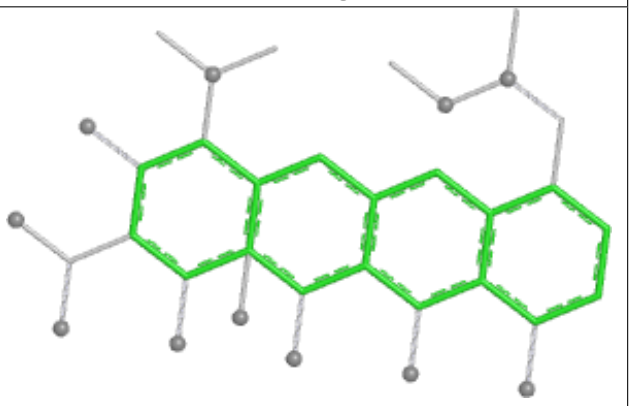
Bond lengths



Bond angles



Torsions



Rings

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.

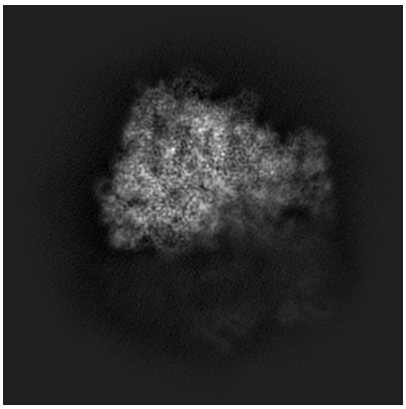
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27009. These allow visual inspection of the internal detail of the map and identification of artifacts.

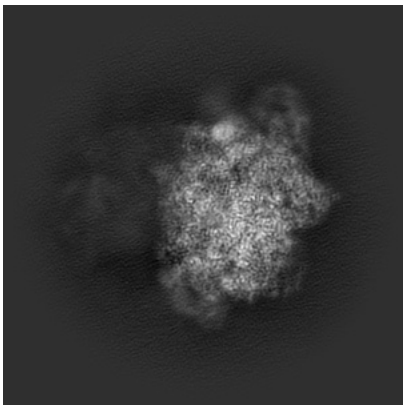
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

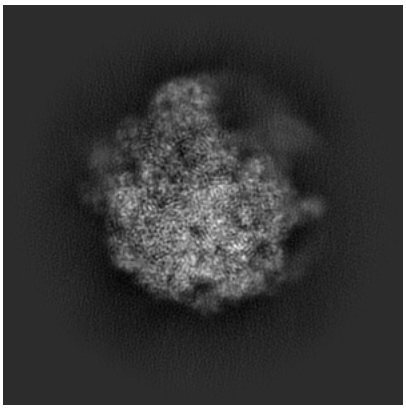
6.1.1 Primary map



X

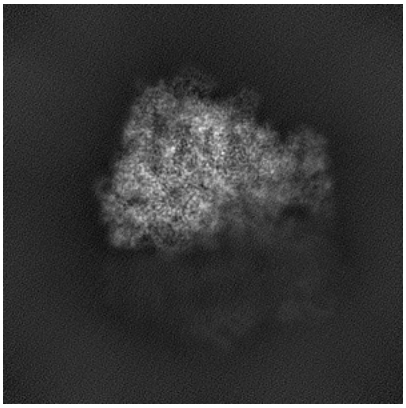


Y

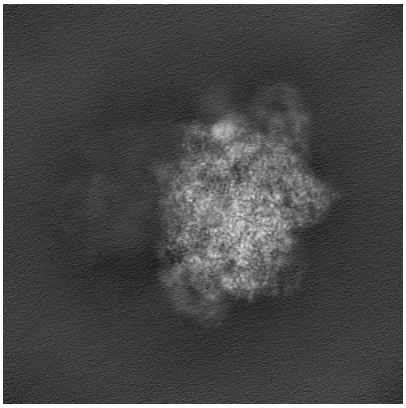


Z

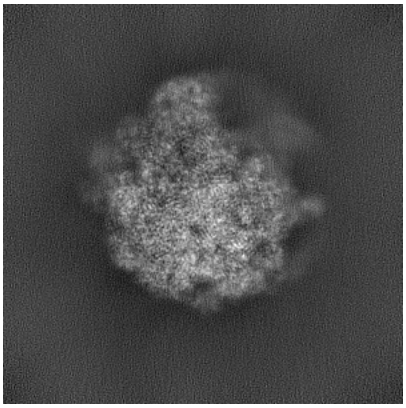
6.1.2 Raw map



X



Y

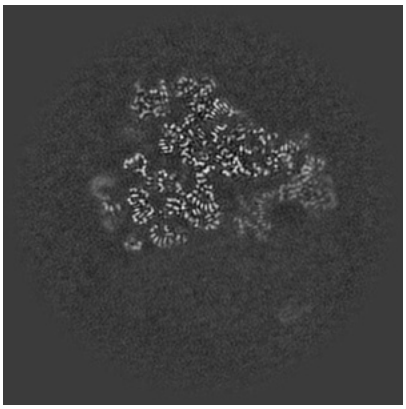


Z

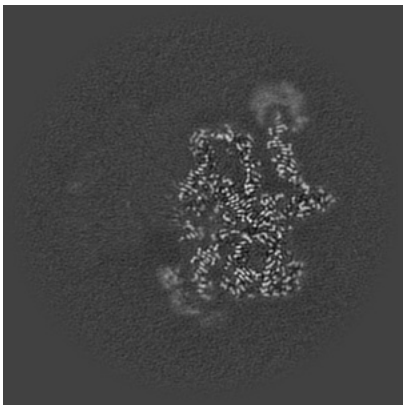
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

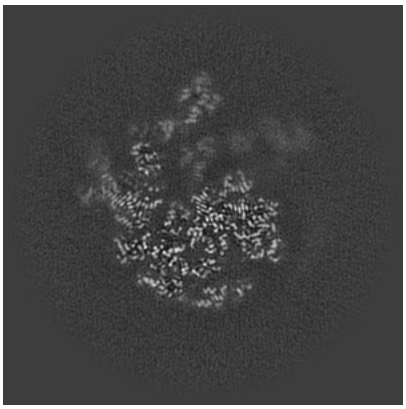
6.2.1 Primary map



X Index: 170

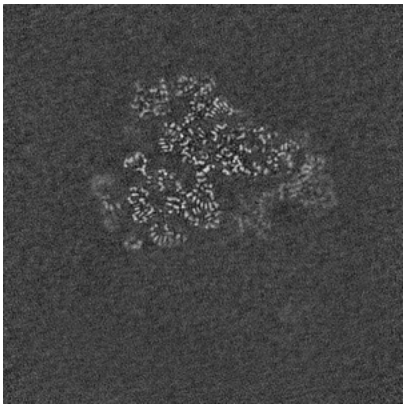


Y Index: 170

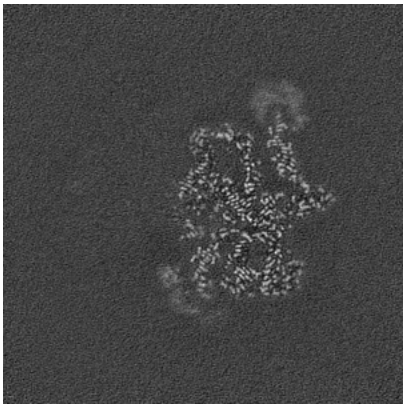


Z Index: 170

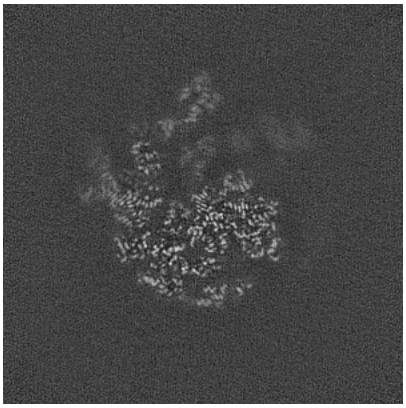
6.2.2 Raw map



X Index: 170



Y Index: 170

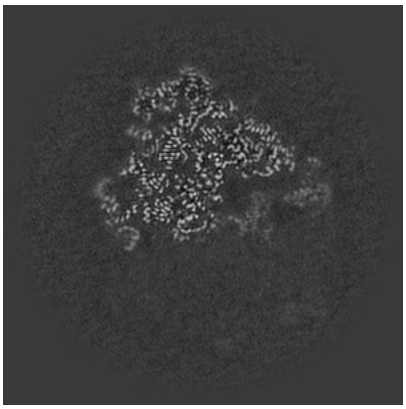


Z Index: 170

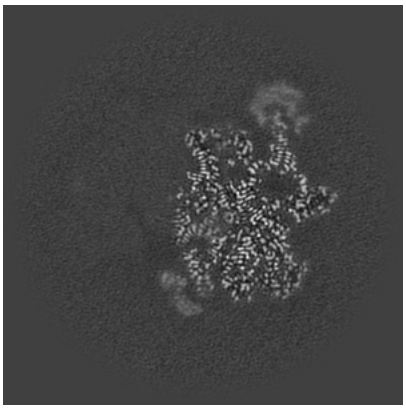
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

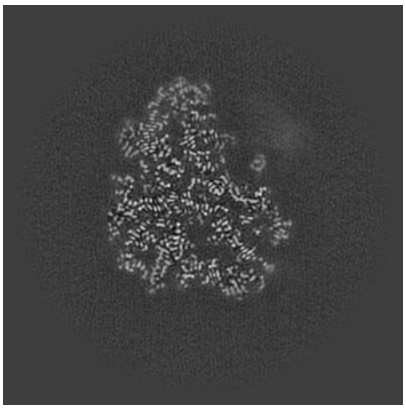
6.3.1 Primary map



X Index: 176

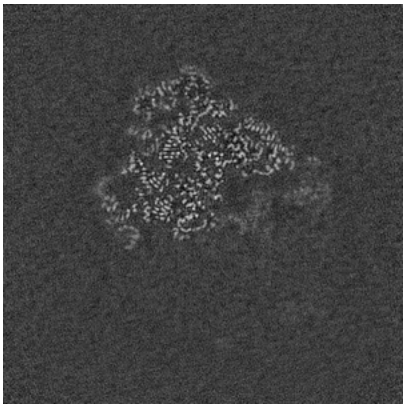


Y Index: 166

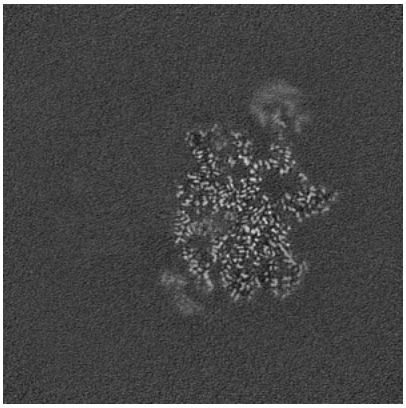


Z Index: 203

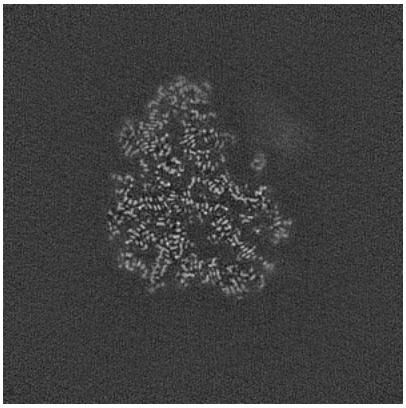
6.3.2 Raw map



X Index: 176



Y Index: 165

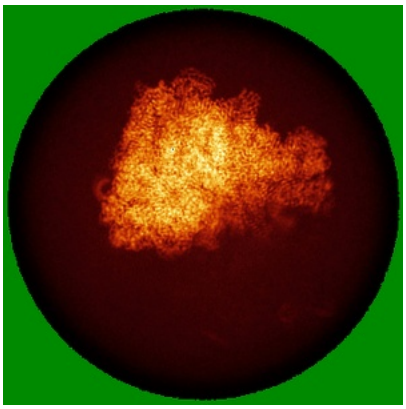


Z Index: 203

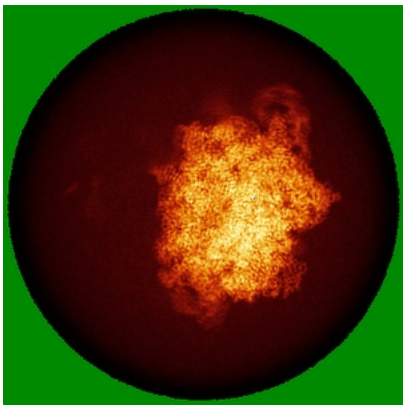
The images above show the largest variance slices of the map in three orthogonal directions.

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

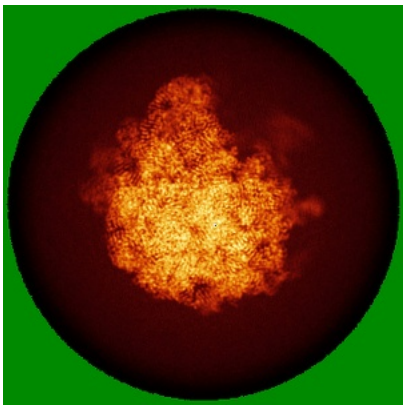
6.4.1 Primary map



X

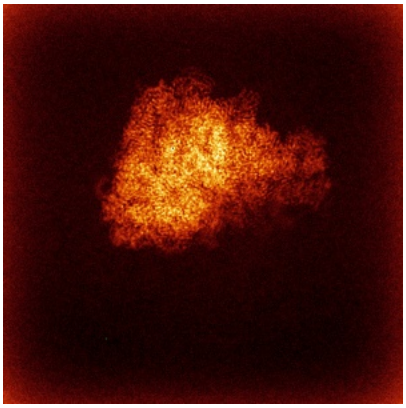


Y

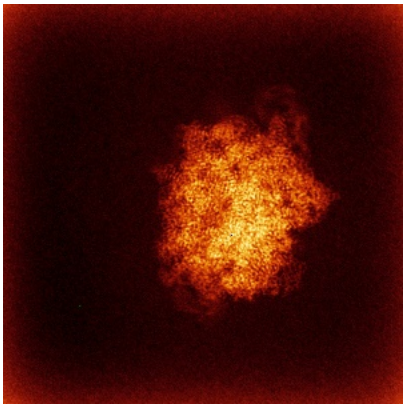


Z

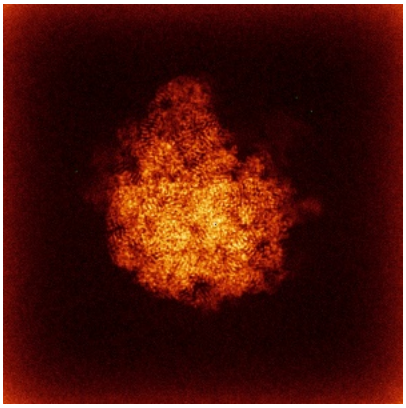
6.4.2 Raw map



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)

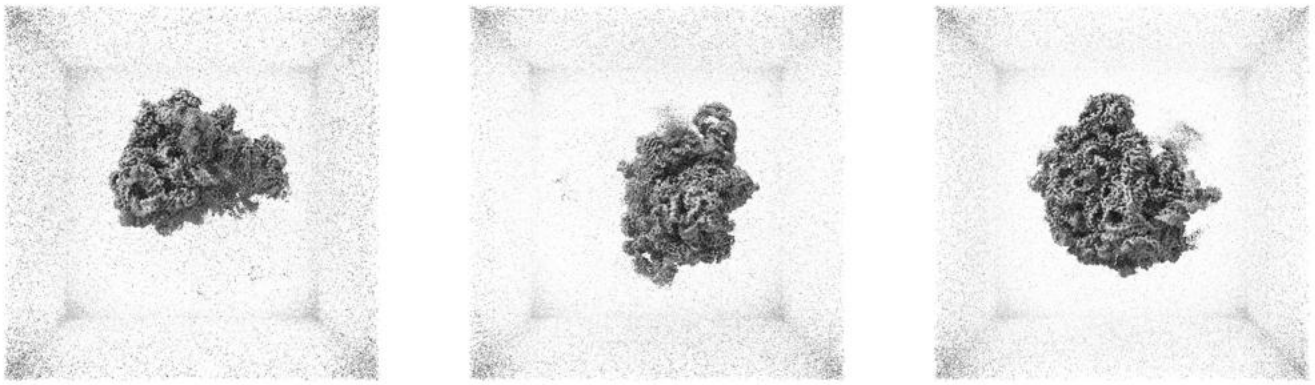
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

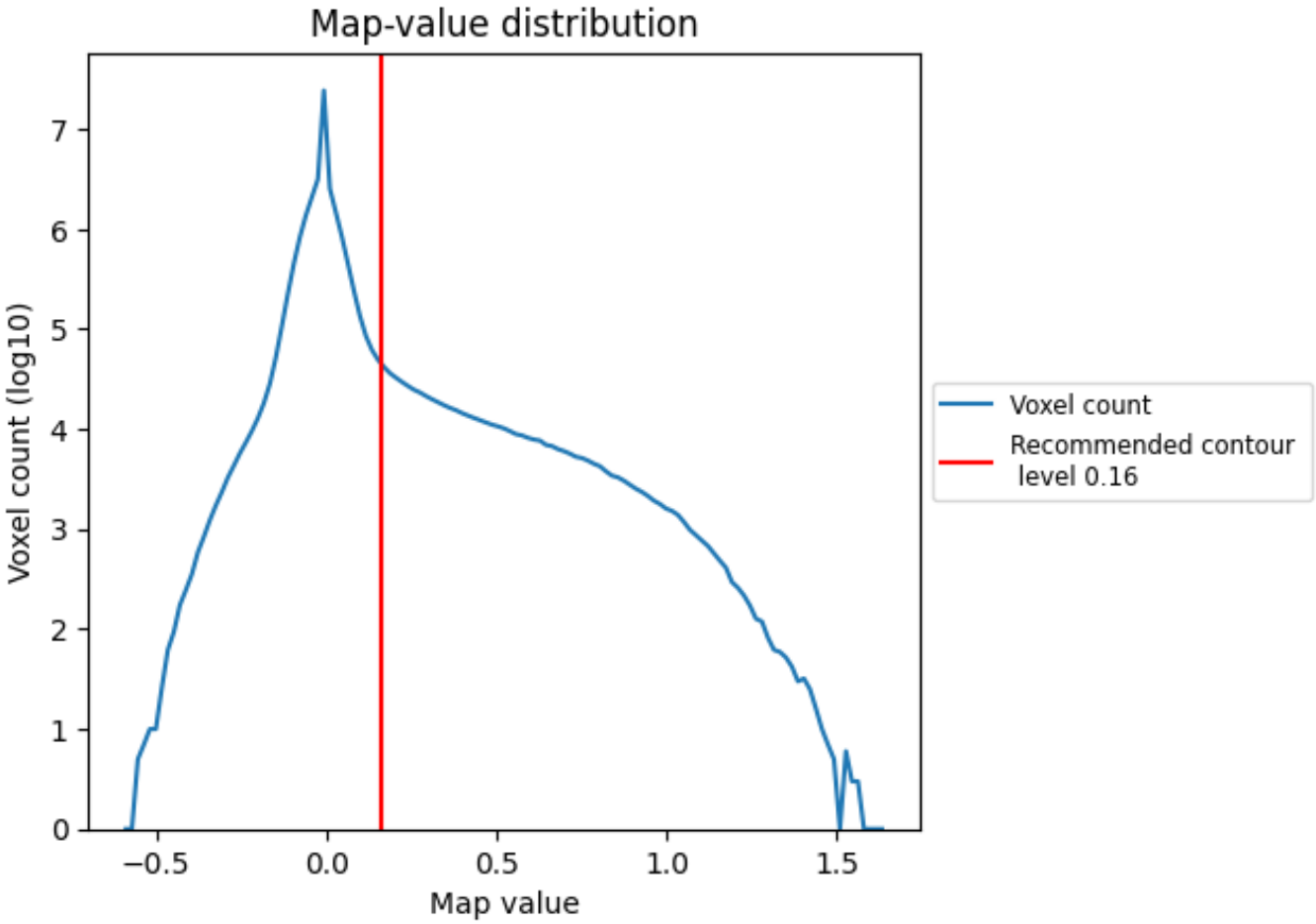
6.6 Mask visualisation (i)

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

7 Map analysis

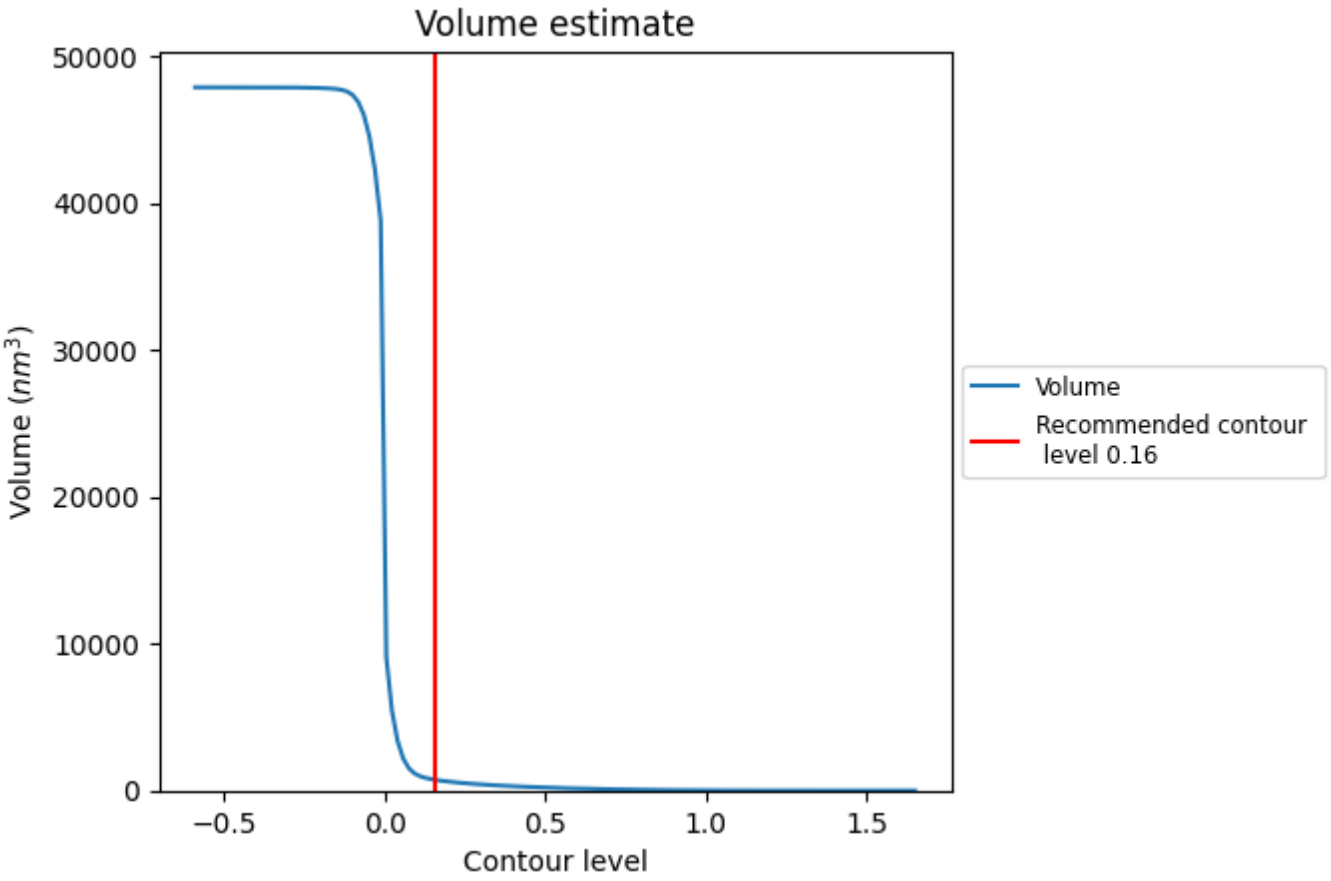
This section contains the results of statistical analysis of the map.

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.

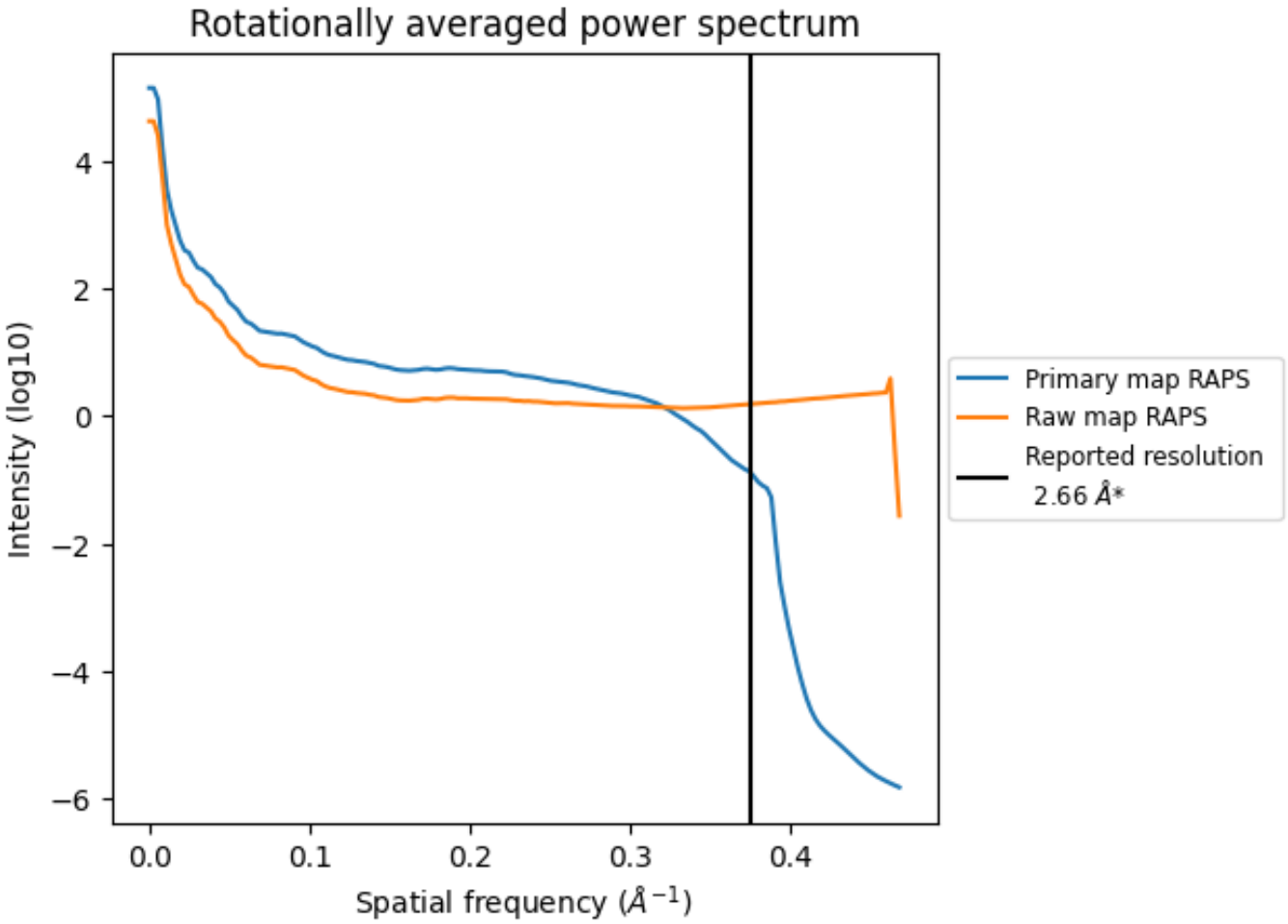
7.2 Volume estimate



The volume at the recommended contour level is 722 nm^3; this corresponds to an approximate mass of 652 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)

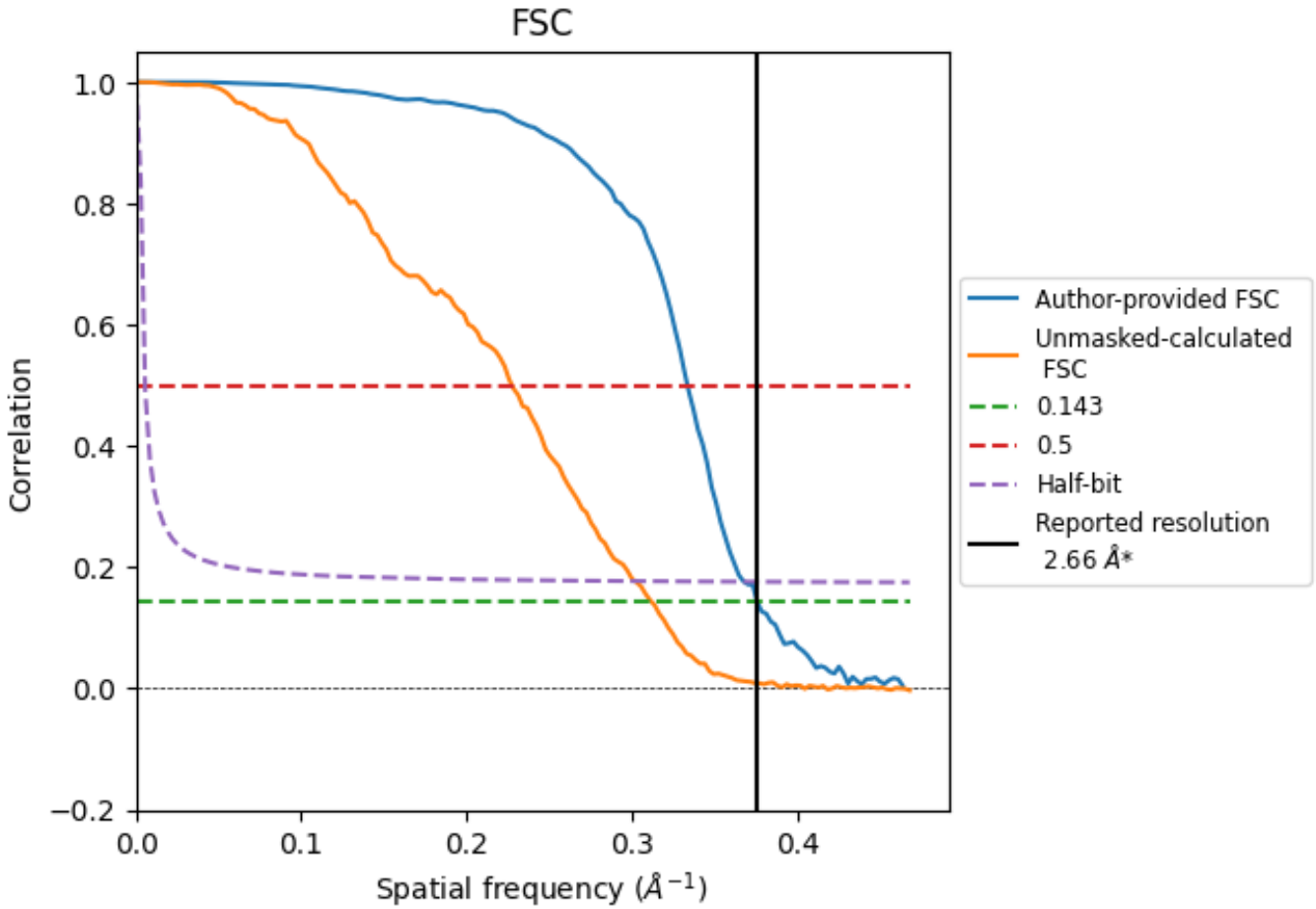


*Reported resolution corresponds to spatial frequency of 0.376 Å^{-1}

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 0.376 Å^{-1}

8.2 Resolution estimates (i)

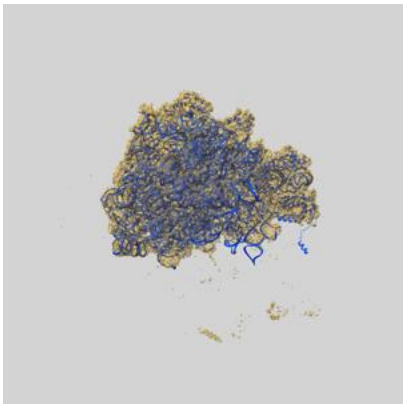
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.66	3.00	2.72
Unmasked-calculated*	3.21	4.40	3.31

*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 3.21 differs from the reported value 2.66 by more than 10 %

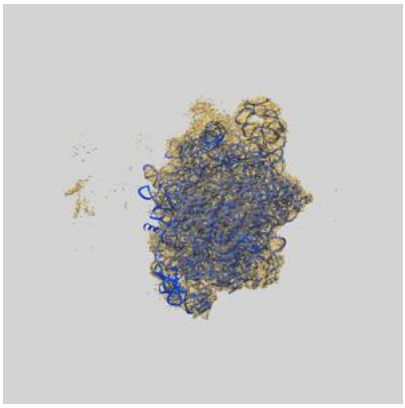
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27009 and PDB model 8CVM. Per-residue inclusion information can be found in section 3 on page 12.

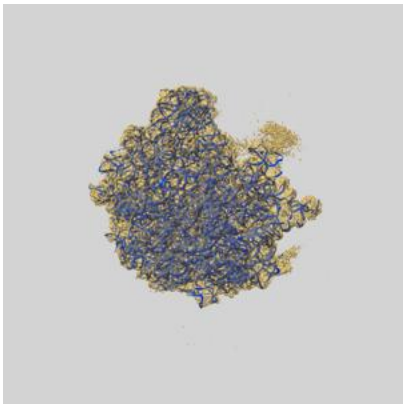
9.1 Map-model overlay



X



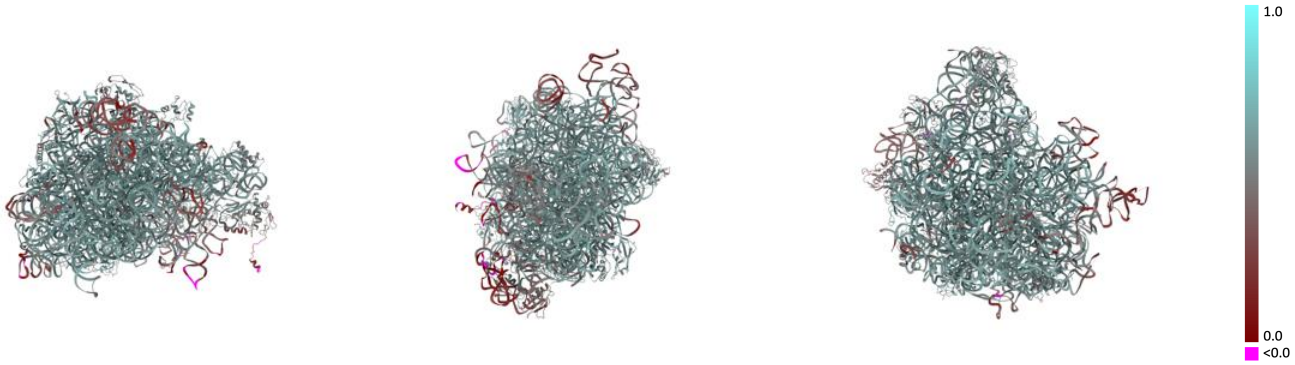
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 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.

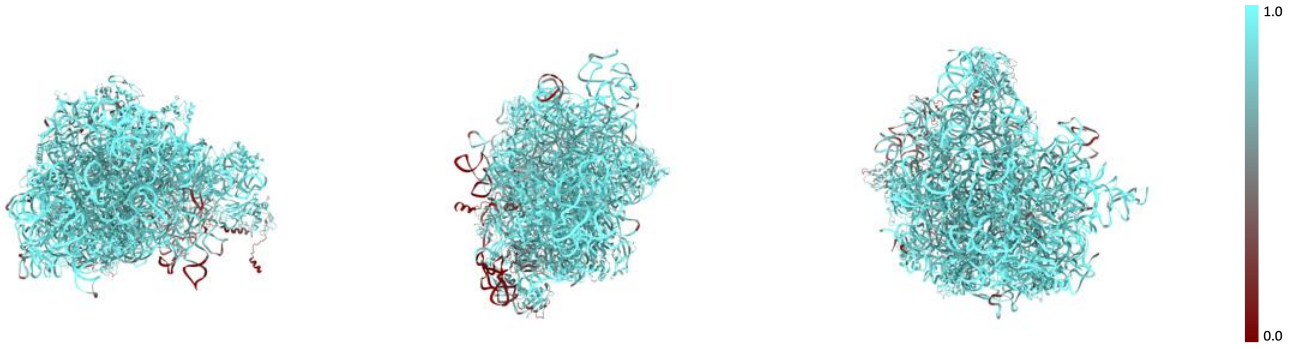
9.2 Q-score mapped to coordinate model (i)



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.

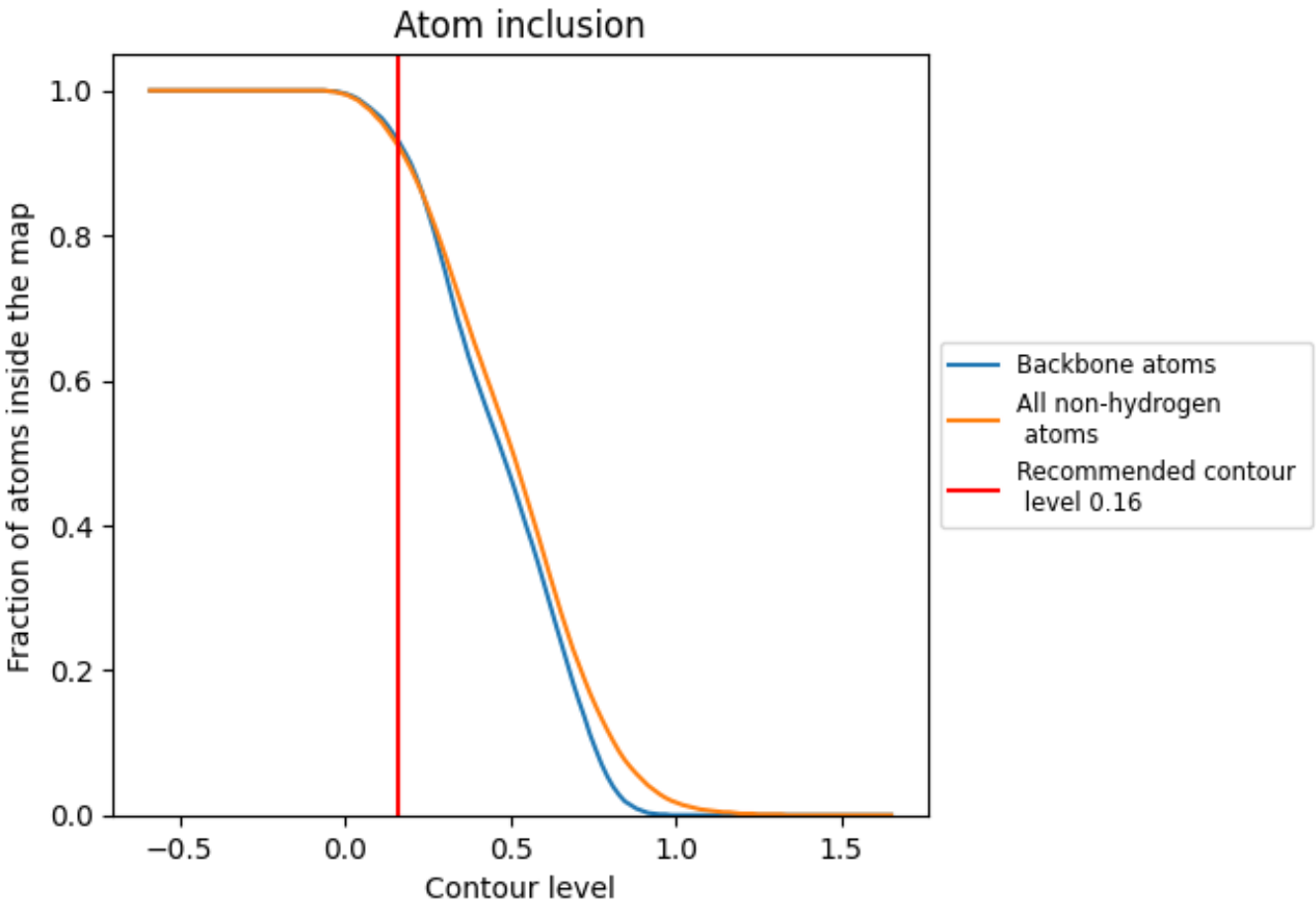
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9240	0.5650
0	0.8910	0.5770
1	0.9670	0.6300
2	0.9640	0.6170
3	0.4250	0.5010
4	0.4580	0.3200
C	0.6210	0.4180
V	0.9590	0.6280
a	0.9460	0.5700
b	0.9950	0.5750
c	0.9520	0.6070
d	0.9540	0.5990
e	0.9210	0.5550
f	0.7690	0.4600
g	0.7380	0.4150
i	0.9640	0.6110
j	0.8690	0.5740
k	0.9390	0.5800
l	0.9550	0.6050
m	0.9490	0.5980
n	0.9190	0.5450
o	0.8000	0.5590
p	0.9610	0.6110
q	0.9170	0.5840
r	0.9410	0.5960
s	0.9300	0.5820
t	0.9380	0.5690
u	0.6720	0.4910
v	0.9560	0.6090
w	0.9780	0.6210
x	0.9140	0.5560
y	0.9600	0.5950
z	0.9480	0.6040

