



## Full wwPDB EM Validation Report ⓘ

Apr 9, 2026 – 12:54 AM UTC

PDB ID : 11FV / pdb\_000011fv  
EMDB ID : EMD-75668  
Title : Chimeric Escherichia coli 70S ribosome containing an evolved 16S rRNA from Pseudomonas aeruginosa (PA-S3.3)  
Authors : Raskar, T.  
Deposited on : 2026-02-21  
Resolution : 2.90 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](mailto: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>.

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

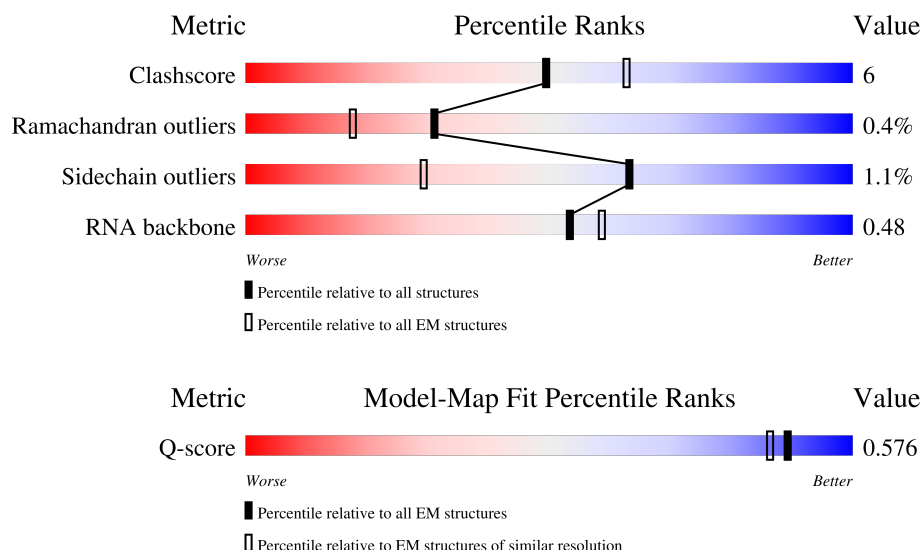
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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.









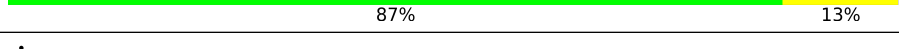
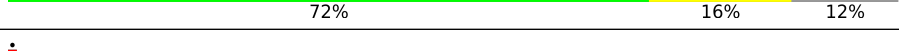
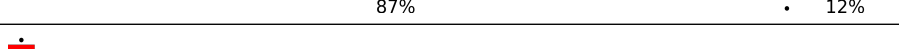
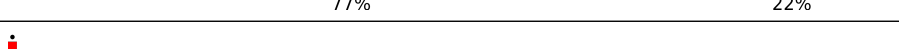
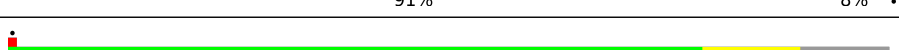

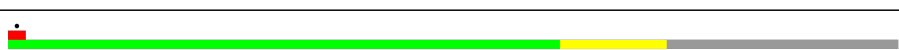
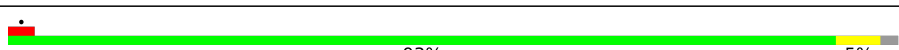
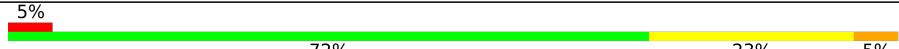




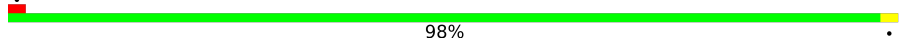
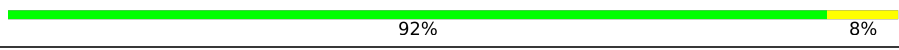
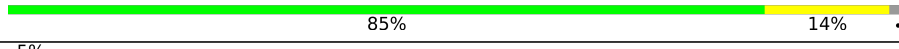

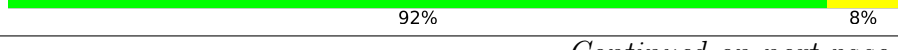

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 ( 2.40 - 3.40 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	1526	
2	0	110	
3	1	81	

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Mol	Chain	Length	Quality of chain
4	Z	103	
5	2	87	
6	3	71	
7	b	100	
8	c	104	
9	D	241	
10	d	94	
11	E	233	
12	e	85	
13	F	206	
14	f	78	
15	G	167	
16	g	63	
17	H	135	
18	h	59	
19	I	2904	
20	i	57	
21	J	120	
22	j	55	
23	K	273	
24	k	46	
25	L	209	
26	l	65	
27	M	201	
28	m	38	

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Mol	Chain	Length	Quality of chain
29	N	179	
30	n	179	
31	O	177	
32	o	130	
33	P	149	
34	p	130	
35	Q	70	
36	q	103	
37	R	142	
38	r	129	
39	S	123	
40	t	124	
41	T	144	
42	u	118	
43	U	136	
44	v	101	
45	V	127	
46	w	89	
47	W	117	
48	x	82	
49	X	115	
50	y	84	
51	Y	118	
52	z	75	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	C	1625	-	-	X	-
53	MG	I	3077	-	-	X	-

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 142151 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1526	Total	C	N	O	P	0	0
			32744	14605	6008	10606	1525		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	434	U	A	conflict	GB 3134256434
C	606	U	C	conflict	GB 3134256434
C	1472	C	U	conflict	GB 3134256434

- Molecule 2 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 3 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	81	Total	C	N	O	S	0	0
			651	416	124	109	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 5 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 6 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 7 is a protein called 50S ribosomal protein L23.

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

- Molecule 8 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 9 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 10 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 12 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	e	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 13 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 14 is a protein called 50S ribosomal protein L28.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 16 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 17 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 18 is a protein called 50S ribosomal protein L30.

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

- Molecule 19 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	2898	Total	C	N	O	P	2	0
			62271	27787	11455	20129	2900		

- Molecule 20 is a protein called 50S ribosomal protein L32.



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

- Molecule 21 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 22 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	j	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 23 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	K	271	Total	C	N	O	S	1	0
			2093	1294	427	365	7		

- Molecule 24 is a protein called Large ribosomal subunit protein bL34.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 28 is a protein called Large ribosomal subunit protein bL36A.

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

- Molecule 29 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 30 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	n	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 32 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 33 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	P	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 34 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 35 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Q	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 36 is a protein called Small ribosomal subunit protein uS10.

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

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

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

- Molecule 38 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	r	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 39 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	S	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 40 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	t	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 41 is a protein called Large ribosomal subunit protein uL15.

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

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

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	U	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 44 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 45 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	w	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

- Molecule 47 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 48 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 49 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 50 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 50S ribosomal protein L20.

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

- Molecule 52 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	C	89	Total	Mg	0
			89	89	
53	I	203	Total	Mg	0
			203	203	
53	J	5	Total	Mg	0
			5	5	
53	K	1	Total	Mg	0
			1	1	
53	L	2	Total	Mg	0
			2	2	
53	l	1	Total	Mg	0
			1	1	

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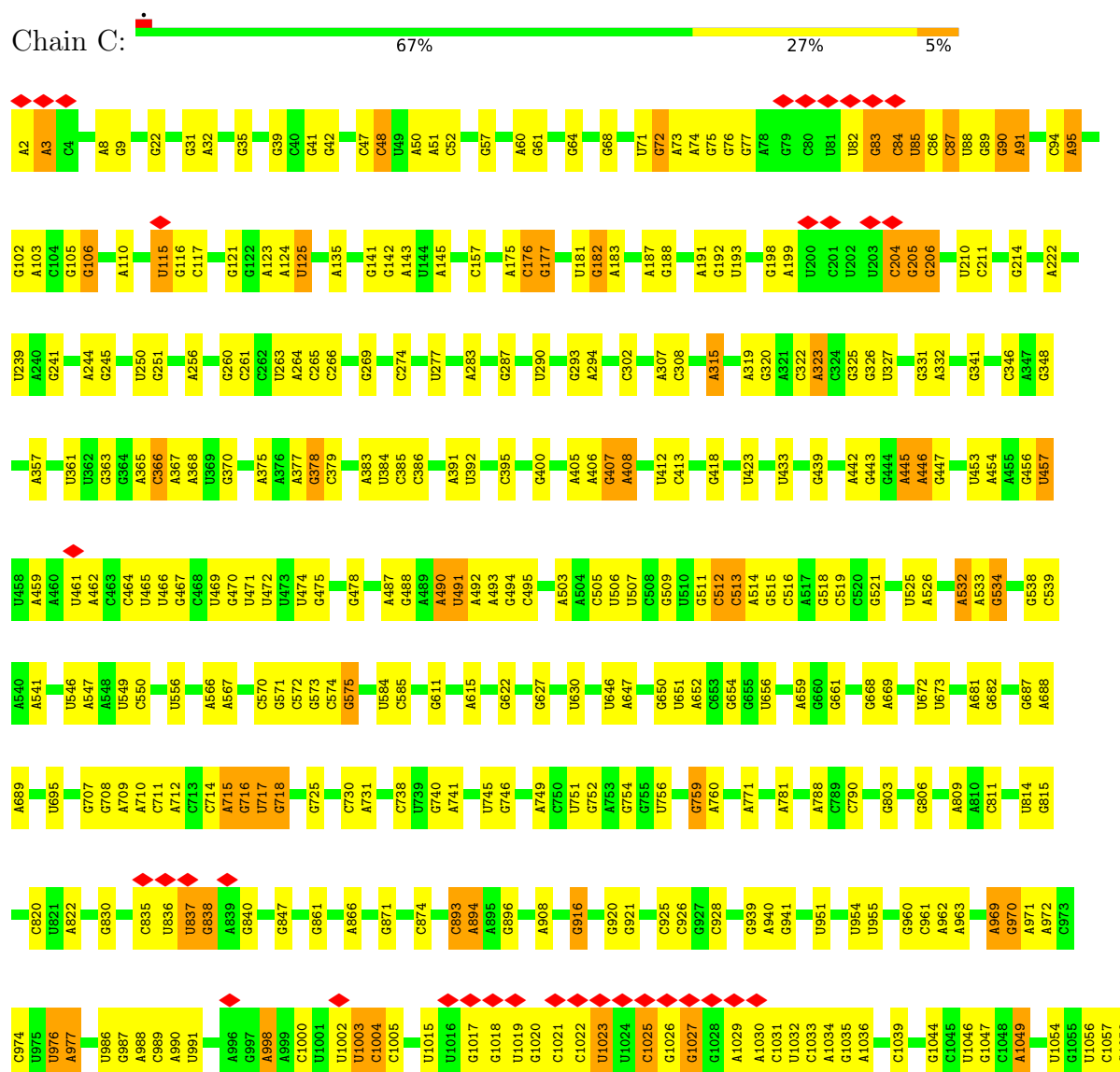
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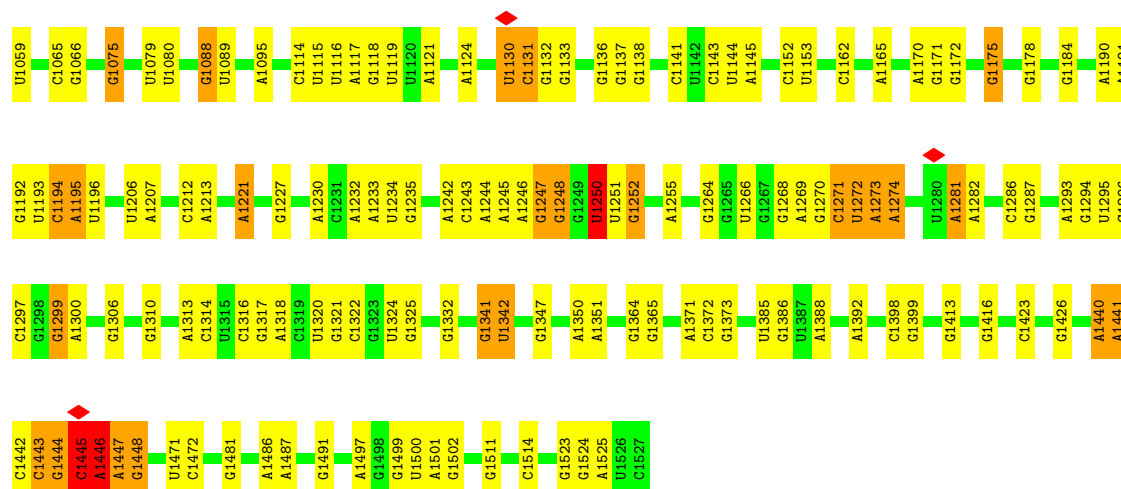
Mol	Chain	Residues	Atoms		AltConf
53	M	1	Total 1	Mg 1	0
53	p	1	Total 1	Mg 1	0
53	T	1	Total 1	Mg 1	0
53	u	1	Total 1	Mg 1	0
53	V	1	Total 1	Mg 1	0
53	Y	1	Total 1	Mg 1	0

### 3 Residue-property plots

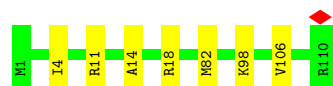
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 16S ribosomal RNA

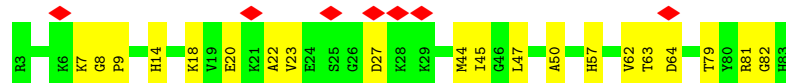
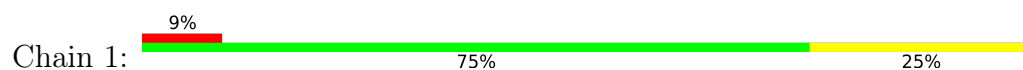




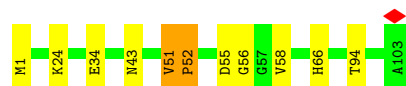
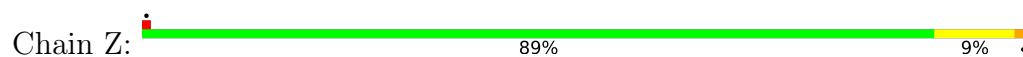
- Molecule 2: Large ribosomal subunit protein uL22



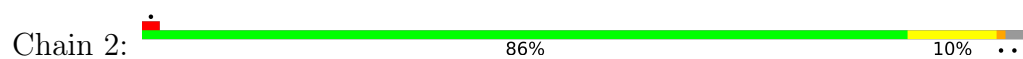
- Molecule 3: Small ribosomal subunit protein uS19



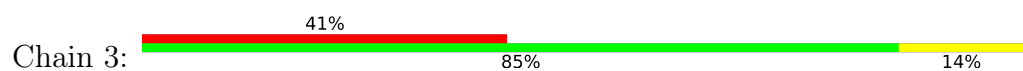
- Molecule 4: Large ribosomal subunit protein bL21



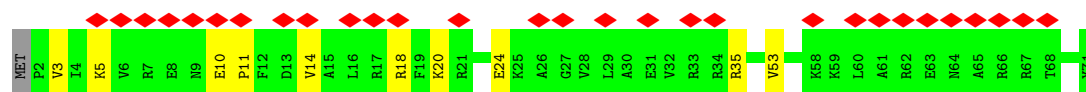
- Molecule 5: Small ribosomal subunit protein bS20



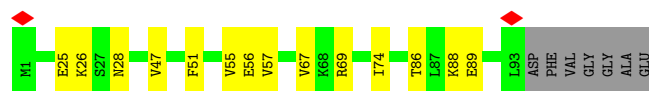
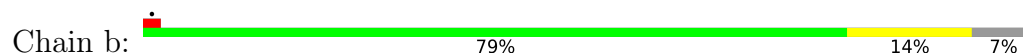
- Molecule 6: Small ribosomal subunit protein bS21



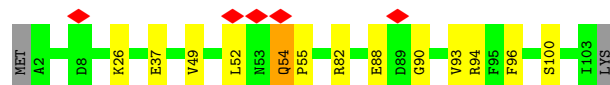
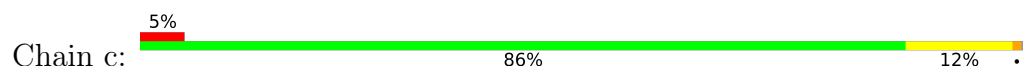




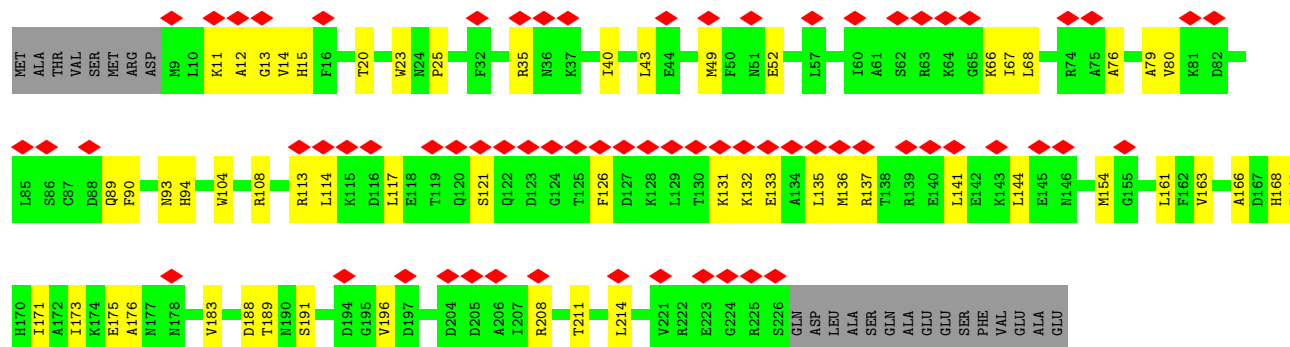
- Molecule 7: 50S ribosomal protein L23



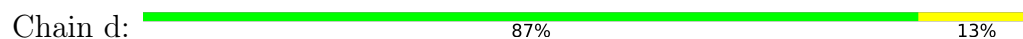
- Molecule 8: 50S ribosomal protein L24



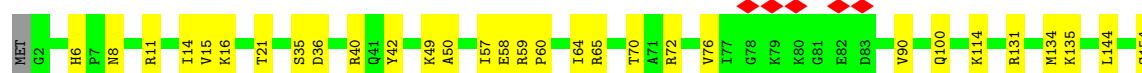
- Molecule 9: Small ribosomal subunit protein uS2

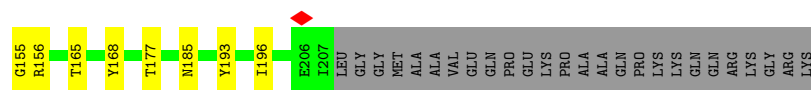


- Molecule 10: Large ribosomal subunit protein bL25

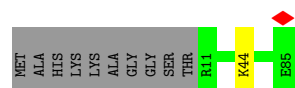
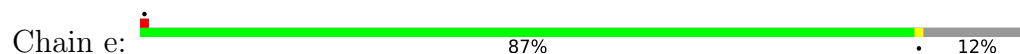


- Molecule 11: Small ribosomal subunit protein uS3

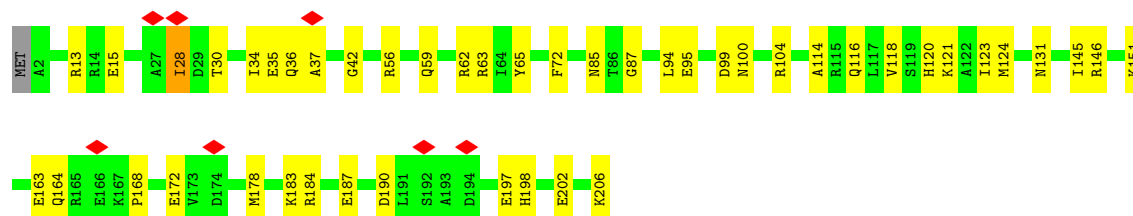
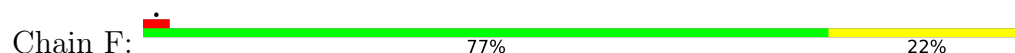




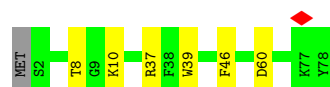
- Molecule 12: 50S ribosomal protein L27



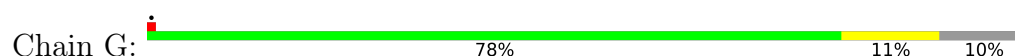
- Molecule 13: Small ribosomal subunit protein uS4



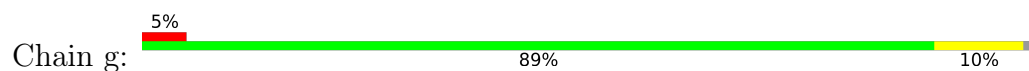
- Molecule 14: 50S ribosomal protein L28



- Molecule 15: Small ribosomal subunit protein uS5



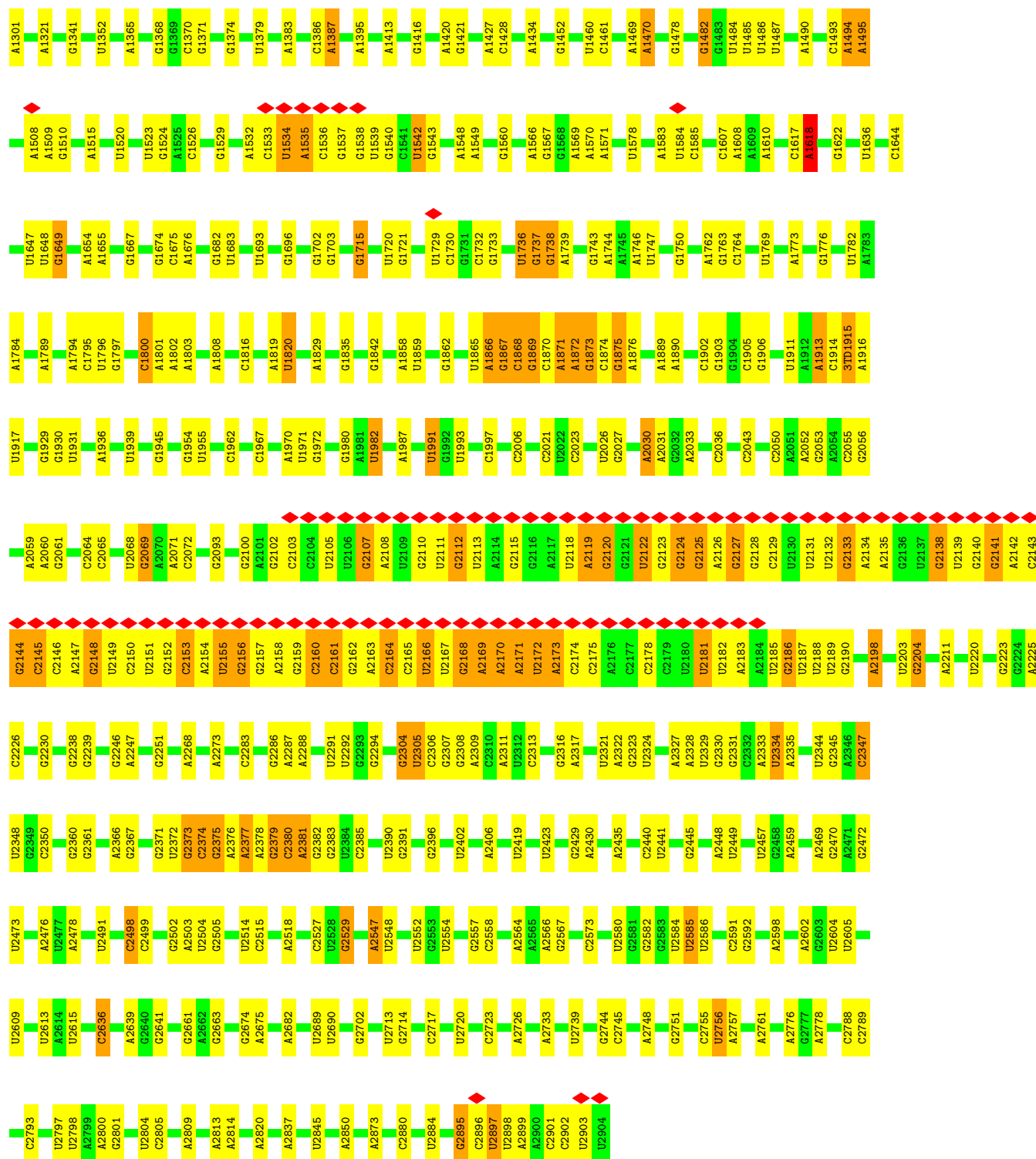
- Molecule 16: Large ribosomal subunit protein uL29



- Molecule 17: Small ribosomal subunit protein bS6







• Molecule 20: 50S ribosomal protein L32

Chain i: 82% 16%



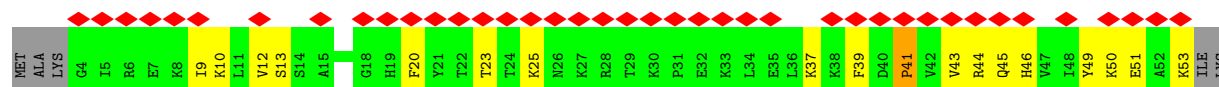
- Molecule 21: 5S ribosomal RNA

Chain J: 




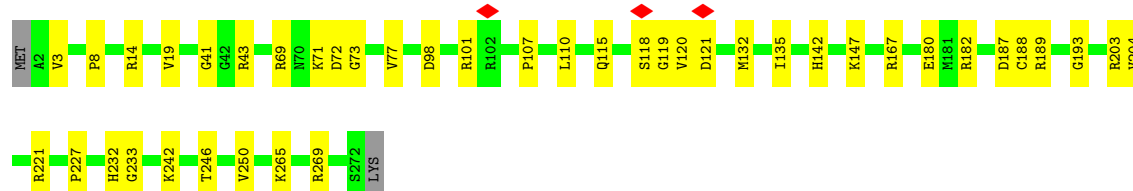
- Molecule 22: 50S ribosomal protein L33

Chain j: 



- Molecule 23: 50S ribosomal protein L2

Chain K: 



- Molecule 24: Large ribosomal subunit protein bL34

Chain k: 




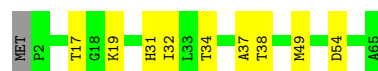
- Molecule 25: Large ribosomal subunit protein uL3

Chain L: 

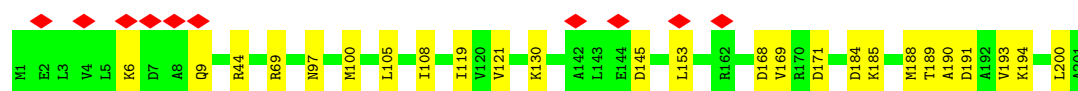
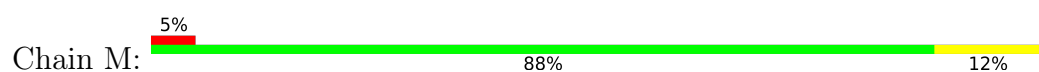


- Molecule 26: 50S ribosomal protein L35

Chain l: 



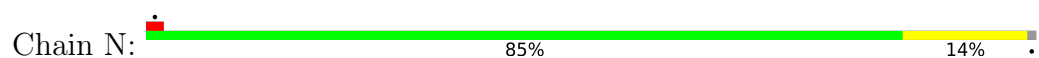
- Molecule 27: Large ribosomal subunit protein uL4



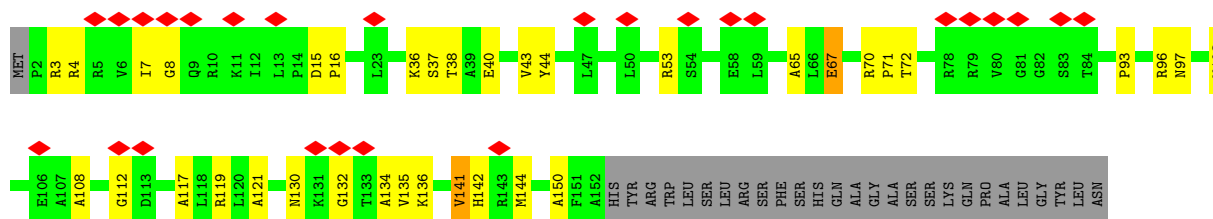
- Molecule 28: Large ribosomal subunit protein bL36A



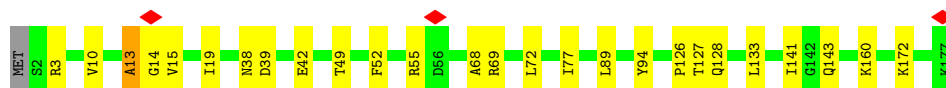
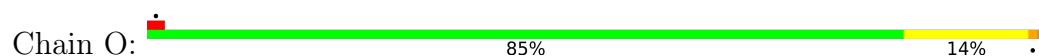
- Molecule 29: Large ribosomal subunit protein uL5



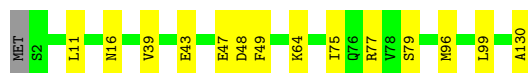
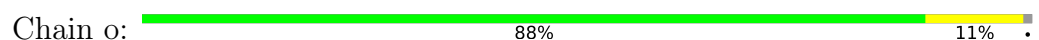
- Molecule 30: Small ribosomal subunit protein uS7



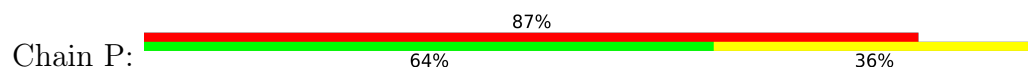
- Molecule 31: Large ribosomal subunit protein uL6

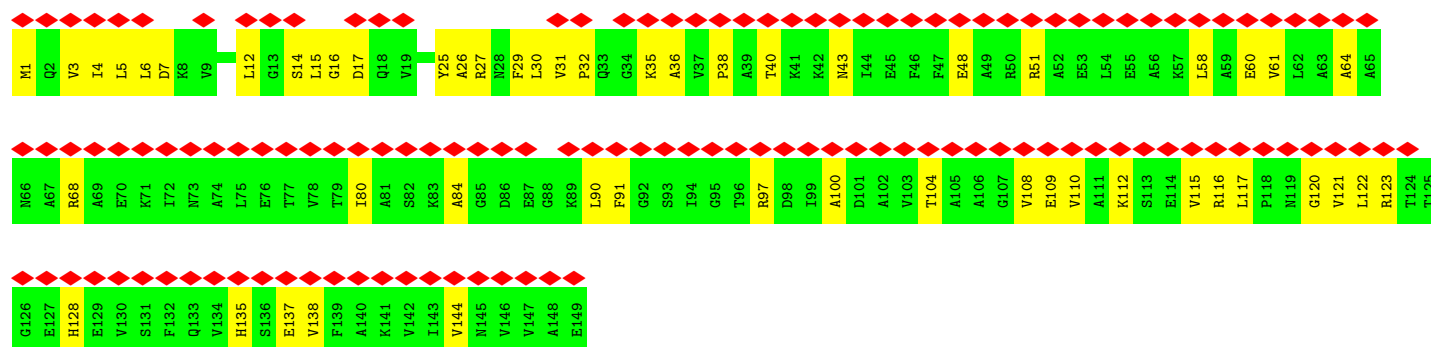


- Molecule 32: Small ribosomal subunit protein uS8

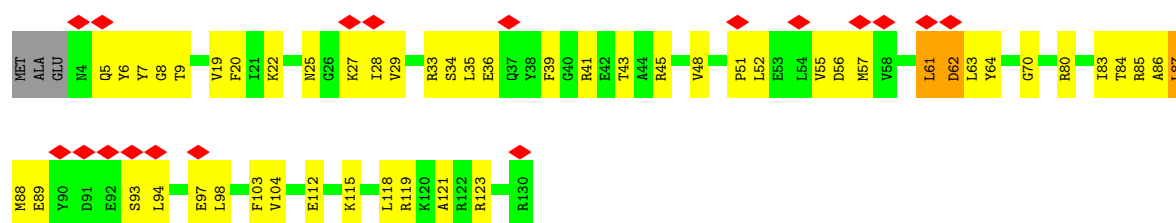


- Molecule 33: Large ribosomal subunit protein bL9

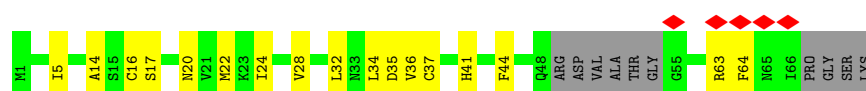




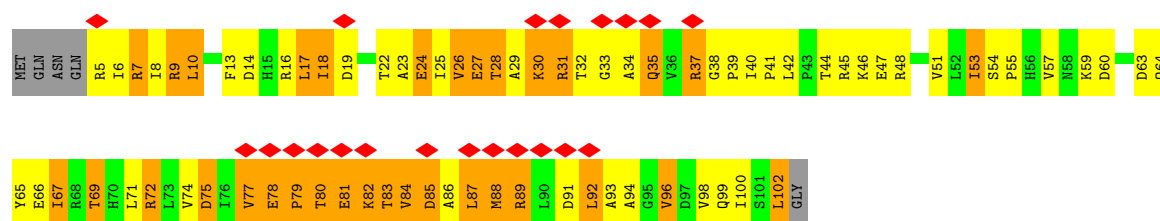
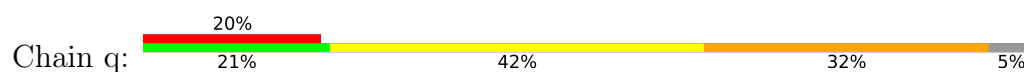
- Molecule 34: Small ribosomal subunit protein uS9



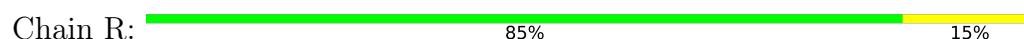
- Molecule 35: 50S ribosomal protein L31



- Molecule 36: Small ribosomal subunit protein uS10

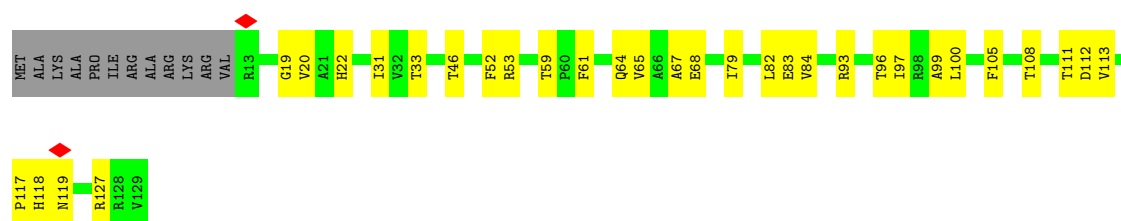


- Molecule 37: Large ribosomal subunit protein uL13




- Molecule 38: 30S ribosomal protein S11

Chain r:  66% 25% 9%




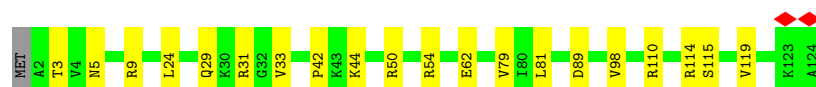
- Molecule 39: Large ribosomal subunit protein uL14

Chain S:  88% 11%




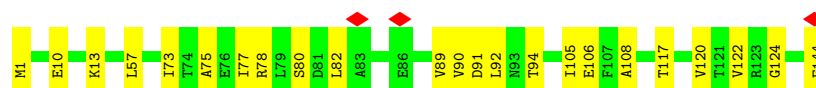
- Molecule 40: 30S ribosomal protein S12

Chain t:  83% 16%




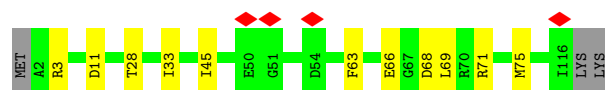
- Molecule 41: Large ribosomal subunit protein uL15

Chain T:  84% 16%




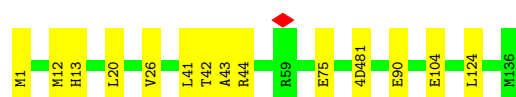
- Molecule 42: Small ribosomal subunit protein uS13

Chain u:  88% 9%



- Molecule 43: Large ribosomal subunit protein uL16

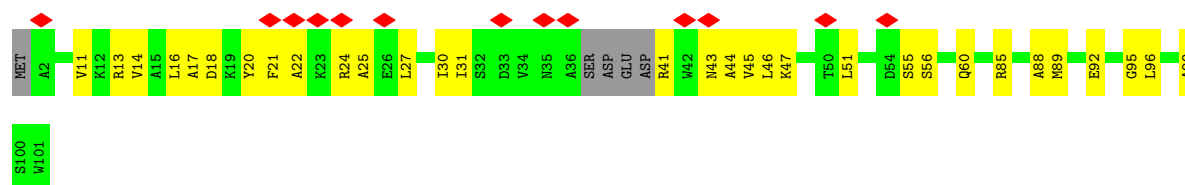
Chain U:  90% 10%



- Molecule 44: Small ribosomal subunit protein uS14

Chain v:  13% 64% 31% 5%

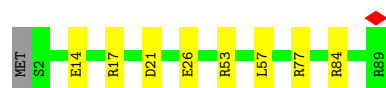




- Molecule 45: Large ribosomal subunit protein bL17



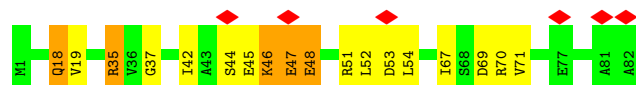
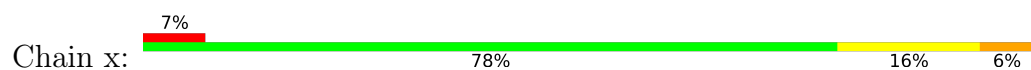
- Molecule 46: Small ribosomal subunit protein uS15



- Molecule 47: Large ribosomal subunit protein uL18



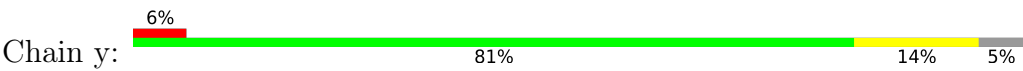
- Molecule 48: Small ribosomal subunit protein bS16



- Molecule 49: Large ribosomal subunit protein bL19



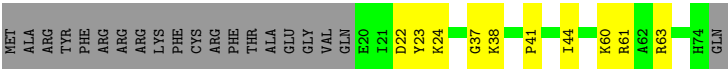
- Molecule 50: Small ribosomal subunit protein uS17



• Molecule 51: 50S ribosomal protein L20



• Molecule 52: Small ribosomal subunit protein bS18



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	312639	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	35.939	Depositor
Minimum map value	-18.973	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size ( $\text{\AA}$ )	455.52, 455.52, 455.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.949, 0.949, 0.949	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.29	0/36666	0.39	12/57201 (0.0%)
2	O	0.31	0/864	0.40	0/1156
3	1	0.30	0/667	0.53	0/897
4	Z	0.30	0/829	0.53	0/1107
5	2	0.30	0/671	0.70	1/888 (0.1%)
6	3	0.19	0/598	0.46	0/792
7	b	0.26	0/744	0.51	0/994
8	c	0.27	0/787	0.57	0/1051
9	D	0.21	0/1735	0.44	0/2338
10	d	0.30	0/766	0.49	0/1025
11	E	0.22	0/1651	0.45	0/2225
12	e	0.32	0/582	0.51	0/769
13	F	0.22	0/1665	0.45	0/2227
14	f	0.34	0/635	0.49	0/848
15	G	0.29	0/1118	0.47	0/1504
16	g	0.23	0/502	0.43	0/667
17	H	0.26	0/835	0.55	0/1128
18	h	0.29	0/453	0.48	0/605
19	I	0.36	0/69168	0.38	21/107901 (0.0%)
20	i	0.31	0/450	0.41	0/599
21	J	0.26	0/2828	0.28	0/4410
22	j	0.26	0/416	0.65	0/554
23	K	0.39	0/2132	0.60	0/2866
24	k	0.35	0/380	0.45	0/498
25	L	0.33	0/1586	0.46	0/2134
26	l	0.34	0/513	0.50	0/676
27	M	0.29	0/1571	0.47	0/2113
28	m	0.33	0/303	0.52	0/397
29	N	0.20	0/1434	0.42	0/1926
30	n	0.25	0/1195	0.89	6/1602 (0.4%)
31	O	0.27	0/1343	0.60	1/1816 (0.1%)
32	o	0.24	0/989	0.42	0/1326

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	P	0.19	0/1122	0.46	0/1515
34	p	0.26	0/1034	0.81	1/1375 (0.1%)
35	Q	0.18	0/488	0.37	0/649
36	q	0.91	0/796	1.24	1/1077 (0.1%)
37	R	0.32	0/1152	0.43	0/1551
38	r	0.23	0/893	0.42	0/1205
39	S	0.36	0/947	0.53	0/1268
40	t	0.31	0/969	0.58	0/1300
41	T	0.31	0/1062	0.50	0/1413
42	u	0.19	0/900	0.40	1/1204 (0.1%)
43	U	0.32	0/1081	0.52	2/1443 (0.1%)
44	v	0.22	0/785	0.45	0/1043
45	V	0.33	0/973	0.44	0/1301
46	w	0.27	0/718	0.42	0/959
47	W	0.30	0/902	0.64	0/1209
48	x	0.37	0/659	0.66	0/884
49	X	0.31	0/929	0.44	0/1242
50	y	0.26	0/657	0.51	0/881
51	Y	0.34	0/960	0.37	0/1278
52	z	0.24	0/462	0.41	0/621
All	All	0.33	0/153565	0.43	46/229658 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	Z	0	1
23	K	0	2
34	p	0	1
40	t	0	1
43	U	0	1
All	All	0	6

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	2717	C	OP1-P-O3'	-9.79	78.63	108.00
19	I	673	C	OP1-P-O3'	-9.20	80.42	108.00
19	I	2598	A	OP1-P-O3'	-8.92	81.24	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	2360	G	OP1-P-O3'	-8.88	81.35	108.00
19	I	2723	C	OP1-P-O3'	-8.88	81.37	108.00
19	I	1655	A	OP2-P-O3'	-8.85	81.46	108.00
19	I	2230	G	OP1-P-O3'	-8.84	81.49	108.00
30	n	108	ALA	N-CA-C	-8.77	104.62	114.62
19	I	2050	C	OP1-P-O3'	-8.69	81.93	108.00
19	I	2674	G	OP1-P-O3'	-8.66	82.02	108.00
19	I	2598	A	OP2-P-O3'	-8.62	82.13	108.00
1	C	325	G	P-O3'-C3'	-8.52	107.42	120.20
19	I	2564	A	OP1-P-O3'	-8.49	82.54	108.00
19	I	2360	G	OP2-P-O3'	-8.45	82.66	108.00
19	I	2564	A	OP2-P-O3'	-8.33	83.02	108.00
19	I	673	C	OP2-P-O3'	-8.31	83.06	108.00
19	I	1655	A	OP1-P-O3'	-8.29	83.12	108.00
19	I	2050	C	OP2-P-O3'	-8.23	83.30	108.00
19	I	2723	C	OP2-P-O3'	-8.20	83.41	108.00
19	I	2674	G	OP2-P-O3'	-8.12	83.63	108.00
19	I	2230	G	OP2-P-O3'	-8.02	83.94	108.00
1	C	307	A	P-O3'-C3'	-7.73	108.61	120.20
19	I	2717	C	OP2-P-O3'	-7.65	85.04	108.00
1	C	1445	C	P-O3'-C3'	-7.42	109.06	120.20
30	n	38	THR	N-CA-C	-7.41	106.17	114.62
30	n	3	ARG	CA-C-N	7.19	133.72	121.14
30	n	3	ARG	C-N-CA	7.19	133.72	121.14
1	C	1250	U	P-O3'-C3'	-6.80	110.00	120.20
1	C	106	G	P-O3'-C3'	-6.66	110.21	120.20
1	C	105	G	P-O3'-C3'	-6.62	110.27	120.20
1	C	1221	A	P-O3'-C3'	-6.09	111.07	120.20
36	q	39	PRO	N-CA-C	-5.83	100.47	112.47
1	C	308	C	P-O3'-C3'	-5.79	111.52	120.20
1	C	1446	A	P-O3'-C3'	-5.78	111.53	120.20
1	C	1443	C	P-O3'-C3'	-5.65	111.72	120.20
19	I	1034	G	C2'-C3'-O3'	5.47	117.71	109.50
42	u	66	GLU	CB-CA-C	-5.44	109.84	117.23
30	n	141	VAL	N-CA-C	-5.27	106.40	112.98
31	O	77	ILE	N-CA-C	-5.25	107.28	113.42
1	C	1445	C	O4'-C1'-C2'	-5.25	102.35	107.60
1	C	525	U	P-O3'-C3'	-5.17	112.45	120.20
5	2	21	ASN	N-CA-C	-5.15	108.26	114.75
34	p	88	MET	N-CA-C	-5.15	108.02	114.56
43	U	12	MET	CA-C-N	-5.12	113.89	123.05
43	U	12	MET	C-N-CA	-5.12	113.89	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	n	67	GLU	N-CA-C	-5.09	106.20	114.09

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	K	101	ARG	Peptide
23	K	232	HIS	Peptide
43	U	13	HIS	Peptide
4	Z	51	VAL	Peptide
34	p	61	LEU	Peptide
40	t	44	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	32744	0	16472	247	0
2	0	857	0	922	4	0
3	1	651	0	675	13	0
4	Z	816	0	839	7	0
5	2	665	0	714	6	0
6	3	590	0	629	9	0
7	b	738	0	807	9	0
8	c	779	0	831	9	0
9	D	1704	0	1732	40	0
10	d	753	0	780	7	0
11	E	1624	0	1696	28	0
12	e	575	0	592	3	0
13	F	1643	0	1707	27	0
14	f	625	0	652	7	0
15	G	1105	0	1148	12	0
16	g	501	0	531	4	0
17	H	817	0	808	12	0
18	h	449	0	488	2	0
19	I	62271	0	31340	375	0
20	i	444	0	458	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	J	2529	0	1281	12	0
22	j	409	0	440	24	0
23	K	2093	0	2166	28	0
24	k	377	0	418	1	0
25	L	1565	0	1616	10	0
26	l	504	0	572	10	0
27	M	1552	0	1619	16	0
28	m	302	0	343	3	0
29	N	1410	0	1444	20	0
30	n	1181	0	1238	27	0
31	O	1323	0	1371	17	0
32	o	979	0	1031	8	0
33	P	1111	0	1148	53	0
34	p	1022	0	1070	48	0
35	Q	480	0	482	13	0
36	q	786	0	828	95	0
37	R	1129	0	1162	14	0
38	r	877	0	887	24	0
39	S	938	0	1012	13	0
40	t	955	0	1016	12	0
41	T	1053	0	1129	16	0
42	u	891	0	952	8	0
43	U	1075	0	1154	7	0
44	v	774	0	824	28	0
45	V	960	0	1000	5	0
46	w	710	0	728	4	0
47	W	892	0	923	87	0
48	x	649	0	666	15	0
49	X	917	0	962	7	0
50	y	648	0	691	8	0
51	Y	947	0	1019	6	0
52	z	455	0	478	8	0
53	C	89	0	0	2	0
53	I	203	0	0	2	0
53	J	5	0	0	0	0
53	K	1	0	0	0	0
53	L	2	0	0	0	0
53	M	1	0	0	0	0
53	T	1	0	0	0	0
53	V	1	0	0	0	0
53	Y	1	0	0	1	0
53	l	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	p	1	0	0	0	0
53	u	1	0	0	0	0
All	All	142151	0	95491	1341	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 6.

All (1341) 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)
36:q:7:ARG:HH11	36:q:7:ARG:CB	1.36	1.37
19:I:1636:U:OP2	53:I:3077:MG:MG	0.78	1.21
36:q:7:ARG:HH11	36:q:7:ARG:HB3	0.97	1.10
36:q:7:ARG:HB3	36:q:7:ARG:NH1	1.68	1.08
1:C:1273:A:H4'	1:C:1274:A:OP1	1.47	1.07
36:q:24:GLU:N	36:q:24:GLU:OE2	1.89	1.05
36:q:7:ARG:CB	36:q:7:ARG:NH1	2.22	1.00
19:I:1047:G:HO2'	19:I:1110:G:H1	1.07	1.00
36:q:85:ASP:OD2	36:q:89:ARG:HD3	1.62	0.99
48:x:44:SER:C	48:x:46:LYS:H	1.70	0.98
36:q:17:LEU:HD11	36:q:93:ALA:HB3	1.45	0.98
19:I:545:U:O2	19:I:549:G:N1	1.96	0.97
36:q:78:GLU:OE1	36:q:78:GLU:C	2.08	0.96
19:I:1866:A:H3'	19:I:1867:G:H4'	1.49	0.92
4:Z:51:VAL:HG23	4:Z:52:PRO:HD2	1.50	0.92
36:q:27:GLU:O	36:q:29:ALA:N	2.03	0.91
47:W:50:ALA:O	47:W:81:ARG:NH1	2.04	0.90
36:q:27:GLU:C	36:q:29:ALA:H	1.81	0.89
1:C:916:G:H21	1:C:1392:A:H8	1.17	0.89
1:C:1088:G:O2'	53:C:1625:MG:MG	1.12	0.89
1:C:1088:G:HO2'	53:C:1625:MG:MG	0.78	0.88
46:w:26:GLU:OE2	46:w:77:ARG:NH1	2.07	0.88
19:I:1032:A:C2	19:I:1034:G:H8	1.93	0.86
36:q:29:ALA:O	36:q:32:THR:N	2.08	0.86
11:E:60:PRO:HB3	36:q:94:ALA:HB1	1.55	0.86
9:D:132:LYS:HG3	9:D:136:MET:HE2	1.58	0.86
19:I:2744:G:O6	19:I:2761:A:N1	2.01	0.85
19:I:1032:A:H2	19:I:1034:G:H8	1.25	0.84
30:n:72:THR:HA	30:n:96:ARG:HH12	1.42	0.83
36:q:17:LEU:CD1	36:q:93:ALA:HB3	2.08	0.83
34:p:55:VAL:HG23	34:p:94:LEU:HD22	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:545:U:O2	19:I:549:G:N2	2.12	0.82
33:P:30:LEU:HA	33:P:35:LYS:HB2	1.61	0.82
9:D:68:LEU:HD12	9:D:154:MET:HE1	1.61	0.82
34:p:51:PRO:HG3	34:p:80:ARG:HG3	1.60	0.82
1:C:1054:U:H5'	36:q:53:ILE:HG22	1.61	0.82
13:F:13:ARG:NH2	13:F:37:ALA:O	2.12	0.82
48:x:44:SER:O	48:x:46:LYS:N	2.13	0.82
19:I:1529:G:H1	19:I:1542:U:H3	1.25	0.81
19:I:545:U:O2	19:I:549:G:C2	2.33	0.81
19:I:2305:U:O2'	29:N:133:ARG:NH1	2.14	0.80
36:q:85:ASP:OD2	36:q:89:ARG:CD	2.28	0.80
19:I:1873:G:C2	19:I:1874:C:H1'	2.16	0.80
47:W:38:GLN:HG2	47:W:51:ALA:H	1.45	0.80
47:W:41:ALA:HB2	47:W:48:LEU:HD21	1.63	0.80
48:x:44:SER:C	48:x:46:LYS:N	2.36	0.80
35:Q:63:ARG:HG3	35:Q:64:PHE:HB2	1.63	0.80
36:q:53:ILE:HD12	44:v:85:ARG:HD2	1.64	0.79
1:C:1444:G:H21	1:C:1447:A:H2	1.31	0.78
19:I:2347:C:N3	19:I:2371:G:N2	2.32	0.77
8:c:26:LYS:HE3	8:c:37:GLU:HG2	1.67	0.77
36:q:78:GLU:OE1	36:q:78:GLU:O	2.02	0.77
15:G:153:VAL:HG11	32:o:99:LEU:HD12	1.67	0.76
26:l:17:THR:HG21	26:l:49:MET:HE1	1.66	0.76
30:n:71:PRO:O	30:n:96:ARG:NH1	2.18	0.76
36:q:17:LEU:CD1	36:q:93:ALA:CB	2.63	0.76
19:I:2151:U:H2'	19:I:2152:G:H8	1.50	0.76
1:C:115:U:O2	1:C:117:C:N4	2.18	0.75
19:I:2162:G:H4'	19:I:2171:A:H2'	1.68	0.75
22:j:44:ARG:O	26:l:38:THR:OG1	2.04	0.75
15:G:103:THR:O	15:G:122:ASN:ND2	2.15	0.75
19:I:1172:C:O2	19:I:1177:G:N2	2.19	0.75
19:I:1913:A:H62	19:I:1915:3TD:H3'	1.49	0.75
1:C:1227:G:OP1	34:p:119:ARG:NH2	2.20	0.75
47:W:26:LEU:HD21	47:W:37:ALA:HB1	1.69	0.75
19:I:2100:G:H1	19:I:2189:U:H3	1.33	0.75
1:C:198:G:C6	1:C:459:A:N6	2.55	0.74
47:W:105:ALA:HA	47:W:108:ASP:HB2	1.67	0.74
36:q:7:ARG:HH11	36:q:7:ARG:CG	1.99	0.74
1:C:204:C:O2'	1:C:206:G:N7	2.19	0.74
19:I:1636:U:P	53:I:3077:MG:MG	1.69	0.74
1:C:1445:C:H1'	1:C:1446:A:H8	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:35:ARG:NH2	38:r:117:PRO:O	2.20	0.73
19:I:2166:U:O4	19:I:2170:A:N6	2.20	0.73
22:j:12:VAL:HG13	22:j:50:LYS:HB3	1.70	0.73
19:I:883:G:N1	19:I:894:U:O2	2.17	0.73
19:I:543:G:H2'	19:I:544:C:H5'	1.71	0.73
39:S:71:ARG:NH1	39:S:106:GLU:OE2	2.17	0.73
38:r:59:THR:HG22	38:r:61:PHE:H	1.54	0.73
47:W:34:HIS:O	47:W:102:ARG:NH2	2.22	0.72
19:I:1871:A:HO2'	19:I:1872:A:H8	1.37	0.72
19:I:2348:U:H5'	22:j:46:HIS:CD2	2.24	0.72
19:I:1039:A:N1	19:I:1116:G:O6	2.23	0.72
44:v:41:ARG:HE	44:v:44:ALA:N	1.87	0.72
16:g:2:LYS:N	19:I:102:U:O4	2.22	0.72
19:I:1867:G:H2'	19:I:1868:C:C5	2.24	0.72
19:I:1875:G:H21	19:I:1876:A:H62	1.38	0.72
11:E:14:ILE:HG22	11:E:15:VAL:HG13	1.72	0.72
44:v:20:TYR:O	44:v:24:ARG:N	2.21	0.72
47:W:18:LEU:HD23	47:W:25:ARG:HA	1.69	0.72
47:W:31:THR:HB	47:W:34:HIS:HB2	1.70	0.71
36:q:41:PRO:HA	36:q:72:ARG:HD2	1.72	0.71
23:K:120:VAL:HG22	33:P:91:PHE:HB3	1.72	0.71
1:C:730:C:OP1	52:z:61:ARG:NH2	2.23	0.71
19:I:2107:G:N1	19:I:2182:U:N3	2.37	0.71
9:D:13:GLY:O	9:D:15:HIS:ND1	2.23	0.71
19:I:52:A:H2	19:I:119:A:H62	1.37	0.71
46:w:14:GLU:OE2	46:w:84:ARG:NH2	2.22	0.71
9:D:13:GLY:HA3	9:D:208:ARG:HH12	1.55	0.71
9:D:114:LEU:HD12	9:D:144:LEU:HB3	1.73	0.71
36:q:17:LEU:HD13	36:q:93:ALA:CB	2.22	0.70
36:q:65:TYR:HB3	44:v:96:LEU:HD11	1.72	0.70
36:q:77:VAL:HG22	36:q:78:GLU:N	2.06	0.70
44:v:16:LEU:HG	44:v:55:SER:HB3	1.72	0.70
1:C:969:A:H4'	1:C:970:G:H5''	1.74	0.70
1:C:974:C:O2'	44:v:13:ARG:NH1	2.25	0.70
19:I:278:A:OP2	19:I:361:G:N1	2.23	0.70
19:I:2134:A:H1'	19:I:2159:G:H1'	1.72	0.70
29:N:38:MET:HE3	29:N:53:ALA:HB1	1.74	0.69
1:C:176:C:H1'	1:C:177:G:H2'	1.73	0.69
47:W:28:VAL:O	47:W:95:SER:HB2	1.92	0.69
19:I:2122:U:OP2	19:I:2169:A:O2'	2.09	0.69
1:C:874:C:OP1	40:t:9:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:896:A:OP2	19:I:897:C:N4	2.25	0.69
1:C:1444:G:H5''	1:C:1445:C:OP2	1.91	0.69
11:E:36:ASP:OD1	11:E:59:ARG:NH2	2.23	0.69
19:I:881:G:N2	19:I:895:U:O2'	2.22	0.69
19:I:1172:C:N3	19:I:1177:G:N1	2.36	0.69
19:I:1913:A:N6	19:I:1916:A:OP2	2.26	0.69
19:I:2895:G:N2	19:I:2896:C:H41	1.90	0.69
17:H:38:ARG:NH1	17:H:98:GLU:O	2.26	0.69
19:I:2291:U:OP1	19:I:2380:C:O2'	2.10	0.69
36:q:34:ALA:CB	36:q:78:GLU:HB3	2.23	0.69
34:p:62:ASP:O	34:p:63:LEU:HD22	1.93	0.68
47:W:7:ARG:HH22	47:W:8:ILE:HD13	1.57	0.68
29:N:158:THR:HG22	29:N:160:ALA:H	1.58	0.68
36:q:53:ILE:HD11	36:q:63:ASP:HB2	1.75	0.68
19:I:1649:G:O2'	45:V:106:ASP:OD2	2.08	0.68
30:n:112:GLY:HA2	30:n:119:ARG:NE	2.08	0.68
9:D:13:GLY:O	9:D:15:HIS:N	2.22	0.68
19:I:1034:G:H3'	19:I:1035:U:C6	2.29	0.68
19:I:290:U:H3	19:I:350:G:H1	0.79	0.68
19:I:1036:G:N2	19:I:1120:G:N3	2.42	0.68
36:q:13:PHE:CD1	36:q:67:ILE:HD11	2.29	0.68
28:m:2:LYS:NZ	28:m:32:LYS:O	2.26	0.67
30:n:16:PRO:HG2	34:p:43:THR:HG22	1.75	0.67
9:D:114:LEU:HB2	9:D:144:LEU:HD23	1.74	0.67
36:q:7:ARG:HH11	36:q:7:ARG:HB2	1.50	0.67
9:D:13:GLY:HA2	9:D:208:ARG:HH22	1.59	0.67
33:P:30:LEU:O	33:P:36:ALA:N	2.27	0.67
47:W:72:ALA:O	47:W:76:LYS:N	2.27	0.67
19:I:1062:G:H3'	19:I:1063:G:H8	1.60	0.67
27:M:108:ILE:HG23	41:T:1:MET:HE1	1.76	0.67
12:e:44:LYS:NZ	19:I:2331:G:OP1	2.29	0.66
22:j:37:LYS:HD3	22:j:46:HIS:HB3	1.77	0.66
36:q:85:ASP:OD2	36:q:89:ARG:NE	2.28	0.66
19:I:2168:G:O2'	19:I:2169:A:O4'	2.13	0.66
33:P:30:LEU:HA	33:P:35:LYS:CB	2.25	0.66
19:I:2306:C:N3	19:I:2307:G:N2	2.43	0.66
19:I:2348:U:H5'	22:j:46:HIS:HD2	1.59	0.66
40:t:54:ARG:HE	40:t:62:GLU:HG3	1.60	0.66
42:u:11:ASP:HA	42:u:45:ILE:HB	1.77	0.66
47:W:34:HIS:ND1	47:W:54:VAL:HG22	2.10	0.66
47:W:99:TYR:OH	47:W:111:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:K:121:ASP:HA	33:P:91:PHE:CD2	2.31	0.65
13:F:85:ASN:HB2	15:G:102:GLY:HA3	1.78	0.65
38:r:20:VAL:HG12	38:r:83:GLU:HB2	1.78	0.65
46:w:17:ARG:N	46:w:21:ASP:OD2	2.28	0.65
48:x:18:GLN:HE22	48:x:35:ARG:HH11	1.43	0.65
7:b:25:GLU:HG2	7:b:26:LYS:HD2	1.78	0.65
22:j:9:ILE:HG21	22:j:25:LYS:HE3	1.79	0.65
1:C:1486:A:HO2'	1:C:1487:A:H8	1.45	0.65
11:E:154:SER:HB3	11:E:165:THR:HG23	1.78	0.65
14:f:39:TRP:HB3	33:P:32:PRO:HA	1.77	0.65
19:I:1173:U:O2	19:I:1176:U:N3	2.19	0.65
33:P:4:ILE:HB	33:P:16:GLY:HA2	1.77	0.65
34:p:84:THR:HG23	34:p:98:LEU:HD23	1.79	0.64
47:W:43:ASN:HD21	47:W:46:GLU:HB2	1.62	0.64
19:I:2895:G:H21	19:I:2896:C:H41	1.45	0.64
34:p:28:ILE:HG12	34:p:63:LEU:HD23	1.78	0.64
19:I:547:A:N3	19:I:548:G:N2	2.45	0.64
1:C:998:A:C6	1:C:1020:G:H1'	2.32	0.64
11:E:65:ARG:HG2	11:E:100:GLN:HB3	1.79	0.64
19:I:2204:G:OP2	23:K:147:LYS:NZ	2.27	0.64
33:P:40:THR:H	33:P:43:ASN:HB3	1.62	0.64
19:I:290:U:O4	19:I:350:G:O6	2.16	0.64
1:C:73:A:H8	1:C:90:G:H21	1.46	0.64
1:C:1273:A:OP1	36:q:9:ARG:NH2	2.31	0.64
19:I:355:U:H2'	19:I:356:G:H8	1.63	0.64
19:I:1068:G:O2'	19:I:1096:A:N3	2.29	0.64
41:T:78:ARG:NH1	41:T:80:SER:OG	2.31	0.64
34:p:52:LEU:HD22	34:p:87:LEU:HD13	1.79	0.64
36:q:5:ARG:HH11	36:q:5:ARG:HG2	1.63	0.64
47:W:68:LYS:HA	47:W:102:ARG:HG2	1.80	0.64
7:b:69:ARG:NH2	7:b:74:ILE:HD13	2.13	0.63
19:I:2305:U:HO2'	29:N:133:ARG:NH1	1.95	0.63
19:I:2313:C:O4'	29:N:37:ASN:ND2	2.31	0.63
1:C:1444:G:N2	1:C:1447:A:H2	1.96	0.63
44:v:41:ARG:HE	44:v:44:ALA:H	1.44	0.63
11:E:40:ARG:NH1	44:v:92:GLU:OE1	2.32	0.63
1:C:86:C:H2'	1:C:87:C:C6	2.33	0.63
34:p:28:ILE:HG21	34:p:35:LEU:HD12	1.81	0.63
1:C:1350:A:H2'	1:C:1351:A:C8	2.33	0.63
19:I:2122:U:H2'	19:I:2123:G:H8	1.63	0.63
1:C:1310:G:N1	1:C:1313:A:OP2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:4:ILE:HG22	2:0:106:VAL:HG22	1.81	0.63
34:p:115:LYS:HB2	34:p:118:LEU:HD12	1.80	0.63
36:q:80:THR:O	36:q:83:THR:HG23	1.99	0.63
47:W:31:THR:HG1	47:W:36:TYR:HE1	1.46	0.63
19:I:1913:A:N6	19:I:1915:3TD:O5'	2.32	0.63
27:M:189:THR:HG22	27:M:191:ASP:H	1.63	0.62
47:W:90:VAL:HG21	47:W:115:LEU:HD13	1.80	0.62
9:D:35:ARG:HB3	9:D:40:ILE:HD11	1.81	0.62
1:C:1172:G:N2	1:C:1175:G:OP2	2.32	0.62
19:I:1914:C:O2'	19:I:1915:3TD:OP2	2.18	0.62
23:K:107:PRO:HD2	23:K:110:LEU:HD22	1.82	0.62
44:v:41:ARG:HD2	44:v:43:ASN:H	1.63	0.62
13:F:184:ARG:NH1	13:F:187:GLU:OE1	2.33	0.62
31:O:13:ALA:O	31:O:15:VAL:N	2.33	0.62
1:C:1445:C:H2'	1:C:1446:A:O5'	2.00	0.62
13:F:163:GLU:OE2	13:F:164:GLN:NE2	2.32	0.62
14:f:60:ASP:HB3	33:P:1:MET:HE2	1.81	0.62
19:I:2139:U:O4	19:I:2152:G:O6	2.18	0.62
21:J:113:C:O2'	47:W:47:VAL:HG11	1.99	0.62
9:D:15:HIS:HB2	9:D:40:ILE:HG23	1.81	0.62
50:y:47:HIS:HB2	50:y:71:LYS:HD3	1.82	0.62
1:C:1017:G:O6	1:C:1018:G:O6	2.18	0.61
49:X:33:VAL:HG22	49:X:38:LYS:HG2	1.82	0.61
47:W:94:ARG:NE	47:W:99:TYR:HB2	2.14	0.61
1:C:1444:G:O3'	1:C:1445:C:O4'	2.18	0.61
10:d:80:HIS:HB2	10:d:85:LYS:HB2	1.82	0.61
22:j:39:PHE:CE2	22:j:41:PRO:HA	2.35	0.61
48:x:47:GLU:C	48:x:48:GLU:HG2	2.25	0.61
19:I:2127:G:H21	19:I:2173:A:H1'	1.65	0.61
4:Z:51:VAL:HG23	4:Z:52:PRO:CD	2.26	0.61
15:G:34:THR:HG22	15:G:52:LYS:HG2	1.83	0.61
13:F:37:ALA:HA	13:F:42:GLY:HA3	1.81	0.61
19:I:2756:U:OP2	28:m:19:ARG:NH1	2.31	0.61
23:K:72:ASP:OD1	23:K:119:GLY:HA2	2.01	0.61
19:I:993:G:OP1	51:Y:50:ARG:NH1	2.33	0.61
19:I:1721:G:N2	19:I:1738:G:O2'	2.34	0.61
25:L:5:VAL:H	25:L:32:ASN:HD21	1.48	0.61
27:M:145:ASP:HB3	27:M:184:ASP:HB2	1.82	0.61
44:v:21:PHE:HE1	44:v:51:LEU:HD23	1.65	0.61
19:I:1122:G:N2	19:I:1123:C:H41	1.99	0.61
31:O:10:VAL:HA	31:O:49:THR:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:R:44:TYR:O	51:Y:64:ARG:NH2	2.32	0.61
38:r:93:ARG:NH2	38:r:112:ASP:OD1	2.34	0.61
1:C:85:U:H2'	1:C:86:C:C6	2.35	0.60
9:D:133:GLU:OE2	9:D:137:ARG:NH2	2.34	0.60
19:I:1175:A:H5'	19:I:1176:U:C6	2.36	0.60
19:I:1277:G:H5'	45:V:20:MET:HE3	1.83	0.60
1:C:1054:U:H5'	36:q:53:ILE:CG2	2.31	0.60
19:I:2144:G:N2	19:I:2147:A:H62	1.99	0.60
19:I:2751:G:OP2	31:O:3:ARG:NH1	2.35	0.60
27:M:168:ASP:OD1	27:M:169:VAL:N	2.34	0.60
19:I:1532:A:H2'	19:I:1533:C:C6	2.37	0.60
4:Z:24:LYS:HA	4:Z:94:THR:HG23	1.82	0.60
19:I:287:G:H2'	19:I:288:U:C6	2.37	0.60
33:P:60:GLU:O	33:P:64:ALA:N	2.31	0.60
9:D:23:TRP:CZ3	9:D:25:PRO:HA	2.37	0.60
1:C:2:A:N7	1:C:3:A:N6	2.49	0.60
19:I:1789:A:OP2	23:K:221:ARG:NH1	2.35	0.60
19:I:2107:G:N2	19:I:2182:U:O2	2.35	0.60
33:P:68:ARG:NH2	33:P:109:GLU:O	2.35	0.60
7:b:56:GLU:HB3	7:b:86:THR:HG23	1.83	0.60
30:n:37:SER:HA	30:n:40:GLU:HG2	1.83	0.60
1:C:538:G:OP1	13:F:56:ARG:NH2	2.34	0.59
19:I:652:U:OP1	19:I:654:A:N6	2.34	0.59
1:C:1272:U:H5'	1:C:1273:A:C8	2.37	0.59
36:q:77:VAL:CG2	36:q:78:GLU:N	2.64	0.59
23:K:41:GLY:O	23:K:43:ARG:NH1	2.36	0.59
30:n:67:GLU:OE2	30:n:70:ARG:NE	2.33	0.59
19:I:1090:A:H2'	19:I:1091:G:C8	2.38	0.59
34:p:29:VAL:HA	34:p:34:SER:HA	1.84	0.59
33:P:15:LEU:HD22	33:P:58:LEU:HD12	1.83	0.59
1:C:1300:A:N6	1:C:1325:G:O2'	2.35	0.59
19:I:1138:G:H21	37:R:108:MET:HE2	1.66	0.59
48:x:69:ASP:OD2	48:x:70:ARG:N	2.35	0.59
1:C:456:G:O2'	1:C:457:U:O5'	2.21	0.58
1:C:1017:G:C6	1:C:1018:G:O6	2.56	0.58
8:c:88:GLU:O	8:c:90:GLY:N	2.36	0.58
23:K:3:VAL:HG12	23:K:19:VAL:HG22	1.85	0.58
33:P:104:THR:HG22	33:P:110:VAL:H	1.68	0.58
1:C:656:U:O2'	1:C:830:G:OP1	2.21	0.58
1:C:961:C:OP2	1:C:962:A:O2'	2.18	0.58
30:n:40:GLU:HA	30:n:43:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:p:29:VAL:HG23	34:p:34:SER:H	1.68	0.58
36:q:6:ILE:HD12	36:q:102:LEU:HB3	1.85	0.58
36:q:80:THR:HB	36:q:82:LYS:HG2	1.85	0.58
47:W:109:ALA:O	47:W:113:ALA:N	2.33	0.58
49:X:53:ARG:H	49:X:57:SER:HB3	1.67	0.58
19:I:1105:U:H2'	19:I:1106:G:C8	2.37	0.58
19:I:2168:G:O2'	19:I:2169:A:O5'	2.20	0.58
27:M:105:LEU:HD23	27:M:200:LEU:HD21	1.86	0.58
33:P:7:ASP:HB2	33:P:35:LYS:HG2	1.86	0.58
47:W:43:ASN:OD1	47:W:44:GLY:N	2.37	0.58
2:0:11:ARG:HH22	2:0:98:LYS:HD3	1.68	0.58
15:G:24:THR:HA	15:G:29:ARG:HA	1.83	0.58
33:P:5:LEU:HD12	33:P:14:SER:O	2.04	0.58
33:P:7:ASP:CB	33:P:35:LYS:HG2	2.33	0.58
37:R:87:ALA:HB3	37:R:92:MET:HE2	1.84	0.58
1:C:740:G:H2'	1:C:741:A:C8	2.38	0.58
19:I:52:A:H2	19:I:119:A:N6	2.02	0.58
19:I:1032:A:C2	19:I:1034:G:C8	2.85	0.58
19:I:2151:U:H2'	19:I:2152:G:C8	2.36	0.58
29:N:37:ASN:OD1	29:N:38:MET:N	2.36	0.58
40:t:114:ARG:HG3	40:t:119:VAL:HB	1.84	0.58
36:q:82:LYS:H	36:q:82:LYS:NZ	2.01	0.58
44:v:21:PHE:CD1	44:v:25:ALA:HB2	2.39	0.58
1:C:319:A:C2	1:C:320:G:H2'	2.39	0.58
13:F:198:HIS:O	13:F:202:GLU:HG3	2.03	0.58
19:I:2223:G:O3'	23:K:265:LYS:NZ	2.37	0.58
19:I:2328:A:H2'	19:I:2329:U:C6	2.39	0.58
27:M:153:LEU:HG	27:M:171:ASP:HB2	1.84	0.58
36:q:33:GLY:HA2	36:q:83:THR:HG22	1.85	0.58
47:W:83:LEU:HD11	47:W:88:LYS:HB3	1.85	0.58
1:C:516:C:H41	40:t:50:ARG:NH2	2.01	0.57
47:W:114:GLY:O	47:W:116:GLN:NE2	2.37	0.57
20:i:54:VAL:HG23	20:i:55:ILE:HG12	1.85	0.57
33:P:26:ALA:HA	33:P:30:LEU:HB2	1.85	0.57
37:R:114:LEU:HG	37:R:118:MET:HE3	1.86	0.57
47:W:94:ARG:NH2	47:W:97:PHE:O	2.37	0.57
1:C:446:A:H62	1:C:474:U:H3	1.51	0.57
34:p:84:THR:HG21	34:p:103:PHE:HB3	1.86	0.57
1:C:453:U:H2'	1:C:454:A:H8	1.70	0.57
1:C:1018:G:H2'	1:C:1019:U:C6	2.39	0.57
36:q:24:GLU:OE2	36:q:24:GLU:CA	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:W:68:LYS:NZ	47:W:101:GLY:HA2	2.19	0.57
1:C:1299:G:H22	1:C:1325:G:H2'	1.70	0.57
19:I:674:G:H1'	27:M:69:ARG:HD3	1.86	0.57
38:r:31:ILE:HG12	38:r:46:THR:HG22	1.85	0.57
1:C:940:A:H2'	1:C:941:G:C8	2.39	0.57
17:H:25:TYR:O	17:H:29:ILE:HD12	2.05	0.57
19:I:1122:G:H21	19:I:1123:C:H41	1.52	0.57
1:C:176:C:N4	1:C:188:G:H22	2.02	0.57
1:C:198:G:C2	1:C:459:A:N1	2.73	0.57
52:z:41:PRO:HD2	52:z:44:ILE:HD12	1.87	0.57
1:C:1117:A:O3'	36:q:37:ARG:NH2	2.38	0.57
1:C:1441:A:H5''	1:C:1442:C:H5	1.68	0.57
1:C:1445:C:O2'	1:C:1446:A:O4'	2.21	0.57
30:n:72:THR:HA	30:n:96:ARG:NH1	2.16	0.57
36:q:29:ALA:O	36:q:33:GLY:N	2.38	0.57
36:q:77:VAL:HG22	36:q:78:GLU:H	1.70	0.57
48:x:18:GLN:NE2	48:x:35:ARG:HH11	2.01	0.57
9:D:67:ILE:H	9:D:89:GLN:NE2	2.03	0.57
19:I:4:U:H2'	19:I:5:A:H8	1.70	0.57
19:I:1118:C:C3'	19:I:1119:U:H4'	2.35	0.57
19:I:2139:U:C4	19:I:2152:G:O6	2.58	0.57
19:I:2159:G:H2'	19:I:2160:C:C2	2.40	0.57
30:n:150:ALA:HB1	38:r:59:THR:HG21	1.86	0.57
19:I:1245:G:OP1	41:T:13:LYS:NZ	2.38	0.56
19:I:1913:A:C5	19:I:1915:3TD:N1	2.65	0.56
19:I:1980:G:O2'	19:I:1982:U:OP2	2.22	0.56
29:N:56:ASP:OD2	29:N:150:ARG:NH2	2.38	0.56
1:C:1141:C:O2'	34:p:7:TYR:OH	2.19	0.56
6:3:10:GLU:OE2	6:3:14:VAL:HG13	2.05	0.56
19:I:2107:G:O6	19:I:2182:U:O4	2.23	0.56
23:K:187:ASP:CG	33:P:123:ARG:HH12	2.13	0.56
25:L:49:GLN:NE2	25:L:79:LEU:HD13	2.21	0.56
33:P:80:ILE:HD12	33:P:144:VAL:HG13	1.87	0.56
1:C:357:A:OP2	40:t:31:ARG:NH1	2.37	0.56
1:C:669:A:H1'	38:r:118:HIS:CD2	2.40	0.56
1:C:1281:A:H2'	1:C:1282:A:C8	2.39	0.56
33:P:30:LEU:HD23	33:P:35:LYS:HB3	1.87	0.56
36:q:5:ARG:HD2	36:q:75:ASP:OD1	2.05	0.56
36:q:78:GLU:OE1	36:q:80:THR:N	2.38	0.56
4:Z:55:ASP:OD1	4:Z:56:GLY:N	2.39	0.56
13:F:99:ASP:OD1	13:F:100:ASN:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:R:62:VAL:HG11	37:R:101:ILE:HD11	1.88	0.56
1:C:135:A:H1'	1:C:177:G:H22	1.70	0.56
34:p:27:LYS:HB3	34:p:62:ASP:CG	2.30	0.56
1:C:2:A:H3'	1:C:3:A:C2	2.41	0.56
13:F:187:GLU:N	13:F:190:ASP:OD2	2.36	0.56
16:g:10:SER:O	16:g:14:LEU:HD13	2.06	0.56
19:I:1:G:O2'	19:I:2:G:O4'	2.21	0.56
19:I:1715:G:O2'	19:I:1743:G:O6	2.18	0.56
23:K:120:VAL:HB	23:K:189:ARG:HH22	1.70	0.56
47:W:15:ARG:NE	47:W:95:SER:OG	2.22	0.56
1:C:456:G:O2'	1:C:457:U:H6	1.89	0.56
1:C:1445:C:H1'	1:C:1446:A:C8	2.38	0.56
19:I:277:G:H2'	19:I:361:G:C6	2.40	0.56
19:I:1070:A:H4'	19:I:1071:G:O5'	2.05	0.56
19:I:2372:U:O2'	19:I:2373:G:H5'	2.06	0.56
32:o:47:GLU:HG2	32:o:64:LYS:HB3	1.86	0.56
36:q:37:ARG:HA	36:q:37:ARG:NE	2.20	0.56
1:C:1320:U:H2'	1:C:1321:G:H8	1.71	0.56
19:I:2529:G:OP1	31:O:172:LYS:NZ	2.39	0.56
33:P:26:ALA:O	33:P:31:VAL:N	2.38	0.56
44:v:21:PHE:HD2	44:v:56:SER:HA	1.69	0.56
19:I:788:A:H1'	24:k:4:THR:HG21	1.88	0.56
37:R:31:GLU:HG2	37:R:142:ILE:HD12	1.87	0.56
47:W:17:LYS:HE3	47:W:21:LEU:HD11	1.88	0.56
47:W:29:HIS:O	47:W:36:TYR:N	2.39	0.56
21:J:9:G:O2'	47:W:44:GLY:O	2.23	0.55
41:T:73:ILE:HG23	41:T:106:GLU:H	1.70	0.55
19:I:2141:G:H2'	19:I:2142:A:C8	2.41	0.55
19:I:2379:G:O2'	19:I:2380:C:O5'	2.25	0.55
47:W:104:GLN:O	47:W:108:ASP:N	2.39	0.55
19:I:4:U:H2'	19:I:5:A:C8	2.41	0.55
22:j:39:PHE:HB2	22:j:46:HIS:CE1	2.41	0.55
36:q:54:SER:OG	36:q:55:PRO:HD2	2.05	0.55
38:r:82:LEU:HD23	38:r:100:LEU:HD21	1.89	0.55
49:X:14:LYS:HD3	49:X:77:HIS:HA	1.88	0.55
47:W:110:ALA:HA	47:W:113:ALA:HB3	1.88	0.55
19:I:1070:A:O2'	19:I:1098:A:OP2	2.23	0.55
29:N:64:LYS:HD3	35:Q:5:ILE:HD12	1.87	0.55
30:n:7:ILE:HG13	30:n:8:GLY:H	1.72	0.55
47:W:15:ARG:HG2	47:W:93:ASP:OD2	2.06	0.55
1:C:141:G:H2'	1:C:142:G:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:5:LYS:NZ	38:r:108:THR:O	2.29	0.55
13:F:15:GLU:OE2	13:F:63:ARG:NH1	2.39	0.55
19:I:544:C:H2'	19:I:545:U:C6	2.42	0.55
1:C:331:G:H2'	1:C:332:A:C8	2.42	0.55
1:C:1020:G:O6	1:C:1029:A:C6	2.60	0.55
11:E:50:ALA:HB1	11:E:76:VAL:HG22	1.88	0.55
13:F:118:VAL:HG22	13:F:123:ILE:HG13	1.88	0.55
22:j:39:PHE:HZ	22:j:44:ARG:HA	1.71	0.55
34:p:86:ALA:O	34:p:87:LEU:HB2	2.05	0.55
47:W:7:ARG:NH2	47:W:8:ILE:HD13	2.21	0.55
1:C:176:C:H42	1:C:188:G:H22	1.54	0.55
34:p:52:LEU:HB2	34:p:55:VAL:HG12	1.89	0.55
47:W:14:ALA:O	47:W:18:LEU:HD13	2.07	0.55
1:C:86:C:H2'	1:C:87:C:H6	1.71	0.55
11:E:57:ILE:HG23	11:E:64:ILE:HD11	1.89	0.55
1:C:1446:A:O2'	1:C:1447:A:O5'	2.25	0.55
10:d:62:THR:HG22	10:d:71:LYS:HD3	1.89	0.55
37:R:68:LYS:HB2	37:R:72:LYS:HG3	1.88	0.55
1:C:1322:C:H5''	42:u:28:THR:HG21	1.89	0.54
17:H:5:GLU:HB3	17:H:90:MET:HB2	1.88	0.54
19:I:878:A:H3'	19:I:879:G:H8	1.72	0.54
19:I:1118:C:H2'	19:I:1119:U:H4'	1.88	0.54
37:R:96:ARG:HD2	37:R:99:ARG:HB2	1.88	0.54
47:W:43:ASN:ND2	47:W:46:GLU:HB2	2.20	0.54
47:W:68:LYS:HG2	47:W:102:ARG:HG3	1.89	0.54
1:C:1295:U:O2'	1:C:1296:C:H5'	2.07	0.54
3:1:8:GLY:C	35:Q:64:PHE:HZ	2.15	0.54
5:2:74:ARG:O	5:2:78:ASN:ND2	2.38	0.54
32:o:48:ASP:OD1	32:o:49:PHE:N	2.38	0.54
47:W:38:GLN:HE21	47:W:50:ALA:HB1	1.71	0.54
1:C:198:G:C2	1:C:199:A:C4	2.95	0.54
19:I:882:G:O6	19:I:894:U:O4	2.25	0.54
19:I:1866:A:N7	19:I:1876:A:N6	2.55	0.54
36:q:18:ILE:O	36:q:22:THR:HG23	2.07	0.54
47:W:26:LEU:O	47:W:93:ASP:HB3	2.06	0.54
19:I:2113:U:O4	19:I:2167:U:O2'	2.26	0.54
27:M:9:GLN:N	27:M:9:GLN:OE1	2.41	0.54
19:I:2125:G:H1	19:I:2170:A:H5''	1.72	0.54
19:I:2163:A:H3'	19:I:2164:C:H5''	1.89	0.54
44:v:27:LEU:HD12	44:v:30:ILE:HD11	1.90	0.54
1:C:708:G:H2'	1:C:709:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:A:C8	38:r:118:HIS:HB3	2.43	0.54
1:C:712:A:H2	52:z:38:LYS:HE2	1.72	0.54
1:C:1244:A:H4'	34:p:70:GLY:H	1.72	0.54
19:I:882:G:N1	19:I:894:U:N3	2.55	0.54
19:I:995:C:OP2	51:Y:54:LYS:NZ	2.41	0.54
19:I:1079:C:HO2'	19:I:1080:A:H8	1.55	0.54
31:O:127:THR:HG22	31:O:128:GLN:H	1.71	0.54
44:v:13:ARG:HB3	44:v:60:GLN:HE21	1.73	0.54
50:y:5:ILE:HD11	50:y:62:ARG:HE	1.72	0.54
19:I:1064:C:H2'	19:I:1065:U:C5	2.42	0.54
52:z:37:GLY:O	52:z:63:ARG:NH2	2.41	0.54
1:C:1446:A:N3	1:C:1446:A:H3'	2.23	0.54
19:I:2745:C:O2	31:O:143:GLN:NE2	2.31	0.54
19:I:2895:G:H21	19:I:2896:C:N4	2.05	0.54
23:K:69:ARG:HH21	23:K:118:SER:HB2	1.72	0.54
23:K:135:ILE:O	23:K:167:ARG:NH2	2.41	0.54
47:W:38:GLN:HG2	47:W:51:ALA:N	2.21	0.54
3:l:50:ALA:HB1	3:l:57:HIS:HB3	1.90	0.54
22:j:43:VAL:HA	26:l:34:THR:O	2.08	0.54
36:q:64:GLN:O	44:v:99:ALA:HB3	2.08	0.54
47:W:99:TYR:HA	47:W:103:VAL:HB	1.89	0.54
1:C:181:U:H2'	1:C:182:G:H3'	1.89	0.53
9:D:20:THR:O	9:D:23:TRP:HD1	1.90	0.53
33:P:122:LEU:HD22	33:P:128:HIS:CG	2.43	0.53
36:q:7:ARG:NH1	36:q:7:ARG:CG	2.62	0.53
25:L:77:ARG:NH2	25:L:200:ASP:OD1	2.35	0.53
30:n:136:LYS:O	30:n:136:LYS:HG2	2.08	0.53
40:t:3:THR:HG22	40:t:5:ASN:H	1.73	0.53
47:W:35:ILE:HG12	47:W:106:LEU:HD12	1.89	0.53
19:I:1120:G:H2'	19:I:1121:C:O4'	2.08	0.53
19:I:1509:A:H2'	19:I:1510:G:C8	2.44	0.53
19:I:2286:G:O6	22:j:41:PRO:HG3	2.09	0.53
36:q:6:ILE:HD12	36:q:102:LEU:HD23	1.90	0.53
19:I:548:G:O2'	19:I:549:G:O4'	2.26	0.53
27:M:188:MET:HE2	27:M:193:VAL:HG22	1.90	0.53
30:n:70:ARG:NH1	30:n:97:ASN:HB3	2.23	0.53
34:p:89:GLU:CD	34:p:89:GLU:H	2.15	0.53
1:C:1445:C:H2'	1:C:1445:C:O2	2.08	0.53
13:F:13:ARG:HG2	13:F:34:ILE:HA	1.89	0.53
17:H:5:GLU:OE1	52:z:24:LYS:NZ	2.28	0.53
19:I:2119:A:N6	19:I:2167:U:O2'	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:2372:U:C2	19:I:2373:G:N7	2.76	0.53
36:q:83:THR:O	36:q:84:VAL:C	2.50	0.53
41:T:124:GLY:H	41:T:144:GLU:HA	1.73	0.53
1:C:926:C:OP1	30:n:4:ARG:NH1	2.40	0.53
1:C:1032:U:H2'	1:C:1033:C:H6	1.72	0.53
9:D:49:MET:HA	9:D:52:GLU:HG3	1.91	0.53
11:E:155:GLY:O	11:E:196:ILE:HG12	2.08	0.53
27:M:119:ILE:HD11	27:M:185:LYS:HD3	1.91	0.53
44:v:17:ALA:O	44:v:22:ALA:N	2.40	0.53
47:W:37:ALA:HB2	47:W:106:LEU:HD21	1.90	0.53
1:C:707:G:H2'	1:C:708:G:C8	2.44	0.53
1:C:712:A:H5'	38:r:119:ASN:OD1	2.09	0.53
1:C:759:G:C4	1:C:806:G:C6	2.96	0.53
19:I:1067:A:H8	19:I:1067:A:OP1	1.92	0.53
19:I:1667:G:O2'	19:I:1991:U:O4	2.21	0.53
19:I:1720:U:H2'	19:I:1721:G:O4'	2.08	0.53
19:I:2379:G:HO2'	19:I:2380:C:H6	1.55	0.53
23:K:187:ASP:OD1	33:P:123:ARG:NH1	2.41	0.53
47:W:18:LEU:HB3	47:W:25:ARG:HB3	1.89	0.53
1:C:990:A:H2'	1:C:991:U:C6	2.44	0.53
9:D:211:THR:HA	9:D:214:LEU:HD23	1.91	0.53
10:d:81:PRO:HG2	43:U:20:LEU:HD11	1.90	0.53
30:n:93:PRO:HA	30:n:96:ARG:HG2	1.89	0.53
4:Z:34:GLU:OE2	4:Z:58:VAL:HG13	2.09	0.53
25:L:16:THR:OG1	25:L:18:ASP:OD1	2.23	0.53
1:C:1255:A:N6	1:C:1268:G:H1'	2.24	0.53
3:1:63:THR:HG22	3:1:64:ASP:H	1.73	0.53
19:I:645:C:H2'	19:I:647:G:N7	2.24	0.53
47:W:38:GLN:CG	47:W:51:ALA:H	2.20	0.53
1:C:1152:C:H5	1:C:1175:G:H1	1.57	0.52
11:E:6:HIS:NE2	44:v:89:MET:SD	2.83	0.52
33:P:115:VAL:O	33:P:116:ARG:NH1	2.40	0.52
35:Q:41:HIS:HB3	35:Q:44:PHE:HD2	1.74	0.52
36:q:67:ILE:HD13	44:v:95:GLY:HA3	1.89	0.52
42:u:33:ILE:HD11	42:u:63:PHE:HE2	1.73	0.52
1:C:1035:G:H2'	1:C:1036:A:C8	2.45	0.52
19:I:848:C:H2'	19:I:849:A:H8	1.75	0.52
1:C:210:U:H2'	1:C:211:C:C6	2.44	0.52
1:C:1034:A:H2'	1:C:1035:G:C8	2.45	0.52
19:I:2134:A:H4'	19:I:2159:G:H21	1.75	0.52
27:M:190:ALA:O	27:M:194:LYS:NZ	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:A:C6	13:F:206:LYS:HB3	2.45	0.52
1:C:175:A:O2'	1:C:176:C:O2	2.27	0.52
9:D:11:LYS:HD3	9:D:12:ALA:N	2.23	0.52
11:E:6:HIS:CE1	11:E:8:ASN:HB3	2.45	0.52
19:I:784:G:H5'	19:I:785:G:OP1	2.10	0.52
19:I:1802:A:H2'	19:I:1803:A:C8	2.44	0.52
41:T:82:LEU:HD21	41:T:120:VAL:HG21	1.91	0.52
47:W:28:VAL:HG11	47:W:103:VAL:HG13	1.92	0.52
1:C:1058:G:H21	1:C:1184:G:H8	1.57	0.52
41:T:117:THR:O	41:T:117:THR:HG22	2.10	0.52
19:I:2304:G:O2'	19:I:2305:U:OP1	2.24	0.52
19:I:856:G:H2'	19:I:857:G:C8	2.44	0.52
19:I:1035:U:O2'	19:I:1036:G:H8	1.91	0.52
23:K:73:GLY:HA2	23:K:121:ASP:OD2	2.09	0.52
36:q:81:GLU:HA	36:q:84:VAL:HB	1.91	0.52
36:q:85:ASP:O	36:q:89:ARG:HG3	2.10	0.52
13:F:87:GLY:HA3	13:F:197:GLU:HG3	1.91	0.52
19:I:848:C:H2'	19:I:849:A:C8	2.45	0.52
19:I:2172:U:H3'	19:I:2173:A:H5'	1.92	0.52
39:S:105:ARG:NH2	49:X:32:VAL:HG21	2.25	0.52
1:C:72:G:H21	1:C:91:A:H62	1.58	0.51
19:I:1047:G:O2'	19:I:1110:G:N1	2.16	0.51
19:I:1532:A:H2'	19:I:1533:C:H6	1.73	0.51
19:I:2144:G:O2'	19:I:2145:C:H3'	2.10	0.51
20:i:38:HIS:ND1	20:i:39:LEU:O	2.37	0.51
30:n:142:HIS:O	30:n:144:MET:N	2.44	0.51
1:C:1271:C:O2'	1:C:1273:A:H8	1.93	0.51
17:H:1:MET:HG3	17:H:65:GLU:OE2	2.10	0.51
19:I:358:U:C2	19:I:359:G:C8	2.98	0.51
33:P:26:ALA:HA	33:P:30:LEU:HD12	1.92	0.51
36:q:85:ASP:O	36:q:86:ALA:C	2.53	0.51
26:l:54:ASP:HB3	41:T:57:LEU:HD22	1.93	0.51
30:n:15:ASP:OD1	30:n:44:TYR:OH	2.27	0.51
36:q:53:ILE:HD12	44:v:85:ARG:CD	2.38	0.51
1:C:1034:A:H2'	1:C:1035:G:H8	1.76	0.51
19:I:2788:C:H2'	19:I:2789:C:C6	2.46	0.51
34:p:83:ILE:HA	34:p:86:ALA:HB3	1.92	0.51
1:C:102:G:H5'	1:C:103:A:H5''	1.91	0.51
1:C:790:C:O3'	38:r:127:ARG:NH1	2.43	0.51
19:I:1141:U:H4'	19:I:1142:A:O4'	2.11	0.51
19:I:2316:G:H2'	19:I:2317:A:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:i:28:LEU:CD1	20:i:37:LYS:HB3	2.41	0.51
19:I:1034:G:O2'	19:I:1035:U:O5'	2.23	0.51
34:p:20:PHE:HB2	34:p:64:TYR:HB3	1.93	0.51
36:q:27:GLU:C	36:q:29:ALA:N	2.48	0.51
41:T:91:ASP:OD1	41:T:92:LEU:N	2.43	0.51
1:C:469:U:H2'	1:C:470:G:H8	1.76	0.51
19:I:299:A:N3	19:I:319:G:O2'	2.40	0.51
19:I:1087:G:N2	19:I:1103:A:N3	2.57	0.51
39:S:18:ARG:HG2	39:S:18:ARG:HH11	1.74	0.51
20:i:28:LEU:HD11	20:i:37:LYS:HD2	1.92	0.51
30:n:53:ARG:NH2	30:n:121:ALA:HB1	2.26	0.51
35:Q:28:VAL:HG11	35:Q:32:LEU:HD11	1.91	0.51
9:D:121:SER:HA	9:D:126:PHE:CD1	2.46	0.51
19:I:2636:C:O2'	25:L:45:TYR:OH	2.26	0.51
48:x:18:GLN:NE2	48:x:35:ARG:HD2	2.26	0.51
1:C:269:G:H5'	50:y:16:LYS:HD2	1.92	0.50
1:C:533:A:H2'	1:C:534:G:C8	2.46	0.50
33:P:40:THR:HG23	33:P:43:ASN:H	1.76	0.50
38:r:84:VAL:HG11	38:r:97:ILE:HD11	1.93	0.50
19:I:1057:A:H2'	19:I:1058:U:C6	2.47	0.50
33:P:135:HIS:ND1	33:P:137:GLU:HG3	2.26	0.50
36:q:22:THR:O	36:q:23:ALA:C	2.54	0.50
7:b:28:ASN:ND2	7:b:88:LYS:O	2.44	0.50
15:G:15:LEU:HD12	15:G:37:THR:HG22	1.92	0.50
19:I:2140:G:H2'	19:I:2141:G:C8	2.45	0.50
19:I:2187:U:H2'	19:I:2188:U:C6	2.46	0.50
33:P:84:ALA:HA	33:P:90:LEU:HA	1.93	0.50
36:q:85:ASP:HA	36:q:88:MET:CE	2.41	0.50
37:R:125:TYR:OH	37:R:132:HIS:NE2	2.40	0.50
1:C:487:A:H2'	1:C:488:G:O4'	2.10	0.50
1:C:512:C:H4'	1:C:513:C:O5'	2.11	0.50
19:I:2162:G:N7	19:I:2164:C:N4	2.60	0.50
19:I:2246:G:H2'	19:I:2247:A:C8	2.47	0.50
19:I:2639:A:H4'	37:R:96:ARG:NH2	2.27	0.50
1:C:470:G:H2'	1:C:471:U:C6	2.46	0.50
14:f:60:ASP:OD2	33:P:27:ARG:NH1	2.44	0.50
19:I:644:A:H2'	19:I:645:C:O4'	2.11	0.50
1:C:972:A:O2'	1:C:1316:C:H5	1.94	0.50
1:C:1026:G:C5	1:C:1027:G:H1'	2.46	0.50
19:I:878:A:H3'	19:I:879:G:C8	2.46	0.50
1:C:1212:C:H2'	1:C:1213:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:2071:A:H2'	19:I:2072:C:C6	2.47	0.50
48:x:46:LYS:HD3	48:x:48:GLU:O	2.11	0.50
1:C:453:U:H2'	1:C:454:A:C8	2.47	0.49
1:C:1286:C:H2'	1:C:1287:G:H8	1.76	0.49
8:c:93:VAL:HG22	8:c:94:ARG:H	1.76	0.49
22:j:10:LYS:O	22:j:53:LYS:N	2.25	0.49
34:p:22:LYS:O	34:p:61:LEU:N	2.45	0.49
23:K:142:HIS:ND1	23:K:193:GLY:O	2.42	0.49
1:C:646:U:O4	1:C:746:G:O2'	2.27	0.49
19:I:1073:A:H3'	19:I:1074:G:H8	1.77	0.49
19:I:2064:C:H2'	19:I:2065:C:C6	2.47	0.49
19:I:2897:U:H2'	19:I:2898:U:H6	1.77	0.49
47:W:28:VAL:HA	47:W:36:TYR:O	2.12	0.49
48:x:67:ILE:HG23	48:x:71:VAL:HG13	1.93	0.49
19:I:1075:C:H2'	19:I:1076:C:H5''	1.94	0.49
19:I:2126:A:C5	19:I:2163:A:H8	2.31	0.49
19:I:2305:U:H5''	29:N:131:GLY:HA3	1.93	0.49
33:P:30:LEU:CD2	33:P:35:LYS:HB3	2.42	0.49
1:C:1056:U:H2'	1:C:1057:C:C6	2.47	0.49
1:C:1446:A:O2'	1:C:1447:A:N3	2.44	0.49
4:Z:66:HIS:ND1	4:Z:94:THR:HG22	2.28	0.49
1:C:125:U:O2'	1:C:256:A:H8	1.96	0.49
1:C:1250:U:H1'	1:C:1252:G:C6	2.48	0.49
9:D:131:LYS:O	9:D:135:LEU:N	2.41	0.49
11:E:131:ARG:O	11:E:135:LYS:HG2	2.12	0.49
1:C:250:U:H2'	1:C:251:G:H8	1.78	0.49
9:D:67:ILE:H	9:D:89:GLN:HE21	1.61	0.49
9:D:166:ALA:HB3	9:D:191:SER:HG	1.78	0.49
11:E:114:LYS:HB2	11:E:185:ASN:HD22	1.78	0.49
11:E:156:ARG:HH11	11:E:193:TYR:HB3	1.77	0.49
29:N:36:LEU:CD1	29:N:57:LEU:HD11	2.42	0.49
47:W:24:THR:HB	47:W:90:VAL:HA	1.93	0.49
9:D:183:VAL:HG12	9:D:196:VAL:HG23	1.94	0.49
14:f:39:TRP:HB2	14:f:46:PHE:CE1	2.48	0.49
19:I:288:U:H2'	19:I:289:G:C8	2.48	0.49
19:I:613:A:O2'	19:I:614:A:H5'	2.12	0.49
19:I:2641:G:H5''	37:R:78:THR:HB	1.95	0.49
1:C:445:A:N6	1:C:474:U:O2'	2.44	0.49
1:C:549:U:H2'	1:C:550:C:C6	2.48	0.49
1:C:1350:A:H2'	1:C:1351:A:H8	1.77	0.49
9:D:66:LYS:HA	9:D:89:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:93:ASN:OD1	9:D:94:HIS:ND1	2.45	0.49
19:I:1873:G:N3	19:I:1874:C:H1'	2.27	0.49
47:W:33:ARG:HG2	47:W:65:THR:O	2.13	0.49
19:I:2119:A:O2'	19:I:2120:G:O5'	2.27	0.49
21:J:28:C:OP1	47:W:34:HIS:CD2	2.65	0.49
35:Q:16:CYS:SG	35:Q:17:SER:N	2.86	0.49
36:q:6:ILE:CD1	36:q:102:LEU:HB3	2.43	0.49
38:r:64:GLN:HG2	38:r:99:ALA:HB2	1.95	0.49
1:C:533:A:H2'	1:C:534:G:H8	1.77	0.48
31:O:42:GLU:OE1	31:O:55:ARG:NH2	2.46	0.48
36:q:71:LEU:O	36:q:72:ARG:HD3	2.12	0.48
1:C:83:G:H2'	1:C:84:C:C6	2.48	0.48
1:C:1245:A:H2'	1:C:1246:A:C8	2.47	0.48
5:2:29:ARG:O	5:2:33:LYS:HG3	2.13	0.48
19:I:2804:U:H2'	19:I:2805:C:C6	2.48	0.48
19:I:2897:U:H2'	19:I:2898:U:C6	2.48	0.48
47:W:7:ARG:HD2	47:W:97:PHE:CE1	2.48	0.48
47:W:68:LYS:HZ3	47:W:101:GLY:HA2	1.77	0.48
9:D:76:ALA:O	9:D:80:VAL:HG23	2.13	0.48
19:I:2379:G:N3	19:I:2380:C:C6	2.80	0.48
21:J:42:C:C5	29:N:66:LEU:HD22	2.48	0.48
36:q:35:GLN:HG2	36:q:77:VAL:HG13	1.95	0.48
5:2:44:LYS:HE3	5:2:86:LEU:HB3	1.95	0.48
19:I:1494:A:H2'	19:I:1495:A:C8	2.49	0.48
19:I:2147:A:N7	19:I:2148:G:H1'	2.28	0.48
19:I:2845:U:H5''	49:X:52:ASN:O	2.12	0.48
34:p:33:ARG:O	34:p:33:ARG:HG2	2.13	0.48
36:q:35:GLN:HG2	36:q:35:GLN:O	2.13	0.48
44:v:41:ARG:NE	44:v:43:ASN:HB3	2.28	0.48
50:y:48:ASP:HA	50:y:75:LEU:HD22	1.94	0.48
21:J:106:G:H2'	21:J:107:G:O4'	2.13	0.48
13:F:145:ILE:HD11	13:F:178:MET:SD	2.53	0.48
19:I:1035:U:OP2	19:I:1035:U:H3'	2.13	0.48
36:q:10:LEU:HD11	36:q:98:VAL:HG23	1.96	0.48
36:q:10:LEU:CD1	36:q:98:VAL:HG23	2.44	0.48
12:e:44:LYS:NZ	19:I:2330:G:O3'	2.45	0.48
19:I:1034:G:O3'	19:I:1035:U:H2'	2.13	0.48
19:I:1913:A:H2'	19:I:1914:C:H2'	1.94	0.48
19:I:2153:C:H2'	19:I:2154:A:C8	2.48	0.48
34:p:118:LEU:HB3	34:p:123:ARG:O	2.13	0.48
41:T:73:ILE:CG2	41:T:106:GLU:H	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:A:H2'	1:C:188:G:C8	2.48	0.48
1:C:893:C:O2'	1:C:894:A:OP1	2.27	0.48
19:I:1118:C:C2'	19:I:1119:U:H4'	2.43	0.48
4:Z:1:MET:HA	4:Z:43:ASN:HA	1.96	0.48
13:F:104:ARG:HG3	13:F:168:PRO:HG3	1.95	0.48
35:Q:35:ASP:OD2	42:u:3:ARG:NH1	2.47	0.48
7:b:56:GLU:HG3	7:b:57:VAL:HG23	1.96	0.48
22:j:43:VAL:HG12	26:l:34:THR:OG1	2.14	0.48
9:D:188:ASP:CG	9:D:189:THR:H	2.22	0.47
19:I:1529:G:O6	19:I:1542:U:O4	2.32	0.47
19:I:1800:C:OP2	23:K:182:ARG:NH2	2.45	0.47
19:I:2327:A:H2'	19:I:2328:A:C8	2.49	0.47
21:J:28:C:OP1	47:W:34:HIS:NE2	2.47	0.47
1:C:407:G:H5''	1:C:408:A:H5'	1.97	0.47
3:1:14:HIS:O	3:1:18:LYS:HG2	2.13	0.47
19:I:1062:G:H3'	19:I:1063:G:C8	2.46	0.47
33:P:3:VAL:HG12	33:P:38:PRO:HA	1.95	0.47
1:C:745:U:H2'	1:C:746:G:O4'	2.15	0.47
3:1:22:ALA:HB1	3:1:27:ASP:HB3	1.95	0.47
9:D:166:ALA:HB3	9:D:191:SER:OG	2.13	0.47
11:E:49:LYS:O	11:E:72:ARG:NH2	2.47	0.47
17:H:43:GLY:HA2	17:H:58:HIS:CD2	2.49	0.47
19:I:45:G:H5'	19:I:46:G:OP1	2.14	0.47
19:I:1248:G:OP1	27:M:44:ARG:NH1	2.40	0.47
29:N:162:SER:OG	29:N:165:GLU:HG3	2.14	0.47
40:t:33:VAL:HG22	40:t:79:VAL:HG12	1.95	0.47
45:V:58:ASP:HB2	45:V:80:PHE:CE1	2.49	0.47
19:I:1105:U:H2'	19:I:1106:G:H8	1.80	0.47
22:j:43:VAL:HG23	22:j:45:GLN:N	2.29	0.47
27:M:97:ASN:HB3	27:M:100:MET:HG2	1.95	0.47
34:p:34:SER:OG	34:p:35:LEU:N	2.45	0.47
47:W:28:VAL:HG13	47:W:106:LEU:HD13	1.96	0.47
48:x:46:LYS:HD3	48:x:48:GLU:H	1.79	0.47
19:I:277:G:H2'	19:I:361:G:C5	2.49	0.47
19:I:2345:G:H21	19:I:2381:A:C2'	2.28	0.47
33:P:5:LEU:HD23	33:P:30:LEU:HD13	1.96	0.47
34:p:87:LEU:O	34:p:87:LEU:HD23	2.15	0.47
36:q:44:THR:HG23	36:q:69:THR:O	2.13	0.47
46:w:53:ARG:O	46:w:57:LEU:HG	2.15	0.47
1:C:204:C:OP2	1:C:205:G:N2	2.48	0.47
1:C:384:U:H2'	1:C:385:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1247:G:H2'	1:C:1248:G:H8	1.78	0.47
1:C:1270:G:H2'	1:C:1271:C:O4'	2.15	0.47
11:E:60:PRO:HB3	36:q:94:ALA:CB	2.36	0.47
13:F:28:ILE:HD12	13:F:30:THR:OG1	2.15	0.47
19:I:1086:A:H5''	19:I:1103:A:H2	1.78	0.47
19:I:1119:U:O2	19:I:1120:G:C8	2.68	0.47
22:j:13:SER:HB2	22:j:49:TYR:CZ	2.50	0.47
40:t:42:PRO:HB3	40:t:89:ASP:OD1	2.14	0.47
43:U:1:MET:HE1	43:U:44:ARG:HA	1.96	0.47
1:C:326:G:C2	1:C:327:U:C6	3.02	0.47
13:F:172:GLU:HB2	13:F:183:LYS:HE2	1.97	0.47
14:f:10:LYS:NZ	19:I:397:U:OP2	2.45	0.47
18:h:4:THR:HG23	18:h:37:GLU:OE2	2.14	0.47
19:I:155:A:H2'	19:I:156:A:H8	1.78	0.47
19:I:544:C:O2'	19:I:545:U:O4'	2.32	0.47
19:I:859:G:O2'	19:I:916:G:O6	2.27	0.47
19:I:1092:C:H2'	19:I:1093:G:O4'	2.15	0.47
19:I:1486:U:H2'	19:I:1487:U:C6	2.50	0.47
19:I:1746:A:H2'	19:I:1747:U:C6	2.50	0.47
21:J:66:A:H61	21:J:107:G:H2'	1.79	0.47
23:K:121:ASP:HA	33:P:91:PHE:CE2	2.50	0.47
33:P:137:GLU:CD	33:P:138:VAL:HG13	2.40	0.47
34:p:9:THR:O	34:p:85:ARG:HD2	2.15	0.47
44:v:31:ILE:HG23	44:v:45:VAL:HG21	1.97	0.47
50:y:75:LEU:H	50:y:75:LEU:HD23	1.78	0.47
1:C:951:U:H4'	3:1:79:THR:HG23	1.97	0.47
6:3:11:PRO:HG2	6:3:14:VAL:HG12	1.97	0.47
19:I:479:A:N3	19:I:481:G:H5''	2.30	0.47
19:I:882:G:H21	19:I:896:A:N6	2.13	0.47
30:n:53:ARG:HH22	30:n:121:ALA:HB1	1.80	0.47
40:t:81:LEU:O	40:t:98:VAL:HG12	2.15	0.47
36:q:29:ALA:O	36:q:31:ARG:N	2.48	0.47
36:q:29:ALA:C	36:q:31:ARG:N	2.69	0.47
47:W:11:ALA:HA	47:W:95:SER:C	2.40	0.47
1:C:1250:U:H1'	1:C:1252:G:C5	2.49	0.47
7:b:47:VAL:HG13	7:b:55:VAL:HG21	1.96	0.47
10:d:77:VAL:HG21	10:d:86:LEU:HD22	1.96	0.47
17:H:9:MET:HB2	17:H:85:ILE:O	2.15	0.47
19:I:155:A:H2'	19:I:156:A:C8	2.50	0.47
19:I:1198:U:H2'	19:I:1199:U:C6	2.49	0.47
34:p:52:LEU:HB2	34:p:55:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:r:117:PRO:HB2	38:r:119:ASN:O	2.15	0.47
1:C:84:C:H2'	1:C:85:U:C6	2.50	0.46
6:3:3:VAL:HG23	38:r:111:THR:HG22	1.97	0.46
8:c:54:GLN:CB	8:c:55:PRO:HD3	2.45	0.46
9:D:168:HIS:ND1	9:D:169:GLU:OE2	2.42	0.46
19:I:2377:A:H3'	19:I:2378:A:C8	2.50	0.46
19:I:2547:A:H2'	19:I:2548:U:C6	2.50	0.46
15:G:150:PRO:HA	15:G:153:VAL:HG12	1.96	0.46
19:I:1176:U:H2'	19:I:1177:G:H8	1.80	0.46
19:I:2134:A:H4'	19:I:2159:G:N2	2.31	0.46
19:I:2380:C:C4	19:I:2381:A:H1'	2.50	0.46
31:O:19:ILE:O	31:O:19:ILE:HG22	2.15	0.46
47:W:34:HIS:CE1	47:W:54:VAL:HG22	2.50	0.46
1:C:1244:A:H2'	1:C:1245:A:C8	2.51	0.46
19:I:1736:U:H2'	19:I:1737:G:C8	2.50	0.46
34:p:6:TYR:O	34:p:7:TYR:HB2	2.15	0.46
36:q:17:LEU:HD11	36:q:96:VAL:HG12	1.97	0.46
1:C:471:U:H2'	1:C:472:U:C6	2.50	0.46
1:C:1032:U:H2'	1:C:1033:C:C6	2.50	0.46
19:I:1386:C:H2'	19:I:1387:A:C8	2.51	0.46
19:I:1867:G:H2'	19:I:1868:C:H5	1.79	0.46
19:I:2720:U:OP1	49:X:53:ARG:NH2	2.48	0.46
22:j:39:PHE:HB2	22:j:46:HIS:HE1	1.81	0.46
31:O:13:ALA:O	31:O:15:VAL:HG12	2.16	0.46
33:P:117:LEU:HD13	33:P:121:VAL:HG22	1.98	0.46
34:p:80:ARG:O	34:p:84:THR:OG1	2.21	0.46
19:I:871:U:H2'	19:I:872:U:C6	2.50	0.46
19:I:1021:A:O2'	19:I:1123:C:OP1	2.24	0.46
22:j:9:ILE:N	22:j:23:THR:O	2.33	0.46
36:q:59:LYS:HG3	36:q:59:LYS:O	2.14	0.46
45:V:20:MET:HE2	45:V:40:LYS:HD3	1.97	0.46
1:C:182:G:H1'	1:C:183:A:C2	2.49	0.46
1:C:1115:U:H2'	1:C:1116:U:C6	2.51	0.46
1:C:1445:C:C1'	1:C:1446:A:H8	2.23	0.46
39:S:104:THR:HG22	39:S:106:GLU:OE1	2.14	0.46
1:C:574:C:H2'	1:C:575:G:O4'	2.16	0.46
1:C:668:G:H2'	1:C:669:A:H8	1.81	0.46
1:C:1341:G:H4'	1:C:1342:U:O5'	2.15	0.46
3:1:9:PRO:HB3	35:Q:64:PHE:HE2	1.80	0.46
19:I:1034:G:H4'	19:I:1035:U:OP1	2.16	0.46
19:I:1079:C:O2'	19:I:1080:A:H8	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:1120:G:C2	19:I:1121:C:C2	3.04	0.46
19:I:1867:G:H2'	19:I:1867:G:N3	2.31	0.46
34:p:39:PHE:O	34:p:45:ARG:NH2	2.48	0.46
36:q:18:ILE:HG23	36:q:19:ASP:N	2.30	0.46
47:W:31:THR:OG1	47:W:36:TYR:HE1	1.98	0.46
1:C:210:U:H2'	1:C:211:C:H6	1.80	0.46
1:C:315:A:N6	1:C:323:A:OP2	2.49	0.46
1:C:319:A:C5	1:C:320:G:C6	3.04	0.46
1:C:378:G:H2'	1:C:379:C:C6	2.51	0.46
1:C:976:U:H4'	1:C:977:A:O5'	2.16	0.46
1:C:1049:A:O2'	11:E:156:ARG:NH2	2.39	0.46
3:1:7:LYS:HD2	3:1:8:GLY:O	2.15	0.46
19:I:1482:G:O6	19:I:1508:A:N6	2.49	0.46
19:I:2323:G:H21	19:I:2324:U:C1'	2.28	0.46
19:I:2377:A:H3'	19:I:2378:A:H8	1.81	0.46
19:I:2472:G:H21	19:I:2478:A:H62	1.62	0.46
27:M:130:LYS:HA	27:M:130:LYS:HD2	1.85	0.46
33:P:5:LEU:HB2	33:P:16:GLY:H	1.81	0.46
39:S:109:SER:O	39:S:113:MET:HG2	2.15	0.46
9:D:117:LEU:HD22	9:D:141:LEU:HD13	1.97	0.46
15:G:25:VAL:HG22	15:G:26:LYS:H	1.81	0.46
19:I:1097:U:H3'	19:I:1098:A:H8	1.81	0.46
19:I:1182:G:H2'	19:I:1183:U:O4'	2.15	0.46
21:J:51:G:OP2	47:W:63:LYS:NZ	2.35	0.46
29:N:40:VAL:HG23	29:N:41:GLY:H	1.81	0.46
34:p:41:ARG:NH1	34:p:43:THR:OG1	2.49	0.46
34:p:94:LEU:HD23	34:p:97:GLU:OE1	2.16	0.46
36:q:33:GLY:HA2	36:q:83:THR:CG2	2.46	0.46
39:S:5:GLN:HA	39:S:20:MET:HE3	1.97	0.46
1:C:94:C:O2'	1:C:95:A:N7	2.44	0.46
1:C:940:A:H2'	1:C:941:G:H8	1.79	0.46
7:b:47:VAL:HG23	7:b:51:PHE:HD2	1.80	0.46
19:I:172:A:H2'	19:I:173:A:H8	1.81	0.46
19:I:880:G:N3	19:I:880:G:H2'	2.31	0.46
19:I:2126:A:N6	19:I:2171:A:OP2	2.49	0.46
36:q:7:ARG:HD2	36:q:75:ASP:OD2	2.16	0.46
48:x:19:VAL:HG12	48:x:37:GLY:C	2.41	0.46
1:C:1124:A:H61	1:C:1138:G:H1'	1.82	0.45
19:I:287:G:H2'	19:I:288:U:H6	1.79	0.45
19:I:703:U:H2'	19:I:704:G:O4'	2.17	0.45
34:p:52:LEU:HD11	34:p:57:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1445:C:O2	1:C:1445:C:C2'	2.64	0.45
8:c:54:GLN:HB2	8:c:55:PRO:HD3	1.98	0.45
17:H:69:GLU:O	17:H:73:GLU:OE1	2.34	0.45
19:I:878:A:N6	19:I:899:A:O2'	2.49	0.45
19:I:1032:A:H2	19:I:1034:G:C8	2.17	0.45
19:I:1534:U:H5''	19:I:1535:A:OP1	2.15	0.45
19:I:1819:A:H4'	19:I:1820:U:H5''	1.98	0.45
29:N:113:ASP:OD1	42:u:71:ARG:NH2	2.50	0.45
36:q:88:MET:HE3	36:q:88:MET:HB3	1.71	0.45
47:W:108:ASP:OD1	47:W:111:ARG:NE	2.44	0.45
48:x:52:LEU:O	48:x:54:LEU:N	2.50	0.45
1:C:198:G:C6	1:C:459:A:C6	3.04	0.45
1:C:365:A:H2'	1:C:366:C:O4'	2.17	0.45
1:C:1130:U:H3'	1:C:1131:C:H6	1.81	0.45
25:L:49:GLN:HE21	25:L:79:LEU:HD13	1.80	0.45
1:C:1118:G:O2'	1:C:1121:A:N6	2.49	0.45
9:D:161:LEU:HD13	9:D:176:ALA:HB2	1.98	0.45
19:I:1179:G:H3'	19:I:1180:U:C5'	2.46	0.45
29:N:40:VAL:HG23	29:N:41:GLY:N	2.32	0.45
1:C:1022:C:H2'	1:C:1023:U:O4'	2.16	0.45
16:g:58:ASN:ND2	19:I:112:U:H5'	2.31	0.45
19:I:827:U:O2'	19:I:2068:U:C2	2.70	0.45
23:K:8:PRO:HB3	23:K:14:ARG:HG3	1.98	0.45
36:q:65:TYR:CB	44:v:96:LEU:HD11	2.42	0.45
41:T:77:ILE:HD11	41:T:108:ALA:HB1	1.97	0.45
47:W:30:ARG:HA	47:W:35:ILE:HA	1.98	0.45
1:C:73:A:N6	1:C:90:G:H4'	2.32	0.45
19:I:1138:G:N2	37:R:108:MET:HE2	2.32	0.45
19:I:1484:U:H2'	19:I:1485:U:H6	1.82	0.45
20:i:9:THR:HG22	20:i:12:LYS:HG2	1.98	0.45
21:J:28:C:H2'	21:J:29:A:C8	2.52	0.45
36:q:30:LYS:HB3	36:q:30:LYS:HE2	1.65	0.45
47:W:38:GLN:HG2	47:W:50:ALA:HB1	1.98	0.45
1:C:1385:U:H2'	1:C:1386:G:C8	2.51	0.45
1:C:1486:A:O2'	1:C:1487:A:H8	1.97	0.45
19:I:1065:U:O2'	19:I:1066:U:O4'	2.35	0.45
19:I:2163:A:N3	19:I:2163:A:H2'	2.32	0.45
33:P:30:LEU:HB3	33:P:36:ALA:CB	2.47	0.45
34:p:22:LYS:HB2	34:p:61:LEU:HD22	1.98	0.45
39:S:5:GLN:HA	39:S:20:MET:CE	2.46	0.45
1:C:1003:U:H5'	1:C:1004:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1371:A:C5	30:n:7:ILE:HD13	2.52	0.45
9:D:79:ALA:HB1	9:D:214:LEU:HD21	1.97	0.45
19:I:278:A:N3	19:I:278:A:H2'	2.32	0.45
19:I:2380:C:OP1	47:W:17:LYS:HE2	2.17	0.45
19:I:2591:C:H2'	19:I:2592:G:C8	2.51	0.45
43:U:41:LEU:HD11	43:U:124:LEU:HD22	1.98	0.45
47:W:41:ALA:HB3	47:W:43:ASN:ND2	2.31	0.45
50:y:60:GLU:OE2	50:y:77:ARG:HG2	2.16	0.45
1:C:836:U:H2'	1:C:837:U:H5''	1.98	0.45
1:C:1445:C:C1'	1:C:1446:A:C8	2.99	0.45
5:2:70:ASN:O	5:2:74:ARG:HG3	2.17	0.45
6:3:5:LYS:O	6:3:18:ARG:NH2	2.49	0.45
7:b:89:GLU:OE2	7:b:89:GLU:N	2.50	0.45
9:D:13:GLY:H	9:D:15:HIS:HE1	1.64	0.45
9:D:171:ILE:O	9:D:175:GLU:HG3	2.17	0.45
19:I:2123:G:H2'	19:I:2124:G:H8	1.81	0.45
19:I:2161:C:H2'	19:I:2162:G:C8	2.52	0.45
19:I:2198:A:N3	33:P:29:PHE:HB2	2.32	0.45
23:K:77:VAL:HG12	23:K:115:GLN:OE1	2.17	0.45
31:O:160:LYS:HB3	31:O:160:LYS:HE3	1.83	0.45
39:S:20:MET:SD	39:S:44:LYS:HE3	2.56	0.45
1:C:1444:G:H3'	1:C:1445:C:H6	1.81	0.45
2:0:11:ARG:NH1	2:0:82:MET:HE2	2.32	0.45
9:D:13:GLY:C	9:D:15:HIS:H	2.16	0.45
19:I:973:A:H5'	19:I:1188:U:H1'	1.99	0.45
19:I:1869:G:N2	19:I:1873:G:N3	2.65	0.45
19:I:2148:G:H2'	19:I:2149:U:C6	2.52	0.45
19:I:2373:G:H2'	19:I:2374:C:C6	2.52	0.45
31:O:133:LEU:HB3	31:O:141:ILE:HD11	1.99	0.45
36:q:37:ARG:NE	36:q:37:ARG:CA	2.79	0.45
36:q:85:ASP:CG	36:q:86:ALA:N	2.75	0.45
42:u:33:ILE:HD11	42:u:63:PHE:CE2	2.50	0.45
13:F:124:MET:SD	13:F:146:ARG:HG2	2.58	0.44
19:I:1056:G:H4'	19:I:1085:A:H2	1.82	0.44
19:I:2379:G:O2'	19:I:2380:C:H6	2.00	0.44
20:i:28:LEU:HD13	20:i:37:LYS:HB3	1.99	0.44
22:j:44:ARG:HE	26:l:37:ALA:HA	1.82	0.44
34:p:112:GLU:OE1	34:p:121:ALA:HB1	2.17	0.44
39:S:79:PHE:CD2	49:X:70:VAL:HG12	2.51	0.44
47:W:7:ARG:O	47:W:10:ARG:N	2.49	0.44
1:C:1416:G:H5''	39:S:48:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:63:ILE:HD11	10:d:72:VAL:HG21	1.98	0.44
36:q:31:ARG:HE	36:q:31:ARG:HB3	1.52	0.44
1:C:41:G:H2'	1:C:42:G:H8	1.83	0.44
1:C:72:G:N2	1:C:90:G:O2'	2.43	0.44
1:C:1471:U:H2'	1:C:1472:C:C6	2.52	0.44
13:F:114:ALA:O	13:F:118:VAL:HG23	2.18	0.44
19:I:2102:G:H3'	19:I:2103:C:C6	2.52	0.44
19:I:2306:C:H5'	29:N:133:ARG:HH12	1.82	0.44
19:I:2898:U:H2'	19:I:2899:A:C8	2.52	0.44
47:W:7:ARG:HH21	47:W:11:ALA:HB2	1.83	0.44
47:W:94:ARG:CD	47:W:99:TYR:HB2	2.47	0.44
6:3:20:LYS:O	6:3:24:GLU:HG2	2.18	0.44
11:E:21:THR:HG23	11:E:58:GLU:OE1	2.16	0.44
19:I:1913:A:N6	19:I:1915:3TD:H3'	2.26	0.44
19:I:2896:C:H2'	19:I:2897:U:H5'	1.98	0.44
33:P:6:LEU:H	33:P:35:LYS:C	2.26	0.44
34:p:8:GLY:HA3	34:p:19:VAL:HB	1.99	0.44
43:U:75:GLU:HB2	43:U:90:GLU:HG3	2.00	0.44
1:C:630:U:H5'	50:y:6:ARG:HH21	1.82	0.44
1:C:672:U:H2'	1:C:673:U:C6	2.51	0.44
1:C:925:C:O3'	30:n:4:ARG:NH1	2.50	0.44
3:1:63:THR:HG22	3:1:64:ASP:N	2.33	0.44
19:I:1682:G:H2'	19:I:1683:U:C6	2.53	0.44
19:I:2163:A:H5''	19:I:2170:A:O2'	2.16	0.44
47:W:29:HIS:HB3	47:W:36:TYR:CD1	2.52	0.44
1:C:72:G:H2'	1:C:90:G:N2	2.33	0.44
1:C:198:G:N2	1:C:199:A:N3	2.65	0.44
1:C:651:U:H2'	1:C:652:A:H8	1.83	0.44
1:C:1268:G:O2'	1:C:1269:A:H8	2.00	0.44
1:C:1324:U:H2'	1:C:1325:G:O4'	2.18	0.44
1:C:1447:A:H2'	1:C:1448:G:O4'	2.18	0.44
19:I:1508:A:H1'	19:I:1509:A:C8	2.52	0.44
19:I:2804:U:H2'	19:I:2805:C:H6	1.81	0.44
36:q:28:THR:O	36:q:28:THR:HG22	2.18	0.44
36:q:86:ALA:O	36:q:87:LEU:C	2.60	0.44
47:W:52:SER:O	47:W:58:ILE:HD13	2.18	0.44
3:1:45:ILE:HD12	3:1:45:ILE:H	1.83	0.44
11:E:144:LEU:O	11:E:144:LEU:HD23	2.17	0.44
19:I:2128:G:H2'	19:I:2129:C:C6	2.52	0.44
19:I:2344:U:H5''	19:I:2373:G:H4'	1.99	0.44
19:I:2813:A:H2'	19:I:2814:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:p:36:GLU:OE2	34:p:45:ARG:NE	2.51	0.44
39:S:38:ILE:HD11	39:S:112:PHE:HZ	1.82	0.44
47:W:30:ARG:HB3	47:W:97:PHE:CG	2.53	0.44
1:C:1020:G:C5	1:C:1021:C:C5	3.06	0.44
1:C:1032:U:C2	1:C:1033:C:C5	3.06	0.44
1:C:1445:C:C2'	1:C:1446:A:C8	3.01	0.44
9:D:104:TRP:HE1	9:D:108:ARG:NH2	2.16	0.44
13:F:121:LYS:HG2	13:F:131:ASN:OD1	2.18	0.44
19:I:414:C:H2'	19:I:415:A:C8	2.53	0.44
19:I:2896:C:C3'	19:I:2897:U:H5'	2.48	0.44
32:o:11:LEU:HD22	32:o:75:ILE:HD11	1.98	0.44
36:q:45:ARG:HG3	36:q:46:LYS:N	2.32	0.44
44:v:18:ASP:HA	44:v:22:ALA:HB2	2.00	0.44
47:W:83:LEU:CD1	47:W:88:LYS:HB3	2.47	0.44
47:W:94:ARG:HD2	47:W:99:TYR:HB2	1.99	0.44
19:I:882:G:H1	19:I:895:U:H1'	1.82	0.44
19:I:2126:A:N3	19:I:2127:G:H1'	2.33	0.44
19:I:2514:U:H2'	19:I:2515:C:C6	2.53	0.44
30:n:132:GLY:O	30:n:134:ALA:N	2.50	0.44
32:o:77:ARG:NE	32:o:79:SER:O	2.51	0.44
34:p:93:SER:C	34:p:94:LEU:HD12	2.43	0.44
35:Q:35:ASP:OD1	35:Q:36:VAL:N	2.50	0.44
38:r:79:ILE:HB	38:r:105:PHE:HE1	1.83	0.44
1:C:1004:C:H2'	1:C:1005:C:C6	2.53	0.43
15:G:115:LEU:HD13	15:G:123:VAL:HG11	2.00	0.43
19:I:593:U:H2'	19:I:594:U:C6	2.54	0.43
36:q:27:GLU:OE2	36:q:31:ARG:HB2	2.18	0.43
43:U:1:MET:HE1	43:U:44:ARG:HD3	2.00	0.43
1:C:331:G:H2'	1:C:332:A:H8	1.82	0.43
1:C:939:G:C2	1:C:940:A:C8	3.06	0.43
13:F:35:GLU:HG2	13:F:36:GLN:HG3	2.00	0.43
19:I:2155:U:H3'	19:I:2156:G:C8	2.54	0.43
34:p:27:LYS:HB3	34:p:62:ASP:OD2	2.19	0.43
36:q:82:LYS:H	36:q:82:LYS:CE	2.31	0.43
36:q:85:ASP:HA	36:q:88:MET:HE1	2.01	0.43
1:C:1049:A:C2'	11:E:156:ARG:HH21	2.30	0.43
7:b:67:VAL:CG1	7:b:74:ILE:HD11	2.48	0.43
18:h:25:LEU:HD21	19:I:930:G:H1'	2.00	0.43
19:I:2152:G:O2'	19:I:2153:C:O4'	2.36	0.43
27:M:121:VAL:O	27:M:189:THR:HA	2.17	0.43
33:P:5:LEU:O	33:P:15:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:P:97:ARG:NE	33:P:112:LYS:HD3	2.33	0.43
38:r:113:VAL:O	38:r:113:VAL:HG12	2.18	0.43
19:I:276:U:O3'	19:I:277:G:H4'	2.18	0.43
21:J:13:G:O2'	21:J:15:A:OP2	2.30	0.43
31:O:38:ASN:OD1	31:O:39:ASP:N	2.51	0.43
31:O:52:PHE:CD1	31:O:69:ARG:HG2	2.53	0.43
38:r:84:VAL:HG11	38:r:97:ILE:CD1	2.49	0.43
44:v:43:ASN:HA	44:v:46:LEU:HB3	1.99	0.43
47:W:11:ALA:HA	47:W:96:GLY:N	2.33	0.43
1:C:1075:G:H21	15:G:52:LYS:HE2	1.83	0.43
1:C:1144:U:O4	1:C:1145:A:N6	2.52	0.43
19:I:279:A:N6	19:I:361:G:H1'	2.34	0.43
19:I:1084:A:H2'	19:I:1085:A:C8	2.54	0.43
19:I:2133:G:H2'	19:I:2157:G:N1	2.34	0.43
19:I:2755:C:H3'	28:m:19:ARG:NH1	2.33	0.43
31:O:127:THR:HG22	31:O:128:GLN:N	2.34	0.43
1:C:668:G:H2'	1:C:669:A:C8	2.54	0.43
1:C:1299:G:HO2'	1:C:1300:A:H8	1.65	0.43
1:C:1440:A:HO2'	1:C:1441:A:P	2.41	0.43
19:I:1064:C:H2'	19:I:1065:U:C6	2.54	0.43
23:K:227:PRO:HA	23:K:233:GLY:HA2	2.00	0.43
38:r:52:PHE:O	38:r:53:ARG:HD2	2.17	0.43
41:T:10:GLU:H	41:T:10:GLU:CD	2.27	0.43
47:W:30:ARG:HB3	47:W:97:PHE:CD1	2.53	0.43
47:W:56:LYS:HD2	47:W:60:GLU:HB3	1.99	0.43
51:Y:30:ARG:HG3	53:Y:201:MG:MG	1.44	0.43
17:H:88:MET:HE2	17:H:90:MET:CE	2.49	0.43
19:I:500:G:N1	19:I:503:A:OP2	2.46	0.43
19:I:1120:G:N1	19:I:1121:C:C2	2.87	0.43
19:I:1509:A:O2'	19:I:1510:G:O4'	2.36	0.43
19:I:1538:G:H2'	19:I:1539:U:C6	2.54	0.43
25:L:28:GLU:O	25:L:28:GLU:HG3	2.18	0.43
29:N:123:ASP:OD1	29:N:123:ASP:N	2.44	0.43
30:n:93:PRO:HA	30:n:96:ARG:CG	2.49	0.43
31:O:126:PRO:O	31:O:127:THR:OG1	2.31	0.43
33:P:31:VAL:HA	33:P:36:ALA:O	2.18	0.43
33:P:100:ALA:HB3	33:P:112:LYS:HG2	2.00	0.43
15:G:108:GLY:O	15:G:112:ARG:HG3	2.19	0.43
19:I:918:A:O2'	19:I:919:U:O5'	2.36	0.43
19:I:2813:A:H2'	19:I:2814:A:H8	1.83	0.43
26:l:31:HIS:ND1	26:l:32:ILE:HG13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:l:32:ILE:O	26:l:32:ILE:HG22	2.17	0.43
33:P:117:LEU:HD22	33:P:120:GLY:O	2.18	0.43
44:v:88:ALA:HB2	44:v:96:LEU:HD23	2.01	0.43
48:x:18:GLN:HE21	48:x:18:GLN:HB3	1.55	0.43
1:C:368:A:H5''	1:C:446:A:C2	2.54	0.43
9:D:15:HIS:HB3	9:D:43:LEU:HD11	2.01	0.43
13:F:59:GLN:OE1	13:F:62:ARG:NH1	2.52	0.43
13:F:116:GLN:HE21	13:F:120:HIS:CE1	2.37	0.43
19:I:172:A:H2'	19:I:173:A:C8	2.54	0.43
19:I:2102:G:H3'	19:I:2103:C:H6	1.83	0.43
27:M:6:LYS:HB2	27:M:119:ILE:HG23	2.00	0.43
1:C:74:A:H3'	1:C:75:G:H8	1.82	0.43
1:C:759:G:C5	1:C:806:G:C5	3.07	0.43
1:C:1116:U:O4	1:C:1117:A:N6	2.51	0.43
6:3:10:GLU:CD	6:3:18:ARG:HH12	2.27	0.43
19:I:2125:G:N1	19:I:2170:A:H5''	2.33	0.43
19:I:2135:A:H61	19:I:2156:G:H1'	1.83	0.43
19:I:2380:C:H2'	19:I:2381:A:C5'	2.48	0.43
19:I:2584:U:H2'	19:I:2585:U:H2'	2.01	0.43
21:J:28:C:OP2	47:W:33:ARG:NH1	2.51	0.43
23:K:72:ASP:HA	23:K:119:GLY:HA2	2.00	0.43
35:Q:22:MET:HG2	35:Q:24:ILE:HG12	2.01	0.43
36:q:48:ARG:HD3	36:q:66:GLU:HB2	1.99	0.43
42:u:71:ARG:O	42:u:75:MET:HG2	2.17	0.43
1:C:319:A:C6	1:C:320:G:C2	3.06	0.42
1:C:998:A:C5	1:C:1020:G:H1'	2.54	0.42
1:C:1242:A:H2'	1:C:1243:C:C6	2.54	0.42
1:C:1398:C:H2'	1:C:1399:G:C8	2.54	0.42
9:D:113:ARG:NH1	9:D:117:LEU:HB2	2.34	0.42
19:I:290:U:O2	19:I:350:G:N2	2.34	0.42
23:K:180:GLU:HG3	23:K:269:ARG:O	2.19	0.42
29:N:8:TYR:HA	29:N:12:VAL:HB	2.01	0.42
32:o:39:VAL:O	32:o:43:GLU:HG2	2.19	0.42
35:Q:20:ASN:OD1	35:Q:37:CYS:SG	2.75	0.42
47:W:3:LYS:O	47:W:7:ARG:HB2	2.19	0.42
1:C:31:G:O2'	1:C:48:C:N4	2.52	0.42
19:I:288:U:H2'	19:I:289:G:H8	1.82	0.42
19:I:365:U:H2'	19:I:366:C:C6	2.55	0.42
19:I:2163:A:H3'	19:I:2164:C:C5'	2.49	0.42
23:K:132:MET:HG2	23:K:188:CYS:O	2.18	0.42
33:P:108:VAL:O	33:P:110:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:q:22:THR:OG1	36:q:23:ALA:N	2.51	0.42
44:v:11:VAL:HA	44:v:14:VAL:HG12	2.01	0.42
1:C:717:U:H4'	1:C:718:G:OP2	2.20	0.42
1:C:1443:C:H2'	1:C:1444:G:O4'	2.19	0.42
5:2:4:ILE:O	5:2:5:LYS:HB2	2.19	0.42
19:I:2144:G:HO2'	19:I:2145:C:P	2.41	0.42
19:I:2291:U:H2'	19:I:2292:U:C6	2.55	0.42
19:I:2334:U:C5	47:W:16:ARG:HG3	2.54	0.42
19:I:2367:G:OP2	19:I:2381:A:N6	2.52	0.42
25:L:99:GLU:OE2	25:L:182:ALA:HB2	2.19	0.42
30:n:65:ALA:C	30:n:67:GLU:H	2.27	0.42
31:O:68:ALA:O	31:O:72:LEU:HD13	2.19	0.42
36:q:34:ALA:HB3	36:q:78:GLU:HB3	1.99	0.42
3:1:44:MET:O	3:1:47:LEU:HD23	2.20	0.42
9:D:13:GLY:H	9:D:15:HIS:CE1	2.37	0.42
11:E:58:GLU:O	11:E:64:ILE:HD12	2.20	0.42
19:I:1179:G:H3'	19:I:1180:U:H5''	2.01	0.42
19:I:1570:A:H2'	19:I:1571:A:C8	2.54	0.42
23:K:71:LYS:NZ	23:K:98:ASP:OD2	2.47	0.42
34:p:86:ALA:HA	34:p:89:GLU:OE2	2.19	0.42
36:q:86:ALA:O	36:q:89:ARG:N	2.51	0.42
1:C:1004:C:H2'	1:C:1005:C:H6	1.84	0.42
1:C:1046:U:O2'	1:C:1049:A:OP2	2.29	0.42
11:E:134:MET:HE2	11:E:168:TYR:HD2	1.84	0.42
17:H:45:ARG:HH11	17:H:45:ARG:HB3	1.84	0.42
19:I:1071:G:H4'	19:I:1088:A:O2'	2.19	0.42
19:I:2030:6MZ:H2	19:I:2499:C:H5''	2.01	0.42
22:j:37:LYS:HD3	22:j:46:HIS:CB	2.49	0.42
51:Y:48:ARG:HH21	51:Y:49:ASP:CG	2.27	0.42
1:C:198:G:N2	1:C:199:A:H1'	2.35	0.42
1:C:546:U:C2	1:C:547:A:C8	3.08	0.42
1:C:998:A:N6	1:C:1020:G:H1'	2.33	0.42
1:C:1143:C:H2'	1:C:1144:U:C6	2.55	0.42
19:I:639:U:H2'	19:I:640:C:C6	2.54	0.42
19:I:1032:A:N1	19:I:1034:G:C8	2.88	0.42
19:I:1120:G:C6	19:I:1121:C:C4	3.07	0.42
19:I:1386:C:H2'	19:I:1387:A:H8	1.85	0.42
19:I:1913:A:O2'	19:I:1914:C:H2'	2.19	0.42
47:W:107:ALA:HB1	47:W:117:PHE:CE1	2.54	0.42
47:W:107:ALA:O	47:W:111:ARG:N	2.51	0.42
19:I:1176:U:H2'	19:I:1177:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:2138:G:H2'	19:I:2139:U:C6	2.54	0.42
1:C:836:U:C5	1:C:838:G:C2	3.07	0.42
1:C:836:U:C5	1:C:838:G:N1	2.88	0.42
1:C:1003:U:H4'	1:C:1004:C:OP2	2.20	0.42
9:D:68:LEU:HA	9:D:90:PHE:O	2.19	0.42
10:d:77:VAL:HG23	10:d:89:ILE:HG12	2.02	0.42
13:F:72:PHE:HE1	13:F:94:LEU:HD11	1.85	0.42
19:I:191:A:H2'	19:I:192:C:C6	2.55	0.42
19:I:620:G:N3	19:I:620:G:H5'	2.35	0.42
19:I:1539:U:H2'	19:I:1540:G:H8	1.83	0.42
22:j:43:VAL:HA	26:l:34:THR:HA	2.00	0.42
30:n:16:PRO:CG	34:p:43:THR:HG22	2.45	0.42
32:o:96:MET:SD	32:o:130:ALA:HB1	2.60	0.42
43:U:42:THR:HG22	43:U:43:ALA:N	2.35	0.42
47:W:18:LEU:HD22	47:W:93:ASP:HB2	2.01	0.42
1:C:714:C:O2	52:z:60:LYS:NZ	2.48	0.42
1:C:717:U:O4	6:3:53:VAL:HG22	2.20	0.42
1:C:1029:A:H2'	1:C:1030:A:H8	1.84	0.42
2:0:14:ALA:O	2:0:18:ARG:HG3	2.20	0.42
19:I:279:A:H61	19:I:361:G:H1'	1.85	0.42
19:I:360:U:H2'	19:I:361:G:C8	2.54	0.42
19:I:542:C:H2'	19:I:543:G:H8	1.85	0.42
19:I:1106:G:H2'	19:I:1107:G:H8	1.83	0.42
19:I:1266:G:OP1	20:i:16:ARG:NE	2.49	0.42
19:I:1902:C:H4'	23:K:242:LYS:O	2.20	0.42
33:P:12:LEU:HD22	33:P:25:TYR:CE2	2.55	0.42
33:P:135:HIS:HB3	33:P:138:VAL:HG22	2.01	0.42
34:p:22:LYS:HE3	34:p:61:LEU:HD22	2.02	0.42
36:q:23:ALA:O	36:q:26:VAL:HG13	2.20	0.42
41:T:77:ILE:CD1	41:T:108:ALA:HB1	2.48	0.42
44:v:43:ASN:O	44:v:47:LYS:HG2	2.20	0.42
47:W:11:ALA:HA	47:W:96:GLY:CA	2.50	0.42
1:C:672:U:H2'	1:C:673:U:H6	1.84	0.42
19:I:896:A:H5''	19:I:897:C:C5	2.54	0.42
19:I:2557:G:H2'	19:I:2558:C:C6	2.55	0.42
38:r:65:VAL:O	38:r:68:GLU:HG2	2.20	0.42
41:T:90:VAL:CG2	41:T:122:VAL:HA	2.49	0.42
43:U:26:VAL:HA	43:U:104:GLU:OE2	2.20	0.42
1:C:465:U:H2'	1:C:466:U:H6	1.85	0.41
1:C:715:A:H4'	1:C:716:G:O5'	2.19	0.41
1:C:1058:G:N2	1:C:1184:G:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1306:G:OP2	35:Q:63:ARG:NH2	2.50	0.41
8:c:96:PHE:O	8:c:100:SER:HA	2.20	0.41
19:I:651:G:H5'	26:l:19:LYS:HG3	2.02	0.41
19:I:2134:A:N6	19:I:2157:G:O4'	2.53	0.41
19:I:2182:U:H2'	19:I:2183:A:N3	2.35	0.41
19:I:2306:C:N3	19:I:2307:G:C2	2.88	0.41
22:j:10:LYS:HG2	22:j:20:PHE:HB2	2.01	0.41
22:j:12:VAL:HG12	22:j:51:GLU:O	2.20	0.41
33:P:48:GLU:HA	33:P:51:ARG:HB2	2.03	0.41
47:W:75:GLY:HA2	47:W:78:VAL:HG12	2.01	0.41
1:C:263:U:H2'	1:C:264:A:C8	2.56	0.41
19:I:1070:A:C8	19:I:1097:U:H4'	2.55	0.41
19:I:1868:C:H6	19:I:1868:C:O5'	2.03	0.41
19:I:2123:G:H2'	19:I:2124:G:C8	2.55	0.41
34:p:5:GLN:OE1	34:p:5:GLN:N	2.47	0.41
44:v:41:ARG:HD2	44:v:43:ASN:N	2.33	0.41
52:z:22:ASP:OD1	52:z:23:TYR:N	2.54	0.41
1:C:751:U:H2'	1:C:752:G:O4'	2.20	0.41
1:C:1136:G:H2'	1:C:1137:G:O4'	2.21	0.41
14:f:8:THR:OG1	14:f:10:LYS:HG3	2.19	0.41
19:I:994:C:H3'	51:Y:54:LYS:HZ2	1.84	0.41
19:I:2149:U:H2'	19:I:2150:C:C6	2.56	0.41
33:P:58:LEU:HA	33:P:61:VAL:HG12	2.01	0.41
34:p:51:PRO:HA	34:p:103:PHE:CZ	2.55	0.41
47:W:25:ARG:NH1	47:W:44:GLY:HA2	2.35	0.41
19:I:1118:C:H3'	19:I:1119:U:H4'	2.00	0.41
1:C:709:A:H2'	1:C:710:A:C8	2.56	0.41
1:C:820:C:O2	32:o:16:ASN:ND2	2.53	0.41
1:C:1065:C:H2'	1:C:1066:G:H8	1.85	0.41
8:c:52:LEU:C	8:c:54:GLN:H	2.27	0.41
13:F:65:TYR:OH	13:F:95:GLU:OE1	2.29	0.41
19:I:357:C:C2	19:I:358:U:C5	3.08	0.41
19:I:1070:A:H2'	19:I:1097:U:P	2.60	0.41
19:I:2112:G:OP1	19:I:2115:G:N2	2.54	0.41
22:j:39:PHE:CZ	22:j:44:ARG:HA	2.52	0.41
33:P:6:LEU:HG	33:P:36:ALA:HA	2.02	0.41
35:Q:14:ALA:HB1	35:Q:34:LEU:HD23	2.02	0.41
41:T:89:VAL:O	41:T:94:THR:HG21	2.20	0.41
47:W:23:ALA:C	47:W:42:PRO:HG3	2.45	0.41
1:C:41:G:H2'	1:C:42:G:C8	2.55	0.41
1:C:383:A:H3'	1:C:384:U:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:G:13:GLU:HB3	15:G:39:VAL:HG22	2.02	0.41
19:I:948:C:H1'	19:I:984:A:C8	2.56	0.41
19:I:2142:A:H2'	19:I:2143:C:C6	2.56	0.41
29:N:100:PHE:CE1	29:N:175:PHE:HZ	2.39	0.41
48:x:42:ILE:O	48:x:42:ILE:HG22	2.20	0.41
9:D:163:VAL:HG21	9:D:173:ILE:HD11	2.02	0.41
19:I:27:G:N2	19:I:512:G:H1'	2.35	0.41
19:I:1086:A:H3'	19:I:1086:A:N3	2.35	0.41
19:I:1119:U:C2	19:I:1120:G:N7	2.88	0.41
19:I:1548:A:H2'	19:I:1549:A:C8	2.56	0.41
19:I:1794:A:H2'	19:I:1795:C:C6	2.56	0.41
30:n:103:TRP:CH2	30:n:141:VAL:HG21	2.56	0.41
31:O:89:LEU:HD23	31:O:94:TYR:HB3	2.01	0.41
33:P:14:SER:HB3	33:P:17:ASP:OD2	2.20	0.41
40:t:24:LEU:HD22	40:t:29:GLN:HA	2.03	0.41
1:C:35:G:N3	40:t:115:SER:OG	2.54	0.41
1:C:412:U:H2'	1:C:413:C:C6	2.55	0.41
1:C:1170:A:H2'	1:C:1171:G:C8	2.55	0.41
8:c:49:VAL:HG23	8:c:52:LEU:HB3	2.03	0.41
19:I:1370:C:H2'	19:I:1371:G:O4'	2.21	0.41
22:j:10:LYS:CG	22:j:20:PHE:HB2	2.50	0.41
23:K:246:THR:HG23	23:K:250:VAL:O	2.21	0.41
25:L:46:ARG:NH1	25:L:85:ALA:O	2.47	0.41
34:p:22:LYS:C	34:p:61:LEU:HB3	2.46	0.41
39:S:104:THR:HG22	39:S:105:ARG:N	2.35	0.41
1:C:74:A:H3'	1:C:75:G:C8	2.56	0.41
1:C:85:U:H2'	1:C:86:C:H6	1.86	0.41
1:C:293:G:H2'	1:C:294:A:C8	2.56	0.41
1:C:464:C:H2'	1:C:465:U:H6	1.86	0.41
1:C:490:A:O2'	1:C:491:U:OP1	2.36	0.41
1:C:518:G:H2'	1:C:519:C:C6	2.56	0.41
11:E:35:SER:OG	11:E:59:ARG:NH2	2.54	0.41
11:E:70:THR:HG21	11:E:76:VAL:HG21	2.03	0.41
13:F:151:LYS:O	13:F:151:LYS:HG3	2.20	0.41
19:I:634:C:H2'	19:I:635:C:C6	2.56	0.41
19:I:866:A:C8	19:I:914:G:C6	3.09	0.41
19:I:1070:A:H8	19:I:1097:U:OP1	2.04	0.41
19:I:1079:C:H41	19:I:1088:A:P	2.44	0.41
19:I:1484:U:H2'	19:I:1485:U:C6	2.55	0.41
19:I:2171:A:H3'	19:I:2173:A:C8	2.56	0.41
19:I:2185:U:C2	19:I:2186:G:C8	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:2347:C:C2	19:I:2371:G:N2	2.88	0.41
25:L:175:LEU:HD22	25:L:190:LYS:O	2.21	0.41
30:n:70:ARG:HH12	30:n:97:ASN:HB3	1.86	0.41
33:P:6:LEU:N	33:P:35:LYS:O	2.49	0.41
34:p:48:VAL:O	34:p:51:PRO:HD2	2.21	0.41
36:q:71:LEU:HD23	36:q:72:ARG:N	2.35	0.41
38:r:22:HIS:HB2	38:r:33:THR:HG23	2.02	0.41
41:T:75:ALA:HB2	41:T:105:ILE:HG21	2.03	0.41
45:V:56:LYS:HE3	45:V:88:ALA:HA	2.03	0.41
1:C:494:G:H2'	1:C:495:C:C6	2.56	0.41
1:C:730:C:H2'	1:C:731:A:C8	2.56	0.41
3:1:20:GLU:O	3:1:23:VAL:HG12	2.21	0.41
12:e:44:LYS:NZ	19:I:2331:G:P	2.94	0.41
17:H:45:ARG:HB3	17:H:45:ARG:NH1	2.35	0.41
17:H:90:MET:HE3	52:z:23:TYR:OH	2.21	0.41
19:I:1796:U:H2'	19:I:1797:G:C8	2.55	0.41
19:I:1866:A:N7	19:I:1867:G:H1'	2.36	0.41
19:I:2181:U:H2'	19:I:2182:U:C6	2.56	0.41
42:u:68:ASP:OD1	42:u:69:LEU:N	2.54	0.41
47:W:34:HIS:ND1	47:W:53:THR:HG23	2.35	0.41
50:y:15:ASP:OD2	50:y:54:GLY:HA2	2.21	0.41
1:C:1114:C:H2'	1:C:1115:U:C6	2.57	0.40
1:C:1268:G:HO2'	1:C:1269:A:H8	1.69	0.40
11:E:6:HIS:HE1	11:E:8:ASN:HB3	1.85	0.40
19:I:1889:A:H2'	19:I:1890:A:C8	2.56	0.40
19:I:2182:U:C2	19:I:2183:A:H2	2.40	0.40
19:I:2374:C:H2'	19:I:2375:G:C8	2.55	0.40
23:K:203[B]:ARG:HG2	23:K:204:VAL:N	2.36	0.40
33:P:6:LEU:HB2	33:P:35:LYS:C	2.46	0.40
1:C:198:G:N1	1:C:459:A:N6	2.69	0.40
5:2:4:ILE:HD12	5:2:4:ILE:H	1.86	0.40
19:I:1469:A:H2'	19:I:1470:A:C8	2.56	0.40
19:I:1607:C:N4	19:I:1622:G:OP2	2.53	0.40
19:I:1913:A:N7	19:I:1915:3TD:C6	2.68	0.40
19:I:2172:U:H3'	19:I:2173:A:C5'	2.51	0.40
34:p:8:GLY:HA3	34:p:86:ALA:HB2	2.03	0.40
37:R:40:HIS:NE2	37:R:41:LYS:HE3	2.36	0.40
38:r:19:GLY:C	38:r:82:LEU:HD12	2.46	0.40
47:W:94:ARG:HD2	47:W:99:TYR:CD1	2.56	0.40
1:C:319:A:H2	1:C:320:G:H2'	1.85	0.40
1:C:465:U:H2'	1:C:466:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:U:C2	1:C:467:G:C2	3.09	0.40
1:C:1194:C:H5''	1:C:1195:A:H3'	2.03	0.40
1:C:1317:G:H2'	1:C:1318:A:C8	2.56	0.40
8:c:82:ARG:NH2	19:I:300:A:OP2	2.53	0.40
10:d:21:ARG:NE	10:d:87:GLN:HB2	2.36	0.40
11:E:11:ARG:NH1	11:E:177:THR:O	2.51	0.40
14:f:37:ARG:HG2	14:f:46:PHE:HB3	2.04	0.40
19:I:279:A:C2	19:I:362:A:H4'	2.56	0.40
19:I:851:C:H2'	19:I:852:U:C6	2.57	0.40
19:I:857:G:H2'	19:I:858:G:O4'	2.22	0.40
19:I:2021:C:OP1	20:i:9:THR:HG21	2.21	0.40
21:J:60:C:H2'	21:J:61:G:H8	1.86	0.40
29:N:44:ILE:HG21	29:N:79:ILE:HG22	2.03	0.40
30:n:130:ASN:HA	30:n:135:VAL:HG21	2.02	0.40
36:q:92:LEU:H	36:q:92:LEU:HD22	1.85	0.40
38:r:67:ALA:HB2	38:r:96:THR:HG23	2.03	0.40
39:S:106:GLU:OE1	39:S:106:GLU:N	2.45	0.40
47:W:28:VAL:HB	47:W:93:ASP:O	2.20	0.40
47:W:35:ILE:O	47:W:53:THR:HG22	2.20	0.40
1:C:395:C:O2'	1:C:615:A:N3	2.50	0.40
1:C:532:A:OP1	40:t:110:ARG:HD2	2.22	0.40
3:1:45:ILE:HA	3:1:62:VAL:HG13	2.04	0.40
11:E:15:VAL:HG23	11:E:16:LYS:HG2	2.03	0.40
19:I:760:G:H2'	19:I:761:A:O4'	2.22	0.40
19:I:1070:A:O2'	19:I:1097:U:H5'	2.22	0.40
19:I:1858:A:H2'	19:I:1859:U:O4'	2.21	0.40
36:q:83:THR:OG1	36:q:84:VAL:N	2.53	0.40
37:R:123:LYS:HE2	37:R:123:LYS:HB3	1.85	0.40
1:C:1023:U:H2'	1:C:1025:C:C4	2.56	0.40
1:C:1192:G:H2'	1:C:1193:U:C6	2.57	0.40
11:E:42:TYR:OH	11:E:90:VAL:HG11	2.22	0.40
16:g:6:LEU:CD2	16:g:53:VAL:HG22	2.52	0.40
19:I:479:A:H1'	19:I:480:A:H5''	2.03	0.40
19:I:742:A:H2'	19:I:743:A:C8	2.57	0.40
19:I:882:G:N1	19:I:895:U:H1'	2.37	0.40
19:I:1063:G:C6	19:I:1064:C:C4	3.09	0.40
19:I:1617:C:O3'	19:I:1618:6MZ:P	2.79	0.40
36:q:42:LEU:HD23	36:q:42:LEU:HA	1.93	0.40
36:q:78:GLU:OE1	36:q:79:PRO:N	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	0	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
3	1	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	9	32
4	Z	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	12	39
5	2	83/87 (95%)	78 (94%)	4 (5%)	1 (1%)	10	34
6	3	68/71 (96%)	68 (100%)	0	0	100	100
7	b	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
8	c	100/104 (96%)	89 (89%)	10 (10%)	1 (1%)	12	39
9	D	216/241 (90%)	208 (96%)	7 (3%)	1 (0%)	24	54
10	d	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
11	E	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
12	e	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
13	F	203/206 (98%)	192 (95%)	10 (5%)	1 (0%)	24	54
14	f	75/78 (96%)	75 (100%)	0	0	100	100
15	G	148/167 (89%)	138 (93%)	10 (7%)	0	100	100
16	g	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
17	H	98/135 (73%)	93 (95%)	5 (5%)	0	100	100
18	h	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
20	i	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
22	j	48/55 (87%)	44 (92%)	3 (6%)	1 (2%)	5	21
23	K	270/273 (99%)	256 (95%)	14 (5%)	0	100	100
24	k	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	L	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
26	l	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
27	M	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
28	m	36/38 (95%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	N	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
30	n	149/179 (83%)	120 (80%)	27 (18%)	2 (1%)	9	32
31	O	174/177 (98%)	157 (90%)	15 (9%)	2 (1%)	11	36
32	o	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
33	P	147/149 (99%)	144 (98%)	3 (2%)	0	100	100
34	p	125/130 (96%)	98 (78%)	22 (18%)	5 (4%)	2	9
35	Q	56/70 (80%)	56 (100%)	0	0	100	100
36	q	96/103 (93%)	75 (78%)	17 (18%)	4 (4%)	2	9
37	R	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
38	r	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
39	S	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
40	t	121/124 (98%)	112 (93%)	9 (7%)	0	100	100
41	T	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
42	u	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
43	U	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
44	v	92/101 (91%)	89 (97%)	3 (3%)	0	100	100
45	V	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
46	w	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	W	114/117 (97%)	103 (90%)	11 (10%)	0	100	100
48	x	80/82 (98%)	76 (95%)	2 (2%)	2 (2%)	4	17
49	X	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
50	y	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
51	Y	115/118 (98%)	115 (100%)	0	0	100	100
52	z	53/75 (71%)	53 (100%)	0	0	100	100
All	All	5556/5902 (94%)	5263 (95%)	271 (5%)	22 (0%)	31	59

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	2	5	LYS
8	c	54	GLN
13	F	28	ILE
31	O	14	GLY
34	p	56	ASP

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Mol	Chain	Res	Type
34	p	87	LEU
34	p	104	VAL
36	q	28	THR
36	q	57	VAL
48	x	45	GLU
9	D	14	VAL
30	n	117	ALA
48	x	53	ASP
3	l	82	GLY
36	q	38	GLY
31	O	13	ALA
34	p	62	ASP
30	n	36	LYS
34	p	25	ASN
36	q	79	PRO
4	Z	52	PRO
22	j	41	PRO

### 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	
2	0	93/93 (100%)	93 (100%)	0	100	100
3	1	71/71 (100%)	70 (99%)	1 (1%)	59	85
4	Z	84/84 (100%)	84 (100%)	0	100	100
5	2	65/66 (98%)	65 (100%)	0	100	100
6	3	60/61 (98%)	60 (100%)	0	100	100
7	b	80/84 (95%)	80 (100%)	0	100	100
8	c	83/85 (98%)	83 (100%)	0	100	100
9	D	180/199 (90%)	180 (100%)	0	100	100
10	d	78/78 (100%)	78 (100%)	0	100	100
11	E	170/190 (90%)	170 (100%)	0	100	100
12	e	57/63 (90%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	F	172/173 (99%)	172 (100%)	0	100	100
14	f	67/68 (98%)	67 (100%)	0	100	100
15	G	113/126 (90%)	113 (100%)	0	100	100
16	g	54/55 (98%)	54 (100%)	0	100	100
17	H	87/116 (75%)	87 (100%)	0	100	100
18	h	48/49 (98%)	48 (100%)	0	100	100
20	i	47/48 (98%)	47 (100%)	0	100	100
22	j	45/49 (92%)	45 (100%)	0	100	100
23	K	217/218 (100%)	217 (100%)	0	100	100
24	k	38/38 (100%)	38 (100%)	0	100	100
25	L	164/164 (100%)	164 (100%)	0	100	100
26	l	51/52 (98%)	51 (100%)	0	100	100
27	M	165/165 (100%)	165 (100%)	0	100	100
28	m	34/34 (100%)	34 (100%)	0	100	100
29	N	148/150 (99%)	148 (100%)	0	100	100
30	n	124/147 (84%)	124 (100%)	0	100	100
31	O	137/138 (99%)	137 (100%)	0	100	100
32	o	104/105 (99%)	104 (100%)	0	100	100
33	P	114/114 (100%)	114 (100%)	0	100	100
34	p	105/107 (98%)	105 (100%)	0	100	100
35	Q	55/62 (89%)	55 (100%)	0	100	100
36	q	86/90 (96%)	43 (50%)	43 (50%)	0	0
37	R	116/116 (100%)	115 (99%)	1 (1%)	70	90
38	r	90/99 (91%)	90 (100%)	0	100	100
39	S	103/104 (99%)	103 (100%)	0	100	100
40	t	103/104 (99%)	103 (100%)	0	100	100
41	T	103/103 (100%)	103 (100%)	0	100	100
42	u	93/96 (97%)	93 (100%)	0	100	100
43	U	108/108 (100%)	108 (100%)	0	100	100
44	v	79/84 (94%)	79 (100%)	0	100	100
45	V	100/103 (97%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	w	75/77 (97%)	75 (100%)	0	100	100
47	W	86/87 (99%)	86 (100%)	0	100	100
48	x	65/65 (100%)	59 (91%)	6 (9%)	8	27
49	X	99/100 (99%)	99 (100%)	0	100	100
50	y	74/78 (95%)	74 (100%)	0	100	100
51	Y	89/90 (99%)	89 (100%)	0	100	100
52	z	48/65 (74%)	48 (100%)	0	100	100
All	All	4627/4821 (96%)	4576 (99%)	51 (1%)	63	88

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1	81	ARG
36	q	7	ARG
36	q	8	ILE
36	q	9	ARG
36	q	10	LEU
36	q	14	ASP
36	q	16	ARG
36	q	17	LEU
36	q	18	ILE
36	q	24	GLU
36	q	25	ILE
36	q	26	VAL
36	q	27	GLU
36	q	30	LYS
36	q	31	ARG
36	q	35	GLN
36	q	37	ARG
36	q	40	ILE
36	q	47	GLU
36	q	51	VAL
36	q	53	ILE
36	q	60	ASP
36	q	67	ILE
36	q	69	THR
36	q	72	ARG
36	q	74	VAL
36	q	75	ASP
36	q	77	VAL

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Mol	Chain	Res	Type
36	q	78	GLU
36	q	80	THR
36	q	81	GLU
36	q	82	LYS
36	q	83	THR
36	q	84	VAL
36	q	85	ASP
36	q	87	LEU
36	q	88	MET
36	q	89	ARG
36	q	91	ASP
36	q	92	LEU
36	q	96	VAL
36	q	99	GLN
36	q	100	ILE
36	q	102	LEU
37	R	128	ASN
48	x	18	GLN
48	x	35	ARG
48	x	46	LYS
48	x	47	GLU
48	x	48	GLU
48	x	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
9	D	58	ASN
9	D	89	GLN
11	E	8	ASN
12	e	50	ASN
13	F	100	ASN
15	G	61	GLN
16	g	58	ASN
17	H	11	HIS
17	H	46	GLN
18	h	20	HIS
23	K	15	HIS
23	K	53	HIS
23	K	70	ASN
23	K	134	ASN
25	L	32	ASN

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Mol	Chain	Res	Type
25	L	67	HIS
25	L	130	GLN
25	L	173	GLN
27	M	165	HIS
28	m	13	ASN
29	N	5	HIS
29	N	52	ASN
31	O	30	ASN
32	o	4	GLN
33	P	73	ASN
34	p	110	GLN
36	q	35	GLN
36	q	56	HIS
37	R	76	HIS
42	u	52	GLN
44	v	4	GLN
44	v	60	GLN
47	W	100	HIS
47	W	104	GLN
48	x	18	GLN
50	y	9	GLN
51	Y	44	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	1525/1526 (99%)	278 (18%)	24 (1%)
19	I	2893/2904 (99%)	529 (18%)	15 (0%)
21	J	117/120 (97%)	14 (11%)	0
All	All	4535/4550 (99%)	821 (18%)	39 (0%)

All (821) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	3	A
1	C	9	G
1	C	22	G
1	C	32	A
1	C	39	G
1	C	47	C
1	C	48	C

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Mol	Chain	Res	Type
1	C	50	A
1	C	51	A
1	C	52	C
1	C	57	G
1	C	60	A
1	C	61	G
1	C	64	G
1	C	68	G
1	C	71	U
1	C	72	G
1	C	76	G
1	C	77	G
1	C	82	U
1	C	83	G
1	C	84	C
1	C	85	U
1	C	88	U
1	C	89	G
1	C	90	G
1	C	91	A
1	C	95	A
1	C	106	G
1	C	110	A
1	C	115	U
1	C	116	G
1	C	121	G
1	C	123	A
1	C	124	A
1	C	125	U
1	C	143	A
1	C	145	A
1	C	157	C
1	C	176	C
1	C	177	G
1	C	182	G
1	C	191	A
1	C	192	G
1	C	193	U
1	C	204	C
1	C	205	G
1	C	206	G
1	C	214	G

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Mol	Chain	Res	Type
1	C	222	A
1	C	239	U
1	C	241	G
1	C	244	A
1	C	245	G
1	C	260	G
1	C	261	C
1	C	265	C
1	C	266	C
1	C	274	C
1	C	277	U
1	C	283	A
1	C	287	G
1	C	290	U
1	C	302	C
1	C	315	A
1	C	322	C
1	C	323	A
1	C	341	G
1	C	346	C
1	C	348	G
1	C	361	U
1	C	363	G
1	C	366	C
1	C	367	A
1	C	370	G
1	C	375	A
1	C	377	A
1	C	378	G
1	C	386	C
1	C	391	A
1	C	392	U
1	C	400	G
1	C	405	A
1	C	406	A
1	C	407	G
1	C	408	A
1	C	418	G
1	C	423	U
1	C	433	U
1	C	439	G
1	C	443	G

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Mol	Chain	Res	Type
1	C	445	A
1	C	446	A
1	C	447	G
1	C	457	U
1	C	461	U
1	C	462	A
1	C	475	G
1	C	478	G
1	C	490	A
1	C	491	U
1	C	492	A
1	C	493	A
1	C	503	A
1	C	505	C
1	C	507	U
1	C	509	G
1	C	511	G
1	C	512	C
1	C	513	C
1	C	514	A
1	C	515	G
1	C	521	G
1	C	526	A
1	C	532	A
1	C	534	G
1	C	539	C
1	C	541	A
1	C	556	U
1	C	566	A
1	C	567	A
1	C	570	C
1	C	571	G
1	C	572	C
1	C	573	G
1	C	575	G
1	C	584	U
1	C	585	C
1	C	611	G
1	C	622	G
1	C	627	G
1	C	647	A
1	C	650	G

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Mol	Chain	Res	Type
1	C	654	G
1	C	659	A
1	C	661	G
1	C	681	A
1	C	682	G
1	C	687	G
1	C	688	A
1	C	689	A
1	C	695	U
1	C	711	C
1	C	715	A
1	C	716	G
1	C	717	U
1	C	718	G
1	C	725	G
1	C	738	C
1	C	749	A
1	C	754	G
1	C	756	U
1	C	759	G
1	C	760	A
1	C	771	A
1	C	781	A
1	C	788	A
1	C	803	G
1	C	809	A
1	C	811	C
1	C	814	U
1	C	815	G
1	C	822	A
1	C	835	C
1	C	837	U
1	C	838	G
1	C	840	G
1	C	847	G
1	C	861	G
1	C	866	A
1	C	871	G
1	C	894	A
1	C	896	G
1	C	908	A
1	C	916	G

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Mol	Chain	Res	Type
1	C	920	G
1	C	921	G
1	C	928	C
1	C	954	U
1	C	955	U
1	C	960	G
1	C	963	A
1	C	969	A
1	C	970	G
1	C	971	A
1	C	977	A
1	C	986	U
1	C	987	G
1	C	988	A
1	C	989	C
1	C	998	A
1	C	1000	C
1	C	1002	U
1	C	1003	U
1	C	1004	C
1	C	1015	U
1	C	1023	U
1	C	1025	C
1	C	1027	G
1	C	1031	C
1	C	1039	C
1	C	1044	G
1	C	1047	G
1	C	1049	A
1	C	1059	U
1	C	1075	G
1	C	1079	U
1	C	1080	U
1	C	1088	G
1	C	1089	U
1	C	1095	A
1	C	1119	U
1	C	1130	U
1	C	1131	C
1	C	1132	G
1	C	1133	G
1	C	1153	U

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Mol	Chain	Res	Type
1	C	1162	C
1	C	1165	A
1	C	1175	G
1	C	1178	G
1	C	1190	A
1	C	1191	A
1	C	1194	C
1	C	1196	U
1	C	1206	U
1	C	1207	A
1	C	1221	A
1	C	1230	A
1	C	1232	A
1	C	1234	U
1	C	1235	G
1	C	1248	G
1	C	1250	U
1	C	1251	U
1	C	1252	G
1	C	1264	G
1	C	1266	U
1	C	1271	C
1	C	1273	A
1	C	1274	A
1	C	1281	A
1	C	1293	A
1	C	1294	G
1	C	1297	C
1	C	1299	G
1	C	1314	C
1	C	1332	G
1	C	1341	G
1	C	1342	U
1	C	1347	G
1	C	1364	G
1	C	1365	G
1	C	1372	C
1	C	1373	G
1	C	1388	A
1	C	1413	G
1	C	1423	C
1	C	1426	G

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Mol	Chain	Res	Type
1	C	1440	A
1	C	1441	A
1	C	1444	G
1	C	1445	C
1	C	1446	A
1	C	1447	A
1	C	1448	G
1	C	1481	G
1	C	1491	G
1	C	1497	A
1	C	1499	G
1	C	1500	U
1	C	1501	A
1	C	1502	G
1	C	1511	G
1	C	1514	C
1	C	1523	G
1	C	1524	G
1	C	1525	A
19	I	2	G
19	I	10	A
19	I	15	G
19	I	34	U
19	I	35	G
19	I	36	G
19	I	46	G
19	I	51	G
19	I	60	G
19	I	63	A
19	I	71	A
19	I	74	A
19	I	75	G
19	I	84	A
19	I	88	G
19	I	100	U
19	I	101	A
19	I	118	A
19	I	119	A
19	I	120	U
19	I	125	A
19	I	136	G
19	I	139	U

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Mol	Chain	Res	Type
19	I	140	C
19	I	149	A
19	I	160	A
19	I	163	C
19	I	165	A
19	I	181	A
19	I	196	A
19	I	199	A
19	I	201	C
19	I	215	G
19	I	216	A
19	I	218	A
19	I	221	A
19	I	222	A
19	I	224	U
19	I	225	C
19	I	227	A
19	I	230	G
19	I	233	A
19	I	245	G
19	I	248	G
19	I	249	C
19	I	264	C
19	I	265	A
19	I	266	G
19	I	271	G
19	I	272	A
19	I	273	G
19	I	277	G
19	I	278	A
19	I	279	A
19	I	284	U
19	I	285	G
19	I	290	U
19	I	291	G
19	I	300	A
19	I	311	A
19	I	330	A
19	I	338	G
19	I	353	C
19	I	359	G
19	I	364	C

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Mol	Chain	Res	Type
19	I	371	A
19	I	372	G
19	I	386	G
19	I	396	G
19	I	403	U
19	I	404	A
19	I	411	G
19	I	412	A
19	I	418	C
19	I	420	C
19	I	457	A
19	I	473	G
19	I	481	G
19	I	491	G
19	I	492	A
19	I	503	A
19	I	504	A
19	I	505	A
19	I	508	A
19	I	509	C
19	I	532	A
19	I	535	G
19	I	543	G
19	I	544	C
19	I	546	U
19	I	547	A
19	I	548	G
19	I	549	G
19	I	550	C
19	I	563	A
19	I	571	U
19	I	573	U
19	I	575	A
19	I	602	A
19	I	603	A
19	I	607	U
19	I	613	A
19	I	615	U
19	I	622	G
19	I	627	A
19	I	637	A
19	I	645	C

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Mol	Chain	Res	Type
19	I	647	G
19	I	653	U
19	I	654	A
19	I	655	A
19	I	686	U
19	I	716	A
19	I	717	C
19	I	730	A
19	I	736	C
19	I	746	PSU
19	I	747	5MU
19	I	764	A
19	I	765	C
19	I	770	G
19	I	774	G
19	I	775	G
19	I	776	G
19	I	782	A
19	I	784	G
19	I	785	G
19	I	789	A
19	I	792	A
19	I	794	A
19	I	805	G
19	I	806	C
19	I	812	C
19	I	819	A
19	I	827	U
19	I	846	U
19	I	858	G
19	I	859	G
19	I	881	G
19	I	884	U
19	I	894	U
19	I	895	U
19	I	896	A
19	I	897	C
19	I	910	A
19	I	915	C
19	I	918	A
19	I	919	U
19	I	932	U

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Mol	Chain	Res	Type
19	I	946	C
19	I	961	C
19	I	974	G
19	I	975	A
19	I	983	A
19	I	988	A
19	I	990	A
19	I	996	A
19	I	997	G
19	I	999	U
19	I	1003	G
19	I	1005	C
19	I	1009	A
19	I	1011	G
19	I	1012	U
19	I	1013	C
19	I	1022	G
19	I	1027	A
19	I	1033	U
19	I	1034	G
19	I	1035	U
19	I	1036	G
19	I	1046	A
19	I	1047	G
19	I	1055	G
19	I	1057	A
19	I	1060	U
19	I	1061	U
19	I	1062	G
19	I	1063	G
19	I	1064	C
19	I	1065	U
19	I	1066	U
19	I	1067	A
19	I	1068	G
19	I	1069	A
19	I	1070	A
19	I	1071	G
19	I	1072	C
19	I	1073	A
19	I	1074	G
19	I	1076	C

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Mol	Chain	Res	Type
19	I	1077	A
19	I	1079	C
19	I	1080	A
19	I	1081	U
19	I	1082	U
19	I	1084	A
19	I	1086	A
19	I	1087	G
19	I	1089	A
19	I	1090	A
19	I	1097	U
19	I	1098	A
19	I	1109	C
19	I	1110	G
19	I	1111	A
19	I	1112	G
19	I	1118	C
19	I	1119	U
19	I	1120	G
19	I	1121	C
19	I	1122	G
19	I	1132	U
19	I	1135	C
19	I	1136	G
19	I	1142	A
19	I	1150	C
19	I	1151	A
19	I	1157	G
19	I	1170	C
19	I	1171	G
19	I	1172	C
19	I	1173	U
19	I	1174	U
19	I	1175	A
19	I	1176	U
19	I	1179	G
19	I	1180	U
19	I	1181	U
19	I	1187	G
19	I	1206	G
19	I	1238	G
19	I	1250	G

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Mol	Chain	Res	Type
19	I	1253	A
19	I	1256	G
19	I	1257	C
19	I	1266	G
19	I	1267	U
19	I	1271	G
19	I	1272	A
19	I	1273	U
19	I	1300	G
19	I	1301	A
19	I	1321	A
19	I	1341	G
19	I	1352	U
19	I	1365	A
19	I	1368	G
19	I	1374	G
19	I	1379	U
19	I	1383	A
19	I	1387	A
19	I	1395	A
19	I	1413	A
19	I	1416	G
19	I	1420	A
19	I	1421	G
19	I	1427	A
19	I	1428	C
19	I	1434	A
19	I	1452	G
19	I	1460	U
19	I	1461	C
19	I	1470	A
19	I	1478	G
19	I	1482	G
19	I	1490	A
19	I	1493	C
19	I	1494	A
19	I	1495	A
19	I	1515	A
19	I	1520	U
19	I	1523	U
19	I	1524	G
19	I	1526	C

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Mol	Chain	Res	Type
19	I	1534	U
19	I	1535	A
19	I	1536	C
19	I	1537	G
19	I	1543	G
19	I	1560	G
19	I	1566	A
19	I	1567	G
19	I	1569	A
19	I	1578	U
19	I	1583	A
19	I	1584	U
19	I	1585	C
19	I	1608	A
19	I	1610	A
19	I	1618	6MZ
19	I	1644	C
19	I	1647	U
19	I	1648	U
19	I	1649	G
19	I	1654	A
19	I	1674	G
19	I	1675	C
19	I	1676	A
19	I	1693	U
19	I	1696	G
19	I	1702	G
19	I	1703	G
19	I	1715	G
19	I	1729	U
19	I	1730	C
19	I	1732	C
19	I	1733	G
19	I	1736	U
19	I	1737	G
19	I	1738	G
19	I	1739	A
19	I	1744	A
19	I	1750	G
19	I	1762	A
19	I	1763	G
19	I	1764	C

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Mol	Chain	Res	Type
19	I	1769	U
19	I	1773	A
19	I	1776	G
19	I	1782	U
19	I	1784	A
19	I	1800	C
19	I	1801	A
19	I	1808	A
19	I	1816	C
19	I	1820	U
19	I	1829	A
19	I	1842	G
19	I	1862	G
19	I	1866	A
19	I	1867	G
19	I	1868	C
19	I	1869	G
19	I	1870	C
19	I	1871	A
19	I	1872	A
19	I	1873	G
19	I	1875	G
19	I	1903	G
19	I	1905	C
19	I	1906	G
19	I	1913	A
19	I	1929	G
19	I	1930	G
19	I	1931	U
19	I	1936	A
19	I	1945	G
19	I	1954	G
19	I	1955	U
19	I	1967	C
19	I	1970	A
19	I	1971	U
19	I	1972	G
19	I	1982	U
19	I	1987	A
19	I	1991	U
19	I	1993	U
19	I	1997	C

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Mol	Chain	Res	Type
19	I	2006	C
19	I	2023	C
19	I	2026	U
19	I	2027	G
19	I	2031	A
19	I	2033	A
19	I	2036	C
19	I	2043	C
19	I	2052	A
19	I	2053	G
19	I	2055	C
19	I	2056	G
19	I	2059	A
19	I	2060	A
19	I	2061	G
19	I	2069	G7M
19	I	2093	G
19	I	2105	U
19	I	2107	G
19	I	2108	A
19	I	2110	G
19	I	2111	U
19	I	2112	G
19	I	2118	U
19	I	2119	A
19	I	2120	G
19	I	2122	U
19	I	2124	G
19	I	2125	G
19	I	2127	G
19	I	2131	U
19	I	2132	U
19	I	2133	G
19	I	2138	G
19	I	2141	G
19	I	2144	G
19	I	2145	C
19	I	2146	C
19	I	2148	G
19	I	2153	C
19	I	2155	U
19	I	2156	G

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Mol	Chain	Res	Type
19	I	2158	A
19	I	2160	C
19	I	2161	C
19	I	2164	C
19	I	2165	C
19	I	2166	U
19	I	2168	G
19	I	2169	A
19	I	2170	A
19	I	2171	A
19	I	2172	U
19	I	2173	A
19	I	2174	C
19	I	2175	C
19	I	2178	C
19	I	2181	U
19	I	2186	G
19	I	2190	G
19	I	2198	A
19	I	2203	U
19	I	2204	G
19	I	2211	A
19	I	2220	U
19	I	2225	A
19	I	2226	C
19	I	2238	G
19	I	2239	G
19	I	2268	A
19	I	2273	A
19	I	2283	C
19	I	2287	A
19	I	2288	A
19	I	2294	G
19	I	2305	U
19	I	2309	A
19	I	2311	A
19	I	2321	U
19	I	2322	A
19	I	2333	A
19	I	2334	U
19	I	2335	A
19	I	2347	C

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Mol	Chain	Res	Type
19	I	2350	C
19	I	2361	G
19	I	2366	A
19	I	2373	G
19	I	2374	C
19	I	2375	G
19	I	2376	A
19	I	2377	A
19	I	2379	G
19	I	2380	C
19	I	2381	A
19	I	2382	G
19	I	2383	G
19	I	2385	C
19	I	2390	U
19	I	2391	G
19	I	2396	G
19	I	2402	U
19	I	2406	A
19	I	2419	U
19	I	2423	U
19	I	2429	G
19	I	2430	A
19	I	2435	A
19	I	2440	C
19	I	2441	U
19	I	2448	A
19	I	2459	A
19	I	2469	A
19	I	2470	G
19	I	2473	U
19	I	2476	A
19	I	2491	U
19	I	2498	OMC
19	I	2502	G
19	I	2505	G
19	I	2518	A
19	I	2527	C
19	I	2529	G
19	I	2547	A
19	I	2554	U
19	I	2566	A

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Mol	Chain	Res	Type
19	I	2567	G
19	I	2573	C
19	I	2582	G
19	I	2585	U
19	I	2586	U
19	I	2602	A
19	I	2609	U
19	I	2613	U
19	I	2615	U
19	I	2636	C
19	I	2661	G
19	I	2663	G
19	I	2675	A
19	I	2682	A
19	I	2689	U
19	I	2690	U
19	I	2702	G
19	I	2713	U
19	I	2714	G
19	I	2726	A
19	I	2733	A
19	I	2739	U
19	I	2748	A
19	I	2756	U
19	I	2757	A
19	I	2776	A
19	I	2778	A
19	I	2793	C
19	I	2797	U
19	I	2798	U
19	I	2800	A
19	I	2801	G
19	I	2809	A
19	I	2820	A
19	I	2837	A
19	I	2850	A
19	I	2873	A
19	I	2880	C
19	I	2884	U
19	I	2895	G
19	I	2897	U
19	I	2901	C

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Mol	Chain	Res	Type
19	I	2902	C
19	I	2903	U
21	J	15	A
21	J	25	U
21	J	32	U
21	J	35	C
21	J	56	G
21	J	67	G
21	J	88	C
21	J	89	U
21	J	90	C
21	J	91	C
21	J	99	A
21	J	105	G
21	J	109	A
21	J	119	A

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	87	C
1	C	90	G
1	C	245	G
1	C	265	C
1	C	322	C
1	C	405	A
1	C	442	A
1	C	491	U
1	C	506	U
1	C	512	C
1	C	717	U
1	C	893	C
1	C	954	U
1	C	976	U
1	C	1003	U
1	C	1195	A
1	C	1233	A
1	C	1247	G
1	C	1250	U
1	C	1251	U
1	C	1272	U
1	C	1273	A

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Mol	Chain	Res	Type
1	C	1341	G
1	C	1440	A
19	I	784	G
19	I	918	A
19	I	1034	G
19	I	1035	U
19	I	1046	A
19	I	1070	A
19	I	1117	C
19	I	1542	U
19	I	1865	U
19	I	1867	G
19	I	1871	A
19	I	2170	A
19	I	2304	G
19	I	2308	G
19	I	2756	U

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

25 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
19	PSU	I	2504	53,19	18,21,22	1.19	3 (16%)	21,30,33	1.95	4 (19%)
19	PSU	I	2605	19	18,21,22	1.33	3 (16%)	21,30,33	2.00	4 (19%)
19	3TD	I	1915	19	19,22,23	1.18	2 (10%)	23,32,35	1.56	4 (17%)
19	PSU	I	955	19	18,21,22	1.23	3 (16%)	21,30,33	1.98	4 (19%)
19	5MC	I	1962	19	19,22,23	1.74	2 (10%)	26,32,35	1.13	2 (7%)
19	6MZ	I	2030	19	22,25,26	1.21	2 (9%)	29,36,39	2.29	9 (31%)
19	PSU	I	1911	19	18,21,22	1.07	2 (11%)	21,30,33	1.99	4 (19%)
19	OMC	I	2498	19	19,22,23	1.08	2 (10%)	25,31,34	1.23	2 (8%)
19	G7M	I	2069	19	23,26,27	0.61	0	34,39,42	0.87	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	OMG	I	2251	19	23,26,27	0.88	2 (8%)	32,38,41	2.03	9 (28%)
19	5MU	I	1939	19	19,22,23	1.32	4 (21%)	27,32,35	2.24	6 (22%)
19	1MG	I	745	19	23,26,27	1.15	2 (8%)	33,39,42	1.79	7 (21%)
19	H2U	I	2449	19	18,21,22	0.58	0	19,30,33	1.08	1 (5%)
19	PSU	I	1917	19	18,21,22	1.07	2 (11%)	21,30,33	1.97	4 (19%)
19	OMU	I	2552	19	19,22,23	1.26	3 (15%)	25,31,34	1.97	6 (24%)
43	4D4	U	81	43	9,11,12	2.06	2 (22%)	7,13,15	1.92	3 (42%)
19	PSU	I	746	19	18,21,22	1.30	4 (22%)	21,30,33	1.95	3 (14%)
19	PSU	I	2604	19	18,21,22	1.23	3 (16%)	21,30,33	2.16	4 (19%)
19	2MA	I	2503	53,19	22,25,26	1.36	4 (18%)	32,37,40	1.96	7 (21%)
19	PSU	I	2457	19	18,21,22	1.29	4 (22%)	21,30,33	2.17	4 (19%)
19	PSU	I	2580	19	18,21,22	1.43	4 (22%)	21,30,33	2.24	5 (23%)
19	2MG	I	2445	19	23,26,27	0.94	2 (8%)	33,38,41	2.35	11 (33%)
19	6MZ	I	1618	19	22,25,26	1.15	2 (9%)	29,36,39	2.32	9 (31%)
19	5MU	I	747	19	19,22,23	1.24	4 (21%)	27,32,35	2.25	7 (25%)
19	2MG	I	1835	19	23,26,27	0.89	1 (4%)	33,38,41	2.25	10 (30%)

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
19	PSU	I	2504	53,19	-	0/7/25/26	0/2/2/2
19	PSU	I	2605	19	-	0/7/25/26	0/2/2/2
19	3TD	I	1915	19	-	0/7/25/26	0/2/2/2
19	PSU	I	955	19	-	0/7/25/26	0/2/2/2
19	5MC	I	1962	19	-	0/7/25/26	0/2/2/2
19	6MZ	I	2030	19	-	2/9/27/28	0/3/3/3
19	PSU	I	1911	19	-	0/7/25/26	0/2/2/2
19	OMC	I	2498	19	-	2/9/27/28	0/2/2/2
19	G7M	I	2069	19	-	1/7/25/26	0/3/3/3
19	OMG	I	2251	19	-	0/9/27/28	0/3/3/3
19	5MU	I	1939	19	-	0/7/25/26	0/2/2/2
19	1MG	I	745	19	-	0/7/25/26	0/3/3/3
19	H2U	I	2449	19	-	0/7/38/39	0/2/2/2
19	PSU	I	1917	19	-	0/7/25/26	0/2/2/2
19	OMU	I	2552	19	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	4D4	U	81	43	-	4/11/12/14	-
19	PSU	I	746	19	-	3/7/25/26	0/2/2/2
19	PSU	I	2604	19	-	0/7/25/26	0/2/2/2
19	2MA	I	2503	53,19	-	0/7/25/26	0/3/3/3
19	PSU	I	2457	19	-	0/7/25/26	0/2/2/2
19	PSU	I	2580	19	-	2/7/25/26	0/2/2/2
19	2MG	I	2445	19	-	0/9/27/28	0/3/3/3
19	6MZ	I	1618	19	-	3/9/27/28	0/3/3/3
19	5MU	I	747	19	-	0/7/25/26	0/2/2/2
19	2MG	I	1835	19	-	0/9/27/28	0/3/3/3

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	I	1962	5MC	C5-C4	-6.08	1.39	1.44
43	U	81	4D4	CZ-NE	5.04	1.43	1.33
19	I	2503	2MA	C6-N1	3.87	1.40	1.35
19	I	2030	6MZ	C6-N6	3.31	1.38	1.34
19	I	1962	5MC	C2-N1	-3.23	1.33	1.40
19	I	745	1MG	C6-N1	-3.23	1.33	1.40
19	I	2503	2MA	C5-N7	-3.22	1.33	1.39
19	I	1618	6MZ	C6-N6	3.19	1.37	1.34
19	I	2552	OMU	C2-N1	-3.03	1.33	1.38
19	I	1939	5MU	C2-N1	-2.97	1.33	1.38
19	I	2580	PSU	C2-N1	-2.88	1.32	1.36
19	I	2498	OMC	C2-N1	-2.81	1.34	1.40
19	I	2605	PSU	C4-N3	-2.80	1.33	1.38
43	U	81	4D4	CZ-NH1	2.77	1.44	1.34
19	I	2605	PSU	C2-N3	-2.74	1.33	1.37
19	I	746	PSU	C2-N3	-2.66	1.33	1.37
19	I	2580	PSU	O4'-C1'	-2.66	1.40	1.43
19	I	2580	PSU	C4-N3	-2.65	1.33	1.38
19	I	747	5MU	C2-N1	-2.63	1.34	1.38
19	I	2552	OMU	C4-N3	-2.62	1.34	1.38
19	I	747	5MU	C4-C5	-2.60	1.40	1.44
19	I	2552	OMU	C2-N3	-2.59	1.33	1.38
19	I	2457	PSU	C4-N3	-2.59	1.34	1.38
19	I	2457	PSU	C2-N1	-2.56	1.33	1.36
19	I	1939	5MU	C4-N3	-2.55	1.34	1.38
19	I	746	PSU	C4-N3	-2.54	1.34	1.38
19	I	1915	3TD	C4-N3	-2.54	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	I	1939	5MU	C4-C5	-2.53	1.40	1.44
19	I	2504	PSU	C4-N3	-2.53	1.34	1.38
19	I	2604	PSU	C2-N3	-2.53	1.33	1.37
19	I	2445	2MG	C6-N1	-2.52	1.34	1.38
19	I	2604	PSU	C4-N3	-2.52	1.34	1.38
19	I	746	PSU	O4'-C1'	-2.51	1.40	1.43
19	I	955	PSU	C4-N3	-2.48	1.34	1.38
19	I	1939	5MU	C2-N3	-2.48	1.33	1.38
19	I	2580	PSU	C2-N3	-2.47	1.33	1.37
19	I	2457	PSU	C2-N3	-2.45	1.33	1.37
19	I	1915	3TD	C4-C5	-2.45	1.42	1.47
19	I	747	5MU	C4-N3	-2.43	1.34	1.38
19	I	2251	OMG	C6-N1	-2.41	1.34	1.38
19	I	2605	PSU	C2-N1	-2.38	1.33	1.36
19	I	2504	PSU	C2-N3	-2.36	1.33	1.37
19	I	1835	2MG	C6-N1	-2.34	1.34	1.38
19	I	2604	PSU	C2-N1	-2.34	1.33	1.36
19	I	2504	PSU	C2-N1	-2.34	1.33	1.36
19	I	955	PSU	C2-N1	-2.33	1.33	1.36
19	I	955	PSU	C2-N3	-2.30	1.33	1.37
19	I	2503	2MA	C2-N3	-2.28	1.30	1.34
19	I	2030	6MZ	C5-N7	-2.25	1.35	1.39
19	I	1911	PSU	C4-N3	-2.23	1.34	1.38
19	I	747	5MU	C2-N3	-2.22	1.34	1.38
19	I	1618	6MZ	C5-N7	-2.18	1.35	1.39
19	I	2503	2MA	C5-C6	2.17	1.47	1.41
19	I	2251	OMG	C5-N7	-2.14	1.34	1.39
19	I	746	PSU	C2-N1	-2.10	1.33	1.36
19	I	1917	PSU	C4-N3	-2.09	1.34	1.38
19	I	1911	PSU	C2-N3	-2.09	1.34	1.37
19	I	1917	PSU	C2-N1	-2.08	1.34	1.36
19	I	745	1MG	C5-N7	-2.04	1.35	1.39
19	I	2445	2MG	C5-N7	-2.04	1.35	1.39
19	I	2457	PSU	O4'-C1'	-2.04	1.41	1.43
19	I	2498	OMC	C2-N3	-2.01	1.32	1.36

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	2445	2MG	C2-N3-C4	7.90	121.88	112.00
19	I	1835	2MG	C2-N3-C4	7.54	121.43	112.00
19	I	2580	PSU	N1-C2-N3	6.30	121.82	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	2457	PSU	N1-C2-N3	6.18	121.69	115.17
19	I	2604	PSU	N1-C2-N3	6.08	121.58	115.17
19	I	2251	OMG	C5-C4-N3	-5.91	118.98	128.39
19	I	2030	6MZ	C5-C4-N3	-5.87	118.64	126.72
19	I	2503	2MA	C5-C4-N3	-5.83	121.03	127.18
19	I	2445	2MG	C5-C4-N3	-5.83	119.11	128.39
19	I	1939	5MU	C4-N3-C2	-5.82	119.71	127.34
19	I	745	1MG	C5-C4-N3	-5.77	119.21	128.39
19	I	1618	6MZ	C5-C4-N3	-5.74	118.82	126.72
19	I	746	PSU	N1-C2-N3	5.62	121.10	115.17
19	I	1835	2MG	C5-C4-N3	-5.62	119.44	128.39
19	I	2605	PSU	N1-C2-N3	5.61	121.09	115.17
19	I	747	5MU	C4-N3-C2	-5.57	120.03	127.34
19	I	955	PSU	N1-C2-N3	5.53	121.00	115.17
19	I	2504	PSU	N1-C2-N3	5.49	120.96	115.17
19	I	1911	PSU	N1-C2-N3	5.46	120.93	115.17
19	I	1917	PSU	N1-C2-N3	5.44	120.91	115.17
19	I	1939	5MU	N3-C2-N1	5.34	121.84	114.89
19	I	2251	OMG	C2-N3-C4	5.24	121.32	112.30
19	I	2552	OMU	C4-N3-C2	-5.23	120.12	126.61
19	I	2604	PSU	C4-N3-C2	-4.97	119.52	126.37
19	I	1939	5MU	C5-C4-N3	4.91	119.59	115.32
19	I	746	PSU	C4-N3-C2	-4.86	119.68	126.37
19	I	2552	OMU	N3-C2-N1	4.85	121.21	114.89
19	I	747	5MU	N3-C2-N1	4.84	121.19	114.89
19	I	747	5MU	C5-C4-N3	4.76	119.46	115.32
19	I	2457	PSU	C4-N3-C2	-4.73	119.86	126.37
19	I	2605	PSU	C4-N3-C2	-4.70	119.90	126.37
19	I	2580	PSU	C4-N3-C2	-4.65	119.97	126.37
19	I	1618	6MZ	C9-N6-C6	-4.61	118.57	122.85
19	I	1911	PSU	C4-N3-C2	-4.59	120.04	126.37
19	I	2503	2MA	N3-C4-N9	4.59	132.81	126.99
19	I	2251	OMG	N9-C4-N3	4.51	134.98	125.95
19	I	2030	6MZ	N3-C4-N9	4.50	134.82	127.17
19	I	1618	6MZ	N3-C4-N9	4.49	134.81	127.17
19	I	747	5MU	O4-C4-C5	-4.48	119.80	124.92
19	I	1917	PSU	C4-N3-C2	-4.46	120.23	126.37
19	I	955	PSU	C4-N3-C2	-4.45	120.24	126.37
19	I	2504	PSU	C4-N3-C2	-4.44	120.25	126.37
19	I	2445	2MG	N9-C4-N3	4.36	134.66	125.95
19	I	745	1MG	N9-C4-N3	4.34	134.63	125.95
19	I	1835	2MG	N9-C4-N3	4.20	134.35	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	1915	3TD	O2-C2-N3	-4.20	115.90	121.82
19	I	2503	2MA	N6-C6-N1	4.20	122.69	117.03
19	I	2030	6MZ	C9-N6-C6	-4.15	119.00	122.85
19	I	745	1MG	C2-N3-C4	4.14	121.29	111.98
19	I	2445	2MG	C2-N1-C6	-4.07	119.63	124.55
19	I	1939	5MU	O4-C4-C5	-4.07	120.26	124.92
19	I	2030	6MZ	C5-N7-C8	3.96	109.67	103.45
19	I	1618	6MZ	N1-C2-N3	-3.95	122.60	128.58
19	I	2030	6MZ	N1-C2-N3	-3.93	122.63	128.58
19	I	2580	PSU	O2-C2-N1	-3.91	118.76	122.79
19	I	1618	6MZ	C5-N7-C8	3.88	109.55	103.45
19	I	2030	6MZ	C2-N3-C4	3.76	121.02	111.83
19	I	1618	6MZ	C2-N3-C4	3.72	120.91	111.83
19	I	1835	2MG	C2-N1-C6	-3.68	120.10	124.55
19	I	2457	PSU	O2-C2-N1	-3.67	119.01	122.79
19	I	2552	OMU	C5-C4-N3	3.65	119.91	114.80
19	I	2503	2MA	C5-N7-C8	3.56	109.05	103.45
43	U	81	4D4	NE-CZ-NH2	3.46	126.61	120.67
19	I	1962	5MC	C5-C6-N1	-3.45	119.56	123.31
19	I	2604	PSU	O2-C2-N1	-3.43	119.25	122.79
19	I	1939	5MU	C5-C6-N1	-3.41	119.61	123.31
19	I	2449	H2U	C5-C4-N3	-3.32	113.15	116.69
19	I	747	5MU	C5-C6-N1	-3.32	119.71	123.31
19	I	2030	6MZ	C4-C5-N7	-3.31	106.80	110.58
19	I	2552	OMU	CM2-O2'-C2'	-3.25	106.13	114.47
19	I	1618	6MZ	C4-C5-N7	-3.24	106.87	110.58
19	I	1911	PSU	O2-C2-N1	-3.23	119.46	122.79
19	I	1917	PSU	O2-C2-N1	-3.20	119.49	122.79
19	I	2503	2MA	N9-C8-N7	-3.11	109.53	113.94
19	I	2580	PSU	C6-N1-C2	-3.10	119.81	122.69
19	I	2504	PSU	O2-C2-N1	-3.07	119.63	122.79
19	I	1915	3TD	C1'-C5-C4	3.03	122.20	117.61
19	I	955	PSU	O2-C2-N1	-2.96	119.73	122.79
19	I	2498	OMC	O2-C2-N3	-2.96	117.67	122.33
19	I	2069	G7M	C8-N7-C5	-2.94	104.11	107.78
19	I	2498	OMC	CM2-O2'-C2'	-2.93	106.97	114.47
19	I	2251	OMG	C2-N1-C6	-2.90	119.84	125.11
19	I	2251	OMG	CM2-O2'-C2'	-2.90	107.03	114.47
19	I	2457	PSU	C6-N1-C2	-2.89	120.01	122.69
19	I	1835	2MG	N1-C2-N2	2.86	119.48	116.56
19	I	1618	6MZ	N9-C8-N7	-2.84	109.91	113.94
19	I	2251	OMG	C8-N7-C5	2.79	109.22	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	2445	2MG	C8-N7-C5	2.74	109.15	104.26
19	I	745	1MG	C8-N7-C5	2.74	109.14	104.26
19	I	2445	2MG	N1-C2-N2	2.72	119.34	116.56
19	I	2503	2MA	C5-C6-N1	-2.72	114.67	118.90
19	I	1835	2MG	C8-N7-C5	2.68	109.04	104.26
19	I	2030	6MZ	N9-C8-N7	-2.67	110.15	113.94
19	I	1915	3TD	C4-N3-C2	-2.64	121.81	124.61
19	I	2552	OMU	O4-C4-C5	-2.64	120.61	125.16
19	I	1939	5MU	O2-C2-N1	-2.63	119.38	122.80
19	I	1915	3TD	C5-C6-N1	-2.55	118.61	122.14
19	I	746	PSU	O2-C2-N1	-2.53	120.18	122.79
43	U	81	4D4	O-C-CA	-2.51	118.31	124.77
19	I	955	PSU	C6-N1-C2	-2.50	120.37	122.69
19	I	1618	6MZ	C6-C5-N7	2.50	135.15	132.43
19	I	747	5MU	C1'-N1-C2	2.43	121.95	117.59
19	I	2580	PSU	O4'-C1'-C2'	2.41	108.49	105.15
19	I	2604	PSU	C6-N1-C2	-2.41	120.45	122.69
19	I	2445	2MG	CM2-N2-C2	-2.41	118.47	123.65
19	I	2030	6MZ	C6-C5-N7	2.40	135.04	132.43
19	I	2445	2MG	C5-C6-N1	2.38	119.31	113.25
19	I	2503	2MA	C4-C5-N7	-2.36	107.88	110.58
19	I	1917	PSU	C6-N1-C2	-2.35	120.51	122.69
19	I	2504	PSU	C6-N1-C2	-2.31	120.54	122.69
19	I	1962	5MC	C5-C4-N3	-2.27	119.43	121.75
19	I	2605	PSU	O2-C2-N1	-2.25	120.47	122.79
19	I	1835	2MG	O6-C6-C5	-2.23	120.66	126.53
19	I	2251	OMG	O6-C6-C5	-2.22	120.66	126.53
19	I	2445	2MG	O6-C6-C5	-2.20	120.73	126.53
19	I	2445	2MG	C6-C5-N7	2.18	134.25	130.29
19	I	2552	OMU	O2-C2-N1	-2.18	119.96	122.80
19	I	2605	PSU	C6-N1-C2	-2.14	120.70	122.69
19	I	1835	2MG	C5-C6-N1	2.13	118.67	113.25
19	I	745	1MG	C6-C5-N7	2.12	134.07	129.36
19	I	745	1MG	C4-C5-N7	-2.10	107.33	110.67
19	I	2251	OMG	C5-C6-N1	2.09	118.58	113.25
19	I	1835	2MG	C6-C5-N7	2.08	134.08	130.29
19	I	1835	2MG	C4-C5-N7	-2.07	107.39	110.67
19	I	745	1MG	C5-C6-N1	2.06	118.82	115.02
19	I	2251	OMG	C4-C5-N7	-2.06	107.41	110.67
19	I	2445	2MG	C4-C5-N7	-2.05	107.42	110.67
19	I	1911	PSU	C6-N1-C2	-2.05	120.79	122.69
19	I	747	5MU	C1'-N1-C6	-2.05	117.78	121.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	U	81	4D4	NH1-CZ-NE	-2.02	114.67	119.27

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	I	746	PSU	O4'-C4'-C5'-O5'
19	I	1618	6MZ	O4'-C4'-C5'-O5'
19	I	2498	OMC	O4'-C4'-C5'-O5'
19	I	2580	PSU	O4'-C4'-C5'-O5'
19	I	746	PSU	C3'-C4'-C5'-O5'
19	I	1618	6MZ	C3'-C4'-C5'-O5'
19	I	2030	6MZ	O4'-C4'-C5'-O5'
19	I	2030	6MZ	C3'-C4'-C5'-O5'
19	I	2580	PSU	C3'-C4'-C5'-O5'
43	U	81	4D4	CG-CD-NE-CZ
19	I	2552	OMU	C3'-C2'-O2'-CM2
19	I	1618	6MZ	C4'-C5'-O5'-P
19	I	2498	OMC	C3'-C4'-C5'-O5'
43	U	81	4D4	OB-CB-CG-CD
19	I	746	PSU	O4'-C1'-C5-C6
19	I	2069	G7M	O4'-C4'-C5'-O5'
43	U	81	4D4	O-C-CA-CB
43	U	81	4D4	CA-CB-CG-CD

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	I	1915	3TD	6	0
19	I	2030	6MZ	1	0
19	I	1618	6MZ	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 307 ligands modelled in this entry, 307 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	1914:C	O3'	1915:3TD	P	5.73
1	I	1617:C	O3'	1618:6MZ	P	2.79

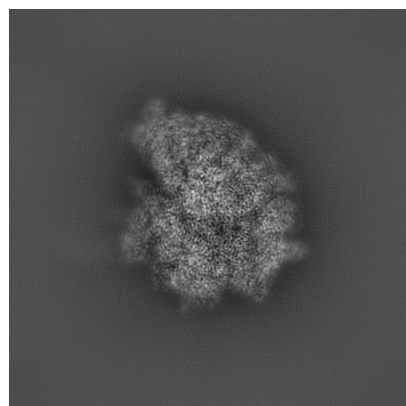
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75668. These allow visual inspection of the internal detail of the map and identification of artifacts.

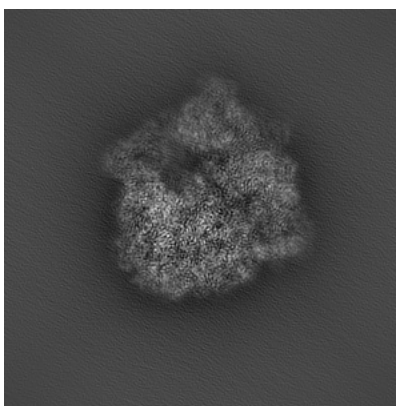
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

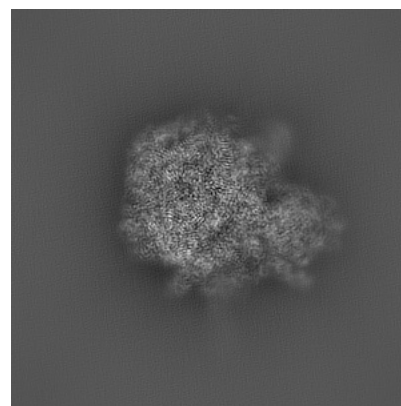
#### 6.1.1 Primary map



X

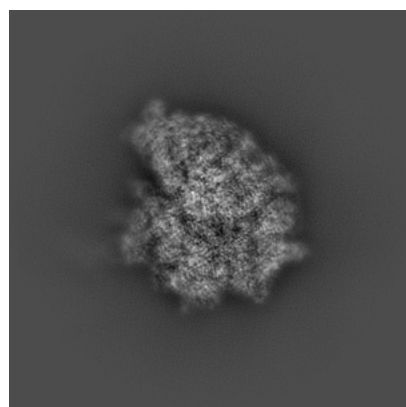


Y

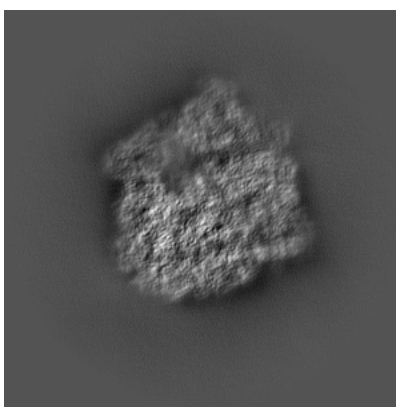


Z

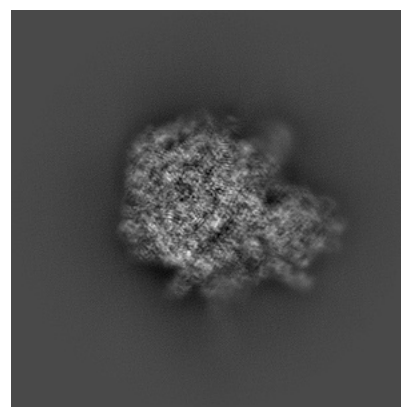
#### 6.1.2 Raw map



X



Y

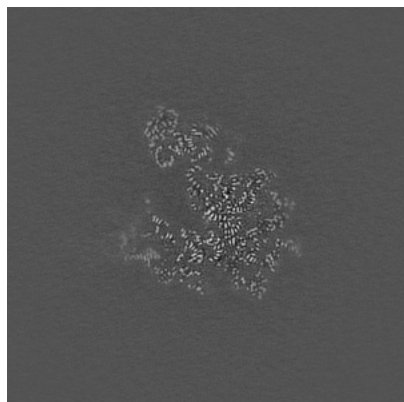


Z

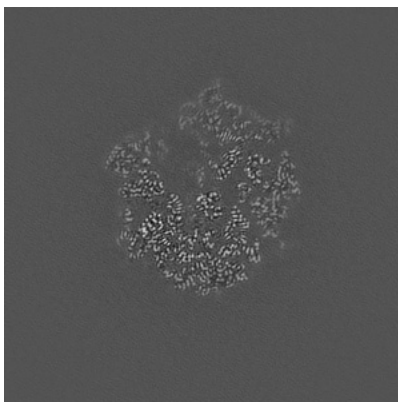
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

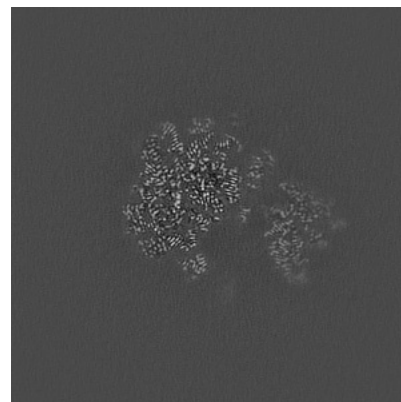
### 6.2.1 Primary map



X Index: 240

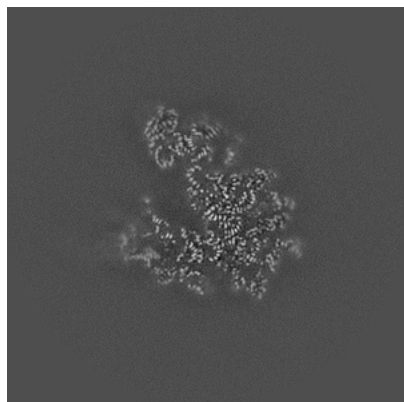


Y Index: 240

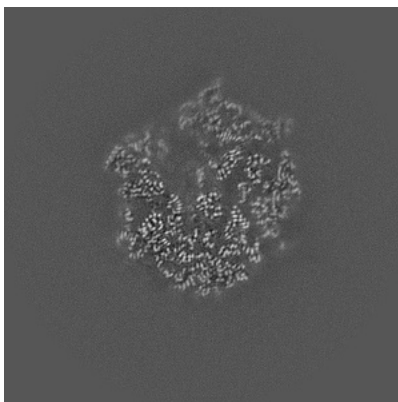


Z Index: 240

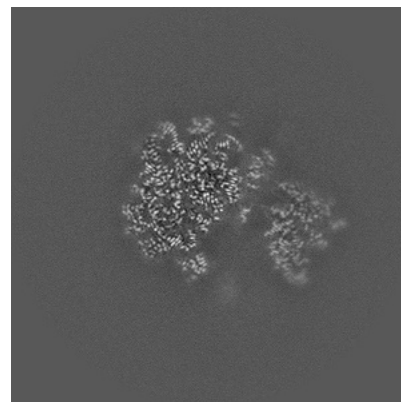
### 6.2.2 Raw map



X Index: 240



Y Index: 240



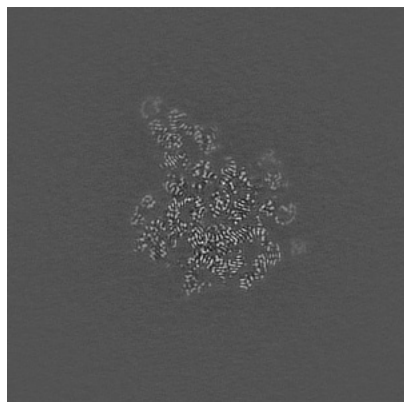
Z Index: 240

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

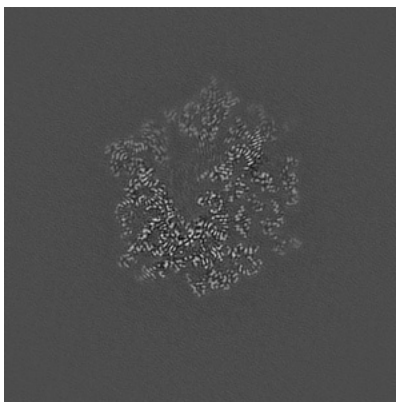


## 6.3 Largest variance slices [i](#)

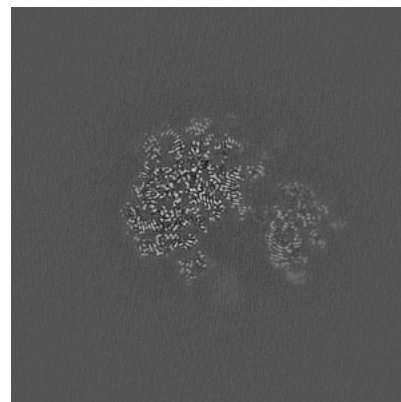
### 6.3.1 Primary map



X Index: 220

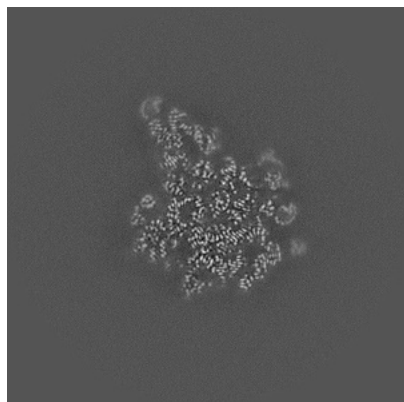


Y Index: 232

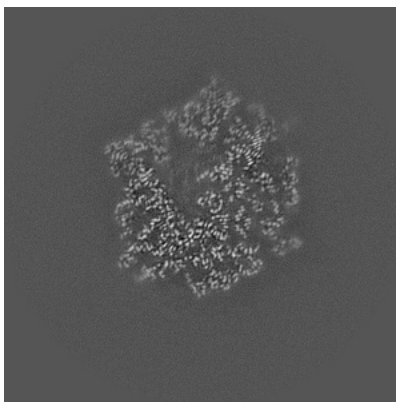


Z Index: 237

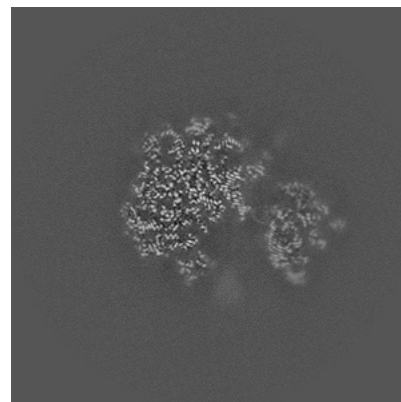
### 6.3.2 Raw map



X Index: 220



Y Index: 232



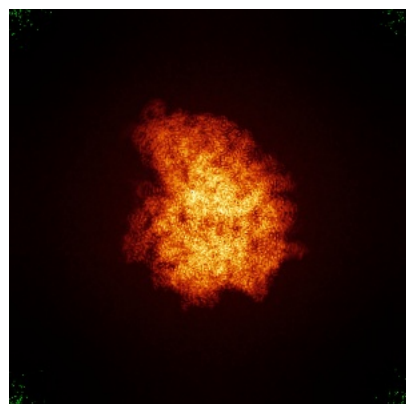
Z Index: 237

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

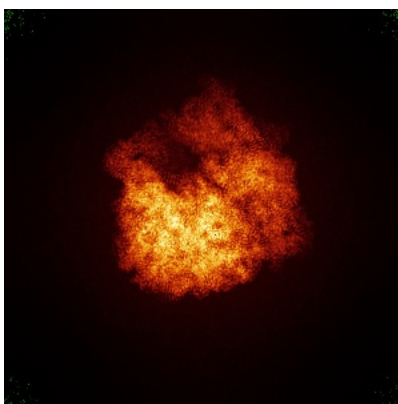


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

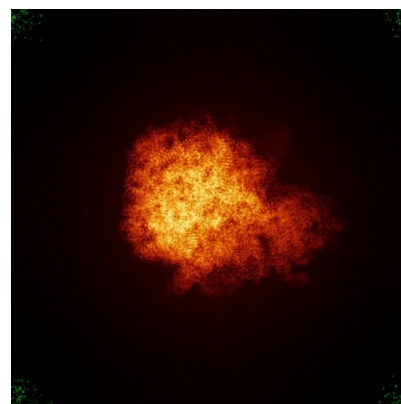
### 6.4.1 Primary map



X

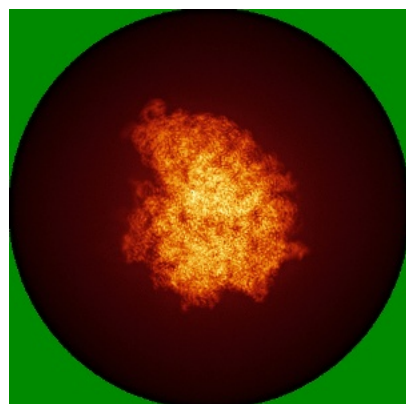


Y

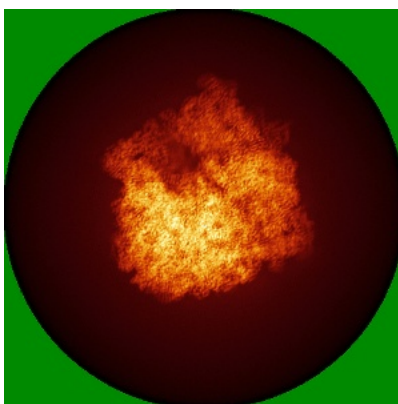


Z

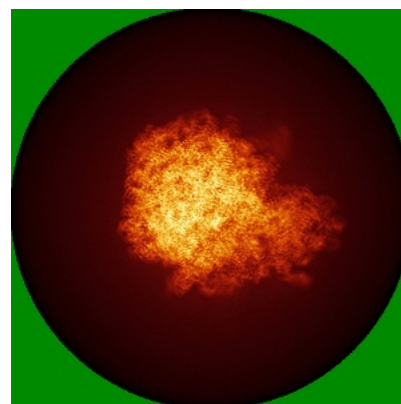
### 6.4.2 Raw map



X



Y

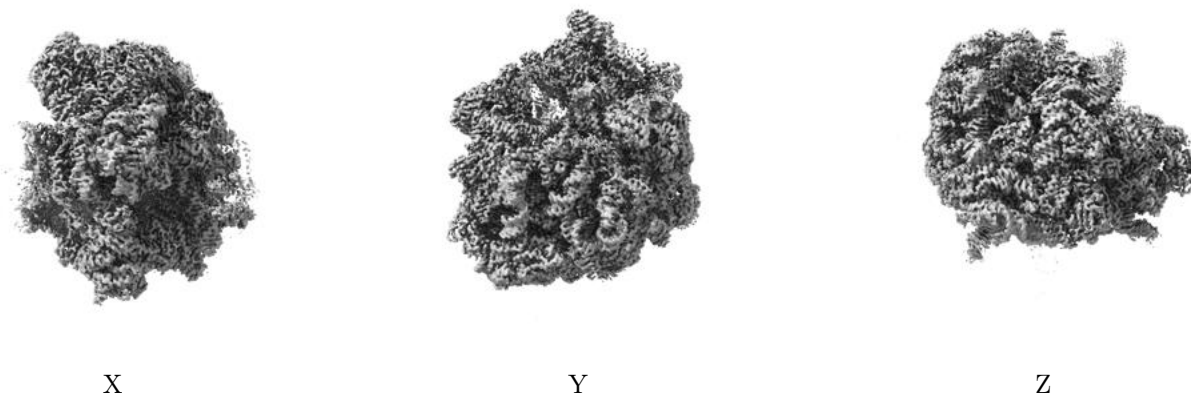


Z

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

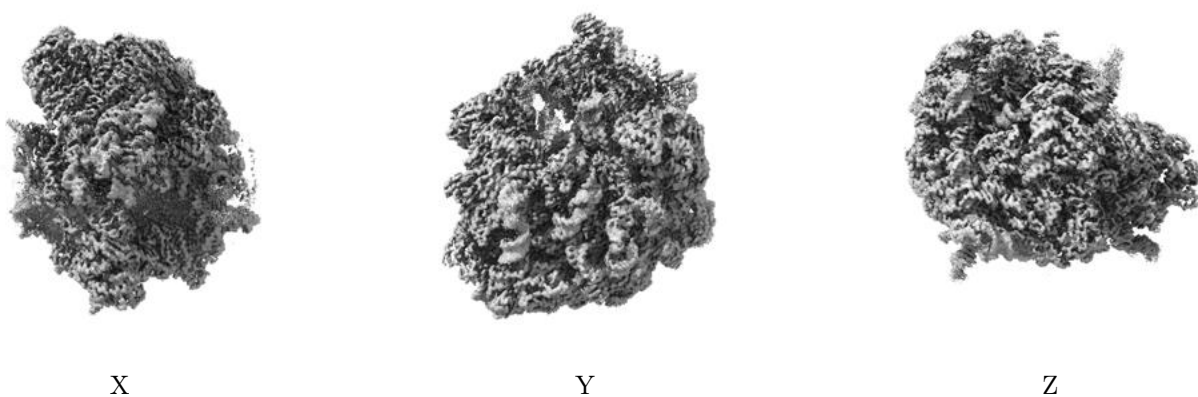
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

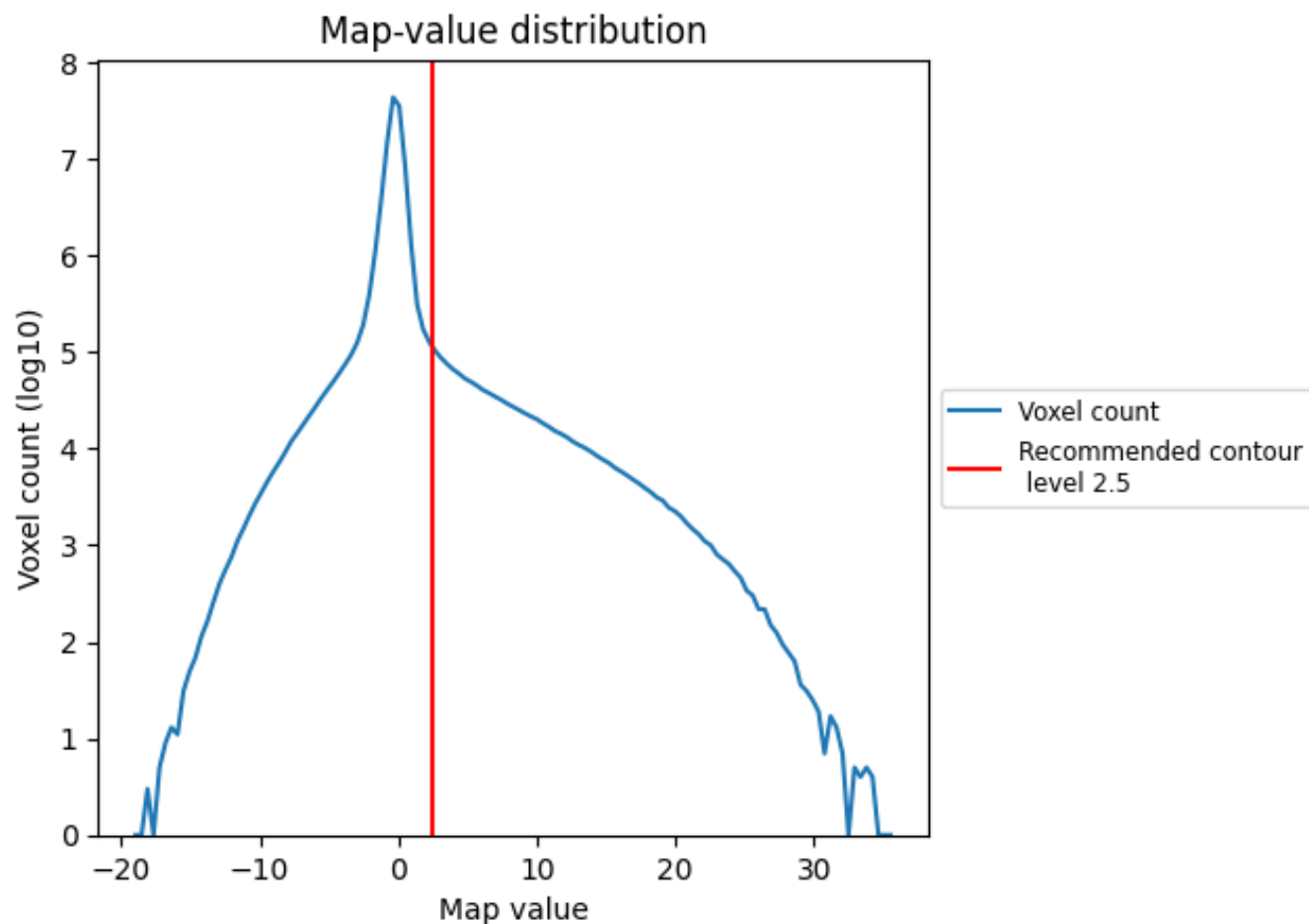
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

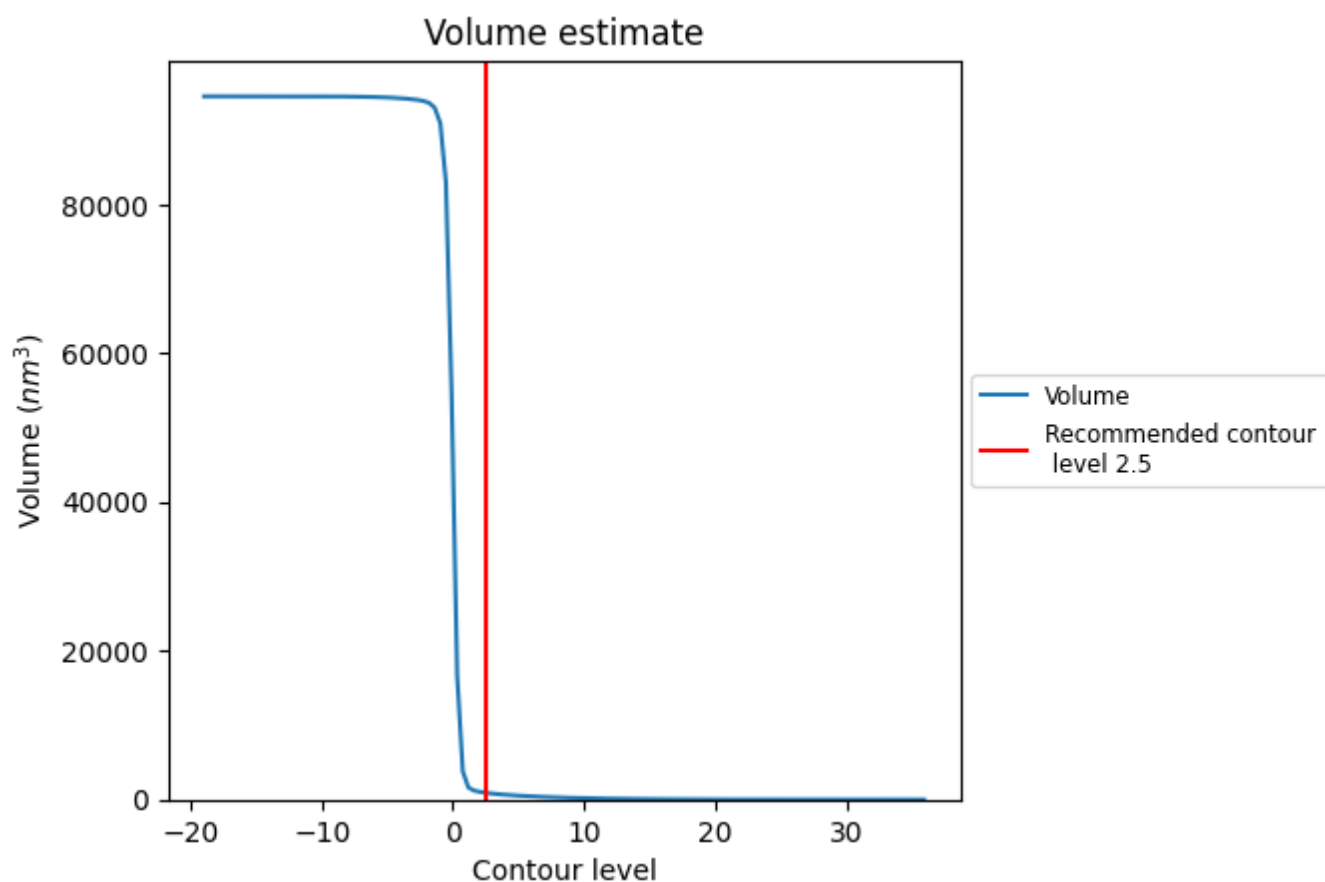
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

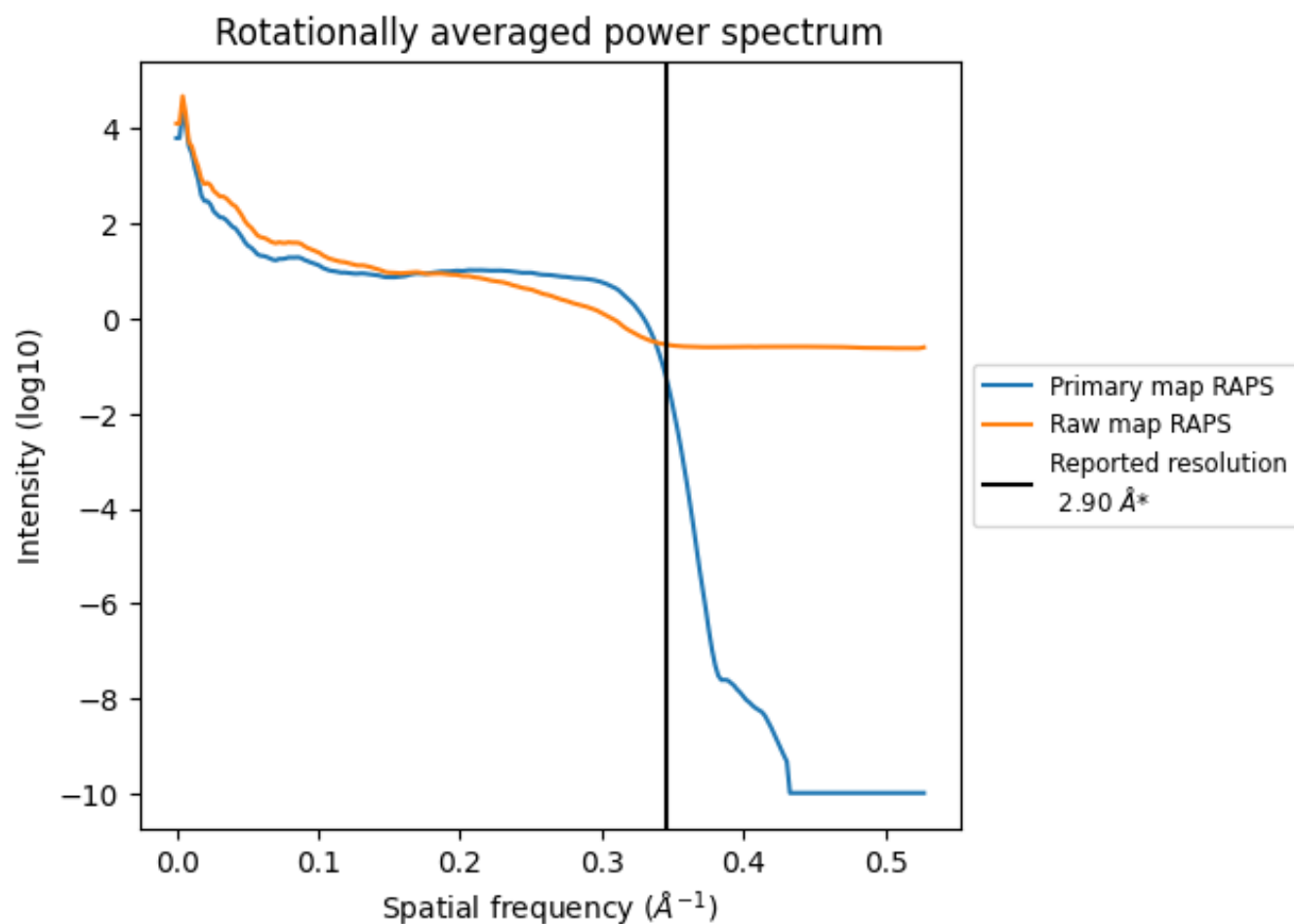
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 914 nm<sup>3</sup>; this corresponds to an approximate mass of 826 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

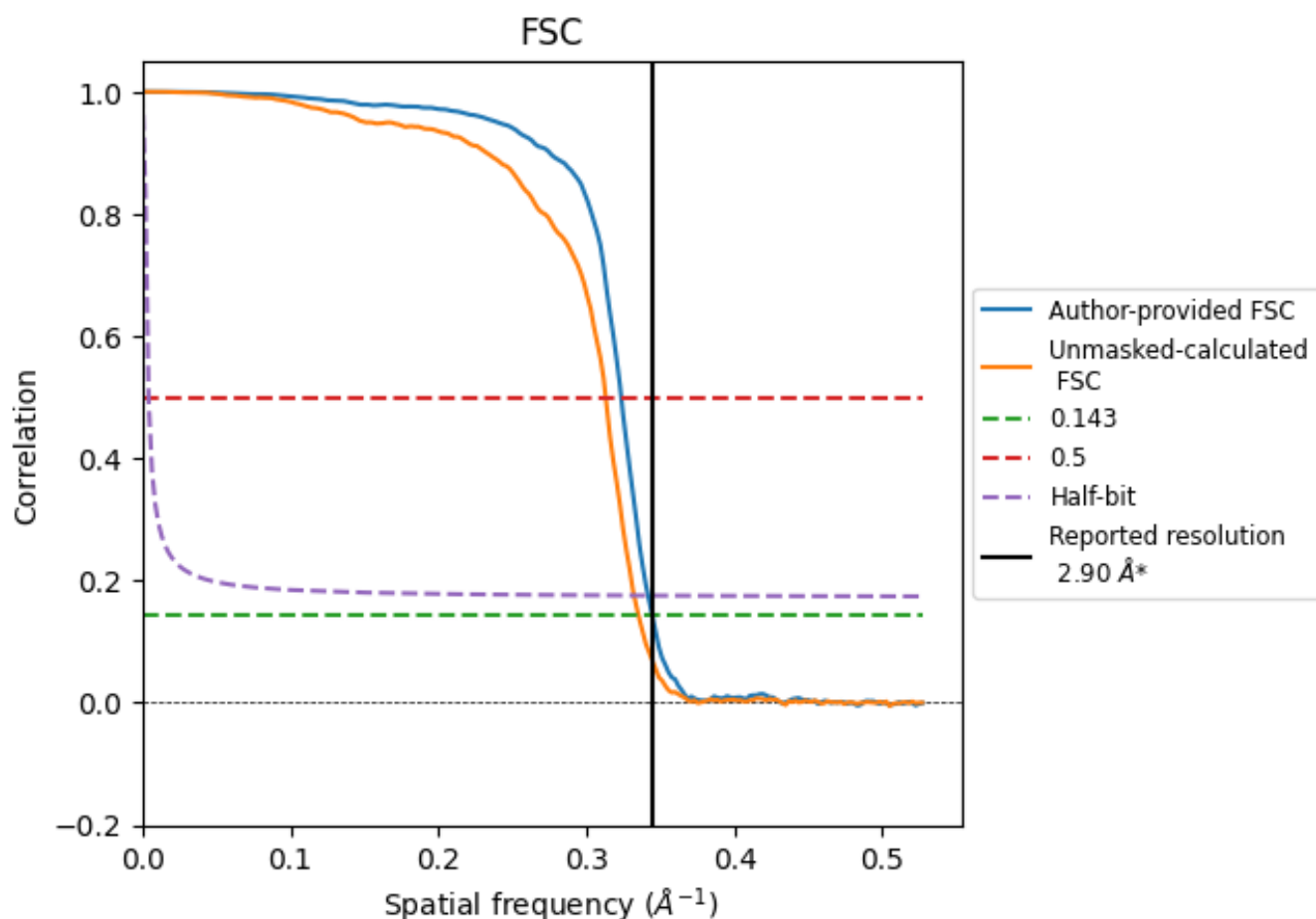


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

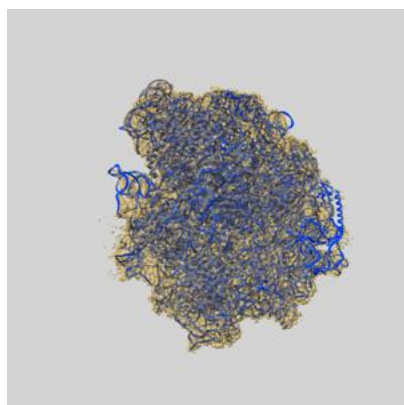
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.09	2.93
Unmasked-calculated*	2.98	3.19	3.01

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

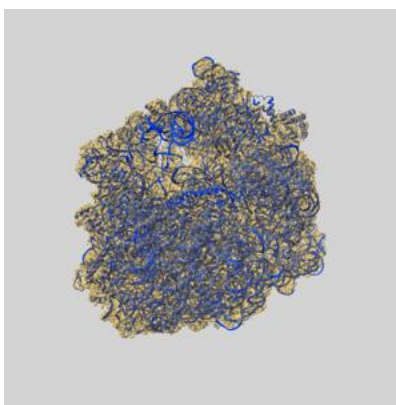
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75668 and PDB model 11FV. Per-residue inclusion information can be found in section [3](#) on page [15](#).

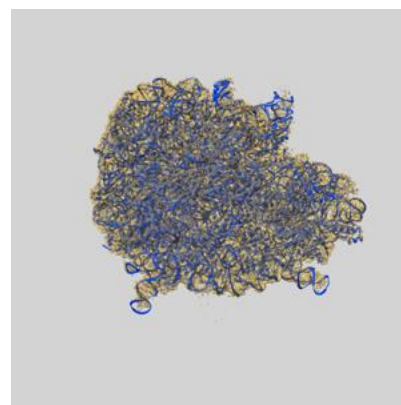
### 9.1 Map-model overlay [i](#)



X



Y

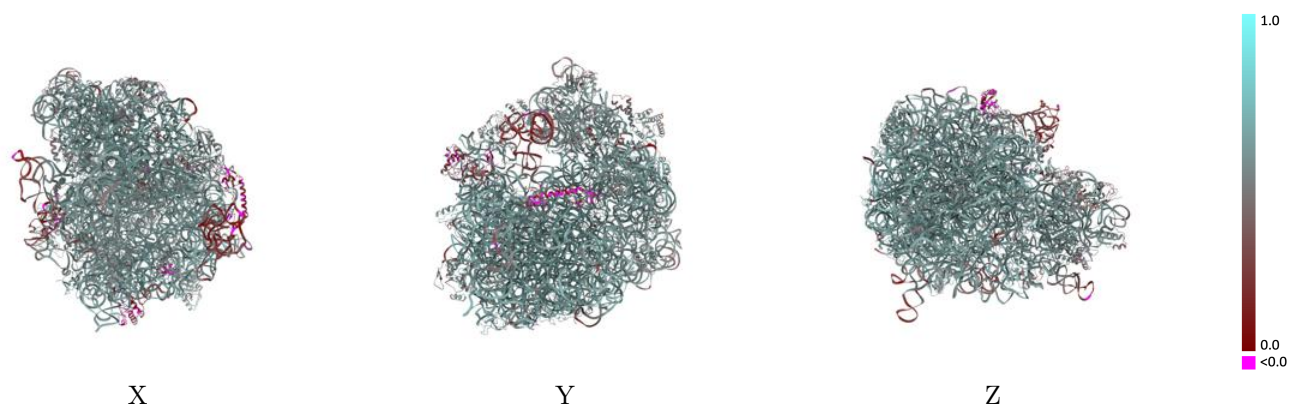


Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

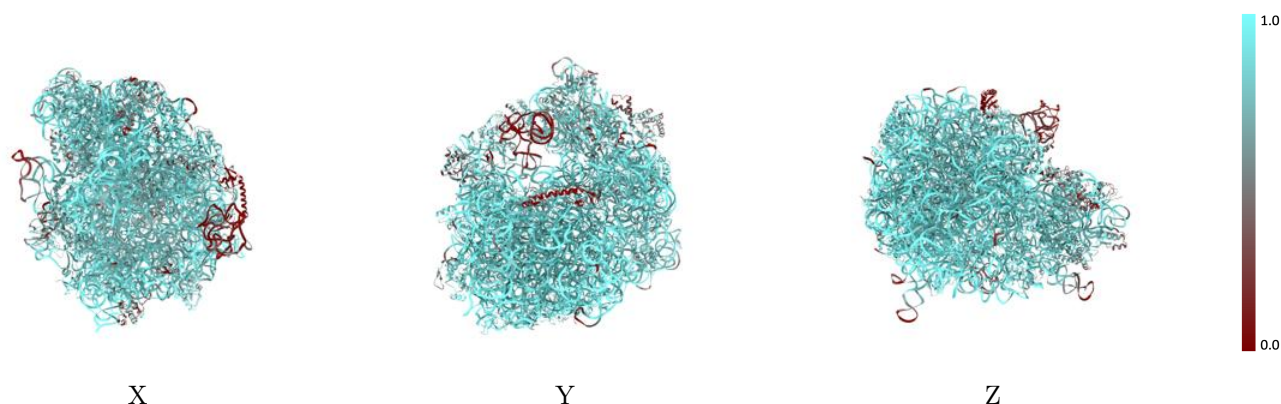


## 9.2 Q-score mapped to coordinate model [i](#)



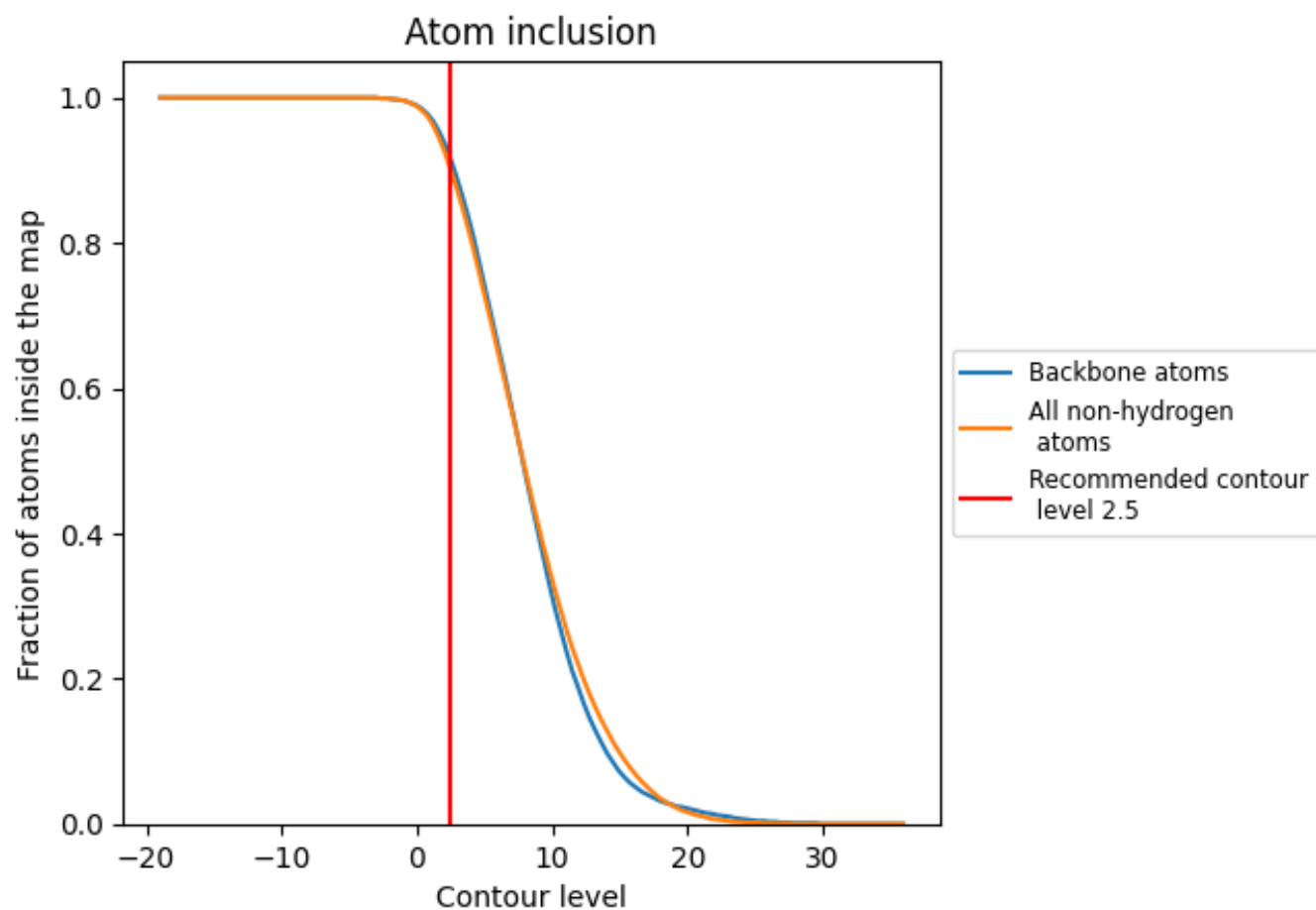
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).







































































## 9.4 Atom inclusion [i](#)



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

## 9.5 Map-model fit summary ⓘ





































The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.5760
0	 0.9160	 0.6130
1	 0.7590	 0.4840
2	 0.8880	 0.5760
3	 0.4860	 0.4210
C	 0.9430	 0.5850
D	 0.5210	 0.4760
E	 0.7840	 0.5410
F	 0.7920	 0.5450
G	 0.9060	 0.5870
H	 0.7950	 0.5070
I	 0.9360	 0.5940
J	 0.9750	 0.6030
K	 0.9480	 0.6130
L	 0.9490	 0.6190
M	 0.8440	 0.5510
N	 0.8050	 0.5440
O	 0.8600	 0.5620
P	 0.1460	 0.1470
Q	 0.7220	 0.5010
R	 0.9440	 0.6220
S	 0.9550	 0.6180
T	 0.9000	 0.5870
U	 0.9370	 0.6050
V	 0.9570	 0.6120
W	 0.4390	 0.1610
X	 0.9350	 0.6180
Y	 0.9700	 0.6230
Z	 0.9120	 0.5950
b	 0.8910	 0.5830
c	 0.8620	 0.5670
d	 0.8930	 0.5820
e	 0.9460	 0.6200
f	 0.9230	 0.6030
g	 0.8430	 0.5450



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Chain	Atom inclusion	Q-score
h	 0.9060	 0.5980
i	 0.9390	 0.6210
j	 0.1950	 0.1140
k	 0.9750	 0.6340
l	 0.9630	 0.6270
m	 0.9490	 0.6090
n	 0.5970	 0.5090
o	 0.9050	 0.5980
p	 0.6880	 0.4900
q	 0.6620	 0.5410
r	 0.8640	 0.5450
t	 0.9000	 0.5890
u	 0.7800	 0.5380
v	 0.7380	 0.4690
w	 0.9100	 0.5790
x	 0.8530	 0.5760
y	 0.8150	 0.5230
z	 0.9060	 0.5710