



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 11:27 AM UTC

PDB ID : 8CD1 / pdb_00008cd1
EMDB ID : EMD-16566
Title : 70S-PHIKZ014
Authors : Gerovac, M.; Vogel, J.
Deposited on : 2023-01-29
Resolution : 3.00 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

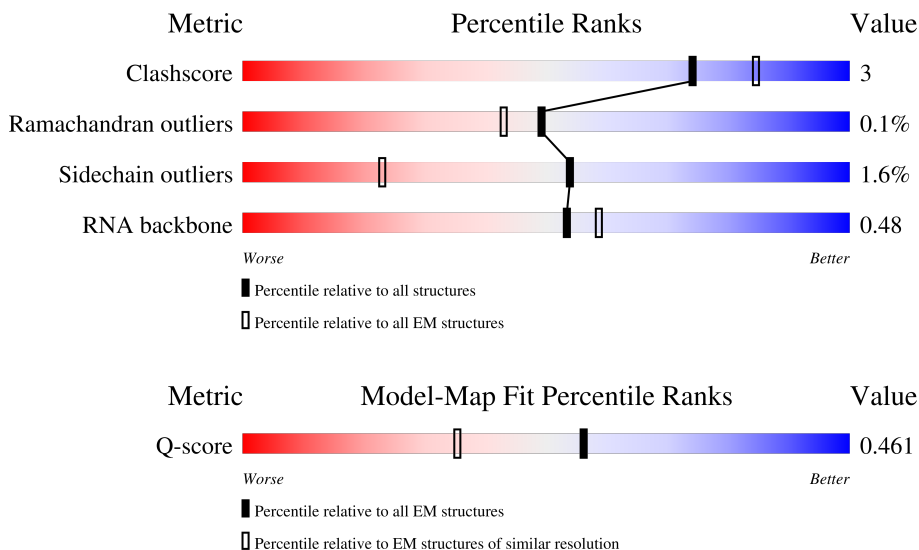
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	2	60	
2	4	44	
3	5	64	

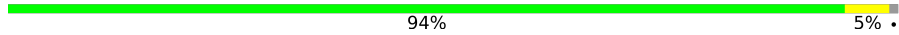
























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Mol	Chain	Length	Quality of chain
4	6	38	95% 5%
5	A	2888	67% 28% 6%
6	B	120	70% 20% 10%
7	C	273	89% 11%
8	D	211	86% 12%
9	Dt	76	57% 38% 5%
10	E	200	91% 8%
11	F	179	84% 12%
12	G	177	94%
13	H	148	45% 51% 47%
14	J	142	88% 11%
15	K	122	86% 12%
16	L	144	94% 5%
17	Le	71	13% 76% 17%
18	M	137	91% 8%
19	N	129	78% 13% 9%
20	O	116	91% 8%
21	P	116	87% 10%
22	Q	118	90% 9%
23	R	103	90% 9%
24	S	110	95% 5%
25	T	99	83% 10% 7%
26	U	104	8% 88% 12%
27	V	204	81% 10% 8%
28	W	85	76% 12% 11%

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Mol	Chain	Length	Quality of chain
29	X	78	 94% 5%
30	Y	63	 57% 22% 13% 6%
31	Z	58	 81% 17%
32	a	1526	 71% 26%
33	b	246	 14% 88% 7% 5%
34	c	228	 87% 10%
35	d	206	 91% 9%
36	e	166	 84% 10% 6%
37	f	139	 68% 7% 24%
38	g	156	 6% 92% 6%
39	h	130	 90% 9%
40	i	130	 75% 21%
41	j	103	 32% 81% 13% 7%
42	k	129	 81% 9% 11%
43	l	123	 88% 10%
44	m	118	 81% 10% 7%
45	n	101	 86% 11%
46	o	89	 92%
47	p	83	 87% 7% 6%
48	q	88	 77% 8% 14%
49	r	76	 12% 83% 8% 7%
50	s	91	 78% 10% 12%
51	t	91	 87% 7% 7%
52	u	71	 35% 82% 6% 13%
53	v	370	 12% 66% 6% 27%

2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 144789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	53	423	254	90	78	1	0	0

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4	44	376	228	91	55	2	1	0

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	5	63	506	314	108	81	3	0	0

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	6	38	303	184	69	46	4	0	0

- Molecule 5 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	A	2883	61859	27600	11347	20030	2882	0	0

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	B	120	2555	1141	455	839	120	0	0

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	271	2048	1258	422	362	6	0	0

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	207	1549	960	297	287	5	0	0

- Molecule 9 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	Dt	76	1623	723	290	534	76	0	0

- Molecule 10 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	E	199	1509	948	281	278	2	0	0

- Molecule 11 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	F	174	1288	811	228	246	3	0	0

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	173	1294	815	238	239	2	0	0

- Molecule 13 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	H	78	577	363	104	110	0	0

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	141	Total	C	N	O	S	0	0
			1122	713	205	201	3		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	120	Total	C	N	O	S	0	0
			922	576	178	162	6		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	143	Total	C	N	O	S	0	0
			1055	648	213	192	2		

- Molecule 17 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Le	68	Total	C	N	O	S	0	0
			531	334	95	96	6		

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	135	Total	C	N	O	S	0	0
			1069	679	209	178	3		

- Molecule 19 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	118	Total	C	N	O	S	0	0
			945	590	190	160	5		

- Molecule 20 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

- Molecule 21 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	P	113	891	563	168	159	1	0	0

- Molecule 22 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Q	117	936	592	196	148		0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	R	102	801	509	154	136	2	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	S	109	825	510	160	152	3	0	0

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	T	92	701	449	124	128		0	0

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	103	800	503	152	143	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	V	188	1396	887	254	253	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	W	76	Total	C	N	O	0	0
			575	364	111	100		

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	77	Total	C	N	O	S	0	0
			626	389	134	101	2		

- Molecule 30 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	59	Total	C	N	O	S	0	0
			473	291	94	87	1		

- Molecule 31 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	57	Total	C	N	O	S	0	0
			445	277	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1526	Total	C	N	O	P	0	0
			32744	14606	6011	10602	1525		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	234	Total	C	N	O	S	0	0
			1821	1145	329	337	10		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	205	Total	C	N	O	S	0	0
			1627	1028	307	287	5		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	205	Total	C	N	O	S	0	0
			1603	991	311	296	5		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	156	Total	C	N	O	S	0	0
			1145	720	209	210	6		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	105	Total	C	N	O	S	0	0
			853	531	158	159	5		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	154	Total	C	N	O	S	0	0
			1190	747	227	211	5		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	129	Total	C	N	O	S	0	0
			982	618	173	185	6		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	127	Total	C	N	O	S	0	0
			1010	625	203	181	1		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	96	Total	C	N	O	S	0	0
			765	479	143	142	1		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	k	115	838	517	163	156	2	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	l	121	949	582	196	167	4	0	0

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	m	110	859	524	174	157	4	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	n	98	777	479	163	132	3	0	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	o	86	686	425	134	126	1	0	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	p	78	610	381	121	108	0	0

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	q	76	619	387	120	110	2	0	0

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	71	Total	C	N	O	S	0	0
			566	361	107	97	1		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	80	Total	C	N	O	S	0	0
			635	405	121	106	3		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	85	Total	C	N	O	S	0	0
			654	404	135	113	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	62	Total	C	N	O	S	0	0
			519	320	112	86	1		

- Molecule 53 is a protein called PHIKZ014.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	271	Total	C	N	O	S	0	0
			2262	1436	410	409	7		


- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

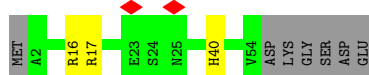
Mol	Chain	Residues	Atoms		AltConf
54	A	150	Total	Mg	0
			150	150	
54	C	1	Total	Mg	0
			1	1	
54	D	1	Total	Mg	0
			1	1	
54	P	1	Total	Mg	0
			1	1	
54	U	1	Total	Mg	0
			1	1	
54	a	17	Total	Mg	0
			17	17	

3 Residue-property plots [i](#)


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

- Molecule 1: 50S ribosomal protein L32

Chain 2:  83% 5% 12%




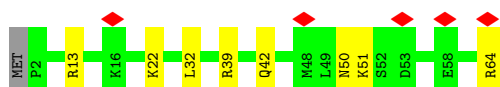
- Molecule 2: 50S ribosomal protein L34

Chain 4:  86% 14%



- Molecule 3: 50S ribosomal protein L35

Chain 5:  8% 86% 12%



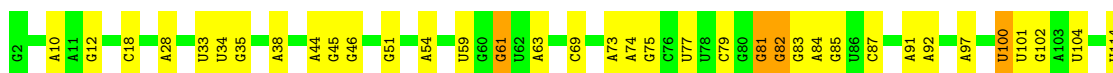
- Molecule 4: 50S ribosomal protein L36

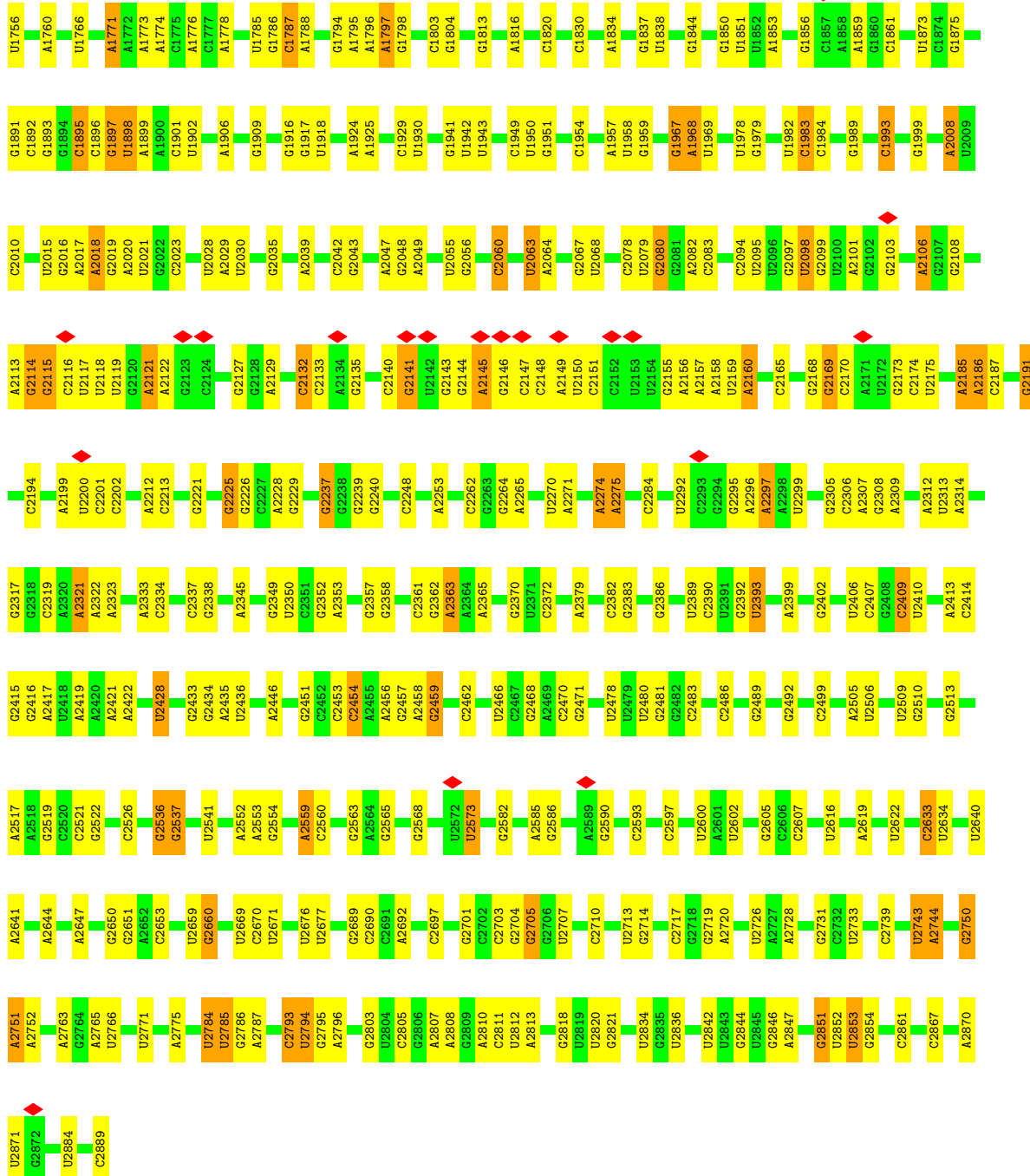
Chain 6:  95% 5%



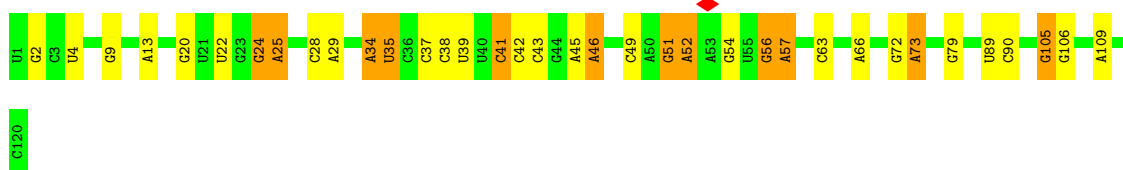
- Molecule 5: 23S rRNA

Chain A:  67% 28% 6%

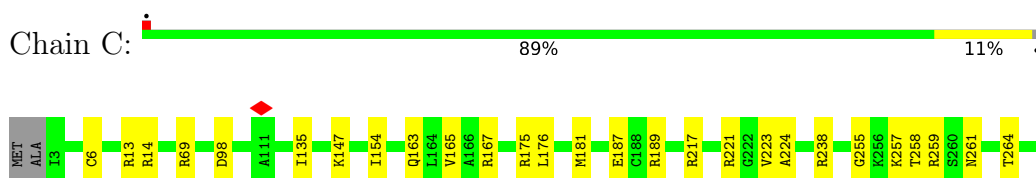




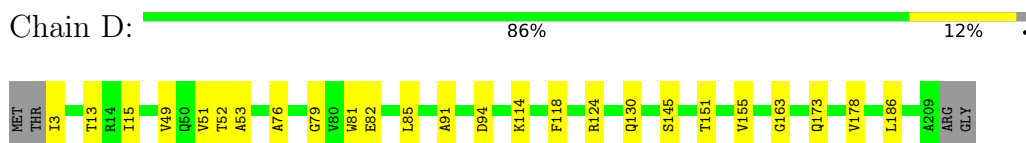
• Molecule 6: 5S rRNA



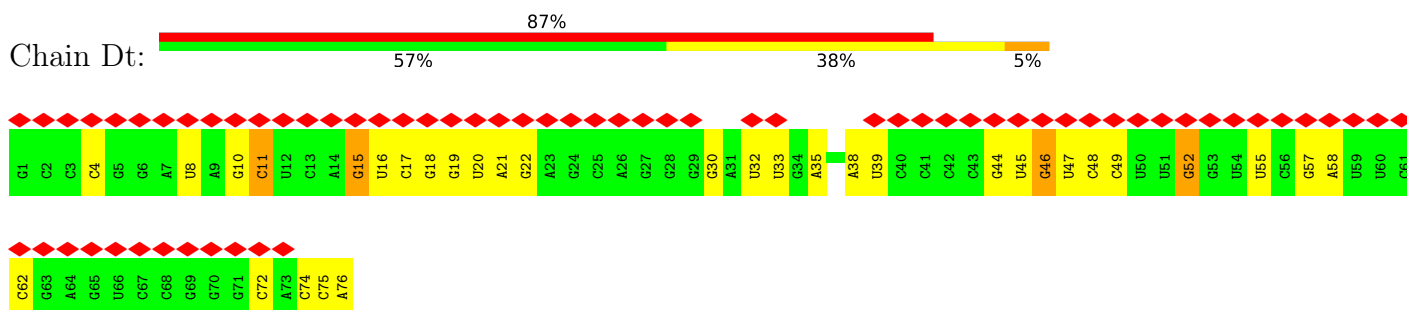
- Molecule 7: 50S ribosomal protein L2



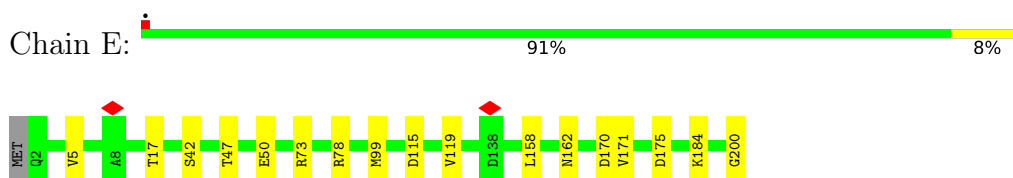
- Molecule 8: 50S ribosomal protein L3



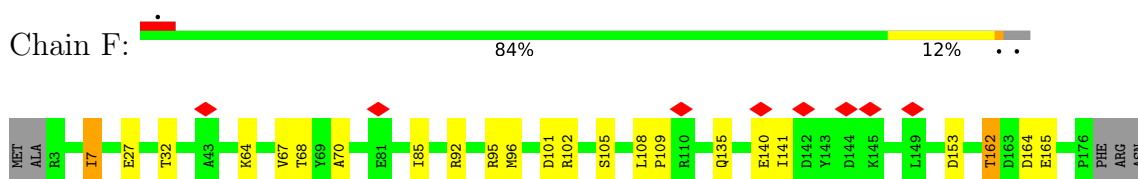
- Molecule 9: tRNA



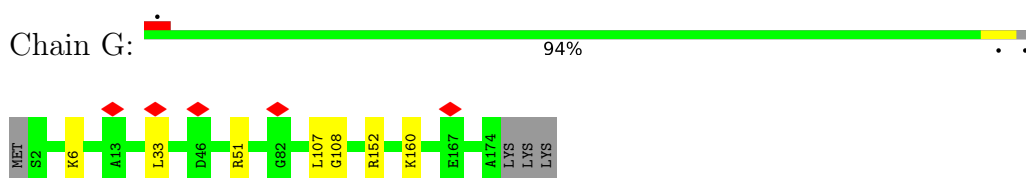
- Molecule 10: 50S ribosomal protein L4



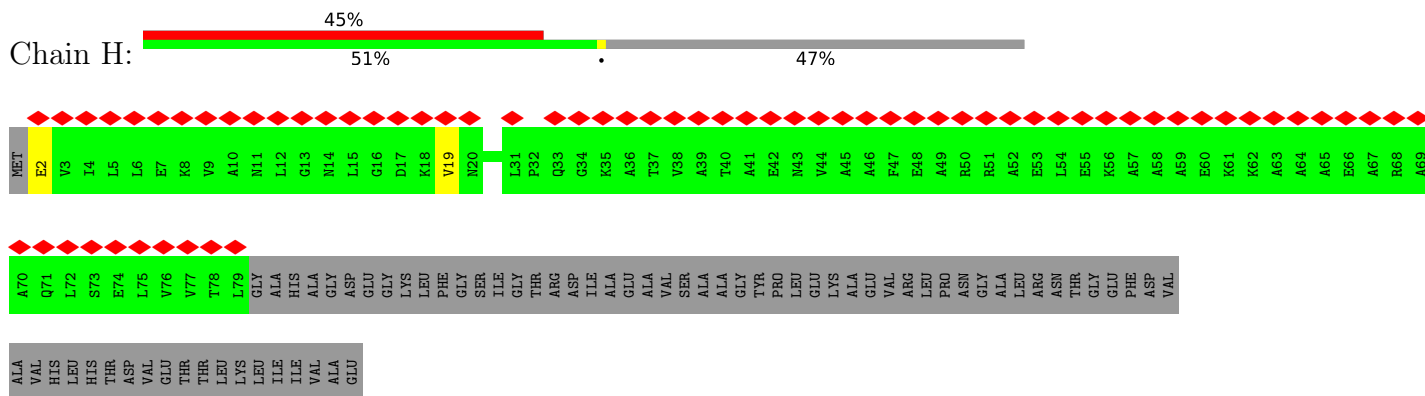
- Molecule 11: 50S ribosomal protein L5



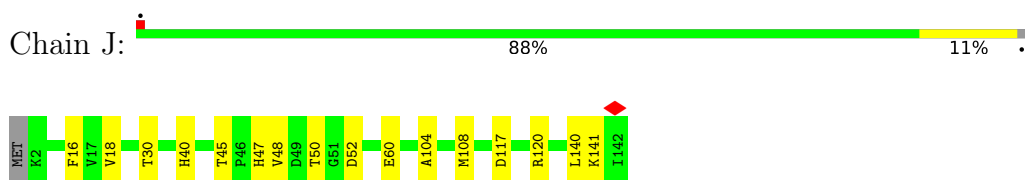
- Molecule 12: 50S ribosomal protein L6



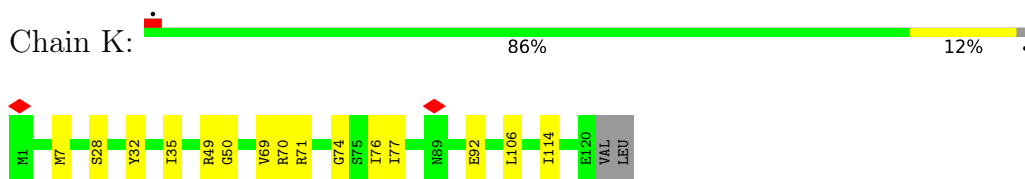
- Molecule 13: 50S ribosomal protein L9



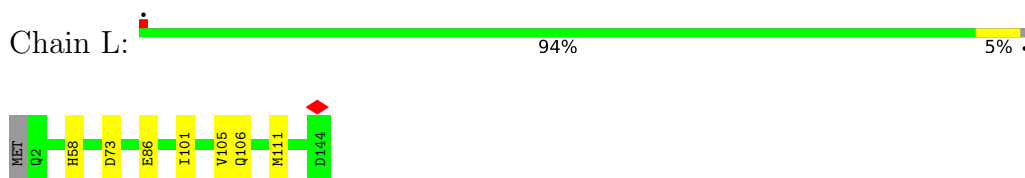
- Molecule 14: 50S ribosomal protein L13



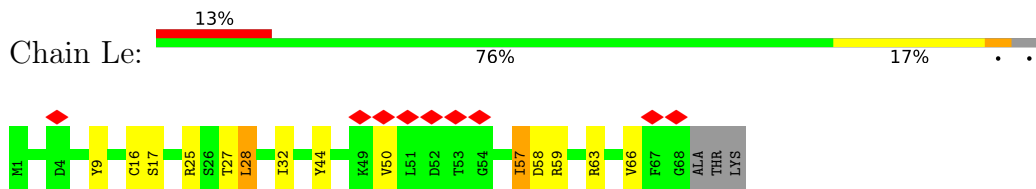
- Molecule 15: 50S ribosomal protein L14



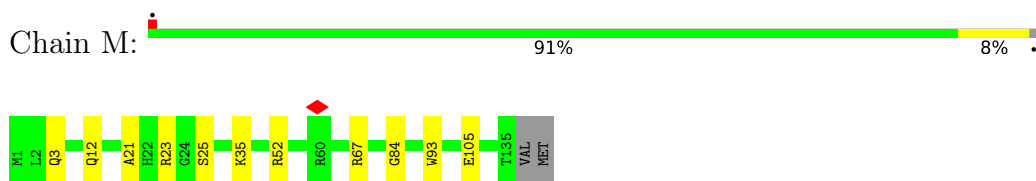
- Molecule 16: 50S ribosomal protein L15




- Molecule 17: 50S ribosomal protein L31



- Molecule 18: 50S ribosomal protein L16



- Molecule 19: 50S ribosomal protein L17

Chain N:  78% 13% 9%




• Molecule 20: 50S ribosomal protein L18

Chain O:  91% 8%




• Molecule 21: 50S ribosomal protein L19

Chain P:  87% 10%




• Molecule 22: 50S ribosomal protein L20

Chain Q:  90% 9%



• Molecule 23: 50S ribosomal protein L21

Chain R:  90% 9%




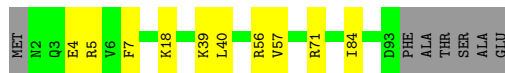
• Molecule 24: Large ribosomal subunit protein uL22

Chain S:  95% 5%

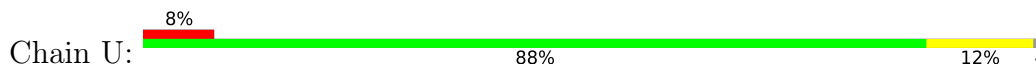


• Molecule 25: 50S ribosomal protein L23

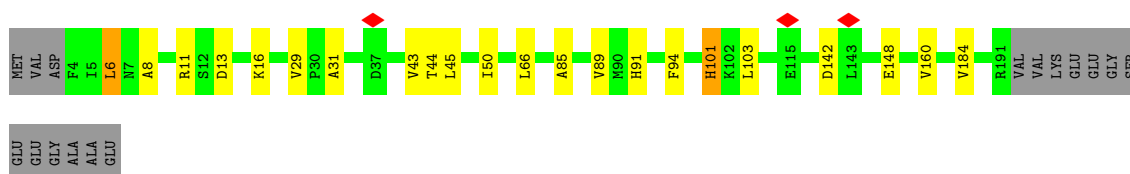
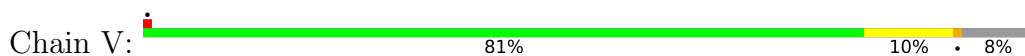
Chain T:  83% 10% 7%



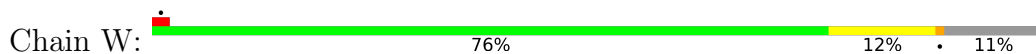
- Molecule 26: 50S ribosomal protein L24



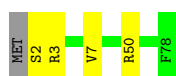
- Molecule 27: 50S ribosomal protein L25



- Molecule 28: 50S ribosomal protein L27



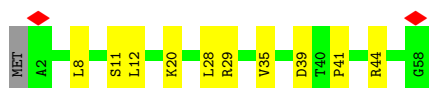
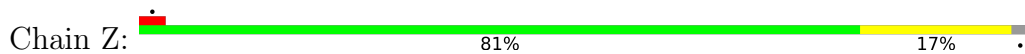
- Molecule 29: 50S ribosomal protein L28



- Molecule 30: 50S ribosomal protein L29

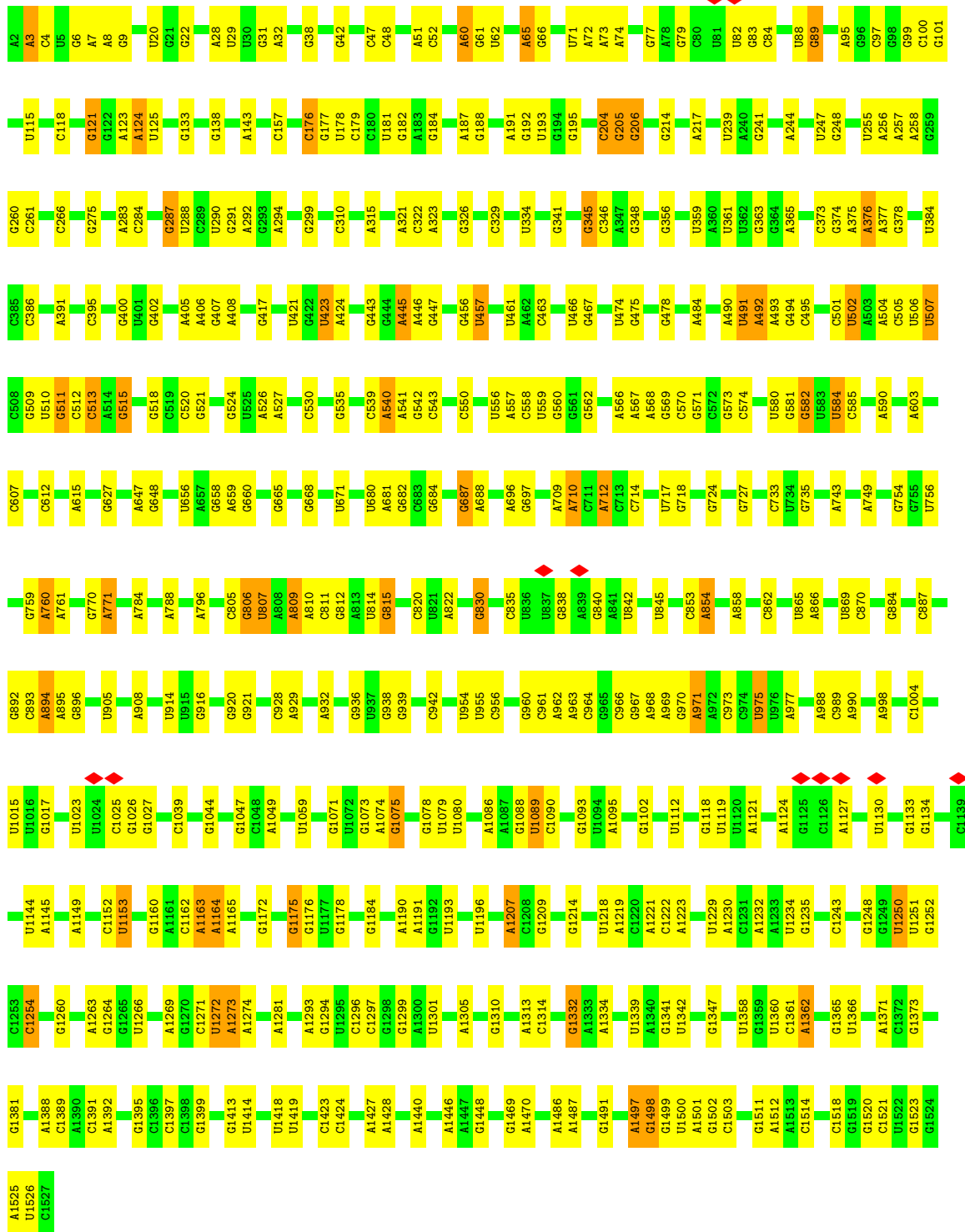


- Molecule 31: 50S ribosomal protein L30

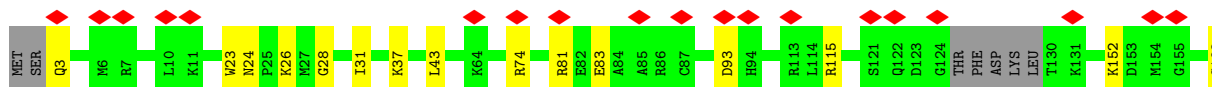
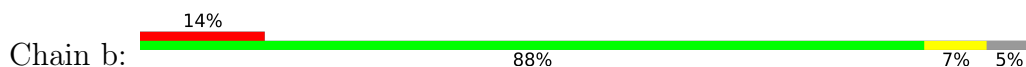


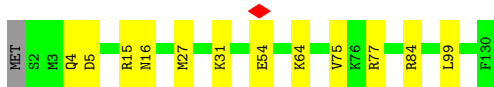
- Molecule 32: 16S rRNA



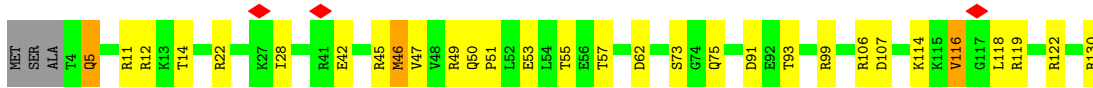
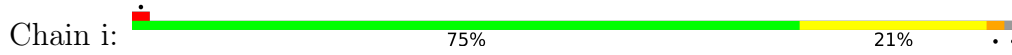


• Molecule 33: 30S ribosomal protein S2

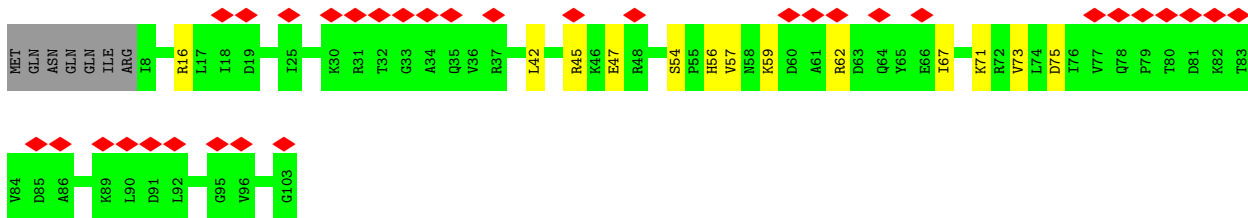
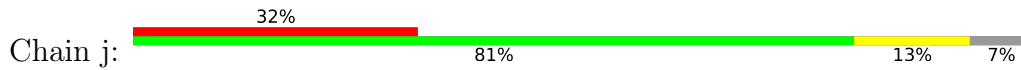




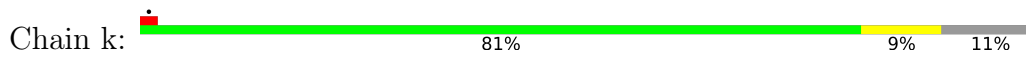
- Molecule 40: 30S ribosomal protein S9



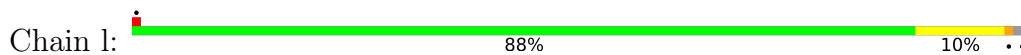
- Molecule 41: 30S ribosomal protein S10



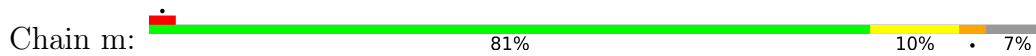
- Molecule 42: 30S ribosomal protein S11



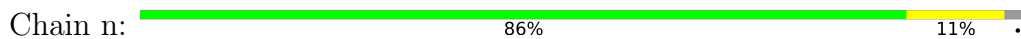
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13

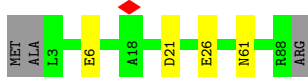
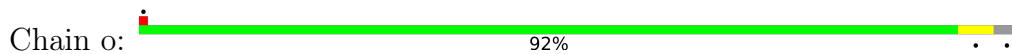


- Molecule 45: 30S ribosomal protein S14

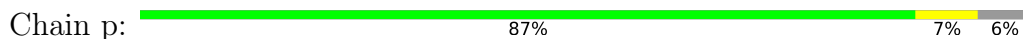




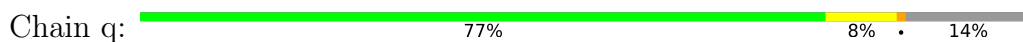
- Molecule 46: 30S ribosomal protein S15



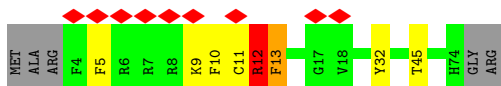
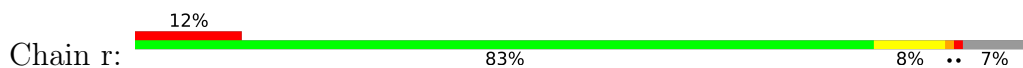
- Molecule 47: 30S ribosomal protein S16



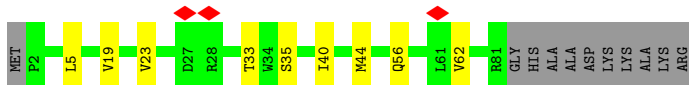
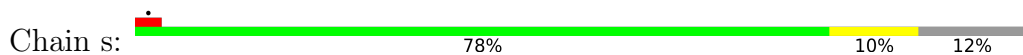
- Molecule 48: 30S ribosomal protein S17



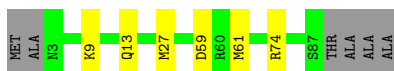
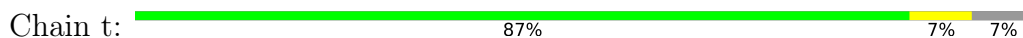
- Molecule 49: 30S ribosomal protein S18



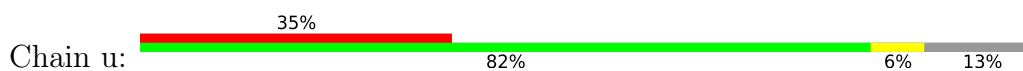
- Molecule 50: 30S ribosomal protein S19

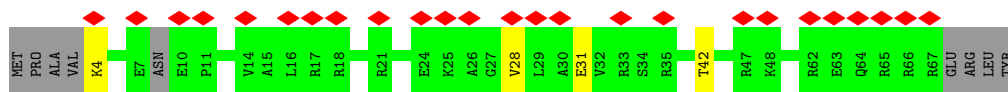


- Molecule 51: 30S ribosomal protein S20

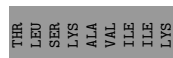
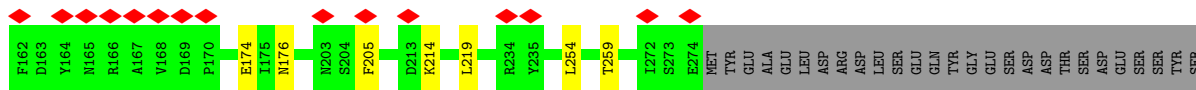
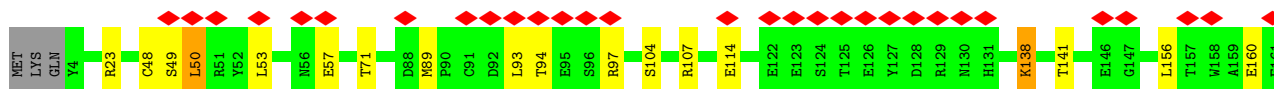


- Molecule 52: 30S ribosomal protein S21





• Molecule 53: PHIKZ014



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	169672	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	88.28	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	26.120	Depositor
Minimum map value	-7.773	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.894	Depositor
Recommended contour level	3.46	Depositor
Map size (Å)	544.512, 544.512, 544.512	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.15	0/429	0.36	0/572
2	4	0.18	0/379	0.43	0/496
3	5	0.15	0/511	0.40	0/668
4	6	0.18	0/304	0.35	0/399
5	A	0.13	0/69275	0.31	2/108063 (0.0%)
6	B	0.12	0/2855	0.31	0/4447
7	C	0.17	0/2084	0.39	0/2800
8	D	0.17	0/1572	0.42	0/2118
9	Dt	0.17	0/1813	0.47	0/2823
10	E	0.15	0/1529	0.38	0/2060
11	F	0.22	0/1304	0.46	0/1766
12	G	0.17	0/1311	0.39	0/1767
13	H	0.15	0/580	0.39	0/781
14	J	0.18	0/1148	0.38	0/1549
15	K	0.19	0/931	0.40	0/1247
16	L	0.16	0/1067	0.40	0/1422
17	Le	0.23	0/542	0.41	0/728
18	M	0.19	0/1089	0.37	0/1456
19	N	0.17	0/960	0.40	0/1282
20	O	0.15	0/888	0.37	0/1183
21	P	0.17	0/900	0.40	0/1203
22	Q	0.17	0/946	0.44	0/1257
23	R	0.18	0/814	0.40	0/1091
24	S	0.16	0/829	0.39	0/1104
25	T	0.17	0/710	0.40	0/953
26	U	0.21	0/808	0.46	0/1079
27	V	0.16	0/1419	0.41	0/1925
28	W	0.22	0/583	0.56	0/774
29	X	0.17	0/637	0.42	0/849
30	Y	0.43	0/474	0.71	2/632 (0.3%)
31	Z	0.16	0/449	0.36	0/602
32	a	0.12	0/36667	0.29	0/57202

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.16	0/1849	0.37	0/2486
34	c	0.16	0/1656	0.41	0/2232
35	d	0.14	0/1622	0.38	0/2171
36	e	0.19	0/1159	0.43	0/1559
37	f	0.15	0/867	0.32	0/1167
38	g	0.15	0/1207	0.39	0/1616
39	h	0.18	0/993	0.39	0/1332
40	i	0.18	0/1022	0.41	0/1365
41	j	0.19	0/775	0.38	0/1046
42	k	0.15	0/854	0.36	0/1159
43	l	0.18	0/963	0.40	0/1292
44	m	0.16	0/867	0.39	0/1165
45	n	0.16	0/787	0.38	0/1048
46	o	0.14	0/693	0.35	0/926
47	p	0.16	0/621	0.34	0/837
48	q	0.17	0/627	0.40	0/844
49	r	0.23	0/575	2.14	3/771 (0.4%)
50	s	0.16	0/649	0.38	0/874
51	t	0.16	0/661	0.43	0/881
52	u	0.15	0/524	0.40	0/689
53	v	0.17	0/2323	0.38	0/3138
All	All	0.14	0/157101	0.35	7/234896 (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
5	A	1	0
8	D	0	1
23	R	0	1
49	r	0	1
All	All	1	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	r	12	ARG	O-C-N	-56.99	31.82	123.00
49	r	12	ARG	CA-C-N	-8.67	104.98	121.54
49	r	12	ARG	C-N-CA	-8.67	104.98	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1895	C	C1'-C2'-O2'	6.80	118.59	108.40
5	A	1895	C	C3'-C2'-O2'	6.69	120.73	110.70
30	Y	15	GLU	N-CA-C	-5.95	106.56	113.88
30	Y	12	GLN	N-CA-C	-5.20	104.87	111.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1897	G	C1'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	151	THR	Peptide
23	R	51	LEU	Peptide
49	r	12	ARG	Mainchain

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	2	423	0	420	4	0
2	4	376	0	421	4	0
3	5	506	0	569	6	0
4	6	303	0	341	2	0
5	A	61859	0	31109	266	0
6	B	2555	0	1294	16	0
7	C	2048	0	2097	21	0
8	D	1549	0	1560	19	0
9	Dt	1623	0	821	10	0
10	E	1509	0	1563	13	0
11	F	1288	0	1254	15	0
12	G	1294	0	1344	4	0
13	H	577	0	606	1	0
14	J	1122	0	1148	10	0
15	K	922	0	992	12	0
16	L	1055	0	1096	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Le	531	0	532	10	0
18	M	1069	0	1139	8	0
19	N	945	0	989	11	0
20	O	881	0	920	10	0
21	P	891	0	950	8	0
22	Q	936	0	1025	11	0
23	R	801	0	830	8	0
24	S	825	0	885	3	0
25	T	701	0	735	5	0
26	U	800	0	864	5	0
27	V	1396	0	1415	14	0
28	W	575	0	598	11	0
29	X	626	0	649	2	0
30	Y	473	0	502	29	0
31	Z	445	0	472	7	0
32	a	32744	0	16477	153	0
33	b	1821	0	1847	10	0
34	c	1627	0	1657	6	0
35	d	1603	0	1624	15	0
36	e	1145	0	1192	12	0
37	f	853	0	828	6	0
38	g	1190	0	1227	5	0
39	h	982	0	1036	10	0
40	i	1010	0	1052	22	0
41	j	765	0	801	9	0
42	k	838	0	830	8	0
43	l	949	0	996	10	0
44	m	859	0	898	9	0
45	n	777	0	818	8	0
46	o	686	0	709	4	0
47	p	610	0	612	3	0
48	q	619	0	659	6	0
49	r	566	0	577	32	0
50	s	635	0	662	6	0
51	t	654	0	699	5	0
52	u	519	0	548	4	0
53	v	2262	0	2213	12	0
54	A	150	0	0	0	0
54	C	1	0	0	0	0
54	D	1	0	0	0	0
54	P	1	0	0	0	0
54	U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	a	17	0	0	0	0
All	All	144789	0	97102	723	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (723) 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)
49:r:9:LYS:O	49:r:12:ARG:CB	1.66	1.40
49:r:5:PHE:CE2	49:r:9:LYS:CE	2.11	1.31
49:r:11:CYS:C	49:r:12:ARG:HA	1.60	1.27
49:r:5:PHE:CE2	49:r:9:LYS:HE3	1.73	1.22
49:r:9:LYS:O	49:r:12:ARG:HB3	1.24	1.13
49:r:5:PHE:HE2	49:r:9:LYS:NZ	1.45	1.12
49:r:5:PHE:CE2	49:r:9:LYS:NZ	2.17	1.10
30:Y:5:LEU:HA	30:Y:8:LYS:HD3	1.42	1.00
49:r:11:CYS:C	49:r:12:ARG:HG3	1.86	0.99
49:r:9:LYS:O	49:r:12:ARG:N	1.95	0.96
49:r:9:LYS:O	49:r:12:ARG:CA	2.14	0.96
49:r:5:PHE:CD2	49:r:9:LYS:HE3	2.00	0.95
49:r:11:CYS:C	49:r:12:ARG:CA	2.39	0.95
30:Y:17:LEU:HD21	30:Y:49:ILE:HG23	1.48	0.92
49:r:11:CYS:CA	49:r:12:ARG:HA	1.91	0.92
5:A:735:G:HO2'	5:A:738:G:HO2'	1.09	0.89
49:r:9:LYS:C	49:r:12:ARG:CB	2.49	0.85
49:r:9:LYS:O	49:r:12:ARG:HB2	1.75	0.85
5:A:626:G:HO2'	5:A:628:G:HO2'	1.19	0.81
49:r:5:PHE:CZ	49:r:9:LYS:CE	2.64	0.80
49:r:9:LYS:C	49:r:12:ARG:HB2	2.06	0.80
5:A:1061:G:HO2'	5:A:1079:A:HO2'	1.26	0.79
5:A:2670:C:O2	15:K:70:ARG:NH2	2.17	0.77
9:Dt:45:U:O2'	9:Dt:46:G:OP1	2.03	0.77
32:a:176:C:N4	32:a:217:A:O2'	2.18	0.76
49:r:5:PHE:HE2	49:r:9:LYS:HZ1	0.77	0.76
5:A:1830:C:O2'	7:C:255:GLY:O	2.02	0.76
5:A:1540:U:OP1	5:A:1708:U:O2'	2.03	0.75
34:c:134:MET:HE2	34:c:151:ILE:HG21	1.68	0.75
40:i:114:LYS:NZ	40:i:118:LEU:O	2.20	0.74
8:D:15:ILE:HD11	8:D:178:VAL:HG11	1.68	0.74
5:A:466:C:O2	5:A:470:A:N6	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1856:G:N2	5:A:1859:A:OP2	2.21	0.74
5:A:2659:U:O2'	5:A:2660:G:O5'	2.04	0.73
32:a:74:A:H62	32:a:89:G:H21	1.34	0.73
32:a:1089:U:OP1	32:a:1102:G:N2	2.21	0.73
49:r:11:CYS:C	49:r:12:ARG:CG	2.59	0.73
5:A:1766:U:OP2	5:A:1771:A:N6	2.21	0.73
9:Dt:52:G:N2	9:Dt:62:C:O2	2.18	0.73
32:a:195:G:O2'	32:a:463:C:O2'	2.06	0.73
5:A:2568:G:N2	5:A:2568:G:OP2	2.20	0.73
32:a:853:C:O2'	32:a:854:A:O5'	2.06	0.72
40:i:5:GLN:OE1	40:i:22:ARG:NH1	2.22	0.72
5:A:2392:G:O2'	5:A:2399:A:N6	2.22	0.72
32:a:291:G:N2	32:a:294:A:OP2	2.21	0.72
32:a:1172:G:N2	32:a:1175:G:OP2	2.22	0.72
5:A:2141:G:OP2	5:A:2143:G:N2	2.23	0.72
5:A:2775:A:O2'	5:A:2796:A:N3	2.21	0.72
3:5:13:ARG:NH1	16:L:58:HIS:O	2.23	0.72
5:A:2262:C:O2'	18:M:84:GLY:O	2.08	0.72
49:r:5:PHE:CZ	49:r:9:LYS:HE2	2.25	0.71
5:A:1191:A:N6	5:A:1227:U:O2'	2.23	0.71
5:A:1786:G:OP1	7:C:259:ARG:NH1	2.23	0.71
5:A:349:U:O2'	5:A:350:G:O5'	2.08	0.71
6:B:37:C:O2	20:O:99:HIS:NE2	2.24	0.71
5:A:1497:G:OP2	5:A:1497:G:N2	2.20	0.71
27:V:8:ALA:HB1	27:V:43:VAL:HG13	1.73	0.71
32:a:491:U:O2'	32:a:492:A:O5'	2.08	0.71
5:A:461:A:OP1	10:E:73:ARG:NH2	2.23	0.70
36:e:47:VAL:HG21	36:e:118:VAL:HG23	1.73	0.70
5:A:2098:U:OP1	5:A:2132:C:N4	2.25	0.70
32:a:971:A:N6	32:a:1218:U:O4'	2.24	0.70
37:f:38:ARG:NH2	37:f:97:THR:O	2.24	0.70
5:A:77:U:OP1	30:Y:51:ARG:NH1	2.24	0.70
49:r:12:ARG:HG2	49:r:13:PHE:H	1.57	0.70
32:a:1296:C:OP2	44:m:21:TYR:OH	2.10	0.70
32:a:356:G:N2	32:a:359:U:OP2	2.24	0.70
25:T:7:PHE:O	30:Y:28:ARG:NH2	2.23	0.69
5:A:2237:G:O2'	5:A:2483:C:OP1	2.09	0.69
5:A:1929:C:OP2	5:A:1930:U:O2'	2.06	0.69
5:A:977:C:O2'	5:A:990:A:N3	2.24	0.69
5:A:402:G:OP2	5:A:2393:U:O2'	2.11	0.69
5:A:2552:A:N6	15:K:28:SER:OG	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1271:C:O2'	32:a:1273:A:N7	2.26	0.69
5:A:1365:A:O2'	5:A:1367:G:OP2	2.10	0.69
4:6:6:SER:OG	5:A:2454:C:OP1	2.09	0.68
11:F:101:ASP:O	11:F:105:SER:OG	2.05	0.68
13:H:2:GLU:N	13:H:19:VAL:O	2.26	0.68
26:U:31:ASP:OD2	26:U:65:HIS:NE2	2.25	0.68
5:A:567:G:O2'	5:A:1241:A:OP1	2.11	0.68
5:A:2861:C:OP1	19:N:4:ARG:NH2	2.26	0.68
6:B:39:U:O2'	6:B:46:A:N1	2.26	0.68
32:a:395:C:O2'	32:a:615:A:N3	2.25	0.68
32:a:445:A:N6	32:a:474:U:O2'	2.26	0.68
32:a:1399:G:O2'	32:a:1512:A:O2'	2.06	0.68
7:C:135:ILE:O	7:C:167:ARG:NH2	2.27	0.68
49:r:10:PHE:O	49:r:12:ARG:C	2.25	0.68
5:A:1350:U:O2'	5:A:1796:A:N3	2.25	0.68
5:A:2456:A:N6	5:A:2468:G:O2'	2.21	0.68
32:a:421:U:O2'	32:a:535:G:OP1	2.08	0.68
5:A:2063:U:OP2	5:A:2225:G:N2	2.26	0.68
5:A:1671:G:OP2	5:A:1671:G:N2	2.26	0.68
16:L:101:ILE:HD11	16:L:105:VAL:HG11	1.76	0.68
5:A:2644:A:O2'	12:G:160:LYS:NZ	2.23	0.68
39:h:5:ASP:OD2	39:h:77:ARG:NH1	2.26	0.68
5:A:1774:A:OP1	7:C:238:ARG:NH2	2.26	0.67
32:a:809:A:N7	32:a:1503:C:O2'	2.26	0.67
34:c:186:THR:OG1	45:n:90:ARG:NH2	2.27	0.67
19:N:12:ARG:NH1	19:N:20:MET:SD	2.67	0.67
6:B:41:C:N4	11:F:67:VAL:O	2.27	0.67
5:A:912:C:O4'	28:W:29:GLN:NE2	2.27	0.67
32:a:204:C:OP2	32:a:205:G:N2	2.28	0.67
3:5:39:ARG:NE	5:A:2349:G:OP1	2.28	0.67
5:A:1017:A:O2'	5:A:1116:A:N6	2.23	0.67
5:A:28:A:N6	5:A:503:G:O2'	2.27	0.67
5:A:1441:U:O2	19:N:63:ARG:NE	2.27	0.67
32:a:176:C:O2'	32:a:178:U:OP2	2.12	0.67
32:a:187:A:O2'	51:t:59:ASP:OD2	2.12	0.67
5:A:248:G:O2'	5:A:2419:A:OP1	2.09	0.67
9:Dt:18:G:O2'	9:Dt:57:G:N2	2.27	0.67
5:A:444:A:O2'	5:A:445:A:OP1	2.12	0.67
5:A:986:A:O2'	22:Q:91:ASP:OD2	2.11	0.67
44:m:66:GLU:OE2	44:m:70:ARG:NE	2.27	0.66
5:A:81:G:HO2'	5:A:82:G:P	2.18	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:964:A:O2'	5:A:979:G:N2	2.27	0.66
5:A:966:G:O2'	5:A:1146:A:O2'	2.12	0.66
32:a:1371:A:O2'	32:a:1373:G:O6	2.13	0.66
7:C:271:ARG:NH1	7:C:272:ARG:O	2.28	0.66
33:b:24:ASN:ND2	33:b:192:SER:OG	2.28	0.66
32:a:687:G:OP1	42:k:127:ARG:NH2	2.28	0.66
5:A:38:A:N3	10:E:42:SER:OG	2.28	0.66
32:a:20:U:OP2	36:e:131:SER:OG	2.12	0.66
36:e:164:GLU:OE1	39:h:64:LYS:NZ	2.28	0.66
5:A:854:C:OP2	18:M:23:ARG:NH1	2.28	0.66
30:Y:8:LYS:HB3	30:Y:12:GLN:HG2	1.78	0.66
5:A:1897:G:O6	5:A:1909:G:N2	2.28	0.66
32:a:1243:C:O2'	40:i:75:GLN:NE2	2.28	0.66
5:A:2510:G:HO2'	5:A:2751:A:HO2'	1.43	0.66
17:Le:59:ARG:NE	32:a:1305:A:OP1	2.23	0.66
5:A:738:G:OP1	24:S:88:ARG:NH2	2.28	0.66
37:f:77:ASN:O	37:f:81:ASN:ND2	2.29	0.66
5:A:12:G:OP2	5:A:12:G:N2	2.29	0.66
5:A:1128:G:H21	14:J:108:MET:HE3	1.61	0.66
5:A:288:A:O2'	5:A:289:G:O4'	2.13	0.65
5:A:1672:G:O2'	5:A:1673:C:OP1	2.15	0.65
32:a:510:U:O2'	32:a:513:C:N3	2.29	0.65
42:k:93:ARG:NH2	42:k:112:ASP:OD1	2.29	0.65
32:a:656:U:O2'	32:a:830:G:OP1	2.10	0.65
5:A:314:A:N3	10:E:162:ASN:ND2	2.44	0.65
32:a:248:G:O2'	48:q:21:ASP:O	2.14	0.65
5:A:2671:U:OP2	21:P:52:ARG:NH1	2.29	0.65
32:a:8:A:N6	35:d:202:GLU:O	2.30	0.65
5:A:2509:U:O2'	5:A:2634:U:OP1	2.08	0.65
5:A:1710:A:O2'	5:A:1711:A:OP1	2.14	0.65
5:A:2106:A:O2'	5:A:2108:G:OP2	2.14	0.65
5:A:2750:G:O2'	5:A:2751:A:OP1	2.14	0.65
32:a:181:U:O2'	32:a:184:G:O6	2.09	0.65
5:A:2115:G:O2'	5:A:2160:A:O2'	2.13	0.65
32:a:1121:A:O2'	32:a:1274:A:N6	2.30	0.65
42:k:17:VAL:O	42:k:37:ARG:NH1	2.30	0.65
42:k:71:GLY:O	42:k:105:TYR:OH	2.12	0.65
5:A:434:A:O2'	5:A:435:C:OP2	2.13	0.64
32:a:1172:G:O6	40:i:99:ARG:NH2	2.30	0.64
32:a:511:G:N2	32:a:524:G:OP1	2.30	0.64
32:a:1389:C:HO2'	32:a:1395:G:HO2'	1.34	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1941:G:O2'	5:A:1943:U:O4	2.07	0.64
5:A:2633:C:OP2	5:A:2719:G:O2'	2.16	0.64
5:A:1061:G:O2'	5:A:1079:A:O2'	2.07	0.64
5:A:2653:C:N4	12:G:108:GLY:O	2.29	0.64
33:b:115:ARG:NH2	33:b:152:LYS:O	2.30	0.64
5:A:619:C:O2	5:A:629:U:O2'	2.16	0.64
32:a:905:U:OP2	43:l:94:ARG:NH2	2.31	0.64
38:g:113:GLU:O	38:g:119:ARG:NH2	2.31	0.64
49:r:11:CYS:C	49:r:12:ARG:CB	2.70	0.64
5:A:177:G:OP2	5:A:177:G:N2	2.24	0.64
14:J:117:ASP:OD1	14:J:120:ARG:NH2	2.31	0.64
49:r:12:ARG:HG2	49:r:13:PHE:N	2.11	0.64
5:A:514:C:O2	5:A:544:U:O2'	2.16	0.63
49:r:5:PHE:CE2	49:r:9:LYS:HE2	2.25	0.63
31:Z:41:PRO:HA	53:v:176:ASN:HD21	1.62	0.63
5:A:681:C:OP1	7:C:217:ARG:NH1	2.30	0.63
5:A:772:A:O2'	7:C:224:ALA:O	2.17	0.63
32:a:842:U:OP1	33:b:37:LYS:NZ	2.21	0.63
40:i:55:THR:HG23	40:i:57:THR:HG22	1.80	0.63
5:A:462:A:OP1	10:E:78:ARG:NH2	2.31	0.63
5:A:356:A:OP2	5:A:416:G:O2'	2.16	0.63
32:a:484:A:OP1	35:d:146:ARG:NH2	2.32	0.63
5:A:1352:A:OP1	29:X:3:ARG:NH1	2.32	0.63
32:a:580:U:O2	39:h:4:GLN:NE2	2.32	0.63
5:A:1144:C:OP1	22:Q:92:ARG:NH2	2.31	0.63
5:A:2458:A:O2'	5:A:2459:G:O5'	2.17	0.63
36:e:116:LEU:HD13	36:e:124:VAL:HG21	1.81	0.63
5:A:1989:G:OP1	19:N:17:ARG:NH2	2.31	0.62
11:F:140:GLU:OE2	17:Le:27:THR:OG1	2.10	0.62
32:a:258:A:O2'	48:q:69:PRO:O	2.17	0.62
32:a:74:A:H62	32:a:89:G:N2	1.96	0.62
30:Y:13:LEU:HA	30:Y:16:GLN:HB2	1.81	0.62
5:A:1162:G:H1	5:A:1167:U:HO2'	1.45	0.62
19:N:77:GLY:O	19:N:81:ASN:ND2	2.33	0.62
32:a:191:A:N1	32:a:214:G:O2'	2.32	0.62
5:A:2510:G:O2'	5:A:2751:A:O2'	2.16	0.62
9:Dt:33:U:OP2	40:i:130:ARG:NH2	2.33	0.62
32:a:806:G:O2'	32:a:807:U:O4'	2.16	0.62
34:c:120:VAL:HG21	34:c:134:MET:HE1	1.80	0.62
5:A:314:A:O2'	5:A:315:U:OP1	2.17	0.62
18:M:21:ALA:O	18:M:25:SER:OG	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2338:G:O2'	5:A:2353:A:N6	2.33	0.61
30:Y:8:LYS:HE3	30:Y:12:GLN:HG3	1.82	0.61
5:A:303:A:N3	5:A:323:G:O2'	2.33	0.61
5:A:1348:G:HO2'	5:A:2202:C:HO2'	1.49	0.61
32:a:421:U:OP1	35:d:13:ARG:NH2	2.32	0.61
5:A:1776:A:OP2	7:C:221:ARG:NH1	2.33	0.61
5:A:1002:U:O4	14:J:30:THR:HG21	2.00	0.61
5:A:2784:U:O2'	5:A:2785:U:O4'	2.18	0.61
6:B:105:G:OP1	27:V:101:HIS:NE2	2.34	0.61
6:B:49:C:OP2	20:O:31:ARG:NH1	2.33	0.61
30:Y:10:VAL:HG12	30:Y:14:ASN:HD21	1.64	0.61
8:D:186:LEU:HD13	21:P:9:ILE:HD11	1.82	0.61
32:a:74:A:N6	32:a:89:G:H21	1.97	0.61
5:A:538:G:O2'	5:A:539:U:OP1	2.17	0.61
5:A:1154:G:OP1	23:R:24:LYS:NZ	2.26	0.61
5:A:219:A:N3	5:A:234:U:O2'	2.33	0.61
5:A:304:A:O2'	5:A:306:G:N7	2.33	0.61
30:Y:17:LEU:HD13	30:Y:21:LEU:HD11	1.83	0.61
5:A:395:A:N6	5:A:412:C:O2'	2.33	0.60
5:A:2433:G:N2	5:A:2436:U:O2	2.32	0.60
32:a:581:G:OP1	39:h:84:ARG:NH2	2.34	0.60
7:C:69:ARG:O	7:C:189:ARG:NH1	2.34	0.60
7:C:163:GLN:OE1	7:C:175:ARG:NH2	2.34	0.60
32:a:1112:U:OP1	40:i:11:ARG:NH1	2.35	0.60
40:i:106:ARG:NH1	40:i:107:ASP:O	2.35	0.60
32:a:820:C:O2	39:h:16:ASN:ND2	2.35	0.60
32:a:961:C:OP2	32:a:962:A:O2'	2.10	0.60
5:A:2808:A:O2'	5:A:2813:A:N1	2.34	0.60
12:G:6:LYS:O	12:G:51:ARG:NH1	2.34	0.60
30:Y:9:SER:O	30:Y:12:GLN:HB3	2.02	0.60
32:a:423:U:O2'	35:d:31:LYS:NZ	2.33	0.60
40:i:53:GLU:OE1	40:i:53:GLU:N	2.35	0.60
5:A:2191:G:OP2	7:C:147:LYS:NZ	2.35	0.60
5:A:2705:G:O2'	5:A:2834:U:OP1	2.19	0.60
32:a:121:G:O2'	48:q:9:ARG:NH1	2.35	0.59
32:a:607:C:O3'	35:d:83:LYS:NZ	2.35	0.59
32:a:1093:G:OP1	33:b:74:ARG:NH2	2.35	0.59
5:A:1010:A:N6	5:A:1132:C:OP2	2.36	0.59
32:a:942:C:OP2	44:m:105:ASN:ND2	2.34	0.59
5:A:1983:C:N4	15:K:32:TYR:OH	2.35	0.59
33:b:81:ARG:NE	33:b:93:ASP:OD2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:R:62:GLU:OE1	23:R:62:GLU:N	2.35	0.59
28:W:40:GLN:CD	28:W:43:THR:HA	2.27	0.59
32:a:671:U:O2	32:a:771:A:O2'	2.19	0.59
5:A:2470:C:O2'	18:M:52:ARG:NH2	2.36	0.59
11:F:27:GLU:N	11:F:27:GLU:OE1	2.36	0.58
5:A:1121:G:N2	5:A:1122:U:O4	2.26	0.58
36:e:39:VAL:HG22	36:e:47:VAL:HG22	1.85	0.58
5:A:2019:G:N2	5:A:2559:A:OP1	2.36	0.58
32:a:290:U:O2'	32:a:550:C:O2	2.20	0.58
5:A:1639:G:O2'	19:N:106:ASP:OD2	2.11	0.58
27:V:31:ALA:N	27:V:43:VAL:O	2.36	0.58
32:a:329:C:O2'	32:a:1427:A:N3	2.29	0.58
32:a:612:C:N4	32:a:615:A:OP2	2.37	0.58
5:A:141:A:O2'	5:A:142:C:O5'	2.18	0.58
17:Le:16:CYS:SG	17:Le:17:SER:N	2.76	0.58
32:a:938:G:N1	32:a:1332:G:OP2	2.37	0.58
5:A:523:A:N7	5:A:2008:A:O2'	2.29	0.58
32:a:1497:A:O2'	32:a:1498:G:OP1	2.17	0.58
53:v:141:THR:OG1	53:v:174:GLU:OE1	2.16	0.57
1:2:17:ARG:NH2	5:A:1253:G:OP2	2.36	0.57
5:A:84:A:N6	5:A:100:U:O4'	2.37	0.57
32:a:584:U:OP1	39:h:31:LYS:N	2.36	0.57
5:A:1627:A:O2'	5:A:1628:C:OP1	2.22	0.57
6:B:56:G:O2'	6:B:57:A:OP2	2.21	0.57
32:a:97:C:OP2	51:t:9:LYS:NZ	2.36	0.57
38:g:86:GLN:O	38:g:148:ASN:ND2	2.37	0.57
5:A:771:A:OP1	7:C:217:ARG:NH2	2.37	0.57
6:B:72:G:O2'	6:B:73:A:O4'	2.19	0.57
5:A:259:G:HO2'	5:A:611:A:HO2'	1.52	0.57
5:A:1967:G:O2'	5:A:1968:A:OP1	2.16	0.57
15:K:70:ARG:HA	15:K:76:ILE:HG22	1.87	0.57
33:b:3:GLN:NE2	33:b:219:GLU:OE1	2.38	0.57
32:a:501:C:OP2	32:a:502:U:O2'	2.15	0.57
47:p:9:GLY:O	47:p:16:PHE:N	2.38	0.57
5:A:1794:G:N2	5:A:1797:A:OP2	2.30	0.57
35:d:160:GLU:N	35:d:160:GLU:OE1	2.37	0.57
5:A:621:A:N3	5:A:2402:G:O2'	2.36	0.56
5:A:1009:U:OP1	5:A:1025:U:O2'	2.21	0.56
5:A:2519:G:N2	5:A:2650:G:O2'	2.37	0.56
28:W:40:GLN:HE21	28:W:57:HIS:HB3	1.69	0.56
32:a:574:C:O2'	46:o:61:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Y:5:LEU:C	30:Y:7:GLU:N	2.61	0.56
35:d:97:ARG:NH2	35:d:99:ASP:OD2	2.38	0.56
5:A:563:U:O4	5:A:2016:G:O2'	2.14	0.56
15:K:74:GLY:O	21:P:76:GLN:NE2	2.38	0.56
30:Y:20:LEU:HD11	30:Y:49:ILE:HG13	1.87	0.56
5:A:1448:C:O2'	5:A:1449:C:OP1	2.21	0.56
32:a:893:C:O2'	32:a:894:A:OP1	2.23	0.56
35:d:147:GLU:OE1	35:d:147:GLU:N	2.39	0.56
32:a:38:G:OP1	43:l:121:ARG:NH2	2.39	0.56
36:e:143:LYS:O	36:e:147:ASN:ND2	2.39	0.56
5:A:2844:G:N2	5:A:2847:A:OP2	2.27	0.56
32:a:559:U:OP2	32:a:560:G:O2'	2.24	0.56
44:m:67:GLY:O	44:m:71:ARG:NH1	2.37	0.56
5:A:966:G:HO2'	5:A:1146:A:HO2'	1.43	0.56
5:A:1657:G:OP1	15:K:7:MET:N	2.38	0.56
5:A:2499:C:O2	8:D:145:SER:OG	2.23	0.56
17:Le:57:ILE:HD12	17:Le:58:ASP:H	1.71	0.56
5:A:1325:G:O2'	5:A:1380:A:N1	2.34	0.55
8:D:52:THR:HG21	8:D:76:ALA:HB1	1.86	0.55
12:G:107:LEU:O	12:G:152:ARG:NH2	2.40	0.55
8:D:91:ALA:N	8:D:94:ASP:OD2	2.40	0.55
43:l:21:VAL:HG11	43:l:24:LEU:HD11	1.88	0.55
32:a:557:A:O2'	32:a:560:G:O2'	2.15	0.55
5:A:547:C:O2'	14:J:47:HIS:O	2.24	0.55
32:a:495:C:OP1	43:l:114:ARG:NH2	2.40	0.55
32:a:506:U:O4'	35:d:41:HIS:NE2	2.34	0.55
32:a:1310:G:N1	32:a:1313:A:OP2	2.40	0.55
32:a:1366:U:OP1	40:i:73:SER:N	2.40	0.55
5:A:456:G:N3	5:A:673:C:O2'	2.32	0.55
49:r:12:ARG:NH2	49:r:32:TYR:OH	2.40	0.55
5:A:1037:G:N2	5:A:1100:G:O2'	2.38	0.54
6:B:4:U:O2'	6:B:25:A:N6	2.39	0.54
5:A:971:A:OP2	5:A:972:C:N4	2.36	0.54
32:a:247:U:O2'	48:q:20:MET:SD	2.63	0.54
51:t:27:MET:HE3	51:t:61:MET:HE3	1.89	0.54
40:i:91:ASP:O	40:i:93:THR:N	2.39	0.54
5:A:2143:G:O2'	5:A:2145:A:N7	2.40	0.54
53:v:205:PHE:CZ	53:v:254:LEU:HD21	2.43	0.54
9:Dt:38:A:O2'	32:a:784:A:OP1	2.24	0.54
5:A:2363:A:N3	20:O:110:ARG:NH2	2.55	0.54
32:a:712:A:O2'	52:u:31:GLU:OE2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:1047:G:O2'	32:a:1193:U:OP2	2.20	0.54
19:N:49:GLU:OE1	19:N:49:GLU:N	2.40	0.54
5:A:983:G:OP1	22:Q:50:ARG:NE	2.41	0.54
5:A:2362:G:N2	5:A:2365:A:OP2	2.34	0.53
19:N:66:ALA:O	19:N:70:THR:HG22	2.08	0.53
36:e:90:HIS:ND1	36:e:136:ASN:OD1	2.37	0.53
53:v:104:SER:O	53:v:107:ARG:NH2	2.42	0.53
5:A:2428:U:OP2	5:A:2573:U:O2'	2.27	0.53
9:Dt:30:G:OP1	32:a:1223:A:O2'	2.25	0.53
32:a:1144:U:O4	32:a:1145:A:N6	2.41	0.53
50:s:56:GLN:N	50:s:56:GLN:OE1	2.41	0.53
23:R:22:VAL:O	23:R:94:THR:N	2.42	0.53
32:a:28:A:O2'	32:a:290:U:OP1	2.12	0.53
5:A:911:C:O2'	28:W:29:GLN:NE2	2.42	0.53
32:a:892:G:N2	32:a:895:A:OP2	2.40	0.53
32:a:1521:C:OP2	52:u:42:THR:HG22	2.09	0.53
1:2:16:ARG:NH2	5:A:1251:G:OP1	2.40	0.53
2:4:24:THR:HG23	2:4:27:GLY:H	1.73	0.53
5:A:1281:A:N3	19:N:23:ASN:ND2	2.56	0.53
26:U:61:GLU:N	26:U:61:GLU:OE1	2.42	0.53
32:a:1520:G:OP2	52:u:42:THR:HG23	2.09	0.53
5:A:69:C:O2	5:A:73:A:O2'	2.27	0.53
5:A:1199:G:O2'	5:A:1224:A:N6	2.42	0.53
5:A:1310:C:O2'	5:A:1311:G:O5'	2.27	0.53
5:A:1573:U:OP1	5:A:1574:U:O2'	2.26	0.53
5:A:2237:G:H21	5:A:2483:C:H4'	1.74	0.53
2:4:26:ASN:ND2	5:A:672:G:O5'	2.43	0.52
3:5:64:ARG:O	5:A:654:G:N2	2.34	0.52
5:A:680:U:O2'	5:A:770:G:OP1	2.27	0.52
5:A:877:C:H41	44:m:92:ARG:HB2	1.74	0.52
49:r:12:ARG:CG	49:r:13:PHE:H	2.23	0.52
32:a:124:A:N3	32:a:257:A:O2'	2.39	0.52
32:a:1365:G:OP1	40:i:14:THR:OG1	2.27	0.52
43:l:15:MET:SD	43:l:15:MET:N	2.81	0.52
53:v:114:GLU:N	53:v:114:GLU:OE1	2.42	0.52
6:B:2:G:O6	53:v:23:ARG:NH2	2.41	0.52
32:a:1361:C:O2'	32:a:1362:A:OP1	2.27	0.52
6:B:38:C:O4'	20:O:99:HIS:NE2	2.42	0.52
32:a:989:C:O4'	45:n:8:ASN:ND2	2.41	0.52
5:A:853:G:H21	5:A:855:A:H61	1.57	0.52
5:A:1741:A:O2'	5:A:1742:A:OP1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:r:9:LYS:HB2	49:r:45:THR:O	2.10	0.51
8:D:124:ARG:NH1	8:D:163:GLY:O	2.43	0.51
30:Y:17:LEU:O	30:Y:21:LEU:HG	2.10	0.51
20:O:6:GLU:N	20:O:6:GLU:OE1	2.42	0.51
32:a:869:U:O2'	39:h:15:ARG:NH1	2.44	0.51
32:a:1071:G:N2	32:a:1074:A:OP2	2.28	0.51
7:C:154:ILE:HG21	7:C:176:LEU:HD22	1.93	0.51
28:W:40:GLN:NE2	28:W:43:THR:HA	2.25	0.51
44:m:54:ASP:OD1	44:m:55:GLN:N	2.43	0.51
49:r:12:ARG:CG	49:r:13:PHE:N	2.74	0.51
32:a:540:A:O2'	32:a:542:G:O2'	2.11	0.51
5:A:1047:A:OP2	5:A:1079:A:N6	2.38	0.51
5:A:1270:G:N2	5:A:1273:A:OP2	2.44	0.51
5:A:872:G:N3	5:A:885:A:N6	2.59	0.50
5:A:1895:C:H2'	5:A:1897:G:N7	2.26	0.50
5:A:1171:G:OP1	31:Z:29:ARG:NE	2.37	0.50
14:J:18:VAL:HG22	14:J:140:LEU:HD21	1.93	0.50
30:Y:8:LYS:HE3	30:Y:12:GLN:CG	2.41	0.50
30:Y:11:GLU:HA	30:Y:14:ASN:HB2	1.93	0.50
32:a:916:G:H21	32:a:1392:A:H8	1.58	0.50
37:f:29:ILE:HD11	37:f:74:LEU:HD11	1.92	0.50
5:A:1785:U:OP1	7:C:257:LYS:NZ	2.36	0.50
14:J:60:GLU:N	14:J:60:GLU:OE1	2.45	0.50
5:A:1654:A:H61	5:A:1983:C:H42	1.58	0.50
7:C:187:GLU:N	7:C:187:GLU:OE1	2.44	0.50
32:a:176:C:H42	32:a:188:G:H22	1.60	0.50
32:a:491:U:O2'	32:a:492:A:O4'	2.28	0.50
32:a:914:U:O2'	32:a:1075:G:O2'	2.12	0.50
5:A:84:A:O2'	26:U:6:ARG:NH2	2.44	0.50
5:A:2851:G:OP2	5:A:2853:U:N3	2.43	0.50
18:M:67:ARG:NH1	18:M:105:GLU:OE2	2.43	0.50
32:a:814:U:O2'	32:a:815:G:OP1	2.27	0.50
9:Dt:15:G:O6	9:Dt:48:C:O2	2.29	0.50
17:Le:28:LEU:HD21	17:Le:32:ILE:HD12	1.93	0.50
11:F:109:PRO:O	44:m:3:ARG:NE	2.45	0.50
32:a:1254:C:O2'	32:a:1269:A:N6	2.45	0.50
7:C:6:CYS:SG	7:C:13:ARG:NH2	2.85	0.49
7:C:261:ASN:ND2	7:C:264:THR:OG1	2.45	0.49
9:Dt:35:A:OP2	40:i:130:ARG:NH1	2.45	0.49
32:a:1361:C:O3'	41:j:62:ARG:NH2	2.45	0.49
5:A:563:U:N3	5:A:2018:A:OP1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:92:ARG:O	11:F:96:MET:N	2.42	0.49
32:a:60:A:N1	32:a:101:G:O2'	2.29	0.49
5:A:245:G:O2'	5:A:375:A:N1	2.33	0.49
5:A:2622:U:O2'	8:D:82:GLU:OE1	2.21	0.49
27:V:29:VAL:N	27:V:45:LEU:O	2.42	0.49
11:F:102:ARG:NH2	17:Le:25:ARG:O	2.46	0.49
42:k:29:ASN:OD1	42:k:30:THR:N	2.44	0.49
6:B:79:G:N7	27:V:16:LYS:NZ	2.61	0.49
30:Y:8:LYS:HB3	30:Y:12:GLN:CG	2.43	0.49
32:a:99:G:OP2	51:t:13:GLN:NE2	2.46	0.49
32:a:1360:U:OP1	40:i:119:ARG:NH1	2.45	0.49
5:A:315:U:H1'	10:E:158:LEU:HD12	1.94	0.49
5:A:1056:U:N3	5:A:1059:A:OP2	2.46	0.49
5:A:2605:G:H21	8:D:155:VAL:HG21	1.78	0.49
21:P:32:LYS:NZ	21:P:80:PRO:O	2.43	0.49
32:a:62:U:O2'	32:a:373:C:O2	2.31	0.49
32:a:724:G:N2	32:a:760:A:OP1	2.40	0.49
32:a:770:G:N2	32:a:796:A:OP2	2.45	0.49
32:a:1250:U:O4'	32:a:1272:U:N3	2.46	0.49
45:n:88:ALA:HB1	45:n:96:LEU:HD23	1.95	0.49
5:A:525:U:O2'	22:Q:49:ASP:OD2	2.22	0.49
32:a:1153:U:O4'	32:a:1176:G:N2	2.46	0.49
43:l:76:GLU:OE1	43:l:76:GLU:N	2.46	0.49
5:A:1494:C:O2'	5:A:1496:A:N6	2.47	0.48
32:a:1361:C:P	40:i:116:VAL:HG12	2.54	0.48
45:n:88:ALA:CB	45:n:96:LEU:HD23	2.44	0.48
46:o:6:GLU:N	46:o:6:GLU:OE1	2.46	0.48
8:D:51:VAL:N	8:D:81:TRP:O	2.44	0.48
11:F:95:ARG:NH1	17:Le:9:TYR:OH	2.46	0.48
5:A:565:A:OP2	5:A:2486:C:O2'	2.31	0.48
5:A:842:U:H4'	53:v:138:LYS:HG3	1.94	0.48
31:Z:39:ASP:O	31:Z:44:ARG:NH2	2.46	0.48
34:c:134:MET:CE	34:c:151:ILE:HG21	2.41	0.48
23:R:31:GLU:N	23:R:31:GLU:OE1	2.47	0.48
5:A:589:G:H21	10:E:99:MET:HE2	1.78	0.48
6:B:51:G:O2'	6:B:52:A:O5'	2.27	0.48
5:A:688:C:O2'	5:A:724:A:N6	2.44	0.48
28:W:12:ASN:OD1	28:W:12:ASN:N	2.47	0.48
34:c:35:ALA:O	34:c:39:VAL:HG23	2.14	0.48
3:5:50:ASN:OD1	3:5:51:LYS:N	2.46	0.48
5:A:266:G:O2'	5:A:267:C:OP1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:783:A:N6	5:A:2060:C:OP1	2.46	0.48
5:A:1404:C:OP1	5:A:1577:G:N2	2.47	0.48
45:n:33:ASN:O	45:n:41:ARG:NH2	2.45	0.48
5:A:564:A:N6	5:A:2021:U:OP1	2.44	0.47
10:E:175:ASP:OD1	10:E:175:ASP:N	2.47	0.47
30:Y:2:ALA:O	30:Y:6:ARG:HG2	2.14	0.47
5:A:293:A:N6	5:A:316:A:O2'	2.46	0.47
32:a:971:A:O2'	32:a:973:C:OP2	2.29	0.47
53:v:48:CYS:SG	53:v:49:SER:N	2.87	0.47
5:A:2186:A:N1	5:A:2213:C:N4	2.63	0.47
8:D:52:THR:HG23	8:D:79:GLY:O	2.13	0.47
35:d:97:ARG:NE	35:d:99:ASP:OD1	2.47	0.47
27:V:142:ASP:OD1	27:V:142:ASP:N	2.46	0.47
27:V:50:ILE:HG21	27:V:89:VAL:HG21	1.96	0.47
32:a:809:A:O2'	32:a:1520:G:N2	2.43	0.47
38:g:41:ARG:O	38:g:45:GLY:N	2.47	0.47
5:A:1310:C:HO2'	5:A:1311:G:P	2.37	0.47
5:A:1856:G:O2'	5:A:1859:A:N6	2.47	0.47
10:E:170:ASP:OD1	10:E:171:VAL:N	2.48	0.47
46:o:26:GLU:OE1	46:o:26:GLU:N	2.45	0.47
5:A:1162:G:N1	5:A:1167:U:O2'	2.47	0.47
5:A:2707:U:OP1	21:P:54:ARG:NH2	2.48	0.47
7:C:165:VAL:HG21	7:C:181:MET:HE1	1.97	0.47
17:Le:57:ILE:H	17:Le:57:ILE:HG13	1.41	0.47
27:V:6:LEU:HD22	27:V:45:LEU:HD22	1.96	0.47
30:Y:13:LEU:HA	30:Y:16:GLN:CB	2.45	0.47
32:a:495:C:O2	32:a:543:C:O2'	2.32	0.47
32:a:1260:G:N2	32:a:1263:A:OP2	2.37	0.47
48:q:28:ILE:HD11	48:q:64:ILE:HD11	1.96	0.47
5:A:466:C:N3	5:A:470:A:N7	2.62	0.47
11:F:135:GLN:O	11:F:141:ILE:HD13	2.14	0.47
5:A:315:U:C1'	10:E:158:LEU:HD12	2.45	0.47
32:a:424:A:OP2	35:d:22:LYS:NZ	2.48	0.47
49:r:9:LYS:HD2	49:r:45:THR:HA	1.96	0.47
20:O:26:ARG:NE	20:O:28:CYS:SG	2.88	0.46
32:a:581:G:O2'	32:a:582:G:OP2	2.27	0.46
5:A:18:C:O2'	5:A:544:U:OP1	2.32	0.46
5:A:355:G:OP2	5:A:356:A:O2'	2.21	0.46
5:A:748:G:H21	5:A:1968:A:H62	1.63	0.46
19:N:26:VAL:HG23	19:N:75:ALA:HB2	1.97	0.46
32:a:1301:U:OP1	44:m:100:GLN:NE2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:j:42:LEU:HD12	41:j:71:LYS:HB3	1.96	0.46
30:Y:15:GLU:HA	30:Y:18:LEU:HG	1.97	0.46
32:a:743:A:O2'	46:o:21:ASP:OD1	2.32	0.46
5:A:1058:G:O2'	5:A:1060:A:N6	2.48	0.46
5:A:1448:C:HO2'	5:A:1449:C:P	2.37	0.46
5:A:1589:C:OP1	25:T:39:LYS:N	2.46	0.46
5:A:1626:U:O2'	5:A:1747:C:O2	2.27	0.46
5:A:1514:G:N1	5:A:1534:A:OP2	2.48	0.46
6:B:34:A:O2'	6:B:35:U:O5'	2.29	0.46
50:s:33:THR:HG22	50:s:35:SER:H	1.81	0.46
5:A:952:G:H21	5:A:2237:G:H1	1.63	0.46
30:Y:17:LEU:HD23	30:Y:17:LEU:HA	1.74	0.46
32:a:402:G:OP1	35:d:110:THR:HG21	2.15	0.46
35:d:138:LYS:N	35:d:141:ASP:OD2	2.47	0.46
5:A:2536:G:O2'	5:A:2537:G:OP1	2.32	0.46
7:C:98:ASP:OD1	7:C:98:ASP:N	2.48	0.46
40:i:22:ARG:O	40:i:62:ASP:N	2.45	0.46
15:K:49:ARG:NH1	15:K:50:GLY:O	2.50	0.45
32:a:557:A:O2'	32:a:560:G:O3'	2.34	0.45
32:a:853:C:HO2'	32:a:854:A:P	2.36	0.45
33:b:43:LEU:HD23	33:b:43:LEU:H	1.81	0.45
5:A:978:A:OP2	31:Z:11:SER:OG	2.32	0.45
5:A:1055:U:O2	5:A:1059:A:O2'	2.32	0.45
5:A:2295:G:O2'	5:A:2297:A:O5'	2.32	0.45
6:B:51:G:OP2	20:O:66:ASN:ND2	2.45	0.45
10:E:115:ASP:O	10:E:184:LYS:NZ	2.49	0.45
15:K:92:GLU:OE1	15:K:92:GLU:N	2.49	0.45
30:Y:11:GLU:O	30:Y:12:GLN:C	2.58	0.45
32:a:805:C:O2'	32:a:895:A:N1	2.49	0.45
40:i:45:ARG:O	40:i:49:ARG:NH1	2.49	0.45
32:a:506:U:O2'	32:a:507:U:OP1	2.32	0.45
32:a:712:A:OP2	32:a:714:C:N4	2.50	0.45
5:A:259:G:O2'	5:A:611:A:O2'	2.25	0.45
5:A:1128:G:O2'	14:J:104:ALA:O	2.35	0.45
29:X:2:SER:O	29:X:50:ARG:NH2	2.48	0.45
34:c:120:VAL:CG2	34:c:134:MET:HE1	2.45	0.45
2:4:39:ARG:NH2	5:A:459:G:N7	2.64	0.45
32:a:65:A:N6	32:a:376:A:O5'	2.50	0.45
11:F:108:LEU:HD22	17:Le:44:TYR:CE2	2.52	0.45
37:f:16:GLU:OE1	37:f:16:GLU:N	2.48	0.45
41:j:54:SER:OG	41:j:56:HIS:O	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1288:A:H2	5:A:1616:G:H21	1.64	0.45
5:A:2350:U:O2	28:W:39:ARG:NH2	2.45	0.45
2:4:33:ARG:NE	5:A:458:G:OP1	2.50	0.45
5:A:1081:G:H22	5:A:1090:C:H42	1.64	0.45
11:F:70:ALA:HB2	11:F:85:ILE:HD12	1.98	0.45
41:j:75:ASP:OD1	41:j:75:ASP:N	2.49	0.45
48:q:51:ASP:OD2	48:q:54:ASN:N	2.47	0.45
5:A:575:G:N7	22:Q:6:ARG:NH2	2.65	0.45
6:B:24:G:O6	6:B:56:G:O2'	2.30	0.45
8:D:3:ILE:HG22	8:D:85:LEU:HD23	1.99	0.45
30:Y:5:LEU:C	30:Y:7:GLU:H	2.25	0.45
32:a:1207:A:O2'	32:a:1209:G:N7	2.39	0.45
32:a:1395:G:O6	32:a:1498:G:N2	2.50	0.45
43:l:27:CYS:SG	43:l:30:ARG:NH2	2.90	0.45
3:5:32:LEU:HD13	5:A:2406:U:OP2	2.17	0.44
5:A:2035:G:H21	8:D:118:PHE:HZ	1.63	0.44
32:a:79:G:H1	32:a:84:C:H42	1.64	0.44
5:A:1253:G:O2'	5:A:1999:G:O6	2.28	0.44
25:T:4:GLU:OE1	25:T:4:GLU:N	2.48	0.44
32:a:854:A:OP1	33:b:26:LYS:NZ	2.50	0.44
5:A:1453:U:O3'	5:A:1536:G:O2'	2.36	0.44
30:Y:10:VAL:HG12	30:Y:14:ASN:ND2	2.29	0.44
44:m:100:GLN:OE1	44:m:100:GLN:N	2.51	0.44
16:L:73:ASP:OD1	16:L:106:GLN:N	2.45	0.44
10:E:5:VAL:HA	10:E:119:VAL:HG13	1.99	0.44
18:M:35:LYS:NZ	27:V:85:ALA:O	2.51	0.44
32:a:374:G:N2	32:a:377:A:OP2	2.51	0.44
33:b:83:GLU:OE2	33:b:215:ASN:ND2	2.51	0.44
5:A:971:A:O2'	5:A:2023:C:O2'	2.32	0.44
5:A:1232:G:O2'	5:A:1233:A:OP1	2.31	0.44
5:A:1386:C:OP2	25:T:56:ARG:NH2	2.51	0.44
17:Le:63:ARG:O	50:s:5:LEU:HD11	2.17	0.44
32:a:310:C:OP2	32:a:345:G:O2'	2.26	0.44
5:A:2078:C:OP2	5:A:2079:U:O2'	2.28	0.44
9:Dt:15:G:H22	9:Dt:48:C:H42	1.64	0.44
22:Q:43:GLY:HA3	23:R:75:ILE:HD12	2.00	0.44
27:V:8:ALA:HB2	27:V:66:LEU:HD11	2.00	0.44
38:g:115:SER:O	38:g:118:LEU:N	2.45	0.44
53:v:156:LEU:HD13	53:v:160:GLU:HB3	1.99	0.44
32:a:1089:U:P	32:a:1102:G:H22	2.39	0.44
49:r:5:PHE:O	49:r:9:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1683:U:O2'	7:C:14:ARG:NH1	2.46	0.44
32:a:255:U:OP2	51:t:74:ARG:NH2	2.51	0.44
15:K:35:ILE:HD12	15:K:69:VAL:HB	2.00	0.43
5:A:316:A:O2'	5:A:317:G:OP1	2.35	0.43
30:Y:6:ARG:HE	30:Y:55:VAL:HG12	1.83	0.43
32:a:515:G:N7	43:l:50:ARG:NH1	2.66	0.43
32:a:658:G:O2'	32:a:660:G:OP2	2.24	0.43
5:A:1813:G:OP1	7:C:223:VAL:HG13	2.19	0.43
32:a:515:G:O2'	32:a:530:C:O2'	2.34	0.43
5:A:227:A:O2'	5:A:228:C:O5'	2.34	0.43
5:A:2108:G:O6	5:A:2165:C:N4	2.52	0.43
5:A:2568:G:O2'	5:A:2597:C:N4	2.52	0.43
47:p:20:THR:HG22	47:p:35:ARG:HG2	2.01	0.43
50:s:19:VAL:HG11	50:s:44:MET:SD	2.58	0.43
5:A:77:U:O2'	30:Y:6:ARG:NH2	2.52	0.43
5:A:1787:C:H5	5:A:1804:G:H22	1.67	0.43
5:A:1993:C:O2'	5:A:2810:A:N3	2.52	0.43
5:A:2317:G:H21	28:W:42:GLY:HA2	1.84	0.43
5:A:626:G:N2	16:L:111:MET:SD	2.92	0.43
5:A:2299:U:O3'	11:F:68:THR:HG21	2.19	0.43
18:M:3:GLN:OE1	18:M:93:TRP:NE1	2.52	0.43
22:Q:112:LYS:CD	23:R:49:ILE:HD11	2.48	0.43
26:U:32:ARG:C	26:U:33:LEU:HD12	2.44	0.43
32:a:1371:A:OP1	38:g:92:ARG:NH2	2.51	0.43
1:2:40:HIS:ND1	5:A:2803:G:O4'	2.52	0.43
11:F:7:ILE:H	11:F:7:ILE:HG12	1.57	0.43
40:i:46:MET:O	40:i:50:GLN:N	2.52	0.43
5:A:2121:A:N6	5:A:2143:G:N3	2.65	0.43
1:2:16:ARG:NH1	5:A:1253:G:OP1	2.52	0.43
5:A:2248:C:OP1	28:W:19:LYS:NZ	2.48	0.43
32:a:562:G:O2'	32:a:568:A:N1	2.52	0.43
35:d:194:ASP:OD1	35:d:195:ILE:N	2.51	0.43
5:A:1142:A:O2'	22:Q:77:SER:O	2.36	0.43
5:A:2168:G:O6	5:A:2169:G:N2	2.52	0.43
6:B:9:G:OP1	20:O:20:ARG:NH2	2.52	0.43
11:F:162:THR:HG23	11:F:164:ASP:OD1	2.19	0.43
32:a:1361:C:OP1	40:i:116:VAL:HG12	2.19	0.43
42:k:88:GLY:O	42:k:93:ARG:NH1	2.50	0.43
5:A:2379:A:OP2	5:A:2409:C:N4	2.52	0.42
32:a:668:G:OP1	37:f:86:ARG:NH2	2.52	0.42
5:A:1016:U:O2'	5:A:1017:A:OP1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Z:8:LEU:HD21	31:Z:12:LEU:CD2	2.49	0.42
32:a:204:C:O2'	32:a:206:G:N7	2.43	0.42
8:D:130:GLN:OE1	8:D:130:GLN:N	2.53	0.42
11:F:164:ASP:OD1	11:F:165:GLU:N	2.52	0.42
14:J:16:PHE:HB3	14:J:140:LEU:HD22	2.00	0.42
24:S:65:ASP:OD1	24:S:66:VAL:N	2.51	0.42
30:Y:20:LEU:HD21	30:Y:49:ILE:HG12	2.02	0.42
32:a:975:U:OP1	45:n:9:ARG:NH2	2.52	0.42
53:v:138:LYS:HA	53:v:138:LYS:HD3	1.39	0.42
5:A:792:A:O2'	5:A:793:U:OP1	2.35	0.42
27:V:8:ALA:HB1	27:V:43:VAL:CG1	2.44	0.42
32:a:684:G:OP2	42:k:29:ASN:ND2	2.48	0.42
5:A:774:G:O2'	5:A:775:G:O5'	2.34	0.42
5:A:2169:G:O2'	5:A:2170:C:O4'	2.36	0.42
50:s:40:ILE:HD12	50:s:62:VAL:HG13	2.02	0.42
5:A:61:G:O2'	30:Y:31:LYS:NZ	2.52	0.42
5:A:139:U:O2'	5:A:140:A:OP2	2.35	0.42
5:A:2717:C:O2'	8:D:173:GLN:O	2.31	0.42
15:K:106:LEU:HD22	15:K:114:ILE:HD11	2.02	0.42
26:U:50:MET:O	26:U:52:GLY:N	2.50	0.42
30:Y:5:LEU:O	30:Y:8:LYS:N	2.44	0.42
50:s:19:VAL:O	50:s:23:VAL:HG23	2.19	0.42
5:A:2607:C:O2'	8:D:124:ARG:NH1	2.53	0.42
15:K:71:ARG:HH12	15:K:77:ILE:HD12	1.84	0.42
16:L:86:GLU:OE1	16:L:86:GLU:N	2.53	0.42
24:S:24:ILE:HD11	24:S:47:MET:SD	2.59	0.42
30:Y:13:LEU:HD13	30:Y:55:VAL:HG23	2.02	0.42
32:a:506:U:OP1	35:d:44:ARG:NE	2.53	0.42
36:e:14:GLU:N	36:e:14:GLU:OE1	2.51	0.42
41:j:42:LEU:HD11	41:j:73:VAL:CG2	2.50	0.42
41:j:57:VAL:HG13	41:j:57:VAL:O	2.20	0.42
5:A:83:G:N1	5:A:101:U:O2'	2.51	0.42
5:A:2582:G:N2	5:A:2585:A:OP2	2.36	0.42
5:A:2743:U:O2'	5:A:2744:A:OP2	2.31	0.42
8:D:52:THR:HG22	8:D:53:ALA:O	2.20	0.42
27:V:13:ASP:N	27:V:13:ASP:OD1	2.51	0.42
42:k:111:THR:HG23	52:u:4:LYS:HG2	2.01	0.42
3:5:42:GLN:NE2	5:A:2352:G:O6	2.53	0.42
21:P:39:GLN:N	21:P:39:GLN:OE1	2.52	0.42
33:b:28:GLY:O	33:b:31:ILE:HG22	2.20	0.42
47:p:54:GLN:N	47:p:54:GLN:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2114:G:H21	5:A:2160:A:C1'	2.33	0.42
8:D:49:VAL:HG23	8:D:85:LEU:HD21	2.02	0.42
32:a:456:G:O2'	32:a:457:U:O5'	2.37	0.42
32:a:466:U:H3'	32:a:467:G:H21	1.84	0.42
5:A:126:A:O2'	5:A:127:A:O4'	2.31	0.41
15:K:71:ARG:NH1	15:K:77:ILE:HD12	2.35	0.41
27:V:160:VAL:O	27:V:184:VAL:N	2.47	0.41
32:a:665:G:O2'	37:f:79:ARG:NH1	2.52	0.41
32:a:1075:G:H21	36:e:53:LYS:NZ	2.16	0.41
32:a:1163:A:O2'	32:a:1164:A:O5'	2.38	0.41
43:l:38:TYR:N	43:l:52:VAL:O	2.53	0.41
5:A:2106:A:H61	5:A:2155:G:H21	1.68	0.41
5:A:2710:C:OP1	8:D:114:LYS:NZ	2.52	0.41
40:i:51:PRO:O	40:i:55:THR:HG22	2.20	0.41
5:A:765:G:N2	5:A:783:A:O2'	2.37	0.41
5:A:2274:A:O2'	5:A:2275:A:O5'	2.38	0.41
14:J:40:HIS:NE2	14:J:52:ASP:OD2	2.51	0.41
28:W:40:GLN:NE2	28:W:57:HIS:O	2.54	0.41
36:e:151:PRO:HG3	39:h:99:LEU:HD13	2.02	0.41
5:A:247:G:OP2	5:A:249:C:N4	2.49	0.41
32:a:658:G:H22	32:a:735:G:H1	1.68	0.41
32:a:709:A:O2'	32:a:710:A:O5'	2.35	0.41
32:a:1341:G:O6	40:i:12:ARG:NH2	2.53	0.41
32:a:1360:U:O2'	41:j:59:LYS:NZ	2.54	0.41
5:A:568:G:OP1	5:A:1242:U:O2'	2.34	0.41
5:A:1239:G:N2	22:Q:33:ARG:O	2.53	0.41
5:A:1628:C:OP2	5:A:2697:C:O2'	2.38	0.41
5:A:1672:G:HO2'	5:A:1673:C:P	2.41	0.41
22:Q:112:LYS:HD2	23:R:49:ILE:HD11	2.01	0.41
32:a:287:G:OP1	32:a:603:A:N6	2.47	0.41
32:a:680:U:O4	32:a:697:G:O2'	2.37	0.41
32:a:761:A:O2'	32:a:1518:C:O2	2.38	0.41
32:a:1362:A:OP2	41:j:62:ARG:NE	2.54	0.41
43:l:70:GLU:N	43:l:70:GLU:OE1	2.53	0.41
5:A:824:G:O2'	5:A:2345:A:O2'	2.35	0.41
5:A:2793:C:O2'	5:A:2794:U:OP1	2.37	0.41
21:P:10:GLU:HG2	21:P:56:LEU:HD12	2.03	0.41
45:n:13:ARG:O	45:n:17:VAL:HG23	2.19	0.41
53:v:57:GLU:N	53:v:57:GLU:OE1	2.54	0.41
5:A:770:G:O2'	5:A:773:A:N6	2.49	0.41
5:A:973:A:N1	5:A:974:A:N6	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2526:C:O2	5:A:2728:A:O2'	2.39	0.41
9:Dt:10:G:O2'	9:Dt:11:C:OP1	2.34	0.41
25:T:57:VAL:HG13	25:T:84:ILE:HD13	2.02	0.41
27:V:148:GLU:OE1	27:V:148:GLU:N	2.53	0.41
32:a:3:A:O2'	32:a:4:C:O4'	2.31	0.41
32:a:1339:U:OP1	40:i:122:ARG:NH1	2.49	0.41
36:e:41:GLY:HA3	36:e:47:VAL:HG23	2.03	0.41
5:A:835:A:O2'	5:A:836:U:O2	2.39	0.41
21:P:51:LYS:NZ	21:P:53:ASN:OD1	2.53	0.41
5:A:899:A:H62	18:M:12:GLN:HA	1.86	0.40
5:A:1605:C:OP2	5:A:1607:C:N4	2.31	0.40
5:A:1896:C:N4	5:A:1898:U:O4'	2.54	0.40
5:A:2363:A:O2'	20:O:110:ARG:NH1	2.50	0.40
10:E:17:THR:OG1	10:E:200:GLY:O	2.36	0.40
22:Q:94:VAL:HG21	23:R:11:GLN:HG3	2.04	0.40
45:n:80:SER:OG	45:n:81:ARG:N	2.53	0.40
4:6:1:MET:N	5:A:2513:G:O2'	2.52	0.40
5:A:184:C:O2'	5:A:217:A:N3	2.51	0.40
5:A:2321:A:O5'	20:O:13:ARG:NE	2.54	0.40
14:J:47:HIS:ND1	14:J:48:VAL:HG13	2.36	0.40
31:Z:12:LEU:HD12	31:Z:20:LYS:HA	2.03	0.40
39:h:27:MET:SD	39:h:27:MET:N	2.93	0.40
49:r:5:PHE:CZ	49:r:9:LYS:HE3	2.37	0.40
5:A:1263:U:OP2	5:A:1635:G:O2'	2.23	0.40
8:D:49:VAL:CG2	8:D:85:LEU:HD21	2.52	0.40
10:E:47:THR:OG1	10:E:50:GLU:OE1	2.21	0.40
19:N:6:SER:OG	19:N:46:ARG:NH1	2.54	0.40
28:W:15:ASP:OD1	28:W:16:SER:N	2.48	0.40
36:e:152:GLU:N	36:e:152:GLU:OE1	2.54	0.40
5:A:1382:A:H2'	5:A:1385:C:H41	1.86	0.40
5:A:2080:G:O2'	5:A:2185:A:N1	2.51	0.40
31:Z:28:LEU:HD21	31:Z:35:VAL:HG22	2.04	0.40
39:h:54:GLU:N	39:h:54:GLU:OE1	2.54	0.40
41:j:45:ARG:NH1	41:j:47:GLU:OE2	2.52	0.40
53:v:50:LEU:HD12	53:v:93:LEU:HD22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	51/60 (85%)	49 (96%)	2 (4%)	0	100	100
2	4	43/44 (98%)	42 (98%)	1 (2%)	0	100	100
3	5	61/64 (95%)	54 (88%)	7 (12%)	0	100	100
4	6	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	C	269/273 (98%)	255 (95%)	14 (5%)	0	100	100
8	D	205/211 (97%)	184 (90%)	21 (10%)	0	100	100
10	E	197/200 (98%)	190 (96%)	7 (4%)	0	100	100
11	F	172/179 (96%)	155 (90%)	17 (10%)	0	100	100
12	G	171/177 (97%)	164 (96%)	7 (4%)	0	100	100
13	H	76/148 (51%)	76 (100%)	0	0	100	100
14	J	139/142 (98%)	134 (96%)	5 (4%)	0	100	100
15	K	118/122 (97%)	111 (94%)	7 (6%)	0	100	100
16	L	141/144 (98%)	130 (92%)	11 (8%)	0	100	100
17	Le	66/71 (93%)	59 (89%)	6 (9%)	1 (2%)	8	35
18	M	133/137 (97%)	132 (99%)	1 (1%)	0	100	100
19	N	116/129 (90%)	105 (90%)	11 (10%)	0	100	100
20	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
21	P	111/116 (96%)	104 (94%)	7 (6%)	0	100	100
22	Q	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
23	R	100/103 (97%)	93 (93%)	7 (7%)	0	100	100
24	S	107/110 (97%)	107 (100%)	0	0	100	100
25	T	90/99 (91%)	84 (93%)	5 (6%)	1 (1%)	11	43
26	U	101/104 (97%)	94 (93%)	7 (7%)	0	100	100
27	V	186/204 (91%)	173 (93%)	13 (7%)	0	100	100
28	W	74/85 (87%)	57 (77%)	17 (23%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	X	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
30	Y	57/63 (90%)	54 (95%)	2 (4%)	1 (2%)	6	31
31	Z	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
33	b	230/246 (94%)	214 (93%)	16 (7%)	0	100	100
34	c	203/228 (89%)	188 (93%)	15 (7%)	0	100	100
35	d	203/206 (98%)	190 (94%)	13 (6%)	0	100	100
36	e	154/166 (93%)	141 (92%)	13 (8%)	0	100	100
37	f	103/139 (74%)	98 (95%)	5 (5%)	0	100	100
38	g	152/156 (97%)	147 (97%)	5 (3%)	0	100	100
39	h	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
40	i	125/130 (96%)	110 (88%)	14 (11%)	1 (1%)	16	50
41	j	94/103 (91%)	88 (94%)	6 (6%)	0	100	100
42	k	113/129 (88%)	110 (97%)	3 (3%)	0	100	100
43	l	119/123 (97%)	111 (93%)	8 (7%)	0	100	100
44	m	108/118 (92%)	103 (95%)	5 (5%)	0	100	100
45	n	96/101 (95%)	91 (95%)	5 (5%)	0	100	100
46	o	84/89 (94%)	83 (99%)	1 (1%)	0	100	100
47	p	76/83 (92%)	73 (96%)	3 (4%)	0	100	100
48	q	74/88 (84%)	72 (97%)	2 (3%)	0	100	100
49	r	67/76 (88%)	65 (97%)	1 (2%)	1 (2%)	8	35
50	s	78/91 (86%)	71 (91%)	7 (9%)	0	100	100
51	t	83/91 (91%)	83 (100%)	0	0	100	100
52	u	58/71 (82%)	56 (97%)	1 (2%)	1 (2%)	7	32
53	v	269/370 (73%)	264 (98%)	5 (2%)	0	100	100
All	All	5794/6327 (92%)	5463 (94%)	325 (6%)	6 (0%)	49	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	T	71	ARG
30	Y	10	VAL
40	i	28	ILE
49	r	13	PHE
17	Le	66	VAL

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Mol	Chain	Res	Type
52	u	28	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	46/52 (88%)	46 (100%)	0	100	100
2	4	38/37 (103%)	37 (97%)	1 (3%)	40	72
3	5	54/55 (98%)	53 (98%)	1 (2%)	50	76
4	6	33/34 (97%)	33 (100%)	0	100	100
7	C	206/213 (97%)	205 (100%)	1 (0%)	81	89
8	D	157/162 (97%)	156 (99%)	1 (1%)	78	88
10	E	155/158 (98%)	155 (100%)	0	100	100
11	F	124/153 (81%)	119 (96%)	5 (4%)	28	62
12	G	133/141 (94%)	132 (99%)	1 (1%)	73	86
13	H	55/107 (51%)	55 (100%)	0	100	100
14	J	118/119 (99%)	115 (98%)	3 (2%)	42	72
15	K	100/102 (98%)	100 (100%)	0	100	100
16	L	104/106 (98%)	104 (100%)	0	100	100
17	Le	59/61 (97%)	56 (95%)	3 (5%)	21	55
18	M	108/110 (98%)	108 (100%)	0	100	100
19	N	97/104 (93%)	96 (99%)	1 (1%)	68	84
20	O	86/87 (99%)	86 (100%)	0	100	100
21	P	94/98 (96%)	93 (99%)	1 (1%)	65	83
22	Q	87/88 (99%)	86 (99%)	1 (1%)	65	83
23	R	82/86 (95%)	82 (100%)	0	100	100
24	S	86/87 (99%)	86 (100%)	0	100	100
25	T	73/82 (89%)	70 (96%)	3 (4%)	27	61
26	U	88/88 (100%)	84 (96%)	4 (4%)	24	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	V	143/164 (87%)	136 (95%)	7 (5%)	22	56
28	W	56/61 (92%)	54 (96%)	2 (4%)	31	65
29	X	65/67 (97%)	64 (98%)	1 (2%)	57	80
30	Y	52/55 (94%)	44 (85%)	8 (15%)	2	13
31	Z	48/49 (98%)	48 (100%)	0	100	100
33	b	191/202 (95%)	190 (100%)	1 (0%)	81	89
34	c	165/187 (88%)	165 (100%)	0	100	100
35	d	166/174 (95%)	165 (99%)	1 (1%)	78	88
36	e	114/124 (92%)	114 (100%)	0	100	100
37	f	88/119 (74%)	87 (99%)	1 (1%)	65	83
38	g	116/122 (95%)	113 (97%)	3 (3%)	40	72
39	h	108/109 (99%)	107 (99%)	1 (1%)	70	85
40	i	104/106 (98%)	99 (95%)	5 (5%)	23	57
41	j	85/92 (92%)	83 (98%)	2 (2%)	43	73
42	k	84/98 (86%)	84 (100%)	0	100	100
43	l	105/107 (98%)	104 (99%)	1 (1%)	68	84
44	m	92/99 (93%)	85 (92%)	7 (8%)	12	41
45	n	78/82 (95%)	78 (100%)	0	100	100
46	o	73/75 (97%)	73 (100%)	0	100	100
47	p	61/65 (94%)	60 (98%)	1 (2%)	55	79
48	q	70/79 (89%)	69 (99%)	1 (1%)	59	80
49	r	56/64 (88%)	56 (100%)	0	100	100
50	s	69/78 (88%)	69 (100%)	0	100	100
51	t	67/70 (96%)	67 (100%)	0	100	100
52	u	51/60 (85%)	51 (100%)	0	100	100
53	v	242/335 (72%)	232 (96%)	10 (4%)	27	61
All	All	4732/5173 (92%)	4654 (98%)	78 (2%)	54	79

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	4	42	LEU
3	5	22	LYS

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Mol	Chain	Res	Type
7	C	258	THR
8	D	13	THR
11	F	7	ILE
11	F	32	THR
11	F	64	LYS
11	F	153	ASP
11	F	162	THR
12	G	33	LEU
14	J	45	THR
14	J	50	THR
14	J	141	LYS
17	Le	28	LEU
17	Le	50	VAL
17	Le	57	ILE
19	N	37	THR
21	P	62	VAL
22	Q	103	LYS
25	T	5	ARG
25	T	18	LYS
25	T	40	LEU
26	U	41	ILE
26	U	45	THR
26	U	82	VAL
26	U	102	VAL
27	V	6	LEU
27	V	11	ARG
27	V	44	THR
27	V	91	HIS
27	V	94	PHE
27	V	101	HIS
27	V	103	LEU
28	W	23	VAL
28	W	40	GLN
29	X	7	VAL
30	Y	8	LYS
30	Y	9	SER
30	Y	15	GLU
30	Y	16	GLN
30	Y	17	LEU
30	Y	18	LEU
30	Y	20	LEU
30	Y	33	THR

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Mol	Chain	Res	Type
33	b	23	TRP
35	d	9	CYS
37	f	9	LEU
38	g	5	ARG
38	g	12	VAL
38	g	148	ASN
39	h	75	VAL
40	i	5	GLN
40	i	42	GLU
40	i	46	MET
40	i	47	VAL
40	i	116	VAL
41	j	16	ARG
41	j	67	ILE
43	l	15	MET
44	m	40	ASN
44	m	71	ARG
44	m	83	LEU
44	m	92	ARG
44	m	102	THR
44	m	105	ASN
44	m	108	THR
47	p	21	VAL
48	q	54	ASN
53	v	50	LEU
53	v	53	LEU
53	v	71	THR
53	v	89	MET
53	v	94	THR
53	v	97	ARG
53	v	138	LYS
53	v	214	LYS
53	v	219	LEU
53	v	259	THR

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

Mol	Chain	Res	Type
2	4	26	ASN
7	C	90	HIS
7	C	226	ASN
10	E	61	GLN

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Mol	Chain	Res	Type
12	G	7	ASN
12	G	81	GLN
14	J	58	ASN
15	K	88	ASN
16	L	54	GLN
16	L	55	GLN
17	Le	33	HIS
18	M	22	HIS
22	Q	44	GLN
23	R	66	HIS
26	U	44	HIS
27	V	25	ASN
27	V	106	HIS
28	W	29	GLN
28	W	40	GLN
30	Y	12	GLN
30	Y	16	GLN
31	Z	43	ASN
33	b	3	GLN
33	b	19	GLN
33	b	24	ASN
34	c	190	HIS
36	e	147	ASN
40	i	75	GLN
42	k	64	GLN
44	m	76	ASN
46	o	61	ASN
47	p	63	GLN
48	q	34	HIS
48	q	54	ASN
50	s	63	ASN
51	t	20	HIS
53	v	102	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	a	1525/1526 (99%)	301 (19%)	0
5	A	2880/2888 (99%)	707 (24%)	49 (1%)
6	B	119/120 (99%)	26 (21%)	2 (1%)
9	Dt	75/76 (98%)	23 (30%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4599/4610 (99%)	1057 (22%)	51 (1%)

All (1057) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	A
5	A	33	U
5	A	34	U
5	A	35	G
5	A	44	A
5	A	45	G
5	A	46	G
5	A	51	G
5	A	54	A
5	A	59	U
5	A	61	G
5	A	63	A
5	A	74	A
5	A	75	G
5	A	79	C
5	A	82	G
5	A	85	G
5	A	91	A
5	A	92	A
5	A	97	A
5	A	100	U
5	A	102	G
5	A	104	U
5	A	114	U
5	A	115	C
5	A	118	A
5	A	120	U
5	A	125	G
5	A	131	A
5	A	137	G
5	A	138	A
5	A	139	U
5	A	141	A
5	A	142	C
5	A	144	U
5	A	146	G
5	A	147	G

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Mol	Chain	Res	Type
5	A	149	A
5	A	150	U
5	A	160	A
5	A	162	U
5	A	163	C
5	A	164	C
5	A	165	A
5	A	166	U
5	A	172	C
5	A	173	A
5	A	181	A
5	A	194	G
5	A	196	A
5	A	199	A
5	A	202	U
5	A	205	G
5	A	215	G
5	A	216	A
5	A	220	G
5	A	222	A
5	A	227	A
5	A	228	C
5	A	230	G
5	A	233	A
5	A	240	U
5	A	241	A
5	A	242	G
5	A	243	U
5	A	244	A
5	A	248	G
5	A	249	C
5	A	252	G
5	A	255	A
5	A	265	A
5	A	266	G
5	A	267	C
5	A	271	U
5	A	273	A
5	A	281	U
5	A	285	U
5	A	289	G
5	A	294	A

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Mol	Chain	Res	Type
5	A	299	C
5	A	305	A
5	A	315	U
5	A	316	A
5	A	317	G
5	A	318	U
5	A	321	G
5	A	322	U
5	A	323	G
5	A	324	A
5	A	325	U
5	A	335	C
5	A	337	C
5	A	338	G
5	A	339	A
5	A	342	G
5	A	347	U
5	A	348	U
5	A	349	U
5	A	350	G
5	A	351	A
5	A	353	G
5	A	358	A
5	A	359	U
5	A	360	C
5	A	361	A
5	A	374	C
5	A	376	C
5	A	377	G
5	A	380	A
5	A	381	A
5	A	385	U
5	A	387	G
5	A	390	U
5	A	391	G
5	A	395	A
5	A	396	U
5	A	397	G
5	A	398	G
5	A	399	G
5	A	400	G
5	A	403	A

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Mol	Chain	Res	Type
5	A	406	A
5	A	407	U
5	A	408	C
5	A	414	A
5	A	428	U
5	A	431	C
5	A	435	C
5	A	438	A
5	A	445	A
5	A	447	C
5	A	448	A
5	A	461	A
5	A	464	G
5	A	466	C
5	A	471	A
5	A	472	G
5	A	481	A
5	A	485	G
5	A	496	A
5	A	499	A
5	A	500	C
5	A	509	G
5	A	519	A
5	A	521	G
5	A	522	C
5	A	523	A
5	A	534	A
5	A	535	C
5	A	536	U
5	A	537	U
5	A	538	G
5	A	539	U
5	A	540	U
5	A	541	A
5	A	550	C
5	A	553	A
5	A	557	U
5	A	558	U
5	A	562	A
5	A	563	U
5	A	564	A
5	A	565	A

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Mol	Chain	Res	Type
5	A	576	A
5	A	586	A
5	A	593	A
5	A	594	G
5	A	599	A
5	A	601	C
5	A	603	U
5	A	604	A
5	A	610	U
5	A	611	A
5	A	618	G
5	A	622	A
5	A	627	A
5	A	635	U
5	A	636	A
5	A	647	U
5	A	659	G
5	A	660	A
5	A	671	G
5	A	672	G
5	A	673	C
5	A	676	U
5	A	687	G
5	A	708	A
5	A	716	G
5	A	720	A
5	A	737	U
5	A	738	G
5	A	743	G
5	A	747	G
5	A	754	A
5	A	755	C
5	A	765	G
5	A	766	G
5	A	767	A
5	A	769	U
5	A	772	A
5	A	774	G
5	A	775	G
5	A	783	A
5	A	784	G
5	A	793	U

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Mol	Chain	Res	Type
5	A	795	G
5	A	802	C
5	A	817	U
5	A	824	G
5	A	827	C
5	A	833	G
5	A	836	U
5	A	841	C
5	A	843	G
5	A	844	G
5	A	846	G
5	A	848	G
5	A	850	A
5	A	855	A
5	A	866	U
5	A	870	G
5	A	875	A
5	A	877	C
5	A	878	C
5	A	880	G
5	A	881	A
5	A	889	A
5	A	899	A
5	A	904	C
5	A	908	U
5	A	911	C
5	A	921	C
5	A	922	G
5	A	931	A
5	A	935	A
5	A	936	C
5	A	949	A
5	A	951	C
5	A	952	G
5	A	954	C
5	A	963	A
5	A	964	A
5	A	972	C
5	A	973	A
5	A	980	A
5	A	986	A
5	A	999	A

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Mol	Chain	Res	Type
5	A	1002	U
5	A	1003	U
5	A	1011	A
5	A	1012	G
5	A	1013	U
5	A	1016	U
5	A	1017	A
5	A	1023	U
5	A	1031	G
5	A	1036	A
5	A	1037	G
5	A	1048	G
5	A	1050	U
5	A	1051	U
5	A	1052	G
5	A	1057	A
5	A	1058	G
5	A	1060	A
5	A	1061	G
5	A	1063	A
5	A	1064	G
5	A	1066	C
5	A	1068	C
5	A	1076	A
5	A	1077	G
5	A	1078	A
5	A	1079	A
5	A	1080	A
5	A	1082	C
5	A	1084	U
5	A	1085	A
5	A	1086	A
5	A	1088	A
5	A	1097	G
5	A	1100	G
5	A	1101	A
5	A	1102	G
5	A	1114	G
5	A	1117	A
5	A	1119	A
5	A	1120	U
5	A	1124	A

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Mol	Chain	Res	Type
5	A	1125	C
5	A	1133	A
5	A	1146	A
5	A	1148	G
5	A	1149	C
5	A	1154	G
5	A	1162	G
5	A	1164	A
5	A	1167	U
5	A	1168	G
5	A	1170	C
5	A	1171	G
5	A	1191	A
5	A	1192	A
5	A	1193	G
5	A	1198	U
5	A	1199	G
5	A	1214	A
5	A	1218	U
5	A	1223	G
5	A	1225	G
5	A	1228	A
5	A	1232	G
5	A	1233	A
5	A	1234	A
5	A	1238	C
5	A	1240	A
5	A	1243	G
5	A	1244	C
5	A	1249	A
5	A	1253	G
5	A	1256	A
5	A	1258	G
5	A	1259	A
5	A	1261	A
5	A	1263	U
5	A	1276	C
5	A	1283	G
5	A	1287	A
5	A	1288	A
5	A	1301	C
5	A	1311	G

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Mol	Chain	Res	Type
5	A	1316	U
5	A	1321	G
5	A	1339	U
5	A	1349	C
5	A	1352	A
5	A	1354	A
5	A	1355	A
5	A	1363	C
5	A	1365	A
5	A	1366	U
5	A	1367	G
5	A	1370	A
5	A	1373	C
5	A	1379	A
5	A	1380	A
5	A	1382	A
5	A	1390	A
5	A	1402	U
5	A	1403	G
5	A	1404	C
5	A	1408	G
5	A	1414	A
5	A	1415	C
5	A	1422	G
5	A	1424	C
5	A	1434	U
5	A	1440	U
5	A	1441	U
5	A	1442	G
5	A	1445	U
5	A	1447	U
5	A	1448	C
5	A	1449	C
5	A	1454	U
5	A	1469	G
5	A	1474	C
5	A	1480	U
5	A	1481	A
5	A	1484	U
5	A	1496	A
5	A	1497	G
5	A	1508	G

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Mol	Chain	Res	Type
5	A	1509	A
5	A	1511	G
5	A	1512	A
5	A	1516	G
5	A	1528	A
5	A	1537	U
5	A	1542	G
5	A	1556	A
5	A	1558	G
5	A	1559	A
5	A	1560	A
5	A	1573	U
5	A	1574	U
5	A	1576	A
5	A	1580	A
5	A	1597	C
5	A	1598	A
5	A	1600	A
5	A	1602	C
5	A	1603	G
5	A	1606	A
5	A	1608	A
5	A	1609	G
5	A	1614	U
5	A	1628	C
5	A	1629	C
5	A	1634	C
5	A	1636	C
5	A	1637	U
5	A	1638	U
5	A	1639	G
5	A	1654	A
5	A	1663	G
5	A	1664	G
5	A	1673	C
5	A	1683	U
5	A	1685	G
5	A	1686	G
5	A	1689	G
5	A	1690	A
5	A	1698	C
5	A	1704	A

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Mol	Chain	Res	Type
5	A	1705	G
5	A	1708	U
5	A	1711	A
5	A	1714	A
5	A	1716	U
5	A	1717	U
5	A	1720	U
5	A	1721	C
5	A	1724	U
5	A	1731	U
5	A	1732	G
5	A	1735	U
5	A	1741	A
5	A	1742	A
5	A	1745	U
5	A	1749	A
5	A	1750	G
5	A	1751	G
5	A	1756	U
5	A	1760	A
5	A	1771	A
5	A	1773	A
5	A	1778	A
5	A	1787	C
5	A	1788	A
5	A	1795	A
5	A	1797	A
5	A	1798	G
5	A	1803	C
5	A	1816	A
5	A	1820	C
5	A	1834	A
5	A	1837	G
5	A	1838	U
5	A	1844	G
5	A	1850	G
5	A	1851	U
5	A	1853	A
5	A	1861	C
5	A	1873	U
5	A	1875	G
5	A	1892	C

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Mol	Chain	Res	Type
5	A	1893	G
5	A	1897	G
5	A	1898	U
5	A	1899	A
5	A	1901	C
5	A	1902	U
5	A	1906	A
5	A	1916	G
5	A	1917	G
5	A	1918	U
5	A	1924	A
5	A	1925	A
5	A	1942	U
5	A	1949	C
5	A	1950	U
5	A	1951	G
5	A	1954	C
5	A	1957	A
5	A	1958	U
5	A	1959	G
5	A	1967	G
5	A	1968	A
5	A	1969	U
5	A	1978	U
5	A	1979	G
5	A	1982	U
5	A	1983	C
5	A	1984	C
5	A	1993	C
5	A	2008	A
5	A	2010	C
5	A	2015	U
5	A	2017	A
5	A	2018	A
5	A	2020	A
5	A	2028	U
5	A	2030	U
5	A	2039	A
5	A	2042	C
5	A	2043	G
5	A	2047	A
5	A	2048	G

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Mol	Chain	Res	Type
5	A	2049	A
5	A	2055	U
5	A	2056	G
5	A	2060	C
5	A	2063	U
5	A	2064	A
5	A	2067	G
5	A	2068	U
5	A	2080	G
5	A	2082	A
5	A	2083	C
5	A	2094	C
5	A	2095	U
5	A	2097	G
5	A	2098	U
5	A	2099	G
5	A	2101	A
5	A	2103	G
5	A	2106	A
5	A	2113	A
5	A	2114	G
5	A	2115	G
5	A	2116	C
5	A	2117	U
5	A	2118	U
5	A	2119	U
5	A	2121	A
5	A	2122	A
5	A	2127	G
5	A	2129	A
5	A	2132	C
5	A	2133	C
5	A	2135	G
5	A	2140	C
5	A	2141	G
5	A	2144	G
5	A	2145	A
5	A	2146	G
5	A	2147	C
5	A	2148	C
5	A	2149	A
5	A	2150	U

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Mol	Chain	Res	Type
5	A	2151	C
5	A	2156	A
5	A	2157	A
5	A	2158	A
5	A	2159	U
5	A	2160	A
5	A	2169	G
5	A	2173	G
5	A	2174	C
5	A	2175	U
5	A	2185	A
5	A	2186	A
5	A	2187	C
5	A	2191	G
5	A	2194	C
5	A	2199	A
5	A	2201	C
5	A	2212	A
5	A	2221	G
5	A	2225	G
5	A	2226	G
5	A	2229	G
5	A	2237	G
5	A	2239	G
5	A	2240	G
5	A	2253	A
5	A	2264	G
5	A	2265	A
5	A	2270	U
5	A	2271	A
5	A	2274	A
5	A	2275	A
5	A	2284	C
5	A	2292	U
5	A	2296	A
5	A	2297	A
5	A	2305	G
5	A	2306	C
5	A	2307	A
5	A	2308	G
5	A	2309	A
5	A	2312	A

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Mol	Chain	Res	Type
5	A	2313	U
5	A	2314	A
5	A	2319	C
5	A	2321	A
5	A	2322	A
5	A	2323	A
5	A	2333	A
5	A	2334	C
5	A	2337	C
5	A	2357	G
5	A	2358	G
5	A	2361	C
5	A	2363	A
5	A	2370	G
5	A	2372	C
5	A	2382	C
5	A	2383	G
5	A	2386	G
5	A	2389	U
5	A	2390	C
5	A	2393	U
5	A	2407	C
5	A	2409	C
5	A	2410	U
5	A	2413	A
5	A	2414	C
5	A	2415	G
5	A	2416	G
5	A	2417	A
5	A	2421	A
5	A	2422	A
5	A	2428	U
5	A	2434	G
5	A	2435	A
5	A	2446	A
5	A	2451	G
5	A	2453	C
5	A	2454	C
5	A	2457	G
5	A	2459	G
5	A	2462	C
5	A	2466	U

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Mol	Chain	Res	Type
5	A	2471	G
5	A	2478	U
5	A	2480	U
5	A	2481	G
5	A	2489	G
5	A	2492	G
5	A	2505	A
5	A	2506	U
5	A	2517	A
5	A	2521	C
5	A	2522	G
5	A	2537	G
5	A	2541	U
5	A	2553	A
5	A	2554	G
5	A	2559	A
5	A	2560	C
5	A	2563	G
5	A	2565	G
5	A	2573	U
5	A	2586	G
5	A	2590	G
5	A	2593	C
5	A	2600	U
5	A	2602	U
5	A	2616	U
5	A	2619	A
5	A	2633	C
5	A	2640	U
5	A	2641	A
5	A	2647	A
5	A	2651	G
5	A	2660	G
5	A	2669	U
5	A	2676	U
5	A	2677	U
5	A	2689	G
5	A	2690	C
5	A	2692	A
5	A	2701	G
5	A	2703	C
5	A	2704	G

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Mol	Chain	Res	Type
5	A	2705	G
5	A	2713	U
5	A	2714	G
5	A	2720	A
5	A	2726	U
5	A	2731	G
5	A	2733	U
5	A	2739	C
5	A	2743	U
5	A	2744	A
5	A	2751	A
5	A	2752	A
5	A	2763	A
5	A	2765	A
5	A	2766	U
5	A	2771	U
5	A	2784	U
5	A	2785	U
5	A	2786	G
5	A	2787	A
5	A	2794	U
5	A	2795	G
5	A	2805	C
5	A	2807	A
5	A	2811	C
5	A	2812	U
5	A	2818	G
5	A	2820	U
5	A	2821	G
5	A	2836	U
5	A	2842	U
5	A	2846	G
5	A	2851	G
5	A	2852	U
5	A	2854	G
5	A	2867	C
5	A	2870	A
5	A	2871	U
5	A	2884	U
5	A	2889	C
6	B	13	A
6	B	20	G

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Mol	Chain	Res	Type
6	B	22	U
6	B	24	G
6	B	25	A
6	B	28	C
6	B	29	A
6	B	35	U
6	B	41	C
6	B	42	C
6	B	43	C
6	B	45	A
6	B	46	A
6	B	51	G
6	B	52	A
6	B	54	G
6	B	56	G
6	B	57	A
6	B	63	C
6	B	66	A
6	B	73	A
6	B	89	U
6	B	90	C
6	B	105	G
6	B	106	G
6	B	109	A
9	Dt	4	C
9	Dt	8	U
9	Dt	11	C
9	Dt	15	G
9	Dt	16	U
9	Dt	17	C
9	Dt	19	G
9	Dt	20	U
9	Dt	21	A
9	Dt	22	G
9	Dt	32	U
9	Dt	39	U
9	Dt	44	G
9	Dt	46	G
9	Dt	47	U
9	Dt	49	C
9	Dt	52	G
9	Dt	55	U

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Mol	Chain	Res	Type
9	Dt	58	A
9	Dt	72	C
9	Dt	74	C
9	Dt	75	C
9	Dt	76	A
32	a	3	A
32	a	6	G
32	a	7	A
32	a	9	G
32	a	22	G
32	a	29	U
32	a	31	G
32	a	32	A
32	a	42	G
32	a	47	C
32	a	48	C
32	a	51	A
32	a	52	C
32	a	60	A
32	a	61	G
32	a	65	A
32	a	66	G
32	a	71	U
32	a	72	A
32	a	73	A
32	a	77	G
32	a	82	U
32	a	83	G
32	a	88	U
32	a	89	G
32	a	95	A
32	a	100	C
32	a	115	U
32	a	118	C
32	a	121	G
32	a	123	A
32	a	124	A
32	a	125	U
32	a	133	G
32	a	138	G
32	a	143	A
32	a	157	C

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Mol	Chain	Res	Type
32	a	176	C
32	a	177	G
32	a	179	C
32	a	182	G
32	a	192	G
32	a	193	U
32	a	204	C
32	a	205	G
32	a	206	G
32	a	239	U
32	a	241	G
32	a	244	A
32	a	256	A
32	a	260	G
32	a	261	C
32	a	266	C
32	a	275	G
32	a	283	A
32	a	284	C
32	a	287	G
32	a	288	U
32	a	292	A
32	a	299	G
32	a	315	A
32	a	321	A
32	a	322	C
32	a	323	A
32	a	326	G
32	a	334	U
32	a	341	G
32	a	345	G
32	a	346	C
32	a	348	G
32	a	361	U
32	a	363	G
32	a	365	A
32	a	375	A
32	a	376	A
32	a	378	G
32	a	384	U
32	a	386	C
32	a	391	A

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Mol	Chain	Res	Type
32	a	400	G
32	a	405	A
32	a	406	A
32	a	407	G
32	a	408	A
32	a	417	G
32	a	423	U
32	a	443	G
32	a	445	A
32	a	446	A
32	a	447	G
32	a	457	U
32	a	461	U
32	a	475	G
32	a	478	G
32	a	490	A
32	a	491	U
32	a	492	A
32	a	493	A
32	a	494	G
32	a	502	U
32	a	504	A
32	a	505	C
32	a	507	U
32	a	509	G
32	a	511	G
32	a	512	C
32	a	513	C
32	a	515	G
32	a	518	G
32	a	520	C
32	a	521	G
32	a	526	A
32	a	527	A
32	a	539	C
32	a	540	A
32	a	541	A
32	a	556	U
32	a	558	C
32	a	566	A
32	a	567	A
32	a	569	G

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Mol	Chain	Res	Type
32	a	570	C
32	a	571	G
32	a	573	G
32	a	582	G
32	a	584	U
32	a	585	C
32	a	590	A
32	a	627	G
32	a	647	A
32	a	648	G
32	a	659	A
32	a	681	A
32	a	682	G
32	a	687	G
32	a	688	A
32	a	696	A
32	a	710	A
32	a	712	A
32	a	717	U
32	a	718	G
32	a	727	G
32	a	733	C
32	a	749	A
32	a	754	G
32	a	756	U
32	a	759	G
32	a	760	A
32	a	771	A
32	a	788	A
32	a	806	G
32	a	807	U
32	a	809	A
32	a	810	A
32	a	811	C
32	a	812	G
32	a	815	G
32	a	822	A
32	a	830	G
32	a	835	C
32	a	838	G
32	a	840	G
32	a	845	U

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Mol	Chain	Res	Type
32	a	854	A
32	a	858	A
32	a	862	C
32	a	865	U
32	a	866	A
32	a	870	C
32	a	884	G
32	a	887	C
32	a	894	A
32	a	896	G
32	a	908	A
32	a	920	G
32	a	921	G
32	a	928	C
32	a	929	A
32	a	932	A
32	a	936	G
32	a	939	G
32	a	954	U
32	a	955	U
32	a	956	C
32	a	960	G
32	a	963	A
32	a	964	C
32	a	966	C
32	a	967	G
32	a	968	A
32	a	969	A
32	a	970	G
32	a	971	A
32	a	975	U
32	a	977	A
32	a	988	A
32	a	990	A
32	a	998	A
32	a	1004	C
32	a	1015	U
32	a	1017	G
32	a	1023	U
32	a	1025	C
32	a	1026	G
32	a	1027	G

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Mol	Chain	Res	Type
32	a	1039	C
32	a	1044	G
32	a	1049	A
32	a	1059	U
32	a	1073	G
32	a	1075	G
32	a	1078	G
32	a	1079	U
32	a	1080	U
32	a	1086	A
32	a	1088	G
32	a	1089	U
32	a	1090	C
32	a	1095	A
32	a	1118	G
32	a	1119	U
32	a	1124	A
32	a	1127	A
32	a	1130	U
32	a	1133	G
32	a	1134	G
32	a	1149	A
32	a	1152	C
32	a	1153	U
32	a	1160	G
32	a	1162	C
32	a	1163	A
32	a	1164	A
32	a	1165	A
32	a	1175	G
32	a	1178	G
32	a	1184	G
32	a	1190	A
32	a	1191	A
32	a	1196	U
32	a	1207	A
32	a	1214	G
32	a	1219	A
32	a	1221	A
32	a	1222	C
32	a	1229	U
32	a	1230	A

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Mol	Chain	Res	Type
32	a	1232	A
32	a	1234	U
32	a	1235	G
32	a	1248	G
32	a	1250	U
32	a	1251	U
32	a	1252	G
32	a	1254	C
32	a	1264	G
32	a	1266	U
32	a	1272	U
32	a	1273	A
32	a	1281	A
32	a	1293	A
32	a	1294	G
32	a	1297	C
32	a	1299	G
32	a	1314	C
32	a	1332	G
32	a	1334	A
32	a	1342	U
32	a	1347	G
32	a	1358	U
32	a	1362	A
32	a	1381	G
32	a	1388	A
32	a	1391	C
32	a	1397	C
32	a	1413	G
32	a	1414	U
32	a	1418	U
32	a	1419	U
32	a	1423	C
32	a	1424	C
32	a	1428	A
32	a	1440	A
32	a	1446	A
32	a	1448	G
32	a	1469	G
32	a	1470	A
32	a	1486	A
32	a	1487	A

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Mol	Chain	Res	Type
32	a	1491	G
32	a	1497	A
32	a	1498	G
32	a	1499	G
32	a	1500	U
32	a	1501	A
32	a	1502	G
32	a	1511	G
32	a	1514	C
32	a	1523	G
32	a	1525	A
32	a	1526	U

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	81	G
5	A	87	C
5	A	114	U
5	A	227	A
5	A	243	U
5	A	266	G
5	A	314	A
5	A	334	A
5	A	348	U
5	A	360	C
5	A	434	A
5	A	444	A
5	A	538	G
5	A	540	U
5	A	774	G
5	A	783	A
5	A	792	A
5	A	840	U
5	A	920	C
5	A	953	U
5	A	963	A
5	A	1003	U
5	A	1016	U
5	A	1051	U
5	A	1169	A
5	A	1232	G

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Mol	Chain	Res	Type
5	A	1233	A
5	A	1378	U
5	A	1448	C
5	A	1627	A
5	A	1653	G
5	A	1672	G
5	A	1710	A
5	A	1715	U
5	A	1741	A
5	A	1891	G
5	A	1897	G
5	A	1917	G
5	A	2029	A
5	A	2149	A
5	A	2200	U
5	A	2228	A
5	A	2274	A
5	A	2536	G
5	A	2703	C
5	A	2750	G
5	A	2784	U
5	A	2793	C
5	A	2853	U
6	B	34	A
6	B	51	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 171 ligands modelled in this entry, 171 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
49	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	11:CYS	C	12:ARG	N	3.53

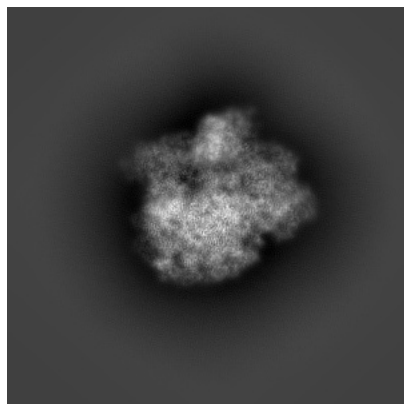
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16566. These allow visual inspection of the internal detail of the map and identification of artifacts.

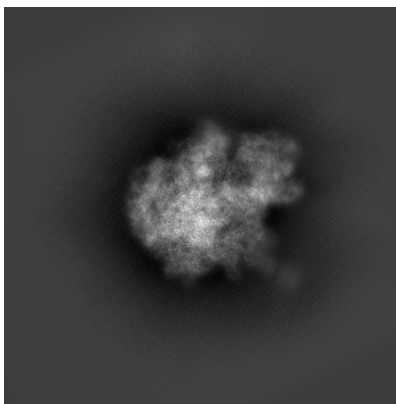
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

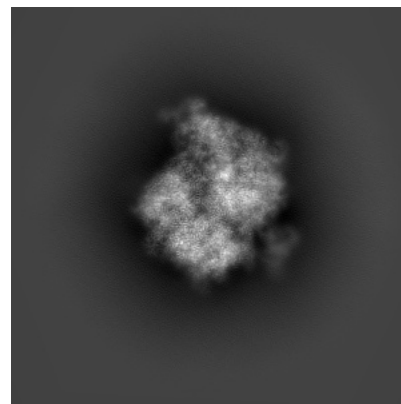
6.1.1 Primary map



X

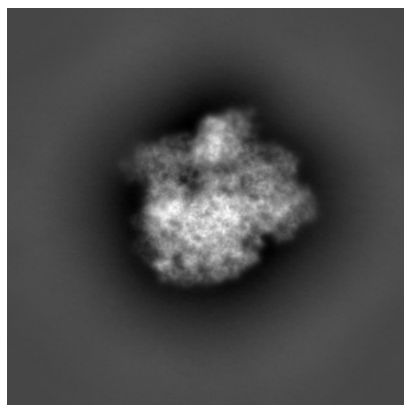


Y

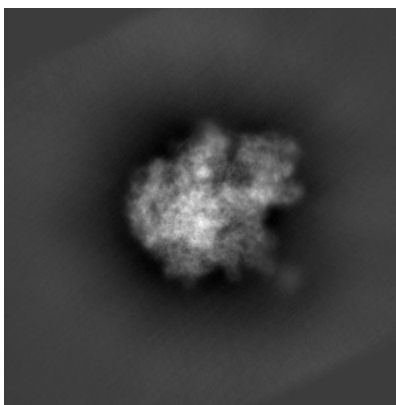


Z

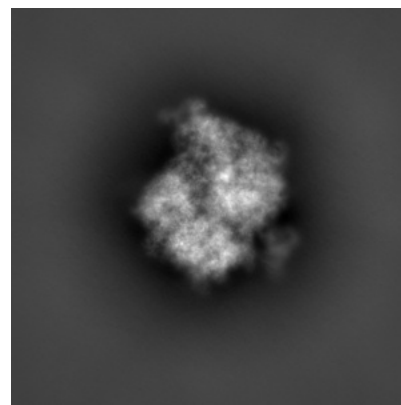
6.1.2 Raw map



X



Y

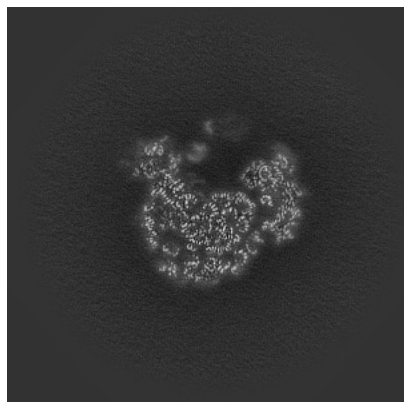


Z

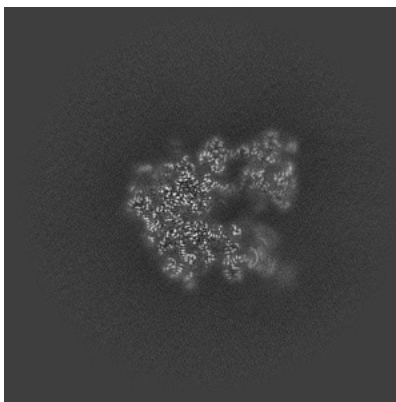
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

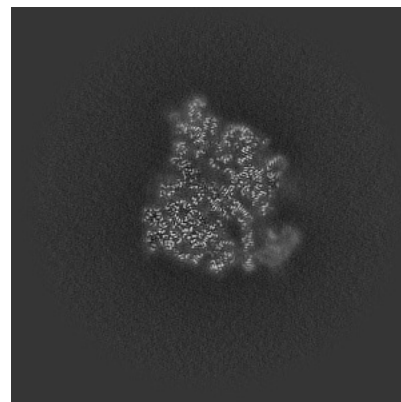
6.2.1 Primary map



X Index: 256

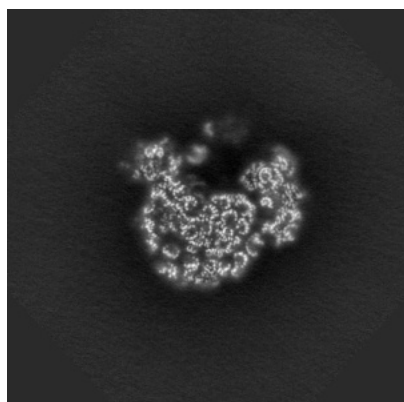


Y Index: 256

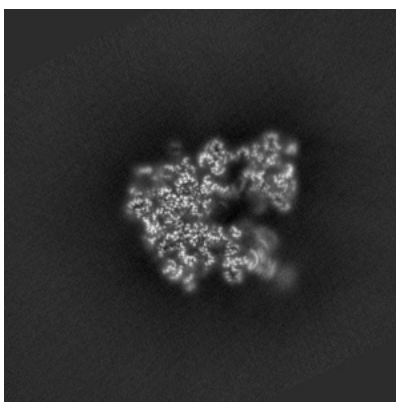


Z Index: 256

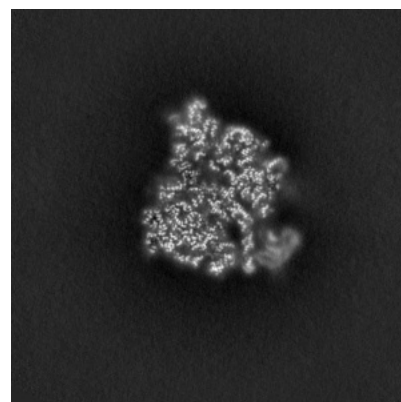
6.2.2 Raw map



X Index: 256



Y Index: 256

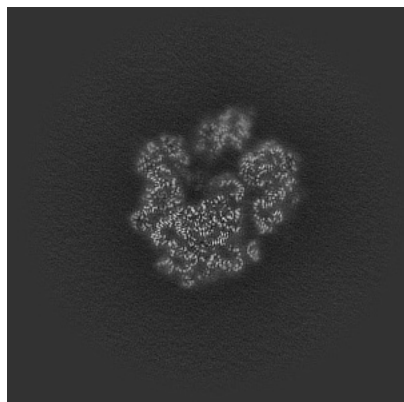


Z Index: 256

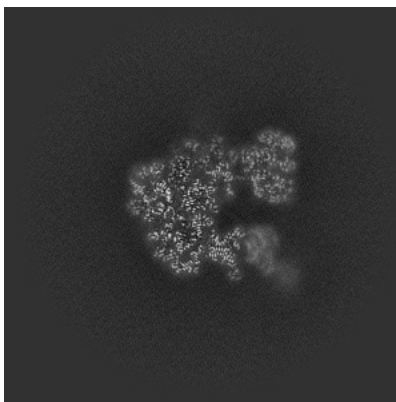
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

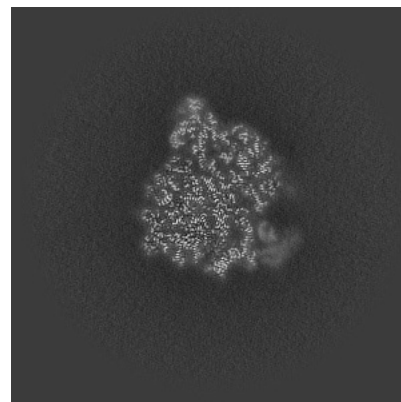
6.3.1 Primary map



X Index: 268

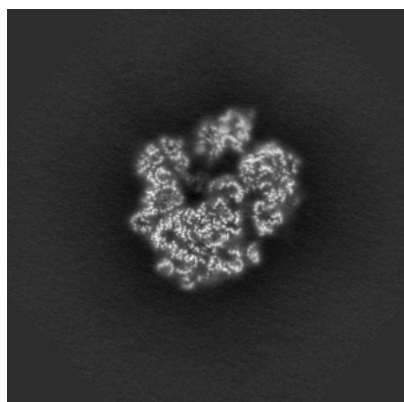


Y Index: 267

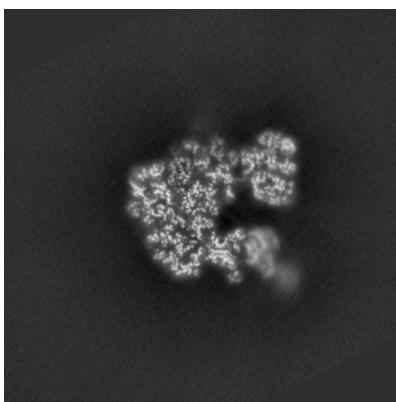


Z Index: 250

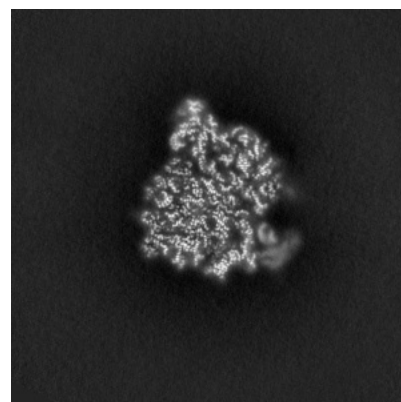
6.3.2 Raw map



X Index: 269



Y Index: 267

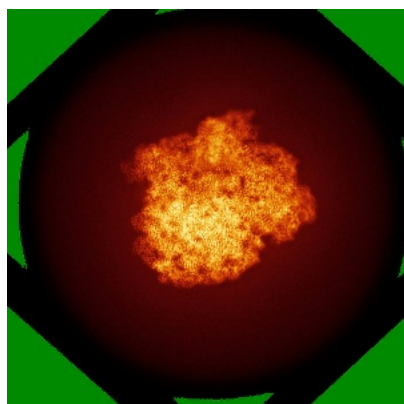


Z Index: 250

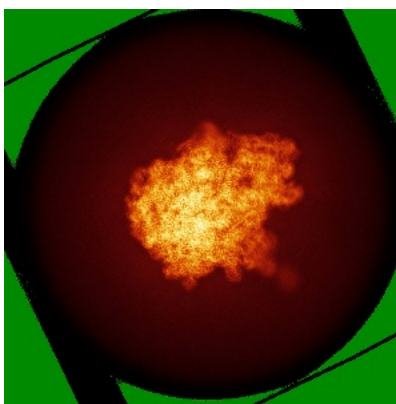
The images above show the largest variance slices of the map in three orthogonal directions.

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

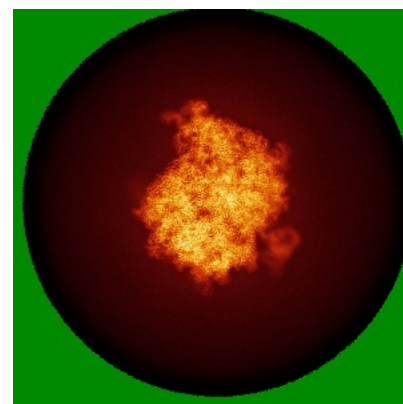
6.4.1 Primary map



X

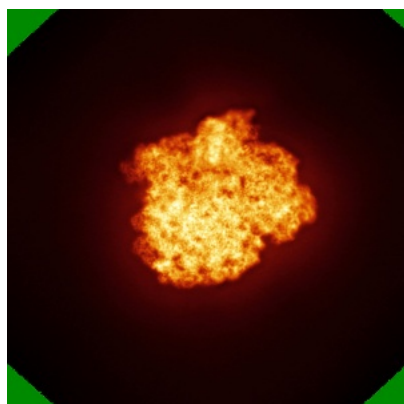


Y

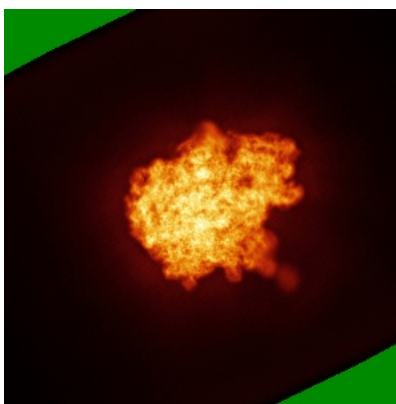


Z

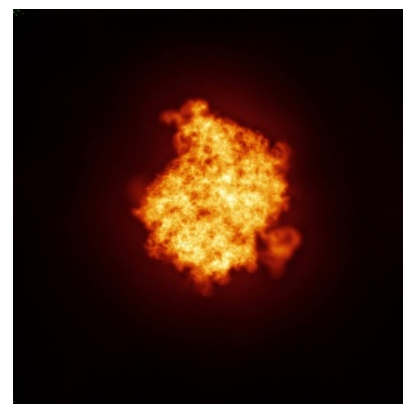
6.4.2 Raw map



X



Y

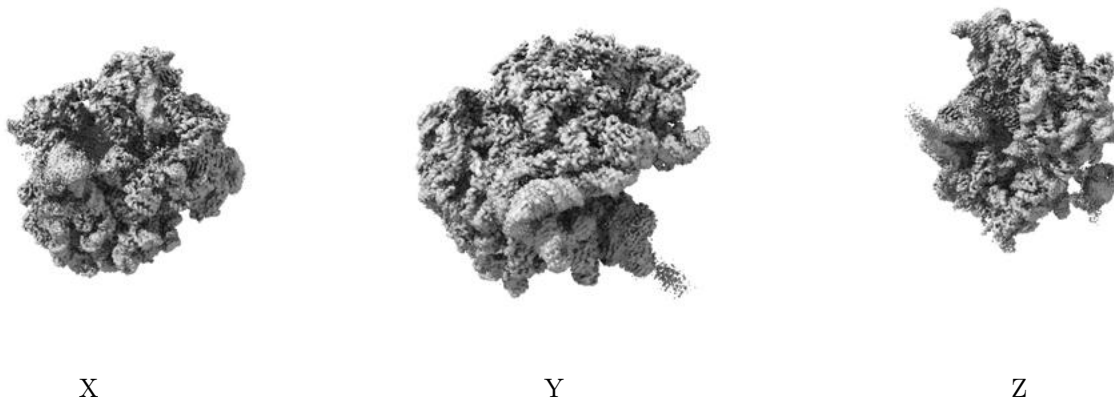


Z

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.

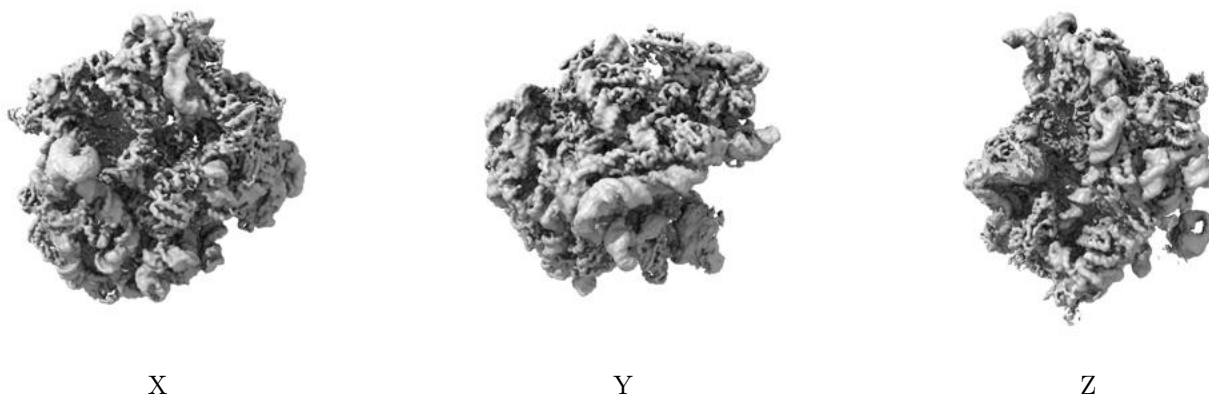
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.46. 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.

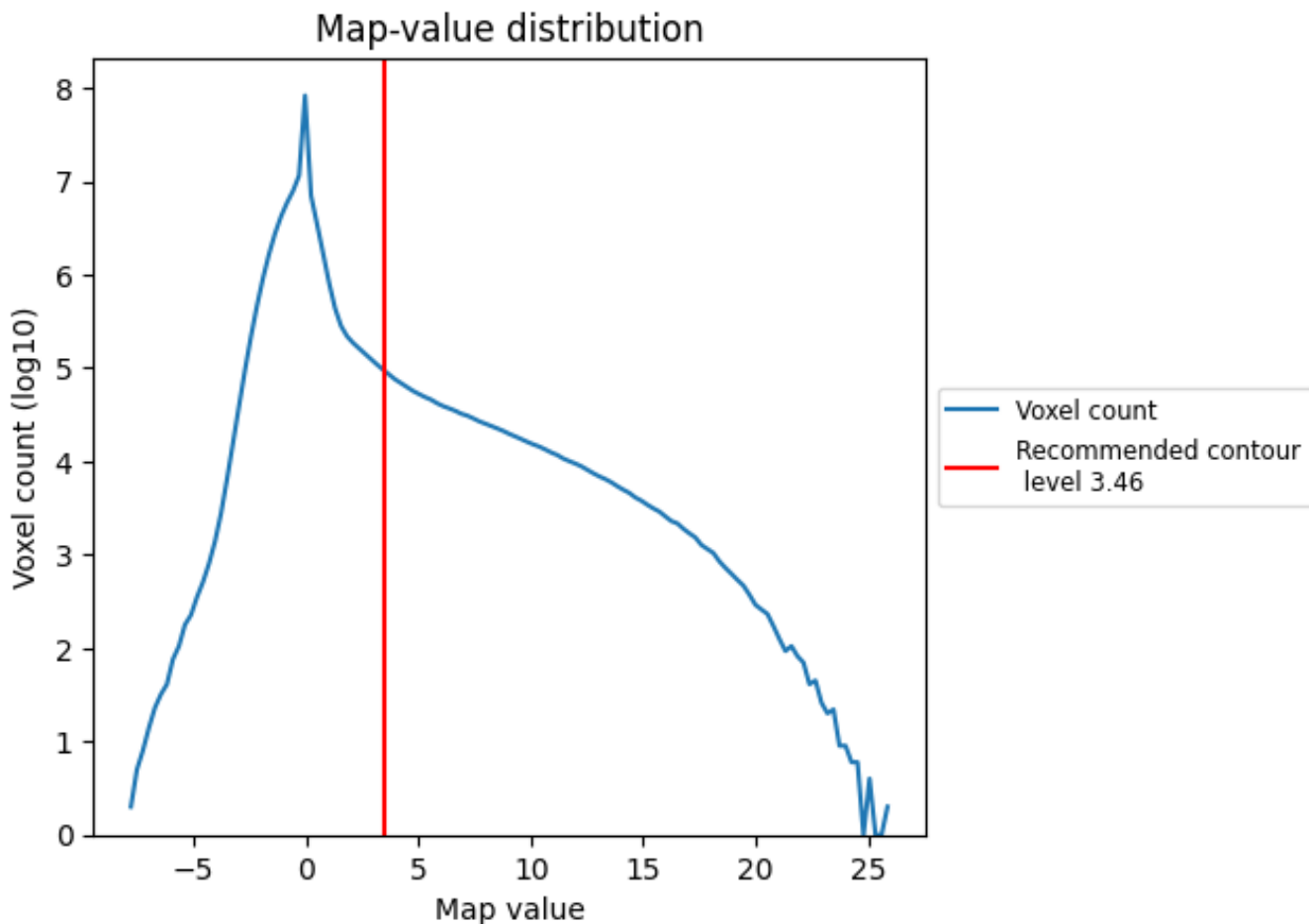
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

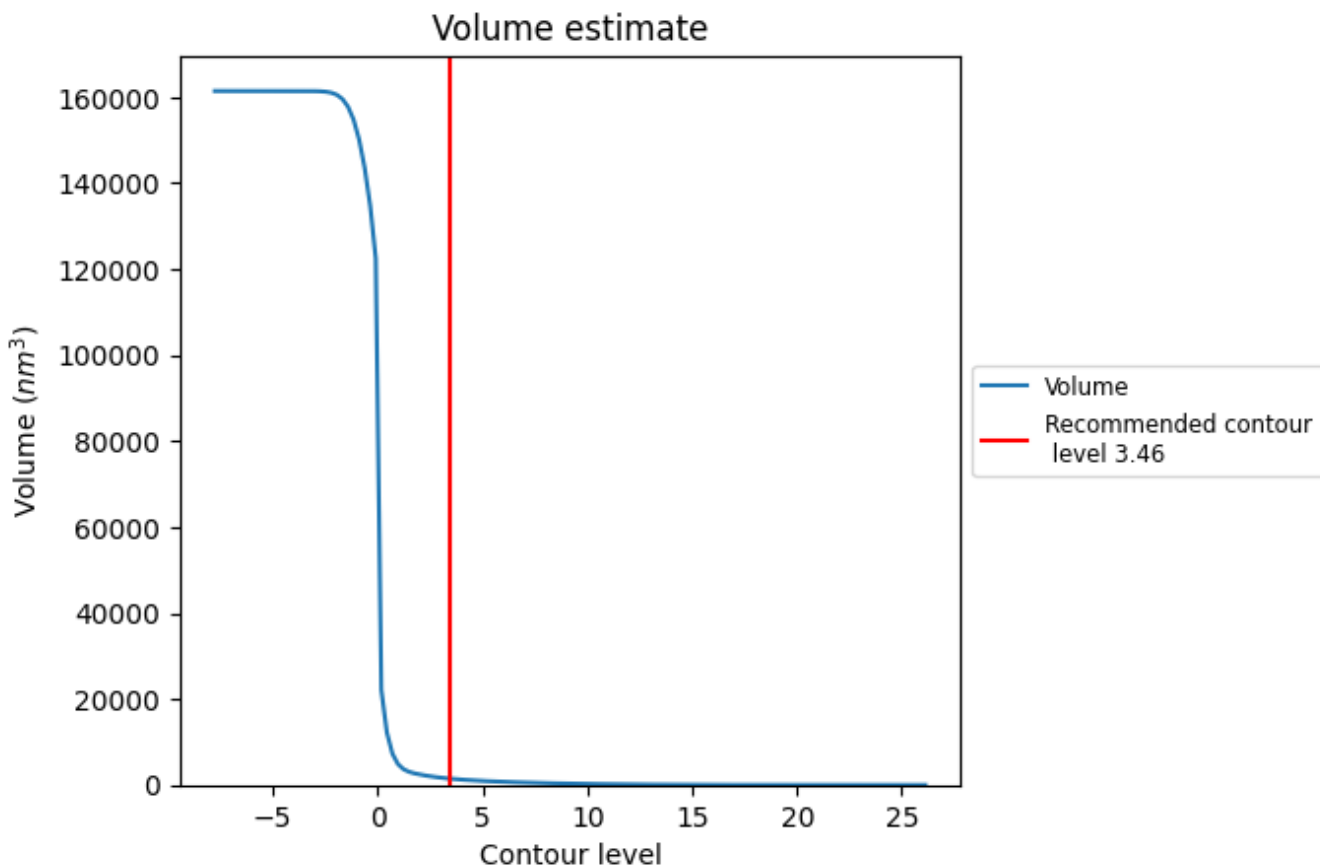
This section contains the results of statistical analysis of the map.

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.

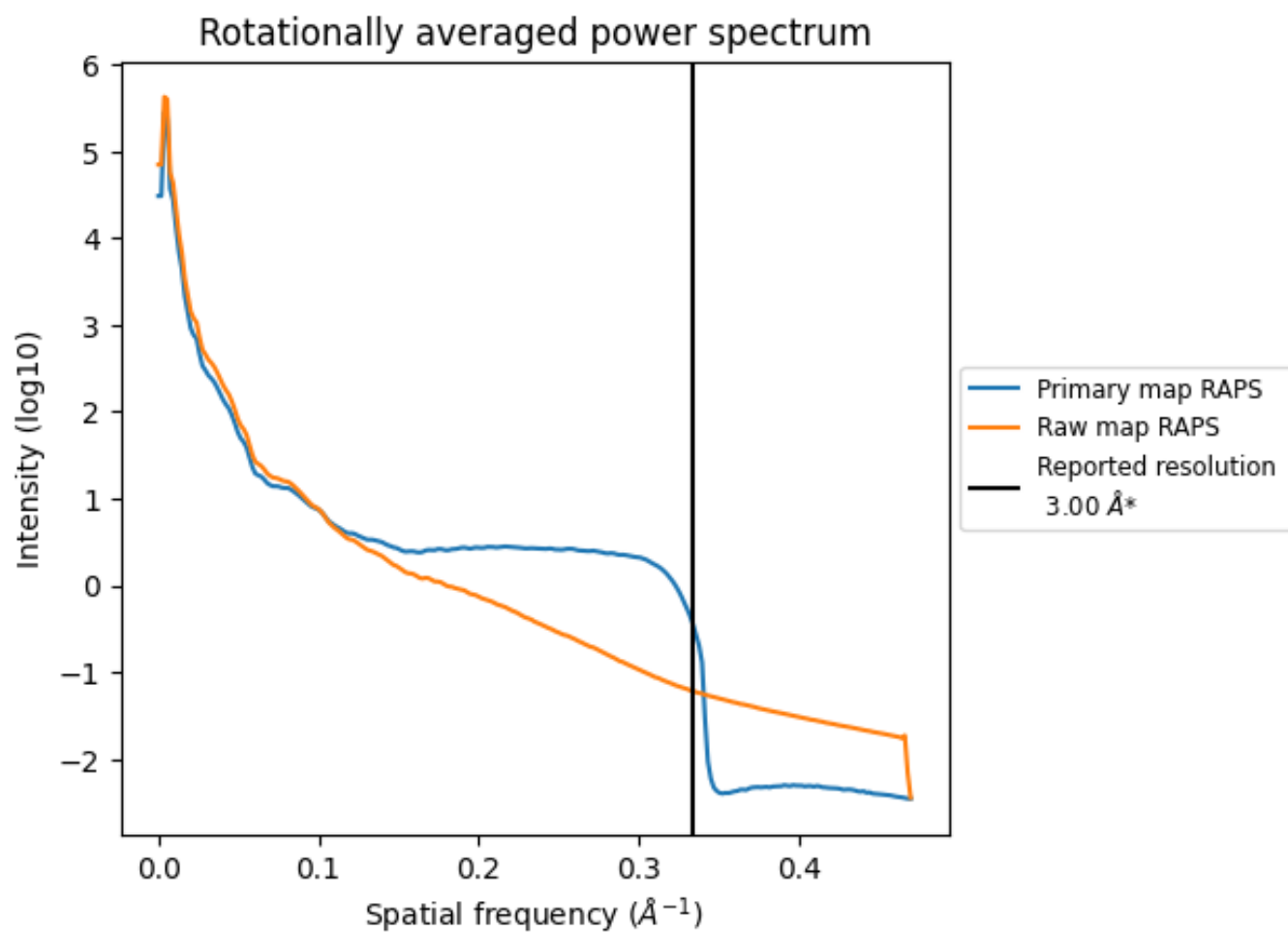
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1459 nm^3 ; this corresponds to an approximate mass of 1318 kDa.

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

7.3 Rotationally averaged power spectrum i

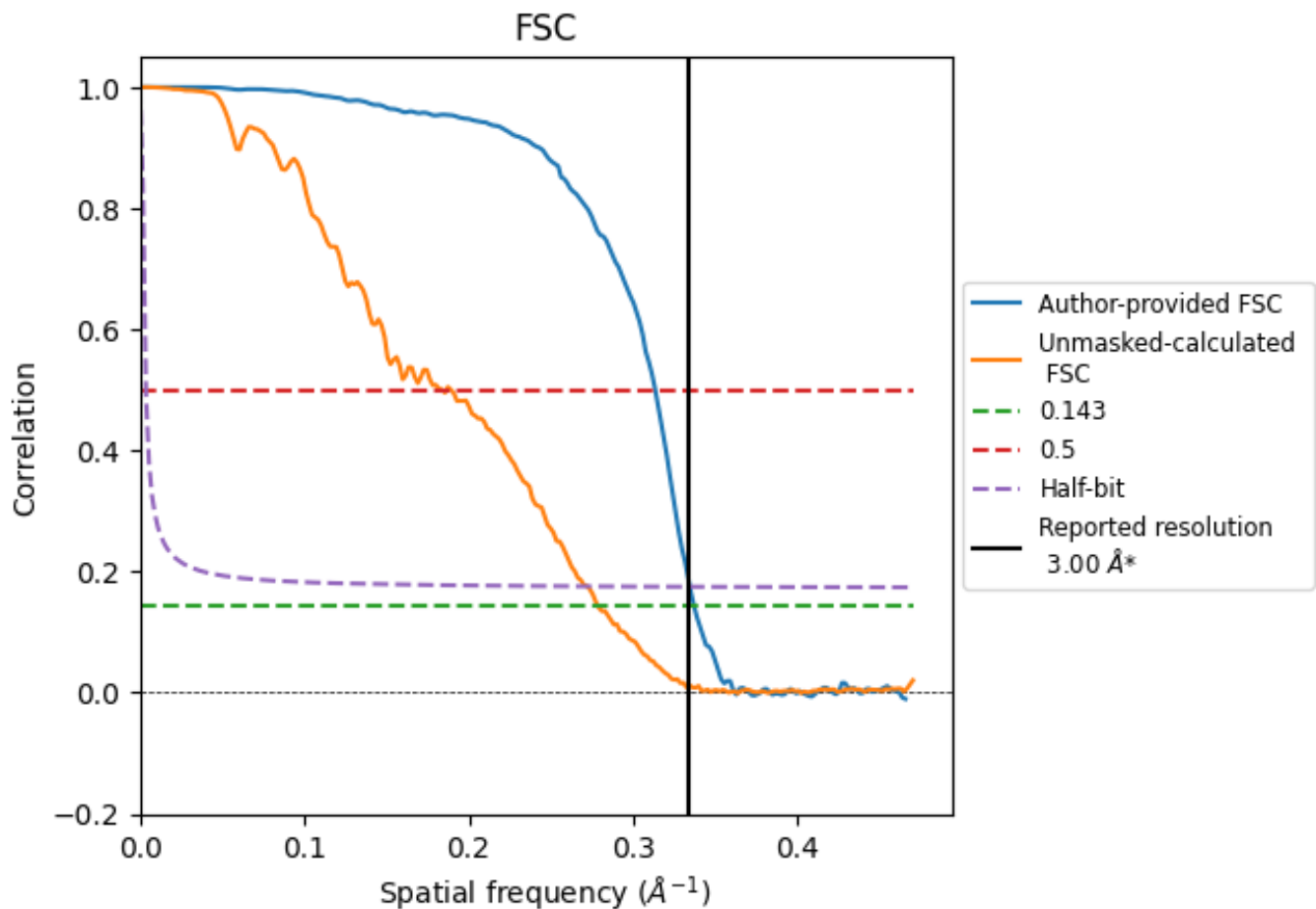


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

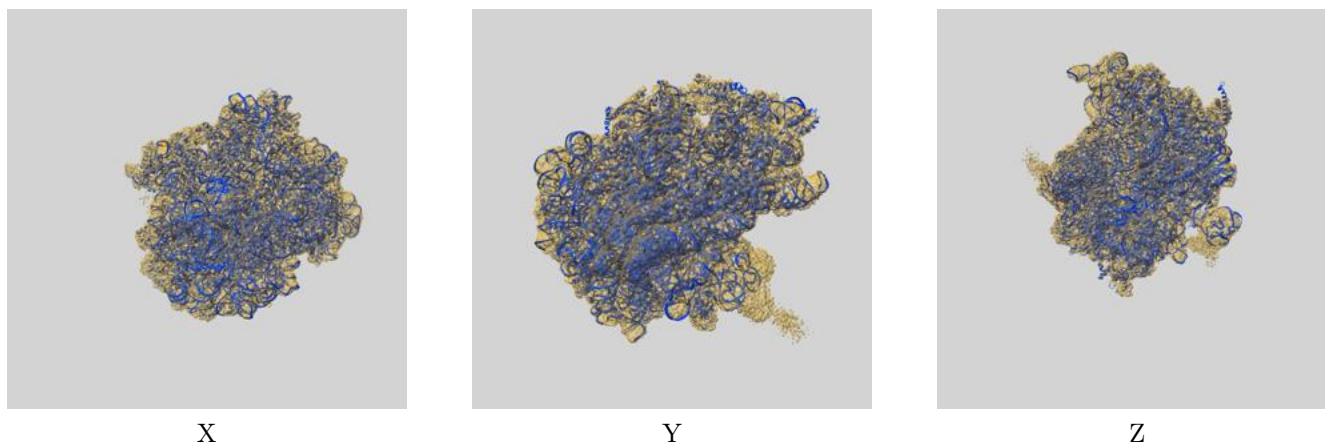
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.97	3.19	2.99
Unmasked-calculated*	3.59	5.44	3.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.59 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

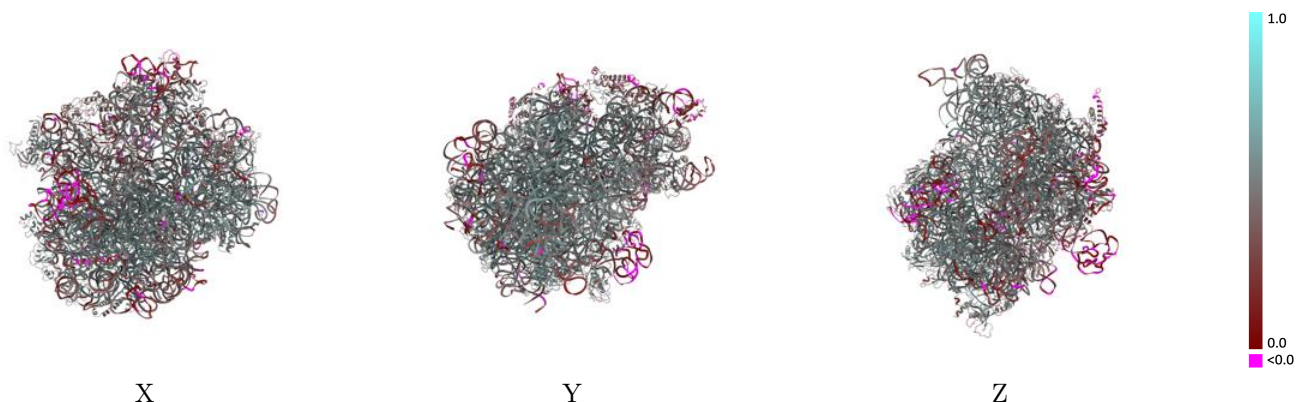
This section contains information regarding the fit between EMDB map EMD-16566 and PDB model 8CD1. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



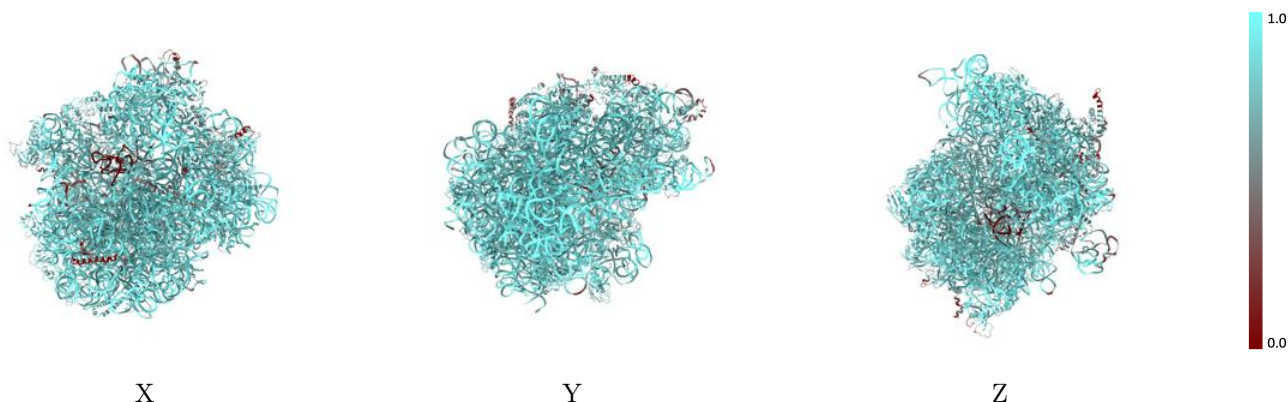
The images above show the 3D surface view of the map at the recommended contour level 3.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



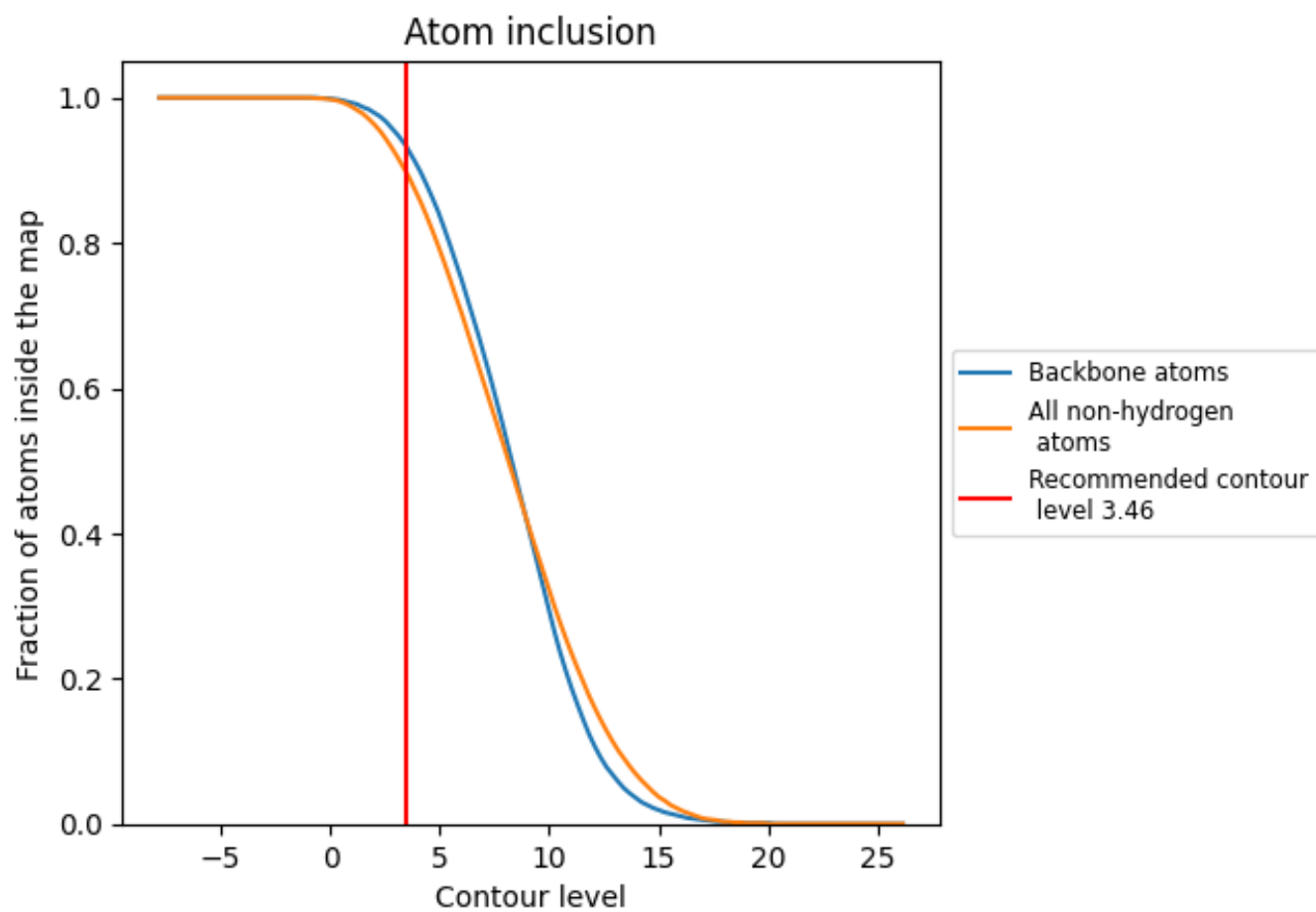
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.46).







































































9.4 Atom inclusion [i](#)

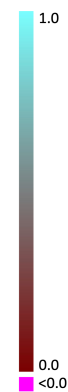


At the recommended contour level, 93% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary







































The table lists the average atom inclusion at the recommended contour level (3.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8980	 0.4610
2	 0.8800	 0.5090
4	 0.9330	 0.5560
5	 0.6800	 0.4950
6	 0.8960	 0.5200
A	 0.9400	 0.4550
B	 0.9300	 0.4200
C	 0.9020	 0.5320
D	 0.8950	 0.5120
Dt	 0.1470	 0.3840
E	 0.8990	 0.5220
F	 0.7810	 0.3700
G	 0.8210	 0.4400
H	 0.1530	 0.2090
J	 0.9060	 0.5310
K	 0.8330	 0.4870
L	 0.8800	 0.4960
Le	 0.7180	 0.3440
M	 0.8750	 0.5400
N	 0.9200	 0.5360
O	 0.8660	 0.4610
P	 0.8550	 0.4940
Q	 0.9290	 0.5520
R	 0.8940	 0.5230
S	 0.8790	 0.5210
T	 0.9020	 0.5250
U	 0.8180	 0.4650
V	 0.8200	 0.4580
W	 0.8750	 0.5090
X	 0.9000	 0.5260
Y	 0.8850	 0.4640
Z	 0.9140	 0.5280
a	 0.9630	 0.4840
b	 0.6390	 0.3340
c	 0.8060	 0.4230



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Chain	Atom inclusion	Q-score
d	 0.8360	 0.4510
e	 0.8150	 0.4450
f	 0.7900	 0.4050
g	 0.7650	 0.3770
h	 0.8740	 0.4970
i	 0.8530	 0.4170
j	 0.5110	 0.1420
k	 0.8480	 0.4720
l	 0.8320	 0.4750
m	 0.7860	 0.3550
n	 0.8650	 0.4270
o	 0.8730	 0.4910
p	 0.9250	 0.5130
q	 0.8600	 0.4860
r	 0.8000	 0.4290
s	 0.8260	 0.3850
t	 0.8990	 0.5050
u	 0.4290	 0.3630
v	 0.6920	 0.4530