



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 06:08 AM UTC

PDB ID : 7ZQ5 / pdb_00007zq5
EMDB ID : EMD-14864
Title : 70S E. coli ribosome with truncated uL23 and uL24 loops
Authors : Mitropoulou, A.; Wlodarski, T.; Ahn, M.; Becker, T.A.; Beckmann, R.; Cabrita, L.D.; Christodoulou, J.
Deposited on : 2022-04-29
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

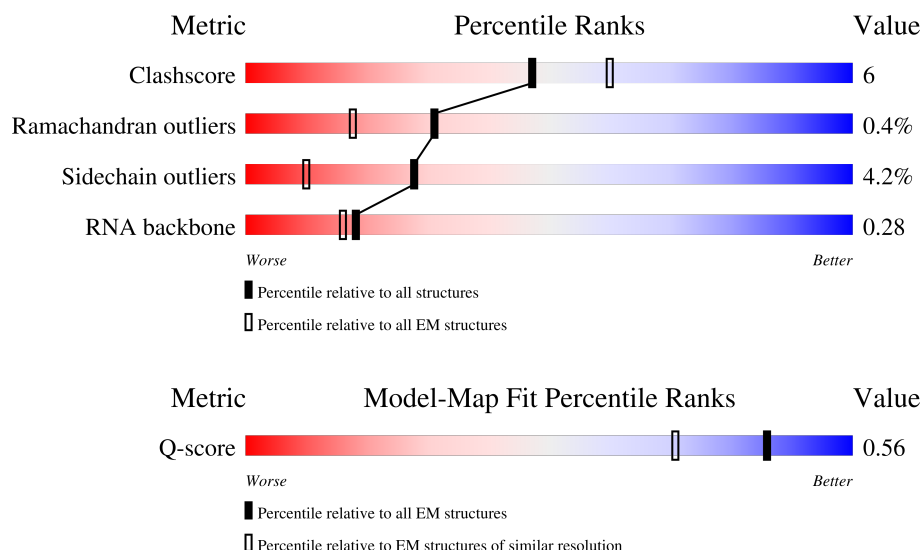
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	0	78	
2	1	63	
3	2	59	

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Mol	Chain	Length	Quality of chain
4	3	57	
5	4	55	
6	6	46	
7	7	65	
8	8	38	
9	a	120	
10	b	2904	
11	c	273	
12	d	209	
13	e	201	
14	f	179	
15	g	177	
16	h	149	
17	j	142	
18	k	123	
19	l	144	
20	m	136	
21	n	127	
22	o	117	
23	p	115	
24	q	118	
25	r	103	
26	s	110	
27	t	93	
28	u	93	

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Mol	Chain	Length	Quality of chain
29	w	94	56% 59% 39%
30	y	85	7% 76% 13% 11%

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 88848 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 L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

- Molecule 4 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 5 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 6 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 9 is a RNA chain called 5S rRNA.

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

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	2900	Total	C	N	O	P	0	0
			62259	27774	11459	20126	2900		

- Molecule 11 is a protein called 50S ribosomal protein L2.

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

- Molecule 12 is a protein called 50S ribosomal protein L3.

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

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

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

- Molecule 15 is a protein called 50S ribosomal protein L6.

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

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	39	Total	C	N	O	S	0	0
			287	184	51	51	1		

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

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

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	l	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	m	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 21 is a protein called 50S ribosomal protein L17.

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

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	p	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	t	86	Total	C	N	O	S	0	0
			681	433	123	123	2		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	?	-	ARG	deletion	UNP P0ADZ0
t	?	-	HIS	deletion	UNP P0ADZ0
t	?	-	GLY	deletion	UNP P0ADZ0
t	?	-	GLN	deletion	UNP P0ADZ0
t	?	-	ARG	deletion	UNP P0ADZ0
t	?	-	ILE	deletion	UNP P0ADZ0
t	?	-	GLY	deletion	UNP P0ADZ0

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	u	91	Total	C	N	O	0	0
			699	441	131	127		

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

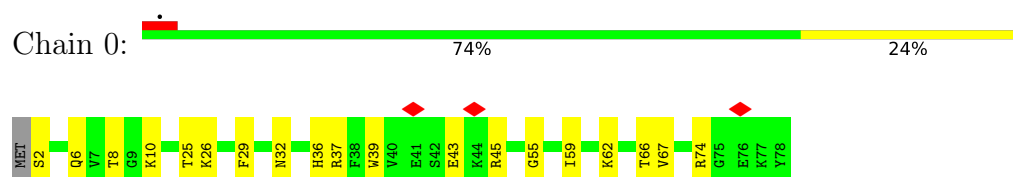
- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	y	76	Total	C	N	O	S	0	0
			578	358	117	102	1		

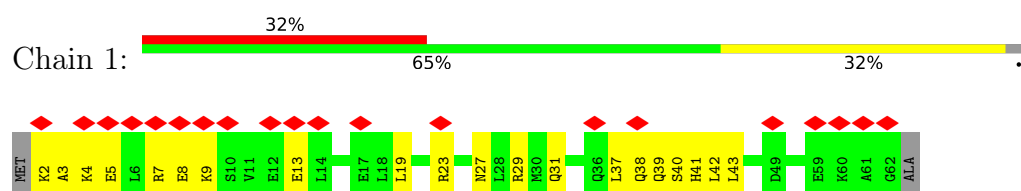
3 Residue-property plots [i](#)

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.

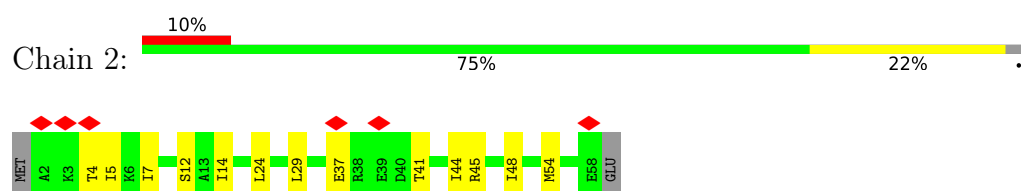
- Molecule 1: 50S ribosomal protein L28



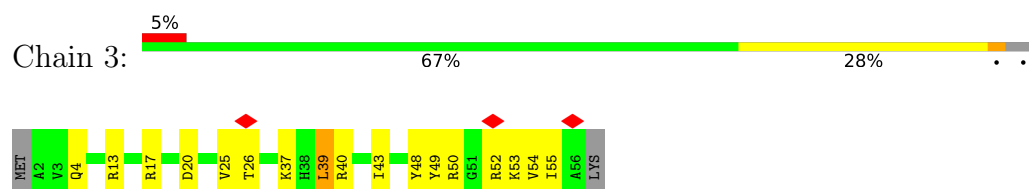
- Molecule 2: 50S ribosomal protein L29



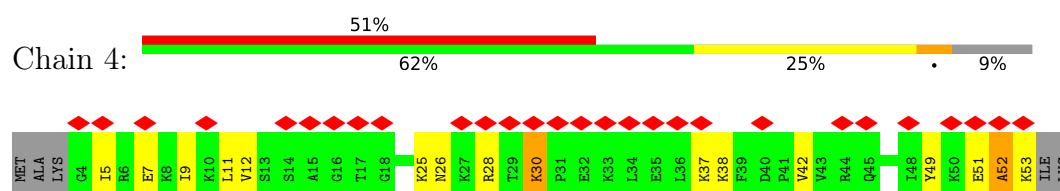
- Molecule 3: 50S ribosomal protein L30



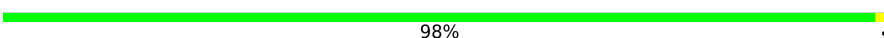
- Molecule 4: 50S ribosomal protein L32

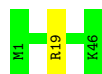


- Molecule 5: 50S ribosomal protein L33



- Molecule 6: 50S ribosomal protein L34

Chain 6:  98% .



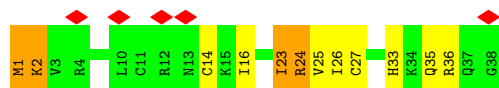
- Molecule 7: 50S ribosomal protein L35

Chain 7:  69% 26% . .



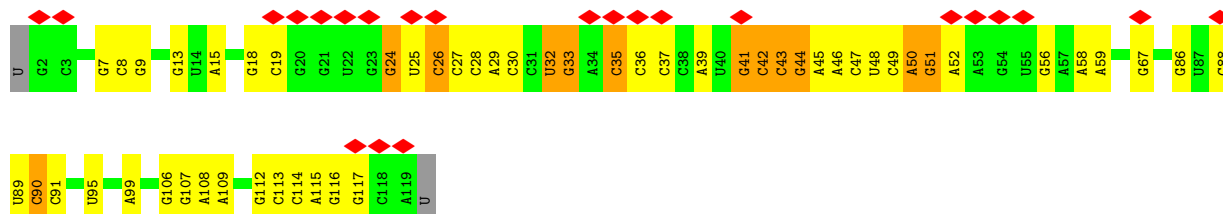
- Molecule 8: 50S ribosomal protein L36

Chain 8:  13% 68% 21% 11%



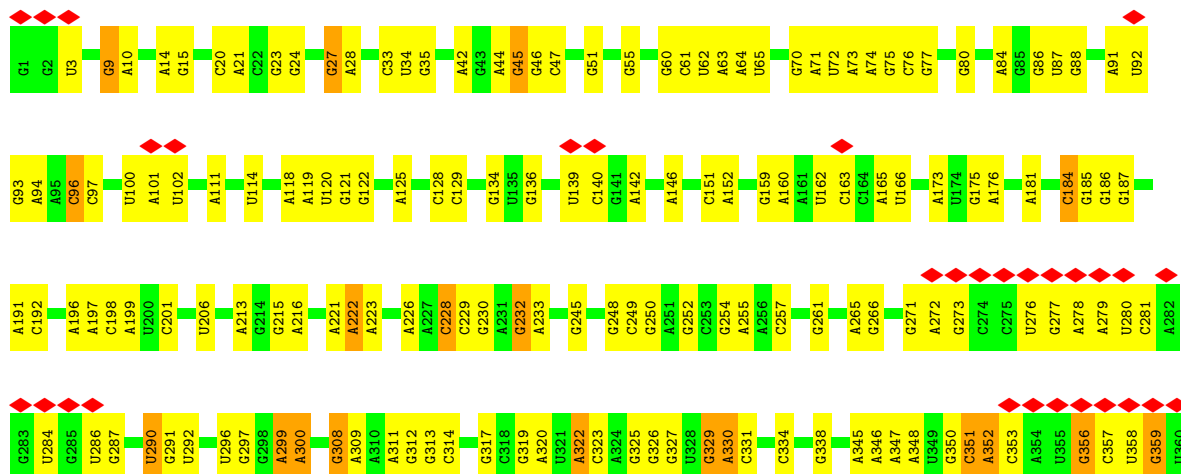
- Molecule 9: 5S rRNA

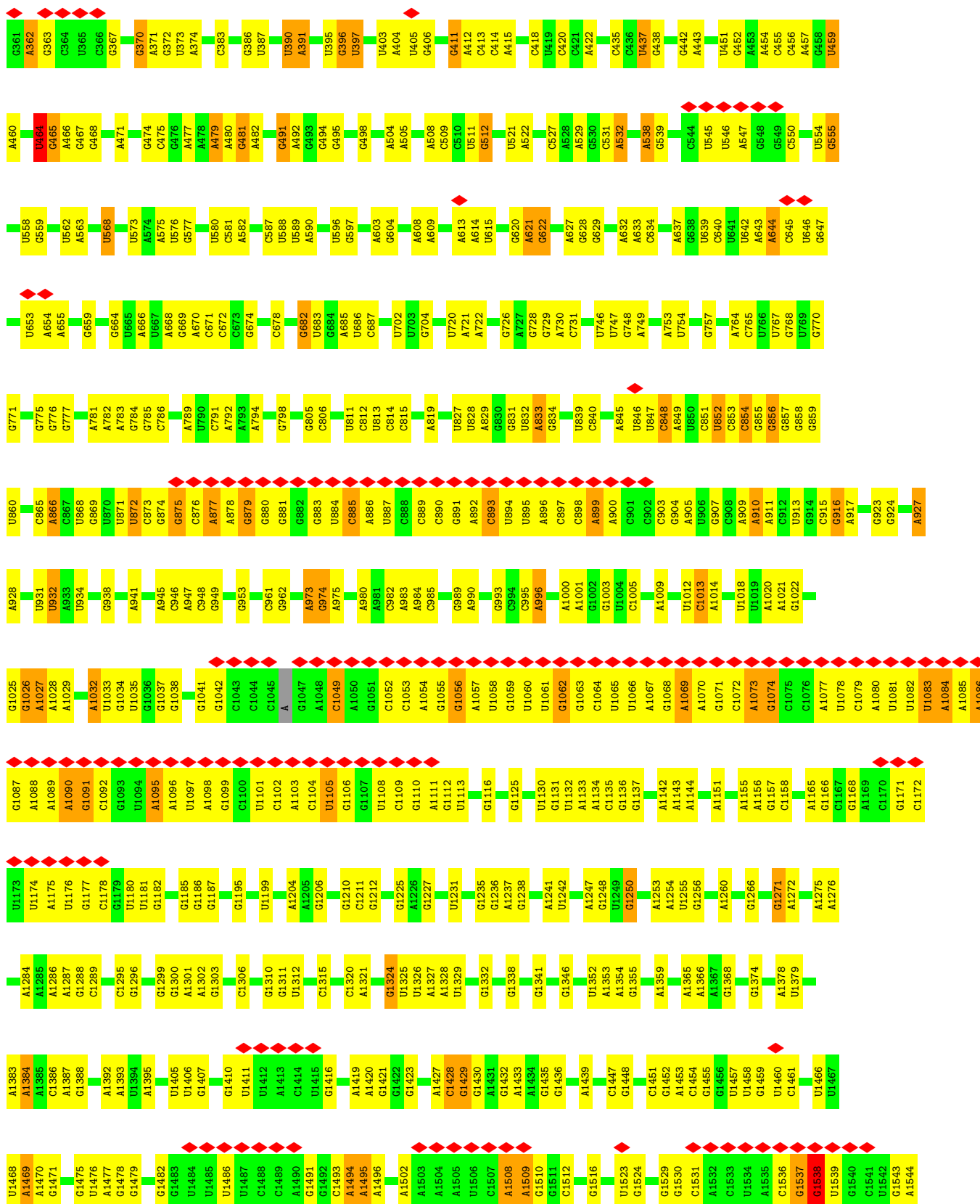
Chain a:  19% 54% 34% 10% .



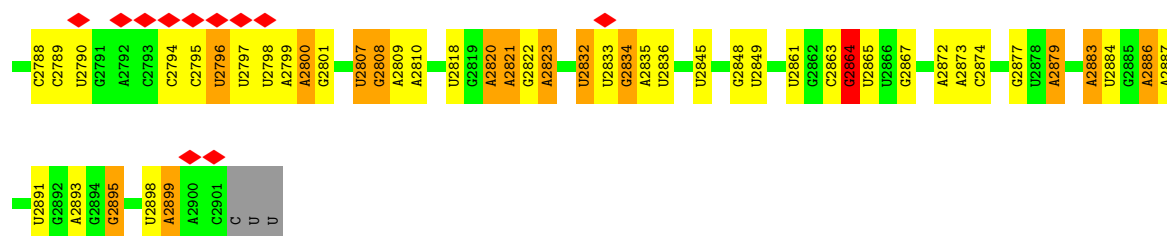
- Molecule 10: 23S rRNA

Chain b:  11% 56% 38% 6%



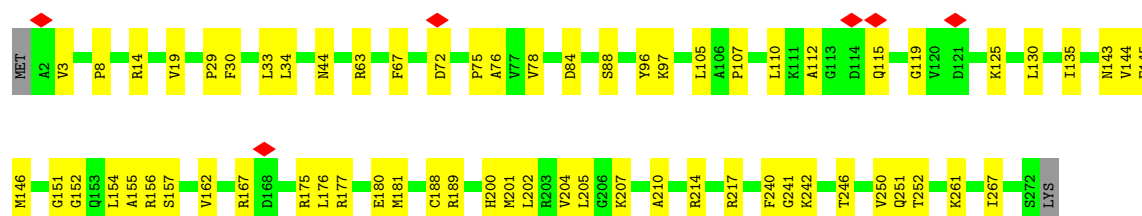






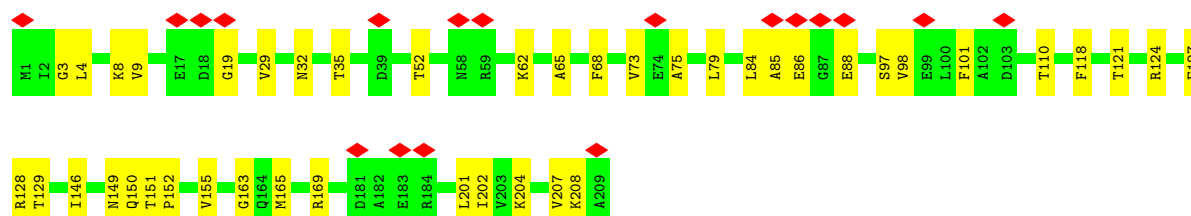
- Molecule 11: 50S ribosomal protein L2

Chain c: 75% 24%



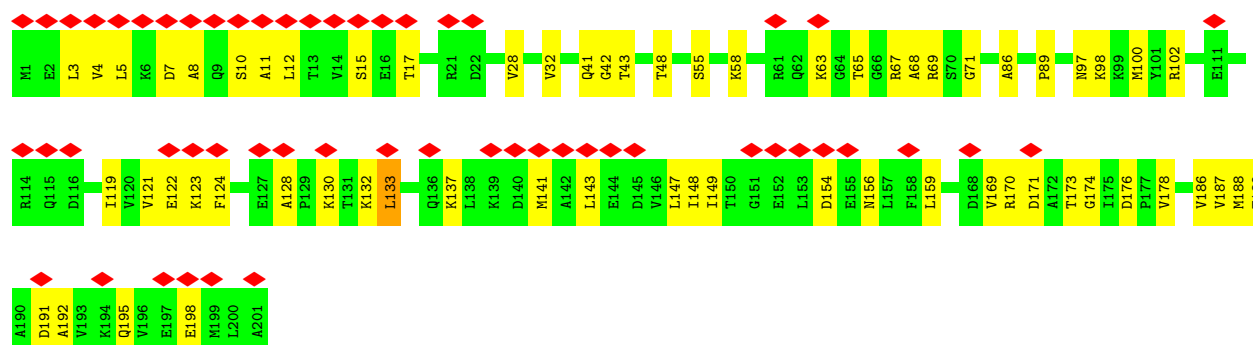
- Molecule 12: 50S ribosomal protein L3

Chain d: 9% 79% 21%



- Molecule 13: 50S ribosomal protein L4

Chain e: 27% 69% 31%

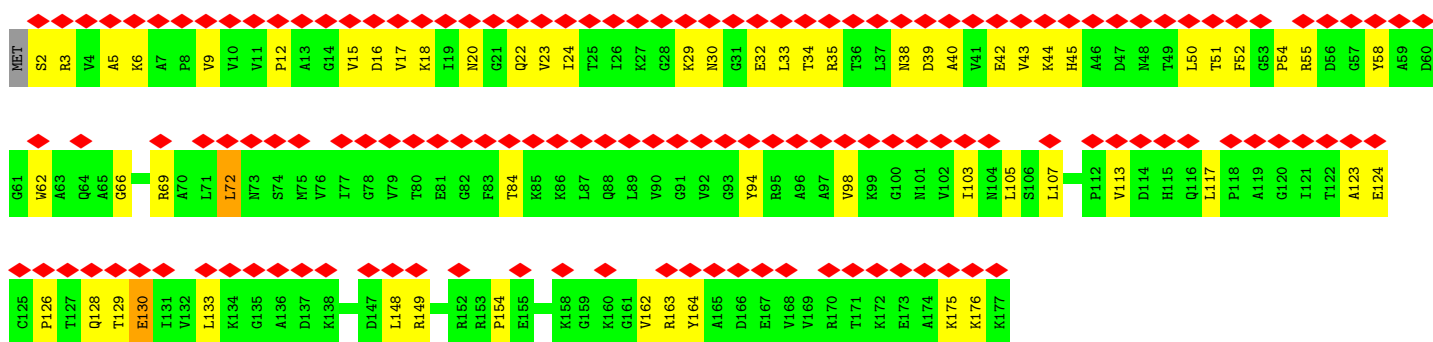
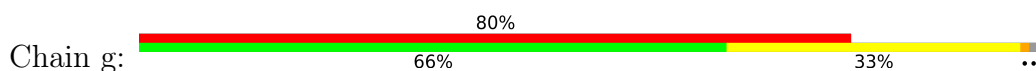


- Molecule 14: 50S ribosomal protein L5

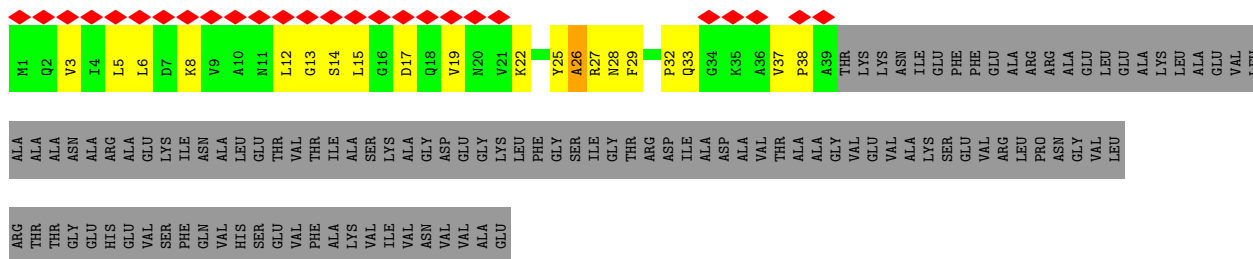
Chain f: 96% 57% 39%



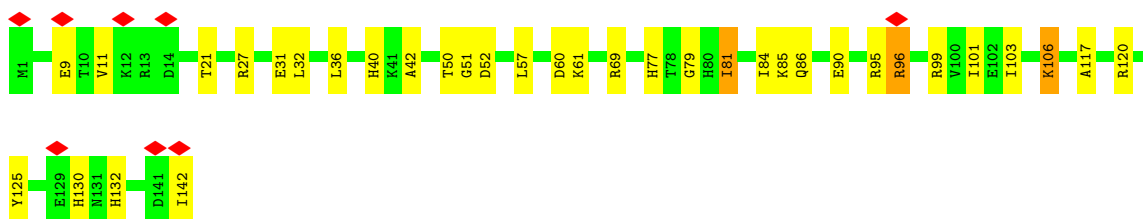
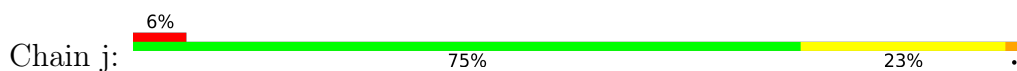
• Molecule 15: 50S ribosomal protein L6



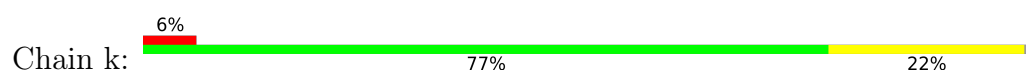
• Molecule 16: 50S ribosomal protein L9



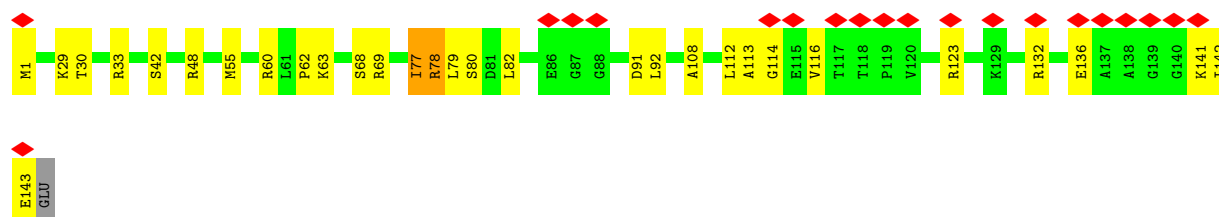
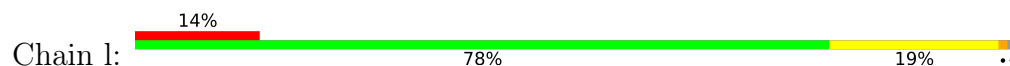
• Molecule 17: 50S ribosomal protein L13



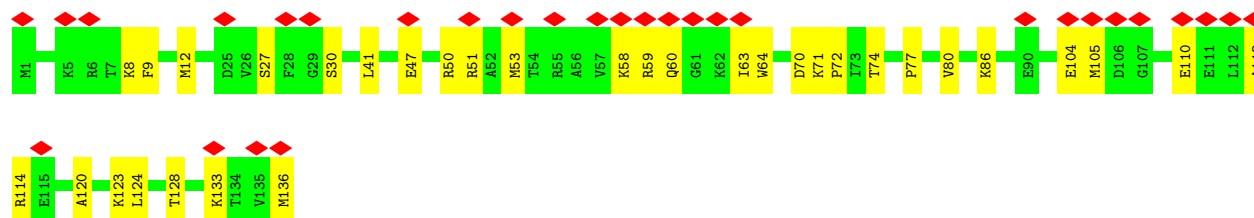
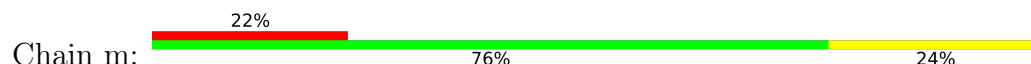
• Molecule 18: 50S ribosomal protein L14



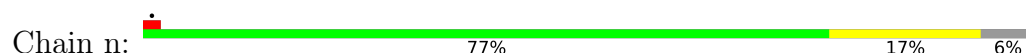
- Molecule 19: 50S ribosomal protein L15



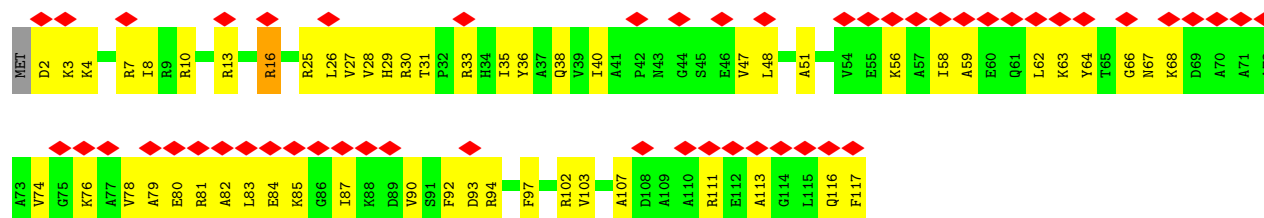
- Molecule 20: 50S ribosomal protein L16



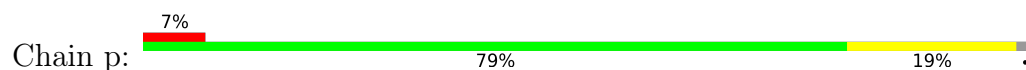
- Molecule 21: 50S ribosomal protein L17



- Molecule 22: 50S ribosomal protein L18

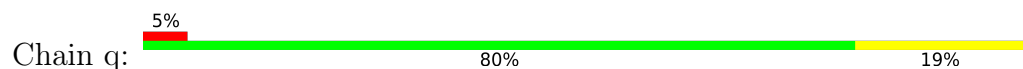


- Molecule 23: 50S ribosomal protein L19

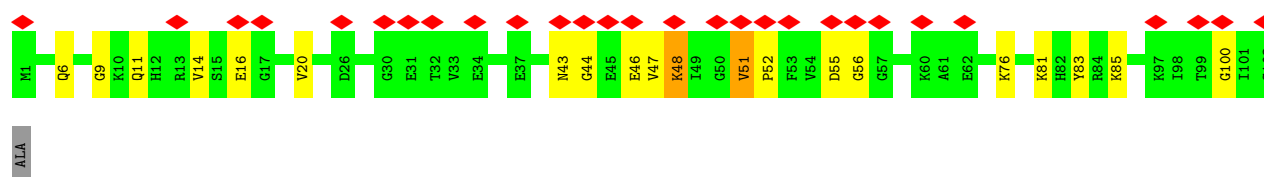
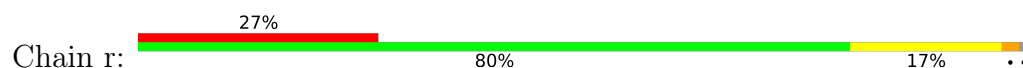




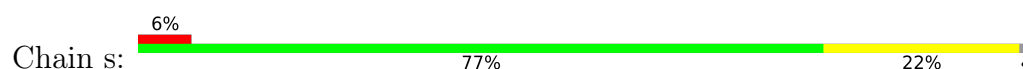
- Molecule 24: 50S ribosomal protein L20



- Molecule 25: 50S ribosomal protein L21



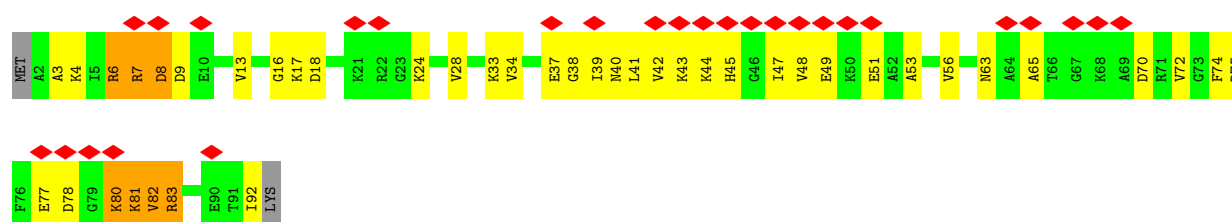
- Molecule 26: 50S ribosomal protein L22



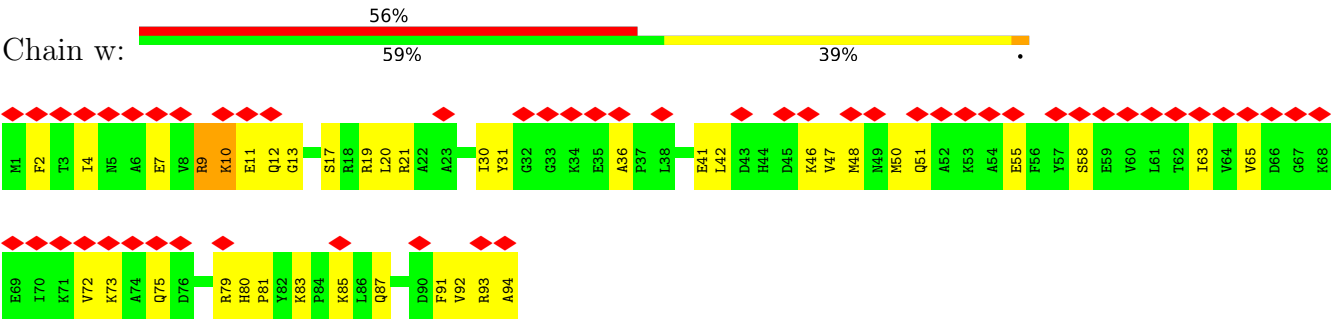
- Molecule 27: 50S ribosomal protein L23



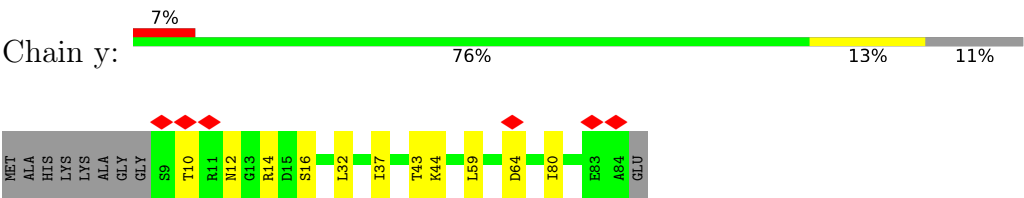
- Molecule 28: 50S ribosomal protein L24



• Molecule 29: 50S ribosomal protein L25



• Molecule 30: 50S ribosomal protein L27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131042	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.9	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.535	Depositor
Minimum map value	-0.136	Depositor
Average map value	-0.009	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.0885	Depositor
Map size ($\text{\AA}$)	399.28003, 399.28003, 399.28003	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.085, 1.085, 1.085	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.86	0/635	0.68	0/848
2	1	0.71	0/496	0.85	0/660
3	2	0.81	0/443	0.66	0/593
4	3	0.88	0/440	0.81	0/588
5	4	0.70	0/416	0.97	0/554
6	6	0.98	0/380	0.71	0/498
7	7	0.93	0/513	0.82	0/676
8	8	0.80	0/302	0.90	0/397
9	a	0.70	0/2828	0.48	0/4410
10	b	0.50	0/69731	0.73	24/108784 (0.0%)
11	c	0.93	0/2121	0.70	0/2852
12	d	0.89	0/1586	0.74	0/2134
13	e	0.76	0/1571	0.71	1/2113 (0.0%)
14	f	0.59	0/1434	0.84	0/1926
15	g	0.61	0/1343	0.75	0/1816
16	h	0.64	0/290	0.81	1/392 (0.3%)
17	j	0.83	0/1152	0.68	0/1551
18	k	0.91	0/947	0.77	0/1268
19	l	0.85	0/1052	0.79	0/1401
20	m	0.76	0/1093	0.71	0/1460
21	n	0.94	0/973	0.78	0/1301
22	o	0.63	0/902	0.72	0/1209
23	p	0.88	0/920	0.66	0/1231
24	q	0.92	0/960	0.73	0/1278
25	r	0.85	0/823	0.72	0/1100
26	s	0.91	0/852	0.68	0/1142
27	t	0.77	0/686	0.85	0/918
28	u	0.70	0/704	0.89	0/936
29	w	0.66	0/766	0.72	1/1025 (0.1%)
30	y	0.87	0/585	0.77	0/775
All	All	0.60	0/96944	0.73	27/145836 (0.0%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	b	2864	G	C2'-C3'-O3'	9.17	127.45	113.70
10	b	390	U	C2'-C3'-O3'	8.13	121.70	109.50
10	b	2820	A	C4'-C3'-O3'	-7.81	101.28	113.00
10	b	1595	C	C2'-C3'-O3'	7.73	125.29	113.70
10	b	1704	C	C2'-C3'-O3'	7.54	125.01	113.70
10	b	546	U	C2'-C3'-O3'	6.95	119.92	109.50
10	b	45	G	C2'-C3'-O3'	-6.88	103.38	113.70
10	b	228	C	C4'-C3'-O3'	6.87	119.70	109.40
10	b	479	A	C2'-C3'-O3'	-6.75	99.37	109.50
10	b	1299	G	C2'-C3'-O3'	6.65	123.67	113.70
10	b	1930	G	C4'-C3'-O3'	6.55	119.22	109.40
10	b	2655	G	C4'-C3'-O3'	6.50	119.15	109.40
10	b	2832	U	C4'-C3'-O3'	6.47	119.11	109.40
29	w	13	GLY	CA-C-O	-6.27	117.79	122.37
10	b	464	U	C2'-C3'-O3'	6.21	123.02	113.70
10	b	1762	A	C4'-C3'-O3'	-6.13	103.80	113.00
10	b	299	A	C3'-C2'-O2'	5.87	123.41	114.60
10	b	9	G	C2'-C3'-O3'	5.66	122.19	113.70
10	b	1538	G	C2'-C3'-O3'	5.60	122.10	113.70
10	b	2655	G	C2'-C3'-O3'	5.51	117.77	109.50
10	b	390	U	C4'-C3'-O3'	5.42	117.53	109.40
10	b	2055	C	C4'-C3'-O3'	5.40	121.09	113.00
16	h	26	ALA	CA-C-O	-5.39	114.87	121.88
10	b	481	G	C1'-O4'-C4'	-5.37	104.53	109.90
10	b	9	G	C4'-C3'-O3'	5.36	121.04	113.00
13	e	128	ALA	O-C-N	-5.25	117.46	121.55
10	b	1872	A	C4'-C3'-O3'	5.04	116.96	109.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	625	0	652	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	495	0	526	15	0
3	2	439	0	482	7	0
4	3	434	0	445	12	0
5	4	409	0	440	12	0
6	6	377	0	418	2	0
7	7	504	0	572	10	0
8	8	301	0	341	7	0
9	a	2529	0	1281	42	0
10	b	62259	0	31313	333	0
11	c	2082	0	2154	44	0
12	d	1565	0	1616	32	0
13	e	1552	0	1619	37	0
14	f	1410	0	1444	56	0
15	g	1323	0	1371	45	0
16	h	287	0	307	11	0
17	j	1129	0	1162	21	0
18	k	938	0	1012	22	0
19	l	1043	0	1123	19	0
20	m	1074	0	1157	25	0
21	n	960	0	1000	12	0
22	o	892	0	923	50	0
23	p	908	0	956	20	0
24	q	947	0	1019	14	0
25	r	810	0	834	12	0
26	s	845	0	909	17	0
27	t	681	0	749	24	0
28	u	699	0	747	29	0
29	w	753	0	780	31	0
30	y	578	0	598	6	0
All	All	88848	0	57950	887	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (887) 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)
10:b:643:A:C2'	10:b:644:A:H5'	1.72	1.17
10:b:643:A:H2'	10:b:644:A:H5'	1.26	1.12
10:b:362:A:C8	10:b:362:A:OP2	2.10	1.04
10:b:892:A:C8	10:b:893:C:C6	2.55	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:892:A:H8	10:b:893:C:C6	1.83	0.95
10:b:875:G:C6	10:b:877:A:N6	2.34	0.94
10:b:851:C:O2'	10:b:852:U:H5'	1.70	0.91
10:b:362:A:OP2	10:b:362:A:H8	1.54	0.88
10:b:874:G:H2'	10:b:875:G:H5''	1.62	0.82
13:e:119:ILE:HB	13:e:187:VAL:HG12	1.62	0.81
21:n:12:ARG:HE	21:n:16:HIS:CE1	1.97	0.81
10:b:2783:U:H2'	10:b:2784:U:C6	2.16	0.81
10:b:329:G:H1	28:u:17:LYS:HZ3	1.28	0.80
10:b:852:U:O2'	10:b:853:C:H5'	1.82	0.79
30:y:10:THR:HG22	30:y:12:ASN:H	1.46	0.79
10:b:851:C:C2'	10:b:852:U:H5'	2.12	0.79
10:b:851:C:H2'	10:b:852:U:C6	2.18	0.78
17:j:77:HIS:HD2	17:j:79:GLY:H	1.32	0.78
10:b:682:G:C8	10:b:682:G:H5''	2.19	0.77
9:a:24:G:H1'	9:a:26:C:H41	1.50	0.77
10:b:2788:C:H2'	10:b:2789:C:C6	2.20	0.76
10:b:643:A:H2'	10:b:644:A:C5'	2.13	0.76
10:b:643:A:O2'	10:b:644:A:H5'	1.86	0.76
10:b:644:A:O2'	10:b:645:C:H2'	1.87	0.74
10:b:1871:A:H4'	10:b:1872:A:OP1	1.86	0.74
10:b:875:G:N1	10:b:877:A:N6	2.35	0.74
10:b:272:A:C6	10:b:273:G:C6	2.76	0.73
10:b:2187:U:H2'	10:b:2188:U:C6	2.23	0.73
18:k:105:ARG:NH1	23:p:34:GLU:OE2	2.22	0.73
20:m:53:MET:HE2	20:m:63:ILE:HD12	1.71	0.73
29:w:73:LYS:HG2	29:w:94:ALA:HB2	1.71	0.73
20:m:41:LEU:HD11	20:m:124:LEU:HD22	1.70	0.73
16:h:12:LEU:HD13	16:h:19:VAL:HG21	1.69	0.72
2:l:27:ASN:O	2:l:31:GLN:NE2	2.22	0.72
10:b:284:U:H3	10:b:356:G:H1	1.33	0.72
29:w:20:LEU:HD21	29:w:41:GLU:HG2	1.70	0.72
9:a:51:G:OP1	22:o:63:LYS:NZ	2.21	0.72
10:b:494:G:H4'	26:s:6:LYS:HB2	1.72	0.71
22:o:29:HIS:HB3	22:o:36:TYR:HB2	1.72	0.71
13:e:58:LYS:HG3	13:e:71:GLY:HA2	1.73	0.71
21:n:58:ASP:OD2	21:n:63:ARG:NH1	2.24	0.70
18:k:107:LEU:HB2	18:k:116:ILE:HD11	1.74	0.70
28:u:43:LYS:HZ3	28:u:48:VAL:HA	1.56	0.70
10:b:1964:G:H4'	10:b:1965:C:OP2	1.91	0.70
9:a:49:C:O3'	22:o:68:LYS:NZ	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:27:G:H22	10:b:512:G:H2'	1.55	0.70
14:f:116:GLY:O	14:f:178:ARG:NH2	2.24	0.70
10:b:356:G:H2'	10:b:357:C:O4'	1.92	0.69
10:b:1439:A:H62	10:b:1552:A:H8	1.40	0.69
17:j:57:LEU:HD21	17:j:130:HIS:HB3	1.74	0.69
14:f:80:ARG:HB3	14:f:83:TYR:CZ	2.27	0.69
22:o:40:ILE:HG12	22:o:47:VAL:HG12	1.75	0.68
28:u:83:ARG:HB3	28:u:92:ILE:HD12	1.76	0.68
10:b:2447:G:H1	10:b:2451:A:H62	1.38	0.68
10:b:682:G:H5''	10:b:682:G:H8	1.57	0.68
10:b:2543:G:H21	10:b:2646:C:H5''	1.58	0.68
20:m:136:MET:O	29:w:79:ARG:NH2	2.27	0.68
9:a:48:U:OP2	22:o:30:ARG:NH2	2.28	0.67
17:j:77:HIS:CD2	17:j:79:GLY:H	2.11	0.66
29:w:21:ARG:NH2	29:w:87:GLN:O	2.28	0.66
10:b:875:G:H8	10:b:875:G:C5'	2.09	0.66
10:b:2682:A:H61	10:b:2728:U:H1'	1.60	0.66
9:a:51:G:OP2	22:o:67:ASN:ND2	2.29	0.66
22:o:48:LEU:O	22:o:85:LYS:NZ	2.27	0.66
27:t:44:LYS:HG3	27:t:55:VAL:HG21	1.77	0.66
14:f:33:LYS:HB3	14:f:92:ARG:HD3	1.77	0.66
27:t:4:GLU:OE1	27:t:49:LYS:HE2	1.96	0.65
1:0:39:TRP:CD1	16:h:32:PRO:HA	2.32	0.65
11:c:105:LEU:HD11	11:c:156:ARG:HG3	1.79	0.65
2:1:29:ARG:NH2	27:t:11:LEU:O	2.30	0.65
10:b:874:G:C2'	10:b:875:G:H5''	2.26	0.65
10:b:1069:A:H4'	10:b:1070:A:H5''	1.79	0.65
25:r:43:ASN:OD1	25:r:44:GLY:N	2.27	0.65
10:b:2123:G:H1	10:b:2176:A:H1'	1.62	0.65
14:f:29:PRO:HB3	14:f:160:ALA:HB2	1.79	0.64
20:m:64:TRP:HB2	20:m:104:GLU:HB2	1.79	0.64
10:b:1884:G:H5''	10:b:1884:G:H8	1.60	0.64
11:c:72:ASP:OD1	11:c:189:ARG:NH1	2.31	0.64
15:g:103:ILE:HD12	15:g:117:LEU:HD11	1.78	0.64
16:h:26:ALA:C	16:h:28:ASN:H	2.05	0.64
22:o:56:LYS:O	22:o:59:ALA:N	2.30	0.64
10:b:2772:C:H2'	10:b:2773:C:C6	2.33	0.64
7:7:26:HIS:CE1	7:7:48:ALA:HB2	2.32	0.64
10:b:666:A:H4'	19:l:48:ARG:HH11	1.61	0.64
10:b:851:C:H2'	10:b:852:U:H6	1.63	0.64
10:b:468:G:H5''	13:e:55:SER:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:134:GLU:OE2	14:f:136:ILE:HG12	1.97	0.64
4:3:54:VAL:HG23	4:3:55:ILE:HG12	1.80	0.63
14:f:29:PRO:HB2	14:f:169:LEU:HD22	1.81	0.63
10:b:2783:U:H2'	10:b:2784:U:H6	1.62	0.63
13:e:141:MET:HE3	13:e:143:LEU:HD12	1.81	0.63
12:d:124:ARG:HA	12:d:165:MET:HE3	1.81	0.63
27:t:53:VAL:HG21	27:t:80:LEU:HD13	1.80	0.63
10:b:1858:A:H61	10:b:1884:G:H1'	1.64	0.63
11:c:175:ARG:HG3	11:c:181:MET:HE1	1.79	0.63
20:m:47:GLU:OE1	20:m:51:ARG:NE	2.32	0.63
14:f:8:TYR:HA	14:f:12:VAL:HG13	1.82	0.62
10:b:2128:G:H1'	10:b:2174:C:H1'	1.80	0.62
11:c:67:PHE:CE1	11:c:156:ARG:HD2	2.34	0.62
15:g:103:ILE:CD1	15:g:117:LEU:HD11	2.30	0.62
13:e:28:VAL:O	13:e:32:VAL:HG23	2.00	0.62
1:0:6:GLN:O	1:0:74:ARG:NH1	2.33	0.62
13:e:147:LEU:HB3	13:e:186:VAL:HG22	1.82	0.62
28:u:39:ILE:HG13	28:u:40:ASN:N	2.15	0.62
11:c:143:ASN:OD1	11:c:152:GLY:HA3	2.00	0.61
18:k:76:VAL:HG12	23:p:73:VAL:HB	1.82	0.61
28:u:51:GLU:N	28:u:51:GLU:OE2	2.33	0.61
15:g:22:GLN:NE2	15:g:39:ASP:HA	2.16	0.61
10:b:2101:A:H61	10:b:2188:U:H3	1.48	0.61
20:m:8:LYS:HG3	20:m:9:PHE:CD1	2.35	0.61
10:b:1858:A:N6	10:b:1884:G:H1'	2.15	0.61
27:t:54:GLU:OE2	27:t:83:GLY:N	2.33	0.61
10:b:27:G:N2	10:b:512:G:H2'	2.14	0.61
29:w:72:VAL:HA	29:w:94:ALA:H	1.65	0.61
11:c:3:VAL:HG12	11:c:19:VAL:HG22	1.82	0.61
15:g:40:ALA:HA	15:g:58:TYR:HD2	1.65	0.61
15:g:42:GLU:OE2	15:g:55:ARG:NE	2.35	0.60
22:o:116:GLN:N	22:o:116:GLN:OE1	2.33	0.60
14:f:135:GLN:NE2	14:f:148:ARG:O	2.33	0.60
20:m:53:MET:HB3	20:m:120:ALA:HB2	1.83	0.60
23:p:7:GLN:O	23:p:11:GLU:HG3	2.02	0.60
15:g:126:PRO:HD2	15:g:130:GLU:HB3	1.82	0.60
21:n:32:GLU:HG2	21:n:115:LEU:HD12	1.82	0.60
9:a:24:G:H1'	9:a:26:C:N4	2.16	0.60
21:n:50:PRO:HA	21:n:53:THR:HG22	1.83	0.60
11:c:251:GLN:NE2	11:c:252:THR:O	2.34	0.60
30:y:37:ILE:HG21	30:y:80:ILE:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:2:SER:O	15:g:5:ALA:N	2.35	0.60
25:r:76:LYS:HB2	25:r:85:LYS:HB3	1.83	0.60
19:l:91:ASP:OD1	19:l:92:LEU:N	2.34	0.59
22:o:7:ARG:HA	22:o:10:ARG:HH21	1.67	0.59
10:b:272:A:C6	10:b:273:G:C5	2.91	0.59
11:c:201:MET:HG3	11:c:202:LEU:HD12	1.84	0.59
12:d:3:GLY:HA3	12:d:204:LYS:HG2	1.83	0.59
10:b:1935:G:H1'	10:b:1964:G:N2	2.18	0.59
10:b:866:A:H61	10:b:913:U:H1'	1.68	0.58
10:b:511:U:H4'	10:b:1235:G:H4'	1.84	0.58
10:b:1028:A:H2'	10:b:1029:A:C8	2.38	0.58
11:c:30:PHE:HD2	11:c:33:LEU:HD12	1.68	0.58
12:d:9:VAL:HG21	23:p:4:ILE:HD11	1.86	0.58
1:0:8:THR:OG1	1:0:10:LYS:HG3	2.04	0.58
12:d:128:ARG:NH1	12:d:129:THR:O	2.36	0.58
10:b:2111:U:H2'	10:b:2143:C:H5''	1.84	0.58
3:2:5:ILE:HG21	3:2:45:ARG:HH11	1.67	0.58
10:b:272:A:N6	10:b:273:G:O6	2.37	0.58
4:3:25:VAL:O	4:3:26:THR:OG1	2.17	0.57
12:d:4:LEU:HD13	12:d:29:VAL:HG11	1.86	0.57
28:u:75:ARG:HG3	28:u:82:VAL:HG23	1.86	0.57
10:b:1952:A:C5	18:k:22:ILE:HD12	2.40	0.57
12:d:151:THR:HG22	12:d:152:PRO:HD3	1.87	0.57
12:d:207:VAL:HG13	12:d:208:LYS:HG3	1.86	0.57
14:f:70:ALA:HB3	14:f:82:GLY:H	1.70	0.57
10:b:581:C:H2'	10:b:582:A:C8	2.39	0.57
11:c:29:PRO:HG2	11:c:34:LEU:HD11	1.86	0.57
11:c:217:ARG:HH11	11:c:217:ARG:HG2	1.69	0.57
12:d:86:GLU:N	12:d:86:GLU:OE1	2.38	0.57
13:e:119:ILE:O	13:e:187:VAL:HA	2.04	0.57
29:w:9:ARG:HG3	29:w:41:GLU:HG3	1.86	0.57
10:b:308:G:H2'	10:b:309:A:C8	2.39	0.57
4:3:13:ARG:O	4:3:17:ARG:HG3	2.05	0.57
9:a:8:C:O3'	22:o:25:ARG:NH1	2.36	0.57
13:e:191:ASP:OD1	13:e:192:ALA:N	2.38	0.57
20:m:27:SER:N	20:m:104:GLU:OE1	2.37	0.57
10:b:875:G:H8	10:b:875:G:H5'	1.68	0.57
9:a:95:U:OP2	29:w:19:ARG:NH2	2.38	0.57
10:b:352:A:H5''	10:b:352:A:H8	1.70	0.57
4:3:4:GLN:HA	10:b:2615:U:C2	2.40	0.56
1:0:36:HIS:CE1	1:0:37:ARG:O	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:290:U:H3	10:b:350:G:H1	1.54	0.56
10:b:329:G:H1	28:u:17:LYS:NZ	2.00	0.56
10:b:370:G:OP2	10:b:370:G:C8	2.59	0.56
10:b:892:A:C8	10:b:893:C:C5	2.93	0.56
15:g:149:ARG:HA	15:g:162:VAL:HG13	1.88	0.56
10:b:915:C:H2'	10:b:915:C:O2	2.04	0.56
14:f:136:ILE:HD11	14:f:146:VAL:HG11	1.87	0.56
10:b:621:A:H2'	10:b:622:G:O4'	2.04	0.56
10:b:1386:C:H2'	10:b:1387:A:C8	2.41	0.56
15:g:52:PHE:CE2	15:g:69:ARG:HA	2.40	0.56
10:b:272:A:H2'	10:b:273:G:C8	2.39	0.56
10:b:2051:A:H4'	12:d:146:ILE:HG12	1.87	0.56
14:f:74:VAL:HB	14:f:79:ILE:HD11	1.88	0.56
9:a:35:C:H2'	9:a:36:C:O4'	2.05	0.56
9:a:49:C:H2'	9:a:50:A:C8	2.41	0.56
11:c:240:PHE:O	11:c:242:LYS:HE3	2.06	0.56
19:l:29:LYS:HD3	19:l:30:THR:HG23	1.88	0.56
10:b:2273:A:H2'	10:b:2274:A:C8	2.41	0.56
12:d:118:PHE:CE1	12:d:163:GLY:HA2	2.40	0.56
11:c:135:ILE:O	11:c:167:ARG:NH1	2.39	0.56
18:k:59:LYS:NZ	18:k:89:ASN:OD1	2.36	0.56
1:0:59:ILE:HD13	1:0:67:VAL:HG21	1.87	0.55
10:b:848:C:H2'	10:b:849:A:C8	2.42	0.55
18:k:5:GLN:HA	18:k:20:MET:HE3	1.88	0.55
26:s:4:ILE:CD1	26:s:106:VAL:HG22	2.37	0.55
17:j:31:GLU:HG2	17:j:142:ILE:HG23	1.89	0.55
10:b:911:A:N6	20:m:9:PHE:CB	2.69	0.55
11:c:205:LEU:HD11	11:c:214:ARG:HH12	1.70	0.55
14:f:36:LEU:HD12	14:f:152:LEU:HD13	1.88	0.55
20:m:58:LYS:C	20:m:59:ARG:HD3	2.30	0.55
10:b:272:A:H2'	10:b:273:G:H8	1.70	0.55
3:2:24:LEU:HD11	3:2:54:MET:SD	2.47	0.55
10:b:2823:A:OP1	12:d:118:PHE:HB2	2.06	0.55
10:b:639:U:H2'	10:b:640:C:C6	2.41	0.55
10:b:1254:A:H5''	10:b:1255:U:H5''	1.89	0.55
18:k:106:GLU:OE1	18:k:106:GLU:N	2.40	0.55
10:b:272:A:N6	10:b:273:G:C6	2.75	0.55
10:b:362:A:OP2	10:b:362:A:N7	2.40	0.54
11:c:180:GLU:OE2	11:c:267:ILE:HG23	2.07	0.54
15:g:149:ARG:HH21	15:g:154:PRO:HD2	1.71	0.54
10:b:2305:U:H5''	14:f:131:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:n:12:ARG:NE	21:n:16:HIS:CE1	2.72	0.54
10:b:2115:G:H22	10:b:2119:A:H62	1.53	0.54
26:s:2:GLU:HA	26:s:108:SER:HB3	1.90	0.54
10:b:885:C:H2'	10:b:886:A:C8	2.43	0.54
14:f:108:VAL:HG23	14:f:109:PRO:HD3	1.90	0.54
21:n:41:ALA:O	21:n:42:LYS:HB2	2.07	0.54
30:y:32:LEU:HA	30:y:64:ASP:OD1	2.07	0.54
14:f:128:TYR:HB3	14:f:156:ILE:HB	1.89	0.54
10:b:672:C:H5	19:l:42:SER:HB2	1.71	0.54
10:b:1199:U:H1'	24:q:4:VAL:HG22	1.88	0.54
9:a:45:A:C4	9:a:46:A:C8	2.95	0.54
10:b:28:A:H62	10:b:512:G:H8	1.56	0.54
10:b:1056:G:H1'	10:b:1086:A:H62	1.72	0.54
10:b:2807:U:H2'	10:b:2808:G:H5'	1.90	0.54
14:f:4:LEU:HD13	14:f:101:GLU:HB2	1.89	0.54
10:b:2233:U:H2'	10:b:2234:G:C8	2.43	0.54
10:b:875:G:C5'	10:b:875:G:C8	2.90	0.54
13:e:32:VAL:HG13	13:e:178:VAL:HG22	1.90	0.53
14:f:73:SER:OG	14:f:81:GLN:N	2.31	0.53
19:l:79:LEU:HG	19:l:112:LEU:HA	1.90	0.53
10:b:2331:G:H21	10:b:2336:A:H8	1.56	0.53
11:c:145:GLU:HB2	11:c:188:CYS:HB3	1.90	0.53
14:f:42:GLU:HG3	14:f:148:ARG:HH12	1.73	0.53
15:g:163:ARG:HG2	15:g:164:TYR:O	2.08	0.53
10:b:2834:G:H2'	10:b:2879:A:H61	1.73	0.53
2:l:2:LYS:HD2	2:l:5:GLU:OE2	2.07	0.53
9:a:45:A:C8	14:f:92:ARG:NH1	2.77	0.53
18:k:121:GLU:OE1	23:p:65:SER:OG	2.25	0.53
10:b:875:G:H5'	10:b:875:G:C8	2.44	0.53
11:c:119:GLY:O	11:c:130:LEU:HD23	2.08	0.53
11:c:155:ALA:HB2	11:c:162:VAL:HG23	1.91	0.53
13:e:98:LYS:HB3	13:e:102:ARG:HH22	1.73	0.53
29:w:46:LYS:O	29:w:50:MET:HG3	2.09	0.53
10:b:1026:G:H2'	10:b:1027:A:C8	2.43	0.53
10:b:1469:A:H2'	10:b:1470:A:C8	2.44	0.53
27:t:8:LEU:HD23	27:t:50:LEU:HD21	1.91	0.53
10:b:1704:C:H2'	10:b:1705:A:C8	2.43	0.53
12:d:19:GLY:HA2	23:p:79:PRO:HG2	1.91	0.53
10:b:1250:G:H5''	24:q:6:ARG:HG2	1.91	0.53
9:a:41:G:H3'	9:a:42:C:H5'	1.92	0.52
10:b:373:U:H2'	10:b:374:A:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:175:LYS:O	15:g:176:LYS:HD3	2.09	0.52
22:o:4:LYS:O	22:o:8:ILE:HG12	2.09	0.52
24:q:81:ASN:OD1	24:q:85:LYS:NZ	2.42	0.52
15:g:175:LYS:HD2	15:g:176:LYS:N	2.24	0.52
23:p:31:TRP:CE3	23:p:38:LYS:HG2	2.45	0.52
9:a:48:U:H2'	9:a:49:C:C6	2.44	0.52
11:c:175:ARG:HG3	11:c:181:MET:CE	2.38	0.52
13:e:63:LYS:O	13:e:65:THR:N	2.41	0.52
22:o:76:LYS:O	22:o:80:GLU:HG3	2.10	0.52
10:b:2720:U:H4'	10:b:2845:U:O2'	2.09	0.52
10:b:2845:U:H5''	23:p:52:ASN:O	2.08	0.52
15:g:5:ALA:HB2	15:g:66:GLY:HA2	1.91	0.52
29:w:30:ILE:HD12	29:w:72:VAL:HG11	1.91	0.52
10:b:2086:U:H2'	10:b:2087:G:C8	2.45	0.52
13:e:41:GLN:HG3	13:e:41:GLN:O	2.07	0.52
14:f:34:ILE:CD1	14:f:156:ILE:HG12	2.39	0.52
23:p:106:LYS:O	23:p:109:ARG:HD3	2.10	0.52
10:b:2125:G:H2'	10:b:2126:A:H4'	1.92	0.52
15:g:45:HIS:HA	15:g:50:LEU:HD23	1.91	0.52
28:u:43:LYS:NZ	28:u:48:VAL:HA	2.22	0.52
8:8:16:ILE:HG12	8:8:25:VAL:HG22	1.91	0.52
10:b:674:G:O2'	13:e:69:ARG:HD2	2.10	0.52
10:b:852:U:H2'	10:b:853:C:C6	2.45	0.52
15:g:2:SER:OG	15:g:3:ARG:N	2.42	0.52
15:g:35:ARG:HG3	15:g:35:ARG:HH11	1.74	0.52
15:g:42:GLU:HG2	15:g:55:ARG:HD3	1.92	0.52
13:e:3:LEU:O	13:e:12:LEU:N	2.27	0.52
14:f:134:GLU:CD	14:f:136:ILE:H	2.18	0.52
22:o:107:ALA:O	22:o:111:ARG:HG2	2.10	0.52
28:u:43:LYS:NZ	28:u:49:GLU:H	2.08	0.52
3:2:12:SER:OG	3:2:14:ILE:HG12	2.10	0.52
10:b:2898:U:H2'	10:b:2899:A:C8	2.45	0.52
4:3:37:LYS:NZ	26:s:34:ASP:OD2	2.37	0.51
13:e:48:THR:HG22	13:e:86:ALA:HB3	1.91	0.51
14:f:36:LEU:HB2	14:f:89:VAL:HG22	1.92	0.51
11:c:8:PRO:HB3	11:c:14:ARG:HG3	1.92	0.51
17:j:117:ALA:HA	17:j:120:ARG:HH21	1.76	0.51
18:k:43:ILE:HD12	18:k:56:ASP:HB2	1.91	0.51
10:b:309:A:H5'	28:u:17:LYS:HD3	1.92	0.51
19:l:80:SER:HB3	19:l:114:GLY:HA3	1.93	0.51
22:o:27:VAL:HG21	22:o:40:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:80:HIS:CD2	29:w:81:PRO:HD2	2.45	0.51
14:f:71:ARG:NH2	14:f:72:LYS:HE3	2.26	0.51
18:k:102:PRO:HD2	23:p:68:GLU:OE2	2.11	0.51
29:w:4:ILE:HB	29:w:63:ILE:HG13	1.92	0.51
5:4:11:LEU:HB3	5:4:49:TYR:HB3	1.93	0.51
10:b:911:A:C6	20:m:9:PHE:CG	2.98	0.51
14:f:56:ASP:OD2	14:f:150:ARG:NH1	2.44	0.51
14:f:175:PHE:HD2	14:f:177:PHE:CE1	2.29	0.51
10:b:1796:U:H2'	10:b:1797:G:C8	2.45	0.51
10:b:2543:G:N2	10:b:2646:C:H5''	2.25	0.51
10:b:2636:C:H2'	10:b:2637:U:C6	2.46	0.51
14:f:33:LYS:HD3	14:f:92:ARG:HH21	1.76	0.51
21:n:70:THR:O	21:n:72:ASP:N	2.44	0.51
22:o:2:ASP:OD1	22:o:3:LYS:N	2.44	0.51
9:a:46:A:O3'	22:o:3:LYS:NZ	2.44	0.51
10:b:589:U:H2'	10:b:590:A:C8	2.46	0.51
10:b:2241:A:H2'	10:b:2242:G:C8	2.46	0.51
10:b:2314:A:H1'	14:f:155:THR:HG21	1.93	0.51
13:e:97:ASN:OD1	13:e:100:MET:HE2	2.11	0.51
16:h:26:ALA:C	16:h:28:ASN:N	2.69	0.51
2:1:41:HIS:CD2	2:1:42:LEU:HD22	2.45	0.51
19:l:78:ARG:HB3	19:l:113:ALA:HB3	1.92	0.51
28:u:44:LYS:HB3	28:u:49:GLU:OE2	2.11	0.51
15:g:123:ALA:HB2	15:g:133:LEU:HD13	1.93	0.50
9:a:43:C:O2	14:f:90:THR:OG1	2.29	0.50
10:b:2294:G:H5''	22:o:10:ARG:HE	1.76	0.50
11:c:76:ALA:HB2	11:c:96:TYR:CD2	2.46	0.50
14:f:73:SER:OG	14:f:80:ARG:HD3	2.11	0.50
9:a:32:U:H2'	9:a:33:G:H8	1.76	0.50
18:k:92:GLU:OE2	18:k:92:GLU:N	2.44	0.50
19:l:79:LEU:HA	19:l:82:LEU:HD13	1.94	0.50
23:p:25:THR:HB	23:p:88:ARG:HG2	1.93	0.50
27:t:14:PRO:HA	27:t:32:LEU:HD23	1.93	0.50
29:w:9:ARG:HH21	29:w:12:GLN:HA	1.77	0.50
8:8:23:ILE:HD12	10:b:1032:A:H1'	1.93	0.50
10:b:300:A:H1'	10:b:319:G:H1'	1.93	0.50
18:k:121:GLU:HG2	18:k:122:VAL:HG23	1.93	0.50
10:b:932:U:O2'	10:b:934:U:O4	2.27	0.50
26:s:84:ARG:HB2	26:s:96:ILE:HB	1.93	0.50
10:b:833:A:H2'	10:b:834:G:C8	2.46	0.50
10:b:2327:A:H2'	10:b:2328:A:C8	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:o:31:THR:HG22	22:o:33:ARG:H	1.77	0.50
26:s:7:HIS:HD2	26:s:10:ALA:HB2	1.76	0.50
10:b:1187:G:H5''	25:r:83:TYR:CE1	2.46	0.50
10:b:1875:G:H8	10:b:1875:G:H5''	1.76	0.50
10:b:2208:C:H2'	10:b:2209:G:C8	2.46	0.50
23:p:6:LYS:O	23:p:10:GLN:HG2	2.11	0.50
6:6:19:ARG:HG2	6:6:19:ARG:HH21	1.76	0.50
10:b:873:C:H4'	20:m:64:TRP:HE1	1.76	0.50
11:c:154:LEU:HD13	11:c:176:LEU:HD21	1.94	0.50
10:b:2377:A:H2'	10:b:2378:A:C8	2.47	0.50
24:q:40:ILE:O	24:q:44:GLN:HG3	2.11	0.50
10:b:1311:G:H21	10:b:1603:A:H62	1.60	0.49
10:b:1667:G:H5''	18:k:5:GLN:O	2.12	0.49
17:j:125:TYR:OH	17:j:132:HIS:NE2	2.41	0.49
26:s:65:ASP:OD1	26:s:67:ASP:HB2	2.11	0.49
28:u:42:VAL:O	28:u:49:GLU:HB2	2.12	0.49
24:q:58:ARG:HA	24:q:61:TRP:CE3	2.47	0.49
28:u:28:VAL:HG22	28:u:34:VAL:HG12	1.94	0.49
10:b:350:G:C2'	10:b:351:C:H5'	2.42	0.49
10:b:1028:A:N6	10:b:1125:G:H2'	2.28	0.49
11:c:78:VAL:HG12	11:c:112:ALA:HA	1.94	0.49
9:a:114:C:H2'	9:a:115:A:C8	2.48	0.49
10:b:1716:U:H2'	10:b:1717:A:H8	1.78	0.49
18:k:109:SER:C	18:k:111:LYS:H	2.20	0.49
19:l:30:THR:O	19:l:33:ARG:HB2	2.13	0.49
2:1:3:ALA:O	2:1:7:ARG:HG3	2.13	0.49
10:b:871:U:H2'	10:b:872:U:C6	2.47	0.49
22:o:28:VAL:HG11	22:o:103:VAL:HG13	1.93	0.49
13:e:122:GLU:HG2	13:e:123:LYS:N	2.26	0.49
27:t:5:GLU:OE2	27:t:5:GLU:N	2.41	0.49
29:w:80:HIS:CB	29:w:85:LYS:HB2	2.43	0.49
10:b:1073:A:H3'	10:b:1074:G:H8	1.78	0.49
12:d:85:ALA:HB3	12:d:88:GLU:HG3	1.94	0.49
13:e:41:GLN:HE21	13:e:43:THR:CG2	2.25	0.49
28:u:38:GLY:HA2	28:u:41:LEU:HD21	1.95	0.49
10:b:1090:A:H2'	10:b:1091:G:C8	2.48	0.48
10:b:2173:A:H5''	10:b:2174:C:H5	1.78	0.48
20:m:30:SER:HA	20:m:133:LYS:HB2	1.94	0.48
22:o:79:ALA:O	22:o:83:LEU:HD23	2.13	0.48
2:1:4:LYS:O	2:1:7:ARG:N	2.45	0.48
10:b:482:A:H1'	10:b:498:G:N2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:48:U:P	22:o:30:ARG:HH21	2.36	0.48
10:b:352:A:H5''	10:b:352:A:C8	2.48	0.48
14:f:132:VAL:HG22	14:f:134:GLU:H	1.78	0.48
29:w:2:PHE:HB3	29:w:50:MET:HE3	1.96	0.48
16:h:3:VAL:HG12	16:h:38:PRO:HA	1.96	0.48
9:a:106:G:H2'	9:a:107:G:O4'	2.13	0.48
10:b:459:U:H2'	10:b:460:A:H8	1.79	0.48
10:b:885:C:H2'	10:b:886:A:H8	1.77	0.48
22:o:81:ARG:HA	22:o:84:GLU:OE1	2.13	0.48
28:u:3:ALA:HB3	28:u:6:ARG:HE	1.79	0.48
6:6:19:ARG:HG2	6:6:19:ARG:NH2	2.28	0.48
8:8:16:ILE:HD13	10:b:1032:A:H5''	1.95	0.48
9:a:7:G:OP1	22:o:4:LYS:NZ	2.34	0.48
10:b:1384:A:H1'	10:b:1405:U:H1'	1.95	0.48
11:c:217:ARG:HG2	11:c:217:ARG:NH1	2.28	0.48
29:w:7:GLU:HA	29:w:65:VAL:HG23	1.94	0.48
11:c:63:ARG:HD3	11:c:84:ASP:OD1	2.14	0.48
12:d:151:THR:CG2	12:d:152:PRO:HD3	2.43	0.48
16:h:8:LYS:O	16:h:13:GLY:HA3	2.13	0.48
10:b:414:C:H2'	10:b:415:A:C8	2.49	0.48
10:b:720:U:H2'	10:b:721:A:C8	2.49	0.48
10:b:1802:A:H2'	10:b:1803:A:C8	2.49	0.48
2:1:5:GLU:HA	2:1:8:GLU:CD	2.39	0.48
10:b:948:C:O4'	10:b:984:A:C2	2.66	0.48
22:o:30:ARG:HB3	22:o:35:ILE:HD12	1.96	0.48
29:w:80:HIS:ND1	29:w:83:LYS:HB2	2.28	0.48
22:o:58:ILE:O	22:o:62:LEU:HD23	2.14	0.47
23:p:10:GLN:C	23:p:12:GLN:H	2.22	0.47
10:b:184:C:H2'	10:b:185:G:C8	2.48	0.47
10:b:1069:A:N1	10:b:1095:A:H5'	2.28	0.47
10:b:1508:A:H5'	10:b:1509:A:C4	2.49	0.47
9:a:29:A:OP2	22:o:31:THR:HG23	2.15	0.47
10:b:852:U:H2'	10:b:853:C:H6	1.79	0.47
11:c:246:THR:HG23	11:c:250:VAL:O	2.14	0.47
27:t:33:LYS:HG2	27:t:73:TRP:CZ3	2.50	0.47
2:1:19:LEU:O	2:1:23:ARG:HG3	2.13	0.47
9:a:29:A:O2'	9:a:58:A:N1	2.44	0.47
13:e:170:ARG:NH2	13:e:174:GLY:O	2.47	0.47
26:s:83:LYS:HB3	26:s:95:ARG:HH21	1.78	0.47
22:o:26:LEU:HB2	22:o:90:VAL:HG11	1.96	0.47
28:u:45:HIS:O	28:u:47:ILE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:107:PRO:HD2	11:c:110:LEU:CD2	2.45	0.47
12:d:121:THR:HB	12:d:127:PHE:CD2	2.48	0.47
15:g:24:ILE:O	15:g:34:THR:OG1	2.31	0.47
21:n:55:ALA:HA	21:n:80:PHE:CE1	2.49	0.47
22:o:82:ALA:HB1	22:o:87:ILE:HB	1.97	0.47
25:r:16:GLU:OE1	25:r:100:GLY:HA2	2.15	0.47
28:u:34:VAL:HG13	28:u:56:VAL:HG12	1.95	0.47
5:4:25:LYS:HD2	5:4:52:ALA:HB1	1.96	0.47
10:b:1000:A:H2'	10:b:1001:A:C8	2.50	0.47
11:c:144:VAL:HB	11:c:154:LEU:HB2	1.96	0.47
13:e:121:VAL:O	13:e:189:THR:HA	2.15	0.47
14:f:123:ASP:OD1	14:f:124:GLY:N	2.47	0.47
15:g:98:VAL:HG11	15:g:124:GLU:HA	1.96	0.47
17:j:60:ASP:OD1	17:j:60:ASP:N	2.31	0.47
17:j:106:LYS:HE3	17:j:106:LYS:HB2	1.53	0.47
18:k:91:SER:O	18:k:93:GLN:N	2.47	0.47
22:o:66:GLY:HA2	22:o:102:ARG:NH1	2.29	0.47
28:u:81:LYS:HB3	28:u:81:LYS:HE3	1.39	0.47
1:0:55:GLY:O	1:0:59:ILE:HG12	2.15	0.47
5:4:5:ILE:HD12	5:4:28:ARG:HH12	1.80	0.47
9:a:32:U:H2'	9:a:33:G:C8	2.50	0.47
10:b:1744:A:H3'	10:b:1745:A:H8	1.79	0.47
10:b:1808:A:H3'	10:b:1809:A:C8	2.50	0.47
10:b:2291:U:H2'	10:b:2292:U:C6	2.50	0.47
17:j:42:ALA:O	24:q:64:ARG:HG2	2.15	0.47
29:w:30:ILE:HD13	29:w:91:PHE:HB2	1.97	0.47
10:b:297:G:H5''	28:u:74:PHE:HB3	1.97	0.47
14:f:36:LEU:HB3	14:f:57:LEU:HD11	1.95	0.47
7:7:55:LEU:O	7:7:59:ILE:HD12	2.15	0.47
9:a:46:A:H5''	22:o:3:LYS:NZ	2.29	0.47
10:b:2134:A:H1'	10:b:2161:C:H5'	1.97	0.47
10:b:2425:A:H4'	10:b:2426:A:H5''	1.95	0.47
11:c:146:MET:HE3	11:c:154:LEU:HD21	1.96	0.47
13:e:67:ARG:HG3	13:e:68:ALA:N	2.30	0.47
23:p:68:GLU:OE1	23:p:68:GLU:N	2.48	0.47
10:b:358:U:H2'	10:b:359:G:C8	2.50	0.46
11:c:107:PRO:HD2	11:c:110:LEU:HD22	1.97	0.46
15:g:43:VAL:HG12	15:g:52:PHE:CD1	2.50	0.46
16:h:5:LEU:HD11	16:h:13:GLY:HA2	1.97	0.46
10:b:1155:A:H5''	24:q:55:ARG:HH11	1.79	0.46
10:b:1792:G:H5'	11:c:204:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:110:THR:HB	12:d:202:ILE:HB	1.97	0.46
21:n:56:LYS:HE2	21:n:87:PHE:O	2.15	0.46
27:t:21:SER:O	27:t:24:MET:N	2.48	0.46
29:w:42:LEU:HD13	29:w:47:VAL:HG21	1.96	0.46
17:j:27:ARG:HH11	17:j:27:ARG:HG2	1.81	0.46
2:l:41:HIS:CE1	10:b:96:C:H4'	2.50	0.46
9:a:33:G:C2	9:a:50:A:C2	3.03	0.46
10:b:853:C:H2'	10:b:854:C:C6	2.50	0.46
10:b:2328:A:H2'	10:b:2329:U:C6	2.51	0.46
12:d:35:THR:HG22	12:d:73:VAL:HG21	1.98	0.46
14:f:106:ILE:C	14:f:109:PRO:HD2	2.41	0.46
20:m:50:ARG:HG2	20:m:50:ARG:NH2	2.29	0.46
22:o:26:LEU:HD23	22:o:92:PHE:CD1	2.50	0.46
4:3:49:TYR:O	4:3:50:ARG:HB2	2.14	0.46
10:b:568:U:H4'	10:b:945:A:N6	2.30	0.46
10:b:813:U:H2'	10:b:814:C:C6	2.51	0.46
13:e:41:GLN:HE21	13:e:43:THR:HG21	1.79	0.46
25:r:6:GLN:HB2	25:r:11:GLN:HG2	1.98	0.46
3:2:24:LEU:HD23	3:2:29:LEU:HD12	1.98	0.46
3:2:41:THR:HG22	3:2:44:ILE:HG12	1.98	0.46
9:a:9:G:P	22:o:25:ARG:HH12	2.38	0.46
9:a:52:A:N7	22:o:64:TYR:OH	2.31	0.46
14:f:38:MET:HB2	14:f:87:CYS:SG	2.56	0.46
17:j:9:GLU:OE1	17:j:9:GLU:N	2.44	0.46
5:4:5:ILE:HG13	5:4:28:ARG:HH22	1.80	0.46
10:b:151:C:H2'	10:b:152:A:C8	2.50	0.46
10:b:839:U:H2'	10:b:840:C:C6	2.51	0.46
10:b:903:C:H2'	10:b:904:G:H8	1.81	0.46
15:g:84:THR:HA	15:g:133:LEU:O	2.15	0.46
19:l:132:ARG:O	19:l:136:GLU:HG3	2.16	0.46
27:t:6:ARG:HD2	27:t:6:ARG:HA	1.70	0.46
10:b:1326:U:H2'	10:b:1327:A:H8	1.81	0.46
11:c:75:PRO:HB2	11:c:97:LYS:HE3	1.97	0.46
15:g:94:TYR:CD1	15:g:107:LEU:HA	2.51	0.46
15:g:149:ARG:HA	15:g:162:VAL:CG1	2.46	0.46
19:l:79:LEU:HD13	19:l:116:VAL:HG12	1.98	0.46
27:t:10:VAL:HG23	27:t:11:LEU:HD13	1.97	0.46
12:d:32:ASN:ND2	12:d:52:THR:HB	2.30	0.46
22:o:2:ASP:OD1	22:o:2:ASP:C	2.58	0.46
10:b:1537:G:C5	10:b:1538:G:H1'	2.51	0.45
10:b:1689:A:H2'	10:b:1690:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:1796:U:H2'	10:b:1797:G:H8	1.80	0.45
10:b:2172:U:H5''	10:b:2174:C:H41	1.81	0.45
20:m:105:MET:HE1	20:m:113:ALA:HA	1.97	0.45
7:7:15:LYS:HB2	7:7:23:LYS:HE2	1.98	0.45
10:b:272:A:C5	10:b:273:G:N7	2.84	0.45
11:c:72:ASP:CG	11:c:189:ARG:HH12	2.24	0.45
13:e:171:ASP:C	13:e:173:THR:H	2.25	0.45
27:t:53:VAL:HG22	27:t:54:GLU:H	1.81	0.45
29:w:9:ARG:HH12	29:w:17:SER:HA	1.81	0.45
1:0:32:ASN:HB2	10:b:397:U:H5''	1.98	0.45
4:3:43:ILE:HG22	4:3:49:TYR:HB2	1.97	0.45
5:4:30:LYS:HB2	5:4:30:LYS:HE2	1.82	0.45
7:7:27:ALA:O	7:7:44:LEU:HD23	2.17	0.45
8:8:1:MET:HE2	8:8:1:MET:HB2	1.64	0.45
22:o:38:GLN:HE21	22:o:47:VAL:HG11	1.81	0.45
26:s:18:ARG:HG2	26:s:76:VAL:HB	1.98	0.45
5:4:26:ASN:C	5:4:26:ASN:ND2	2.70	0.45
10:b:309:A:H4'	28:u:16:GLY:HA2	1.98	0.45
10:b:621:A:C4	10:b:622:G:H1'	2.52	0.45
10:b:1447:C:H2'	10:b:1448:G:C8	2.51	0.45
10:b:1996:C:H4'	10:b:1997:C:OP1	2.16	0.45
15:g:16:ASP:OD1	15:g:16:ASP:N	2.48	0.45
10:b:947:A:O2'	10:b:984:A:H2	1.99	0.45
14:f:64:LYS:HE3	14:f:64:LYS:HB3	1.65	0.45
15:g:20:ASN:HB3	15:g:23:VAL:HG13	1.99	0.45
26:s:7:HIS:CD2	26:s:10:ALA:HB2	2.51	0.45
2:1:39:GLN:HB3	2:1:42:LEU:HD23	1.99	0.45
13:e:7:ASP:OD1	13:e:8:ALA:N	2.49	0.45
14:f:14:LYS:HB2	14:f:14:LYS:HE2	1.45	0.45
8:8:2:LYS:HB2	8:8:35:GLN:HG2	1.99	0.45
10:b:1818:U:H5''	11:c:157:SER:HB2	1.99	0.45
10:b:1965:C:H2'	10:b:1966:A:C8	2.51	0.45
12:d:149:ASN:OD1	12:d:150:GLN:N	2.50	0.45
29:w:7:GLU:OE1	29:w:7:GLU:N	2.50	0.45
10:b:973:A:H5''	25:r:81:LYS:HD2	1.98	0.45
10:b:1884:G:H5''	10:b:1884:G:C8	2.44	0.45
10:b:2408:U:H2'	10:b:2409:G:C8	2.52	0.45
13:e:149:ILE:HB	13:e:188:MET:HG2	1.99	0.45
18:k:104:THR:HG22	18:k:106:GLU:OE1	2.17	0.45
9:a:28:C:C2	9:a:29:A:C8	3.04	0.45
10:b:521:U:H2'	10:b:522:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:853:C:H2'	10:b:854:C:H6	1.82	0.45
10:b:1752:C:H2'	10:b:1753:G:C8	2.52	0.45
10:b:2261:C:C6	30:y:16:SER:HB3	2.51	0.45
10:b:2394:C:H5''	19:l:63:LYS:HE2	1.99	0.45
14:f:70:ALA:C	14:f:72:LYS:H	2.25	0.45
14:f:108:VAL:CG2	14:f:109:PRO:HD3	2.46	0.45
15:g:175:LYS:C	15:g:176:LYS:HD3	2.42	0.45
18:k:105:ARG:HH22	23:p:32:VAL:HG11	1.81	0.45
25:r:55:ASP:OD1	25:r:56:GLY:N	2.48	0.45
27:t:31:VAL:HG22	27:t:77:TYR:CD1	2.52	0.45
28:u:33:LYS:HB3	28:u:53:ALA:HB1	1.98	0.45
4:3:39:LEU:HD23	4:3:39:LEU:HA	1.75	0.45
10:b:191:A:H2'	10:b:192:C:C6	2.52	0.45
10:b:1085:A:H1'	10:b:1105:U:H4'	1.99	0.45
22:o:90:VAL:O	22:o:117:PHE:HB3	2.17	0.45
29:w:31:TYR:O	29:w:92:VAL:HA	2.18	0.45
10:b:2618:G:H21	12:d:155:VAL:HG21	1.82	0.44
13:e:148:ILE:HB	13:e:169:VAL:HG22	1.99	0.44
13:e:195:GLN:O	13:e:198:GLU:HG2	2.17	0.44
14:f:66:LEU:HD23	14:f:66:LEU:HA	1.74	0.44
28:u:80:LYS:HE3	28:u:80:LYS:HB3	1.80	0.44
29:w:72:VAL:HG12	29:w:93:ARG:HA	1.98	0.44
10:b:911:A:N6	20:m:9:PHE:HB2	2.31	0.44
10:b:1592:C:H2'	10:b:1593:A:C8	2.53	0.44
10:b:2740:A:H2'	10:b:2741:A:C8	2.52	0.44
10:b:2789:C:H2'	10:b:2893:A:N7	2.33	0.44
17:j:99:ARG:O	17:j:103:ILE:HG13	2.17	0.44
10:b:2458:G:H8	10:b:2459:A:H62	1.65	0.44
25:r:14:VAL:HG11	25:r:20:VAL:HG21	1.99	0.44
29:w:10:LYS:HB3	29:w:10:LYS:HE3	1.36	0.44
30:y:59:LEU:HD12	30:y:80:ILE:HD12	2.00	0.44
10:b:464:U:H2'	10:b:465:G:C8	2.52	0.44
10:b:891:G:H4'	10:b:892:A:C4	2.52	0.44
10:b:1636:U:H2'	10:b:1637:A:C8	2.53	0.44
1:0:26:LYS:HD3	1:0:26:LYS:HA	1.81	0.44
13:e:5:LEU:HD23	13:e:10:SER:O	2.18	0.44
9:a:52:A:C8	22:o:33:ARG:NH1	2.86	0.44
10:b:184:C:H2'	10:b:185:G:H8	1.80	0.44
10:b:608:A:H2'	10:b:609:A:C8	2.53	0.44
10:b:910:A:H2'	10:b:911:A:C8	2.52	0.44
10:b:915:C:H3'	10:b:916:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:f:57:LEU:HD21	14:f:89:VAL:HG22	2.00	0.44
19:l:1:MET:HE2	19:l:1:MET:HB3	1.81	0.44
26:s:14:ALA:O	26:s:18:ARG:HG3	2.18	0.44
10:b:1595:C:H2'	10:b:1596:A:C8	2.53	0.44
11:c:115:GLN:O	11:c:125:LYS:NZ	2.33	0.44
15:g:2:SER:O	15:g:6:LYS:N	2.50	0.44
16:h:5:LEU:HD22	16:h:15:LEU:HA	1.99	0.44
19:l:55:MET:O	19:l:60:ARG:NH2	2.51	0.44
20:m:74:THR:HG21	20:m:86:LYS:HE3	1.99	0.44
1:0:29:PHE:HB3	10:b:396:G:H1'	1.99	0.44
8:8:24:ARG:HH11	8:8:36:ARG:HE	1.66	0.44
10:b:621:A:C5	10:b:622:G:H1'	2.53	0.44
10:b:2765:A:N3	10:b:2765:A:H2'	2.32	0.44
13:e:133:LEU:HD12	13:e:133:LEU:HA	1.74	0.44
20:m:58:LYS:O	20:m:59:ARG:HD3	2.18	0.44
24:q:14:HIS:HD2	24:q:32:TYR:CG	2.36	0.44
27:t:6:ARG:NH1	27:t:42:GLU:OE1	2.50	0.44
28:u:24:LYS:H	28:u:37:GLU:HB3	1.82	0.44
29:w:36:ALA:O	29:w:93:ARG:NH2	2.51	0.44
10:b:437:U:H2'	10:b:438:G:C8	2.53	0.43
10:b:580:U:H2'	10:b:581:C:C6	2.52	0.43
10:b:1026:G:H2'	10:b:1027:A:H8	1.83	0.43
10:b:1326:U:H2'	10:b:1327:A:C8	2.53	0.43
10:b:1964:G:C4'	10:b:1965:C:OP2	2.62	0.43
4:3:48:TYR:CE1	4:3:53:LYS:HD3	2.53	0.43
10:b:729:G:C6	11:c:207:LYS:HB2	2.53	0.43
10:b:851:C:H2'	10:b:852:U:H5'	1.97	0.43
10:b:879:G:H2'	10:b:880:G:C8	2.53	0.43
10:b:1306:C:H5''	10:b:1606:C:N4	2.33	0.43
10:b:2663:G:H3'	10:b:2664:G:H8	1.84	0.43
11:c:78:VAL:HG21	11:c:110:LEU:HD21	1.99	0.43
12:d:110:THR:HG21	12:d:169:ARG:HE	1.82	0.43
13:e:4:VAL:HA	13:e:11:ALA:HA	2.00	0.43
13:e:15:SER:OG	13:e:17:THR:HG22	2.19	0.43
13:e:176:ASP:OD1	13:e:176:ASP:N	2.51	0.43
16:h:14:SER:OG	16:h:17:ASP:OD2	2.24	0.43
23:p:44:GLU:OE2	23:p:87:LYS:HG3	2.18	0.43
3:2:7:ILE:HD11	3:2:48:ILE:HD11	2.00	0.43
4:3:52:ARG:NH2	4:3:54:VAL:HG12	2.33	0.43
10:b:632:A:H2'	10:b:633:A:C8	2.54	0.43
14:f:91:LEU:C	14:f:96:MET:HB2	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:j:96:ARG:HD2	17:j:99:ARG:HB2	2.00	0.43
3:2:4:THR:HB	3:2:37:GLU:OE2	2.18	0.43
12:d:8:LYS:HB2	12:d:201:LEU:HD11	2.00	0.43
14:f:106:ILE:HG21	14:f:139:PRO:HG3	1.99	0.43
21:n:44:LEU:HD12	21:n:44:LEU:HA	1.84	0.43
22:o:51:ALA:HB3	22:o:78:VAL:HB	2.00	0.43
22:o:79:ALA:HB3	22:o:113:ALA:HB3	1.99	0.43
27:t:54:GLU:O	27:t:54:GLU:HG2	2.17	0.43
28:u:39:ILE:HG13	28:u:40:ASN:H	1.82	0.43
28:u:42:VAL:O	28:u:42:VAL:HG13	2.19	0.43
10:b:962:G:H21	10:b:2250:G:H1	1.66	0.43
22:o:29:HIS:O	22:o:36:TYR:N	2.44	0.43
9:a:48:U:P	22:o:30:ARG:NH2	2.92	0.43
10:b:915:C:H3'	10:b:916:G:H8	1.83	0.43
10:b:2279:G:N7	30:y:14:ARG:NH2	2.61	0.43
10:b:2547:G:H4'	18:k:29:HIS:NE2	2.34	0.43
10:b:2756:U:H1'	10:b:2757:A:H5''	1.99	0.43
14:f:52:ASN:C	14:f:150:ARG:HH12	2.27	0.43
19:l:123:ARG:HE	19:l:123:ARG:HB2	1.59	0.43
22:o:16:ARG:HA	22:o:16:ARG:HD3	1.62	0.43
26:s:88:ARG:HD2	26:s:88:ARG:HA	1.79	0.43
9:a:42:C:H2'	9:a:43:C:C6	2.54	0.43
10:b:558:U:H2'	10:b:559:G:H8	1.84	0.43
10:b:671:C:H2'	10:b:672:C:C6	2.54	0.43
10:b:1310:G:H1'	10:b:1611:C:H5''	2.00	0.43
10:b:1683:U:H2'	10:b:1684:G:C8	2.53	0.43
10:b:2030:A:C2	10:b:2499:C:H5''	2.53	0.43
10:b:2794:C:H2'	10:b:2795:C:C6	2.53	0.43
14:f:91:LEU:HB3	14:f:96:MET:HA	2.00	0.43
14:f:125:ARG:HE	14:f:125:ARG:HB2	1.44	0.43
15:g:94:TYR:HD1	15:g:107:LEU:HA	1.84	0.43
22:o:38:GLN:NE2	22:o:47:VAL:HG11	2.33	0.43
24:q:95:LEU:HD23	24:q:95:LEU:HA	1.81	0.43
2:l:5:GLU:HA	2:l:8:GLU:OE1	2.19	0.43
10:b:749:A:H4'	10:b:1271:G:N3	2.33	0.43
10:b:1083:U:H2'	10:b:1084:A:H2'	2.00	0.43
10:b:2096:C:H2'	10:b:2097:A:C8	2.54	0.43
13:e:97:ASN:HB2	13:e:100:MET:HG3	1.99	0.43
14:f:36:LEU:HD13	14:f:154:ILE:HG13	2.01	0.43
17:j:11:VAL:HG11	17:j:50:THR:HG22	2.00	0.43
20:m:50:ARG:HG2	20:m:50:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:u:4:LYS:HA	28:u:83:ARG:HE	1.84	0.43
7:7:25:LYS:HD3	19:l:62:PRO:HG2	1.99	0.43
7:7:33:LEU:HD23	7:7:36:LYS:HE2	1.99	0.43
10:b:2115:G:N2	10:b:2119:A:H62	2.16	0.43
15:g:72:LEU:HA	15:g:72:LEU:HD13	1.72	0.43
7:7:18:GLY:N	10:b:629:G:OP1	2.52	0.43
10:b:576:U:H2'	10:b:577:G:C8	2.54	0.43
10:b:856:G:H2'	10:b:857:G:C8	2.54	0.43
19:l:68:SER:O	19:l:69:ARG:HB3	2.18	0.43
10:b:64:A:H5'	27:t:70:ARG:HH21	1.84	0.42
10:b:948:C:H2'	10:b:949:G:C8	2.53	0.42
10:b:1432:G:H2'	10:b:1433:A:C8	2.54	0.42
10:b:1494:A:HO2'	10:b:1495:A:H8	1.64	0.42
10:b:2461:A:H1'	10:b:2492:U:C2	2.54	0.42
17:j:21:THR:HA	17:j:61:LYS:HB2	2.01	0.42
27:t:44:LYS:HG3	27:t:55:VAL:CG2	2.47	0.42
1:0:62:LYS:HB3	1:0:66:THR:CG2	2.49	0.42
2:1:37:LEU:HD23	2:1:37:LEU:O	2.19	0.42
9:a:95:U:P	29:w:19:ARG:HH22	2.41	0.42
10:b:581:C:H2'	10:b:582:A:H8	1.84	0.42
10:b:874:G:C3'	10:b:875:G:H5''	2.49	0.42
10:b:927:A:H2'	10:b:928:A:C8	2.54	0.42
10:b:1927:A:H2'	10:b:1928:A:C8	2.54	0.42
10:b:2014:A:H2'	10:b:2015:A:C8	2.54	0.42
20:m:77:PRO:HD2	20:m:80:VAL:HG11	2.01	0.42
29:w:21:ARG:HE	29:w:87:GLN:HA	1.84	0.42
1:0:43:GLU:HB3	1:0:45:ARG:HG2	2.00	0.42
7:7:32:ILE:HG22	7:7:35:LYS:HE3	2.01	0.42
10:b:848:C:H2'	10:b:849:A:H8	1.81	0.42
10:b:2116:G:H1'	10:b:2148:G:H21	1.84	0.42
10:b:2795:C:H2'	10:b:2796:U:C6	2.54	0.42
14:f:110:ARG:NH1	14:f:137:ILE:O	2.35	0.42
15:g:5:ALA:HB2	15:g:66:GLY:CA	2.50	0.42
15:g:17:VAL:HG21	15:g:50:LEU:HD11	2.01	0.42
19:l:77:ILE:CD1	19:l:108:ALA:HB1	2.49	0.42
9:a:39:A:C2	9:a:44:G:C2	3.07	0.42
12:d:9:VAL:HG11	23:p:4:ILE:HD11	2.01	0.42
14:f:134:GLU:CD	14:f:136:ILE:HG12	2.44	0.42
14:f:147:ASP:OD1	14:f:148:ARG:N	2.53	0.42
9:a:44:G:N2	9:a:48:U:C2	2.87	0.42
10:b:330:A:H2'	10:b:330:A:N3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:596:U:H2'	10:b:597:G:C8	2.54	0.42
10:b:2302:U:H2'	10:b:2303:G:C8	2.54	0.42
10:b:2312:U:H5'	14:f:85:ILE:HD11	2.01	0.42
10:b:2324:U:H1'	10:b:2337:G:H5''	2.01	0.42
10:b:2698:U:H2'	10:b:2699:C:C6	2.54	0.42
14:f:34:ILE:HD12	14:f:156:ILE:HG12	2.01	0.42
15:g:12:PRO:HD2	15:g:15:VAL:HG11	2.01	0.42
24:q:24:TYR:HB3	24:q:28:ARG:HB2	2.01	0.42
27:t:25:GLU:C	27:t:26:LYS:HD3	2.44	0.42
4:3:49:TYR:HE2	10:b:2883:A:OP1	2.01	0.42
10:b:373:U:H2'	10:b:374:A:C8	2.54	0.42
10:b:1428:C:C5	10:b:1569:A:H5''	2.55	0.42
10:b:2313:C:H2'	10:b:2314:A:C8	2.54	0.42
10:b:2783:U:O2'	10:b:2784:U:H5'	2.19	0.42
15:g:22:GLN:NE2	15:g:38:ASN:O	2.52	0.42
17:j:32:LEU:HD23	17:j:32:LEU:HA	1.81	0.42
20:m:8:LYS:HG3	20:m:9:PHE:CE1	2.55	0.42
20:m:110:GLU:OE2	20:m:114:ARG:NH2	2.53	0.42
26:s:82:MET:HB2	26:s:98:LYS:HB2	2.01	0.42
10:b:554:U:H2'	10:b:555:G:O4'	2.19	0.42
10:b:767:U:H2'	10:b:768:G:H8	1.84	0.42
10:b:1853:A:N1	10:b:2087:G:H1'	2.35	0.42
10:b:2081:U:H2'	10:b:2082:A:H8	1.85	0.42
11:c:207:LYS:HG3	11:c:210:ALA:H	1.84	0.42
15:g:9:VAL:CG1	15:g:50:LEU:HB2	2.49	0.42
17:j:36:LEU:O	17:j:51:GLY:HA3	2.20	0.42
20:m:12:MET:SD	20:m:72:PRO:HD2	2.60	0.42
7:7:5:LYS:HE2	10:b:254:G:N7	2.35	0.42
11:c:44:ASN:OD1	11:c:44:ASN:C	2.63	0.42
12:d:68:PHE:CD2	12:d:75:ALA:HA	2.55	0.42
15:g:22:GLN:HE21	15:g:39:ASP:HA	1.83	0.42
27:t:69:ARG:HD2	27:t:69:ARG:HA	1.64	0.42
10:b:20:C:H2'	10:b:21:A:C8	2.55	0.42
10:b:1724:G:H1	10:b:1736:U:H3	1.68	0.42
10:b:1779:U:H5	10:b:1784:A:N7	2.18	0.42
10:b:2886:A:H3'	10:b:2887:A:H8	1.84	0.42
27:t:67:VAL:O	27:t:68:LYS:C	2.62	0.42
5:4:38:LYS:HB2	5:4:49:TYR:CD2	2.55	0.42
10:b:532:A:N1	10:b:2020:A:H1'	2.35	0.42
10:b:538:A:H3'	10:b:539:G:H8	1.84	0.42
10:b:2710:C:H2'	10:b:2711:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:154:ASP:OD2	13:e:156:ASN:HB3	2.20	0.42
15:g:44:LYS:HB2	15:g:51:THR:CG2	2.50	0.42
9:a:51:G:H5''	22:o:64:TYR:CD2	2.55	0.41
10:b:128:C:H2'	10:b:129:C:C6	2.55	0.41
10:b:362:A:C4	10:b:363:G:C8	3.07	0.41
10:b:898:C:H2'	10:b:899:A:O5'	2.20	0.41
10:b:1548:A:H2'	10:b:1549:A:C8	2.54	0.41
10:b:2006:C:H5''	10:b:2048:G:H5''	2.02	0.41
12:d:4:LEU:HD12	12:d:101:PHE:CE2	2.54	0.41
22:o:94:ARG:HD2	22:o:97:PHE:O	2.20	0.41
10:b:917:A:H5''	10:b:2268:A:H61	1.85	0.41
10:b:1799:G:H8	11:c:180:GLU:OE1	2.02	0.41
13:e:98:LYS:HB3	13:e:102:ARG:NH2	2.34	0.41
15:g:148:LEU:O	15:g:162:VAL:HG11	2.19	0.41
16:h:6:LEU:HD11	16:h:37:VAL:HG23	2.03	0.41
28:u:63:ASN:C	28:u:65:ALA:H	2.28	0.41
10:b:222:A:N6	10:b:232:G:H1'	2.34	0.41
10:b:296:U:H2'	10:b:297:G:C8	2.55	0.41
10:b:1049:C:H1'	10:b:1113:U:H4'	2.01	0.41
10:b:1447:C:H2'	10:b:1448:G:H8	1.85	0.41
10:b:2515:C:H2'	10:b:2516:A:H8	1.85	0.41
10:b:2863:C:H2'	10:b:2864:G:C8	2.55	0.41
12:d:68:PHE:CE1	12:d:79:LEU:HD21	2.55	0.41
12:d:84:LEU:HA	12:d:84:LEU:HD23	1.70	0.41
18:k:14:SER:OG	18:k:86:LEU:HD12	2.19	0.41
18:k:70:ARG:HA	18:k:70:ARG:HD2	1.77	0.41
25:r:46:GLU:HB3	25:r:48:LYS:NZ	2.35	0.41
28:u:77:GLU:HB2	28:u:82:VAL:HG21	2.02	0.41
29:w:41:GLU:O	29:w:42:LEU:HD23	2.20	0.41
10:b:2809:A:H2'	10:b:2810:A:C8	2.55	0.41
14:f:71:ARG:HD3	14:f:71:ARG:O	2.20	0.41
22:o:35:ILE:HG23	22:o:74:VAL:HG11	2.03	0.41
24:q:80:ILE:O	24:q:84:LYS:HG2	2.20	0.41
27:t:80:LEU:HD23	27:t:80:LEU:HA	1.78	0.41
28:u:13:VAL:HB	28:u:18:ASP:O	2.20	0.41
4:3:20:ASP:O	26:s:19:LEU:HD11	2.21	0.41
9:a:18:G:H2'	9:a:19:C:C6	2.56	0.41
10:b:1794:A:H2'	10:b:1795:C:C6	2.56	0.41
15:g:9:VAL:HG12	15:g:50:LEU:HB2	2.01	0.41
5:4:12:VAL:HG12	5:4:51:GLU:HG3	2.02	0.41
7:7:50:VAL:HG11	7:7:58:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:28:C:P	22:o:31:THR:HG21	2.60	0.41
10:b:666:A:H4'	19:l:48:ARG:NH1	2.34	0.41
10:b:786:C:H5''	10:b:1780:A:N7	2.35	0.41
10:b:996:A:H1'	25:r:9:GLY:O	2.20	0.41
15:g:43:VAL:HG12	15:g:52:PHE:CE1	2.55	0.41
17:j:69:ARG:O	17:j:90:GLU:HG3	2.21	0.41
21:n:42:LYS:HA	21:n:45:ARG:NE	2.36	0.41
24:q:19:LYS:O	24:q:22:LYS:HG2	2.21	0.41
27:t:53:VAL:HG22	27:t:54:GLU:N	2.35	0.41
10:b:721:A:H2'	10:b:722:A:C8	2.55	0.41
10:b:947:A:O2'	10:b:984:A:C2	2.67	0.41
10:b:1429:G:H2'	10:b:1430:G:C8	2.56	0.41
10:b:1744:A:H3'	10:b:1745:A:C8	2.56	0.41
10:b:1875:G:H5''	10:b:1875:G:C8	2.54	0.41
10:b:2100:G:H1	10:b:2189:U:H3	1.69	0.41
10:b:2597:G:H5'	11:c:241:GLY:HA3	2.03	0.41
10:b:2749:A:H3'	10:b:2750:A:H2'	2.02	0.41
12:d:62:LYS:HA	12:d:65:ALA:HB3	2.02	0.41
2:1:43:LEU:HD12	10:b:61:C:H5''	2.01	0.41
10:b:974:G:H1'	10:b:975:A:C8	2.55	0.41
10:b:1168:G:H1	10:b:1181:U:H3	1.69	0.41
10:b:1723:A:H62	10:b:1737:G:H21	1.69	0.41
10:b:2512:C:OP1	12:d:128:ARG:HB3	2.21	0.41
12:d:149:ASN:CG	12:d:150:GLN:H	2.27	0.41
20:m:58:LYS:O	20:m:60:GLN:HG2	2.21	0.41
22:o:80:GLU:O	22:o:84:GLU:OE1	2.38	0.41
23:p:4:ILE:HG21	23:p:4:ILE:HD13	1.84	0.41
23:p:100:LEU:HD23	23:p:100:LEU:HA	1.90	0.41
27:t:23:ALA:HB1	27:t:29:THR:CG2	2.50	0.41
2:1:27:ASN:C	2:1:31:GLN:HE22	2.29	0.41
5:4:7:GLU:N	5:4:7:GLU:OE1	2.54	0.41
9:a:46:A:C5	9:a:47:C:C4	3.09	0.41
10:b:272:A:C4	10:b:273:G:C8	3.09	0.41
10:b:391:A:H1'	10:b:411:G:O4'	2.20	0.41
10:b:753:A:H2'	10:b:754:U:C6	2.56	0.41
10:b:1013:C:H2'	10:b:1014:A:C8	2.56	0.41
10:b:1062:G:H3'	10:b:1070:A:H8	1.85	0.41
10:b:1324:G:H1'	10:b:1616:A:N6	2.35	0.41
10:b:2114:A:H5''	10:b:2146:C:H41	1.85	0.41
10:b:2339:C:H2'	10:b:2340:A:C8	2.56	0.41
10:b:2483:C:N3	20:m:123:LYS:NZ	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:2765:A:N3	10:b:2765:A:C2'	2.84	0.41
10:b:2821:A:H2'	10:b:2822:G:C8	2.55	0.41
12:d:32:ASN:HD22	12:d:52:THR:HB	1.86	0.41
14:f:108:VAL:HA	14:f:111:ILE:CD1	2.51	0.41
14:f:119:ALA:O	14:f:167:ARG:NE	2.53	0.41
24:q:109:LEU:HD23	24:q:109:LEU:HA	1.82	0.41
26:s:86:MET:HB2	26:s:96:ILE:CG1	2.51	0.41
10:b:1353:A:H2'	10:b:1354:A:C8	2.56	0.41
10:b:1405:U:H2'	10:b:1406:U:C6	2.56	0.41
10:b:2169:A:N3	10:b:2169:A:H2'	2.36	0.41
13:e:42:GLY:O	13:e:89:PRO:HA	2.21	0.41
13:e:124:PHE:CE1	13:e:137:LYS:NZ	2.89	0.41
15:g:39:ASP:O	15:g:55:ARG:HG3	2.21	0.41
18:k:105:ARG:O	18:k:108:ARG:HG3	2.21	0.41
22:o:93:ASP:C	22:o:93:ASP:OD1	2.63	0.41
25:r:55:ASP:OD1	25:r:55:ASP:N	2.51	0.41
5:4:9:ILE:HD12	5:4:52:ALA:HA	2.01	0.40
9:a:41:G:H2'	14:f:66:LEU:HD21	2.04	0.40
10:b:491:G:H3'	10:b:492:A:H8	1.86	0.40
10:b:2074:U:H2'	10:b:2075:U:C6	2.56	0.40
10:b:2173:A:H5''	10:b:2174:C:C5	2.55	0.40
11:c:88:SER:HB2	11:c:200:HIS:CE1	2.56	0.40
12:d:97:SER:OG	12:d:98:VAL:N	2.53	0.40
15:g:17:VAL:C	15:g:18:LYS:HD3	2.47	0.40
16:h:29:PHE:CE1	16:h:33:GLN:NE2	2.89	0.40
23:p:106:LYS:HB3	23:p:109:ARG:HH21	1.87	0.40
24:q:61:TRP:O	24:q:65:ILE:HG13	2.21	0.40
26:s:72:THR:HG21	26:s:108:SER:OG	2.21	0.40
2:1:38:GLN:O	2:1:40:SER:N	2.54	0.40
5:4:26:ASN:C	5:4:26:ASN:HD22	2.29	0.40
9:a:89:U:H5'	9:a:90:C:C6	2.55	0.40
10:b:350:G:O2'	10:b:351:C:H5'	2.21	0.40
10:b:413:C:H2'	10:b:414:C:C6	2.57	0.40
10:b:588:U:H2'	10:b:589:U:C6	2.56	0.40
10:b:832:U:H2'	10:b:833:A:C8	2.56	0.40
10:b:891:G:O2'	10:b:893:C:N4	2.53	0.40
14:f:135:GLN:O	14:f:141:ILE:HD11	2.20	0.40
9:a:27:C:C4	9:a:28:C:C4	3.09	0.40
10:b:495:G:H5''	26:s:4:ILE:HG23	2.03	0.40
11:c:145:GLU:HG2	11:c:151:GLY:C	2.46	0.40
21:n:41:ALA:C	21:n:43:GLU:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:48:MET:O	29:w:51:GLN:NE2	2.49	0.40
10:b:320:A:H4'	10:b:322:A:N7	2.35	0.40
10:b:1470:A:H3'	10:b:1471:G:H8	1.86	0.40
10:b:1790:C:H2'	10:b:1791:A:C5	2.56	0.40
10:b:2229:U:H2'	10:b:2230:G:C8	2.56	0.40
11:c:177:ARG:HH21	11:c:177:ARG:HD2	1.75	0.40
15:g:54:PRO:HD3	15:g:62:TRP:CH2	2.56	0.40
25:r:85:LYS:HB2	25:r:85:LYS:HE3	1.70	0.40
29:w:75:GLN:HB2	29:w:92:VAL:HG13	2.02	0.40
29:w:80:HIS:HB3	29:w:85:LYS:HB2	2.04	0.40
5:4:51:GLU:O	5:4:53:LYS:N	2.54	0.40
8:8:14:CYS:SG	8:8:33:HIS:HB3	2.62	0.40
10:b:915:C:O2	10:b:915:C:C2'	2.67	0.40
10:b:2233:U:H2'	10:b:2234:G:H8	1.86	0.40
10:b:2345:G:H4'	10:b:2346:A:H5''	2.02	0.40
10:b:2514:U:H5''	17:j:81:ILE:HG21	2.01	0.40
10:b:2800:A:N7	10:b:2895:G:H1'	2.37	0.40
15:g:44:LYS:HB2	15:g:51:THR:HG22	2.04	0.40
17:j:40:HIS:NE2	17:j:52:ASP:OD2	2.54	0.40
17:j:101:ILE:HD12	17:j:101:ILE:HG23	1.84	0.40
18:k:88:ASN:HB3	18:k:91:SER:O	2.21	0.40
29:w:10:LYS:H	29:w:10:LYS:HG2	1.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
2	1	59/63 (94%)	55 (93%)	4 (7%)	0	100	100
3	2	55/59 (93%)	53 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	3	53/57 (93%)	49 (92%)	4 (8%)	0	100	100
5	4	48/55 (87%)	44 (92%)	3 (6%)	1 (2%)	5	15
6	6	44/46 (96%)	44 (100%)	0	0	100	100
7	7	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
8	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
12	d	207/209 (99%)	192 (93%)	15 (7%)	0	100	100
13	e	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
14	f	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
15	g	174/177 (98%)	155 (89%)	19 (11%)	0	100	100
16	h	37/149 (25%)	30 (81%)	6 (16%)	1 (3%)	4	10
17	j	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	18	41
18	k	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
19	l	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
20	m	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
21	n	118/127 (93%)	110 (93%)	8 (7%)	0	100	100
22	o	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
23	p	111/115 (96%)	106 (96%)	5 (4%)	0	100	100
24	q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
25	r	100/103 (97%)	92 (92%)	6 (6%)	2 (2%)	6	16
26	s	107/110 (97%)	100 (94%)	7 (6%)	0	100	100
27	t	84/93 (90%)	75 (89%)	6 (7%)	3 (4%)	2	6
28	u	89/93 (96%)	74 (83%)	13 (15%)	2 (2%)	5	14
29	w	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
30	y	74/85 (87%)	71 (96%)	2 (3%)	1 (1%)	9	23
All	All	3032/3249 (93%)	2845 (94%)	176 (6%)	11 (0%)	31	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	r	52	PRO
27	t	68	LYS
27	t	67	VAL

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Mol	Chain	Res	Type
27	t	69	ARG
16	h	27	ARG
25	r	51	VAL
28	u	7	ARG
28	u	8	ASP
30	y	44	LYS
5	4	52	ALA
17	j	84	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	67/68 (98%)	65 (97%)	2 (3%)	36	66
2	1	54/55 (98%)	52 (96%)	2 (4%)	30	59
3	2	47/49 (96%)	47 (100%)	0	100	100
4	3	46/48 (96%)	44 (96%)	2 (4%)	26	54
5	4	45/49 (92%)	42 (93%)	3 (7%)	15	36
6	6	38/38 (100%)	38 (100%)	0	100	100
7	7	51/52 (98%)	47 (92%)	4 (8%)	11	29
8	8	34/34 (100%)	28 (82%)	6 (18%)	2	5
11	c	216/218 (99%)	215 (100%)	1 (0%)	81	92
12	d	164/164 (100%)	164 (100%)	0	100	100
13	e	165/165 (100%)	161 (98%)	4 (2%)	43	72
14	f	148/150 (99%)	133 (90%)	15 (10%)	7	18
15	g	137/138 (99%)	127 (93%)	10 (7%)	13	32
16	h	30/114 (26%)	28 (93%)	2 (7%)	15	36
17	j	116/116 (100%)	110 (95%)	6 (5%)	21	47
18	k	103/104 (99%)	103 (100%)	0	100	100
19	l	102/103 (99%)	97 (95%)	5 (5%)	22	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	m	109/109 (100%)	106 (97%)	3 (3%)	38	68
21	n	100/103 (97%)	97 (97%)	3 (3%)	36	66
22	o	86/87 (99%)	84 (98%)	2 (2%)	44	73
23	p	98/100 (98%)	98 (100%)	0	100	100
24	q	89/90 (99%)	87 (98%)	2 (2%)	45	74
25	r	84/84 (100%)	81 (96%)	3 (4%)	31	60
26	s	92/93 (99%)	91 (99%)	1 (1%)	65	85
27	t	75/79 (95%)	64 (85%)	11 (15%)	3	8
28	u	74/76 (97%)	63 (85%)	11 (15%)	3	8
29	w	78/78 (100%)	73 (94%)	5 (6%)	16	38
30	y	58/63 (92%)	57 (98%)	1 (2%)	53	79
All	All	2506/2627 (95%)	2402 (96%)	104 (4%)	28	55

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	2	SER
1	0	25	THR
2	1	9	LYS
2	1	13	GLU
4	3	39	LEU
4	3	40	ARG
5	4	30	LYS
5	4	37	LYS
5	4	42	VAL
7	7	32	ILE
7	7	52	LYS
7	7	54	ASP
7	7	55	LEU
8	8	1	MET
8	8	2	LYS
8	8	23	ILE
8	8	24	ARG
8	8	26	ILE
8	8	27	CYS
11	c	261	LYS
13	e	130	LYS
13	e	132	LYS

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Mol	Chain	Res	Type
13	e	133	LEU
13	e	159	LEU
14	f	9	LYS
14	f	12	VAL
14	f	13	VAL
14	f	14	LYS
14	f	17	MET
14	f	23	ASN
14	f	24	SER
14	f	26	MET
14	f	27	GLN
14	f	38	MET
14	f	64	LYS
14	f	66	LEU
14	f	125	ARG
14	f	129	SER
14	f	158	THR
15	g	29	LYS
15	g	30	ASN
15	g	32	GLU
15	g	33	LEU
15	g	72	LEU
15	g	105	LEU
15	g	113	VAL
15	g	128	GLN
15	g	129	THR
15	g	130	GLU
16	h	22	LYS
16	h	25	TYR
17	j	81	ILE
17	j	85	LYS
17	j	86	GLN
17	j	95	ARG
17	j	96	ARG
17	j	106	LYS
19	l	77	ILE
19	l	78	ARG
19	l	141	LYS
19	l	142	ILE
19	l	143	GLU
20	m	70	ASP
20	m	71	LYS

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Mol	Chain	Res	Type
20	m	128	THR
21	n	103	ARG
21	n	118	ARG
21	n	120	GLU
22	o	13	ARG
22	o	16	ARG
24	q	89	GLU
24	q	90	ILE
25	r	47	VAL
25	r	48	LYS
25	r	51	VAL
26	s	13	SER
27	t	16	VAL
27	t	18	GLU
27	t	19	LYS
27	t	61	LEU
27	t	62	VAL
27	t	64	LYS
27	t	66	LYS
27	t	67	VAL
27	t	68	LYS
27	t	69	ARG
27	t	70	ARG
28	u	6	ARG
28	u	7	ARG
28	u	8	ASP
28	u	9	ASP
28	u	70	ASP
28	u	72	VAL
28	u	78	ASP
28	u	80	LYS
28	u	81	LYS
28	u	82	VAL
28	u	83	ARG
29	w	9	ARG
29	w	10	LYS
29	w	11	GLU
29	w	55	GLU
29	w	58	SER
30	y	43	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	34	HIS
1	0	36	HIS
2	1	25	GLN
2	1	31	GLN
2	1	41	HIS
2	1	45	GLN
4	3	19	HIS
5	4	46	HIS
7	7	26	HIS
7	7	31	HIS
11	c	37	ASN
11	c	60	GLN
11	c	86	ASN
11	c	142	HIS
12	d	140	HIS
13	e	41	GLN
13	e	115	GLN
13	e	136	GLN
15	g	22	GLN
15	g	38	ASN
15	g	115	HIS
16	h	11	ASN
17	j	77	HIS
17	j	80	HIS
18	k	93	GLN
19	l	99	ASN
20	m	60	GLN
21	n	16	HIS
21	n	81	ASN
22	o	43	ASN
23	p	66	ASN
24	q	44	GLN
25	r	66	HIS
26	s	15	GLN
27	t	48	GLN
28	u	45	HIS
28	u	63	ASN
29	w	87	GLN
30	y	57	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	2898/2904 (99%)	1008 (34%)	0
9	a	117/120 (97%)	30 (25%)	0
All	All	3015/3024 (99%)	1038 (34%)	0

All (1038) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	a	13	G
9	a	15	A
9	a	24	G
9	a	25	U
9	a	26	C
9	a	30	C
9	a	32	U
9	a	33	G
9	a	35	C
9	a	37	C
9	a	41	G
9	a	42	C
9	a	43	C
9	a	44	G
9	a	50	A
9	a	51	G
9	a	56	G
9	a	59	A
9	a	67	G
9	a	86	G
9	a	88	C
9	a	90	C
9	a	91	C
9	a	99	A
9	a	108	A
9	a	109	A
9	a	112	G
9	a	113	C
9	a	116	G
9	a	117	G
10	b	3	U
10	b	9	G
10	b	10	A
10	b	14	A
10	b	15	G
10	b	23	G

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Mol	Chain	Res	Type
10	b	24	G
10	b	27	G
10	b	33	C
10	b	34	U
10	b	35	G
10	b	42	A
10	b	44	A
10	b	45	G
10	b	46	G
10	b	47	C
10	b	51	G
10	b	55	G
10	b	60	G
10	b	62	U
10	b	63	A
10	b	65	U
10	b	70	G
10	b	71	A
10	b	72	U
10	b	73	A
10	b	74	A
10	b	75	G
10	b	76	C
10	b	77	G
10	b	80	G
10	b	84	A
10	b	86	G
10	b	87	U
10	b	88	G
10	b	91	A
10	b	92	U
10	b	93	G
10	b	94	A
10	b	96	C
10	b	97	C
10	b	100	U
10	b	101	A
10	b	102	U
10	b	111	A
10	b	114	U
10	b	118	A
10	b	119	A

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Mol	Chain	Res	Type
10	b	120	U
10	b	121	G
10	b	122	G
10	b	125	A
10	b	134	G
10	b	136	G
10	b	139	U
10	b	140	C
10	b	142	A
10	b	146	A
10	b	159	G
10	b	160	A
10	b	162	U
10	b	163	C
10	b	165	A
10	b	166	U
10	b	173	A
10	b	175	G
10	b	176	A
10	b	181	A
10	b	184	C
10	b	186	G
10	b	187	G
10	b	196	A
10	b	197	A
10	b	198	C
10	b	199	A
10	b	201	C
10	b	206	U
10	b	213	A
10	b	215	G
10	b	216	A
10	b	221	A
10	b	222	A
10	b	223	A
10	b	226	A
10	b	228	C
10	b	229	C
10	b	230	G
10	b	232	G
10	b	233	A
10	b	245	G

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Mol	Chain	Res	Type
10	b	248	G
10	b	249	C
10	b	250	G
10	b	252	G
10	b	255	A
10	b	257	C
10	b	261	G
10	b	265	A
10	b	266	G
10	b	271	G
10	b	276	U
10	b	277	G
10	b	278	A
10	b	279	A
10	b	280	U
10	b	281	C
10	b	286	U
10	b	287	G
10	b	290	U
10	b	291	G
10	b	292	U
10	b	299	A
10	b	300	A
10	b	308	G
10	b	311	A
10	b	312	G
10	b	313	G
10	b	314	C
10	b	317	G
10	b	322	A
10	b	323	C
10	b	325	G
10	b	326	G
10	b	327	G
10	b	329	G
10	b	330	A
10	b	331	C
10	b	334	C
10	b	338	G
10	b	345	A
10	b	346	A
10	b	347	A

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Mol	Chain	Res	Type
10	b	348	A
10	b	351	C
10	b	352	A
10	b	353	C
10	b	356	G
10	b	359	G
10	b	362	A
10	b	367	G
10	b	370	G
10	b	371	A
10	b	372	G
10	b	383	C
10	b	386	G
10	b	387	U
10	b	390	U
10	b	391	A
10	b	395	U
10	b	396	G
10	b	397	U
10	b	403	U
10	b	404	A
10	b	405	U
10	b	406	G
10	b	411	G
10	b	412	A
10	b	418	C
10	b	420	C
10	b	422	A
10	b	435	C
10	b	437	U
10	b	442	G
10	b	443	A
10	b	451	U
10	b	452	G
10	b	454	A
10	b	455	C
10	b	456	C
10	b	457	A
10	b	459	U
10	b	464	U
10	b	465	G
10	b	466	A

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Mol	Chain	Res	Type
10	b	467	G
10	b	471	A
10	b	474	G
10	b	475	C
10	b	477	A
10	b	479	A
10	b	480	A
10	b	481	G
10	b	491	G
10	b	504	A
10	b	505	A
10	b	508	A
10	b	509	C
10	b	512	G
10	b	527	C
10	b	529	A
10	b	531	C
10	b	532	A
10	b	538	A
10	b	545	U
10	b	547	A
10	b	550	C
10	b	555	G
10	b	562	U
10	b	563	A
10	b	568	U
10	b	573	U
10	b	575	A
10	b	587	C
10	b	603	A
10	b	604	G
10	b	613	A
10	b	614	A
10	b	615	U
10	b	620	G
10	b	621	A
10	b	622	G
10	b	627	A
10	b	628	G
10	b	634	C
10	b	637	A
10	b	642	U

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Mol	Chain	Res	Type
10	b	644	A
10	b	646	U
10	b	647	G
10	b	653	U
10	b	654	A
10	b	655	A
10	b	659	G
10	b	664	G
10	b	668	A
10	b	669	G
10	b	670	A
10	b	678	C
10	b	682	G
10	b	683	U
10	b	685	A
10	b	686	U
10	b	687	C
10	b	702	U
10	b	704	G
10	b	726	G
10	b	728	G
10	b	730	A
10	b	731	C
10	b	746	U
10	b	747	U
10	b	748	G
10	b	757	G
10	b	764	A
10	b	765	C
10	b	770	G
10	b	771	G
10	b	775	G
10	b	776	G
10	b	777	G
10	b	781	A
10	b	782	A
10	b	783	A
10	b	784	G
10	b	785	G
10	b	789	A
10	b	791	C
10	b	792	A

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Mol	Chain	Res	Type
10	b	794	A
10	b	798	G
10	b	805	G
10	b	806	C
10	b	811	U
10	b	812	C
10	b	815	C
10	b	819	A
10	b	827	U
10	b	828	U
10	b	829	A
10	b	831	G
10	b	833	A
10	b	845	A
10	b	846	U
10	b	847	U
10	b	848	C
10	b	852	U
10	b	854	C
10	b	855	G
10	b	856	G
10	b	858	G
10	b	859	G
10	b	860	U
10	b	865	C
10	b	866	A
10	b	868	U
10	b	869	G
10	b	872	U
10	b	875	G
10	b	876	C
10	b	877	A
10	b	878	A
10	b	879	G
10	b	881	G
10	b	883	G
10	b	884	U
10	b	885	C
10	b	887	U
10	b	889	C
10	b	890	C
10	b	893	C

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Mol	Chain	Res	Type
10	b	894	U
10	b	895	U
10	b	896	A
10	b	897	C
10	b	899	A
10	b	900	A
10	b	905	A
10	b	907	G
10	b	909	A
10	b	910	A
10	b	916	G
10	b	923	G
10	b	924	G
10	b	927	A
10	b	931	U
10	b	932	U
10	b	938	G
10	b	941	A
10	b	946	C
10	b	953	G
10	b	961	C
10	b	973	A
10	b	974	G
10	b	980	A
10	b	982	C
10	b	983	A
10	b	985	C
10	b	989	G
10	b	990	A
10	b	993	G
10	b	995	C
10	b	996	A
10	b	1003	G
10	b	1005	C
10	b	1009	A
10	b	1012	U
10	b	1013	C
10	b	1018	U
10	b	1020	A
10	b	1021	A
10	b	1022	G
10	b	1025	G

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Mol	Chain	Res	Type
10	b	1026	G
10	b	1027	A
10	b	1032	A
10	b	1033	U
10	b	1034	G
10	b	1035	U
10	b	1037	G
10	b	1038	G
10	b	1041	G
10	b	1042	G
10	b	1049	C
10	b	1052	C
10	b	1053	C
10	b	1054	A
10	b	1055	G
10	b	1056	G
10	b	1057	A
10	b	1058	U
10	b	1059	G
10	b	1060	U
10	b	1061	U
10	b	1062	G
10	b	1063	G
10	b	1064	C
10	b	1065	U
10	b	1066	U
10	b	1067	A
10	b	1068	G
10	b	1069	A
10	b	1071	G
10	b	1072	C
10	b	1073	A
10	b	1074	G
10	b	1077	A
10	b	1078	U
10	b	1079	C
10	b	1080	A
10	b	1081	U
10	b	1082	U
10	b	1083	U
10	b	1084	A
10	b	1086	A

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Mol	Chain	Res	Type
10	b	1087	G
10	b	1088	A
10	b	1089	A
10	b	1090	A
10	b	1091	G
10	b	1092	C
10	b	1095	A
10	b	1096	A
10	b	1097	U
10	b	1098	A
10	b	1099	G
10	b	1101	U
10	b	1102	C
10	b	1103	A
10	b	1104	C
10	b	1105	U
10	b	1106	G
10	b	1108	U
10	b	1109	C
10	b	1110	G
10	b	1111	A
10	b	1112	G
10	b	1116	G
10	b	1130	U
10	b	1131	G
10	b	1132	U
10	b	1133	A
10	b	1134	A
10	b	1135	C
10	b	1136	G
10	b	1137	G
10	b	1142	A
10	b	1143	A
10	b	1144	A
10	b	1151	A
10	b	1156	A
10	b	1157	G
10	b	1158	C
10	b	1165	A
10	b	1166	G
10	b	1171	G
10	b	1172	C

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Mol	Chain	Res	Type
10	b	1174	U
10	b	1175	A
10	b	1176	U
10	b	1177	G
10	b	1178	C
10	b	1180	U
10	b	1182	G
10	b	1185	G
10	b	1186	G
10	b	1195	G
10	b	1204	A
10	b	1206	G
10	b	1210	G
10	b	1211	C
10	b	1212	G
10	b	1225	G
10	b	1227	G
10	b	1231	U
10	b	1236	G
10	b	1237	A
10	b	1238	G
10	b	1241	A
10	b	1242	U
10	b	1247	A
10	b	1248	G
10	b	1250	G
10	b	1253	A
10	b	1256	G
10	b	1260	A
10	b	1266	G
10	b	1271	G
10	b	1272	A
10	b	1275	A
10	b	1276	A
10	b	1284	A
10	b	1286	A
10	b	1287	A
10	b	1288	G
10	b	1289	C
10	b	1295	C
10	b	1296	G
10	b	1300	G

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Mol	Chain	Res	Type
10	b	1301	A
10	b	1302	A
10	b	1303	G
10	b	1312	U
10	b	1315	C
10	b	1320	C
10	b	1321	A
10	b	1324	G
10	b	1325	U
10	b	1328	A
10	b	1329	U
10	b	1332	G
10	b	1338	G
10	b	1341	G
10	b	1346	G
10	b	1352	U
10	b	1355	G
10	b	1359	A
10	b	1365	A
10	b	1366	A
10	b	1368	G
10	b	1374	G
10	b	1378	A
10	b	1379	U
10	b	1383	A
10	b	1384	A
10	b	1388	G
10	b	1392	A
10	b	1393	A
10	b	1395	A
10	b	1407	G
10	b	1410	G
10	b	1411	U
10	b	1416	G
10	b	1419	A
10	b	1420	A
10	b	1421	G
10	b	1423	G
10	b	1427	A
10	b	1428	C
10	b	1429	G
10	b	1435	G

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Mol	Chain	Res	Type
10	b	1436	G
10	b	1451	C
10	b	1452	G
10	b	1453	A
10	b	1454	C
10	b	1455	G
10	b	1457	U
10	b	1458	U
10	b	1459	G
10	b	1460	U
10	b	1461	C
10	b	1466	U
10	b	1468	U
10	b	1469	A
10	b	1475	G
10	b	1476	U
10	b	1477	A
10	b	1478	G
10	b	1479	G
10	b	1482	G
10	b	1486	U
10	b	1491	G
10	b	1493	C
10	b	1494	A
10	b	1495	A
10	b	1496	A
10	b	1502	A
10	b	1508	A
10	b	1509	A
10	b	1510	G
10	b	1512	C
10	b	1516	G
10	b	1523	U
10	b	1524	G
10	b	1529	G
10	b	1530	G
10	b	1531	C
10	b	1536	C
10	b	1537	G
10	b	1538	G
10	b	1539	U
10	b	1543	G

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Mol	Chain	Res	Type
10	b	1544	A
10	b	1552	A
10	b	1554	U
10	b	1559	U
10	b	1560	G
10	b	1565	C
10	b	1566	A
10	b	1568	G
10	b	1569	A
10	b	1575	C
10	b	1578	U
10	b	1581	G
10	b	1582	C
10	b	1583	A
10	b	1584	U
10	b	1585	C
10	b	1588	G
10	b	1589	U
10	b	1595	C
10	b	1596	A
10	b	1607	C
10	b	1608	A
10	b	1610	A
10	b	1611	C
10	b	1618	A
10	b	1619	G
10	b	1622	G
10	b	1630	A
10	b	1632	A
10	b	1634	A
10	b	1647	U
10	b	1648	U
10	b	1649	G
10	b	1664	A
10	b	1667	G
10	b	1672	A
10	b	1674	G
10	b	1675	C
10	b	1694	C
10	b	1698	A
10	b	1699	G
10	b	1700	A

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Mol	Chain	Res	Type
10	b	1703	G
10	b	1705	A
10	b	1706	C
10	b	1707	G
10	b	1715	G
10	b	1716	U
10	b	1726	G
10	b	1729	U
10	b	1731	G
10	b	1732	C
10	b	1733	U
10	b	1737	G
10	b	1753	G
10	b	1754	A
10	b	1755	A
10	b	1756	G
10	b	1758	U
10	b	1759	A
10	b	1763	G
10	b	1764	C
10	b	1773	A
10	b	1776	G
10	b	1779	U
10	b	1782	U
10	b	1784	A
10	b	1786	A
10	b	1799	G
10	b	1800	C
10	b	1801	A
10	b	1805	A
10	b	1808	A
10	b	1809	A
10	b	1811	G
10	b	1816	C
10	b	1817	G
10	b	1820	U
10	b	1821	A
10	b	1829	A
10	b	1833	C
10	b	1848	A
10	b	1853	A
10	b	1857	G

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Mol	Chain	Res	Type
10	b	1862	G
10	b	1864	U
10	b	1867	G
10	b	1869	G
10	b	1870	C
10	b	1871	A
10	b	1872	A
10	b	1873	G
10	b	1874	C
10	b	1875	G
10	b	1876	A
10	b	1881	C
10	b	1882	U
10	b	1884	G
10	b	1885	A
10	b	1887	C
10	b	1890	A
10	b	1895	C
10	b	1899	A
10	b	1900	A
10	b	1902	C
10	b	1906	G
10	b	1907	G
10	b	1908	C
10	b	1913	A
10	b	1918	A
10	b	1927	A
10	b	1929	G
10	b	1930	G
10	b	1931	U
10	b	1936	A
10	b	1937	A
10	b	1938	A
10	b	1939	U
10	b	1955	U
10	b	1958	C
10	b	1964	G
10	b	1965	C
10	b	1966	A
10	b	1967	C
10	b	1970	A
10	b	1971	U

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Mol	Chain	Res	Type
10	b	1972	G
10	b	1975	G
10	b	1980	G
10	b	1981	A
10	b	1982	U
10	b	1991	U
10	b	1992	G
10	b	1993	U
10	b	1996	C
10	b	1997	C
10	b	2002	G
10	b	2020	A
10	b	2023	C
10	b	2024	G
10	b	2031	A
10	b	2032	G
10	b	2033	A
10	b	2035	G
10	b	2036	C
10	b	2039	U
10	b	2043	C
10	b	2049	G
10	b	2051	A
10	b	2052	A
10	b	2055	C
10	b	2056	G
10	b	2059	A
10	b	2060	A
10	b	2061	G
10	b	2062	A
10	b	2068	U
10	b	2069	G
10	b	2076	U
10	b	2077	A
10	b	2078	C
10	b	2080	A
10	b	2093	G
10	b	2099	U
10	b	2101	A
10	b	2102	G
10	b	2104	C
10	b	2105	U

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Mol	Chain	Res	Type
10	b	2106	U
10	b	2107	G
10	b	2109	U
10	b	2111	U
10	b	2112	G
10	b	2113	U
10	b	2114	A
10	b	2115	G
10	b	2116	G
10	b	2117	A
10	b	2118	U
10	b	2119	A
10	b	2120	G
10	b	2121	G
10	b	2123	G
10	b	2124	G
10	b	2126	A
10	b	2127	G
10	b	2128	G
10	b	2129	C
10	b	2130	U
10	b	2131	U
10	b	2133	G
10	b	2134	A
10	b	2135	A
10	b	2136	G
10	b	2137	U
10	b	2138	G
10	b	2139	U
10	b	2140	G
10	b	2141	G
10	b	2142	A
10	b	2143	C
10	b	2145	C
10	b	2146	C
10	b	2147	A
10	b	2148	G
10	b	2149	U
10	b	2150	C
10	b	2151	U
10	b	2152	G
10	b	2154	A

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Mol	Chain	Res	Type
10	b	2157	G
10	b	2158	A
10	b	2159	G
10	b	2160	C
10	b	2161	C
10	b	2162	G
10	b	2163	A
10	b	2164	C
10	b	2165	C
10	b	2166	U
10	b	2169	A
10	b	2170	A
10	b	2171	A
10	b	2172	U
10	b	2174	C
10	b	2175	C
10	b	2176	A
10	b	2177	C
10	b	2178	C
10	b	2180	U
10	b	2183	A
10	b	2186	G
10	b	2189	U
10	b	2192	U
10	b	2193	G
10	b	2197	U
10	b	2198	A
10	b	2203	U
10	b	2204	G
10	b	2210	U
10	b	2212	A
10	b	2213	U
10	b	2214	C
10	b	2225	A
10	b	2238	G
10	b	2239	G
10	b	2243	U
10	b	2249	U
10	b	2250	G
10	b	2258	C
10	b	2259	U
10	b	2266	A

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Mol	Chain	Res	Type
10	b	2268	A
10	b	2278	A
10	b	2279	G
10	b	2282	G
10	b	2283	C
10	b	2287	A
10	b	2288	A
10	b	2294	G
10	b	2296	U
10	b	2297	A
10	b	2305	U
10	b	2307	G
10	b	2308	G
10	b	2309	A
10	b	2311	A
10	b	2312	U
10	b	2319	G
10	b	2320	U
10	b	2321	U
10	b	2322	A
10	b	2325	G
10	b	2327	A
10	b	2331	G
10	b	2332	C
10	b	2333	A
10	b	2334	U
10	b	2335	A
10	b	2336	A
10	b	2337	G
10	b	2340	A
10	b	2344	U
10	b	2345	G
10	b	2347	C
10	b	2350	C
10	b	2352	A
10	b	2354	C
10	b	2355	G
10	b	2357	G
10	b	2361	G
10	b	2371	G
10	b	2374	C
10	b	2377	A

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Mol	Chain	Res	Type
10	b	2379	G
10	b	2383	G
10	b	2385	C
10	b	2389	G
10	b	2391	G
10	b	2396	G
10	b	2397	G
10	b	2402	U
10	b	2403	C
10	b	2406	A
10	b	2407	A
10	b	2410	G
10	b	2419	U
10	b	2420	C
10	b	2422	C
10	b	2423	U
10	b	2424	C
10	b	2425	A
10	b	2426	A
10	b	2427	C
10	b	2428	G
10	b	2429	G
10	b	2430	A
10	b	2431	U
10	b	2432	A
10	b	2434	A
10	b	2435	A
10	b	2439	A
10	b	2441	U
10	b	2444	G
10	b	2445	G
10	b	2448	A
10	b	2458	G
10	b	2459	A
10	b	2468	A
10	b	2470	G
10	b	2474	U
10	b	2475	C
10	b	2476	A
10	b	2481	G
10	b	2483	C
10	b	2484	G

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Mol	Chain	Res	Type
10	b	2486	C
10	b	2491	U
10	b	2492	U
10	b	2498	C
10	b	2502	G
10	b	2504	U
10	b	2505	G
10	b	2511	U
10	b	2513	A
10	b	2517	C
10	b	2518	A
10	b	2519	U
10	b	2520	C
10	b	2525	G
10	b	2528	U
10	b	2529	G
10	b	2532	G
10	b	2533	U
10	b	2534	A
10	b	2535	G
10	b	2547	G
10	b	2554	U
10	b	2559	C
10	b	2560	A
10	b	2562	U
10	b	2564	A
10	b	2566	A
10	b	2567	G
10	b	2573	C
10	b	2574	G
10	b	2579	C
10	b	2581	G
10	b	2582	G
10	b	2583	G
10	b	2585	U
10	b	2586	U
10	b	2601	C
10	b	2602	A
10	b	2609	U
10	b	2610	C
10	b	2613	U
10	b	2614	A

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Mol	Chain	Res	Type
10	b	2615	U
10	b	2623	G
10	b	2629	U
10	b	2630	G
10	b	2635	A
10	b	2638	G
10	b	2639	A
10	b	2641	G
10	b	2643	G
10	b	2646	C
10	b	2655	G
10	b	2656	U
10	b	2662	A
10	b	2663	G
10	b	2669	G
10	b	2673	G
10	b	2674	G
10	b	2681	C
10	b	2682	A
10	b	2684	U
10	b	2689	U
10	b	2690	U
10	b	2691	C
10	b	2714	G
10	b	2716	C
10	b	2718	G
10	b	2720	U
10	b	2726	A
10	b	2731	G
10	b	2733	A
10	b	2736	A
10	b	2737	G
10	b	2744	G
10	b	2748	A
10	b	2751	G
10	b	2754	U
10	b	2755	C
10	b	2757	A
10	b	2761	A
10	b	2765	A
10	b	2778	A
10	b	2779	U

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Mol	Chain	Res	Type
10	b	2784	U
10	b	2790	U
10	b	2796	U
10	b	2797	U
10	b	2798	U
10	b	2799	A
10	b	2800	A
10	b	2801	G
10	b	2807	U
10	b	2808	G
10	b	2818	U
10	b	2820	A
10	b	2821	A
10	b	2823	A
10	b	2832	U
10	b	2833	U
10	b	2834	G
10	b	2835	A
10	b	2836	U
10	b	2848	G
10	b	2849	U
10	b	2861	U
10	b	2864	G
10	b	2865	U
10	b	2867	G
10	b	2872	A
10	b	2873	A
10	b	2874	C
10	b	2877	G
10	b	2879	A
10	b	2883	A
10	b	2884	U
10	b	2886	A
10	b	2891	U
10	b	2895	G
10	b	2899	A

There are no RNA pucker outliers to report.

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

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

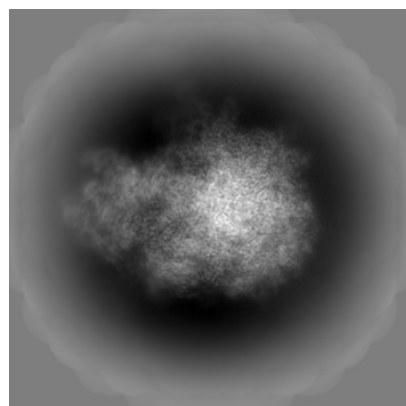
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14864. These allow visual inspection of the internal detail of the map and identification of artifacts.

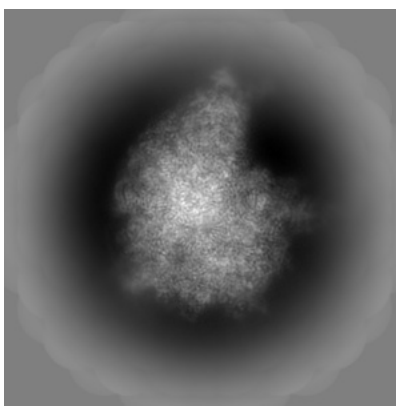
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

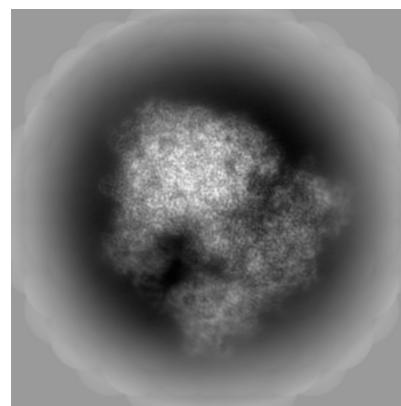
6.1.1 Primary map



X

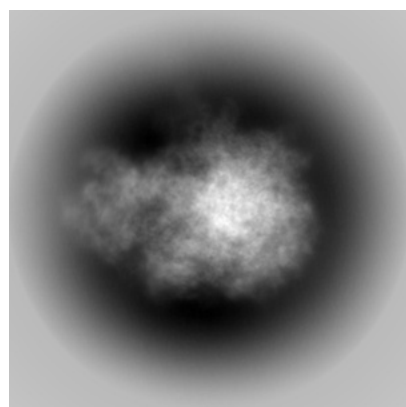


Y

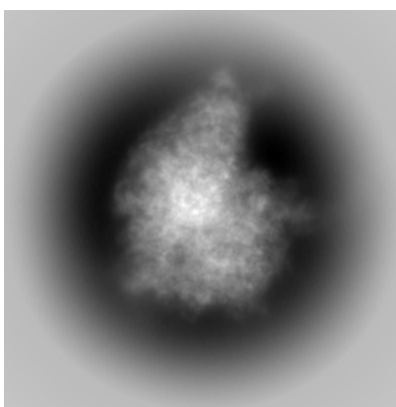


Z

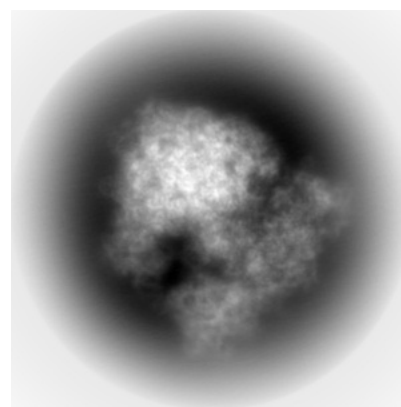
6.1.2 Raw map



X



Y

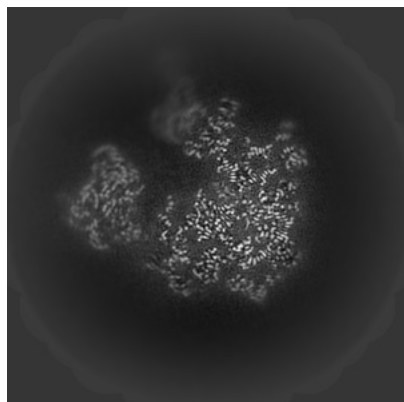


Z

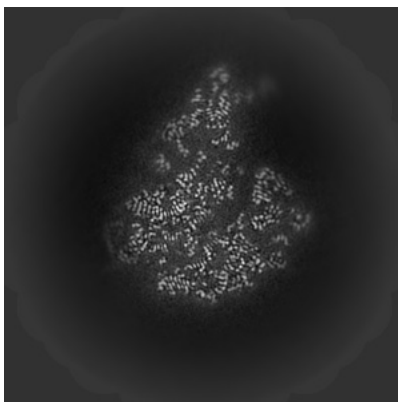
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

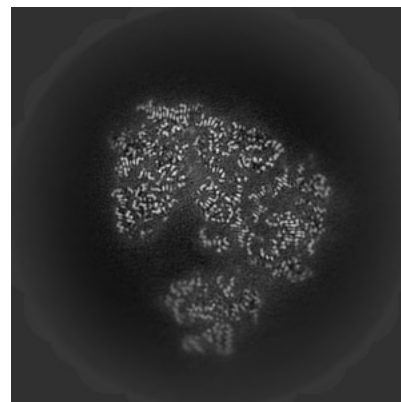
6.2.1 Primary map



X Index: 184

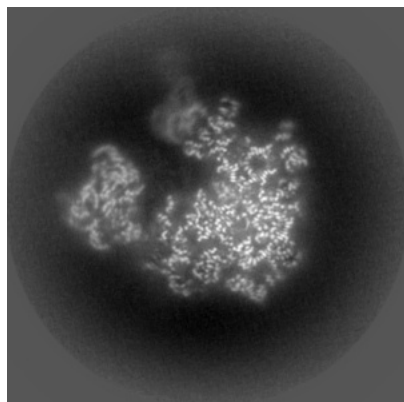


Y Index: 184

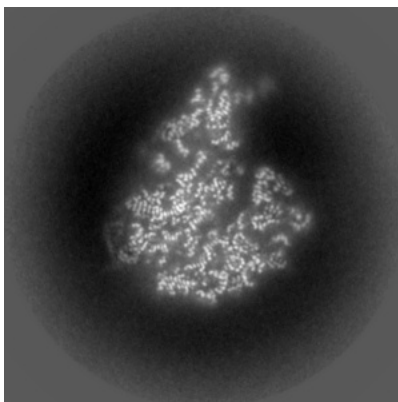


Z Index: 184

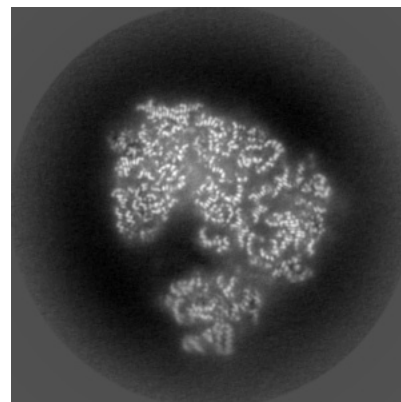
6.2.2 Raw map



X Index: 184



Y Index: 184

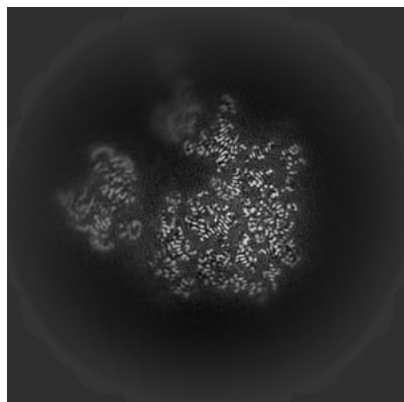


Z Index: 184

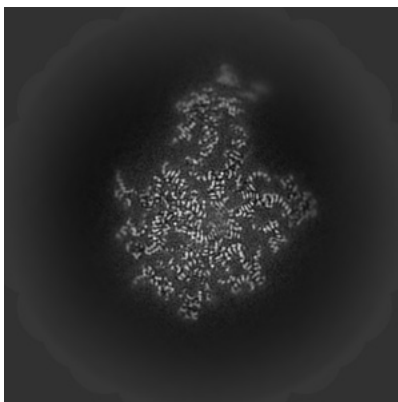
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

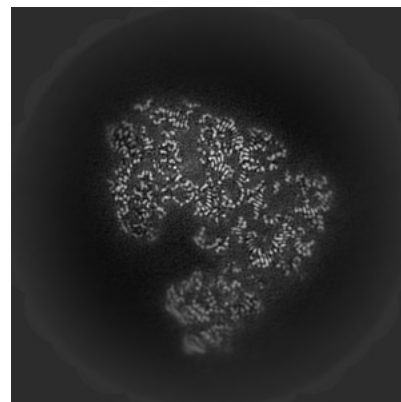
6.3.1 Primary map



X Index: 188

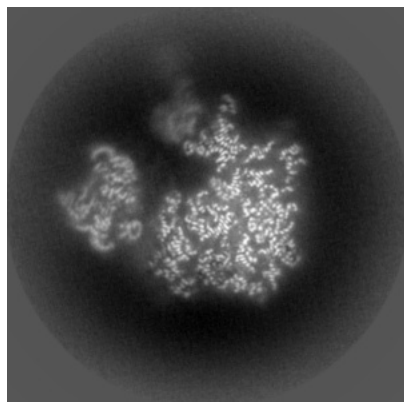


Y Index: 202

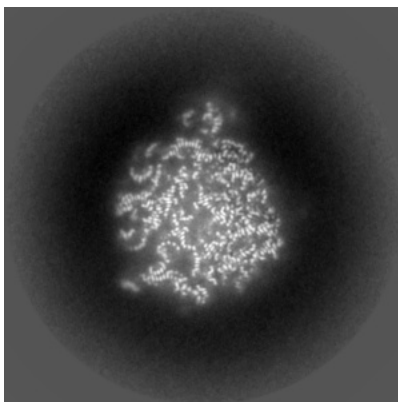


Z Index: 180

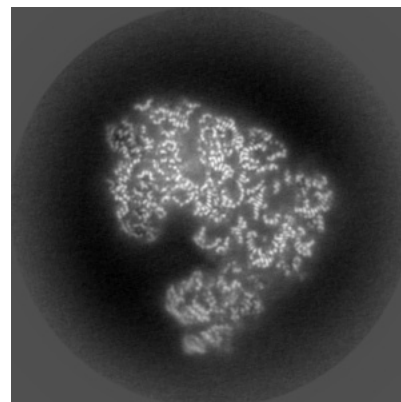
6.3.2 Raw map



X Index: 188



Y Index: 218

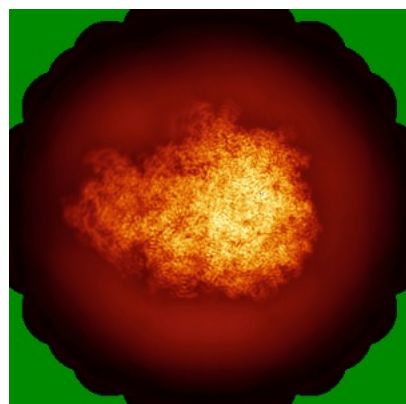


Z Index: 180

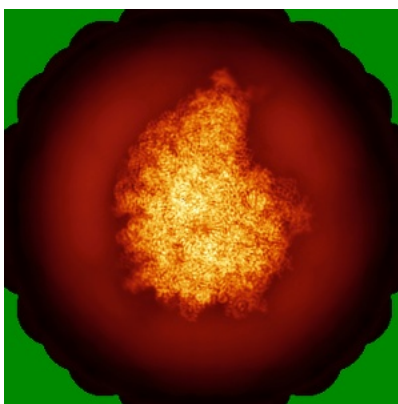
The images above show the largest variance slices of the map in three orthogonal directions.

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

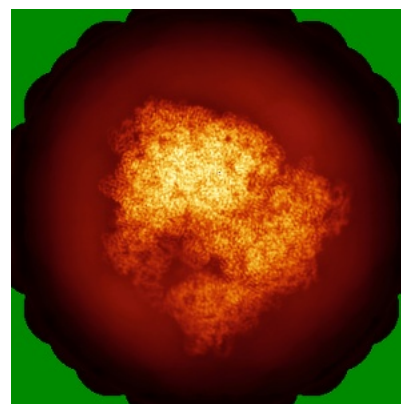
6.4.1 Primary map



X

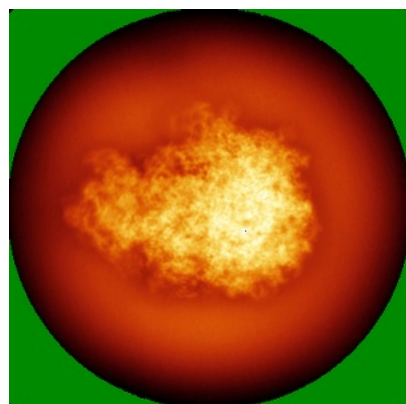


Y

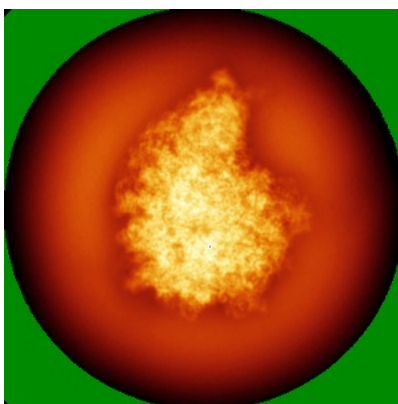


Z

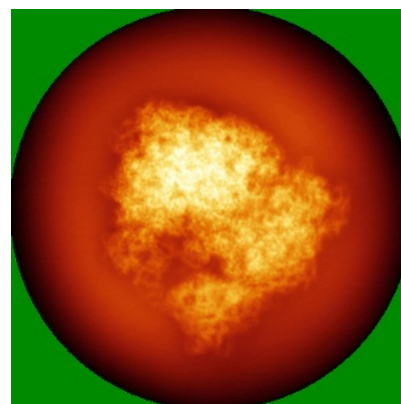
6.4.2 Raw map



X



Y

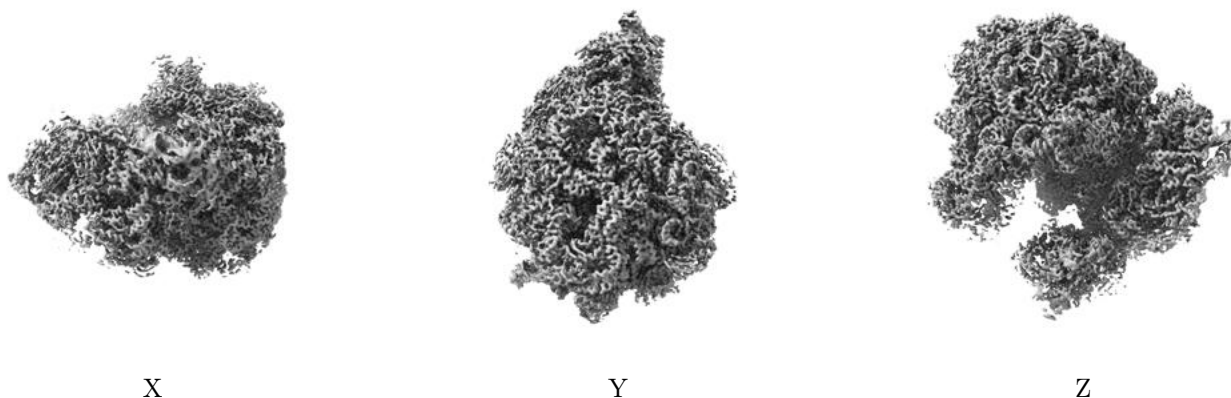


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0885. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

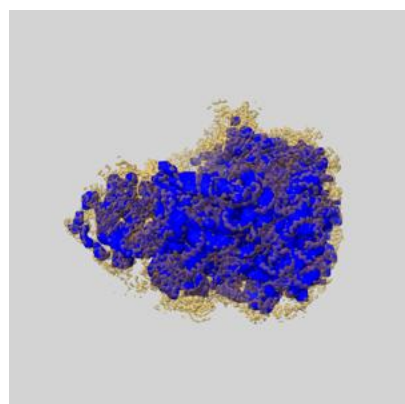
6.6 Mask visualisation [i](#)

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

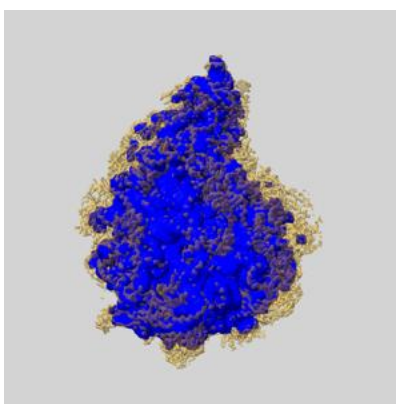
A mask typically either:

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

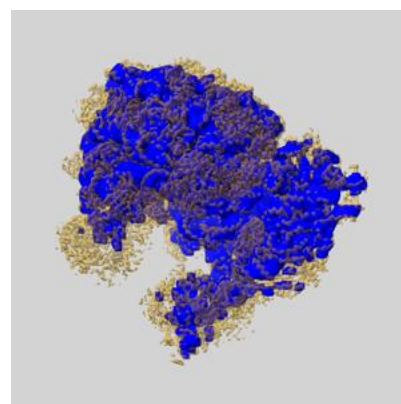
6.6.1 emd_14864_msk_1.map [i](#)



X



Y

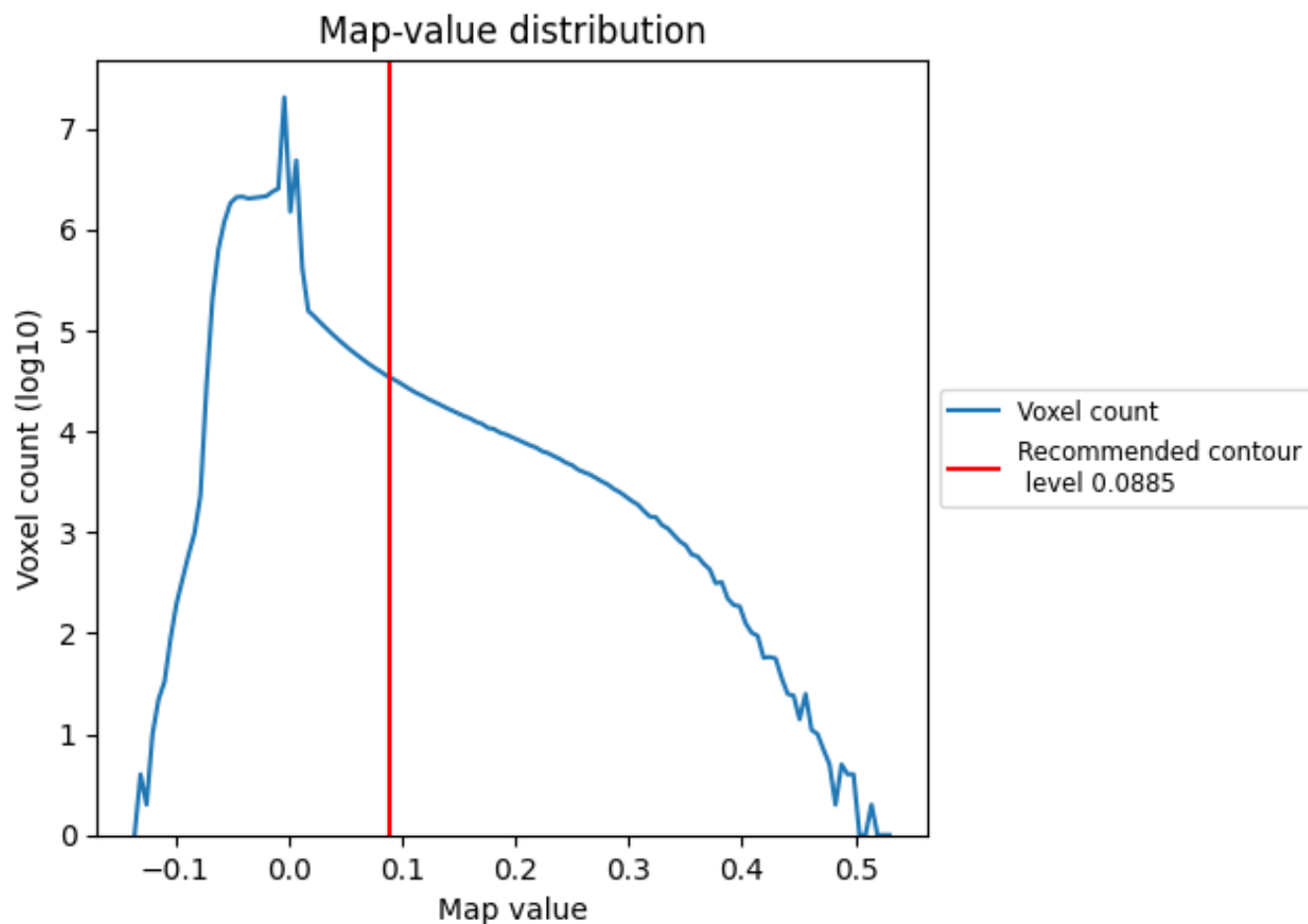


Z

7 Map analysis [i](#)

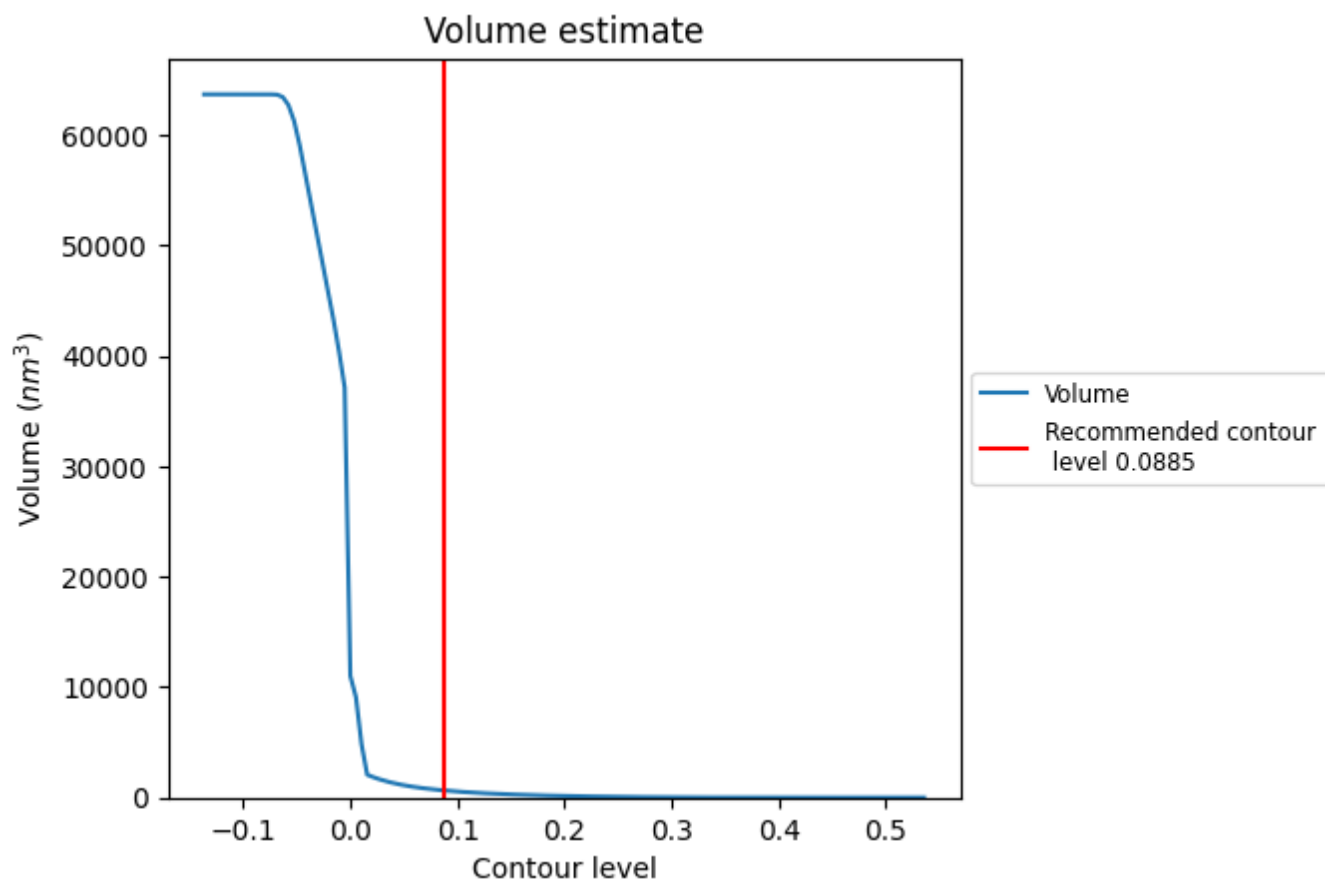
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

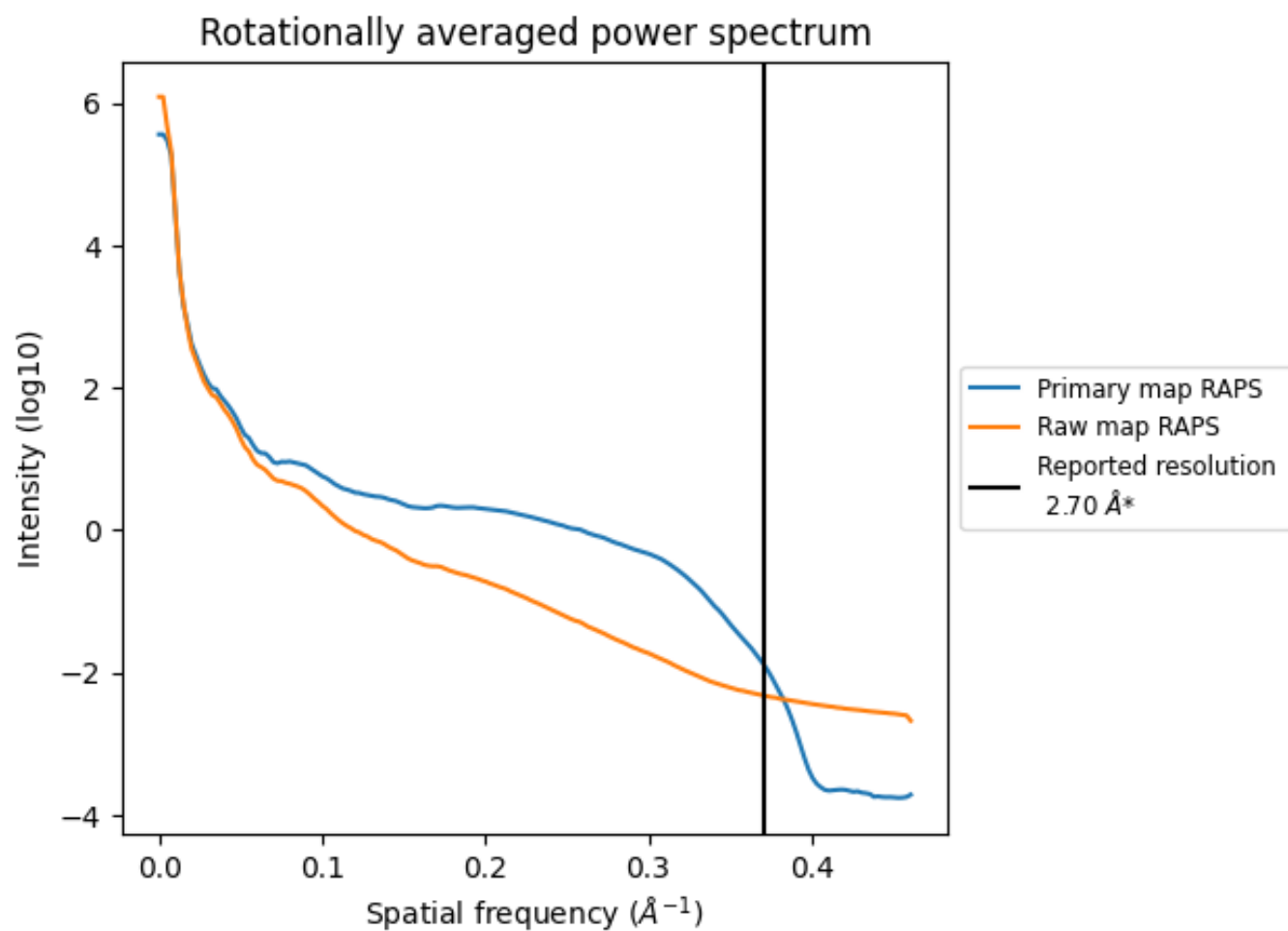
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 637 nm³; this corresponds to an approximate mass of 576 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

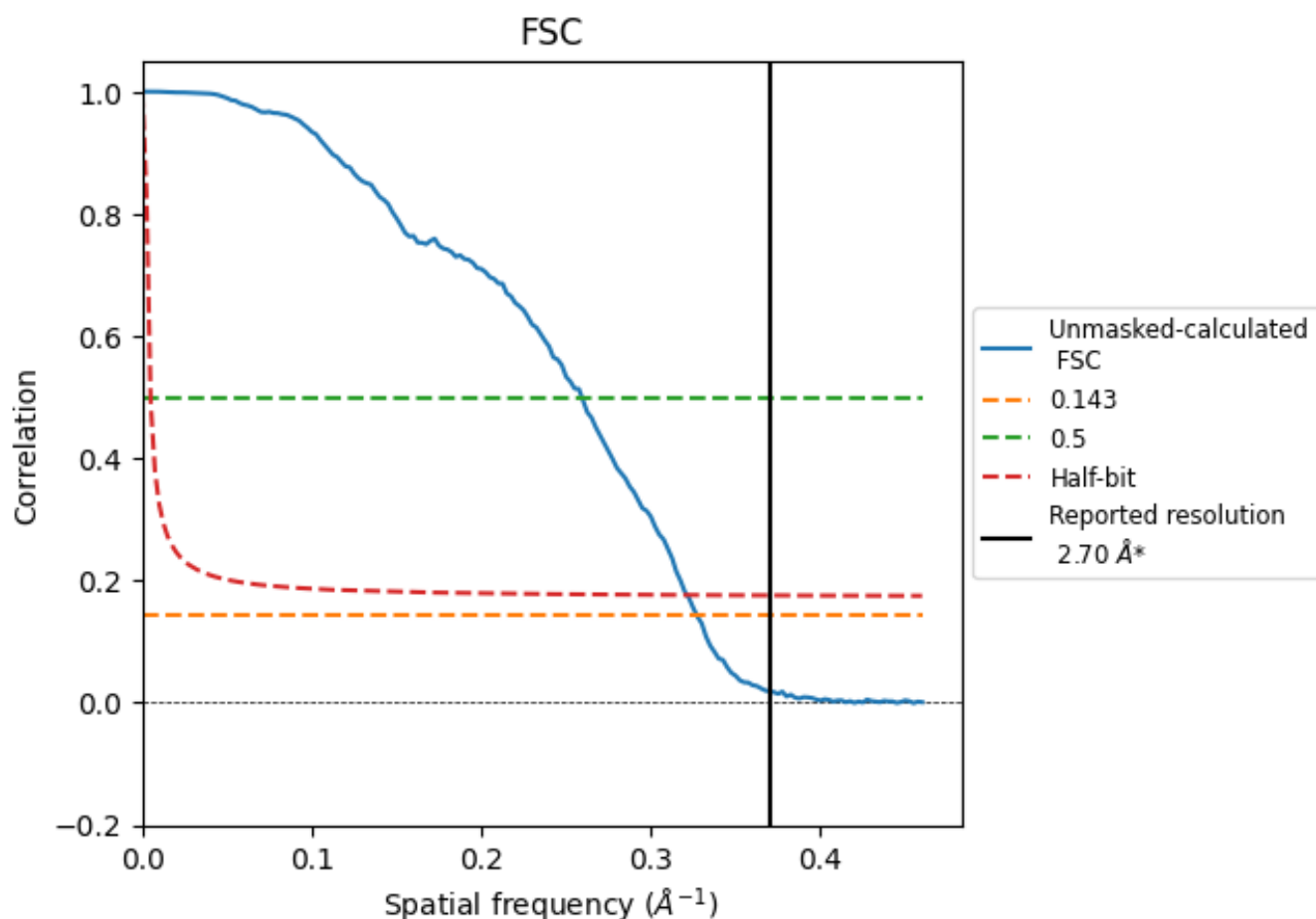


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

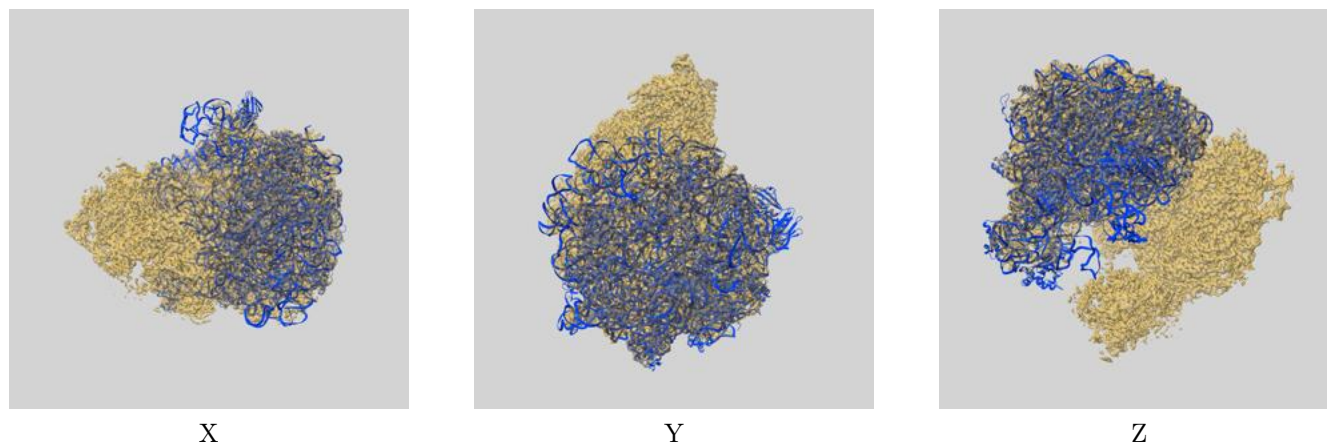
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.05	3.85	3.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.05 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

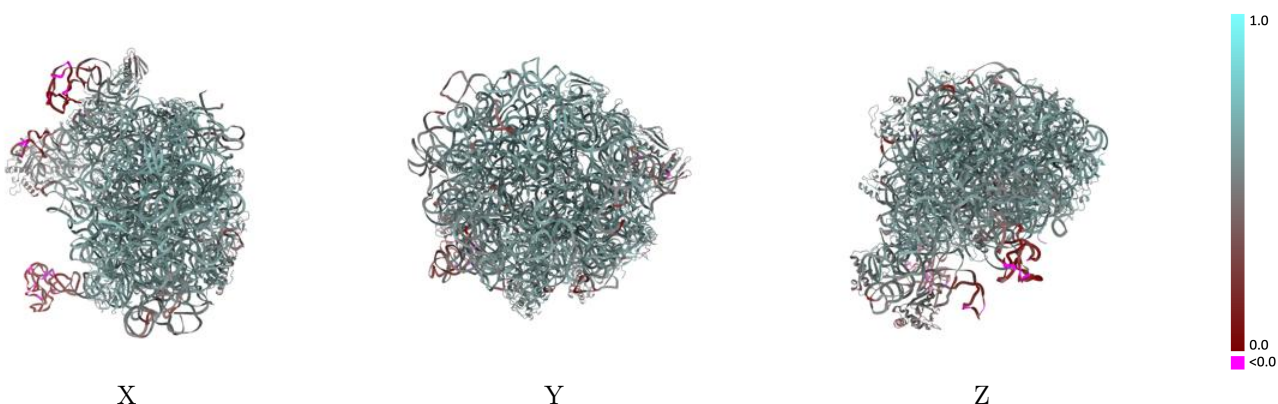
This section contains information regarding the fit between EMDB map EMD-14864 and PDB model 7ZQ5. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



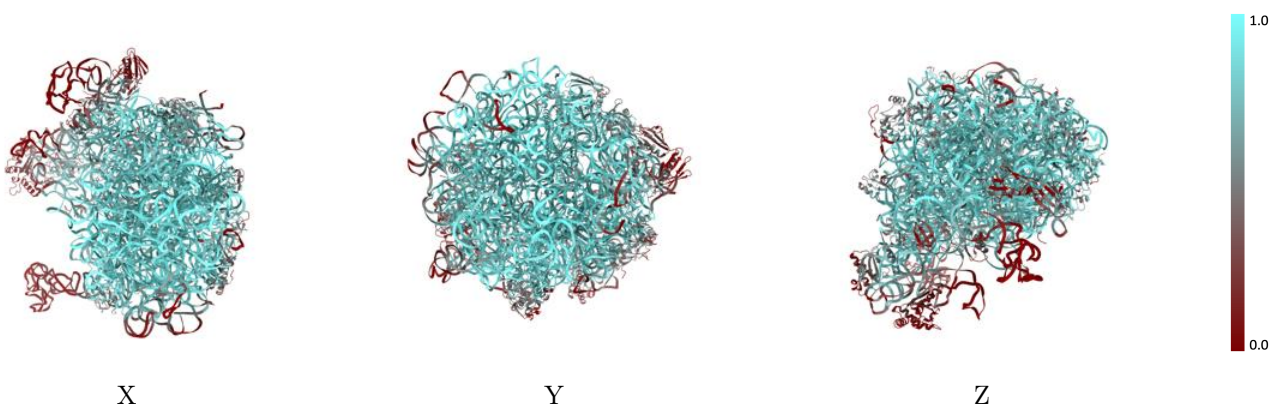
The images above show the 3D surface view of the map at the recommended contour level 0.0885 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



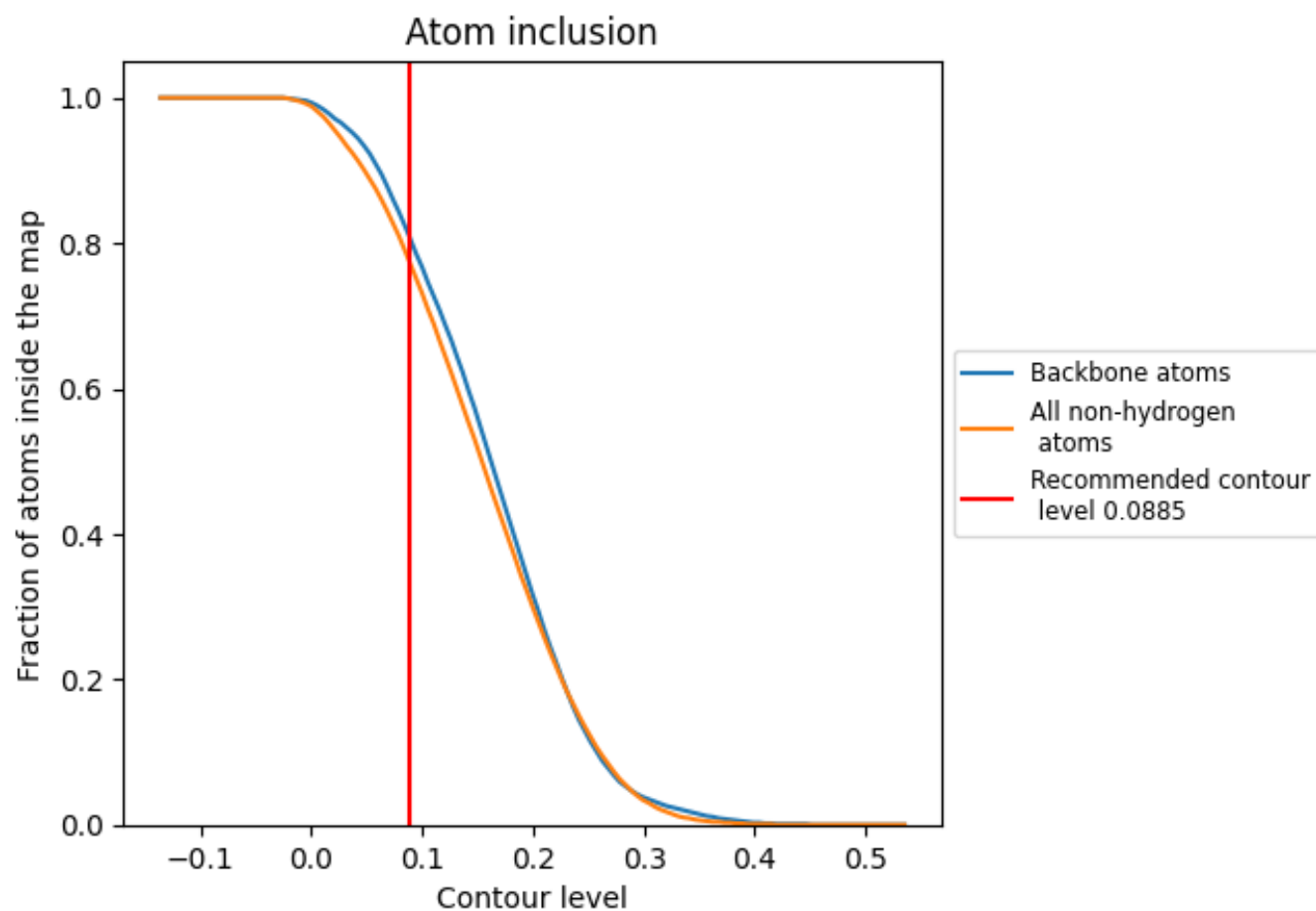
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0885).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0885) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7750	 0.5600
0	 0.8300	 0.6090
1	 0.5340	 0.5180
2	 0.7400	 0.5950
3	 0.7890	 0.6060
4	 0.3790	 0.5450
6	 0.9830	 0.6470
7	 0.9100	 0.6300
8	 0.6010	 0.5810
a	 0.6470	 0.5310
b	 0.8320	 0.5550
c	 0.8460	 0.6260
d	 0.7340	 0.6120
e	 0.6300	 0.5630
f	 0.0810	 0.4390
g	 0.2010	 0.5000
h	 0.2890	 0.4960
j	 0.7690	 0.6030
k	 0.7570	 0.6100
l	 0.7570	 0.5990
m	 0.5980	 0.5900
n	 0.8380	 0.6160
o	 0.3910	 0.5060
p	 0.7380	 0.6100
q	 0.8220	 0.6160
r	 0.6160	 0.5750
s	 0.8320	 0.6080
t	 0.6670	 0.5550
u	 0.4900	 0.5250
w	 0.3790	 0.5460
y	 0.7650	 0.6020

