



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2022 – 10:21 AM EDT

PDB ID : 5V7Q  
EMDB ID : EMD-8641  
Title : Cryo-EM structure of the large ribosomal subunit from Mycobacterium tuberculosis bound with a potent linezolid analog  
Authors : Yang, K.; Chang, J.-Y.; Cui, Z.; Zhang, J.  
Deposited on : 2017-03-20  
Resolution : 3.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

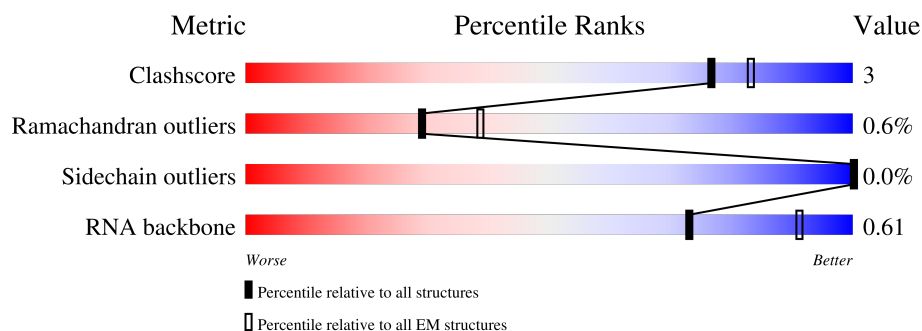
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	57	<div> <div>60%</div> <div>86% 7% 7%</div> </div>
2	1	55	<div> <div>56%</div> <div>82% 5% 13%</div> </div>
3	2	47	<div> <div>32%</div> <div>79% 11% 11%</div> </div>
4	3	64	<div> <div>59%</div> <div>86% 11% .</div> </div>
5	4	37	<div> <div>86%</div> <div>81% 19%</div> </div>
6	6	80	<div> <div>56%</div> <div>51% 5% 44%</div> </div>
7	A	3138	<div> <div>33%</div> <div>76% 20% . .</div> </div>

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Mol	Chain	Length	Quality of chain
8	B	115	
9	C	280	
10	D	217	
11	E	223	
12	F	187	
13	G	179	
14	H	152	
15	J	147	
16	K	122	
17	L	146	
18	M	138	
19	N	180	
20	O	122	
21	P	113	
22	Q	129	
23	R	104	
24	S	197	
25	T	100	
26	U	105	
27	V	215	
28	W	86	
29	X	64	
30	Y	77	
31	Z	65	

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 94306 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	53	Total	C	N	O	0	0
			421	262	93	66		

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			400	245	84	67	4		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	42	Total	C	N	O	S	0	0
			358	212	94	51	1		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	62	Total	C	N	O	0	0
			494	298	112	84		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			299	182	66	47	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	VAL	MET	conflict	UNP A0A1L6JSF4

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	45	Total	C	N	O	S	0	0
			345	214	60	66	5		

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	3118	Total	C	N	O	P	0	0
			66956	29845	12340	21653	3118		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	115	Total	C	N	O	P	0	0
			2458	1097	456	790	115		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	272	Total	C	N	O	S	0	0
			2088	1277	437	369	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	213	Total	C	N	O	S	0	0
			1590	985	307	292	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	207	Total	C	N	O	S	0	0
			1552	958	303	289	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	170	Total	C	N	O	S	0	0
			1335	834	254	242	5		

- Molecule 13 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	174	Total	C	N	O	S	0	0
			1330	836	249	244	1		

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	47	Total	C	N	O	S	0	0
			350	220	64	65	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	146	Total	C	N	O	S	0	0
			1143	724	217	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	121	Total	C	N	O	S	0	0
			934	585	179	168	2		

- Molecule 17 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	142	Total	C	N	O	S	0	0
			1060	656	215	187	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	VAL	MET	conflict	UNP A0A0T7M0A0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	134	Total	C	N	O	S	0	0
			1072	679	215	177	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	116	Total	C	N	O	S	0	0
			908	574	175	158	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	116	Total	C	N	O		0	0
			886	541	188	157			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	112	Total	C	N	O	S	0	0
			907	573	174	159	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	122	Total	C	N	O		0	0
			980	608	205	167			

- Molecule 23 is a protein called LSU ribosomal protein L21p.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	98	Total	C	N	O		0	0
			742	472	136	134			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	113	Total	C	N	O		0	0
			860	533	178	149			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	98	Total	C	N	O		0	0
			759	480	141	138			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	90	Total	C	N	O	S	0	0
			699	430	138	129	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	177	Total	C	N	O		0	0
			1319	822	243	254			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	74	Total	C	N	O		0	0
			546	336	111	99			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	63	Total	C	N	O	S	0	0
			476	289	101	81	5		

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

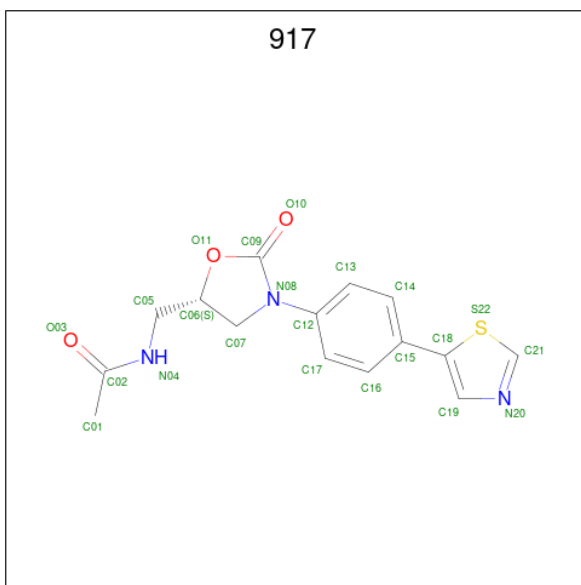
Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	65	Total	C	N	O	S	0	0
			541	331	106	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	59	Total	C	N	O		0	0
			476	293	101	82			

- Molecule 32 is N-((5S)-2-oxo-3-[4-(1,3-thiazol-5-yl)phenyl]-1,3-oxazolidin-5-yl)methyl)acetamide (three-letter code: 917) (formula: C<sub>15</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub>S).



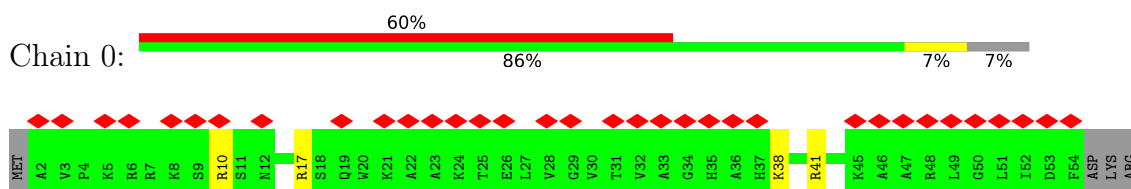


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
32	A	1	22	15	3	3	1	0

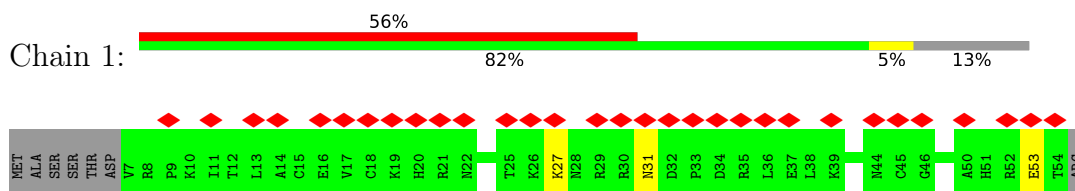
### 3 Residue-property plots [i](#)

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

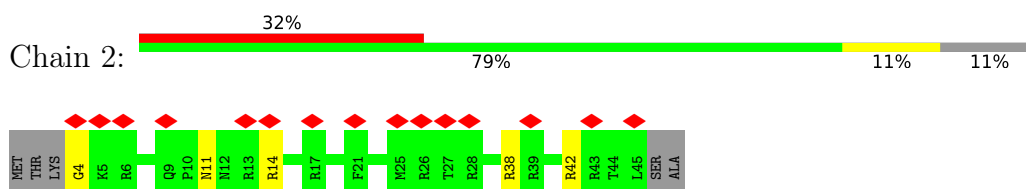
- Molecule 1: 50S ribosomal protein L32



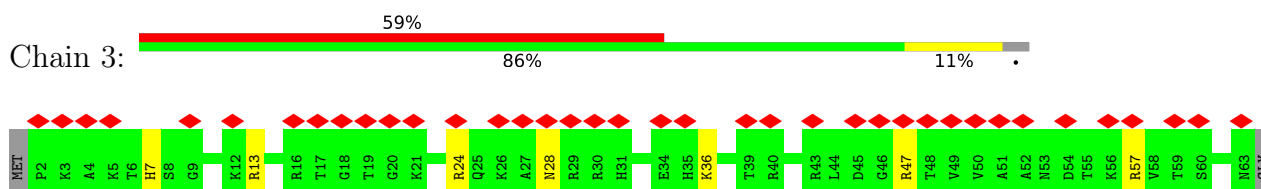
- Molecule 2: 50S ribosomal protein L33



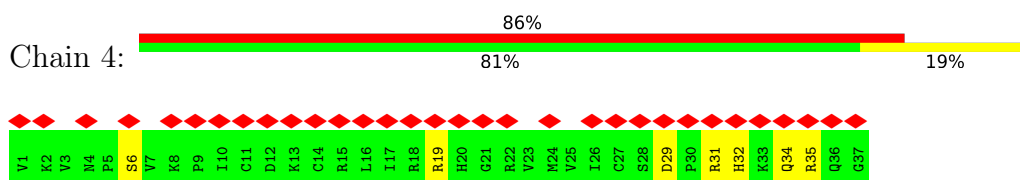
- Molecule 3: 50S ribosomal protein L34



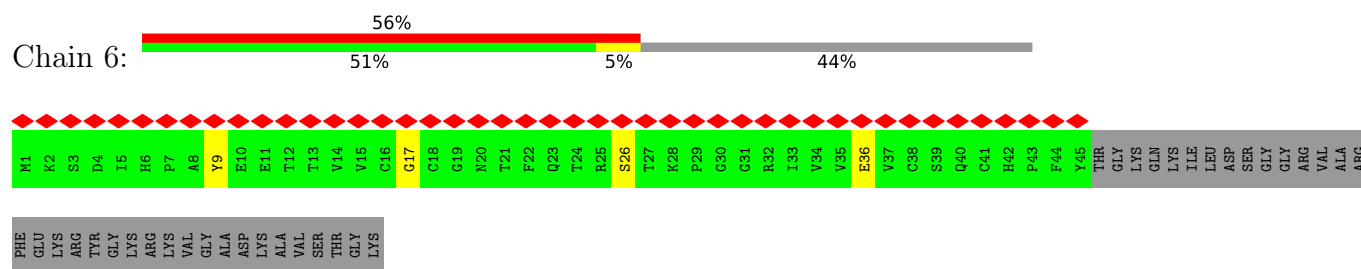
- Molecule 4: 50S ribosomal protein L35



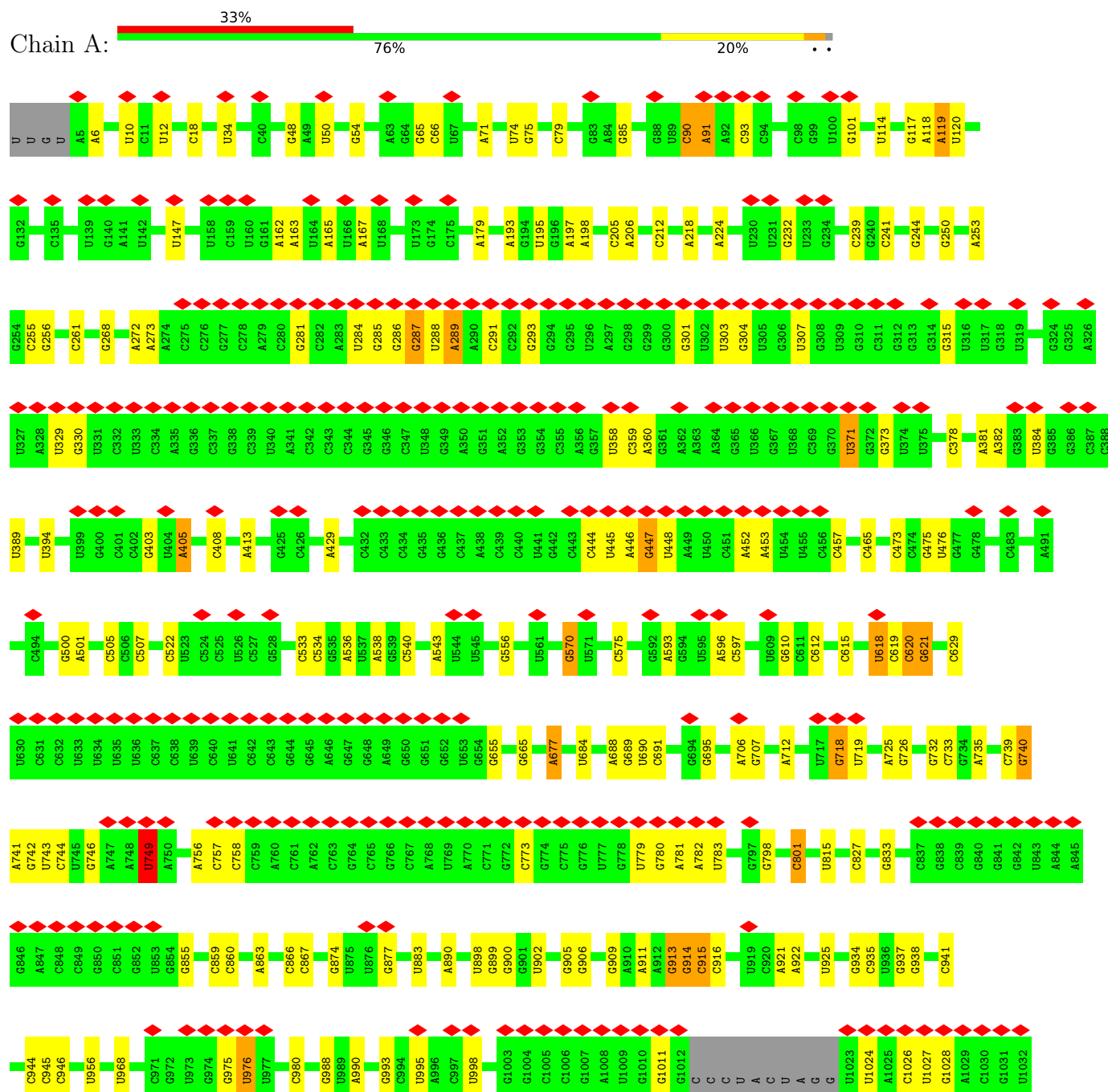
- Molecule 5: 50S ribosomal protein L36

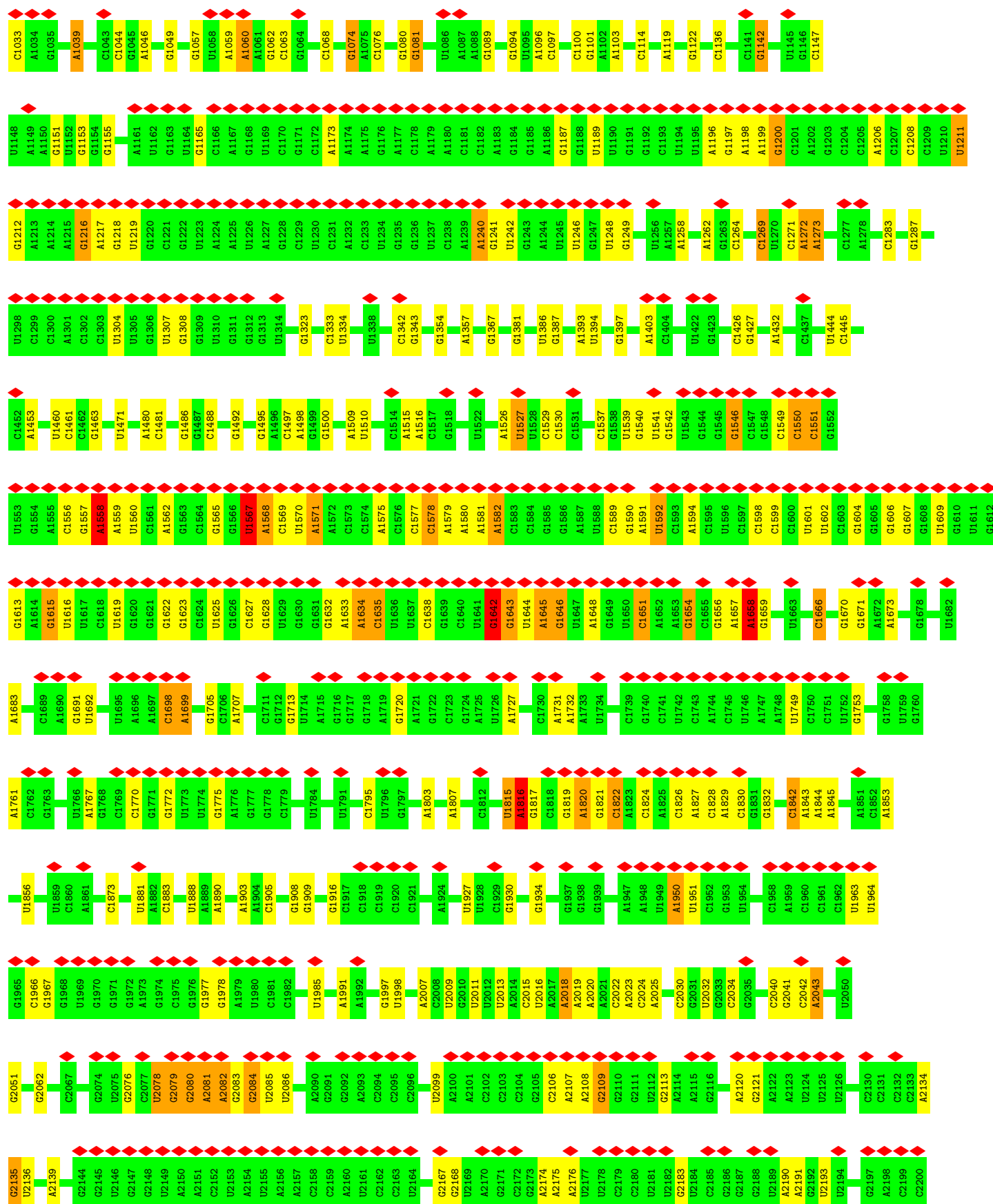


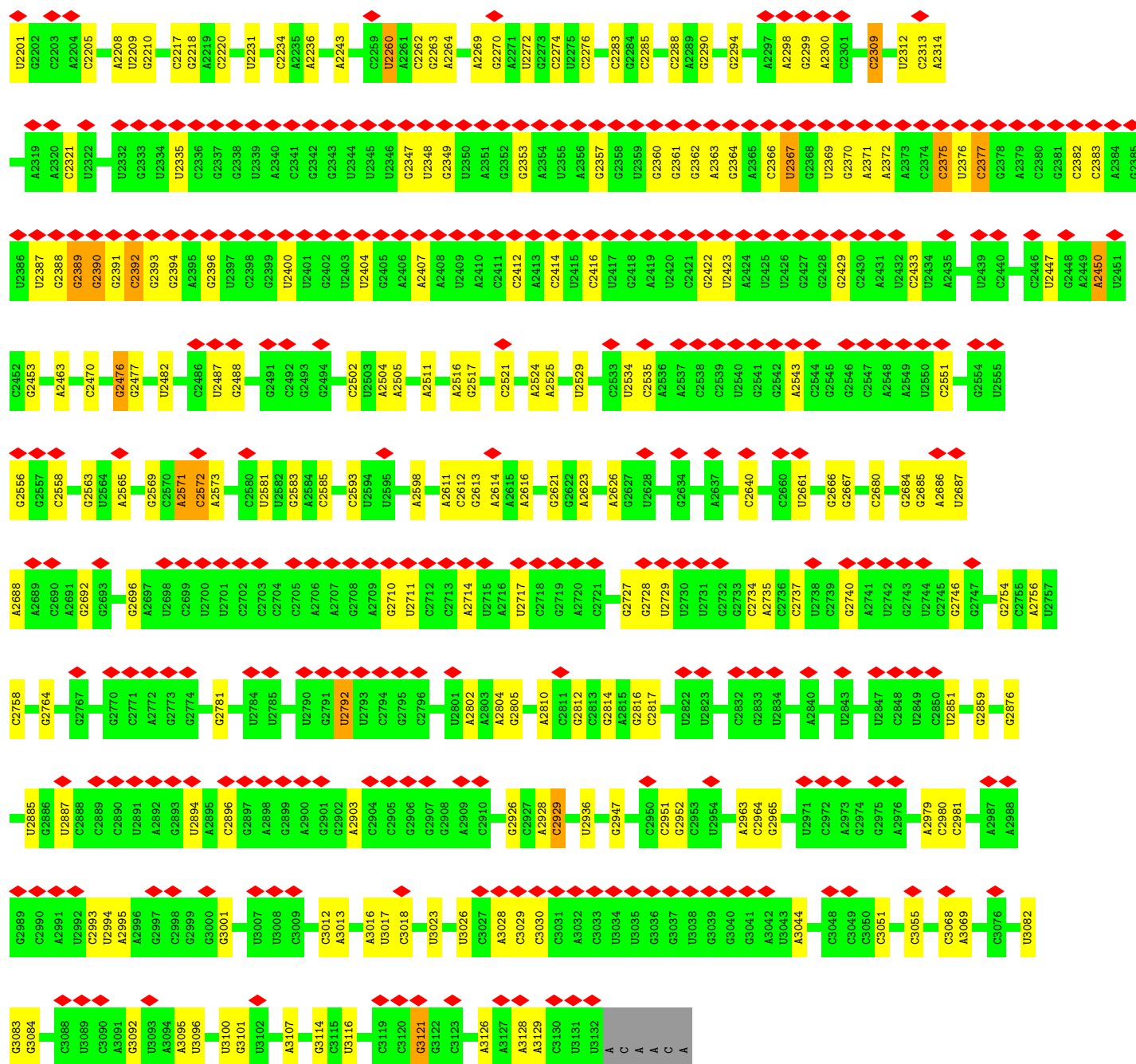
- Molecule 6: 50S ribosomal protein L31



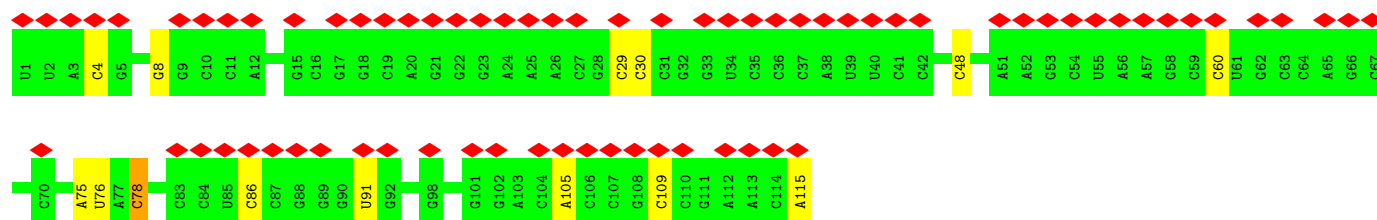
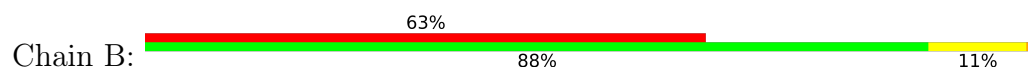
- Molecule 7: 23S rRNA







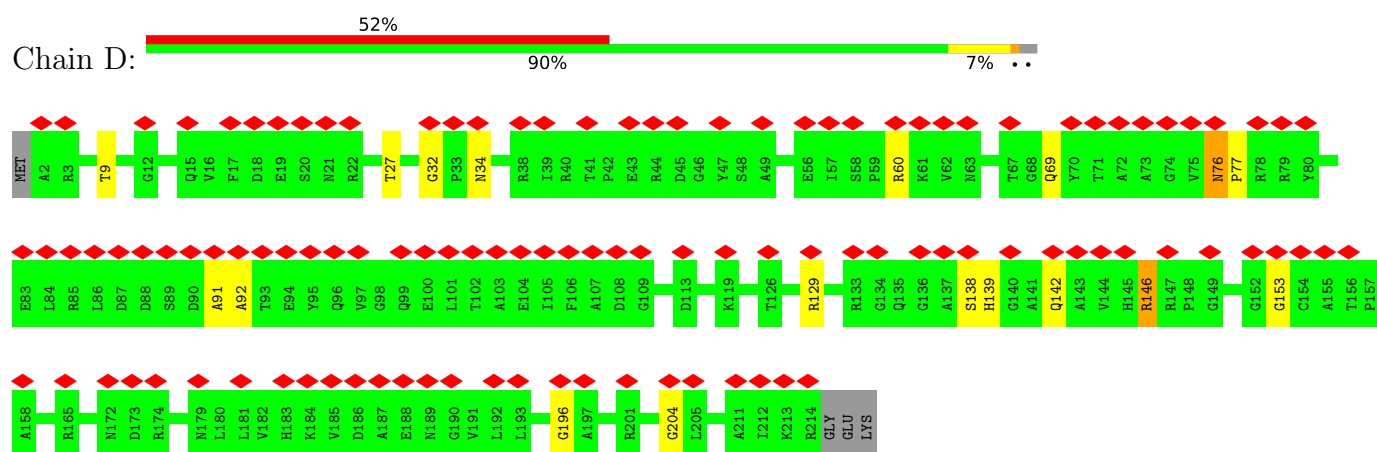
• Molecule 8: 5S ribosomal RNA



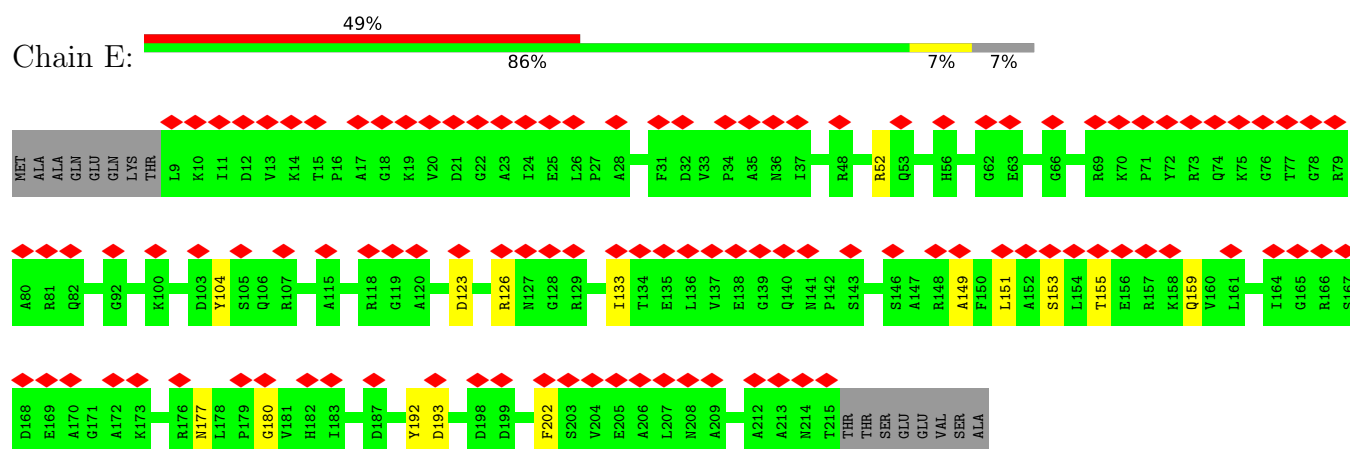
- Molecule 9: 50S ribosomal protein L2



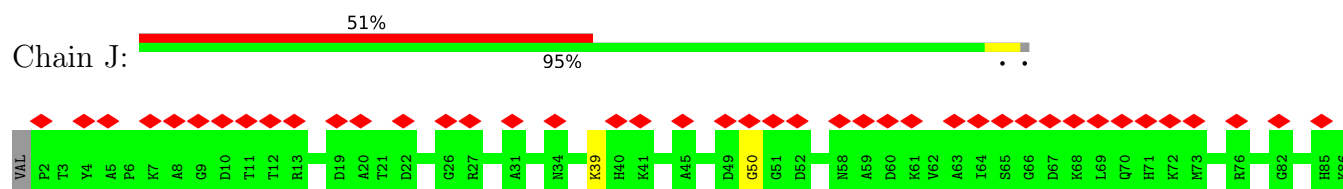
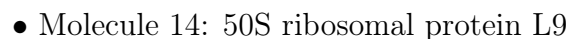
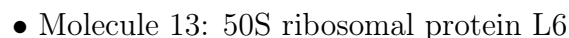
- Molecule 10: 50S ribosomal protein L3

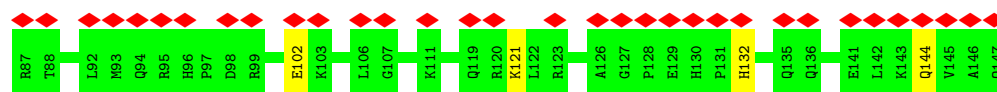


- Molecule 11: 50S ribosomal protein L4

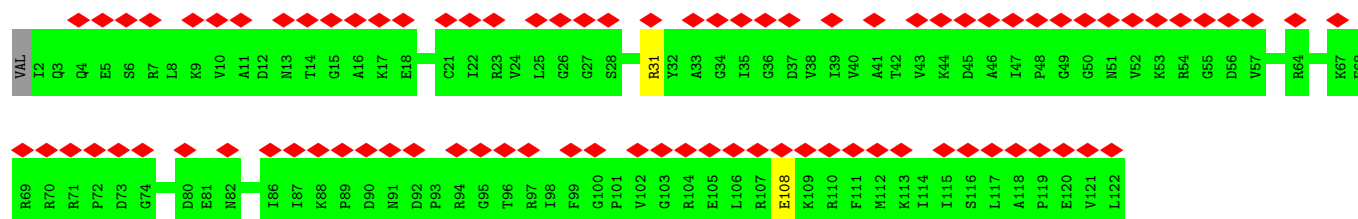


- Molecule 12: 50S ribosomal protein L5

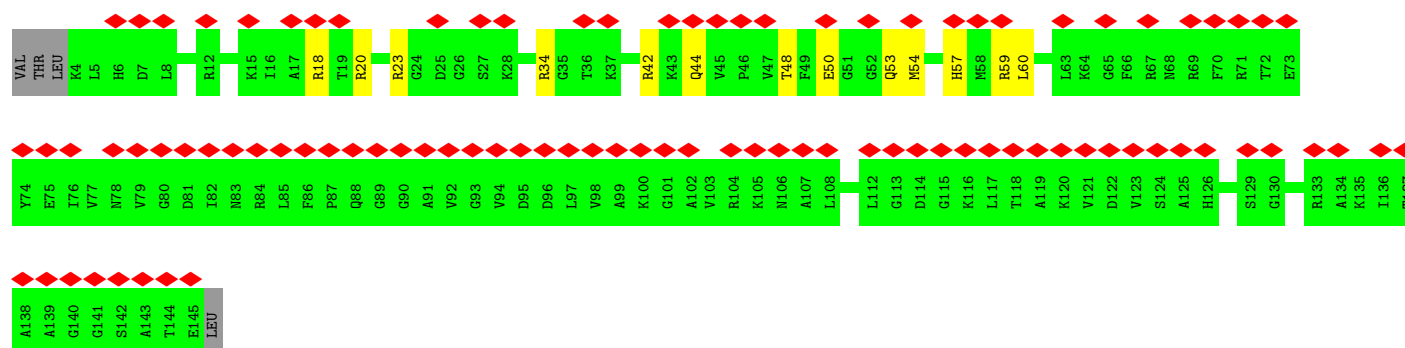
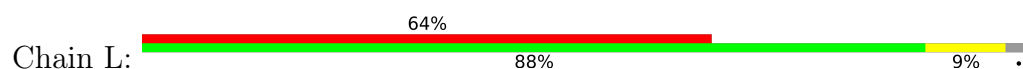




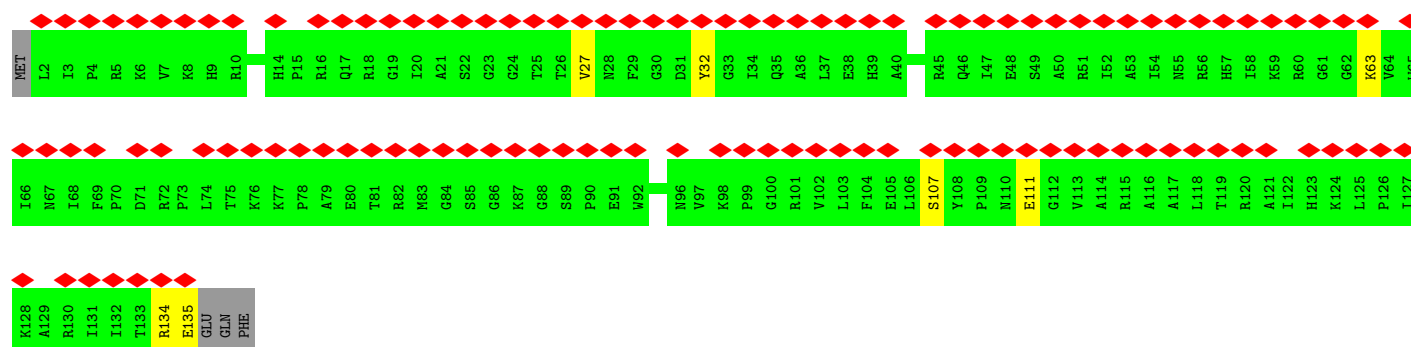
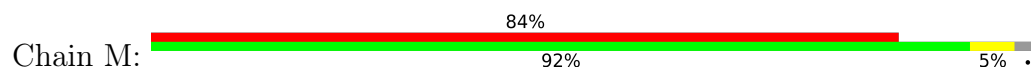
- Molecule 16: 50S ribosomal protein L14



- Molecule 17: 50S ribosomal protein L15



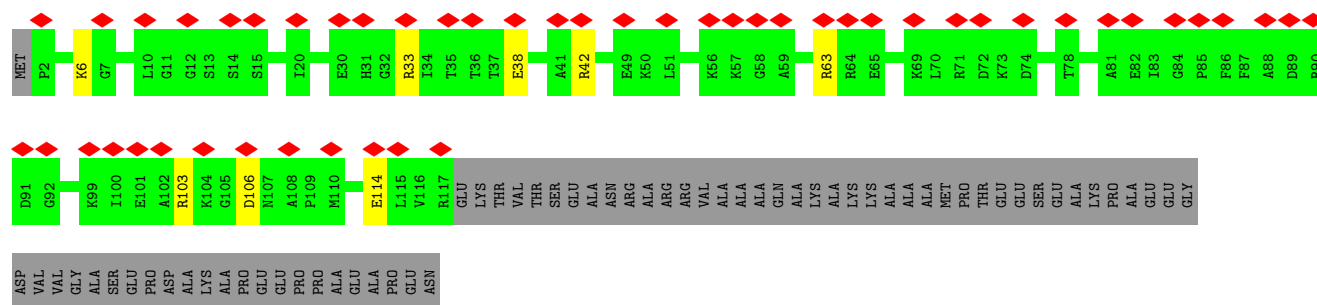
- Molecule 18: 50S ribosomal protein L16



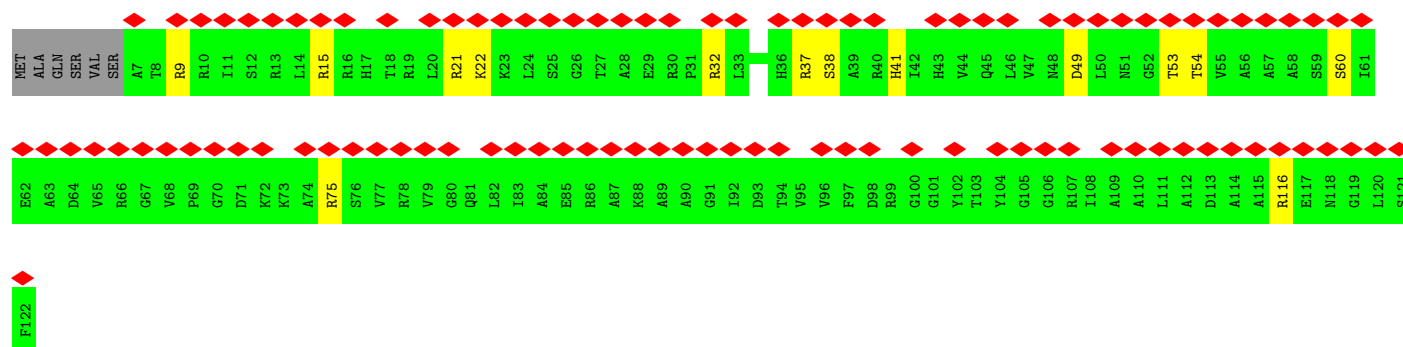
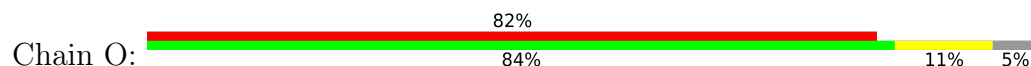
- Molecule 19: 50S ribosomal protein L17



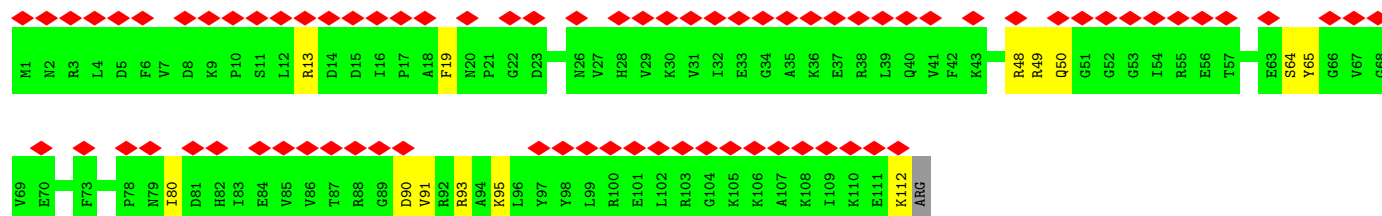
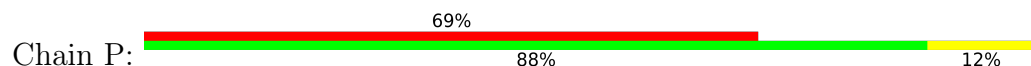




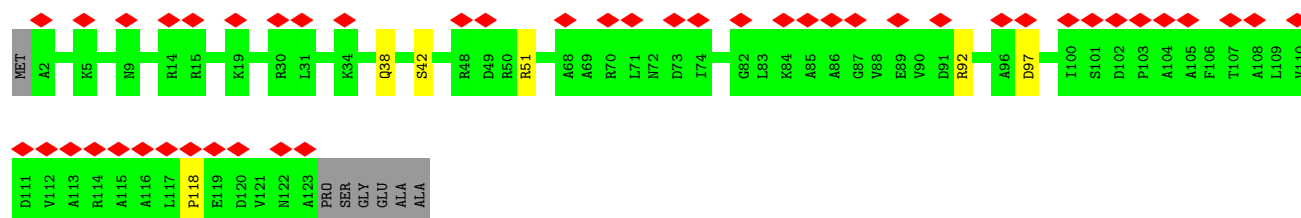
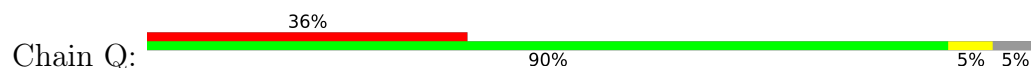
• Molecule 20: 50S ribosomal protein L18



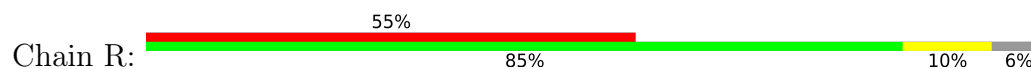
• Molecule 21: 50S ribosomal protein L19

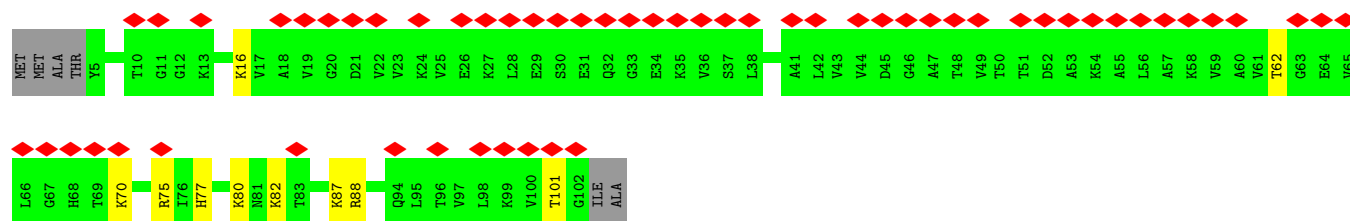


• Molecule 22: 50S ribosomal protein L20

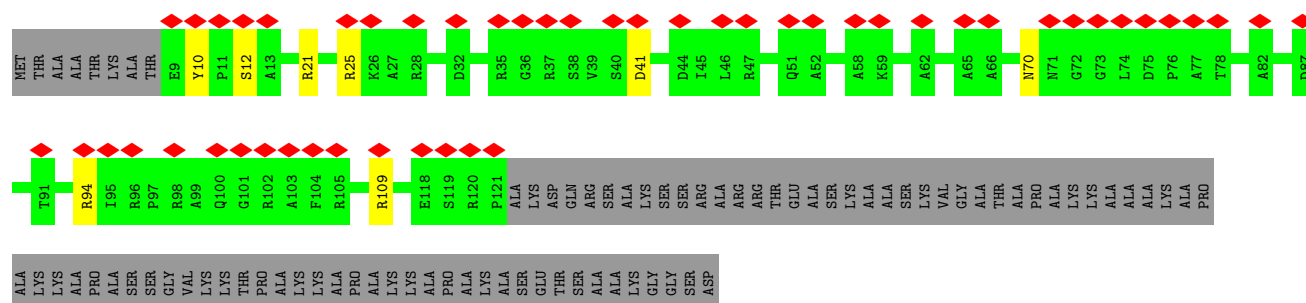


• Molecule 23: LSU ribosomal protein L21p

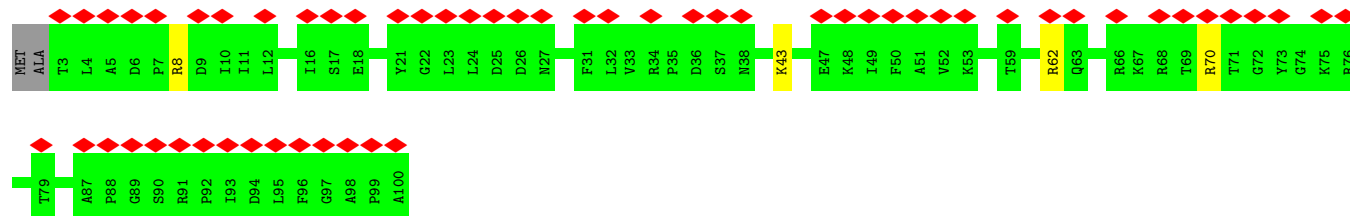




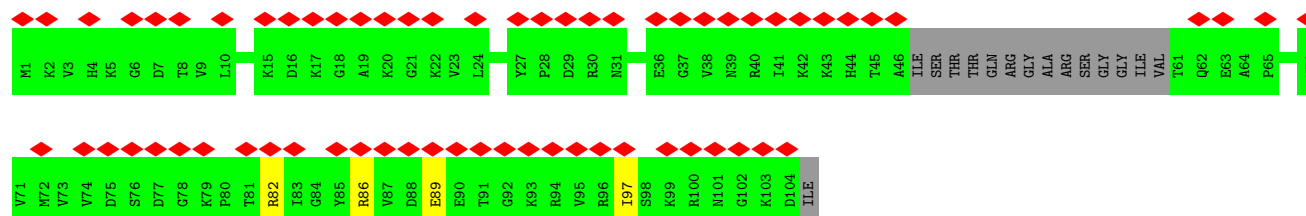
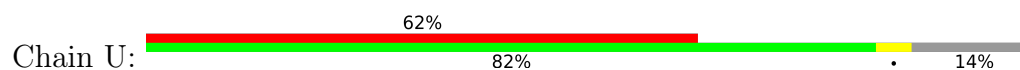
• Molecule 24: 50S ribosomal protein L22



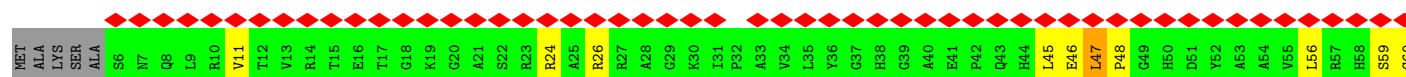
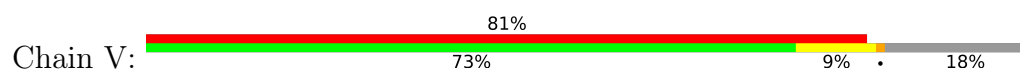
• Molecule 25: 50S ribosomal protein L23

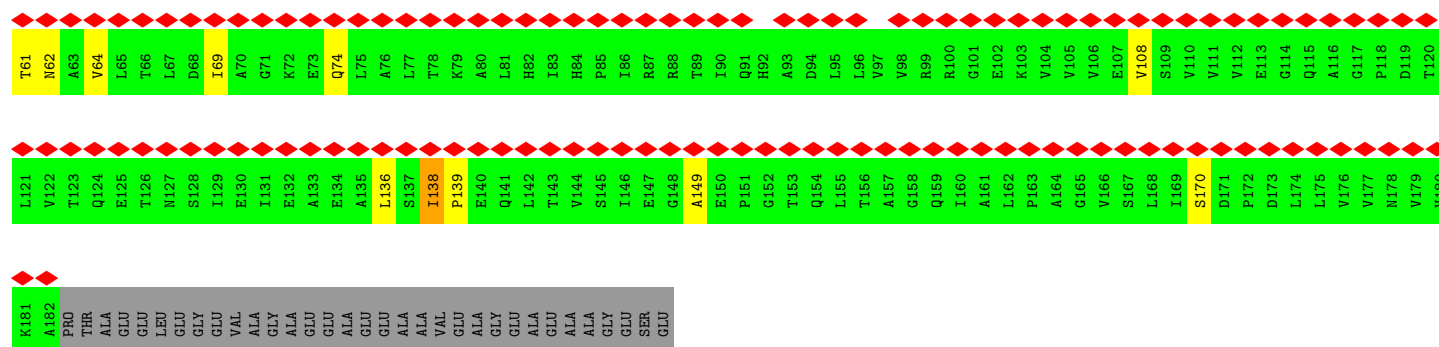


• Molecule 26: 50S ribosomal protein L24

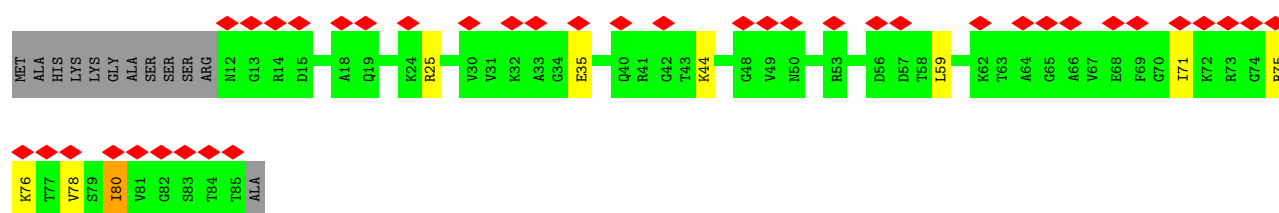
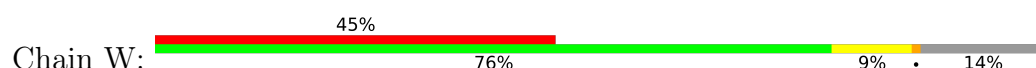


• Molecule 27: 50S ribosomal protein L25

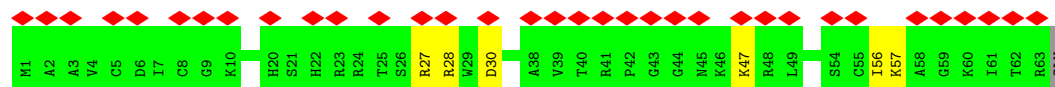
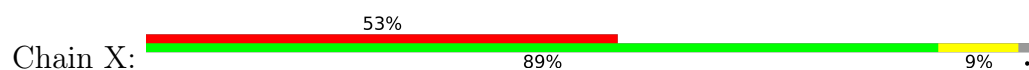




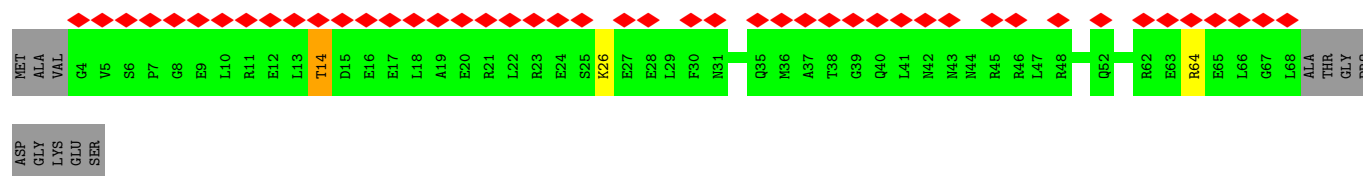
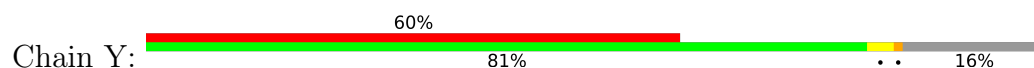
• Molecule 28: 50S ribosomal protein L27



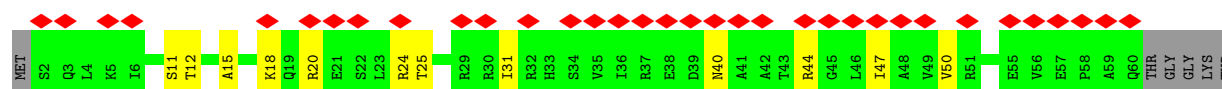
• Molecule 29: 50S ribosomal protein L28



• Molecule 30: 50S ribosomal protein L29



• Molecule 31: 50S ribosomal protein L30



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2.37	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.307	Depositor
Minimum map value	-0.145	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.06	Depositor
Map size ( $\text{\AA}$ )	298.47998, 298.47998, 298.47998	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.435, 1.435, 1.435	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:  
917

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	0.40	0/427	0.66	0/570
2	1	0.41	0/407	0.64	0/543
3	2	0.54	0/361	0.78	0/473
4	3	0.43	0/499	0.68	0/664
5	4	0.37	0/303	0.74	0/402
6	6	0.31	0/353	0.56	0/478
7	A	0.72	2/74973 (0.0%)	1.10	219/116979 (0.2%)
8	B	0.54	0/2749	1.02	7/4284 (0.2%)
9	C	0.42	0/2129	0.69	1/2861 (0.0%)
10	D	0.43	1/1613 (0.1%)	0.68	0/2174
11	E	0.41	0/1575	0.63	0/2129
12	F	0.31	0/1352	0.67	0/1817
13	G	0.31	0/1351	0.58	0/1824
14	H	0.32	0/353	0.58	0/474
15	J	0.43	0/1170	0.67	0/1584
16	K	0.40	0/944	0.67	0/1268
17	L	0.40	0/1073	0.67	0/1432
18	M	0.36	0/1098	0.62	0/1481
19	N	0.42	0/925	0.64	0/1242
20	O	0.35	0/895	0.69	0/1202
21	P	0.37	0/922	0.59	0/1236
22	Q	0.47	0/992	0.68	0/1329
23	R	0.42	0/751	0.61	0/1009
24	S	0.42	0/874	0.68	0/1186
25	T	0.37	0/770	0.67	0/1038
26	U	0.33	0/705	0.53	0/941
27	V	0.27	0/1336	0.57	0/1820
28	W	0.40	0/551	0.69	0/735
29	X	0.52	0/484	0.73	0/648
30	Y	0.37	0/544	0.65	0/727
31	Z	0.39	0/480	0.71	0/645
All	All	0.65	3/102959 (0.0%)	1.01	227/155195 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	146	ARG	C-N	5.43	1.46	1.34
7	A	1658	A	N9-C4	5.22	1.41	1.37
7	A	1816	A	N7-C5	-5.04	1.36	1.39

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	507	C	N3-C4-N4	9.97	124.98	118.00
7	A	507	C	C5-C4-N4	-9.80	113.34	120.20
7	A	866	C	N3-C4-N4	9.44	124.61	118.00
7	A	946	C	N3-C2-O2	-9.28	115.41	121.90
7	A	3012	C	N3-C4-N4	9.28	124.49	118.00
7	A	1026	C	C6-N1-C2	-9.14	116.64	120.30
7	A	1068	C	C5-C4-N4	-9.14	113.80	120.20
7	A	946	C	N1-C2-O2	9.02	124.31	118.90
7	A	3012	C	C5-C4-N4	-9.01	113.89	120.20
7	A	1026	C	C2-N1-C1'	8.99	128.69	118.80
7	A	2433	C	N3-C4-N4	8.86	124.20	118.00
7	A	1068	C	N3-C4-N4	8.84	124.19	118.00
7	A	866	C	C5-C4-N4	-8.52	114.23	120.20
7	A	890	A	N1-C6-N6	8.52	123.71	118.60
7	A	1567	U	N1-C2-O2	-8.27	117.01	122.80
7	A	1272	A	O4'-C1'-N9	8.10	114.68	108.20
7	A	739	C	C2-N1-C1'	7.91	127.50	118.80
7	A	2009	U	C5-C4-O4	-7.91	121.16	125.90
7	A	998	U	C5-C4-O4	-7.91	121.16	125.90
7	A	2433	C	C5-C4-N4	-7.79	114.74	120.20
7	A	1480	A	C8-N9-C4	-7.77	102.69	105.80
8	B	78	C	N3-C4-N4	7.74	123.42	118.00
7	A	2482	U	C5-C4-O4	-7.73	121.26	125.90
7	A	719	U	O4'-C1'-N1	7.66	114.33	108.20
7	A	1480	A	N7-C8-N9	7.65	117.63	113.80
7	A	2593	C	C5-C4-N4	-7.65	114.84	120.20
7	A	2482	U	N3-C4-O4	7.48	124.64	119.40
7	A	707	G	C5-C6-O6	-7.43	124.14	128.60
7	A	2593	C	N3-C4-N4	7.41	123.18	118.00
7	A	1658	A	C8-N9-C4	-7.34	102.86	105.80
8	B	78	C	C5-C4-N4	-7.34	115.06	120.20
7	A	534	C	N3-C2-O2	-7.33	116.77	121.90
7	A	12	U	C2-N1-C1'	7.29	126.45	117.70
7	A	1598	C	N1-C2-O2	7.29	123.27	118.90
7	A	2011	U	N3-C4-O4	7.29	124.50	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	890	A	C5-C6-N6	-7.29	117.87	123.70
7	A	3116	U	C5-C4-O4	-7.23	121.56	125.90
7	A	2288	C	C6-N1-C2	-7.21	117.41	120.30
7	A	1488	C	C5-C4-N4	-7.17	115.18	120.20
7	A	534	C	N1-C2-O2	7.06	123.14	118.90
7	A	570	G	O4'-C1'-N9	7.05	113.84	108.20
7	A	3116	U	N3-C4-O4	7.05	124.33	119.40
7	A	739	C	N3-C2-O2	-7.03	116.98	121.90
7	A	2011	U	C5-C4-O4	-6.92	121.75	125.90
7	A	2276	C	C5-C4-N4	-6.88	115.39	120.20
7	A	3083	G	O4'-C1'-N9	6.86	113.69	108.20
7	A	2309	C	N3-C2-O2	-6.81	117.13	121.90
7	A	998	U	N3-C4-O4	6.81	124.16	119.40
8	B	86	C	N1-C2-O2	6.77	122.97	118.90
7	A	1269	C	N3-C4-N4	6.72	122.70	118.00
7	A	945	C	C5-C4-N4	-6.65	115.55	120.20
7	A	147	U	N3-C4-O4	6.63	124.04	119.40
7	A	147	U	C5-C4-O4	-6.62	121.93	125.90
7	A	707	G	N1-C6-O6	6.56	123.83	119.90
7	A	2309	C	C2-N1-C1'	6.55	126.01	118.80
7	A	1643	G	N3-C4-N9	-6.53	122.08	126.00
7	A	1598	C	N3-C2-O2	-6.45	117.39	121.90
7	A	739	C	N1-C2-O2	6.40	122.74	118.90
7	A	1488	C	N3-C4-N4	6.39	122.47	118.00
7	A	473	C	C6-N1-C2	-6.38	117.75	120.30
7	A	1966	C	N3-C2-O2	-6.37	117.44	121.90
7	A	902	U	C5-C4-O4	-6.37	122.08	125.90
7	A	2887	U	C5-C4-O4	-6.36	122.09	125.90
7	A	1642	G	C4-C5-N7	6.33	113.33	110.80
7	A	610	G	N9-C4-C5	-6.30	102.88	105.40
7	A	291	C	C5-C4-N4	-6.27	115.81	120.20
7	A	1575	A	N1-C6-N6	6.26	122.35	118.60
7	A	1658	A	N3-C4-C5	-6.23	122.44	126.80
7	A	408	C	C5-C4-N4	-6.21	115.85	120.20
7	A	291	C	N3-C4-N4	6.21	122.35	118.00
7	A	935	C	N3-C4-N4	6.20	122.34	118.00
7	A	1556	C	N3-C4-C5	6.15	124.36	121.90
7	A	1824	C	N3-C4-N4	-6.14	113.70	118.00
7	A	378	C	N3-C4-N4	6.13	122.29	118.00
7	A	935	C	C5-C4-N4	-6.13	115.91	120.20
7	A	945	C	N3-C4-N4	6.11	122.28	118.00
7	A	1114	C	C6-N1-C2	-6.11	117.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1642	G	N9-C4-C5	-6.10	102.96	105.40
7	A	255	C	N3-C4-N4	6.09	122.26	118.00
7	A	2321	C	C5-C4-N4	-6.05	115.97	120.20
7	A	408	C	N3-C4-N4	6.04	122.22	118.00
7	A	2285	C	N3-C4-N4	6.02	122.22	118.00
7	A	12	U	N3-C2-O2	-6.02	117.98	122.20
7	A	1567	U	N3-C2-O2	6.02	126.42	122.20
7	A	1269	C	C5-C4-N4	-6.01	115.99	120.20
7	A	946	C	C6-N1-C2	-6.00	117.90	120.30
7	A	2387	U	C5-C6-N1	5.99	125.70	122.70
7	A	2680	C	N3-C4-N4	5.99	122.19	118.00
7	A	1575	A	C5-C6-N6	-5.98	118.91	123.70
7	A	378	C	C5-C4-N4	-5.97	116.02	120.20
7	A	1575	A	C4-C5-N7	5.97	113.69	110.70
7	A	2009	U	N3-C4-O4	5.96	123.58	119.40
7	A	212	C	C5-C4-N4	-5.96	116.03	120.20
7	A	2309	C	N1-C2-O2	5.95	122.47	118.90
7	A	1820	A	N1-C6-N6	-5.94	115.03	118.60
7	A	1816	A	C5-N7-C8	-5.93	100.94	103.90
7	A	444	C	C5-C6-N1	5.91	123.95	121.00
7	A	444	C	C6-N1-C2	-5.91	117.94	120.30
7	A	1816	A	N7-C8-N9	5.91	116.75	113.80
7	A	2263	G	C5-C6-O6	-5.86	125.08	128.60
7	A	612	C	C5-C4-N4	-5.85	116.11	120.20
7	A	1575	A	N9-C4-C5	-5.83	103.47	105.80
7	A	2283	C	C5-C4-N4	-5.83	116.12	120.20
7	A	522	C	N1-C2-O2	5.82	122.39	118.90
8	B	86	C	N3-C2-O2	-5.82	117.83	121.90
7	A	739	C	C6-N1-C2	-5.80	117.98	120.30
7	A	1246	U	C5-C4-O4	-5.80	122.42	125.90
7	A	1658	A	C5-C6-N1	5.80	120.60	117.70
7	A	534	C	C6-N1-C2	-5.79	117.98	120.30
7	A	90	C	N3-C2-O2	-5.79	117.85	121.90
7	A	2680	C	C5-C4-N4	-5.79	116.15	120.20
7	A	610	G	C6-C5-N7	-5.78	126.93	130.40
7	A	2285	C	C5-C4-N4	-5.75	116.17	120.20
7	A	2262	C	C5-C4-N4	-5.69	116.21	120.20
7	A	1749	U	C5-C6-N1	5.69	125.54	122.70
7	A	980	C	C5-C4-N4	-5.66	116.24	120.20
7	A	2727	G	N1-C6-O6	5.65	123.29	119.90
7	A	1076	C	C6-N1-C2	-5.64	118.04	120.30
8	B	86	C	C2-N1-C1'	5.64	125.00	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	197	A	N1-C6-N6	5.64	121.98	118.60
7	A	91	A	O4'-C1'-N9	5.63	112.71	108.20
7	A	1824	C	C5-C4-N4	5.61	124.13	120.20
7	A	2135	G	C6-C5-N7	-5.61	127.03	130.40
7	A	2816	G	N1-C6-O6	-5.61	116.53	119.90
7	A	66	C	C5-C4-N4	-5.59	116.29	120.20
7	A	2734	C	C5-C4-N4	-5.58	116.29	120.20
7	A	212	C	N3-C4-N4	5.58	121.90	118.00
7	A	1643	G	N3-C4-C5	5.57	131.38	128.60
7	A	2264	A	C4-C5-N7	5.57	113.48	110.70
7	A	3051	C	N3-C2-O2	-5.57	118.00	121.90
7	A	744	C	N1-C2-O2	5.56	122.24	118.90
7	A	684	U	N3-C4-O4	5.56	123.29	119.40
7	A	946	C	C2-N1-C1'	5.55	124.91	118.80
7	A	2412	C	C6-N1-C2	-5.55	118.08	120.30
7	A	1666	C	C6-N1-C2	-5.54	118.08	120.30
7	A	2288	C	C2-N1-C1'	5.54	124.89	118.80
7	A	1550	C	C5-C4-N4	-5.54	116.32	120.20
7	A	2264	A	N9-C4-C5	-5.53	103.59	105.80
7	A	1529	C	C5-C4-N4	-5.51	116.34	120.20
7	A	1063	C	C5-C4-N4	-5.51	116.34	120.20
7	A	976	U	N3-C2-O2	-5.50	118.35	122.20
7	A	740	G	O4'-C1'-N9	5.50	112.60	108.20
7	A	473	C	C2-N1-C1'	5.49	124.84	118.80
7	A	2321	C	N3-C4-N4	5.49	121.84	118.00
7	A	2754	G	N7-C8-N9	5.48	115.84	113.10
7	A	2390	G	C5-C6-O6	-5.48	125.31	128.60
7	A	1594	A	N9-C4-C5	-5.48	103.61	105.80
7	A	2288	C	N1-C2-O2	5.48	122.19	118.90
7	A	2040	C	C5-C4-N4	-5.48	116.37	120.20
7	A	890	A	C5-N7-C8	-5.45	101.18	103.90
7	A	1530	C	C5-C4-N4	-5.44	116.39	120.20
7	A	757	C	C6-N1-C2	-5.43	118.13	120.30
7	A	1654	G	C2-N3-C4	-5.42	109.19	111.90
7	A	371	U	C2-N1-C1'	5.41	124.19	117.70
7	A	2262	C	N3-C4-N4	5.40	121.78	118.00
7	A	1153	G	C5-C6-O6	5.40	131.84	128.60
7	A	1546	G	N3-C4-C5	5.40	131.30	128.60
7	A	801	C	C5-C4-N4	-5.39	116.43	120.20
7	A	1558	A	N1-C6-N6	5.38	121.83	118.60
7	A	2887	U	N3-C4-O4	5.38	123.17	119.40
7	A	1643	G	C2-N3-C4	-5.38	109.21	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1658	A	C6-N1-C2	-5.38	115.37	118.60
7	A	465	C	C5-C4-N4	-5.37	116.44	120.20
7	A	1658	A	C4-N9-C1'	5.37	135.96	126.30
7	A	1114	C	C2-N1-C1'	5.36	124.70	118.80
7	A	1822	C	C5-C4-N4	-5.35	116.45	120.20
7	A	1656	G	C2-N3-C4	-5.33	109.23	111.90
7	A	287	G	N3-C4-C5	-5.33	125.94	128.60
7	A	610	G	N3-C4-N9	5.32	129.19	126.00
7	A	2711	U	N3-C2-O2	-5.31	118.48	122.20
7	A	1500	G	N3-C4-N9	5.30	129.18	126.00
7	A	916	C	N1-C2-O2	5.29	122.08	118.90
7	A	916	C	N3-C2-O2	-5.29	118.19	121.90
7	A	1333	C	N3-C4-N4	5.29	121.70	118.00
7	A	2929	C	N1-C2-O2	5.28	122.07	118.90
7	A	1445	C	C6-N1-C2	-5.28	118.19	120.30
7	A	444	C	C2-N1-C1'	5.27	124.60	118.80
7	A	2276	C	N3-C4-N4	5.26	121.68	118.00
7	A	2217	C	N3-C2-O2	-5.25	118.22	121.90
7	A	522	C	N3-C2-O2	-5.25	118.22	121.90
7	A	2030	C	N1-C2-O2	5.24	122.05	118.90
7	A	1770	C	C6-N1-C2	-5.24	118.20	120.30
7	A	739	C	C6-N1-C1'	-5.24	114.52	120.80
7	A	993	G	C6-C5-N7	-5.23	127.26	130.40
7	A	1651	C	C6-N1-C2	-5.22	118.21	120.30
7	A	1550	C	N3-C4-N4	5.22	121.66	118.00
7	A	1616	U	C5-C4-O4	-5.22	122.77	125.90
7	A	287	G	C4-N9-C1'	5.22	133.28	126.50
7	A	2217	C	C6-N1-C2	-5.20	118.22	120.30
7	A	197	A	C5-C6-N6	-5.20	119.54	123.70
7	A	2283	C	N3-C4-N4	5.20	121.64	118.00
7	A	757	C	N1-C2-O2	5.19	122.01	118.90
7	A	898	U	N3-C2-O2	-5.18	118.57	122.20
7	A	12	U	C6-N1-C2	-5.18	117.89	121.00
7	A	1480	A	C4-N9-C1'	5.18	135.62	126.30
7	A	114	U	C2-N1-C1'	5.18	123.91	117.70
7	A	2727	G	C5-C6-O6	-5.17	125.50	128.60
7	A	757	C	N3-C2-O2	-5.17	118.28	121.90
7	A	1830	C	N3-C2-O2	-5.15	118.30	121.90
7	A	902	U	N3-C4-O4	5.14	123.00	119.40
7	A	1026	C	C6-N1-C1'	-5.13	114.64	120.80
7	A	2375	C	N3-C4-N4	-5.13	114.41	118.00
7	A	1819	G	N3-C4-C5	5.13	131.16	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1153	G	N1-C6-O6	-5.12	116.83	119.90
7	A	505	C	C5-C4-N4	-5.12	116.62	120.20
7	A	1445	C	C2-N1-C1'	5.12	124.43	118.80
7	A	1287	G	C6-C5-N7	-5.11	127.34	130.40
7	A	1426	C	C6-N1-C2	-5.11	118.26	120.30
7	A	2018	A	N1-C6-N6	5.10	121.66	118.60
8	B	30	C	C2-N1-C1'	5.09	124.40	118.80
7	A	255	C	C5-C4-N4	-5.09	116.64	120.20
7	A	890	A	C4-C5-N7	5.09	113.25	110.70
7	A	1615	G	N3-C2-N2	5.08	123.46	119.90
9	C	69	ARG	NE-CZ-NH2	-5.08	117.76	120.30
7	A	1100	C	N1-C2-O2	5.07	121.94	118.90
7	A	2309	C	C6-N1-C2	-5.07	118.27	120.30
7	A	749	U	N3-C2-O2	-5.07	118.66	122.20
7	A	2288	C	N3-C2-O2	-5.05	118.36	121.90
7	A	1645	A	C8-N9-C4	5.04	107.82	105.80
7	A	610	G	C4-C5-N7	5.04	112.81	110.80
7	A	860	C	N3-C4-N4	5.03	121.52	118.00
7	A	1824	C	N3-C2-O2	-5.02	118.39	121.90
8	B	30	C	C6-N1-C2	-5.02	118.29	120.30
7	A	1500	G	C6-C5-N7	-5.01	127.39	130.40
7	A	1026	C	C5-C6-N1	5.01	123.51	121.00
7	A	1578	C	N1-C2-O2	5.01	121.91	118.90
7	A	1461	C	C5-C4-N4	-5.00	116.70	120.20

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	421	0	461	4	0
2	1	400	0	413	3	0
3	2	358	0	390	5	0
4	3	494	0	533	7	0
5	4	299	0	326	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	6	345	0	332	2	0
7	A	66956	0	33720	280	0
8	B	2458	0	1253	10	0
9	C	2088	0	2123	21	0
10	D	1590	0	1633	12	0
11	E	1552	0	1593	12	0
12	F	1335	0	1372	7	0
13	G	1330	0	1390	16	0
14	H	350	0	367	2	0
15	J	1143	0	1173	5	0
16	K	934	0	993	2	0
17	L	1060	0	1119	12	0
18	M	1072	0	1115	4	0
19	N	908	0	956	5	0
20	O	886	0	924	11	0
21	P	907	0	947	7	0
22	Q	980	0	1028	5	0
23	R	742	0	799	8	0
24	S	860	0	903	7	0
25	T	759	0	809	4	0
26	U	699	0	738	2	0
27	V	1319	0	1365	13	0
28	W	546	0	567	5	0
29	X	476	0	496	4	0
30	Y	541	0	551	2	0
31	Z	476	0	509	8	0
32	A	22	0	0	0	0
All	All	94306	0	60898	391	0

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

All (391) 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)
7:A:1557:G:N3	7:A:1648:A:N6	2.10	0.97
13:G:103:ASN:ND2	13:G:116:ILE:O	2.10	0.84
7:A:1731:A:C2	7:A:1816:A:O2'	2.31	0.83
7:A:1627:C:N3	9:C:134:ARG:NH2	2.30	0.78
7:A:2746:G:O2'	7:A:2792:U:O2'	2.02	0.78
31:Z:40:ASN:O	31:Z:44:ARG:NH1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:162:A:OP2	7:A:167:A:N6	2.17	0.77
3:2:14:ARG:NH2	7:A:899:G:OP2	2.17	0.77
4:3:7:HIS:NE2	7:A:253:A:OP1	2.17	0.77
7:A:1577:C:O2	7:A:1627:C:N4	2.16	0.77
7:A:1732:A:H2	7:A:1815:U:O2	1.68	0.77
20:O:38:SER:OG	20:O:41:HIS:O	2.03	0.77
7:A:874:G:O2'	7:A:877:G:O2'	2.03	0.76
1:0:38:LYS:NZ	24:S:41:ASP:OD1	2.19	0.76
7:A:1471:U:OP2	25:T:62:ARG:NH2	2.20	0.75
7:A:2083:G:O2'	7:A:2084:G:H5'	1.87	0.75
7:A:1559:A:N6	7:A:1645:A:C8	2.54	0.74
7:A:718:G:N2	11:E:193:ASP:OD2	2.20	0.74
7:A:1173:A:O2'	7:A:1240:A:N1	2.21	0.74
5:4:6:SER:O	5:4:34:GLN:NE2	2.20	0.74
7:A:403:G:N2	11:E:177:ASN:O	2.20	0.74
9:C:260:ALA:O	9:C:265:ASN:ND2	2.20	0.74
21:P:19:PHE:O	21:P:49:ARG:NH1	2.20	0.74
7:A:1731:A:H2	7:A:1816:A:O2'	1.70	0.73
7:A:3069:A:N6	7:A:3114:G:O2'	2.21	0.73
7:A:2896:C:OP1	13:G:159:LYS:NZ	2.22	0.73
7:A:3055:C:OP1	19:N:6:LYS:NZ	2.21	0.73
19:N:38:GLU:OE2	19:N:42:ARG:NH2	2.23	0.72
4:3:13:ARG:NH1	17:L:60:LEU:O	2.22	0.71
7:A:1283:C:OP1	22:Q:92:ARG:NH2	2.24	0.71
7:A:1049:G:OP1	31:Z:18:LYS:NZ	2.22	0.71
7:A:1060:A:OP2	31:Z:24:ARG:NH2	2.22	0.71
7:A:3018:C:N4	15:J:102:GLU:OE2	2.24	0.71
7:A:1950:A:N6	7:A:1977:G:N7	2.39	0.70
7:A:2051:G:OP1	9:C:88:ARG:NH2	2.24	0.70
7:A:1951:U:O4	7:A:1978:G:O6	2.08	0.70
7:A:1453:A:O2'	24:S:94:ARG:NH2	2.25	0.69
7:A:2013:U:OP2	7:A:2018:A:N6	2.26	0.69
7:A:615:C:N4	7:A:3017:U:OP2	2.26	0.68
7:A:1381:G:OP2	17:L:23:ARG:NE	2.26	0.68
7:A:976:U:O2'	7:A:1062:G:N2	2.26	0.68
7:A:746:G:N2	7:A:749:U:O5'	2.27	0.68
7:A:1927:U:O2	7:A:1930:G:O6	2.11	0.68
13:G:7:GLN:O	13:G:70:ARG:NH1	2.26	0.67
7:A:3026:U:O2'	7:A:3044:A:N3	2.23	0.67
7:A:1216:G:N2	7:A:1219:U:OP1	2.26	0.67
7:A:833:G:HO2'	7:A:855:G:H1	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2534:U:OP2	20:O:15:ARG:NH1	2.28	0.67
7:A:827:C:O2'	7:A:863:A:N6	2.27	0.67
7:A:2218:G:O2'	7:A:2220:C:OP2	2.12	0.66
7:A:2710:G:N2	7:A:2717:U:O4	2.28	0.66
14:H:23:ASP:OD2	29:X:57:LYS:NZ	2.26	0.66
7:A:284:U:O2	7:A:304:G:O6	2.14	0.66
15:J:50:GLY:O	15:J:121:LYS:NZ	2.29	0.66
8:B:8:G:OP2	20:O:21:ARG:NH2	2.28	0.66
7:A:2981:C:OP2	7:A:2993:C:N4	2.29	0.65
7:A:2581:U:O2'	7:A:2611:A:O2'	2.14	0.65
8:B:48:C:OP2	20:O:37:ARG:NH2	2.30	0.65
13:G:53:VAL:O	13:G:66:HIS:NE2	2.30	0.65
1:O:17:ARG:NH2	7:A:1394:U:OP1	2.29	0.65
4:3:47:ARG:NH2	7:A:735:A:OP2	2.30	0.65
7:A:3092:G:N2	7:A:3095:A:OP2	2.30	0.65
11:E:123:ASP:OD1	11:E:126:ARG:NH1	2.30	0.64
7:A:1713:G:O2'	7:A:1753:G:O6	2.14	0.64
7:A:2613:G:N2	7:A:2616:A:OP2	2.31	0.64
7:A:3100:U:OP2	7:A:3101:G:O2'	2.13	0.64
7:A:995:U:N3	7:A:1033:C:OP2	2.31	0.64
5:4:35:ARG:NH1	7:A:2980:C:OP1	2.31	0.64
7:A:117:G:OP2	7:A:119:A:O2'	2.14	0.64
8:B:29:C:OP1	20:O:9:ARG:NH2	2.30	0.64
19:N:33:ARG:NE	19:N:114:GLU:OE2	2.30	0.64
7:A:2470:C:OP2	29:X:27:ARG:NH2	2.30	0.64
7:A:1334:U:O2'	11:E:192:TYR:OH	2.05	0.63
7:A:2083:G:C2'	7:A:2084:G:H5'	2.28	0.63
7:A:2894:U:O2	7:A:2903:A:N7	2.31	0.63
7:A:1658:A:H61	7:A:1815:U:H3	1.46	0.63
18:M:32:TYR:OH	18:M:111:GLU:OE1	2.12	0.63
7:A:1492:G:O2'	7:A:2453:G:O2'	2.16	0.63
7:A:944:C:OP1	23:R:87:LYS:NZ	2.28	0.63
7:A:2082:A:OP2	7:A:2082:A:H3'	1.98	0.63
13:G:75:ASN:O	13:G:84:TYR:OH	2.16	0.63
3:2:11:ASN:ND2	7:A:899:G:OP1	2.31	0.63
7:A:2876:G:O2'	7:A:3013:A:N1	2.30	0.63
7:A:2312:U:OP2	7:A:2476:G:O2'	2.09	0.62
7:A:2859:G:OP1	10:D:129:ARG:NH2	2.32	0.62
7:A:575:C:O2'	24:S:70:ASN:ND2	2.32	0.62
21:P:48:ARG:NH2	21:P:50:GLN:OE1	2.33	0.62
7:A:382:A:N7	26:U:82:ARG:NH1	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2684:G:N2	7:A:2687:U:O2	2.34	0.61
7:A:1549:C:OP2	7:A:1551:C:N4	2.33	0.61
7:A:1557:G:H1'	7:A:1648:A:H61	1.64	0.61
7:A:2376:U:O2'	7:A:2377:C:O2	2.18	0.61
20:O:49:ASP:OD2	20:O:53:THR:OG1	2.17	0.61
4:3:28:ASN:O	4:3:36:LYS:NZ	2.34	0.61
7:A:1211:U:OP2	7:A:1212:G:N1	2.34	0.60
7:A:2024:C:OP1	9:C:220:SER:OG	2.17	0.60
7:A:732:G:N1	7:A:740:G:N7	2.50	0.60
7:A:1634:A:OP2	7:A:1635:C:N4	2.33	0.60
7:A:1142:G:OP1	15:J:144:GLN:NE2	2.35	0.60
30:Y:14:THR:O	30:Y:64:ARG:NH1	2.34	0.59
7:A:1269:C:O2	7:A:1273:A:O2'	2.19	0.59
7:A:2025:A:O2'	9:C:206:TRP:O	2.12	0.59
7:A:2894:U:C2	7:A:2903:A:N7	2.69	0.59
7:A:1397:G:O5'	24:S:25:ARG:NH2	2.35	0.59
7:A:1165:G:O6	7:A:1248:U:O4	2.21	0.59
7:A:1567:U:O2'	7:A:1569:C:OP2	2.19	0.58
7:A:1772:G:O2'	7:A:1775:G:O6	2.22	0.58
7:A:629:C:N4	7:A:655:G:O6	2.36	0.58
7:A:2106:C:N4	7:A:2109:G:N3	2.51	0.58
7:A:2022:C:OP1	9:C:222:ARG:NH2	2.37	0.58
12:F:136:THR:OG1	12:F:162:ASN:OD1	2.07	0.58
11:E:159:GLN:NE2	11:E:180:GLY:O	2.36	0.58
7:A:556:G:HO2'	7:A:925:U:HO2'	1.50	0.57
7:A:1707:A:OP2	7:A:1761:A:N6	2.37	0.57
7:A:1732:A:C2	7:A:1815:U:O2	2.54	0.57
7:A:798:G:N2	7:A:801:C:OP1	2.36	0.57
7:A:1039:A:N3	7:A:2502:C:O2'	2.36	0.57
7:A:677:A:OP2	7:A:2737:C:O2'	2.23	0.57
6:6:17:GLY:N	6:6:36:GLU:O	2.36	0.57
11:E:151:LEU:O	11:E:155:THR:OG1	2.15	0.57
7:A:1537:C:C4	7:A:1832:G:N2	2.73	0.56
7:A:913:G:O4'	9:C:227:ASN:ND2	2.38	0.56
7:A:2082:A:H2'	7:A:2083:G:C8	2.40	0.56
7:A:1044:C:OP1	28:W:76:LYS:NZ	2.37	0.56
7:A:1832:G:OP2	25:T:43:LYS:NZ	2.38	0.56
7:A:2979:A:N6	7:A:3001:G:O2'	2.38	0.56
8:B:4:C:OP1	8:B:60:C:O2'	2.24	0.56
13:G:55:ARG:HH11	13:G:56:PRO:HD2	1.71	0.56
4:3:24:ARG:NH2	7:A:2598:A:OP1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1516:A:O2'	7:A:1527:U:O2	2.23	0.56
7:A:1579:A:O2'	9:C:170:ALA:HA	2.06	0.56
7:A:2504:A:N6	7:A:2511:A:OP2	2.36	0.56
2:1:53:GLU:OE1	2:1:53:GLU:N	2.38	0.56
7:A:261:C:O2	7:A:725:A:O2'	2.23	0.56
7:A:1628:G:H1'	9:C:134:ARG:NH1	2.20	0.56
8:B:109:C:O2'	20:O:54:THR:O	2.24	0.55
4:3:13:ARG:NE	17:L:57:HIS:O	2.40	0.55
7:A:289:A:O2'	7:A:304:G:N3	2.39	0.55
7:A:1570:U:N3	7:A:1633:A:OP2	2.39	0.55
7:A:2764:G:OP2	13:G:154:ARG:NH1	2.39	0.55
7:A:1119:A:N1	23:R:80:LYS:NZ	2.52	0.55
12:F:50:ALA:O	12:F:87:ARG:NH1	2.39	0.55
7:A:244:G:O2'	7:A:256:G:O6	2.23	0.55
28:W:59:LEU:HD13	28:W:80:ILE:HD11	1.89	0.55
7:A:2535:C:OP2	7:A:2556:G:N1	2.38	0.55
3:2:4:GLY:N	7:A:867:C:OP1	2.39	0.55
7:A:1842:C:N4	7:A:1856:U:OP2	2.40	0.55
7:A:2083:G:H2'	7:A:2084:G:H8	1.72	0.55
7:A:2083:G:H2'	7:A:2084:G:C8	2.42	0.54
7:A:1147:C:O2'	7:A:1249:G:N2	2.40	0.54
7:A:1826:C:H2'	7:A:1827:A:C8	2.43	0.54
8:B:8:G:OP1	20:O:32:ARG:NH2	2.41	0.54
7:A:281:G:N2	7:A:307:U:O2	2.39	0.54
1:0:10:ARG:NH2	7:A:18:C:OP1	2.40	0.54
7:A:1683:A:OP2	7:A:1698:C:N4	2.41	0.54
7:A:733:C:O2	7:A:743:U:O2'	2.26	0.54
31:Z:11:SER:OG	31:Z:12:THR:N	2.38	0.53
7:A:2135:G:H2'	7:A:2136:U:C6	2.43	0.53
7:A:2042:C:O2'	7:A:2043:A:O4'	2.26	0.53
27:V:47:LEU:H	27:V:48:PRO:HD2	1.72	0.53
27:V:138:ILE:H	27:V:139:PRO:HD2	1.72	0.53
31:Z:47:ILE:O	31:Z:50:VAL:C	2.47	0.53
12:F:63:ASP:OD2	12:F:157:ARG:NH2	2.42	0.53
7:A:6:A:HO2'	15:J:132:HIS:HD1	1.56	0.53
7:A:272:A:OP2	7:A:315:G:N1	2.37	0.53
7:A:1557:G:O6	7:A:1646:G:O2'	2.18	0.53
13:G:116:ILE:HD11	13:G:149:ILE:HD13	1.90	0.53
7:A:905:G:N1	7:A:2309:C:OP1	2.40	0.52
7:A:2082:A:H2'	7:A:2083:G:H8	1.74	0.52
7:A:3084:G:O2'	7:A:3101:G:N2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:330:G:O2'	7:A:446:A:OP2	2.22	0.52
8:B:76:U:OP1	27:V:26:ARG:NH1	2.43	0.52
7:A:1654:G:O2'	7:A:1822:C:O2'	2.26	0.52
7:A:1074:G:O6	7:A:1101:G:N2	2.42	0.52
7:A:1985:U:O2'	7:A:3096:U:O2'	2.28	0.52
11:E:149:ALA:O	11:E:153:SER:OG	2.27	0.52
7:A:1826:C:H2'	7:A:1827:A:H8	1.74	0.52
7:A:284:U:C2	7:A:304:G:O6	2.63	0.52
29:X:28:ARG:NH1	29:X:30:ASP:OD1	2.42	0.52
7:A:1903:A:N3	7:A:1905:C:N4	2.58	0.52
17:L:54:MET:O	17:L:59:ARG:NH2	2.42	0.51
7:A:2814:G:O2'	7:A:2817:C:OP2	2.28	0.51
5:4:29:ASP:O	5:4:31:ARG:N	2.44	0.51
7:A:2963:A:O2'	7:A:2965:G:N7	2.39	0.51
7:A:691:C:OP1	17:L:18:ARG:NH1	2.44	0.51
7:A:2078:U:H2'	7:A:2079:G:O4'	2.11	0.51
26:U:86:ARG:HD3	26:U:97:ILE:HD13	1.91	0.51
7:A:1197:G:O2'	7:A:1199:A:N6	2.44	0.51
7:A:3082:U:OP1	21:P:95:LYS:NZ	2.42	0.51
7:A:2190:A:O2'	7:A:2191:A:O4'	2.28	0.51
7:A:2572:C:O2	20:O:22:LYS:NZ	2.39	0.51
13:G:112:HIS:O	13:G:112:HIS:ND1	2.44	0.51
7:A:34:U:O4	7:A:543:A:O2'	2.29	0.51
7:A:1027:U:O2'	7:A:1028:G:O4'	2.28	0.51
27:V:60:GLY:O	27:V:62:ASN:N	2.44	0.51
7:A:1546:G:H1	7:A:1822:C:H42	1.59	0.50
7:A:1627:C:O2	9:C:134:ARG:NE	2.43	0.50
8:B:75:A:O3'	27:V:26:ARG:NH2	2.43	0.50
7:A:329:U:O2	7:A:447:G:O6	2.29	0.50
13:G:57:ASP:OD1	13:G:62:ASN:ND2	2.45	0.50
7:A:749:U:O2	7:A:749:U:O2'	2.29	0.50
7:A:900:G:O2'	7:A:1486:G:O2'	2.27	0.50
7:A:2081:A:O2'	7:A:2082:A:OP1	2.26	0.50
13:G:17:VAL:O	13:G:45:ARG:NH2	2.42	0.50
19:N:103:ARG:NH2	19:N:106:ASP:OD2	2.45	0.50
7:A:874:G:HO2'	7:A:877:G:HO2'	1.48	0.50
7:A:2135:G:H2'	7:A:2136:U:H6	1.77	0.50
7:A:1558:A:H5'	7:A:1645:A:H61	1.77	0.50
7:A:2032:U:OP2	9:C:272:ARG:NH2	2.43	0.50
7:A:1200:G:O6	7:A:1218:G:O2'	2.12	0.49
7:A:1444:U:O2'	7:A:1463:G:O4'	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:9:THR:OG1	10:D:204:GLY:O	2.15	0.49
7:A:909:G:OP1	9:C:218:ARG:NH1	2.41	0.49
7:A:1453:A:OP1	24:S:21:ARG:NH1	2.42	0.49
7:A:1567:U:H4'	7:A:1568:A:C5'	2.43	0.49
7:A:1539:U:H2'	7:A:1540:G:C8	2.48	0.49
7:A:1557:G:N2	7:A:1648:A:H62	2.11	0.49
7:A:2079:G:C2	7:A:2080:G:H1'	2.48	0.49
7:A:1592:U:O4	7:A:1613:G:O6	2.30	0.49
7:A:3084:G:O3'	7:A:3101:G:N2	2.45	0.49
12:F:70:GLN:NE2	12:F:97:THR:O	2.43	0.49
9:C:69:ARG:NH1	9:C:97:TYR:OH	2.46	0.49
7:A:968:U:O2'	7:A:1323:G:N3	2.46	0.49
7:A:2234:C:OP1	16:K:31:ARG:NH1	2.42	0.49
7:A:1581:A:N7	7:A:1623:G:O2'	2.46	0.48
7:A:2082:A:O2'	7:A:2083:G:H5'	2.13	0.48
7:A:2696:G:O6	7:A:2728:G:O2'	2.28	0.48
7:A:1011:G:C6	7:A:1024:U:C2	3.01	0.48
12:F:87:ARG:NH2	12:F:91:PRO:O	2.47	0.48
7:A:2023:A:OP2	9:C:222:ARG:NH2	2.46	0.48
7:A:2392:C:O2'	7:A:2393:G:N2	2.47	0.48
7:A:2558:C:N4	7:A:2571:A:O2'	2.46	0.48
7:A:2269:A:O2'	7:A:2692:G:N2	2.44	0.48
21:P:64:SER:OG	21:P:65:TYR:N	2.45	0.48
23:R:62:THR:O	23:R:101:THR:OG1	2.30	0.48
7:A:2569:G:OP1	28:W:44:LYS:NZ	2.25	0.47
7:A:1873:C:O2	7:A:2936:U:O2'	2.31	0.47
7:A:2236:A:OP2	10:D:146:ARG:NH1	2.47	0.47
7:A:883:U:HO2'	7:A:1853:A:H2	1.59	0.47
7:A:1122:G:OP2	22:Q:51:ARG:NH2	2.47	0.47
7:A:1731:A:H2	7:A:1816:A:HO2'	1.49	0.47
7:A:1354:G:O6	23:R:75:ARG:NH1	2.42	0.47
7:A:2926:G:OP1	7:A:2951:C:N4	2.47	0.47
7:A:1495:G:N2	7:A:1498:A:OP2	2.42	0.47
7:A:2517:G:O2'	7:A:2565:A:O2'	2.31	0.47
10:D:76:ASN:HD22	10:D:77:PRO:N	2.13	0.47
6:6:9:TYR:O	6:6:26:SER:OG	2.24	0.47
7:A:1386:U:O4'	7:A:2740:G:N2	2.48	0.47
7:A:1343:G:N2	7:A:1367:G:O2'	2.47	0.47
7:A:1562:A:N6	7:A:1642:G:O6	2.48	0.47
7:A:1908:G:O6	10:D:139:HIS:ND1	2.48	0.47
7:A:273:A:H2	7:A:457:C:HO2'	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:446:A:O2'	7:A:447:G:O4'	2.28	0.46
7:A:914:G:O2'	7:A:915:C:O5'	2.33	0.46
7:A:2375:C:N4	7:A:2391:G:O6	2.48	0.46
9:C:258:ARG:NH2	9:C:264:SER:OG	2.47	0.46
7:A:1057:G:O2'	31:Z:25:THR:O	2.33	0.46
7:A:2024:C:OP2	7:A:2062:G:N1	2.48	0.46
12:F:171:ASP:OD1	12:F:174:ARG:NH2	2.44	0.46
7:A:1890:A:N6	7:A:2243:A:O2'	2.49	0.46
31:Z:47:ILE:O	31:Z:50:VAL:O	2.33	0.46
7:A:2260:U:O2	7:A:2272:U:N3	2.48	0.46
8:B:91:U:OP1	27:V:24:ARG:NH1	2.45	0.46
28:W:71:ILE:HG22	28:W:78:VAL:HG22	1.97	0.46
7:A:1916:G:OP2	7:A:1991:A:N6	2.49	0.46
10:D:138:SER:OG	10:D:139:HIS:N	2.48	0.46
7:A:405:A:OP2	11:E:177:ASN:ND2	2.45	0.46
7:A:1427:G:OP1	7:A:2947:G:O2'	2.25	0.46
7:A:1463:G:N7	7:A:1844:A:O2'	2.36	0.46
7:A:2367:U:OP1	7:A:2396:G:N1	2.48	0.46
22:Q:97:ASP:OD2	23:R:16:LYS:NZ	2.40	0.45
3:2:38:ARG:NH1	7:A:54:G:O2'	2.49	0.45
7:A:988:G:N2	7:A:1046:A:OP2	2.46	0.45
3:2:42:ARG:NH1	7:A:556:G:N7	2.60	0.45
18:M:27:VAL:O	18:M:134:ARG:NH1	2.44	0.45
7:A:2082:A:H2'	7:A:2083:G:O4'	2.16	0.45
7:A:2688:A:OP1	7:A:2735:A:O2'	2.21	0.45
5:4:19:ARG:NE	7:A:2994:U:OP2	2.46	0.45
7:A:359:C:H4'	7:A:360:A:H5''	1.99	0.45
7:A:688:A:N1	7:A:938:G:O2'	2.42	0.45
9:C:85:ASP:OD2	9:C:88:ARG:NH1	2.48	0.45
17:L:34:ARG:HH21	17:L:44:GLN:HE21	1.64	0.45
17:L:34:ARG:NH2	17:L:44:GLN:HE21	2.14	0.45
7:A:65:G:N1	7:A:90:C:O2	2.49	0.45
7:A:1094:G:O4'	7:A:2505:A:N6	2.49	0.45
7:A:1381:G:O6	17:L:20:ARG:NH2	2.49	0.45
7:A:3068:C:N3	10:D:60:ARG:NE	2.65	0.45
20:O:60:SER:O	20:O:75:ARG:NH2	2.49	0.45
7:A:536:A:O4'	7:A:538:A:N6	2.50	0.45
7:A:1558:A:OP2	7:A:1646:G:N2	2.41	0.45
7:A:2389:G:N2	7:A:2390:G:O6	2.50	0.45
13:G:170:ILE:O	13:G:172:ARG:NH1	2.50	0.45
7:A:195:U:N3	7:A:205:C:O2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:452:A:N6	7:A:453:A:N1	2.65	0.44
9:C:130:ASN:O	9:C:190:ARG:NH2	2.50	0.44
7:A:2894:U:N3	7:A:2903:A:C8	2.86	0.44
27:V:62:ASN:HD21	27:V:108:VAL:HG12	1.83	0.44
23:R:77:HIS:HB3	23:R:88:ARG:HA	1.98	0.44
7:A:937:G:O6	17:L:42:ARG:NH1	2.47	0.44
27:V:64:VAL:HG21	27:V:136:LEU:HB3	2.00	0.44
27:V:47:LEU:H	27:V:48:PRO:CD	2.30	0.44
7:A:620:C:OP2	22:Q:38:GLN:NE2	2.45	0.44
11:E:133:ILE:N	11:E:202:PHE:O	2.50	0.44
21:P:91:VAL:HG23	21:P:93:ARG:H	1.82	0.44
2:1:27:LYS:HD2	7:A:2524:A:H5''	1.98	0.44
7:A:48:G:N2	7:A:179:A:OP2	2.50	0.44
7:A:91:A:OP1	25:T:70:ARG:NH2	2.51	0.44
7:A:358:U:O2'	7:A:359:C:O4'	2.32	0.44
18:M:135:GLU:HG3	27:V:56:LEU:HD22	2.00	0.44
7:A:1540:G:C2	7:A:1829:A:C2	3.06	0.44
7:A:79:C:HO2'	7:A:429:A:H8	1.63	0.44
7:A:1200:G:O4'	7:A:1206:A:N6	2.51	0.44
7:A:1673:A:N1	7:A:1795:C:N4	2.65	0.43
7:A:2551:C:O4'	12:F:44:ASN:ND2	2.51	0.43
27:V:11:VAL:HG11	27:V:45:LEU:HD23	1.99	0.43
7:A:833:G:HO2'	7:A:855:G:N2	2.15	0.43
9:C:7:LYS:O	9:C:9:THR:N	2.50	0.43
7:A:1628:G:H1'	9:C:134:ARG:CZ	2.48	0.43
21:P:13:ARG:NH1	21:P:80:ILE:O	2.48	0.43
7:A:193:A:OP2	7:A:206:A:N6	2.46	0.43
7:A:2076:G:C2	7:A:2139:A:C2	3.07	0.43
7:A:2529:U:O2'	7:A:2612:C:O2	2.37	0.43
4:3:57:ARG:NH2	17:L:48:THR:O	2.51	0.43
7:A:1558:A:C5'	7:A:1645:A:H61	2.31	0.43
7:A:1670:G:H2'	7:A:1671:G:O4'	2.19	0.43
13:G:46:ASN:ND2	13:G:48:ASP:OD1	2.52	0.43
24:S:10:TYR:O	24:S:12:SER:N	2.51	0.42
7:A:1357:A:H5'	23:R:88:ARG:HE	1.84	0.42
7:A:2447:U:O2'	7:A:2450:A:N7	2.38	0.42
7:A:1096:A:H4'	7:A:1097:C:H5'	2.00	0.42
7:A:1698:C:O2'	7:A:1699:A:N7	2.52	0.42
7:A:2802:A:N7	7:A:2885:U:O2'	2.52	0.42
7:A:2085:U:C5	7:A:2086:U:C5	3.07	0.42
14:H:27:ARG:NH1	29:X:56:ILE:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:27:LYS:CE	2:1:31:ASN:HD22	2.33	0.42
7:A:3023:U:O2	10:D:69:GLN:NE2	2.51	0.42
7:A:285:G:OP2	7:A:286:G:N2	2.52	0.42
7:A:1582:A:H61	7:A:1622:G:C2'	2.33	0.42
7:A:2174:A:O2'	7:A:2183:G:N7	2.46	0.42
10:D:32:GLY:O	10:D:34:ASN:N	2.49	0.42
11:E:52:ARG:NH1	11:E:104:TYR:OH	2.53	0.42
17:L:50:GLU:CD	17:L:53:GLN:HE21	2.23	0.42
7:A:2041:G:OP1	9:C:48:ARG:NH1	2.52	0.42
7:A:2290:G:O2'	10:D:153:GLY:O	2.32	0.42
16:K:108:GLU:OE1	16:K:108:GLU:N	2.47	0.42
1:0:41:ARG:NH1	7:A:3121:G:N3	2.68	0.42
7:A:389:U:HO2'	7:A:1342:C:H5	1.63	0.42
7:A:2810:A:OP1	7:A:2812:G:O2'	2.33	0.42
7:A:1559:A:N6	7:A:1645:A:H8	2.12	0.42
31:Z:15:ALA:O	31:Z:20:ARG:NH1	2.53	0.42
7:A:239:C:O2	7:A:712:A:O2'	2.35	0.41
7:A:618:U:O2'	7:A:2274:C:OP1	2.36	0.41
7:A:1692:U:O4'	19:N:63:ARG:NH1	2.52	0.41
7:A:2085:U:C5	7:A:2086:U:C4	3.08	0.41
27:V:46:GLU:HB3	27:V:48:PRO:HD2	2.02	0.41
7:A:990:A:H2	8:B:78:C:HO2'	1.66	0.41
7:A:1354:G:OP1	23:R:70:LYS:NZ	2.49	0.41
18:M:63:LYS:N	18:M:107:SER:OG	2.53	0.41
5:4:32:HIS:HD1	5:4:34:GLN:H	1.68	0.41
7:A:1828:C:O2'	7:A:1829:A:H5'	2.20	0.41
7:A:689:G:H3'	7:A:690:U:H5'	2.02	0.41
7:A:1393:A:OP1	24:S:109:ARG:NH2	2.54	0.41
7:A:2076:G:N3	7:A:2139:A:C2	2.89	0.41
7:A:2614:A:O2'	20:O:116:ARG:NH1	2.52	0.41
25:T:8:ARG:HD2	30:Y:26:LYS:HB3	2.01	0.41
28:W:25:ARG:NE	28:W:35:GLU:OE2	2.46	0.41
7:A:405:A:C5'	11:E:177:ASN:HD21	2.34	0.41
13:G:58:ASP:OD1	13:G:63:ARG:NH1	2.36	0.41
7:A:2099:U:O2'	7:A:2113:G:N2	2.53	0.41
10:D:27:THR:OG1	10:D:196:GLY:O	2.30	0.41
7:A:1557:G:H21	7:A:1648:A:H62	1.68	0.41
7:A:2120:A:H2'	7:A:2121:G:O4'	2.21	0.41
7:A:2335:U:O2	7:A:2429:G:N2	2.53	0.41
11:E:149:ALA:O	11:E:153:SER:CB	2.69	0.41
17:L:50:GLU:OE2	17:L:53:GLN:NE2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:59:GLU:O	13:G:61:ARG:N	2.48	0.41
7:A:1463:G:HO2'	7:A:1844:A:H2	1.64	0.40
7:A:1136:C:OP1	15:J:39:LYS:NZ	2.41	0.40
7:A:2083:G:H2'	7:A:2084:G:O4'	2.20	0.40
27:V:69:ILE:HD12	27:V:74:GLN:HG3	2.03	0.40
7:A:381:A:N6	7:A:382:A:N1	2.70	0.40
7:A:621:G:HO2'	22:Q:42:SER:HG	1.57	0.40
7:A:1080:G:H3'	7:A:1081:G:H5''	2.03	0.40
13:G:66:HIS:HE2	13:G:70:ARG:HH21	1.69	0.40
7:A:163:A:N6	7:A:167:A:C2	2.90	0.40
7:A:241:C:O2'	7:A:726:G:O2'	2.32	0.40
7:A:1571:A:OP2	7:A:1632:G:N1	2.45	0.40
7:A:2020:A:O2'	7:A:2176:A:N6	2.55	0.40
10:D:76:ASN:HD22	10:D:77:PRO:CD	2.34	0.40
9:C:66:ASP:OD2	9:C:103:ARG:NH1	2.47	0.40
21:P:90:ASP:HB2	21:P:112:LYS:HD3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
2	1	46/55 (84%)	41 (89%)	5 (11%)	0	100	100
3	2	40/47 (85%)	39 (98%)	1 (2%)	0	100	100
4	3	60/64 (94%)	53 (88%)	7 (12%)	0	100	100
5	4	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
6	6	43/80 (54%)	36 (84%)	7 (16%)	0	100	100
9	C	270/280 (96%)	240 (89%)	29 (11%)	1 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	D	211/217 (97%)	186 (88%)	22 (10%)	3 (1%)	11	45
11	E	205/223 (92%)	176 (86%)	29 (14%)	0	100	100
12	F	168/187 (90%)	152 (90%)	16 (10%)	0	100	100
13	G	172/179 (96%)	147 (86%)	24 (14%)	1 (1%)	25	62
14	H	45/152 (30%)	39 (87%)	6 (13%)	0	100	100
15	J	144/147 (98%)	135 (94%)	9 (6%)	0	100	100
16	K	119/122 (98%)	113 (95%)	6 (5%)	0	100	100
17	L	140/146 (96%)	130 (93%)	10 (7%)	0	100	100
18	M	132/138 (96%)	116 (88%)	16 (12%)	0	100	100
19	N	114/180 (63%)	108 (95%)	6 (5%)	0	100	100
20	O	114/122 (93%)	102 (90%)	12 (10%)	0	100	100
21	P	110/113 (97%)	96 (87%)	14 (13%)	0	100	100
22	Q	120/129 (93%)	112 (93%)	7 (6%)	1 (1%)	19	56
23	R	96/104 (92%)	87 (91%)	8 (8%)	1 (1%)	15	51
24	S	111/197 (56%)	104 (94%)	7 (6%)	0	100	100
25	T	96/100 (96%)	88 (92%)	8 (8%)	0	100	100
26	U	86/105 (82%)	71 (83%)	14 (16%)	1 (1%)	13	48
27	V	175/215 (81%)	143 (82%)	26 (15%)	6 (3%)	3	30
28	W	72/86 (84%)	65 (90%)	5 (7%)	2 (3%)	5	33
29	X	61/64 (95%)	50 (82%)	10 (16%)	1 (2%)	9	43
30	Y	63/77 (82%)	60 (95%)	2 (3%)	1 (2%)	9	43
31	Z	57/65 (88%)	51 (90%)	5 (9%)	1 (2%)	8	41
All	All	3156/3688 (86%)	2815 (89%)	322 (10%)	19 (1%)	29	62

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	108	PRO
10	D	91	ALA
10	D	92	ALA
22	Q	118	PRO
27	V	61	THR
28	W	75	ARG
28	W	80	ILE

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Mol	Chain	Res	Type
29	X	47	LYS
30	Y	14	THR
31	Z	31	ILE
10	D	142	GLN
27	V	59	SER
27	V	149	ALA
13	G	158	TYR
23	R	82	LYS
26	U	89	GLU
27	V	47	LEU
27	V	138	ILE
27	V	170	SER

### 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	43/47 (92%)	43 (100%)	0	100	100
2	1	45/51 (88%)	45 (100%)	0	100	100
3	2	36/40 (90%)	36 (100%)	0	100	100
4	3	53/54 (98%)	53 (100%)	0	100	100
5	4	35/35 (100%)	35 (100%)	0	100	100
6	6	40/66 (61%)	40 (100%)	0	100	100
9	C	212/219 (97%)	212 (100%)	0	100	100
10	D	163/166 (98%)	162 (99%)	1 (1%)	86	93
11	E	159/172 (92%)	159 (100%)	0	100	100
12	F	139/155 (90%)	139 (100%)	0	100	100
13	G	143/147 (97%)	143 (100%)	0	100	100
14	H	36/121 (30%)	36 (100%)	0	100	100
15	J	120/121 (99%)	120 (100%)	0	100	100
16	K	100/101 (99%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	L	106/110 (96%)	106 (100%)	0	100	100
18	M	110/114 (96%)	110 (100%)	0	100	100
19	N	94/139 (68%)	94 (100%)	0	100	100
20	O	88/93 (95%)	88 (100%)	0	100	100
21	P	98/99 (99%)	98 (100%)	0	100	100
22	Q	95/99 (96%)	95 (100%)	0	100	100
23	R	79/83 (95%)	79 (100%)	0	100	100
24	S	87/140 (62%)	87 (100%)	0	100	100
25	T	82/83 (99%)	82 (100%)	0	100	100
26	U	77/88 (88%)	77 (100%)	0	100	100
27	V	142/164 (87%)	142 (100%)	0	100	100
28	W	54/62 (87%)	54 (100%)	0	100	100
29	X	52/52 (100%)	52 (100%)	0	100	100
30	Y	58/66 (88%)	58 (100%)	0	100	100
31	Z	51/55 (93%)	51 (100%)	0	100	100
All	All	2597/2942 (88%)	2596 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	D	76	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	20	HIS
2	1	44	ASN
4	3	53	ASN
9	C	227	ASN
10	D	76	ASN
11	E	159	GLN
17	L	44	GLN
18	M	123	HIS
24	S	70	ASN
27	V	62	ASN

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	A	3116/3138 (99%)	297 (9%)	1 (0%)
8	B	114/115 (99%)	2 (1%)	0
All	All	3230/3253 (99%)	299 (9%)	1 (0%)

All (299) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	10	U
7	A	50	U
7	A	71	A
7	A	74	U
7	A	75	G
7	A	85	G
7	A	93	C
7	A	101	G
7	A	118	A
7	A	119	A
7	A	120	U
7	A	165	A
7	A	198	A
7	A	218	A
7	A	224	A
7	A	232	G
7	A	250	G
7	A	268	G
7	A	287	G
7	A	288	U
7	A	289	A
7	A	293	G
7	A	301	G
7	A	303	U
7	A	371	U
7	A	373	G
7	A	384	U
7	A	394	U
7	A	405	A
7	A	413	A
7	A	445	U
7	A	447	G
7	A	448	U
7	A	475	G

*Continued on next page...*

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Mol	Chain	Res	Type
7	A	476	U
7	A	500	G
7	A	501	A
7	A	533	C
7	A	540	C
7	A	570	G
7	A	593	A
7	A	596	A
7	A	597	C
7	A	618	U
7	A	619	C
7	A	620	C
7	A	621	G
7	A	665	G
7	A	677	A
7	A	695	G
7	A	706	A
7	A	718	G
7	A	741	A
7	A	742	G
7	A	749	U
7	A	756	A
7	A	758	C
7	A	773	C
7	A	779	U
7	A	780	G
7	A	781	A
7	A	782	A
7	A	783	U
7	A	815	U
7	A	859	C
7	A	906	G
7	A	911	A
7	A	913	G
7	A	914	G
7	A	915	C
7	A	921	A
7	A	922	A
7	A	934	G
7	A	941	C
7	A	956	U
7	A	975	G

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Mol	Chain	Res	Type
7	A	1039	A
7	A	1059	A
7	A	1060	A
7	A	1074	G
7	A	1081	G
7	A	1089	G
7	A	1103	A
7	A	1142	G
7	A	1151	G
7	A	1155	G
7	A	1187	G
7	A	1189	U
7	A	1196	A
7	A	1198	A
7	A	1200	G
7	A	1208	C
7	A	1211	U
7	A	1216	G
7	A	1217	A
7	A	1240	A
7	A	1241	G
7	A	1242	U
7	A	1258	A
7	A	1262	A
7	A	1264	C
7	A	1271	C
7	A	1272	A
7	A	1273	A
7	A	1304	U
7	A	1307	U
7	A	1308	G
7	A	1387	G
7	A	1403	A
7	A	1432	A
7	A	1460	U
7	A	1481	C
7	A	1497	C
7	A	1509	A
7	A	1510	U
7	A	1515	A
7	A	1526	A
7	A	1527	U

*Continued on next page...*

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Mol	Chain	Res	Type
7	A	1541	U
7	A	1542	G
7	A	1550	C
7	A	1551	C
7	A	1558	A
7	A	1560	U
7	A	1565	G
7	A	1567	U
7	A	1568	A
7	A	1571	A
7	A	1578	C
7	A	1580	A
7	A	1582	A
7	A	1589	C
7	A	1590	G
7	A	1591	A
7	A	1592	U
7	A	1599	C
7	A	1601	U
7	A	1602	U
7	A	1604	G
7	A	1606	G
7	A	1607	G
7	A	1609	U
7	A	1615	G
7	A	1619	U
7	A	1625	U
7	A	1634	A
7	A	1635	C
7	A	1638	C
7	A	1642	G
7	A	1643	G
7	A	1644	U
7	A	1646	G
7	A	1651	C
7	A	1657	A
7	A	1658	A
7	A	1659	G
7	A	1666	C
7	A	1691	G
7	A	1698	C
7	A	1699	A

*Continued on next page...*

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Mol	Chain	Res	Type
7	A	1705	G
7	A	1720	G
7	A	1727	A
7	A	1767	A
7	A	1803	A
7	A	1807	A
7	A	1815	U
7	A	1816	A
7	A	1817	G
7	A	1820	A
7	A	1821	G
7	A	1842	C
7	A	1843	A
7	A	1845	A
7	A	1881	U
7	A	1883	C
7	A	1888	U
7	A	1909	G
7	A	1934	G
7	A	1950	A
7	A	1963	U
7	A	1964	U
7	A	1967	G
7	A	1997	G
7	A	1998	U
7	A	2007	A
7	A	2015	C
7	A	2016	U
7	A	2019	A
7	A	2034	C
7	A	2043	A
7	A	2078	U
7	A	2079	G
7	A	2080	G
7	A	2081	A
7	A	2082	A
7	A	2084	G
7	A	2107	A
7	A	2108	A
7	A	2109	G
7	A	2134	A
7	A	2167	G

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Mol	Chain	Res	Type
7	A	2168	G
7	A	2175	A
7	A	2193	U
7	A	2201	U
7	A	2205	C
7	A	2208	A
7	A	2209	U
7	A	2210	G
7	A	2231	U
7	A	2260	U
7	A	2270	G
7	A	2294	G
7	A	2298	A
7	A	2299	G
7	A	2300	A
7	A	2313	C
7	A	2314	A
7	A	2347	G
7	A	2348	U
7	A	2349	G
7	A	2353	G
7	A	2357	G
7	A	2360	G
7	A	2361	G
7	A	2362	G
7	A	2363	A
7	A	2364	G
7	A	2366	C
7	A	2367	U
7	A	2369	U
7	A	2370	G
7	A	2371	A
7	A	2372	A
7	A	2377	C
7	A	2382	C
7	A	2383	C
7	A	2388	G
7	A	2389	G
7	A	2392	C
7	A	2394	G
7	A	2400	U
7	A	2404	U

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Mol	Chain	Res	Type
7	A	2407	A
7	A	2414	C
7	A	2416	C
7	A	2422	G
7	A	2423	U
7	A	2450	A
7	A	2463	A
7	A	2476	G
7	A	2477	G
7	A	2487	U
7	A	2488	G
7	A	2516	A
7	A	2521	C
7	A	2525	A
7	A	2543	A
7	A	2563	G
7	A	2571	A
7	A	2572	C
7	A	2573	A
7	A	2583	G
7	A	2585	C
7	A	2621	G
7	A	2623	A
7	A	2626	A
7	A	2640	C
7	A	2661	U
7	A	2666	G
7	A	2667	G
7	A	2685	G
7	A	2686	A
7	A	2714	A
7	A	2729	U
7	A	2756	A
7	A	2758	C
7	A	2781	G
7	A	2792	U
7	A	2804	A
7	A	2805	G
7	A	2851	U
7	A	2928	A
7	A	2929	C
7	A	2952	G

*Continued on next page...*



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Mol	Chain	Res	Type
7	A	2964	C
7	A	2995	A
7	A	3016	A
7	A	3028	A
7	A	3029	C
7	A	3030	C
7	A	3107	A
7	A	3121	G
7	A	3126	A
7	A	3128	A
7	A	3129	A
8	B	105	A
8	B	115	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	1567	U

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	917	A	5001	-	21,24,24	3.02	7 (33%)	28,33,33	3.16	12 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	917	A	5001	-	-	4/13/25/25	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	5001	917	C09-N08	9.37	1.45	1.36
32	A	5001	917	O11-C09	6.78	1.44	1.35
32	A	5001	917	C02-N04	3.93	1.45	1.34
32	A	5001	917	C07-N08	-3.30	1.41	1.47
32	A	5001	917	C07-C06	-3.07	1.47	1.52
32	A	5001	917	O11-C06	-2.92	1.42	1.46
32	A	5001	917	O03-C02	-2.01	1.18	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	5001	917	C07-N08-C09	-8.15	106.56	111.28
32	A	5001	917	C19-N20-C21	6.66	116.17	105.78
32	A	5001	917	C06-C07-N08	5.41	107.26	101.81
32	A	5001	917	C07-C06-C05	-4.85	107.71	113.08
32	A	5001	917	C18-C19-N20	4.26	117.43	108.94
32	A	5001	917	O11-C09-O10	3.98	126.78	122.37
32	A	5001	917	C06-O11-C09	-3.97	107.01	110.15
32	A	5001	917	O11-C09-N08	-3.94	107.12	109.83
32	A	5001	917	O10-C09-N08	-3.55	126.09	128.91
32	A	5001	917	C07-N08-C12	3.30	127.02	121.45
32	A	5001	917	O11-C06-C07	3.11	107.71	104.57
32	A	5001	917	C01-C02-N04	2.05	119.73	116.09

There are no chirality outliers.

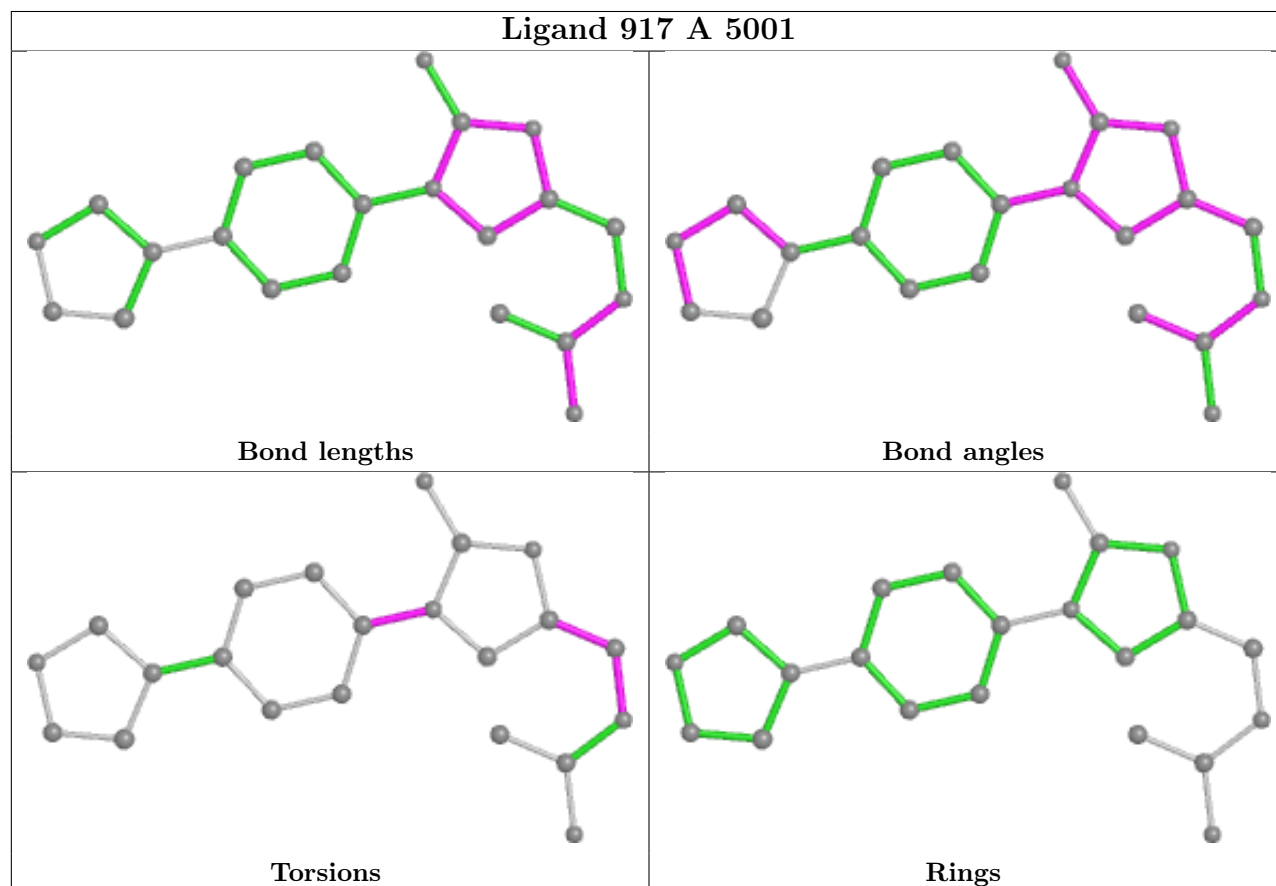
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	5001	917	N04-C05-C06-C07
32	A	5001	917	C13-C12-N08-C09
32	A	5001	917	C17-C12-N08-C09
32	A	5001	917	C06-C05-N04-C02

There are no ring outliers.

No monomer is involved in short contacts.

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



## 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.

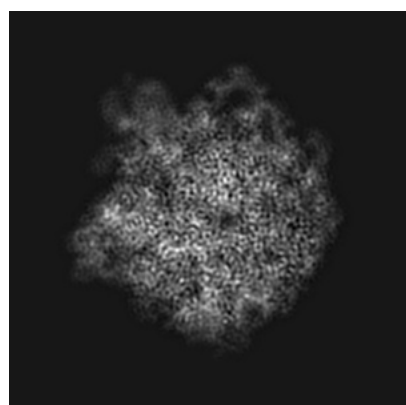
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8641. These allow visual inspection of the internal detail of the map and identification of artifacts.

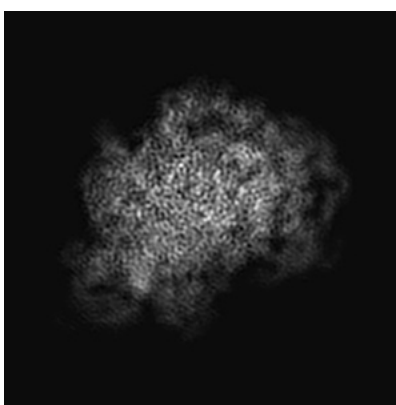
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

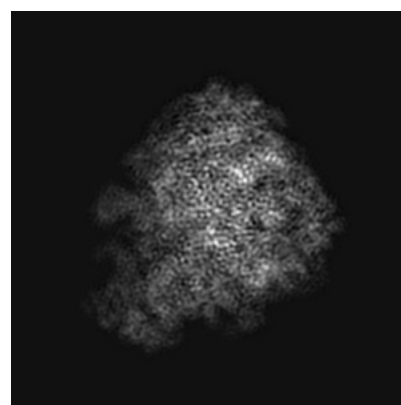
#### 6.1.1 Primary map



X



Y

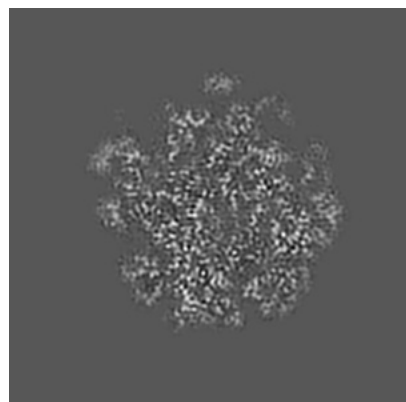


Z

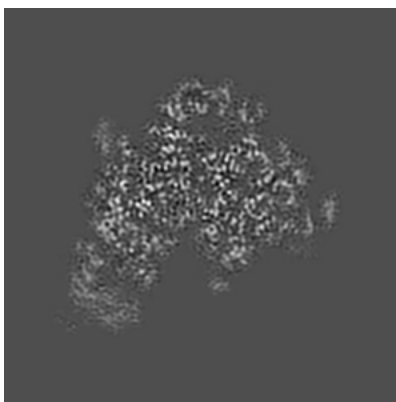
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

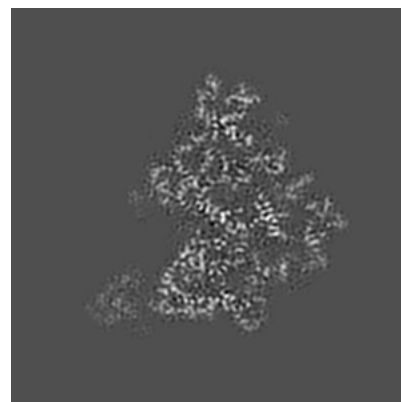
#### 6.2.1 Primary map



X Index: 104



Y Index: 104

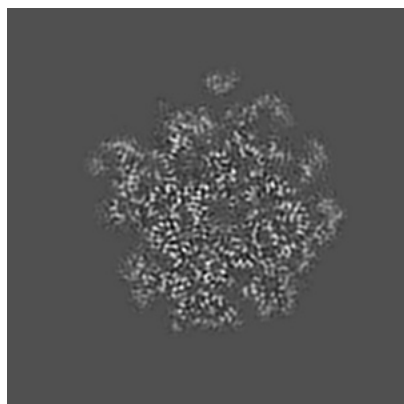


Z Index: 104

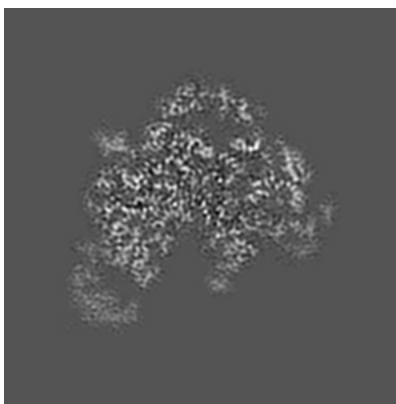
The images above show central slices of the map in three orthogonal directions.

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

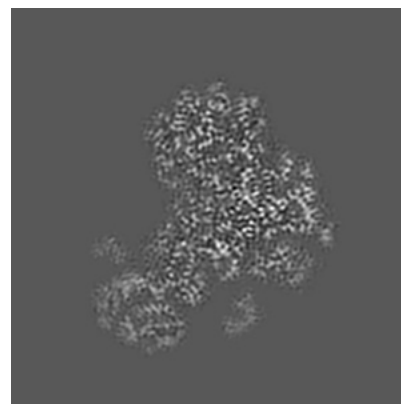
### 6.3.1 Primary map



X Index: 106



Y Index: 102



Z Index: 87

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

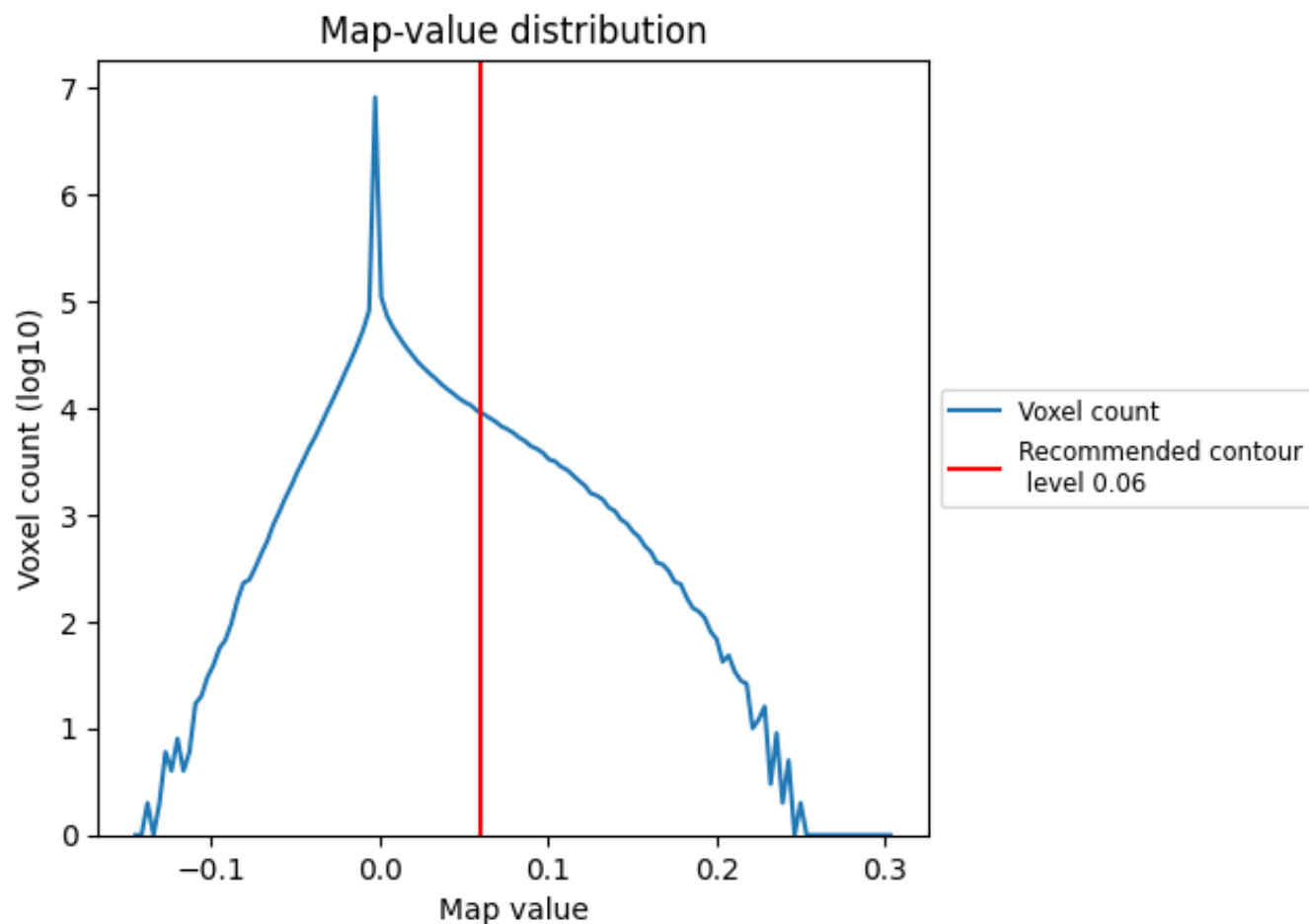
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

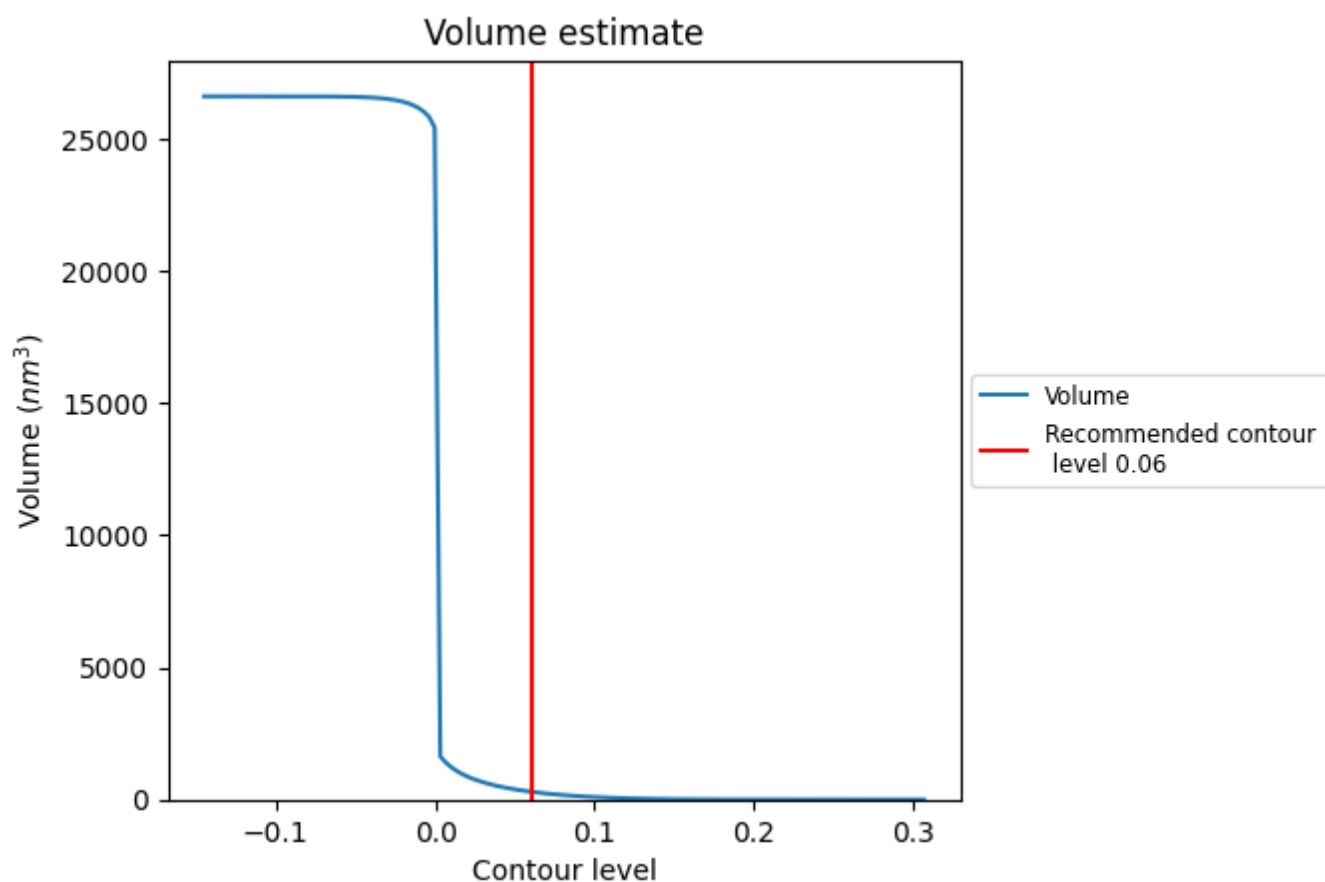
### 7.1 Map-value distribution [i](#)



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



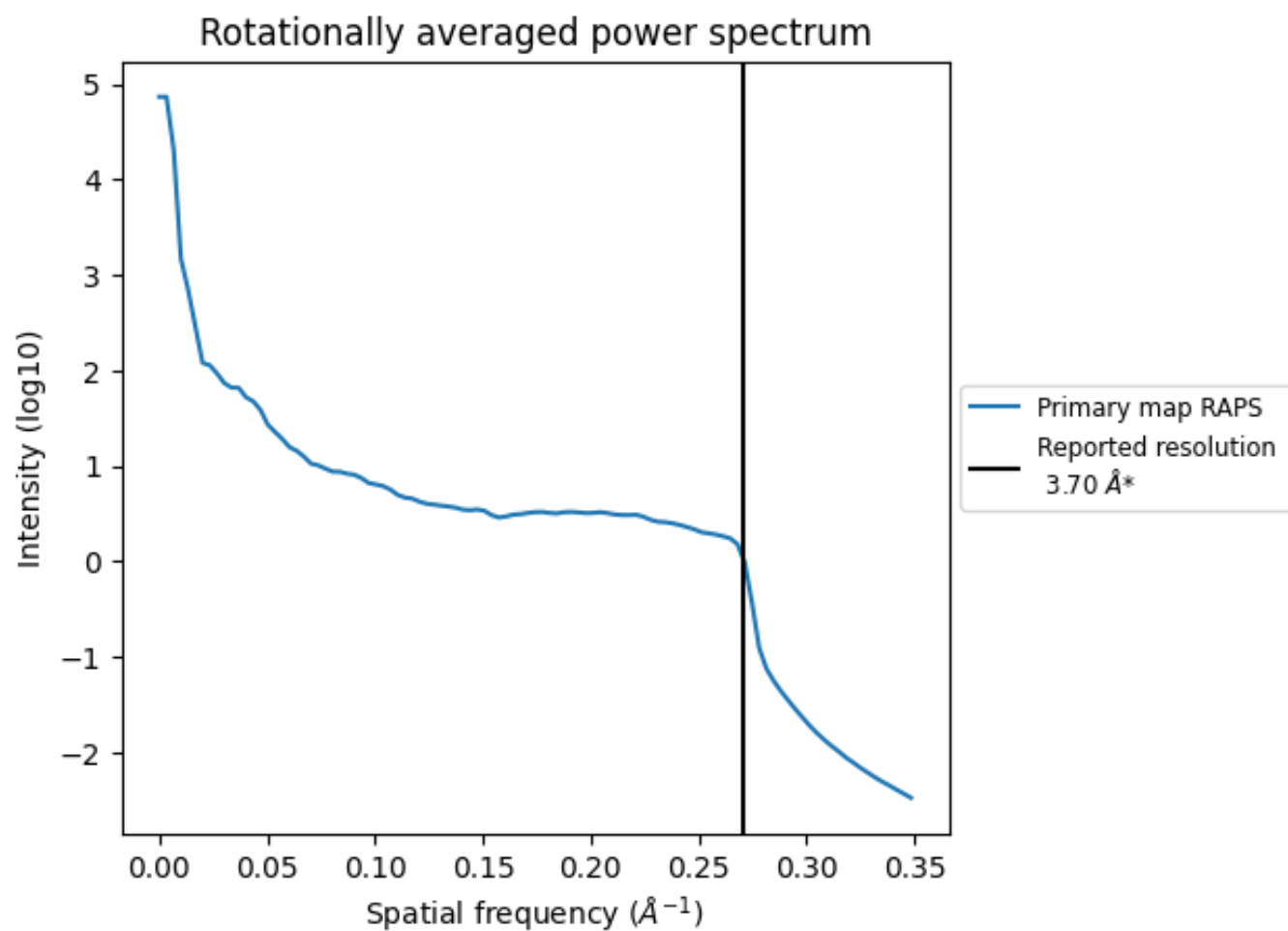
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296 nm<sup>3</sup>; this corresponds to an approximate mass of 268 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 ⓘ

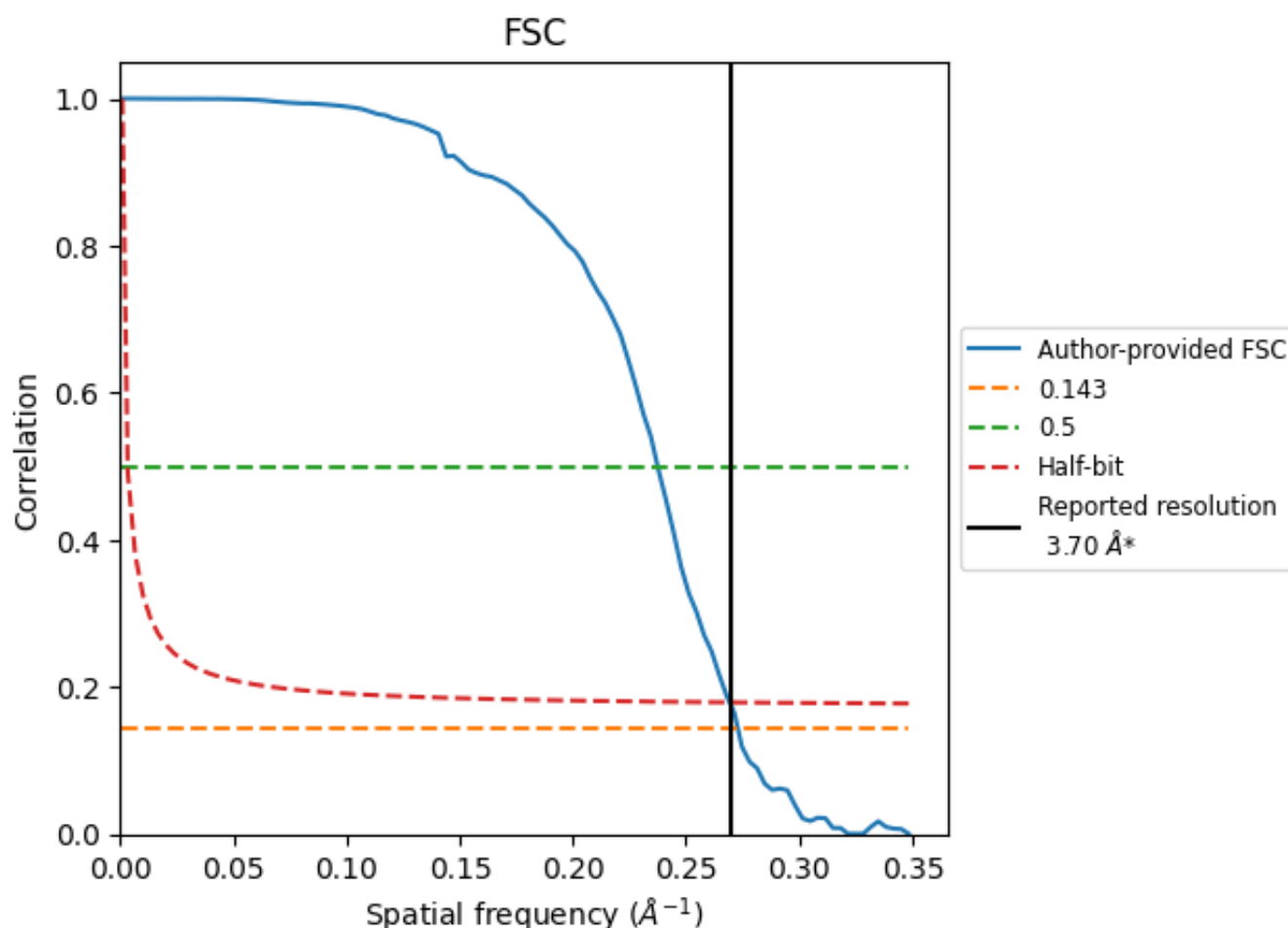


\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$

## 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 0.270  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

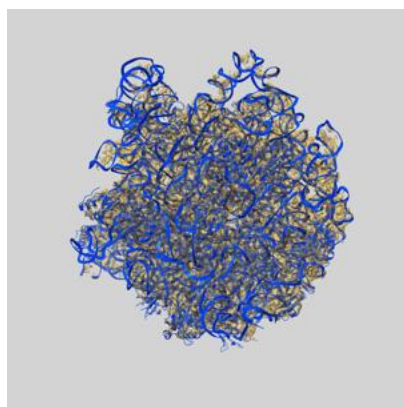
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.66	4.21	3.71
Unmasked-calculated*	-	-	-

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

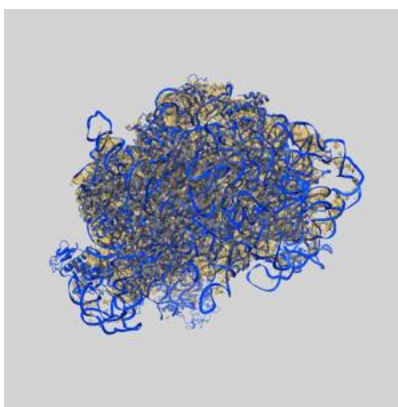
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8641 and PDB model 5V7Q. Per-residue inclusion information can be found in section 3 on page 10.

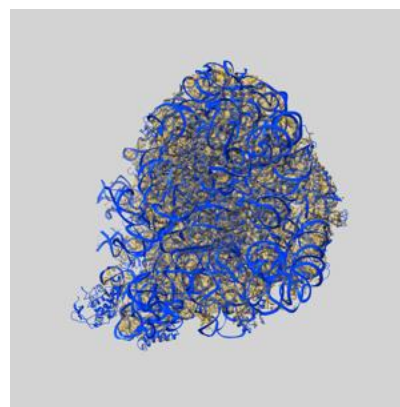
### 9.1 Map-model overlay [i](#)



X



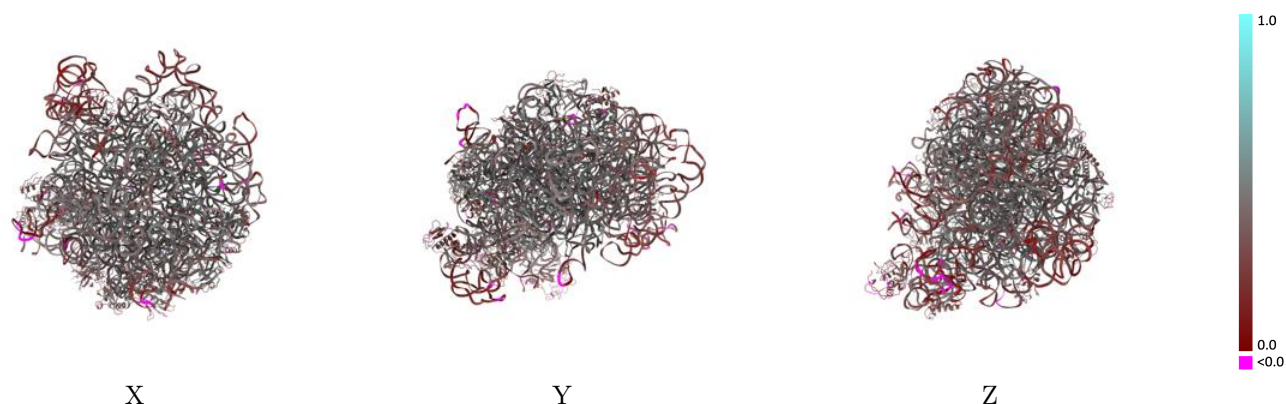
Y



Z

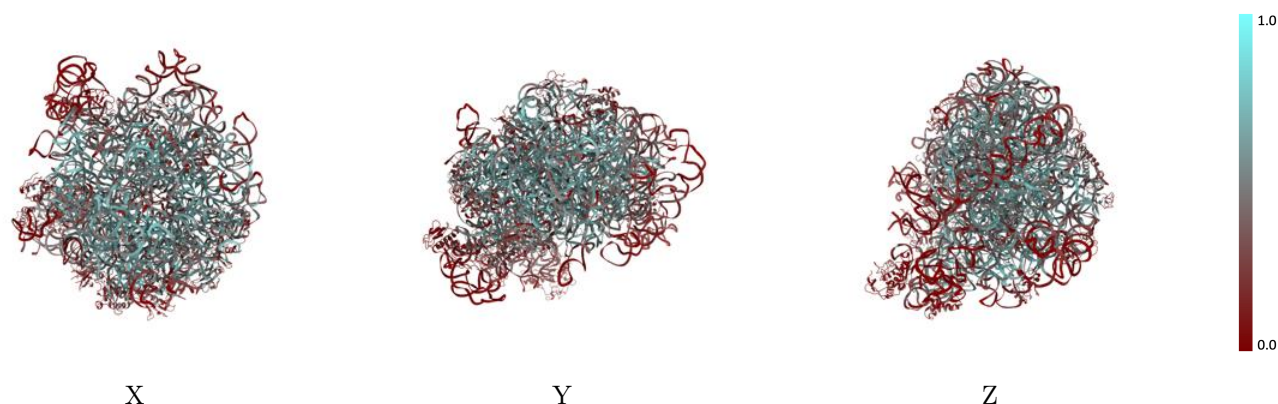
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



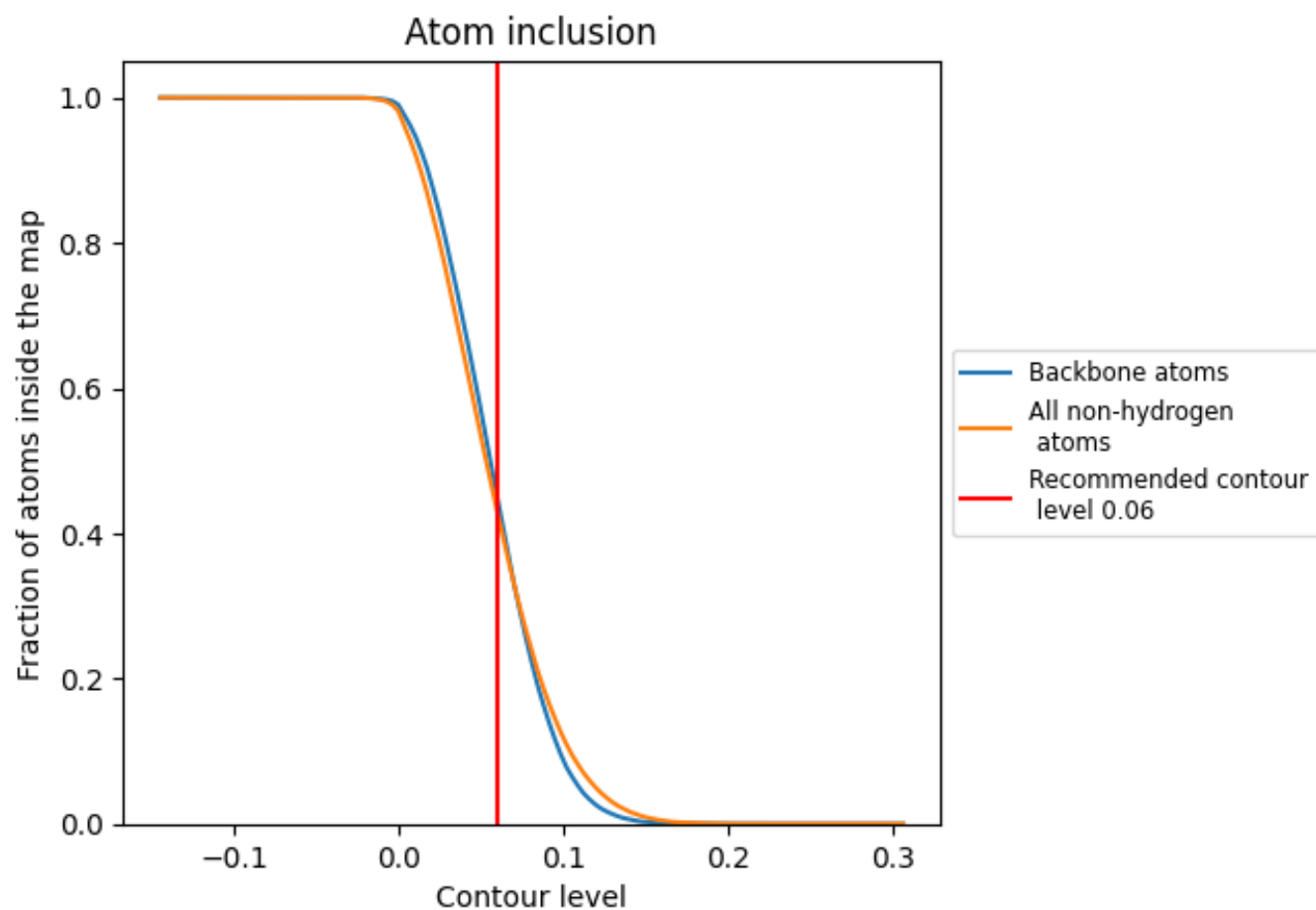
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 43% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4282	 0.3840
0	 0.3234	 0.3740
1	 0.3307	 0.4080
2	 0.5213	 0.4160
3	 0.3771	 0.4140
4	 0.2160	 0.3840
6	 0.0059	 0.1110
A	 0.4807	 0.3920
B	 0.3552	 0.3550
C	 0.4092	 0.4180
D	 0.3776	 0.4180
E	 0.3709	 0.3890
F	 0.0279	 0.2370
G	 0.0610	 0.2710
H	 0.0204	 0.2620
J	 0.3842	 0.3960
K	 0.2788	 0.3770
L	 0.3343	 0.4010
M	 0.1853	 0.3590
N	 0.4434	 0.4180
O	 0.2087	 0.3260
P	 0.2563	 0.3540
Q	 0.4882	 0.4220
R	 0.3083	 0.3730
S	 0.4143	 0.4100
T	 0.3103	 0.3710
U	 0.2570	 0.3490
V	 0.0425	 0.2480
W	 0.3894	 0.4110
X	 0.4013	 0.4050
Y	 0.3282	 0.3690
Z	 0.3538	 0.4160

