Full wwPDB EM Validation Report ⓘ

Nov 7, 2023 – 12:18 PM EST

PDB ID	:	6PJ6
EMDB ID	:	EMD-20353
Title	:	High resolution cryo-EM structure of E.coli 50S
Authors	:	Stojkovic, V.; Myasnikov, A.; Frost, A.; Fujimori, D.G.
Deposited on	:	2019-06-27
Resolution	:	2.20 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:

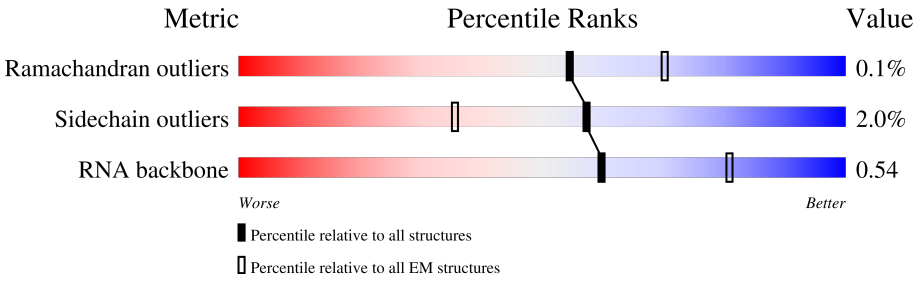
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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)
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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	2904	13% 83% 16%
2	J	118	9% 88% 12%
3	K	271	97%
4	L	209	9% 97%
5	M	201	15% 99%
6	N	177	94% 99%
7	O	176	41% 97%
8	P	149	87% 98%

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Mol	Chain	Length	Quality of chain
9	Q	134	100% 99%
10	R	142	97%
11	S	122	13% 97%
12	T	144	6% 98%
13	U	136	7% 96%
14	V	120	95% 5%
15	W	117	25% 98%
16	X	114	20% 100%
17	Y	117	94% 6%
18	Z	103	12% 96%
19	a	110	7% 100%
20	b	93	16% 99%
21	c	102	21% 98%
22	d	94	19% 100%
23	e	75	97%
24	f	77	13% 96%
25	g	62	29% 98%
26	h	58	7% 98%
27	i	56	9% 100%
28	j	50	20% 100%
29	k	46	96%
30	l	64	97%
31	m	38	8% 97%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 154828 atoms, of which 59910 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	I	2898	93536	27768	31307	11448	20115	2898	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	J	118	3810	1126	1281	464	821	118	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	K	271	4261	1294	2167	427	366	7	1	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	L	209	3175	979	1610	288	294	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	M	201	3171	974	1619	283	290	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	N	177	2855	899	1444	249	257	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	O	176	Total	C	H	N	O	S	0	0
			2694	832	1371	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	149	Total	C	H	N	O	S	0	0
			2258	699	1148	197	213	1		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Q	134	Total	C	H	N	O	S	0	0
			2007	619	1028	169	185	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	R	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	S	122	Total	C	H	N	O	S	0	0
			1950	587	1012	180	165	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	T	144	Total	C	H	N	O	S	0	0
			2169	654	1116	207	190	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	U	136	Total	C	H	N	O	S	0	0
			2229	686	1154	205	178	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	V	120	Total	C	H	N	O	S	0	0
			1960	593	1000	196	166	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	116	Total	C	H	N	O	0	0
			1815	552	923	178	162		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	X	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	117	Total	C	H	N	O	0	0
			1967	604	1020	192	151		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Z	103	Total	C	H	N	O	S	0	0
			1582	516	766	153	145	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	a	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	b	93	Total	C	H	N	O	S	0	0
			1546	466	807	139	132	2		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	102	Total	C	H	N	O	0	0
			1611	492	831	146	142		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	d	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	e	75	Total	C	H	N	O	S	0	0
			1156	356	581	116	102	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	f	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	g	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	h	58	Total	C	H	N	O	S	0	0
			937	281	488	87	79	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	i	56	Total	C	H	N	O	S	0	0
			902	269	458	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	50	Total	C	H	N	O	0	0
			849	263	440	75	71		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	k	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	l	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	m	38	Total	C	H	N	O	S	0	0
			642	185	340	65	48	4		

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	I	182	Total	Mg	0
			182	182	
32	J	1	Total	Mg	0
			1	1	
32	K	1	Total	Mg	0
			1	1	
32	L	1	Total	Mg	0
			1	1	

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
33	K	1	Total	Na	0
			1	1	

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
34	m	1	Total Zn 1 1	0

- Molecule 35 is water.

Mol	Chain	Residues	Atoms	AltConf
35	I	3347	Total O 3347 3347	0
35	J	62	Total O 62 62	0
35	K	59	Total O 59 59	0
35	L	41	Total O 41 41	0
35	M	42	Total O 42 42	0
35	N	14	Total O 14 14	0
35	O	13	Total O 13 13	0
35	P	6	Total O 6 6	0
35	Q	10	Total O 10 10	0
35	R	17	Total O 17 17	0
35	S	7	Total O 7 7	0
35	T	33	Total O 33 33	0
35	U	13	Total O 13 13	0
35	V	23	Total O 23 23	0
35	W	11	Total O 11 11	0
35	X	14	Total O 14 14	0
35	Y	33	Total O 33 33	0
35	Z	16	Total O 16 16	0
35	a	18	Total O 18 18	0

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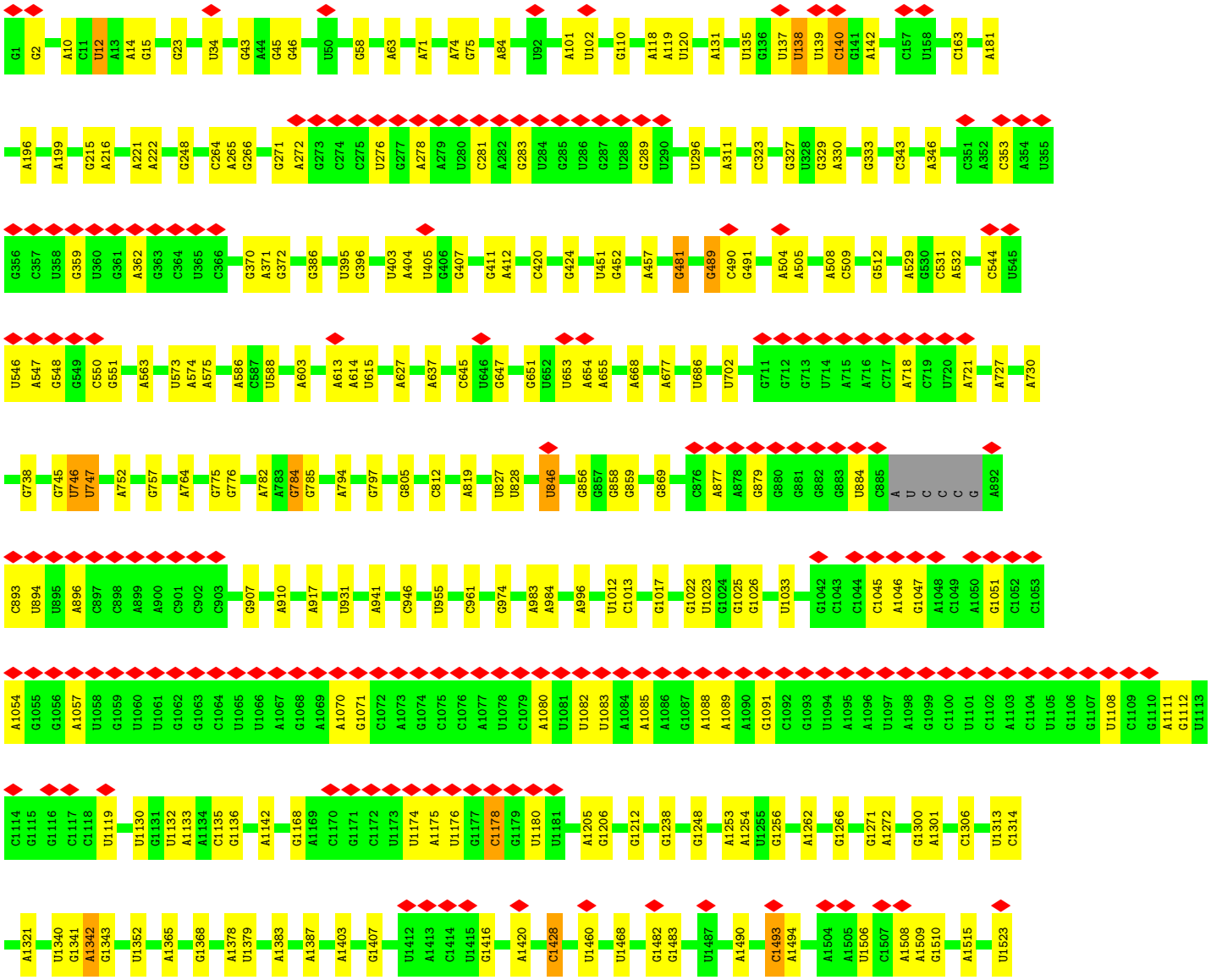
Mol	Chain	Residues	Atoms	AltConf
35	b	15	Total O 15 15	0
35	c	7	Total O 7 7	0
35	d	9	Total O 9 9	0
35	e	13	Total O 13 13	0
35	f	9	Total O 9 9	0
35	g	6	Total O 6 6	0
35	h	4	Total O 4 4	0
35	i	12	Total O 12 12	0
35	j	9	Total O 9 9	0
35	k	11	Total O 11 11	0
35	l	19	Total O 19 19	0
35	m	4	Total O 4 4	0

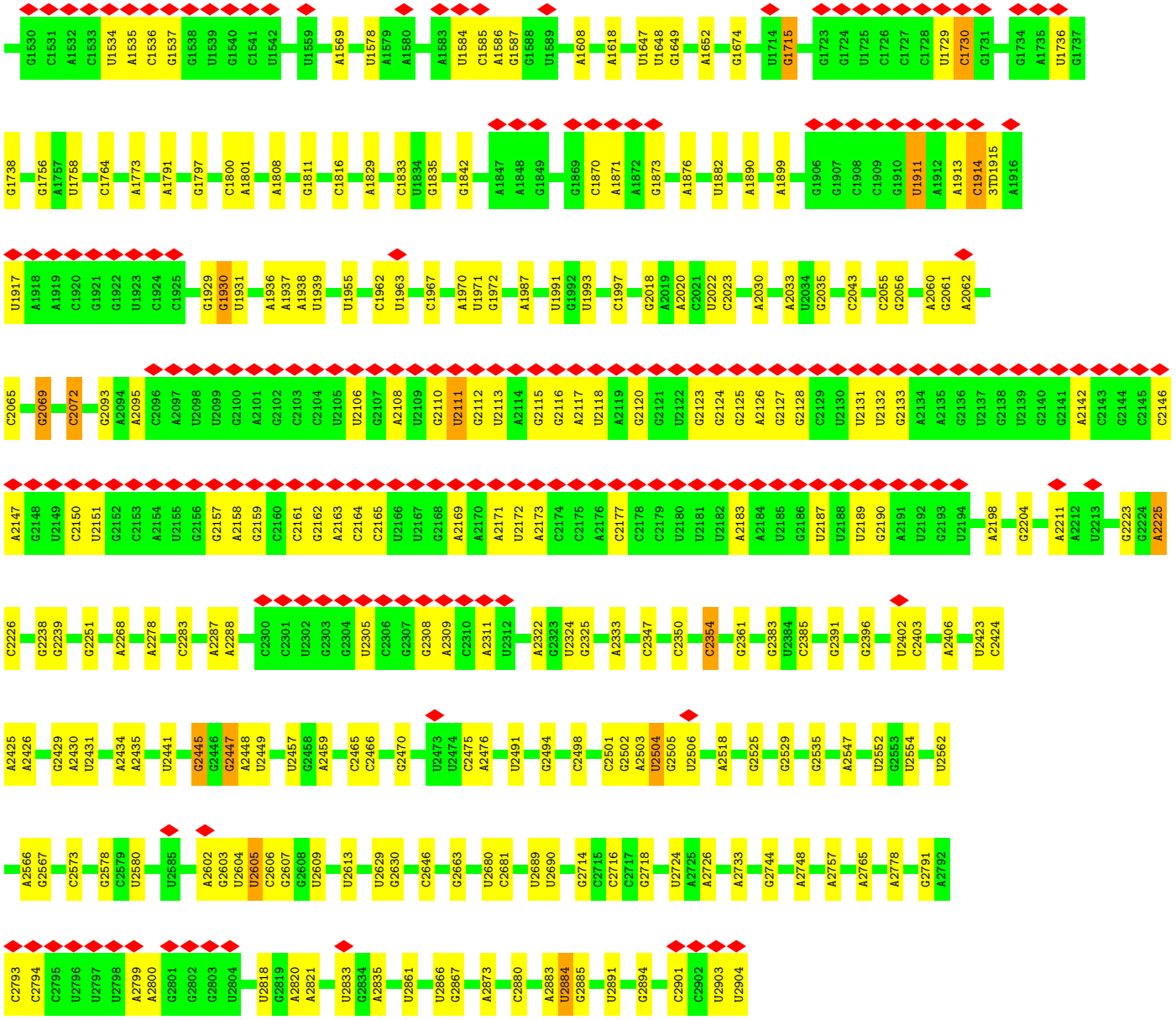
3 Residue-property plots (i)

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: 23S rRNA

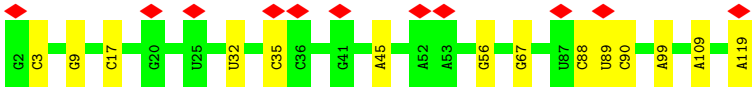
Chain I:





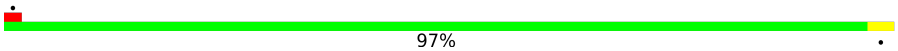
• Molecule 2: 5S rRNA

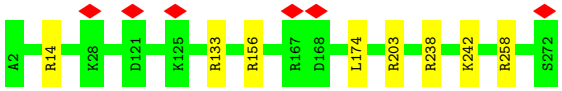
Chain J:



• Molecule 3: 50S ribosomal protein L2

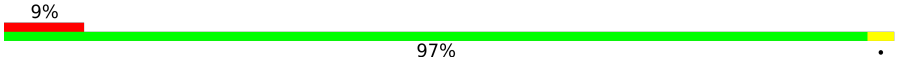
Chain K:

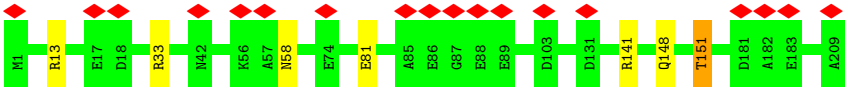




• Molecule 4: 50S ribosomal protein L3

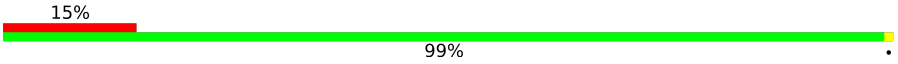
Chain L:

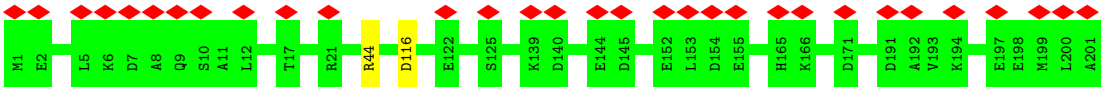




• Molecule 5: 50S ribosomal protein L4

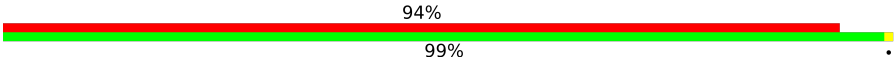
Chain M:

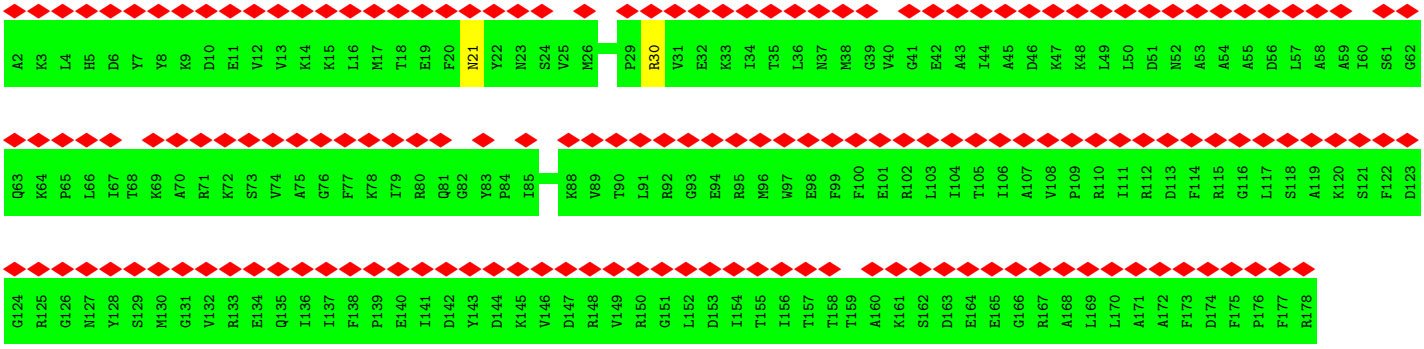




• Molecule 6: 50S ribosomal protein L5

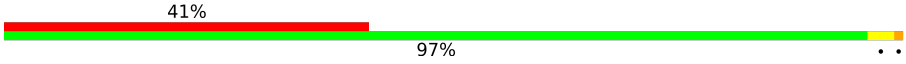
Chain N:

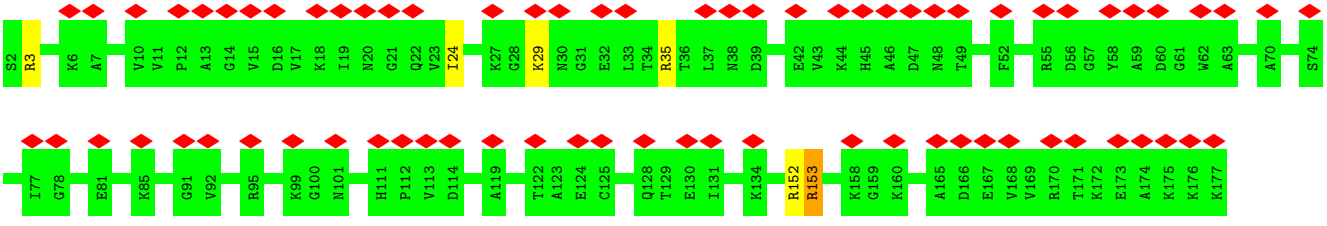




• Molecule 7: 50S ribosomal protein L6

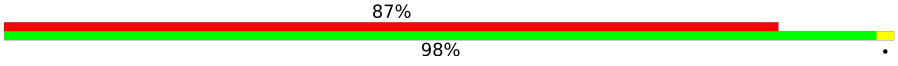
Chain O:

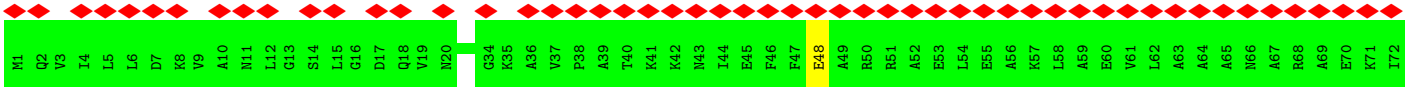


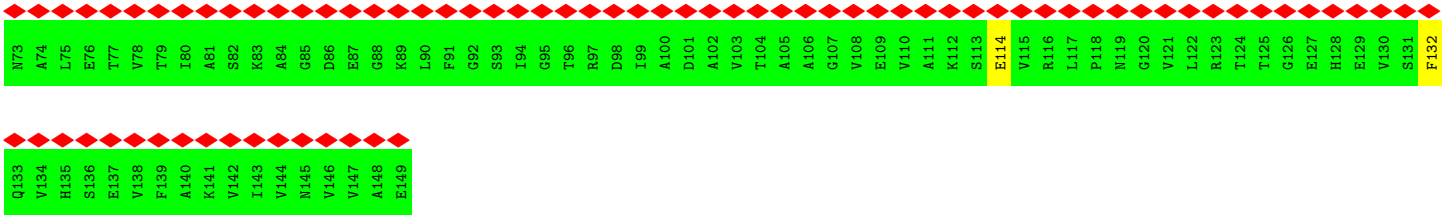


• Molecule 8: 50S ribosomal protein L9

Chain P:

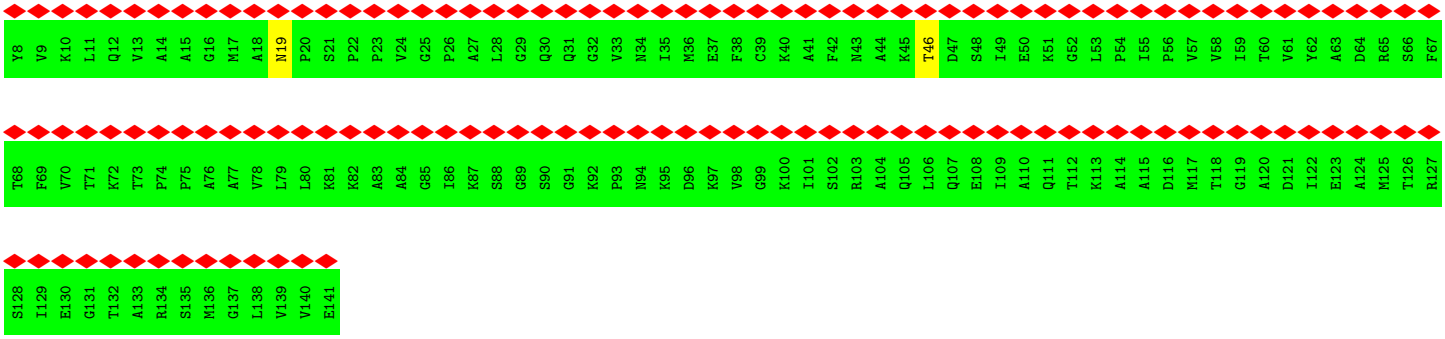






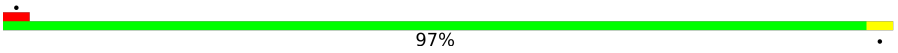
• Molecule 9: 50S ribosomal protein L11

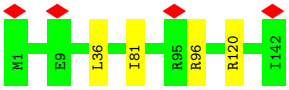
Chain Q:



• Molecule 10: 50S ribosomal protein L13

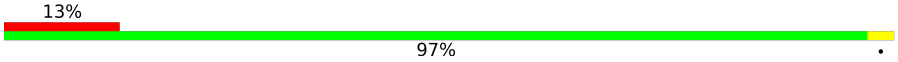
Chain R:

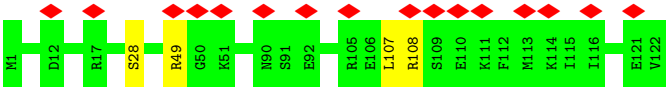




• Molecule 11: 50S ribosomal protein L14

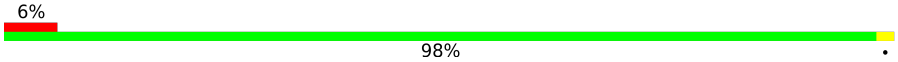
Chain S:

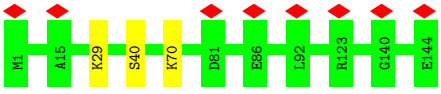




• Molecule 12: 50S ribosomal protein L15

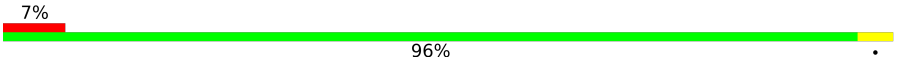
Chain T:

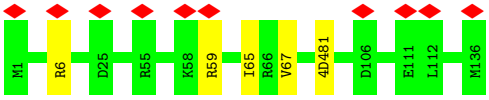




• Molecule 13: 50S ribosomal protein L16

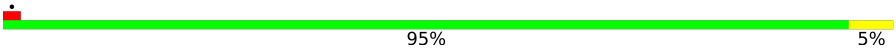
Chain U:





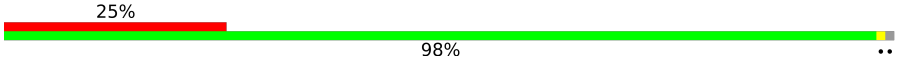
• Molecule 14: 50S ribosomal protein L17

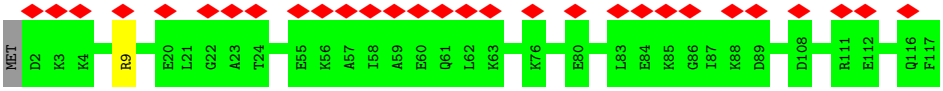
Chain V:



• Molecule 15: 50S ribosomal protein L18

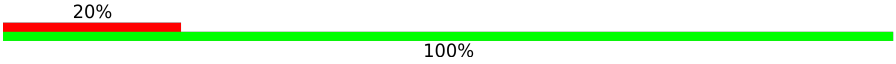
Chain W:

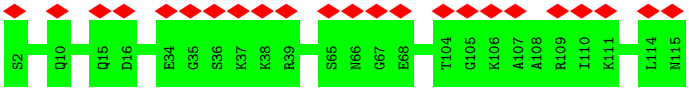




• Molecule 16: 50S ribosomal protein L19

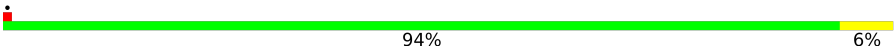
Chain X:

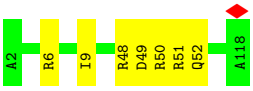




• Molecule 17: 50S ribosomal protein L20

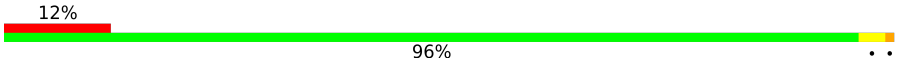
Chain Y:

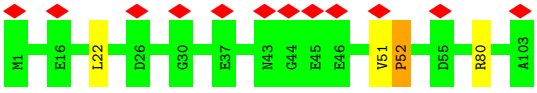




• Molecule 18: 50S ribosomal protein L21

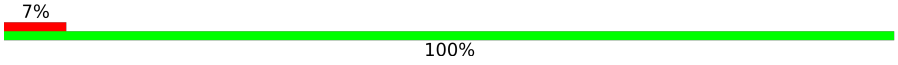
Chain Z:

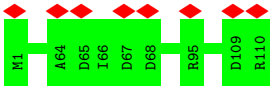




• Molecule 19: 50S ribosomal protein L22

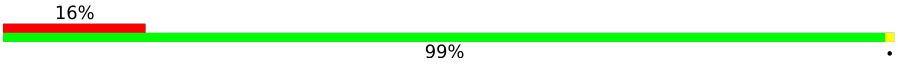
Chain a:

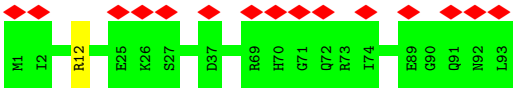




• Molecule 20: 50S ribosomal protein L23

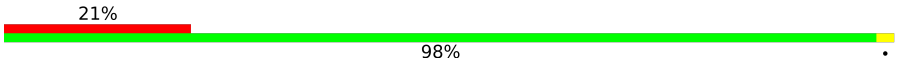
Chain b:

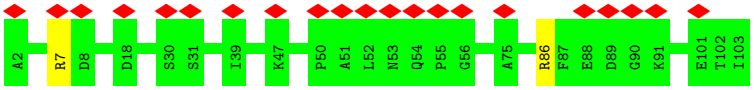




• Molecule 21: 50S ribosomal protein L24

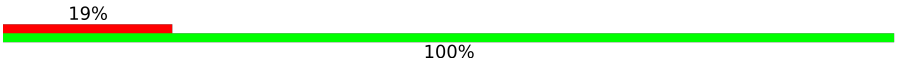
Chain c:

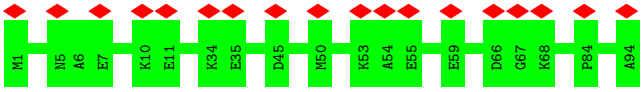




• Molecule 22: 50S ribosomal protein L25

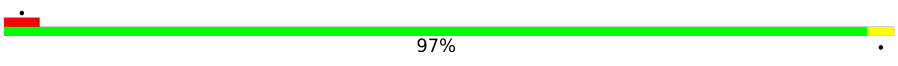
Chain d:

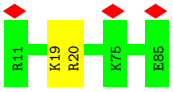




• Molecule 23: 50S ribosomal protein L27

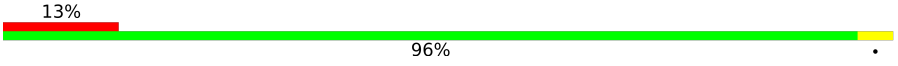
Chain e:

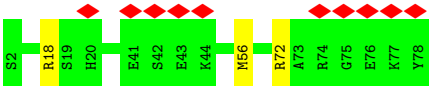




• Molecule 24: 50S ribosomal protein L28

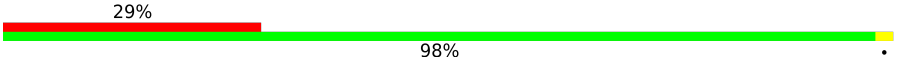
Chain f:

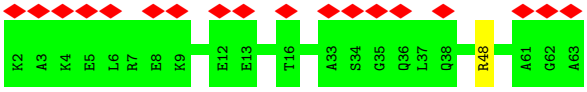




• Molecule 25: 50S ribosomal protein L29

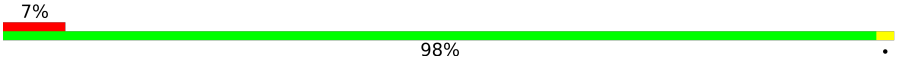
Chain g:

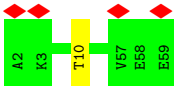




• Molecule 26: 50S ribosomal protein L30

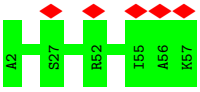
Chain h:





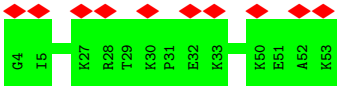
• Molecule 27: 50S ribosomal protein L32

Chain i:



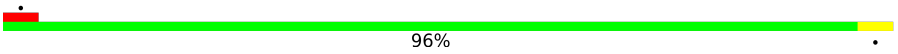
• Molecule 28: 50S ribosomal protein L33

Chain j:



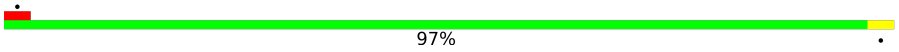
• Molecule 29: 50S ribosomal protein L34

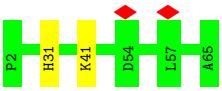
Chain k:



• Molecule 30: 50S ribosomal protein L35

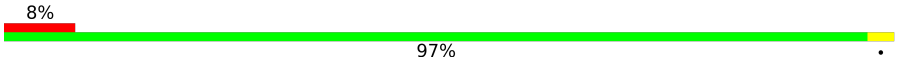
Chain l:

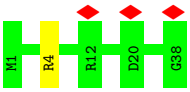




• Molecule 31: 50S ribosomal protein L36

Chain m:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141549	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	60827	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	66.611	Depositor
Minimum map value	-32.287	Depositor
Average map value	-0.035	Depositor
Map value standard deviation	2.434	Depositor
Recommended contour level	10.0	Depositor
Map size (Å)	420.864, 420.864, 420.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

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

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	I	1.15	4/69121 (0.0%)	1.06	63/107828 (0.1%)
2	J	0.94	0/2828	0.99	0/4410
3	K	0.69	0/2133	0.81	3/2866 (0.1%)
4	L	0.70	1/1586 (0.1%)	0.80	1/2134 (0.0%)
5	M	0.64	0/1571	0.71	0/2113
6	N	0.37	0/1435	0.68	0/1926
7	O	0.49	0/1343	0.70	1/1816 (0.1%)
8	P	0.44	0/1121	0.71	0/1515
9	Q	0.36	0/993	0.67	0/1341
10	R	0.67	0/1152	0.75	1/1551 (0.1%)
11	S	0.62	0/947	0.81	0/1268
12	T	0.73	0/1062	0.86	1/1413 (0.1%)
13	U	0.67	0/1081	0.80	0/1443
14	V	0.79	0/973	0.91	1/1301 (0.1%)
15	W	0.54	0/902	0.74	0/1209
16	X	0.59	0/929	0.71	0/1242
17	Y	0.81	0/960	0.99	7/1278 (0.5%)
18	Z	0.64	0/829	0.86	4/1107 (0.4%)
19	a	0.58	0/864	0.70	0/1156
20	b	0.55	0/745	0.62	0/994
21	c	0.52	0/788	0.71	0/1051
22	d	0.55	0/766	0.61	0/1025
23	e	0.70	0/582	0.79	1/769 (0.1%)
24	f	0.68	0/635	0.88	3/848 (0.4%)
25	g	0.46	0/502	0.62	0/667
26	h	0.59	0/453	0.69	0/605
27	i	0.68	0/450	0.84	0/599
28	j	0.60	0/416	0.67	0/554
29	k	0.75	0/380	1.06	2/498 (0.4%)
30	l	0.70	0/513	0.76	0/676
31	m	0.60	0/303	0.76	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	1.03	5/98363 (0.0%)	1.00	88/147600 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	1
8	P	0	1
9	Q	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2605	PSU	O3'-P	-6.01	1.53	1.61
1	I	1254	A	N9-C4	-5.43	1.34	1.37
1	I	727	A	N9-C4	-5.35	1.34	1.37
4	L	81	GLU	CD-OE2	-5.05	1.20	1.25
1	I	1652	A	N9-C4	-5.00	1.34	1.37

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	2607	G	N9-C1'-C2'	-10.93	99.80	114.00
1	I	12	U	C2-N1-C1'	10.18	129.91	117.70
1	I	846	U	C2-N1-C1'	9.83	129.49	117.70
1	I	2606	C	N1-C1'-C2'	-9.79	101.24	112.00
17	Y	6	ARG	NE-CZ-NH1	-8.52	116.04	120.30
1	I	12	U	N3-C2-O2	-8.32	116.38	122.20
1	I	2606	C	C4'-C3'-O3'	8.06	129.12	113.00
1	I	12	U	N1-C2-O2	7.59	128.12	122.80
18	Z	52	PRO	CA-N-CD	-7.55	100.93	111.50
1	I	2065	C	C6-N1-C2	-7.36	117.36	120.30
1	I	138	U	C5'-C4'-O4'	7.31	117.87	109.10
17	Y	48	ARG	NE-CZ-NH1	-7.27	116.66	120.30
1	I	512	G	O4'-C1'-N9	7.23	113.98	108.20
29	k	21	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	I	2072	C	C5-C4-N4	-6.75	115.48	120.20
1	I	846	U	C6-N1-C1'	-6.70	111.82	121.20
1	I	2065	C	N3-C2-O2	-6.62	117.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	140	C	N1-C2-O2	6.53	122.82	118.90
1	I	489	G	P-O3'-C3'	6.52	127.52	119.70
17	Y	50	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	I	1914	C	C2-N1-C1'	6.44	125.89	118.80
1	I	2225	A	P-O3'-C3'	6.37	127.34	119.70
1	I	846	U	N3-C2-O2	-6.31	117.78	122.20
1	I	12	U	C6-N1-C1'	-6.29	112.40	121.20
1	I	2501	C	N3-C2-O2	-6.11	117.63	121.90
1	I	846	U	N1-C2-O2	6.04	127.03	122.80
17	Y	49	ASP	CB-CA-C	6.02	122.43	110.40
1	I	140	C	N3-C2-O2	-5.98	117.72	121.90
1	I	2072	C	N3-C4-N4	5.98	122.18	118.00
1	I	1313	U	C2-N1-C1'	5.95	124.83	117.70
12	T	29	LYS	CB-CA-C	5.94	122.28	110.40
24	f	18	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	I	2501	C	N1-C2-O2	5.85	122.41	118.90
1	I	323	C	C5-C4-N4	-5.84	116.11	120.20
1	I	395	U	O4'-C1'-N1	5.84	112.87	108.20
17	Y	51	ARG	CG-CD-NE	-5.82	99.57	111.80
1	I	12	U	C6-N1-C2	-5.77	117.54	121.00
3	K	156	ARG	CB-CG-CD	-5.74	96.69	111.60
1	I	2607	G	C4'-C3'-O3'	5.72	124.45	113.00
23	e	20	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	I	2606	C	C1'-C2'-O2'	-5.68	93.56	110.60
1	I	12	U	C5-C6-N1	5.64	125.52	122.70
1	I	2018	G	C2-N3-C4	-5.61	109.10	111.90
10	R	120	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	I	333	G	N3-C2-N2	-5.51	116.04	119.90
18	Z	80	ARG	NE-CZ-NH2	-5.46	117.57	120.30
7	O	153	ARG	CB-CA-C	5.43	121.27	110.40
1	I	2884	U	N3-C4-O4	-5.43	115.60	119.40
1	I	1730	C	C6-N1-C2	-5.42	118.13	120.30
1	I	1342	A	P-O3'-C3'	5.39	126.17	119.70
1	I	2354	C	C6-N1-C2	-5.36	118.16	120.30
1	I	1715	G	N3-C2-N2	-5.35	116.15	119.90
3	K	258	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	I	797	G	C2-N3-C4	-5.34	109.23	111.90
29	k	21	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	I	2035	G	N3-C2-N2	-5.33	116.17	119.90
1	I	1930	G	P-O3'-C3'	5.31	126.07	119.70
1	I	1936	A	O4'-C1'-N9	5.31	112.45	108.20
3	K	238	ARG	NE-CZ-NH1	5.30	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	1178	C	C6-N1-C2	-5.28	118.19	120.30
1	I	2646	C	C6-N1-C2	-5.27	118.19	120.30
24	f	72	ARG	NE-CZ-NH1	5.26	122.93	120.30
24	f	18	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	I	1493	C	C2-N1-C1'	5.25	124.57	118.80
18	Z	80	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	I	2607	G	C1'-C2'-O2'	-5.23	94.90	110.60
1	I	784	G	P-O3'-C3'	5.21	125.95	119.70
14	V	114	GLU	CB-CA-C	-5.21	99.98	110.40
1	I	2111	U	N3-C2-O2	-5.20	118.56	122.20
1	I	2324	U	C5-C6-N1	5.17	125.28	122.70
4	L	148	GLN	CB-CA-C	5.16	120.71	110.40
17	Y	50	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	I	1314	C	C5-C4-N4	-5.12	116.62	120.20
1	I	452	G	N7-C8-N9	5.10	115.65	113.10
1	I	481	G	O4'-C1'-N9	5.09	112.28	108.20
1	I	2894	G	N3-C4-N9	-5.09	122.94	126.00
18	Z	51	VAL	C-N-CD	5.08	139.07	128.40
1	I	1936	A	N9-C4-C5	-5.08	103.77	105.80
1	I	1914	C	C6-N1-C2	-5.06	118.27	120.30
1	I	370	G	O4'-C1'-N9	-5.06	104.15	108.20
1	I	2447	G	P-O3'-C3'	5.06	125.77	119.70
1	I	140	C	C6-N1-C2	-5.05	118.28	120.30
17	Y	6	ARG	CB-CG-CD	-5.03	98.53	111.60
1	I	752	A	C5'-C4'-O4'	5.02	115.13	109.10
1	I	1797	G	N7-C8-N9	5.02	115.61	113.10
1	I	1428	C	C6-N1-C2	-5.01	118.30	120.30
1	I	278	A	C4-N9-C1'	5.00	135.31	126.30
1	I	1025	G	C8-N9-C4	-5.00	104.40	106.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	203[B]	ARG	Mainchain
8	P	114	GLU	Peptide
9	Q	19	ASN	Peptide
9	Q	46	THR	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
3	K	270/271 (100%)	254 (94%)	16 (6%)	0	100	100
4	L	207/209 (99%)	195 (94%)	11 (5%)	1 (0%)	29	31
5	M	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
6	N	175/177 (99%)	152 (87%)	23 (13%)	0	100	100
7	O	174/176 (99%)	162 (93%)	12 (7%)	0	100	100
8	P	147/149 (99%)	126 (86%)	21 (14%)	0	100	100
9	Q	132/134 (98%)	110 (83%)	22 (17%)	0	100	100
10	R	140/142 (99%)	140 (100%)	0	0	100	100
11	S	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
12	T	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
13	U	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
14	V	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
15	W	114/117 (97%)	105 (92%)	9 (8%)	0	100	100
16	X	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
17	Y	115/117 (98%)	115 (100%)	0	0	100	100
18	Z	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	15	14
19	a	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
20	b	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
21	c	100/102 (98%)	90 (90%)	10 (10%)	0	100	100
22	d	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
23	e	73/75 (97%)	73 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	f	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
25	g	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
26	h	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
27	i	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
28	j	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
29	k	44/46 (96%)	44 (100%)	0	0	100	100
30	l	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	m	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	3298/3357 (98%)	3112 (94%)	184 (6%)	2 (0%)	54	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	Z	52	PRO
4	L	151	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	217/216 (100%)	213 (98%)	4 (2%)	59	72
4	L	164/164 (100%)	159 (97%)	5 (3%)	41	53
5	M	165/165 (100%)	163 (99%)	2 (1%)	71	83
6	N	148/148 (100%)	146 (99%)	2 (1%)	67	80
7	O	137/137 (100%)	131 (96%)	6 (4%)	28	35
8	P	114/114 (100%)	112 (98%)	2 (2%)	59	72
9	Q	104/104 (100%)	104 (100%)	0	100	100
10	R	116/116 (100%)	113 (97%)	3 (3%)	46	58
11	S	103/103 (100%)	99 (96%)	4 (4%)	32	41
12	T	103/103 (100%)	101 (98%)	2 (2%)	57	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	U	108/108 (100%)	104 (96%)	4 (4%)	34 43
14	V	100/100 (100%)	95 (95%)	5 (5%)	24 30
15	W	86/87 (99%)	85 (99%)	1 (1%)	71 83
16	X	99/99 (100%)	99 (100%)	0	100 100
17	Y	89/89 (100%)	87 (98%)	2 (2%)	52 65
18	Z	84/84 (100%)	83 (99%)	1 (1%)	71 83
19	a	93/93 (100%)	93 (100%)	0	100 100
20	b	80/80 (100%)	79 (99%)	1 (1%)	69 81
21	c	83/83 (100%)	81 (98%)	2 (2%)	49 62
22	d	78/78 (100%)	78 (100%)	0	100 100
23	e	57/57 (100%)	56 (98%)	1 (2%)	59 72
24	f	67/67 (100%)	66 (98%)	1 (2%)	65 78
25	g	54/54 (100%)	53 (98%)	1 (2%)	57 71
26	h	48/48 (100%)	47 (98%)	1 (2%)	53 67
27	i	47/47 (100%)	47 (100%)	0	100 100
28	j	45/45 (100%)	45 (100%)	0	100 100
29	k	38/38 (100%)	37 (97%)	1 (3%)	46 58
30	l	51/51 (100%)	49 (96%)	2 (4%)	32 41
31	m	34/34 (100%)	33 (97%)	1 (3%)	42 54
All	All	2712/2712 (100%)	2658 (98%)	54 (2%)	57 69

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	14	ARG
3	K	133	ARG
3	K	174	LEU
3	K	242	LYS
4	L	13	ARG
4	L	33	ARG
4	L	58	ASN
4	L	141	ARG
4	L	151	THR
5	M	44	ARG
5	M	116	ASP

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Mol	Chain	Res	Type
6	N	21	ASN
6	N	30	ARG
7	O	3	ARG
7	O	24	ILE
7	O	29	LYS
7	O	35	ARG
7	O	152	ARG
7	O	153	ARG
8	P	48	GLU
8	P	132	PHE
10	R	36	LEU
10	R	81	ILE
10	R	96	ARG
11	S	28	SER
11	S	49	ARG
11	S	107	LEU
11	S	108	ARG
12	T	40	SER
12	T	70	LYS
13	U	6	ARG
13	U	59	ARG
13	U	65	ILE
13	U	67	VAL
14	V	1	MET
14	V	14	SER
14	V	20	MET
14	V	65	LEU
14	V	69	ARG
15	W	9	ARG
17	Y	9	ILE
17	Y	52	GLN
18	Z	22	LEU
20	b	12	ARG
21	c	7	ARG
21	c	86	ARG
23	e	19	LYS
24	f	56	MET
25	g	48	ARG
26	h	10	THR
29	k	44	VAL
30	l	31	HIS
30	l	41	LYS

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Mol	Chain	Res	Type
31	m	4	ARG

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

Mol	Chain	Res	Type
3	K	134	ASN
3	K	153	GLN
5	M	115	GLN
7	O	115	HIS
9	Q	30	GLN
12	T	35	HIS
14	V	11	ASN
17	Y	52	GLN
25	g	15	ASN
30	l	31	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2892/2904 (99%)	449 (15%)	23 (0%)
2	J	117/118 (99%)	14 (11%)	0
All	All	3009/3022 (99%)	463 (15%)	23 (0%)

All (463) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	2	G
1	I	10	A
1	I	12	U
1	I	14	A
1	I	15	G
1	I	23	G
1	I	34	U
1	I	43	G
1	I	45	G
1	I	46	G
1	I	58	G
1	I	63	A
1	I	71	A
1	I	74	A

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Mol	Chain	Res	Type
1	I	75	G
1	I	84	A
1	I	101	A
1	I	102	U
1	I	110	G
1	I	118	A
1	I	119	A
1	I	120	U
1	I	131	A
1	I	135	U
1	I	137	U
1	I	139	U
1	I	140	C
1	I	142	A
1	I	163	C
1	I	181	A
1	I	196	A
1	I	215	G
1	I	216	A
1	I	221	A
1	I	222	A
1	I	248	G
1	I	264	C
1	I	265	A
1	I	266	G
1	I	272	A
1	I	276	U
1	I	281	C
1	I	283	G
1	I	289	G
1	I	296	U
1	I	311	A
1	I	327	G
1	I	329	G
1	I	330	A
1	I	343	C
1	I	346	A
1	I	353	C
1	I	359	G
1	I	362	A
1	I	371	A
1	I	372	G

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Mol	Chain	Res	Type
1	I	386	G
1	I	396	G
1	I	403	U
1	I	405	U
1	I	407	G
1	I	411	G
1	I	412	A
1	I	420	C
1	I	424	G
1	I	451	U
1	I	457	A
1	I	481	G
1	I	490	C
1	I	491	G
1	I	504	A
1	I	505	A
1	I	508	A
1	I	509	C
1	I	529	A
1	I	531	C
1	I	532	A
1	I	544	C
1	I	546	U
1	I	547	A
1	I	548	G
1	I	550	C
1	I	551	G
1	I	563	A
1	I	573	U
1	I	574	A
1	I	575	A
1	I	586	A
1	I	588	U
1	I	603	A
1	I	613	A
1	I	614	A
1	I	615	U
1	I	627	A
1	I	637	A
1	I	645	C
1	I	647	G
1	I	651	G

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Mol	Chain	Res	Type
1	I	653	U
1	I	654	A
1	I	655	A
1	I	668	A
1	I	677	A
1	I	686	U
1	I	702	U
1	I	718	A
1	I	721	A
1	I	730	A
1	I	738	G
1	I	746	PSU
1	I	747	5MU
1	I	757	G
1	I	764	A
1	I	775	G
1	I	776	G
1	I	782	A
1	I	784	G
1	I	785	G
1	I	794	A
1	I	805	G
1	I	812	C
1	I	819	A
1	I	827	U
1	I	828	U
1	I	846	U
1	I	856	G
1	I	858	G
1	I	859	G
1	I	869	G
1	I	877	A
1	I	879	G
1	I	884	U
1	I	893	C
1	I	894	U
1	I	896	A
1	I	907	G
1	I	910	A
1	I	917	A
1	I	931	U
1	I	941	A

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Mol	Chain	Res	Type
1	I	946	C
1	I	961	C
1	I	974	G
1	I	983	A
1	I	996	A
1	I	1012	U
1	I	1013	C
1	I	1017	G
1	I	1022	G
1	I	1023	U
1	I	1026	G
1	I	1033	U
1	I	1045	C
1	I	1046	A
1	I	1047	G
1	I	1051	G
1	I	1054	A
1	I	1057	A
1	I	1070	A
1	I	1071	G
1	I	1080	A
1	I	1082	U
1	I	1083	U
1	I	1085	A
1	I	1088	A
1	I	1089	A
1	I	1091	G
1	I	1108	U
1	I	1111	A
1	I	1112	G
1	I	1119	U
1	I	1130	U
1	I	1132	U
1	I	1133	A
1	I	1135	C
1	I	1136	G
1	I	1142	A
1	I	1168	G
1	I	1174	U
1	I	1175	A
1	I	1176	U
1	I	1178	C

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Mol	Chain	Res	Type
1	I	1180	U
1	I	1206	G
1	I	1212	G
1	I	1238	G
1	I	1248	G
1	I	1253	A
1	I	1256	G
1	I	1262	A
1	I	1266	G
1	I	1271	G
1	I	1272	A
1	I	1300	G
1	I	1301	A
1	I	1306	C
1	I	1321	A
1	I	1340	U
1	I	1341	G
1	I	1343	G
1	I	1352	U
1	I	1365	A
1	I	1368	G
1	I	1378	A
1	I	1379	U
1	I	1383	A
1	I	1387	A
1	I	1403	A
1	I	1407	G
1	I	1416	G
1	I	1420	A
1	I	1428	C
1	I	1460	U
1	I	1468	U
1	I	1482	G
1	I	1483	G
1	I	1490	A
1	I	1493	C
1	I	1494	A
1	I	1506	U
1	I	1508	A
1	I	1509	A
1	I	1510	G
1	I	1515	A

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Mol	Chain	Res	Type
1	I	1523	U
1	I	1534	U
1	I	1535	A
1	I	1536	C
1	I	1537	G
1	I	1569	A
1	I	1578	U
1	I	1584	U
1	I	1585	C
1	I	1586	A
1	I	1587	G
1	I	1608	A
1	I	1647	U
1	I	1648	U
1	I	1649	G
1	I	1674	G
1	I	1715	G
1	I	1729	U
1	I	1730	C
1	I	1736	U
1	I	1738	G
1	I	1756	G
1	I	1758	U
1	I	1764	C
1	I	1773	A
1	I	1791	A
1	I	1800	C
1	I	1801	A
1	I	1808	A
1	I	1811	G
1	I	1816	C
1	I	1829	A
1	I	1833	C
1	I	1842	G
1	I	1870	C
1	I	1871	A
1	I	1873	G
1	I	1876	A
1	I	1882	U
1	I	1890	A
1	I	1899	A
1	I	1911	PSU

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Mol	Chain	Res	Type
1	I	1913	A
1	I	1914	C
1	I	1929	G
1	I	1930	G
1	I	1931	U
1	I	1937	A
1	I	1938	A
1	I	1955	U
1	I	1963	U
1	I	1967	C
1	I	1970	A
1	I	1971	U
1	I	1972	G
1	I	1987	A
1	I	1991	U
1	I	1993	U
1	I	1997	C
1	I	2020	A
1	I	2022	U
1	I	2023	C
1	I	2033	A
1	I	2043	C
1	I	2055	C
1	I	2056	G
1	I	2060	A
1	I	2061	G
1	I	2062	A
1	I	2069	G7M
1	I	2072	C
1	I	2093	G
1	I	2095	A
1	I	2106	U
1	I	2108	A
1	I	2110	G
1	I	2111	U
1	I	2112	G
1	I	2113	U
1	I	2115	G
1	I	2116	G
1	I	2117	A
1	I	2118	U
1	I	2120	G

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Mol	Chain	Res	Type
1	I	2123	G
1	I	2124	G
1	I	2125	G
1	I	2126	A
1	I	2127	G
1	I	2128	G
1	I	2131	U
1	I	2132	U
1	I	2133	G
1	I	2142	A
1	I	2146	C
1	I	2147	A
1	I	2150	C
1	I	2151	U
1	I	2157	G
1	I	2158	A
1	I	2159	G
1	I	2161	C
1	I	2162	G
1	I	2163	A
1	I	2164	C
1	I	2165	C
1	I	2169	A
1	I	2171	A
1	I	2172	U
1	I	2173	A
1	I	2177	C
1	I	2183	A
1	I	2187	U
1	I	2189	U
1	I	2190	G
1	I	2198	A
1	I	2204	G
1	I	2211	A
1	I	2223	G
1	I	2225	A
1	I	2226	C
1	I	2238	G
1	I	2239	G
1	I	2268	A
1	I	2278	A
1	I	2283	C

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Mol	Chain	Res	Type
1	I	2287	A
1	I	2288	A
1	I	2305	U
1	I	2308	G
1	I	2309	A
1	I	2311	A
1	I	2322	A
1	I	2325	G
1	I	2333	A
1	I	2347	C
1	I	2350	C
1	I	2354	C
1	I	2361	G
1	I	2383	G
1	I	2385	C
1	I	2391	G
1	I	2396	G
1	I	2402	U
1	I	2403	C
1	I	2406	A
1	I	2423	U
1	I	2424	C
1	I	2425	A
1	I	2426	A
1	I	2429	G
1	I	2430	A
1	I	2431	U
1	I	2434	A
1	I	2435	A
1	I	2441	U
1	I	2445	2MG
1	I	2447	G
1	I	2448	A
1	I	2459	A
1	I	2465	C
1	I	2466	C
1	I	2470	G
1	I	2475	C
1	I	2476	A
1	I	2491	U
1	I	2494	G
1	I	2502	G

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Mol	Chain	Res	Type
1	I	2504	PSU
1	I	2505	G
1	I	2506	U
1	I	2518	A
1	I	2525	G
1	I	2529	G
1	I	2535	G
1	I	2547	A
1	I	2554	U
1	I	2562	U
1	I	2566	A
1	I	2567	G
1	I	2573	C
1	I	2578	G
1	I	2602	A
1	I	2603	G
1	I	2605	PSU
1	I	2609	U
1	I	2613	U
1	I	2629	U
1	I	2630	G
1	I	2663	G
1	I	2681	C
1	I	2689	U
1	I	2690	U
1	I	2714	G
1	I	2716	C
1	I	2718	G
1	I	2724	U
1	I	2726	A
1	I	2733	A
1	I	2744	G
1	I	2748	A
1	I	2757	A
1	I	2765	A
1	I	2778	A
1	I	2791	G
1	I	2793	C
1	I	2794	C
1	I	2799	A
1	I	2800	A
1	I	2818	U

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Mol	Chain	Res	Type
1	I	2820	A
1	I	2821	A
1	I	2833	U
1	I	2835	A
1	I	2861	U
1	I	2867	G
1	I	2873	A
1	I	2880	C
1	I	2883	A
1	I	2884	U
1	I	2885	G
1	I	2891	U
1	I	2901	C
1	I	2903	U
1	I	2904	U
2	J	3	C
2	J	9	G
2	J	17	C
2	J	32	U
2	J	35	C
2	J	45	A
2	J	56	G
2	J	67	G
2	J	88	C
2	J	89	U
2	J	90	C
2	J	99	A
2	J	109	A
2	J	119	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	138	U
1	I	199	A
1	I	271	G
1	I	404	A
1	I	489	G
1	I	504	A
1	I	784	G
1	I	984	A
1	I	1205	A

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Mol	Chain	Res	Type
1	I	1340	U
1	I	1342	A
1	I	1608	A
1	I	1930	G
1	I	2146	C
1	I	2162	G
1	I	2225	A
1	I	2425	A
1	I	2430	A
1	I	2447	G
1	I	2680	U
1	I	2866	U
1	I	2873	A
1	I	2903	U

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	4D4	U	81	13	9,11,12	2.58	3 (33%)	8,13,15	1.14	0
1	1MG	I	745	1	18,26,27	2.66	5 (27%)	19,39,42	1.50	5 (26%)
1	OMC	I	2498	32,1	19,22,23	2.70	7 (36%)	26,31,34	0.68	0
1	PSU	I	955	1	18,21,22	1.65	5 (27%)	22,30,33	1.77	4 (18%)
1	OMU	I	2552	1	19,22,23	2.84	8 (42%)	26,31,34	1.67	5 (19%)
1	5MC	I	1962	1	18,22,23	3.11	7 (38%)	26,32,35	1.16	2 (7%)
1	PSU	I	2605	1	18,21,22	3.03	10 (55%)	22,30,33	2.54	6 (27%)
1	PSU	I	2604	1	18,21,22	2.65	9 (50%)	22,30,33	2.65	5 (22%)
1	PSU	I	2580	1	18,21,22	1.84	6 (33%)	22,30,33	1.69	5 (22%)
1	5MU	I	1939	1	19,22,23	4.71	7 (36%)	28,32,35	3.59	9 (32%)
1	2MA	I	2503	1	17,25,26	2.33	5 (29%)	17,37,40	1.51	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MU	I	747	1	19,22,23	4.56	7 (36%)	28,32,35	3.59	8 (28%)
1	3TD	I	1915	1	18,22,23	4.18	6 (33%)	22,32,35	1.53	2 (9%)
1	PSU	I	746	1	18,21,22	1.64	6 (33%)	22,30,33	1.71	4 (18%)
1	6MZ	I	1618	1	18,25,26	1.85	3 (16%)	16,36,39	2.61	3 (18%)
1	2MG	I	1835	1	18,26,27	2.22	7 (38%)	16,38,41	1.25	3 (18%)
1	PSU	I	2457	1	18,21,22	1.65	4 (22%)	22,30,33	1.89	3 (13%)
1	H2U	I	2449	1	18,21,22	1.56	3 (16%)	21,30,33	0.60	0
1	PSU	I	1911	1	18,21,22	1.37	3 (16%)	22,30,33	2.17	3 (13%)
1	2MG	I	2445	1	18,26,27	2.23	7 (38%)	16,38,41	1.15	2 (12%)
1	PSU	I	1917	1	18,21,22	1.43	2 (11%)	22,30,33	1.87	4 (18%)
1	6MZ	I	2030	1	18,25,26	1.91	4 (22%)	16,36,39	2.98	4 (25%)
1	G7M	I	2069	1	20,26,27	2.10	7 (35%)	17,39,42	1.10	2 (11%)
1	OMG	I	2251	1	18,26,27	2.25	8 (44%)	19,38,41	1.32	3 (15%)
1	PSU	I	2504	32,1	18,21,22	1.69	5 (27%)	22,30,33	1.66	4 (18%)

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
13	4D4	U	81	13	-	2/11/12/14	-
1	1MG	I	745	1	-	0/3/25/26	0/3/3/3
1	OMC	I	2498	32,1	-	0/9/27/28	0/2/2/2
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2
1	5MC	I	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2605	1	-	2/7/25/26	0/2/2/2
1	PSU	I	2604	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	2MA	I	2503	1	-	1/3/25/26	0/3/3/3
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
1	3TD	I	1915	1	-	3/7/25/26	0/2/2/2
1	PSU	I	746	1	-	2/7/25/26	0/2/2/2
1	6MZ	I	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	I	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	H2U	I	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	I	1911	1	-	2/7/25/26	0/2/2/2
1	2MG	I	2445	1	-	2/5/27/28	0/3/3/3
1	PSU	I	1917	1	-	2/7/25/26	0/2/2/2
1	6MZ	I	2030	1	-	2/5/27/28	0/3/3/3
1	G7M	I	2069	1	-	2/3/25/26	0/3/3/3
1	OMG	I	2251	1	-	0/5/27/28	0/3/3/3
1	PSU	I	2504	32,1	-	2/7/25/26	0/2/2/2

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1915	3TD	C6-C5	12.30	1.49	1.35
1	I	1939	5MU	C2-N1	10.56	1.55	1.38
1	I	747	5MU	C2-N1	10.13	1.54	1.38
1	I	1939	5MU	C6-N1	10.11	1.55	1.38
1	I	747	5MU	C6-N1	9.91	1.55	1.38
1	I	1939	5MU	C4-C5	9.78	1.61	1.44
1	I	747	5MU	C4-C5	9.09	1.59	1.44
1	I	1915	3TD	C2-N1	9.04	1.48	1.37
1	I	745	1MG	C2-N2	7.89	1.48	1.34
1	I	1962	5MC	C6-C5	7.55	1.47	1.34
1	I	1939	5MU	C4-N3	-7.52	1.24	1.38
1	I	747	5MU	C4-N3	-7.50	1.24	1.38
1	I	2503	2MA	C2-N3	6.68	1.45	1.31
1	I	2552	OMU	C2-N1	6.47	1.48	1.38
1	I	2552	OMU	C2-N3	6.23	1.49	1.38
13	U	81	4D4	CZ-NE	6.12	1.45	1.33
1	I	1962	5MC	C4-N3	5.91	1.44	1.34
1	I	2030	6MZ	C6-N6	5.87	1.44	1.35
1	I	1618	6MZ	C6-N6	5.87	1.44	1.35
1	I	2605	PSU	C2-N1	-5.85	1.28	1.36
1	I	1939	5MU	C6-C5	5.84	1.44	1.34
1	I	1915	3TD	C6-N1	5.74	1.45	1.36
1	I	2498	OMC	C2-N3	5.66	1.47	1.36
1	I	747	5MU	C6-C5	5.62	1.43	1.34
1	I	1962	5MC	C2-N3	5.52	1.47	1.36
1	I	2498	OMC	C6-C5	5.34	1.47	1.35
1	I	2605	PSU	C4-N3	-5.34	1.28	1.38
1	I	2604	PSU	C4-N3	-5.28	1.29	1.38
1	I	2605	PSU	C2-N3	-5.06	1.28	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2251	OMG	C2-N3	5.02	1.45	1.33
1	I	1915	3TD	C2-N3	4.99	1.49	1.38
1	I	2552	OMU	C6-C5	4.91	1.46	1.35
1	I	2445	2MG	C2-N2	4.83	1.44	1.33
1	I	1835	2MG	C2-N2	4.74	1.43	1.33
1	I	2604	PSU	C2-N3	-4.58	1.29	1.37
1	I	2498	OMC	C4-N3	4.56	1.43	1.34
1	I	1835	2MG	C4-N3	4.48	1.48	1.37
1	I	2069	G7M	C2-N3	4.36	1.43	1.33
1	I	745	1MG	C2-N3	4.34	1.42	1.34
1	I	2503	2MA	C4-N3	4.33	1.47	1.37
1	I	2445	2MG	C4-N3	4.19	1.47	1.37
1	I	2251	OMG	C4-N3	4.17	1.47	1.37
1	I	2498	OMC	C4-N4	4.17	1.43	1.33
1	I	745	1MG	C4-N3	4.13	1.47	1.37
1	I	2552	OMU	C4-N3	4.07	1.45	1.38
1	I	2605	PSU	C6-N1	-4.07	1.29	1.36
1	I	2604	PSU	C6-N1	-4.06	1.29	1.36
1	I	2604	PSU	C2-N1	-4.05	1.31	1.36
1	I	1835	2MG	C2-N1	4.03	1.43	1.36
1	I	2445	2MG	C2-N1	4.02	1.43	1.36
1	I	2069	G7M	C4-N3	4.01	1.47	1.37
1	I	2580	PSU	C4-N3	-3.91	1.31	1.38
1	I	1962	5MC	C2-N1	3.83	1.48	1.40
1	I	2504	PSU	C4-N3	-3.83	1.31	1.38
1	I	2069	G7M	C2-N2	3.80	1.43	1.34
1	I	1917	PSU	C6-C5	3.78	1.39	1.35
1	I	2449	H2U	C2-N3	-3.75	1.31	1.38
1	I	745	1MG	O6-C6	-3.72	1.15	1.22
1	I	746	PSU	C4-N3	-3.71	1.32	1.38
1	I	2498	OMC	C2-N1	3.67	1.47	1.40
1	I	2449	H2U	C4-N3	-3.62	1.31	1.37
1	I	1962	5MC	C6-N1	3.59	1.44	1.38
1	I	2605	PSU	O5'-C5'	-3.57	1.36	1.44
1	I	1962	5MC	C4-N4	3.57	1.43	1.34
1	I	2251	OMG	C2-N2	3.53	1.42	1.34
1	I	2580	PSU	C2-N1	-3.43	1.32	1.36
1	I	2457	PSU	C4-N3	-3.43	1.32	1.38
1	I	2503	2MA	C5-C4	-3.43	1.34	1.43
1	I	2580	PSU	C6-C5	3.42	1.39	1.35
1	I	955	PSU	C2-N1	-3.35	1.32	1.36
1	I	1911	PSU	C6-C5	3.33	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	U	81	4D4	CZ-NH2	3.33	1.45	1.32
1	I	955	PSU	C4-N3	-3.32	1.32	1.38
1	I	747	5MU	O4-C4	-3.28	1.17	1.23
1	I	2605	PSU	C2'-C1'	-3.23	1.49	1.53
1	I	2449	H2U	C2-N1	-3.20	1.31	1.35
1	I	747	5MU	O2-C2	-3.19	1.17	1.23
1	I	2604	PSU	C1'-C5	-3.16	1.43	1.50
1	I	2552	OMU	O4-C4	-3.15	1.18	1.24
1	I	2498	OMC	O2-C2	-3.15	1.17	1.23
1	I	1939	5MU	O4-C4	-3.15	1.17	1.23
1	I	2069	G7M	C6-N1	3.10	1.42	1.37
1	I	1962	5MC	O2-C2	-3.08	1.18	1.23
1	I	2457	PSU	C2-N3	-3.05	1.32	1.37
1	I	1915	3TD	C4-N3	3.02	1.46	1.40
1	I	2457	PSU	C2-N1	-3.01	1.32	1.36
1	I	2504	PSU	C6-C5	2.99	1.38	1.35
1	I	2445	2MG	C5-C4	-2.98	1.35	1.43
1	I	2604	PSU	C2'-C1'	-2.98	1.49	1.53
1	I	746	PSU	C2-N3	-2.97	1.32	1.37
1	I	2580	PSU	C2-N3	-2.95	1.32	1.37
1	I	2030	6MZ	C5-C4	-2.93	1.33	1.40
1	I	1939	5MU	O2-C2	-2.92	1.17	1.23
1	I	1618	6MZ	C5-C4	-2.91	1.33	1.40
1	I	2498	OMC	C6-N1	2.88	1.44	1.38
1	I	2251	OMG	C5-C4	-2.83	1.35	1.43
1	I	2069	G7M	C5-C6	2.77	1.52	1.45
1	I	1835	2MG	C5-C4	-2.76	1.36	1.43
1	I	2445	2MG	O6-C6	-2.73	1.17	1.23
1	I	955	PSU	C2-N3	-2.72	1.32	1.37
1	I	746	PSU	O4'-C1'	-2.70	1.40	1.43
1	I	2504	PSU	C2-N1	-2.70	1.33	1.36
1	I	1917	PSU	C4-N3	-2.69	1.33	1.38
1	I	2552	OMU	O2-C2	-2.68	1.18	1.23
1	I	2503	2MA	C6-N1	2.67	1.43	1.38
1	I	2251	OMG	O6-C6	-2.65	1.17	1.23
1	I	2504	PSU	C2-N3	-2.61	1.33	1.37
1	I	2069	G7M	O6-C6	-2.60	1.18	1.23
1	I	2251	OMG	C5-C6	2.58	1.52	1.47
1	I	2604	PSU	O4-C4	-2.56	1.18	1.23
1	I	2251	OMG	C6-N1	2.53	1.41	1.37
1	I	2457	PSU	C6-C5	2.53	1.38	1.35
1	I	2030	6MZ	C6-N1	-2.51	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2552	OMU	C6-N1	2.50	1.44	1.38
1	I	1835	2MG	O6-C6	-2.49	1.18	1.23
1	I	2604	PSU	O2-C2	-2.48	1.18	1.23
1	I	2445	2MG	C5-C6	2.46	1.52	1.47
1	I	1835	2MG	C5-C6	2.45	1.52	1.47
1	I	1911	PSU	C4-N3	-2.44	1.34	1.38
1	I	2605	PSU	O4'-C4'	-2.43	1.39	1.45
1	I	1915	3TD	O2-C2	-2.42	1.18	1.23
1	I	1835	2MG	C6-N1	2.40	1.41	1.37
1	I	2504	PSU	C6-N1	-2.37	1.32	1.36
1	I	955	PSU	C6-N1	-2.37	1.32	1.36
1	I	745	1MG	C5-C4	-2.35	1.37	1.43
1	I	2030	6MZ	C5-N7	-2.33	1.31	1.39
1	I	2604	PSU	O4'-C1'	-2.32	1.40	1.43
1	I	746	PSU	C6-C5	2.32	1.38	1.35
1	I	2445	2MG	C6-N1	2.31	1.41	1.37
13	U	81	4D4	CZ-NH1	-2.28	1.25	1.34
1	I	2605	PSU	O4-C4	-2.23	1.19	1.23
1	I	2580	PSU	O4'-C1'	-2.22	1.40	1.43
1	I	2251	OMG	C2-N1	2.19	1.43	1.37
1	I	2552	OMU	C5-C4	2.15	1.48	1.43
1	I	2580	PSU	C6-N1	-2.15	1.32	1.36
1	I	1618	6MZ	C5-N7	-2.14	1.31	1.39
1	I	2605	PSU	C3'-C2'	-2.13	1.47	1.53
1	I	955	PSU	C6-C5	2.11	1.37	1.35
1	I	2069	G7M	C5-C4	-2.10	1.34	1.39
1	I	746	PSU	C6-N1	-2.09	1.32	1.36
1	I	2605	PSU	C3'-C4'	-2.07	1.47	1.53
1	I	2503	2MA	C2-N1	2.05	1.42	1.36
1	I	746	PSU	C2-N1	-2.04	1.34	1.36
1	I	1911	PSU	C2-N1	-2.01	1.34	1.36

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	1939	5MU	C5-C4-N3	12.20	125.73	115.31
1	I	747	5MU	C5-C4-N3	11.59	125.20	115.31
1	I	747	5MU	C5-C6-N1	-9.34	113.73	123.34
1	I	2030	6MZ	C1'-N9-C4	-9.14	110.59	126.64
1	I	1939	5MU	C5-C6-N1	-9.06	114.02	123.34
1	I	1618	6MZ	C1'-N9-C4	-8.51	111.69	126.64
1	I	2604	PSU	N1-C2-N3	8.05	124.25	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	2605	PSU	N1-C2-N3	7.20	123.29	115.13
1	I	1911	PSU	N1-C2-N3	6.87	122.91	115.13
1	I	2457	PSU	N1-C2-N3	6.20	122.15	115.13
1	I	1917	PSU	N1-C2-N3	5.92	121.84	115.13
1	I	747	5MU	O4-C4-C5	-5.80	118.18	124.90
1	I	2604	PSU	C4-N3-C2	-5.70	118.12	126.34
1	I	955	PSU	N1-C2-N3	5.36	121.20	115.13
1	I	746	PSU	N1-C2-N3	5.31	121.14	115.13
1	I	2504	PSU	N1-C2-N3	5.25	121.08	115.13
1	I	2552	OMU	C4-N3-C2	-5.17	119.76	126.58
1	I	747	5MU	C4-N3-C2	-5.13	120.70	127.35
1	I	2580	PSU	N1-C2-N3	5.05	120.85	115.13
1	I	1939	5MU	O4-C4-C5	-4.98	119.13	124.90
1	I	1618	6MZ	N3-C2-N1	-4.92	120.99	128.68
1	I	747	5MU	N3-C2-N1	4.92	121.42	114.89
1	I	1939	5MU	C4-N3-C2	-4.90	121.01	127.35
1	I	2030	6MZ	C9-N6-C6	4.76	126.97	122.87
1	I	1915	3TD	N1-C2-N3	4.71	119.85	116.14
1	I	2030	6MZ	N3-C2-N1	-4.63	121.45	128.68
1	I	2605	PSU	C4-N3-C2	-4.52	119.83	126.34
1	I	1939	5MU	C5M-C5-C4	4.47	123.69	118.77
1	I	1911	PSU	C4-N3-C2	-4.44	119.94	126.34
1	I	1939	5MU	N3-C2-N1	4.38	120.70	114.89
1	I	747	5MU	O2-C2-N1	-4.32	117.05	122.79
1	I	1911	PSU	O2-C2-N1	-4.24	118.12	122.79
1	I	1915	3TD	C4-N3-C2	-4.17	120.08	124.61
1	I	1939	5MU	C5M-C5-C6	-3.97	117.54	122.85
1	I	2605	PSU	C5'-C4'-C3'	-3.85	100.75	115.18
1	I	955	PSU	O2-C2-N1	-3.82	118.59	122.79
1	I	2503	2MA	C5-C6-N1	3.81	120.60	114.02
1	I	2605	PSU	C6-C5-C4	-3.77	115.56	118.20
1	I	2604	PSU	O2-C2-N3	-3.71	114.81	121.82
1	I	1917	PSU	C4-N3-C2	-3.71	121.00	126.34
1	I	2552	OMU	N3-C2-N1	3.67	119.77	114.89
1	I	747	5MU	C5M-C5-C6	-3.53	118.14	122.85
1	I	1962	5MC	CM5-C5-C6	-3.49	118.18	122.85
1	I	2457	PSU	C4-N3-C2	-3.48	121.32	126.34
1	I	745	1MG	C5-C6-N1	3.42	119.04	113.90
1	I	746	PSU	C4-N3-C2	-3.35	121.51	126.34
1	I	2457	PSU	O2-C2-N1	-3.34	119.11	122.79
1	I	2580	PSU	O2-C2-N1	-3.32	119.14	122.79
1	I	1939	5MU	O2-C2-N1	-3.30	118.41	122.79

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	745	1MG	CM1-N1-C6	3.20	121.92	117.55
1	I	747	5MU	C5M-C5-C4	3.15	122.23	118.77
1	I	2552	OMU	C5-C4-N3	3.13	119.52	114.84
1	I	1835	2MG	C5-C6-N1	3.10	119.42	113.95
1	I	1917	PSU	O2-C2-N1	-3.06	119.42	122.79
1	I	746	PSU	C6-C5-C4	-3.01	116.09	118.20
1	I	2580	PSU	C6-C5-C4	-2.98	116.11	118.20
1	I	1618	6MZ	C9-N6-C6	2.97	125.43	122.87
1	I	2605	PSU	O2-C2-N3	-2.96	116.23	121.82
1	I	2251	OMG	C5-C6-N1	2.96	119.18	113.95
1	I	2030	6MZ	C2-N1-C6	2.93	119.10	116.59
1	I	2504	PSU	O2-C2-N1	-2.89	119.61	122.79
1	I	2445	2MG	C5-C6-N1	2.88	119.05	113.95
1	I	955	PSU	C4-N3-C2	-2.85	122.24	126.34
1	I	2552	OMU	O4-C4-C5	-2.82	120.20	125.16
1	I	2251	OMG	C2-N1-C6	-2.79	119.96	125.10
1	I	2503	2MA	CM2-C2-N1	2.73	122.30	116.23
1	I	1962	5MC	C5-C6-N1	-2.64	120.62	123.34
1	I	1939	5MU	O4-C4-N3	-2.60	115.14	120.12
1	I	2503	2MA	C8-N7-C5	2.56	107.87	102.99
1	I	745	1MG	O6-C6-C5	-2.55	119.67	124.19
1	I	2504	PSU	C4-N3-C2	-2.53	122.69	126.34
1	I	2604	PSU	O4'-C4'-C3'	-2.52	100.12	105.11
1	I	2445	2MG	C8-N7-C5	2.51	107.77	102.99
1	I	2504	PSU	C6-C5-C4	-2.45	116.48	118.20
1	I	2069	G7M	N2-C2-N1	2.45	121.93	116.71
1	I	955	PSU	C6-C5-C4	-2.39	116.53	118.20
1	I	2503	2MA	N1-C2-N3	-2.36	119.14	123.06
1	I	1917	PSU	C6-C5-C4	-2.33	116.57	118.20
1	I	2069	G7M	C2-N1-C6	-2.31	120.85	125.10
1	I	2580	PSU	C4-N3-C2	-2.27	123.06	126.34
1	I	745	1MG	CM1-N1-C2	-2.27	118.36	120.72
1	I	2251	OMG	C8-N7-C5	2.26	107.30	102.99
1	I	1835	2MG	O6-C6-C5	-2.22	120.04	124.37
1	I	2552	OMU	O2-C2-N1	-2.20	119.86	122.79
1	I	2604	PSU	O4-C4-C5	-2.14	118.46	124.05
1	I	745	1MG	C8-N7-C5	2.13	107.06	102.99
1	I	2605	PSU	O2-C2-N1	-2.10	120.48	122.79
1	I	1835	2MG	C8-N7-C5	2.08	106.95	102.99
1	I	2580	PSU	O4'-C1'-C2'	2.06	108.05	105.14
1	I	746	PSU	O2-C2-N1	-2.04	120.54	122.79

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	1911	PSU	O4'-C4'-C5'-O5'
1	I	1915	3TD	C3'-C4'-C5'-O5'
1	I	1915	3TD	O4'-C4'-C5'-O5'
1	I	2445	2MG	C3'-C4'-C5'-O5'
1	I	2504	PSU	O4'-C4'-C5'-O5'
1	I	2605	PSU	C3'-C4'-C5'-O5'
1	I	1911	PSU	C3'-C4'-C5'-O5'
1	I	1917	PSU	O4'-C4'-C5'-O5'
1	I	2030	6MZ	O4'-C4'-C5'-O5'
1	I	2030	6MZ	C3'-C4'-C5'-O5'
1	I	2504	PSU	C3'-C4'-C5'-O5'
1	I	1917	PSU	C3'-C4'-C5'-O5'
1	I	2605	PSU	O4'-C4'-C5'-O5'
1	I	2445	2MG	O4'-C4'-C5'-O5'
1	I	2069	G7M	C4'-C5'-O5'-P
13	U	81	4D4	CG-CD-NE-CZ
1	I	1915	3TD	O4'-C1'-C5-C4
1	I	2503	2MA	O4'-C4'-C5'-O5'
1	I	746	PSU	O4'-C4'-C5'-O5'
1	I	746	PSU	C3'-C4'-C5'-O5'
1	I	2069	G7M	O4'-C4'-C5'-O5'
13	U	81	4D4	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 187 ligands modelled in this entry, 187 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

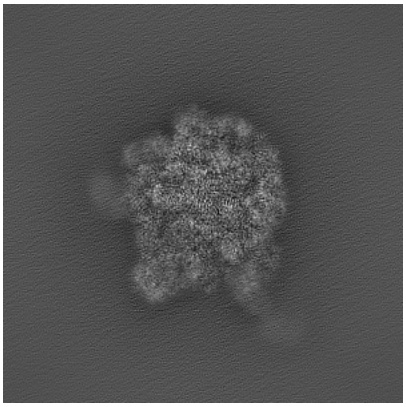
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20353. These allow visual inspection of the internal detail of the map and identification of artifacts.

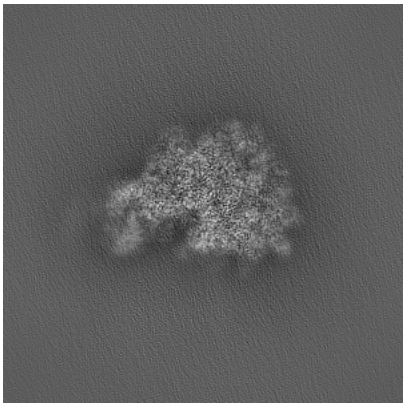
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

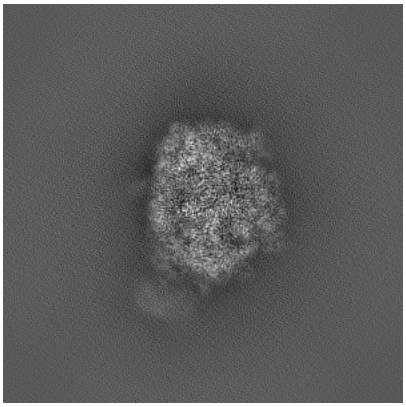
6.1.1 Primary map



X



Y

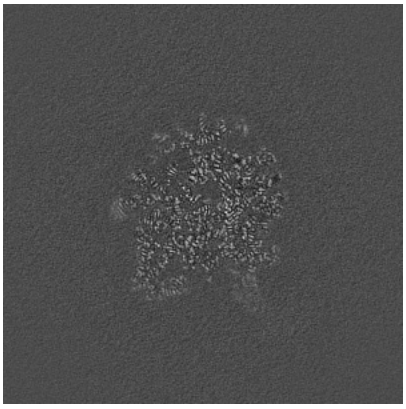


Z

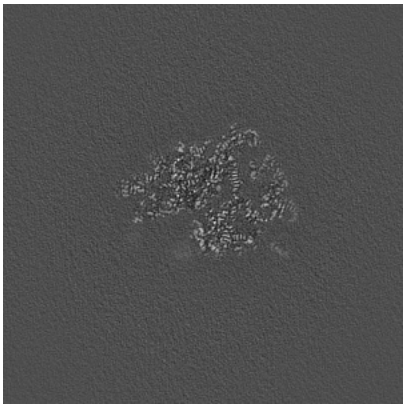
The images above show the map projected in three orthogonal directions.

6.2 Central slices

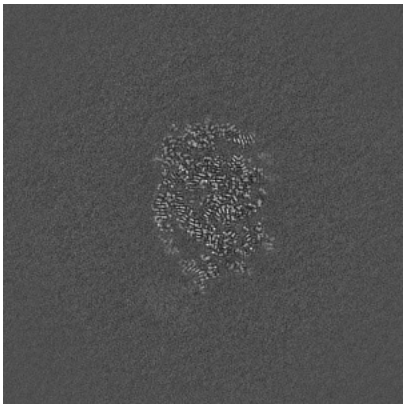
6.2.1 Primary map



X Index: 256



Y Index: 256

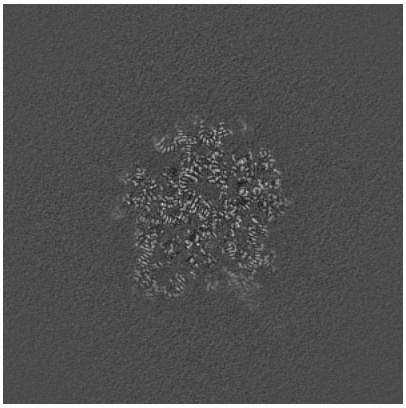


Z Index: 256

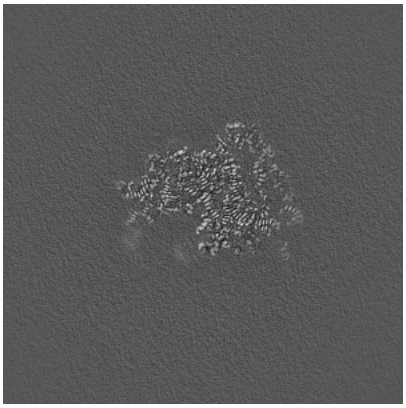
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

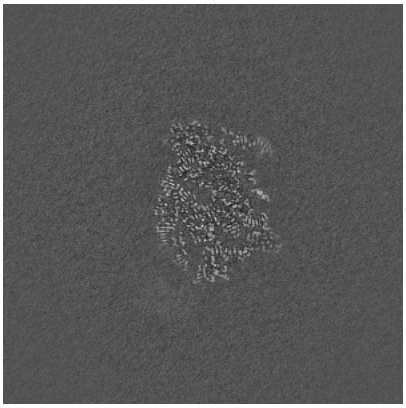
6.3.1 Primary map



X Index: 261



Y Index: 247

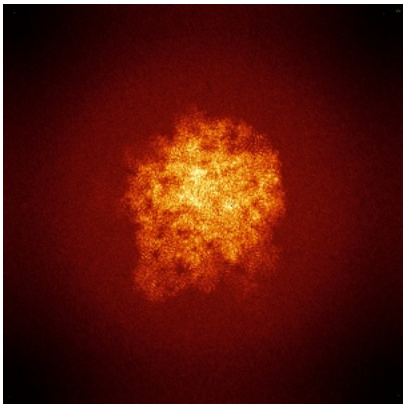


Z Index: 266

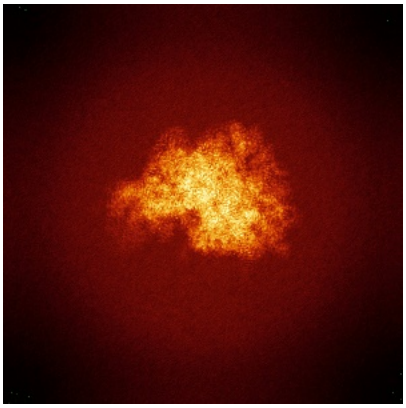
The images above show the largest variance slices of the map in three orthogonal directions.

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

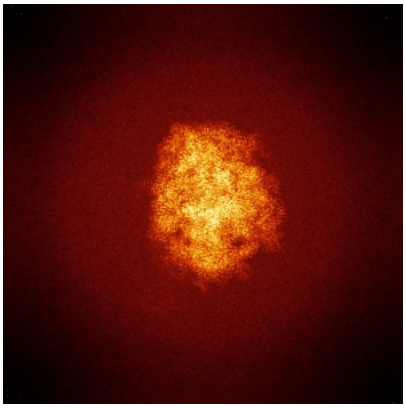
6.4.1 Primary map



X



Y

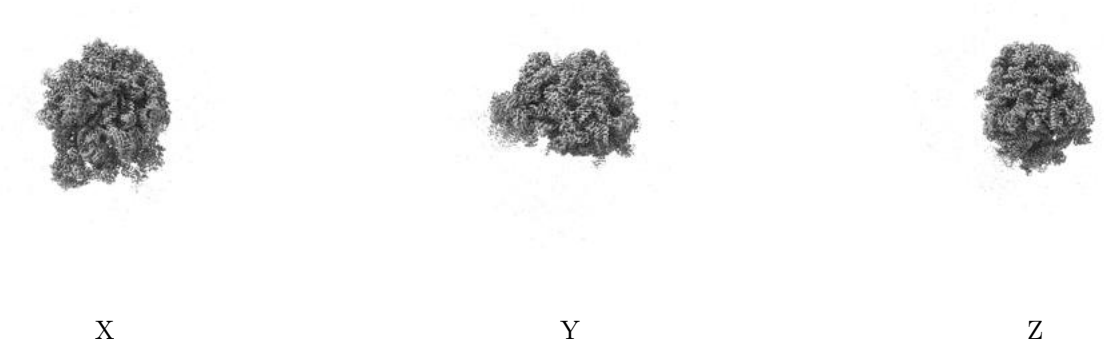


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

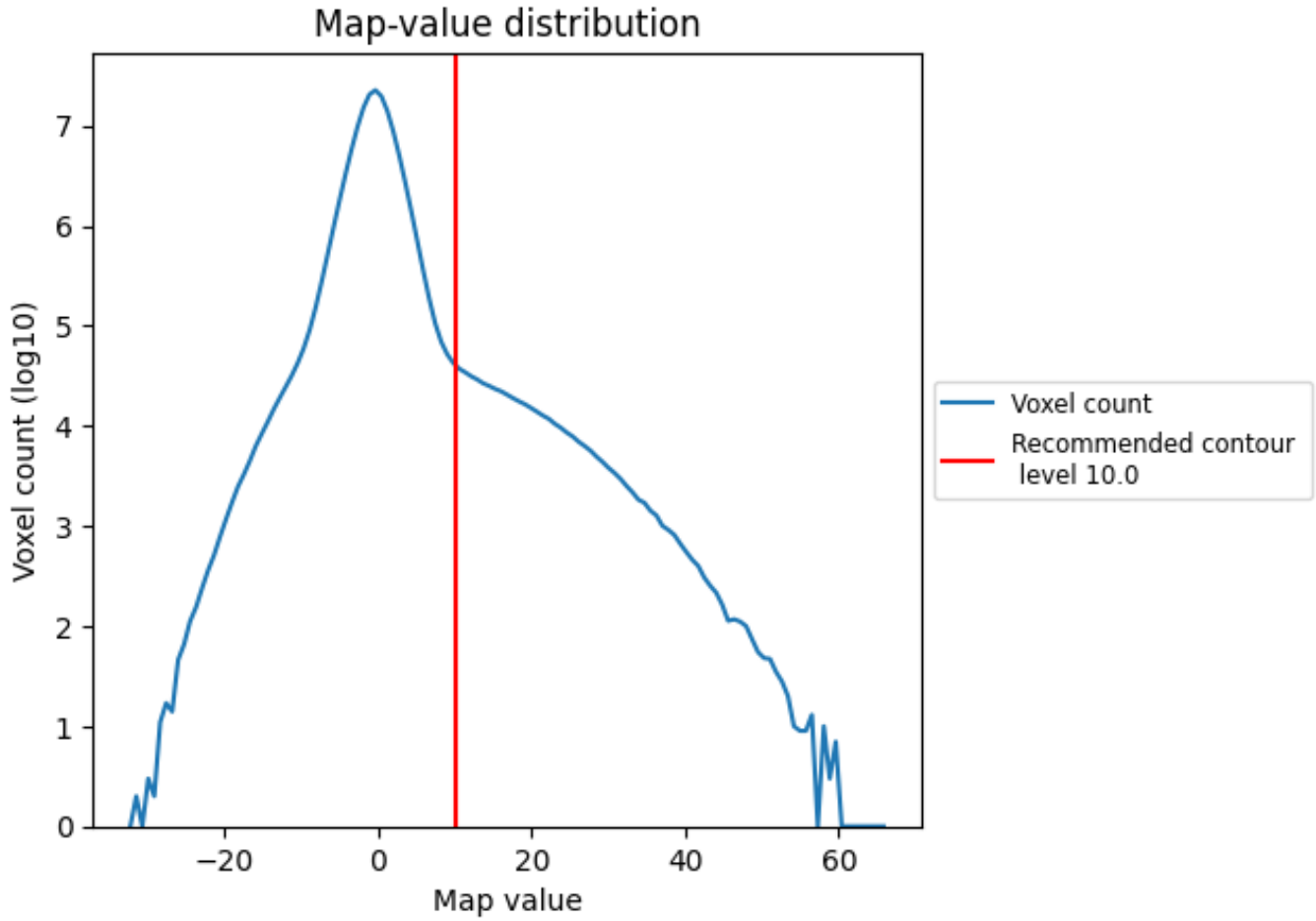
6.6 Mask visualisation (i)

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

7 Map analysis

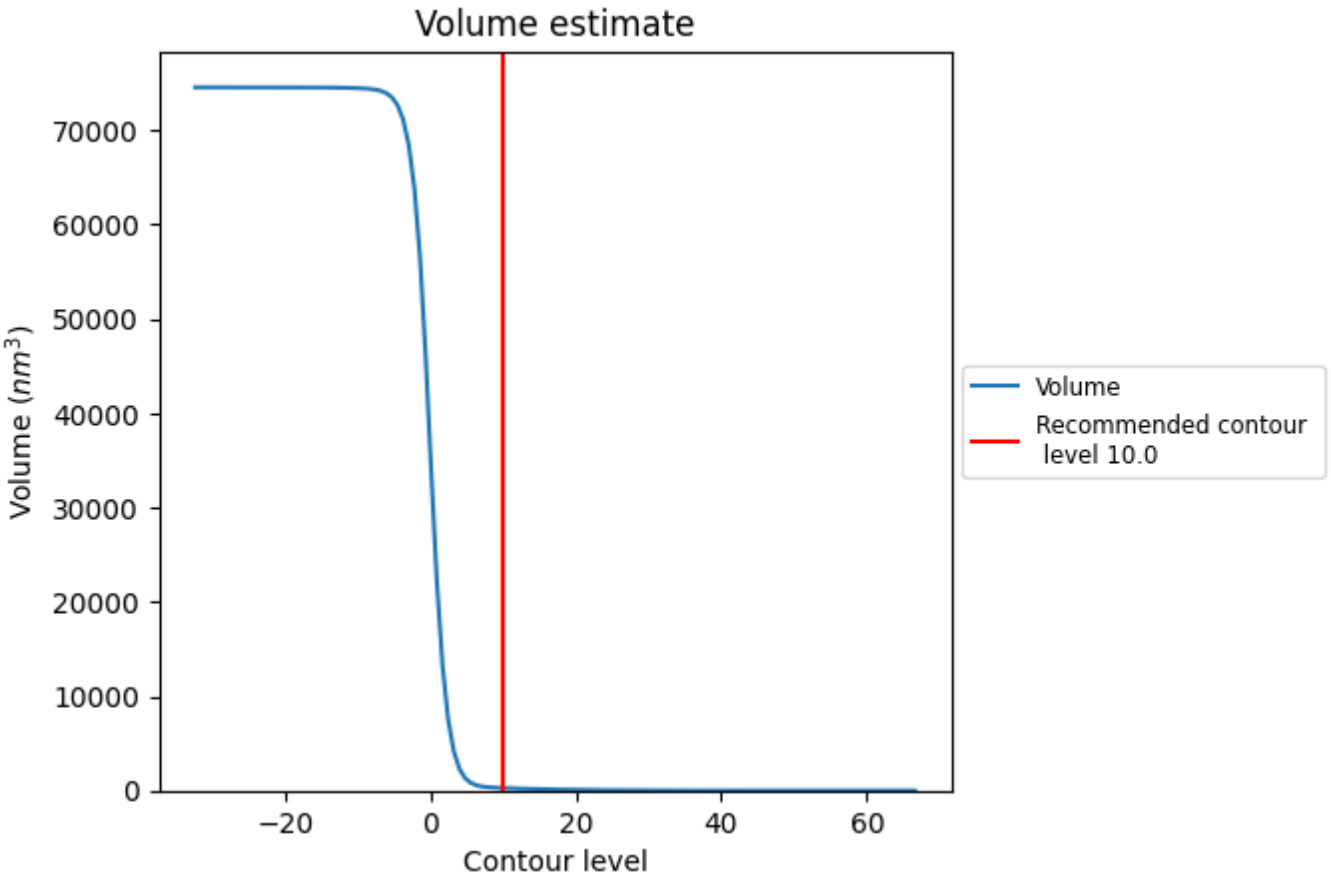
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

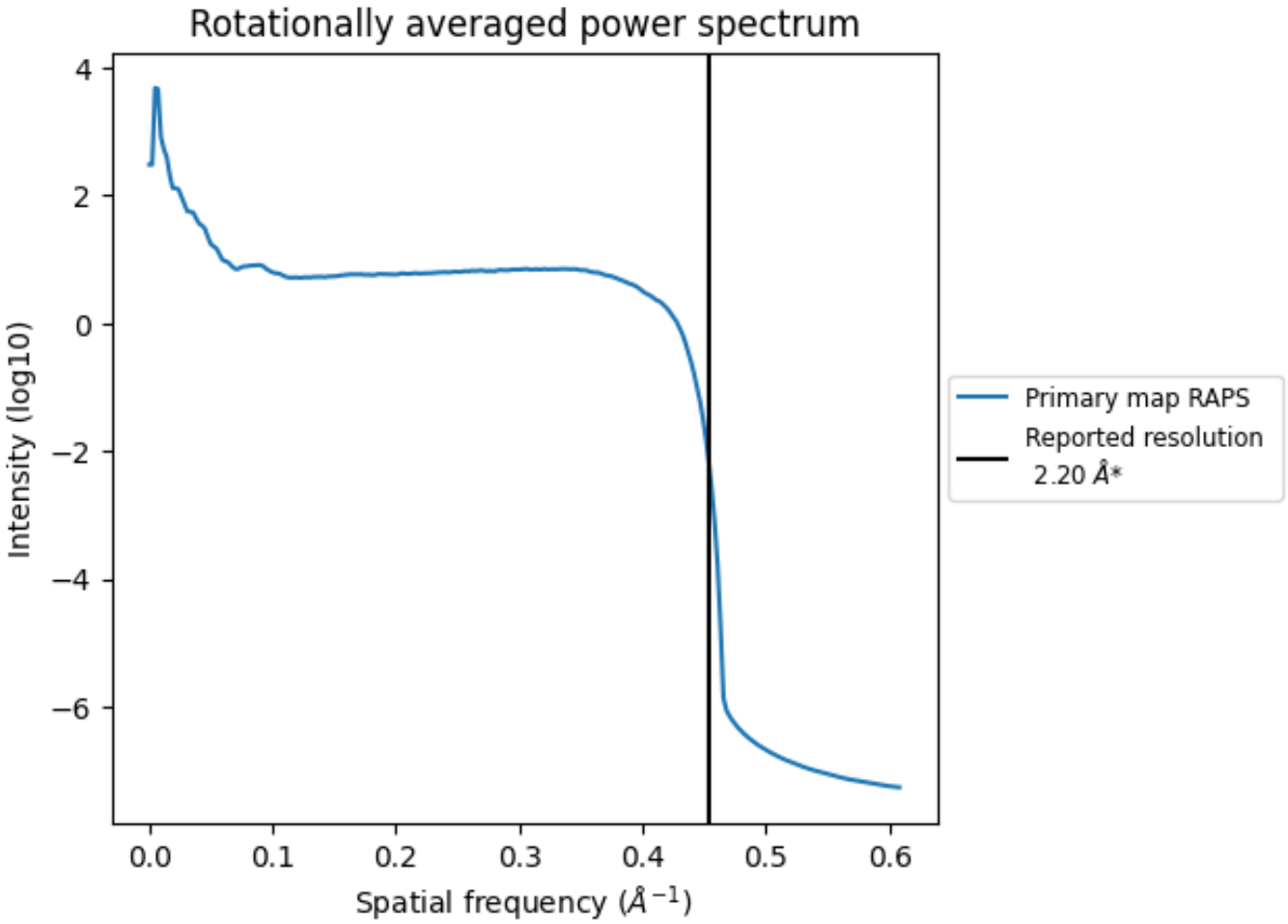
7.2 Volume estimate



The volume at the recommended contour level is 266 nm^3; this corresponds to an approximate mass of 240 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

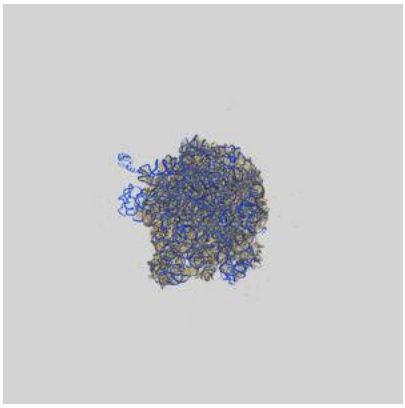
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

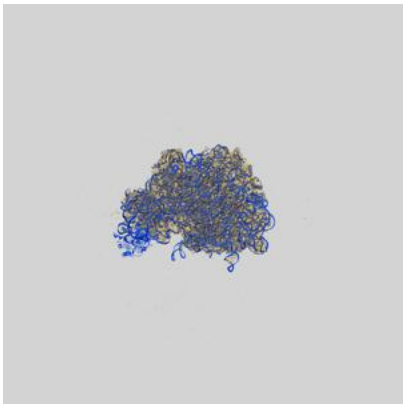
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20353 and PDB model 6PJ6. Per-residue inclusion information can be found in section 3 on page 11.

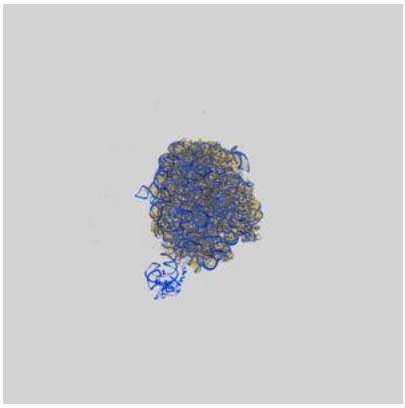
9.1 Map-model overlay



X



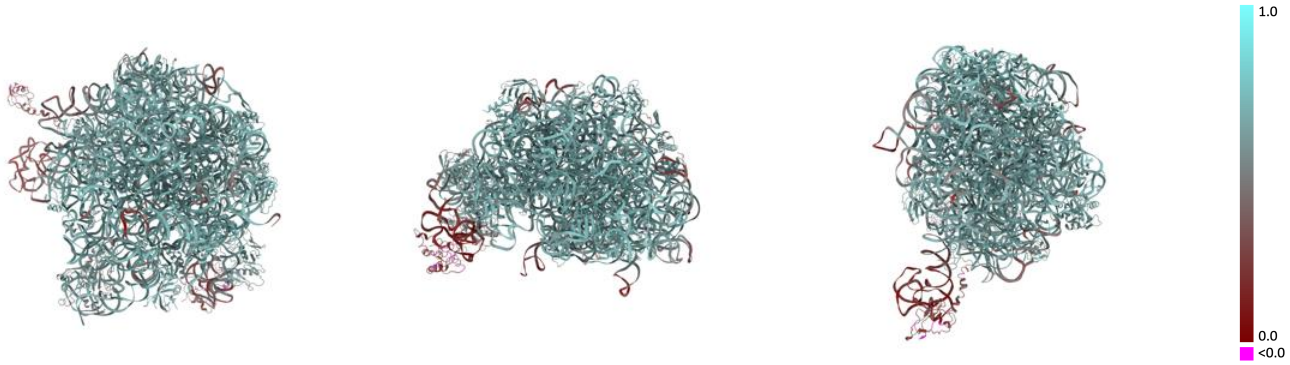
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

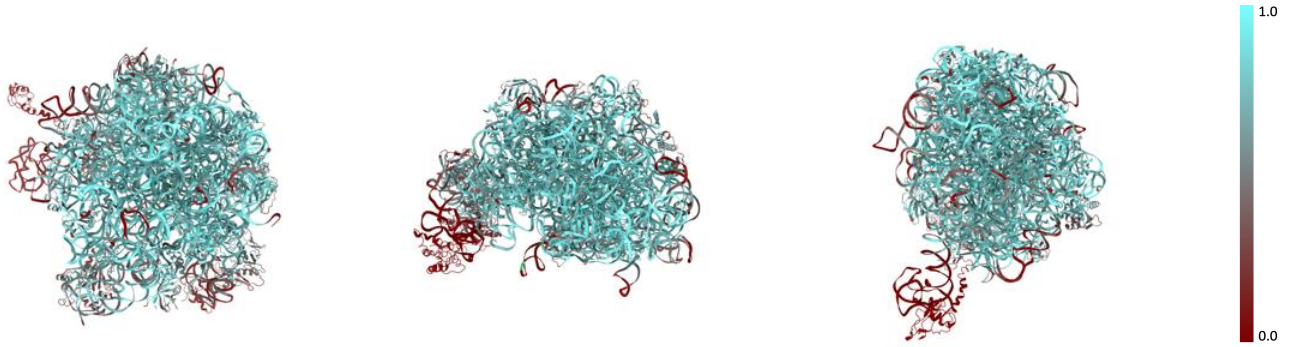
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

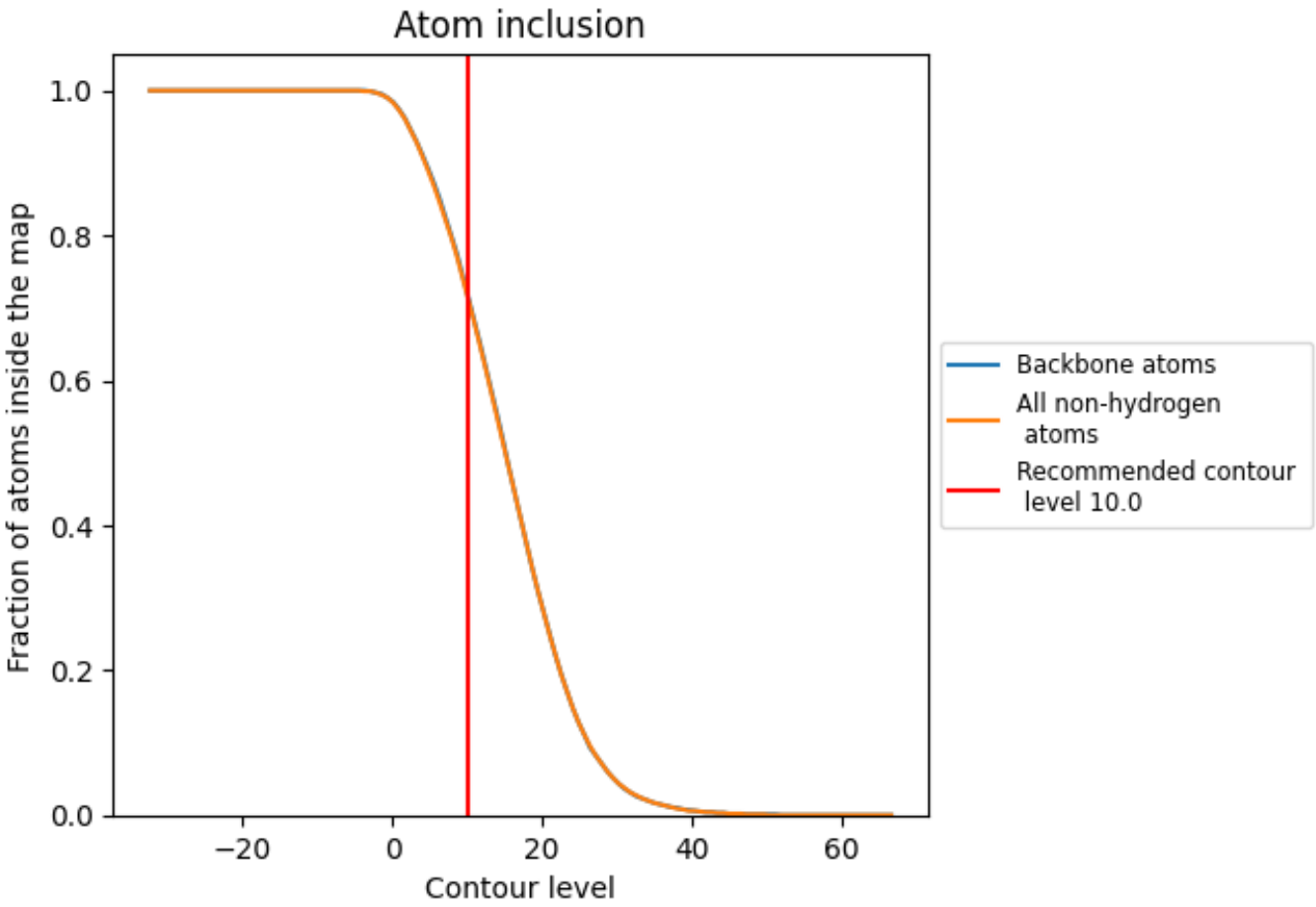
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (10.0).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (10.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7190	0.6160
I	0.7610	0.6180
J	0.6860	0.6150
K	0.7910	0.6730
L	0.7800	0.6700
M	0.6780	0.6470
N	0.1220	0.4500
O	0.4460	0.5820
P	0.1270	0.3310
Q	0.0000	0.2260
R	0.7690	0.6740
S	0.6980	0.6520
T	0.7520	0.6650
U	0.7400	0.6650
V	0.8400	0.6810
W	0.5700	0.6060
X	0.6670	0.6330
Y	0.8390	0.6930
Z	0.7290	0.6440
a	0.7490	0.6570
b	0.6390	0.6360
c	0.5990	0.6150
d	0.6350	0.6360
e	0.7910	0.6630
f	0.7140	0.6620
g	0.5400	0.6070
h	0.7480	0.6580
i	0.7520	0.6600
j	0.5960	0.6200
k	0.8370	0.6900
l	0.8370	0.6870
m	0.7070	0.6500