Full wwPDB EM Validation Report (i)

Jan 9, 2024 – 03:05 PM JST

PDB ID	:	7YLA
EMDB ID	:	EMD-33904
Title	:	Cryo-EM structure of 50S-HflX complex
Authors	:	Damu, W.; Ning, G.
Deposited on	:	2022-07-25
Resolution	:	2.52 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 (i) 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 (i)) were used in the production of this report:

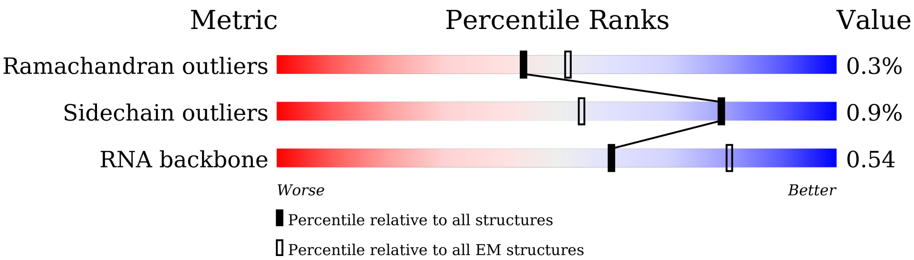
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.52 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	6	426	10% 98% • •
2	I	2904	5% 81% 18% • •
3	J	118	89% 11%
4	K	271	99% •
5	L	209	100%
6	M	201	100%
7	N	177	• 100%
8	O	176	• 99% •

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Mol	Chain	Length	Quality of chain
9	P	149	45% 99%
10	Q	134	81% 100%
11	R	142	97%
12	S	122	98%
13	T	144	98%
14	U	136	98%
15	V	120	100%
16	W	116	100%
17	X	114	100%
18	Y	117	100%
19	Z	103	97%
20	a	110	96%
21	b	93	99%
22	c	102	95%
23	d	94	100%
24	e	75	100%
25	f	77	100%
26	g	62	97%
27	h	58	100%
28	i	56	100%
29	j	50	100%
30	k	46	100%
31	l	64	97%
32	m	38	100%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 125796 atoms, of which 32064 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 GTPase HflX.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	6	419	Total 6704	C 2088	H 3366	N 614	O 628	S 8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	19	ALA	THR	conflict	UNP P25519

- Molecule 2 is a RNA chain called Escherichia coli strain K-12 substr. MG1655_TMP32XR1 chromosome, complete genome.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	2876	Total 61752	C 27546	N 11370	O 19960	P 2876	0	0

- Molecule 3 is a RNA chain called 5S rRNA.

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

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	K	271	Total 4261	C 1294	H 2167	N 427	O 366	S 7	2	0

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	L	209	Total 3182	C 979	H 1617	N 288	O 294	S 4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	P	149	2251	699	1140	197	214	1	0	0

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	Q	134	2003	619	1024	169	185	6	0	0

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	T	144	Total 2182	C 654	H 1129	N 207	O 190	S 2	0	0

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	U	136	Total 2218	C 686	H 1144	N 205	O 177	S 6	0	0

- Molecule 15 is a protein called 50S ribosomal protein L17.

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

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	Z	103	Total 1655	C 516	H 839	N 153	O 145	S 2	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

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

- Molecule 22 is a protein called 50S ribosomal protein L24.

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

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	e	75	Total 1167	C 356	H 592	N 116	O 102	S 1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L32.

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

- Molecule 29 is a protein called 50S ribosomal protein L33.

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

- Molecule 30 is a protein called 50S ribosomal protein L34.

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

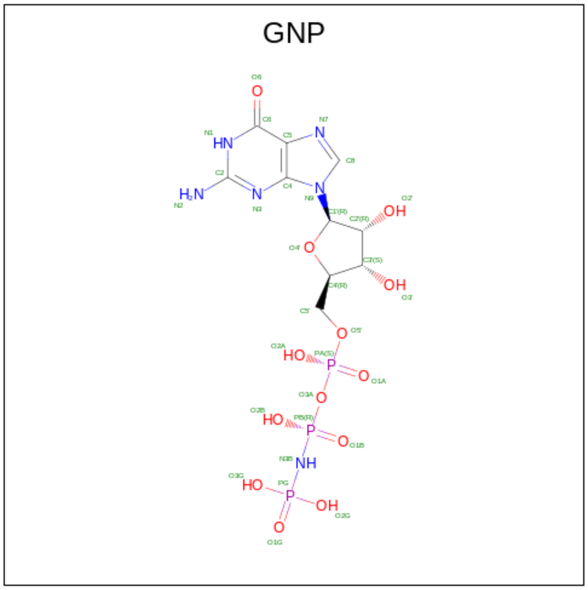
- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
31	l	64	1077	323	573	105	74	2	0	0

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
33	6	1	44	10	12	6	13	3	0

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
34	6	1	1	1	0
34	K	1	1	1	0
34	L	1	1	1	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

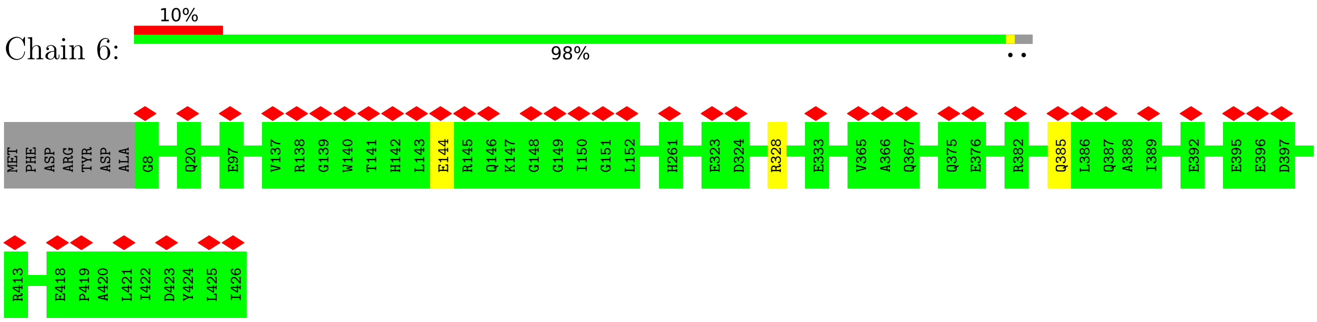
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
36	m	1	1	1	0

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.

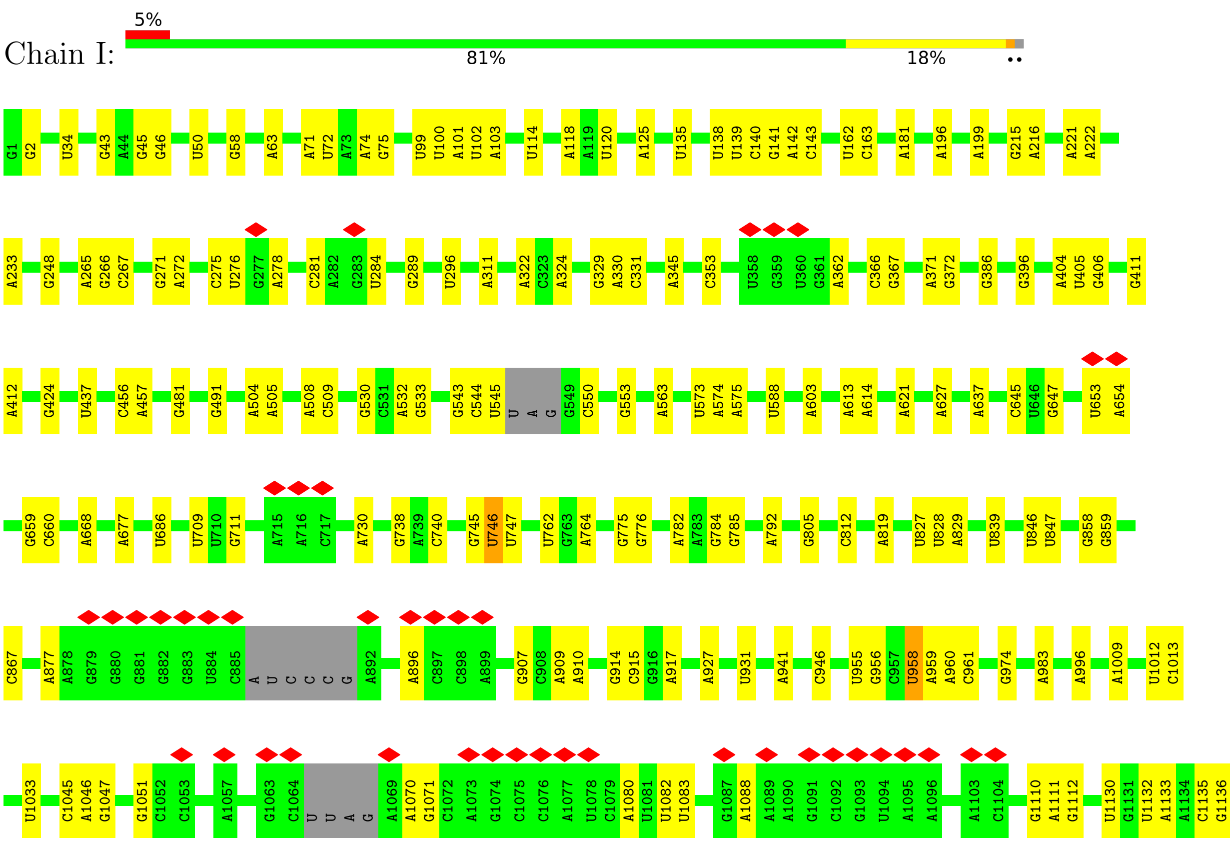
- Molecule 1: GTPase HflX

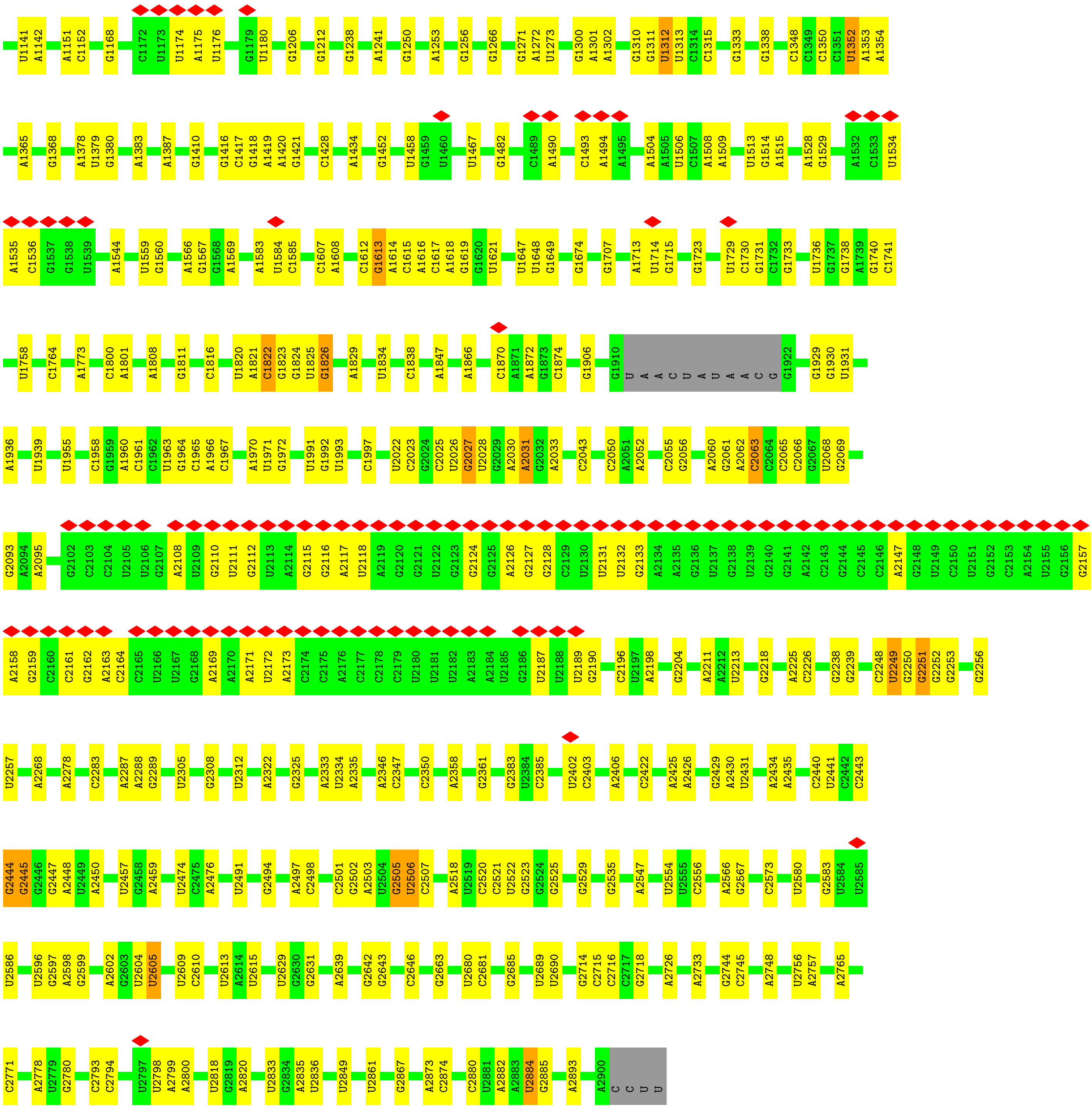
Chain 6:



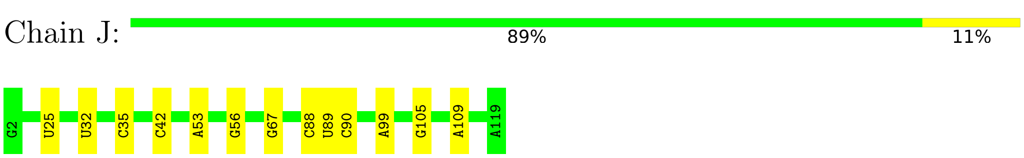
- Molecule 2: Escherichia coli strain K-12 substr. MG1655_TMP32XR1 chromosome, complete genome

Chain I:

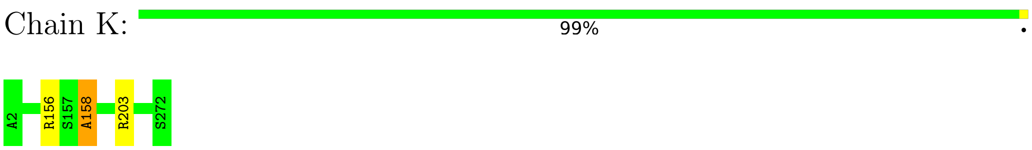




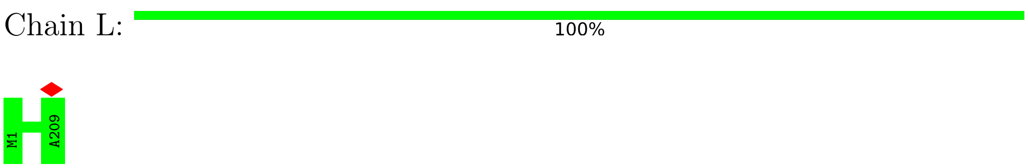
• Molecule 3: 5S rRNA



• Molecule 4: 50S ribosomal protein L2



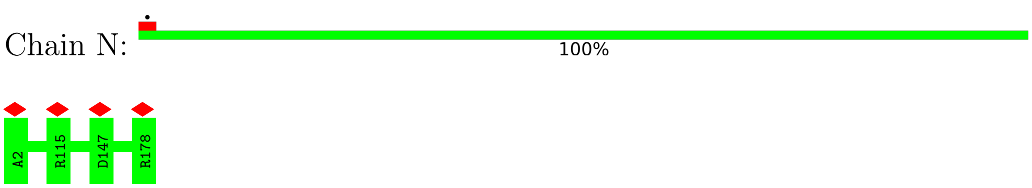
• Molecule 5: 50S ribosomal protein L3



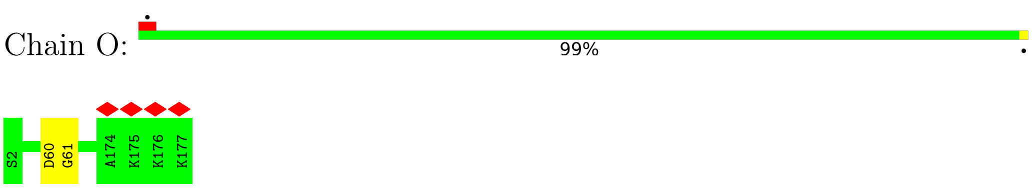
• Molecule 6: 50S ribosomal protein L4

There are no outlier residues recorded for this chain.

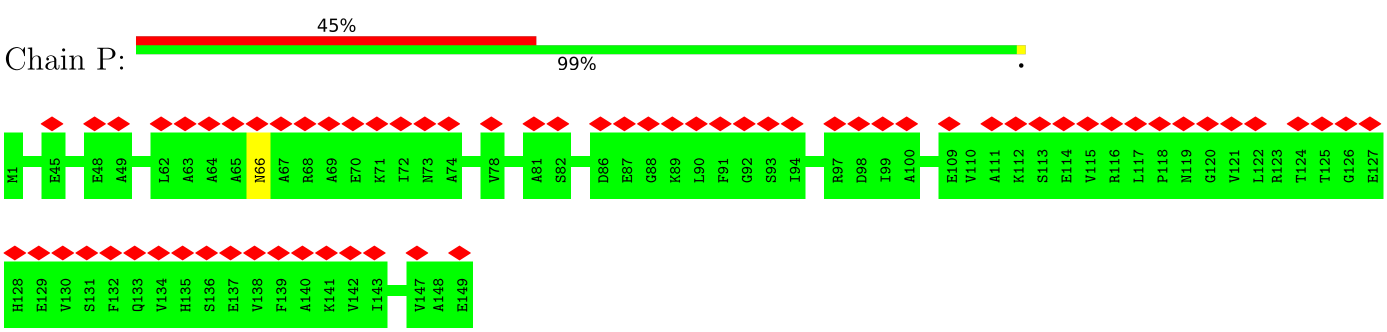
• Molecule 7: 50S ribosomal protein L5



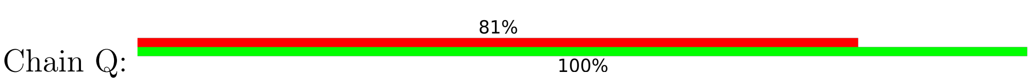
• Molecule 8: 50S ribosomal protein L6

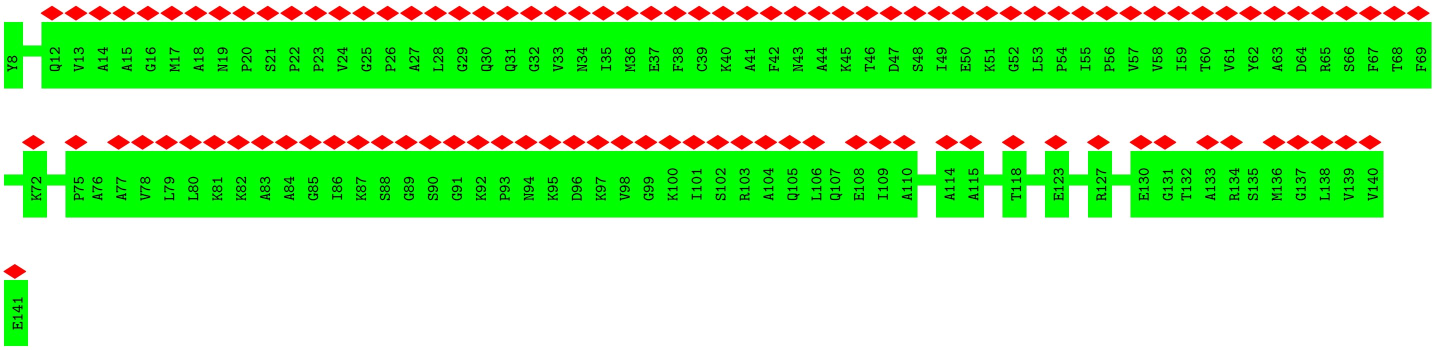


• Molecule 9: 50S ribosomal protein L9

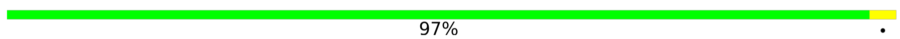


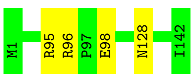
• Molecule 10: 50S ribosomal protein L11



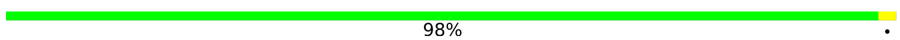


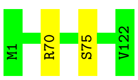
• Molecule 11: 50S ribosomal protein L13

Chain R:


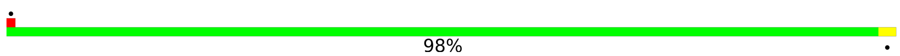


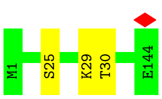
• Molecule 12: 50S ribosomal protein L14

Chain S:


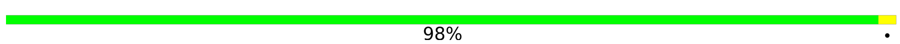


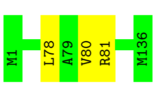
• Molecule 13: 50S ribosomal protein L15

Chain T:




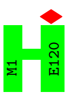
• Molecule 14: 50S ribosomal protein L16

Chain U:




• Molecule 15: 50S ribosomal protein L17

Chain V:

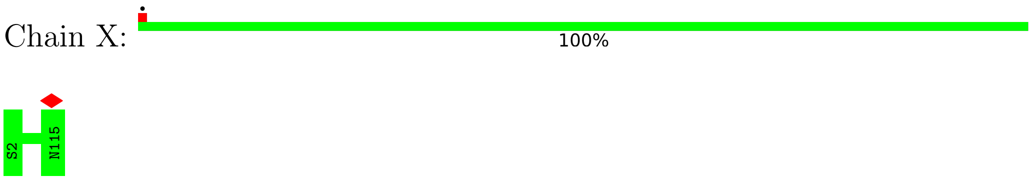
• Molecule 16: 50S ribosomal protein L18

Chain W:

There are no outlier residues recorded for this chain.

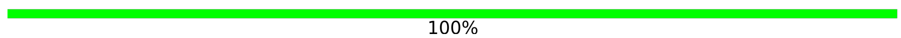
- Molecule 17: 50S ribosomal protein L19

Chain X:



- Molecule 18: 50S ribosomal protein L20

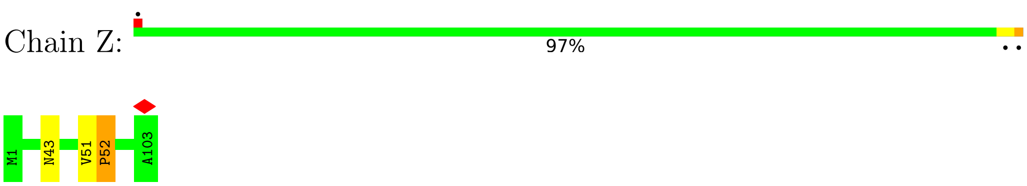
Chain Y:



There are no outlier residues recorded for this chain.

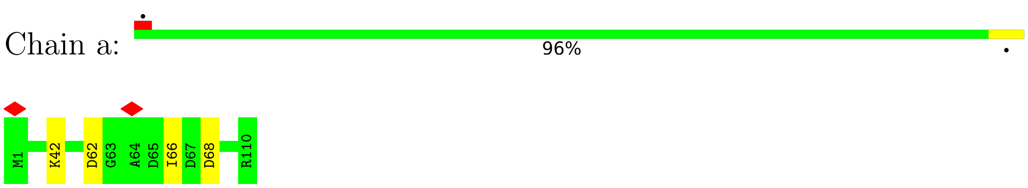
- Molecule 19: 50S ribosomal protein L21

Chain Z:



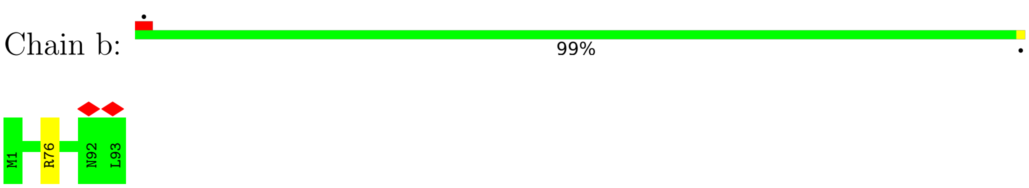
- Molecule 20: 50S ribosomal protein L22

Chain a:



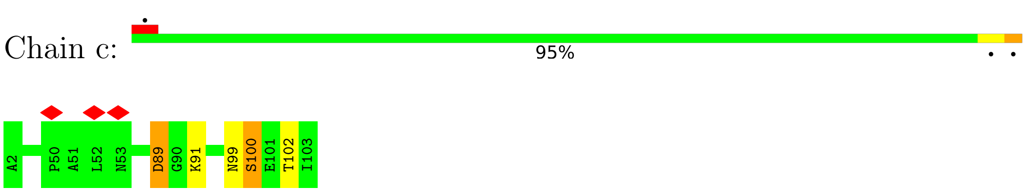
- Molecule 21: 50S ribosomal protein L23

Chain b:



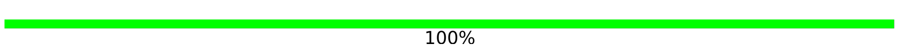
- Molecule 22: 50S ribosomal protein L24

Chain c:



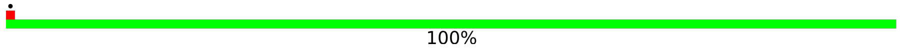
- Molecule 23: 50S ribosomal protein L25

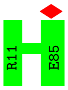
Chain d:



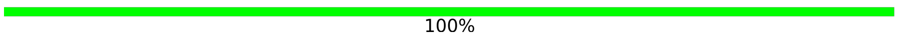
There are no outlier residues recorded for this chain.

• Molecule 24: 50S ribosomal protein L27

Chain e: 

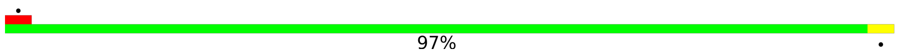


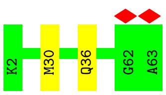
• Molecule 25: 50S ribosomal protein L28

Chain f: 

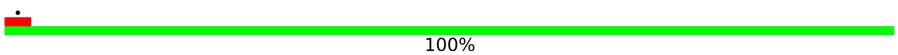
There are no outlier residues recorded for this chain.

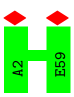
• Molecule 26: 50S ribosomal protein L29

Chain g: 

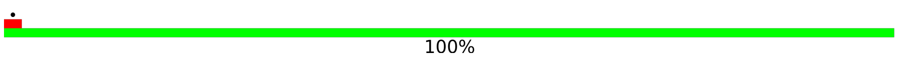


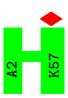
• Molecule 27: 50S ribosomal protein L30

Chain h: 

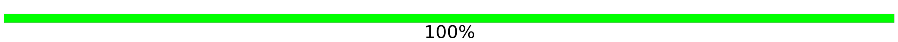


• Molecule 28: 50S ribosomal protein L32

Chain i: 

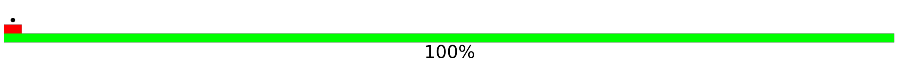


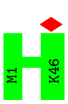
• Molecule 29: 50S ribosomal protein L33

Chain j: 

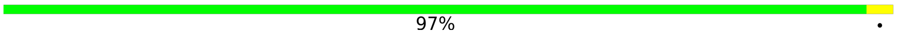
There are no outlier residues recorded for this chain.

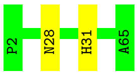
• Molecule 30: 50S ribosomal protein L34

Chain k: 

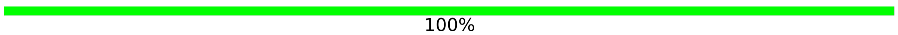


• Molecule 31: 50S ribosomal protein L35

Chain l: 



• Molecule 32: 50S ribosomal protein L36

Chain m: 

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93913	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	1.8	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.650	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	315.6, 315.6, 315.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, ZN, NA, PSU, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	6	0.28	0/3389	0.65	0/4585
2	I	0.58	66/69029 (0.1%)	0.79	14/107686 (0.0%)
3	J	0.42	0/2828	0.81	0/4410
4	K	0.37	1/2140 (0.0%)	0.74	2/2876 (0.1%)
5	L	0.29	0/1586	0.62	0/2134
6	M	0.29	0/1571	0.60	0/2113
7	N	0.27	0/1435	0.62	0/1926
8	O	0.30	0/1343	0.62	0/1816
9	P	0.29	0/1122	0.56	0/1515
10	Q	0.27	0/993	0.57	0/1341
11	R	0.35	0/1152	0.60	0/1551
12	S	0.36	0/947	0.68	0/1268
13	T	0.32	0/1062	0.69	0/1413
14	U	0.36	0/1093	0.68	0/1460
15	V	0.30	0/973	0.69	0/1301
16	W	0.30	0/902	0.69	0/1209
17	X	0.29	0/929	0.65	0/1242
18	Y	0.33	0/960	0.66	0/1278
19	Z	0.39	0/829	0.77	1/1107 (0.1%)
20	a	0.45	0/864	0.73	0/1156
21	b	0.27	0/745	0.58	0/994
22	c	0.40	0/788	0.69	0/1051
23	d	0.39	0/766	0.64	0/1025
24	e	0.32	0/582	0.68	0/769
25	f	0.27	0/635	0.71	0/848
26	g	0.36	0/502	0.72	0/667
27	h	0.26	0/453	0.64	0/605
28	i	0.30	0/450	0.68	0/599
29	j	0.33	0/416	0.62	0/554
30	k	0.27	0/380	0.78	0/498
31	l	0.40	0/513	0.80	0/676
32	m	0.32	0/303	0.70	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.52	67/101680 (0.1%)	0.76	17/152070 (0.0%)

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	959	A	O3'-P	-10.48	1.48	1.61
2	I	2444	G	P-OP2	-8.86	1.33	1.49
2	I	2444	G	O3'-P	-8.48	1.50	1.61
2	I	2503	A	O3'-P	-8.19	1.51	1.61
2	I	1313	U	O3'-P	-8.04	1.51	1.61
2	I	322	A	O3'-P	-7.99	1.51	1.61
2	I	1348	C	O3'-P	-7.93	1.51	1.61
2	I	2507	C	O3'-P	-7.84	1.51	1.61
2	I	2642	G	O3'-P	-7.83	1.51	1.61
2	I	2583	G	O3'-P	-7.81	1.51	1.61
2	I	955	PSU	O3'-P	-7.58	1.52	1.61
2	I	1312	U	O3'-P	-7.48	1.52	1.61
2	I	956	G	O3'-P	-7.29	1.52	1.61
2	I	1822	C	O3'-P	-7.28	1.52	1.61
2	I	1825	U	O3'-P	-7.27	1.52	1.61
2	I	2256	G	O3'-P	-7.26	1.52	1.61
2	I	2596	U	O3'-P	-7.20	1.52	1.61
2	I	1354	A	O3'-P	-7.10	1.52	1.61
2	I	1310	G	O3'-P	-7.10	1.52	1.61
2	I	2025	C	O3'-P	-7.09	1.52	1.61
2	I	1311	G	O3'-P	-7.03	1.52	1.61
2	I	2249	U	O3'-P	-6.98	1.52	1.61
2	I	2063	C	O3'-P	-6.92	1.52	1.61
2	I	1615	C	O3'-P	-6.81	1.52	1.61
2	I	1825	U	P-OP2	-6.74	1.37	1.49
2	I	2031	A	O3'-P	-6.62	1.53	1.61
2	I	2250	G	O3'-P	-6.57	1.53	1.61
2	I	2523	G	O3'-P	-6.53	1.53	1.61
2	I	2066	C	O3'-P	-6.51	1.53	1.61
2	I	1821	A	O3'-P	-6.49	1.53	1.61
2	I	1823	G	O3'-P	-6.40	1.53	1.61
2	I	553	G	O3'-P	-6.34	1.53	1.61
2	I	1826	G	P-OP1	-6.25	1.38	1.49
2	I	958	U	P-OP1	-6.22	1.38	1.49
2	I	1353	A	O3'-P	-6.22	1.53	1.61
2	I	1612	C	P-OP2	-6.21	1.38	1.49
4	K	158	ALA	C-O	-6.15	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1614	A	P-OP2	-6.12	1.38	1.49
2	I	1613	G	O3'-P	-5.99	1.53	1.61
2	I	2443	C	P-OP2	-5.94	1.38	1.49
2	I	1824	G	O3'-P	-5.87	1.54	1.61
2	I	960	A	P-OP1	-5.85	1.39	1.49
2	I	2257	U	O3'-P	-5.77	1.54	1.61
2	I	1960	A	O3'-P	-5.77	1.54	1.61
2	I	2598	A	O3'-P	-5.67	1.54	1.61
2	I	2252	G	P-OP2	-5.65	1.39	1.49
2	I	2882	A	O3'-P	-5.52	1.54	1.61
2	I	2521	C	P-OP1	-5.52	1.39	1.49
2	I	2522	U	P-OP2	-5.51	1.39	1.49
2	I	2251	G	P-OP2	-5.51	1.39	1.49
2	I	1958	C	O3'-P	-5.48	1.54	1.61
2	I	2501	C	O3'-P	-5.46	1.54	1.61
2	I	2253	G	O3'-P	-5.45	1.54	1.61
2	I	1352	U	O3'-P	-5.38	1.54	1.61
2	I	1354	A	P-OP1	-5.37	1.39	1.49
2	I	2522	U	O3'-P	-5.35	1.54	1.61
2	I	2445	G	O3'-P	-5.30	1.54	1.61
2	I	2065	C	P-OP2	-5.28	1.40	1.49
2	I	2248	C	O3'-P	-5.25	1.54	1.61
2	I	2027	G	O3'-P	-5.20	1.54	1.61
2	I	2028	U	O3'-P	-5.17	1.54	1.61
2	I	2250	G	P-OP1	-5.16	1.40	1.49
2	I	2597	G	O3'-P	-5.13	1.54	1.61
2	I	1352	U	P-OP2	-5.13	1.40	1.49
2	I	1824	G	P-OP2	-5.09	1.40	1.49
2	I	2248	C	P-OP2	-5.04	1.40	1.49
2	I	2026	U	O3'-P	-5.02	1.55	1.61

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1614	A	O5'-P-OP1	10.53	123.33	110.70
2	I	2066	C	O5'-P-OP1	-7.25	99.17	105.70
2	I	1614	A	O5'-P-OP2	-6.90	99.49	105.70
2	I	2505	G	O5'-P-OP2	-6.85	99.54	105.70
2	I	322	A	O5'-P-OP1	-6.57	99.78	105.70
2	I	2598	A	O5'-P-OP2	-6.44	99.90	105.70
2	I	2440	C	P-O3'-C3'	6.10	127.02	119.70
2	I	2884	U	O4'-C1'-C2'	-6.02	99.78	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2506	U	O4'-C1'-N1	5.92	112.94	108.20
2	I	1315	C	O5'-P-OP2	-5.86	100.43	105.70
2	I	2599	G	O5'-P-OP2	-5.80	100.48	105.70
2	I	1613	G	O5'-P-OP2	5.78	117.64	110.70
4	K	158	ALA	CA-C-N	5.61	127.42	116.20
2	I	2884	U	C1'-C2'-O2'	-5.43	94.31	110.60
19	Z	52	PRO	N-CA-CB	5.15	109.48	103.30
2	I	1311	G	O4'-C1'-N9	5.08	112.27	108.20
4	K	156	ARG	CB-CG-CD	-5.01	98.57	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	417/426 (98%)	397 (95%)	19 (5%)	1 (0%)	47	67
4	K	271/271 (100%)	261 (96%)	9 (3%)	1 (0%)	34	53
5	L	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
6	M	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
7	N	175/177 (99%)	162 (93%)	13 (7%)	0	100	100
8	O	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	25	41
9	P	147/149 (99%)	128 (87%)	19 (13%)	0	100	100
10	Q	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
11	R	140/142 (99%)	137 (98%)	2 (1%)	1 (1%)	22	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	S	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
13	T	142/144 (99%)	139 (98%)	2 (1%)	1 (1%)	22	37
14	U	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
15	V	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
16	W	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
17	X	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
18	Y	115/117 (98%)	115 (100%)	0	0	100	100
19	Z	101/103 (98%)	92 (91%)	7 (7%)	2 (2%)	7	11
20	a	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17	30
21	b	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
22	c	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	7	11
23	d	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	e	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
25	f	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
26	g	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
27	h	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
28	i	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	j	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
30	k	44/46 (96%)	44 (100%)	0	0	100	100
31	l	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
32	m	36/38 (95%)	36 (100%)	0	0	100	100
All	All	3717/3782 (98%)	3548 (96%)	159 (4%)	10 (0%)	44	59

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	K	158	ALA
8	O	61	GLY
22	c	100	SER
22	c	89	ASP
13	T	29	LYS
19	Z	52	PRO
1	6	144	GLU
11	R	95	ARG
19	Z	51	VAL

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Mol	Chain	Res	Type
20	a	66	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6	357/363 (98%)	355 (99%)	2 (1%)	86	94
4	K	218/216 (101%)	216 (99%)	2 (1%)	78	91
5	L	164/164 (100%)	164 (100%)	0	100	100
6	M	165/165 (100%)	165 (100%)	0	100	100
7	N	148/148 (100%)	148 (100%)	0	100	100
8	O	137/137 (100%)	136 (99%)	1 (1%)	84	93
9	P	114/114 (100%)	113 (99%)	1 (1%)	78	91
10	Q	104/104 (100%)	104 (100%)	0	100	100
11	R	116/116 (100%)	113 (97%)	3 (3%)	46	70
12	S	103/103 (100%)	101 (98%)	2 (2%)	57	79
13	T	103/103 (100%)	101 (98%)	2 (2%)	57	79
14	U	109/109 (100%)	106 (97%)	3 (3%)	43	68
15	V	100/100 (100%)	100 (100%)	0	100	100
16	W	86/86 (100%)	86 (100%)	0	100	100
17	X	99/99 (100%)	99 (100%)	0	100	100
18	Y	89/89 (100%)	89 (100%)	0	100	100
19	Z	84/84 (100%)	83 (99%)	1 (1%)	71	87
20	a	93/93 (100%)	90 (97%)	3 (3%)	39	63
21	b	80/80 (100%)	79 (99%)	1 (1%)	69	86
22	c	83/83 (100%)	78 (94%)	5 (6%)	19	34
23	d	78/78 (100%)	78 (100%)	0	100	100
24	e	57/57 (100%)	57 (100%)	0	100	100
25	f	67/67 (100%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	g	54/54 (100%)	52 (96%)	2 (4%)	34	57
27	h	48/48 (100%)	48 (100%)	0	100	100
28	i	47/47 (100%)	47 (100%)	0	100	100
29	j	45/45 (100%)	45 (100%)	0	100	100
30	k	38/38 (100%)	38 (100%)	0	100	100
31	l	51/51 (100%)	49 (96%)	2 (4%)	32	55
32	m	34/34 (100%)	34 (100%)	0	100	100
All	All	3071/3075 (100%)	3041 (99%)	30 (1%)	79	89

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	6	328	ARG
1	6	385	GLN
4	K	203[A]	ARG
4	K	203[B]	ARG
8	O	60	ASP
9	P	66	ASN
11	R	96	ARG
11	R	98	GLU
11	R	128	ASN
12	S	70	ARG
12	S	75	SER
13	T	25	SER
13	T	30	THR
14	U	78	LEU
14	U	80	VAL
14	U	81	ARG
19	Z	43	ASN
20	a	42	LYS
20	a	62	ASP
20	a	68	ASP
21	b	76	ARG
22	c	89	ASP
22	c	91	LYS
22	c	99	ASN
22	c	100	SER
22	c	102	THR
26	g	30	MET
26	g	36	GLN

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Mol	Chain	Res	Type
31	l	28	ASN
31	l	31	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	6	385	GLN
19	Z	43	ASN
21	b	59	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	2871/2904 (98%)	473 (16%)	20 (0%)
3	J	117/118 (99%)	13 (11%)	0
All	All	2988/3022 (98%)	486 (16%)	20 (0%)

All (486) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	2	G
2	I	34	U
2	I	43	G
2	I	45	G
2	I	46	G
2	I	50	U
2	I	58	G
2	I	63	A
2	I	71	A
2	I	72	U
2	I	74	A
2	I	75	G
2	I	99	U
2	I	101	A
2	I	102	U
2	I	103	A
2	I	114	U
2	I	118	A
2	I	120	U
2	I	125	A

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Mol	Chain	Res	Type
2	I	135	U
2	I	139	U
2	I	140	C
2	I	141	G
2	I	142	A
2	I	143	C
2	I	162	U
2	I	163	C
2	I	181	A
2	I	196	A
2	I	199	A
2	I	215	G
2	I	216	A
2	I	221	A
2	I	222	A
2	I	233	A
2	I	248	G
2	I	265	A
2	I	266	G
2	I	267	C
2	I	272	A
2	I	275	C
2	I	276	U
2	I	278	A
2	I	281	C
2	I	284	U
2	I	289	G
2	I	296	U
2	I	311	A
2	I	324	A
2	I	329	G
2	I	330	A
2	I	331	C
2	I	345	A
2	I	353	C
2	I	362	A
2	I	366	C
2	I	367	G
2	I	371	A
2	I	372	G
2	I	386	G
2	I	396	G

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Mol	Chain	Res	Type
2	I	405	U
2	I	406	G
2	I	411	G
2	I	412	A
2	I	424	G
2	I	437	U
2	I	456	C
2	I	457	A
2	I	481	G
2	I	491	G
2	I	504	A
2	I	505	A
2	I	508	A
2	I	509	C
2	I	530	G
2	I	532	A
2	I	533	G
2	I	543	G
2	I	544	C
2	I	545	U
2	I	550	C
2	I	563	A
2	I	573	U
2	I	574	A
2	I	575	A
2	I	588	U
2	I	603	A
2	I	613	A
2	I	614	A
2	I	621	A
2	I	627	A
2	I	637	A
2	I	645	C
2	I	647	G
2	I	653	U
2	I	654	A
2	I	659	G
2	I	660	C
2	I	668	A
2	I	677	A
2	I	686	U
2	I	709	U

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Mol	Chain	Res	Type
2	I	711	G
2	I	730	A
2	I	738	G
2	I	740	C
2	I	745	G
2	I	746	PSU
2	I	747	U
2	I	762	U
2	I	764	A
2	I	775	G
2	I	776	G
2	I	782	A
2	I	784	G
2	I	785	G
2	I	792	A
2	I	805	G
2	I	812	C
2	I	819	A
2	I	827	U
2	I	828	U
2	I	829	A
2	I	839	U
2	I	846	U
2	I	847	U
2	I	858	G
2	I	859	G
2	I	867	C
2	I	877	A
2	I	896	A
2	I	907	G
2	I	909	A
2	I	910	A
2	I	914	G
2	I	915	C
2	I	917	A
2	I	927	A
2	I	931	U
2	I	941	A
2	I	946	C
2	I	958	U
2	I	961	C
2	I	974	G

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Mol	Chain	Res	Type
2	I	983	A
2	I	996	A
2	I	1009	A
2	I	1012	U
2	I	1013	C
2	I	1033	U
2	I	1045	C
2	I	1046	A
2	I	1047	G
2	I	1051	G
2	I	1070	A
2	I	1071	G
2	I	1080	A
2	I	1082	U
2	I	1083	U
2	I	1088	A
2	I	1110	G
2	I	1111	A
2	I	1112	G
2	I	1130	U
2	I	1132	U
2	I	1133	A
2	I	1135	C
2	I	1136	G
2	I	1141	U
2	I	1142	A
2	I	1151	A
2	I	1152	C
2	I	1168	G
2	I	1174	U
2	I	1175	A
2	I	1176	U
2	I	1180	U
2	I	1206	G
2	I	1212	G
2	I	1238	G
2	I	1241	A
2	I	1250	G
2	I	1253	A
2	I	1256	G
2	I	1266	G
2	I	1271	G

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Mol	Chain	Res	Type
2	I	1272	A
2	I	1273	U
2	I	1300	G
2	I	1301	A
2	I	1302	A
2	I	1312	U
2	I	1333	G
2	I	1338	G
2	I	1350	C
2	I	1352	U
2	I	1365	A
2	I	1368	G
2	I	1378	A
2	I	1379	U
2	I	1380	G
2	I	1383	A
2	I	1387	A
2	I	1410	G
2	I	1416	G
2	I	1417	C
2	I	1418	G
2	I	1419	A
2	I	1420	A
2	I	1421	G
2	I	1428	C
2	I	1434	A
2	I	1452	G
2	I	1458	U
2	I	1467	U
2	I	1482	G
2	I	1490	A
2	I	1493	C
2	I	1494	A
2	I	1504	A
2	I	1506	U
2	I	1508	A
2	I	1509	A
2	I	1513	U
2	I	1514	G
2	I	1515	A
2	I	1528	A
2	I	1529	G

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Mol	Chain	Res	Type
2	I	1534	U
2	I	1535	A
2	I	1536	C
2	I	1544	A
2	I	1559	U
2	I	1560	G
2	I	1566	A
2	I	1567	G
2	I	1569	A
2	I	1583	A
2	I	1584	U
2	I	1585	C
2	I	1607	C
2	I	1608	A
2	I	1613	G
2	I	1616	A
2	I	1617	C
2	I	1618	A
2	I	1619	G
2	I	1621	U
2	I	1647	U
2	I	1648	U
2	I	1649	G
2	I	1674	G
2	I	1707	G
2	I	1713	A
2	I	1714	U
2	I	1715	G
2	I	1723	G
2	I	1729	U
2	I	1730	C
2	I	1731	G
2	I	1733	G
2	I	1736	U
2	I	1738	G
2	I	1740	G
2	I	1741	C
2	I	1758	U
2	I	1764	C
2	I	1773	A
2	I	1800	C
2	I	1801	A

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Mol	Chain	Res	Type
2	I	1808	A
2	I	1811	G
2	I	1816	C
2	I	1820	U
2	I	1822	C
2	I	1826	G
2	I	1829	A
2	I	1834	U
2	I	1838	C
2	I	1847	A
2	I	1866	A
2	I	1870	C
2	I	1872	A
2	I	1874	C
2	I	1906	G
2	I	1929	G
2	I	1930	G
2	I	1931	U
2	I	1936	A
2	I	1939	U
2	I	1955	U
2	I	1961	C
2	I	1963	U
2	I	1964	G
2	I	1965	C
2	I	1966	A
2	I	1967	C
2	I	1970	A
2	I	1971	U
2	I	1972	G
2	I	1991	U
2	I	1992	G
2	I	1993	U
2	I	1997	C
2	I	2022	U
2	I	2023	C
2	I	2027	G
2	I	2030	A
2	I	2031	A
2	I	2033	A
2	I	2043	C
2	I	2050	C

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Mol	Chain	Res	Type
2	I	2052	A
2	I	2055	C
2	I	2056	G
2	I	2060	A
2	I	2061	G
2	I	2062	A
2	I	2063	C
2	I	2068	U
2	I	2069	G
2	I	2093	G
2	I	2095	A
2	I	2108	A
2	I	2110	G
2	I	2111	U
2	I	2112	G
2	I	2115	G
2	I	2116	G
2	I	2117	A
2	I	2118	U
2	I	2124	G
2	I	2126	A
2	I	2127	G
2	I	2128	G
2	I	2131	U
2	I	2132	U
2	I	2133	G
2	I	2147	A
2	I	2157	G
2	I	2158	A
2	I	2159	G
2	I	2161	C
2	I	2163	A
2	I	2164	C
2	I	2169	A
2	I	2171	A
2	I	2172	U
2	I	2173	A
2	I	2187	U
2	I	2189	U
2	I	2190	G
2	I	2196	C
2	I	2198	A

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Mol	Chain	Res	Type
2	I	2204	G
2	I	2211	A
2	I	2213	U
2	I	2218	G
2	I	2225	A
2	I	2226	C
2	I	2238	G
2	I	2239	G
2	I	2249	U
2	I	2251	G
2	I	2268	A
2	I	2278	A
2	I	2283	C
2	I	2287	A
2	I	2288	A
2	I	2289	G
2	I	2305	U
2	I	2308	G
2	I	2312	U
2	I	2322	A
2	I	2325	G
2	I	2333	A
2	I	2334	U
2	I	2335	A
2	I	2346	A
2	I	2347	C
2	I	2350	C
2	I	2358	A
2	I	2361	G
2	I	2383	G
2	I	2385	C
2	I	2402	U
2	I	2403	C
2	I	2406	A
2	I	2422	C
2	I	2425	A
2	I	2426	A
2	I	2429	G
2	I	2430	A
2	I	2431	U
2	I	2434	A
2	I	2435	A

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Mol	Chain	Res	Type
2	I	2441	U
2	I	2444	G
2	I	2445	G
2	I	2448	A
2	I	2450	A
2	I	2459	A
2	I	2474	U
2	I	2476	A
2	I	2491	U
2	I	2494	G
2	I	2498	C
2	I	2502	G
2	I	2505	G
2	I	2506	U
2	I	2518	A
2	I	2520	C
2	I	2525	G
2	I	2529	G
2	I	2535	G
2	I	2547	A
2	I	2554	U
2	I	2556	C
2	I	2566	A
2	I	2567	G
2	I	2573	C
2	I	2586	U
2	I	2602	A
2	I	2605	PSU
2	I	2609	U
2	I	2610	C
2	I	2613	U
2	I	2615	U
2	I	2629	U
2	I	2631	G
2	I	2639	A
2	I	2643	G
2	I	2646	C
2	I	2663	G
2	I	2681	C
2	I	2685	G
2	I	2689	U
2	I	2690	U

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Mol	Chain	Res	Type
2	I	2714	G
2	I	2715	C
2	I	2716	C
2	I	2718	G
2	I	2726	A
2	I	2733	A
2	I	2744	G
2	I	2745	C
2	I	2748	A
2	I	2757	A
2	I	2765	A
2	I	2771	C
2	I	2778	A
2	I	2780	G
2	I	2793	C
2	I	2794	C
2	I	2798	U
2	I	2799	A
2	I	2800	A
2	I	2818	U
2	I	2820	A
2	I	2833	U
2	I	2835	A
2	I	2836	U
2	I	2849	U
2	I	2861	U
2	I	2867	G
2	I	2873	A
2	I	2874	C
2	I	2880	C
2	I	2884	U
2	I	2885	G
2	I	2893	A
3	J	25	U
3	J	32	U
3	J	35	C
3	J	42	C
3	J	53	A
3	J	56	G
3	J	67	G
3	J	88	C
3	J	89	U

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Mol	Chain	Res	Type
3	J	90	C
3	J	99	A
3	J	105	G
3	J	109	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	I	100	U
2	I	138	U
2	I	271	G
2	I	404	A
2	I	504	A
2	I	550	C
2	I	746	PSU
2	I	784	G
2	I	846	U
2	I	958	U
2	I	1616	A
2	I	1963	U
2	I	2030	A
2	I	2162	G
2	I	2425	A
2	I	2447	G
2	I	2497	A
2	I	2586	U
2	I	2680	U
2	I	2756	U

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

6 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
2	PSU	I	2605	2	18,21,22	1.10	2 (11%)	22,30,33	1.83	5 (22%)
2	PSU	I	955	2	18,21,22	2.71	8 (44%)	22,30,33	3.19	11 (50%)
2	PSU	I	746	2	18,21,22	2.97	7 (38%)	22,30,33	2.40	5 (22%)
2	PSU	I	2604	2	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
2	PSU	I	2580	2	18,21,22	1.16	3 (16%)	22,30,33	1.86	6 (27%)
2	PSU	I	2457	2	18,21,22	1.09	1 (5%)	22,30,33	1.84	6 (27%)

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
2	PSU	I	2605	2	-	3/7/25/26	0/2/2/2
2	PSU	I	955	2	-	0/7/25/26	0/2/2/2
2	PSU	I	746	2	-	3/7/25/26	0/2/2/2
2	PSU	I	2604	2	-	0/7/25/26	0/2/2/2
2	PSU	I	2580	2	-	0/7/25/26	0/2/2/2
2	PSU	I	2457	2	-	0/7/25/26	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	746	PSU	C2-N3	-6.88	1.25	1.37
2	I	746	PSU	C4-N3	-6.06	1.27	1.38
2	I	955	PSU	C2-N3	-5.45	1.28	1.37
2	I	955	PSU	C4-N3	-5.35	1.28	1.38
2	I	746	PSU	C2-N1	-4.71	1.30	1.36
2	I	955	PSU	C6-N1	-3.75	1.30	1.36
2	I	746	PSU	C6-N1	-3.59	1.30	1.36
2	I	955	PSU	O4-C4	-3.40	1.17	1.23
2	I	746	PSU	O2-C2	-3.36	1.16	1.23
2	I	955	PSU	O4'-C1'	-3.33	1.39	1.43
2	I	955	PSU	C2-N1	-3.33	1.32	1.36
2	I	2457	PSU	C6-C5	3.25	1.39	1.35
2	I	2580	PSU	C6-C5	3.19	1.39	1.35
2	I	2605	PSU	C6-C5	3.19	1.39	1.35
2	I	2604	PSU	C6-C5	3.08	1.38	1.35
2	I	746	PSU	O5'-C5'	-2.92	1.37	1.44
2	I	955	PSU	C2'-C1'	-2.71	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	955	PSU	O2-C2	-2.61	1.17	1.23
2	I	2580	PSU	O4'-C1'	-2.43	1.40	1.43
2	I	746	PSU	C2'-C1'	-2.17	1.50	1.53
2	I	2605	PSU	O4'-C1'	-2.06	1.41	1.43
2	I	2580	PSU	C4-C5	-2.03	1.38	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	955	PSU	N1-C2-N3	8.92	125.24	115.13
2	I	746	PSU	N1-C2-N3	7.63	123.78	115.13
2	I	955	PSU	C4-N3-C2	-5.97	117.73	126.34
2	I	955	PSU	C3'-C2'-C1'	5.72	108.30	101.64
2	I	955	PSU	O2-C2-N3	-5.10	112.21	121.82
2	I	2605	PSU	C4-N3-C2	-4.73	119.53	126.34
2	I	2457	PSU	C4-N3-C2	-4.71	119.55	126.34
2	I	746	PSU	O2-C2-N3	-4.67	113.02	121.82
2	I	2604	PSU	C4-N3-C2	-4.67	119.61	126.34
2	I	2457	PSU	N1-C2-N3	4.63	120.38	115.13
2	I	2605	PSU	N1-C2-N3	4.60	120.34	115.13
2	I	2580	PSU	C4-N3-C2	-4.57	119.75	126.34
2	I	2604	PSU	N1-C2-N3	4.47	120.19	115.13
2	I	2580	PSU	N1-C2-N3	4.41	120.12	115.13
2	I	746	PSU	C4-N3-C2	-3.74	120.95	126.34
2	I	746	PSU	C6-C5-C4	-3.45	115.79	118.20
2	I	2580	PSU	O2-C2-N1	-2.62	119.91	122.79
2	I	2580	PSU	O4'-C1'-C2'	2.60	108.82	105.14
2	I	955	PSU	C6-C5-C4	-2.59	116.38	118.20
2	I	2457	PSU	O2-C2-N1	-2.58	119.95	122.79
2	I	955	PSU	C5-C6-N1	-2.51	118.34	122.11
2	I	746	PSU	C6-N1-C2	-2.40	120.23	122.68
2	I	2604	PSU	O2-C2-N1	-2.37	120.19	122.79
2	I	955	PSU	O4-C4-N3	-2.35	115.62	120.12
2	I	2605	PSU	O2-C2-N1	-2.29	120.27	122.79
2	I	2580	PSU	C6-C5-C4	2.26	119.78	118.20
2	I	955	PSU	O2'-C2'-C1'	-2.26	105.85	111.23
2	I	2457	PSU	O4'-C1'-C2'	2.16	108.19	105.14
2	I	955	PSU	O4'-C1'-C2'	-2.14	102.12	105.14
2	I	2605	PSU	C6-N1-C2	-2.13	120.50	122.68
2	I	2457	PSU	C6-N1-C2	-2.13	120.51	122.68
2	I	2604	PSU	C6-C5-C4	2.10	119.67	118.20
2	I	955	PSU	C2'-C3'-C4'	-2.10	98.57	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	955	PSU	C4'-O4'-C1'	2.08	113.79	108.55
2	I	2457	PSU	C6-C5-C4	2.08	119.65	118.20
2	I	2580	PSU	C6-N1-C2	-2.07	120.57	122.68
2	I	2605	PSU	C6-C5-C4	2.05	119.63	118.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	2605	PSU	O4'-C4'-C5'-O5'
2	I	2605	PSU	C3'-C4'-C5'-O5'
2	I	746	PSU	C3'-C4'-C5'-O5'
2	I	746	PSU	O4'-C4'-C5'-O5'
2	I	2605	PSU	O4'-C1'-C5-C4
2	I	746	PSU	O4'-C1'-C5-C6

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 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
33	GNP	6	501	34	29,34,34	1.56	7 (24%)	33,54,54	2.23	6 (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
33	GNP	6	501	34	-	4/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	6	501	GNP	PB-O3A	4.17	1.64	1.59
33	6	501	GNP	C6-N1	3.06	1.38	1.33
33	6	501	GNP	PB-O1B	2.90	1.50	1.46
33	6	501	GNP	PG-N3B	2.81	1.70	1.63
33	6	501	GNP	PG-O1G	2.51	1.50	1.46
33	6	501	GNP	PB-O2B	-2.29	1.50	1.56
33	6	501	GNP	C5-C6	2.00	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	6	501	GNP	C5-C6-N1	-8.40	111.94	123.43
33	6	501	GNP	C2-N1-C6	5.82	125.17	115.93
33	6	501	GNP	PB-O3A-PA	-2.77	122.86	132.62
33	6	501	GNP	N3-C2-N1	-2.74	123.56	127.22
33	6	501	GNP	C4-C5-C6	-2.55	118.36	120.80
33	6	501	GNP	C2-N3-C4	-2.20	112.84	115.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

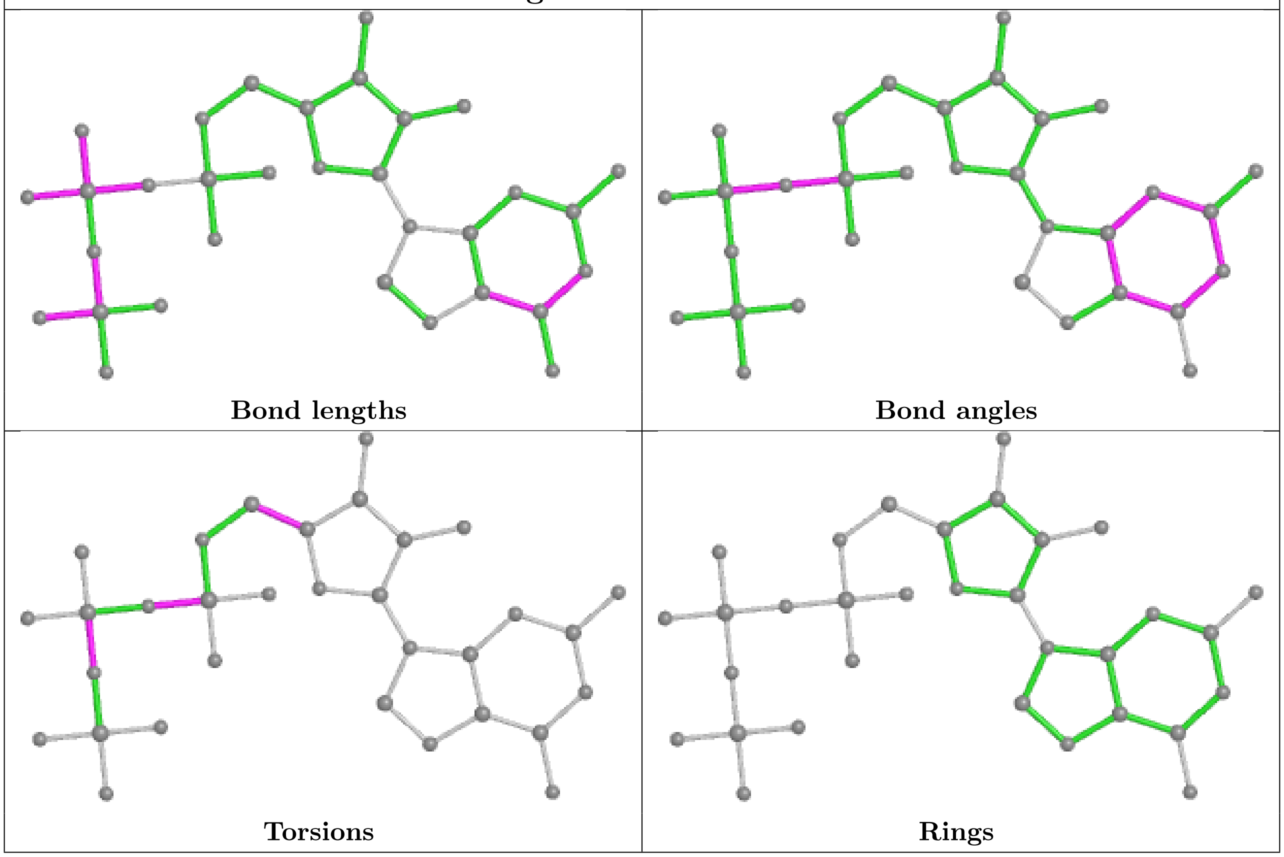
Mol	Chain	Res	Type	Atoms
33	6	501	GNP	PG-N3B-PB-O1B
33	6	501	GNP	PG-N3B-PB-O3A
33	6	501	GNP	PB-O3A-PA-O2A
33	6	501	GNP	O4'-C4'-C5'-O5'

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 then 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.

Ligand GNP 6 501



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.

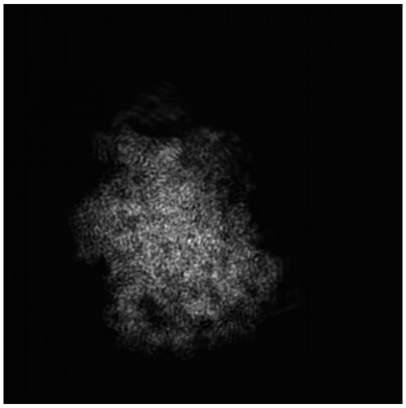
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-33904. These allow visual inspection of the internal detail of the map and identification of artifacts.

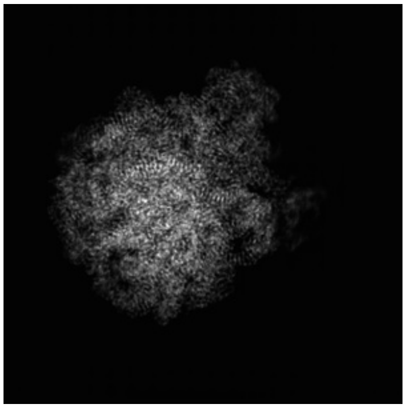
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

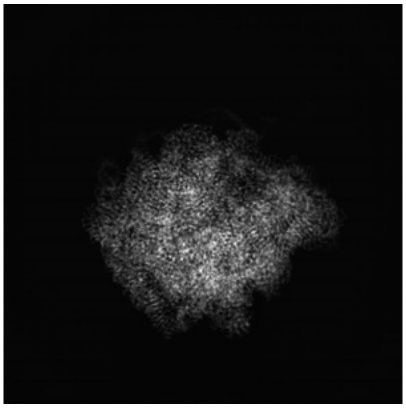
6.1.1 Primary map



X

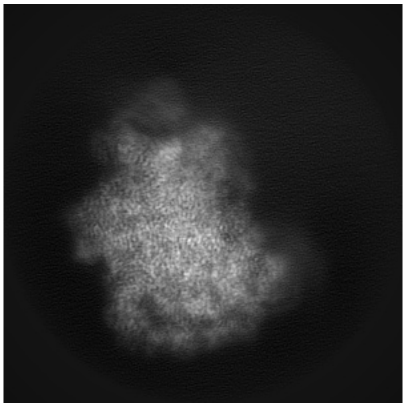


Y

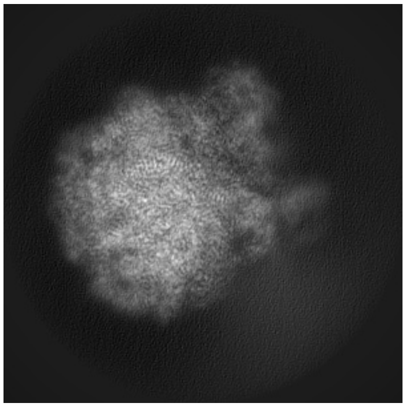


Z

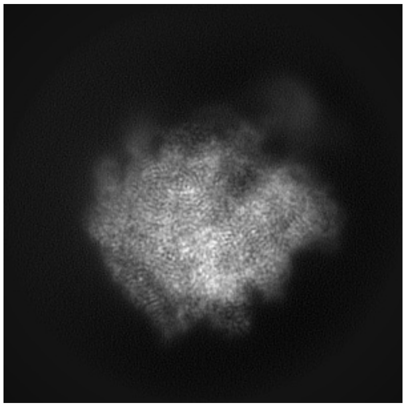
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices ⓘ

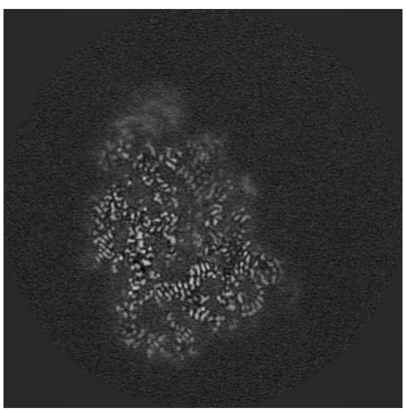
6.2.1 Primary map

X Index: 150

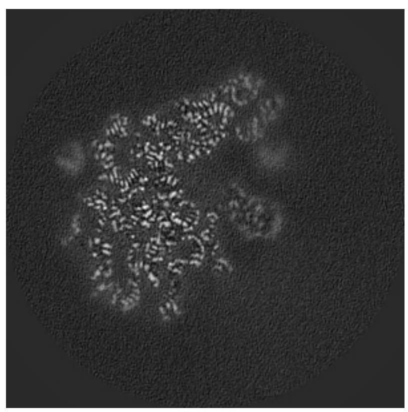
Y Index: 150

Z Index: 150

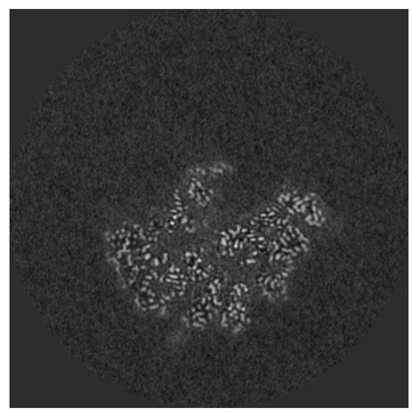
6.2.2 Raw map



X Index: 150



Y Index: 150



Z Index: 150

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

6.3 Largest variance slices (i)

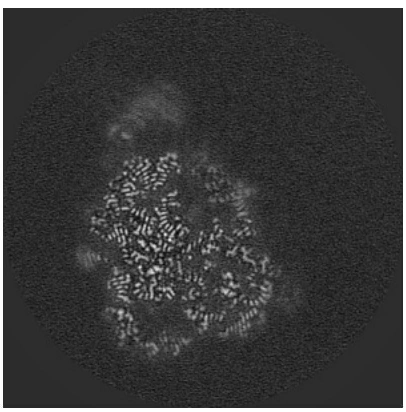
6.3.1 Primary map

X Index: 153

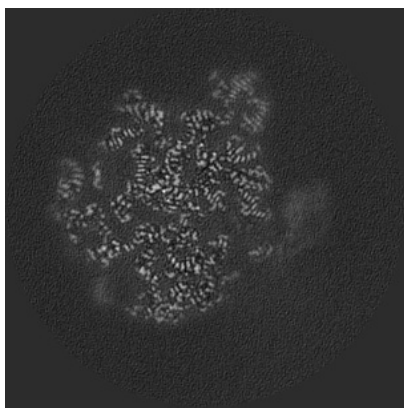
Y Index: 129

Z Index: 122

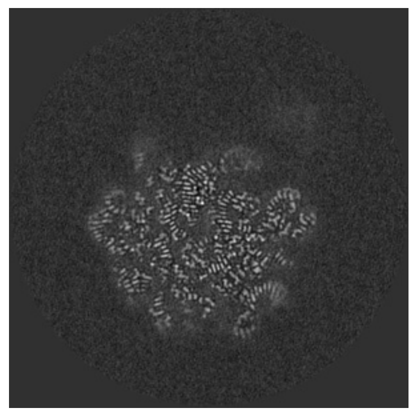
6.3.2 Raw map



X Index: 157



Y Index: 127

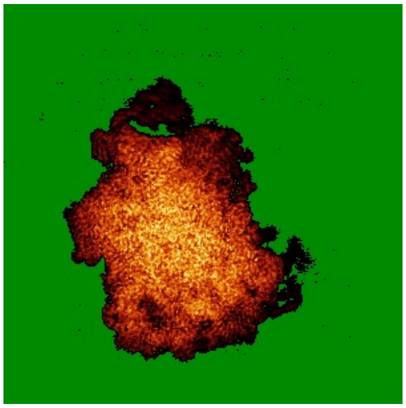


Z Index: 122

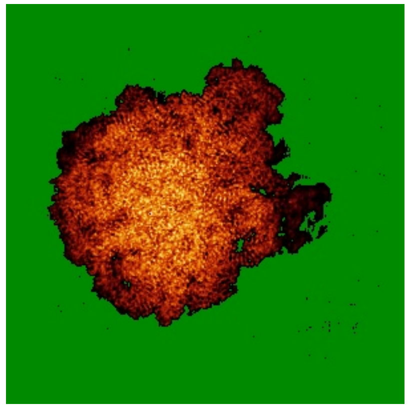
The images above show the largest variance slices of the map in three orthogonal directions.

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

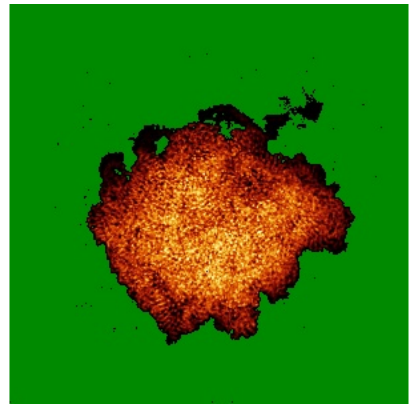
6.4.1 Primary map



X

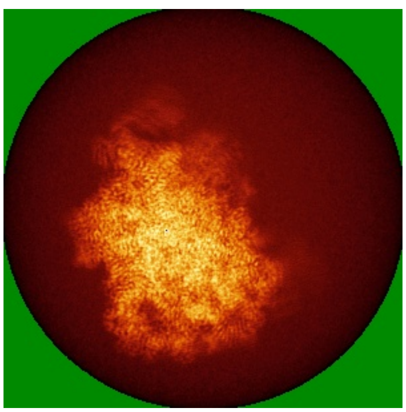


Y

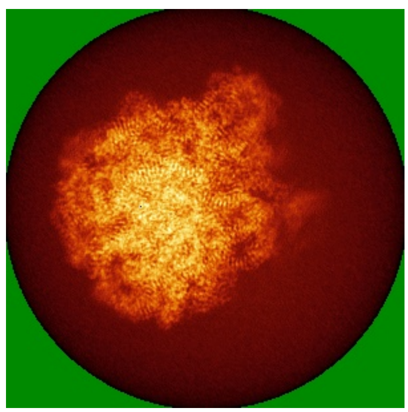


Z

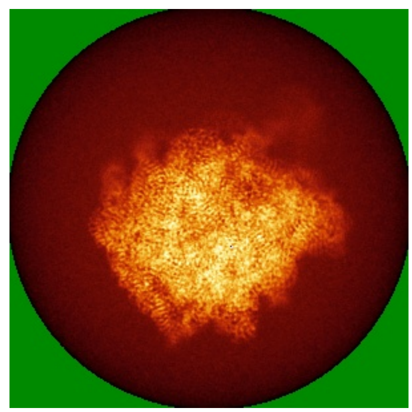
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

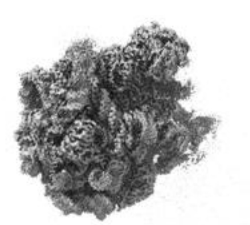
Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X



Y

Z

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

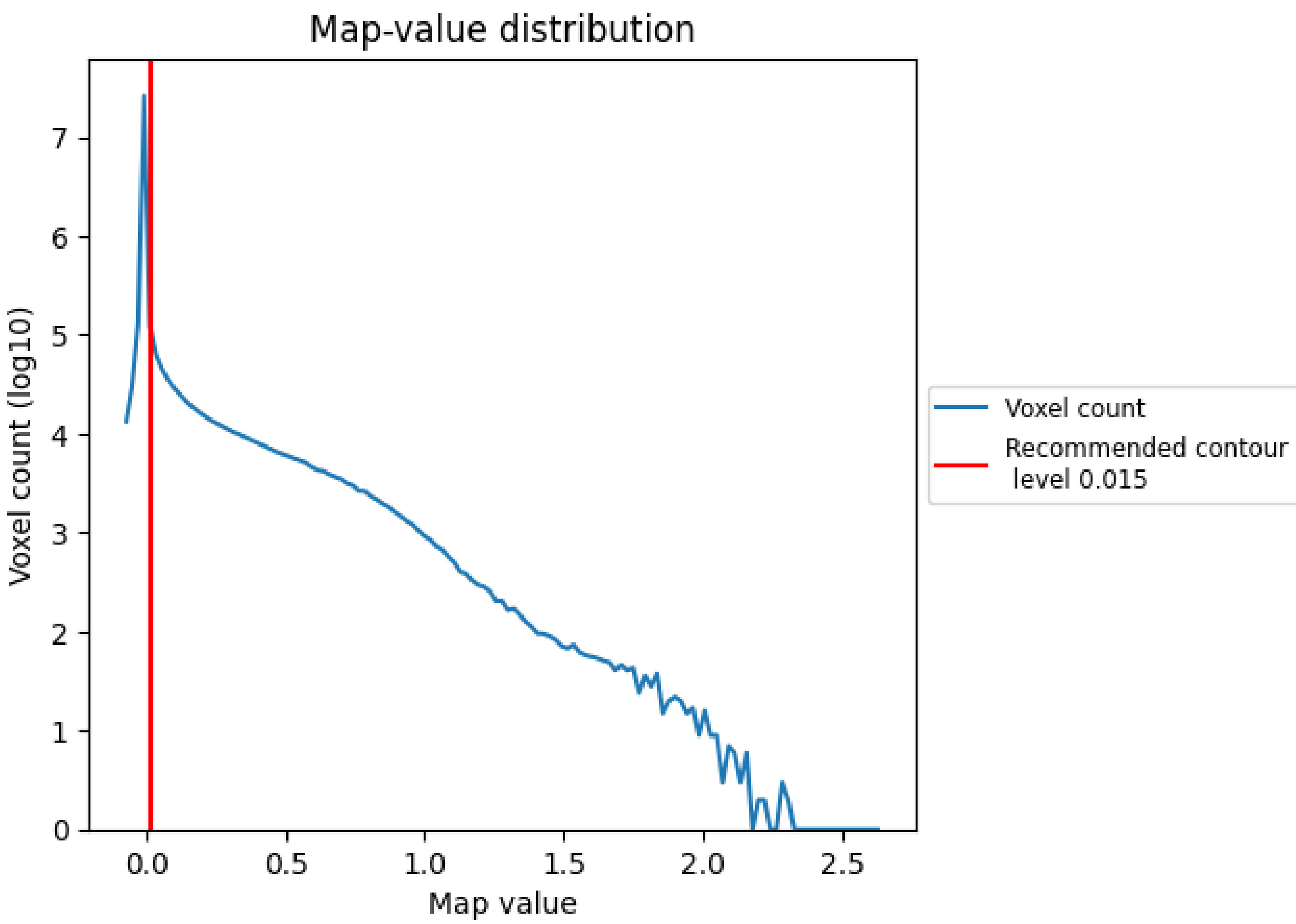
6.6 Mask visualisation (i)

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

7 Map analysis (i)

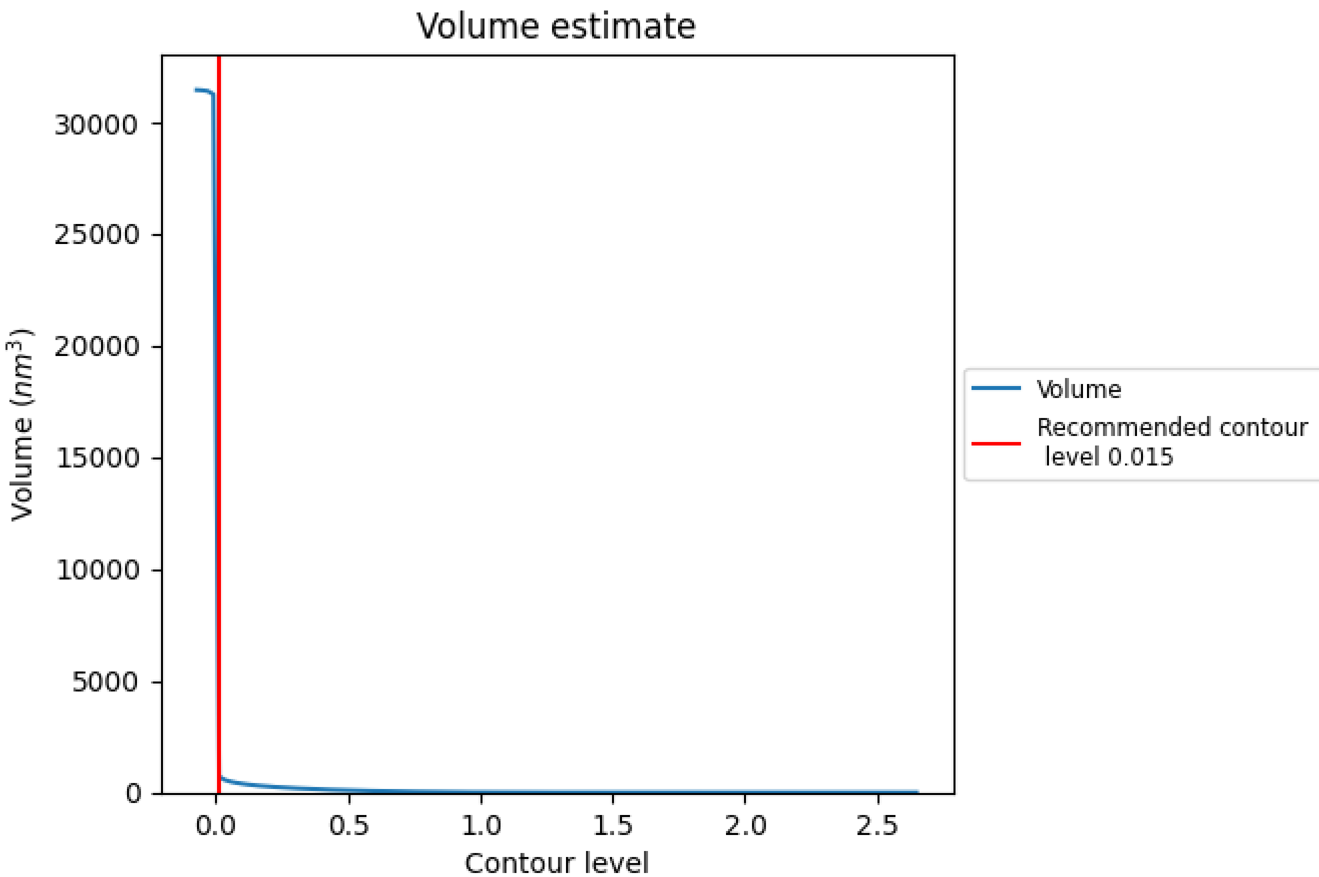
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

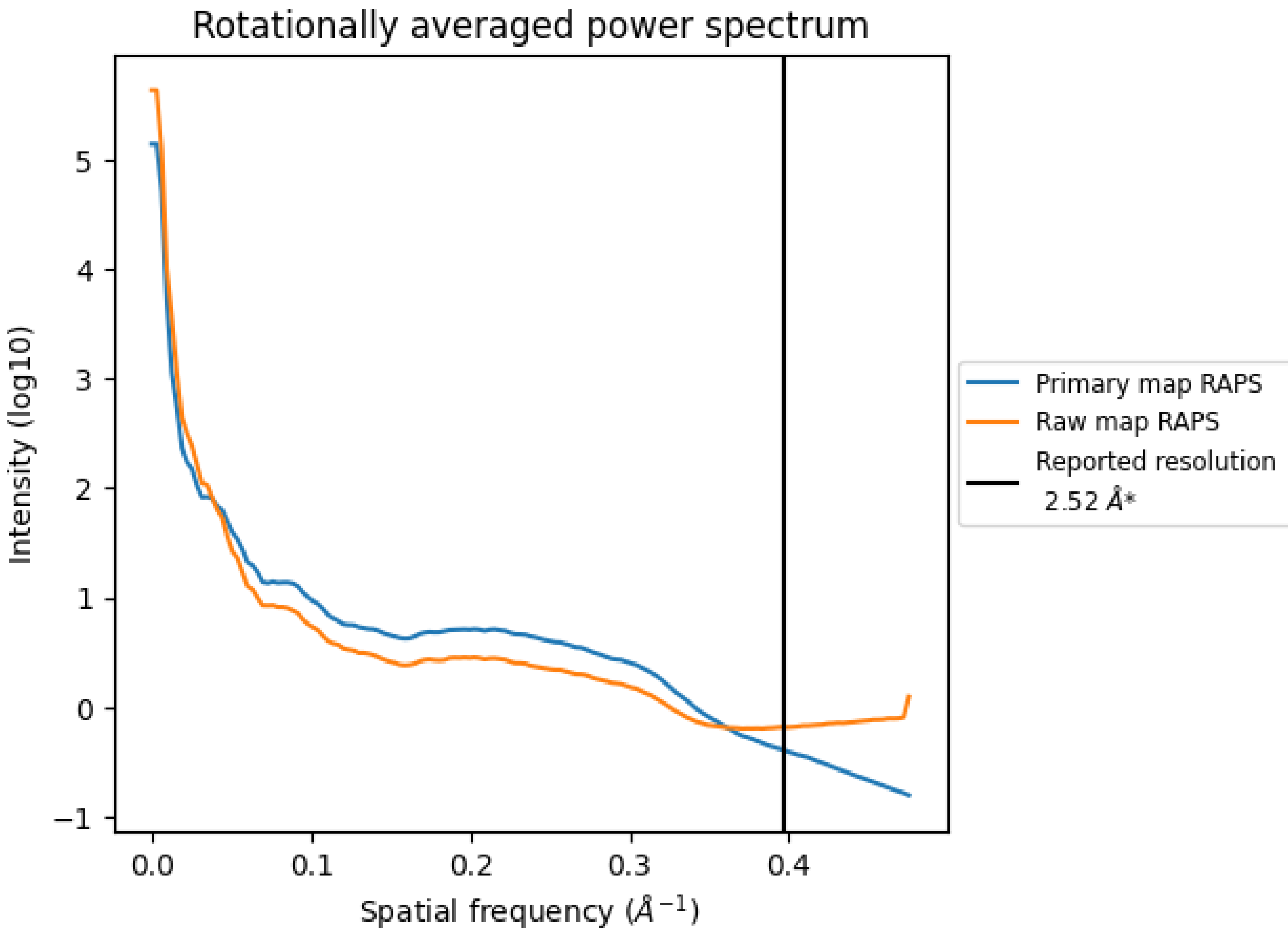
7.2 Volume estimate



The volume at the recommended contour level is 688 nm^3; this corresponds to an approximate mass of 621 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)

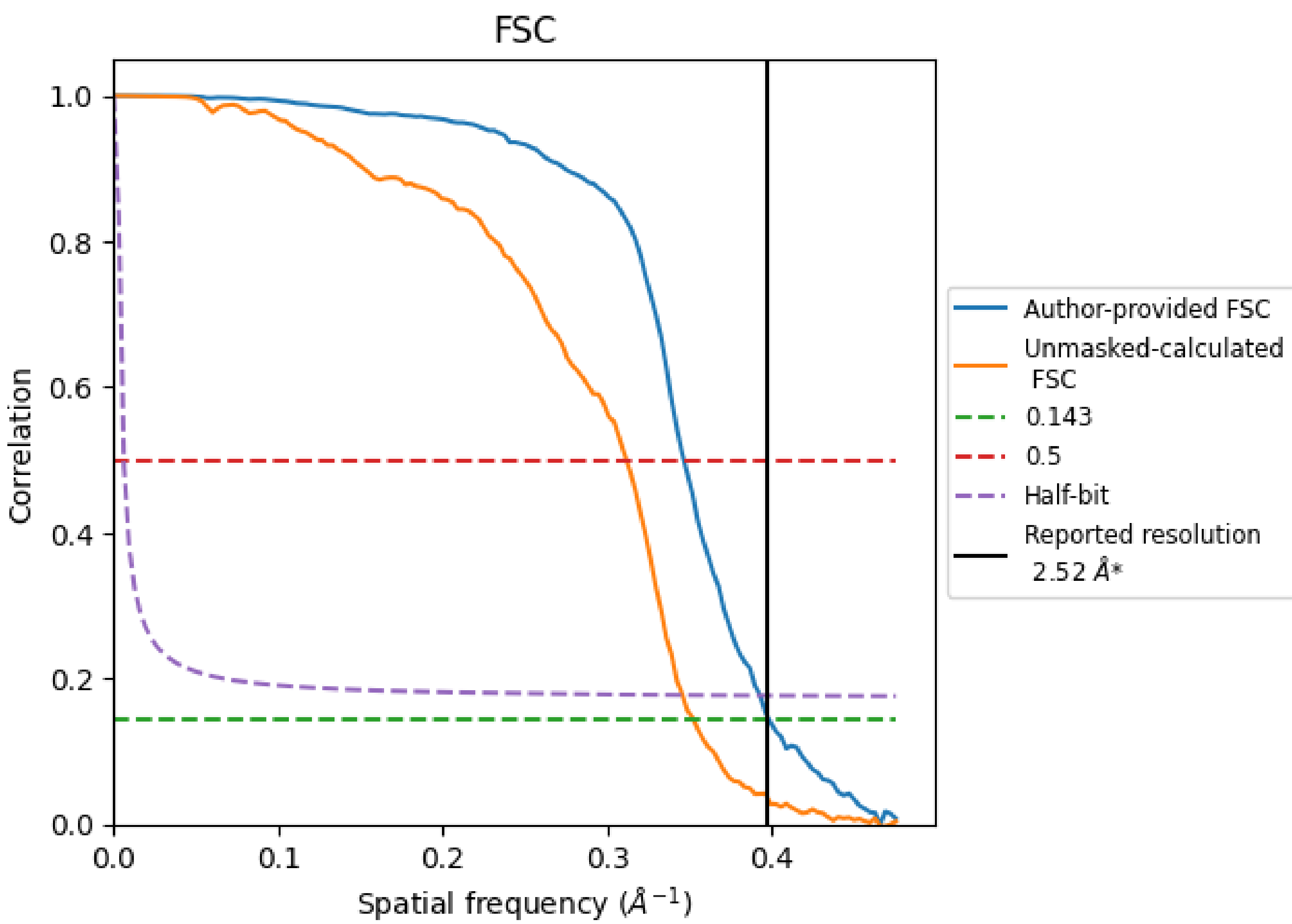


*Reported resolution corresponds to spatial frequency of 0.397 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.397 $Å^{-1}$

8.2 Resolution estimates (i)

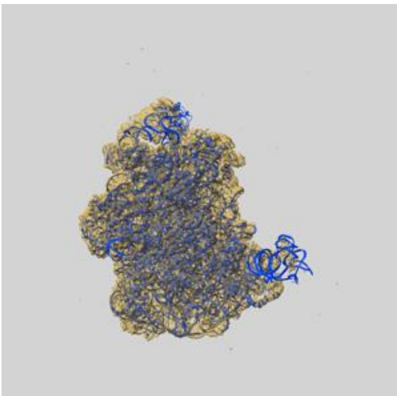
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	2.51	2.89	2.55
Unmasked-calculated*	2.84	3.21	2.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.84 differs from the reported value 2.52 by more than 10 %

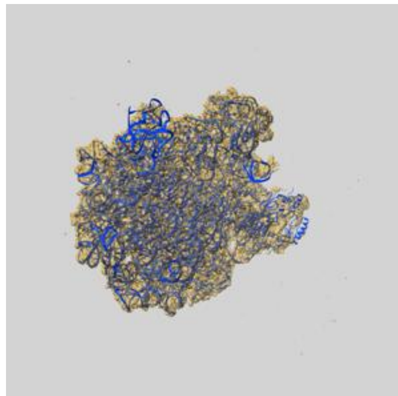
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-33904 and PDB model 7YLA. Per-residue inclusion information can be found in section 3 on page 10.

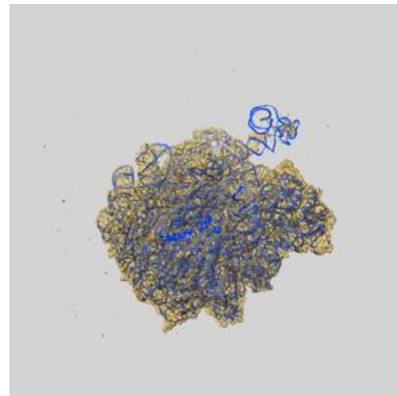
9.1 Map-model overlay (i)



X



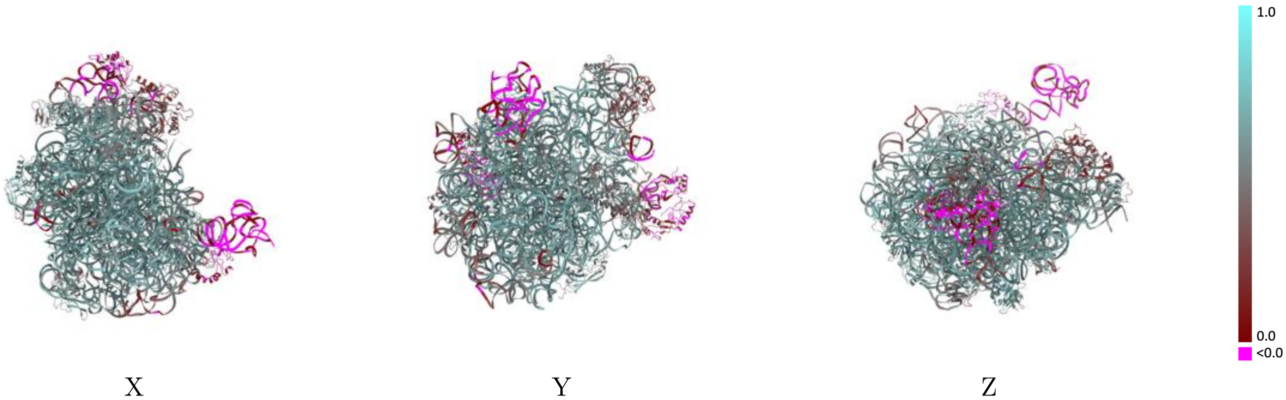
Y



Z

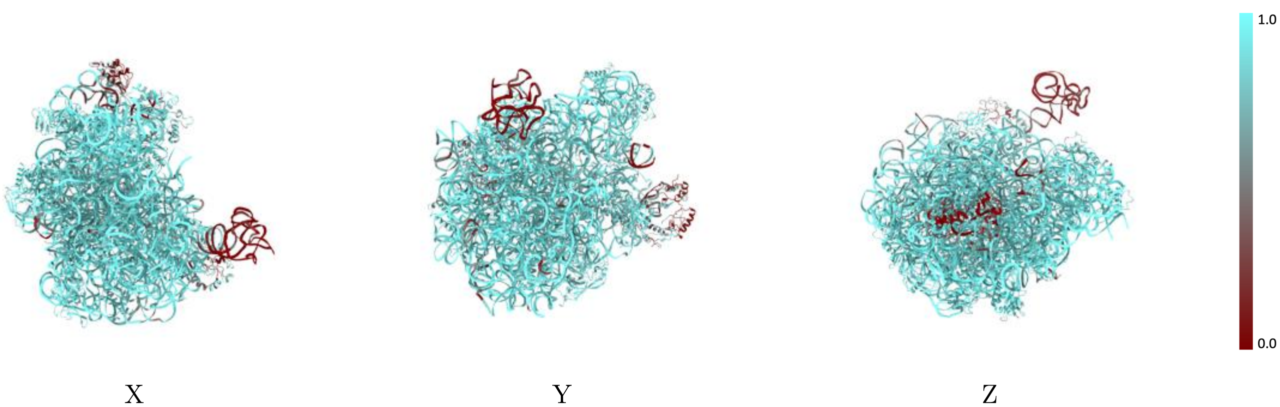
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



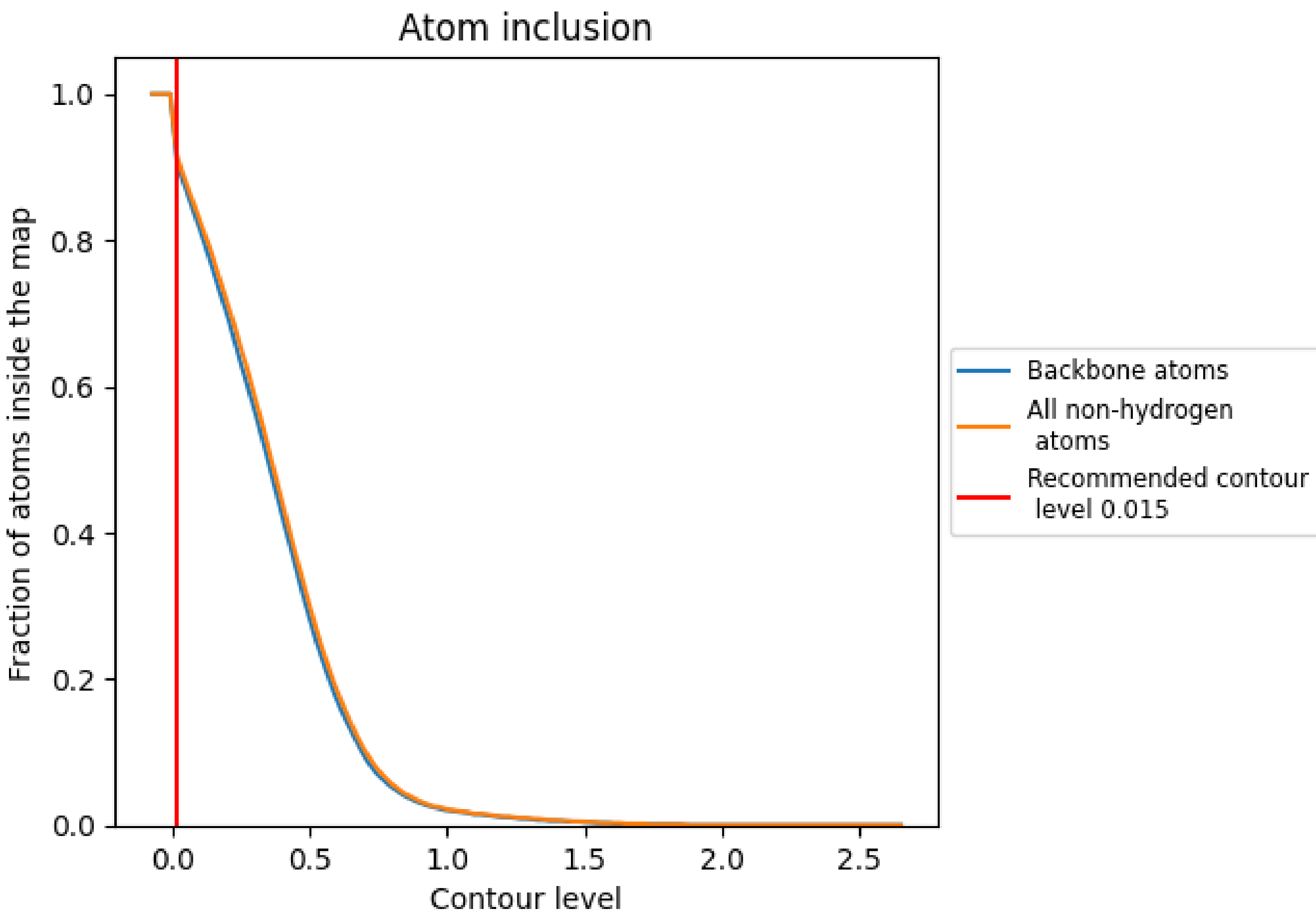
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.5550
6	0.7600	0.3570
I	0.9290	0.5740
J	0.9780	0.5580
K	0.9610	0.6260
L	0.9520	0.6190
M	0.9340	0.5800
N	0.8020	0.3080
O	0.8890	0.4800
P	0.4400	0.1220
Q	0.1540	-0.0160
R	0.9540	0.6270
S	0.9380	0.5970
T	0.9500	0.6170
U	0.9510	0.6080
V	0.9650	0.6340
W	0.9080	0.5110
X	0.9210	0.5820
Y	0.9730	0.6530
Z	0.9260	0.6080
a	0.9320	0.6070
b	0.8950	0.5460
c	0.9060	0.5360
d	0.9120	0.5600
e	0.9370	0.6100
f	0.9350	0.5760
g	0.8850	0.5220
h	0.9270	0.6110
i	0.9320	0.5960
j	0.9400	0.5920
k	0.9550	0.6450
l	0.9650	0.6510
m	0.9520	0.6070