



wwPDB EM Validation Summary Report ⓘ

May 20, 2024 – 05:07 PM EDT

PDB ID : 3J7Y
EMDB ID : EMD-2762
Title : Structure of the large ribosomal subunit from human mitochondria
Authors : Brown, A.; Amunts, A.; Bai, X.C.; Sugimoto, Y.; Edwards, P.C.; Murshudov, G.; Scheres, S.H.W.; Ramakrishnan, V.
Deposited on : 2014-08-26
Resolution : 3.40 Å(reported)

This is a wwPDB EM Validation Summary 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:

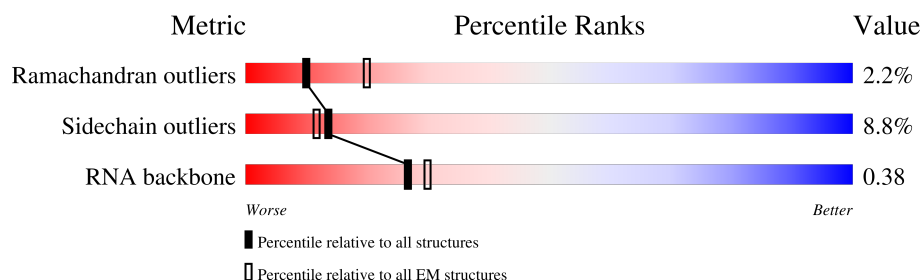
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.














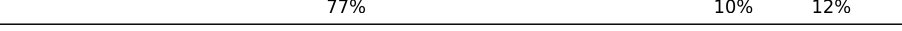




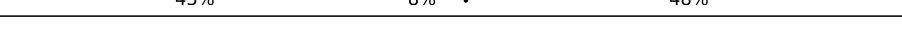


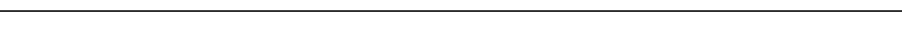

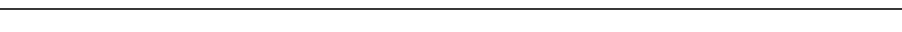
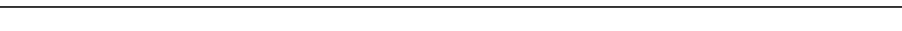


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1559	
2	B	73	
3	D	305	
4	E	348	
5	F	311	
6	H	267	
7	I	261	
8	J	192	










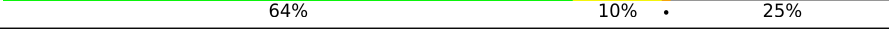



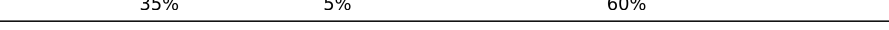



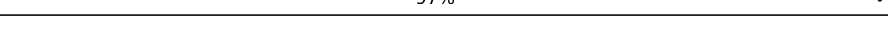
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Mol	Chain	Length	Quality of chain
9	K	178	
10	L	145	
11	M	296	
12	N	251	
13	O	175	
14	P	179	
15	Q	292	
16	R	149	
17	S	205	
18	T	212	
19	U	153	
20	V	216	
21	W	148	
22	X	256	
23	Y	250	
24	Z	161	
25	0	188	
26	1	65	
27	2	92	
28	3	188	
29	4	103	
30	5	423	
31	6	380	
32	7	338	
33	8	206	

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Mol	Chain	Length	Quality of chain
34	9	137	
35	a	142	
36	b	155	
37	c	332	
38	d	306	
39	e	279	
40	f	211	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	112	
46	o	102	
47	p	206	
48	q	222	
49	r	196	
50	s	439	
51	t	127	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 94121 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1472	Total	C	N	O	P	0	0
			31261	14025	5642	10122	1472		

- Molecule 2 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	57	Total	C	N	O	P	0	0
			1211	543	217	394	57		

- Molecule 3 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	236	Total	C	N	O	S	0	0
			1842	1145	373	315	9		

- Molecule 4 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	300	Total	C	N	O	S	0	0
			2365	1523	410	422	10		

- Molecule 5 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 6 is a protein called bL9.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	95	Total	C	N	O	0	0
			784	498	152	134		

- Molecule 7 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 8 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 9 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 10 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 11 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 12 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 13 is a protein called bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 14 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	133	Total	C	N	O	S	0	0
			1080	677	209	189	5		

- Molecule 15 is a protein called bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	204	Total	C	N	O	S	0	0
			1704	1094	303	299	8		

- Molecule 16 is a protein called bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 17 is a protein called bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 18 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 19 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	111	Total	C	N	O	S	0	0
			922	591	176	153	2		

- Molecule 20 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	189	Total	C	N	O	S	0	0
			1551	987	278	278	8		

- Molecule 21 is a protein called bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	107	Total	C	N	O	S	0	0
			842	542	158	139	3		

- Molecule 22 is a protein called bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	243	Total	C	N	O	S	0	0
			2027	1310	350	362	5		

- Molecule 23 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 24 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 25 is a protein called bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	98	Total	C	N	O	S	0	0
			803	501	159	137	6		

- Molecule 26 is a protein called bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 27 is a protein called bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	43	Total	C	N	O	S	0	0
			351	218	76	56	1		

- Molecule 28 is a protein called bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	36	Total	C	N	O	S	0	0
			322	203	70	46	3		

- Molecule 30 is a protein called mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	376	Total	C	N	O	S	0	0
			3064	1987	529	538	10		

- Molecule 31 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	325	Total	C	N	O	S	0	0
			2636	1692	465	470	9		

- Molecule 32 is a protein called mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	266	Total	C	N	O	S	0	0
			2158	1383	371	388	16		

- Molecule 33 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	8	57	Total	C	N	O	S	0	0
			482	302	86	92	2		

- Molecule 34 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	9	109	Total	C	N	O	S	0	0
			873	565	152	154	2		

- Molecule 35 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	39	Total	C	N	O	S	0	0
			343	217	68	55	3		

- Molecule 36 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 37 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 38 is a protein called mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	162	Total	C	N	O	S	0	0
			1347	870	234	235	8		

- Molecule 39 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	134	Total	C	N	O	S	0	0
			1082	690	193	196	3		

- Molecule 40 is a protein called mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	95	Total	C	N	O	S	0	0
			703	448	119	133	3		

- Molecule 41 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 42 is a protein called mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 43 is a protein called mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	96	Total	C	N	O	S	0	0
			816	526	161	125	4		

- Molecule 44 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 45 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	84	Total	C	N	O	S	0	0
			655	407	122	121	5		

- Molecule 46 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 47 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	83	Total	C	N	O	S	0	0
			674	421	125	125	3		

- Molecule 48 is a protein called CRIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 49 is a protein called bS18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

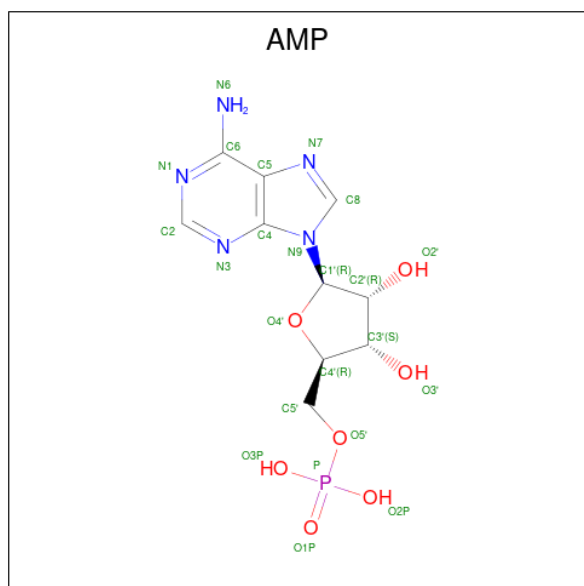
- Molecule 50 is a protein called mS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 51 is a protein called unknown protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	123	Total	C	N	O		0	0
			615	369	123	123			

- Molecule 52 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					AltConf
52	A	1	Total	C	N	O	P	0
			22	10	5	6	1	

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	A	65	Total	Mg	0
			65	65	

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Mol	Chain	Residues	Atoms		AltConf
53	E	1	Total	Mg	0
			1	1	

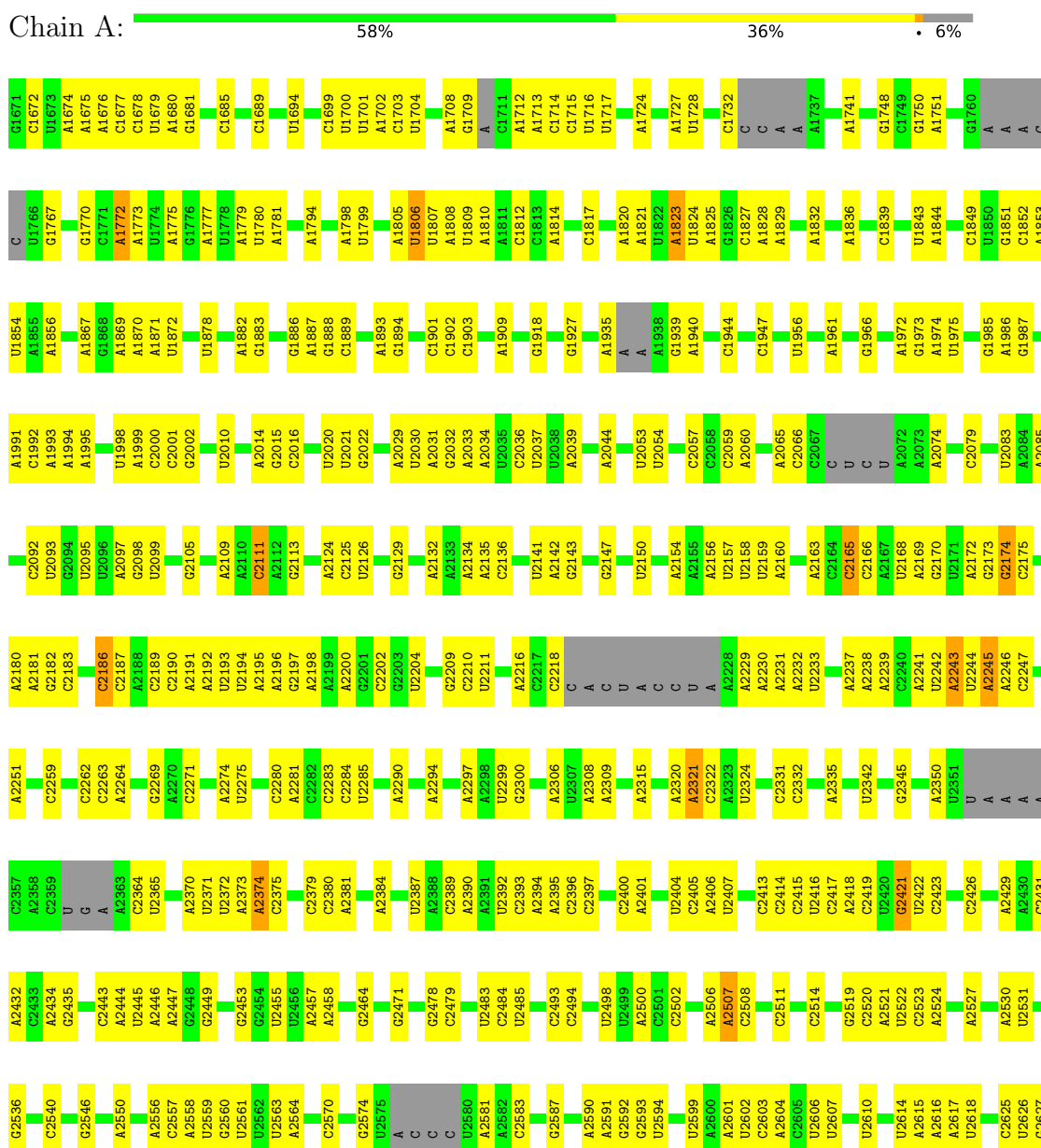
- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

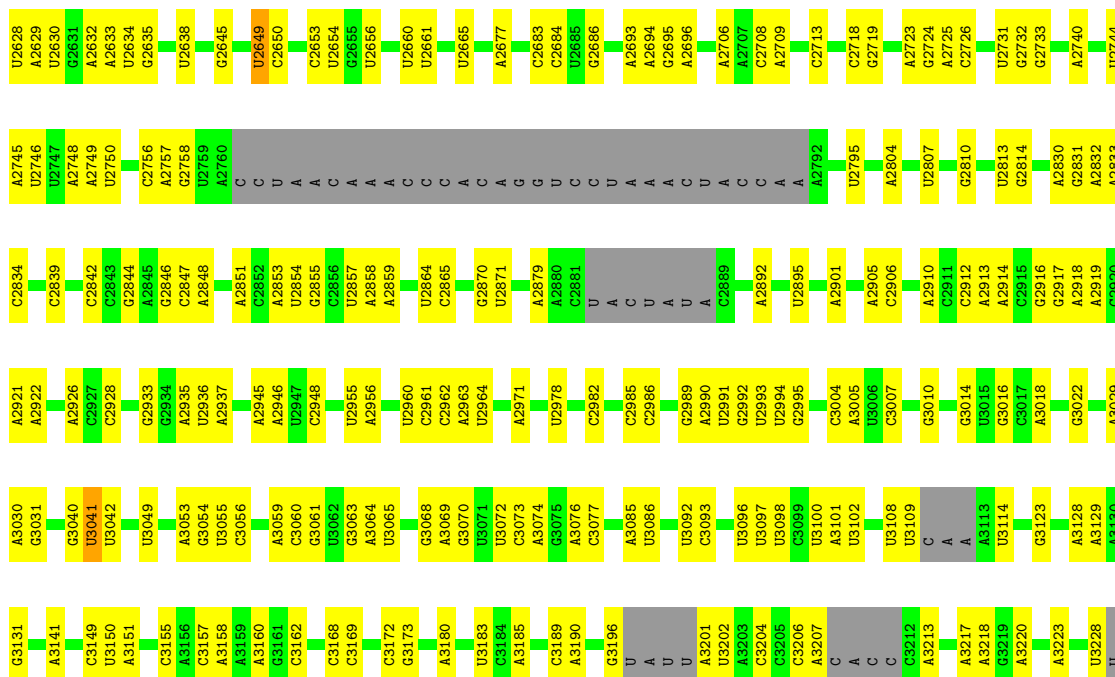
Mol	Chain	Residues	Atoms		AltConf
54	0	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	
54	r	1	Total	Zn	0
			1	1	

3 Residue-property plots

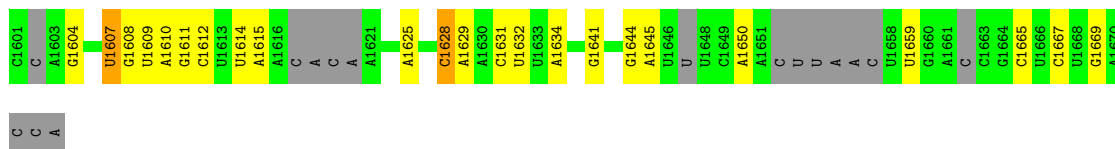
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

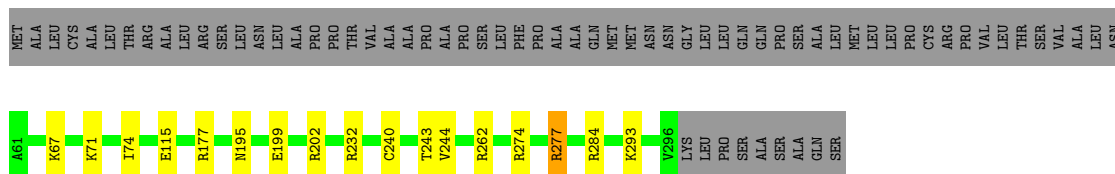




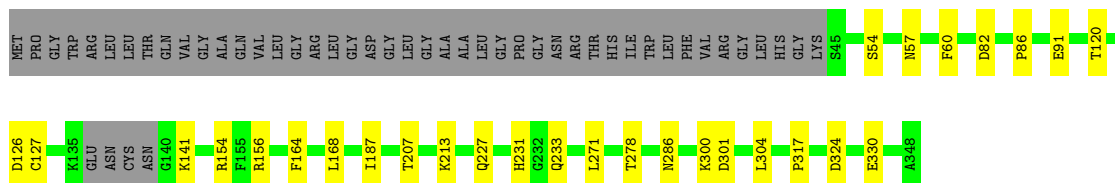
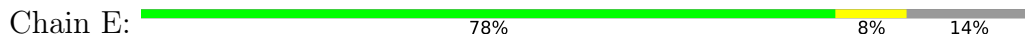
• Molecule 2: mt-tRNAVal



• Molecule 3: uL2

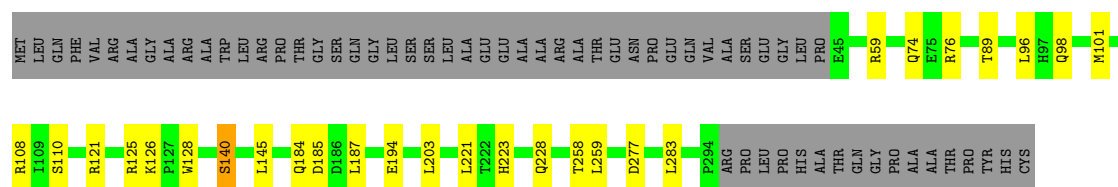


• Molecule 4: uL3



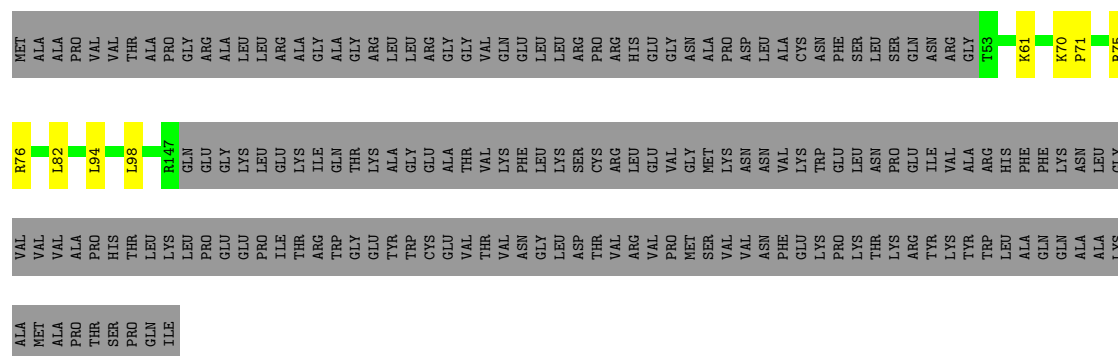
• Molecule 5: uL4

Chain F:  72% 8% 20%



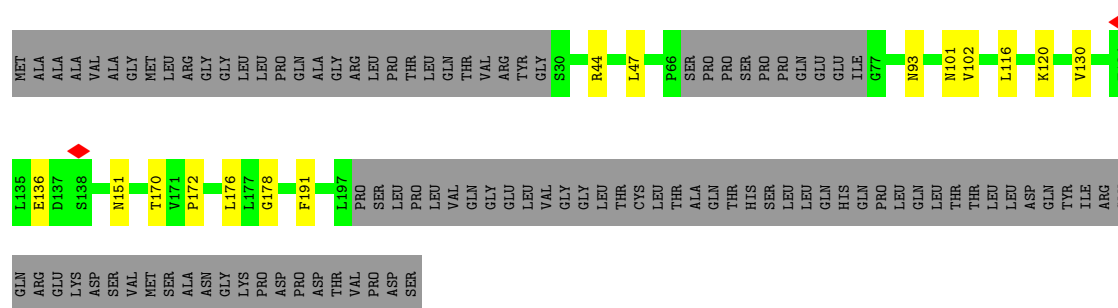
• Molecule 6: bL9

Chain H:  33% 64%



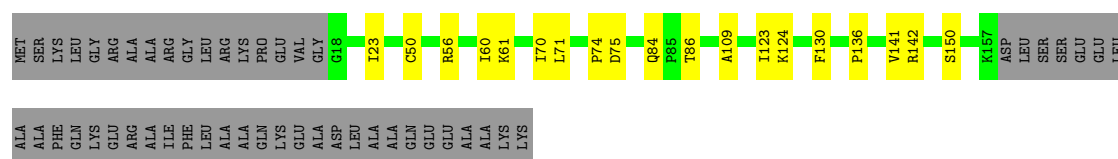
• Molecule 7: uL10

Chain I:  55% 6% 39%




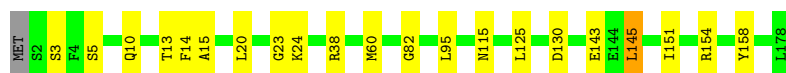
• Molecule 8: uL11

Chain J:  63% 10% 27%



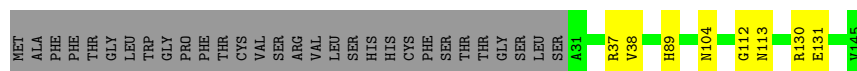
• Molecule 9: uL13

Chain K:  88% 11% ..



- Molecule 10: uL14

Chain L: 74% 6% 21%



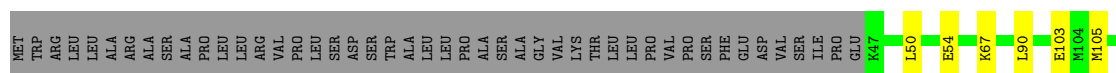
- Molecule 11: uL15

Chain M: 86% 11% .



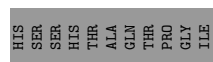
- Molecule 12: uL16

Chain N: 75% 7% 18%



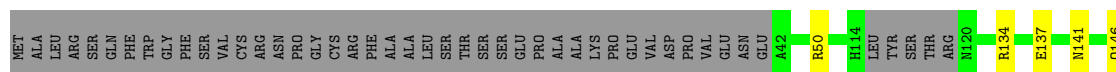
- Molecule 13: bL17

Chain O: 74% 13% . 13%



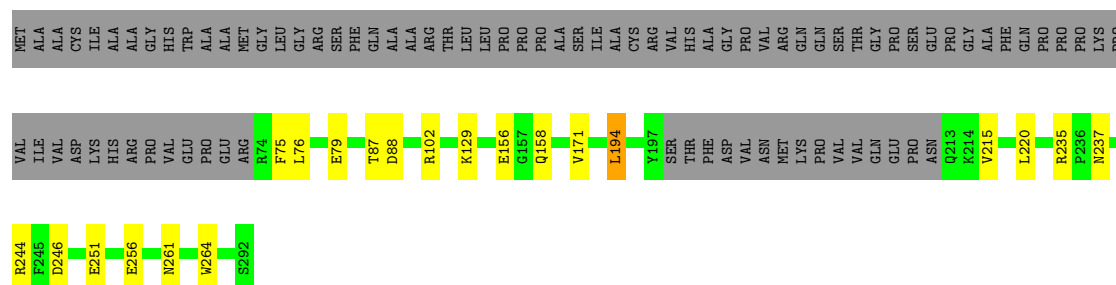
- Molecule 14: uL18

Chain P: 69% 6% 26%




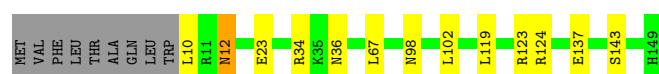
- Molecule 15: bL19

Chain Q:  63% 7% 30%



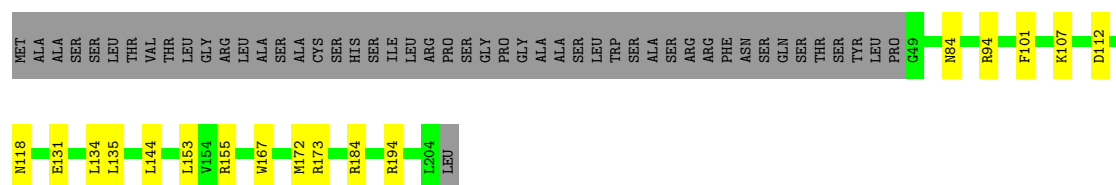
- Molecule 16: bL20

Chain R:  85% 8% 6%



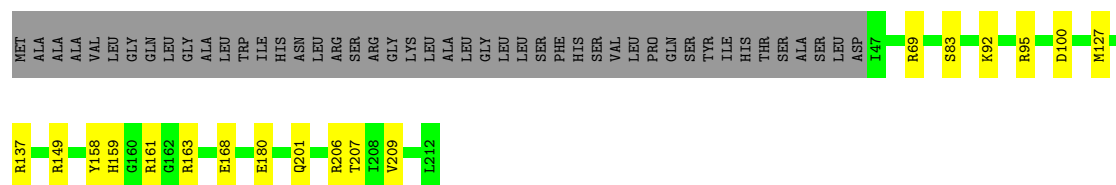
- Molecule 17: bL21

Chain S:  68% 8% 24%



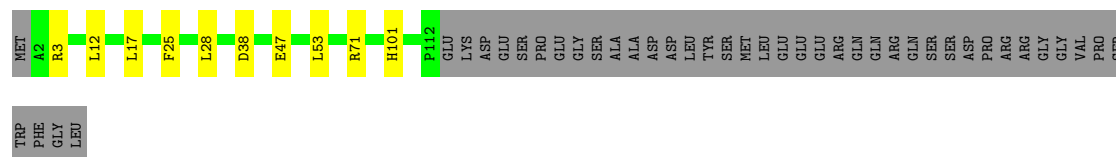
- Molecule 18: uL22

Chain T:  70% 8% 22%




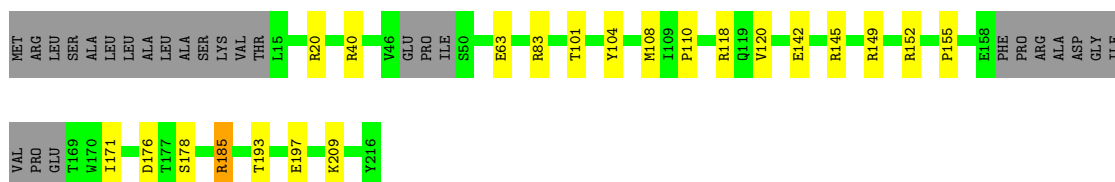
- Molecule 19: uL23

Chain U:  66% 7% 27%



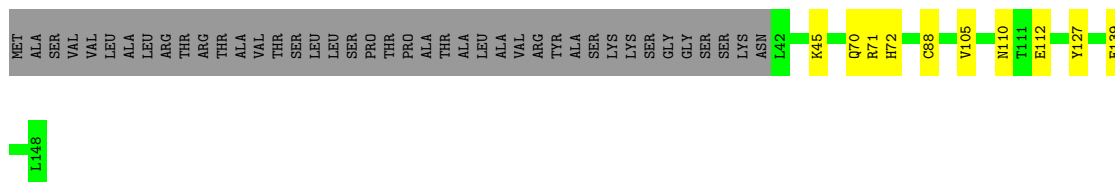
- Molecule 20: uL24

Chain V:  77% 10% 12%



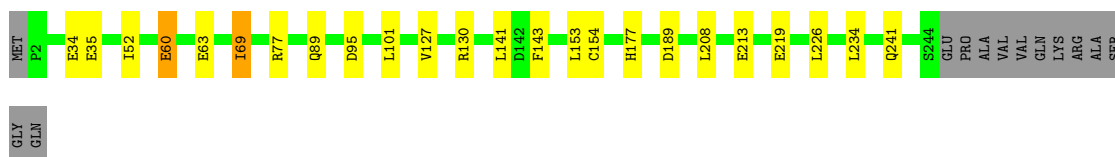
• Molecule 21: bL27

Chain W: 66% 7% 28%



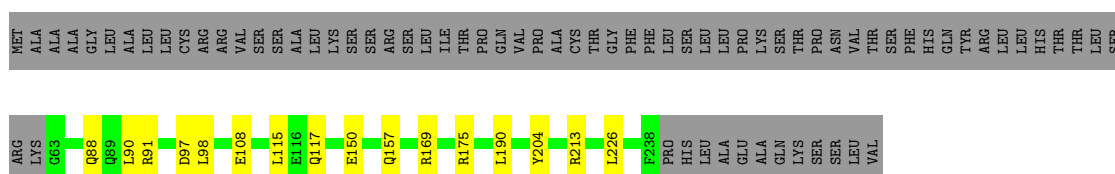
• Molecule 22: bL28

Chain X: 86% 9% 5%



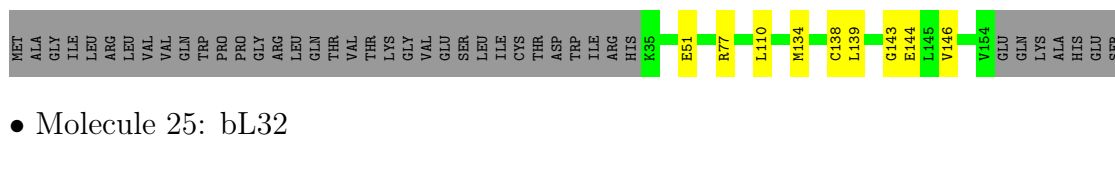
• Molecule 23: uL29

Chain Y: 64% 6% 30%



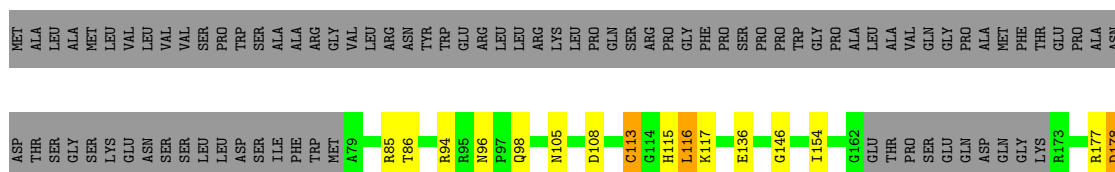
• Molecule 24: uL30

Chain Z: 69% 6% 25%



• Molecule 25: bL32

Chain 0: 43% 8% 48%



14%



21%



72%

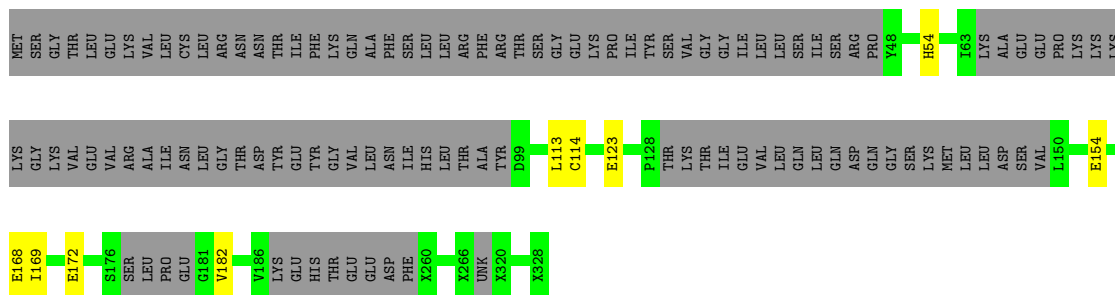


20%



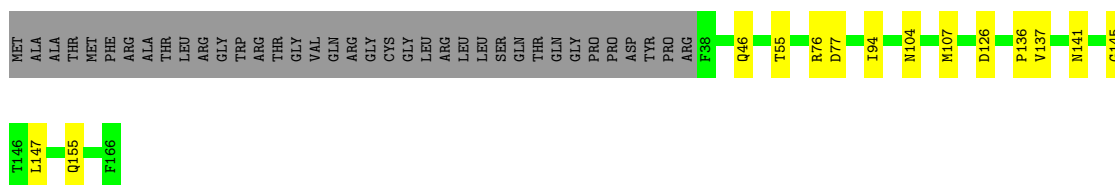
73%





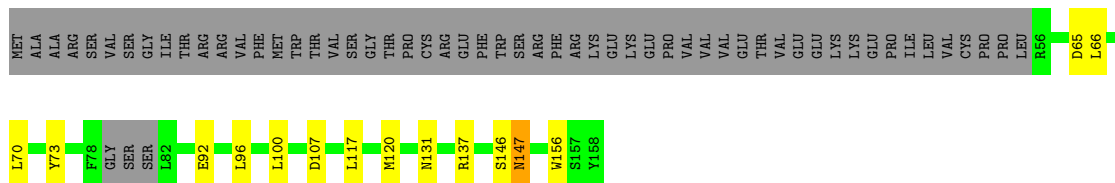
• Molecule 41: mL49

Chain g: 69% 8% 22%



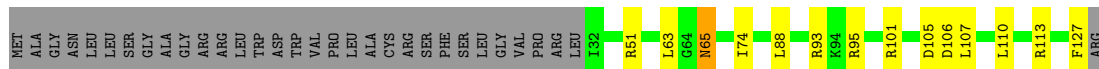
• Molecule 42: mL50

Chain h: 54% 9% 37%



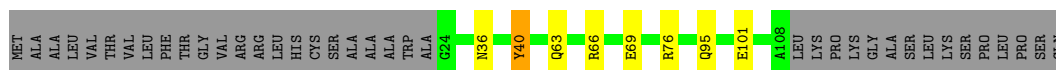
• Molecule 43: mL51

Chain i: 64% 10% 25%



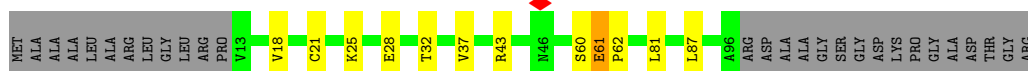
• Molecule 44: mL52

Chain j: 63% 6% 31%




• Molecule 45: mL53

Chain k: 64% 10% 25%



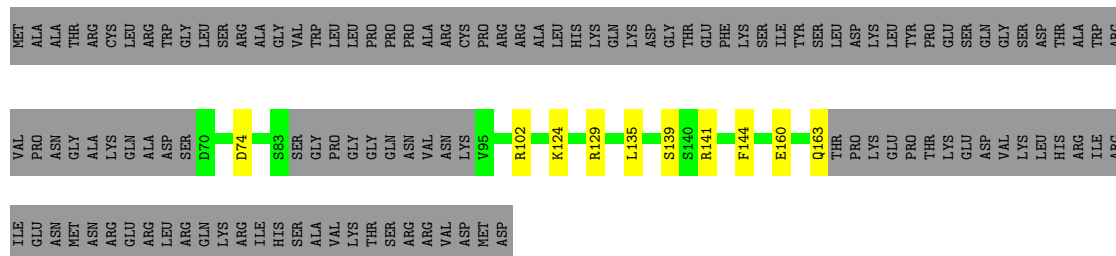
- Molecule 46: mL63

Chain o:  80% 11% 8%



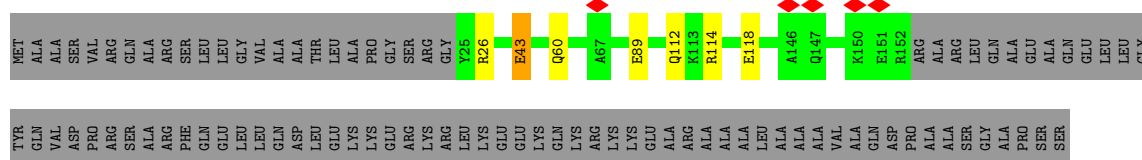
- Molecule 47: ICT1

Chain p:  35% 5% 60%



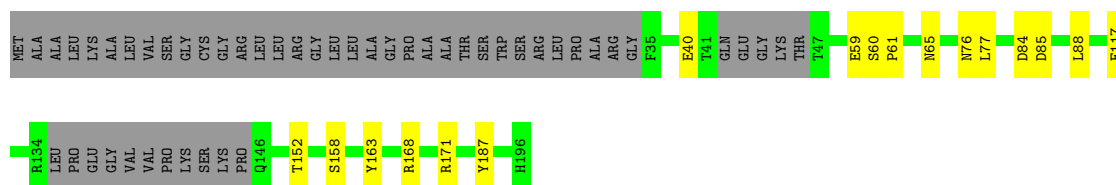
- Molecule 48: CRIF1

Chain q:  55% 42%



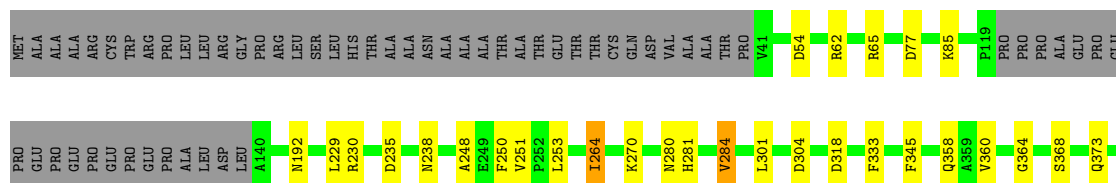
- Molecule 49: bS18a

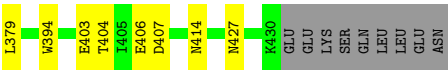
Chain r:  66% 9% 26%



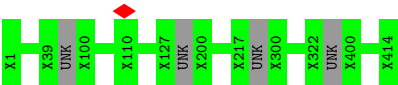
- Molecule 50: mS30

Chain s:  76% 8% 16%





• Molecule 51: unknown protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107679	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.968	Depositor
Minimum map value	-0.779	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.0175	Depositor
Map size (\AA)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, ZN, 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	A	0.29	0/34967	0.76	15/54407 (0.0%)
2	B	0.23	0/1349	0.71	2/2086 (0.1%)
3	D	0.47	1/1879 (0.1%)	0.76	1/2527 (0.0%)
4	E	0.42	1/2433 (0.0%)	0.72	0/3299
5	F	0.41	0/2071	0.73	0/2817
6	H	0.46	0/798	0.78	1/1073 (0.1%)
7	I	0.45	0/1308	0.79	0/1761
8	J	0.46	0/1077	0.77	0/1452
9	K	0.48	1/1495 (0.1%)	0.76	1/2029 (0.0%)
10	L	0.39	0/904	0.71	0/1218
11	M	0.44	2/2359 (0.1%)	0.79	0/3185
12	N	0.45	1/1697 (0.1%)	0.76	1/2281 (0.0%)
13	O	0.58	3/1269 (0.2%)	0.85	0/1708
14	P	0.80	2/1103 (0.2%)	0.73	0/1491
15	Q	0.55	3/1741 (0.2%)	0.73	1/2340 (0.0%)
16	R	0.77	2/1174 (0.2%)	0.85	0/1572
17	S	0.37	0/1276	0.72	0/1729
18	T	0.47	0/1402	0.78	0/1886
19	U	0.63	2/946 (0.2%)	0.77	0/1283
20	V	0.44	1/1590 (0.1%)	0.71	0/2151
21	W	0.47	0/864	0.76	0/1166
22	X	0.48	2/2081 (0.1%)	0.72	0/2812
23	Y	0.50	1/1552 (0.1%)	0.83	1/2079 (0.0%)
24	Z	0.50	1/1003 (0.1%)	0.64	0/1354
25	0	0.57	2/816 (0.2%)	0.80	1/1093 (0.1%)
26	1	0.53	1/438 (0.2%)	0.81	0/583
27	2	0.46	0/357	0.92	0/475
28	3	0.42	0/852	0.81	1/1136 (0.1%)
29	4	0.33	0/329	0.68	0/435
30	5	0.44	0/3154	0.75	1/4295 (0.0%)
31	6	0.51	3/2722 (0.1%)	0.74	0/3709
32	7	0.49	1/2207 (0.0%)	0.71	0/2978

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	8	0.52	0/487	0.83	0/649
34	9	0.75	6/896 (0.7%)	0.72	0/1205
35	a	0.46	0/355	0.76	0/475
36	b	0.80	4/1202 (0.3%)	0.73	0/1626
37	c	0.54	3/2264 (0.1%)	0.78	2/3059 (0.1%)
38	d	0.43	0/1385	0.67	0/1877
39	e	0.67	1/1107 (0.1%)	0.72	0/1494
40	f	0.97	3/632 (0.5%)	0.70	0/850
41	g	0.42	0/1102	0.72	1/1503 (0.1%)
42	h	0.45	0/847	0.73	0/1150
43	i	0.46	0/838	0.85	0/1121
44	j	0.61	3/698 (0.4%)	0.79	0/940
45	k	0.61	0/665	0.77	0/897
46	o	0.56	1/818 (0.1%)	0.97	1/1097 (0.1%)
47	p	0.48	1/682 (0.1%)	0.75	0/917
48	q	0.55	2/1107 (0.2%)	0.78	0/1498
49	r	0.39	0/1238	0.67	0/1676
50	s	0.55	4/3114 (0.1%)	0.77	2/4225 (0.0%)
All	All	0.45	58/98650 (0.1%)	0.76	32/140669 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	F	0	1
9	K	0	1
31	6	0	1
45	k	0	1
46	o	0	1
All	All	0	5

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	R	23	GLU	CD-OE2	18.73	1.46	1.25
14	P	151	GLU	CD-OE2	18.14	1.45	1.25
39	e	180	GLU	CD-OE2	15.19	1.42	1.25
36	b	78	GLU	CD-OE2	14.77	1.41	1.25
40	f	123	GLU	CD-OE1	14.32	1.41	1.25

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	o	15	ARG	NE-CZ-NH2	-7.78	116.41	120.30
25	0	108	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	A	1772	A	C2'-C3'-O3'	7.47	125.93	109.50
28	3	169	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	2174	G	C2'-C3'-O3'	7.26	125.47	109.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	6	191	ASN	Sidechain
5	F	140	SER	Peptide
9	K	82	GLY	Peptide
45	k	61	GLU	Peptide
46	o	63	ALA	Peptide

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	
3	D	234/305 (77%)	222 (95%)	11 (5%)	1 (0%)	34	67
4	E	296/348 (85%)	268 (90%)	21 (7%)	7 (2%)	6	28
5	F	248/311 (80%)	228 (92%)	17 (7%)	3 (1%)	13	41
6	H	93/267 (35%)	81 (87%)	10 (11%)	2 (2%)	6	29
7	I	154/261 (59%)	143 (93%)	6 (4%)	5 (3%)	4	22
8	J	138/192 (72%)	115 (83%)	16 (12%)	7 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	K	175/178 (98%)	157 (90%)	10 (6%)	8 (5%)	2	15
10	L	113/145 (78%)	100 (88%)	10 (9%)	3 (3%)	5	26
11	M	285/296 (96%)	256 (90%)	23 (8%)	6 (2%)	7	30
12	N	203/251 (81%)	186 (92%)	15 (7%)	2 (1%)	15	46
13	O	150/175 (86%)	133 (89%)	15 (10%)	2 (1%)	12	39
14	P	129/179 (72%)	115 (89%)	12 (9%)	2 (2%)	9	34
15	Q	200/292 (68%)	179 (90%)	17 (8%)	4 (2%)	7	30
16	R	138/149 (93%)	128 (93%)	7 (5%)	3 (2%)	6	29
17	S	154/205 (75%)	144 (94%)	9 (6%)	1 (1%)	25	57
18	T	164/212 (77%)	152 (93%)	9 (6%)	3 (2%)	8	32
19	U	109/153 (71%)	96 (88%)	12 (11%)	1 (1%)	17	49
20	V	183/216 (85%)	161 (88%)	15 (8%)	7 (4%)	3	19
21	W	105/148 (71%)	102 (97%)	2 (2%)	1 (1%)	15	46
22	X	241/256 (94%)	220 (91%)	16 (7%)	5 (2%)	7	30
23	Y	174/250 (70%)	157 (90%)	17 (10%)	0	100	100
24	Z	118/161 (73%)	107 (91%)	9 (8%)	2 (2%)	9	34
25	0	94/188 (50%)	81 (86%)	7 (7%)	6 (6%)	1	9
26	1	50/65 (77%)	46 (92%)	2 (4%)	2 (4%)	3	18
27	2	41/92 (45%)	40 (98%)	0	1 (2%)	6	28
28	3	93/188 (50%)	88 (95%)	5 (5%)	0	100	100
29	4	34/103 (33%)	34 (100%)	0	0	100	100
30	5	368/423 (87%)	329 (89%)	26 (7%)	13 (4%)	3	21
31	6	313/380 (82%)	274 (88%)	30 (10%)	9 (3%)	4	24
32	7	258/338 (76%)	236 (92%)	21 (8%)	1 (0%)	34	67
33	8	55/206 (27%)	53 (96%)	2 (4%)	0	100	100
34	9	105/137 (77%)	93 (89%)	9 (9%)	3 (3%)	4	24
35	a	37/142 (26%)	35 (95%)	2 (5%)	0	100	100
36	b	146/155 (94%)	125 (86%)	17 (12%)	4 (3%)	5	26
37	c	271/332 (82%)	238 (88%)	27 (10%)	6 (2%)	6	29
38	d	156/306 (51%)	139 (89%)	11 (7%)	6 (4%)	3	19
39	e	132/279 (47%)	103 (78%)	25 (19%)	4 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	f	71/211 (34%)	63 (89%)	7 (10%)	1 (1%)	11	37
41	g	127/166 (76%)	116 (91%)	8 (6%)	3 (2%)	6	28
42	h	96/158 (61%)	82 (85%)	10 (10%)	4 (4%)	3	18
43	i	94/128 (73%)	80 (85%)	13 (14%)	1 (1%)	14	44
44	j	83/123 (68%)	79 (95%)	3 (4%)	1 (1%)	13	41
45	k	82/112 (73%)	64 (78%)	13 (16%)	5 (6%)	1	10
46	o	92/102 (90%)	80 (87%)	9 (10%)	3 (3%)	4	22
47	p	79/206 (38%)	73 (92%)	5 (6%)	1 (1%)	12	39
48	q	126/222 (57%)	120 (95%)	5 (4%)	1 (1%)	19	51
49	r	140/196 (71%)	125 (89%)	12 (9%)	3 (2%)	7	30
50	s	366/439 (83%)	326 (89%)	32 (9%)	8 (2%)	6	29
All	All	7313/10347 (71%)	6572 (90%)	580 (8%)	161 (2%)	10	29

5 of 161 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	I	102	VAL
8	J	70	ILE
12	N	67	LYS
16	R	12	ASN
22	X	69	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	190/245 (78%)	175 (92%)	15 (8%)	12	39
4	E	255/290 (88%)	234 (92%)	21 (8%)	11	37
5	F	217/262 (83%)	193 (89%)	24 (11%)	6	22
6	H	86/228 (38%)	81 (94%)	5 (6%)	20	50
7	I	145/232 (62%)	135 (93%)	10 (7%)	15	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	113/150 (75%)	101 (89%)	12 (11%)	6	24
9	K	155/156 (99%)	144 (93%)	11 (7%)	14	44
10	L	98/124 (79%)	93 (95%)	5 (5%)	24	54
11	M	245/249 (98%)	218 (89%)	27 (11%)	6	23
12	N	172/211 (82%)	158 (92%)	14 (8%)	11	38
13	O	133/150 (89%)	113 (85%)	20 (15%)	3	12
14	P	115/154 (75%)	108 (94%)	7 (6%)	18	48
15	Q	186/256 (73%)	171 (92%)	15 (8%)	11	38
16	R	118/126 (94%)	108 (92%)	10 (8%)	10	35
17	S	141/180 (78%)	125 (89%)	16 (11%)	6	21
18	T	146/182 (80%)	131 (90%)	15 (10%)	7	26
19	U	99/135 (73%)	91 (92%)	8 (8%)	11	38
20	V	169/191 (88%)	154 (91%)	15 (9%)	9	33
21	W	87/119 (73%)	78 (90%)	9 (10%)	7	26
22	X	217/227 (96%)	198 (91%)	19 (9%)	10	33
23	Y	159/223 (71%)	144 (91%)	15 (9%)	8	30
24	Z	111/147 (76%)	105 (95%)	6 (5%)	22	52
25	0	88/164 (54%)	74 (84%)	14 (16%)	2	10
26	1	49/60 (82%)	41 (84%)	8 (16%)	2	9
27	2	38/72 (53%)	34 (90%)	4 (10%)	7	25
28	3	88/166 (53%)	83 (94%)	5 (6%)	20	50
29	4	35/89 (39%)	33 (94%)	2 (6%)	20	50
30	5	337/368 (92%)	306 (91%)	31 (9%)	9	31
31	6	266/332 (80%)	230 (86%)	36 (14%)	4	14
32	7	242/303 (80%)	231 (96%)	11 (4%)	27	58
33	8	51/190 (27%)	49 (96%)	2 (4%)	32	61
34	9	91/112 (81%)	87 (96%)	4 (4%)	28	58
35	a	37/133 (28%)	34 (92%)	3 (8%)	11	38
36	b	130/135 (96%)	120 (92%)	10 (8%)	13	40
37	c	241/288 (84%)	227 (94%)	14 (6%)	20	50
38	d	151/274 (55%)	148 (98%)	3 (2%)	55	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	e	114/236 (48%)	99 (87%)	15 (13%)	4	15
40	f	70/173 (40%)	64 (91%)	6 (9%)	10	35
41	g	119/148 (80%)	109 (92%)	10 (8%)	11	36
42	h	95/148 (64%)	83 (87%)	12 (13%)	4	17
43	i	85/110 (77%)	71 (84%)	14 (16%)	2	9
44	j	68/97 (70%)	63 (93%)	5 (7%)	13	42
45	k	74/90 (82%)	67 (90%)	7 (10%)	8	29
46	o	80/87 (92%)	72 (90%)	8 (10%)	7	27
47	p	75/181 (41%)	67 (89%)	8 (11%)	6	24
48	q	110/178 (62%)	104 (94%)	6 (6%)	21	51
49	r	133/169 (79%)	119 (90%)	14 (10%)	7	25
50	s	326/381 (86%)	300 (92%)	26 (8%)	12	38
All	All	6550/8921 (73%)	5973 (91%)	577 (9%)	13	33

5 of 577 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	f	114	CYS
50	s	394	TRP
41	g	155	GLN
40	f	113	LEU
46	o	69	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
42	h	147	ASN
46	o	85	HIS
50	s	164	HIS
19	U	101	HIS
19	U	82	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1458/1559 (93%)	550 (37%)	118 (8%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	51/73 (69%)	21 (41%)	3 (5%)
All	All	1509/1632 (92%)	571 (37%)	121 (8%)

5 of 571 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1672	C
1	A	1674	A
1	A	1675	A
1	A	1676	A
1	A	1677	C

5 of 121 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2370	A
1	A	3068	G
1	A	2519	G
1	A	3063	G
2	B	1607	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 69 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
52	AMP	A	3301	-	18,24,25	0.58	0	18,35,38	0.92	1 (5%)

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
52	AMP	A	3301	-	-	1/3/25/26	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A	3301	AMP	C5-C6-N6	2.15	123.62	120.35

There are no chirality outliers.

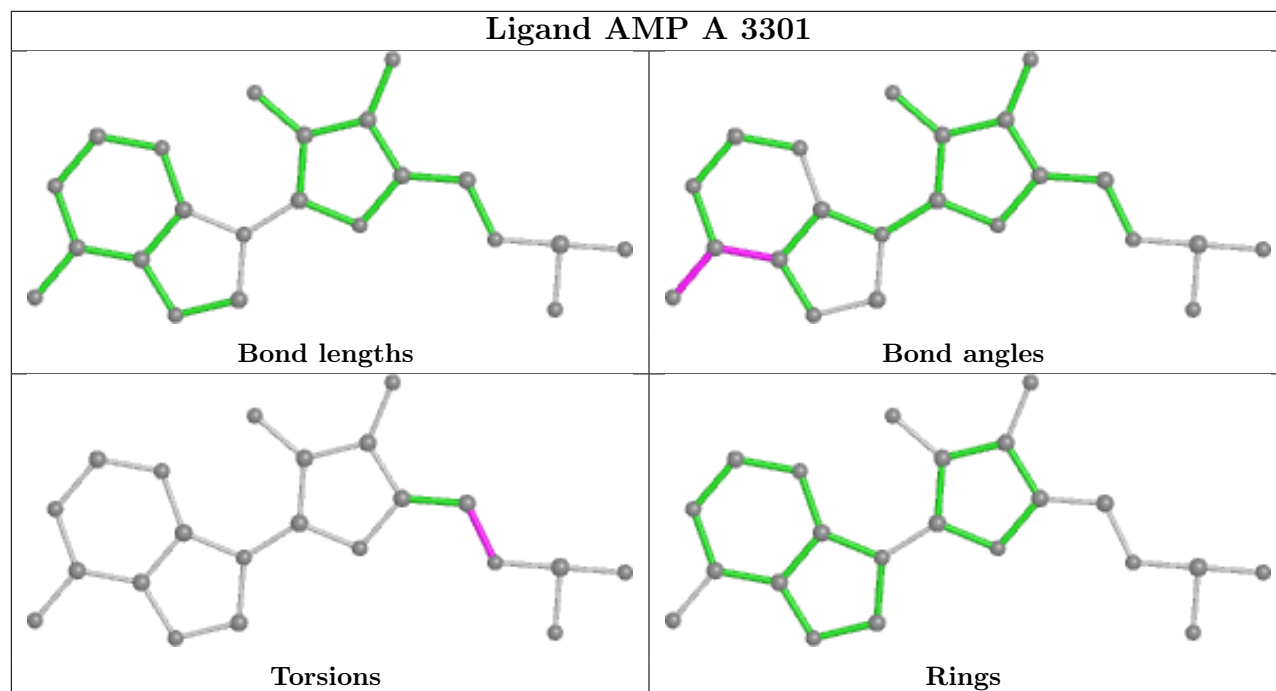
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	A	3301	AMP	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

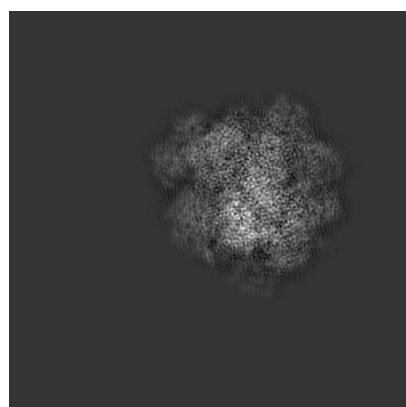
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2762. These allow visual inspection of the internal detail of the map and identification of artifacts.

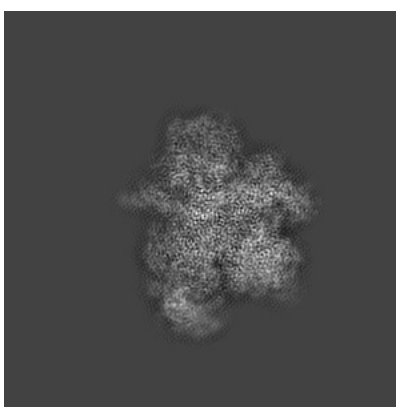
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

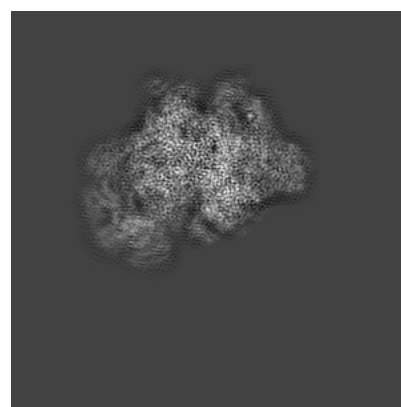
6.1.1 Primary map



X



Y

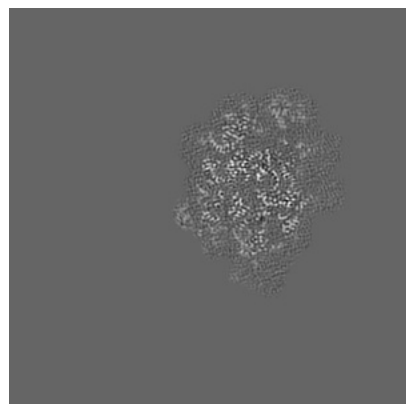


Z

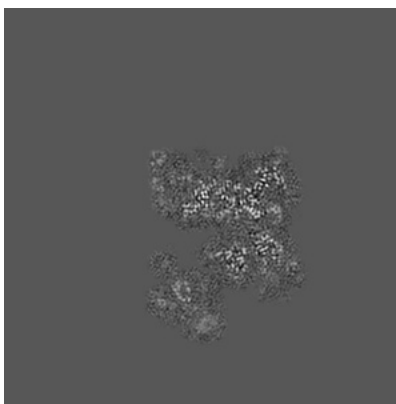
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

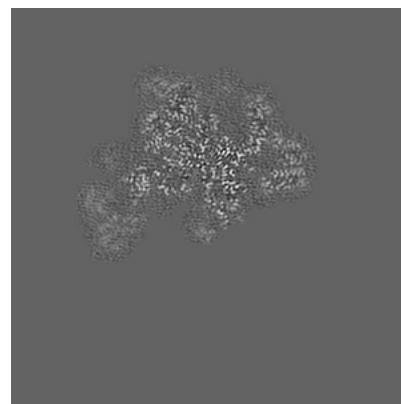
6.2.1 Primary map



X Index: 160



Y Index: 160

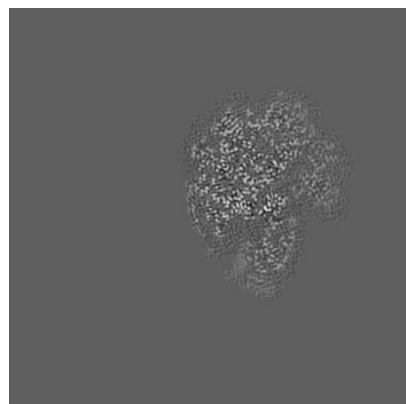


Z Index: 160

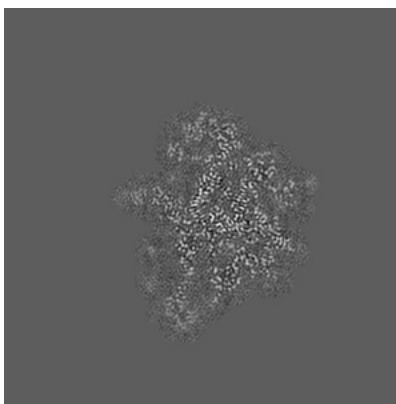
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

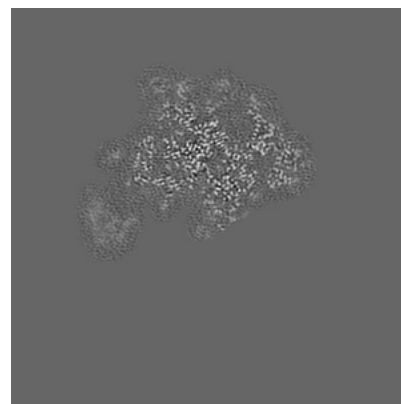
6.3.1 Primary map



X Index: 170



Y Index: 202

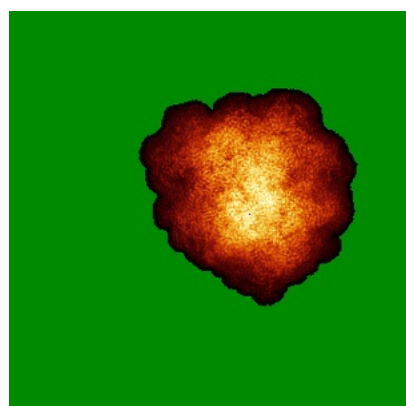


Z Index: 166

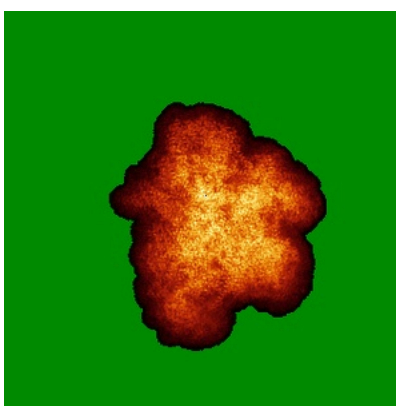
The images above show the largest variance slices of the map in three orthogonal directions.

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

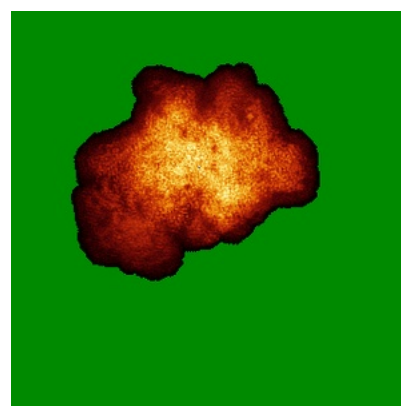
6.4.1 Primary map



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](#)

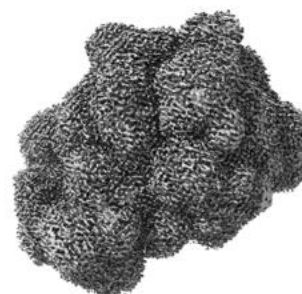
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

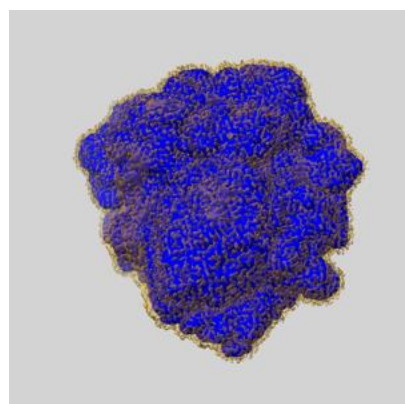
6.6 Mask visualisation [i](#)

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

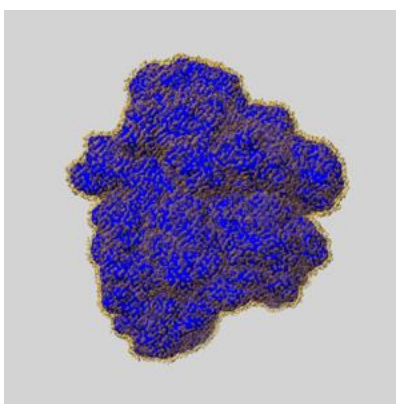
A mask typically either:

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

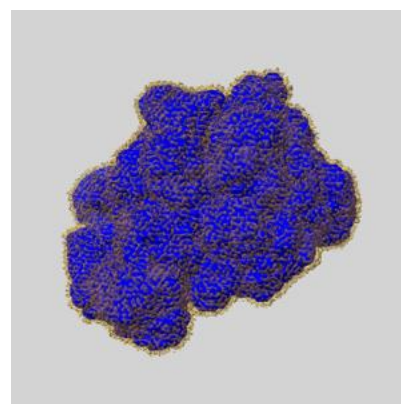
6.6.1 emd_2762_msk_1.map [i](#)



X



Y

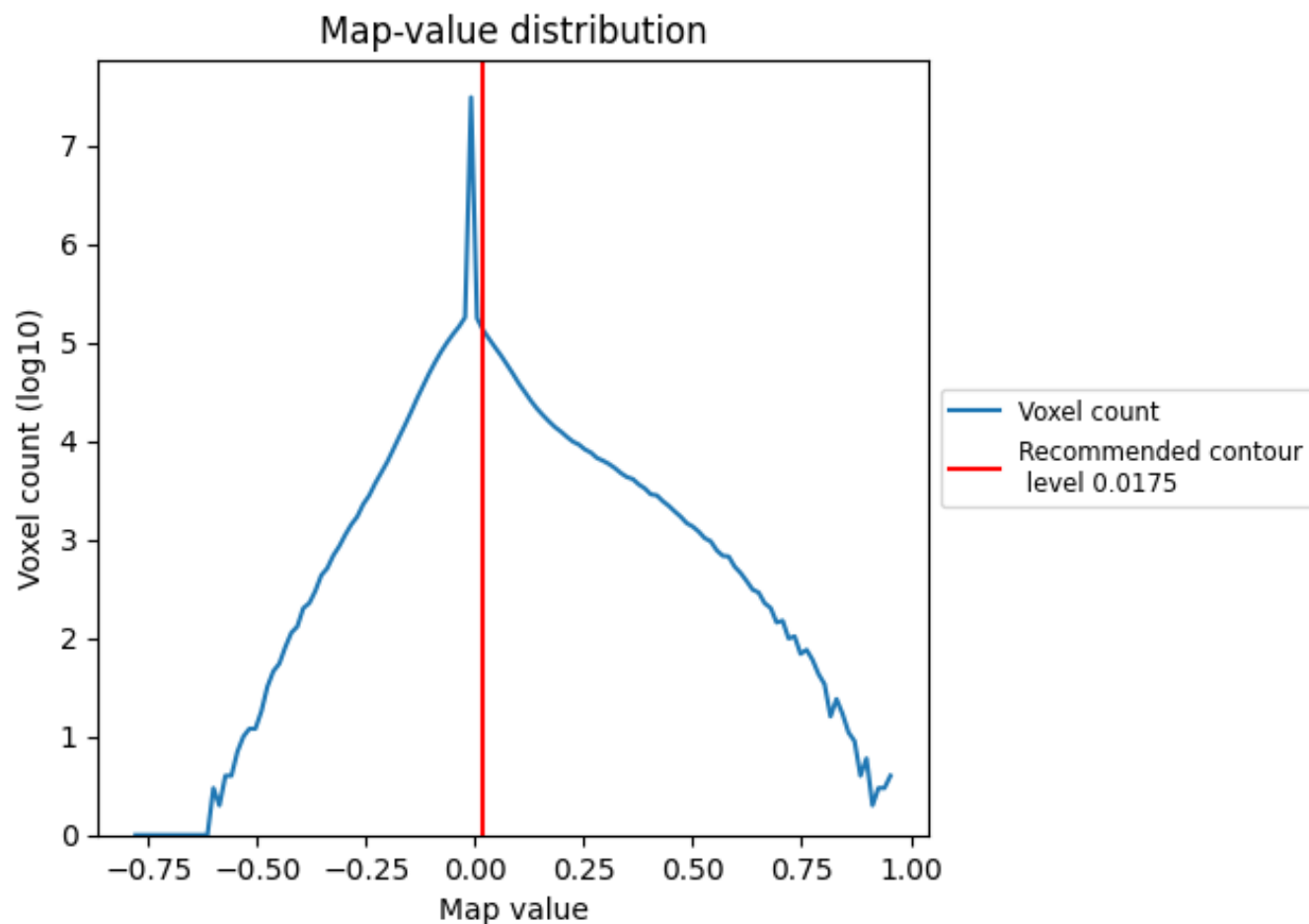


Z

7 Map analysis [i](#)

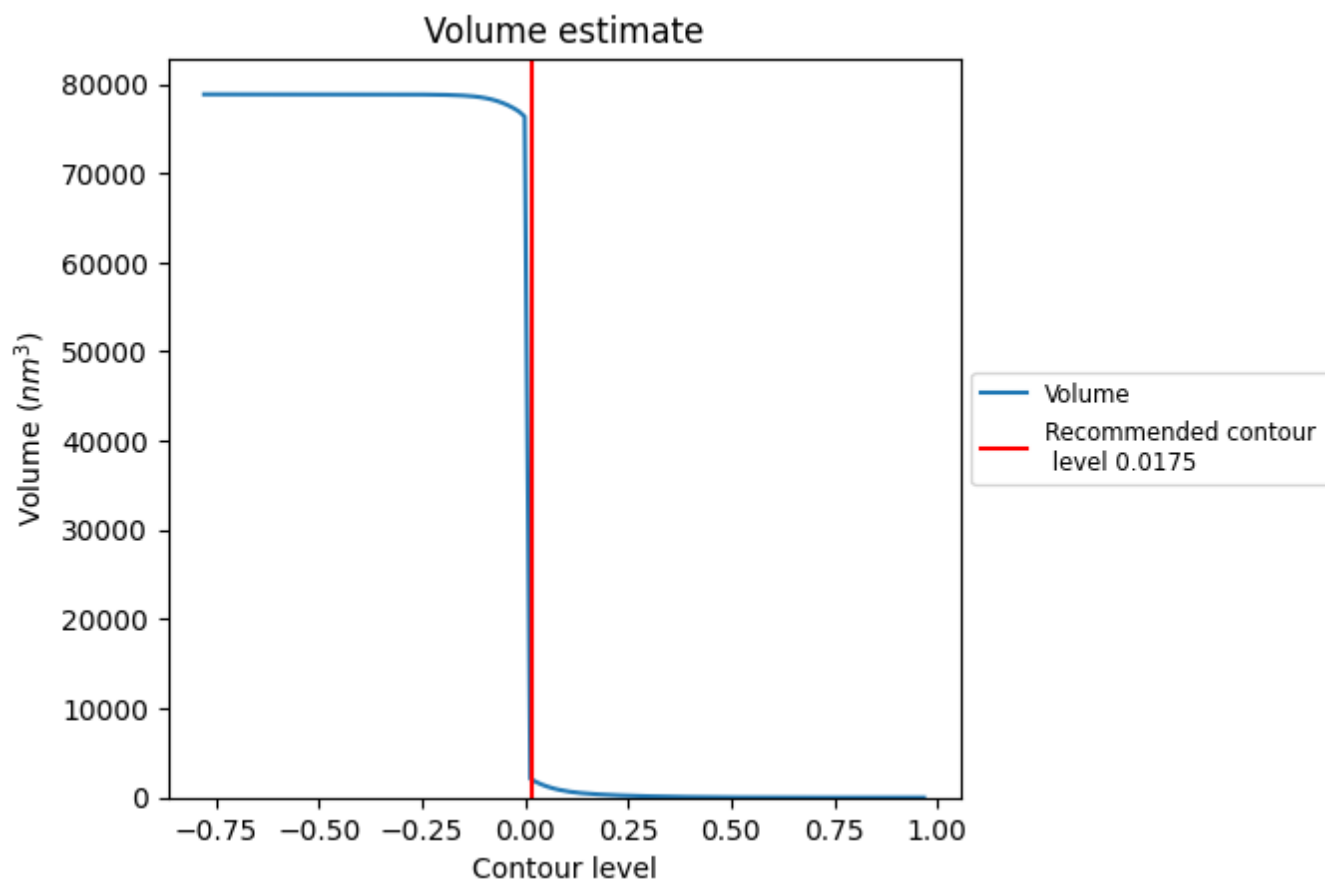
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

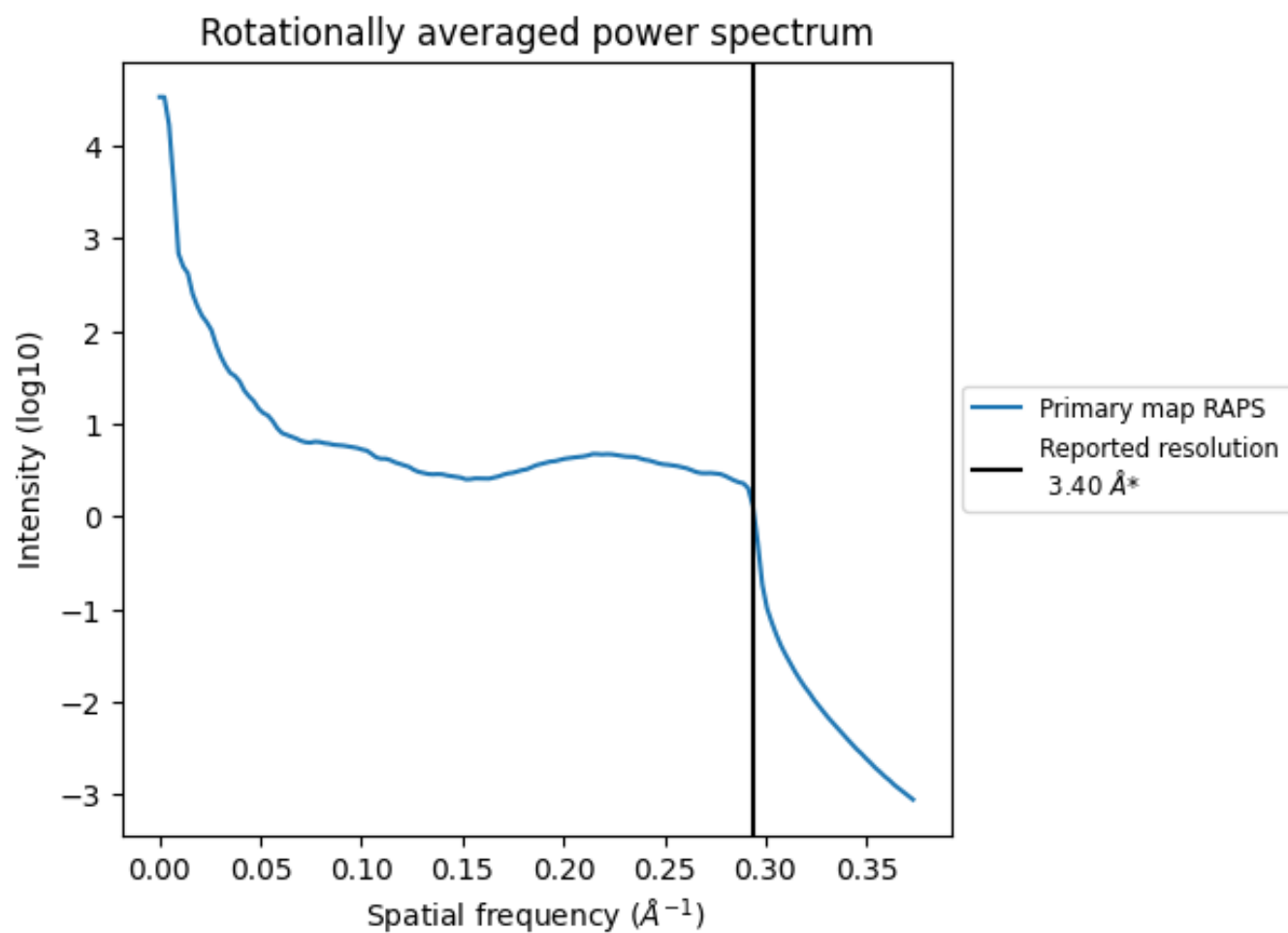
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1982 nm³; this corresponds to an approximate mass of 1791 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

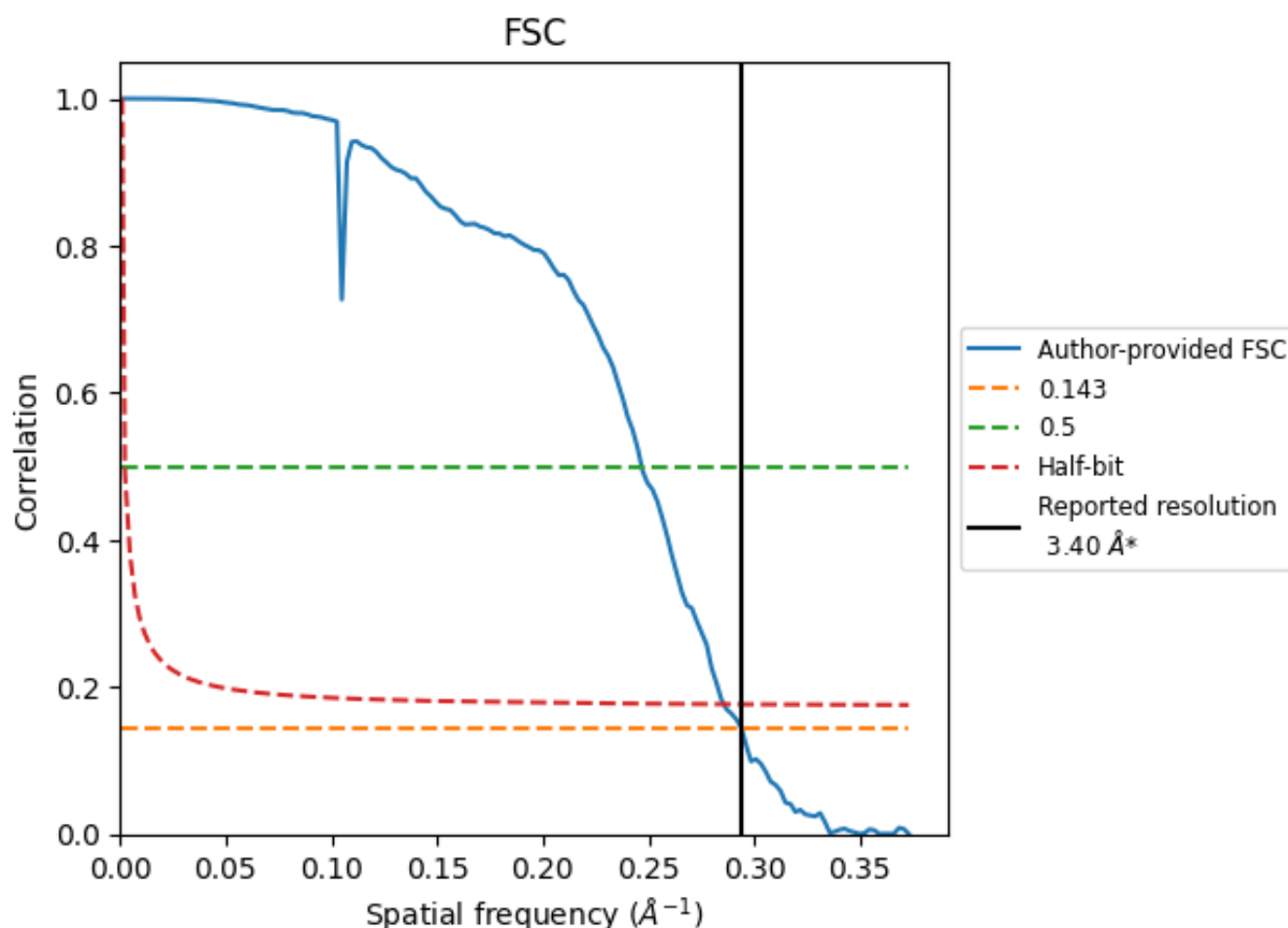


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

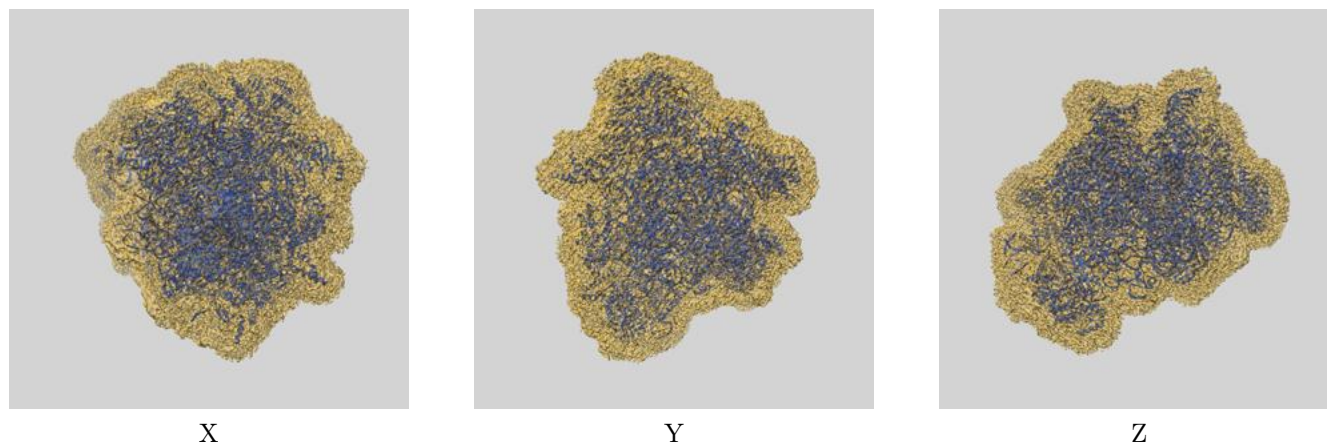
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	4.05	3.50
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

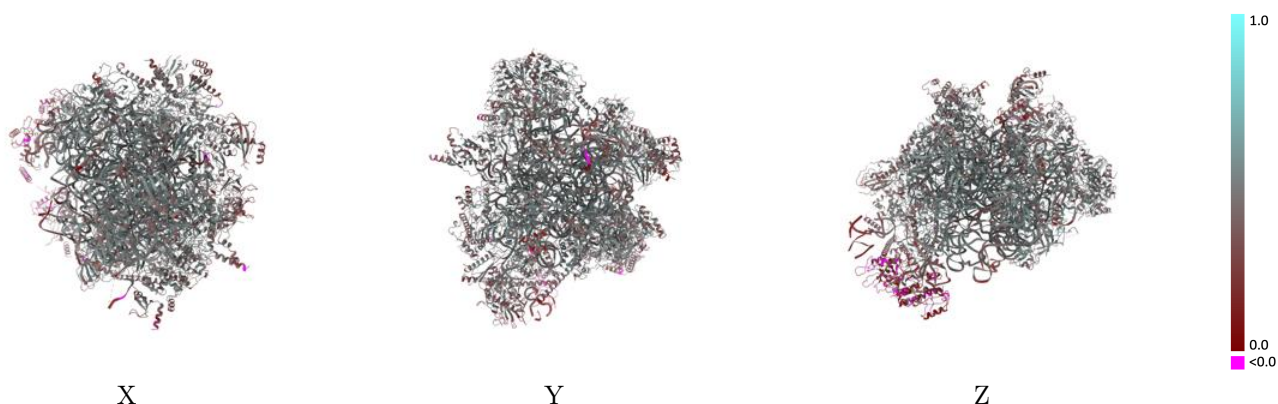
This section contains information regarding the fit between EMDB map EMD-2762 and PDB model 3J7Y. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



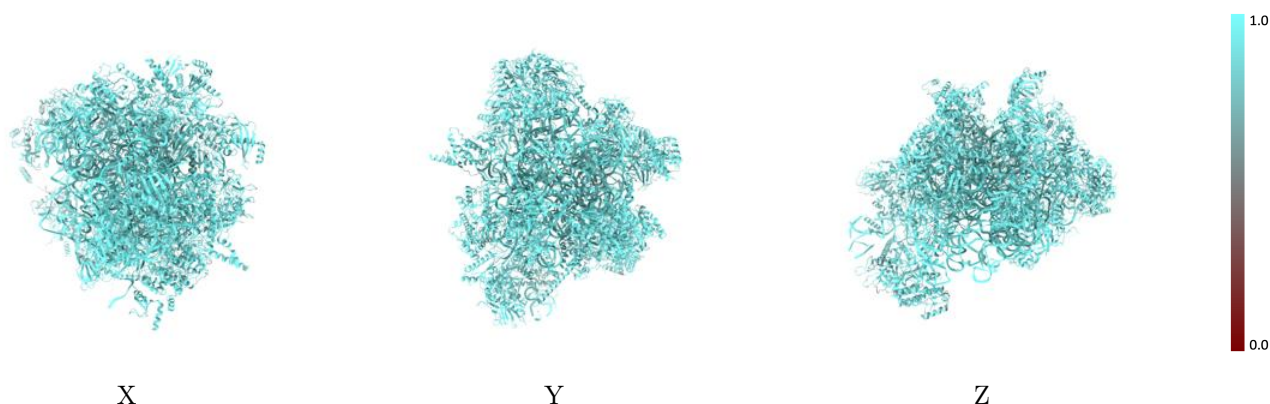
The images above show the 3D surface view of the map at the recommended contour level 0.0175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



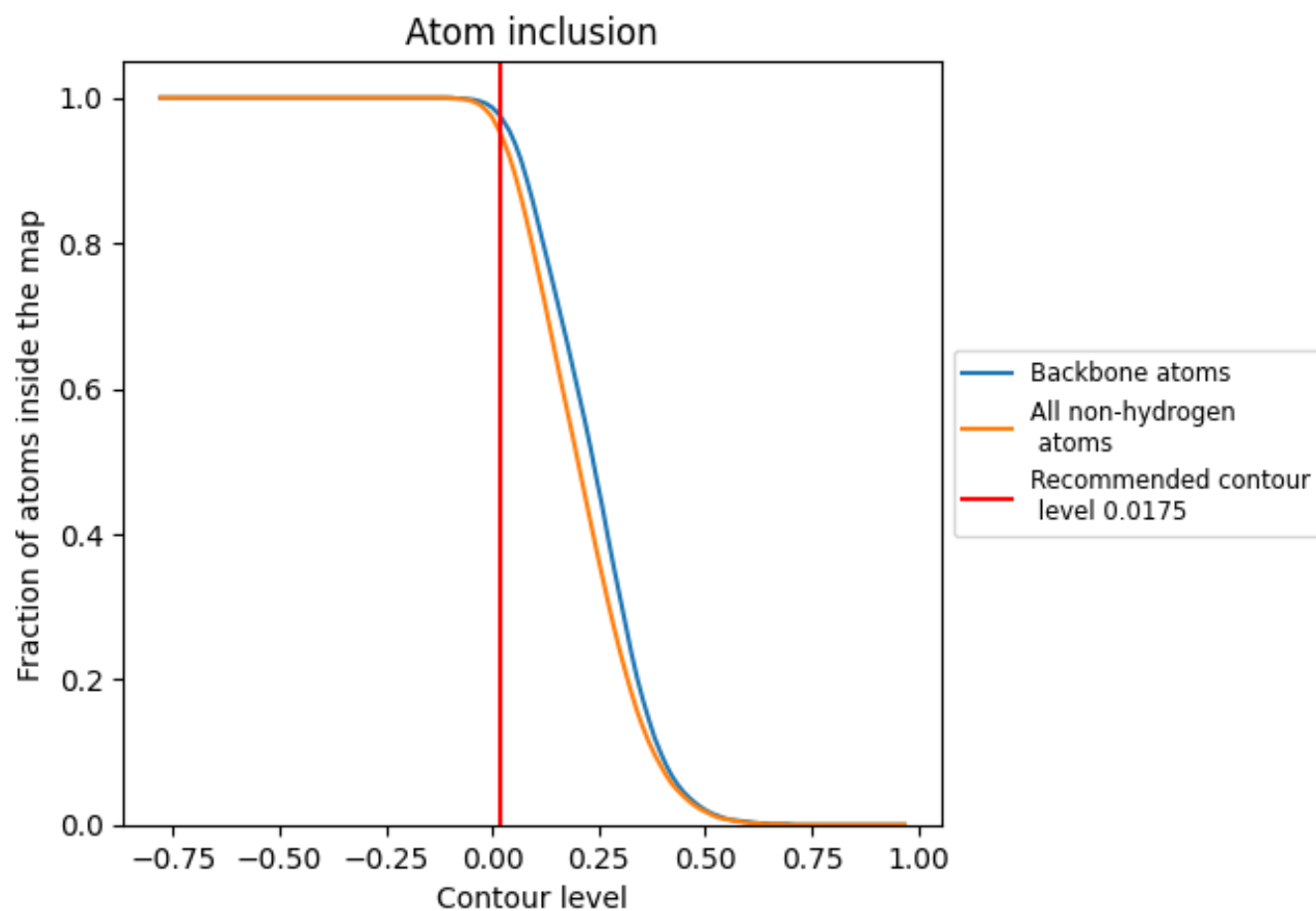
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0175).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



































The table lists the average atom inclusion at the recommended contour level (0.0175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.4520
0	 0.9500	 0.4750
1	 0.9210	 0.4440
2	 0.9700	 0.5260
3	 0.9620	 0.5220
4	 0.9900	 0.5340
5	 0.9470	 0.4580
6	 0.9430	 0.3940
7	 0.9370	 0.4160
8	 0.9150	 0.2700
9	 0.9440	 0.4500
A	 0.9800	 0.4820
B	 0.9690	 0.2970
D	 0.9620	 0.4980
E	 0.9660	 0.4970
F	 0.9630	 0.4920
H	 0.9250	 0.4050
I	 0.8760	 0.2750
J	 0.8450	 0.1910
K	 0.9530	 0.4890
L	 0.9530	 0.4810
M	 0.9540	 0.4830
N	 0.9450	 0.4730
O	 0.9480	 0.4780
P	 0.9470	 0.4510
Q	 0.9400	 0.4680
R	 0.9500	 0.5070
S	 0.9540	 0.4870
T	 0.9460	 0.5000
U	 0.9660	 0.4920
V	 0.9170	 0.3870
W	 0.9770	 0.5160
X	 0.9370	 0.4550
Y	 0.9380	 0.4630
Z	 0.9600	 0.4950



Continued on next page...

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Chain	Atom inclusion	Q-score
a	 0.9330	 0.4640
b	 0.9650	 0.4890
c	 0.9450	 0.4390
d	 0.9200	 0.3860
e	 0.7980	 0.0950
f	 0.9540	 0.4060
g	 0.9510	 0.4790
h	 0.8920	 0.3280
i	 0.9530	 0.5080
j	 0.9400	 0.4500
k	 0.8600	 0.2400
o	 0.9500	 0.4860
p	 0.9300	 0.4080
q	 0.8720	 0.3490
r	 0.9620	 0.4780
s	 0.9510	 0.4710
t	 0.9590	 0.3610