



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:45 PM EST

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

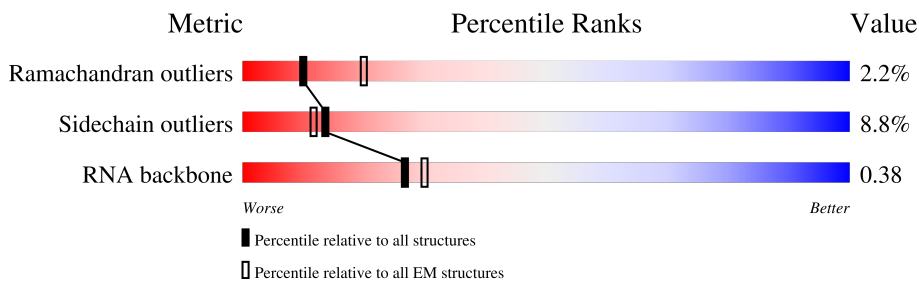
1 Overall quality at a glance

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.














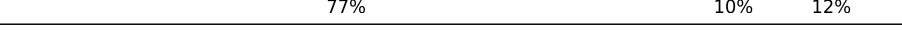




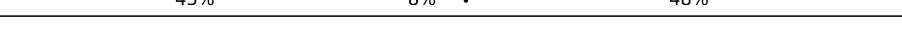


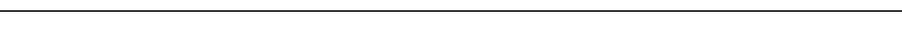

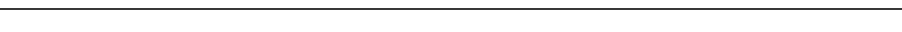
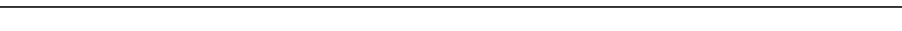


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	










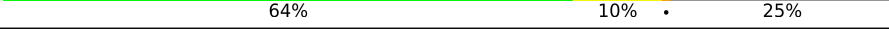



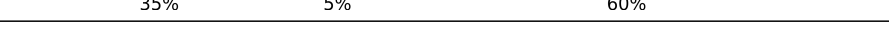



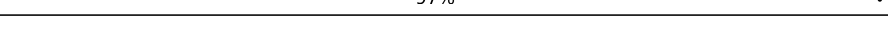
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Mol	Chain	Length	Quality of chain
9	K	178	 88% 11% ..
10	L	145	 74% 6% 21%
11	M	296	 86% 11% .
12	N	251	 75% 7% 18%
13	O	175	 74% 13% . 13%
14	P	179	 69% 6% 26%
15	Q	292	 63% 7% 30%
16	R	149	 85% 8% . 6%
17	S	205	 68% 8% 24%
18	T	212	 70% 8% 22%
19	U	153	 66% 7% 27%
20	V	216	 77% 10% 12%
21	W	148	 66% 7% 28%
22	X	256	 86% 9% . 5%
23	Y	250	 64% 6% 30%
24	Z	161	 69% 6% 25%
25	0	188	 43% 8% . 48%
26	1	65	 65% 14% . 20%
27	2	92	 41% 5% 53%
28	3	188	 48% .. 49%
29	4	103	 33% . 65%
30	5	423	 79% 9% . 11%
31	6	380	 73% 11% . 14%
32	7	338	 75% . 21%
33	8	206	 27% . 72%

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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		

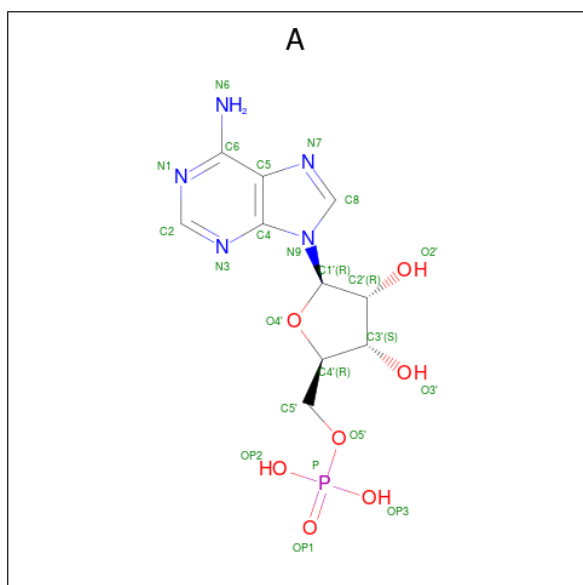
- Molecule 50 is a protein called mS30.

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-5'-MONOPHOSPHATE (three-letter code: A) (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	

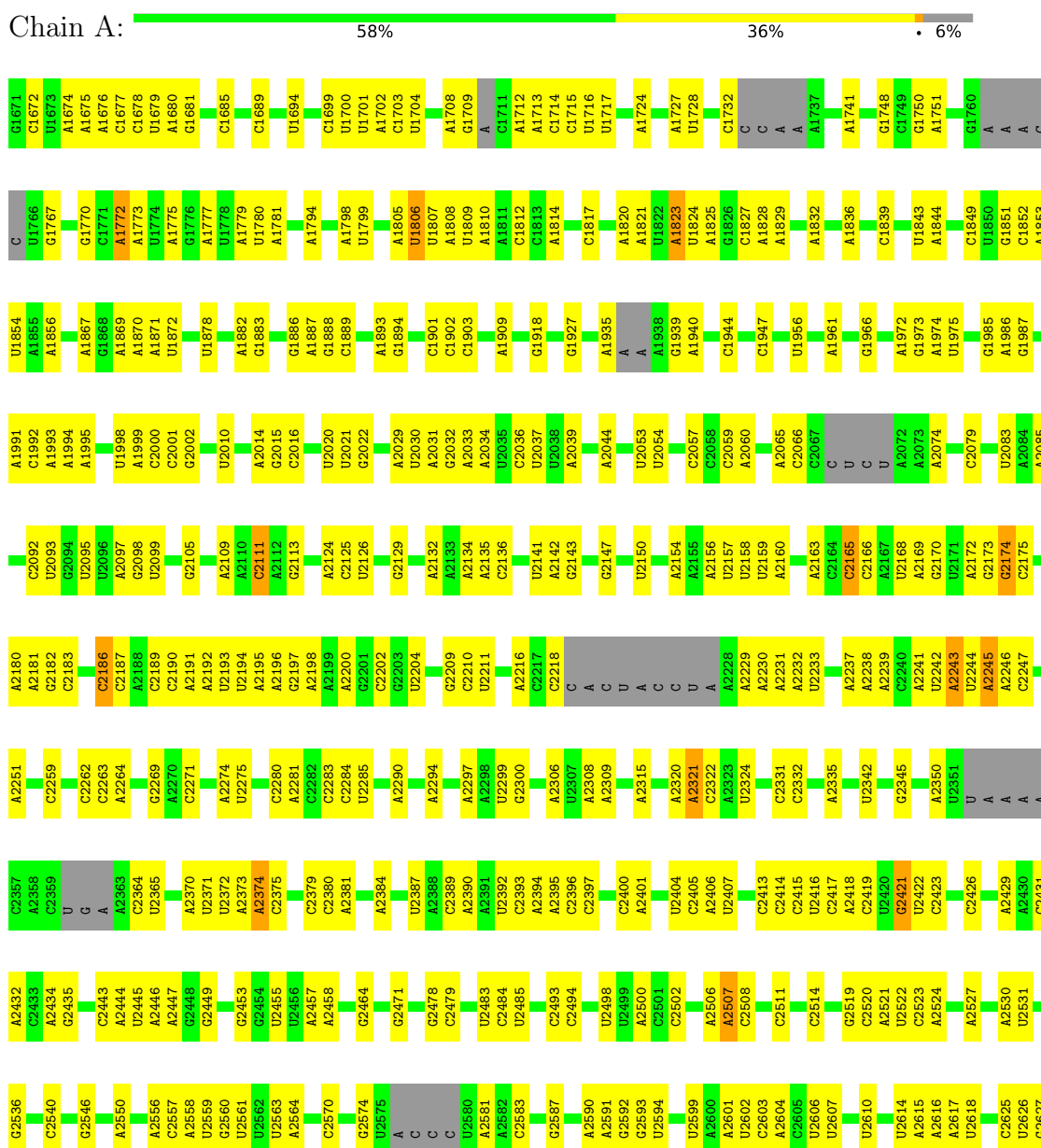
- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

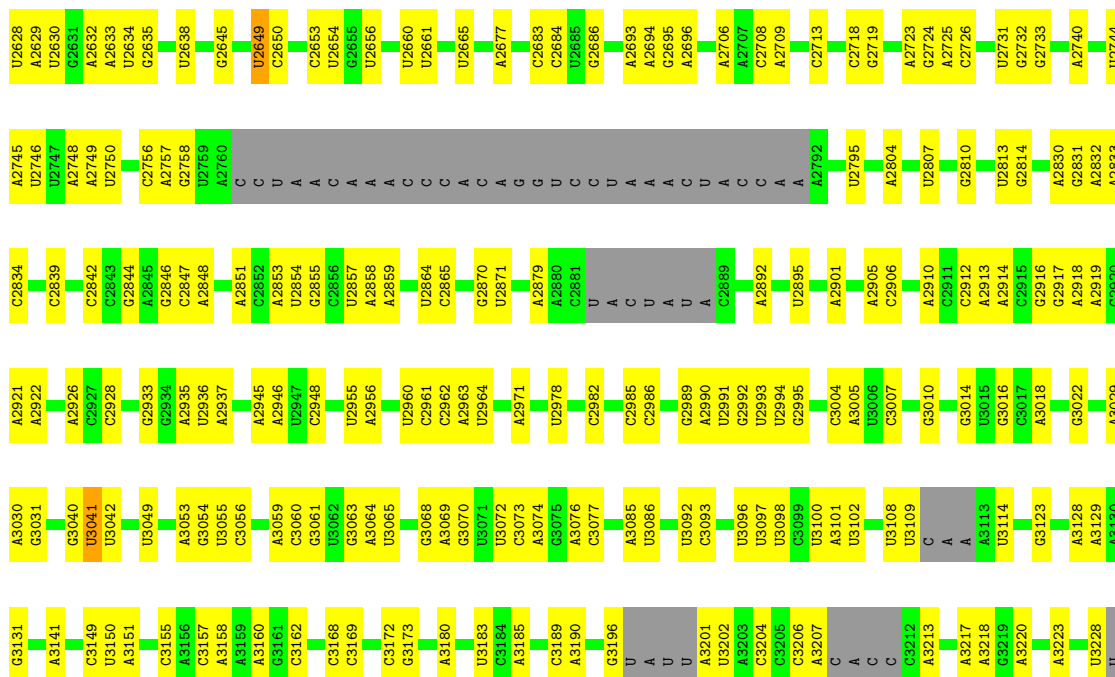
Mol	Chain	Residues	Atoms		AltConf
54	0	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	
54	r	1	Total	Zn	0
			1	1	

3 Residue-property plots

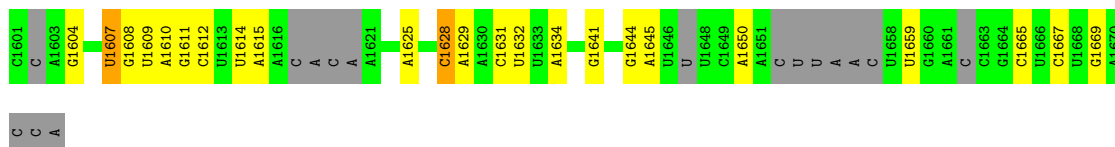
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

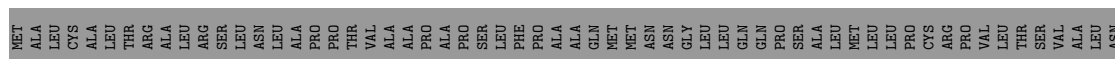




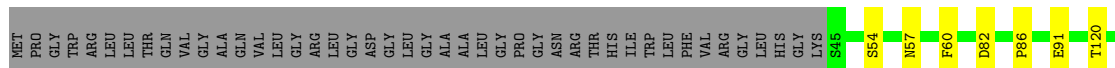
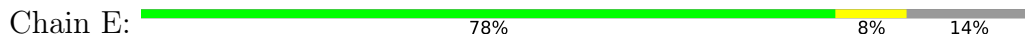
• Molecule 2: mt-tRNAVal



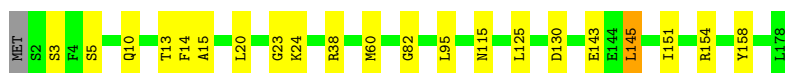
• Molecule 3: uL2



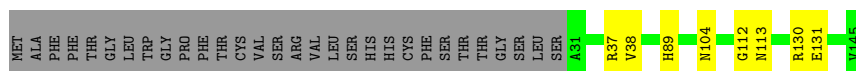
• Molecule 4: uL3



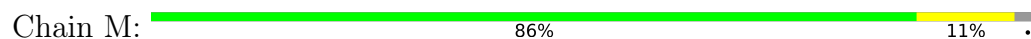
• Molecule 5: uL4



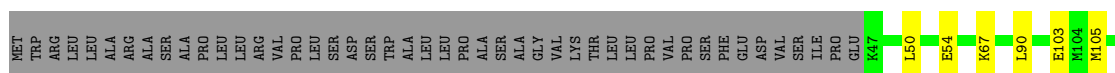
- Molecule 10: uL14



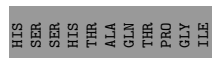
- Molecule 11: uL15



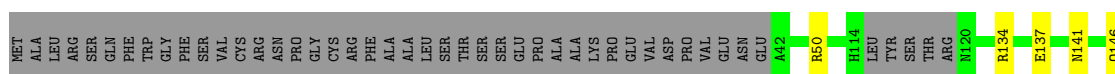
- Molecule 12: uL16



- Molecule 13: bL17

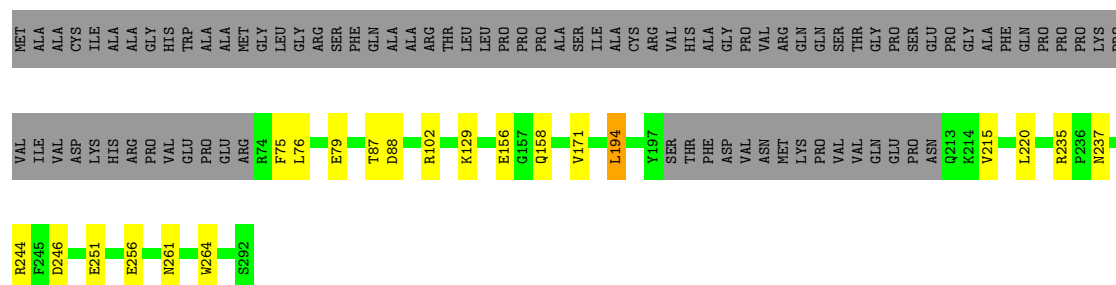


- Molecule 14: uL18




- Molecule 15: bL19

Chain Q:  63% 7% 30%



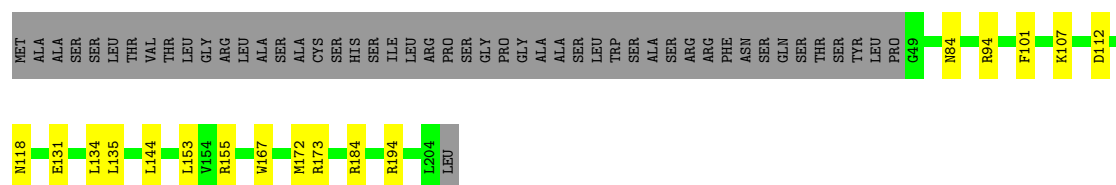
- Molecule 16: bL20

Chain R:  85% 8% 6%



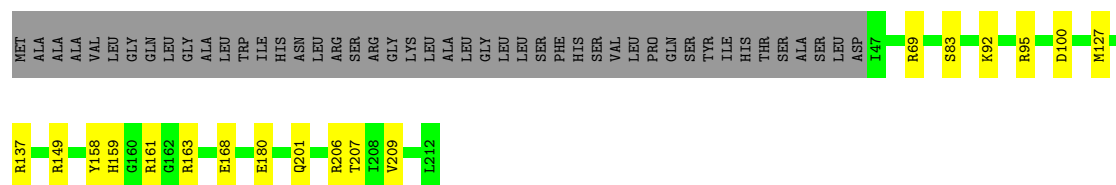
- Molecule 17: bL21

Chain S:  68% 8% 24%



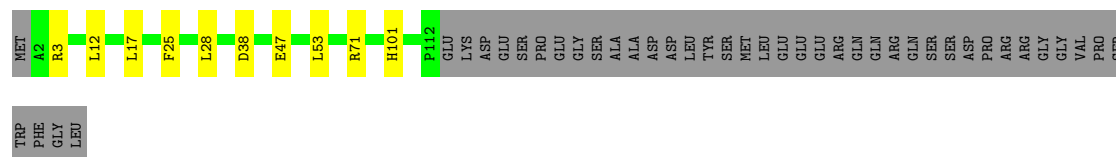
- Molecule 18: uL22

Chain T:  70% 8% 22%




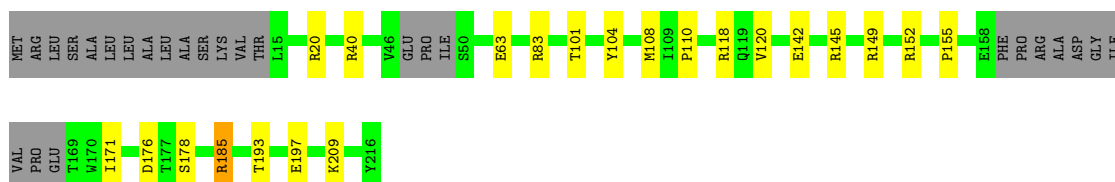
- Molecule 19: uL23

Chain U:  66% 7% 27%



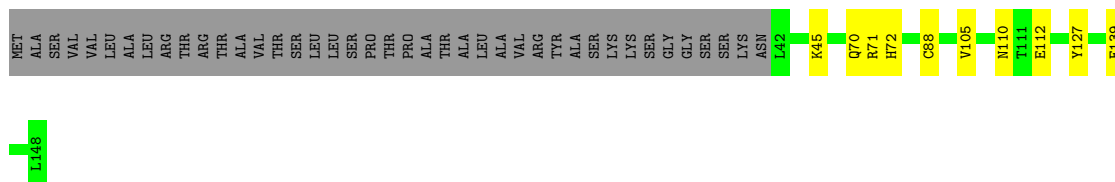
- Molecule 20: uL24

Chain V:  77% 10% 12%



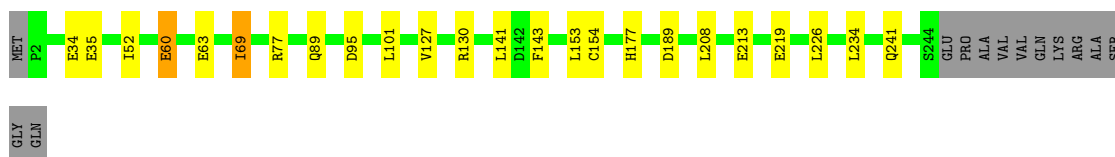
• Molecule 21: bL27

Chain W: 66% 7% 28%



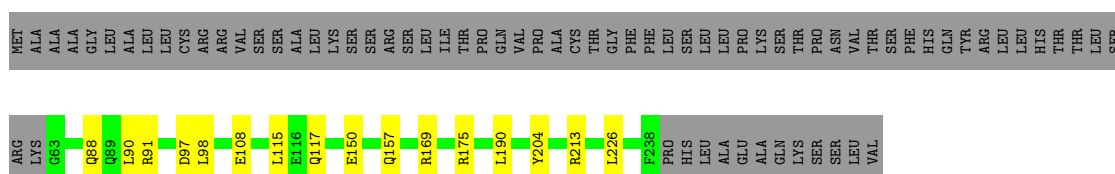
• Molecule 22: bL28

Chain X: 86% 9% 5%



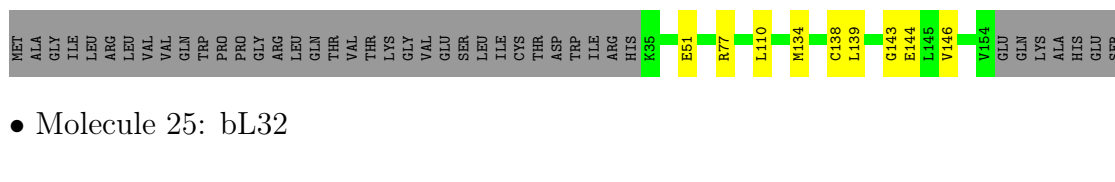
• Molecule 23: uL29

Chain Y: 64% 6% 30%



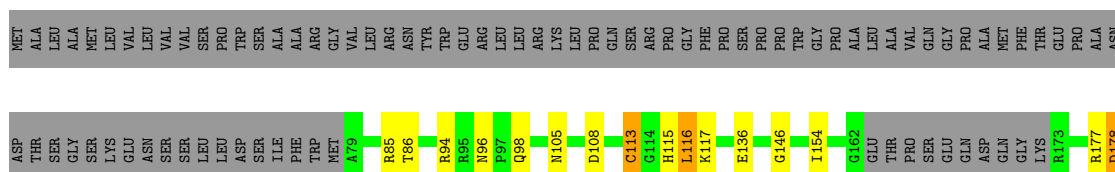
• Molecule 24: uL30

Chain Z: 69% 6% 25%



• Molecule 25: bL32

Chain 0: 43% 8% 48%



Response	Percentage
Yes	73%
No	11%
Don't know	14%



Response	Percentage
Yes, I have used a mobile app to book a flight	75%
No, I have not used a mobile app to book a flight	21%



Opinion	Percentage
Doing a good job	27%
Doing a bad job	72%




Response	Percentage
Yes	72%
No	7%
Don't know	20%



Response	Percentage
Yes, it is a crisis	25%
No, it is not a crisis	73%



- Molecule 36: mL43

Chain b:  85% 10% 5%



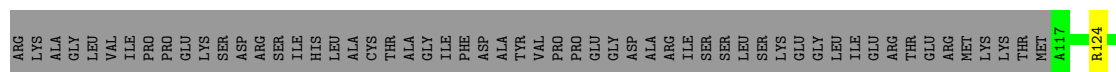
- Molecule 37: mL44

Chain c:  76% 7% 17%




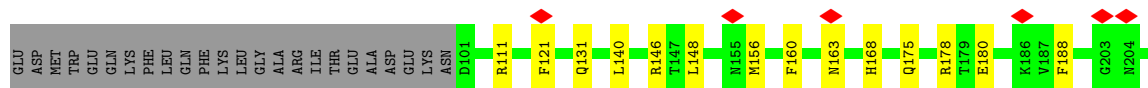
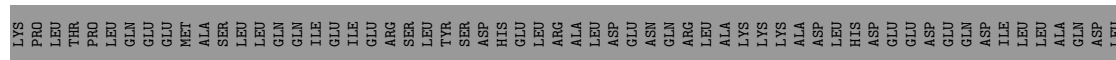
- Molecule 38: mL45

Chain d:  50% 47%



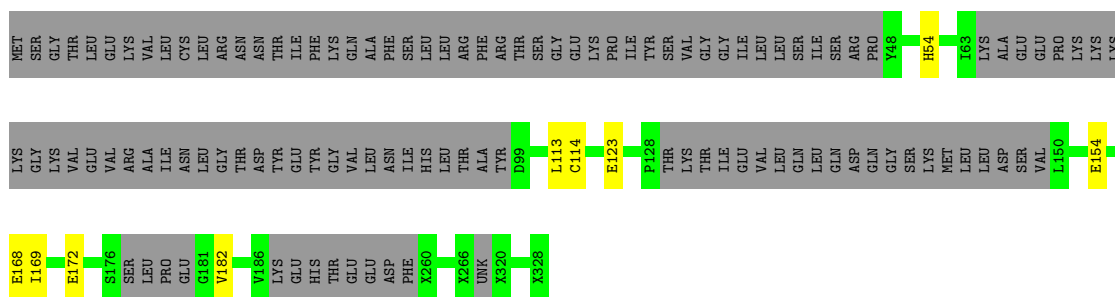
- Molecule 39: mL46

Chain e:  41% 6% 52%



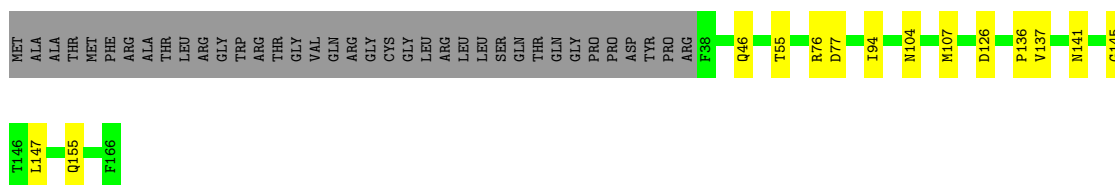
- Molecule 40: mL48

Chain f:  41% 55%



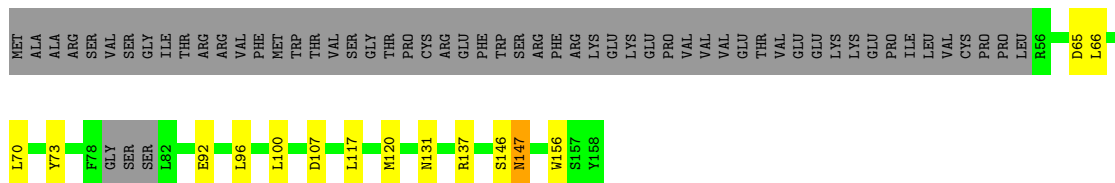
• Molecule 41: mL49

Chain g: 69% 8% 22%



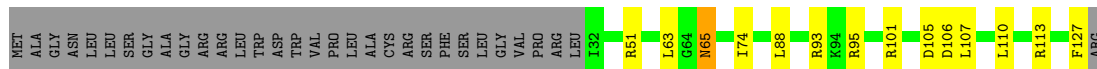
• Molecule 42: mL50

Chain h: 54% 9% 37%



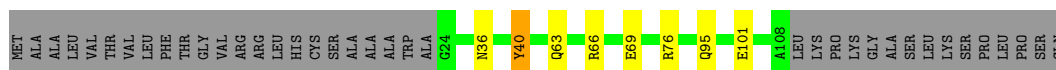
• Molecule 43: mL51

Chain i: 64% 10% 25%



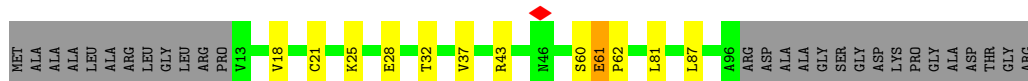
• Molecule 44: mL52

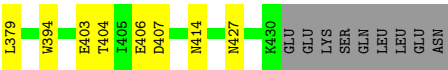
Chain j: 63% 6% 31%



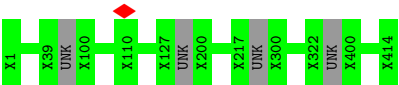
• Molecule 45: mL53

Chain k: 64% 10% 25%





• Molecule 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 [i](#)

5.1 Standard geometry [i](#)

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

All (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
40	f	123	GLU	CD-OE2	14.31	1.41	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	151	GLU	CD-OE1	13.91	1.41	1.25
36	b	86	GLU	CD-OE1	13.62	1.40	1.25
19	U	47	GLU	CD-OE2	12.06	1.39	1.25
34	9	94	GLU	CD-OE1	11.41	1.38	1.25
3	D	199	GLU	CD-OE1	11.20	1.38	1.25
36	b	86	GLU	CD-OE2	10.04	1.36	1.25
15	Q	256	GLU	CG-CD	9.35	1.66	1.51
19	U	47	GLU	CD-OE1	8.95	1.35	1.25
31	6	191	ASN	CG-OD1	8.67	1.43	1.24
50	s	318	ASP	CG-OD2	8.62	1.45	1.25
16	R	23	GLU	CD-OE1	8.29	1.34	1.25
36	b	78	GLU	CD-OE1	8.08	1.34	1.25
37	c	44	GLU	CD-OE1	8.08	1.34	1.25
24	Z	51	GLU	CD-OE1	7.47	1.33	1.25
25	0	108	ASP	CG-OD2	7.45	1.42	1.25
13	O	43	GLU	CD-OE1	7.44	1.33	1.25
13	O	70	GLU	CD-OE2	7.39	1.33	1.25
23	Y	97	ASP	CG-OD2	7.24	1.42	1.25
34	9	90	GLN	CD-OE1	7.19	1.39	1.24
31	6	63	GLN	CD-NE2	7.16	1.50	1.32
50	s	403	GLU	CD-OE2	7.16	1.33	1.25
25	0	108	ASP	CG-OD1	7.10	1.41	1.25
46	o	15	ARG	CZ-NH1	6.88	1.42	1.33
40	f	168	GLU	CD-OE1	6.79	1.33	1.25
34	9	120	GLU	CD-OE1	6.75	1.33	1.25
48	q	118	GLU	CG-CD	6.70	1.62	1.51
50	s	318	ASP	CG-OD1	6.70	1.40	1.25
32	7	259	ASP	CG-OD2	6.65	1.40	1.25
34	9	94	GLU	CD-OE2	6.39	1.32	1.25
20	V	176	ASP	CG-OD1	6.39	1.40	1.25
31	6	140	GLU	CD-OE1	6.25	1.32	1.25
34	9	120	GLU	CD-OE2	6.21	1.32	1.25
37	c	295	GLU	CD-OE2	6.19	1.32	1.25
44	j	95	GLN	CD-OE1	5.76	1.36	1.24
44	j	69	GLU	CD-OE1	5.75	1.31	1.25
34	9	90	GLN	CD-NE2	5.66	1.47	1.32
50	s	406	GLU	CG-CD	5.61	1.60	1.51
15	Q	79	GLU	CD-OE1	5.61	1.31	1.25
4	E	91	GLU	CD-OE1	5.48	1.31	1.25
12	N	202	GLN	CD-NE2	5.39	1.46	1.32
22	X	60	GLU	CD-OE2	5.38	1.31	1.25
11	M	139	GLN	CD-OE1	5.36	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	p	74	ASP	CG-OD1	5.33	1.37	1.25
37	c	101	GLU	CD-OE1	5.23	1.31	1.25
11	M	139	GLN	CD-NE2	5.22	1.45	1.32
13	O	70	GLU	CD-OE1	5.20	1.31	1.25
26	l	39	GLU	CD-OE2	5.19	1.31	1.25
48	q	118	GLU	CD-OE2	5.14	1.31	1.25
9	K	130	ASP	CG-OD2	5.12	1.37	1.25
22	X	35	GLU	CD-OE1	5.07	1.31	1.25
15	Q	79	GLU	CD-OE2	5.06	1.31	1.25
44	j	101	GLU	CD-OE2	5.03	1.31	1.25

All (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
1	A	2374	A	C2'-C3'-O3'	7.01	124.93	109.50
37	c	241	LEU	CA-CB-CG	6.51	130.28	115.30
1	A	2507	A	C2'-C3'-O3'	6.28	123.75	113.70
1	A	2421	G	C2'-C3'-O3'	6.08	123.42	113.70
1	A	2165	C	C2'-C3'-O3'	5.82	123.01	113.70
2	B	1628	C	C2'-C3'-O3'	5.64	122.72	113.70
23	Y	97	ASP	CB-CG-OD1	-5.56	113.30	118.30
6	H	70	LYS	C-N-CD	5.41	139.75	128.40
50	s	62	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	3041	U	C2'-C3'-O3'	5.34	122.24	113.70
1	A	2321	A	N9-C1'-C2'	5.34	120.94	114.00
9	K	145	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	1823	A	C2'-C3'-O3'	5.30	122.18	113.70
1	A	2649	U	C2'-C3'-O3'	5.25	122.11	113.70
1	A	2111	C	N1-C1'-C2'	5.25	120.83	114.00
41	g	77	ASP	CB-CG-OD2	5.24	123.01	118.30
12	N	199	ARG	NE-CZ-NH2	-5.22	117.69	120.30
50	s	54	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	2245	A	N9-C1'-C2'	5.20	120.76	114.00
1	A	2243	A	C2'-C3'-O3'	5.18	121.99	113.70
30	5	116	GLY	N-CA-C	-5.18	100.14	113.10
1	A	2186	C	C2'-C3'-O3'	5.13	121.91	113.70
2	B	1607	U	C2'-C3'-O3'	5.09	121.85	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	194	LEU	CA-CB-CG	5.06	126.94	115.30
37	c	241	LEU	CB-CA-C	-5.06	100.58	110.20
1	A	1806	U	C2'-C3'-O3'	5.06	121.80	113.70
3	D	277	ARG	NE-CZ-NH1	5.03	122.82	120.30

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
9	K	175/178 (98%)	157 (90%)	10 (6%)	8 (5%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
40	f	71/211 (34%)	63 (89%)	7 (10%)	1 (1%)	11	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
22	X	127	VAL
24	Z	146	VAL
26	1	39	GLU
30	5	383	TYR
30	5	420	HIS
31	6	344	PHE
36	b	69	PRO
37	c	123	GLN
38	d	164	VAL
38	d	187	GLU
38	d	268	PRO
38	d	272	PRO
39	e	221	LYS
42	h	65	ASP
42	h	147	ASN
45	k	61	GLU
45	k	62	PRO
49	r	76	ASN

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Mol	Chain	Res	Type
49	r	158	SER
4	E	231	HIS
4	E	317	PRO
5	F	223	HIS
9	K	115	ASN
15	Q	264	TRP
17	S	94	ARG
20	V	155	PRO
22	X	177	HIS
25	0	146	GLY
25	0	178	ASP
30	5	35	VAL
30	5	263	ILE
30	5	359	LEU
31	6	379	ILE
37	c	64	PRO
37	c	264	THR
38	d	195	VAL
41	g	145	GLY
44	j	40	TYR
45	k	18	VAL
46	o	15	ARG
48	q	43	GLU
50	s	345	PHE
3	D	67	LYS
7	I	120	LYS
7	I	172	PRO
7	I	178	GLY
8	J	61	LYS
9	K	3	SER
9	K	15	ALA
11	M	287	ASP
13	O	112	ASN
15	Q	76	LEU
18	T	209	VAL
20	V	118	ARG
20	V	178	SER
30	5	272	ASP
31	6	51	TYR
31	6	72	ARG
34	9	46	SER
34	9	131	TYR

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Mol	Chain	Res	Type
36	b	14	VAL
36	b	116	ARG
40	f	182	VAL
42	h	146	SER
46	o	50	SER
47	p	139	SER
50	s	85	LYS
50	s	250	PHE
50	s	407	ASP
4	E	82	ASP
4	E	127	CYS
4	E	141	LYS
7	I	176	LEU
9	K	151	ILE
11	M	125	ARG
11	M	208	GLU
12	N	240	LYS
15	Q	215	VAL
18	T	158	TYR
20	V	171	ILE
21	W	127	TYR
22	X	34	GLU
25	0	177	ARG
25	0	184	TRP
26	1	60	LYS
30	5	296	LYS
30	5	297	ALA
31	6	165	ALA
31	6	307	HIS
36	b	117	LYS
37	c	35	PHE
39	e	160	PHE
43	i	65	ASN
45	k	37	VAL
45	k	60	SER
50	s	248	ALA
50	s	264	ILE
4	E	126	ASP
4	E	324	ASP
5	F	74	GLN
8	J	60	ILE
8	J	84	GLN

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Mol	Chain	Res	Type
8	J	109	ALA
9	K	14	PHE
9	K	24	LYS
9	K	143	GLU
14	P	173	GLU
14	P	177	ILE
15	Q	171	VAL
16	R	137	GLU
16	R	143	SER
19	U	12	LEU
20	V	142	GLU
20	V	185	ARG
30	5	70	LEU
30	5	170	ILE
30	5	256	PHE
31	6	68	PRO
31	6	351	HIS
32	7	157	ALA
34	9	39	LYS
37	c	314	TRP
39	e	219	TYR
41	g	137	VAL
42	h	66	LEU
6	H	61	LYS
9	K	23	GLY
10	L	113	ASN
10	L	131	GLU
11	M	110	VAL
11	M	242	TYR
22	X	52	ILE
25	0	113	CYS
25	0	116	LEU
27	2	51	ASN
30	5	381	LEU
37	c	229	PHE
39	e	178	ARG
41	g	136	PRO
50	s	284	VAL
50	s	364	GLY
30	5	305	GLN
49	r	61	PRO
6	H	71	PRO

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Mol	Chain	Res	Type
38	d	208	VAL
5	F	128	TRP
8	J	74	PRO
8	J	136	PRO
10	L	112	GLY
31	6	130	VAL
11	M	265	ILE
13	O	12	GLY
18	T	69	ARG
20	V	110	PRO
24	Z	143	GLY
46	o	13	PRO

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (577) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	71	LYS
3	D	74	ILE
3	D	115	GLU
3	D	177	ARG
3	D	195	ASN
3	D	202	ARG
3	D	232	ARG
3	D	240	CYS
3	D	243	THR
3	D	244	VAL
3	D	262	ARG
3	D	274	ARG
3	D	277	ARG
3	D	284	ARG
3	D	293	LYS
4	E	54	SER
4	E	57	ASN
4	E	60	PHE
4	E	86	PRO
4	E	120	THR
4	E	154	ARG
4	E	156	ARG
4	E	164	PHE
4	E	168	LEU
4	E	187	ILE
4	E	207	THR
4	E	213	LYS
4	E	227	GLN
4	E	233	GLN
4	E	271	LEU
4	E	278	THR
4	E	286	ASN
4	E	300	LYS

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Mol	Chain	Res	Type
4	E	301	ASP
4	E	304	LEU
4	E	330	GLU
5	F	59	ARG
5	F	76	ARG
5	F	89	THR
5	F	96	LEU
5	F	98	GLN
5	F	101	MET
5	F	108	ARG
5	F	110	SER
5	F	121	ARG
5	F	125	ARG
5	F	126	LYS
5	F	140	SER
5	F	145	LEU
5	F	184	GLN
5	F	185	ASP
5	F	187	LEU
5	F	194	GLU
5	F	203	LEU
5	F	221	LEU
5	F	228	GLN
5	F	258	THR
5	F	259	LEU
5	F	277	ASP
5	F	283	LEU
6	H	75	ARG
6	H	76	ARG
6	H	82	LEU
6	H	94	LEU
6	H	98	LEU
7	I	44	ARG
7	I	47	LEU
7	I	93	ASN
7	I	101	ASN
7	I	116	LEU
7	I	130	VAL
7	I	136	GLU
7	I	151	ASN
7	I	170	THR
7	I	191	PHE

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Mol	Chain	Res	Type
8	J	23	ILE
8	J	50	CYS
8	J	56	ARG
8	J	71	LEU
8	J	75	ASP
8	J	86	THR
8	J	123	ILE
8	J	124	LYS
8	J	130	PHE
8	J	141	VAL
8	J	142	ARG
8	J	150	SER
9	K	5	SER
9	K	10	GLN
9	K	13	THR
9	K	20	LEU
9	K	38	ARG
9	K	60	MET
9	K	95	LEU
9	K	125	LEU
9	K	145	LEU
9	K	154	ARG
9	K	158	TYR
10	L	37	ARG
10	L	38	VAL
10	L	89	HIS
10	L	104	ASN
10	L	130	ARG
11	M	19	LEU
11	M	28	LYS
11	M	41	ARG
11	M	57	ARG
11	M	64	ARG
11	M	87	HIS
11	M	96	LEU
11	M	100	ARG
11	M	101	LEU
11	M	114	GLN
11	M	118	LEU
11	M	130	GLN
11	M	132	LEU
11	M	142	GLU

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Mol	Chain	Res	Type
11	M	156	VAL
11	M	162	LEU
11	M	179	TYR
11	M	182	ARG
11	M	184	LEU
11	M	195	LEU
11	M	208	GLU
11	M	222	TYR
11	M	233	ARG
11	M	234	LEU
11	M	255	MET
11	M	273	TRP
11	M	279	ASP
12	N	50	LEU
12	N	54	GLU
12	N	90	LEU
12	N	103	GLU
12	N	105	MET
12	N	113	MET
12	N	123	ARG
12	N	151	VAL
12	N	158	ARG
12	N	168	GLU
12	N	198	MET
12	N	206	GLU
12	N	226	ILE
12	N	250	ARG
13	O	14	VAL
13	O	17	ARG
13	O	20	LEU
13	O	23	GLU
13	O	26	ILE
13	O	30	ARG
13	O	33	LEU
13	O	36	LEU
13	O	75	MET
13	O	89	LEU
13	O	104	TYR
13	O	112	ASN
13	O	123	ILE
13	O	129	CYS
13	O	138	ARG

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Mol	Chain	Res	Type
13	O	141	HIS
13	O	144	LEU
13	O	146	ASN
13	O	152	LEU
13	O	153	ARG
14	P	50	ARG
14	P	134	ARG
14	P	137	GLU
14	P	141	ASN
14	P	146	GLN
14	P	155	ASP
14	P	160	LEU
15	Q	75	PHE
15	Q	87	THR
15	Q	88	ASP
15	Q	102	ARG
15	Q	129	LYS
15	Q	156	GLU
15	Q	158	GLN
15	Q	194	LEU
15	Q	220	LEU
15	Q	235	ARG
15	Q	237	ASN
15	Q	244	ARG
15	Q	246	ASP
15	Q	251	GLU
15	Q	261	ASN
16	R	10	LEU
16	R	12	ASN
16	R	34	ARG
16	R	36	ASN
16	R	67	LEU
16	R	98	ASN
16	R	102	LEU
16	R	119	LEU
16	R	123	ARG
16	R	124	ARG
17	S	84	ASN
17	S	101	PHE
17	S	107	LYS
17	S	112	ASP
17	S	118	ASN

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Mol	Chain	Res	Type
17	S	131	GLU
17	S	134	LEU
17	S	135	LEU
17	S	144	LEU
17	S	153	LEU
17	S	155	ARG
17	S	167	TRP
17	S	172	MET
17	S	173	ARG
17	S	184	ARG
17	S	194	ARG
18	T	83	SER
18	T	92	LYS
18	T	95	ARG
18	T	100	ASP
18	T	127	MET
18	T	137	ARG
18	T	149	ARG
18	T	159	HIS
18	T	161	ARG
18	T	163	ARG
18	T	168	GLU
18	T	180	GLU
18	T	201	GLN
18	T	206	ARG
18	T	207	THR
19	U	3	ARG
19	U	17	LEU
19	U	25	PHE
19	U	28	LEU
19	U	38	ASP
19	U	53	LEU
19	U	71	ARG
19	U	101	HIS
20	V	20	ARG
20	V	40	ARG
20	V	63	GLU
20	V	83	ARG
20	V	101	THR
20	V	104	TYR
20	V	108	MET
20	V	120	VAL

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Mol	Chain	Res	Type
20	V	145	ARG
20	V	149	ARG
20	V	152	ARG
20	V	185	ARG
20	V	193	THR
20	V	197	GLU
20	V	209	LYS
21	W	45	LYS
21	W	70	GLN
21	W	71	ARG
21	W	72	HIS
21	W	88	CYS
21	W	105	VAL
21	W	110	ASN
21	W	112	GLU
21	W	139	GLU
22	X	60	GLU
22	X	63	GLU
22	X	69	ILE
22	X	77	ARG
22	X	89	GLN
22	X	95	ASP
22	X	101	LEU
22	X	130	ARG
22	X	141	LEU
22	X	143	PHE
22	X	153	LEU
22	X	154	CYS
22	X	189	ASP
22	X	208	LEU
22	X	213	GLU
22	X	219	GLU
22	X	226	LEU
22	X	234	LEU
22	X	241	GLN
23	Y	88	GLN
23	Y	90	LEU
23	Y	91	ARG
23	Y	98	LEU
23	Y	108	GLU
23	Y	115	LEU
23	Y	117	GLN

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Mol	Chain	Res	Type
23	Y	150	GLU
23	Y	157	GLN
23	Y	169	ARG
23	Y	175	ARG
23	Y	190	LEU
23	Y	204	TYR
23	Y	213	ARG
23	Y	226	LEU
24	Z	77	ARG
24	Z	110	LEU
24	Z	134	MET
24	Z	138	CYS
24	Z	139	LEU
24	Z	144	GLU
25	0	85	ARG
25	0	86	THR
25	0	94	ARG
25	0	96	ASN
25	0	98	GLN
25	0	105	ASN
25	0	113	CYS
25	0	115	HIS
25	0	116	LEU
25	0	117	LYS
25	0	136	GLU
25	0	154	ILE
25	0	178	ASP
25	0	185	PHE
26	1	18	VAL
26	1	22	SER
26	1	30	PHE
26	1	34	ARG
26	1	41	LEU
26	1	47	ASP
26	1	58	GLU
26	1	65	LEU
27	2	54	GLN
27	2	72	THR
27	2	87	ARG
27	2	92	HIS
28	3	94	LEU
28	3	112	ASP

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Mol	Chain	Res	Type
28	3	129	TYR
28	3	168	ARG
28	3	169	ARG
29	4	76	CYS
29	4	85	ARG
30	5	55	LEU
30	5	96	HIS
30	5	98	LEU
30	5	106	ILE
30	5	110	ARG
30	5	113	LEU
30	5	167	THR
30	5	168	GLU
30	5	201	ARG
30	5	218	LEU
30	5	220	LEU
30	5	223	ARG
30	5	229	ARG
30	5	230	LEU
30	5	256	PHE
30	5	269	ASN
30	5	272	ASP
30	5	293	LEU
30	5	294	LEU
30	5	305	GLN
30	5	309	LEU
30	5	312	LYS
30	5	315	LEU
30	5	322	LEU
30	5	345	VAL
30	5	358	GLN
30	5	365	ASP
30	5	371	LYS
30	5	375	TRP
30	5	381	LEU
30	5	382	LEU
31	6	40	ILE
31	6	42	LEU
31	6	51	TYR
31	6	52	ARG
31	6	60	ARG
31	6	73	THR

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Mol	Chain	Res	Type
31	6	74	TYR
31	6	130	VAL
31	6	136	ARG
31	6	142	THR
31	6	146	TYR
31	6	157	LEU
31	6	173	LEU
31	6	182	ASP
31	6	185	MET
31	6	192	GLU
31	6	200	GLN
31	6	206	TYR
31	6	218	LEU
31	6	222	ASP
31	6	233	LEU
31	6	235	TRP
31	6	267	ARG
31	6	272	LEU
31	6	292	GLN
31	6	298	PHE
31	6	303	PHE
31	6	318	PHE
31	6	324	ASP
31	6	334	LEU
31	6	339	GLU
31	6	354	GLN
31	6	356	ARG
31	6	370	ARG
31	6	371	ASP
31	6	372	SER
32	7	54	ARG
32	7	55	GLN
32	7	64	LYS
32	7	65	ILE
32	7	81	MET
32	7	114	ASP
32	7	143	TRP
32	7	168	ARG
32	7	234	LYS
32	7	300	VAL
32	7	313	TRP
33	8	77	TRP

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Mol	Chain	Res	Type
33	8	85	ARG
34	9	17	ARG
34	9	23	SER
34	9	54	LYS
34	9	96	VAL
35	a	109	ILE
35	a	122	ARG
35	a	132	CYS
36	b	15	LEU
36	b	26	LEU
36	b	62	VAL
36	b	68	ARG
36	b	71	CYS
36	b	81	ASN
36	b	96	GLU
36	b	103	LYS
36	b	131	HIS
36	b	135	ASN
37	c	65	ASN
37	c	88	LEU
37	c	94	ASN
37	c	123	GLN
37	c	145	TYR
37	c	180	LEU
37	c	202	LEU
37	c	203	LEU
37	c	211	THR
37	c	227	GLU
37	c	269	LEU
37	c	271	PHE
37	c	283	GLU
37	c	315	ASN
38	d	124	ARG
38	d	166	GLU
38	d	209	TYR
39	e	111	ARG
39	e	121	PHE
39	e	131	GLN
39	e	140	LEU
39	e	146	ARG
39	e	148	LEU
39	e	156	MET

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Mol	Chain	Res	Type
39	e	163	ASN
39	e	168	HIS
39	e	175	GLN
39	e	188	PHE
39	e	219	TYR
39	e	220	LEU
39	e	225	LEU
39	e	227	GLN
40	f	54	HIS
40	f	113	LEU
40	f	114	CYS
40	f	154	GLU
40	f	169	ILE
40	f	172	GLU
41	g	46	GLN
41	g	55	THR
41	g	76	ARG
41	g	94	ILE
41	g	104	ASN
41	g	107	MET
41	g	126	ASP
41	g	141	ASN
41	g	147	LEU
41	g	155	GLN
42	h	70	LEU
42	h	73	TYR
42	h	92	GLU
42	h	96	LEU
42	h	100	LEU
42	h	107	ASP
42	h	117	LEU
42	h	120	MET
42	h	131	ASN
42	h	137	ARG
42	h	147	ASN
42	h	156	TRP
43	i	51	ARG
43	i	63	LEU
43	i	65	ASN
43	i	74	ILE
43	i	88	LEU
43	i	93	ARG

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Mol	Chain	Res	Type
43	i	95	ARG
43	i	101	ARG
43	i	105	ASP
43	i	106	ASP
43	i	107	LEU
43	i	110	LEU
43	i	113	ARG
43	i	127	PHE
44	j	36	ASN
44	j	40	TYR
44	j	63	GLN
44	j	66	ARG
44	j	76	ARG
45	k	21	CYS
45	k	25	LYS
45	k	28	GLU
45	k	32	THR
45	k	43	ARG
45	k	81	LEU
45	k	87	LEU
46	o	22	ARG
46	o	23	ARG
46	o	59	GLU
46	o	60	ARG
46	o	68	ARG
46	o	69	GLU
46	o	82	PHE
46	o	87	PHE
47	p	102	ARG
47	p	124	LYS
47	p	129	ARG
47	p	135	LEU
47	p	141	ARG
47	p	144	PHE
47	p	160	GLU
47	p	163	GLN
48	q	26	ARG
48	q	43	GLU
48	q	60	GLN
48	q	89	GLU
48	q	112	GLN
48	q	114	ARG

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Mol	Chain	Res	Type
49	r	40	GLU
49	r	59	GLU
49	r	60	SER
49	r	65	ASN
49	r	77	LEU
49	r	84	ASP
49	r	85	ASP
49	r	88	LEU
49	r	117	GLU
49	r	152	THR
49	r	163	TYR
49	r	168	ARG
49	r	171	ARG
49	r	187	TYR
50	s	65	ARG
50	s	77	ASP
50	s	192	ASN
50	s	229	LEU
50	s	230	ARG
50	s	235	ASP
50	s	238	ASN
50	s	251	VAL
50	s	253	LEU
50	s	264	ILE
50	s	270	LYS
50	s	280	ASN
50	s	281	HIS
50	s	284	VAL
50	s	301	LEU
50	s	304	ASP
50	s	333	PHE
50	s	358	GLN
50	s	360	VAL
50	s	368	SER
50	s	373	GLN
50	s	379	LEU
50	s	394	TRP
50	s	404	THR
50	s	414	ASN
50	s	427	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	276	HIS
4	E	57	ASN
4	E	128	HIS
4	E	231	HIS
5	F	58	HIS
5	F	74	GLN
5	F	97	HIS
5	F	228	GLN
5	F	249	ASN
7	I	189	GLN
10	L	64	ASN
11	M	26	ASN
11	M	102	GLN
13	O	146	ASN
14	P	78	HIS
14	P	95	HIS
14	P	120	ASN
15	Q	139	GLN
15	Q	258	GLN
15	Q	261	ASN
16	R	36	ASN
16	R	98	ASN
18	T	210	HIS
19	U	82	HIS
19	U	101	HIS
21	W	80	HIS
21	W	110	ASN
22	X	241	GLN
23	Y	225	ASN
24	Z	47	GLN
26	1	15	ASN
29	4	98	HIS
30	5	102	GLN
30	5	119	GLN
30	5	186	GLN
30	5	251	HIS
30	5	305	GLN
30	5	358	GLN
30	5	380	GLN
30	5	384	GLN
31	6	292	GLN
32	7	246	GLN
32	7	298	GLN

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Mol	Chain	Res	Type
33	8	99	GLN
34	9	129	GLN
36	b	24	GLN
36	b	131	HIS
37	c	193	GLN
37	c	222	GLN
38	d	235	GLN
38	d	286	GLN
39	e	124	GLN
39	e	182	ASN
40	f	158	GLN
41	g	104	ASN
42	h	99	ASN
42	h	103	HIS
42	h	147	ASN
46	o	62	HIS
46	o	85	HIS
47	p	96	ASN
47	p	146	ASN
48	q	60	GLN
48	q	137	GLN
50	s	71	HIS
50	s	164	HIS
50	s	373	GLN
50	s	385	GLN
50	s	420	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1458/1559 (93%)	550 (37%)	118 (8%)
2	B	51/73 (69%)	21 (41%)	3 (5%)
All	All	1509/1632 (92%)	571 (37%)	121 (8%)

All (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

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Mol	Chain	Res	Type
1	A	1677	C
1	A	1678	C
1	A	1679	U
1	A	1680	A
1	A	1681	G
1	A	1685	C
1	A	1689	C
1	A	1694	U
1	A	1699	C
1	A	1700	U
1	A	1701	U
1	A	1702	A
1	A	1703	C
1	A	1704	U
1	A	1708	A
1	A	1709	G
1	A	1712	A
1	A	1713	A
1	A	1714	C
1	A	1715	C
1	A	1716	U
1	A	1717	U
1	A	1724	A
1	A	1727	A
1	A	1728	U
1	A	1732	C
1	A	1741	A
1	A	1748	G
1	A	1750	G
1	A	1751	A
1	A	1767	G
1	A	1770	G
1	A	1773	A
1	A	1775	A
1	A	1777	A
1	A	1779	A
1	A	1780	U
1	A	1781	A
1	A	1794	A
1	A	1799	U
1	A	1805	A
1	A	1806	U

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Mol	Chain	Res	Type
1	A	1807	U
1	A	1808	A
1	A	1809	U
1	A	1810	A
1	A	1812	C
1	A	1814	A
1	A	1817	C
1	A	1820	A
1	A	1821	A
1	A	1823	A
1	A	1824	U
1	A	1825	A
1	A	1827	C
1	A	1828	A
1	A	1829	A
1	A	1832	A
1	A	1836	A
1	A	1839	C
1	A	1843	U
1	A	1844	A
1	A	1849	C
1	A	1851	G
1	A	1852	C
1	A	1853	A
1	A	1854	U
1	A	1856	A
1	A	1867	A
1	A	1869	A
1	A	1871	A
1	A	1872	U
1	A	1878	U
1	A	1882	A
1	A	1883	G
1	A	1886	G
1	A	1887	A
1	A	1888	G
1	A	1889	C
1	A	1893	A
1	A	1894	G
1	A	1901	C
1	A	1902	C
1	A	1903	C

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Mol	Chain	Res	Type
1	A	1909	A
1	A	1918	G
1	A	1927	G
1	A	1935	A
1	A	1939	G
1	A	1940	A
1	A	1944	C
1	A	1947	C
1	A	1956	U
1	A	1961	A
1	A	1966	G
1	A	1972	A
1	A	1973	G
1	A	1974	A
1	A	1975	U
1	A	1985	G
1	A	1986	A
1	A	1987	G
1	A	1991	A
1	A	1992	C
1	A	1993	A
1	A	1994	A
1	A	1995	A
1	A	1998	U
1	A	1999	A
1	A	2000	C
1	A	2001	C
1	A	2002	G
1	A	2010	U
1	A	2014	A
1	A	2015	G
1	A	2016	C
1	A	2020	U
1	A	2021	U
1	A	2022	G
1	A	2029	A
1	A	2030	U
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2034	A
1	A	2036	C

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Mol	Chain	Res	Type
1	A	2037	U
1	A	2039	A
1	A	2044	A
1	A	2053	U
1	A	2054	U
1	A	2057	C
1	A	2059	C
1	A	2060	A
1	A	2065	A
1	A	2066	C
1	A	2074	A
1	A	2079	C
1	A	2083	U
1	A	2085	A
1	A	2092	C
1	A	2093	U
1	A	2095	U
1	A	2097	A
1	A	2098	G
1	A	2099	U
1	A	2105	G
1	A	2111	C
1	A	2113	G
1	A	2124	A
1	A	2125	C
1	A	2126	U
1	A	2129	G
1	A	2132	A
1	A	2134	A
1	A	2135	A
1	A	2136	C
1	A	2141	U
1	A	2142	A
1	A	2143	G
1	A	2147	G
1	A	2150	U
1	A	2154	A
1	A	2156	A
1	A	2157	U
1	A	2158	U
1	A	2159	U
1	A	2160	A

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Mol	Chain	Res	Type
1	A	2163	A
1	A	2165	C
1	A	2166	C
1	A	2168	U
1	A	2169	A
1	A	2170	G
1	A	2172	A
1	A	2173	G
1	A	2174	G
1	A	2175	C
1	A	2180	A
1	A	2181	A
1	A	2182	G
1	A	2183	C
1	A	2187	C
1	A	2189	C
1	A	2190	C
1	A	2191	A
1	A	2192	A
1	A	2193	U
1	A	2194	U
1	A	2195	A
1	A	2196	A
1	A	2197	G
1	A	2198	A
1	A	2200	A
1	A	2202	C
1	A	2204	U
1	A	2210	C
1	A	2211	U
1	A	2216	A
1	A	2218	C
1	A	2229	A
1	A	2230	A
1	A	2232	A
1	A	2233	U
1	A	2237	A
1	A	2238	A
1	A	2239	A
1	A	2241	A
1	A	2242	U
1	A	2243	A

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Mol	Chain	Res	Type
1	A	2244	U
1	A	2245	A
1	A	2246	A
1	A	2247	C
1	A	2259	C
1	A	2262	C
1	A	2263	C
1	A	2264	A
1	A	2269	G
1	A	2271	C
1	A	2275	U
1	A	2280	C
1	A	2281	A
1	A	2283	C
1	A	2284	C
1	A	2285	U
1	A	2290	A
1	A	2294	A
1	A	2297	A
1	A	2299	U
1	A	2300	G
1	A	2306	A
1	A	2308	A
1	A	2309	A
1	A	2315	A
1	A	2320	A
1	A	2321	A
1	A	2322	C
1	A	2324	U
1	A	2331	C
1	A	2332	C
1	A	2335	A
1	A	2342	U
1	A	2345	G
1	A	2350	A
1	A	2364	C
1	A	2365	U
1	A	2370	A
1	A	2371	U
1	A	2372	U
1	A	2373	A
1	A	2374	A

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Mol	Chain	Res	Type
1	A	2375	C
1	A	2379	C
1	A	2381	A
1	A	2384	A
1	A	2387	U
1	A	2389	C
1	A	2390	A
1	A	2392	U
1	A	2393	C
1	A	2394	A
1	A	2395	A
1	A	2396	C
1	A	2397	C
1	A	2401	A
1	A	2404	U
1	A	2405	C
1	A	2406	A
1	A	2407	U
1	A	2413	C
1	A	2414	C
1	A	2415	C
1	A	2416	U
1	A	2417	C
1	A	2418	A
1	A	2419	C
1	A	2421	G
1	A	2422	U
1	A	2423	C
1	A	2426	C
1	A	2429	A
1	A	2432	A
1	A	2434	A
1	A	2435	G
1	A	2443	C
1	A	2444	A
1	A	2445	U
1	A	2446	A
1	A	2447	A
1	A	2449	G
1	A	2453	G
1	A	2455	U
1	A	2458	A

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Mol	Chain	Res	Type
1	A	2464	G
1	A	2471	G
1	A	2478	G
1	A	2479	C
1	A	2483	U
1	A	2484	C
1	A	2485	U
1	A	2493	C
1	A	2494	C
1	A	2498	U
1	A	2500	A
1	A	2502	C
1	A	2506	A
1	A	2507	A
1	A	2508	C
1	A	2511	C
1	A	2514	C
1	A	2520	C
1	A	2521	A
1	A	2522	U
1	A	2523	C
1	A	2524	A
1	A	2527	A
1	A	2530	A
1	A	2531	U
1	A	2536	G
1	A	2540	C
1	A	2546	G
1	A	2550	A
1	A	2556	A
1	A	2557	C
1	A	2558	A
1	A	2559	U
1	A	2560	G
1	A	2561	U
1	A	2563	U
1	A	2564	A
1	A	2570	C
1	A	2574	G
1	A	2581	A
1	A	2583	C
1	A	2587	G

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Mol	Chain	Res	Type
1	A	2590	A
1	A	2591	A
1	A	2592	G
1	A	2593	G
1	A	2594	U
1	A	2599	U
1	A	2601	A
1	A	2602	U
1	A	2603	C
1	A	2604	A
1	A	2606	U
1	A	2607	U
1	A	2610	U
1	A	2614	U
1	A	2615	A
1	A	2616	A
1	A	2618	U
1	A	2626	U
1	A	2627	G
1	A	2629	A
1	A	2630	U
1	A	2632	A
1	A	2633	A
1	A	2634	U
1	A	2635	G
1	A	2638	U
1	A	2645	G
1	A	2649	U
1	A	2650	C
1	A	2654	U
1	A	2656	U
1	A	2660	U
1	A	2661	U
1	A	2665	U
1	A	2677	A
1	A	2683	C
1	A	2684	C
1	A	2686	G
1	A	2693	A
1	A	2694	A
1	A	2695	G
1	A	2696	A

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Mol	Chain	Res	Type
1	A	2706	A
1	A	2708	C
1	A	2709	A
1	A	2713	C
1	A	2718	C
1	A	2719	G
1	A	2723	A
1	A	2724	G
1	A	2725	A
1	A	2726	C
1	A	2731	U
1	A	2732	G
1	A	2733	G
1	A	2740	A
1	A	2744	U
1	A	2745	A
1	A	2746	U
1	A	2748	A
1	A	2749	A
1	A	2750	U
1	A	2756	C
1	A	2757	A
1	A	2758	G
1	A	2795	U
1	A	2804	A
1	A	2807	U
1	A	2810	G
1	A	2813	U
1	A	2814	G
1	A	2830	A
1	A	2831	G
1	A	2832	A
1	A	2833	A
1	A	2834	C
1	A	2842	C
1	A	2844	G
1	A	2846	G
1	A	2847	C
1	A	2848	A
1	A	2851	A
1	A	2854	U
1	A	2855	G

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Mol	Chain	Res	Type
1	A	2857	U
1	A	2858	A
1	A	2859	A
1	A	2864	U
1	A	2865	C
1	A	2870	G
1	A	2871	U
1	A	2879	A
1	A	2892	A
1	A	2895	U
1	A	2901	A
1	A	2906	C
1	A	2910	A
1	A	2912	C
1	A	2913	A
1	A	2914	A
1	A	2916	G
1	A	2917	G
1	A	2919	A
1	A	2921	A
1	A	2922	A
1	A	2926	A
1	A	2928	C
1	A	2933	G
1	A	2935	A
1	A	2936	U
1	A	2937	A
1	A	2945	A
1	A	2946	A
1	A	2948	C
1	A	2955	U
1	A	2956	A
1	A	2960	U
1	A	2961	C
1	A	2962	C
1	A	2963	A
1	A	2964	U
1	A	2971	A
1	A	2978	U
1	A	2982	C
1	A	2985	C
1	A	2986	C

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Mol	Chain	Res	Type
1	A	2989	G
1	A	2990	A
1	A	2991	U
1	A	2992	G
1	A	2993	U
1	A	2994	U
1	A	2995	G
1	A	3004	C
1	A	3005	A
1	A	3007	C
1	A	3010	G
1	A	3014	G
1	A	3016	G
1	A	3018	A
1	A	3022	G
1	A	3029	A
1	A	3030	A
1	A	3031	G
1	A	3040	G
1	A	3041	U
1	A	3042	U
1	A	3049	U
1	A	3053	A
1	A	3054	G
1	A	3055	U
1	A	3056	C
1	A	3059	A
1	A	3060	C
1	A	3061	G
1	A	3063	G
1	A	3064	A
1	A	3065	U
1	A	3068	G
1	A	3069	A
1	A	3070	G
1	A	3072	U
1	A	3073	C
1	A	3074	A
1	A	3076	A
1	A	3077	C
1	A	3085	A
1	A	3086	U

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Mol	Chain	Res	Type
1	A	3093	C
1	A	3096	U
1	A	3097	U
1	A	3098	U
1	A	3100	U
1	A	3101	A
1	A	3102	U
1	A	3108	U
1	A	3109	U
1	A	3114	U
1	A	3123	G
1	A	3128	A
1	A	3129	A
1	A	3131	G
1	A	3141	A
1	A	3150	U
1	A	3151	A
1	A	3155	C
1	A	3157	C
1	A	3158	A
1	A	3160	A
1	A	3162	C
1	A	3168	C
1	A	3169	C
1	A	3172	C
1	A	3173	G
1	A	3180	A
1	A	3183	U
1	A	3185	A
1	A	3189	C
1	A	3190	A
1	A	3196	G
1	A	3202	U
1	A	3204	C
1	A	3206	C
1	A	3207	A
1	A	3213	A
1	A	3217	A
1	A	3218	A
1	A	3220	A
1	A	3223	A
1	A	3228	U

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Mol	Chain	Res	Type
2	B	1604	G
2	B	1608	G
2	B	1609	U
2	B	1610	A
2	B	1611	G
2	B	1612	C
2	B	1614	U
2	B	1615	A
2	B	1625	A
2	B	1629	A
2	B	1631	C
2	B	1632	U
2	B	1634	A
2	B	1641	G
2	B	1644	G
2	B	1645	A
2	B	1650	A
2	B	1659	U
2	B	1665	C
2	B	1667	C
2	B	1669	G

All (121) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1677	C
1	A	1700	U
1	A	1702	A
1	A	1703	C
1	A	1708	A
1	A	1713	A
1	A	1715	C
1	A	1724	A
1	A	1727	A
1	A	1772	A
1	A	1780	U
1	A	1798	A
1	A	1805	A
1	A	1806	U
1	A	1807	U
1	A	1809	U
1	A	1820	A

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Mol	Chain	Res	Type
1	A	1823	A
1	A	1824	U
1	A	1852	C
1	A	1870	A
1	A	1871	A
1	A	1882	A
1	A	1887	A
1	A	1888	G
1	A	1901	C
1	A	1918	G
1	A	1972	A
1	A	1974	A
1	A	1985	G
1	A	1998	U
1	A	2001	C
1	A	2021	U
1	A	2029	A
1	A	2059	C
1	A	2065	A
1	A	2109	A
1	A	2135	A
1	A	2154	A
1	A	2158	U
1	A	2160	A
1	A	2165	C
1	A	2172	A
1	A	2174	G
1	A	2186	C
1	A	2189	C
1	A	2193	U
1	A	2196	A
1	A	2197	G
1	A	2209	G
1	A	2231	A
1	A	2243	A
1	A	2245	A
1	A	2251	A
1	A	2274	A
1	A	2284	C
1	A	2321	A
1	A	2370	A
1	A	2372	U

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Mol	Chain	Res	Type
1	A	2373	A
1	A	2374	A
1	A	2380	C
1	A	2400	C
1	A	2404	U
1	A	2421	G
1	A	2422	U
1	A	2431	C
1	A	2444	A
1	A	2457	A
1	A	2506	A
1	A	2507	A
1	A	2519	G
1	A	2523	C
1	A	2530	A
1	A	2531	U
1	A	2540	C
1	A	2558	A
1	A	2559	U
1	A	2601	A
1	A	2606	U
1	A	2607	U
1	A	2615	A
1	A	2617	A
1	A	2618	U
1	A	2625	C
1	A	2628	U
1	A	2649	U
1	A	2653	C
1	A	2693	A
1	A	2695	G
1	A	2744	U
1	A	2807	U
1	A	2813	U
1	A	2831	G
1	A	2839	C
1	A	2853	A
1	A	2865	C
1	A	2870	G
1	A	2905	A
1	A	2918	A
1	A	2936	U

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Mol	Chain	Res	Type
1	A	2945	A
1	A	2955	U
1	A	2989	G
1	A	2990	A
1	A	2993	U
1	A	3016	G
1	A	3030	A
1	A	3041	U
1	A	3063	G
1	A	3068	G
1	A	3092	U
1	A	3096	U
1	A	3149	C
1	A	3160	A
1	A	3162	C
1	A	3168	C
1	A	3201	A
2	B	1607	U
2	B	1608	G
2	B	1628	C

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	A	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	A	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	A	C5-C6-N6	2.15	123.62	120.35

There are no chirality outliers.

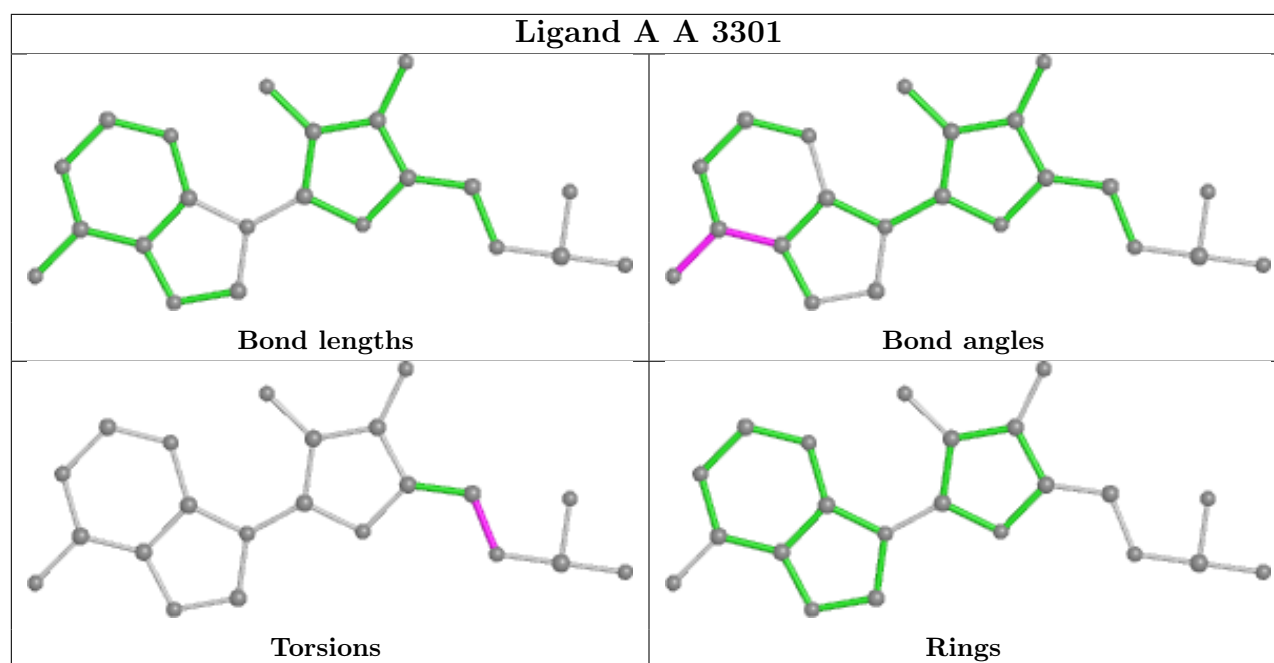
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	A	3301	A	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.

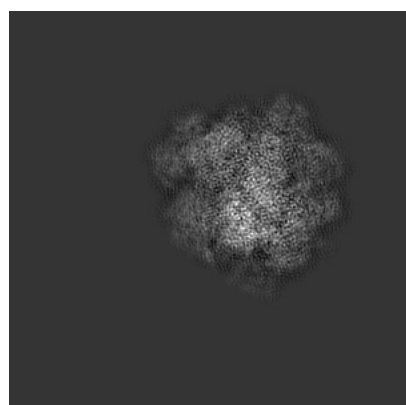
6 Map visualisation [i](#)

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.

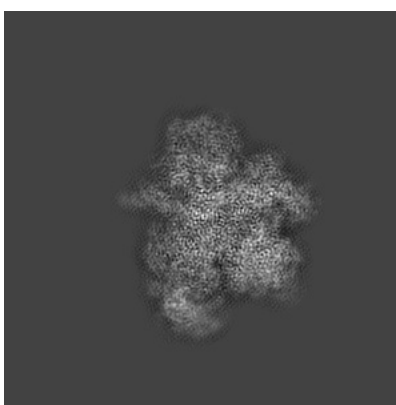
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

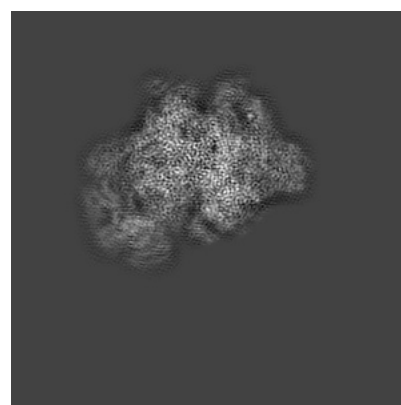
6.1.1 Primary map



X



Y

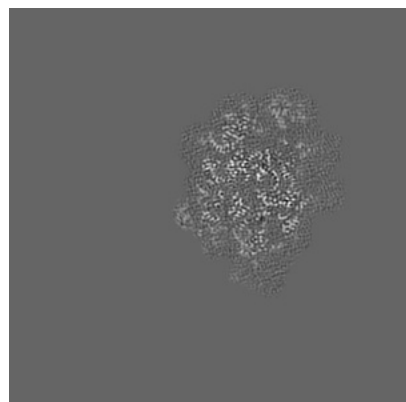


Z

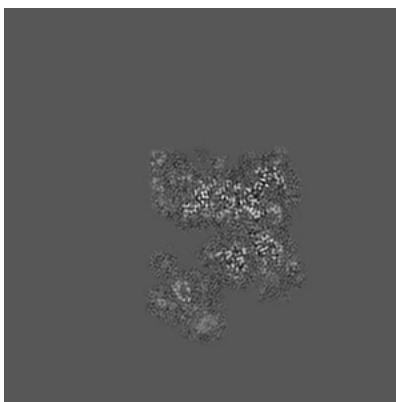
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

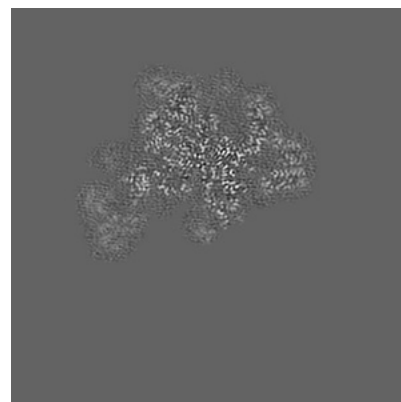
6.2.1 Primary map



X Index: 160



Y Index: 160

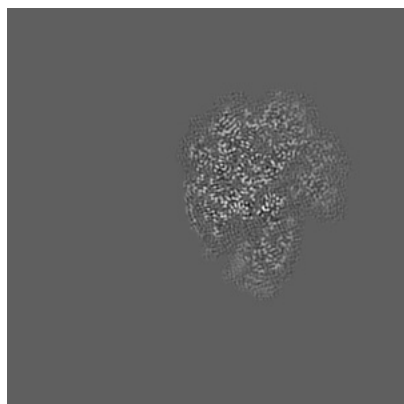


Z Index: 160

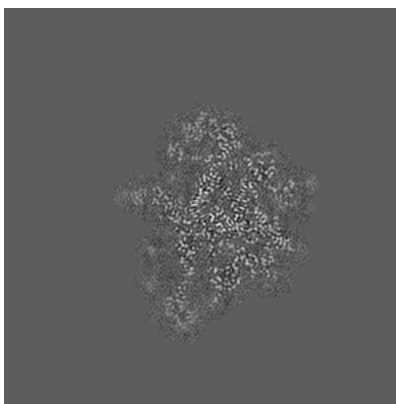
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

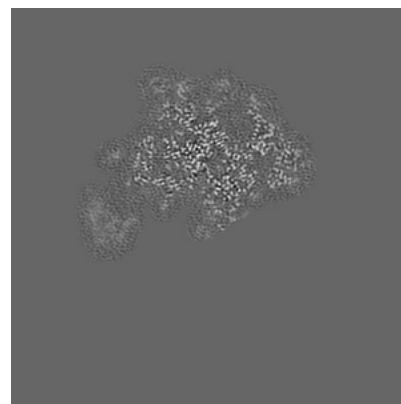
6.3.1 Primary map



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 surface views [i](#)

6.4.1 Primary map



X



Y



Z

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

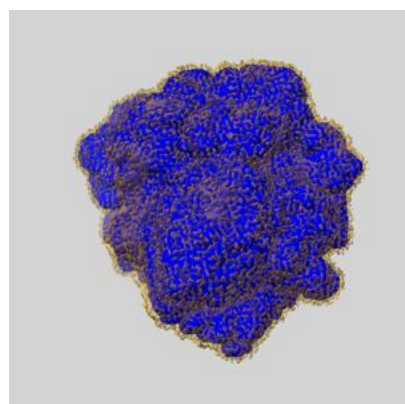
6.5 Mask visualisation [i](#)

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

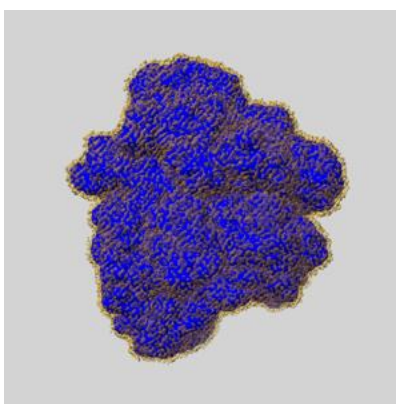
A mask typically either:

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

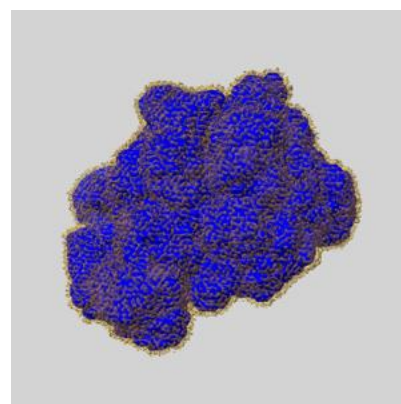
6.5.1 emd_2762_msk.map [i](#)



X



Y

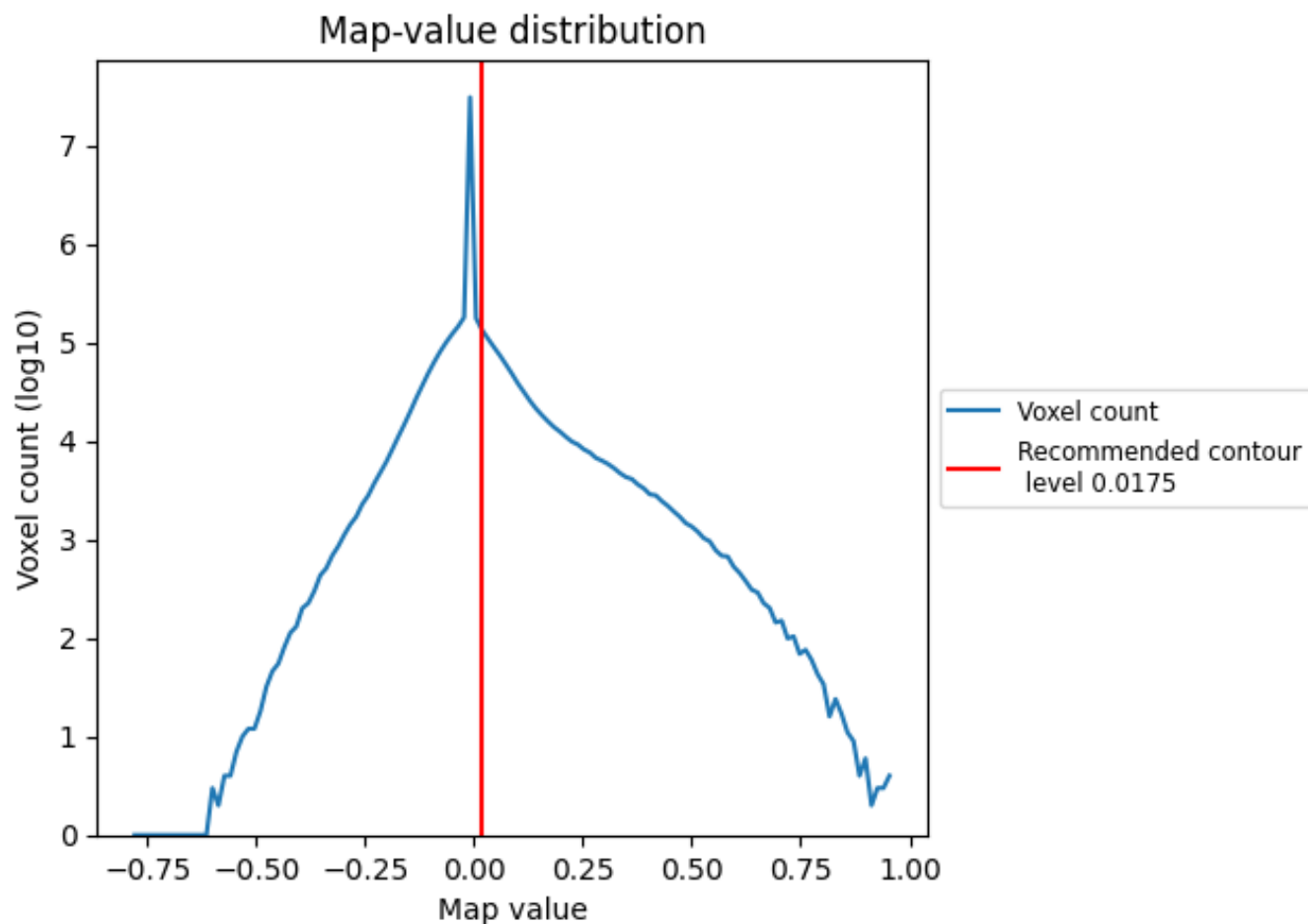


Z

7 Map analysis [i](#)

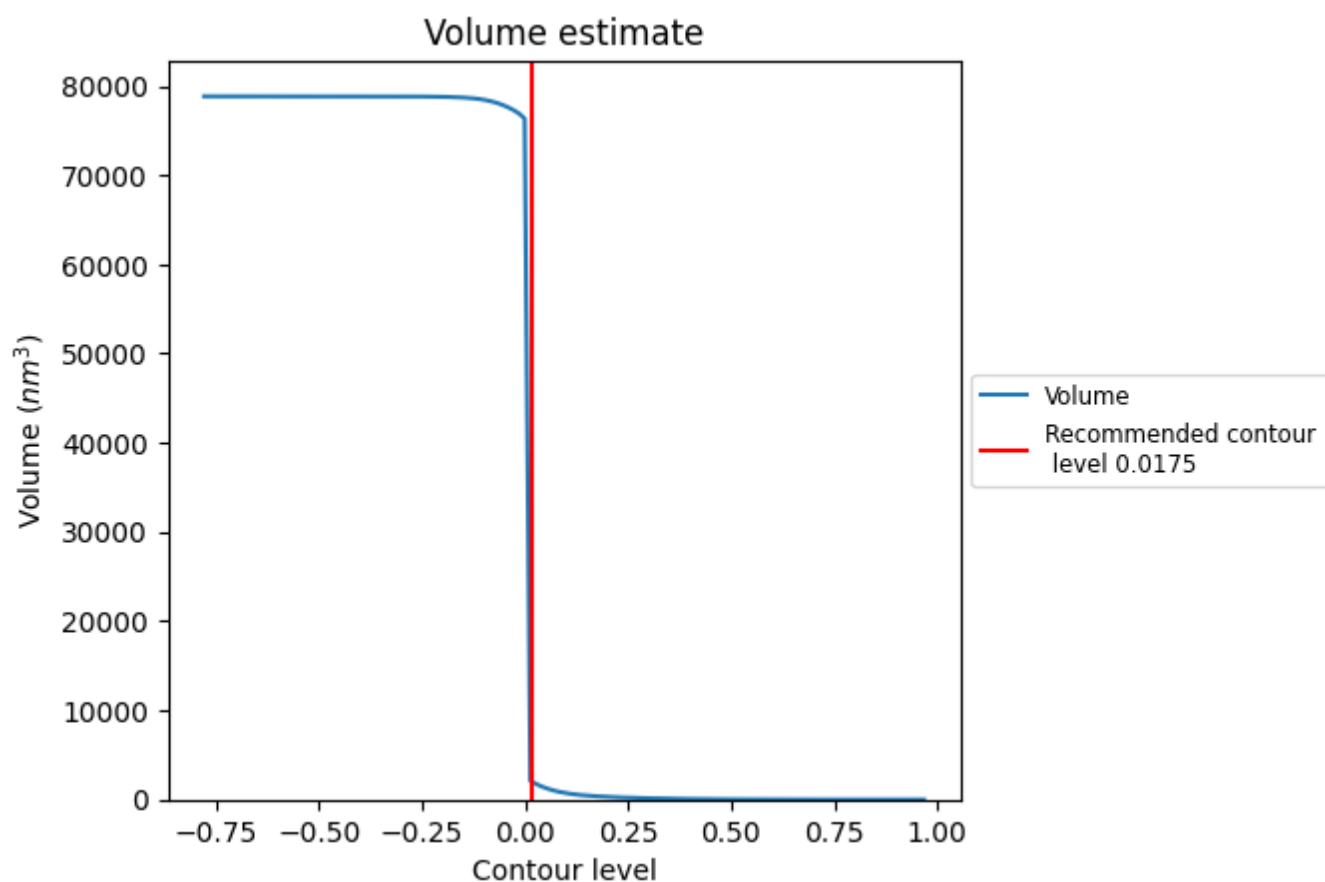
This section contains the results of statistical analysis of the map.

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.

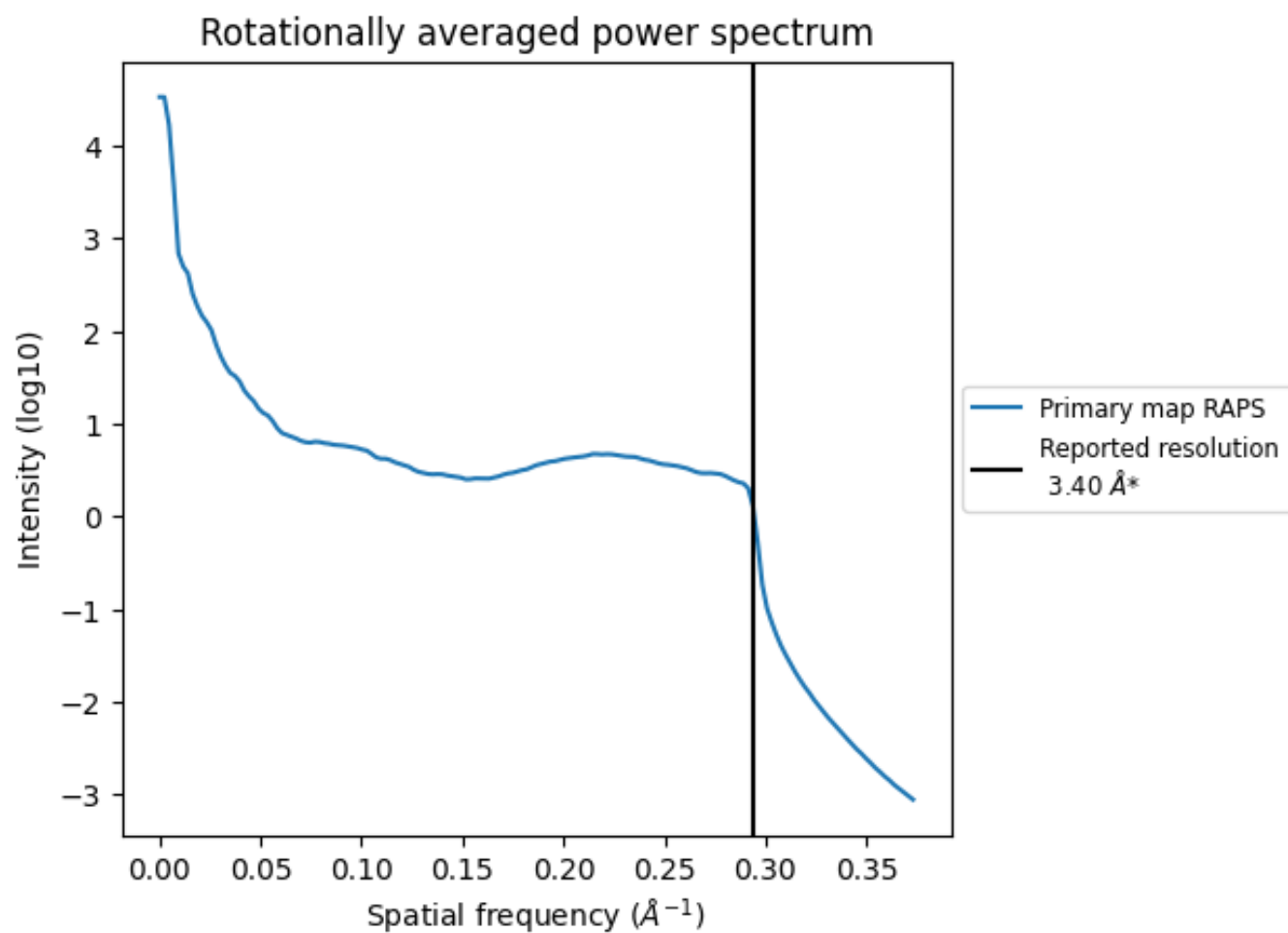
7.2 Volume estimate [i](#)



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 ⓘ

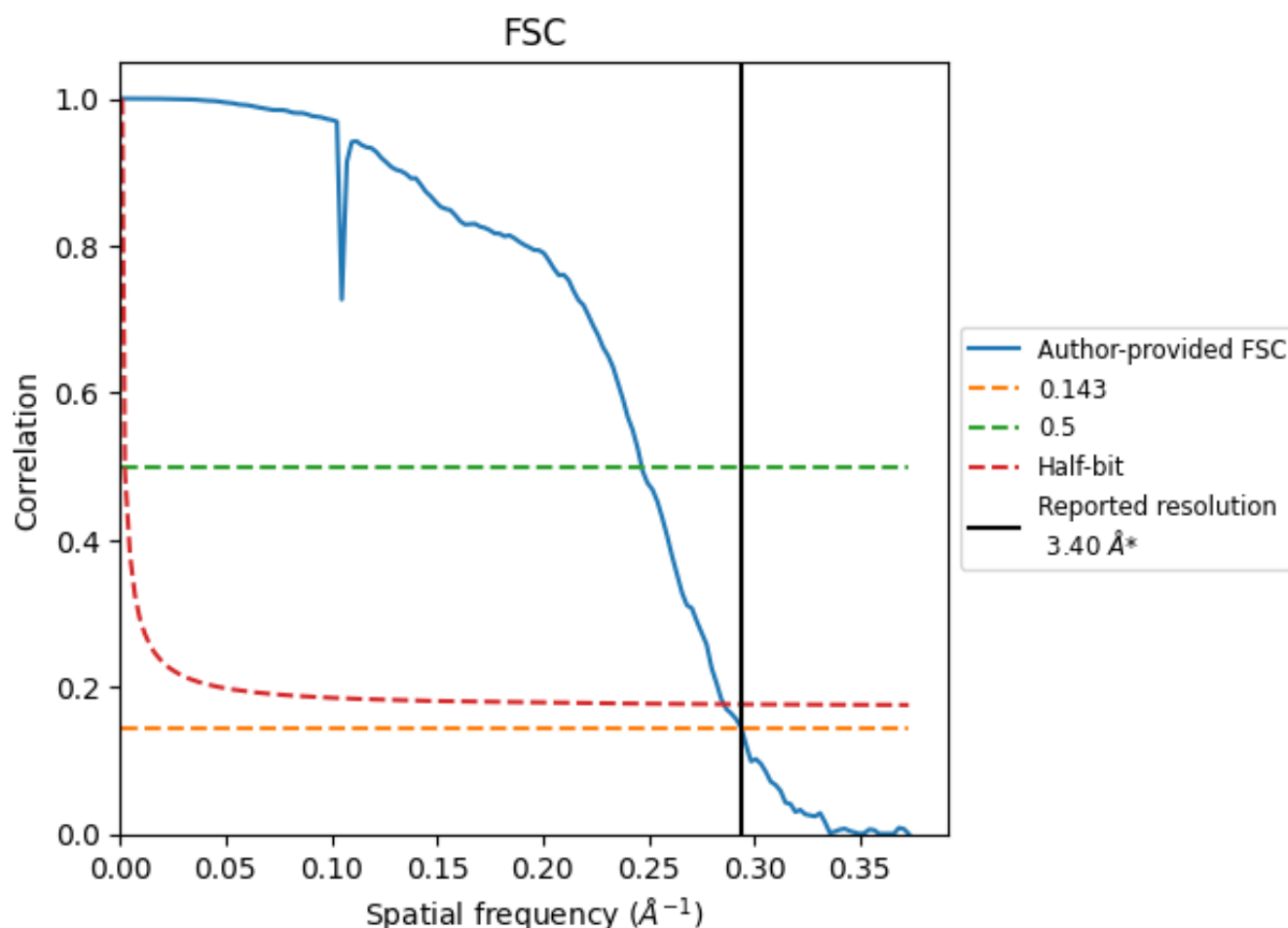


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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](#)

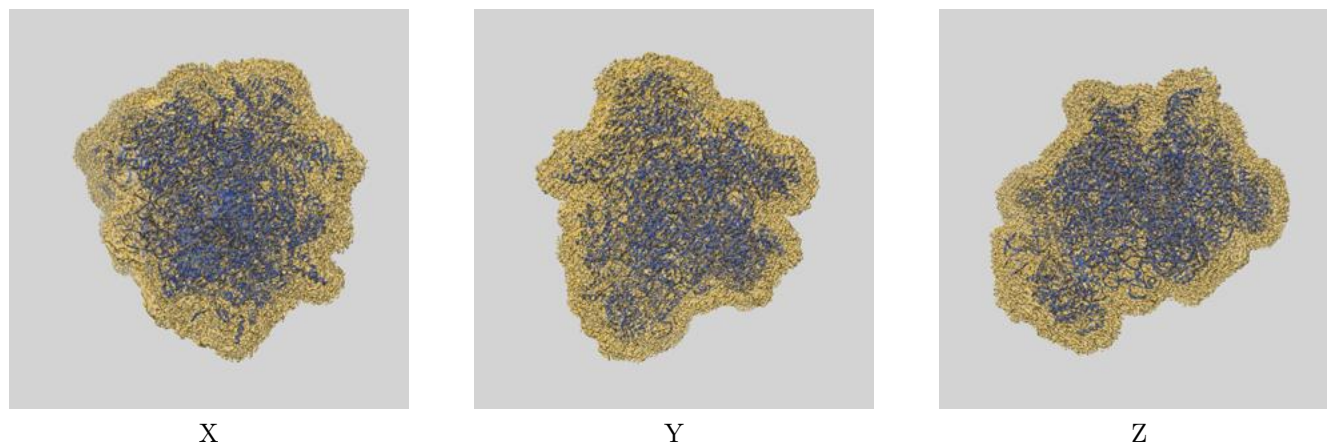
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	4.05	3.50
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

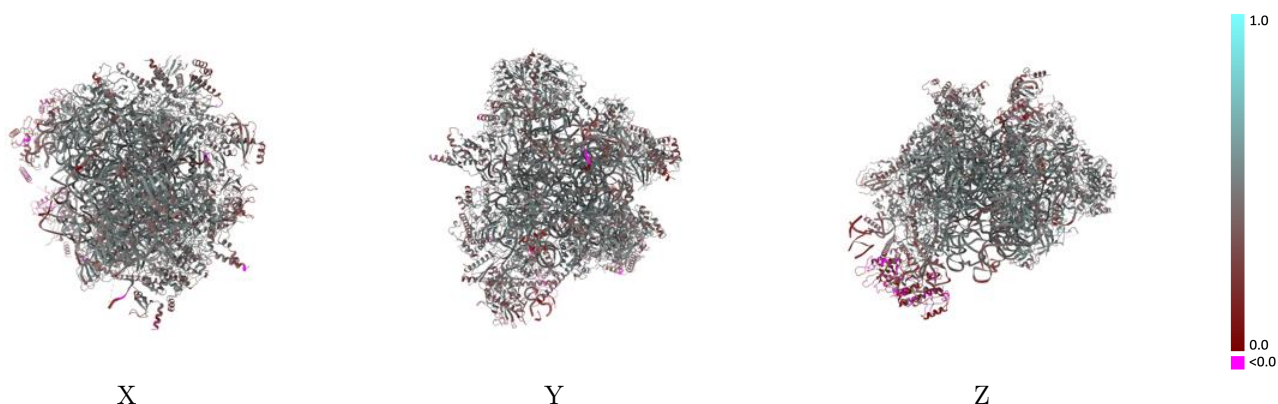
This section contains information regarding the fit between EMDB map EMD-2762 and PDB model 3J7Y. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



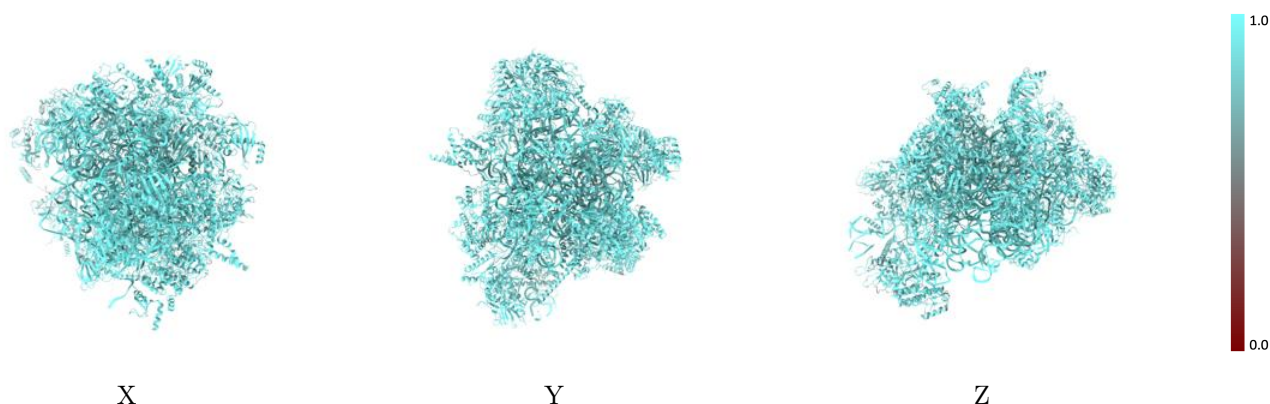
The images above show the 3D surface view of the map at the recommended contour level 0.0175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



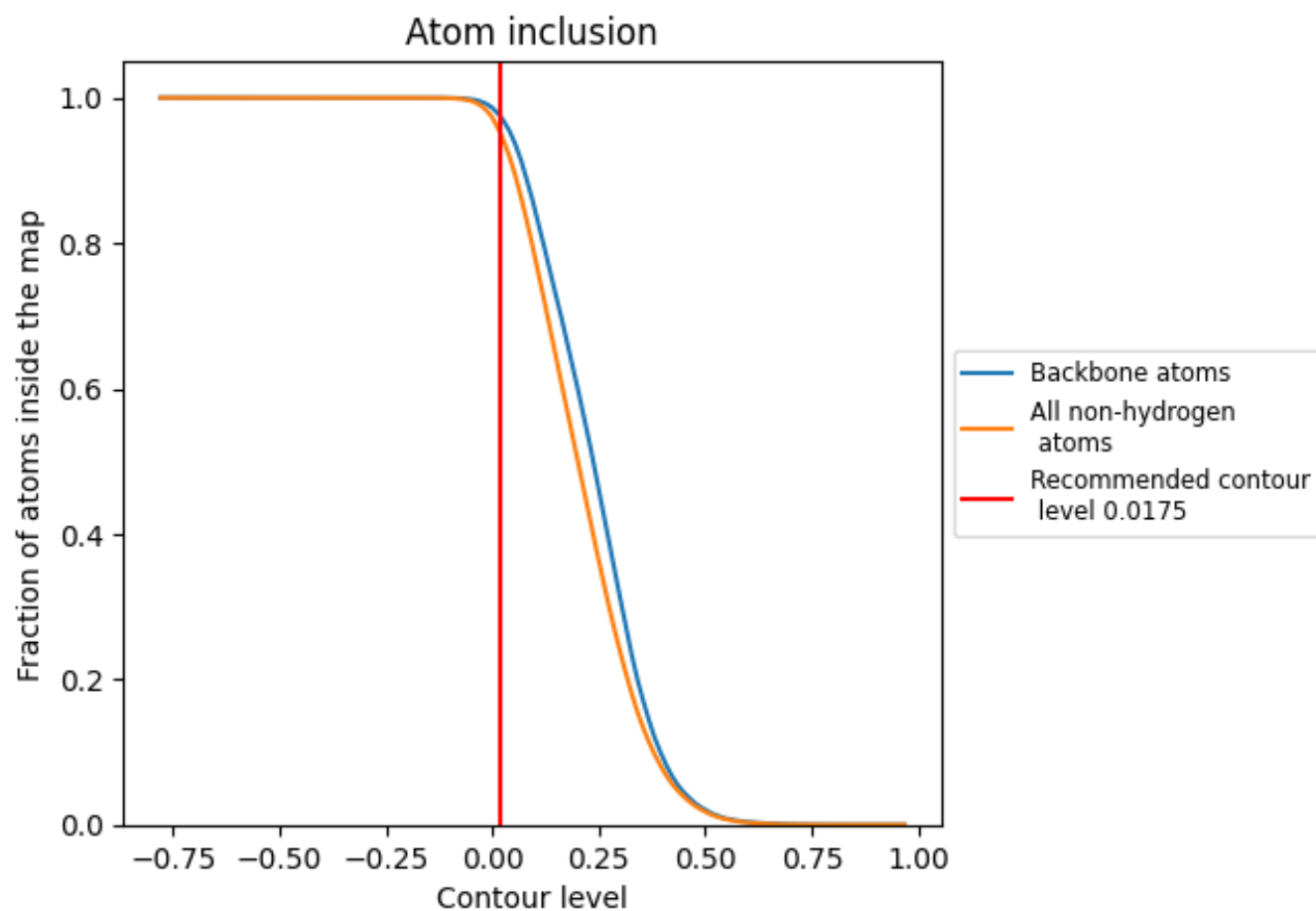
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9534	 0.4520
0	 0.9497	 0.4750
1	 0.9214	 0.4440
2	 0.9703	 0.5260
3	 0.9624	 0.5220
4	 0.9902	 0.5340
5	 0.9472	 0.4580
6	 0.9428	 0.3940
7	 0.9366	 0.4160
8	 0.9149	 0.2700
9	 0.9435	 0.4500
A	 0.9797	 0.4820
B	 0.9686	 0.2970
D	 0.9617	 0.4980
E	 0.9660	 0.4970
F	 0.9627	 0.4920
H	 0.9248	 0.4050
I	 0.8756	 0.2750
J	 0.8450	 0.1910
K	 0.9526	 0.4890
L	 0.9528	 0.4810
M	 0.9543	 0.4830
N	 0.9446	 0.4730
O	 0.9475	 0.4780
P	 0.9473	 0.4510
Q	 0.9402	 0.4680
R	 0.9504	 0.5070
S	 0.9542	 0.4870
T	 0.9457	 0.5000
U	 0.9662	 0.4920
V	 0.9166	 0.3870
W	 0.9769	 0.5160
X	 0.9367	 0.4550
Y	 0.9379	 0.4630
Z	 0.9604	 0.4950



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Chain	Atom inclusion	Q-score
a	 0.9333	 0.4640
b	 0.9649	 0.4890
c	 0.9447	 0.4390
d	 0.9202	 0.3860
e	 0.7977	 0.0950
f	 0.9539	 0.4060
g	 0.9510	 0.4790
h	 0.8919	 0.3280
i	 0.9529	 0.5080
j	 0.9395	 0.4500
k	 0.8596	 0.2400
o	 0.9501	 0.4860
p	 0.9298	 0.4080
q	 0.8721	 0.3490
r	 0.9621	 0.4780
s	 0.9512	 0.4710
t	 0.9593	 0.3610