



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 02:40 PM EST

PDB ID : 3JCS
EMDB ID : EMD-6583
Title : 2.8 Angstrom cryo-EM structure of the large ribosomal subunit from the eukaryotic parasite Leishmania
Authors : Shalev-Benami, M.; Zhang, Y.; Matzov, D.; Halfon, Y.; Zackay, A.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Jaffe, C.L.; Yonath, A.; Skiniotis, G.
Deposited on : 2016-01-21
Resolution : 2.80 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:

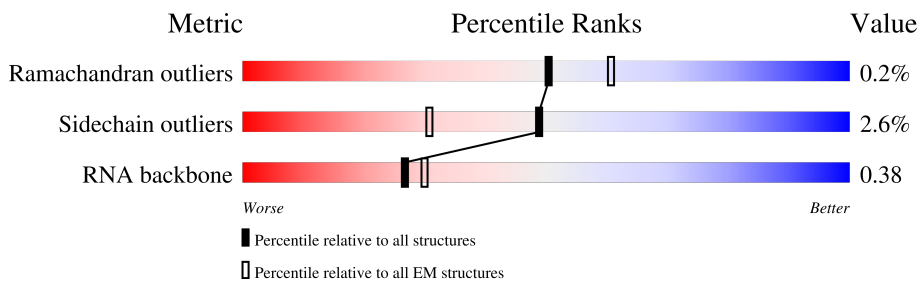
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al.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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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	1	1782	8% (red) 52% (green) 33% (yellow) 13% (grey)
2	2	1527	11% (red) 43% (green) 29% (yellow) 27% (grey)
3	3	213	17% (red) 45% (green) 41% (yellow) 14% (grey)
4	4	183	9% (red) 55% (green) 26% (yellow) 19% (grey)
5	5	133	36% (green) 23% (yellow) 40% (grey)
6	6	76	17% (red) 16% (red) 59% (green) 5% (orange) 20% (grey)
7	7	171	60% (green) 29% (yellow) 10% (grey)
8	8	121	53% (green) 45% (yellow) 2% (grey)

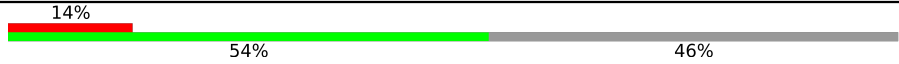
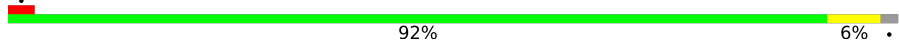




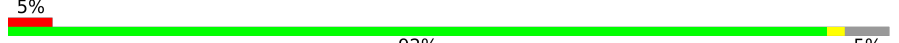

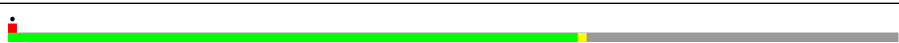

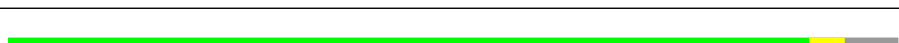


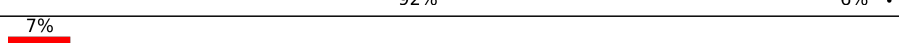
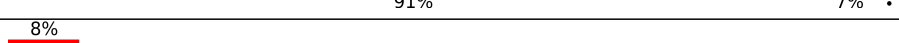
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Mol	Chain	Length	Quality of chain
9	A	260	91% 6%
10	B	419	92% 5%
11	C	373	80% 19%
12	D	188	40% 86% 14%
13	E	190	96% 98%
14	F	195	70% 30%
15	G	348	62% 35%
16	H	222	89% 9%
17	I	220	58% 40%
18	J	139	90% 8%
19	K	233	12% 61% 5% 33%
20	L	145	5% 98%
21	M	204	98%
22	N	213	99% 99%
23	O	305	7% 76% 23%
24	P	198	96%
25	Q	245	6% 63% 36%
26	R	179	71% 27%
27	S	159	13% 92% 6%
28	T	166	92% 7%
29	U	129	40% 78% 22%
30	V	145	80% 19%
31	W	143	82% 18%
32	X	124	50% 48%
33	Y	134	7% 98%

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Mol	Chain	Length	Quality of chain
34	Z	147	 14% 54% 46%
35	a	127	 92% 6%
36	b	70	 87% 6% 7%
37	c	252	 87% 12%
38	d	104	 11% 69% 28%
39	e	183	 5% 61% 39%
40	f	133	 5% 92% 5%
41	g	144	 85% 13%
42	h	168	 64% 35%
43	i	105	 57% 40%
44	j	83	 90% 6%
45	k	83	 24% 69% 30%
46	l	51	 92% 6%
47	m	92	 7% 91% 7%
48	n	106	 8% 80% 19%

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 117257 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 26S alpha ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	1554	33313	14886	6081	10792	1554	0	0

- Molecule 2 is a RNA chain called 26S delta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1119	23926	10702	4308	7797	1119	0	0

- Molecule 3 is a RNA chain called 26S gamma ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	184	3893	1740	662	1307	184	0	0

- Molecule 4 is a RNA chain called 26S delta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	149	3177	1418	570	1040	149	0	0

- Molecule 5 is a RNA chain called 26S epsilon ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	5	80	1708	763	310	555	80	0	0

- Molecule 6 is a RNA chain called 26S zeta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	6	61	1288	577	225	425	61	0	0

- Molecule 7 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	7	154	3280	1469	584	1074	153	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	8	119	2531	1132	450	830	119	0	0

- Molecule 9 is a protein called ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	245	1859	1158	384	307	10	2	0

- Molecule 10 is a protein called ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B	396	3020	1908	592	508	12	2	0

- Molecule 11 is a protein called ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	301	2237	1413	428	384	12	1	0

- Molecule 12 is a protein called ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	D	161	799	476	161	162	0	0

- Molecule 13 is a protein called ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	190	1509	953	276	272	8	0	0

- Molecule 14 is a protein called ribosomal protein L6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	137	1002	641	192	167	2	1	0

- Molecule 15 is a protein called ribosomal protein L8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	226	1772	1113	353	299	7	1	0

- Molecule 16 is a protein called ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H	202	1596	1019	307	263	7	0	0

- Molecule 17 is a protein called ribosomal protein L13e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	132	1061	666	221	169	5	0	0

- Molecule 18 is a protein called ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	J	128	924	588	171	160	5	0	0

- Molecule 19 is a protein called ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	K	156	1061	661	212	184	4	0	0

- Molecule 20 is a protein called ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	144	1096	691	223	177	5	0	0

- Molecule 21 is a protein called ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M	203	1714	1080	362	264	8	0	0

- Molecule 22 is a protein called ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	N	213	1714	1077	340	281	16	0	0

- Molecule 23 is a protein called ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	O	235	1557	986	300	268	3	0	0

- Molecule 24 is a protein called ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	P	195	1494	942	299	247	6	1	0

- Molecule 25 is a protein called ribosomal protein L19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q	156	1162	730	243	186	3	0	0

- Molecule 26 is a protein called ribosomal protein L20e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	131	1019	651	197	167	4	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	158	ILE	LEU	VARIANT	UNP E9BRT7

- Molecule 27 is a protein called ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	S	149	1112	704	218	187	3	2	0

- Molecule 28 is a protein called ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	154	1221	763	241	206	11	2	0

- Molecule 29 is a protein called ribosomal protein L22e.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	U	100	541	331	101	109	0	0

- Molecule 30 is a protein called ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	V	118	892	566	171	153	2	0	0

- Molecule 31 is a protein called ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	W	117	896	562	187	144	3	1	0

- Molecule 32 is a protein called ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	X	64	508	333	96	76	3	0	0

- Molecule 33 is a protein called ribosomal protein L27e.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	Y	132	914	589	174	151	0	0

- Molecule 34 is a protein called ribosomal protein L28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Z	79	538	329	111	95	3	0	0

- Molecule 35 is a protein called ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	a	124	982	613	203	163	3	0	0

- Molecule 36 is a protein called ribosomal protein L29e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	b	65	503	309	113	80	1	0	0

- Molecule 37 is a protein called ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	c	222	1732	1105	327	289	11	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	49	ALA	GLY	VARIANT	UNP E9BI29

- Molecule 38 is a protein called ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	d	75	518	325	93	97	3	0	0

- Molecule 39 is a protein called ribosomal protein L31e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	e	112	824	531	155	136	2	1	0

- Molecule 40 is a protein called ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	f	126	982	616	195	167	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	105	LYS	THR	VARIANT	UNP E9BFJ5

- Molecule 41 is a protein called ribosomal protein L33e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	g	125	983	612	205	161	5	0	0

- Molecule 42 is a protein called ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	h	109	856	529	182	140	5	0	0

- Molecule 43 is a protein called ribosomal protein L36e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	i	63	494	316	100	76	2	1	0

- Molecule 44 is a protein called ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	j	78	639	385	149	99	6	0	0

- Molecule 45 is a protein called ribosomal protein L38e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	k	58	373	234	71	66	2	0	0

- Molecule 46 is a protein called ribosomal protein L39e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	l	50	457	294	98	64	1	1	0

- Molecule 47 is a protein called ribosomal protein L43e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	m	90	668	414	135	113	6	0	0

- Molecule 48 is a protein called ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	n	86	659	418	129	110	2	0	0

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	1	51	Total	Mg	0
			51	51	
49	2	25	Total	Mg	0
			25	25	
49	3	3	Total	Mg	0
			3	3	
49	4	2	Total	Mg	0
			2	2	
49	5	4	Total	Mg	0
			4	4	
49	7	9	Total	Mg	0
			9	9	
49	C	1	Total	Mg	0
			1	1	
49	K	1	Total	Mg	0
			1	1	
49	M	3	Total	Mg	0
			3	3	
49	V	1	Total	Mg	0
			1	1	
49	a	1	Total	Mg	0
			1	1	
49	f	2	Total	Mg	0
			2	2	

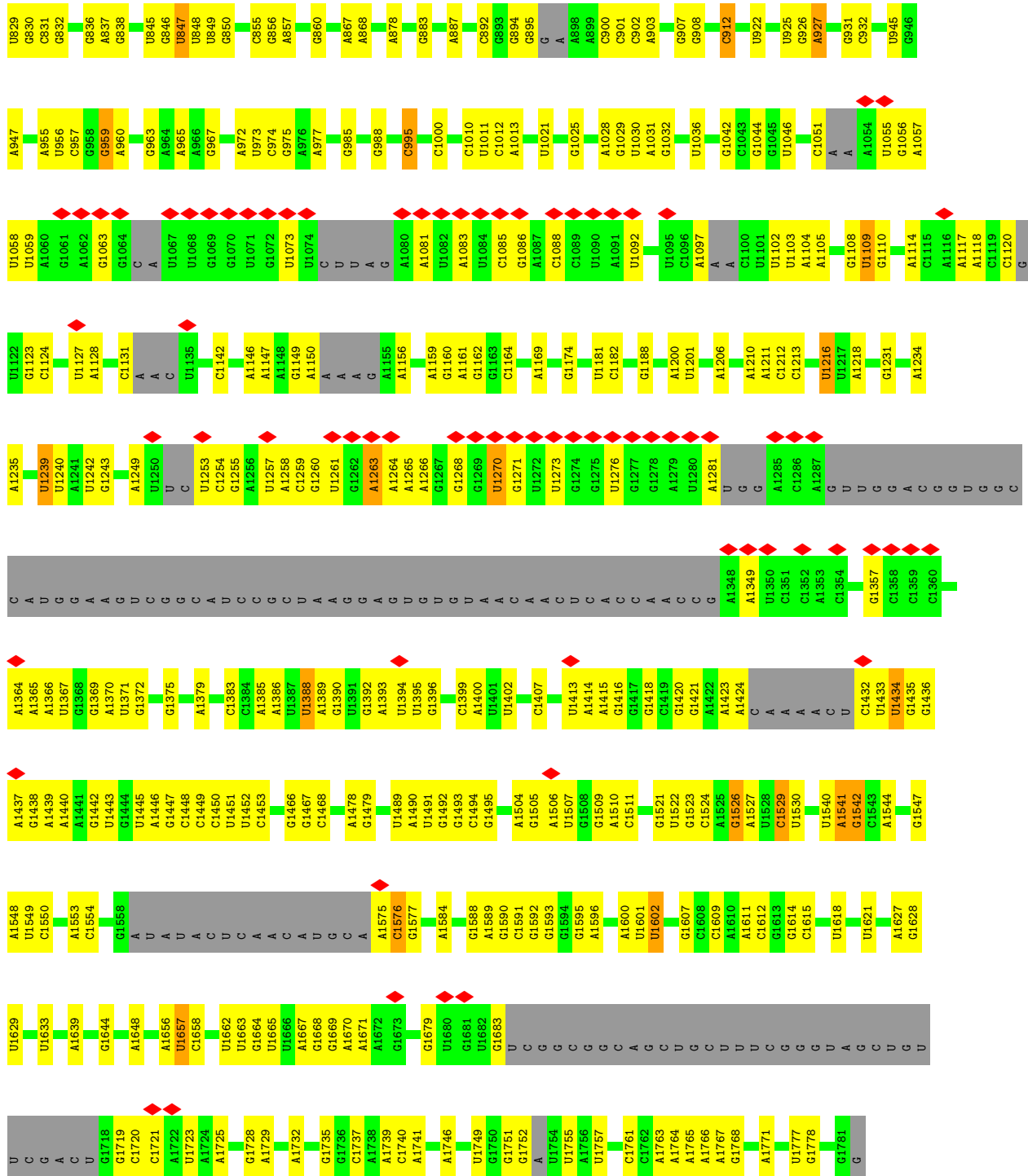
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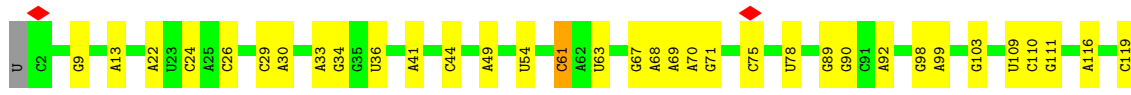
Mol	Chain	Residues	Atoms		AltConf
49	g	1	Total 1	Mg 1	0
49	h	1	Total 1	Mg 1	0
49	j	4	Total 4	Mg 4	0

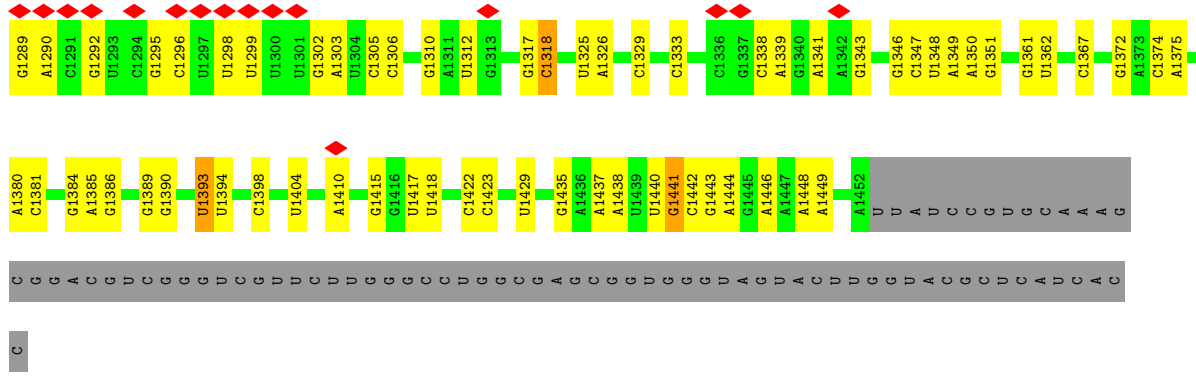
- Molecule 50 is water.

Mol	Chain	Residues	Atoms		AltConf
50	1	72	Total 72	O 72	0
50	2	40	Total 40	O 40	0
50	4	4	Total 4	O 4	0
50	5	4	Total 4	O 4	0
50	7	16	Total 16	O 16	0
50	8	1	Total 1	O 1	0
50	A	2	Total 2	O 2	0
50	G	1	Total 1	O 1	0
50	M	2	Total 2	O 2	0
50	i	1	Total 1	O 1	0
50	j	1	Total 1	O 1	0

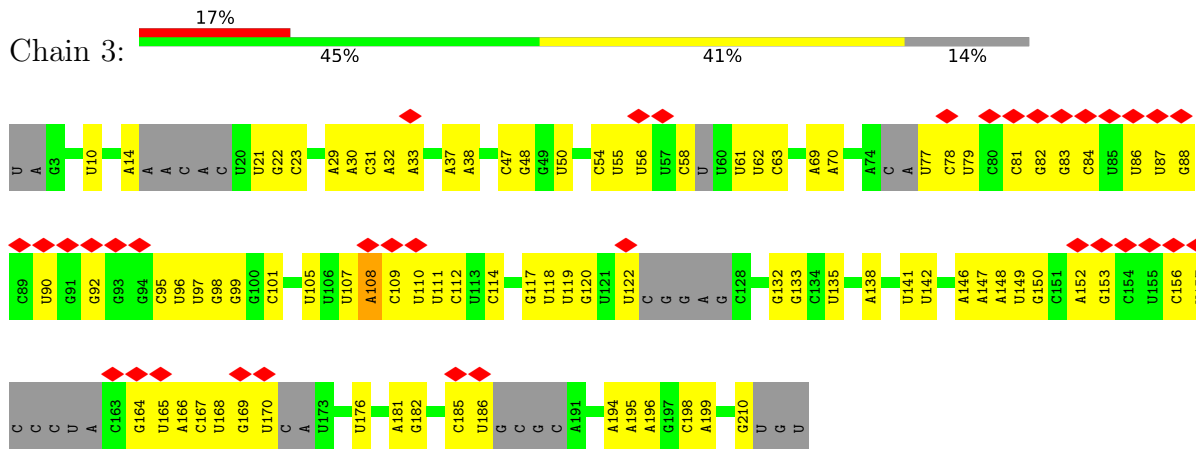


• Molecule 2: 26S delta ribosomal RNA

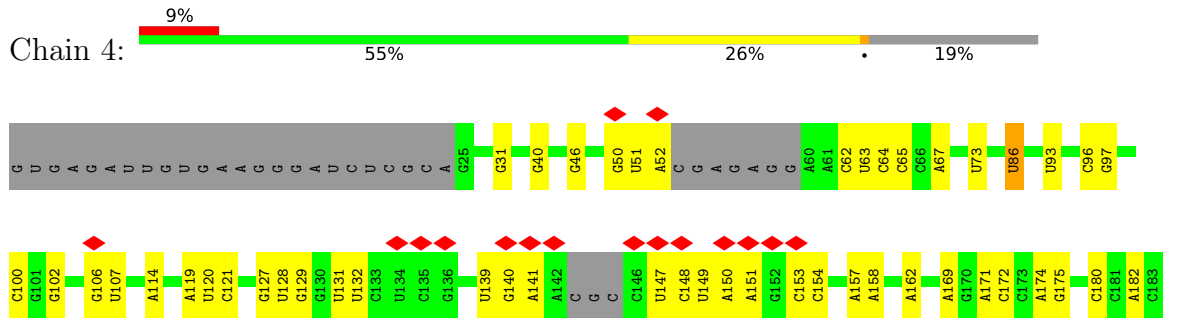




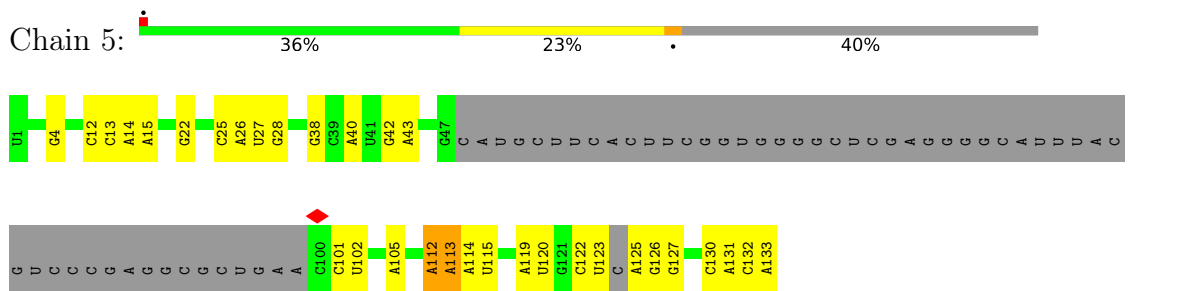
• Molecule 3: 26S gamma ribosomal RNA



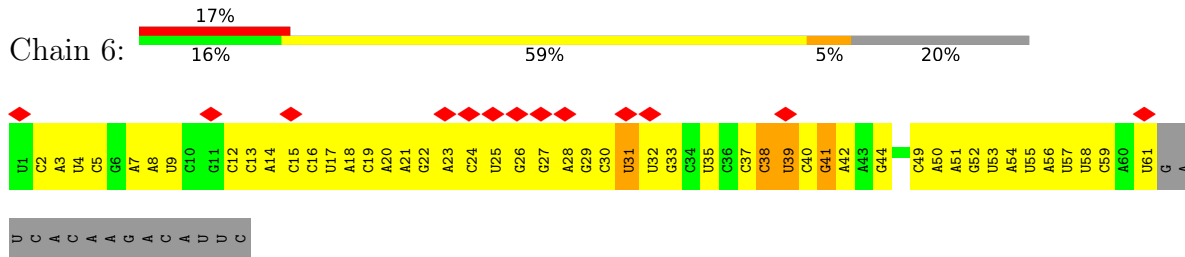
• Molecule 4: 26S delta ribosomal RNA



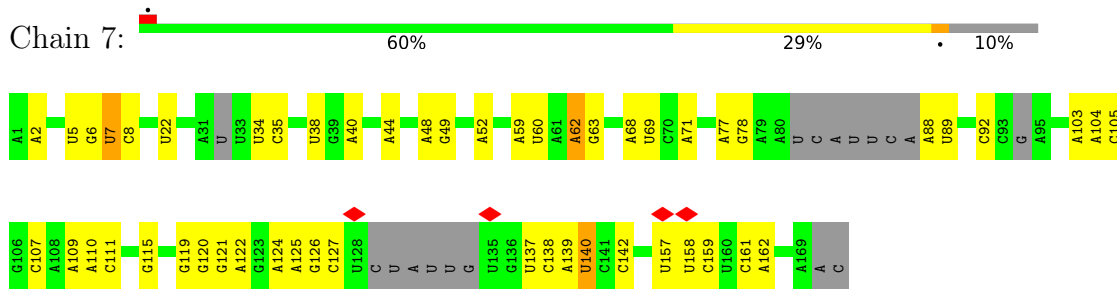
• Molecule 5: 26S epsilon ribosomal RNA



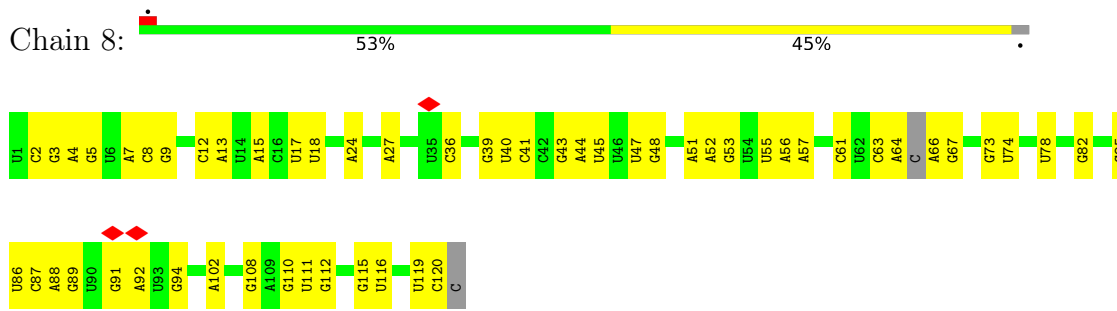
• Molecule 6: 26S zeta ribosomal RNA



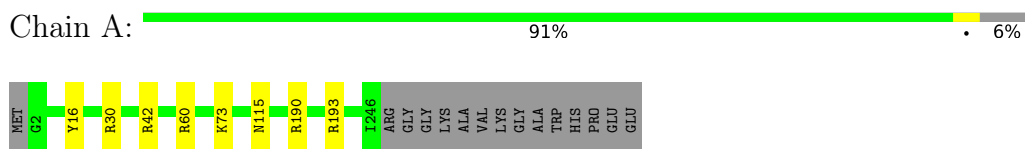
• Molecule 7: 5.8S ribosomal RNA



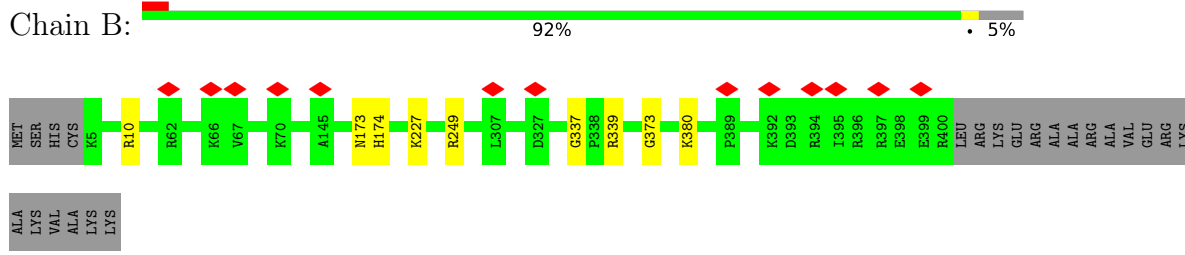
• Molecule 8: 5S ribosomal RNA



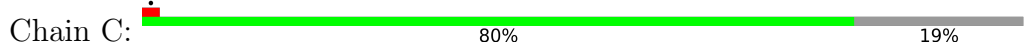
• Molecule 9: ribosomal protein L2

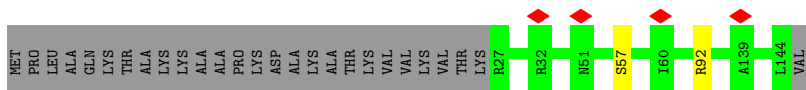


• Molecule 10: ribosomal protein L3

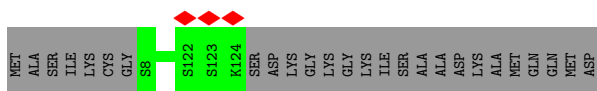
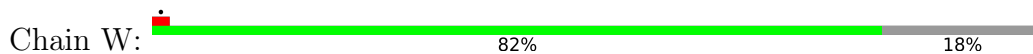


• Molecule 11: ribosomal protein L4

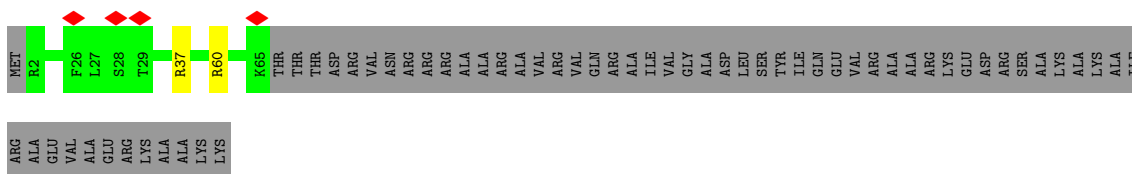




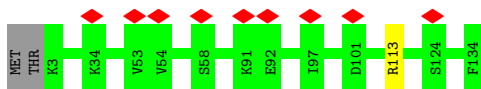
• Molecule 31: ribosomal protein L24



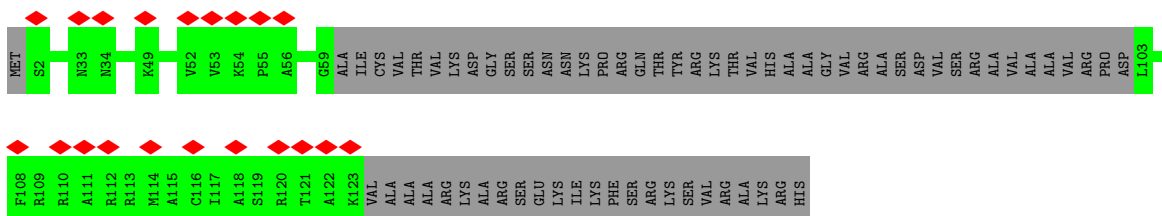
• Molecule 32: ribosomal protein L24e



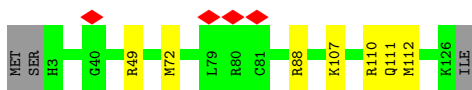
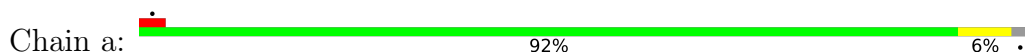
• Molecule 33: ribosomal protein L27e



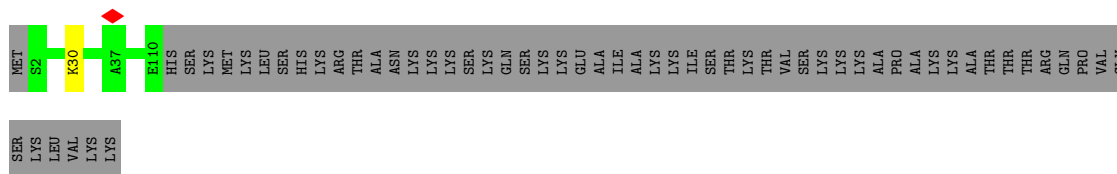
• Molecule 34: ribosomal protein L28e



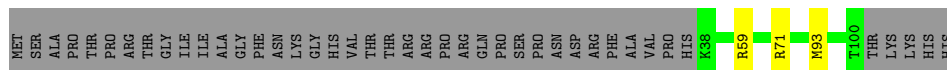
• Molecule 35: ribosomal protein L29



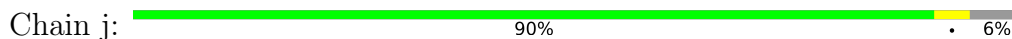
• Molecule 36: ribosomal protein L29e



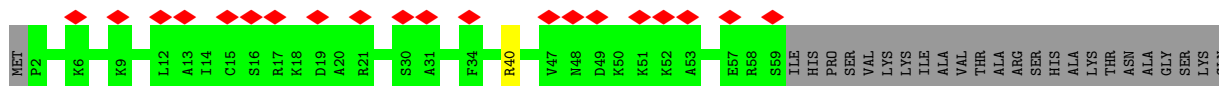
• Molecule 43: ribosomal protein L36e



• Molecule 44: ribosomal protein L37e



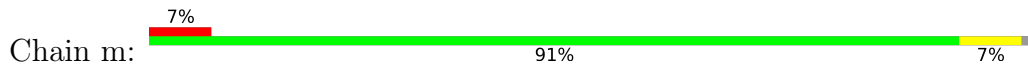
• Molecule 45: ribosomal protein L38e



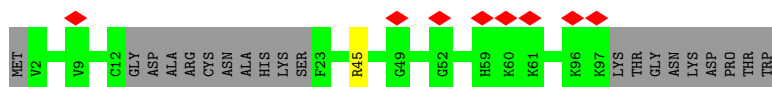
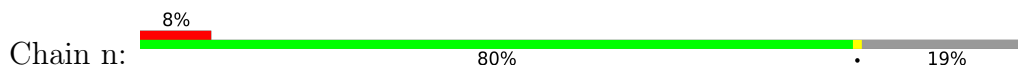
• Molecule 46: ribosomal protein L39e



• Molecule 47: ribosomal protein L43e



• Molecule 48: ribosomal protein L44e



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107134	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	25000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.231	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	384.0, 384.0, 384.0	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0, 1.0, 1.0	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: OMC, H2U, OMU, OMG, MG, A2M

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	1	0.75	8/36881 (0.0%)	0.90	48/57466 (0.1%)
2	2	0.60	0/26109	0.86	28/40668 (0.1%)
3	3	0.48	0/4337	0.84	1/6734 (0.0%)
4	4	0.69	0/3549	0.88	3/5525 (0.1%)
5	5	0.69	0/1908	0.91	3/2967 (0.1%)
6	6	0.39	2/1437 (0.1%)	0.79	4/2234 (0.2%)
7	7	0.76	0/3615	0.87	2/5622 (0.0%)
8	8	0.47	0/2828	0.82	0/4401
9	A	0.47	0/1903	0.56	0/2559
10	B	0.44	0/3086	0.55	0/4176
11	C	0.45	0/2284	0.60	0/3092
12	D	0.25	0/800	0.49	0/1111
13	E	0.29	0/1529	0.56	0/2056
14	F	0.40	0/1023	0.56	0/1390
15	G	0.38	0/1798	0.59	1/2423 (0.0%)
16	H	0.42	0/1628	0.60	0/2194
17	I	0.40	0/1084	0.57	0/1454
18	J	0.39	0/941	0.61	2/1277 (0.2%)
19	K	0.27	0/1077	0.59	1/1475 (0.1%)
20	L	0.43	0/1123	0.56	0/1505
21	M	0.49	0/1754	0.57	0/2342
22	N	0.27	0/1747	0.54	0/2338
23	O	0.32	0/1583	0.50	0/2157
24	P	0.42	0/1519	0.57	0/2040
25	Q	0.35	0/1179	0.53	0/1588
26	R	0.42	0/1044	0.59	1/1415 (0.1%)
27	S	0.43	0/1142	0.60	0/1547
28	T	0.45	0/1249	0.65	1/1679 (0.1%)
29	U	0.26	0/545	0.49	0/754
30	V	0.42	0/907	0.51	0/1227
31	W	0.37	0/910	0.56	0/1224
32	X	0.40	0/527	0.53	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Y	0.37	0/934	0.51	0/1274
34	Z	0.28	0/545	0.52	0/739
35	a	0.32	0/992	0.53	0/1326
36	b	0.34	0/514	0.50	0/690
37	c	0.42	0/1763	0.52	0/2374
38	d	0.31	0/525	0.50	0/719
39	e	0.37	0/838	0.57	0/1131
40	f	0.46	0/1002	0.55	0/1346
41	g	0.49	0/1003	0.53	0/1352
42	h	0.38	0/868	0.55	0/1160
43	i	0.38	0/499	0.56	0/662
44	j	0.50	0/651	0.61	0/869
45	k	0.30	0/378	0.57	0/518
46	l	0.43	0/470	0.51	0/627
47	m	0.43	0/680	0.53	0/913
48	n	0.34	0/667	0.56	0/889
All	All	0.59	10/125375 (0.0%)	0.79	95/185945 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	A	0	1
10	B	0	2
13	E	0	1
15	G	0	1
16	H	0	1
19	K	0	3
26	R	0	1
27	S	0	1
28	T	0	1
40	f	0	1
All	All	0	13

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	634	G	C1'-N9	-6.69	1.37	1.46
1	1	159	U	C1'-N1	6.17	1.58	1.48
1	1	568	U	C1'-N1	6.06	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	564	U	C1'-N1	5.95	1.57	1.48
1	1	565	U	C1'-N1	5.91	1.57	1.48

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	45	SER	C-N-CD	-11.87	94.48	120.60
1	1	1575	A	OP1-P-O3'	-11.81	79.22	105.20
1	1	1757	U	C2-N1-C1'	8.96	128.45	117.70
2	2	776	C	N1-C2-O2	8.91	124.25	118.90
2	2	776	C	C2-N1-C1'	8.72	128.39	118.80

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	A	60[B]	ARG	Mainchain
10	B	337	GLY	Peptide
10	B	373	GLY	Peptide
13	E	136	PRO	Peptide
15	G	114	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	
9	A	245/260 (94%)	220 (90%)	25 (10%)	0	100	100
10	B	396/419 (94%)	352 (89%)	43 (11%)	1 (0%)	41	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	C	300/373 (80%)	269 (90%)	31 (10%)	0	100	100
12	D	159/188 (85%)	136 (86%)	23 (14%)	0	100	100
13	E	188/190 (99%)	160 (85%)	28 (15%)	0	100	100
14	F	134/195 (69%)	112 (84%)	22 (16%)	0	100	100
15	G	225/348 (65%)	205 (91%)	18 (8%)	2 (1%)	17	46
16	H	200/222 (90%)	175 (88%)	24 (12%)	1 (0%)	29	61
17	I	130/220 (59%)	120 (92%)	10 (8%)	0	100	100
18	J	126/139 (91%)	115 (91%)	11 (9%)	0	100	100
19	K	154/233 (66%)	136 (88%)	17 (11%)	1 (1%)	25	56
20	L	142/145 (98%)	127 (89%)	15 (11%)	0	100	100
21	M	201/204 (98%)	187 (93%)	14 (7%)	0	100	100
22	N	211/213 (99%)	186 (88%)	25 (12%)	0	100	100
23	O	229/305 (75%)	205 (90%)	24 (10%)	0	100	100
24	P	194/198 (98%)	179 (92%)	15 (8%)	0	100	100
25	Q	154/245 (63%)	141 (92%)	13 (8%)	0	100	100
26	R	130/179 (73%)	104 (80%)	25 (19%)	1 (1%)	19	49
27	S	149/159 (94%)	125 (84%)	22 (15%)	2 (1%)	12	36
28	T	154/166 (93%)	127 (82%)	27 (18%)	0	100	100
29	U	98/129 (76%)	81 (83%)	17 (17%)	0	100	100
30	V	116/145 (80%)	99 (85%)	17 (15%)	0	100	100
31	W	116/143 (81%)	106 (91%)	10 (9%)	0	100	100
32	X	62/124 (50%)	59 (95%)	3 (5%)	0	100	100
33	Y	130/134 (97%)	111 (85%)	19 (15%)	0	100	100
34	Z	75/147 (51%)	65 (87%)	10 (13%)	0	100	100
35	a	122/127 (96%)	105 (86%)	17 (14%)	0	100	100
36	b	63/70 (90%)	53 (84%)	10 (16%)	0	100	100
37	c	220/252 (87%)	190 (86%)	30 (14%)	0	100	100
38	d	71/104 (68%)	63 (89%)	8 (11%)	0	100	100
39	e	111/183 (61%)	92 (83%)	19 (17%)	0	100	100
40	f	124/133 (93%)	110 (89%)	14 (11%)	0	100	100
41	g	123/144 (85%)	112 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	h	106/168 (63%)	91 (86%)	15 (14%)	0	100	100
43	i	62/105 (59%)	57 (92%)	5 (8%)	0	100	100
44	j	76/83 (92%)	68 (90%)	8 (10%)	0	100	100
45	k	56/83 (68%)	52 (93%)	4 (7%)	0	100	100
46	l	49/51 (96%)	46 (94%)	2 (4%)	1 (2%)	7	24
47	m	88/92 (96%)	71 (81%)	16 (18%)	1 (1%)	14	41
48	n	82/106 (77%)	66 (80%)	16 (20%)	0	100	100
All	All	5771/7124 (81%)	5078 (88%)	683 (12%)	10 (0%)	50	78

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	G	132	SER
26	R	22	PRO
27	S	101	CYS
47	m	40	SER
10	B	380	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	A	188/204 (92%)	181 (96%)	7 (4%)	34	68
10	B	296/352 (84%)	288 (97%)	8 (3%)	44	78
11	C	222/302 (74%)	221 (100%)	1 (0%)	88	96
12	D	4/163 (2%)	4 (100%)	0	100	100
13	E	172/172 (100%)	169 (98%)	3 (2%)	60	87
14	F	92/154 (60%)	91 (99%)	1 (1%)	73	92
15	G	179/292 (61%)	173 (97%)	6 (3%)	37	71
16	H	166/188 (88%)	164 (99%)	2 (1%)	71	92
17	I	114/181 (63%)	110 (96%)	4 (4%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	J	91/111 (82%)	88 (97%)	3 (3%)	38	72
19	K	79/195 (40%)	68 (86%)	11 (14%)	3	11
20	L	105/115 (91%)	103 (98%)	2 (2%)	57	85
21	M	179/180 (99%)	176 (98%)	3 (2%)	60	87
22	N	178/179 (99%)	175 (98%)	3 (2%)	60	87
23	O	103/242 (43%)	100 (97%)	3 (3%)	42	76
24	P	149/164 (91%)	145 (97%)	4 (3%)	44	78
25	Q	100/196 (51%)	98 (98%)	2 (2%)	55	84
26	R	98/158 (62%)	96 (98%)	2 (2%)	55	84
27	S	100/133 (75%)	100 (100%)	0	100	100
28	T	125/144 (87%)	125 (100%)	0	100	100
29	U	13/114 (11%)	13 (100%)	0	100	100
30	V	86/124 (69%)	84 (98%)	2 (2%)	50	82
31	W	87/122 (71%)	87 (100%)	0	100	100
32	X	48/104 (46%)	46 (96%)	2 (4%)	30	63
33	Y	70/115 (61%)	69 (99%)	1 (1%)	67	90
34	Z	44/119 (37%)	44 (100%)	0	100	100
35	a	99/117 (85%)	92 (93%)	7 (7%)	14	39
36	b	48/58 (83%)	44 (92%)	4 (8%)	11	32
37	c	168/209 (80%)	164 (98%)	4 (2%)	49	81
38	d	47/90 (52%)	44 (94%)	3 (6%)	17	45
39	e	79/156 (51%)	79 (100%)	0	100	100
40	f	97/114 (85%)	95 (98%)	2 (2%)	53	84
41	g	98/121 (81%)	96 (98%)	2 (2%)	55	84
42	h	85/145 (59%)	84 (99%)	1 (1%)	71	92
43	i	47/89 (53%)	44 (94%)	3 (6%)	17	45
44	j	63/70 (90%)	60 (95%)	3 (5%)	25	58
45	k	26/74 (35%)	25 (96%)	1 (4%)	33	67
46	l	46/47 (98%)	44 (96%)	2 (4%)	29	62
47	m	63/74 (85%)	58 (92%)	5 (8%)	12	34
48	n	64/92 (70%)	63 (98%)	1 (2%)	62	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4118/5979 (69%)	4010 (97%)	108 (3%)	49 79

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	P	56	ARG
35	a	72	MET
45	k	40	ARG
24	P	147	ARG
30	V	57	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
23	O	31	HIS
44	j	16	HIS
27	S	58	HIS
44	j	12	HIS
37	c	196	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1535/1782 (86%)	588 (38%)	57 (3%)
2	2	1106/1527 (72%)	445 (40%)	28 (2%)
3	3	177/213 (83%)	83 (46%)	10 (5%)
4	4	146/183 (79%)	48 (32%)	5 (3%)
5	5	78/133 (58%)	30 (38%)	4 (5%)
6	6	60/76 (78%)	48 (80%)	15 (25%)
7	7	150/171 (87%)	50 (33%)	2 (1%)
8	8	118/121 (97%)	54 (45%)	5 (4%)
All	All	3370/4206 (80%)	1346 (39%)	126 (3%)

5 of 1346 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	G
1	1	10	A
1	1	13	G
1	1	23	U

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Mol	Chain	Res	Type
1	1	24	A

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	29	C
6	6	29	G
2	2	815	G
6	6	24	C
6	6	58	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	2	1079	2	18,26,27	0.99	1 (5%)	19,38,41	1.13	2 (10%)
2	H2U	2	1404	2	18,21,22	1.10	2 (11%)	21,30,33	1.65	2 (9%)
2	OMC	2	583	2	19,22,23	0.87	0	26,31,34	1.02	1 (3%)
2	A2M	2	591	2	18,25,26	0.98	1 (5%)	18,36,39	1.33	2 (11%)
1	A2M	1	1541	2,1	18,25,26	0.96	1 (5%)	18,36,39	1.21	2 (11%)
2	OMG	2	1254	2	18,26,27	1.04	1 (5%)	19,38,41	1.05	2 (10%)
1	OMC	1	1529	1	19,22,23	0.88	0	26,31,34	0.99	1 (3%)
1	OMG	1	1628	1	18,26,27	1.01	1 (5%)	19,38,41	1.18	2 (10%)
7	OMU	7	7	7,1	19,22,23	1.25	2 (10%)	26,31,34	2.12	6 (23%)
7	A2M	7	162	7,1	18,25,26	1.02	1 (5%)	18,36,39	1.22	2 (11%)
2	OMG	2	71	2	18,26,27	1.03	1 (5%)	19,38,41	1.05	2 (10%)
2	A2M	2	572	2	18,25,26	0.98	1 (5%)	18,36,39	1.19	2 (11%)
1	OMG	1	959	1	18,26,27	1.07	1 (5%)	19,38,41	1.25	2 (10%)
2	OMU	2	667	2	19,22,23	1.26	3 (15%)	26,31,34	1.83	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	2	382	2	18,25,26	0.93	1 (5%)	18,36,39	1.20	2 (11%)
2	OMG	2	1230	2	18,26,27	1.03	1 (5%)	19,38,41	1.05	2 (10%)
2	A2M	2	628	2	18,25,26	0.93	1 (5%)	18,36,39	1.24	2 (11%)
1	OMU	1	847	1	19,22,23	1.25	3 (15%)	26,31,34	1.81	6 (23%)
2	OMG	2	534	2	18,26,27	1.01	1 (5%)	19,38,41	1.04	2 (10%)
2	OMC	2	554	2	19,22,23	0.85	0	26,31,34	1.01	1 (3%)
2	OMG	2	641	2	18,26,27	1.04	1 (5%)	19,38,41	1.03	2 (10%)
2	OMG	2	655	2	18,26,27	1.02	1 (5%)	19,38,41	1.13	2 (10%)
2	OMU	2	656	2	19,22,23	1.23	3 (15%)	26,31,34	1.97	6 (23%)
2	OMU	2	1153	2	19,22,23	1.30	3 (15%)	26,31,34	1.99	6 (23%)
2	OMC	2	1318	2	19,22,23	0.86	0	26,31,34	0.99	2 (7%)
2	OMG	2	571	2	18,26,27	0.98	1 (5%)	19,38,41	1.10	2 (10%)
1	A2M	1	955	1	18,25,26	0.96	1 (5%)	18,36,39	1.33	2 (11%)
1	A2M	1	681	1	18,25,26	0.93	1 (5%)	18,36,39	1.24	2 (11%)
1	A2M	1	927	1	18,25,26	1.02	1 (5%)	18,36,39	1.29	2 (11%)
2	OMC	2	443	2	19,22,23	0.85	0	26,31,34	0.87	0
1	OMU	1	48	1	19,22,23	1.36	3 (15%)	26,31,34	1.84	6 (23%)
1	OMG	1	1526	1	18,26,27	1.00	1 (5%)	19,38,41	1.21	2 (10%)
1	OMU	1	36	1	19,22,23	1.31	3 (15%)	26,31,34	1.85	6 (23%)
1	OMG	1	1542	2,1	18,26,27	1.00	1 (5%)	19,38,41	1.17	2 (10%)
2	OMC	2	1398	2	19,22,23	0.86	0	26,31,34	1.06	1 (3%)
1	OMC	1	695	1	19,22,23	0.92	1 (5%)	26,31,34	1.19	2 (7%)
1	OMU	1	845	1	19,22,23	1.32	4 (21%)	26,31,34	1.97	6 (23%)
2	OMC	2	1249	2	19,22,23	0.85	0	26,31,34	1.00	1 (3%)
2	A2M	2	1186	2	18,25,26	0.95	1 (5%)	18,36,39	1.27	2 (11%)
1	A2M	1	678	2,1	18,25,26	0.97	1 (5%)	18,36,39	1.29	2 (11%)
1	OMG	1	856	1	18,26,27	1.01	1 (5%)	19,38,41	1.05	2 (10%)
2	A2M	2	527	2	18,25,26	0.95	1 (5%)	18,36,39	1.38	2 (11%)
2	OMU	2	1078	2	19,22,23	1.27	2 (10%)	26,31,34	1.81	6 (23%)
2	OMC	2	1160	2	19,22,23	0.86	0	26,31,34	0.97	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	2	1079	2	-	2/5/27/28	0/3/3/3
2	H2U	2	1404	2	-	3/7/38/39	0/2/2/2
2	OMC	2	583	2	-	2/9/27/28	0/2/2/2
2	A2M	2	591	2	-	3/5/27/28	0/3/3/3
1	A2M	1	1541	2,1	-	3/5/27/28	0/3/3/3
2	OMG	2	1254	2	-	4/5/27/28	0/3/3/3
1	OMC	1	1529	1	-	2/9/27/28	0/2/2/2
1	OMG	1	1628	1	-	0/5/27/28	0/3/3/3
7	OMU	7	7	7,1	-	4/9/27/28	0/2/2/2
7	A2M	7	162	7,1	-	1/5/27/28	0/3/3/3
2	OMG	2	71	2	-	2/5/27/28	0/3/3/3
2	A2M	2	572	2	-	2/5/27/28	0/3/3/3
1	OMG	1	959	1	-	0/5/27/28	0/3/3/3
2	OMU	2	667	2	-	3/9/27/28	0/2/2/2
2	A2M	2	382	2	-	1/5/27/28	0/3/3/3
2	OMG	2	1230	2	-	3/5/27/28	0/3/3/3
2	A2M	2	628	2	-	0/5/27/28	0/3/3/3
1	OMU	1	847	1	-	3/9/27/28	0/2/2/2
2	OMG	2	534	2	-	0/5/27/28	0/3/3/3
2	OMC	2	554	2	-	2/9/27/28	0/2/2/2
2	OMG	2	641	2	-	2/5/27/28	0/3/3/3
2	OMG	2	655	2	-	0/5/27/28	0/3/3/3
2	OMU	2	656	2	-	4/9/27/28	0/2/2/2
2	OMU	2	1153	2	-	2/9/27/28	0/2/2/2
2	OMC	2	1318	2	-	2/9/27/28	0/2/2/2
2	OMG	2	571	2	-	2/5/27/28	0/3/3/3
1	A2M	1	955	1	-	3/5/27/28	0/3/3/3
1	A2M	1	681	1	-	3/5/27/28	0/3/3/3
1	A2M	1	927	1	-	1/5/27/28	0/3/3/3
2	OMC	2	443	2	-	5/9/27/28	0/2/2/2
1	OMU	1	48	1	-	3/9/27/28	0/2/2/2
1	OMG	1	1526	1	-	1/5/27/28	0/3/3/3
1	OMU	1	36	1	-	2/9/27/28	0/2/2/2
1	OMG	1	1542	2,1	-	2/5/27/28	0/3/3/3
2	OMC	2	1398	2	-	0/9/27/28	0/2/2/2
1	OMC	1	695	1	-	0/9/27/28	0/2/2/2
1	OMU	1	845	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	2	1249	2	-	3/9/27/28	0/2/2/2
2	A2M	2	1186	2	-	3/5/27/28	0/3/3/3
1	A2M	1	678	2,1	-	4/5/27/28	0/3/3/3
1	OMG	1	856	1	-	0/5/27/28	0/3/3/3
2	A2M	2	527	2	-	1/5/27/28	0/3/3/3
2	OMU	2	1078	2	-	0/9/27/28	0/2/2/2
2	OMC	2	1160	2	-	0/9/27/28	0/2/2/2

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	36	OMU	C4-N3	-2.96	1.33	1.38
1	1	48	OMU	C4-N3	-2.95	1.33	1.38
1	1	845	OMU	C4-N3	-2.94	1.33	1.38
1	1	856	OMG	C6-N1	-2.89	1.33	1.37
2	2	1153	OMU	C4-N3	-2.83	1.33	1.38

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1404	H2U	C4-N3-C2	-6.13	120.71	125.79
7	7	7	OMU	C2'-C1'-N1	-5.47	103.60	114.22
7	7	7	OMU	C4-N3-C2	-4.79	120.26	126.58
2	2	656	OMU	C4-N3-C2	-4.76	120.31	126.58
1	1	845	OMU	C4-N3-C2	-4.75	120.31	126.58

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	48	OMU	C3'-C4'-C5'-O5'
1	1	48	OMU	O4'-C4'-C5'-O5'
1	1	681	A2M	O4'-C4'-C5'-O5'
1	1	681	A2M	C3'-C4'-C5'-O5'
1	1	1529	OMC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 109 ligands modelled in this entry, 109 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

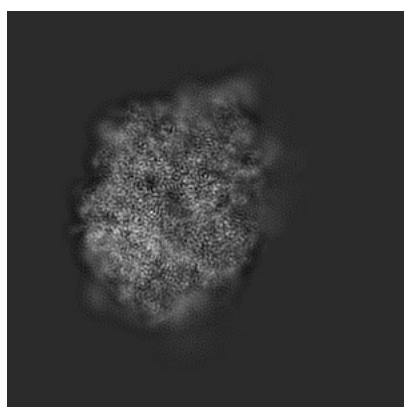
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6583. These allow visual inspection of the internal detail of the map and identification of artifacts.

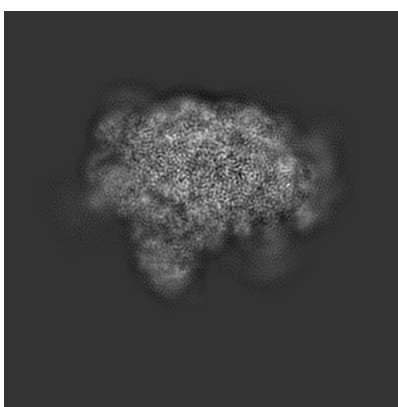
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

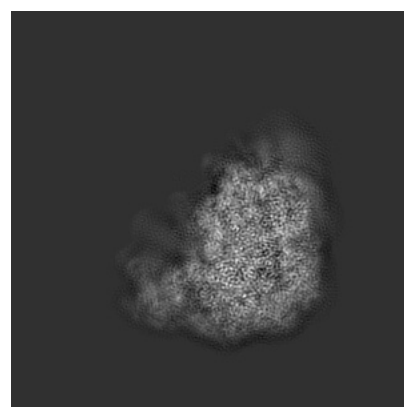
6.1.1 Primary map



X



Y

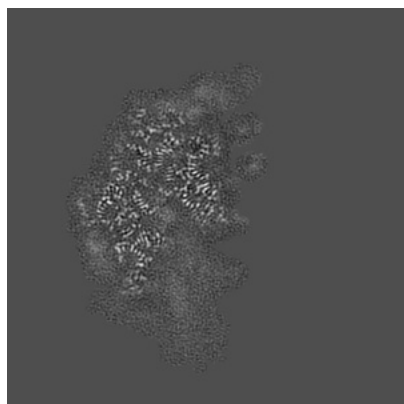


Z

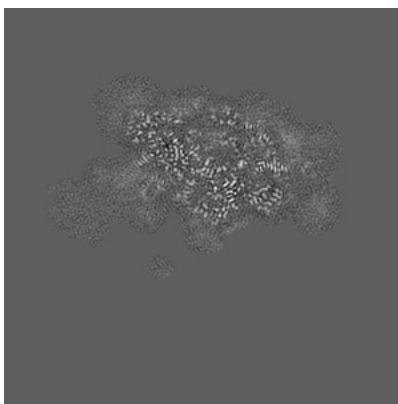
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

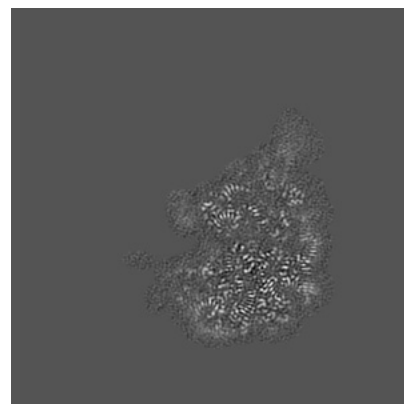
6.2.1 Primary map



X Index: 192



Y Index: 192

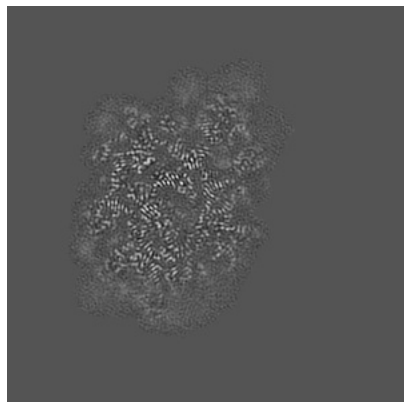


Z Index: 192

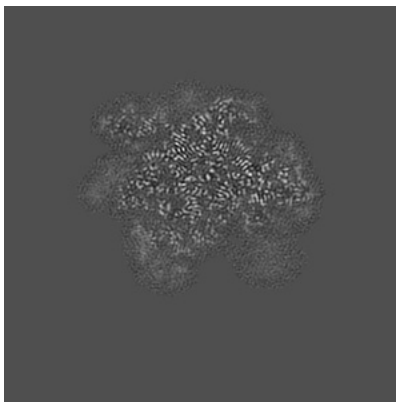
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

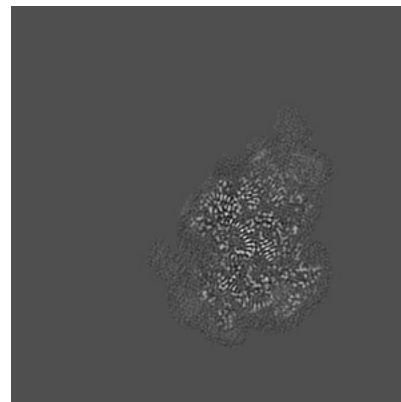
6.3.1 Primary map



X Index: 228



Y Index: 123



Z Index: 213

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

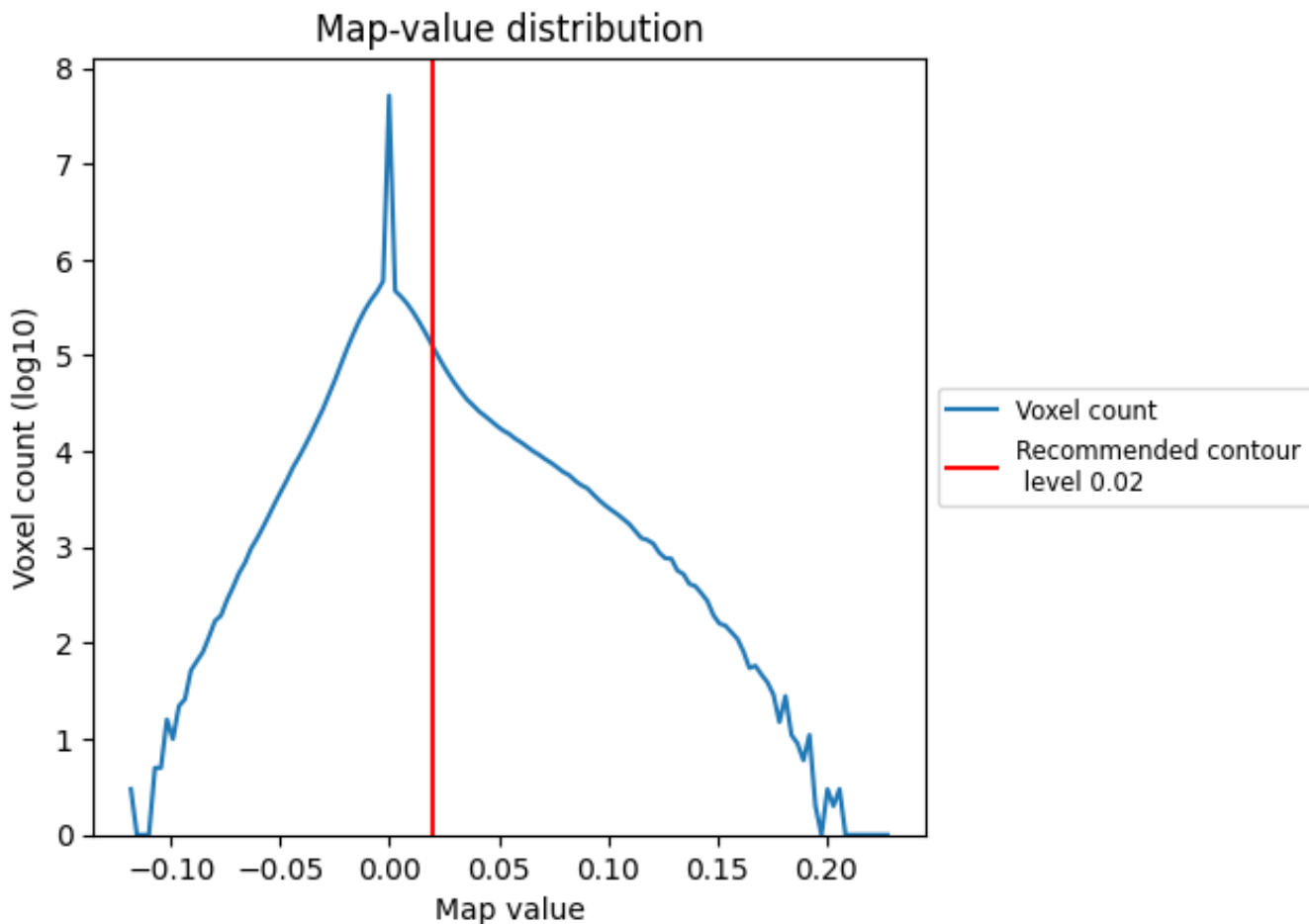
6.5 Mask visualisation

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

7 Map analysis [i](#)

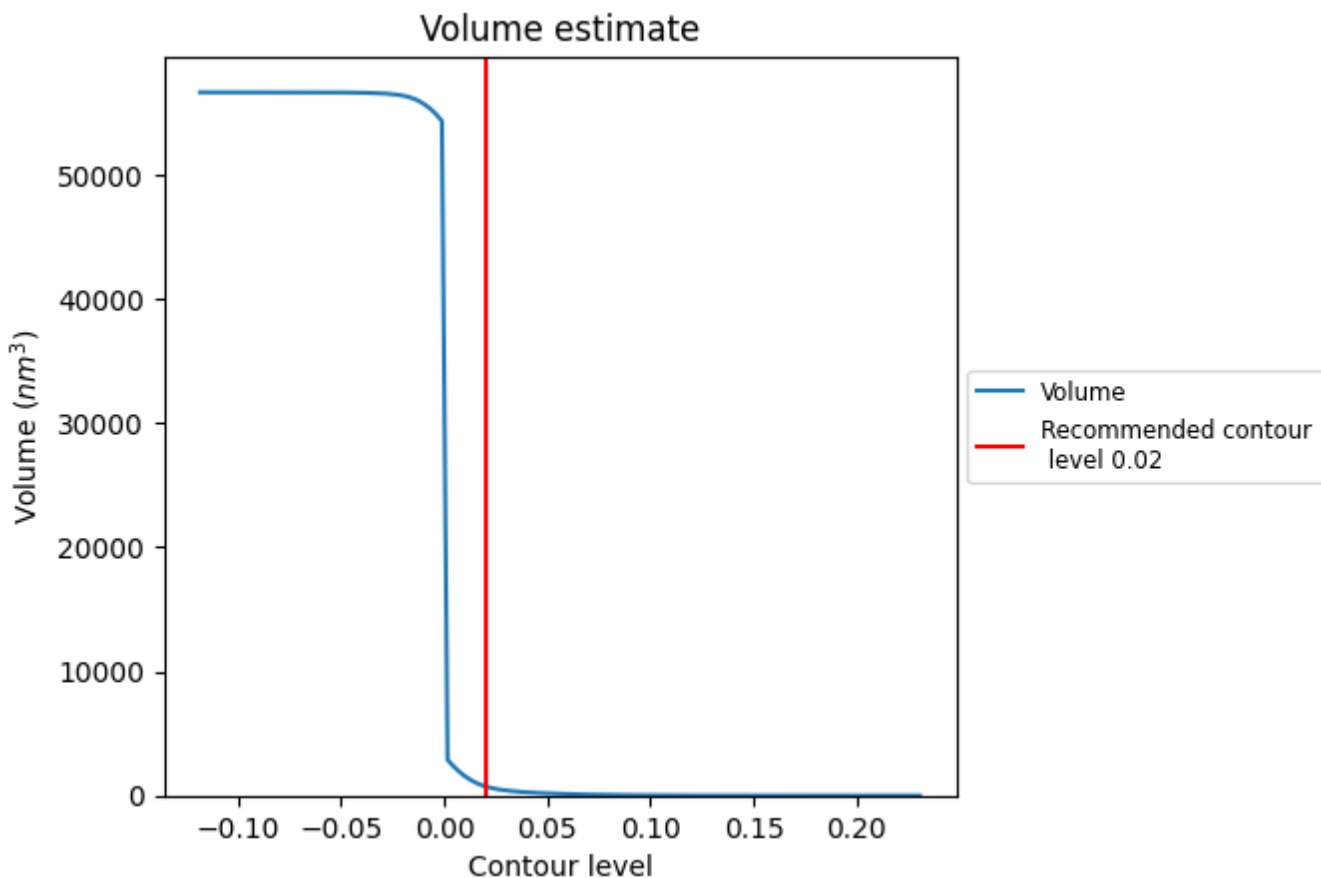
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

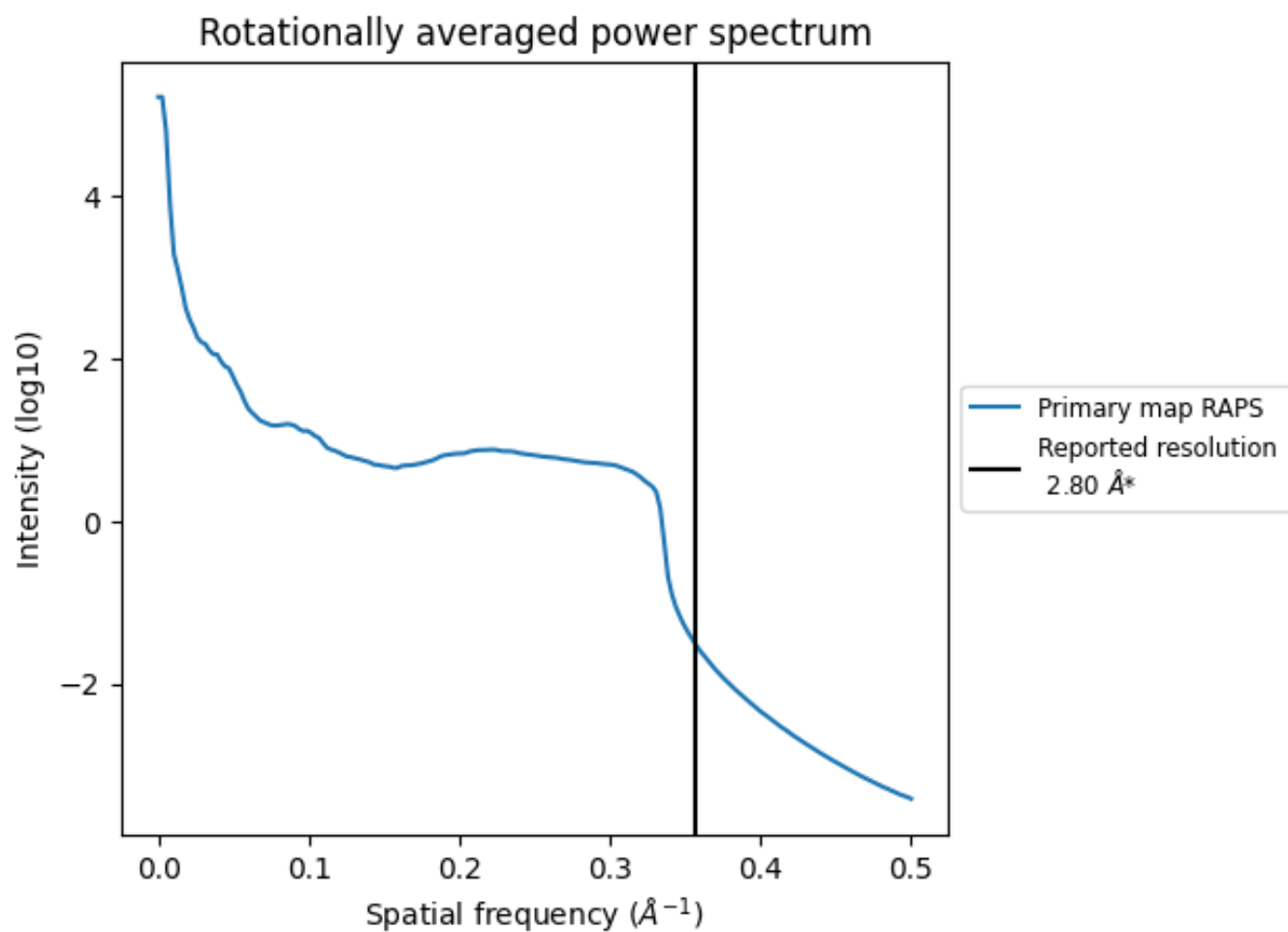
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 742 nm^3 ; this corresponds to an approximate mass of 670 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.357\AA^{-1}

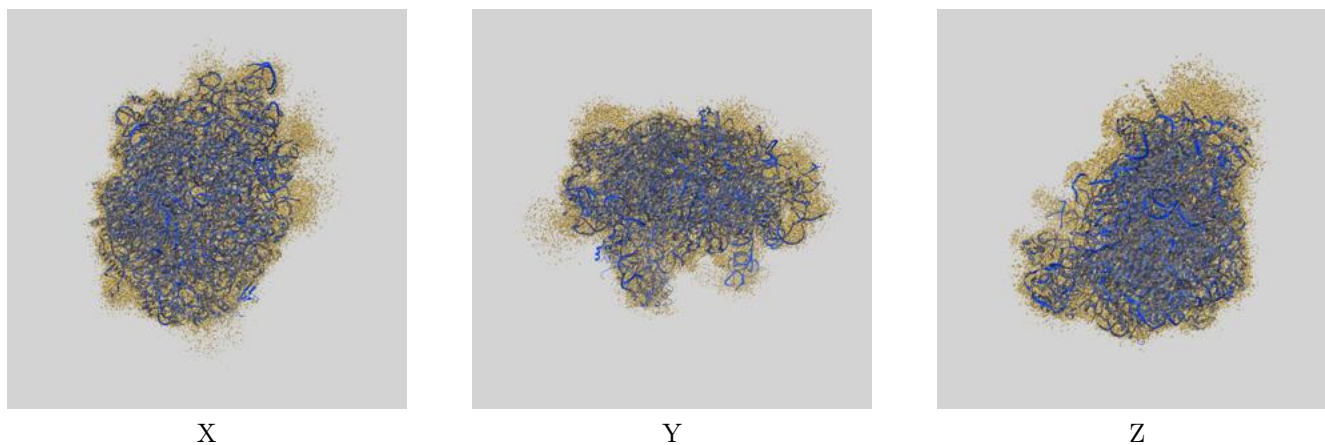
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

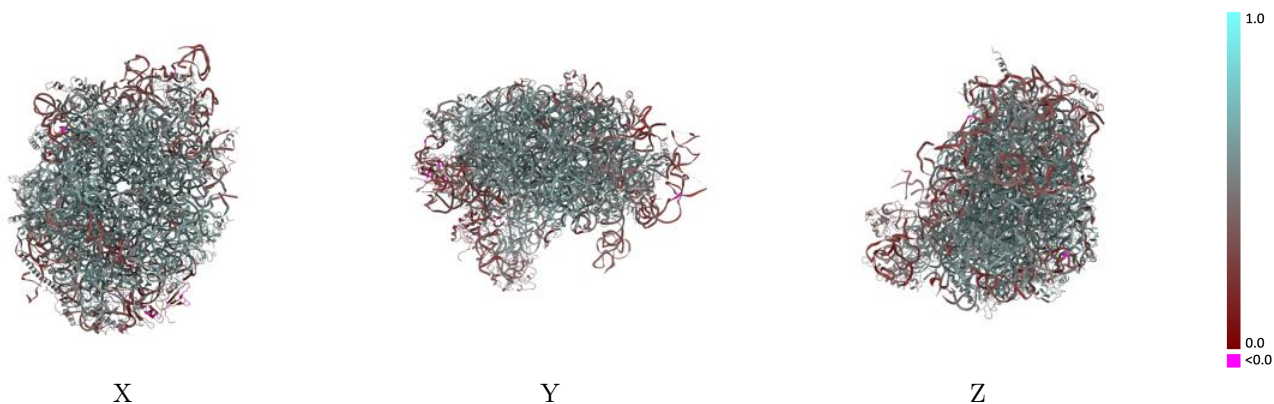
This section contains information regarding the fit between EMDB map EMD-6583 and PDB model 3JCS. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



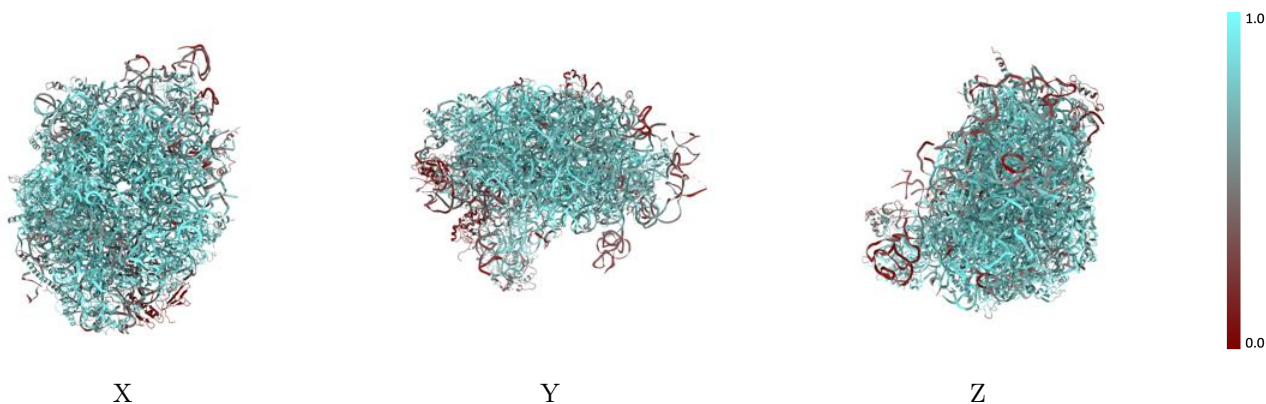
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



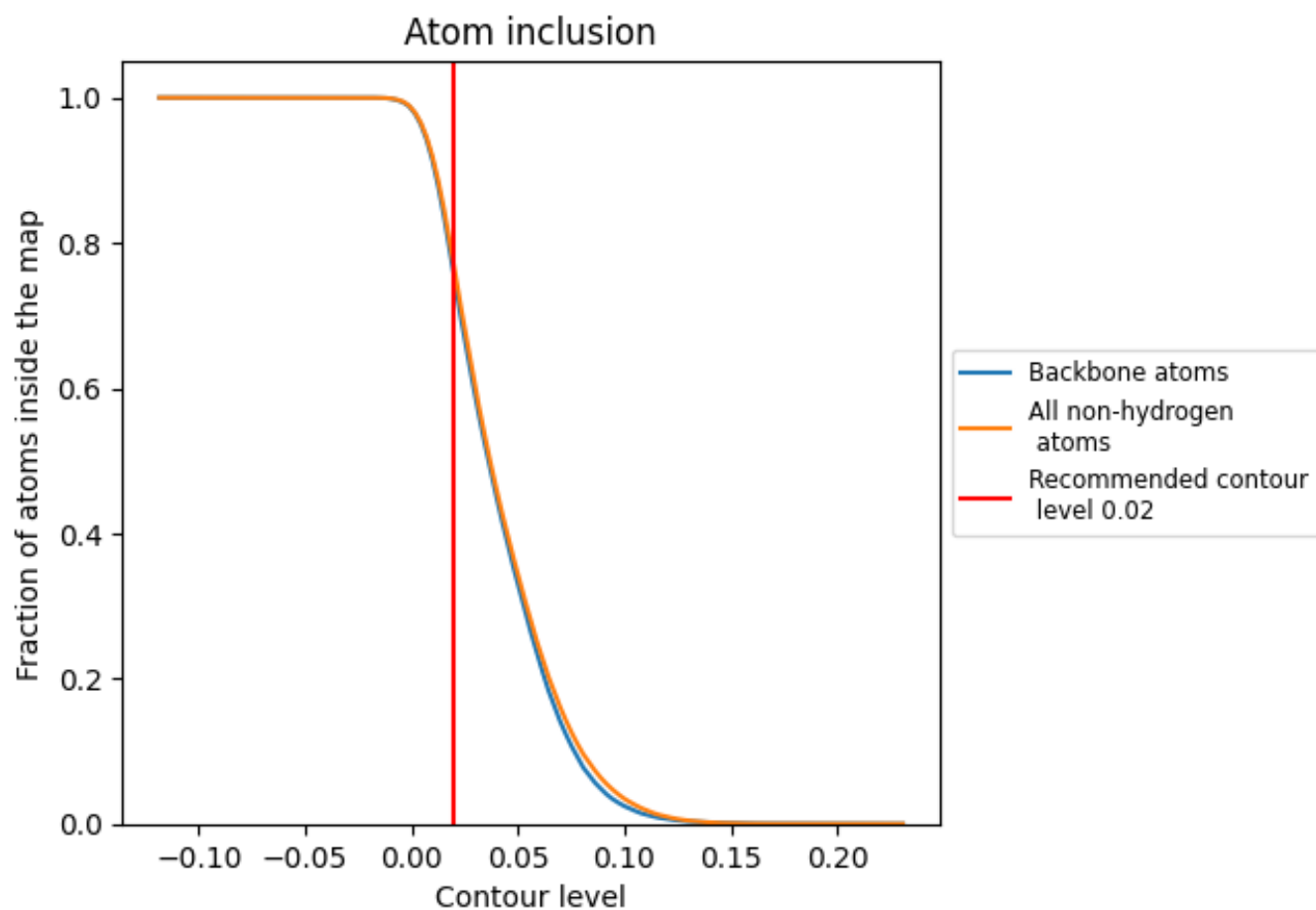
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 77% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7677	 0.4990
1	 0.8182	 0.5060
2	 0.7556	 0.4850
3	 0.6910	 0.4460
4	 0.7952	 0.4970
5	 0.8879	 0.5440
6	 0.6724	 0.3910
7	 0.8930	 0.5550
8	 0.8056	 0.4420
A	 0.8575	 0.5770
B	 0.8237	 0.5530
C	 0.8482	 0.5580
D	 0.4593	 0.3530
E	 0.1210	 0.2290
F	 0.8041	 0.5200
G	 0.7575	 0.5140
H	 0.7841	 0.5300
I	 0.8463	 0.5620
J	 0.8232	 0.5510
K	 0.7090	 0.4450
L	 0.8397	 0.5570
M	 0.8664	 0.5820
N	 0.0709	 0.2100
O	 0.7577	 0.4740
P	 0.8268	 0.5570
Q	 0.7303	 0.5080
R	 0.8151	 0.5220
S	 0.7307	 0.5060
T	 0.8349	 0.5590
U	 0.4480	 0.3960
V	 0.8283	 0.5500
W	 0.8306	 0.5460
X	 0.7286	 0.5210
Y	 0.7685	 0.4950
Z	 0.6279	 0.4930



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Chain	Atom inclusion	Q-score
a	 0.8038	 0.5310
b	 0.8320	 0.5530
c	 0.8069	 0.5410
d	 0.6437	 0.4540
e	 0.7910	 0.5220
f	 0.8237	 0.5580
g	 0.8669	 0.5780
h	 0.7497	 0.5290
i	 0.7340	 0.5140
j	 0.8740	 0.5930
k	 0.5531	 0.4250
l	 0.8278	 0.5680
m	 0.7578	 0.5320
n	 0.6646	 0.4980