



wwPDB EM Validation Summary Report ⓘ

Aug 3, 2026 – 01:03 pm BST

PDB ID : 9SRE / pdb_00009sre
EMDB ID : EMD-55139
Title : Cryo-EM structure of *P. abyssi* 70S ribosome in complex with hibernation factor HibA (PTC conformation with E-site tRNA)
Authors : Madru, C.M.; Bourgeois, G.B.; Mechulam, Y.M.; Schmitt, E.S.
Deposited on : 2025-09-24
Resolution : 2.11 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:

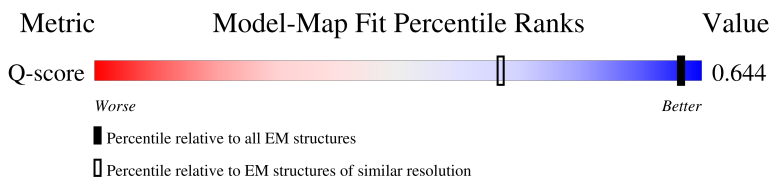
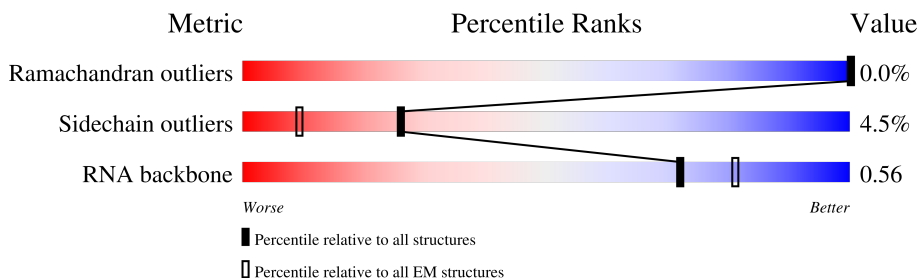
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.11 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)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2361 (1.64 - 2.61)

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	3	128	
2	4	77	
3	H	392	
4	AA	199	

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Mol	Chain	Length	Quality of chain
5	AB	202	94%
6	AC	63	90%
7	AD	180	94%
8	AE	243	99%
9	AF	236	95%
10	AG	125	95%
11	AH	215	96%
12	AI	130	98%
13	AJ	127	95%
14	AK	135	95%
15	AL	102	24%
16	AM	137	90%
17	AN	147	97%
18	AP	56	89%
19	AQ	158	96%
20	AR	113	94%
21	AS	67	88%
22	AU	150	96%
23	AV	99	96%
23	B6	99	5%
24	AW	65	92%
25	AX	71	83%
26	AY	51	90%
27	AZ	210	6%
28	A0	37	95%

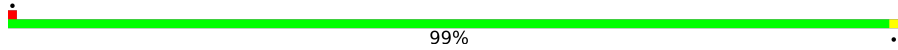
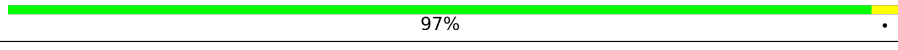
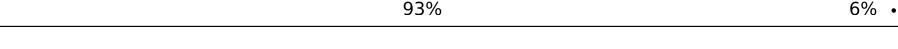
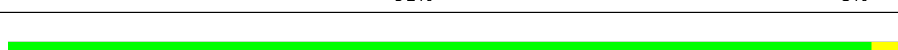
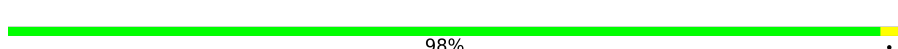
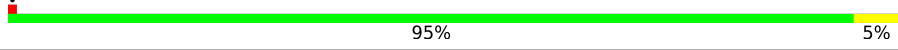
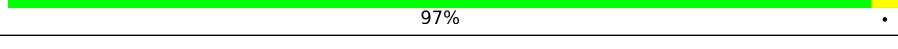
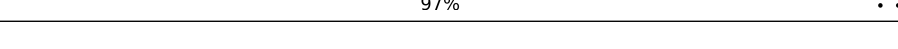
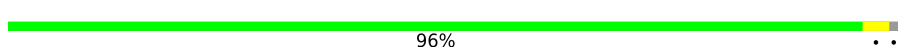
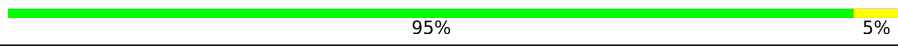
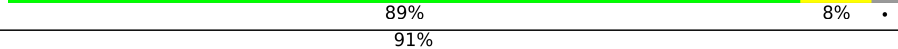
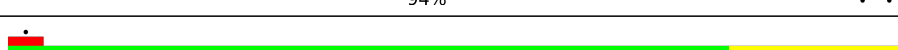
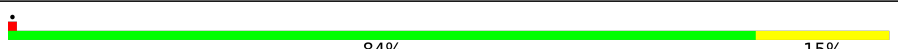
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Mol	Chain	Length	Quality of chain
29	A3	123	97%
29	B4	123	25% 94% 5%
29	BG	123	91% 8%
30	AT	132	5% 94% 5%
31	AO	148	91% 7%
32	BB	239	96%
33	BY	155	97%
34	BO	203	91% 7%
35	BC	361	98%
36	B5	82	94% 5%
36	BK	82	91% 6%
37	BL	147	93% 7%
38	Bf	51	94%
39	BU	121	96%
40	Bb	130	98%
41	Be	62	97%
42	BE	188	87% 12%
43	Ba	94	98%
44	BT	86	99%
45	BW	68	97%
46	Bi	83	95%
47	BI	142	99%
48	BR	97	97%
49	BQ	151	98%
50	BV	67	91% 6%

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Mol	Chain	Length	Quality of chain
51	Bj	94	 99%
52	BD	255	 97%
53	BF	184	 93% 6%
54	BZ	99	 91% 8%
55	BP	120	 97%
56	BM	194	 98%
57	BS	155	 95% 5%
58	Bd	91	 97%
59	BN	181	 97%
60	Bg	51	 94% 6%
61	Bc	87	 98%
62	BJ	141	 96%
63	Bl	77	 95% 5%
64	Bk	65	 89% 8%
65	BA	219	 91% 9%
66	1	3018	 81% 19%
67	2	1496	 84% 15%

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 198152 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 rRNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	126	Total	C	N	O	P	0	0
			2703	1203	498	876	126		

- Molecule 2 is a RNA chain called tRNAMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	4	77	Total	C	N	O	P	S	0	0
			1644	734	296	536	77	1		

- Molecule 3 is a protein called Dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	386	Total	C	N	O	S	0	0
			3074	1962	535	567	10		

- Molecule 4 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AA	188	Total	C	N	O	S	0	0
			1531	993	268	266	4		

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AB	196	Total	C	N	O	S	0	0
			1571	1017	269	281	4		

- Molecule 6 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AC	57	Total	C	N	O	S	0	0
			449	285	80	76	8		

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AD	173	Total	C	N	O	S	0	0
			1452	913	280	255	4		

- Molecule 8 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AE	242	Total	C	N	O	S	0	0
			1983	1281	358	339	5		

- Molecule 9 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AF	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 10 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AG	124	Total	C	N	O	S	0	0
			977	621	178	176	2		

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AH	214	Total	C	N	O	S	0	0
			1725	1095	323	300	7		

- Molecule 12 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AI	129	Total	C	N	O	S	0	0
			1034	668	184	180	2		

- Molecule 13 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	AJ	125	Total	C	N	O	0	0
			986	612	205	169		

- Molecule 14 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AK	135	Total	C	N	O	S	0	0
			1073	673	207	189	4		

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AL	100	Total	C	N	O	S	0	0
			809	502	157	147	3		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AM	127	Total	C	N	O	S	0	0
			955	591	190	172	2		

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AN	146	Total	C	N	O	S	0	0
			1148	727	224	194	3		

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AP	55	Total	C	N	O	S	0	0
			455	288	95	67	5		

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AQ	157	Total	C	N	O	S	0	0
			1305	833	249	219	4		

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AR	107	Total	C	N	O	S	0	0
			884	562	172	147	3		

- Molecule 21 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AS	64	Total	C	N	O	S	0	0
			541	343	104	93	1		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AU	149	Total	C	N	O		0	0
			1223	790	221	212			

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AV	96	Total	C	N	O	S	0	0
			808	528	129	148	3		
23	B6	94	Total	C	N	O	S	0	0
			790	516	125	146	3		

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AW	61	Total	C	N	O	S	0	0
			470	294	91	80	5		

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AX	65	Total	C	N	O		0	0
			516	316	103	97			

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AY	49	Total	C	N	O	S	0	0
			400	257	76	62	5		

- Molecule 27 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AZ	196	Total	C	N	O	S	0	0
			1541	983	284	270	4		

- Molecule 28 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A0	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A3	122	Total	C	N	O	S	0	0
			933	594	156	180	3		
29	BG	122	Total	C	N	O	S	0	0
			932	594	156	179	3		
29	B4	122	Total	C	N	O	S	0	0
			933	594	156	180	3		

- Molecule 30 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AT	130	Total	C	N	O	S	0	0
			1057	675	201	174	7		

- Molecule 31 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AO	138	Total	C	N	O	S	0	0
			1116	700	221	190	5		

- Molecule 32 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BB	238	Total	C	N	O	S	0	0
			1838	1163	354	317	4		

- Molecule 33 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BY	154	Total	C	N	O	S	0	0
			1235	783	234	212	6		

- Molecule 34 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BO	198	Total	C	N	O	S	0	0
			1607	1024	302	279	2		

- Molecule 35 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BC	360	Total	C	N	O	S	0	0
			2870	1843	522	494	11		

- Molecule 36 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B5	81	Total	C	N	O	S	0	0
			614	388	116	108	2		
36	BK	80	Total	C	N	O	S	0	0
			607	383	115	107	2		

- Molecule 37 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	147	Total	C	N	O	S	0	0
			1149	720	224	202	3		

- Molecule 38 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bf	50	Total	C	N	O	S	0	0
			435	275	99	60	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BU	121	Total	C	N	O	S	0	0
			1011	638	198	170	5		

- Molecule 40 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bb	129	Total	C	N	O	S	0	0
			1095	702	221	171	1		

- Molecule 41 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Be	61	Total	C	N	O	S	0	0
			503	312	112	75	4		

- Molecule 42 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BE	185	Total	C	N	O	S	0	0
			1485	934	277	265	9		

- Molecule 43 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ba	94	Total	C	N	O	S	0	0
			778	503	147	127	1		

- Molecule 44 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BT	86	Total	C	N	O	S	0	0
			696	451	118	126	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BW	68	Total	C	N	O	S	0	0
			565	349	111	99	6		

- Molecule 46 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bi	82	Total	C	N	O	S	0	0
			620	389	129	97	5		

- Molecule 47 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BI	142	Total	C	N	O	S	0	0
			1148	734	217	194	3		

- Molecule 48 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BR	96	Total	C	N	O	S	0	0
			797	507	164	125	1		

- Molecule 49 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BQ	150	Total	C	N	O	S	0	0
			1265	795	261	203	6		

- Molecule 50 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BV	63	Total	C	N	O	S	0	0
			532	339	103	84	6		

- Molecule 51 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bj	94	Total	C	N	O	S	0	0
			789	502	163	119	5		

- Molecule 52 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BD	255	Total	C	N	O	S	0	0
			2026	1290	388	343	5		

- Molecule 53 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BF	183	Total	C	N	O	S	0	0
			1456	943	251	261	1		

- Molecule 54 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BZ	98	Total	C	N	O		0	0
			749	486	122	141			

- Molecule 55 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BP	120	Total	C	N	O	S	0	0
			971	610	188	170	3		

- Molecule 56 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BM	193	Total	C	N	O	S	0	0
			1588	1014	318	251	5		

- Molecule 57 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BS	154	Total	C	N	O	S	0	0
			1247	786	246	211	4		

- Molecule 58 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bd	91	Total	C	N	O	S	0	0
			759	477	163	109	10		

- Molecule 59 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BN	178	Total	C	N	O	S	0	0
			1452	920	281	246	5		

- Molecule 60 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bg	48	Total	C	N	O	S	0	0
			387	243	80	60	4		

- Molecule 61 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bc	87	Total	C	N	O	S	0	0
			684	435	132	115	2		

- Molecule 62 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BJ	140	Total	C	N	O	S	0	0
			1066	664	214	185	3		

- Molecule 63 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bl	77	Total	C	N	O	S	0	0
			659	425	120	113	1		

- Molecule 64 is a protein called C2H2-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bk	63	Total	C	N	O	S	0	0
			528	339	108	78	3		

- Molecule 65 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BA	215	Total	C	N	O	S	0	0
			1675	1065	301	304	5		

- Molecule 66 is a RNA chain called rRNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	1	3018	Total	C	N	O	P	0	0
			65181	29055	12094	21014	3018		

- Molecule 67 is a RNA chain called rRNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	2	1496	Total	C	N	O	P	0	0
			32291	14408	5957	10430	1496		

- Molecule 68 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
68	3	1	Total	Mg	0
			1	1	
68	AK	1	Total	Mg	0
			1	1	
68	AN	1	Total	Mg	0
			1	1	
68	BB	2	Total	Mg	0
			2	2	
68	Bb	1	Total	Mg	0
			1	1	
68	BD	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
68	BM	1	Total 1	Mg 1	0
68	BS	1	Total 1	Mg 1	0
68	1	166	Total 166	Mg 166	0
68	2	69	Total 69	Mg 69	0

- Molecule 69 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
69	AC	2	Total 2	Zn 2	0
69	AF	1	Total 1	Zn 1	0
69	AP	1	Total 1	Zn 1	0
69	AR	1	Total 1	Zn 1	0
69	AW	1	Total 1	Zn 1	0
69	Be	1	Total 1	Zn 1	0
69	Bi	1	Total 1	Zn 1	0
69	BV	1	Total 1	Zn 1	0
69	Bj	1	Total 1	Zn 1	0
69	Bd	1	Total 1	Zn 1	0
69	Bg	1	Total 1	Zn 1	0
69	Bk	1	Total 1	Zn 1	0

- Molecule 70 is water.

Mol	Chain	Residues	Atoms		AltConf
70	3	424	Total 424	O 424	0

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Mol	Chain	Residues	Atoms		AltConf
70	4	4	Total 4	O 4	0
70	H	474	Total 474	O 474	0
70	AA	288	Total 288	O 288	0
70	AB	295	Total 295	O 295	0
70	AC	61	Total 61	O 61	0
70	AD	190	Total 190	O 190	0
70	AE	207	Total 207	O 207	0
70	AF	194	Total 194	O 194	0
70	AG	227	Total 227	O 227	0
70	AH	249	Total 249	O 249	0
70	AI	109	Total 109	O 109	0
70	AJ	125	Total 125	O 125	0
70	AK	113	Total 113	O 113	0
70	AL	136	Total 136	O 136	0
70	AM	88	Total 88	O 88	0
70	AN	142	Total 142	O 142	0
70	AP	61	Total 61	O 61	0
70	AQ	162	Total 162	O 162	0
70	AR	67	Total 67	O 67	0
70	AU	172	Total 172	O 172	0
70	AV	165	Total 165	O 165	0

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Mol	Chain	Residues	Atoms		AltConf
70	AW	85	Total 85	O 85	0
70	AX	82	Total 82	O 82	0
70	AZ	4	Total 4	O 4	0
70	A0	42	Total 42	O 42	0
70	AT	230	Total 230	O 230	0
70	AO	1	Total 1	O 1	0
70	BB	170	Total 170	O 170	0
70	BY	115	Total 115	O 115	0
70	BO	204	Total 204	O 204	0
70	BC	238	Total 238	O 238	0
70	B5	77	Total 77	O 77	0
70	BL	101	Total 101	O 101	0
70	Bf	36	Total 36	O 36	0
70	BU	95	Total 95	O 95	0
70	Bb	120	Total 120	O 120	0
70	Be	56	Total 56	O 56	0
70	BE	6	Total 6	O 6	0
70	Ba	77	Total 77	O 77	0
70	BT	67	Total 67	O 67	0
70	BW	67	Total 67	O 67	0
70	Bi	62	Total 62	O 62	0

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Mol	Chain	Residues	Atoms		AltConf
70	BI	93	Total 93	O 93	0
70	BR	78	Total 78	O 78	0
70	BK	121	Total 121	O 121	0
70	BQ	119	Total 119	O 119	0
70	BV	47	Total 47	O 47	0
70	Bj	85	Total 85	O 85	0
70	BG	231	Total 231	O 231	0
70	BD	197	Total 197	O 197	0
70	BF	224	Total 224	O 224	0
70	BZ	102	Total 102	O 102	0
70	B6	214	Total 214	O 214	0
70	BP	99	Total 99	O 99	0
70	BM	138	Total 138	O 138	0
70	BS	119	Total 119	O 119	0
70	Bd	69	Total 69	O 69	0
70	BN	133	Total 133	O 133	0
70	Bg	44	Total 44	O 44	0
70	Bc	61	Total 61	O 61	0
70	BJ	84	Total 84	O 84	0
70	Bl	107	Total 107	O 107	0
70	B4	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
70	Bk	47	Total 47	O 47	0
70	1	10842	Total 10842	O 10842	0
70	2	5225	Total 5225	O 5225	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: rRNA 5S

Chain 3: 

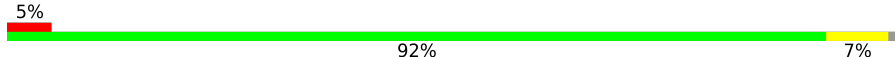


- Molecule 2: tRNA^{Met}

Chain 4: 



- Molecule 3: Dehydrogenase

Chain H: 

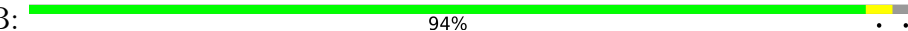


- Molecule 4: 30S ribosomal protein S3Ae

Chain AA: 

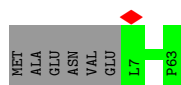


- Molecule 5: 30S ribosomal protein S2

Chain AB: 



- Molecule 6: Zn-ribbon RNA-binding protein involved in translation



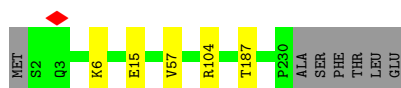
- Molecule 7: 30S ribosomal protein S4



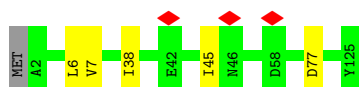
- Molecule 8: 30S ribosomal protein S4e



- Molecule 9: 30S ribosomal protein S5



- Molecule 10: 30S ribosomal protein S6e



- Molecule 11: 30S ribosomal protein S7



- Molecule 12: 30S ribosomal protein S8





- Molecule 13: 30S ribosomal protein S8e

Chain AJ: 95%



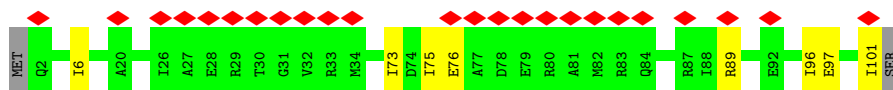
- Molecule 14: 30S ribosomal protein S9

Chain AK: 95%



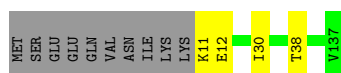
- Molecule 15: 30S ribosomal protein S10

Chain AL: 24% 90% 8%



- Molecule 16: 30S ribosomal protein S11

Chain AM: 90% 7%



- Molecule 17: 30S ribosomal protein S12

Chain AN: 97%



- Molecule 18: 30S ribosomal protein S14 type Z

Chain AP: 89% 9%



- Molecule 19: 30S ribosomal protein S15

Chain AQ: 96%



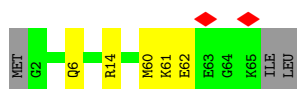
- Molecule 20: 30S ribosomal protein S17

Chain AR: 94% 5%



- Molecule 21: 30S ribosomal protein S17e

Chain AS: 88% 7% 5%



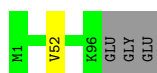
- Molecule 22: 30S ribosomal protein S19e

Chain AU: 96% 4%



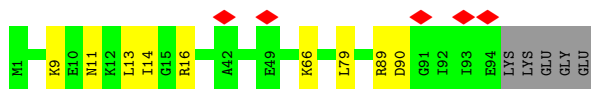
- Molecule 23: 30S ribosomal protein S24e

Chain AV: 96% 4%



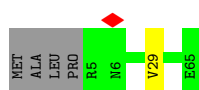
- Molecule 23: 30S ribosomal protein S24e

Chain B6: 5% 86% 9% 5%



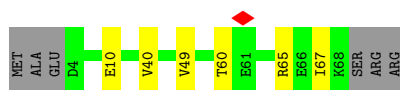
- Molecule 24: 30S ribosomal protein S27e

Chain AW: 92% 6% 2%

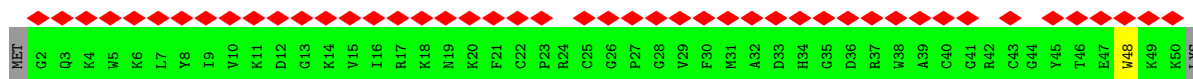


- Molecule 25: 30S ribosomal protein S28e

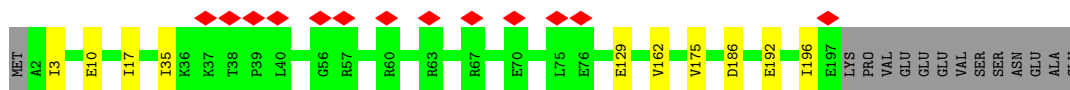
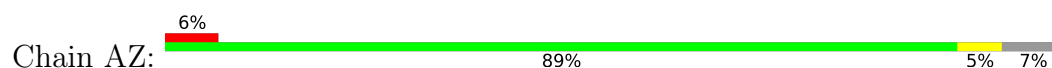
Chain AX: 83% 8% 8%



- Molecule 26: 30S ribosomal protein S27ae



- Molecule 27: 30S ribosomal protein S3



- Molecule 28: Small ribosomal subunit protein eS32



- Molecule 29: 50S ribosomal protein L7Ae

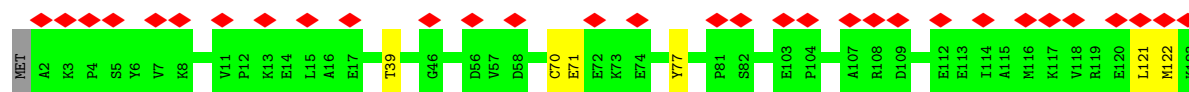


- Molecule 29: 50S ribosomal protein L7Ae



- Molecule 29: 50S ribosomal protein L7Ae





- Molecule 30: 30S ribosomal protein S19



- Molecule 31: 30S ribosomal protein S13



- Molecule 32: Large ribosomal subunit protein uL2



- Molecule 33: Large ribosomal subunit protein uL30



- Molecule 34: Large ribosomal subunit protein uL18



- Molecule 35: Large ribosomal subunit protein uL3



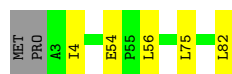
- Molecule 36: Large ribosomal subunit protein eL14

Chain B5:  94% 5%



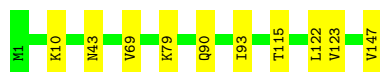
- Molecule 36: Large ribosomal subunit protein eL14

Chain BK:  91% 6%



- Molecule 37: Large ribosomal subunit protein uL15

Chain BL:  93% 7%

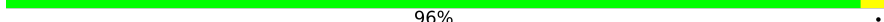


- Molecule 38: Large ribosomal subunit protein eL39

Chain Bf:  94%

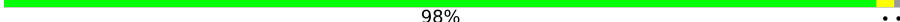


- Molecule 39: Large ribosomal subunit protein uL24

Chain BU:  96%

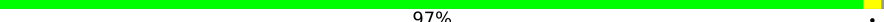


- Molecule 40: Large ribosomal subunit protein eL32

Chain Bb:  98%



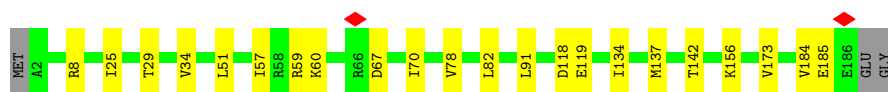
- Molecule 41: Large ribosomal subunit protein eL37

Chain Be:  97%

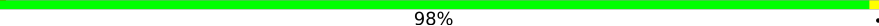


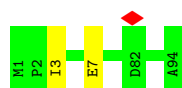
- Molecule 42: Large ribosomal subunit protein uL5

Chain BE:  87% 12%

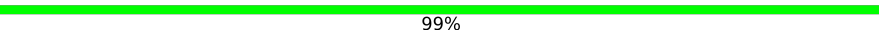


- Molecule 43: Large ribosomal subunit protein eL31

Chain Ba:  98%

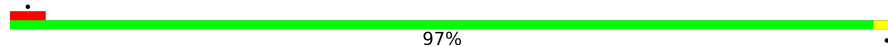


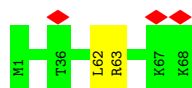
- Molecule 44: Large ribosomal subunit protein uL23

Chain BT:  99%

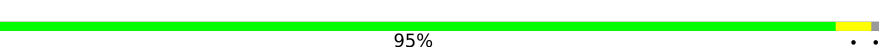


- Molecule 45: Large ribosomal subunit protein uL29

Chain BW:  97%

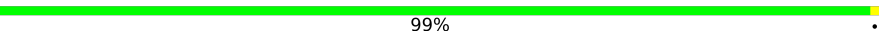


- Molecule 46: Large ribosomal subunit protein eL43

Chain Bi:  95%

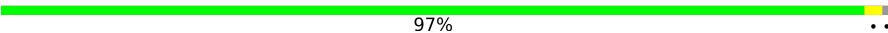


- Molecule 47: Large ribosomal subunit protein uL13

Chain BI:  99%

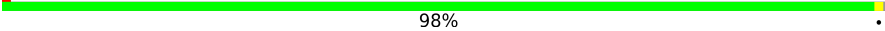


- Molecule 48: Large ribosomal subunit protein eL21

Chain BR:  97%



- Molecule 49: Large ribosomal subunit protein eL19

Chain BQ:  98% ..



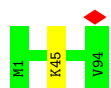
- Molecule 50: Large ribosomal subunit protein eL24

Chain BV:  91% • 6%

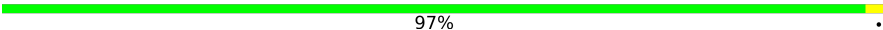


- Molecule 51: Large ribosomal subunit protein eL42

Chain Bj:  99% .

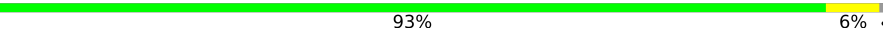


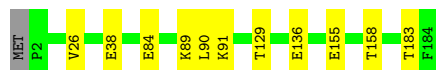
- Molecule 52: Large ribosomal subunit protein uL4

Chain BD:  97% .



- Molecule 53: Large ribosomal subunit protein uL6

Chain BF:  93% • 6% .

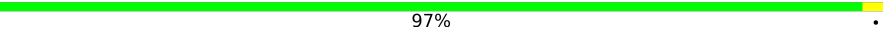


- Molecule 54: Large ribosomal subunit protein eL30

Chain BZ:  91% • 8% .

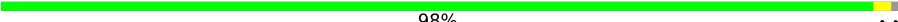


- Molecule 55: Large ribosomal subunit protein eL18

Chain BP:  97% .



- Molecule 56: Large ribosomal subunit protein eL15

Chain BM:  98% ..

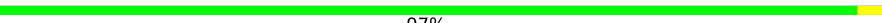


- Molecule 57: Large ribosomal subunit protein uL22

Chain BS:  95% 5% .

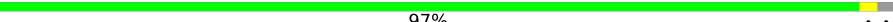


- Molecule 58: Large ribosomal subunit protein eL34

Chain Bd:  97% .



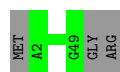
- Molecule 59: Large ribosomal subunit protein uL16

Chain BN:  97% ..

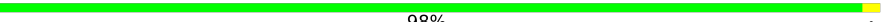


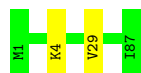
- Molecule 60: Large ribosomal subunit protein eL40

Chain Bg:  94% 6%



- Molecule 61: Large ribosomal subunit protein eL33

Chain Bc:  98% .



- Molecule 62: Large ribosomal subunit protein uL14

Chain BJ:  96% ..



- Molecule 63: Large ribosomal subunit protein eL20

```

graph LR
    M1[M1] --- R7[R7]
    R7 --- E13[E13]
    E13 --- R17[R17]
    R17 --- K20[K20]
    K20 --- L77[L77]
    style M1 fill:#00FF00
    style R7 fill:#FFFF00
    style E13 fill:#FFFF00
    style R17 fill:#FFFF00
    style K20 fill:#FFFF00
    style L77 fill:#00FF00
  
```

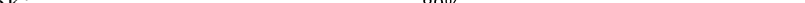
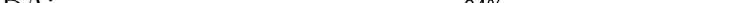
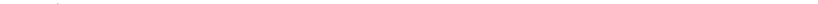
- Chain Bk:  89% 8%

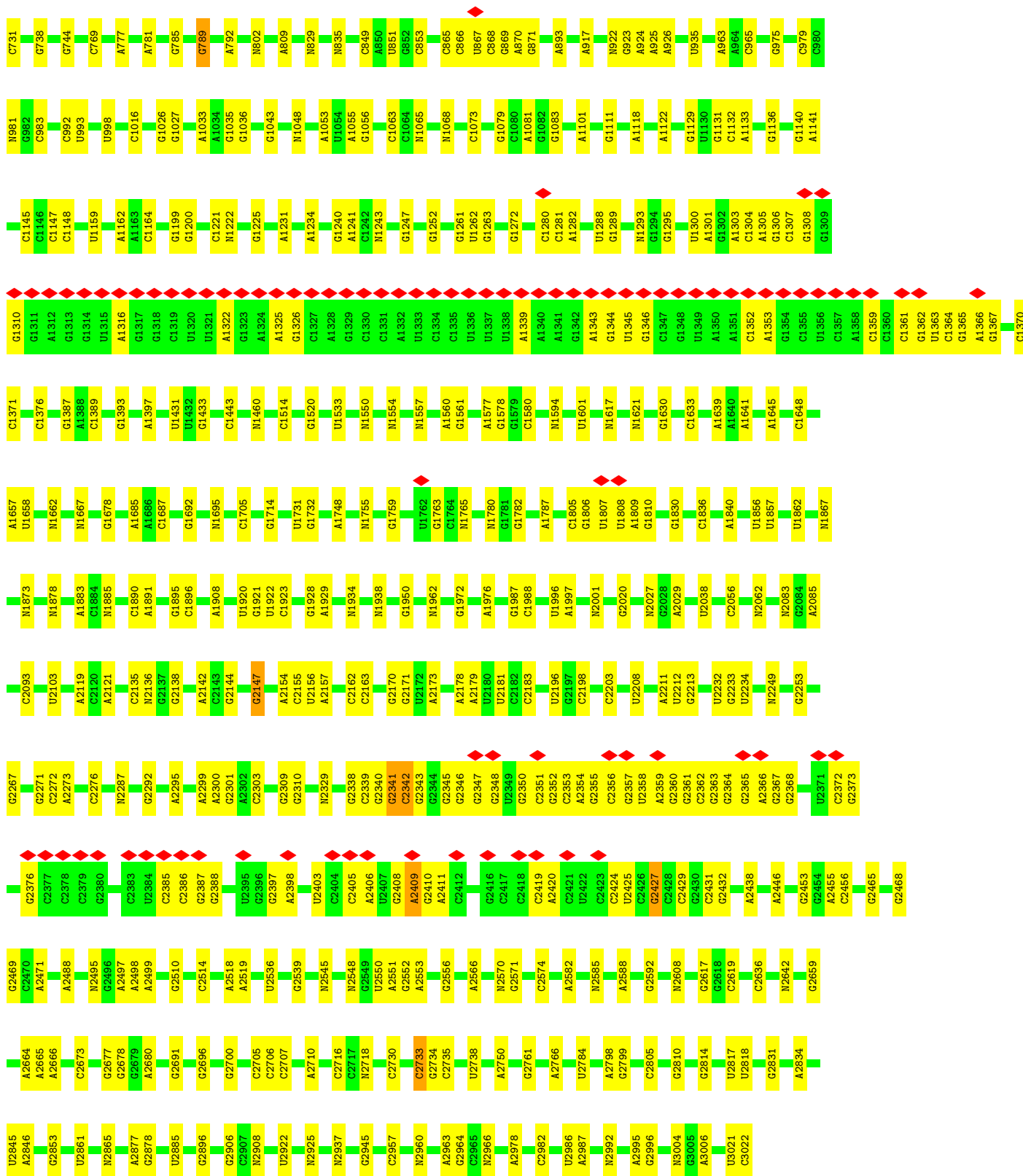
Diagram illustrating the structure of the C-terminal domain of the human p53 protein. The protein is shown as a yellow bar with green segments representing alpha-helices and loops. The residues MET, V2, E16, C23, K39, L44, K49, L63, S64, and GLN are labeled. A red diamond is placed above the L63/S64 region, indicating a site of interest.

- Chain BA:  91% 94%

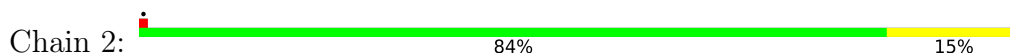
[illegible]

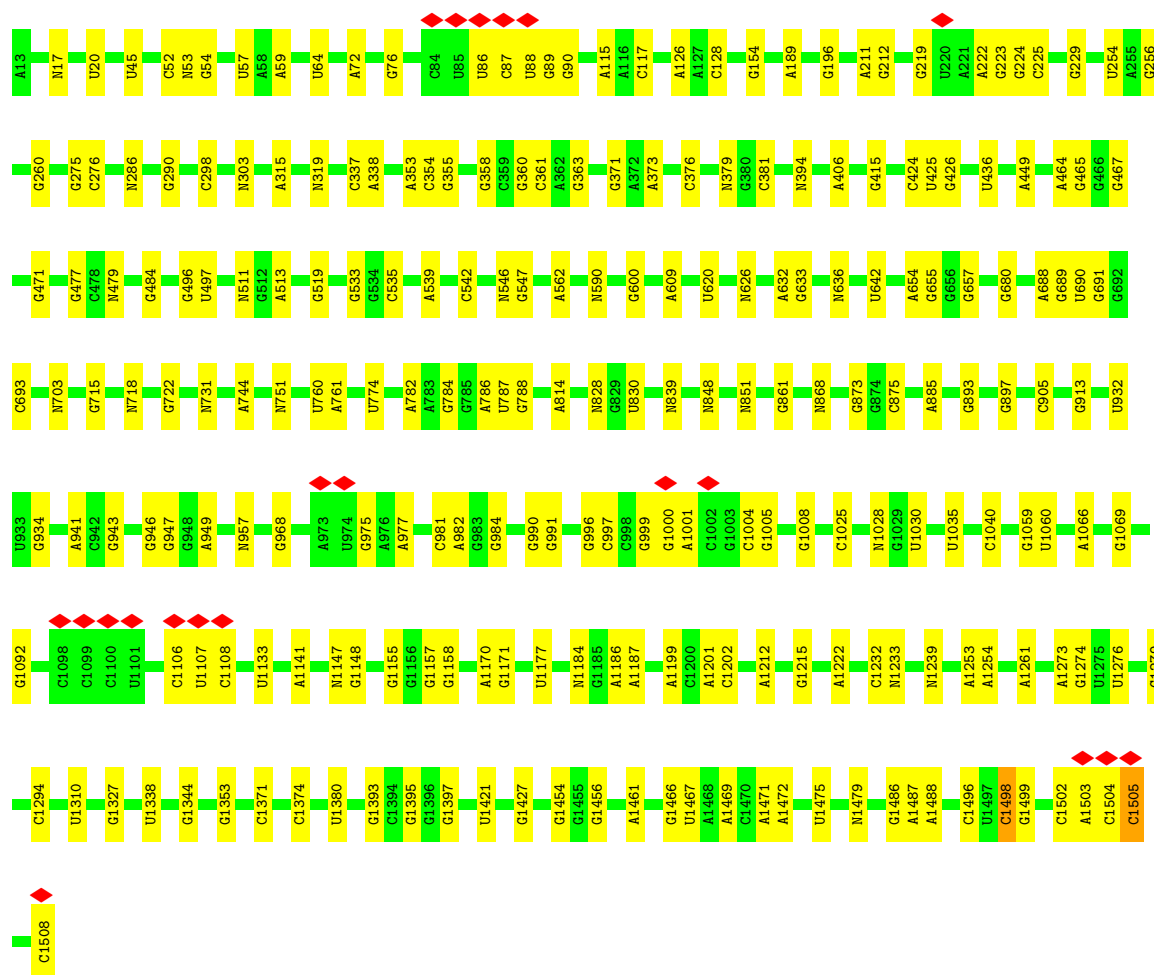
- Chain 1:  81% 19%

U456	G272	G121	C1
U457	C273	G122	G12
U458	C274	A123	A16
C466	A279	N136	N22
G484	A285	G137	A28
A485	A300	G138	A39
A501	A310	C148	U40
G507	N314	G154	A43
G517	G319	C160	A51
A522	A326	N161	G52
C523	A327	A178	G53
C524	G328	A185	G54
G529	A332	A188	U55
N533	A333	G189	C56
U544	A337	G199	A57
A545	U338	G205	A58
A560	G340	N211	C59
G565	N341	C214	N60
A608	G352	G229	U68
A611	N357	G230	U69
G621	G370	A231	G75
G635	A392	A232	C92
N641	C393	U233	G88
A656	G416	C238	N91
A657	C422	C239	G94
C661	C423	U240	G95
A683	C424	C241	U96
G684	U428	N242	C97
G685	A430	G244	C98
C689	U439	C245	U99
N694	U440	G246	G100
A696	G440	G247	U101
G699	A447	C248	C102
G704	A448	U249	G103
	G450	U250	C104
	N451	A251	C105
		U252	G106
		C254	G107
		G264	A112
		A268	G113
		U269	G114
		A270	G115
		A271	G116
			G117
			U118
			C119
			A120



● Molecule 67: rRNA 16S





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0015	Depositor
Map size (Å)	302.04, 302.04, 302.04	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83900005, 0.83900005, 0.83900005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU, ZN, 4SU, OMG, OMU, MA6, A2M, LHH, B8H, UR3, 4AC, 6MZ, MG, H2U, OMC, 5MC

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	3	0.20	0/2995	0.32	0/4669
2	4	0.21	1/1724 (0.1%)	0.42	0/2687
3	H	0.17	0/3120	0.33	0/4209
4	AA	0.15	0/1557	0.29	0/2087
5	AB	0.14	0/1602	0.29	0/2165
6	AC	0.14	0/463	0.30	0/628
7	AD	0.13	0/1476	0.25	0/1980
8	AE	0.15	0/2032	0.31	0/2742
9	AF	0.15	0/1838	0.30	0/2478
10	AG	0.16	0/993	0.33	0/1329
11	AH	0.13	0/1762	0.29	0/2366
12	AI	0.16	0/1055	0.29	0/1415
13	AJ	0.16	0/995	0.27	0/1327
14	AK	0.14	0/1089	0.29	0/1459
15	AL	0.14	0/817	0.31	0/1097
16	AM	0.16	0/973	0.34	0/1311
17	AN	0.15	0/1165	0.30	0/1547
18	AP	0.15	0/465	0.34	0/613
19	AQ	0.14	0/1333	0.29	0/1791
20	AR	0.16	0/907	0.31	0/1225
21	AS	0.13	0/548	0.29	0/725
22	AU	0.14	0/1253	0.29	0/1689
23	AV	0.13	0/826	0.26	0/1108
23	B6	0.16	0/808	0.36	0/1086
24	AW	0.14	0/476	0.31	0/641
25	AX	0.10	0/518	0.25	0/694
26	AY	0.09	0/412	0.25	0/549
27	AZ	0.12	0/1563	0.26	0/2099
28	A0	0.20	0/349	0.40	0/451
29	A3	0.11	0/945	0.32	0/1274
29	B4	0.15	0/945	0.35	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	BG	0.19	0/944	0.34	0/1274
30	AT	0.15	0/1077	0.30	0/1439
31	AO	0.12	0/1135	0.29	0/1526
32	BB	0.21	0/1882	0.37	0/2538
33	BY	0.19	0/1254	0.33	0/1677
34	BO	0.18	0/1645	0.34	0/2209
35	BC	0.18	0/2933	0.36	0/3943
36	B5	0.17	0/619	0.35	0/830
36	BK	0.15	0/611	0.35	0/819
37	BL	0.19	0/1167	0.38	0/1552
38	Bf	0.21	0/443	0.35	0/589
39	BU	0.34	0/1027	0.44	0/1368
40	Bb	0.18	0/1120	0.32	0/1494
41	Be	0.20	0/514	0.35	0/676
42	BE	0.20	0/1509	0.39	0/2022
43	Ba	0.17	0/793	0.33	0/1064
44	BT	0.17	0/705	0.33	0/945
45	BW	0.17	0/566	0.31	0/747
46	Bi	0.15	0/630	0.35	0/839
47	BI	0.17	0/1166	0.32	0/1559
48	BR	0.18	0/819	0.33	0/1098
49	BQ	0.17	0/1281	0.32	0/1689
50	BV	0.17	0/547	0.33	0/729
51	Bj	0.18	0/807	0.32	0/1070
52	BD	0.20	0/2069	0.37	0/2787
53	BF	0.18	0/1485	0.31	0/2003
54	BZ	0.17	0/759	0.36	0/1023
55	BP	0.16	0/984	0.30	0/1314
56	BM	0.21	0/1627	0.35	0/2170
57	BS	0.28	0/1275	0.49	2/1715 (0.1%)
58	Bd	0.18	0/778	0.31	0/1036
59	BN	0.17	0/1483	0.32	0/1992
60	Bg	0.18	0/396	0.30	0/526
61	Bc	0.17	0/693	0.35	0/926
62	BJ	0.20	0/1080	0.34	0/1456
63	Bl	0.18	0/669	0.32	0/886
64	Bk	0.21	0/538	0.33	0/709
65	BA	0.15	0/1700	0.38	0/2288
66	1	0.26	1/70601 (0.0%)	0.38	5/110066 (0.0%)
67	2	0.21	0/34413	0.31	0/53647
All	All	0.22	2/182748 (0.0%)	0.35	7/268955 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	1	96	U	C1'-N1	5.75	1.57	1.48
2	4	8	4SU	O3'-P	5.01	1.61	1.56

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	1	2341	G	C2'-C3'-O3'	9.21	127.52	113.70
57	BS	79	GLY	N-CA-C	-8.59	94.82	112.34
66	1	2409	A	C2'-C3'-O3'	7.07	124.30	113.70
66	1	2427	G	C4'-C3'-O3'	6.09	122.14	113.00
57	BS	78	PHE	N-CA-C	5.85	118.06	108.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	384/392 (98%)	382 (100%)	2 (0%)	0	100	100
4	AA	186/199 (94%)	181 (97%)	5 (3%)	0	100	100
5	AB	194/202 (96%)	192 (99%)	2 (1%)	0	100	100
6	AC	55/63 (87%)	53 (96%)	2 (4%)	0	100	100
7	AD	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
8	AE	240/243 (99%)	238 (99%)	2 (1%)	0	100	100
9	AF	227/236 (96%)	221 (97%)	6 (3%)	0	100	100
10	AG	122/125 (98%)	117 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AH	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
12	AI	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
13	AJ	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
14	AK	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
15	AL	98/102 (96%)	96 (98%)	2 (2%)	0	100	100
16	AM	125/137 (91%)	122 (98%)	3 (2%)	0	100	100
17	AN	144/147 (98%)	143 (99%)	1 (1%)	0	100	100
18	AP	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
19	AQ	155/158 (98%)	151 (97%)	4 (3%)	0	100	100
20	AR	105/113 (93%)	104 (99%)	1 (1%)	0	100	100
21	AS	62/67 (92%)	58 (94%)	4 (6%)	0	100	100
22	AU	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
23	AV	94/99 (95%)	92 (98%)	2 (2%)	0	100	100
23	B6	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
24	AW	59/65 (91%)	56 (95%)	3 (5%)	0	100	100
25	AX	63/71 (89%)	63 (100%)	0	0	100	100
26	AY	47/51 (92%)	42 (89%)	5 (11%)	0	100	100
27	AZ	194/210 (92%)	182 (94%)	12 (6%)	0	100	100
28	A0	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
29	A3	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
29	B4	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
29	BG	120/123 (98%)	120 (100%)	0	0	100	100
30	AT	128/132 (97%)	127 (99%)	1 (1%)	0	100	100
31	AO	136/148 (92%)	129 (95%)	7 (5%)	0	100	100
32	BB	236/239 (99%)	229 (97%)	6 (2%)	1 (0%)	30	28
33	BY	152/155 (98%)	150 (99%)	2 (1%)	0	100	100
34	BO	196/203 (97%)	195 (100%)	1 (0%)	0	100	100
35	BC	358/361 (99%)	348 (97%)	10 (3%)	0	100	100
36	B5	79/82 (96%)	78 (99%)	1 (1%)	0	100	100
36	BK	78/82 (95%)	75 (96%)	3 (4%)	0	100	100
37	BL	145/147 (99%)	139 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	Bf	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
39	BU	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
40	Bb	127/130 (98%)	127 (100%)	0	0	100	100
41	Be	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
42	BE	183/188 (97%)	183 (100%)	0	0	100	100
43	Ba	92/94 (98%)	92 (100%)	0	0	100	100
44	BT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
45	BW	66/68 (97%)	66 (100%)	0	0	100	100
46	Bi	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
47	BI	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
48	BR	94/97 (97%)	94 (100%)	0	0	100	100
49	BQ	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
50	BV	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
51	Bj	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
52	BD	253/255 (99%)	250 (99%)	3 (1%)	0	100	100
53	BF	181/184 (98%)	181 (100%)	0	0	100	100
54	BZ	96/99 (97%)	95 (99%)	1 (1%)	0	100	100
55	BP	118/120 (98%)	118 (100%)	0	0	100	100
56	BM	191/194 (98%)	189 (99%)	2 (1%)	0	100	100
57	BS	152/155 (98%)	149 (98%)	3 (2%)	0	100	100
58	Bd	89/91 (98%)	89 (100%)	0	0	100	100
59	BN	176/181 (97%)	171 (97%)	5 (3%)	0	100	100
60	Bg	46/51 (90%)	46 (100%)	0	0	100	100
61	Bc	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
62	BJ	138/141 (98%)	138 (100%)	0	0	100	100
63	Bl	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
64	Bk	61/65 (94%)	61 (100%)	0	0	100	100
65	BA	213/219 (97%)	206 (97%)	7 (3%)	0	100	100
All	All	8781/9080 (97%)	8612 (98%)	168 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	BB	122	VAL

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	H	332/338 (98%)	305 (92%)	27 (8%)	11	8
4	AA	160/167 (96%)	151 (94%)	9 (6%)	19	17
5	AB	168/173 (97%)	162 (96%)	6 (4%)	31	33
6	AC	50/55 (91%)	50 (100%)	0	100	100
7	AD	156/160 (98%)	153 (98%)	3 (2%)	50	57
8	AE	213/214 (100%)	211 (99%)	2 (1%)	70	78
9	AF	192/198 (97%)	187 (97%)	5 (3%)	40	45
10	AG	107/108 (99%)	102 (95%)	5 (5%)	23	23
11	AH	183/184 (100%)	175 (96%)	8 (4%)	25	25
12	AI	106/107 (99%)	104 (98%)	2 (2%)	50	57
13	AJ	101/103 (98%)	97 (96%)	4 (4%)	28	28
14	AK	111/111 (100%)	104 (94%)	7 (6%)	16	13
15	AL	89/91 (98%)	81 (91%)	8 (9%)	9	6
16	AM	94/104 (90%)	90 (96%)	4 (4%)	26	26
17	AN	120/121 (99%)	117 (98%)	3 (2%)	42	47
18	AP	45/46 (98%)	40 (89%)	5 (11%)	6	3
19	AQ	142/143 (99%)	136 (96%)	6 (4%)	26	27
20	AR	96/102 (94%)	95 (99%)	1 (1%)	68	76
21	AS	58/61 (95%)	53 (91%)	5 (9%)	10	7
22	AU	126/127 (99%)	121 (96%)	5 (4%)	28	28
23	AV	88/90 (98%)	87 (99%)	1 (1%)	65	74
23	B6	86/90 (96%)	77 (90%)	9 (10%)	6	4
24	AW	53/56 (95%)	52 (98%)	1 (2%)	50	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AX	55/60 (92%)	49 (89%)	6 (11%)	6	3
26	AY	40/42 (95%)	39 (98%)	1 (2%)	42	47
27	AZ	155/168 (92%)	145 (94%)	10 (6%)	15	13
28	A0	34/35 (97%)	33 (97%)	1 (3%)	37	41
29	A3	98/99 (99%)	95 (97%)	3 (3%)	35	38
29	B4	98/99 (99%)	92 (94%)	6 (6%)	17	14
29	BG	98/99 (99%)	88 (90%)	10 (10%)	7	4
30	AT	113/114 (99%)	107 (95%)	6 (5%)	20	18
31	AO	115/123 (94%)	111 (96%)	4 (4%)	32	34
32	BB	188/189 (100%)	181 (96%)	7 (4%)	30	31
33	BY	132/133 (99%)	128 (97%)	4 (3%)	36	40
34	BO	167/170 (98%)	153 (92%)	14 (8%)	10	7
35	BC	306/307 (100%)	299 (98%)	7 (2%)	44	50
36	B5	65/66 (98%)	61 (94%)	4 (6%)	16	14
36	BK	64/66 (97%)	59 (92%)	5 (8%)	11	9
37	BL	118/118 (100%)	108 (92%)	10 (8%)	10	7
38	Bf	46/47 (98%)	44 (96%)	2 (4%)	26	26
39	BU	109/109 (100%)	104 (95%)	5 (5%)	24	24
40	Bb	117/118 (99%)	115 (98%)	2 (2%)	53	61
41	Be	52/53 (98%)	51 (98%)	1 (2%)	50	57
42	BE	158/160 (99%)	136 (86%)	22 (14%)	3	1
43	Ba	84/84 (100%)	82 (98%)	2 (2%)	43	48
44	BT	77/77 (100%)	76 (99%)	1 (1%)	61	69
45	BW	63/63 (100%)	61 (97%)	2 (3%)	34	37
46	Bi	61/62 (98%)	58 (95%)	3 (5%)	22	21
47	BI	122/122 (100%)	120 (98%)	2 (2%)	55	63
48	BR	86/87 (99%)	84 (98%)	2 (2%)	44	50
49	BQ	132/133 (99%)	130 (98%)	2 (2%)	57	65
50	BV	54/58 (93%)	52 (96%)	2 (4%)	30	31
51	Bj	83/84 (99%)	82 (99%)	1 (1%)	63	71
52	BD	212/212 (100%)	205 (97%)	7 (3%)	33	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	BF	156/157 (99%)	145 (93%)	11 (7%)	13	10
54	BZ	79/80 (99%)	71 (90%)	8 (10%)	7	4
55	BP	102/102 (100%)	98 (96%)	4 (4%)	28	29
56	BM	160/161 (99%)	157 (98%)	3 (2%)	50	57
57	BS	130/131 (99%)	125 (96%)	5 (4%)	29	30
58	Bd	82/82 (100%)	79 (96%)	3 (4%)	30	31
59	BN	149/151 (99%)	146 (98%)	3 (2%)	48	55
60	Bg	37/39 (95%)	37 (100%)	0	100	100
61	Bc	74/74 (100%)	72 (97%)	2 (3%)	39	44
62	BJ	108/109 (99%)	104 (96%)	4 (4%)	30	31
63	Bl	72/72 (100%)	68 (94%)	4 (6%)	19	17
64	Bk	55/57 (96%)	50 (91%)	5 (9%)	9	6
65	BA	182/186 (98%)	173 (95%)	9 (5%)	22	21
All	All	7564/7707 (98%)	7223 (96%)	341 (4%)	26	24

5 of 341 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	Bi	2	SER
23	B6	13	LEU
36	BK	4	ILE
52	BD	92	THR
57	BS	65	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

Mol	Chain	Res	Type
43	Ba	46	GLN
23	B6	11	ASN
47	BI	51	GLN
49	BQ	75	HIS
56	BM	154	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	125/128 (97%)	17 (13%)	0
2	4	76/77 (98%)	29 (38%)	1 (1%)
66	1	3016/3018 (99%)	491 (16%)	33 (1%)
67	2	1495/1496 (99%)	170 (11%)	4 (0%)
All	All	4712/4719 (99%)	707 (15%)	38 (0%)

5 of 707 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	5	C
1	3	24	G
1	3	25	C
1	3	26	C
1	3	30	C

5 of 38 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
66	1	2455	A
67	2	688	A
66	1	2551	A
66	1	2986	U
67	2	1502	C

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

165 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	$\# Z > 2$
67	OMG	2	467	67	23,26,27	1.21	3 (13%)	33,38,41	1.97	6 (18%)
67	4AC	2	731	67	21,24,25	1.05	2 (9%)	29,34,37	1.33	4 (13%)
66	4AC	1	1662	66	21,24,25	1.00	2 (9%)	29,34,37	1.32	4 (13%)
66	4AC	1	2329	66	21,24,25	1.05	2 (9%)	29,34,37	1.36	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
66	4AC	1	2001	66	21,24,25	1.07	2 (9%)	29,34,37	1.31	4 (13%)
67	OMG	2	873	67	23,26,27	1.20	3 (13%)	33,38,41	1.98	6 (18%)
67	OMG	2	913	67	23,26,27	1.21	3 (13%)	33,38,41	1.96	6 (18%)
67	4AC	2	53	67	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
67	4AC	2	379	67	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
66	4AC	1	2495	66	21,24,25	1.09	2 (9%)	29,34,37	1.35	5 (17%)
66	4AC	1	2570	66	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
67	4AC	2	286	67	21,24,25	1.04	2 (9%)	29,34,37	1.36	4 (13%)
66	OMG	1	328	66	23,26,27	1.22	3 (13%)	33,38,41	1.97	6 (18%)
67	OMG	2	519	67	23,26,27	1.17	3 (13%)	33,38,41	2.01	7 (21%)
67	OMC	2	773	67	19,22,23	0.81	0	26,31,34	0.81	0
67	OMU	2	830	67	19,22,23	1.26	4 (21%)	26,31,34	1.69	5 (19%)
66	4AC	1	2548	66	21,24,25	1.03	2 (9%)	29,34,37	1.39	4 (13%)
66	4AC	1	2585	66	21,24,25	1.07	2 (9%)	29,34,37	1.79	5 (17%)
66	4AC	1	533	66	21,24,25	1.07	2 (9%)	29,34,37	1.37	4 (13%)
66	OMG	1	2144	66	23,26,27	1.21	3 (13%)	33,38,41	1.99	6 (18%)
66	4AC	1	22	66	21,24,25	1.05	2 (9%)	29,34,37	1.39	4 (13%)
66	4AC	1	1048	66	21,24,25	1.09	2 (9%)	29,34,37	1.34	3 (10%)
66	4AC	1	2608	66	21,24,25	1.08	2 (9%)	29,34,37	1.77	5 (17%)
66	4AC	1	451	66	21,24,25	1.06	2 (9%)	29,34,37	1.37	4 (13%)
66	OMG	1	2147	66	23,26,27	1.21	3 (13%)	33,38,41	1.88	6 (18%)
66	4AC	1	2992	66	21,24,25	1.04	2 (9%)	29,34,37	0.88	1 (3%)
67	4AC	2	718	67	21,24,25	1.02	2 (9%)	29,34,37	1.26	4 (13%)
67	4AC	2	1239	67	21,24,25	1.04	2 (9%)	29,34,37	1.33	4 (13%)
67	OMU	2	774	67	19,22,23	1.23	3 (15%)	26,31,34	1.70	4 (15%)
67	OMC	2	846	67	19,22,23	0.81	0	26,31,34	0.79	0
67	4AC	2	1028	67	21,24,25	1.03	2 (9%)	29,34,37	1.36	4 (13%)
66	4AC	1	981	66	21,24,25	1.03	2 (9%)	29,34,37	1.19	4 (13%)
66	4AC	1	1885	66	21,24,25	1.04	2 (9%)	29,34,37	1.22	4 (13%)
66	4AC	1	694	66	21,24,25	1.03	2 (9%)	29,34,37	1.27	4 (13%)
66	4AC	1	3004	66	21,24,25	1.06	2 (9%)	29,34,37	1.23	4 (13%)
66	4AC	1	829	66	21,24,25	1.04	2 (9%)	29,34,37	1.31	4 (13%)
67	5MC	2	1374	67	18,22,23	0.91	2 (11%)	26,32,35	1.12	2 (7%)
66	4AC	1	2966	66	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
66	OMC	1	615	66	19,22,23	0.77	0	26,31,34	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	OMU	2	1380	67	19,22,23	1.33	3 (15%)	26,31,34	1.75	4 (15%)
66	4AC	1	2545	66	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
67	5MC	2	693	67	18,22,23	0.93	2 (11%)	26,32,35	1.17	3 (11%)
66	4AC	1	1878	66	21,24,25	1.06	2 (9%)	29,34,37	1.53	4 (13%)
66	4AC	1	802	66	21,24,25	1.05	2 (9%)	29,34,37	1.28	4 (13%)
66	OMG	1	923	68,66	23,26,27	1.20	3 (13%)	33,38,41	1.98	8 (24%)
66	4AC	1	1222	68,66	21,24,25	1.06	2 (9%)	29,34,37	1.21	4 (13%)
66	4AC	1	1867	66	21,24,25	1.03	2 (9%)	29,34,37	1.29	4 (13%)
67	4AC	2	479	67	21,24,25	1.02	2 (9%)	29,34,37	1.40	4 (13%)
67	4AC	2	394	67	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
66	4AC	1	161	66	21,24,25	1.05	2 (9%)	29,34,37	1.31	4 (13%)
67	5MC	2	875	67	18,22,23	0.91	2 (11%)	26,32,35	1.13	3 (11%)
2	PSU	4	55	2	18,21,22	1.38	3 (16%)	22,30,33	2.31	7 (31%)
2	OMC	4	32	2	19,22,23	0.82	0	26,31,34	0.73	0
66	4AC	1	1293	66	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
67	4AC	2	1233	67	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
67	A2M	2	373	67	22,25,26	1.44	4 (18%)	31,36,39	2.06	8 (25%)
66	4AC	1	2718	66	21,24,25	1.04	2 (9%)	29,34,37	1.28	4 (13%)
66	5MC	1	2198	66	18,22,23	0.88	2 (11%)	26,32,35	1.10	2 (7%)
66	OMU	1	2784	66	19,22,23	1.20	2 (10%)	26,31,34	1.74	5 (19%)
67	5MC	2	1496	67	18,22,23	0.94	2 (11%)	26,32,35	1.16	3 (11%)
66	4AC	1	2960	66	21,24,25	1.05	2 (9%)	29,34,37	1.27	4 (13%)
67	4AC	2	303	67	21,24,25	1.04	2 (9%)	29,34,37	1.31	4 (13%)
67	4AC	2	1147	67	21,24,25	1.05	2 (9%)	29,34,37	1.56	5 (17%)
67	MA6	2	1488	67	23,26,27	1.45	5 (21%)	34,38,41	2.11	10 (29%)
66	5MC	1	2183	66	18,22,23	0.93	2 (11%)	26,32,35	1.09	2 (7%)
66	OMC	1	1948	66	19,22,23	0.76	0	26,31,34	0.76	0
67	4AC	2	868	67	21,24,25	1.03	2 (9%)	29,34,37	1.29	4 (13%)
2	5MU	4	54	2	19,22,23	1.43	6 (31%)	28,32,35	2.04	5 (17%)
67	LHH	2	250	67	22,25,26	0.33	0	29,35,38	0.48	0
66	4AC	1	1243	66	21,24,25	1.06	2 (9%)	29,34,37	1.35	4 (13%)
66	4AC	1	136	66	21,24,25	1.06	2 (9%)	29,34,37	1.27	4 (13%)
66	4AC	1	2908	66	21,24,25	1.06	2 (9%)	29,34,37	1.28	4 (13%)
66	OMG	1	2138	66	23,26,27	1.20	3 (13%)	33,38,41	1.90	6 (18%)
67	6MZ	2	1469	68,67	22,25,26	1.48	4 (18%)	30,36,39	2.18	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
66	A2M	1	1055	66	22,25,26	1.44	4 (18%)	31,36,39	2.10	8 (25%)
66	4AC	1	835	66	21,24,25	1.08	2 (9%)	29,34,37	1.28	5 (17%)
67	OMC	2	1036	67	19,22,23	0.80	0	26,31,34	0.79	0
66	4AC	1	1554	66	21,24,25	1.07	2 (9%)	29,34,37	1.24	4 (13%)
66	4AC	1	2136	66	21,24,25	1.06	2 (9%)	29,34,37	1.44	5 (17%)
67	UR3	2	1467	67	19,22,23	0.92	0	26,32,35	1.41	3 (11%)
67	4AC	2	626	67	21,24,25	1.02	2 (9%)	29,34,37	1.40	4 (13%)
66	4AC	1	641	66	21,24,25	1.07	2 (9%)	29,34,37	1.34	4 (13%)
67	OMU	2	20	67	19,22,23	1.26	3 (15%)	26,31,34	1.77	5 (19%)
66	4AC	1	341	66	21,24,25	1.06	2 (9%)	29,34,37	1.30	4 (13%)
67	4AC	2	957	67	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
66	4AC	1	1934	66	21,24,25	1.06	2 (9%)	29,34,37	1.30	4 (13%)
66	5MC	1	2203	66	18,22,23	0.92	2 (11%)	26,32,35	1.18	2 (7%)
66	4AC	1	1938	66	21,24,25	1.11	2 (9%)	29,34,37	1.32	5 (17%)
67	5MC	2	1498	67	18,22,23	0.93	2 (11%)	26,32,35	1.30	4 (15%)
66	4AC	1	1780	66	21,24,25	1.07	2 (9%)	29,34,37	1.80	5 (17%)
67	OMG	2	657	67	23,26,27	1.23	3 (13%)	33,38,41	1.97	6 (18%)
66	4AC	1	1873	66	21,24,25	1.08	2 (9%)	29,34,37	1.29	4 (13%)
67	4AC	2	319	67	21,24,25	1.05	2 (9%)	29,34,37	1.29	4 (13%)
66	A2M	1	2173	66	22,25,26	1.46	4 (18%)	31,36,39	2.02	8 (25%)
66	4AC	1	243	66	21,24,25	1.04	2 (9%)	29,34,37	1.30	4 (13%)
66	4AC	1	458	66	21,24,25	1.00	2 (9%)	29,34,37	1.37	4 (13%)
66	4AC	1	1065	66	21,24,25	1.05	2 (9%)	29,34,37	1.33	4 (13%)
67	4AC	2	751	67	21,24,25	1.04	2 (9%)	29,34,37	1.31	4 (13%)
67	4AC	2	851	67	21,24,25	1.05	2 (9%)	29,34,37	1.32	4 (13%)
2	4SU	4	8	2	18,21,22	1.80	5 (27%)	26,30,33	2.25	5 (19%)
66	4AC	1	2249	66	21,24,25	1.10	2 (9%)	29,34,37	1.38	4 (13%)
66	4AC	1	314	66	21,24,25	1.07	2 (9%)	29,34,37	1.25	4 (13%)
66	4AC	1	1962	66	21,24,25	1.02	2 (9%)	29,34,37	1.35	4 (13%)
66	LHH	1	616	66	22,25,26	0.33	0	29,35,38	0.41	0
66	5MC	1	2162	66	18,22,23	0.95	2 (11%)	26,32,35	1.28	4 (15%)
66	4AC	1	2865	66	21,24,25	1.04	2 (9%)	29,34,37	1.28	4 (13%)
66	4AC	1	1557	66	21,24,25	1.01	2 (9%)	29,34,37	1.27	4 (13%)
66	4AC	1	1695	66	21,24,25	1.03	2 (9%)	29,34,37	1.32	4 (13%)
66	4AC	1	1765	66	21,24,25	1.06	2 (9%)	29,34,37	1.28	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	4AC	2	703	67	21,24,25	1.03	2 (9%)	29,34,37	1.46	4 (13%)
67	OMG	2	471	67	23,26,27	1.22	3 (13%)	33,38,41	1.93	6 (18%)
66	4AC	1	2937	68,66	21,24,25	1.05	2 (9%)	29,34,37	1.47	3 (10%)
67	B8H	2	938	67	19,22,23	0.57	0	22,32,35	0.62	0
66	4AC	1	229	66	21,24,25	1.10	2 (9%)	29,34,37	1.32	3 (10%)
66	OMG	1	789	66	23,26,27	1.27	3 (13%)	33,38,41	2.00	6 (18%)
67	OMC	2	1376	67	19,22,23	0.79	0	26,31,34	0.76	0
67	OMU	2	1177	67	19,22,23	1.25	3 (15%)	26,31,34	1.72	4 (15%)
67	5MC	2	1025	67	18,22,23	0.93	2 (11%)	26,32,35	1.08	2 (7%)
66	OMG	1	2678	66	23,26,27	1.22	4 (17%)	33,38,41	1.92	6 (18%)
66	5MC	1	2093	66	18,22,23	0.96	2 (11%)	26,32,35	1.12	2 (7%)
67	4AC	2	590	67	21,24,25	1.02	2 (9%)	29,34,37	1.27	4 (13%)
67	OMG	2	680	67	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
67	OMU	2	787	67	19,22,23	1.22	2 (10%)	26,31,34	1.86	6 (23%)
67	OMG	2	934	67	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
1	4AC	3	32	1	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
66	4AC	1	211	66	21,24,25	1.08	2 (9%)	29,34,37	1.30	4 (13%)
66	4AC	1	922	66	21,24,25	1.07	2 (9%)	29,34,37	1.40	4 (13%)
67	4AC	2	546	67	21,24,25	1.03	2 (9%)	29,34,37	1.27	4 (13%)
67	4AC	2	828	67	21,24,25	1.03	2 (9%)	29,34,37	1.27	4 (13%)
67	LHH	2	1041	67	21,24,26	0.33	0	29,34,38	0.35	0
66	4AC	1	2027	66	21,24,25	1.05	2 (9%)	29,34,37	1.24	4 (13%)
67	4AC	2	17	67	21,24,25	1.04	2 (9%)	29,34,37	1.35	4 (13%)
66	4AC	1	2925	66	21,24,25	1.07	2 (9%)	29,34,37	1.32	4 (13%)
66	4AC	1	1460	66	21,24,25	1.04	2 (9%)	29,34,37	1.29	4 (13%)
67	OMU	2	64	67	19,22,23	1.25	4 (21%)	26,31,34	1.68	5 (19%)
66	4AC	1	1594	68,66	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
67	MA6	2	1487	67	23,26,27	1.48	5 (21%)	34,38,41	2.12	11 (32%)
66	4AC	1	2642	66	21,24,25	1.05	2 (9%)	29,34,37	1.29	4 (13%)
67	OMC	2	1040	67	19,22,23	0.81	0	26,31,34	0.89	1 (3%)
66	4AC	1	2083	66	21,24,25	1.12	2 (9%)	29,34,37	1.24	2 (6%)
66	4AC	1	1621	66	21,24,25	1.08	2 (9%)	29,34,37	1.32	4 (13%)
67	OMG	2	1069	67	23,26,27	1.18	3 (13%)	33,38,41	1.95	6 (18%)
67	4AC	2	1479	67	21,24,25	0.99	2 (9%)	29,34,37	1.27	4 (13%)
66	4AC	1	2287	66	21,24,25	1.03	2 (9%)	29,34,37	1.31	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	4AC	2	848	67	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
67	4AC	2	636	67	21,24,25	1.02	2 (9%)	29,34,37	1.54	4 (13%)
67	4AC	2	839	67	21,24,25	1.04	2 (9%)	29,34,37	1.38	4 (13%)
66	4AC	1	2062	66	21,24,25	1.05	2 (9%)	29,34,37	1.27	4 (13%)
66	5MC	1	2163	66	18,22,23	0.95	2 (11%)	26,32,35	1.17	3 (11%)
66	4AC	1	91	66	21,24,25	1.04	2 (9%)	29,34,37	1.45	4 (13%)
67	5MC	2	535	67	18,22,23	0.93	2 (11%)	26,32,35	1.15	3 (11%)
67	4AC	2	1184	67	21,24,25	1.05	2 (9%)	29,34,37	1.45	4 (13%)
66	4AC	1	1667	66	21,24,25	1.06	2 (9%)	29,34,37	1.30	4 (13%)
66	4AC	1	60	66	21,24,25	1.01	2 (9%)	29,34,37	1.40	5 (17%)
67	5MC	2	1505	67	18,22,23	0.97	2 (11%)	26,32,35	1.38	4 (15%)
67	OMC	2	129	67	19,22,23	0.81	0	26,31,34	0.81	0
66	4AC	1	1550	66	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
66	4AC	1	1068	66	21,24,25	1.09	2 (9%)	29,34,37	1.36	5 (17%)
66	4AC	1	357	66	21,24,25	1.08	2 (9%)	29,34,37	1.25	4 (13%)
67	4AC	2	511	67	21,24,25	1.04	2 (9%)	29,34,37	1.40	4 (13%)
66	4AC	1	1755	66	21,24,25	1.07	2 (9%)	29,34,37	1.76	4 (13%)
67	5MC	2	1202	67	18,22,23	0.97	2 (11%)	26,32,35	1.14	3 (11%)
2	H2U	4	20	2	18,21,22	0.98	2 (11%)	21,30,33	2.01	5 (23%)
66	4AC	1	1617	66	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
66	5MC	1	2733	66	18,22,23	0.96	2 (11%)	26,32,35	1.30	3 (11%)

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
67	OMG	2	467	67	-	0/9/27/28	0/3/3/3
67	4AC	2	731	67	-	0/11/29/30	0/2/2/2
66	4AC	1	1662	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2329	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2001	66	-	0/11/29/30	0/2/2/2
67	OMG	2	873	67	-	1/9/27/28	0/3/3/3
67	OMG	2	913	67	-	0/9/27/28	0/3/3/3
67	4AC	2	53	67	-	0/11/29/30	0/2/2/2
67	4AC	2	379	67	-	0/11/29/30	0/2/2/2
66	4AC	1	2495	66	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	4AC	1	2570	66	-	0/11/29/30	0/2/2/2
67	4AC	2	286	67	-	0/11/29/30	0/2/2/2
66	OMG	1	328	66	-	0/9/27/28	0/3/3/3
67	OMG	2	519	67	-	0/9/27/28	0/3/3/3
67	OMC	2	773	67	-	0/9/27/28	0/2/2/2
67	OMU	2	830	67	-	0/9/27/28	0/2/2/2
66	4AC	1	2548	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2585	66	-	3/11/29/30	0/2/2/2
66	4AC	1	533	66	-	0/11/29/30	0/2/2/2
66	OMG	1	2144	66	-	0/9/27/28	0/3/3/3
66	4AC	1	22	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1048	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2608	66	-	3/11/29/30	0/2/2/2
66	4AC	1	451	66	-	0/11/29/30	0/2/2/2
66	OMG	1	2147	66	-	2/9/27/28	0/3/3/3
66	4AC	1	2992	66	-	2/11/29/30	0/2/2/2
67	4AC	2	718	67	-	0/11/29/30	0/2/2/2
67	4AC	2	1239	67	-	0/11/29/30	0/2/2/2
67	OMU	2	774	67	-	0/9/27/28	0/2/2/2
67	OMC	2	846	67	-	0/9/27/28	0/2/2/2
67	4AC	2	1028	67	-	0/11/29/30	0/2/2/2
66	4AC	1	981	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1885	66	-	0/11/29/30	0/2/2/2
66	4AC	1	694	66	-	0/11/29/30	0/2/2/2
66	4AC	1	3004	66	-	0/11/29/30	0/2/2/2
66	4AC	1	829	66	-	0/11/29/30	0/2/2/2
67	5MC	2	1374	67	-	0/7/25/26	0/2/2/2
66	4AC	1	2966	66	-	0/11/29/30	0/2/2/2
66	OMC	1	615	66	-	0/9/27/28	0/2/2/2
67	OMU	2	1380	67	-	0/9/27/28	0/2/2/2
66	4AC	1	2545	66	-	0/11/29/30	0/2/2/2
67	5MC	2	693	67	-	0/7/25/26	0/2/2/2
66	4AC	1	1878	66	-	0/11/29/30	0/2/2/2
66	4AC	1	802	66	-	0/11/29/30	0/2/2/2
66	OMG	1	923	68,66	-	0/9/27/28	0/3/3/3
66	4AC	1	1222	68,66	-	0/11/29/30	0/2/2/2
66	4AC	1	1867	66	-	0/11/29/30	0/2/2/2
67	4AC	2	479	67	-	0/11/29/30	0/2/2/2
67	4AC	2	394	67	-	0/11/29/30	0/2/2/2
66	4AC	1	161	66	-	0/11/29/30	0/2/2/2
67	5MC	2	875	67	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	4	55	2	-	2/7/25/26	0/2/2/2
2	OMC	4	32	2	-	0/9/27/28	0/2/2/2
66	4AC	1	1293	66	-	0/11/29/30	0/2/2/2
67	4AC	2	1233	67	-	0/11/29/30	0/2/2/2
67	A2M	2	373	67	-	0/9/27/28	0/3/3/3
66	4AC	1	2718	66	-	0/11/29/30	0/2/2/2
66	5MC	1	2198	66	-	0/7/25/26	0/2/2/2
66	OMU	1	2784	66	-	0/9/27/28	0/2/2/2
67	5MC	2	1496	67	-	0/7/25/26	0/2/2/2
66	4AC	1	2960	66	-	0/11/29/30	0/2/2/2
67	4AC	2	303	67	-	0/11/29/30	0/2/2/2
67	4AC	2	1147	67	-	1/11/29/30	0/2/2/2
67	MA6	2	1488	67	-	2/11/29/30	0/3/3/3
66	5MC	1	2183	66	-	0/7/25/26	0/2/2/2
66	OMC	1	1948	66	-	0/9/27/28	0/2/2/2
67	4AC	2	868	67	-	0/11/29/30	0/2/2/2
2	5MU	4	54	2	-	0/7/25/26	0/2/2/2
67	LHH	2	250	67	-	0/13/31/32	0/2/2/2
66	4AC	1	1243	66	-	0/11/29/30	0/2/2/2
66	4AC	1	136	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2908	66	-	0/11/29/30	0/2/2/2
66	OMG	1	2138	66	-	0/9/27/28	0/3/3/3
67	6MZ	2	1469	68,67	-	0/9/27/28	0/3/3/3
66	A2M	1	1055	66	-	0/9/27/28	0/3/3/3
66	4AC	1	835	66	-	0/11/29/30	0/2/2/2
67	OMC	2	1036	67	-	0/9/27/28	0/2/2/2
66	4AC	1	1554	66	-	0/11/29/30	0/2/2/2
66	4AC	1	2136	66	-	0/11/29/30	0/2/2/2
67	UR3	2	1467	67	-	0/7/25/26	0/2/2/2
67	4AC	2	626	67	-	0/11/29/30	0/2/2/2
66	4AC	1	641	66	-	0/11/29/30	0/2/2/2
67	OMU	2	20	67	-	5/9/27/28	0/2/2/2
66	4AC	1	341	66	-	0/11/29/30	0/2/2/2
67	4AC	2	957	67	-	0/11/29/30	0/2/2/2
66	4AC	1	1934	66	-	0/11/29/30	0/2/2/2
66	5MC	1	2203	66	-	0/7/25/26	0/2/2/2
66	4AC	1	1938	66	-	0/11/29/30	0/2/2/2
67	5MC	2	1498	67	-	4/7/25/26	0/2/2/2
66	4AC	1	1780	66	-	0/11/29/30	0/2/2/2
67	OMG	2	657	67	-	0/9/27/28	0/3/3/3
66	4AC	1	1873	66	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	4AC	2	319	67	-	0/11/29/30	0/2/2/2
66	A2M	1	2173	66	-	0/9/27/28	0/3/3/3
66	4AC	1	243	66	-	0/11/29/30	0/2/2/2
66	4AC	1	458	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1065	66	-	0/11/29/30	0/2/2/2
67	4AC	2	751	67	-	0/11/29/30	0/2/2/2
67	4AC	2	851	67	-	0/11/29/30	0/2/2/2
2	4SU	4	8	2	-	2/7/25/26	0/2/2/2
66	4AC	1	2249	66	-	0/11/29/30	0/2/2/2
66	4AC	1	314	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1962	66	-	0/11/29/30	0/2/2/2
66	LHH	1	616	66	-	0/13/31/32	0/2/2/2
66	5MC	1	2162	66	-	0/7/25/26	0/2/2/2
66	4AC	1	2865	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1557	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1695	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1765	66	-	0/11/29/30	0/2/2/2
67	4AC	2	703	67	-	0/11/29/30	0/2/2/2
67	OMG	2	471	67	-	0/9/27/28	0/3/3/3
66	4AC	1	2937	68,66	-	1/11/29/30	0/2/2/2
67	B8H	2	938	67	-	0/7/25/26	0/2/2/2
66	4AC	1	229	66	-	0/11/29/30	0/2/2/2
66	OMG	1	789	66	-	2/9/27/28	0/3/3/3
67	OMC	2	1376	67	-	0/9/27/28	0/2/2/2
67	OMU	2	1177	67	-	0/9/27/28	0/2/2/2
67	5MC	2	1025	67	-	0/7/25/26	0/2/2/2
66	OMG	1	2678	66	-	0/9/27/28	0/3/3/3
66	5MC	1	2093	66	-	0/7/25/26	0/2/2/2
67	4AC	2	590	67	-	0/11/29/30	0/2/2/2
67	OMG	2	680	67	-	0/9/27/28	0/3/3/3
67	OMU	2	787	67	-	4/9/27/28	0/2/2/2
67	OMG	2	934	67	-	0/9/27/28	0/3/3/3
1	4AC	3	32	1	-	2/11/29/30	0/2/2/2
66	4AC	1	211	66	-	0/11/29/30	0/2/2/2
66	4AC	1	922	66	-	0/11/29/30	0/2/2/2
67	4AC	2	546	67	-	0/11/29/30	0/2/2/2
67	4AC	2	828	67	-	0/11/29/30	0/2/2/2
67	LHH	2	1041	67	-	0/11/29/32	0/2/2/2
66	4AC	1	2027	66	-	0/11/29/30	0/2/2/2
67	4AC	2	17	67	-	0/11/29/30	0/2/2/2
66	4AC	1	2925	66	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	4AC	1	1460	66	-	0/11/29/30	0/2/2/2
67	OMU	2	64	67	-	0/9/27/28	0/2/2/2
66	4AC	1	1594	68,66	-	0/11/29/30	0/2/2/2
67	MA6	2	1487	67	-	0/11/29/30	0/3/3/3
66	4AC	1	2642	66	-	0/11/29/30	0/2/2/2
67	OMC	2	1040	67	-	0/9/27/28	0/2/2/2
66	4AC	1	2083	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1621	66	-	0/11/29/30	0/2/2/2
67	OMG	2	1069	67	-	1/9/27/28	0/3/3/3
67	4AC	2	1479	67	-	0/11/29/30	0/2/2/2
66	4AC	1	2287	66	-	0/11/29/30	0/2/2/2
67	4AC	2	848	67	-	0/11/29/30	0/2/2/2
67	4AC	2	636	67	-	0/11/29/30	0/2/2/2
67	4AC	2	839	67	-	0/11/29/30	0/2/2/2
66	4AC	1	2062	66	-	0/11/29/30	0/2/2/2
66	5MC	1	2163	66	-	0/7/25/26	0/2/2/2
66	4AC	1	91	66	-	0/11/29/30	0/2/2/2
67	5MC	2	535	67	-	0/7/25/26	0/2/2/2
67	4AC	2	1184	67	-	0/11/29/30	0/2/2/2
66	4AC	1	1667	66	-	0/11/29/30	0/2/2/2
66	4AC	1	60	66	-	0/11/29/30	0/2/2/2
67	5MC	2	1505	67	-	2/7/25/26	0/2/2/2
67	OMC	2	129	67	-	0/9/27/28	0/2/2/2
66	4AC	1	1550	66	-	0/11/29/30	0/2/2/2
66	4AC	1	1068	66	-	0/11/29/30	0/2/2/2
66	4AC	1	357	66	-	0/11/29/30	0/2/2/2
67	4AC	2	511	67	-	0/11/29/30	0/2/2/2
66	4AC	1	1755	66	-	0/11/29/30	0/2/2/2
67	5MC	2	1202	67	-	1/7/25/26	0/2/2/2
2	H2U	4	20	2	-	3/7/38/39	0/2/2/2
66	4AC	1	1617	66	-	0/11/29/30	0/2/2/2
66	5MC	1	2733	66	-	5/7/25/26	0/2/2/2

The worst 5 of 349 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4	8	4SU	C4-S4	-4.63	1.59	1.68
67	2	1469	6MZ	C5-C4	4.58	1.47	1.39
66	1	1055	A2M	C5-C4	4.33	1.47	1.39
67	2	1487	MA6	C5-C4	4.31	1.47	1.39
67	2	373	A2M	C5-C4	4.27	1.47	1.39

The worst 5 of 668 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4	20	H2U	C4-N3-C2	-7.53	119.55	125.79
67	2	657	OMG	C5-C4-N3	-6.50	117.92	128.46
2	4	8	4SU	C4-N3-C2	-6.46	121.07	127.34
66	1	1055	A2M	C5-C4-N3	-6.31	118.52	126.75
67	2	471	OMG	C5-C4-N3	-6.28	118.28	128.46

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	4	20	H2U	O4'-C1'-N1-C6
66	1	789	OMG	O4'-C4'-C5'-O5'
66	1	789	OMG	C3'-C4'-C5'-O5'
66	1	2147	OMG	C3'-C4'-C5'-O5'
66	1	2585	4AC	O4'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 257 ligands modelled in this entry, 257 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
66	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	107:G	O3'	112:A	P	11.57

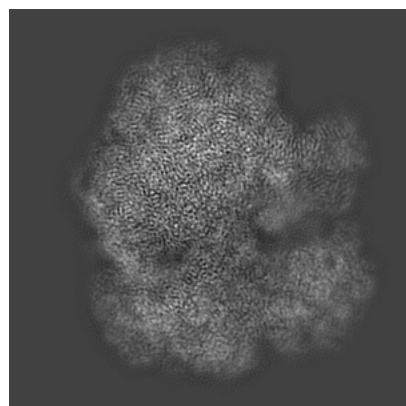
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55139. These allow visual inspection of the internal detail of the map and identification of artifacts.

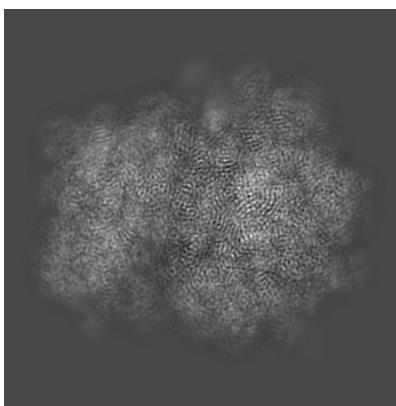
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

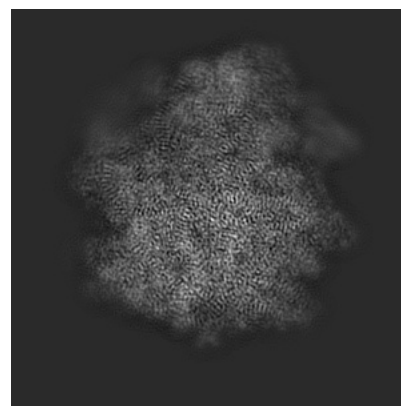
6.1.1 Primary map



X

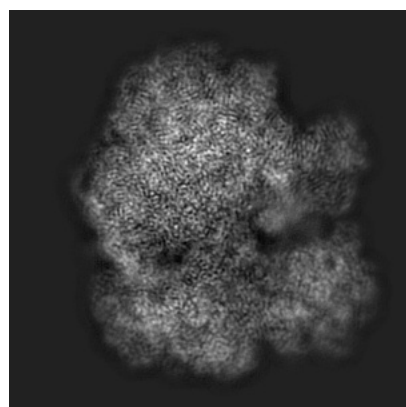


Y

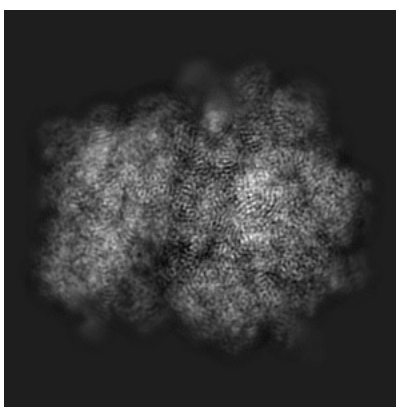


Z

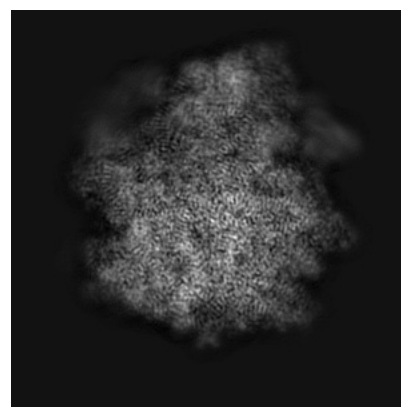
6.1.2 Raw map



X



Y

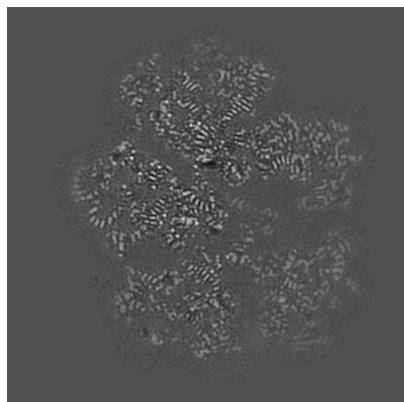


Z

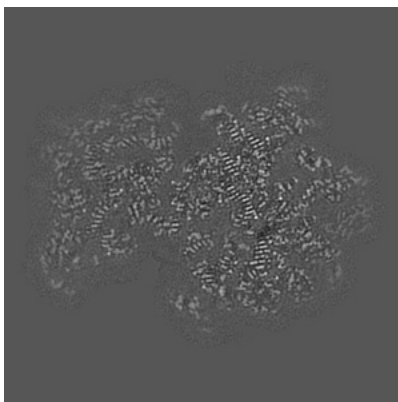
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

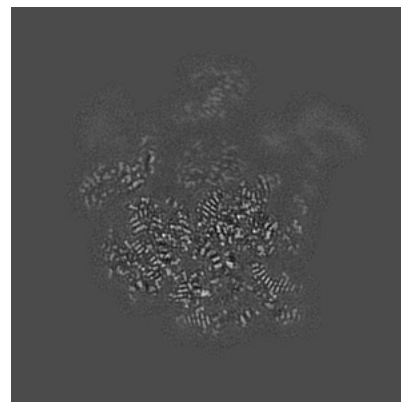
6.2.1 Primary map



X Index: 180

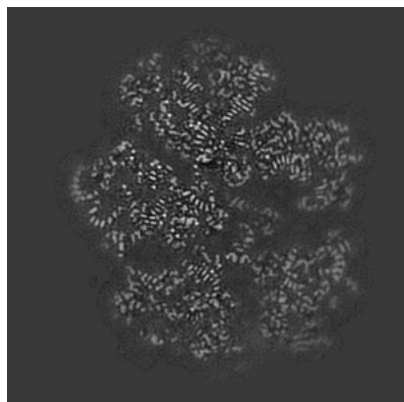


Y Index: 180

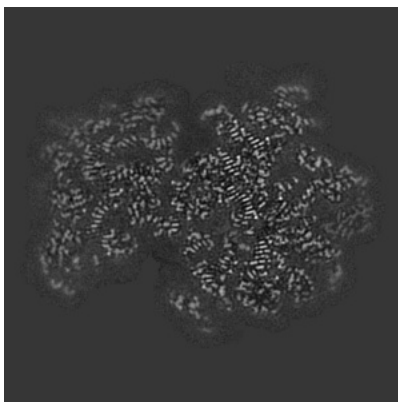


Z Index: 180

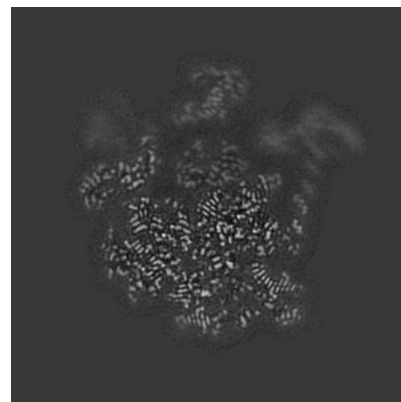
6.2.2 Raw map



X Index: 180



Y Index: 180

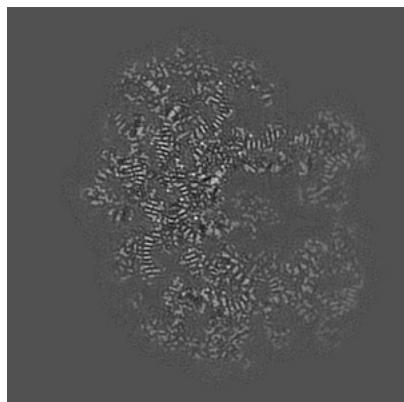


Z Index: 180

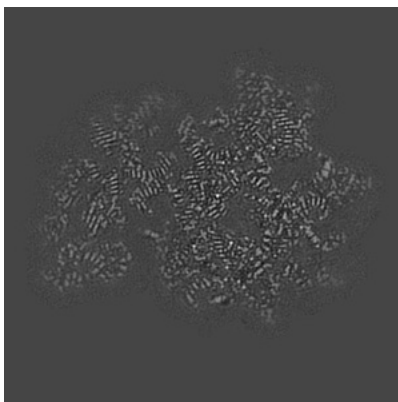
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

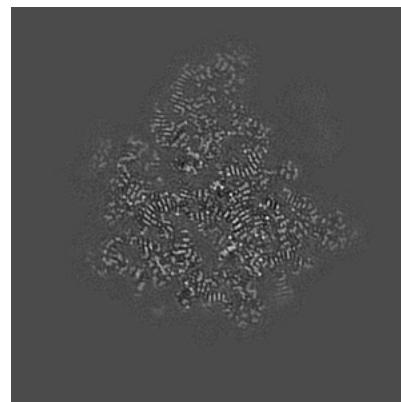
6.3.1 Primary map



X Index: 195

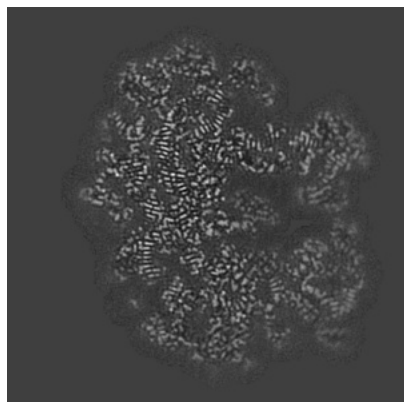


Y Index: 166

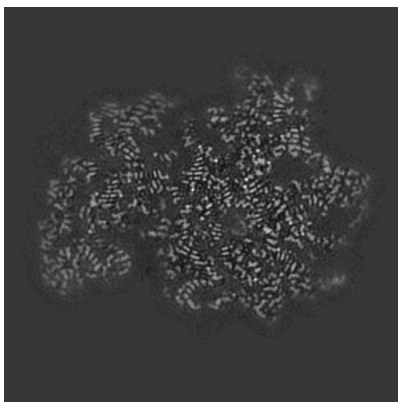


Z Index: 228

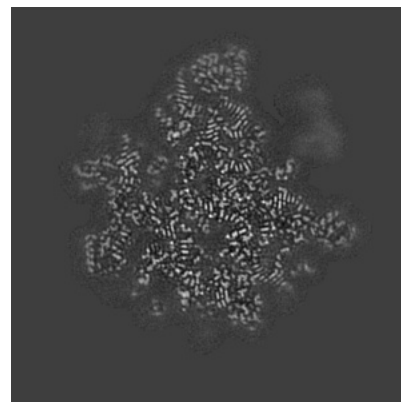
6.3.2 Raw map



X Index: 196



Y Index: 170

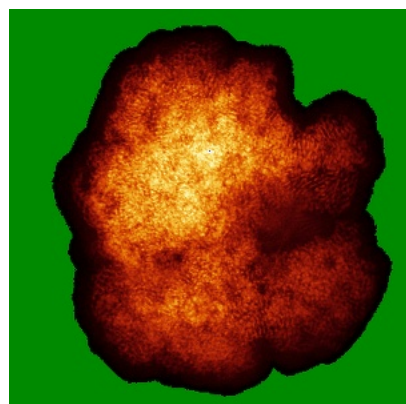


Z Index: 222

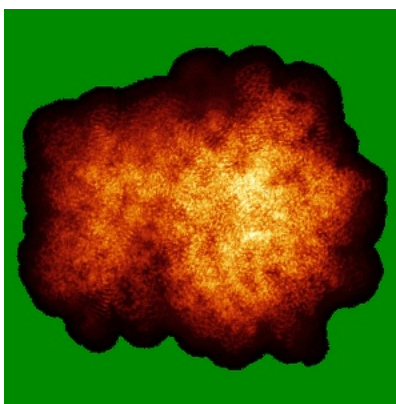
The images above show the largest variance slices of the map in three orthogonal directions.

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

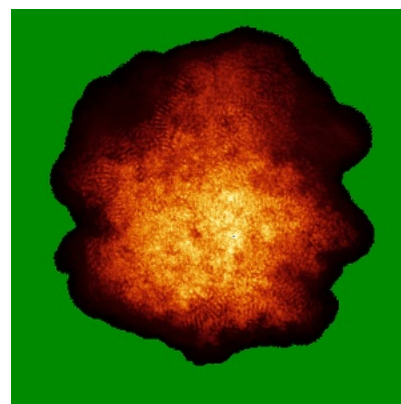
6.4.1 Primary map



X

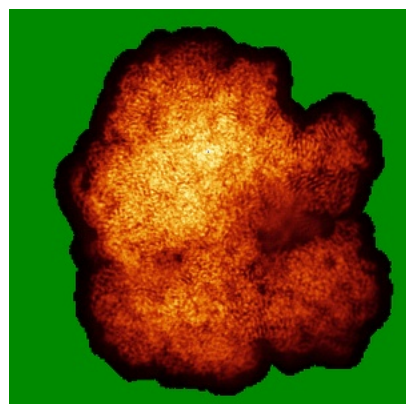


Y

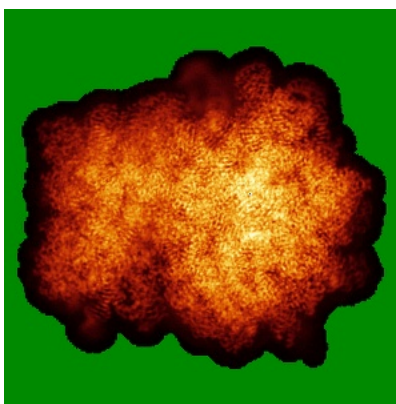


Z

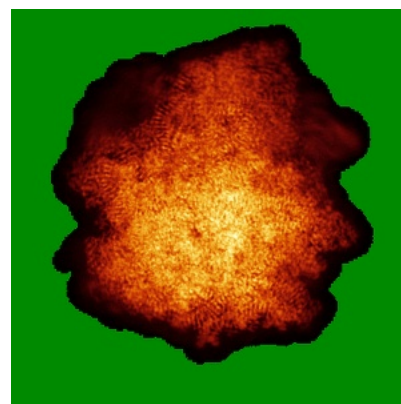
6.4.2 Raw map



X



Y

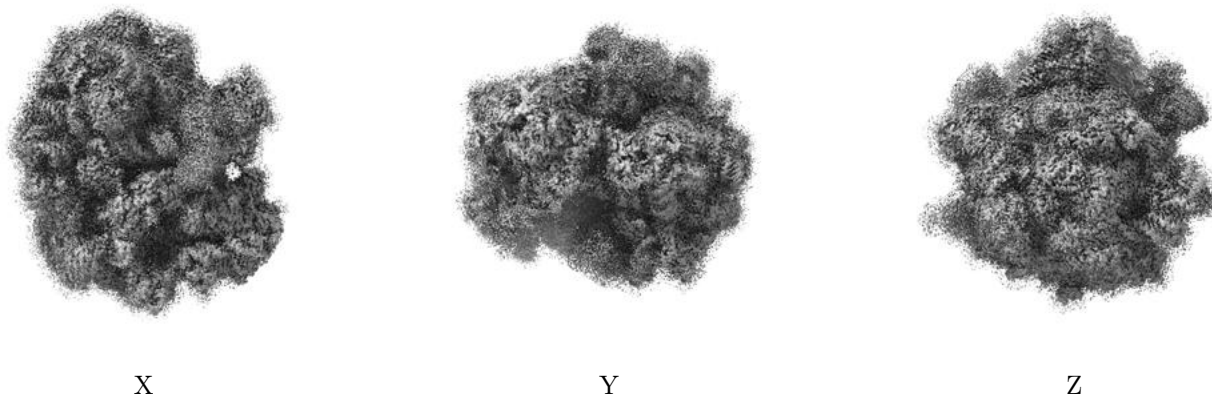


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

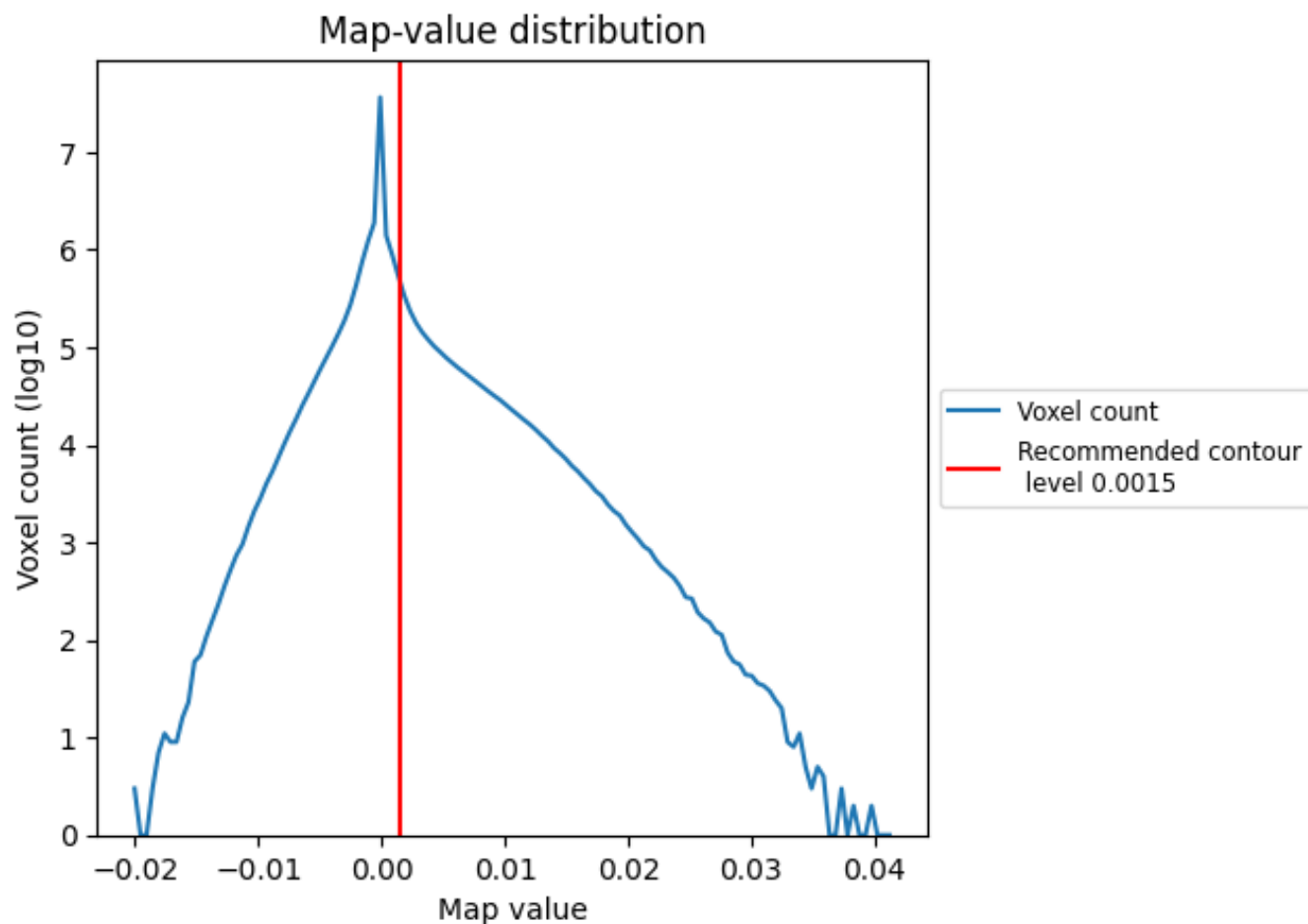
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

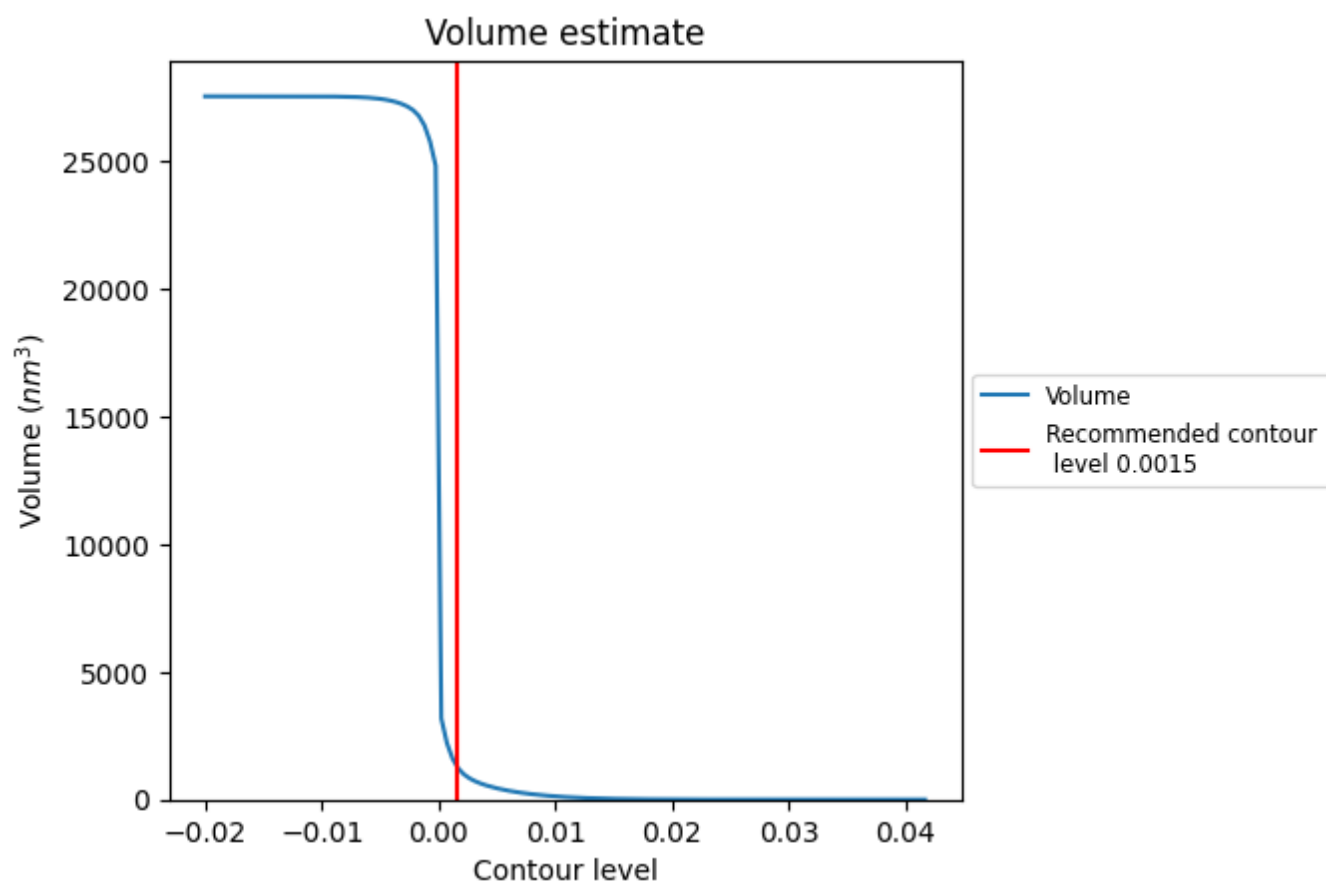
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

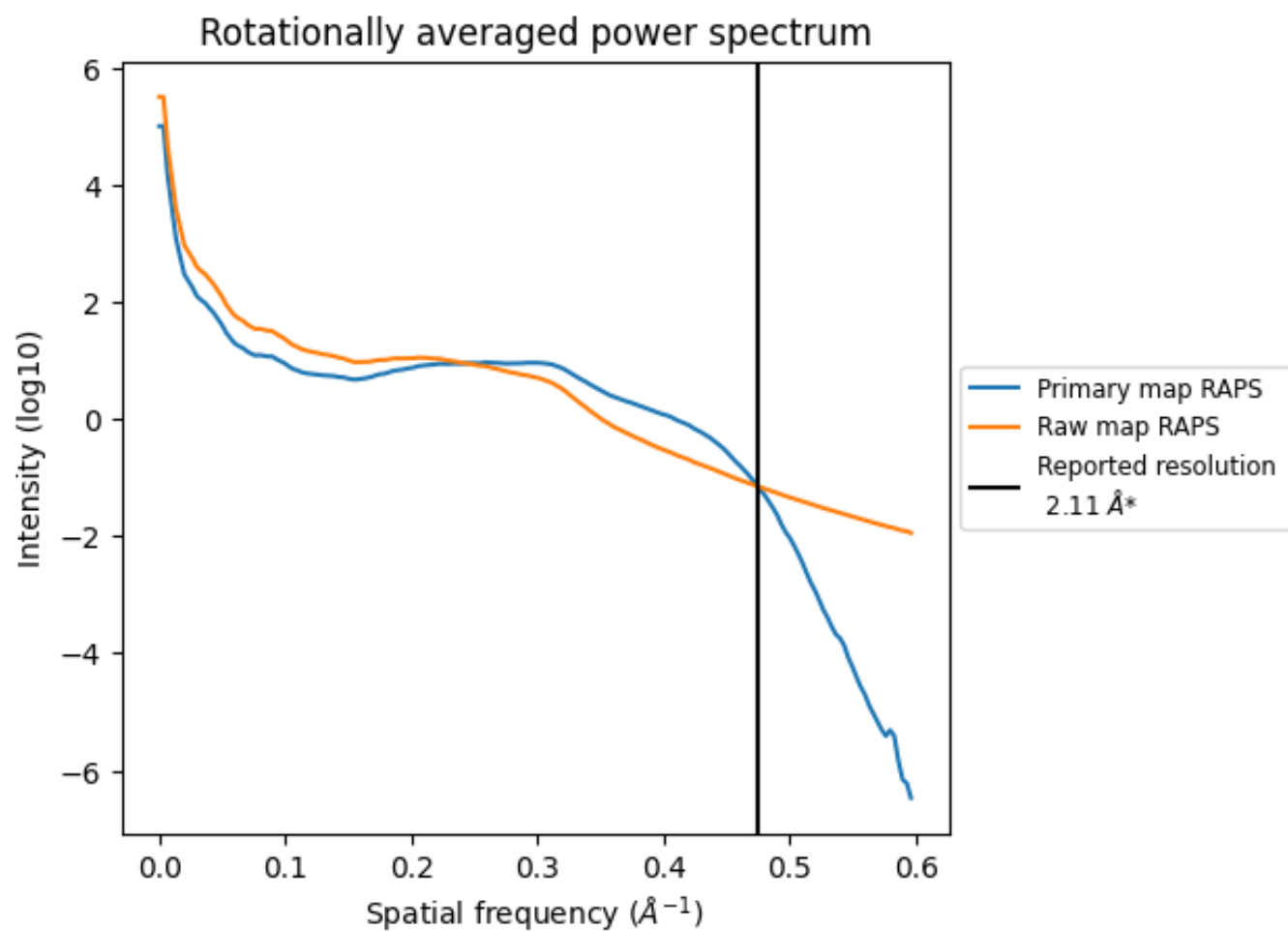
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1353 nm^3 ; this corresponds to an approximate mass of 1222 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 ⓘ

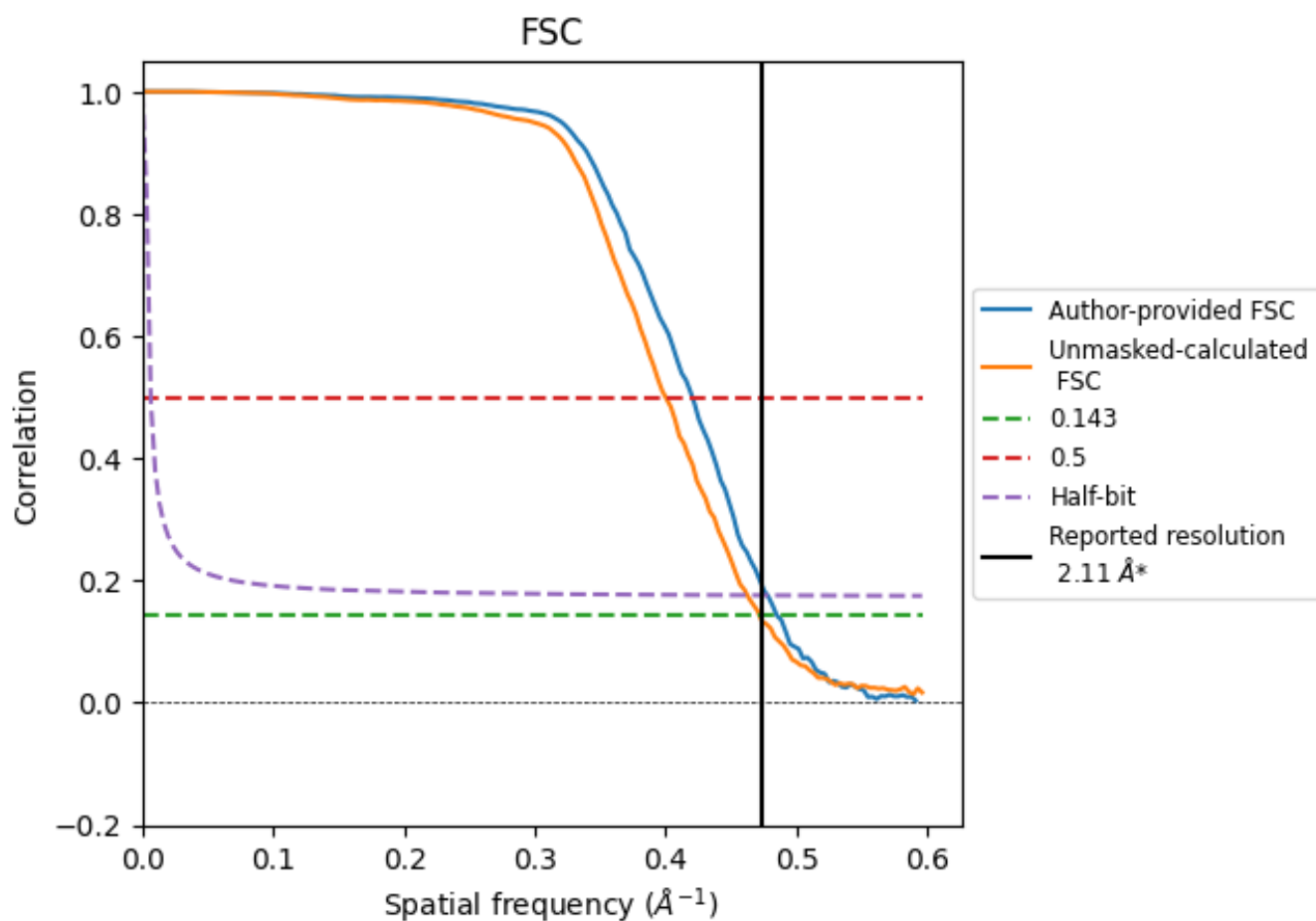


*Reported resolution corresponds to spatial frequency of $0.474 \text{ \AA}^{-1}$

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 0.474 Å⁻¹

8.2 Resolution estimates [i](#)

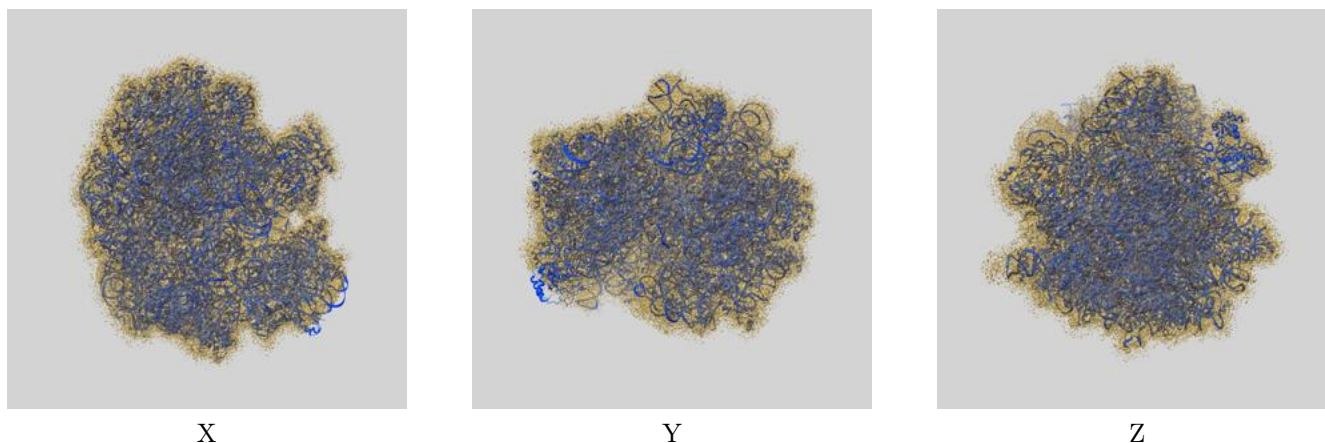
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.11	-	-
Author-provided FSC curve	2.06	2.38	2.09
Unmasked-calculated*	2.12	2.50	2.16

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

9 Map-model fit [i](#)

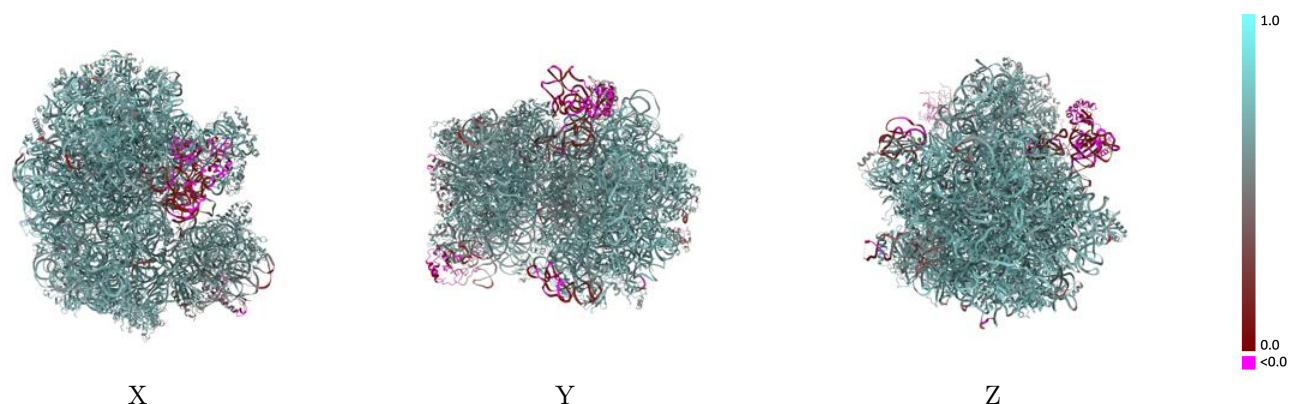
This section contains information regarding the fit between EMDB map EMD-55139 and PDB model 9SRE. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



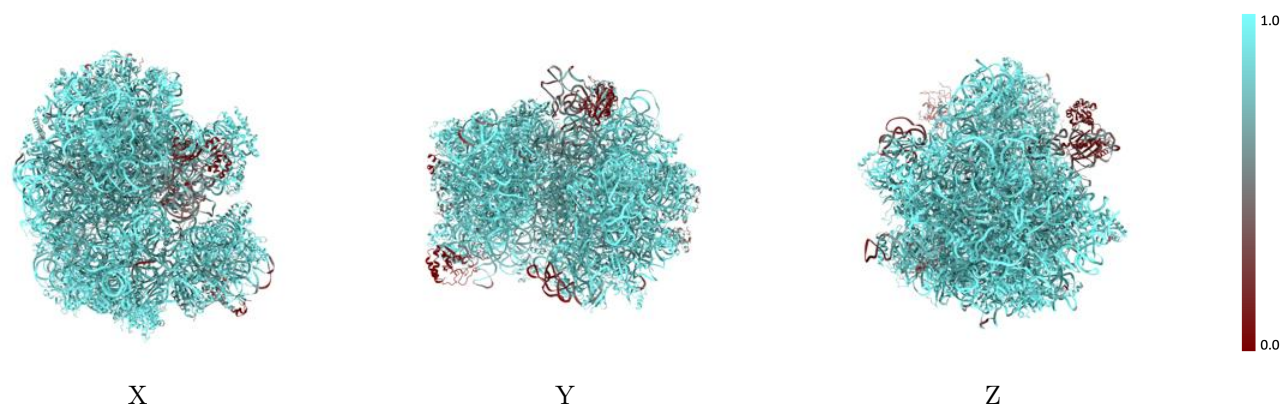
The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



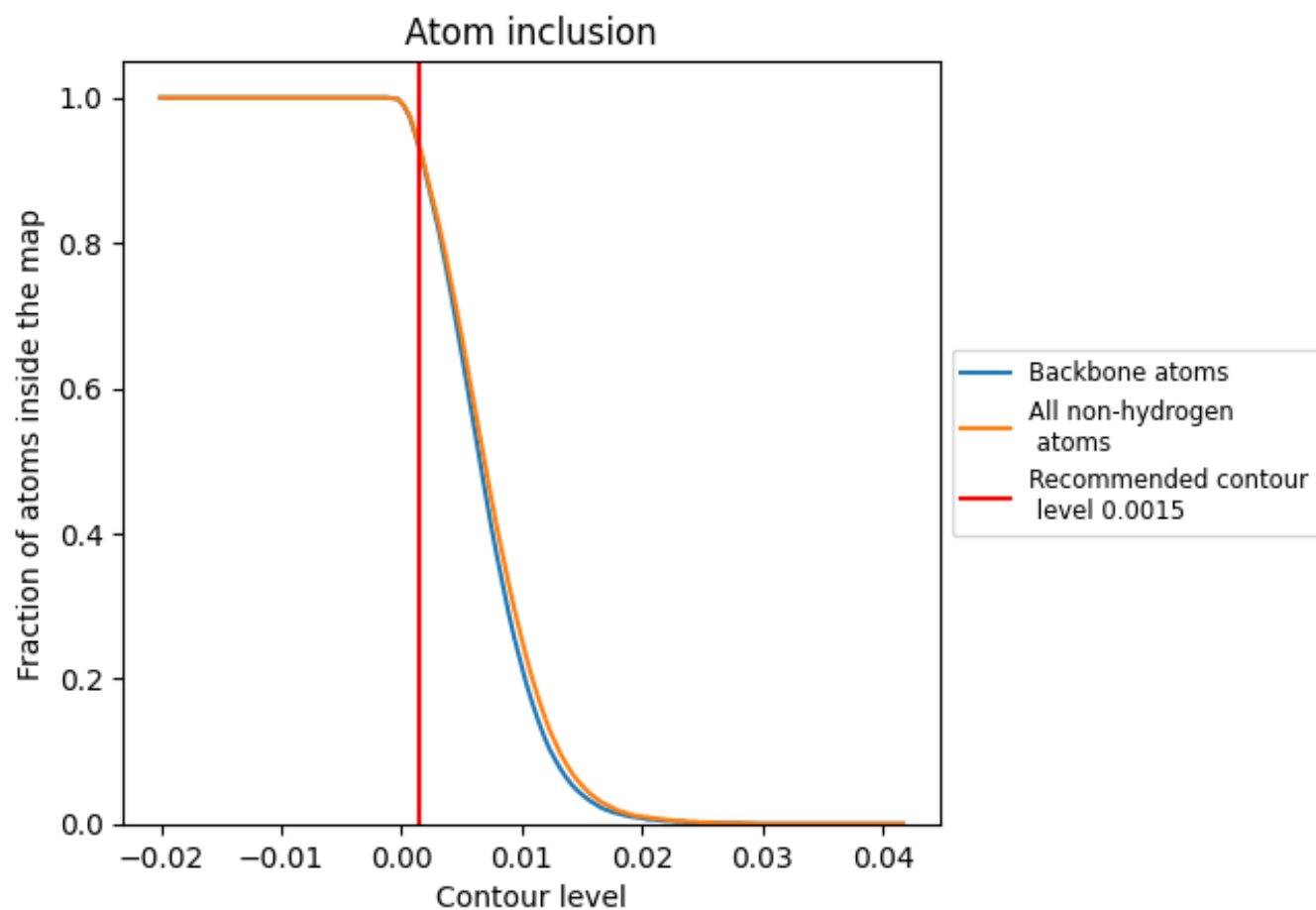
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.0015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.6440
1	 0.9510	 0.6610
2	 0.9710	 0.6530
3	 0.9890	 0.6570
4	 0.5780	 0.2760
A0	 0.9780	 0.7200
A3	 0.0620	 0.0830
AA	 0.9100	 0.6190
AB	 0.9490	 0.6240
AC	 0.9430	 0.6470
AD	 0.9710	 0.6700
AE	 0.9740	 0.6750
AF	 0.9610	 0.6670
AG	 0.8860	 0.5720
AH	 0.9440	 0.6180
AI	 0.9830	 0.6910
AJ	 0.9680	 0.6870
AK	 0.9420	 0.6100
AL	 0.6820	 0.4510
AM	 0.9570	 0.6600
AN	 0.9750	 0.6940
AO	 0.9220	 0.6070
AP	 0.9260	 0.6170
AQ	 0.9520	 0.6600
AR	 0.9750	 0.6930
AS	 0.8800	 0.5390
AT	 0.8820	 0.5770
AU	 0.9400	 0.6040
AV	 0.9500	 0.6330
AW	 0.9190	 0.5930
AX	 0.8990	 0.5940
AY	 0.1010	 0.1260
AZ	 0.8440	 0.5420
B4	 0.5960	 0.4050
B5	 0.9680	 0.6580



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Chain	Atom inclusion	Q-score
B6	 0.8060	 0.6150
BA	 0.1380	 0.0390
BB	 0.9800	 0.7290
BC	 0.9800	 0.7170
BD	 0.9820	 0.7090
BE	 0.9130	 0.5960
BF	 0.9480	 0.6600
BG	 0.9490	 0.6640
BI	 0.9790	 0.7150
BJ	 0.9810	 0.7170
BK	 0.9390	 0.6160
BL	 0.9540	 0.6780
BM	 0.9930	 0.7350
BN	 0.9640	 0.6860
BO	 0.9610	 0.6480
BP	 0.9840	 0.7130
BQ	 0.9760	 0.7080
BR	 0.9880	 0.7150
BS	 0.9860	 0.7170
BT	 0.9800	 0.7000
BU	 0.9730	 0.6850
BV	 0.9650	 0.6940
BW	 0.8890	 0.6320
BY	 0.9820	 0.7110
BZ	 0.9510	 0.6520
Ba	 0.9550	 0.6820
Bb	 0.9770	 0.7160
Bc	 0.9790	 0.7140
Bd	 0.9750	 0.7040
Be	 0.9980	 0.7350
Bf	 0.9980	 0.7240
Bg	 0.9780	 0.6780
Bi	 0.9720	 0.7230
Bj	 0.9540	 0.6970
Bk	 0.9510	 0.6740
Bl	 0.9410	 0.6410
H	 0.8240	 0.6120