wwPDB EM Validation Summary Report (i)

Sep 15, 2026 – 11:55 PM EDT

PDB ID	:	9PJ9 / pdb_00009pj9
EMDB ID	:	EMD-71684
Title	:	C. acnes 70S ribosome bound to Minocycline
Authors	:	Devarkar, S.C.; Lomakin, I.B.; Bunick, C.G.
Deposited on	:	2025-07-12
Resolution	:	2.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

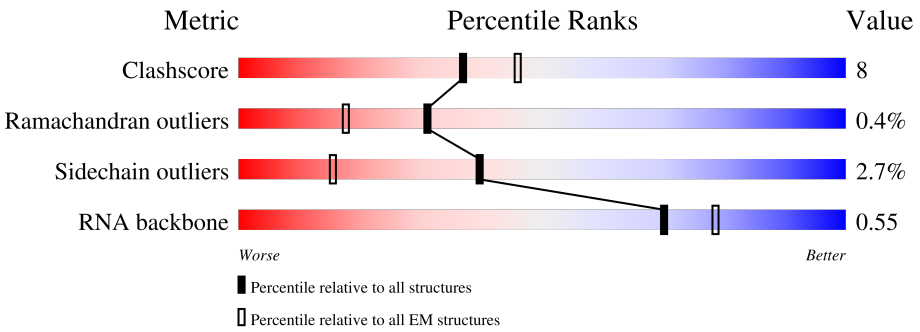
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

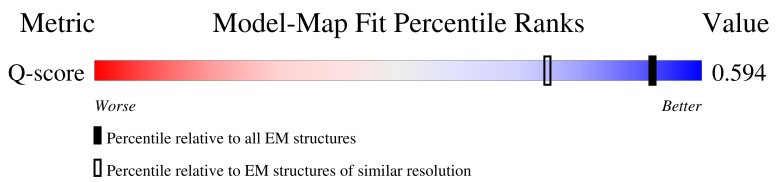
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	56	77% 12% 11%
2	1	44	86% 14%
3	2	68	94%

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Mol	Chain	Length	Quality of chain
4	3	37	81% 16%
5	4	69	7% 75% 17%
6	A	1537	58% 34% 6%
7	B	283	70% 46% 34% 18%
8	C	76	72% 20% 7%
9	D	201	68% 31%
10	E	215	59% 24% 17%
11	F	96	70% 28%
12	G	269	57% 19% 23%
13	H	135	76% 24%
14	I	156	68% 31%
15	J	173	49% 28% 23%
16	K	135	66% 20% 13%
17	L	123	85% 15%
18	M	103	6% 49% 43% 5%
19	N	123	5% 69% 30%
20	O	87	80% 20%
21	P	147	9% 64% 20% 13%
22	Q	90	6% 72% 27%
23	R	79	5% 58% 23% 15%
24	S	61	77% 21%
25	T	88	86% 13%
26	U	93	69% 20% 10%
27	V	24	96%
28	X	33	79% 18%

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Mol	Chain	Length	Quality of chain
29	Y	22	5% 14% 23% 9% 55%
30	a	3086	62% 26% 6% 6%
31	b	120	80% 18%
32	c	278	87% 12%
33	d	223	84% 12%
34	e	301	52% 14% 30%
35	f	210	64% 23% 12%
36	g	180	73% 24%
37	i	147	91% 8%
38	j	122	78% 21%
39	k	146	77% 19%
40	l	139	78% 19%
41	m	187	51% 12% 36%
42	n	127	74% 24%
43	o	117	79% 17%
44	p	123	84% 12%
45	q	102	74% 25%
46	r	153	69% 16% 14%
47	s	102	75% 18% 7%
48	t	122	76% 10% 12%
49	u	205	20% 73% 14% 13%
50	v	89	72% 15% 12%
51	w	61	75% 20%
52	x	77	74% 16% 10%
53	y	60	87% 10%

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Mol	Chain	Length	Quality of chain
54	z	63	89% 10%

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 144436 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 protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	50	423	253	91	73	6	0	0

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	44	362	213	91	56	2	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	67	513	315	110	87	1	0	0

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	37	302	184	66	47	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	66	512	313	97	97	5	0	0

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	A	1505	32340	14408	5893	10534	1505	0	0

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	233	1836	1163	326	338	9	0	0

- Molecule 8 is a RNA chain called initiator tRNA Met.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
8	C	75	1605	716	291	522	75	1	0	0

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	D	200	1632	1021	313	297	1	0	0

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	E	179	1309	816	244	245	4	0	0

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	F	96	785	496	134	149	6	0	0

- Molecule 12 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	206	1613	1010	305	294	4	0	0

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	H	134	1021	642	182	194	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	I	155	1225	764	235	220	6	0	0

- Molecule 15 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	J	134	1012	629	204	177	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	K	117	858	532	168	154	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	L	122	948	587	195	164	2	0	0

- Molecule 18 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	M	98	786	496	146	141	3	0	0

- Molecule 19 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	N	122	976	598	205	173	0	0

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	O	87	708	440	140	125	3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	P	128	994	621	185	187	1	0	0

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Q	90	728	446	142	134	6	0	0

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	R	67	527	334	103	90	0	0

- Molecule 24 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	S	60	474	298	98	73	5	0	0

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	T	87	673	408	144	121	0	0

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	84	658	416	126	113	3	0	0

- Molecule 27 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	V	23	183	106	50	27	0	0

- Molecule 28 is a protein called AURKAIP1/COX24 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	X	32	277	170	71	35	1	0	0

- Molecule 29 is a RNA chain called mRNA 32MF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	Y	10	211	95	35	71	10	0	0

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	a	2903	62450	27813	11394	20338	2905	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	63	A	G	conflict	GB CP012350
a	524	C	G	conflict	GB CP012350
a	1038	PSU	G	conflict	GB CP012350

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	b	120	2567	1145	466	836	120	0	0

- Molecule 32 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	c	274	2091	1289	425	372	5	0	0

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	d	214	1586	984	304	291	7	0	0

- Molecule 34 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	e	210	1577	979	301	295	2	0	0

- Molecule 35 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	f	184	1468	924	269	266	9	0	0

- Molecule 36 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	g	177	1376	867	250	258	1	0	0

- Molecule 37 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	i	146	1139	718	213	205	3	0	0

- Molecule 38 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	j	122	946	596	177	169	4	0	0

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	k	144	1072	675	196	199	2	0	0

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	l	136	1082	685	210	181	6	0	0

- Molecule 41 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	m	120	936	583	188	163	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	124	ALA	THR	conflict	UNP A0A8B2VJI7
m	185	PRO	SER	conflict	UNP A0A8B2VJI7

- Molecule 42 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	n	126	952	583	190	176	3	0	0

- Molecule 43 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	114	896	559	174	162	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	119	958	589	196	171	2	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	q	102	778	487	140	150	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	52	ALA	VAL	conflict	UNP Q6A9I3

- Molecule 46 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	r	132	1017	624	204	182	7	0	0

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	s	95	751	474	138	138	1	0	0

- Molecule 48 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	t	107	833	516	163	153	1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	u	179	1376	865	240	268	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	v	78	591	355	127	109	0	0

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	w	60	474	290	102	77	5	0	0

- Molecule 52 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	x	69	564	348	108	108	0	0

- Molecule 53 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	y	58	467	290	91	83	3	0	0

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	z	62	477	287	102	83	5	0	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	0	1	1	1	0
55	3	1	1	1	0
55	4	1	1	1	0
55	S	1	1	1	0
55	w	1	1	1	0
55	z	1	1	1	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	0	1	1	1	0
56	A	54	54	54	0
56	S	1	1	1	0
56	T	1	1	1	0
56	a	262	262	262	0
56	b	2	2	2	0
56	c	1	1	1	0

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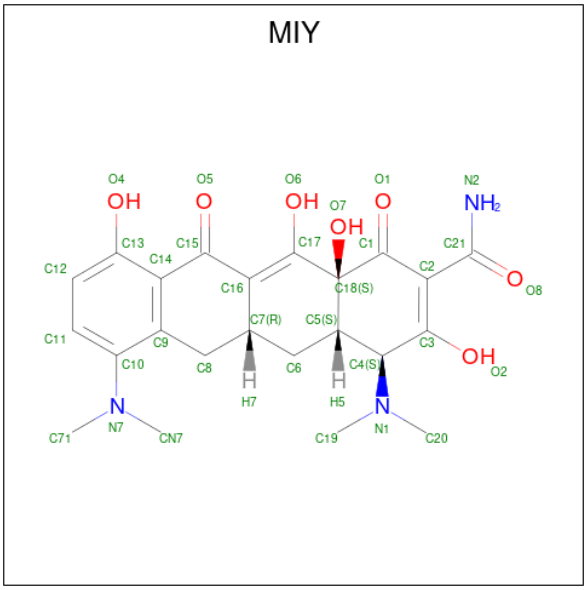
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	d	1	1	1	0
56	k	1	1	1	0

- Molecule 57 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: MIY) (formula: $C_{23}H_{27}N_3O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
57	A	1	33	23	3	7	0
57	a	1	33	23	3	7	0
57	a	1	33	23	3	7	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
58	1	1	1	1	0
58	A	9	9	9	0
58	a	80	80	80	0

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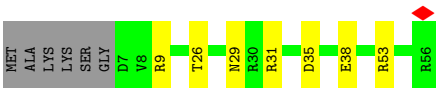
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
58	b	1	1	1	0
			Total	O	
58	c	1	1	1	0

3 Residue-property plots (i)

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

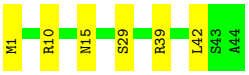
- Molecule 1: 50S ribosomal protein L33

Chain 0:



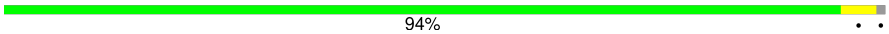
- Molecule 2: 50S ribosomal protein L34

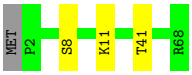
Chain 1:



- Molecule 3: Large ribosomal subunit protein bL35

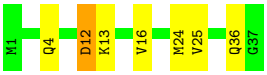
Chain 2:





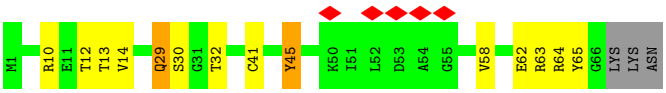
- Molecule 4: 50S ribosomal protein L36

Chain 3:



- Molecule 5: 50S ribosomal protein L31

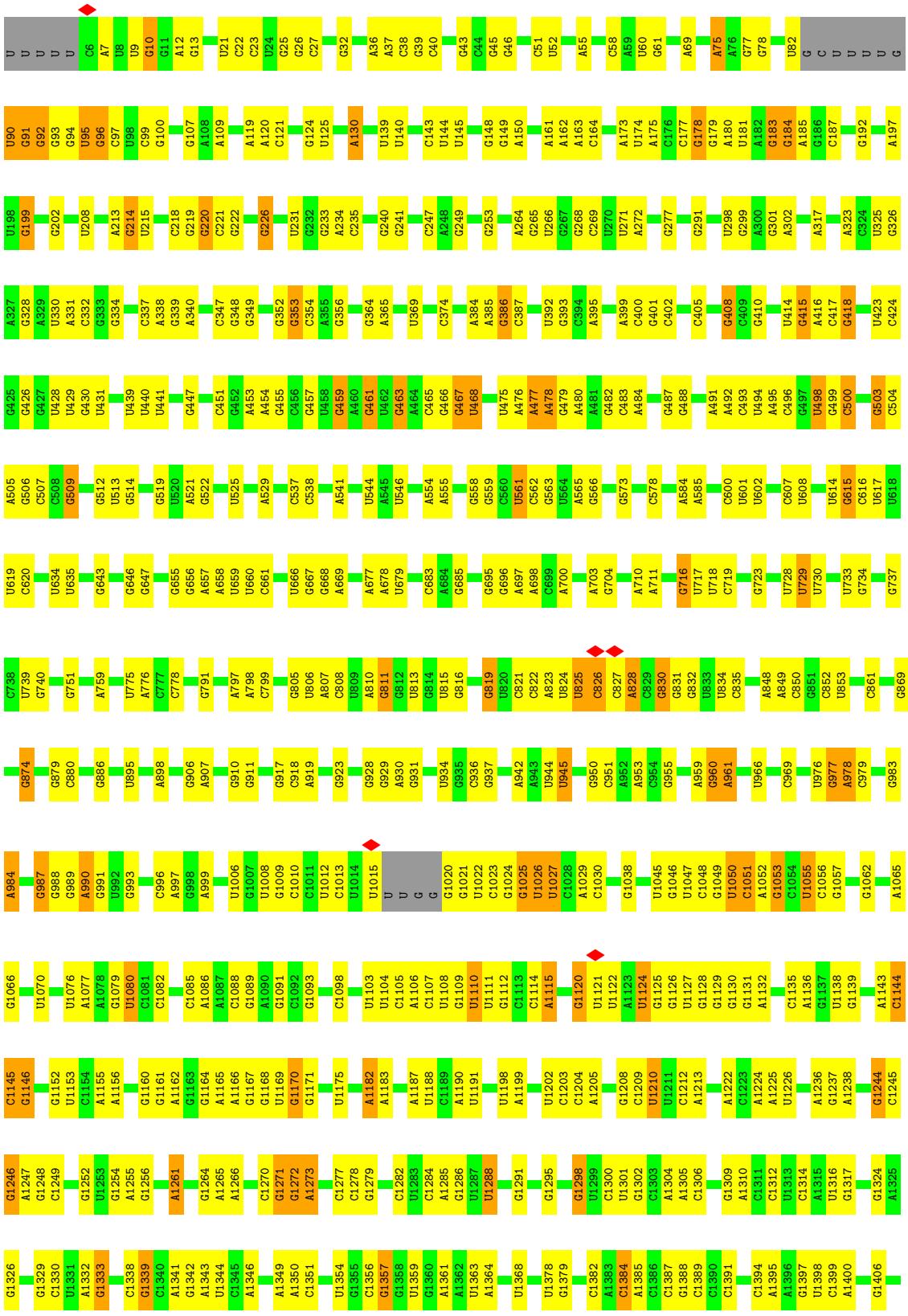
Chain 4:



- Molecule 6: 16S rRNA

Chain A:

58%
34%
6%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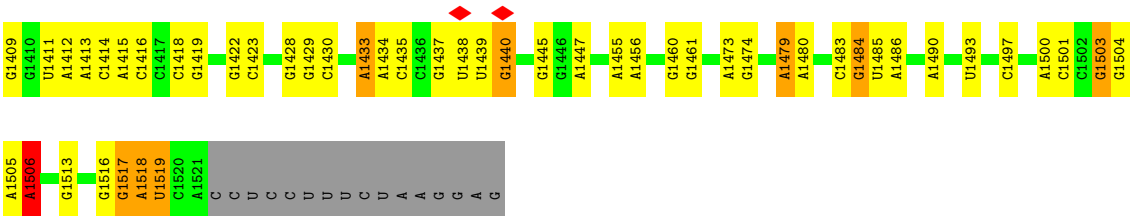
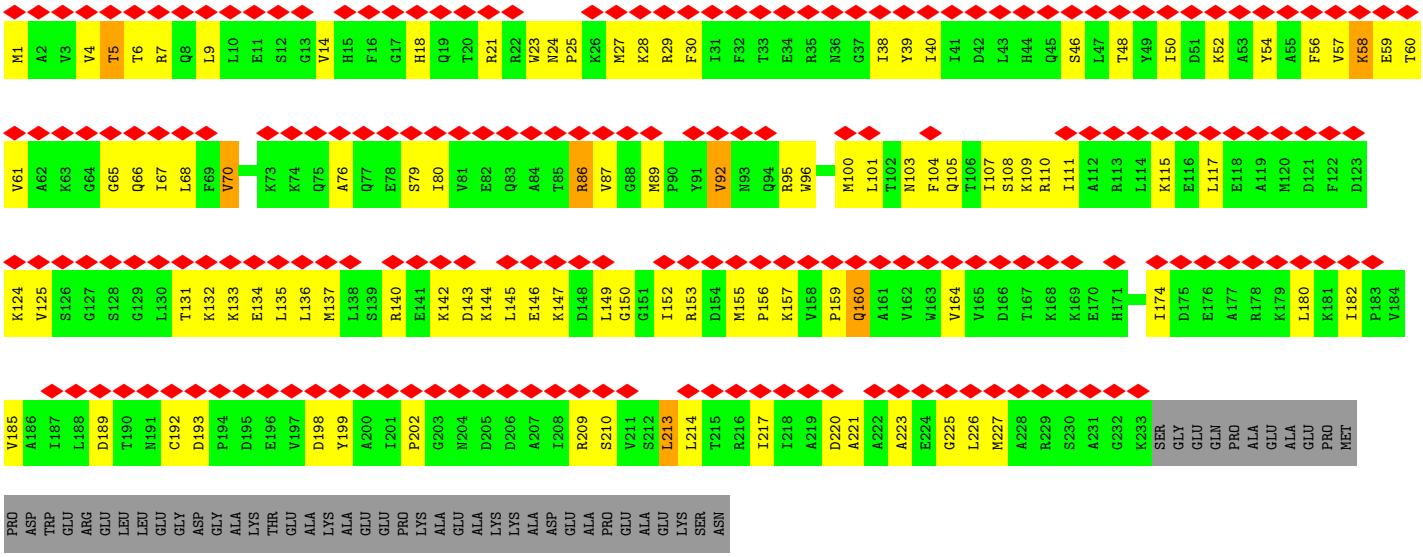


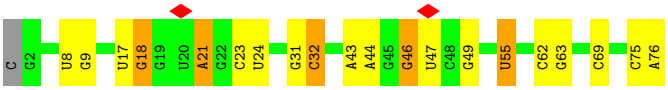
- Molecule 7: 30S ribosomal protein S2

Chain B:



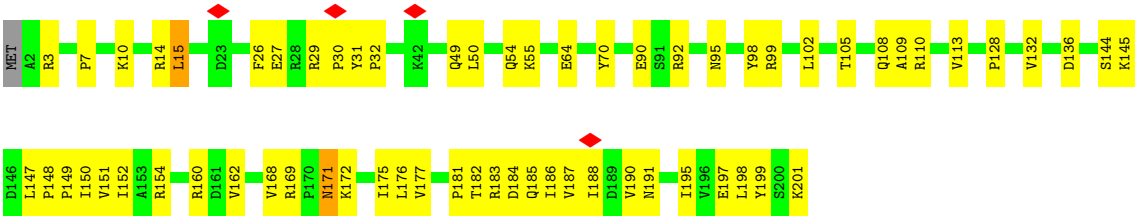
- Molecule 8: initiator tRNA Met

Chain C:



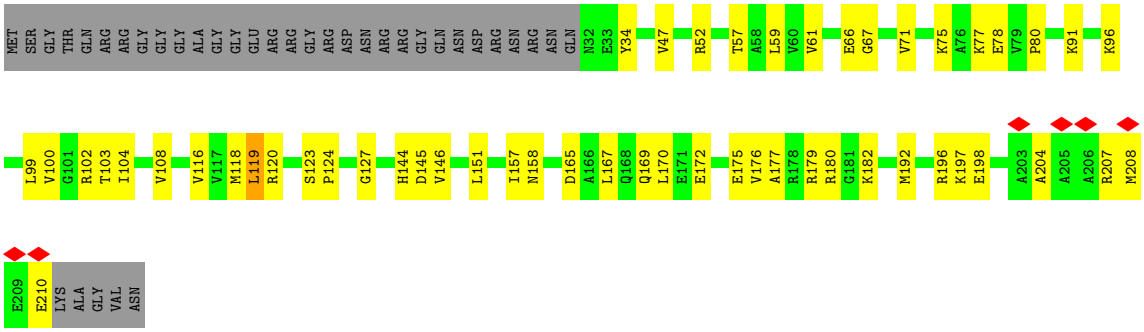
- Molecule 9: 30S ribosomal protein S4

Chain D:



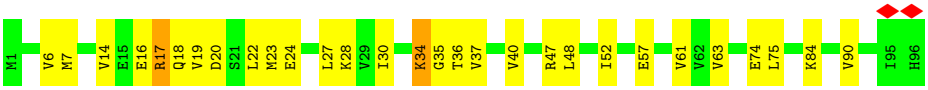
- Molecule 10: Small ribosomal subunit protein uS5

Chain E:



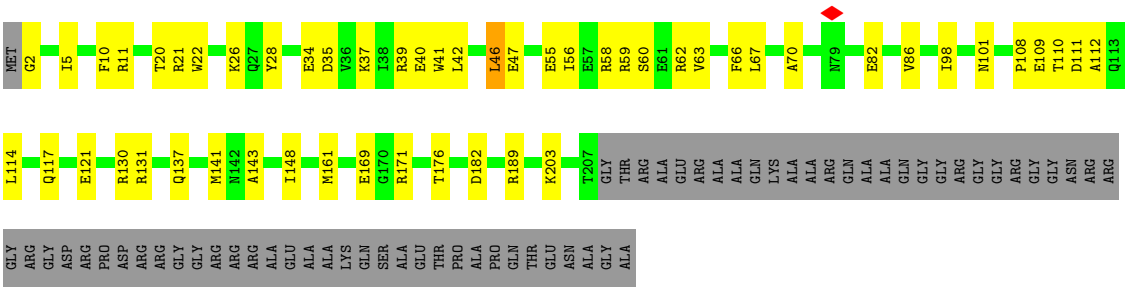
- Molecule 11: 30S ribosomal protein S6

Chain F:



- Molecule 12: 30S ribosomal protein S3

Chain G:

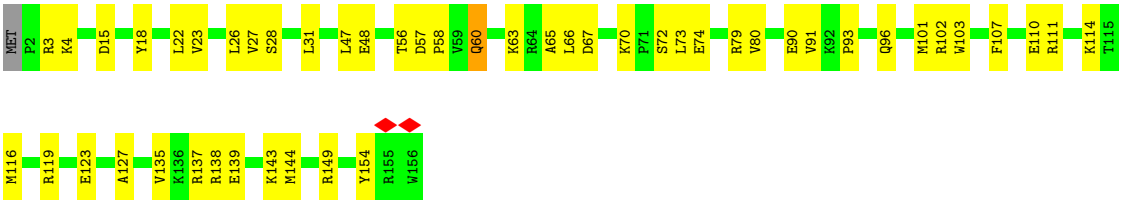


- Molecule 13: 30S ribosomal protein S8

Chain H:

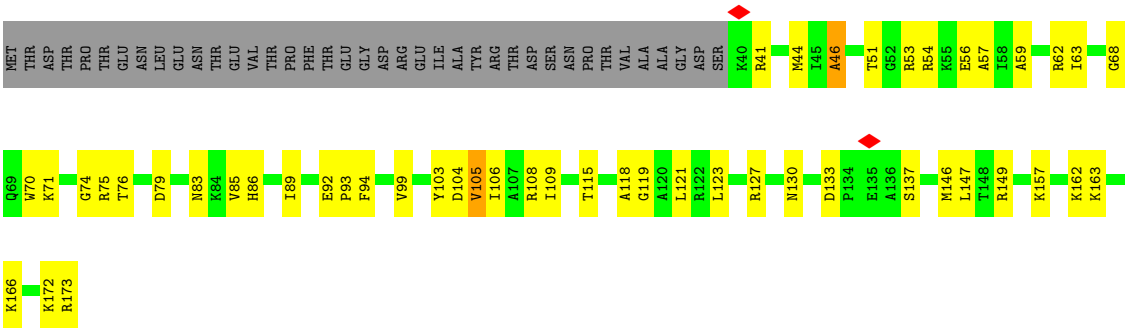
- Molecule 14: 30S ribosomal protein S7

Chain I:



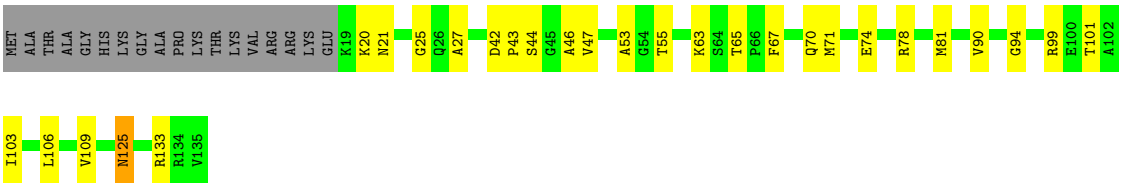
- Molecule 15: 30S ribosomal protein S9

Chain J:



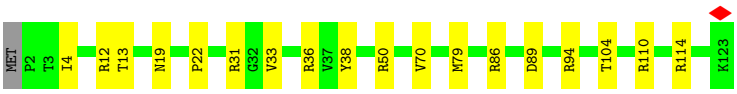
- Molecule 16: 30S ribosomal protein S11

Chain K:



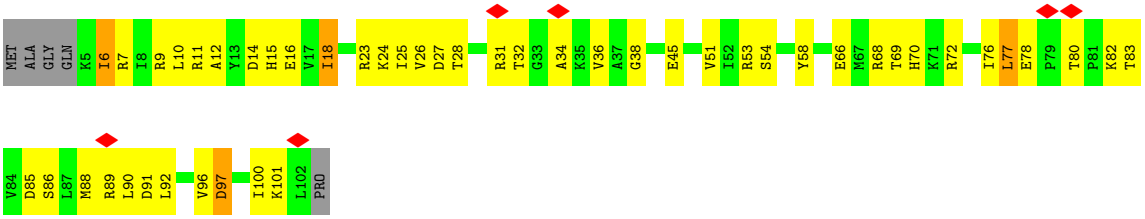
- Molecule 17: 30S ribosomal protein S12

Chain L:



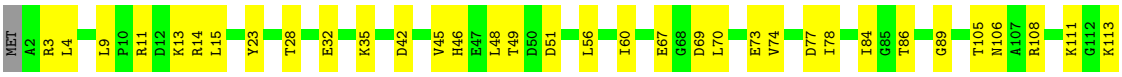
- Molecule 18: Small ribosomal subunit protein uS10

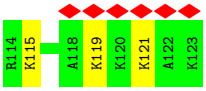
Chain M:



- Molecule 19: 30S ribosomal protein S13

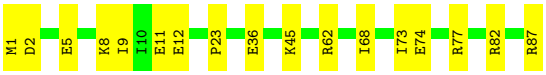
Chain N:





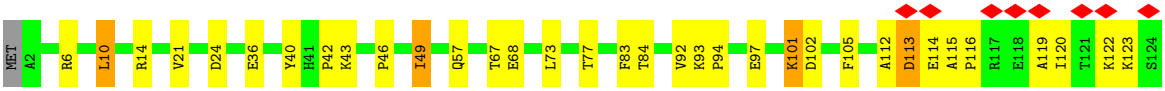
- Molecule 20: 30S ribosomal protein S15

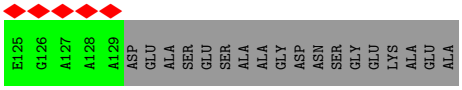
Chain O:



- Molecule 21: 30S ribosomal protein S16

Chain P:



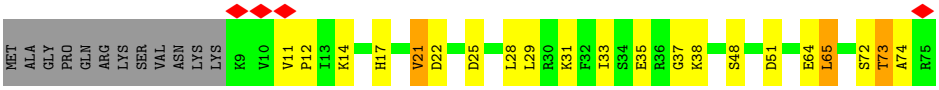


- Molecule 22: 30S ribosomal protein S17

Chain Q:

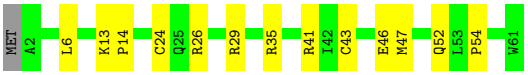
- Molecule 23: 30S ribosomal protein S18

Chain R:



- Molecule 24: 30S ribosomal protein S14 type Z

Chain S:

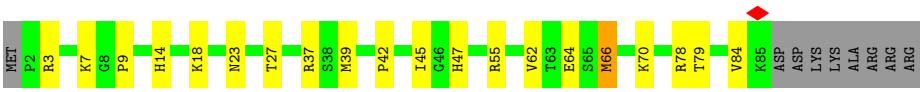


- Molecule 25: 30S ribosomal protein S20

Chain T:

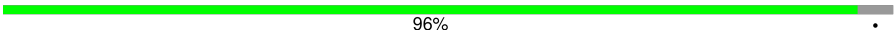
• Molecule 26: 30S ribosomal protein S19

Chain U:



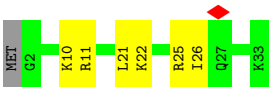
• Molecule 27: 50S ribosomal protein bL37

Chain V:



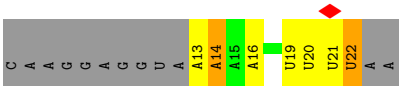
• Molecule 28: AURKAIP1/COX24 domain-containing protein

Chain X:



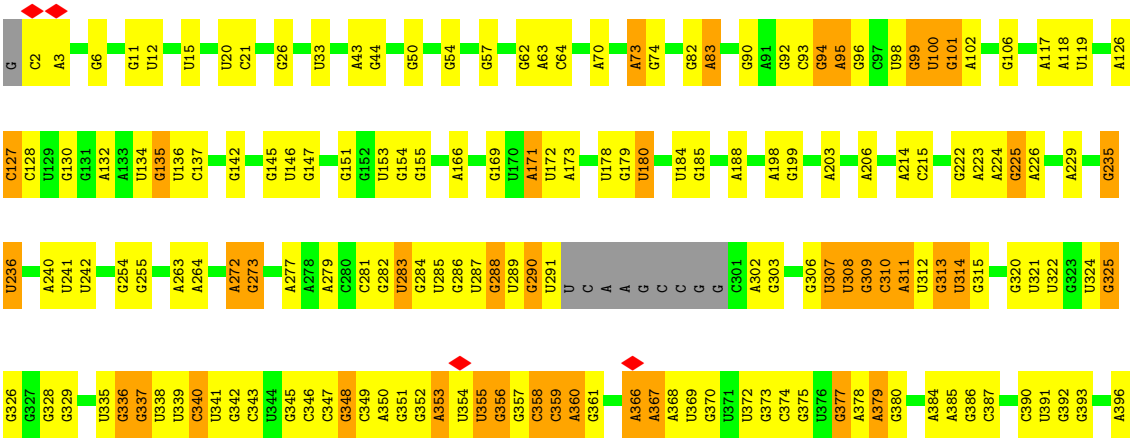
• Molecule 29: mRNA 32MF

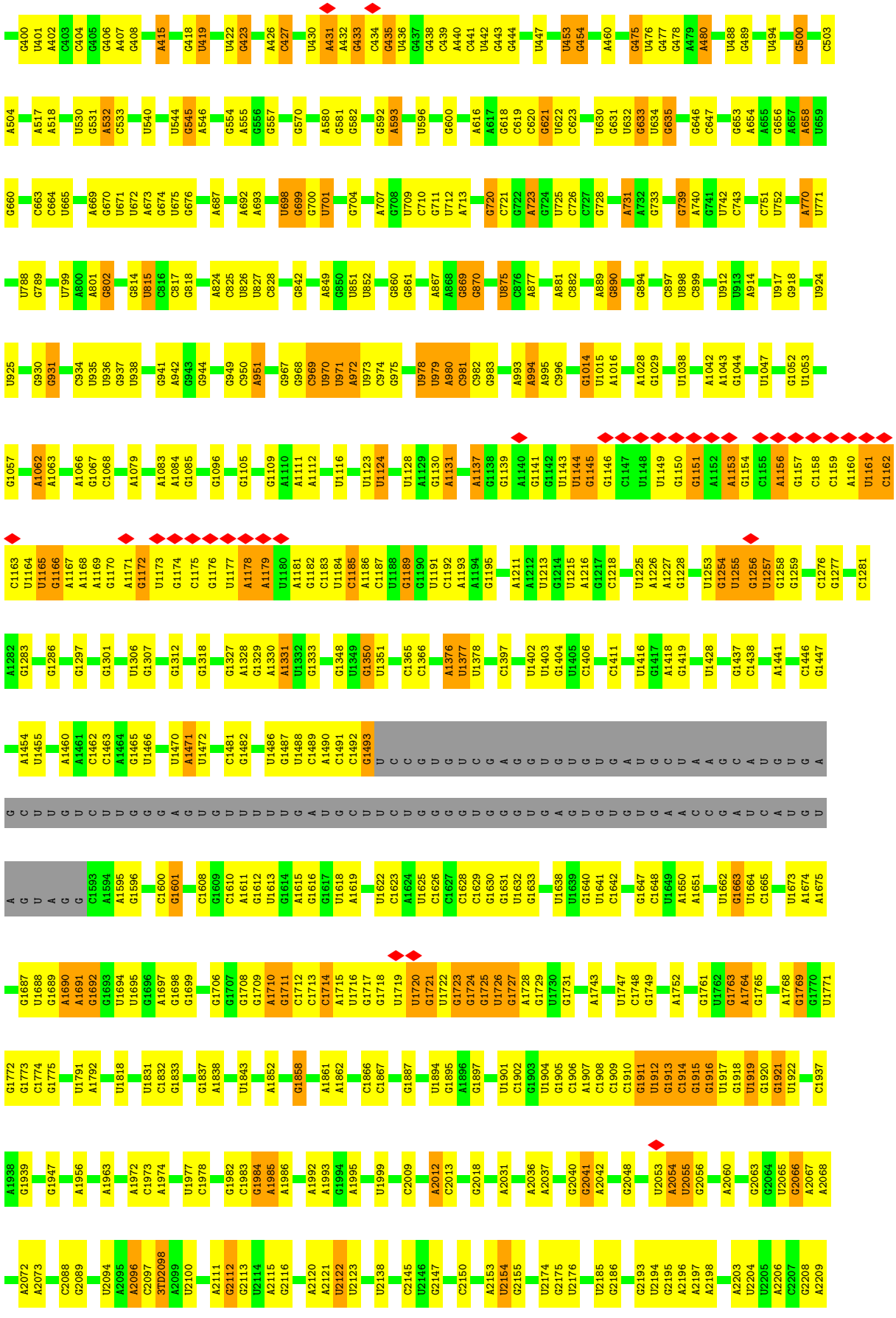
Chain Y:



• Molecule 30: 23S rRNA

Chain a:

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A504 A517 A518 U530 G531 A532 C533 U540 U544 G545 A546 G554 A555 G556 G557 G570 A580 G581 G582 G592 A593 U596 G600 A616 A617 G618 C619 C620 G621 U622 C623 U630 G631 U632 G633 U634 G635 G646 C647 G653 A654 A655 G656 A657 A658 U659
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G C U U G U C U U G G G A G U G U U U U G A U G U C U C U G G U G U U U G U G U G U G A U G U G U G A C U A A C C G G A C A U U C A U G G U
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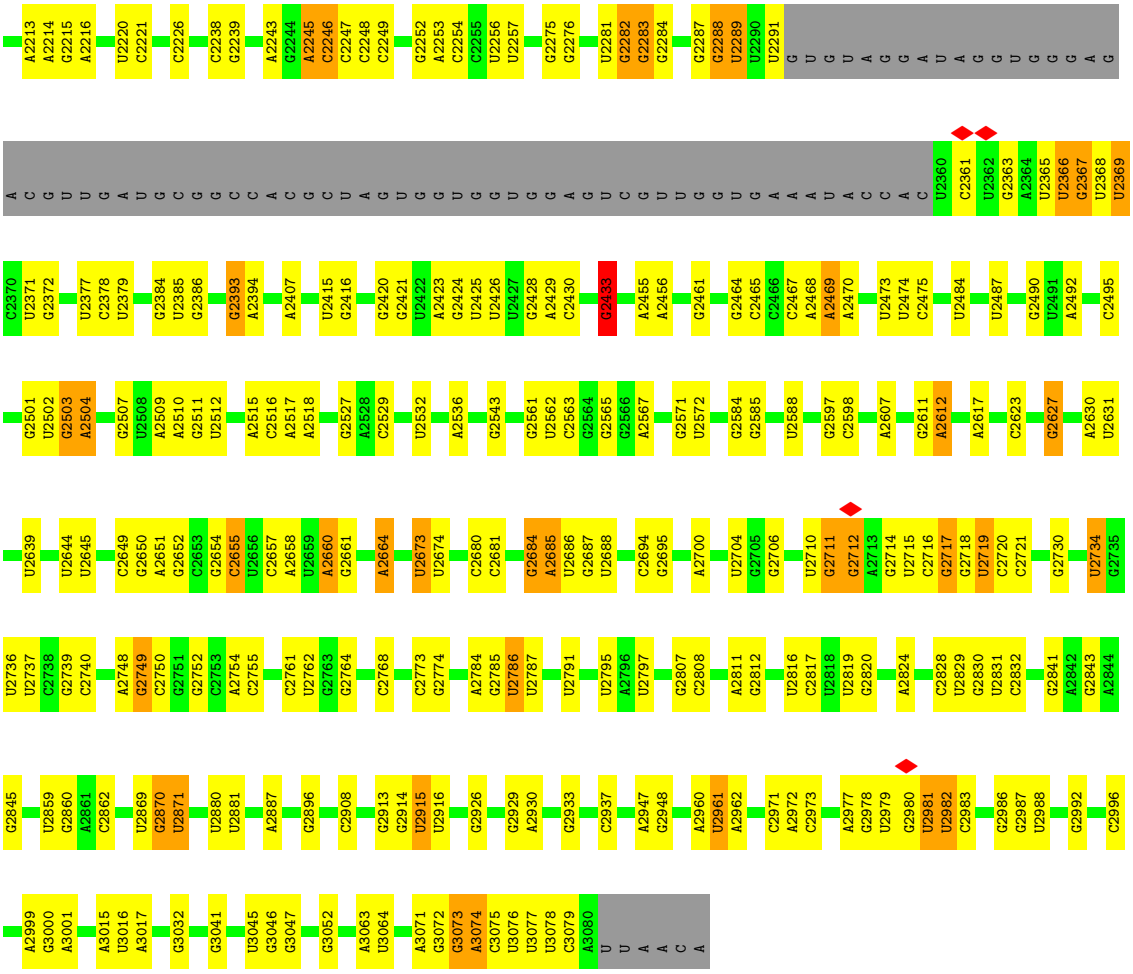
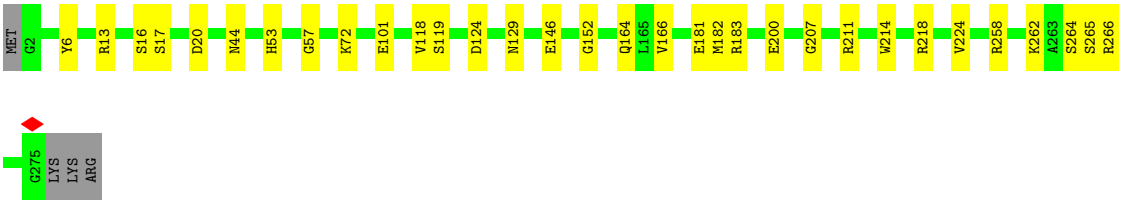


• Molecule 31: 5S rRNA

Chain b:

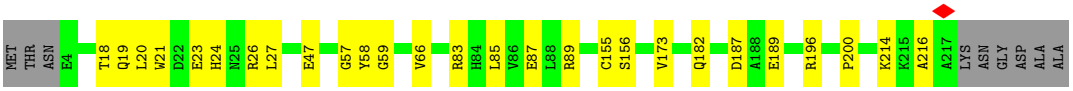
• Molecule 32: 50S ribosomal protein L2

Chain c:



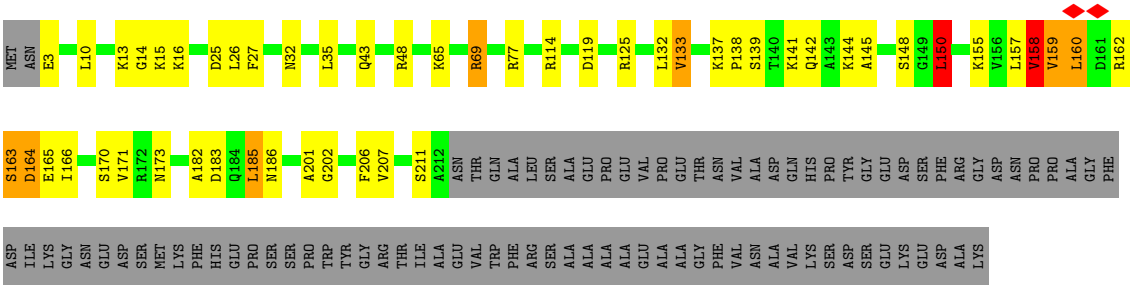
• Molecule 33: 50S ribosomal protein L3

Chain d:



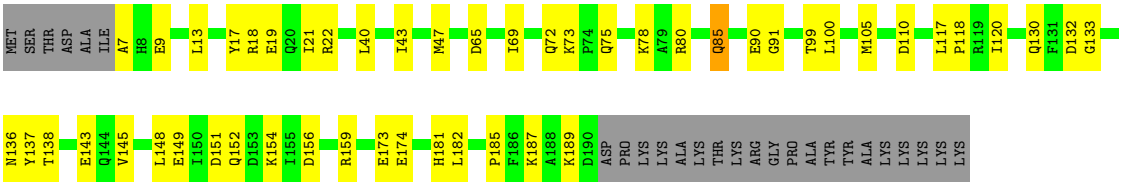
• Molecule 34: 50S ribosomal protein L4

Chain e:



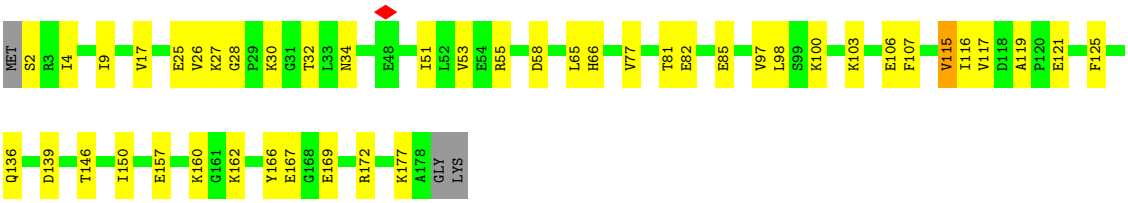
• Molecule 35: 50S ribosomal protein L5

Chain f:



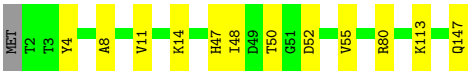
• Molecule 36: 50S ribosomal protein L6

Chain g:



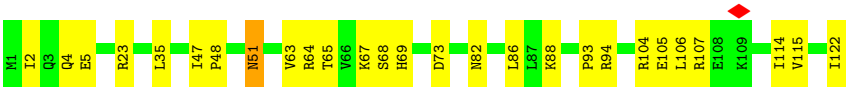
• Molecule 37: 50S ribosomal protein L13

Chain i:



• Molecule 38: 50S ribosomal protein L14

Chain j:

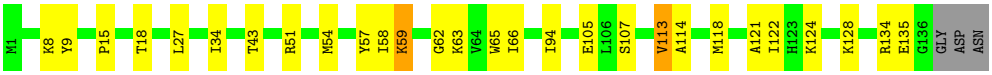


• Molecule 39: 50S ribosomal protein L15

Chain k:

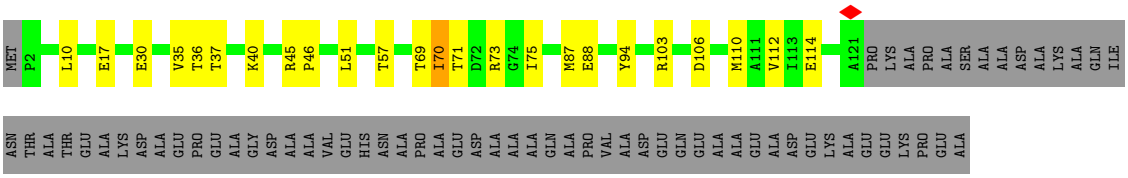
• Molecule 40: 50S ribosomal protein L16

Chain l:



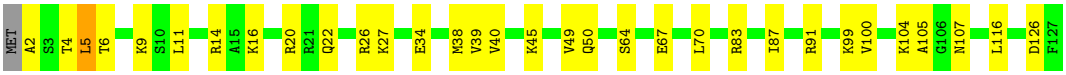
• Molecule 41: Large ribosomal subunit protein bL17

Chain m:



• Molecule 42: 50S ribosomal protein L18

Chain n:

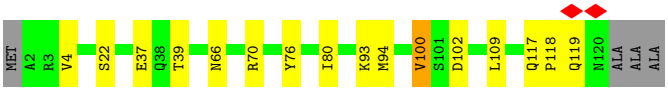


• Molecule 43: 50S ribosomal protein L19

Chain o:

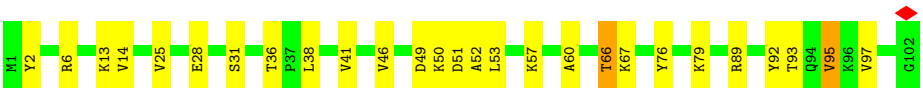
• Molecule 44: 50S ribosomal protein L20

Chain p:



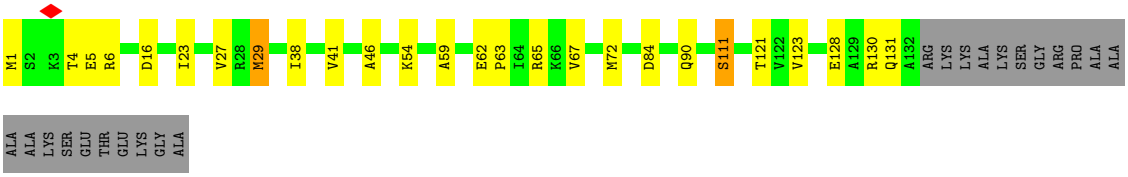
• Molecule 45: Large ribosomal subunit protein bL21

Chain q:



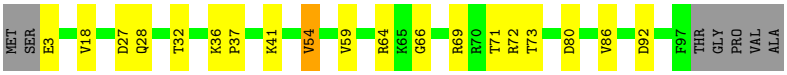
- Molecule 46: 50S ribosomal protein L22

Chain r:



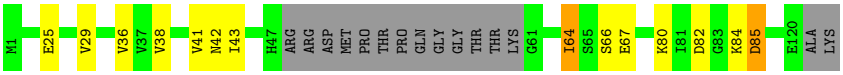
- Molecule 47: 50S ribosomal protein L23

Chain s:



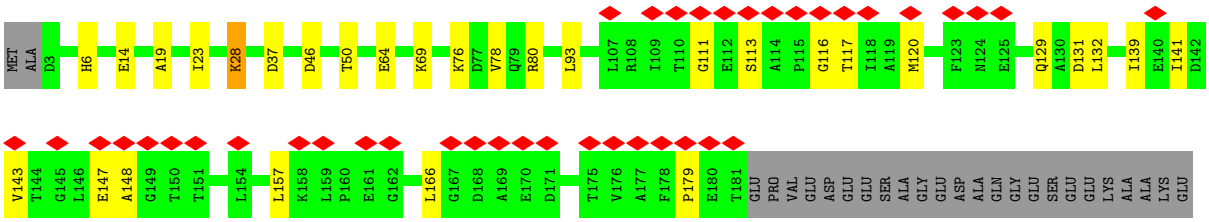
- Molecule 48: Large ribosomal subunit protein uL24

Chain t:



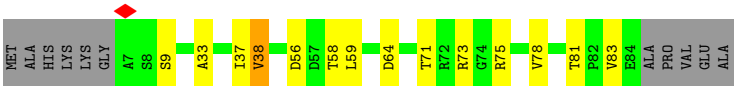
- Molecule 49: 50S ribosomal protein L25

Chain u:



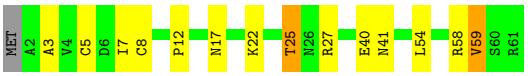
- Molecule 50: 50S ribosomal protein L27

Chain v:



- Molecule 51: 50S ribosomal protein L28

Chain w:

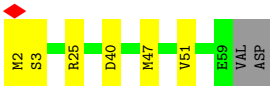


- Molecule 52: 50S ribosomal protein L29

Chain x:

- Molecule 53: 50S ribosomal protein L30

Chain y:



- Molecule 54: 50S ribosomal protein L32

Chain z:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105824	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.812	Depositor
Minimum map value	-0.244	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: 3TD, OMG, 5MC, 5MU, MIY, H2U, 2MA, 4SU, PSU, 4OC, MG, 2MG, UR3, MA6, OMU, OMC, ZN, G7M

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	0	0.29	0/429	0.33	0/569
2	1	0.34	0/365	0.31	0/478
3	2	0.34	0/519	0.40	0/682
4	3	0.33	0/305	0.35	0/401
5	4	0.70	0/521	0.97	0/700
6	A	0.28	0/35898	0.30	0/56012
7	B	0.29	0/1864	0.56	1/2509 (0.0%)
8	C	0.29	0/1703	0.35	0/2655
9	D	0.27	0/1662	0.43	0/2239
10	E	0.28	0/1325	0.46	0/1789
11	F	0.26	0/794	0.52	0/1069
12	G	0.17	0/1638	0.35	0/2201
13	H	0.26	0/1036	0.41	0/1395
14	I	0.20	0/1246	0.45	0/1679
15	J	0.20	0/1027	0.45	0/1376
16	K	0.24	0/874	0.53	0/1177
17	L	0.23	0/960	0.32	0/1283
18	M	0.31	0/800	0.58	0/1080
19	N	0.20	0/985	0.43	0/1317
20	O	0.35	0/718	0.51	0/959
21	P	0.24	0/1013	0.45	0/1370
22	Q	0.24	0/734	0.42	0/978
23	R	0.24	0/532	0.42	0/713
24	S	0.17	0/484	0.36	0/644
25	T	0.24	0/676	0.31	0/897
26	U	0.33	0/675	0.49	0/908
27	V	0.34	0/184	0.40	0/236
28	X	0.30	0/277	0.46	0/355
29	Y	0.22	0/235	0.34	0/363
30	a	0.43	0/69490	0.41	3/108431 (0.0%)
31	b	0.37	0/2871	0.34	0/4475

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	c	0.35	0/2132	0.43	0/2871
33	d	0.33	0/1611	0.39	0/2172
34	e	0.55	0/1600	0.78	5/2165 (0.2%)
35	f	0.33	0/1493	0.49	0/2001
36	g	0.22	0/1398	0.38	0/1884
37	i	0.35	0/1164	0.35	0/1574
38	j	0.34	0/957	0.40	0/1282
39	k	0.35	0/1090	0.50	0/1465
40	l	0.34	0/1108	0.39	0/1488
41	m	0.41	0/949	0.50	0/1277
42	n	0.27	0/959	0.40	0/1281
43	o	0.31	0/909	0.33	0/1216
44	p	0.36	0/969	0.36	0/1292
45	q	0.31	0/785	0.40	0/1050
46	r	0.40	0/1028	0.52	0/1379
47	s	0.32	0/759	0.40	0/1022
48	t	0.27	0/840	0.43	0/1123
49	u	0.22	0/1396	0.40	0/1896
50	v	0.35	0/598	0.38	0/800
51	w	0.34	0/483	0.39	0/648
52	x	0.26	0/567	0.40	0/759
53	y	0.32	0/471	0.40	0/627
54	z	0.32	0/487	0.32	0/654
All	All	0.37	0/155593	0.40	9/232866 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
41	m	0	1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	2097	C	C4'-C3'-O3'	6.53	122.80	113.00
7	B	109	LYS	N-CA-C	-6.29	103.72	111.33
34	e	163	SER	N-CA-C	-6.15	106.32	113.88
34	e	159	VAL	N-CA-CB	6.01	117.58	110.55
30	a	2122	5MU	O3'-P-O5'	-5.69	95.46	104.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	m	73	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	423	0	429	5	0
2	1	362	0	388	4	0
3	2	513	0	565	1	0
4	3	302	0	330	4	0
5	4	512	0	498	16	0
6	A	32340	0	16267	390	0
7	B	1836	0	1902	75	0
8	C	1605	0	818	9	0
9	D	1632	0	1663	53	0
10	E	1309	0	1349	42	0
11	F	785	0	818	28	0
12	G	1613	0	1626	38	0
13	H	1021	0	1059	25	0
14	I	1225	0	1275	34	0
15	J	1012	0	1069	41	0
16	K	858	0	884	20	0
17	L	948	0	1031	13	0
18	M	786	0	823	41	0
19	N	976	0	1031	25	0
20	O	708	0	737	16	0
21	P	994	0	1008	24	0
22	Q	728	0	772	20	0
23	R	527	0	580	17	0
24	S	474	0	499	11	0
25	T	673	0	726	11	0
26	U	658	0	671	15	0
27	V	183	0	202	0	0
28	X	277	0	338	6	0
29	Y	211	0	106	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	62450	0	31319	580	0
31	b	2567	0	1297	14	0
32	c	2091	0	2150	20	0
33	d	1586	0	1634	20	0
34	e	1577	0	1619	53	0
35	f	1468	0	1487	39	0
36	g	1376	0	1421	31	0
37	i	1139	0	1163	6	0
38	j	946	0	1011	17	0
39	k	1072	0	1106	29	0
40	l	1082	0	1117	18	0
41	m	936	0	997	14	0
42	n	952	0	995	23	0
43	o	896	0	928	14	0
44	p	958	0	986	12	0
45	q	778	0	824	19	0
46	r	1017	0	1070	18	0
47	s	751	0	803	12	0
48	t	833	0	883	10	0
49	u	1376	0	1397	18	0
50	v	591	0	581	7	0
51	w	474	0	487	10	0
52	x	564	0	582	7	0
53	y	467	0	504	4	0
54	z	477	0	479	3	0
55	0	1	0	0	0	0
55	3	1	0	0	0	0
55	4	1	0	0	0	0
55	S	1	0	0	0	0
55	w	1	0	0	0	0
55	z	1	0	0	0	0
56	0	1	0	0	0	0
56	A	54	0	0	0	0
56	S	1	0	0	0	0
56	T	1	0	0	0	0
56	a	262	0	0	0	0
56	b	2	0	0	0	0
56	c	1	0	0	0	0
56	d	1	0	0	0	0
56	k	1	0	0	0	0
57	A	33	0	24	0	0
57	a	66	0	49	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1	1	0	0	0	0
58	A	9	0	0	1	0
58	a	80	0	0	0	0
58	b	1	0	0	0	0
58	c	1	0	0	0	0
All	All	144436	0	96377	1793	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1793 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:361:G:H21	30:a:368:A:N6	1.57	1.01
34:e:160:LEU:HB3	34:e:164:ASP:HB2	1.40	1.01
30:a:2706:G:H1	30:a:2721:C:H5	1.11	0.97
30:a:1281:C:H5	30:a:1318:G:H1	1.03	0.94
10:E:116:VAL:HB	10:E:151:LEU:O	1.67	0.94

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	48/56 (86%)	45 (94%)	3 (6%)	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	65/68 (96%)	64 (98%)	1 (2%)	0	100	100
4	3	35/37 (95%)	35 (100%)	0	0	100	100
5	4	64/69 (93%)	56 (88%)	8 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	B	231/283 (82%)	213 (92%)	16 (7%)	2 (1%)	14	27
9	D	198/201 (98%)	189 (96%)	9 (4%)	0	100	100
10	E	177/215 (82%)	171 (97%)	6 (3%)	0	100	100
11	F	94/96 (98%)	88 (94%)	4 (4%)	2 (2%)	5	9
12	G	204/269 (76%)	196 (96%)	8 (4%)	0	100	100
13	H	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
14	I	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
15	J	132/173 (76%)	118 (89%)	13 (10%)	1 (1%)	16	31
16	K	115/135 (85%)	104 (90%)	11 (10%)	0	100	100
17	L	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
18	M	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	12	24
19	N	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
20	O	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
21	P	126/147 (86%)	115 (91%)	8 (6%)	3 (2%)	4	8
22	Q	88/90 (98%)	80 (91%)	8 (9%)	0	100	100
23	R	65/79 (82%)	60 (92%)	4 (6%)	1 (2%)	8	16
24	S	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
25	T	85/88 (97%)	85 (100%)	0	0	100	100
26	U	82/93 (88%)	72 (88%)	9 (11%)	1 (1%)	10	20
27	V	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
28	X	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
32	c	272/278 (98%)	257 (94%)	15 (6%)	0	100	100
33	d	212/223 (95%)	200 (94%)	12 (6%)	0	100	100
34	e	208/301 (69%)	186 (89%)	18 (9%)	4 (2%)	6	11
35	f	182/210 (87%)	171 (94%)	11 (6%)	0	100	100
36	g	175/180 (97%)	166 (95%)	9 (5%)	0	100	100
37	i	144/147 (98%)	143 (99%)	0	1 (1%)	18	34
38	j	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
39	k	142/146 (97%)	123 (87%)	18 (13%)	1 (1%)	18	34
40	l	134/139 (96%)	129 (96%)	5 (4%)	0	100	100
41	m	118/187 (63%)	109 (92%)	7 (6%)	2 (2%)	7	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	n	124/127 (98%)	120 (97%)	3 (2%)	1 (1%)	16	31
43	o	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
44	p	117/123 (95%)	114 (97%)	2 (2%)	1 (1%)	14	27
45	q	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
46	r	130/153 (85%)	128 (98%)	2 (2%)	0	100	100
47	s	93/102 (91%)	87 (94%)	6 (6%)	0	100	100
48	t	103/122 (84%)	96 (93%)	6 (6%)	1 (1%)	12	24
49	u	177/205 (86%)	169 (96%)	8 (4%)	0	100	100
50	v	76/89 (85%)	73 (96%)	3 (4%)	0	100	100
51	w	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
52	x	67/77 (87%)	62 (92%)	5 (8%)	0	100	100
53	y	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
54	z	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
All	All	5646/6322 (89%)	5326 (94%)	298 (5%)	22 (0%)	31	49

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	F	17	ARG
21	P	46	PRO
21	P	113	ASP
23	R	73	THR
34	e	133	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/51 (92%)	46 (98%)	1 (2%)	47	74
2	1	36/36 (100%)	34 (94%)	2 (6%)	19	39
3	2	54/55 (98%)	53 (98%)	1 (2%)	50	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	35/35 (100%)	33 (94%)	2 (6%)	18	39
5	4	56/59 (95%)	53 (95%)	3 (5%)	20	41
7	B	197/234 (84%)	185 (94%)	12 (6%)	17	35
9	D	175/176 (99%)	173 (99%)	2 (1%)	65	84
10	E	130/155 (84%)	127 (98%)	3 (2%)	44	72
11	F	89/89 (100%)	87 (98%)	2 (2%)	45	73
12	G	160/200 (80%)	157 (98%)	3 (2%)	50	76
13	H	108/109 (99%)	107 (99%)	1 (1%)	70	87
14	I	132/133 (99%)	128 (97%)	4 (3%)	36	64
15	J	97/131 (74%)	95 (98%)	2 (2%)	47	74
16	K	88/101 (87%)	87 (99%)	1 (1%)	65	84
17	L	103/104 (99%)	101 (98%)	2 (2%)	50	76
18	M	89/93 (96%)	86 (97%)	3 (3%)	32	60
19	N	99/100 (99%)	97 (98%)	2 (2%)	48	75
20	O	74/74 (100%)	73 (99%)	1 (1%)	59	81
21	P	103/115 (90%)	97 (94%)	6 (6%)	18	38
22	Q	81/81 (100%)	80 (99%)	1 (1%)	63	83
23	R	55/65 (85%)	53 (96%)	2 (4%)	31	58
24	S	48/49 (98%)	48 (100%)	0	100	100
25	T	68/69 (99%)	68 (100%)	0	100	100
26	U	72/80 (90%)	70 (97%)	2 (3%)	38	66
27	V	16/17 (94%)	16 (100%)	0	100	100
28	X	28/29 (97%)	28 (100%)	0	100	100
32	c	216/220 (98%)	213 (99%)	3 (1%)	59	81
33	d	166/172 (96%)	164 (99%)	2 (1%)	63	83
34	e	165/237 (70%)	157 (95%)	8 (5%)	23	46
35	f	154/175 (88%)	151 (98%)	3 (2%)	50	76
36	g	150/152 (99%)	147 (98%)	3 (2%)	48	75
37	i	118/120 (98%)	116 (98%)	2 (2%)	53	78
38	j	101/101 (100%)	98 (97%)	3 (3%)	36	64
39	k	111/113 (98%)	107 (96%)	4 (4%)	31	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	l	108/110 (98%)	106 (98%)	2 (2%)	50	76
41	m	100/142 (70%)	98 (98%)	2 (2%)	48	75
42	n	95/96 (99%)	93 (98%)	2 (2%)	47	74
43	o	97/99 (98%)	93 (96%)	4 (4%)	27	53
44	p	98/99 (99%)	96 (98%)	2 (2%)	48	75
45	q	84/84 (100%)	79 (94%)	5 (6%)	17	36
46	r	105/118 (89%)	98 (93%)	7 (7%)	15	31
47	s	84/89 (94%)	81 (96%)	3 (4%)	31	58
48	t	91/103 (88%)	89 (98%)	2 (2%)	45	73
49	u	149/168 (89%)	147 (99%)	2 (1%)	61	82
50	v	60/67 (90%)	55 (92%)	5 (8%)	10	22
51	w	52/53 (98%)	50 (96%)	2 (4%)	29	56
52	x	61/68 (90%)	61 (100%)	0	100	100
53	y	53/55 (96%)	53 (100%)	0	100	100
54	z	51/52 (98%)	50 (98%)	1 (2%)	48	75
All	All	4709/5133 (92%)	4584 (97%)	125 (3%)	40	67

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	U	79	THR
47	s	18	VAL
35	f	85	GLN
46	r	130	ARG
50	v	38	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
43	o	41	GLN
49	u	48	HIS
44	p	27	GLN
48	t	76	GLN
51	w	17	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	Y	9/22 (40%)	6 (66%)	0
30	a	2890/3086 (93%)	479 (16%)	0
31	b	117/120 (97%)	10 (8%)	0
6	A	1503/1537 (97%)	234 (15%)	15 (0%)
8	C	74/76 (97%)	10 (13%)	0
All	All	4593/4841 (94%)	739 (16%)	15 (0%)

5 of 739 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	7	A
6	A	9	U
6	A	10	G
6	A	13	G
6	A	36	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	825	U
6	A	1350	A
6	A	869	G
6	A	1518	A
6	A	1187	A

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

34 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	$\#\|Z\| > 2$
6	4OC	A	1389	6	20,23,24	2.99	8 (40%)	25,32,35	0.97	2 (8%)
6	2MG	A	950	6	23,26,27	0.37	0	33,38,41	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	5MC	A	1391	6	19,22,23	4.26	8 (42%)	26,32,35	1.01	1 (3%)
30	5MC	a	2145	30	19,22,23	4.13	8 (42%)	26,32,35	1.11	3 (11%)
6	MA6	A	1506	6	23,26,27	0.28	0	33,38,41	0.72	1 (3%)
30	PSU	a	1038	56,30	18,21,22	0.90	1 (5%)	21,30,33	0.94	0
30	PSU	a	2787	30	18,21,22	0.93	1 (5%)	21,30,33	0.78	1 (4%)
30	3TD	a	2098	30	19,22,23	1.27	2 (10%)	23,32,35	1.09	1 (4%)
6	5MC	A	1387	6	19,22,23	4.38	8 (42%)	26,32,35	1.08	2 (7%)
30	5MU	a	2122	30	19,22,23	0.31	0	27,32,35	0.52	0
30	OMG	a	2433	8,30	23,26,27	2.49	9 (39%)	32,38,41	2.34	11 (34%)
30	PSU	a	2094	30	18,21,22	0.94	1 (5%)	21,30,33	0.67	0
6	PSU	A	498	6	18,21,22	0.93	1 (5%)	21,30,33	0.69	0
30	PSU	a	2762	30	18,21,22	0.92	1 (5%)	21,30,33	0.87	1 (4%)
30	2MA	a	2685	56,30	22,25,26	0.85	1 (4%)	32,37,40	1.22	5 (15%)
6	UR3	A	1485	6	19,22,23	2.67	8 (42%)	26,32,35	1.62	3 (11%)
6	5MC	A	1394	6	19,22,23	4.29	8 (42%)	26,32,35	1.08	2 (7%)
30	PSU	a	2100	30	18,21,22	0.93	1 (5%)	21,30,33	0.72	0
8	5MU	C	54	8	19,22,23	0.24	0	27,32,35	0.35	0
30	2MG	a	2627	56,30	23,26,27	2.96	7 (30%)	33,38,41	2.43	11 (33%)
30	PSU	a	2786	30	18,21,22	0.94	1 (5%)	21,30,33	0.83	1 (4%)
8	4SU	C	8	8	18,21,22	3.71	7 (38%)	25,30,33	2.36	5 (20%)
30	OMU	a	2734	30	19,22,23	2.79	6 (31%)	25,31,34	1.97	5 (20%)
30	2MG	a	2018	30	23,26,27	2.99	8 (34%)	33,38,41	2.53	12 (36%)
8	5MC	C	32	8	19,22,23	4.29	8 (42%)	26,32,35	1.11	1 (3%)
6	G7M	A	509	6	23,26,27	2.58	9 (39%)	34,39,42	1.70	7 (20%)
30	H2U	a	2631	30	18,21,22	2.94	5 (27%)	19,30,33	1.51	4 (21%)
6	MA6	A	1505	6	23,26,27	0.30	0	33,38,41	0.69	1 (3%)
30	PSU	a	2639	30	18,21,22	0.97	1 (5%)	21,30,33	0.75	0
6	5MC	A	951	6	19,22,23	0.78	1 (5%)	26,32,35	0.45	0
8	PSU	C	55	8	18,21,22	0.92	1 (5%)	21,30,33	0.75	0
30	OMC	a	2680	56,30	19,22,23	3.11	8 (42%)	25,31,34	0.95	0
30	PSU	a	2686	30	18,21,22	0.94	1 (5%)	21,30,33	0.78	1 (4%)
6	2MG	A	1503	6	23,26,27	3.01	8 (34%)	33,38,41	2.63	12 (36%)

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
6	4OC	A	1389	6	-	2/9/29/30	0/2/2/2
6	2MG	A	950	6	-	4/9/27/28	0/3/3/3
6	5MC	A	1391	6	-	0/7/25/26	0/2/2/2
30	5MC	a	2145	30	-	0/7/25/26	0/2/2/2
6	MA6	A	1506	6	-	3/11/29/30	0/3/3/3
30	PSU	a	1038	56,30	-	0/7/25/26	0/2/2/2
30	PSU	a	2787	30	-	0/7/25/26	0/2/2/2
30	3TD	a	2098	30	-	2/7/25/26	0/2/2/2
6	5MC	A	1387	6	-	0/7/25/26	0/2/2/2
30	5MU	a	2122	30	-	0/7/25/26	0/2/2/2
30	OMG	a	2433	8,30	-	2/9/27/28	0/3/3/3
30	PSU	a	2094	30	-	0/7/25/26	0/2/2/2
6	PSU	A	498	6	-	2/7/25/26	0/2/2/2
30	PSU	a	2762	30	-	0/7/25/26	0/2/2/2
30	2MA	a	2685	56,30	-	1/7/25/26	0/3/3/3
6	UR3	A	1485	6	-	0/7/25/26	0/2/2/2
6	5MC	A	1394	6	-	0/7/25/26	0/2/2/2
30	PSU	a	2100	30	-	0/7/25/26	0/2/2/2
8	5MU	C	54	8	-	0/7/25/26	0/2/2/2
30	2MG	a	2627	56,30	-	2/9/27/28	0/3/3/3
30	PSU	a	2786	30	-	0/7/25/26	0/2/2/2
8	4SU	C	8	8	-	0/7/25/26	0/2/2/2
30	OMU	a	2734	30	-	0/9/27/28	0/2/2/2
30	2MG	a	2018	30	-	2/9/27/28	0/3/3/3
8	5MC	C	32	8	-	0/7/25/26	0/2/2/2
6	G7M	A	509	6	-	3/7/25/26	0/3/3/3
30	H2U	a	2631	30	-	0/7/38/39	0/2/2/2
6	MA6	A	1505	6	-	0/11/29/30	0/3/3/3
30	PSU	a	2639	30	-	0/7/25/26	0/2/2/2
6	5MC	A	951	6	-	0/7/25/26	0/2/2/2
8	PSU	C	55	8	-	0/7/25/26	0/2/2/2
30	OMC	a	2680	56,30	-	0/9/27/28	0/2/2/2
30	PSU	a	2686	30	-	1/7/25/26	0/2/2/2
6	2MG	A	1503	6	-	0/9/27/28	0/3/3/3

The worst 5 of 137 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	32	5MC	C6-C5	9.47	1.50	1.34
6	A	1394	5MC	C6-C5	9.43	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1387	5MC	C6-C5	9.33	1.49	1.34
6	A	1391	5MC	C6-C5	9.33	1.49	1.34
6	A	1387	5MC	C5-C4	9.00	1.50	1.44

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	8	4SU	C4-N3-C2	-8.05	119.60	127.31
30	a	2018	2MG	C2-N3-C4	7.04	120.81	112.00
30	a	2627	2MG	C2-N3-C4	6.56	120.20	112.00
6	A	1503	2MG	C2-N3-C4	6.51	120.15	112.00
30	a	2433	OMG	C1'-N9-C8	-6.32	108.77	126.73

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	950	2MG	N1-C2-N2-CM2
6	A	950	2MG	N3-C2-N2-CM2
6	A	1506	MA6	O4'-C4'-C5'-O5'
30	a	2098	3TD	O4'-C4'-C5'-O5'
30	a	2433	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1506	MA6	1	0
30	a	2122	5MU	1	0
30	a	2433	OMG	1	0
30	a	2685	2MA	1	0
30	a	2627	2MG	1	0
30	a	2786	PSU	1	0
30	a	2734	OMU	1	0
8	C	32	5MC	1	0
8	C	55	PSU	1	0
6	A	1503	2MG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 333 ligands modelled in this entry, 330 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	MIY	a	3364	-	36,36,36	1.11	2 (5%)	42,58,58	1.20	4 (9%)
57	MIY	A	1647	56	36,36,36	1.39	5 (13%)	42,58,58	1.82	10 (23%)
57	MIY	a	3344	56	36,36,36	1.41	7 (19%)	42,58,58	1.94	11 (26%)

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
57	MIY	a	3364	-	-	8/12/70/70	0/4/4/4
57	MIY	A	1647	56	-	2/12/70/70	0/4/4/4
57	MIY	a	3344	56	-	1/12/70/70	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	a	3364	MIY	C21-N2	5.07	1.48	1.33
57	A	1647	MIY	C18-C1	-3.63	1.50	1.55
57	a	3344	MIY	C7-C16	-3.42	1.48	1.51
57	A	1647	MIY	C7-C16	-3.22	1.48	1.51
57	a	3344	MIY	C5-C4	2.79	1.57	1.54

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	a	3344	MIY	C21-C2-C1	-5.12	114.91	120.97
57	A	1647	MIY	C21-C2-C1	-4.76	115.33	120.97
57	a	3344	MIY	C11-C10-N7	-4.43	115.56	121.65
57	a	3344	MIY	C11-C12-C13	-4.16	116.33	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	A	1647	MIY	C11-C12-C13	-4.05	116.45	120.50

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	1647	MIY	C1-C2-C21-O8
57	A	1647	MIY	C1-C2-C21-N2
57	a	3364	MIY	C1-C2-C21-O8
57	a	3364	MIY	C3-C2-C21-O8
57	a	3364	MIY	C3-C2-C21-N2

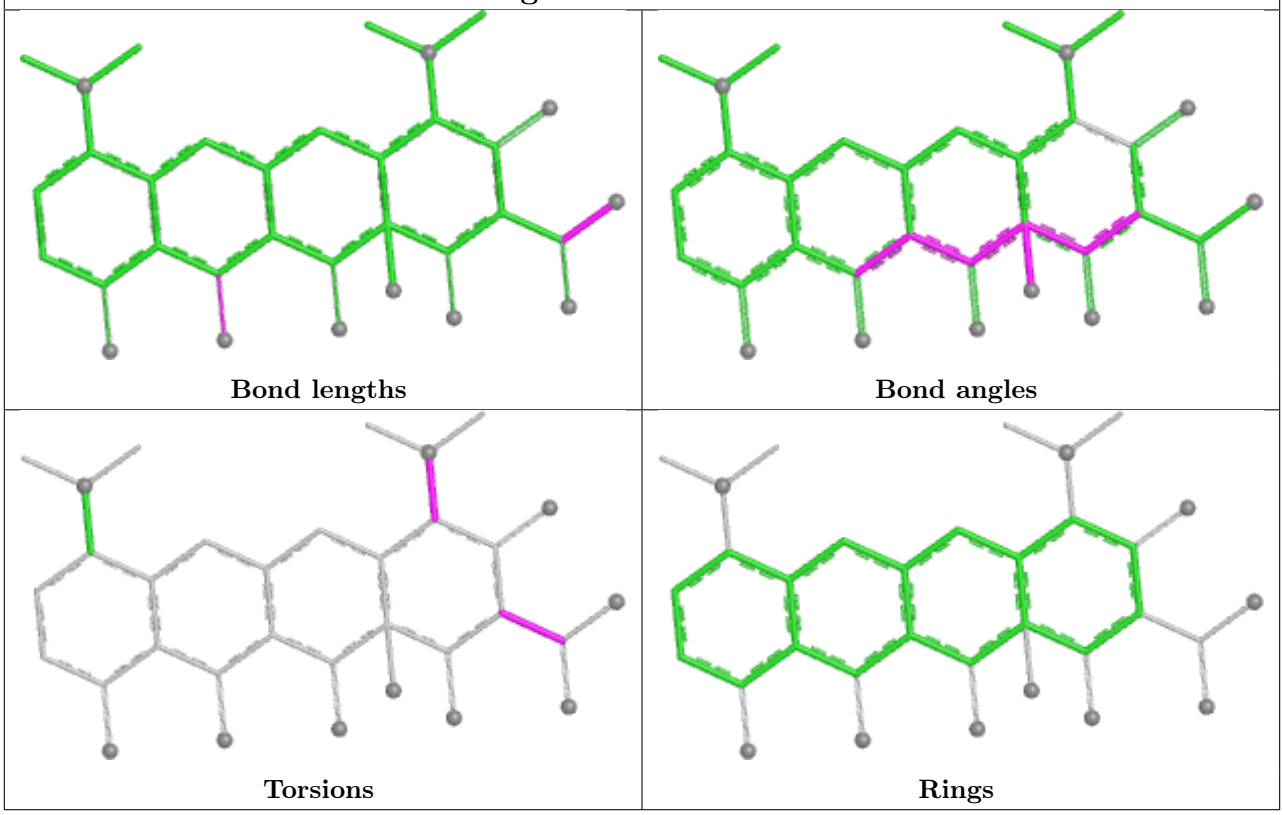
There are no ring outliers.

1 monomer is involved in 2 short contacts:

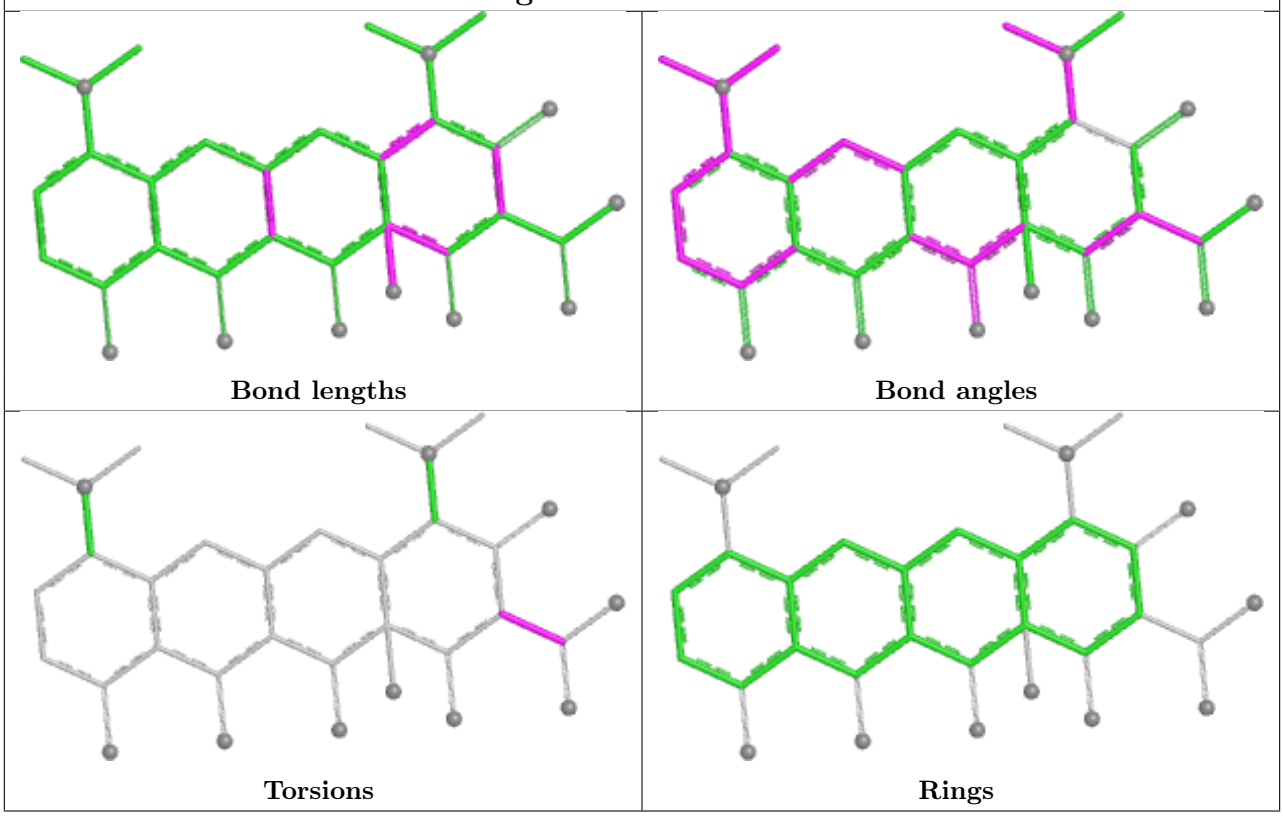
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	a	3344	MIY	2	0

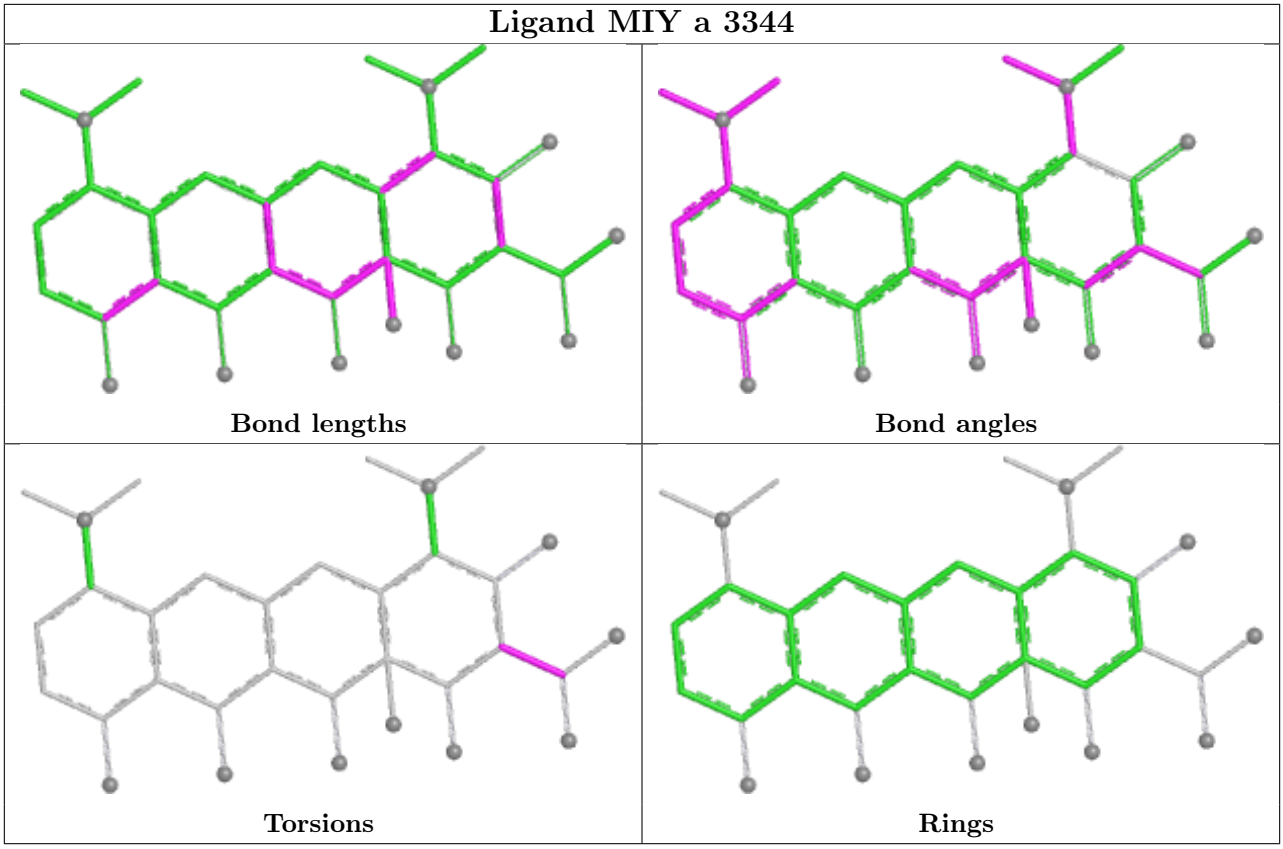
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand MIY a 3364



Ligand MIY A 1647





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.

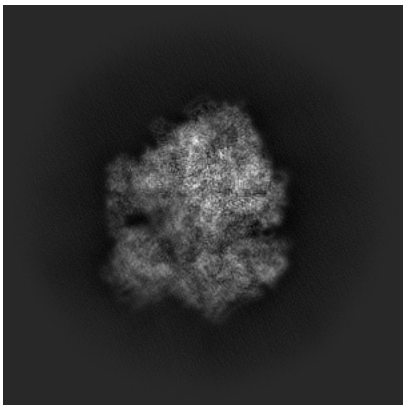
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-71684. These allow visual inspection of the internal detail of the map and identification of artifacts.

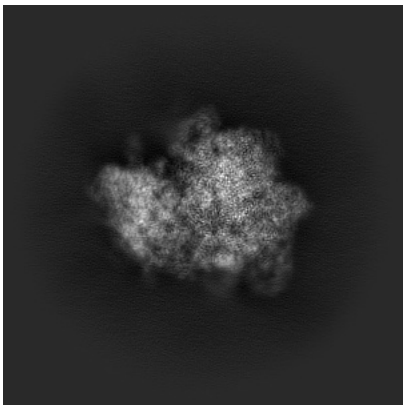
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

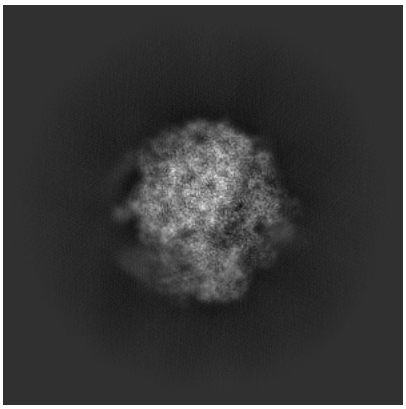
6.1.1 Primary map



X

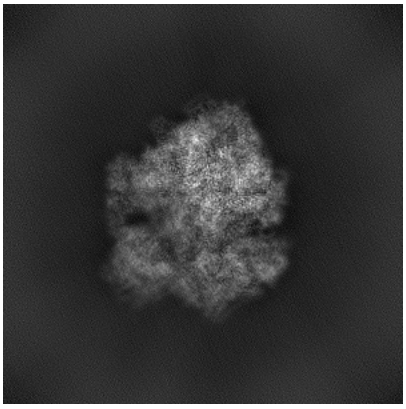


Y

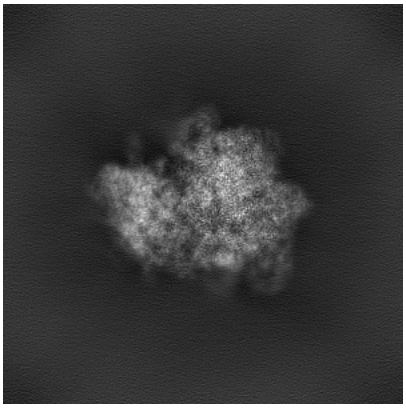


Z

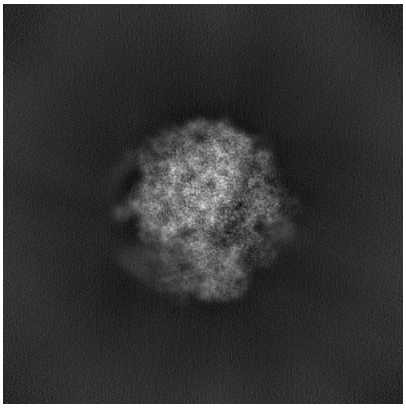
6.1.2 Raw map



X



Y

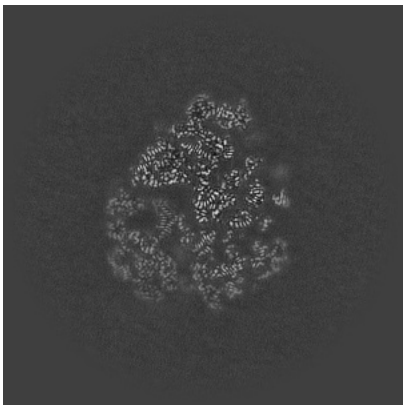


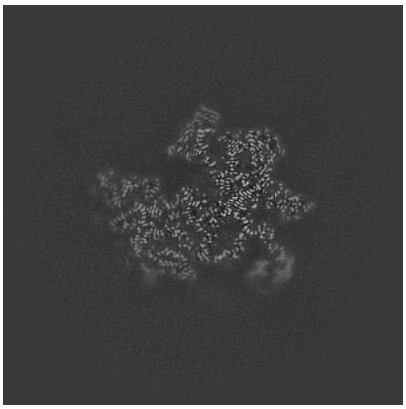
Z

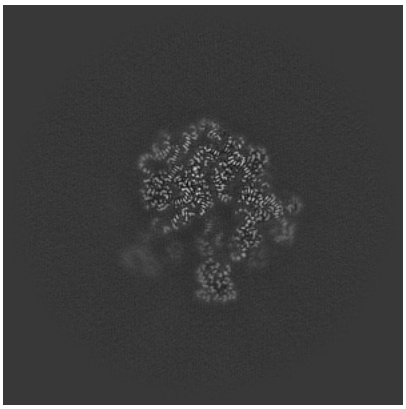
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

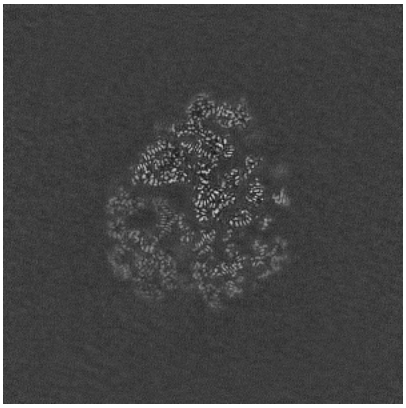
6.2.1 Primary map

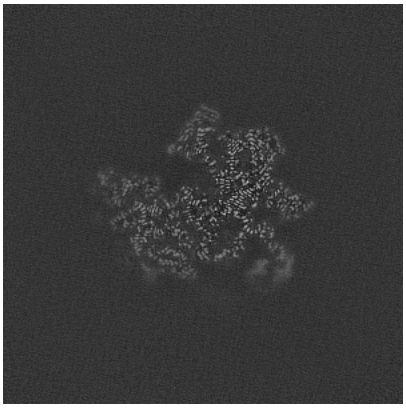

X Index: 220

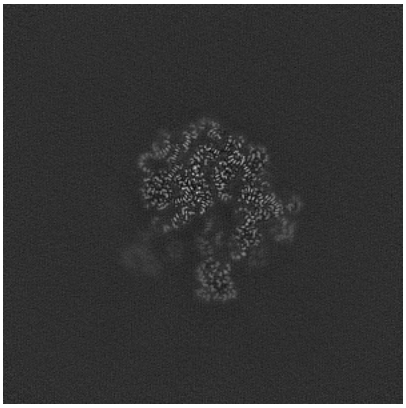

Y Index: 220


Z Index: 220

6.2.2 Raw map


X Index: 220

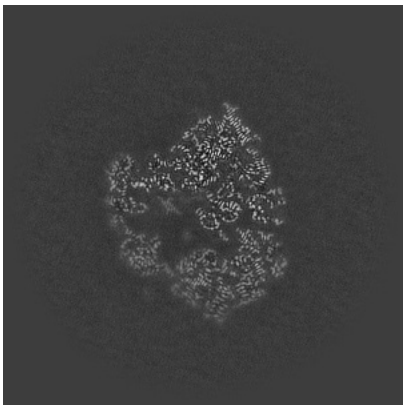

Y Index: 220


Z Index: 220

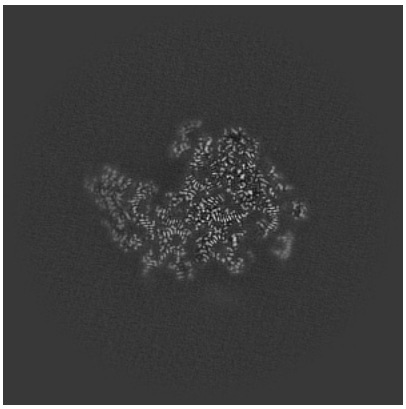
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

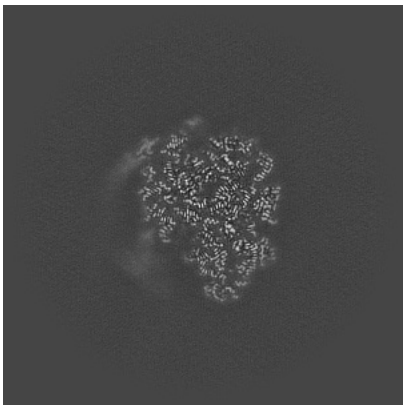
6.3.1 Primary map



X Index: 235

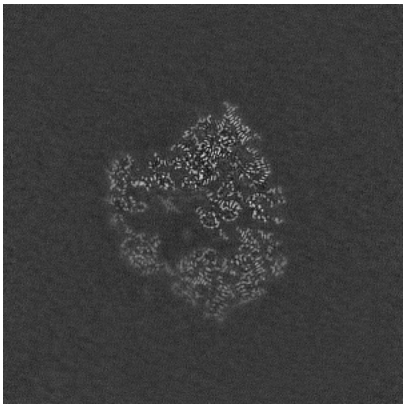


Y Index: 232

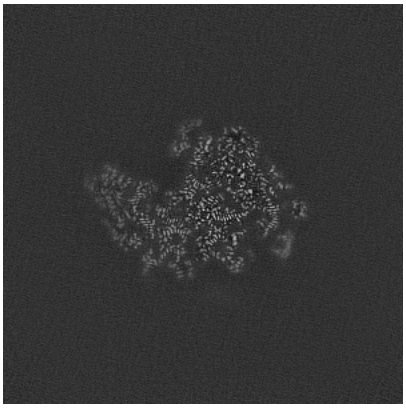


Z Index: 248

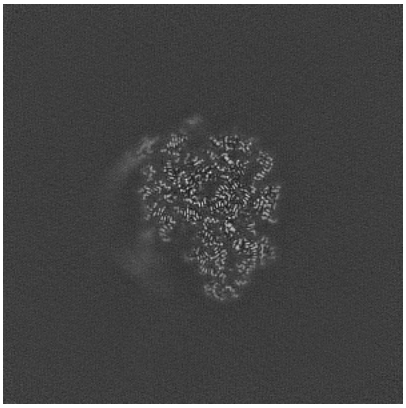
6.3.2 Raw map



X Index: 235



Y Index: 232

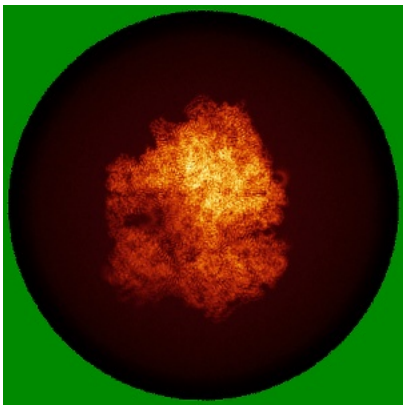


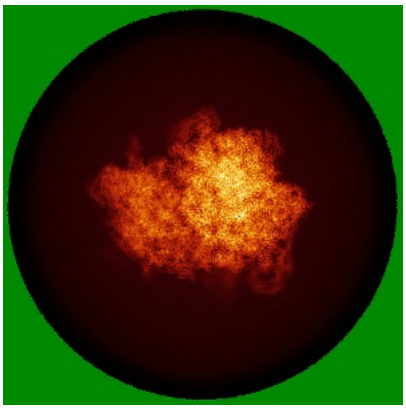
Z Index: 248

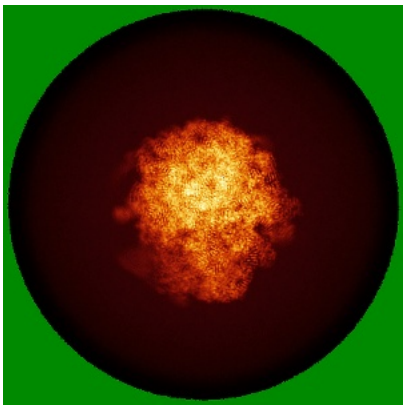
The images above show the largest variance slices of the map in three orthogonal directions.

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

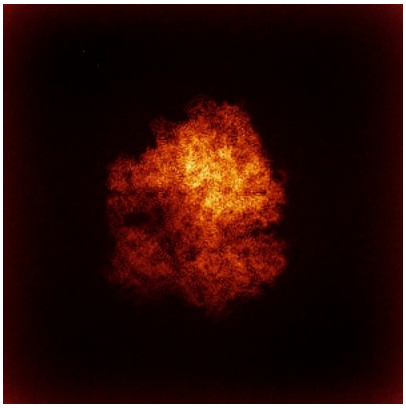
6.4.1 Primary map

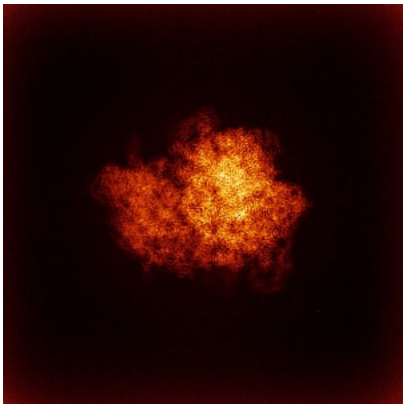

X

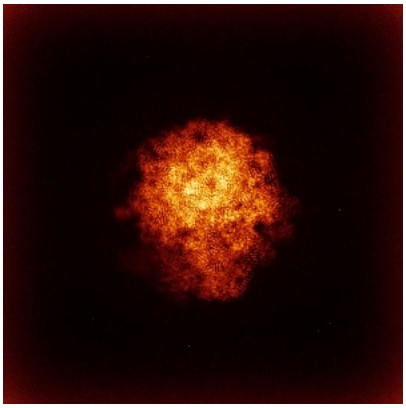

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

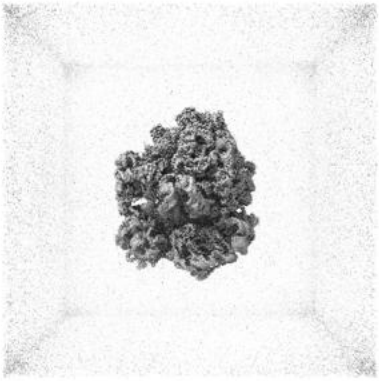
X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X

Y

Z

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

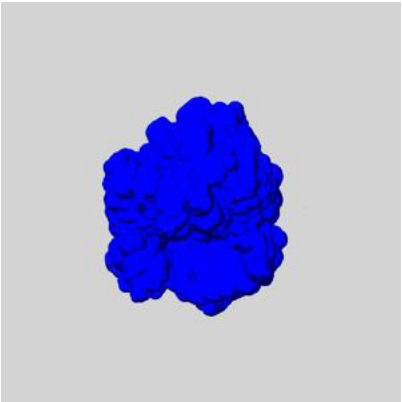
6.6 Mask visualisation (i)

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

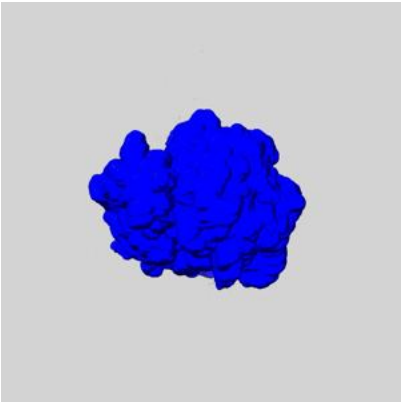
A mask typically either:

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

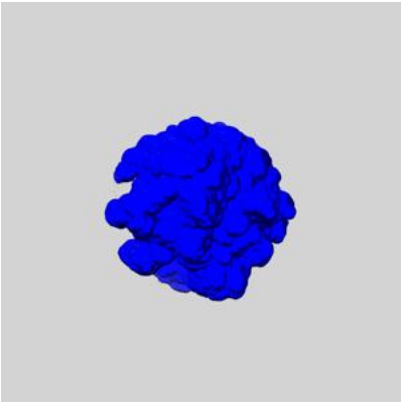
6.6.1 emd_71684_msk_1.map (i)



X



Y

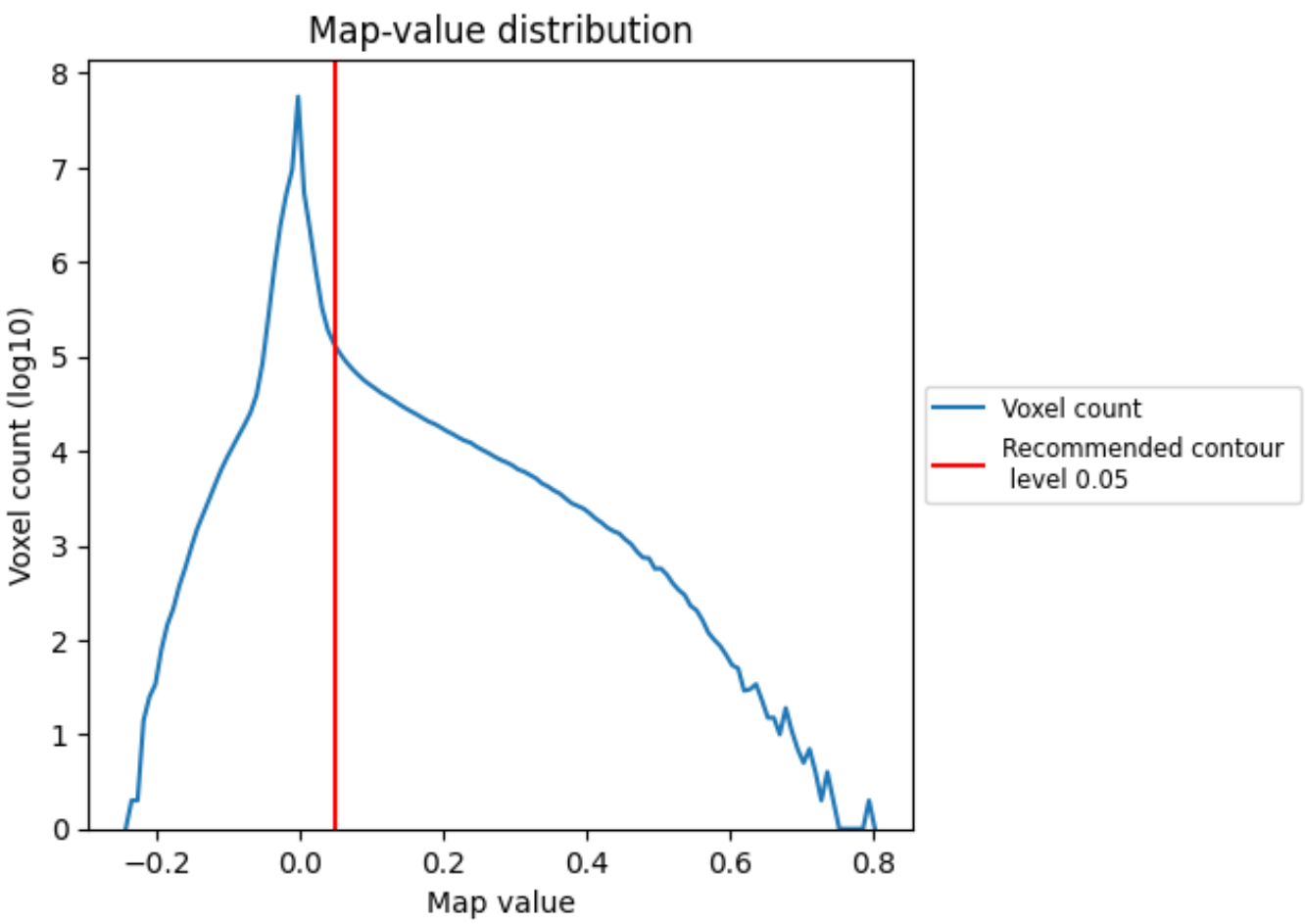


Z

7 Map analysis (i)

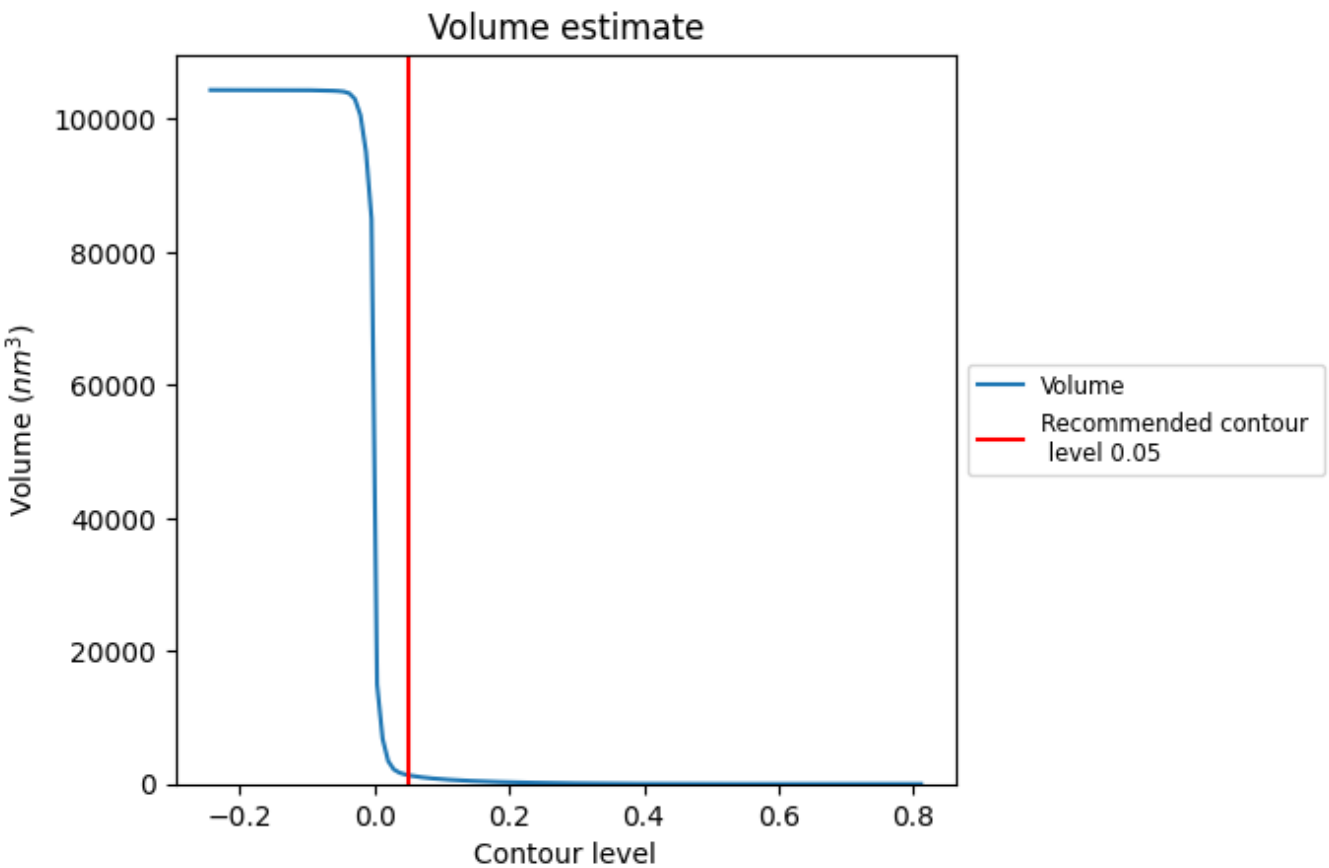
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

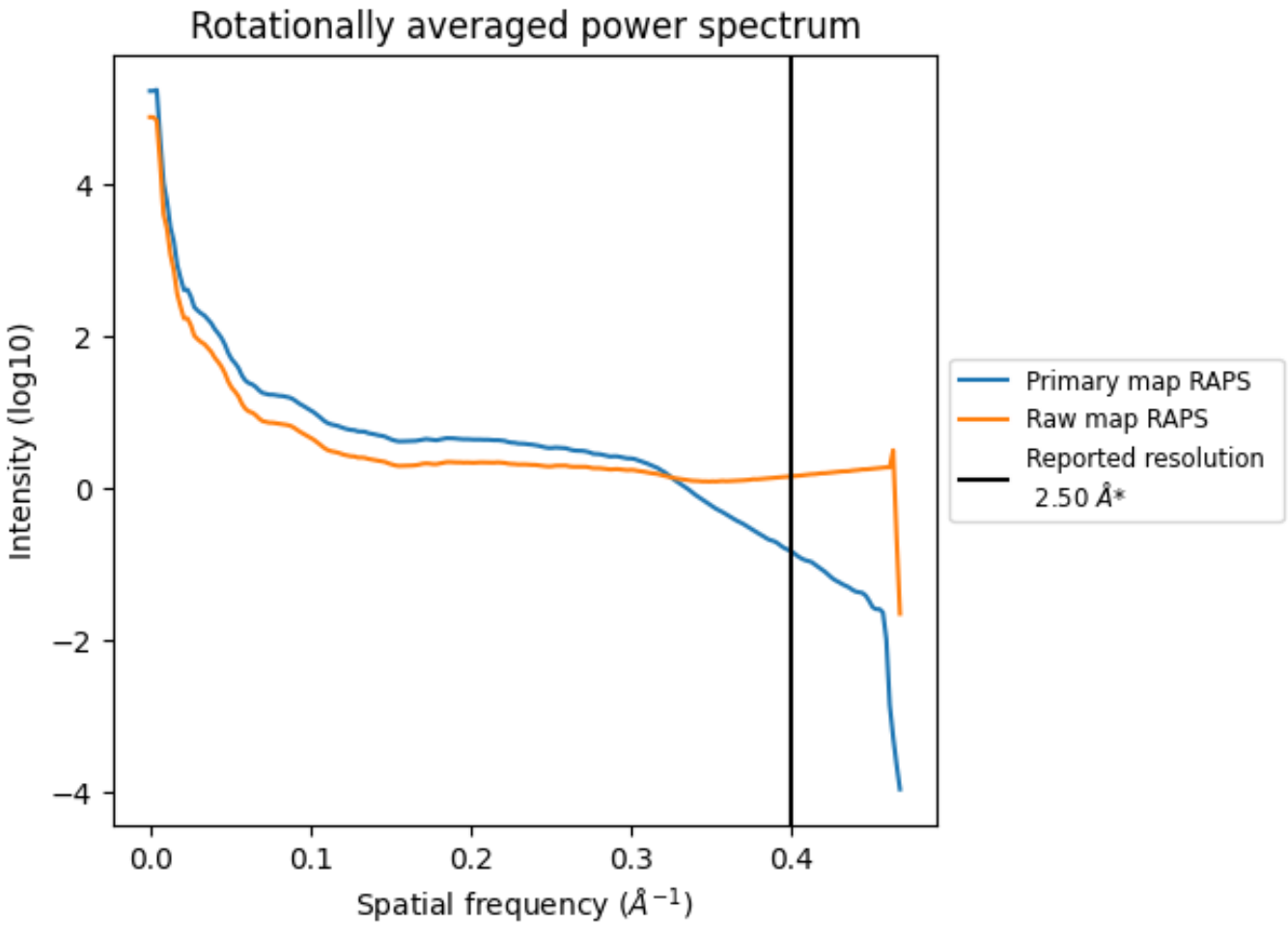
7.2 Volume estimate (i)



The volume at the recommended contour level is 1332 nm^3; this corresponds to an approximate mass of 1203 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)

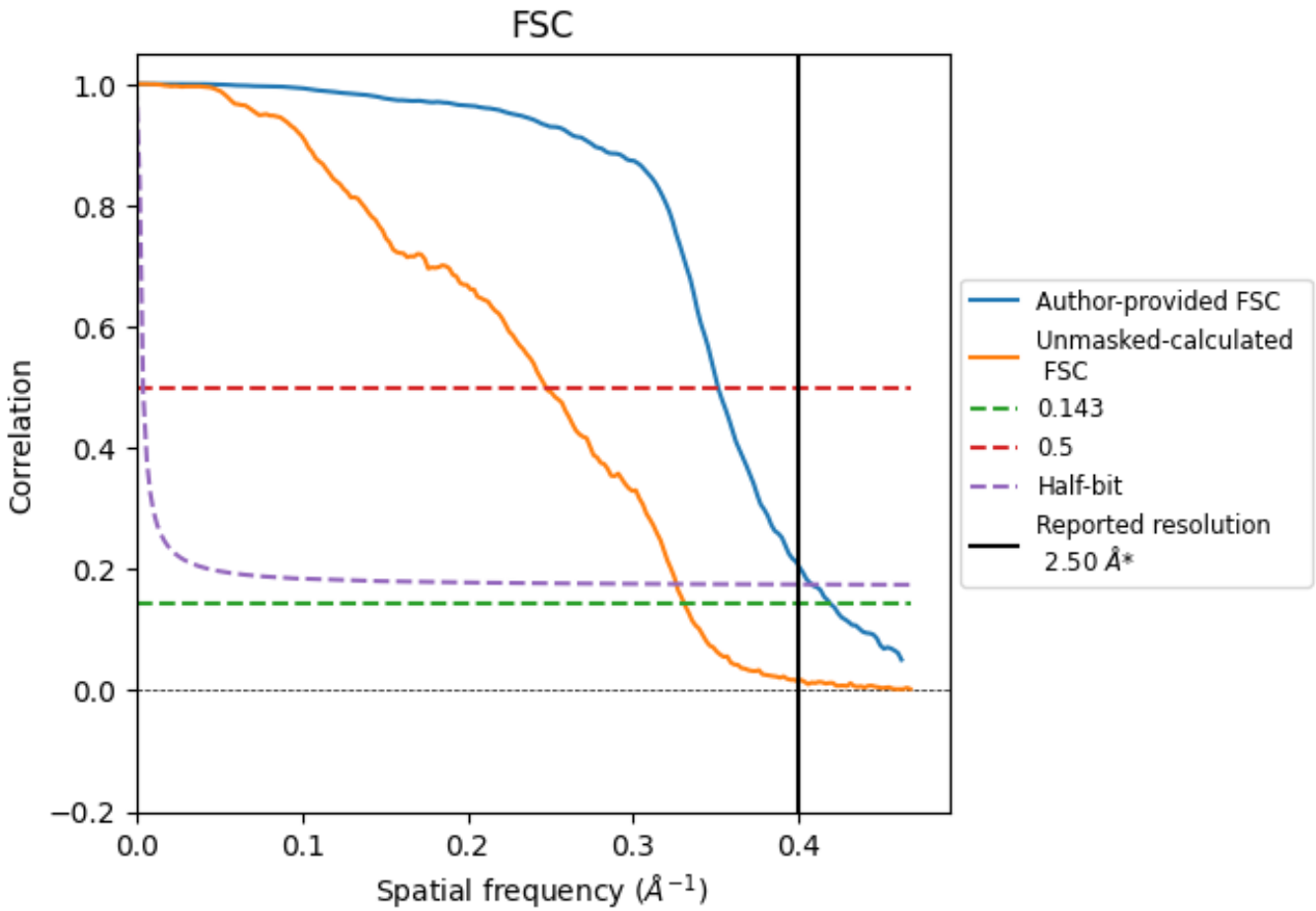


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

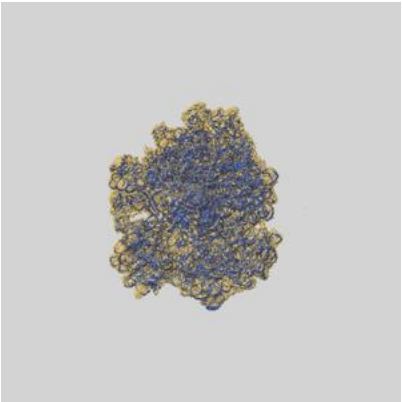
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.39	2.85	2.45
Unmasked-calculated*	3.02	4.04	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 2.5 by more than 10 %

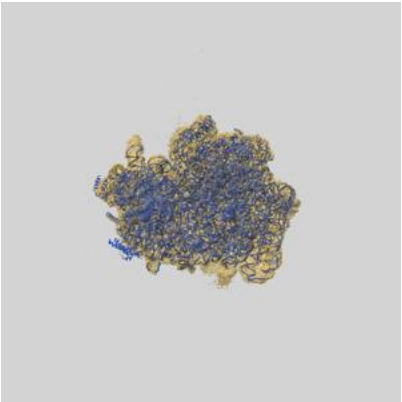
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-71684 and PDB model 9PJ9. Per-residue inclusion information can be found in section 3 on page 17.

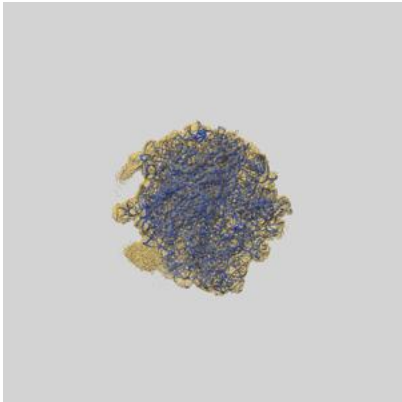
9.1 Map-model overlay (i)



X



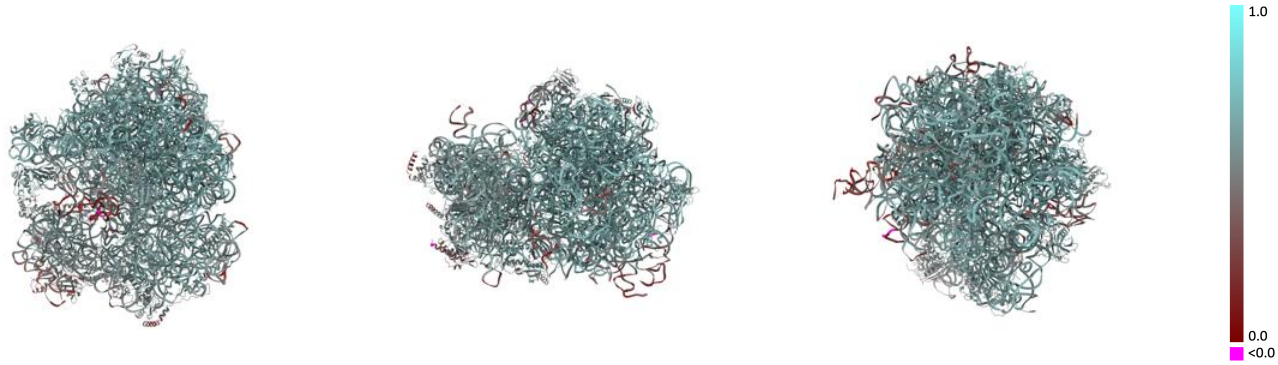
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

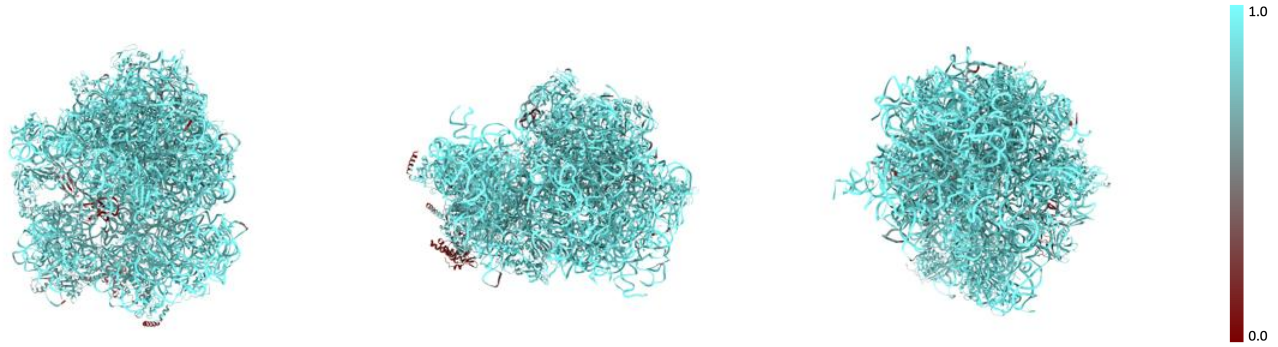
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

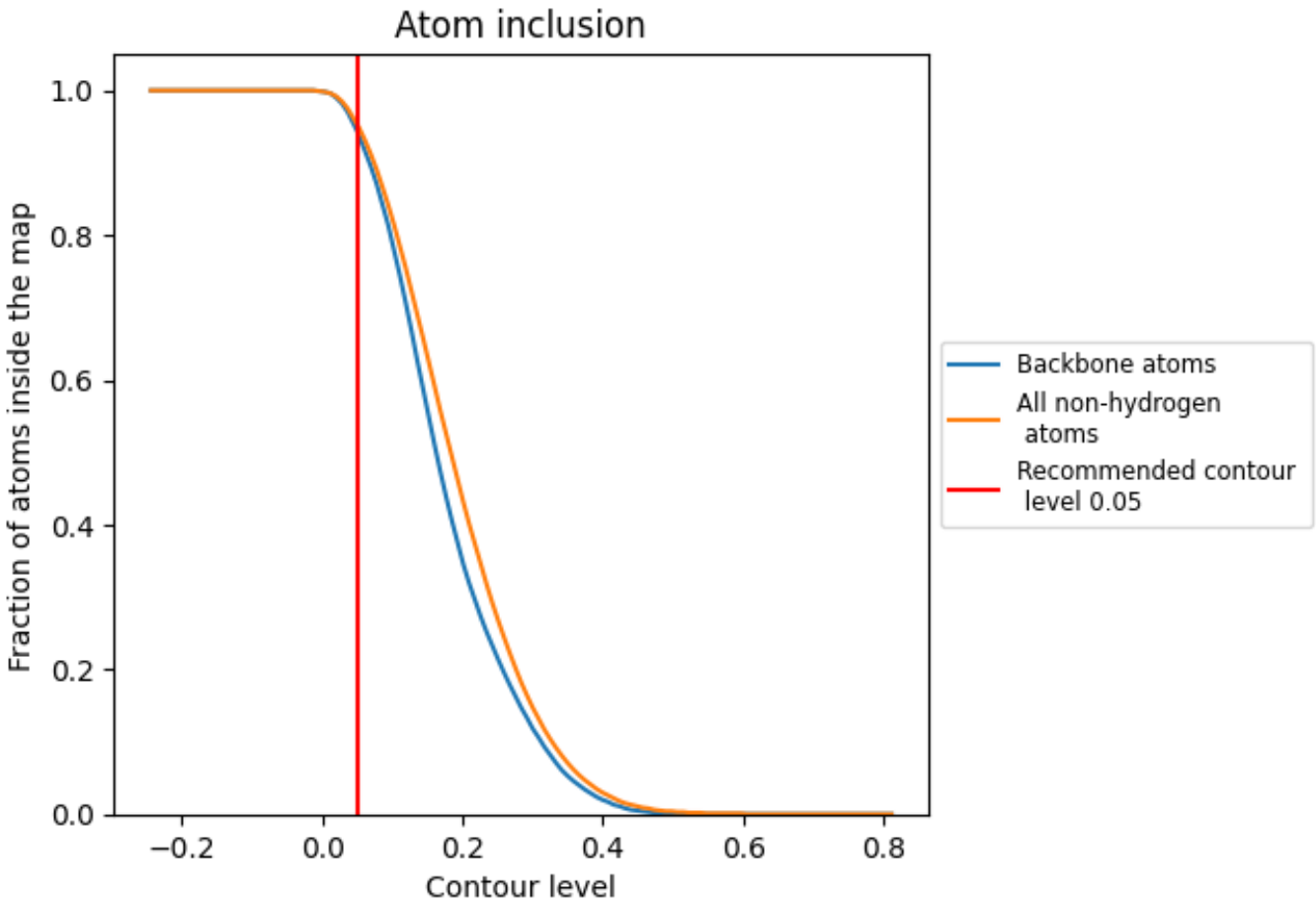
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9530	0.5940
0	0.9660	0.6400
1	0.9910	0.6770
2	0.9800	0.6610
3	0.9730	0.6440
4	0.8810	0.5140
A	0.9860	0.5790
B	0.1920	0.4020
C	0.9160	0.5780
D	0.9230	0.5330
E	0.8830	0.5710
F	0.9190	0.5520
G	0.8360	0.5240
H	0.9580	0.5930
I	0.9050	0.5270
J	0.9000	0.4810
K	0.9650	0.5720
L	0.9490	0.6080
M	0.7660	0.4690
N	0.8890	0.5420
O	0.9470	0.5780
P	0.8730	0.5220
Q	0.8880	0.5730
R	0.8980	0.5430
S	0.9280	0.5720
T	0.9500	0.5760
U	0.9240	0.5150
V	0.9830	0.6670
X	0.8730	0.5830
Y	0.7490	0.4380
a	0.9740	0.6100
b	0.9970	0.6180
c	0.9780	0.6560
d	0.9770	0.6420
e	0.9580	0.6100

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.9530	0.5770
g	0.9450	0.5370
i	0.9820	0.6510
j	0.9500	0.6300
k	0.9700	0.6290
l	0.9790	0.6410
m	0.9730	0.6430
n	0.9770	0.6020
o	0.9600	0.6390
p	0.9700	0.6510
q	0.9540	0.6210
r	0.9600	0.6390
s	0.9730	0.6220
t	0.9670	0.5970
u	0.7320	0.5150
v	0.9650	0.6520
w	0.9890	0.6560
x	0.9620	0.6050
y	0.9670	0.6290
z	0.9670	0.6510