wwPDB EM Validation Summary Report (i)

Mar 5, 2024 – 04:00 AM EST

PDB ID	:	8UU8
EMDB ID	:	EMD-42571
Title	:	Cryo-EM structure of the Listeria innocua 70S ribosome (head-swiveled) in complex with HflXr and pe/E-tRNA (structure II-C)
Authors	:	Seely, S.M.; Basu, R.S.; Gagnon, M.G.
Deposited on	:	2023-10-31
Resolution	:	3.10 Å(reported)
Based on initial model	:	7NHN

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:

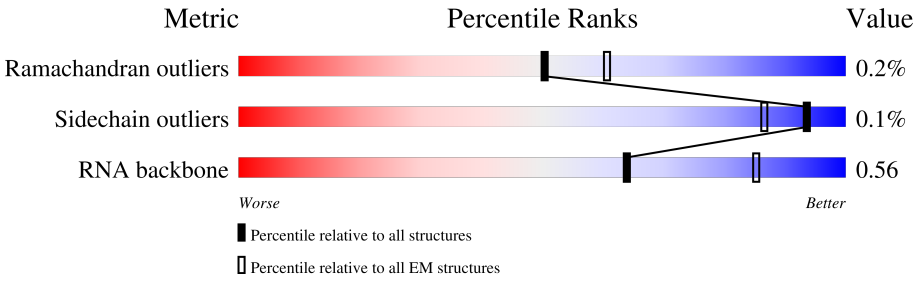
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	a	1550	5% 76% 22%
2	b	249	13% 83% 16%
3	c	218	39% 94% 6%
4	d	200	100%
5	e	167	91% 9%
6	f	97	13% 97%
7	g	156	51% 83% 17%
8	h	132	99%

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Mol	Chain	Length	Quality of chain
9	i	130	28% 98%
10	j	102	32% 93% 6%
11	k	129	9% 88% 12%
12	l	137	96%
13	m	121	54% 89% 11%
14	n	61	18% 82% 18%
15	o	89	98%
16	p	90	96%
17	q	87	92% 8%
18	r	79	81% 19%
19	s	92	68% 80% 20%
20	t	84	96%
21	x	76	87% 67% 28%
22	w	21	24% 14% 29% 57%
23	v	418	9% 100%
24	A	2932	83% 16%
25	B	116	88% 10%
26	C	277	99%
27	D	209	99%
28	E	207	99%
29	F	179	34% 97%
30	G	178	8% 96%
31	I	166	68% 78% 22%
32	H	141	60% 94%
33	L	145	99%

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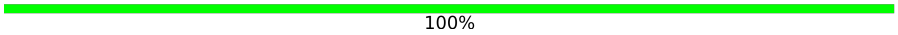
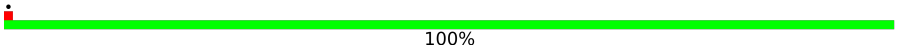
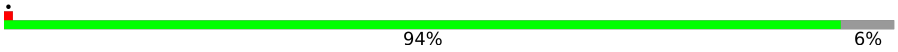
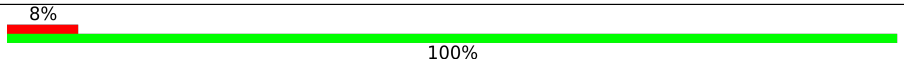
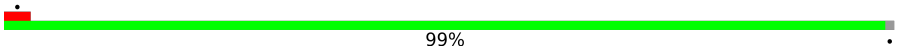
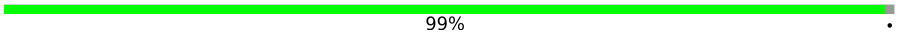
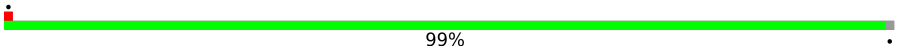
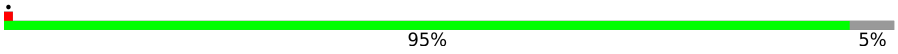
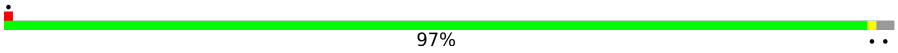
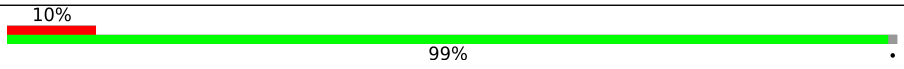
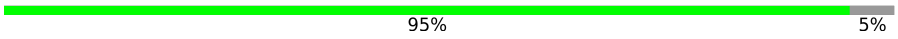
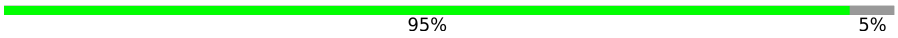
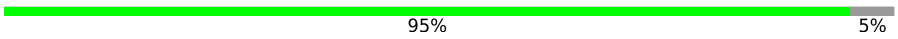
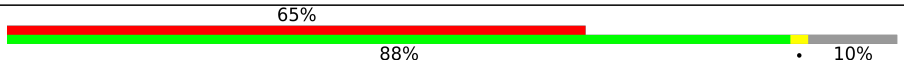
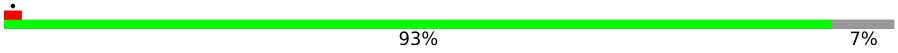
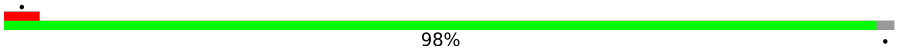
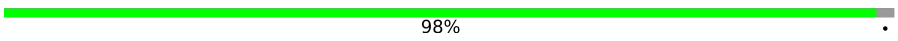
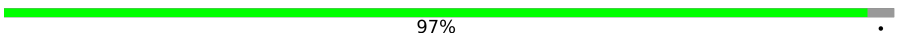
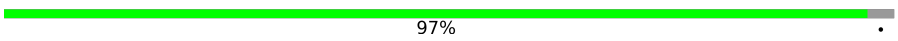
Mol	Chain	Length	Quality of chain
34	M	122	
35	N	146	
36	O	144	
37	P	135	
38	Q	119	
39	R	114	
40	S	119	
41	T	102	
42	U	118	
43	V	94	
44	W	103	
45	Y	96	
46	Z	62	
47	1	63	
48	2	59	
49	3	81	
50	4	57	
51	5	49	
52	6	44	
53	7	66	
54	8	37	

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 142031 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1516	32515	14504	5960	10535	1516	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	209	1396	888	249	255	4	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	c	204	1003	595	204	204	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	199	1562	978	289	293	2	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	152	1057	666	197	192	2	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	95	785	496	138	149	2	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	130	Total	C	N	O	S	0	0
			650	387	130	132	1		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	131	Total	C	N	O	S	0	0
			1022	651	180	189	2		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	i	127	Total	C	N	O	0	0
			635	377	128	130		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	96	Total	C	N	O	0	0
			477	285	96	96		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	114	Total	C	N	O	S	0	0
			748	455	149	141	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	135	Total	C	N	O	S	0	0
			993	615	198	179	1		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	m	108	Total	C	N	O	0	0
			529	313	108	108		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	50	Total	C	N	O	S	0	0
			260	154	53	50	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	87	Total	C	N	O	S	0	0
			695	431	137	125	2		

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	88	Total	C	N	O	S	0	0
			661	418	126	114	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			650	410	120	119	1		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	64	Total	C	N	O	S	0	0
			494	319	93	81	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	s	74	Total	C	N	O	0	0
			365	217	74	74		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	81	Total	C	N	O	S	0	0
			583	353	117	112	1		

- Molecule 21 is a RNA chain called pe/E Hybrid State Phenylalanine tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	x	74	Total	C	N	O	P	S	0	0
			1591	713	285	517	74	2		

- Molecule 22 is a RNA chain called F-Stop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	w	9	Total	C	N	O	P	0	0
			190	86	34	61	9		

- Molecule 23 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	v	417	Total	C	N	O	S	0	0
			3282	2067	566	639	10		

- Molecule 24 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	2901	Total	C	N	O	P	0	0
			62318	27812	11528	20077	2901		

- Molecule 25 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	114	Total	C	N	O	P	0	0
			2428	1082	428	804	114		

- Molecule 26 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C	274	Total	C	N	O	S	0	0
			2084	1293	408	376	7		

- Molecule 27 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D	206	Total	C	N	O	S	0	0
			1544	975	288	277	4		

- Molecule 28 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	E	205	Total 1536	C 976	N 286	O 274	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	175	Total 1173	C 732	N 215	O 222	S 4	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	G	171	Total 1305	C 822	N 241	O 241	S 1	0	0

- Molecule 31 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	I	129	Total 636	C 378	N 129	O 129	0	0

- Molecule 32 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	H	135	Total 673	C 403	N 135	O 135	0	0

- Molecule 33 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	143	Total 1112	C 707	N 205	O 197	S 3	0	0

- Molecule 34 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	122	Total 893	C 554	N 170	O 165	S 4	0	0

- Molecule 35 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N	146	Total	C	N	O	S	0	0
			1071	662	209	199	1		

- Molecule 36 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	O	135	Total	C	N	O	S	0	0
			1062	679	203	174	6		

- Molecule 37 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	P	122	Total	C	N	O	S	0	0
			982	616	193	172	1		

- Molecule 38 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Q	119	Total	C	N	O	S	0	0
			884	545	172	166	1		

- Molecule 39 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	R	113	Total	C	N	O	S	0	0
			885	560	171	153	1		

- Molecule 40 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	S	118	Total	C	N	O	S	0	0
			949	602	187	156	4		

- Molecule 41 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	T	101	Total	C	N	O	S	0	0
			774	502	134	137	1		

- Molecule 42 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	U	112	Total	C	N	O	0	0
			850	537	159	154		

- Molecule 43 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	V	92	Total	C	N	O	S	0	0
			726	463	126	134	3		

- Molecule 44 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	102	Total	C	N	O	S	0	0
			760	482	140	135	3		

- Molecule 45 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Y	76	Total	C	N	O	S	0	0
			567	347	110	109	1		

- Molecule 46 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Z	59	Total	C	N	O	S	0	0
			444	274	92	76	2		

- Molecule 47 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1	60	Total	C	N	O	S	0	0
			477	295	94	87	1		

- Molecule 48 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	2	56	Total	C	N	O	S	0	0
			433	272	82	78	1		

- Molecule 49 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3	73	Total	C	N	O	S	0	0
			523	328	90	104	1		

- Molecule 50 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	4	53	Total	C	N	O	S	0	0
			417	256	86	70	5		

- Molecule 51 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	5	48	Total	C	N	O	S	0	0
			394	241	79	70	4		

- Molecule 52 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	6	43	Total	C	N	O	S	0	0
			365	222	88	53	2		

- Molecule 53 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	7	64	Total	C	N	O	S	0	0
			520	322	114	79	5		

- Molecule 54 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	8	36	Total	C	N	O	S	0	0
			280	174	56	44	6		

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	a	151	Total	Mg	0
			151	151	
55	b	1	Total	Mg	0
			1	1	
55	c	1	Total	Mg	0
			1	1	

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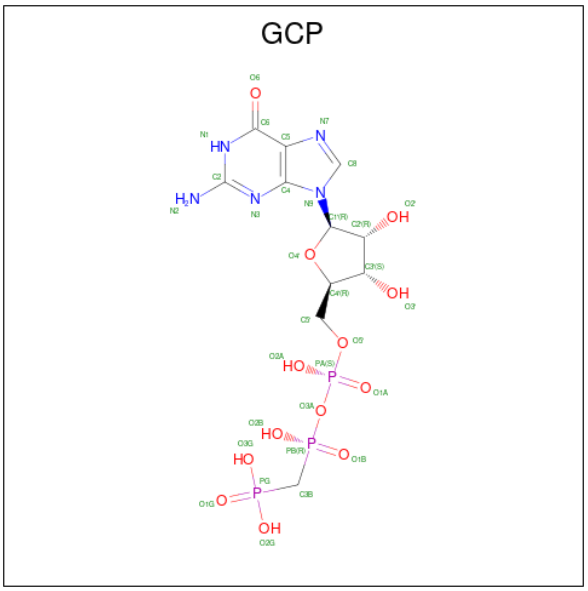
Mol	Chain	Residues	Atoms	AltConf
55	g	1	Total Mg 1 1	0
55	i	2	Total Mg 2 2	0
55	m	1	Total Mg 1 1	0
55	n	2	Total Mg 2 2	0
55	o	1	Total Mg 1 1	0
55	v	2	Total Mg 2 2	0
55	A	249	Total Mg 249 249	0
55	B	5	Total Mg 5 5	0
55	C	1	Total Mg 1 1	0
55	D	2	Total Mg 2 2	0
55	M	1	Total Mg 1 1	0
55	N	1	Total Mg 1 1	0
55	S	1	Total Mg 1 1	0
55	W	1	Total Mg 1 1	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
56	n	1	Total Zn 1 1	0
56	4	1	Total Zn 1 1	0
56	5	1	Total Zn 1 1	0
56	8	1	Total Zn 1 1	0

- Molecule 57 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
57	v	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	a	94	Total	O	0
			94	94	
58	d	1	Total	O	0
			1	1	
58	e	1	Total	O	0
			1	1	
58	f	1	Total	O	0
			1	1	
58	i	1	Total	O	0
			1	1	
58	p	3	Total	O	0
			3	3	
58	t	1	Total	O	0
			1	1	
58	v	2	Total	O	0
			2	2	
58	A	235	Total	O	0
			235	235	
58	B	6	Total	O	0
			6	6	
58	C	2	Total	O	0
			2	2	

Continued on next page...

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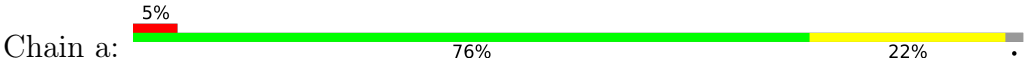
Mol	Chain	Residues	Atoms	AltConf
58	D	1	Total O 1 1	0
58	N	5	Total O 5 5	0
58	O	1	Total O 1 1	0
58	P	1	Total O 1 1	0
58	S	2	Total O 2 2	0
58	T	1	Total O 1 1	0
58	U	2	Total O 2 2	0
58	V	1	Total O 1 1	0
58	Z	2	Total O 2 2	0
58	2	1	Total O 1 1	0

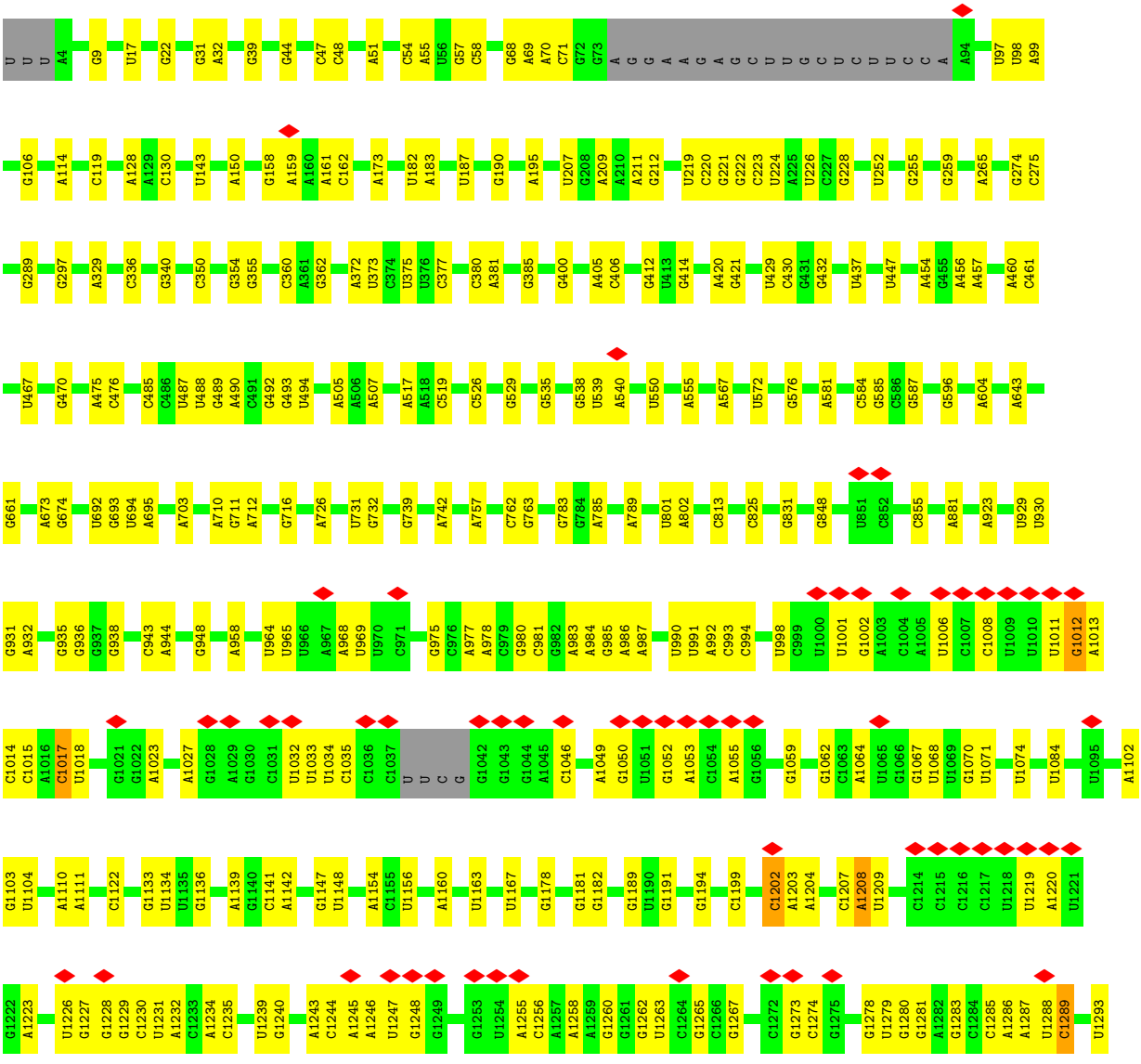
3 Residue-property plots (i)

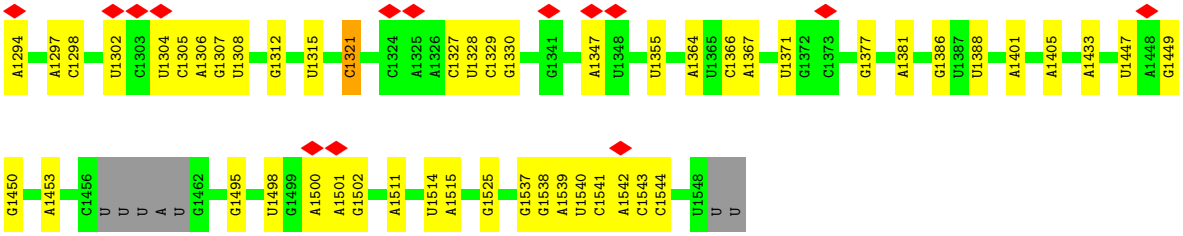
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain a:

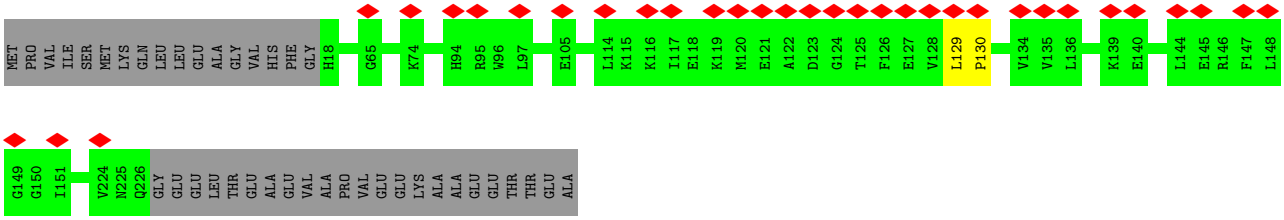






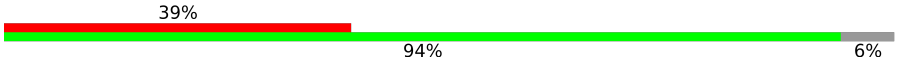
• Molecule 2: Small ribosomal subunit protein uS2

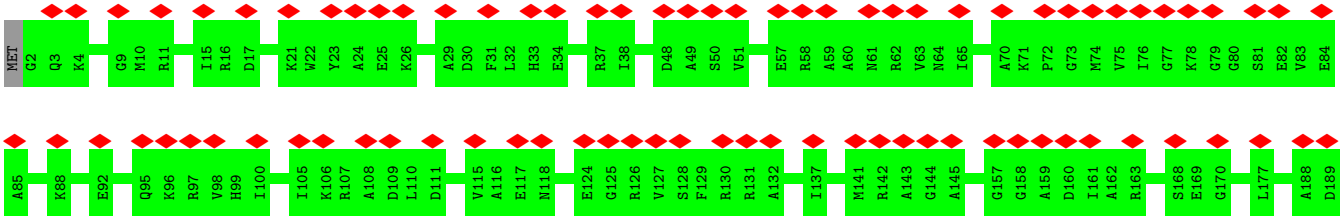
Chain b:



• Molecule 3: Small ribosomal subunit protein uS3

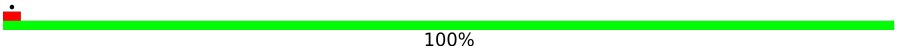
Chain c:

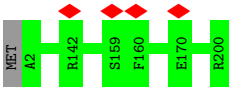




• Molecule 4: Small ribosomal subunit protein uS4

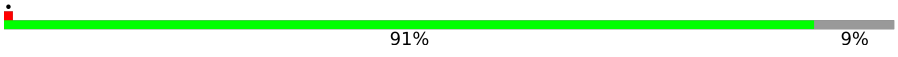
Chain d:

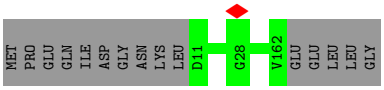




• Molecule 5: Small ribosomal subunit protein uS5

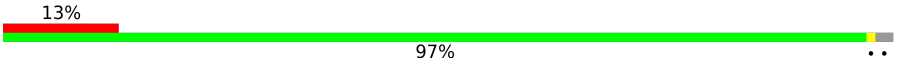
Chain e:

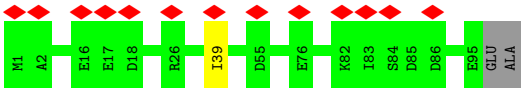




• Molecule 6: Small ribosomal subunit protein bS6

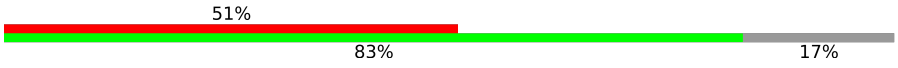
Chain f:

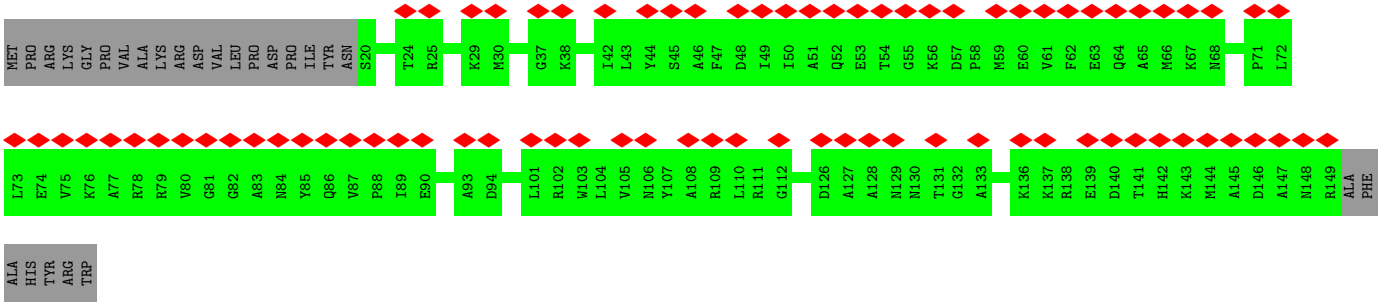




• Molecule 7: Small ribosomal subunit protein uS7

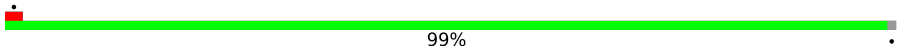
Chain g:

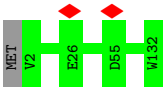




• Molecule 8: Small ribosomal subunit protein uS8

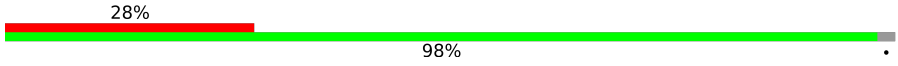
Chain h:

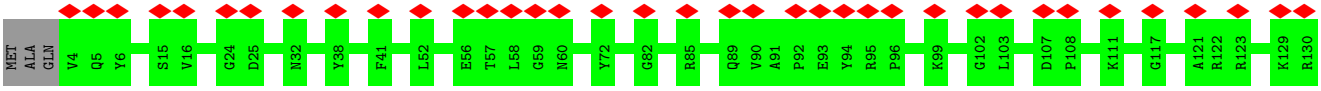




• Molecule 9: Small ribosomal subunit protein uS9

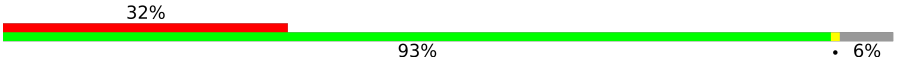
Chain i:

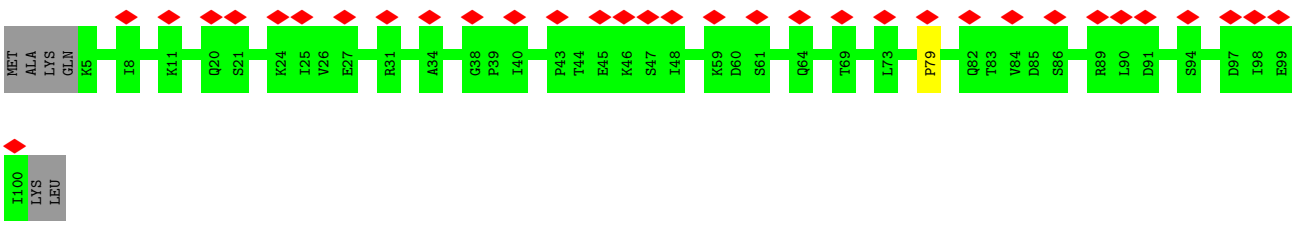




• Molecule 10: Small ribosomal subunit protein uS10

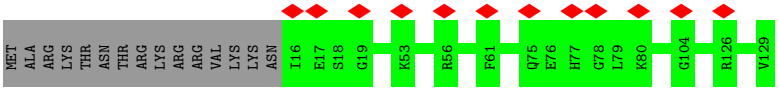
Chain j:





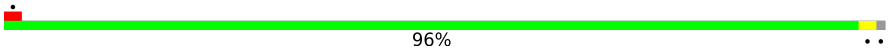
• Molecule 11: Small ribosomal subunit protein uS11

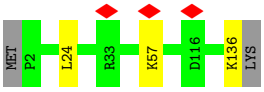
Chain k:



• Molecule 12: Small ribosomal subunit protein uS12

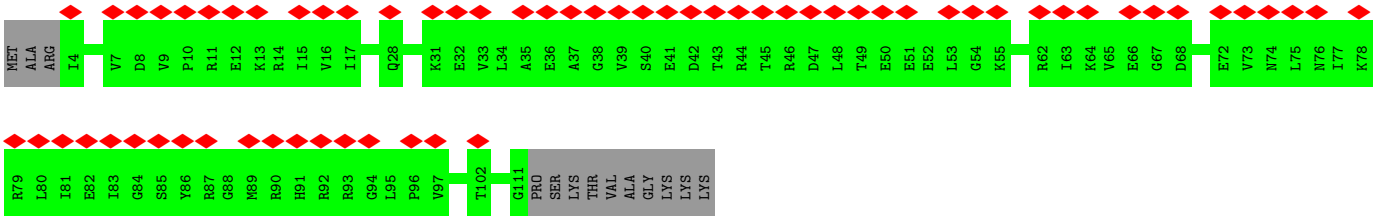
Chain l:





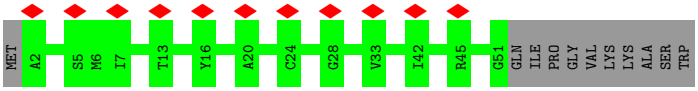
• Molecule 13: Small ribosomal subunit protein uS13

Chain m:



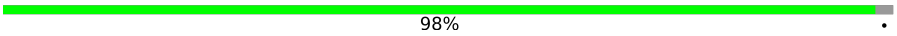
• Molecule 14: Small ribosomal subunit protein uS14

Chain n:



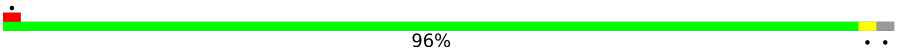
• Molecule 15: Small ribosomal subunit protein uS15

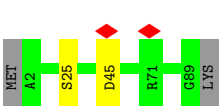
Chain o:



• Molecule 16: Small ribosomal subunit protein bS16

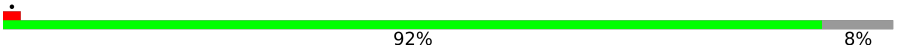
Chain p:

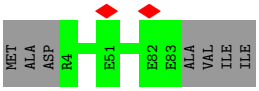




• Molecule 17: Small ribosomal subunit protein uS17

Chain q:



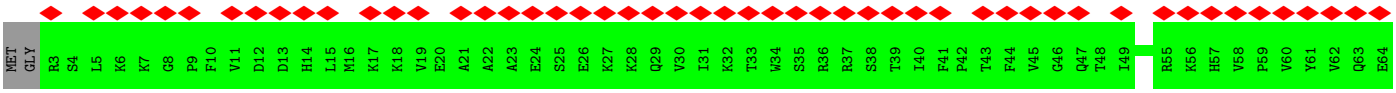


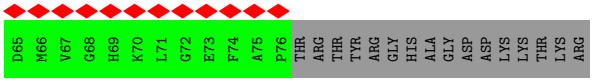
• Molecule 18: Small ribosomal subunit protein bS18

Chain r:

• Molecule 19: Small ribosomal subunit protein uS19

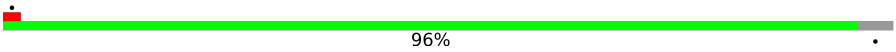
Chain s:

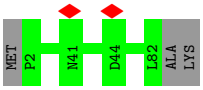




• Molecule 20: Small ribosomal subunit protein bS20

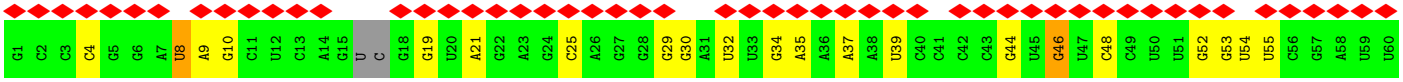
Chain t:

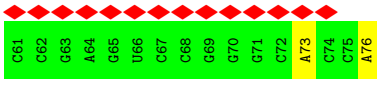




• Molecule 21: pe/E Hybrid State Phenylalanine tRNA

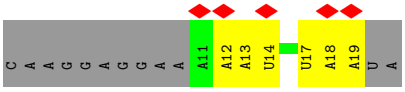
Chain x:





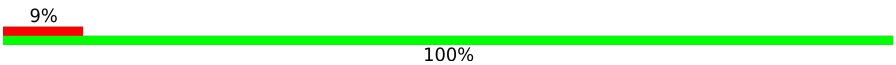
• Molecule 22: F-Stop mRNA

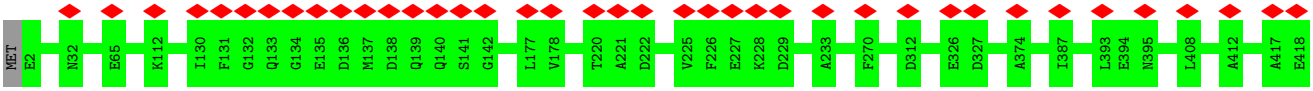
Chain w:



• Molecule 23: GTPase HflX

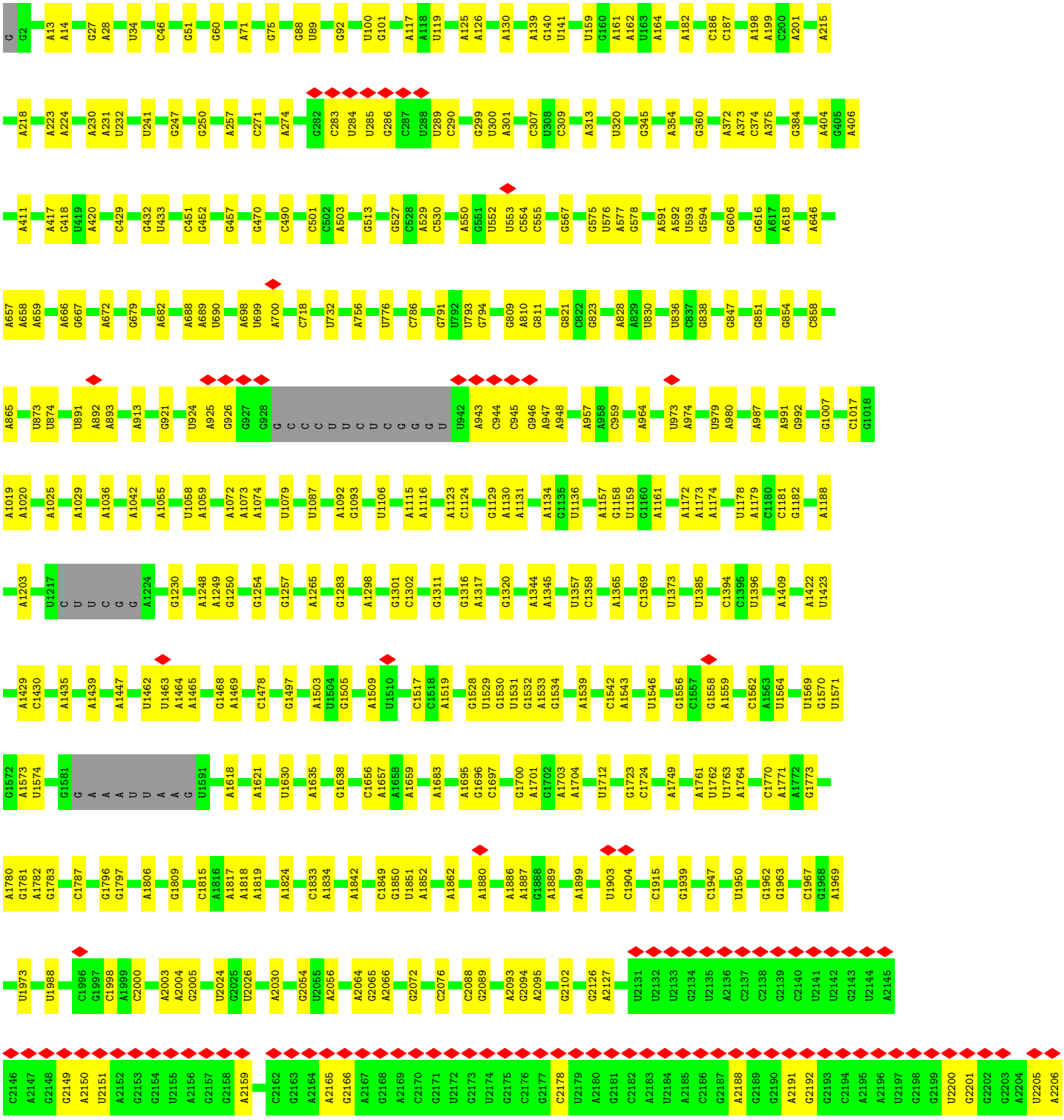
Chain v:

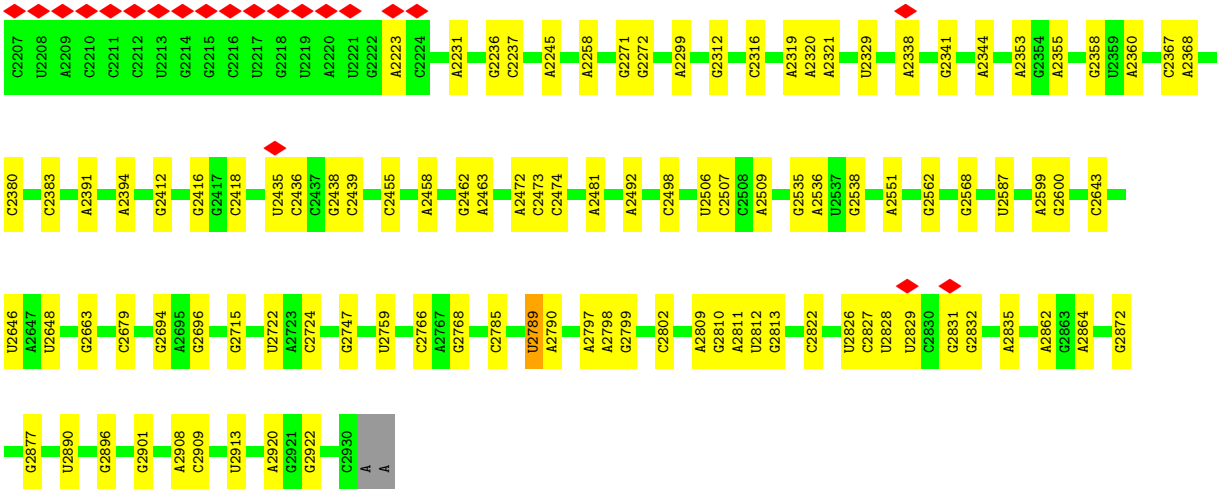




• Molecule 24: 23S Ribosomal RNA

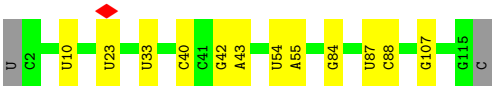
Chain A:





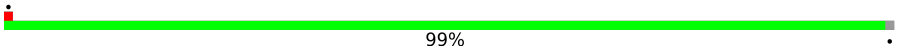
• Molecule 25: 5S Ribosomal RNA

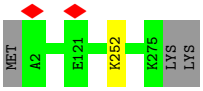
Chain B:



• Molecule 26: Large ribosomal subunit protein uL2

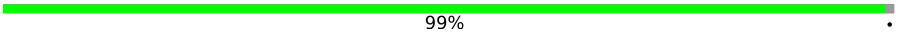
Chain C:

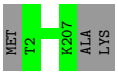




• Molecule 27: Large ribosomal subunit protein uL3

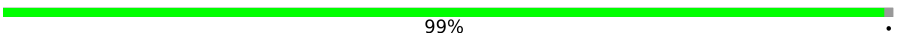
Chain D:





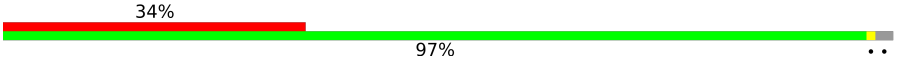
• Molecule 28: Large ribosomal subunit protein uL4

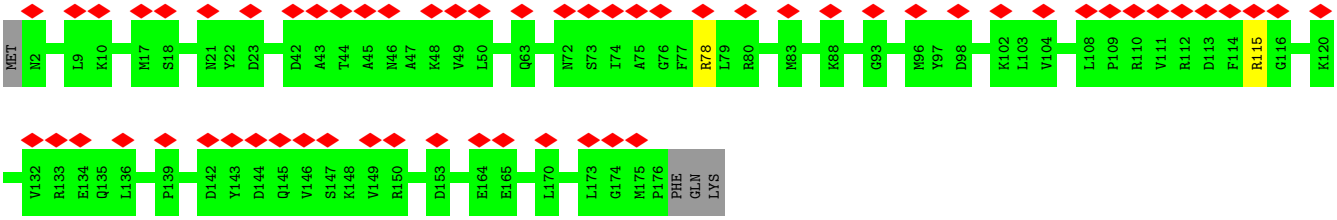
Chain E:



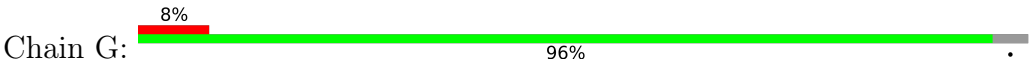
• Molecule 29: Large ribosomal subunit protein uL5

Chain F:

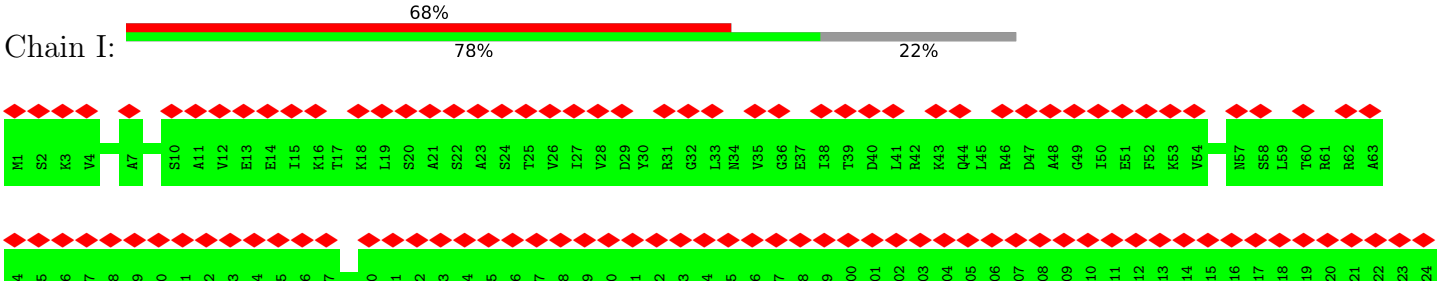




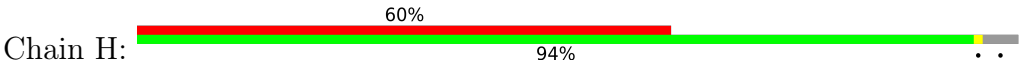
• Molecule 30: Large ribosomal subunit protein uL6



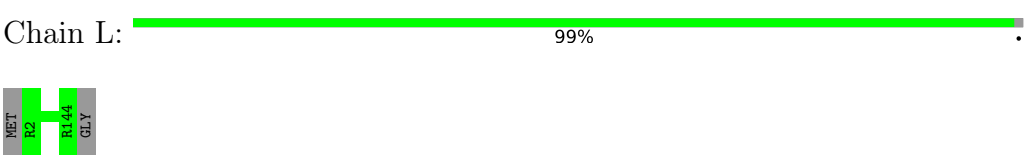
• Molecule 31: Large ribosomal subunit protein uL10



• Molecule 32: Large ribosomal subunit protein uL11



• Molecule 33: Large ribosomal subunit protein uL13



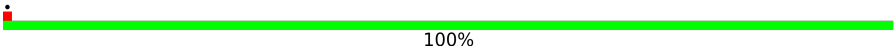
• Molecule 34: Large ribosomal subunit protein uL14

Chain M:

There are no outlier residues recorded for this chain.

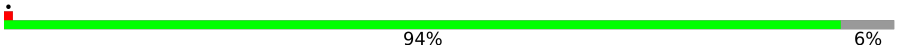
• Molecule 35: Large ribosomal subunit protein uL15

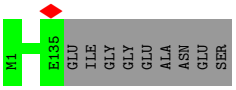
Chain N:



• Molecule 36: Large ribosomal subunit protein uL16

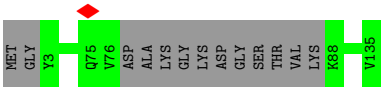
Chain O:





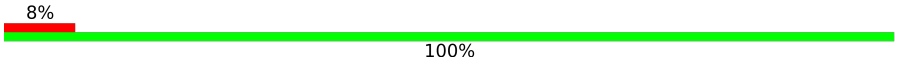
• Molecule 37: Large ribosomal subunit protein bL17

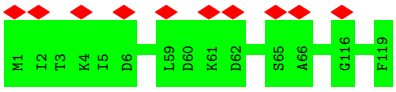
Chain P:



• Molecule 38: Large ribosomal subunit protein uL18

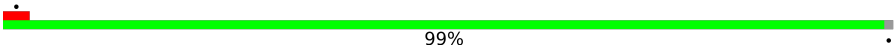
Chain Q:

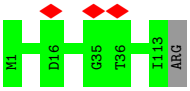




• Molecule 39: Large ribosomal subunit protein bL19

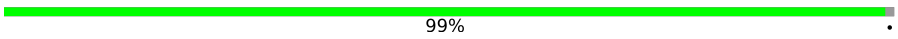
Chain R:





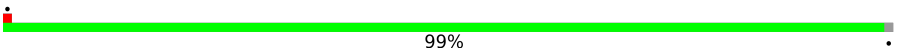
• Molecule 40: Large ribosomal subunit protein bL20

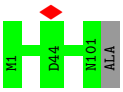
Chain S:



• Molecule 41: Large ribosomal subunit protein bL21

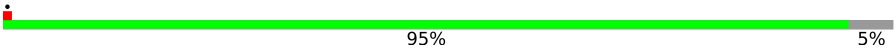
Chain T:

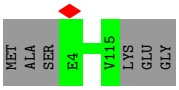




• Molecule 42: Large ribosomal subunit protein uL22

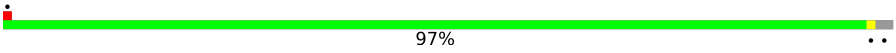
Chain U:

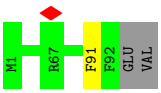




• Molecule 43: Large ribosomal subunit protein uL23

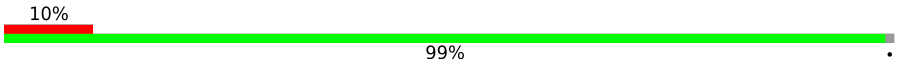
Chain V:

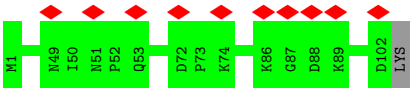




• Molecule 44: Large ribosomal subunit protein uL24

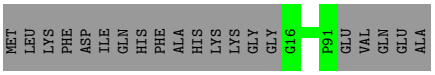
Chain W:





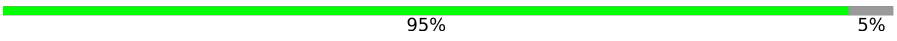
• Molecule 45: Large ribosomal subunit protein bL27

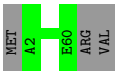
Chain Y:



• Molecule 46: Large ribosomal subunit protein bL28

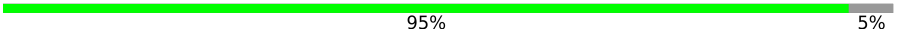
Chain Z:

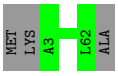




• Molecule 47: Large ribosomal subunit protein uL29

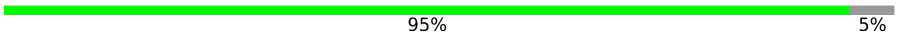
Chain 1:

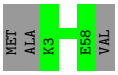




• Molecule 48: Large ribosomal subunit protein uL30

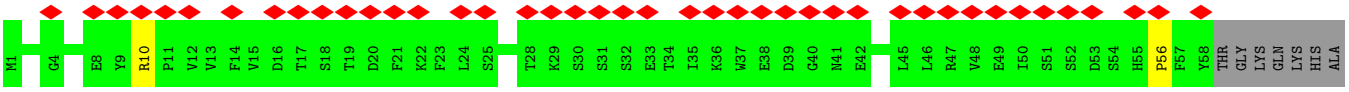
Chain 2:

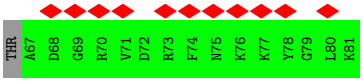




• Molecule 49: Large ribosomal subunit protein bL31B

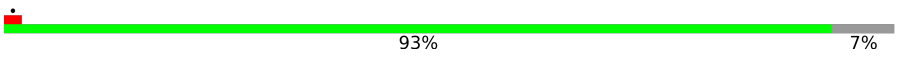
Chain 3:

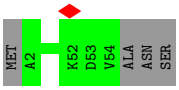




• Molecule 50: Large ribosomal subunit protein bL32

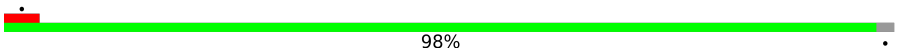
Chain 4:

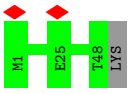




• Molecule 51: Large ribosomal subunit protein bL33

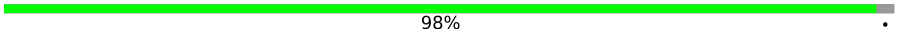
Chain 5:





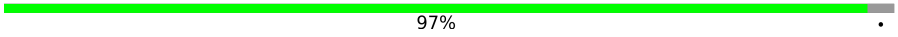
• Molecule 52: Large ribosomal subunit protein bL34

Chain 6:



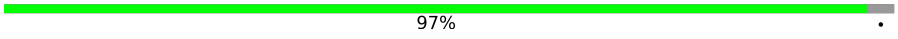
• Molecule 53: Large ribosomal subunit protein bL35

Chain 7:



• Molecule 54: Large ribosomal subunit protein bL36

Chain 8:




M1
Q36
GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55099	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 ($e^-/Å^2$)	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	34.334	Depositor
Minimum map value	-17.982	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.124	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, PSU, MIA, GCP, MG, 4SU, ZN, 5MU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	a	0.54	0/36403	0.88	12/56778 (0.0%)
2	b	0.29	0/1419	0.55	1/1945 (0.1%)
3	c	0.24	0/1002	0.45	0/1391
4	d	0.32	0/1590	0.56	0/2142
5	e	0.34	0/1069	0.55	0/1451
6	f	0.32	0/797	0.60	0/1068
7	g	0.24	0/649	0.41	0/901
8	h	0.37	0/1035	0.61	0/1392
9	i	0.27	0/636	0.49	0/878
10	j	0.24	0/476	0.48	0/663
11	k	0.27	0/760	0.53	0/1031
12	l	0.33	0/1009	0.61	1/1365 (0.1%)
13	m	0.24	0/528	0.45	0/731
14	n	0.27	0/259	0.56	0/357
15	o	0.33	0/705	0.63	0/949
16	p	0.33	0/674	0.59	0/909
17	q	0.32	0/659	0.57	0/882
18	r	0.34	0/502	0.60	0/673
19	s	0.24	0/364	0.45	0/505
20	t	0.29	0/586	0.55	0/788
21	x	0.26	0/1605	0.82	0/2497
22	w	0.29	0/212	0.81	0/327
23	v	0.30	0/3324	0.54	0/4483
24	A	0.51	0/69819	0.79	3/108917 (0.0%)
25	B	0.32	0/2711	0.75	0/4224
26	C	0.32	0/2120	0.54	0/2848
27	D	0.35	0/1566	0.55	0/2108
28	E	0.31	0/1557	0.52	0/2103
29	F	0.26	0/1186	0.56	0/1615
30	G	0.28	0/1327	0.52	0/1793
31	I	0.23	0/635	0.40	0/882
32	H	0.26	0/676	0.42	0/942

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	L	0.33	0/1135	0.50	0/1526
34	M	0.33	0/900	0.56	0/1212
35	N	0.31	0/1082	0.54	0/1446
36	O	0.32	0/1084	0.55	0/1450
37	P	0.32	0/993	0.57	0/1328
38	Q	0.26	0/893	0.54	0/1201
39	R	0.32	0/897	0.57	0/1206
40	S	0.34	0/962	0.50	0/1280
41	T	0.37	0/787	0.50	0/1057
42	U	0.32	0/860	0.54	0/1165
43	V	0.32	0/735	0.51	0/988
44	W	0.30	0/770	0.50	0/1032
45	Y	0.33	0/574	0.58	0/766
46	Z	0.30	0/449	0.56	0/597
47	1	0.26	0/478	0.52	0/640
48	2	0.28	0/436	0.53	0/585
49	3	0.26	0/532	0.49	0/720
50	4	0.36	0/425	0.58	0/567
51	5	0.30	0/398	0.58	0/534
52	6	0.33	0/368	0.64	0/479
53	7	0.31	0/527	0.62	0/685
54	8	0.32	0/283	0.53	0/375
All	All	0.47	0/153428	0.76	17/230377 (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
12	l	0	1
16	p	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	130	PRO	CA-N-CD	-7.68	100.75	111.50
1	a	1012	G	O4'-C1'-N9	6.58	113.47	108.20
1	a	1260	G	C6-C5-N7	-6.52	126.49	130.40
1	a	1017	C	C2-N1-C1'	6.21	125.63	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1260	G	N3-C4-N9	6.14	129.69	126.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	l	57	LYS	Peptide
16	p	45	ASP	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	b	207/249 (83%)	180 (87%)	26 (13%)	1 (0%)	29 64
3	c	202/218 (93%)	176 (87%)	26 (13%)	0	100 100
4	d	197/200 (98%)	181 (92%)	16 (8%)	0	100 100
5	e	150/167 (90%)	137 (91%)	13 (9%)	0	100 100
6	f	93/97 (96%)	72 (77%)	20 (22%)	1 (1%)	14 46
7	g	128/156 (82%)	118 (92%)	10 (8%)	0	100 100
8	h	129/132 (98%)	115 (89%)	14 (11%)	0	100 100
9	i	125/130 (96%)	105 (84%)	20 (16%)	0	100 100
10	j	94/102 (92%)	71 (76%)	22 (23%)	1 (1%)	14 46
11	k	112/129 (87%)	100 (89%)	12 (11%)	0	100 100
12	l	133/137 (97%)	120 (90%)	13 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	106/121 (88%)	92 (87%)	14 (13%)	0	100	100
14	n	48/61 (79%)	33 (69%)	15 (31%)	0	100	100
15	o	85/89 (96%)	78 (92%)	7 (8%)	0	100	100
16	p	86/90 (96%)	74 (86%)	11 (13%)	1 (1%)	13	44
17	q	78/87 (90%)	71 (91%)	7 (9%)	0	100	100
18	r	62/79 (78%)	56 (90%)	6 (10%)	0	100	100
19	s	72/92 (78%)	65 (90%)	7 (10%)	0	100	100
20	t	79/84 (94%)	77 (98%)	2 (2%)	0	100	100
23	v	415/418 (99%)	382 (92%)	33 (8%)	0	100	100
26	C	272/277 (98%)	261 (96%)	10 (4%)	1 (0%)	34	69
27	D	204/209 (98%)	194 (95%)	10 (5%)	0	100	100
28	E	203/207 (98%)	189 (93%)	14 (7%)	0	100	100
29	F	173/179 (97%)	161 (93%)	12 (7%)	0	100	100
30	G	169/178 (95%)	156 (92%)	13 (8%)	0	100	100
31	I	127/166 (76%)	122 (96%)	5 (4%)	0	100	100
32	H	133/141 (94%)	122 (92%)	9 (7%)	2 (2%)	10	39
33	L	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
34	M	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
35	N	144/146 (99%)	133 (92%)	11 (8%)	0	100	100
36	O	133/144 (92%)	129 (97%)	4 (3%)	0	100	100
37	P	118/135 (87%)	113 (96%)	5 (4%)	0	100	100
38	Q	117/119 (98%)	107 (92%)	10 (8%)	0	100	100
39	R	111/114 (97%)	104 (94%)	7 (6%)	0	100	100
40	S	116/119 (98%)	113 (97%)	3 (3%)	0	100	100
41	T	99/102 (97%)	96 (97%)	3 (3%)	0	100	100
42	U	110/118 (93%)	107 (97%)	3 (3%)	0	100	100
43	V	90/94 (96%)	84 (93%)	5 (6%)	1 (1%)	14	46
44	W	100/103 (97%)	98 (98%)	2 (2%)	0	100	100
45	Y	74/96 (77%)	68 (92%)	6 (8%)	0	100	100
46	Z	57/62 (92%)	53 (93%)	4 (7%)	0	100	100
47	1	58/63 (92%)	56 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
48	2	54/59 (92%)	51 (94%)	3 (6%)	0	100 100
49	3	69/81 (85%)	61 (88%)	7 (10%)	1 (1%)	11 40
50	4	51/57 (90%)	44 (86%)	7 (14%)	0	100 100
51	5	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
52	6	41/44 (93%)	41 (100%)	0	0	100 100
53	7	62/66 (94%)	57 (92%)	5 (8%)	0	100 100
54	8	34/37 (92%)	32 (94%)	2 (6%)	0	100 100
All	All	5827/6270 (93%)	5350 (92%)	468 (8%)	9 (0%)	50 79

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	j	79	PRO
16	p	25	SER
32	H	92	PRO
49	3	56	PRO
2	b	129	LEU

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
2	b	104/214 (49%)	104 (100%)	0	100 100
4	d	162/170 (95%)	162 (100%)	0	100 100
5	e	104/131 (79%)	104 (100%)	0	100 100
6	f	81/85 (95%)	81 (100%)	0	100 100
7	g	4/130 (3%)	4 (100%)	0	100 100
8	h	109/110 (99%)	109 (100%)	0	100 100
9	i	4/102 (4%)	4 (100%)	0	100 100
11	k	58/100 (58%)	58 (100%)	0	100 100
12	l	101/118 (86%)	100 (99%)	1 (1%)	76 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	n	5/52 (10%)	5 (100%)	0	100	100
15	o	71/81 (88%)	71 (100%)	0	100	100
16	p	63/80 (79%)	63 (100%)	0	100	100
17	q	72/78 (92%)	72 (100%)	0	100	100
18	r	47/67 (70%)	47 (100%)	0	100	100
20	t	55/66 (83%)	55 (100%)	0	100	100
23	v	351/365 (96%)	351 (100%)	0	100	100
26	C	215/225 (96%)	215 (100%)	0	100	100
27	D	158/171 (92%)	158 (100%)	0	100	100
28	E	161/174 (92%)	161 (100%)	0	100	100
29	F	93/155 (60%)	91 (98%)	2 (2%)	52	78
30	G	139/147 (95%)	139 (100%)	0	100	100
32	H	4/111 (4%)	4 (100%)	0	100	100
33	L	116/121 (96%)	116 (100%)	0	100	100
34	M	92/101 (91%)	92 (100%)	0	100	100
35	N	105/115 (91%)	105 (100%)	0	100	100
36	O	105/113 (93%)	105 (100%)	0	100	100
37	P	102/111 (92%)	102 (100%)	0	100	100
38	Q	88/97 (91%)	88 (100%)	0	100	100
39	R	93/99 (94%)	93 (100%)	0	100	100
40	S	95/97 (98%)	95 (100%)	0	100	100
41	T	78/82 (95%)	78 (100%)	0	100	100
42	U	90/97 (93%)	90 (100%)	0	100	100
43	V	76/84 (90%)	76 (100%)	0	100	100
44	W	83/88 (94%)	83 (100%)	0	100	100
45	Y	57/76 (75%)	57 (100%)	0	100	100
46	Z	45/53 (85%)	45 (100%)	0	100	100
47	1	48/55 (87%)	48 (100%)	0	100	100
48	2	50/52 (96%)	50 (100%)	0	100	100
49	3	48/73 (66%)	47 (98%)	1 (2%)	53	79
50	4	44/50 (88%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	5	44/48 (92%)	44 (100%)	0	100	100
52	6	39/39 (100%)	39 (100%)	0	100	100
53	7	54/56 (96%)	54 (100%)	0	100	100
54	8	32/35 (91%)	32 (100%)	0	100	100
All	All	3745/4674 (80%)	3741 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	l	136	LYS
29	F	78	ARG
29	F	115	ARG
49	3	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
35	N	27	ASN
44	W	67	ASN
35	N	126	ASN
38	Q	43	GLN
45	Y	58	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1512/1550 (97%)	340 (22%)	0
21	x	71/76 (93%)	18 (25%)	0
22	w	8/21 (38%)	6 (75%)	0
24	A	2897/2932 (98%)	457 (15%)	29 (1%)
25	B	113/116 (97%)	12 (10%)	0
All	All	4601/4695 (97%)	833 (18%)	29 (0%)

5 of 833 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	17	U

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Mol	Chain	Res	Type
1	a	22	G
1	a	31	G
1	a	32	A

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	1468	G
24	A	2809	A
24	A	1530	G
24	A	2438	G
24	A	1528	G

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

7 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	$\#\|Z\| > 2$
21	PSU	x	55	21	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
21	PSU	x	39	21	18,21,22	1.28	2 (11%)	22,30,33	1.97	4 (18%)
21	G7M	x	46	21	20,26,27	2.64	4 (20%)	17,39,42	0.90	1 (5%)
21	MIA	x	37	21	24,31,32	2.18	3 (12%)	26,44,47	2.51	8 (30%)
21	PSU	x	32	21	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
21	4SU	x	8	21	18,21,22	1.77	5 (27%)	26,30,33	2.39	6 (23%)
21	5MU	x	54	21	19,22,23	1.36	5 (26%)	28,32,35	2.11	6 (21%)

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
21	PSU	x	55	21	-	0/7/25/26	0/2/2/2
21	PSU	x	39	21	-	0/7/25/26	0/2/2/2
21	G7M	x	46	21	-	2/3/25/26	0/3/3/3
21	MIA	x	37	21	-	1/11/33/34	0/3/3/3
21	PSU	x	32	21	-	0/7/25/26	0/2/2/2
21	4SU	x	8	21	-	2/7/25/26	0/2/2/2
21	5MU	x	54	21	-	0/7/25/26	0/2/2/2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	x	46	G7M	C8-N9	7.50	1.46	1.33
21	x	37	MIA	C13-C14	7.10	1.52	1.32
21	x	46	G7M	C8-N7	6.96	1.45	1.33
21	x	37	MIA	C2-S10	-6.46	1.70	1.75
21	x	8	4SU	C4-S4	-4.54	1.59	1.68

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	x	37	MIA	C12-C13-C14	-8.40	110.80	127.14
21	x	8	4SU	C4-N3-C2	-7.09	120.46	127.34
21	x	39	PSU	N1-C2-N3	6.05	121.99	115.13
21	x	8	4SU	C5-C4-N3	6.01	120.26	114.69
21	x	32	PSU	N1-C2-N3	5.96	121.88	115.13

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	x	37	MIA	C12-C13-C14-C16
21	x	46	G7M	O4'-C4'-C5'-O5'
21	x	8	4SU	C3'-C4'-C5'-O5'
21	x	8	4SU	O4'-C4'-C5'-O5'
21	x	46	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 428 ligands modelled in this entry, 427 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	GCP	v	503	55	27,34,34	1.40	5 (18%)	34,54,54	1.90	8 (23%)

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	GCP	v	503	55	-	5/15/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	v	503	GCP	C5-C6	3.75	1.47	1.41
57	v	503	GCP	PG-O3G	2.71	1.61	1.54
57	v	503	GCP	PG-O2G	2.66	1.61	1.54
57	v	503	GCP	C5-C4	2.18	1.46	1.40
57	v	503	GCP	PB-O3A	2.18	1.60	1.58

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	v	503	GCP	C2-N3-C4	4.81	120.86	115.36
57	v	503	GCP	C4-C5-C6	-3.87	117.10	120.80
57	v	503	GCP	C5-C6-N1	-3.82	118.21	123.43
57	v	503	GCP	C2-N1-C6	3.79	121.96	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	v	503	GCP	N3-C2-N1	-3.19	122.97	127.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

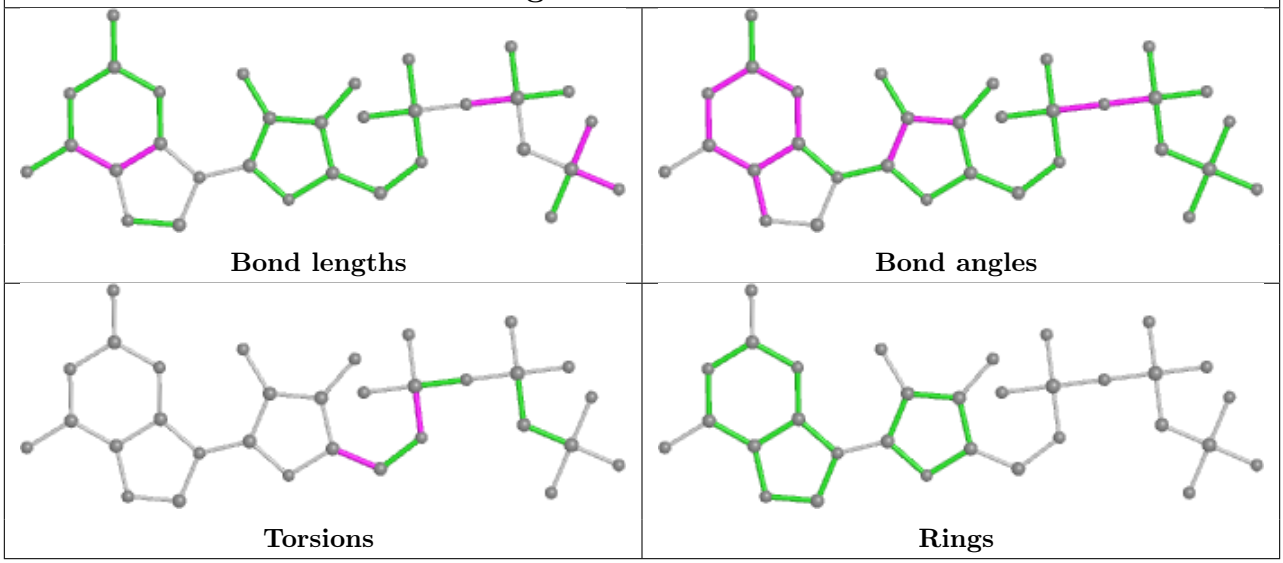
Mol	Chain	Res	Type	Atoms
57	v	503	GCP	C5'-O5'-PA-O1A
57	v	503	GCP	O4'-C4'-C5'-O5'
57	v	503	GCP	C3'-C4'-C5'-O5'
57	v	503	GCP	C5'-O5'-PA-O3A
57	v	503	GCP	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 GCP v 503



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.

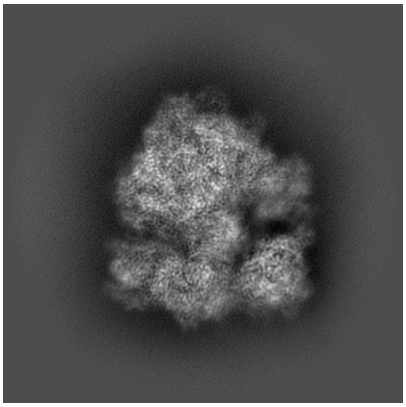
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42571. These allow visual inspection of the internal detail of the map and identification of artifacts.

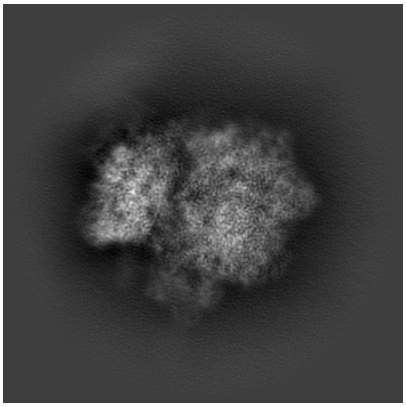
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

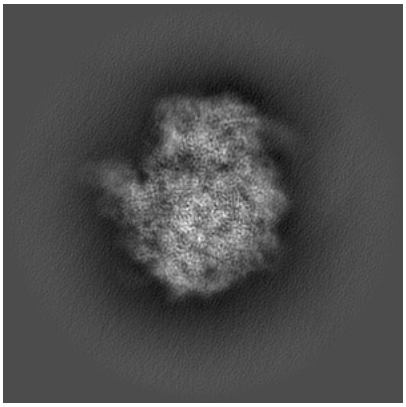
6.1.1 Primary map



X



Y

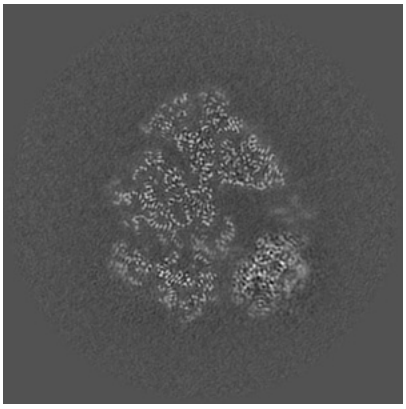


Z

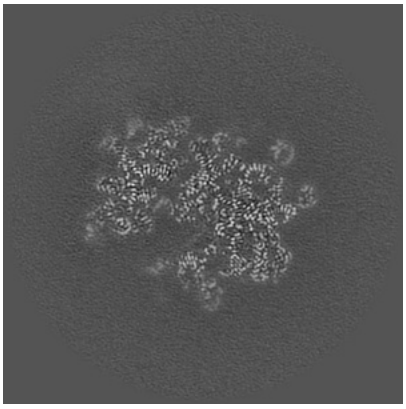
The images above show the map projected in three orthogonal directions.

6.2 Central slices

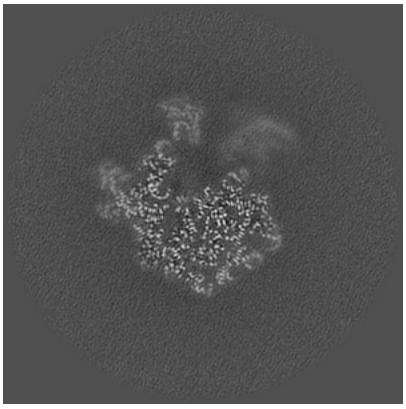
6.2.1 Primary map



X Index: 256



Y Index: 256

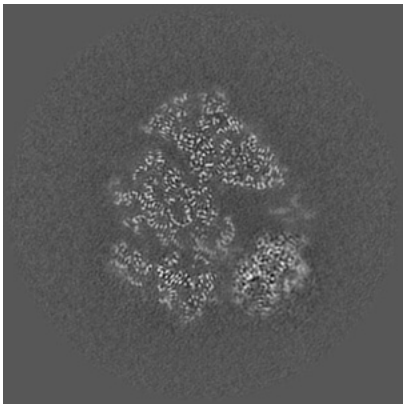


Z Index: 256

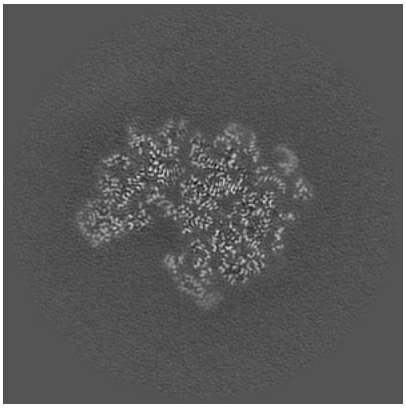
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

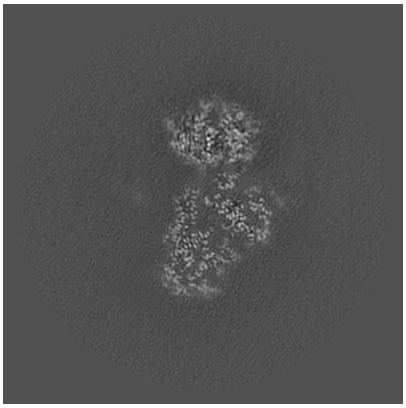
6.3.1 Primary map



X Index: 255



Y Index: 244

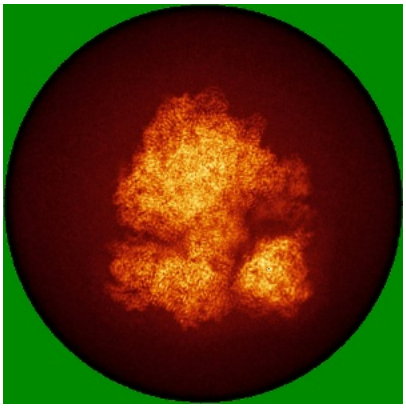


Z Index: 178

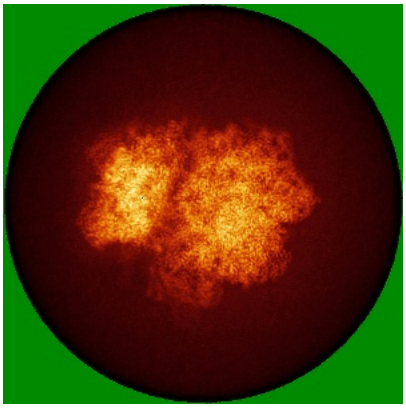
The images above show the largest variance slices of the map in three orthogonal directions.

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

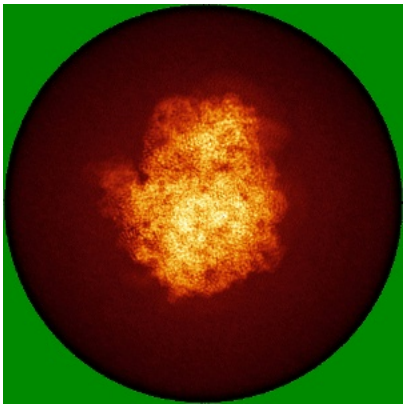
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

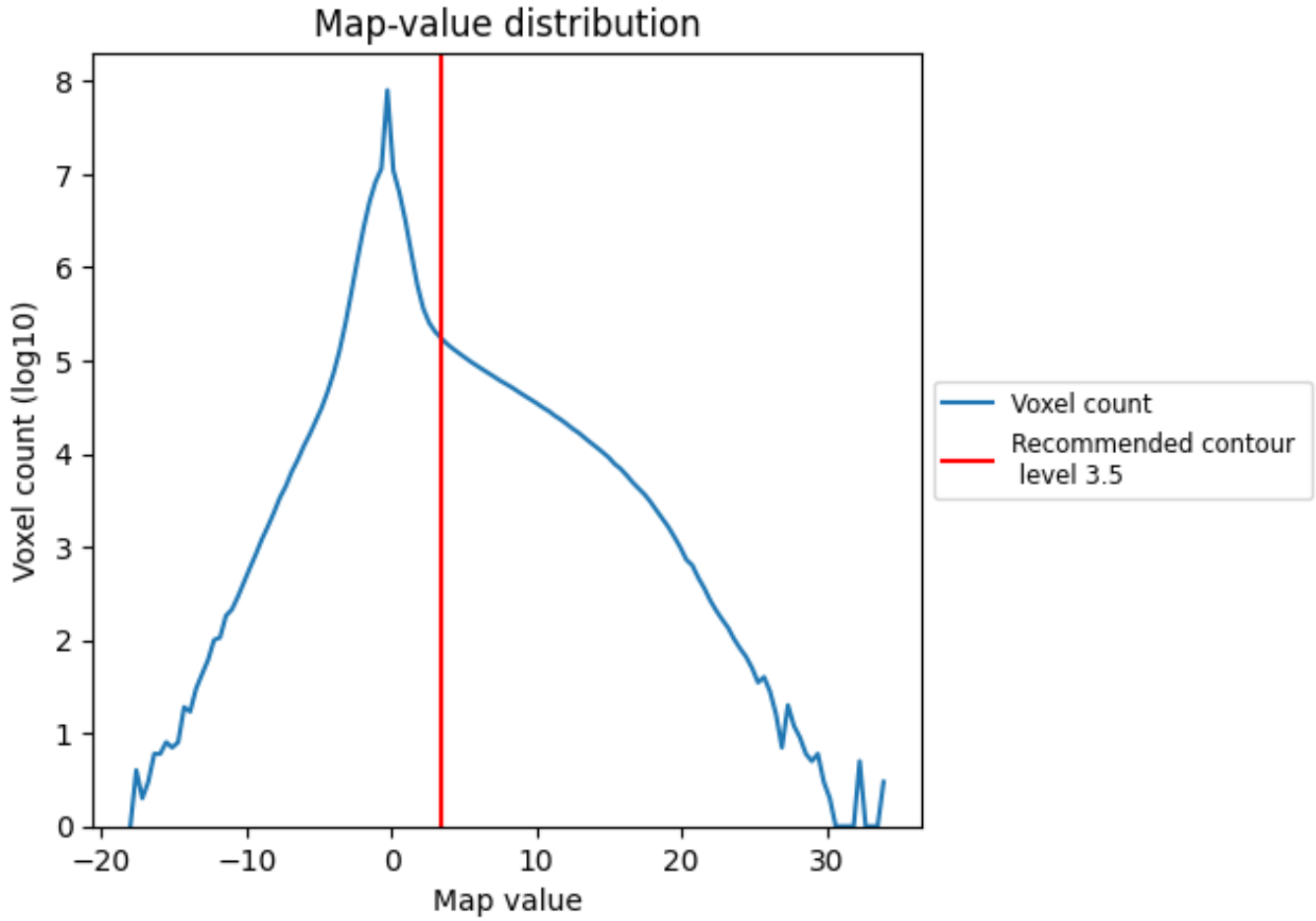
6.6 Mask visualisation (i)

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

7 Map analysis

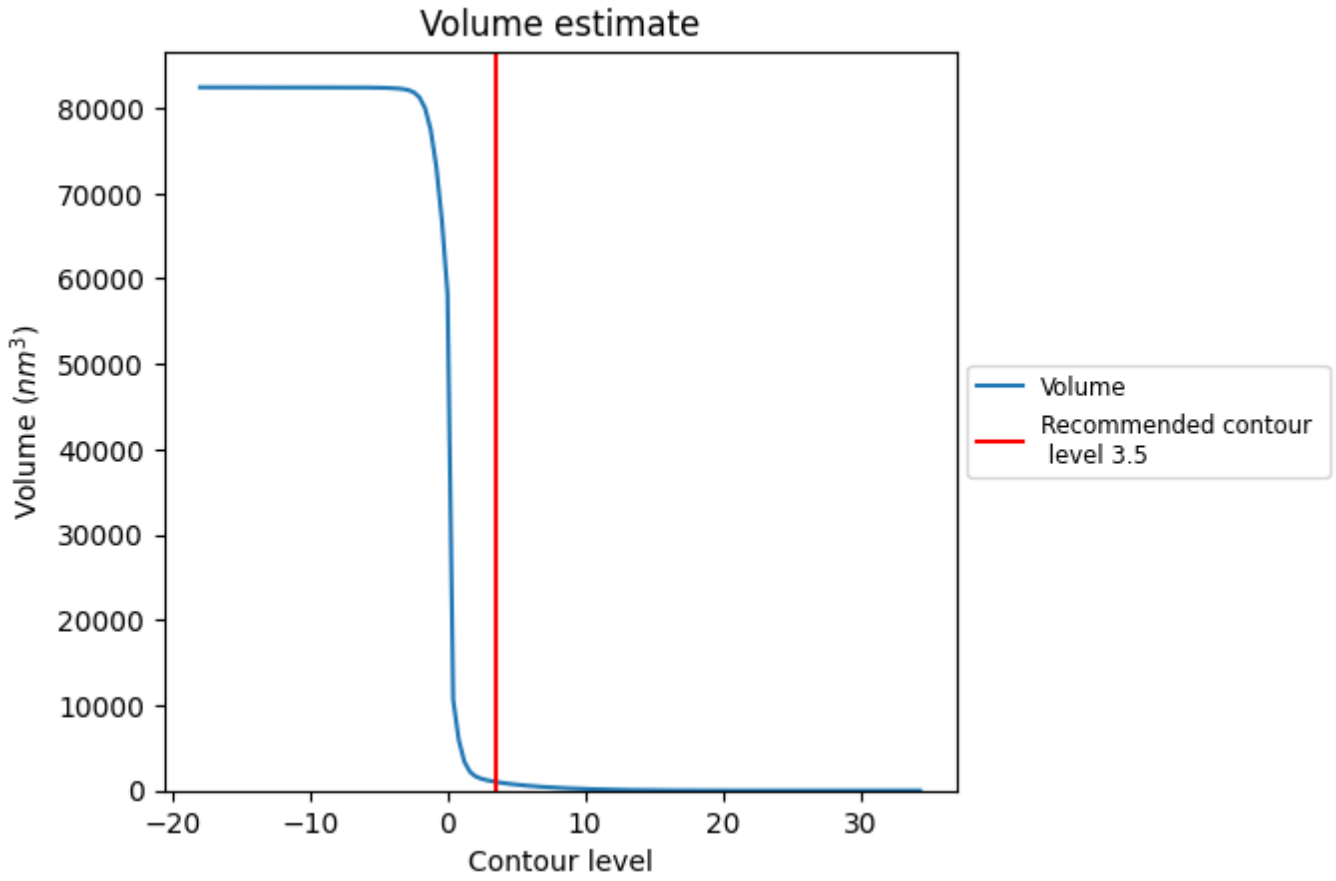
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

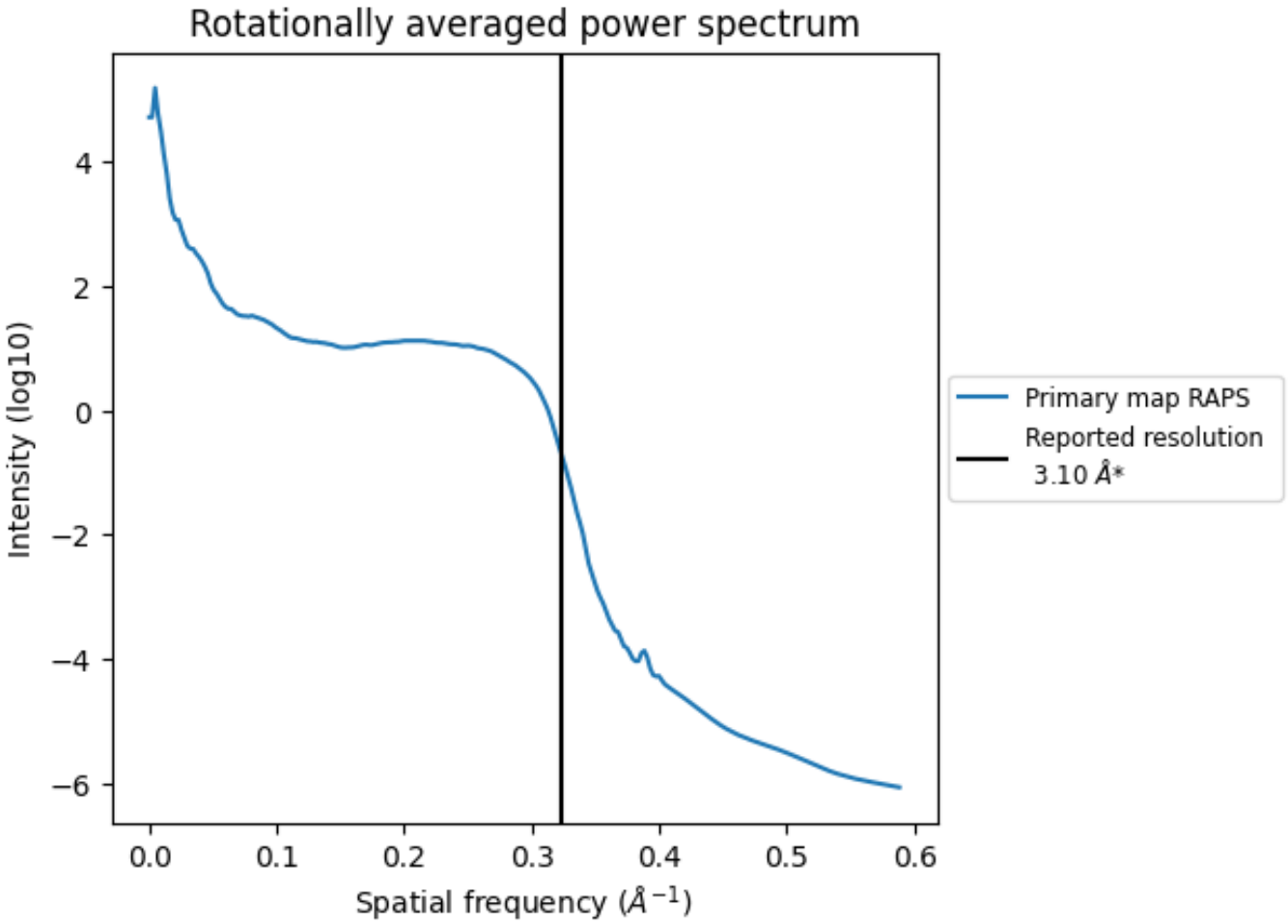
7.2 Volume estimate (i)



The volume at the recommended contour level is 1018 nm^3; this corresponds to an approximate mass of 919 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 0.323 Å^{-1}

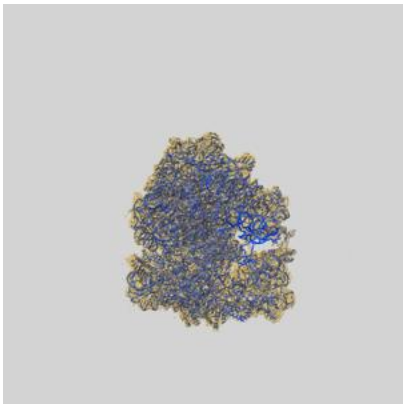
8 Fourier-Shell correlation (i)

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

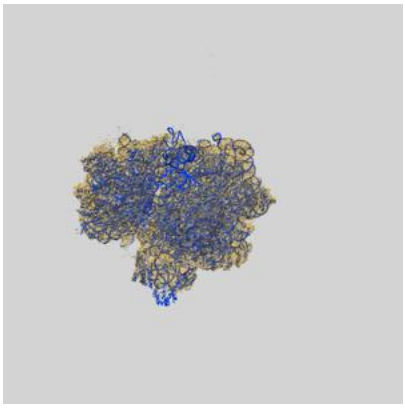
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42571 and PDB model 8UU8. Per-residue inclusion information can be found in section 3 on page 16.

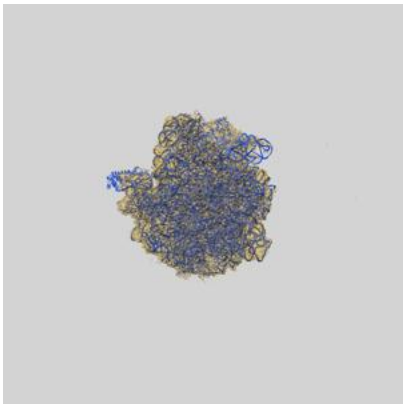
9.1 Map-model overlay



X



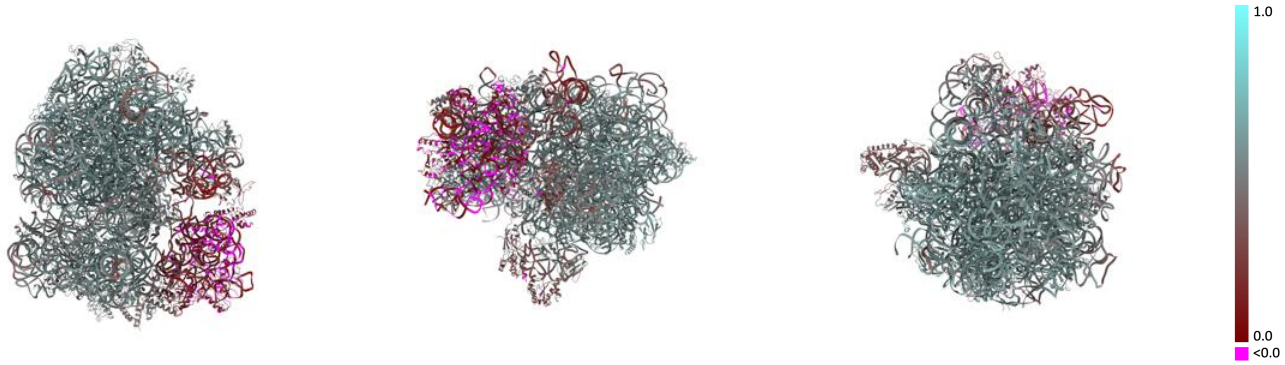
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5 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.

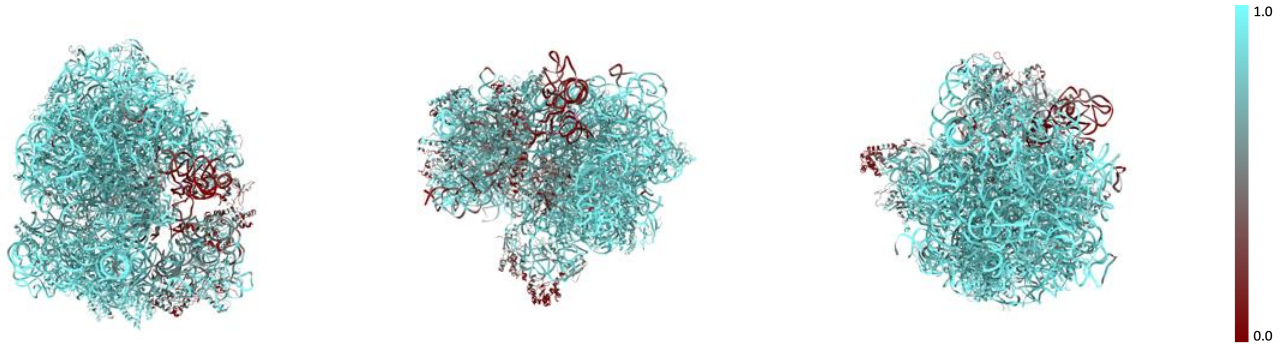
9.2 Q-score mapped to coordinate model (i)



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.

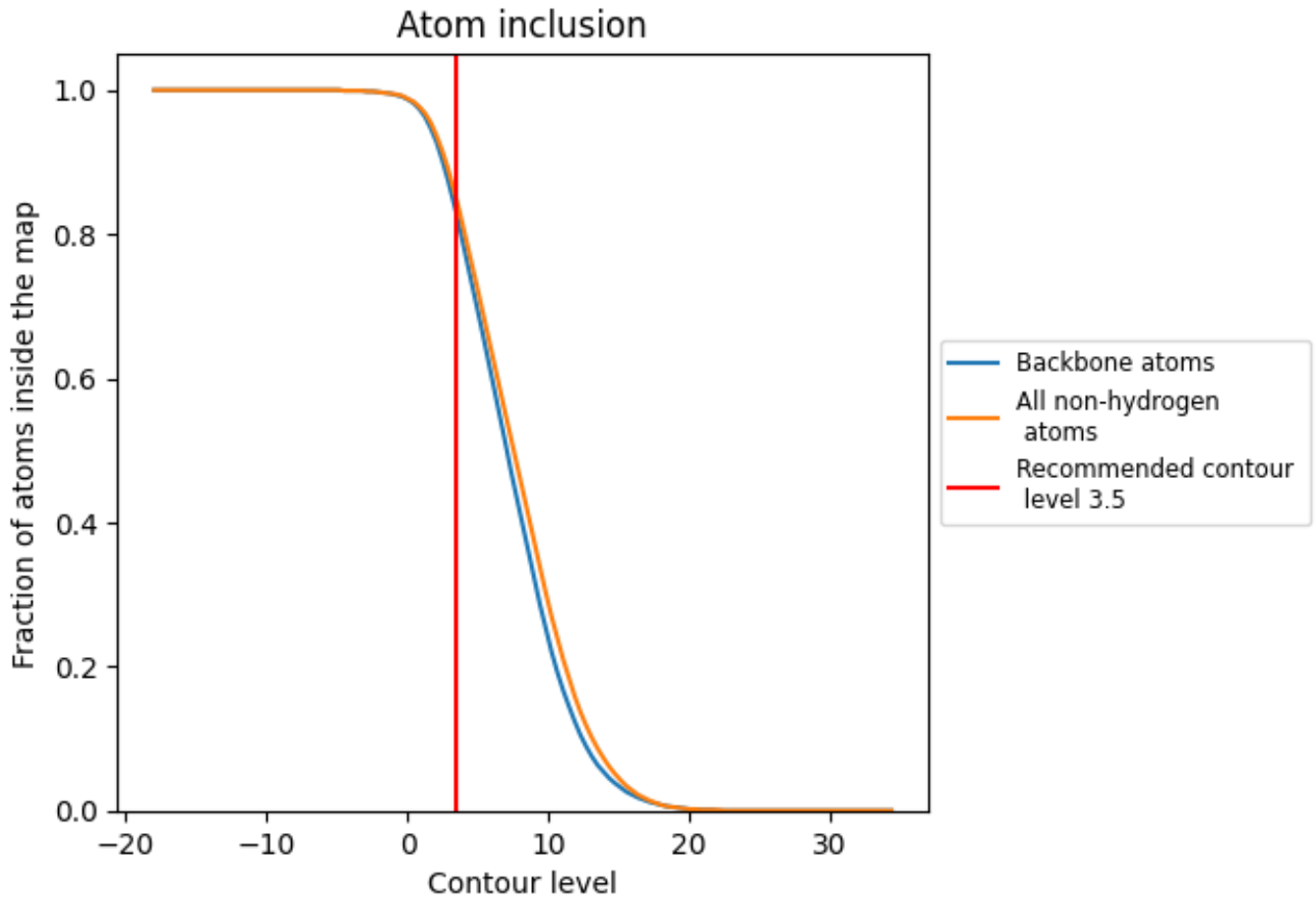
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.5).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 85% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8460	0.4960
1	0.8590	0.5500
2	0.8820	0.5800
3	0.3020	0.2860
4	0.8910	0.5710
5	0.8390	0.5660
6	0.9360	0.6050
7	0.9240	0.6010
8	0.8910	0.5920
A	0.9200	0.5500
B	0.9080	0.4850
C	0.8710	0.5900
D	0.8960	0.5870
E	0.8740	0.5700
F	0.5140	0.4000
G	0.6820	0.4780
H	0.3860	0.3430
I	0.1510	0.3370
L	0.9260	0.5950
M	0.8450	0.5760
N	0.8600	0.5600
O	0.8680	0.5810
P	0.8770	0.5780
Q	0.7450	0.5010
R	0.8400	0.5760
S	0.9230	0.5940
T	0.9200	0.5940
U	0.8840	0.5870
V	0.8720	0.5720
W	0.7820	0.5250
Y	0.9120	0.5890
Z	0.8730	0.5650
a	0.8410	0.4110
b	0.6710	0.4360
c	0.5490	0.1920

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Chain	Atom inclusion	Q-score
d	0.8700	0.5170
e	0.8670	0.5350
f	0.7060	0.4520
g	0.3860	0.0340
h	0.8590	0.5290
i	0.6450	0.1130
j	0.6020	0.0820
k	0.7420	0.4800
l	0.8530	0.5560
m	0.4170	0.1220
n	0.6900	0.0940
o	0.7910	0.5200
p	0.8960	0.5470
q	0.8040	0.5060
r	0.8750	0.5140
s	0.2050	0.0830
t	0.8370	0.5190
v	0.7140	0.4890
w	0.3630	0.3800
x	0.1390	0.3140