wwPDB EM Validation Summary Report

Sep 15, 2026 – 11:52 PM EDT

PDB ID	:	7UNU / pdb_00007unu
EMDB ID	:	EMD-26633
Title	:	Pseudomonas aeruginosa 70S ribosome initiation complex bound to compact IF2-GDP (composite structure I-B)
Authors	:	Basu, R.S.; Sherman, M.B.; Gagnon, M.G.
Deposited on	:	2022-04-11
Resolution	:	2.90 Å(reported)
Based on initial models	:	6SPG, 3JCJ

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:

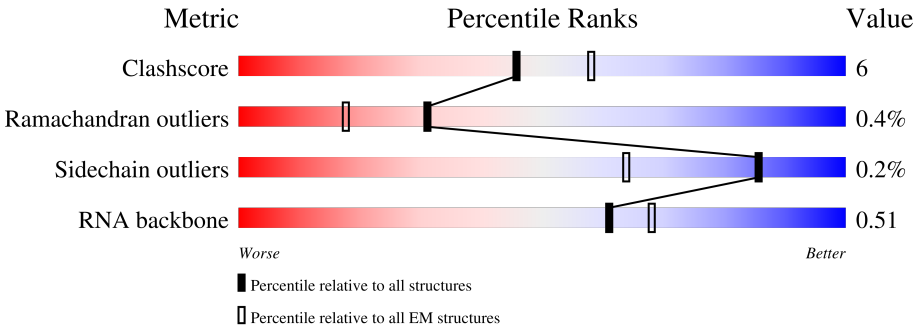
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

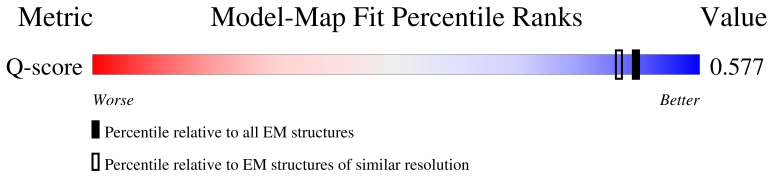
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	1536	62% 31% 6%
2	b	246	19% 70% 21% 9%
3	c	228	11% 78% 14% 9%

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Mol	Chain	Length	Quality of chain
4	d	206	11% 71% 28%
5	e	166	72% 21% 7%
6	f	139	7% 47% 28% 24%
7	g	156	15% 69% 28%
8	h	130	76% 23%
9	i	130	8% 59% 38%
10	j	103	23% 68% 28%
11	k	129	5% 77% 16% 8%
12	l	123	76% 23%
13	m	118	10% 63% 33%
14	n	101	8% 67% 32%
15	o	89	76% 22%
16	p	83	83% 14%
17	q	88	81% 10% 9%
18	r	76	12% 66% 16% 18%
19	s	91	11% 69% 22% 9%
20	t	91	86% 10%
21	u	71	15% 66% 20% 13%
22	v	77	71% 22%
23	w	24	25% 75%
24	x	840	45% 11% 44%
25	A	2891	67% 27% 6%
26	B	120	73% 21%
27	C	273	89% 10%
28	D	211	82% 18%

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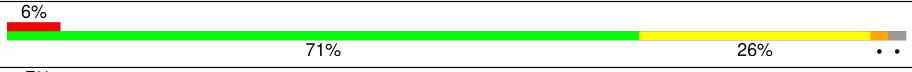
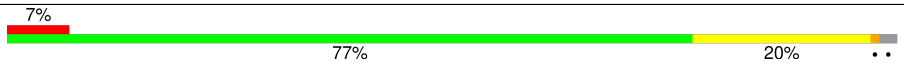
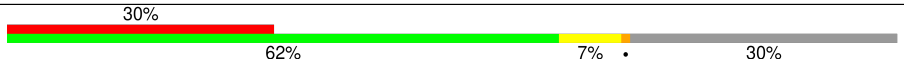
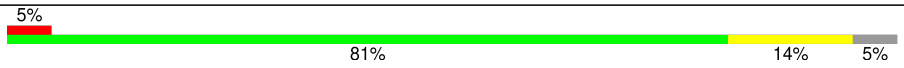
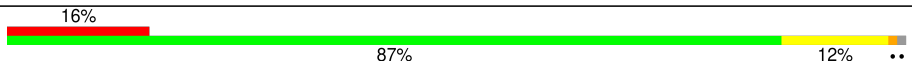
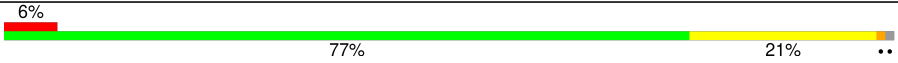
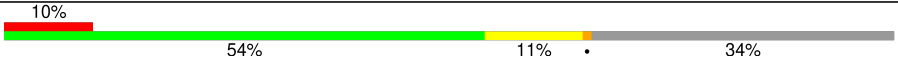
Mol	Chain	Length	Quality of chain
29	E	200	
30	F	179	
31	G	177	
32	H	148	
33	I	166	
34	J	143	
35	L	142	
36	M	122	
37	N	144	
38	O	137	
39	P	129	
40	Q	116	
41	R	116	
42	S	118	
43	T	103	
44	U	110	
45	V	99	
46	W	104	
47	X	204	
48	Y	85	
49	Z	78	
50	1	63	
51	2	58	
52	3	71	
53	4	60	

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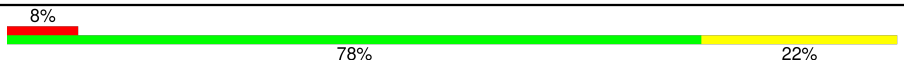
Mol	Chain	Length	Quality of chain
54	5	51	
55	6	44	
56	7	64	
57	8	38	

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 149259 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	1522	32675	14581	5999	10574	1521	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	224	1751	1104	320	317	10	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	208	1656	1047	313	291	5	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	205	1617	998	313	301	5	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	154	1134	711	210	207	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	106	857	534	159	158	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	152	Total	C	N	O	S	0	0
			1187	743	231	208	5		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			982	618	173	185	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1010	625	203	181	1		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	99	Total	C	N	O	S	0	0
			793	496	150	146	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	119	Total	C	N	O	S	0	0
			879	545	171	161	2		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	122	Total	C	N	O	S	0	0
			956	587	197	168	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			891	544	182	161	4		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			800	494	167	136	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			703	434	139	129	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	81	Total	C	N	O	S	0	0
			636	397	125	113	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			645	404	124	115	2		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	62	Total	C	N	O	0	0
			480	307	85	88		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	83	Total	C	N	O	S	0	0
			663	422	129	109	3		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	87	Total	C	N	O	S	0	0
			671	414	138	117	2		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	62	Total	C	N	O	S	0	0
			506	316	103	86	1		

- Molecule 22 is a RNA chain called P-site initiator tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	w	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 24 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	x	472	Total	C	N	O	S	0	0
			3235	2046	591	587	11		

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2884	Total	C	N	O	P	0	0
			61891	27621	11346	20041	2883		

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	117	Total	C	N	O	P	0	0
			2495	1114	448	816	117		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	C	272	Total	C	N	O	S	0	0
			2072	1276	426	364	6		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	211	Total	C	N	O	S	0	0
			1588	981	304	297	6		

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	E	200	Total	C	N	O	S	0	0
			1521	955	283	280	3		

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	176	Total	C	N	O	S	0	0
			1407	899	249	255	4		

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	174	Total	C	N	O	S	0	0
			1307	824	241	240	2		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	148	Total	C	N	O	S	0	0
			964	598	178	187	1		

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	I	117	Total	C	N	O	S	0	0
			718	454	134	129	1		

- Molecule 34 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	J	135	Total	C	N	O	S	0	0
			911	573	163	173	2		

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	142	Total	C	N	O	S	0	0
			1130	718	206	202	4		

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	144	Total	C	N	O	S	0	0
			1066	654	215	194	3		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	137	Total	C	N	O	S	0	0
			1085	689	211	181	4		

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P	120	Total	C	N	O	S	0	0
			956	599	192	160	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Q	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	114	Total	C	N	O	S	0	0
			901	568	171	161	1		

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	S	117	Total	C	N	O	0	0
			936	592	196	148		

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	T	103	Total	C	N	O	S	0	0
			822	521	156	143	2		

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	U	110	Total	C	N	O	S	0	0
			833	515	161	153	4		

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	94	Total	C	N	O	S	0	0
			739	472	134	132	1		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	W	103	Total	C	N	O	S	0	0
			786	494	150	141	1		

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	X	190	Total	C	N	O	S	0	0
			1445	915	262	265	3		

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Y	76	Total	C	N	O	0	0
			575	364	111	100		

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Z	77	Total	C	N	O	S	0	0
			630	391	134	103	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	61	Total	C	N	O	S	0	0
			490	301	96	91	2		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	2	57	Total	C	N	O	S	0	0
			445	277	87	79	2		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3	47	Total	C	N	O	S	0	0
			356	222	60	68	6		

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	55	Total	C	N	O	S	0	0
			436	262	93	80	1		

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	5	51	Total	C	N	O	S	0	0
			426	272	78	75	1		

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	44	Total	C	N	O	S	0	0
			365	222	87	54	2		

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	7	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	8	38	Total	C	N	O	S	0	0
			307	186	69	48	4		

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
58	a	120	Total	Mg	0
			120	120	
58	i	1	Total	Mg	0
			1	1	
58	t	1	Total	Mg	0
			1	1	
58	v	2	Total	Mg	0
			2	2	
58	w	1	Total	Mg	0
			1	1	
58	A	456	Total	Mg	0
			456	456	
58	B	7	Total	Mg	0
			7	7	
58	C	2	Total	Mg	0
			2	2	
58	D	1	Total	Mg	0
			1	1	
58	E	3	Total	Mg	0
			3	3	
58	M	1	Total	Mg	0
			1	1	
58	N	1	Total	Mg	0
			1	1	
58	Q	1	Total	Mg	0
			1	1	
58	S	3	Total	Mg	0
			3	3	
58	Y	1	Total	Mg	0
			1	1	

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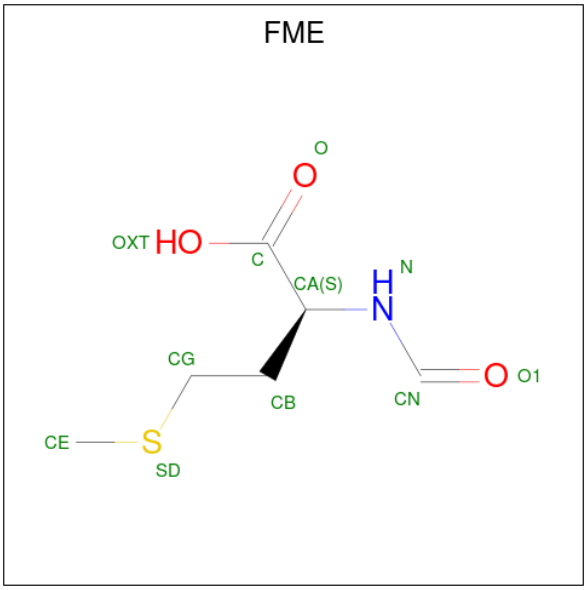
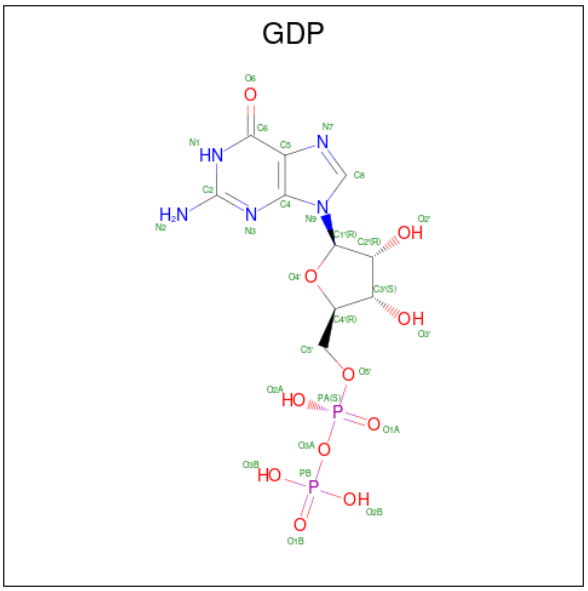
Mol	Chain	Residues	Atoms	AltConf
58	4	4	Total Mg 4 4	0
58	7	1	Total Mg 1 1	0
58	8	1	Total Mg 1 1	0

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms	AltConf
59	v	1	Total C N O S 10 6 1 2 1	0

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
60	x	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
61	3	1	Total	Zn	0
			1	1	
61	8	1	Total	Zn	0
			1	1	

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
62	a	22	Total	O	0
			22	22	
62	k	1	Total	O	0
			1	1	
62	w	1	Total	O	0
			1	1	
62	A	169	Total	O	0
			169	169	
62	C	1	Total	O	0
			1	1	
62	E	1	Total	O	0
			1	1	

Continued on next page...

Continued from previous page...

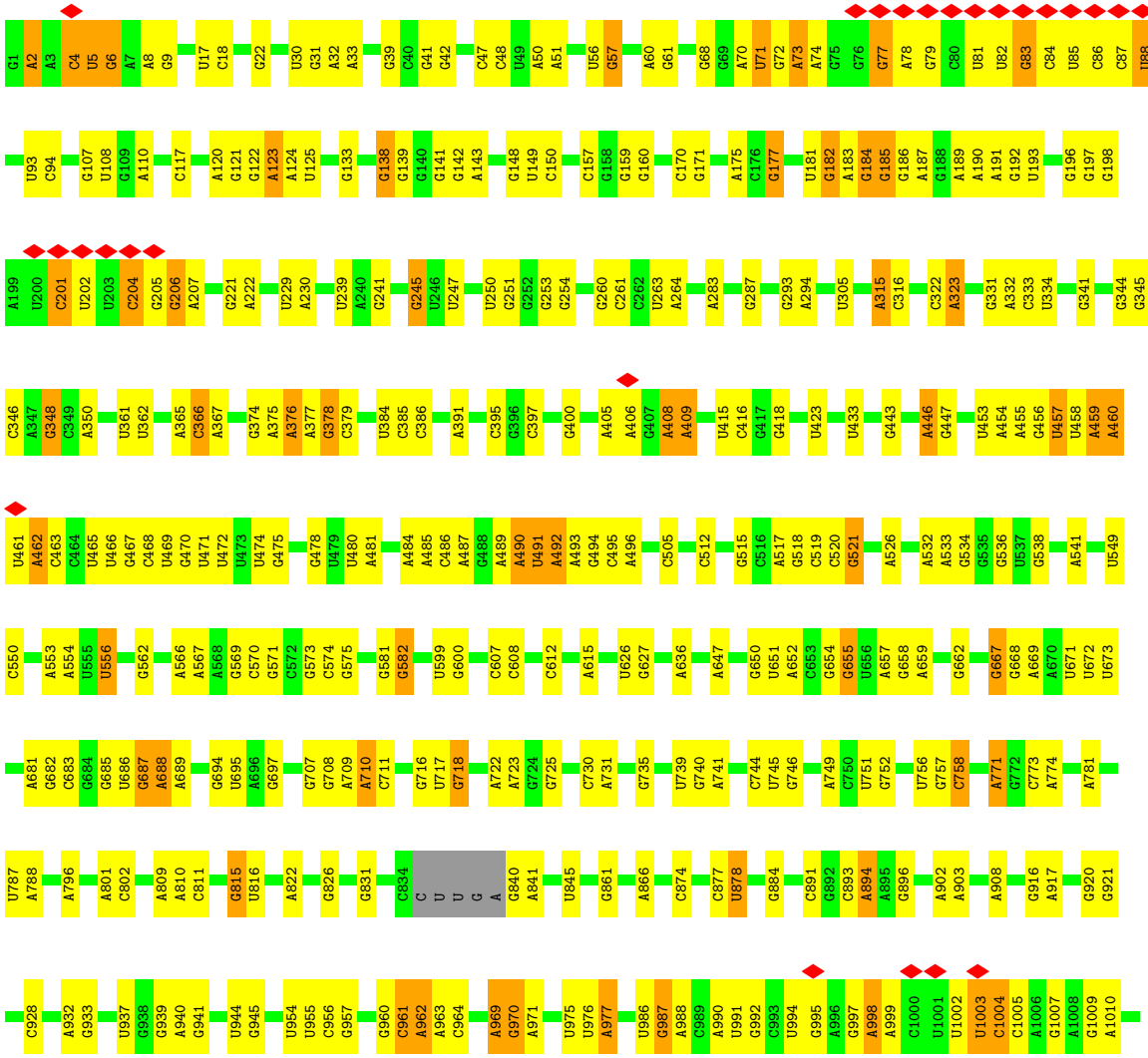
Mol	Chain	Residues	Atoms	AltConf
62	P	2	Total O 2 2	0
62	S	1	Total O 1 1	0
62	4	3	Total O 3 3	0

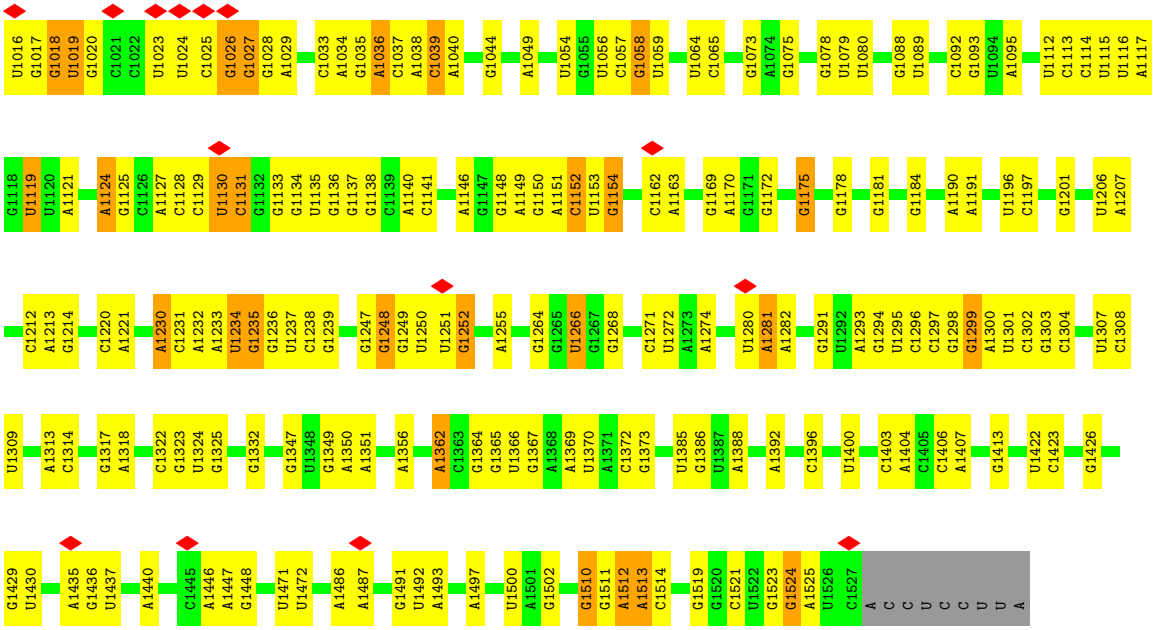
3 Residue-property plots (i)

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

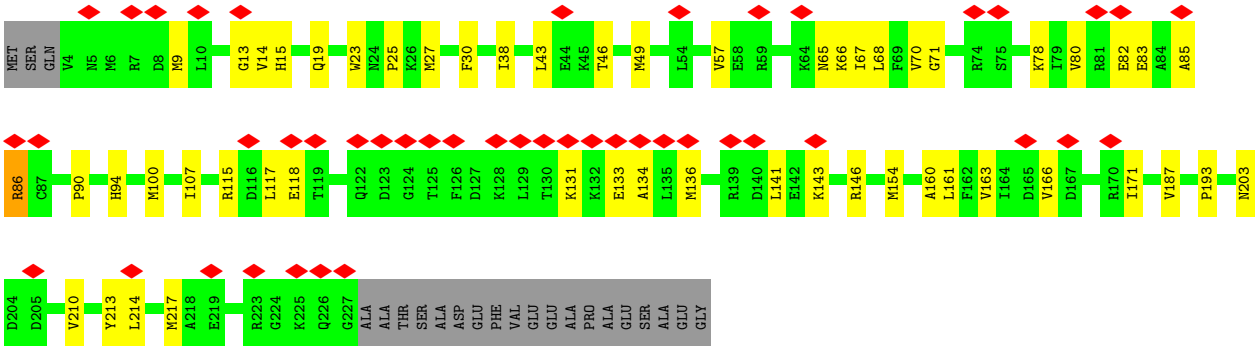
Chain a:





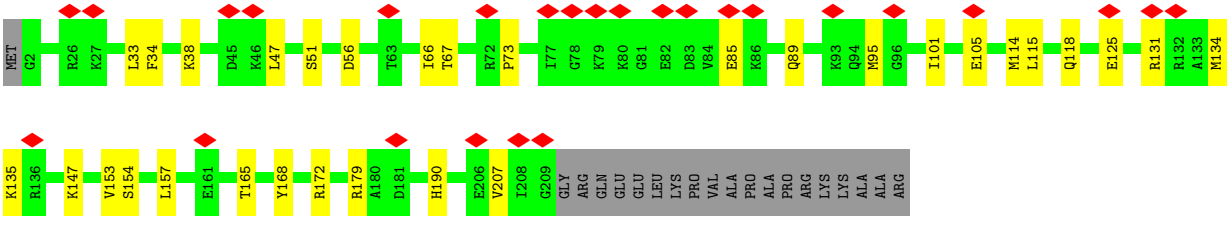
• Molecule 2: 30S ribosomal protein S2

Chain b:



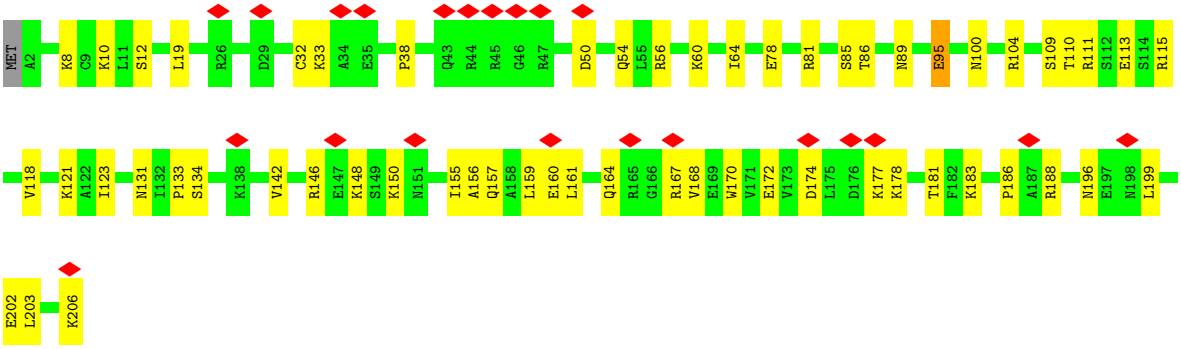
• Molecule 3: 30S ribosomal protein S3

Chain c:

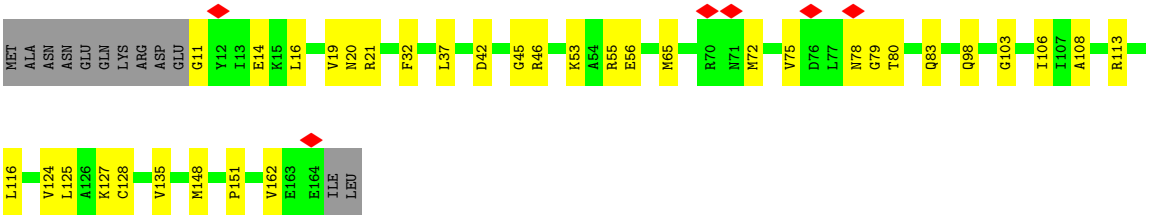


• Molecule 4: 30S ribosomal protein S4

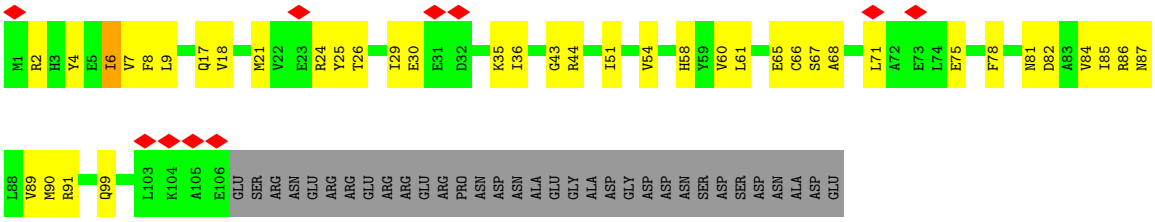
Chain d:



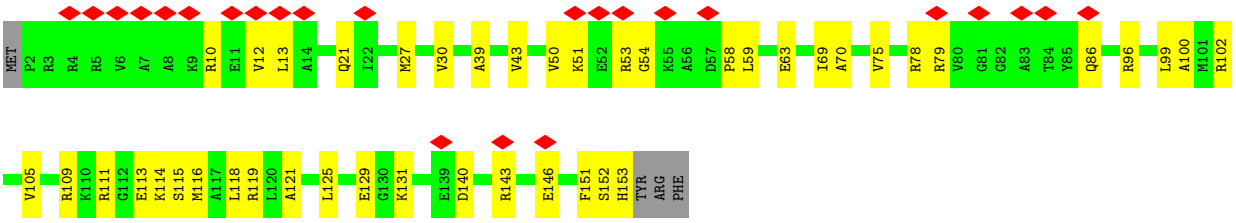
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6



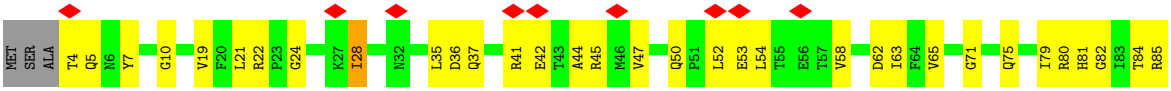
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

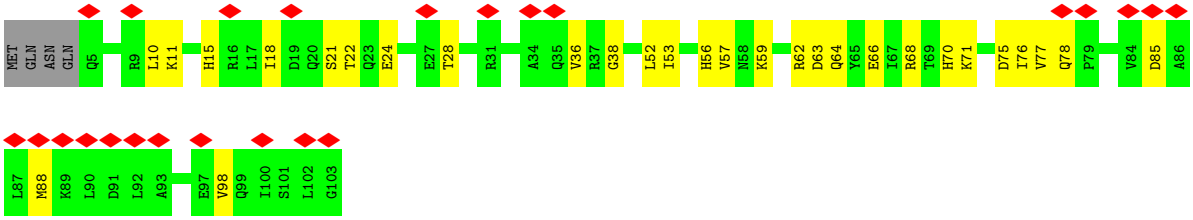
• Molecule 9: 30S ribosomal protein S9

Chain i:



• Molecule 10: 30S ribosomal protein S10

Chain j:

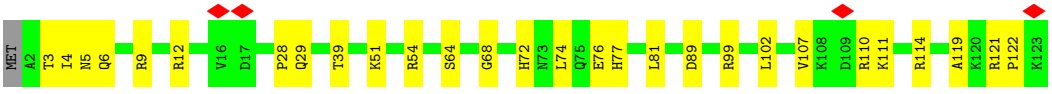


• Molecule 11: 30S ribosomal protein S11

Chain k:

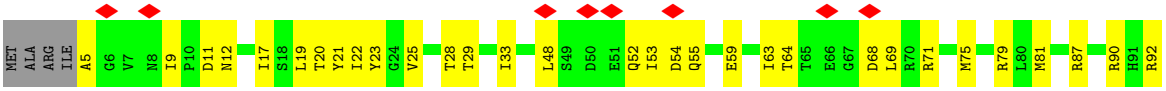
• Molecule 12: 30S ribosomal protein S12

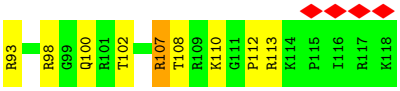
Chain l:



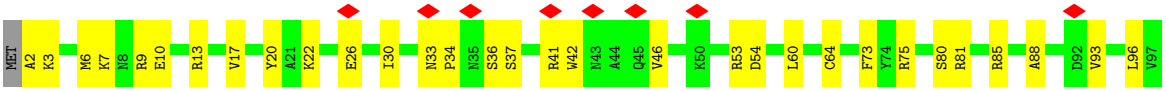
• Molecule 13: 30S ribosomal protein S13

Chain m:

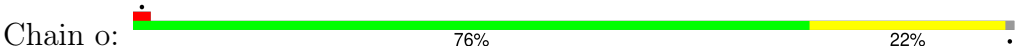


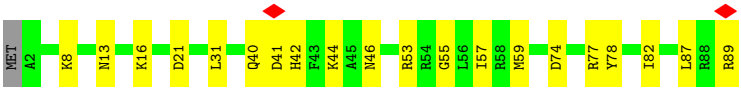


• Molecule 14: 30S ribosomal protein S14

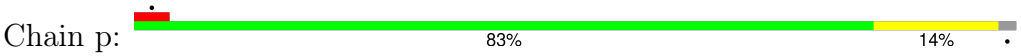


• Molecule 15: 30S ribosomal protein S15

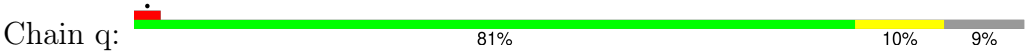


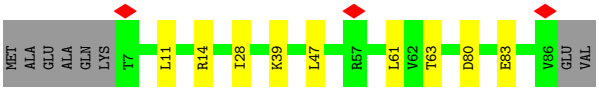


• Molecule 16: 30S ribosomal protein S16

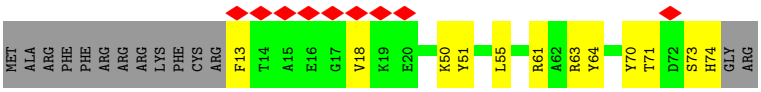


• Molecule 17: 30S ribosomal protein S17

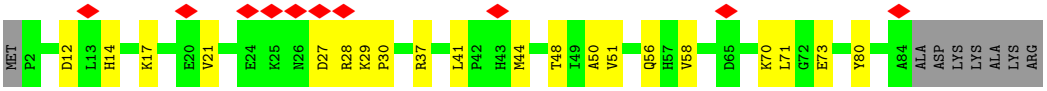




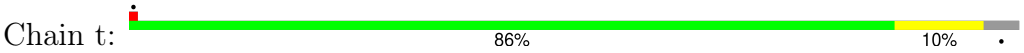
• Molecule 18: 30S ribosomal protein S18

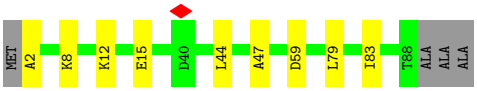


• Molecule 19: 30S ribosomal protein S19

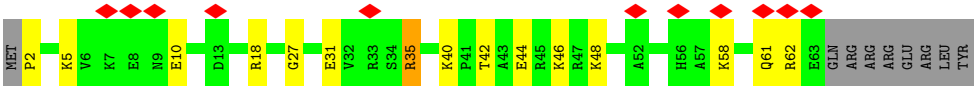


• Molecule 20: 30S ribosomal protein S20

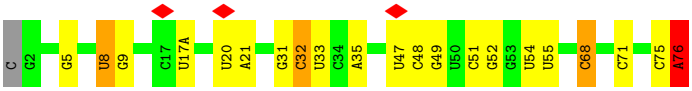




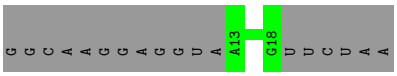
• Molecule 21: 30S ribosomal protein S21



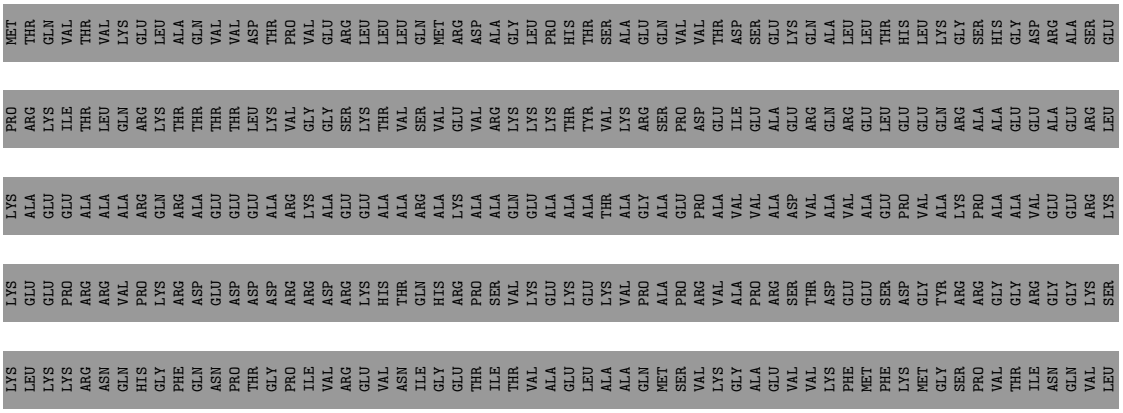
• Molecule 22: P-site initiator tRNA

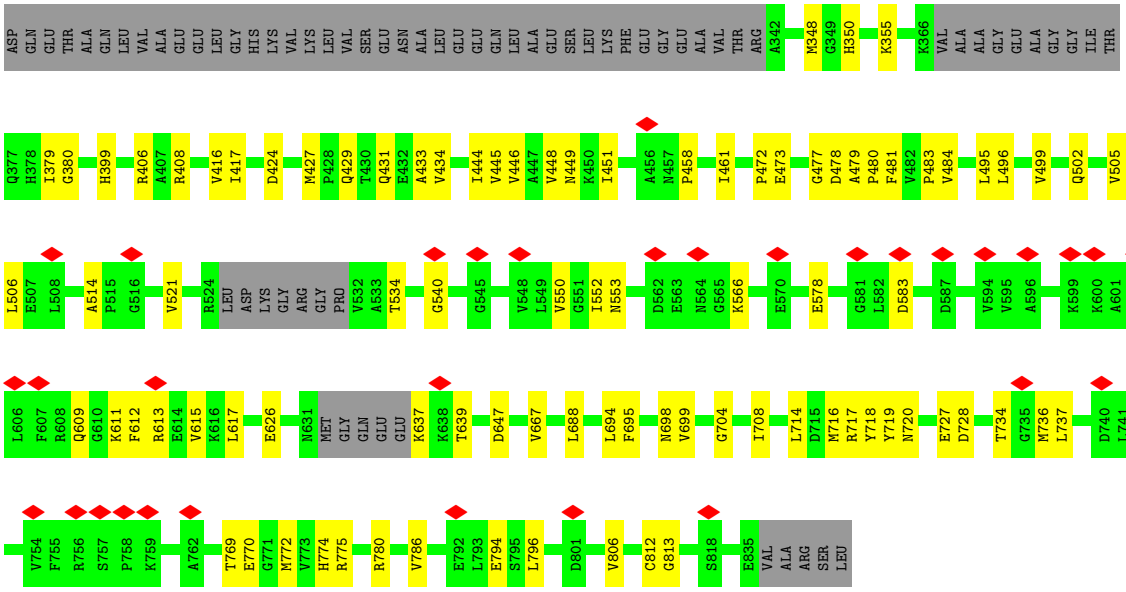


• Molecule 23: mRNA



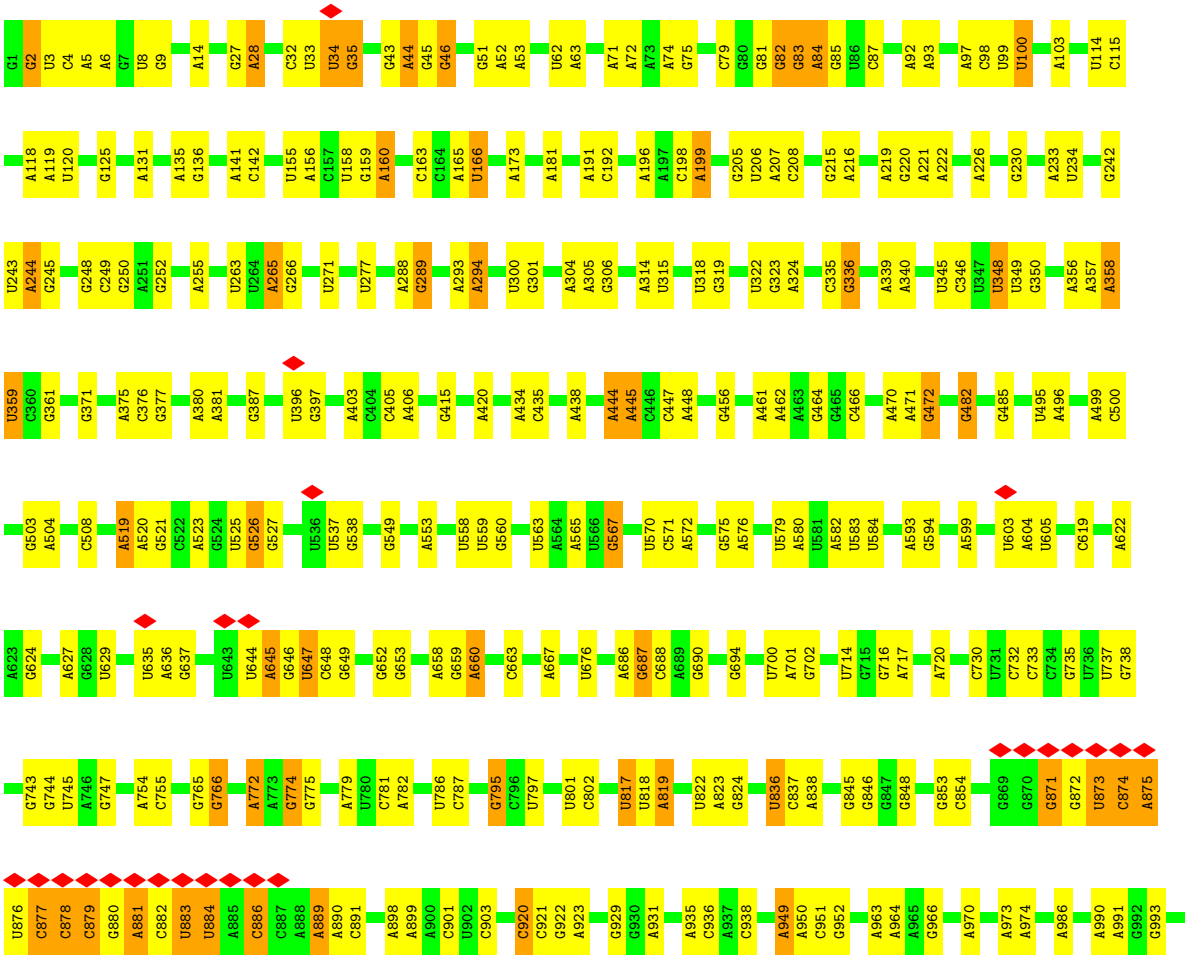
• Molecule 24: Translation initiation factor IF-2

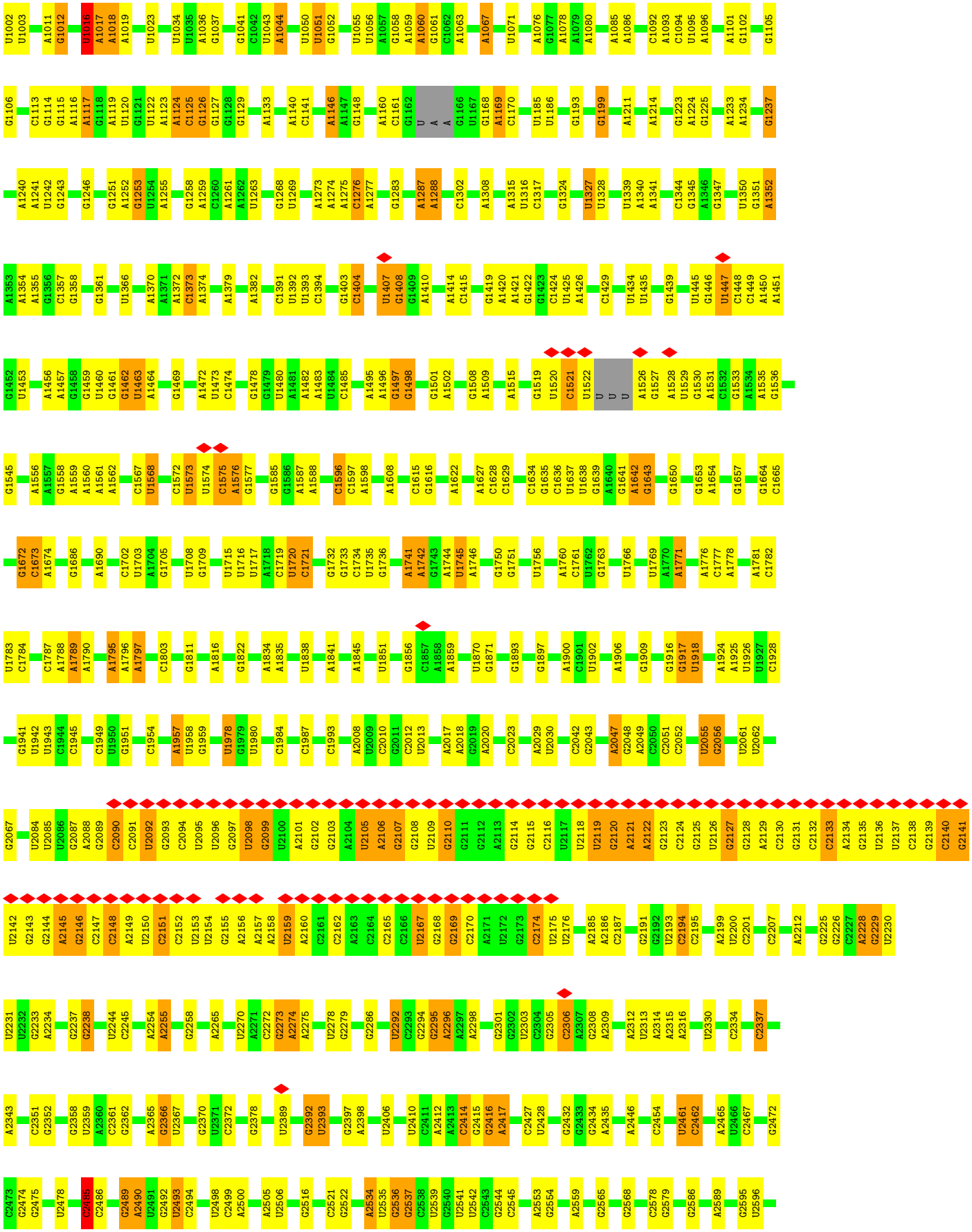


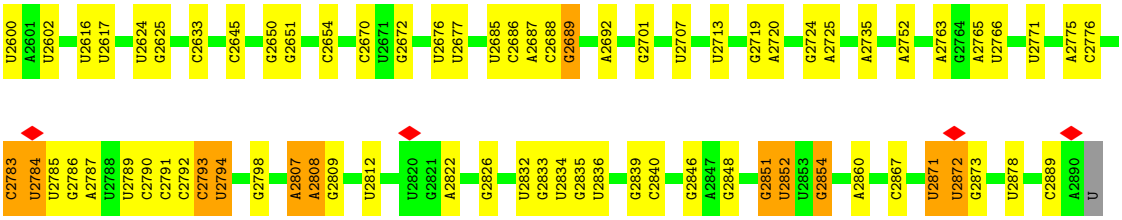


• Molecule 25: 23S Ribosomal RNA

Chain A:

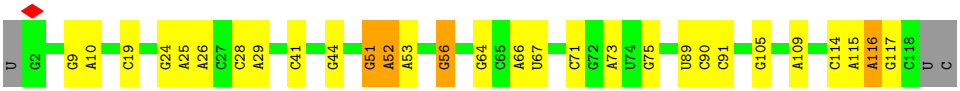






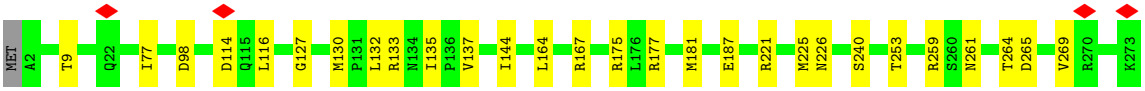
• Molecule 26: 5S Ribosomal RNA

Chain B:



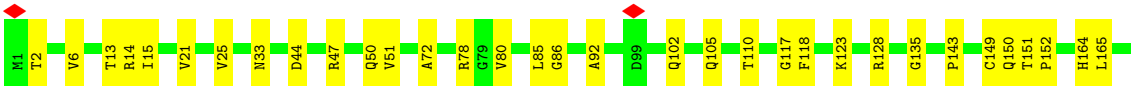
• Molecule 27: 50S ribosomal protein L2

Chain C:



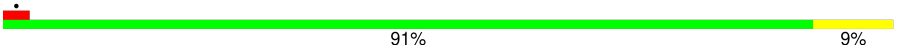
• Molecule 28: 50S ribosomal protein L3

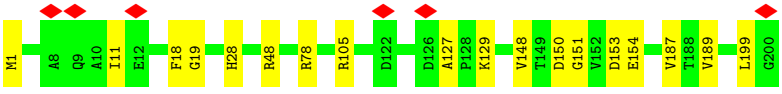
Chain D:



• Molecule 29: 50S ribosomal protein L4

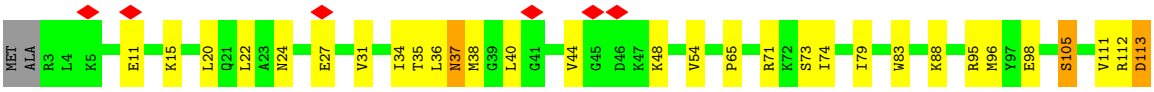
Chain E:

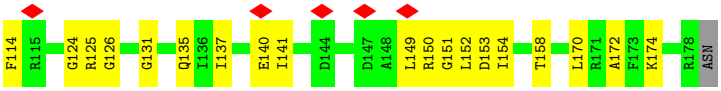




• Molecule 30: 50S ribosomal protein L5

Chain F:



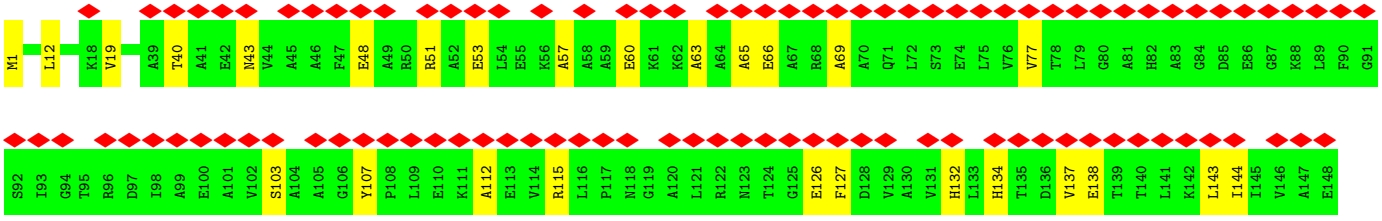


• Molecule 31: 50S ribosomal protein L6

Chain G:

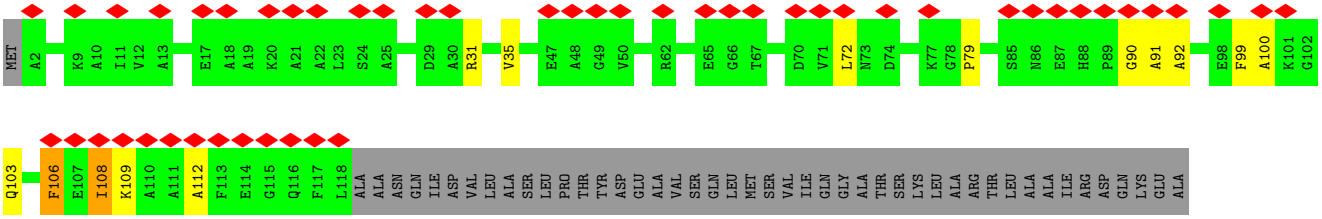
• Molecule 32: 50S ribosomal protein L9

Chain H:



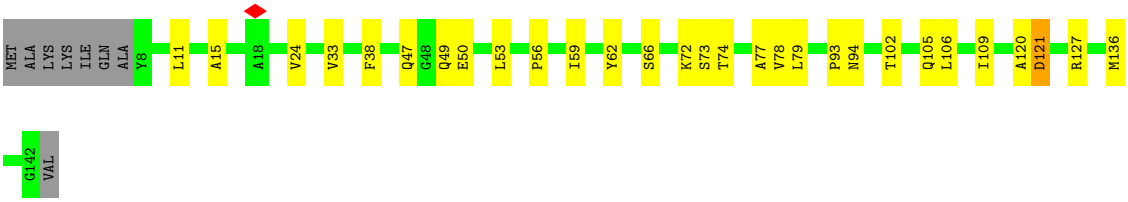
• Molecule 33: 50S ribosomal protein L10

Chain I:



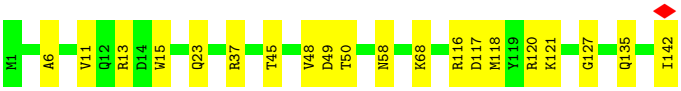
• Molecule 34: 50S ribosomal protein L11

Chain J:



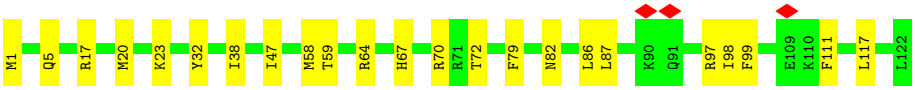
• Molecule 35: 50S ribosomal protein L13

Chain L:



• Molecule 36: 50S ribosomal protein L14

Chain M:

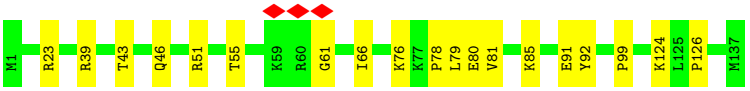


• Molecule 37: 50S ribosomal protein L15

Chain N:

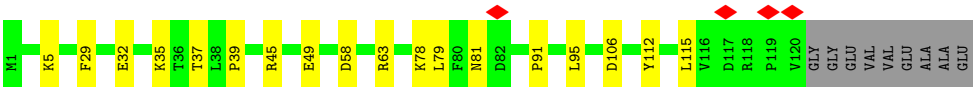
• Molecule 38: 50S ribosomal protein L16

Chain O:



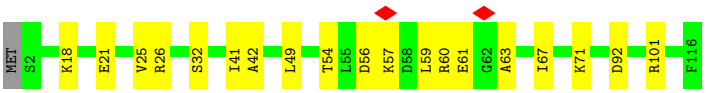
• Molecule 39: 50S ribosomal protein L17

Chain P:



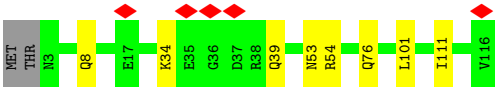
• Molecule 40: 50S ribosomal protein L18

Chain Q:



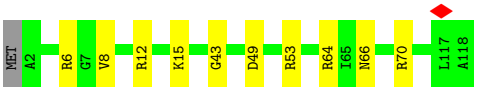
• Molecule 41: 50S ribosomal protein L19

Chain R:



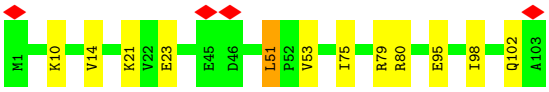
• Molecule 42: 50S ribosomal protein L20

Chain S:



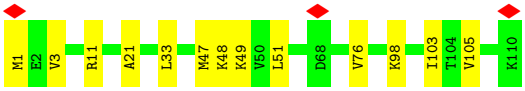
• Molecule 43: 50S ribosomal protein L21

Chain T:



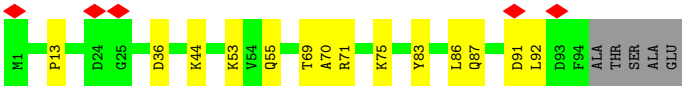
• Molecule 44: 50S ribosomal protein L22

Chain U:



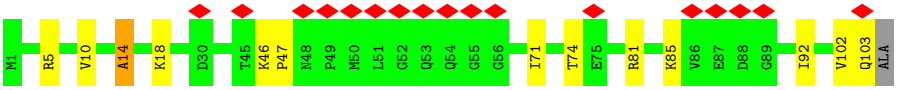
• Molecule 45: 50S ribosomal protein L23

Chain V:



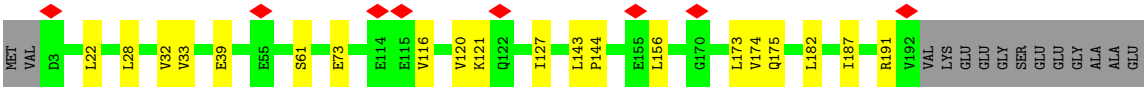
• Molecule 46: 50S ribosomal protein L24

Chain W:



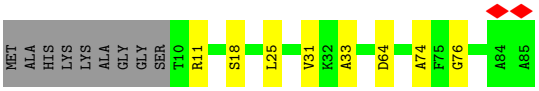
• Molecule 47: 50S ribosomal protein L25

Chain X:



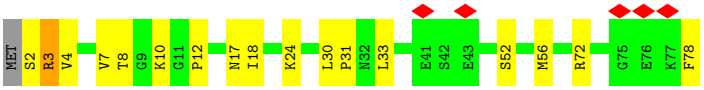
• Molecule 48: 50S ribosomal protein L27

Chain Y:



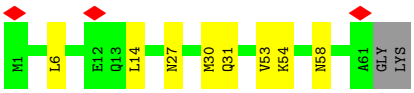
• Molecule 49: 50S ribosomal protein L28

Chain Z:



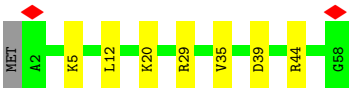
• Molecule 50: 50S ribosomal protein L29

Chain 1:



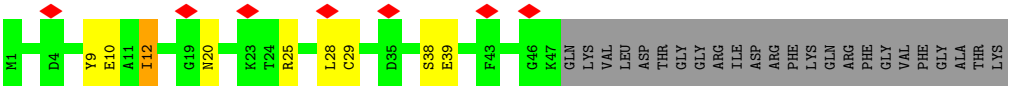
• Molecule 51: 50S ribosomal protein L30

Chain 2:



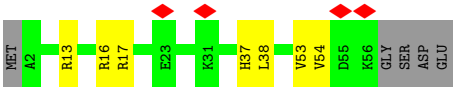
• Molecule 52: 50S ribosomal protein L31

Chain 3:



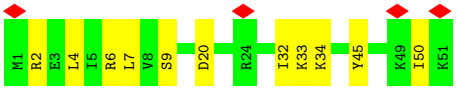
• Molecule 53: 50S ribosomal protein L32

Chain 4:



• Molecule 54: 50S ribosomal protein L33

Chain 5:

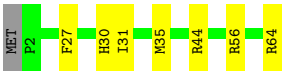


• Molecule 55: 50S ribosomal protein L34

Chain 6:

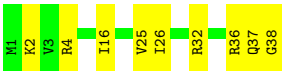
• Molecule 56: 50S ribosomal protein L35

Chain 7:



• Molecule 57: 50S ribosomal protein L36

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24614	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 ($e^-/Å^2$)	31	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	29.769	Depositor
Minimum map value	-17.350	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.012	Depositor
Recommended contour level	3.6	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MA6, ZN, OMC, 4SU, 2MG, PSU, 6MZ, 2MA, OMU, 7MG, FME, 5MU, 4OC, 5MC, GDP, 1MG, UR3, OMG

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	0.26	0/36354	0.32	1/56707 (0.0%)
2	b	0.19	0/1779	0.42	0/2392
3	c	0.19	0/1685	0.35	0/2270
4	d	0.23	0/1636	0.43	0/2189
5	e	0.24	0/1148	0.43	0/1544
6	f	0.28	0/871	0.52	0/1172
7	g	0.22	0/1204	0.45	0/1609
8	h	0.22	0/993	0.37	0/1332
9	i	0.20	0/1022	0.39	0/1365
10	j	0.20	0/803	0.39	0/1083
11	k	0.23	0/895	0.38	0/1209
12	l	0.23	0/970	0.40	0/1299
13	m	0.26	0/900	0.48	0/1209
14	n	0.20	0/812	0.39	0/1082
15	o	0.22	0/710	0.29	0/947
16	p	0.22	0/647	0.38	0/870
17	q	0.21	0/653	0.36	0/881
18	r	0.24	0/488	0.37	0/660
19	s	0.20	0/678	0.40	0/912
20	t	0.22	0/678	0.36	0/904
21	u	0.25	0/513	0.43	0/680
22	v	0.31	0/1725	0.42	2/2689 (0.1%)
23	w	0.24	0/147	0.20	0/227
24	x	0.30	0/3274	0.47	0/4452
25	A	0.32	0/68977	0.36	4/107590 (0.0%)
26	B	0.24	0/2789	0.30	0/4345
27	C	0.30	0/2108	0.40	0/2831
28	D	0.31	0/1611	0.44	0/2167
29	E	0.26	0/1541	0.35	0/2075
30	F	0.23	0/1428	0.52	2/1918 (0.1%)
31	G	0.27	0/1325	0.44	0/1786

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
32	H	0.14	0/971	0.34	0/1324
33	I	0.15	0/725	0.36	0/992
34	J	0.30	0/925	0.58	0/1263
35	L	0.26	0/1156	0.33	0/1559
36	M	0.27	0/947	0.37	0/1268
37	N	0.26	0/1078	0.40	0/1436
38	O	0.26	0/1105	0.36	0/1476
39	P	0.29	0/972	0.37	0/1300
40	Q	0.21	0/888	0.32	0/1183
41	R	0.26	0/910	0.29	0/1217
42	S	0.29	0/946	0.32	0/1257
43	T	0.25	0/835	0.35	0/1117
44	U	0.25	0/837	0.29	0/1114
45	V	0.23	0/749	0.35	0/1002
46	W	0.20	0/794	0.35	0/1062
47	X	0.21	0/1468	0.35	0/1987
48	Y	0.27	0/583	0.35	0/774
49	Z	0.34	0/641	0.42	0/854
50	1	0.20	0/491	0.30	0/654
51	2	0.34	0/449	0.42	0/602
52	3	0.20	0/364	0.46	0/494
53	4	0.27	0/442	0.33	0/589
54	5	0.22	0/433	0.30	0/576
55	6	0.31	0/368	0.40	0/482
56	7	0.27	0/511	0.32	0/668
57	8	0.28	0/308	0.34	0/404
All	All	0.28	0/160260	0.36	9/239050 (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
28	D	0	1
30	F	0	1
43	T	0	1
All	All	0	3

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})
22	v	76	A	O4'-C1'-N9	9.21	122.02	108.20
25	A	1094	C	OP1-P-O3'	-9.14	80.57	108.00
25	A	1094	C	OP2-P-O3'	-8.03	83.92	108.00
25	A	1016	U	C2'-C3'-O3'	6.48	123.42	113.70
22	v	76	A	C1'-O4'-C4'	-6.39	103.31	109.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	D	151	THR	Peptide
30	F	105	SER	Peptide
43	T	51	LEU	Peptide

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	a	32675	0	16462	326	0
2	b	1751	0	1785	32	0
3	c	1656	0	1706	20	0
4	d	1617	0	1650	44	0
5	e	1134	0	1181	21	0
6	f	857	0	836	30	0
7	g	1187	0	1244	29	0
8	h	982	0	1036	19	0
9	i	1010	0	1052	38	0
10	j	793	0	833	22	0
11	k	879	0	896	14	0
12	l	956	0	1005	19	0
13	m	891	0	933	38	0
14	n	800	0	837	23	0
15	o	703	0	727	12	0
16	p	636	0	646	8	0
17	q	645	0	689	6	0
18	r	480	0	488	9	0
19	s	663	0	697	15	0
20	t	671	0	722	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	u	506	0	537	12	0
22	v	1625	0	828	9	0
23	w	131	0	66	0	0
24	x	3235	0	3115	62	0
25	A	61891	0	31142	461	0
26	B	2495	0	1263	12	0
27	C	2072	0	2152	21	0
28	D	1588	0	1603	26	0
29	E	1521	0	1580	11	0
30	F	1407	0	1470	37	0
31	G	1307	0	1360	33	0
32	H	964	0	886	14	0
33	I	718	0	600	10	0
34	J	911	0	876	20	0
35	L	1130	0	1160	14	0
36	M	938	0	1012	15	0
37	N	1066	0	1112	14	0
38	O	1085	0	1157	13	0
39	P	956	0	1003	12	0
40	Q	881	0	920	12	0
41	R	901	0	957	8	0
42	S	936	0	1025	11	0
43	T	822	0	858	7	0
44	U	833	0	897	8	0
45	V	739	0	788	10	0
46	W	786	0	836	8	0
47	X	1445	0	1486	12	0
48	Y	575	0	598	5	0
49	Z	630	0	653	14	0
50	1	490	0	520	6	0
51	2	445	0	472	3	0
52	3	356	0	342	9	0
53	4	436	0	433	7	0
54	5	426	0	457	9	0
55	6	365	0	409	3	0
56	7	506	0	569	5	0
57	8	307	0	342	6	0
58	4	4	0	0	0	0
58	7	1	0	0	0	0
58	8	1	0	0	0	0
58	A	456	0	0	0	0
58	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	C	2	0	0	0	0
58	D	1	0	0	0	0
58	E	3	0	0	0	0
58	M	1	0	0	0	0
58	N	1	0	0	0	0
58	Q	1	0	0	0	0
58	S	3	0	0	0	0
58	Y	1	0	0	0	0
58	a	120	0	0	0	0
58	i	1	0	0	0	0
58	t	1	0	0	0	0
58	v	2	0	0	0	0
58	w	1	0	0	0	0
59	v	10	0	10	2	0
60	x	28	0	12	0	0
61	3	1	0	0	0	0
61	8	1	0	0	0	0
62	4	3	0	0	0	0
62	A	169	0	0	3	0
62	C	1	0	0	0	0
62	E	1	0	0	0	0
62	P	2	0	0	0	0
62	S	1	0	0	0	0
62	a	22	0	0	0	0
62	k	1	0	0	0	0
62	w	1	0	0	0	0
All	All	149259	0	100931	1512	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 6.

The worst 5 of 1512 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)
31:G:9:VAL:C	31:G:10:LYS:HD3	1.70	1.16
1:a:1020:G:H1	1:a:1029:A:N6	1.56	1.03
22:v:5:G:H1	22:v:68:C:H42	1.05	1.03
25:A:2106:A:H61	25:A:2155:G:N2	1.58	1.00
25:A:2106:A:N6	25:A:2155:G:H21	1.60	0.99

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
2	b	222/246 (90%)	200 (90%)	21 (10%)	1 (0%)	24 54
3	c	206/228 (90%)	190 (92%)	16 (8%)	0	100 100
4	d	203/206 (98%)	179 (88%)	24 (12%)	0	100 100
5	e	152/166 (92%)	142 (93%)	10 (7%)	0	100 100
6	f	104/139 (75%)	92 (88%)	10 (10%)	2 (2%)	6 23
7	g	150/156 (96%)	138 (92%)	11 (7%)	1 (1%)	18 48
8	h	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	16 44
9	i	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	16 44
10	j	97/103 (94%)	89 (92%)	8 (8%)	0	100 100
11	k	117/129 (91%)	109 (93%)	8 (7%)	0	100 100
12	l	120/123 (98%)	112 (93%)	8 (7%)	0	100 100
13	m	112/118 (95%)	96 (86%)	16 (14%)	0	100 100
14	n	98/101 (97%)	92 (94%)	6 (6%)	0	100 100
15	o	86/89 (97%)	82 (95%)	4 (5%)	0	100 100
16	p	79/83 (95%)	74 (94%)	4 (5%)	1 (1%)	9 32
17	q	78/88 (89%)	77 (99%)	1 (1%)	0	100 100
18	r	60/76 (79%)	56 (93%)	3 (5%)	1 (2%)	7 26
19	s	81/91 (89%)	74 (91%)	7 (9%)	0	100 100
20	t	85/91 (93%)	84 (99%)	1 (1%)	0	100 100
21	u	60/71 (84%)	57 (95%)	3 (5%)	0	100 100
24	x	464/840 (55%)	400 (86%)	63 (14%)	1 (0%)	43 72
27	C	270/273 (99%)	249 (92%)	21 (8%)	0	100 100
28	D	209/211 (99%)	181 (87%)	26 (12%)	2 (1%)	12 39
29	E	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	24 54
30	F	174/179 (97%)	145 (83%)	27 (16%)	2 (1%)	11 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	G	172/177 (97%)	156 (91%)	16 (9%)	0	100	100
32	H	146/148 (99%)	126 (86%)	19 (13%)	1 (1%)	18	48
33	I	115/166 (69%)	102 (89%)	9 (8%)	4 (4%)	3	12
34	J	133/143 (93%)	96 (72%)	34 (26%)	3 (2%)	5	19
35	L	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
36	M	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
37	N	142/144 (99%)	124 (87%)	17 (12%)	1 (1%)	18	48
38	O	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
39	P	118/129 (92%)	109 (92%)	9 (8%)	0	100	100
40	Q	113/116 (97%)	103 (91%)	10 (9%)	0	100	100
41	R	112/116 (97%)	105 (94%)	7 (6%)	0	100	100
42	S	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
43	T	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
44	U	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
45	V	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
46	W	101/104 (97%)	93 (92%)	7 (7%)	1 (1%)	12	39
47	X	188/204 (92%)	177 (94%)	10 (5%)	1 (0%)	24	54
48	Y	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
49	Z	75/78 (96%)	75 (100%)	0	0	100	100
50	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
51	2	55/58 (95%)	55 (100%)	0	0	100	100
52	3	45/71 (63%)	39 (87%)	5 (11%)	1 (2%)	5	20
53	4	53/60 (88%)	51 (96%)	2 (4%)	0	100	100
54	5	49/51 (96%)	46 (94%)	3 (6%)	0	100	100
55	6	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
56	7	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
57	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	6377/7157 (89%)	5841 (92%)	510 (8%)	26 (0%)	31	59

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	86	ARG

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Mol	Chain	Res	Type
7	g	152	SER
28	D	152	PRO
30	F	74	ILE
33	I	106	PHE

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	184/202 (91%)	184 (100%)	0	100 100
3	c	170/187 (91%)	170 (100%)	0	100 100
4	d	171/174 (98%)	170 (99%)	1 (1%)	78 93
5	e	113/124 (91%)	113 (100%)	0	100 100
6	f	88/119 (74%)	87 (99%)	1 (1%)	65 88
7	g	118/122 (97%)	118 (100%)	0	100 100
8	h	108/109 (99%)	108 (100%)	0	100 100
9	i	104/106 (98%)	104 (100%)	0	100 100
10	j	88/92 (96%)	88 (100%)	0	100 100
11	k	90/98 (92%)	90 (100%)	0	100 100
12	l	105/107 (98%)	105 (100%)	0	100 100
13	m	95/99 (96%)	94 (99%)	1 (1%)	65 88
14	n	80/82 (98%)	80 (100%)	0	100 100
15	o	74/75 (99%)	74 (100%)	0	100 100
16	p	64/65 (98%)	64 (100%)	0	100 100
17	q	73/79 (92%)	73 (100%)	0	100 100
18	r	48/64 (75%)	48 (100%)	0	100 100
19	s	72/78 (92%)	72 (100%)	0	100 100
20	t	69/70 (99%)	69 (100%)	0	100 100
21	u	51/60 (85%)	50 (98%)	1 (2%)	48 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	x	284/668 (42%)	284 (100%)	0	100	100
27	C	212/213 (100%)	212 (100%)	0	100	100
28	D	162/162 (100%)	162 (100%)	0	100	100
29	E	157/158 (99%)	157 (100%)	0	100	100
30	F	150/153 (98%)	150 (100%)	0	100	100
31	G	135/141 (96%)	132 (98%)	3 (2%)	45	77
32	H	72/107 (67%)	72 (100%)	0	100	100
33	I	39/122 (32%)	39 (100%)	0	100	100
34	J	82/110 (74%)	82 (100%)	0	100	100
35	L	119/119 (100%)	119 (100%)	0	100	100
36	M	102/102 (100%)	102 (100%)	0	100	100
37	N	106/106 (100%)	106 (100%)	0	100	100
38	O	110/110 (100%)	110 (100%)	0	100	100
39	P	98/104 (94%)	98 (100%)	0	100	100
40	Q	86/87 (99%)	86 (100%)	0	100	100
41	R	95/98 (97%)	95 (100%)	0	100	100
42	S	87/88 (99%)	87 (100%)	0	100	100
43	T	86/86 (100%)	86 (100%)	0	100	100
44	U	87/87 (100%)	87 (100%)	0	100	100
45	V	79/82 (96%)	79 (100%)	0	100	100
46	W	84/88 (96%)	84 (100%)	0	100	100
47	X	154/164 (94%)	154 (100%)	0	100	100
48	Y	56/61 (92%)	56 (100%)	0	100	100
49	Z	66/67 (98%)	65 (98%)	1 (2%)	57	84
50	1	54/55 (98%)	54 (100%)	0	100	100
51	2	48/49 (98%)	46 (96%)	2 (4%)	26	60
52	3	41/61 (67%)	41 (100%)	0	100	100
53	4	47/52 (90%)	47 (100%)	0	100	100
54	5	47/47 (100%)	47 (100%)	0	100	100
55	6	37/37 (100%)	37 (100%)	0	100	100
56	7	54/55 (98%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
57	8	34/34 (100%)	34 (100%)	0	100 100
All	All	5035/5785 (87%)	5025 (100%)	10 (0%)	85 96

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	Z	3	ARG
51	2	5	LYS
51	2	35	VAL
21	u	35	ARG
31	G	10	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
35	L	58	ASN
42	S	72	ASN
36	M	67	HIS
40	Q	39	GLN
46	W	99	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1520/1536 (98%)	252 (16%)	0
22	v	75/77 (97%)	10 (13%)	0
23	w	5/24 (20%)	0	0
25	A	2881/2891 (99%)	539 (18%)	41 (1%)
26	B	116/120 (96%)	18 (15%)	2 (1%)
All	All	4597/4648 (98%)	819 (17%)	43 (0%)

5 of 819 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	2	A
1	a	4	C
1	a	5	U
1	a	6	G
1	a	9	G

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	1741	A
25	A	2392	G
25	A	1917	G
25	A	2273	G
25	A	2536	G

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

26 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	$\#\|Z\| > 2$
25	5MU	A	1926	25	19,22,23	1.40	4 (21%)	27,32,35	2.22	6 (22%)
1	2MG	a	1510	1	23,26,27	1.26	4 (17%)	33,38,41	2.22	8 (24%)
25	2MG	A	1822	25	23,26,27	1.28	3 (13%)	33,38,41	2.23	8 (24%)
25	2MG	A	2432	58,25	23,26,27	1.33	4 (17%)	33,38,41	2.23	9 (27%)
22	PSU	v	55	22	18,21,22	1.38	3 (16%)	21,30,33	2.06	4 (19%)
25	2MA	A	2490	58,25	22,25,26	1.44	5 (22%)	32,37,40	2.32	9 (28%)
22	4SU	v	8	22	18,21,22	2.15	4 (22%)	25,30,33	1.62	4 (16%)
1	7MG	a	521	1	23,26,27	1.30	3 (13%)	27,39,42	2.72	6 (22%)
1	2MG	a	960	1	23,26,27	1.27	3 (13%)	33,38,41	2.18	9 (27%)
25	OMG	A	2238	58,22,25	23,26,27	1.25	3 (13%)	32,38,41	1.99	6 (18%)
1	MA6	a	1512	1	23,26,27	1.45	4 (17%)	33,38,41	2.39	13 (39%)
22	5MC	v	32	22	19,22,23	1.42	3 (15%)	26,32,35	1.30	3 (11%)
1	4OC	a	1396	1	20,23,24	0.77	0	25,32,35	0.98	2 (8%)
25	6MZ	A	2017	25	22,25,26	1.86	6 (27%)	29,36,39	3.41	10 (34%)
25	7MG	A	2056	58,25	23,26,27	1.33	3 (13%)	27,39,42	2.70	7 (25%)
25	6MZ	A	1608	25	22,25,26	1.83	6 (27%)	29,36,39	3.43	10 (34%)
1	5MC	a	961	1	19,22,23	1.45	3 (15%)	26,32,35	1.10	3 (11%)
1	MA6	a	1513	1	23,26,27	1.44	5 (21%)	33,38,41	2.47	15 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	OMU	A	2539	25	19,22,23	1.35	4 (21%)	25,31,34	1.91	5 (20%)
1	UR3	a	1492	1	19,22,23	0.96	1 (5%)	26,32,35	1.76	2 (7%)
25	UR3	A	1902	25	19,22,23	0.98	1 (5%)	26,32,35	1.72	4 (15%)
25	1MG	A	735	25	23,26,27	1.13	3 (13%)	33,39,42	1.72	5 (15%)
22	5MU	v	54	22	19,22,23	1.41	6 (31%)	27,32,35	2.05	6 (22%)
1	2MG	a	1201	1	23,26,27	1.26	3 (13%)	33,38,41	2.16	6 (18%)
25	5MC	A	1949	25	19,22,23	1.36	3 (15%)	26,32,35	1.11	2 (7%)
25	OMC	A	2485	58,25	19,22,23	0.85	2 (10%)	25,31,34	1.03	1 (4%)

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
25	5MU	A	1926	25	-	0/7/25/26	0/2/2/2
1	2MG	a	1510	1	-	0/9/27/28	0/3/3/3
25	2MG	A	1822	25	-	0/9/27/28	0/3/3/3
25	2MG	A	2432	58,25	-	0/9/27/28	0/3/3/3
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2
25	2MA	A	2490	58,25	-	1/7/25/26	0/3/3/3
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
1	7MG	a	521	1	-	2/7/37/38	0/3/3/3
1	2MG	a	960	1	-	0/9/27/28	0/3/3/3
25	OMG	A	2238	58,22,25	-	2/9/27/28	0/3/3/3
1	MA6	a	1512	1	-	2/11/29/30	0/3/3/3
22	5MC	v	32	22	-	0/7/25/26	0/2/2/2
1	4OC	a	1396	1	-	0/9/29/30	0/2/2/2
25	6MZ	A	2017	25	-	2/9/27/28	0/3/3/3
25	7MG	A	2056	58,25	-	2/7/37/38	0/3/3/3
25	6MZ	A	1608	25	-	0/9/27/28	0/3/3/3
1	5MC	a	961	1	-	0/7/25/26	0/2/2/2
1	MA6	a	1513	1	-	4/11/29/30	0/3/3/3
25	OMU	A	2539	25	-	0/9/27/28	0/2/2/2
1	UR3	a	1492	1	-	0/7/25/26	0/2/2/2
25	UR3	A	1902	25	-	0/7/25/26	0/2/2/2
25	1MG	A	735	25	-	0/7/25/26	0/3/3/3
22	5MU	v	54	22	-	0/7/25/26	0/2/2/2
1	2MG	a	1201	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	5MC	A	1949	25	-	0/7/25/26	0/2/2/2
25	OMC	A	2485	58,25	-	3/9/27/28	0/2/2/2

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2017	6MZ	C6-N6	5.45	1.40	1.34
25	A	1608	6MZ	C6-N6	5.34	1.40	1.34
22	v	8	4SU	C4-S4	-5.05	1.59	1.68
1	a	961	5MC	C5-C4	4.87	1.47	1.44
22	v	32	5MC	C5-C4	4.72	1.47	1.44

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1608	6MZ	C9-N6-C6	-14.40	109.49	122.85
25	A	2017	6MZ	C9-N6-C6	-14.36	109.53	122.85
1	a	521	7MG	N9-C4-N3	9.31	139.10	125.46
25	A	2056	7MG	N9-C4-N3	9.09	138.79	125.46
25	A	2490	2MA	C5-C4-N3	-8.25	118.49	127.18

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1513	MA6	C5-C6-N6-C9
25	A	2238	OMG	O4'-C4'-C5'-O5'
1	a	521	7MG	O4'-C4'-C5'-O5'
1	a	521	7MG	C3'-C4'-C5'-O5'
1	a	1513	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1510	2MG	1	0
25	A	2490	2MA	1	0
22	v	8	4SU	1	0
1	a	1512	MA6	2	0
22	v	32	5MC	1	0
1	a	961	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1513	MA6	3	0
25	A	2485	OMC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 611 ligands modelled in this entry, 609 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
59	FME	v	103	22	8,9,10	0.29	0	8,9,11	1.41	1 (12%)
60	GDP	x	901	-	29,30,30	1.16	4 (13%)	45,47,47	1.76	6 (13%)

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
59	FME	v	103	22	-	2/7/9/11	-
60	GDP	x	901	-	-	3/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	x	901	GDP	C5-C4	2.80	1.46	1.38
60	x	901	GDP	C6-N1	-2.58	1.34	1.38
60	x	901	GDP	C5-N7	-2.32	1.34	1.39
60	x	901	GDP	C4-N9	-2.07	1.32	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	x	901	GDP	C5-C4-N3	-5.80	119.15	128.39
60	x	901	GDP	C2-N3-C4	4.91	120.76	112.30
60	x	901	GDP	N9-C4-N3	4.18	134.31	125.95
60	x	901	GDP	C6-C5-N7	3.52	136.69	130.29
60	x	901	GDP	C4-C5-N7	-2.75	106.31	110.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	v	103	FME	O1-CN-N-CA
59	v	103	FME	CB-CA-N-CN
60	x	901	GDP	C5'-O5'-PA-O3A
60	x	901	GDP	C5'-O5'-PA-O1A
60	x	901	GDP	C5'-O5'-PA-O2A

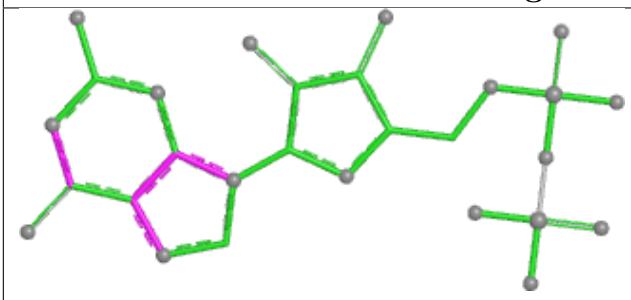
There are no ring outliers.

1 monomer is involved in 2 short contacts:

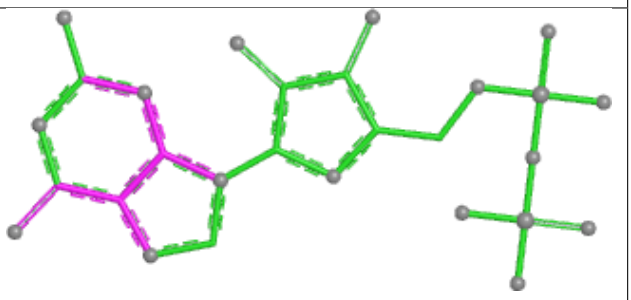
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	v	103	FME	2	0

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.

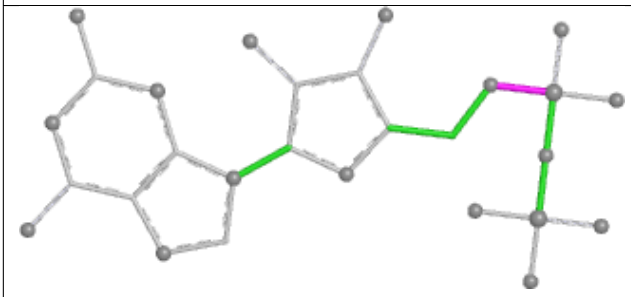
Ligand GDP x 901



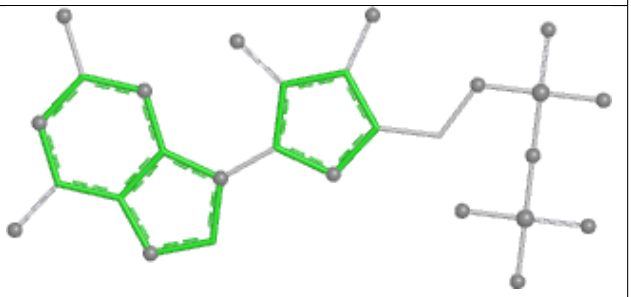
Bond lengths



Bond angles



Torsions



Rings

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.

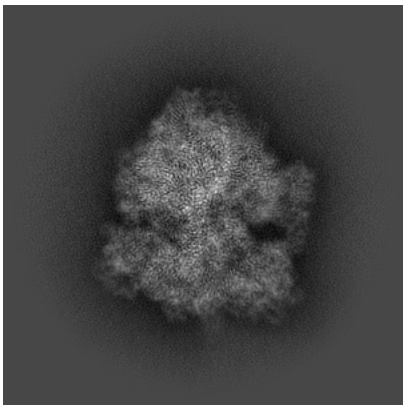
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26633. These allow visual inspection of the internal detail of the map and identification of artifacts.

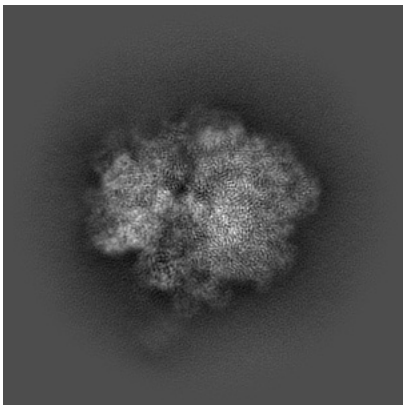
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



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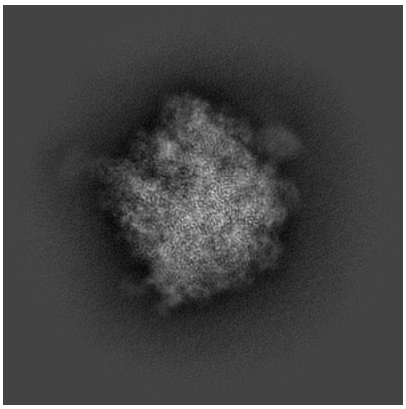
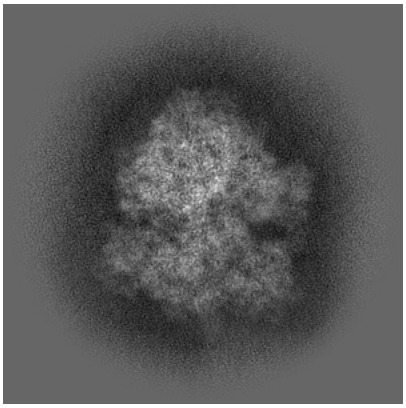
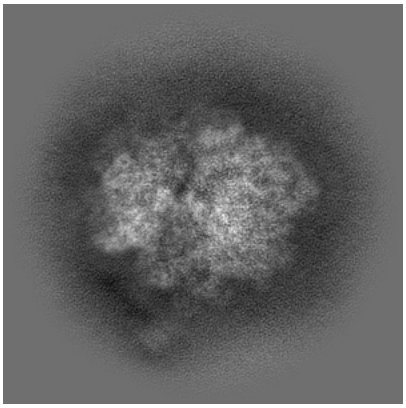


Z

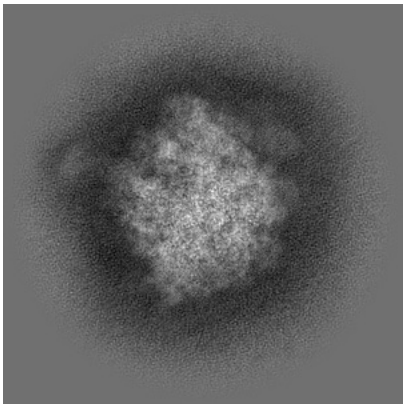
6.1.2 Raw map



X



Y

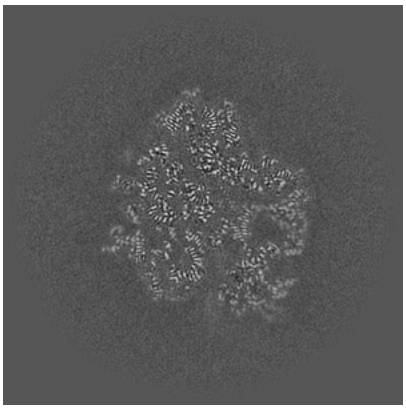


Z

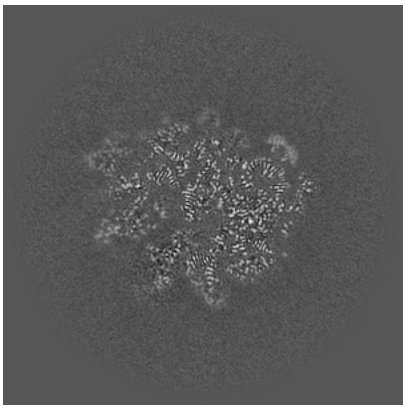
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

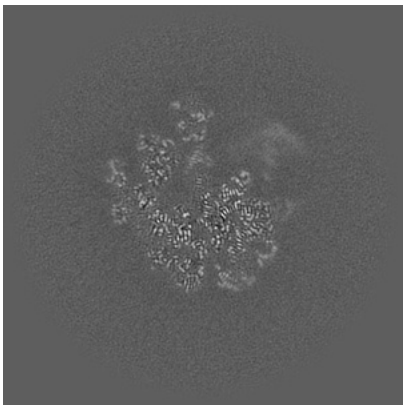
6.2.1 Primary map



X Index: 256

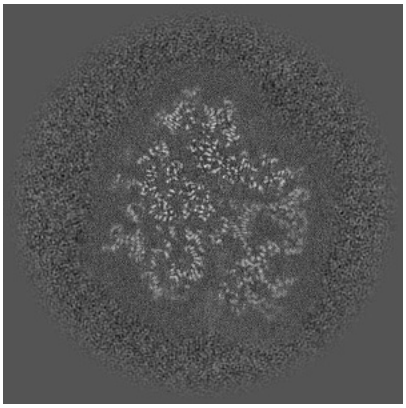


Y Index: 256

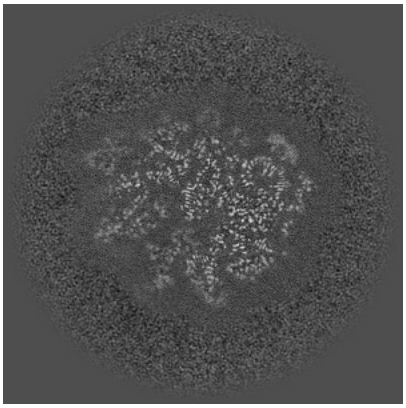


Z Index: 256

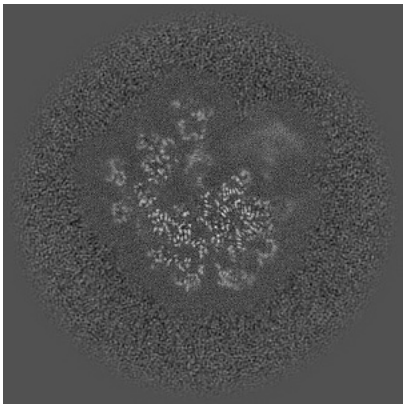
6.2.2 Raw map



X Index: 256



Y Index: 256

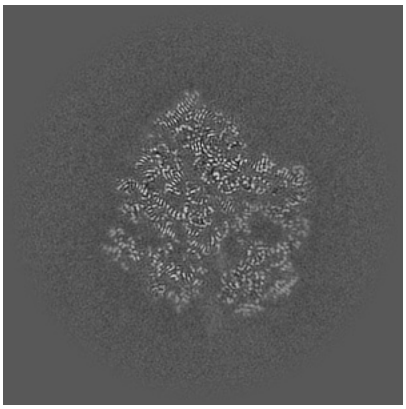


Z Index: 256

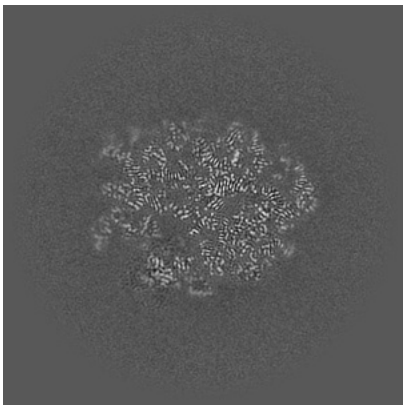
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

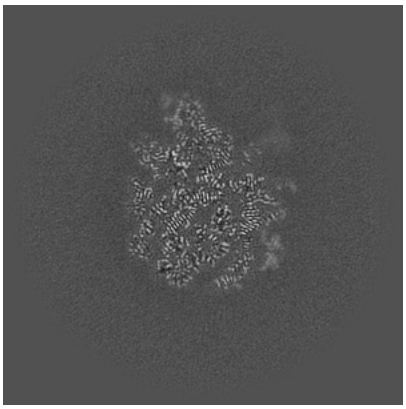
6.3.1 Primary map



X Index: 251

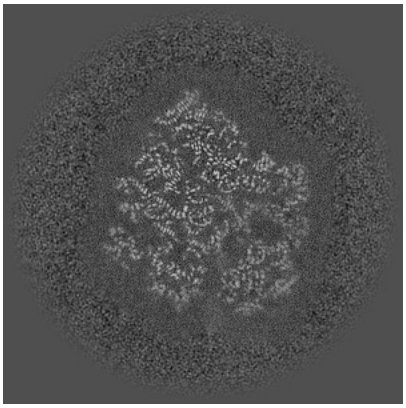


Y Index: 243

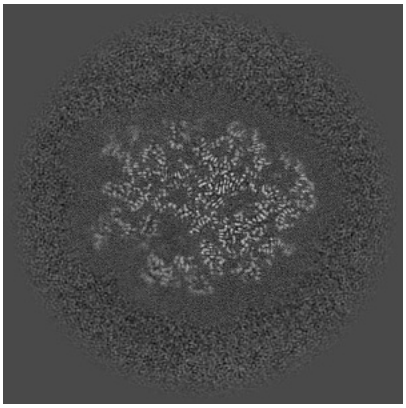


Z Index: 297

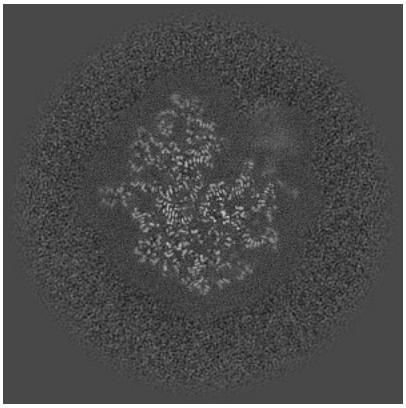
6.3.2 Raw map



X Index: 251



Y Index: 242

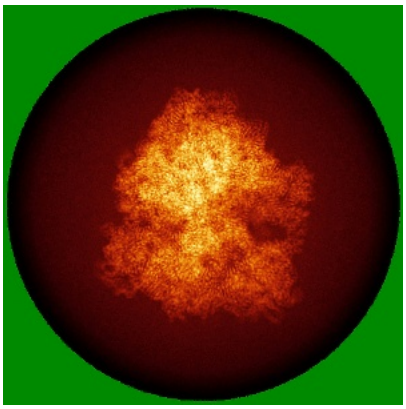


Z Index: 279

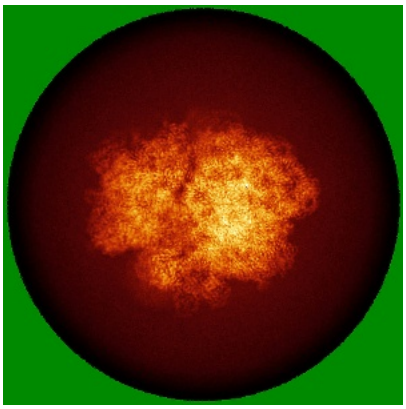
The images above show the largest variance slices of the map in three orthogonal directions.

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

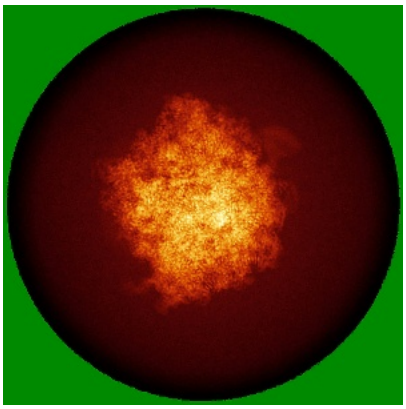
6.4.1 Primary map



X

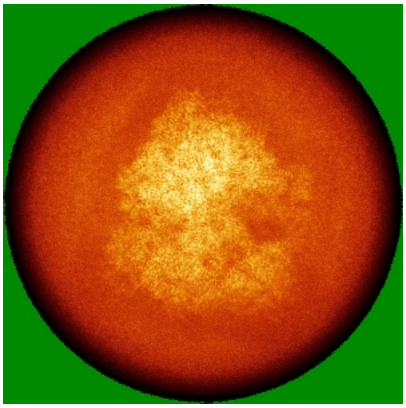


Y

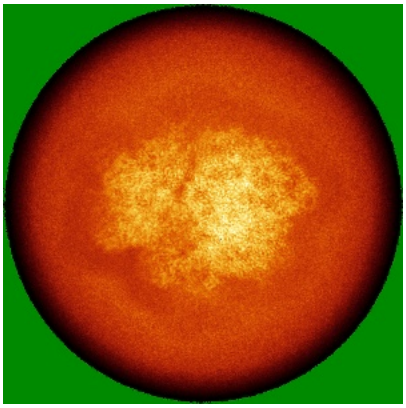


Z

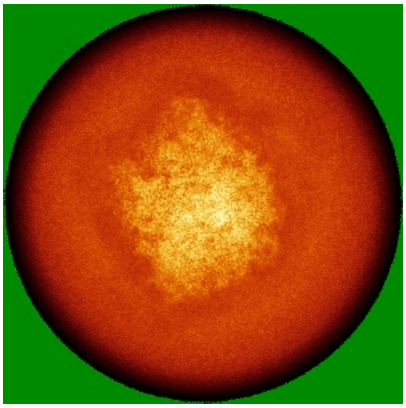
6.4.2 Raw map



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.

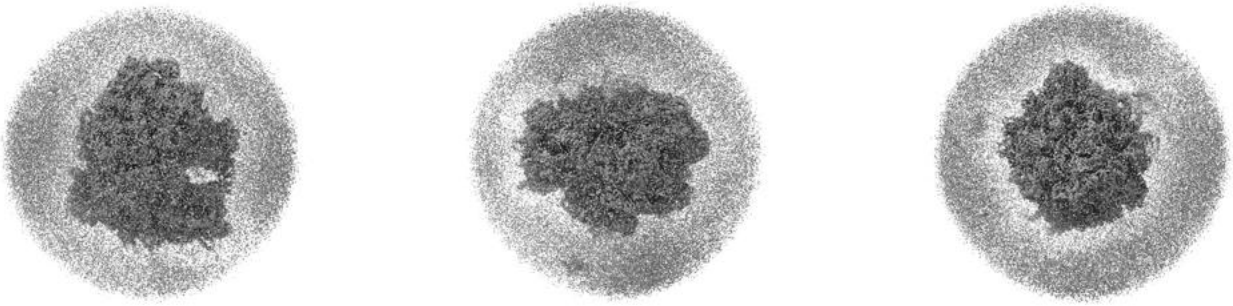
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.6. 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.

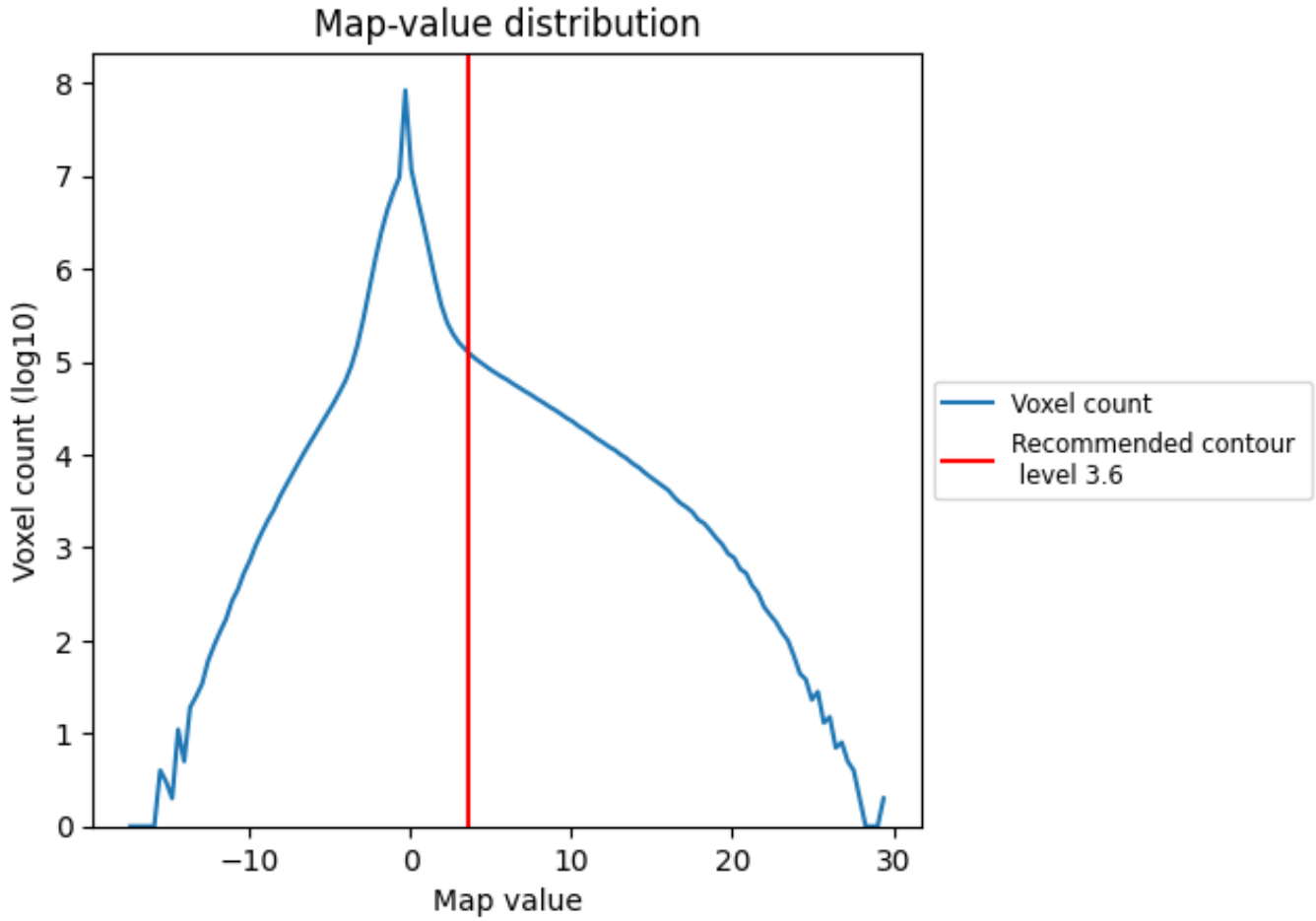
6.6 Mask visualisation (i)

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

7 Map analysis

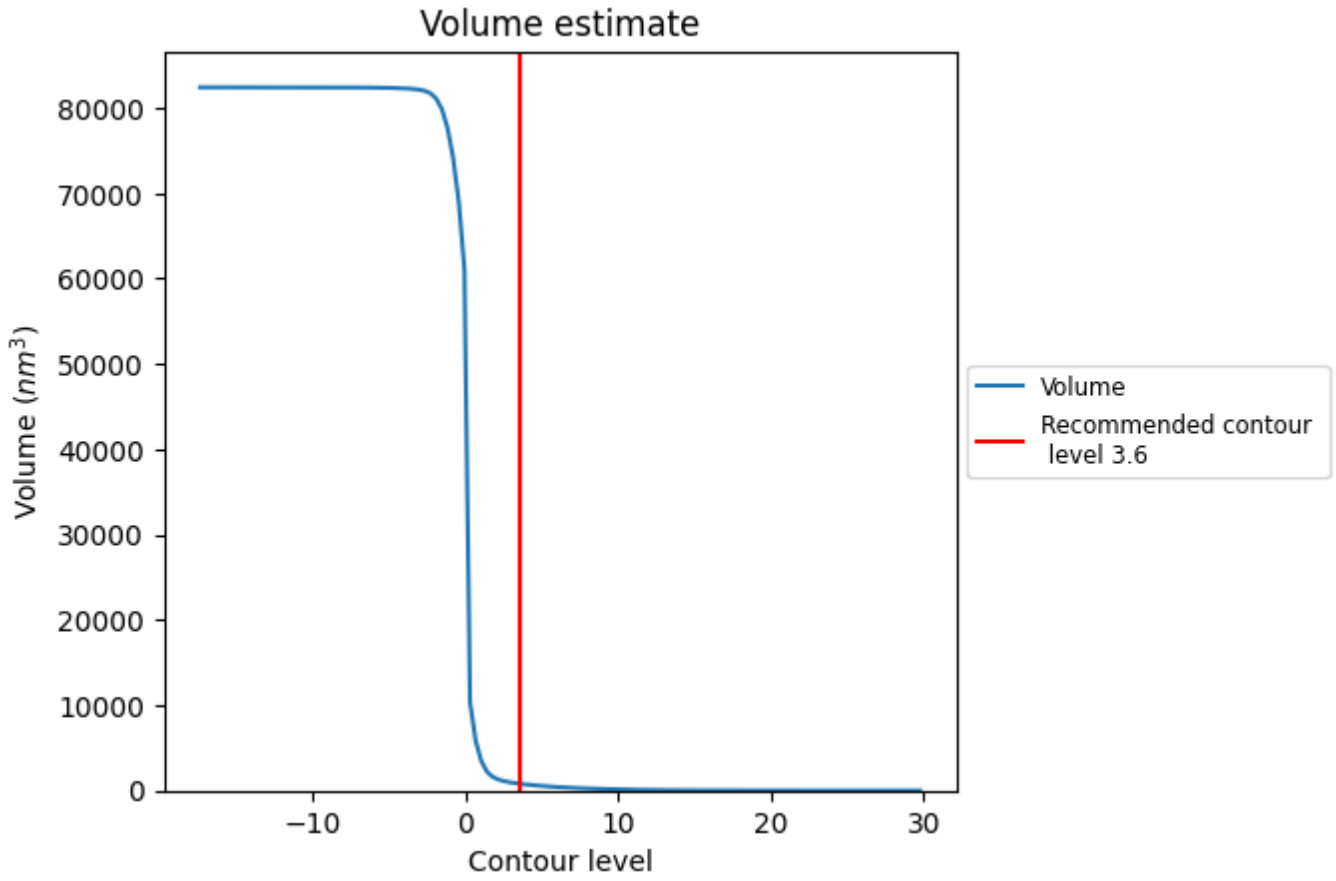
This section contains the results of statistical analysis of the map.

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.

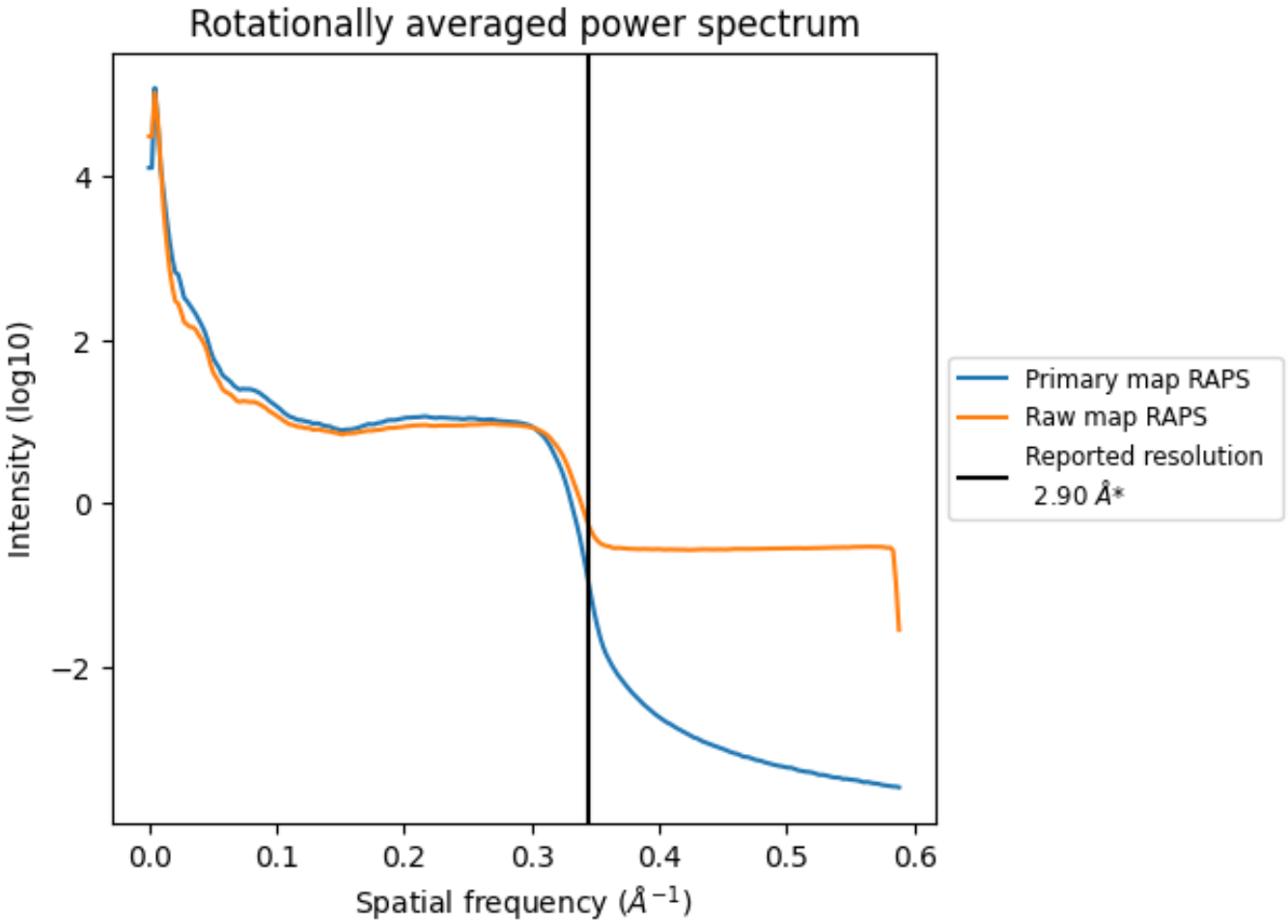
7.2 Volume estimate (i)



The volume at the recommended contour level is 791 nm^3; this corresponds to an approximate mass of 715 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)

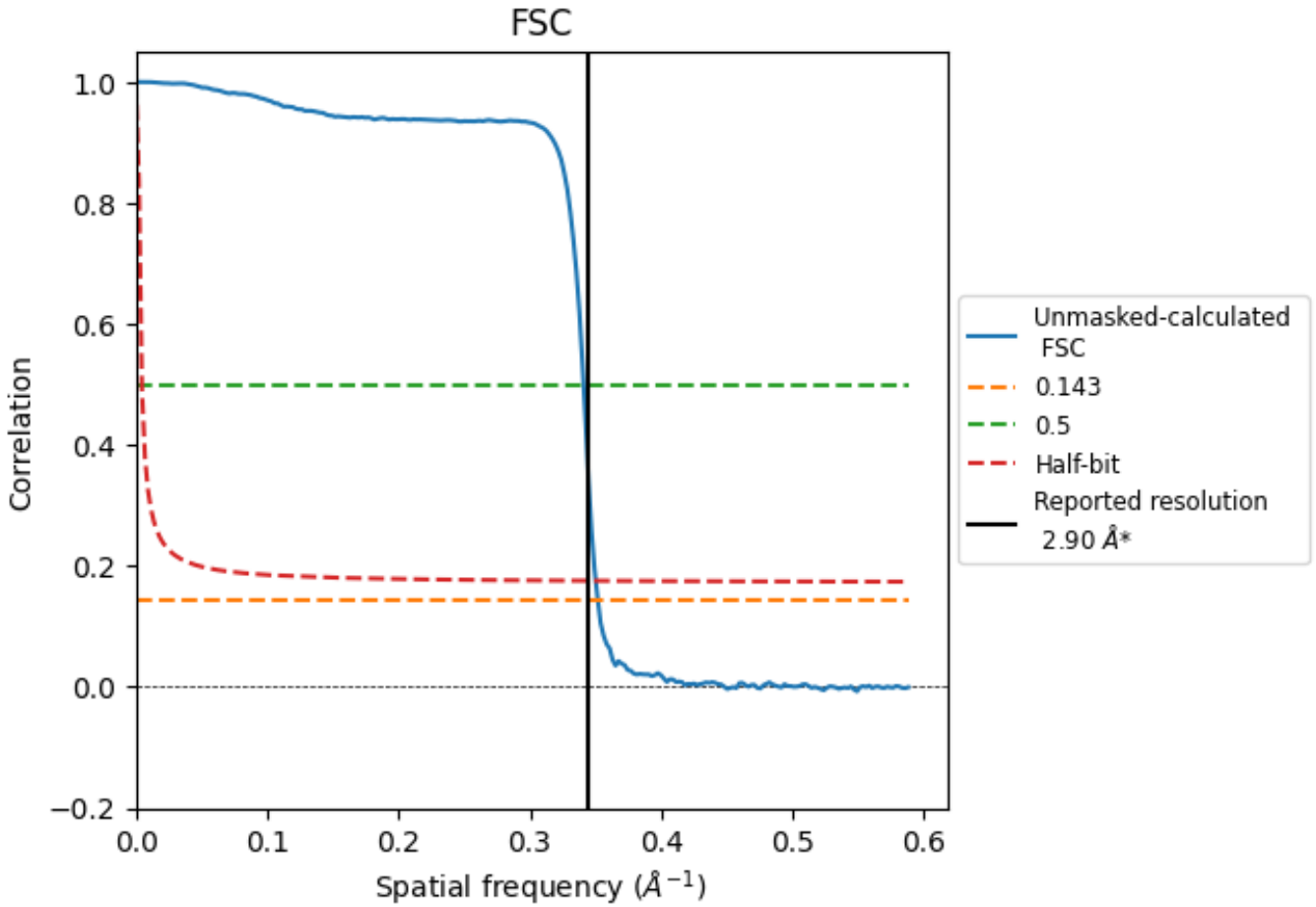


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

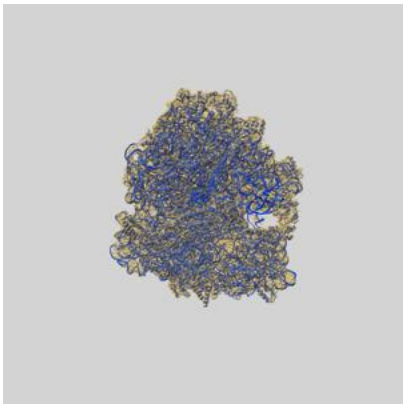
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.84	2.93	2.86

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

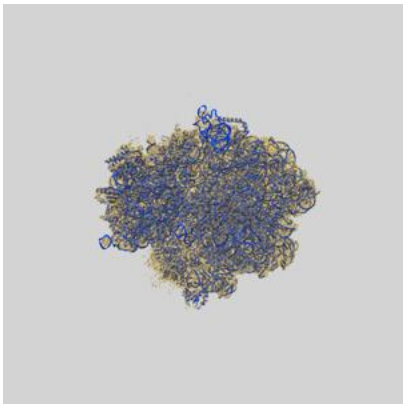
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26633 and PDB model 7UNU. Per-residue inclusion information can be found in section 3 on page 18.

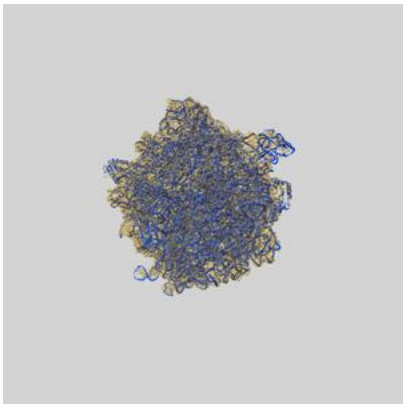
9.1 Map-model overlay



X



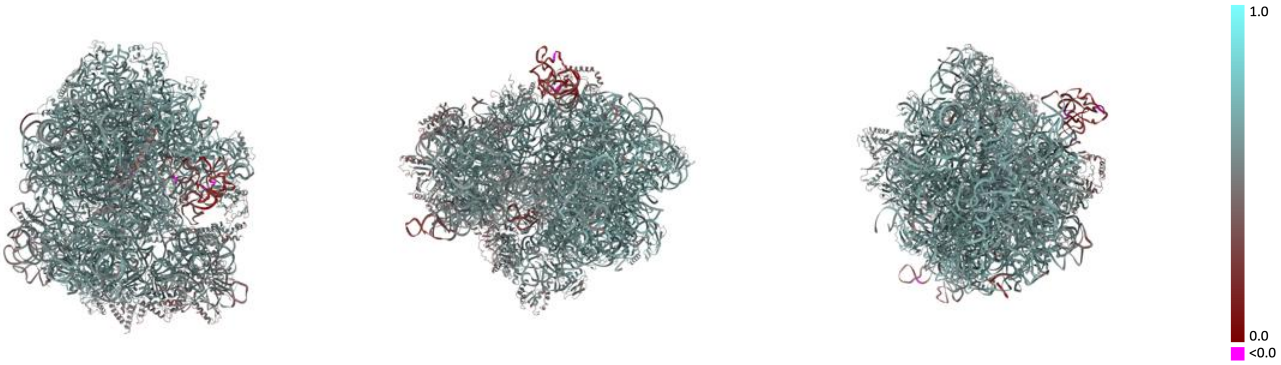
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.6 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.

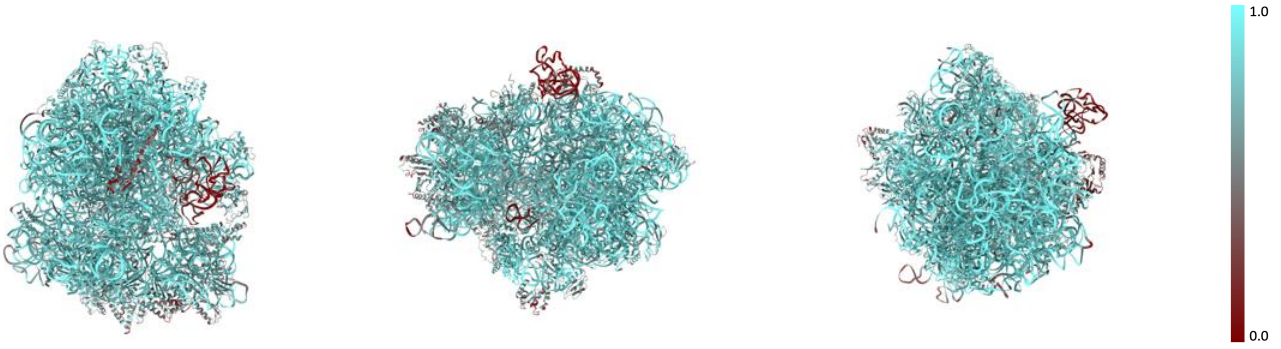
9.2 Q-score mapped to coordinate model (i)



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.

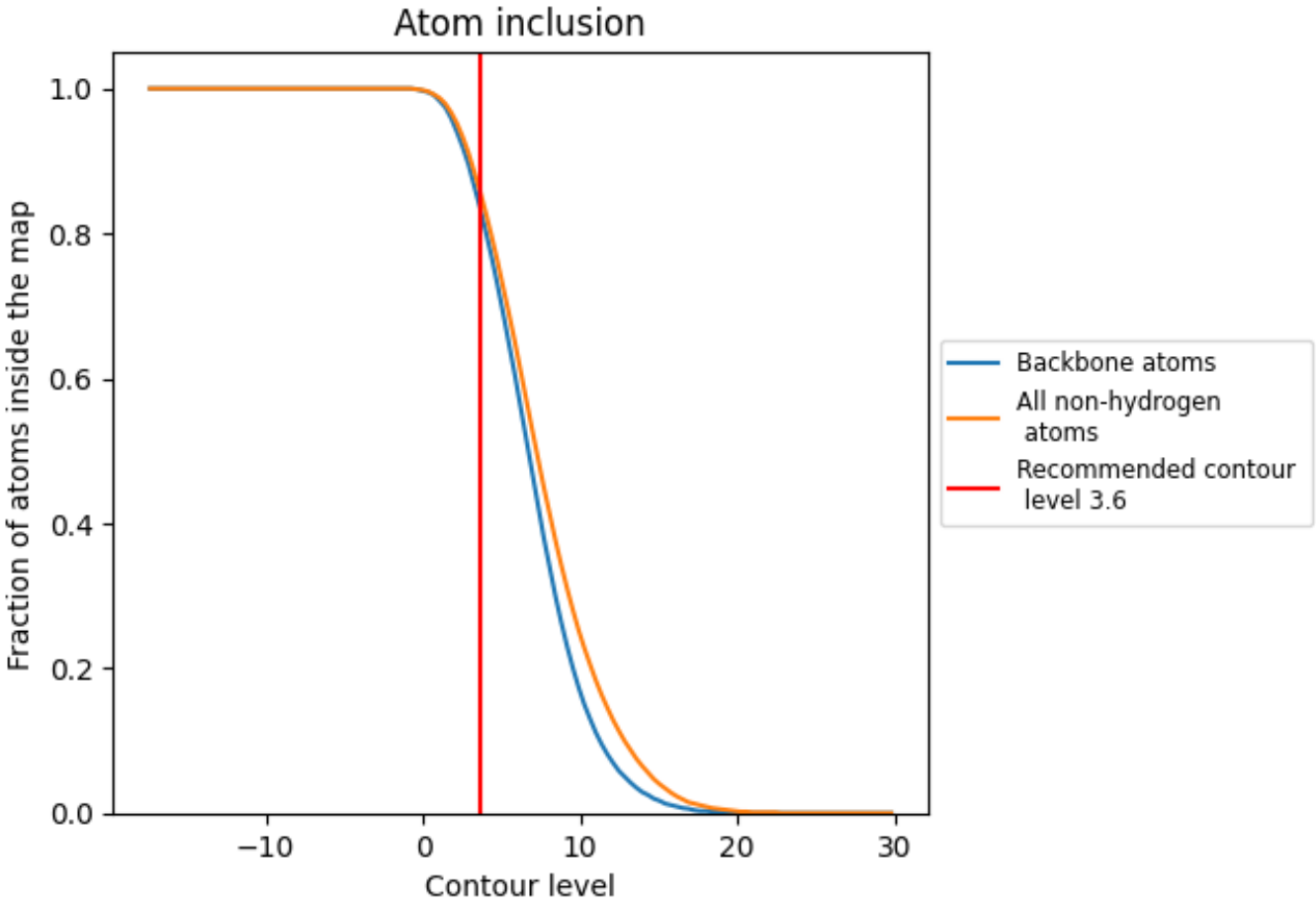
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.6).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 86% 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 (3.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8600	0.5770
1	0.7480	0.5480
2	0.8380	0.6110
3	0.6120	0.4750
4	0.8210	0.6000
5	0.7470	0.5810
6	0.8980	0.6290
7	0.9040	0.6300
8	0.9020	0.6080
A	0.9240	0.5990
B	0.9120	0.5840
C	0.8900	0.6200
D	0.8570	0.6030
E	0.8240	0.5970
F	0.7060	0.5250
G	0.7070	0.5410
H	0.3510	0.4320
I	0.4740	0.4720
J	0.8540	0.4910
L	0.8750	0.6190
M	0.8510	0.6130
N	0.8460	0.5990
O	0.8510	0.6150
P	0.8880	0.6160
Q	0.7680	0.5650
R	0.8310	0.6080
S	0.9020	0.6230
T	0.8110	0.5860
U	0.8450	0.6080
V	0.7690	0.5910
W	0.6850	0.5240
X	0.7250	0.5630
Y	0.8650	0.6150
Z	0.8280	0.6050
a	0.9060	0.5720

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Chain	Atom inclusion	Q-score
b	0.6070	0.4840
c	0.6670	0.5100
d	0.6520	0.5140
e	0.7750	0.5640
f	0.6920	0.5090
g	0.6220	0.4850
h	0.8070	0.5770
i	0.6700	0.4950
j	0.5730	0.4780
k	0.7650	0.5610
l	0.7620	0.5700
m	0.6860	0.5030
n	0.7110	0.5240
o	0.7930	0.5760
p	0.7830	0.5590
q	0.7610	0.5590
r	0.7260	0.5620
s	0.6540	0.4940
t	0.8010	0.5510
u	0.6000	0.5300
v	0.7730	0.5620
w	0.8180	0.5800
x	0.7880	0.4860