wwPDB EM Validation Summary Report ⓘ

Apr 20, 2024 – 10:09 pm BST

PDB ID : 7ABZ
EMDB ID : EMD-11710
Title : Structure of pre-accomodated trans-translation complex on E. coli stalled ribosome.
Authors : Guyomar, C.; D'Urso, G.; Chat, S.; Giudice, E.; Gillet, R.
Deposited on : 2020-09-09
Resolution : 3.21 Å(reported)
Based on initial model : 4YBB

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

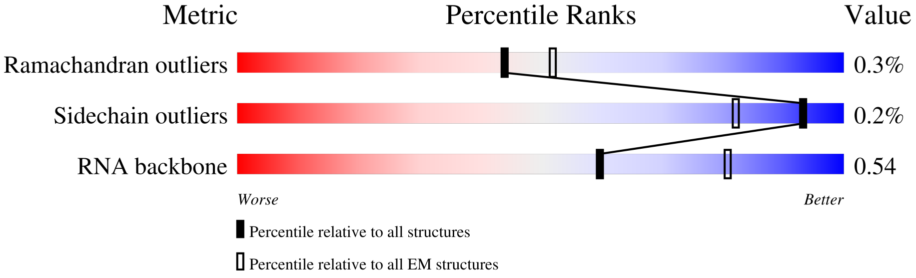
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance ⓘ

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

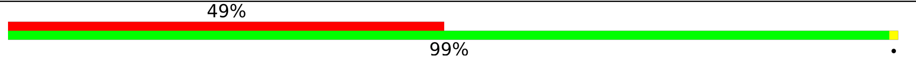
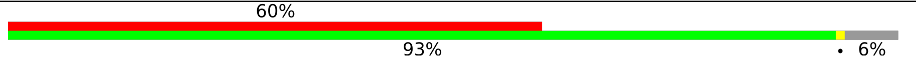
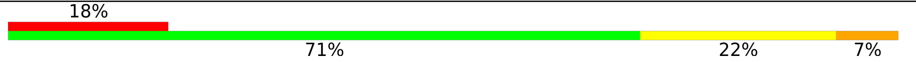
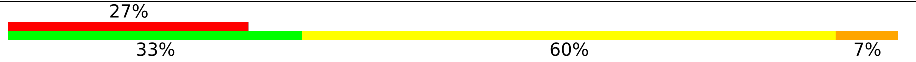
The reported resolution of this entry is 3.21 Å.

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	1	2904	 • 80% 20%
2	2	1540	 • 77% 23% •
3	3	118	 81% 19%
4	4	363	 71% 49% 50% •
5	5	146	 49% 99% •
6	6	394	 60% 93% • 6%
7	7	76	 18% 71% 22% 7%
8	8	15	 27% 33% 60% 7%

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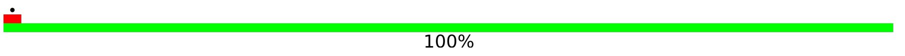
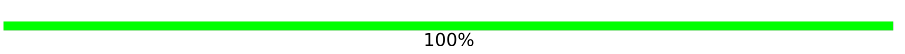
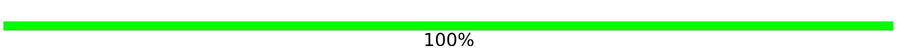
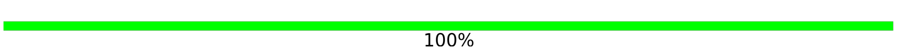
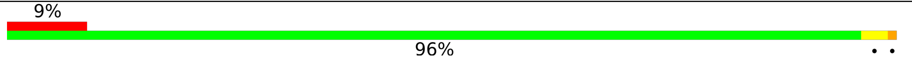
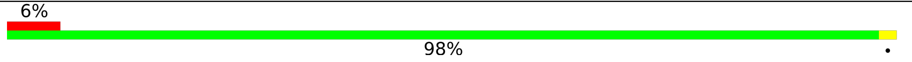
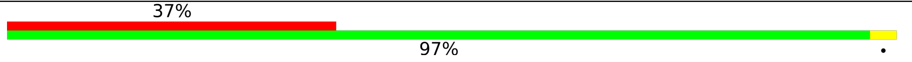
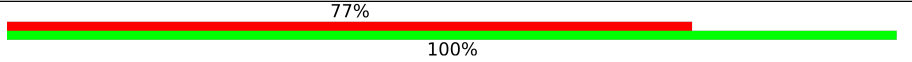
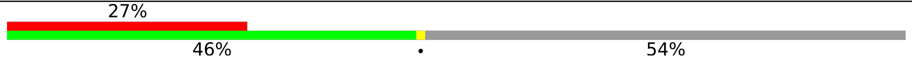
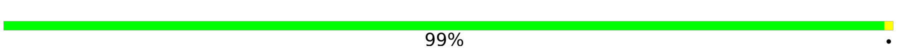
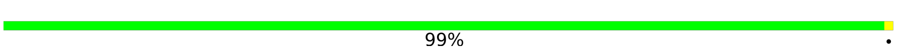
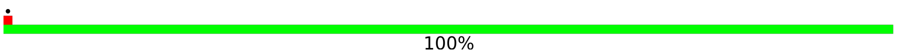
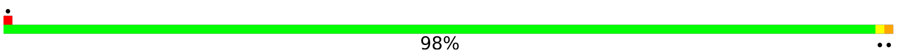
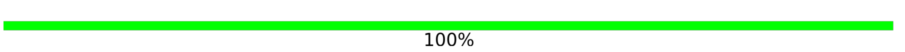
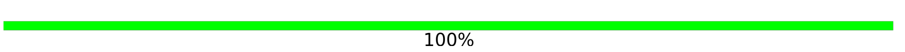
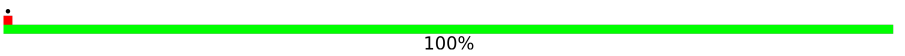
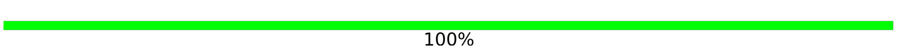
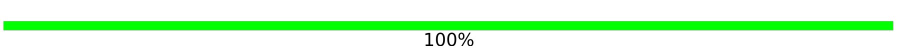
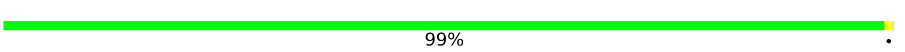
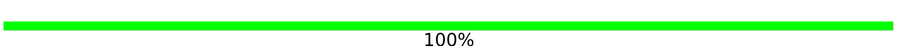
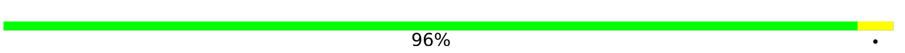
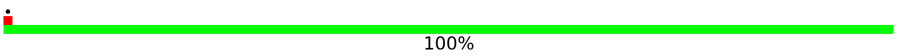
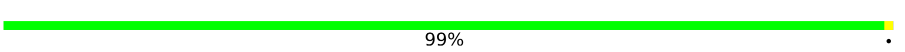
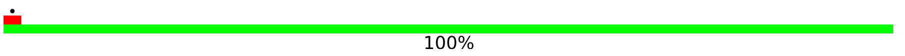
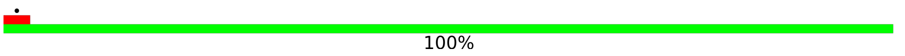
Mol	Chain	Length	Quality of chain
9	A	80	
10	B	271	
11	C	209	
12	D	201	
13	E	177	
14	F	176	
15	G	149	
16	H	130	
17	I	142	
18	J	142	
19	K	122	
20	L	144	
21	M	136	
22	N	120	
23	O	116	
24	P	114	
25	Q	117	
26	R	103	
27	S	110	
28	T	93	
29	U	102	
30	V	94	
31	X	77	
32	Y	62	
33	Z	58	

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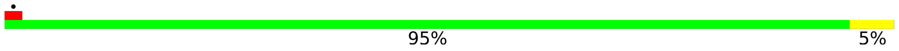
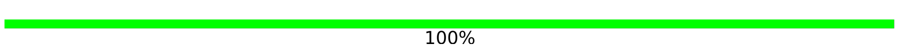
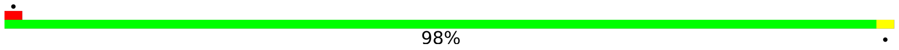
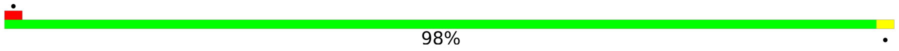
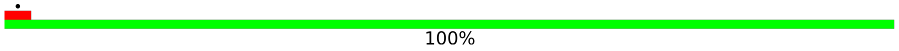
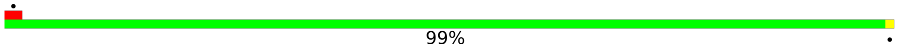
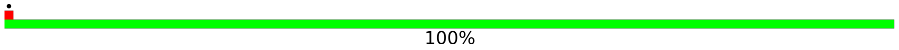
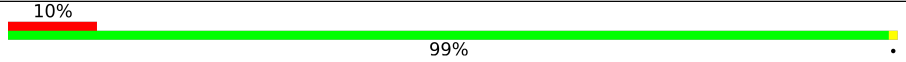
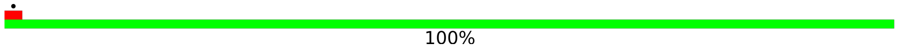
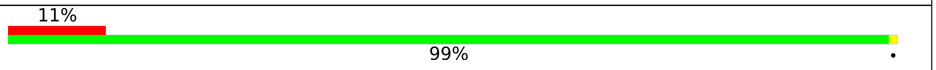
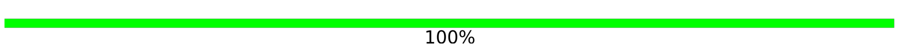
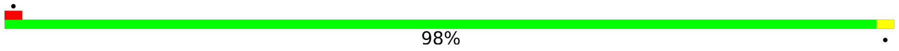
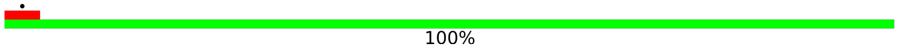
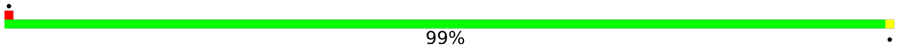
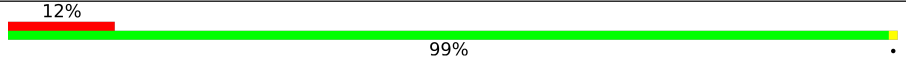
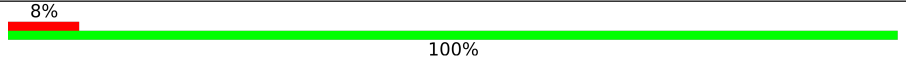
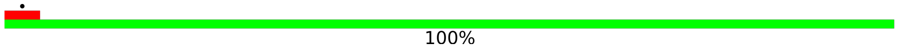
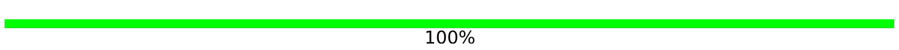
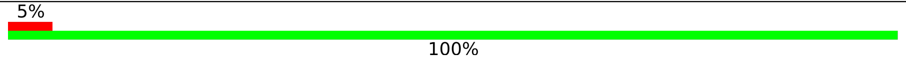
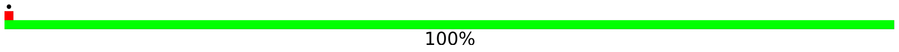
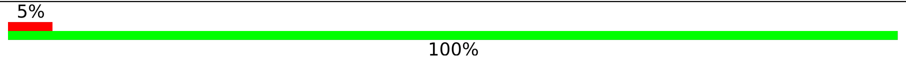
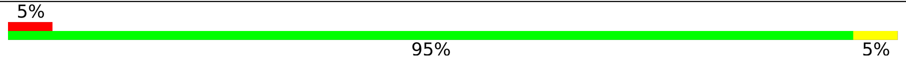
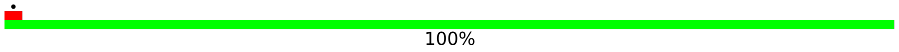
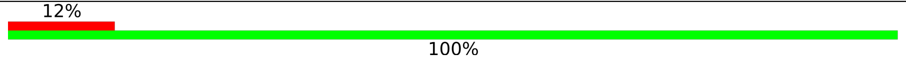
Mol	Chain	Length	Quality of chain
34	b	56	
35	c	50	
36	d	46	
37	e	64	
38	f	38	
39	g	224	
40	h	206	
41	i	205	
42	j	167	
43	k	100	
44	l	151	
45	m	129	
46	n	127	
47	o	98	
48	p	117	
49	q	123	
50	r	114	
51	s	100	
52	t	88	
53	u	82	
54	v	80	
55	w	55	
56	x	79	
57	y	85	
58	z	56	

2 Entry composition ⓘ

There are 62 unique types of molecules in this entry. The entry contains 157227 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2904	62355	27825	11472	20154	2904	0	0

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1540	33048	14747	6054	10707	1540	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	118	2529	1126	464	821	118	0	0

- Molecule 4 is a RNA chain called transfer-messenger RNA (tmRNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	363	7760	3466	1410	2521	363	0	0

- Molecule 5 is a protein called SsrA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	146	1181	747	219	211	4	0	0

- Molecule 6 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	371	2871	1818	492	548	13	0	0

- Molecule 7 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
7	7	76	1635	735	291	532	75	2	0	0

- Molecule 8 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	8	15	327	145	60	107	15	0	0

- Molecule 9 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	80	601	370	121	109	1	0	0

- Molecule 10 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B	271	2082	1288	423	364	7	0	0

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	209	1565	979	288	294	4	0	0

- Molecule 12 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	201	1552	974	283	290	5	0	0

- Molecule 13 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	177	1410	899	249	256	6	0	0

- Molecule 14 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	176	1322	832	243	245	2	0	0

- Molecule 15 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	149	1111	699	197	214	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H	130	980	620	174	182	4	0	0

- Molecule 17 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	66	470	289	87	91	3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	J	142	1129	714	212	199	4	0	0

- Molecule 19 is a protein called 50S ribosomal protein L14.

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

- Molecule 20 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	144	1053	654	207	190	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M	136	1075	686	205	178	6	0	0

- Molecule 22 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	N	120	960	593	196	166	5	0	0

- Molecule 23 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	O	116	892	552	178	162	0	0

- Molecule 24 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	P	114	917	574	179	163	1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	Q	117	947	604	192	151	0	0

- Molecule 26 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	103	816	516	153	145	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	S	110	857	532	166	156	3	0	0

- Molecule 28 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	93	739	466	139	132	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	U	102	780	492	146	142	0	0

- Molecule 30 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	V	94	753	479	137	134	3	0	0

- Molecule 31 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	X	77	625	388	129	106	2	0	0

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Y	62	501	308	98	94	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Z	58	449	281	87	79	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	b	56	444	269	94	80	1	0	0

- Molecule 35 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	c	50	Total 409	C 263	N 75	O 71	0	0

- Molecule 36 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	46	Total 377	C 228	N 90	O 57	S 2	0	0

- Molecule 37 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	64	Total 504	C 323	N 105	O 74	S 2	0	0

- Molecule 38 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	38	Total 302	C 185	N 65	O 48	S 4	0	0

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	224	Total 1753	C 1109	N 315	O 321	S 8	0	0

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	206	Total 1625	C 1028	N 305	O 289	S 3	0	0

- Molecule 41 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	205	Total 1643	C 1026	N 315	O 298	S 4	0	0

- Molecule 42 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	j	152	1118	695	214	203	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	161	LYS	VAL	conflict	UNP P0A7W1

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	k	100	817	515	148	148	6	0	0

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	l	151	1182	735	227	216	4	0	0

- Molecule 45 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	m	129	979	616	173	184	6	0	0

- Molecule 46 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	n	127	1022	634	206	179	3	0	0

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	o	98	787	493	150	143	1	0	0

- Molecule 48 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	117	Total	C	N	O	S	0	0
			876	540	174	159	3		

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	123	Total	C	N	O	S	0	0
			956	591	196	164	5		

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 51 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 52 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 53 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	w	55	456	288	86	82	0	0

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	x	79	638	408	120	108	2	0	0

- Molecule 57 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	y	85	665	411	137	114	3	0	0

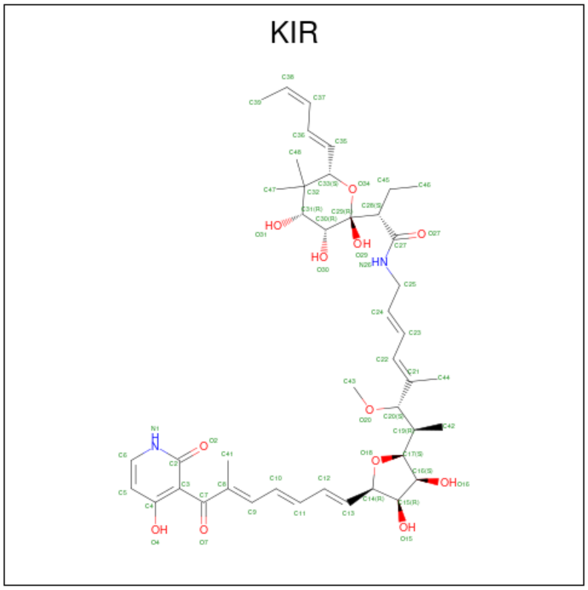
- Molecule 58 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	z	56	466	290	96	79	1	0	0

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

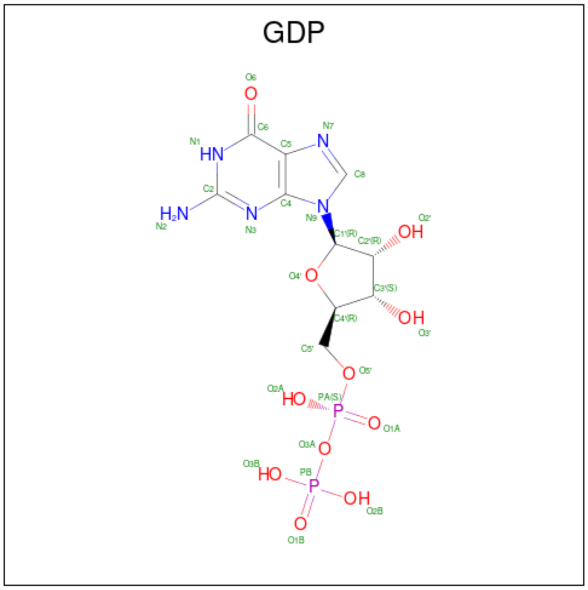
Mol	Chain	Residues	Atoms		AltConf
59	1	168	Total 168	Mg 168	0
59	2	18	Total 18	Mg 18	0
59	3	3	Total 3	Mg 3	0
59	B	1	Total 1	Mg 1	0
59	C	1	Total 1	Mg 1	0
59	O	1	Total 1	Mg 1	0

- Molecule 60 is KIRROMYCIN (three-letter code: KIR) (formula: $C_{43}H_{60}N_2O_{12}$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
60	6	1	57	43	2	12	0

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
61	6	1	28	10	5	11	2	0

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

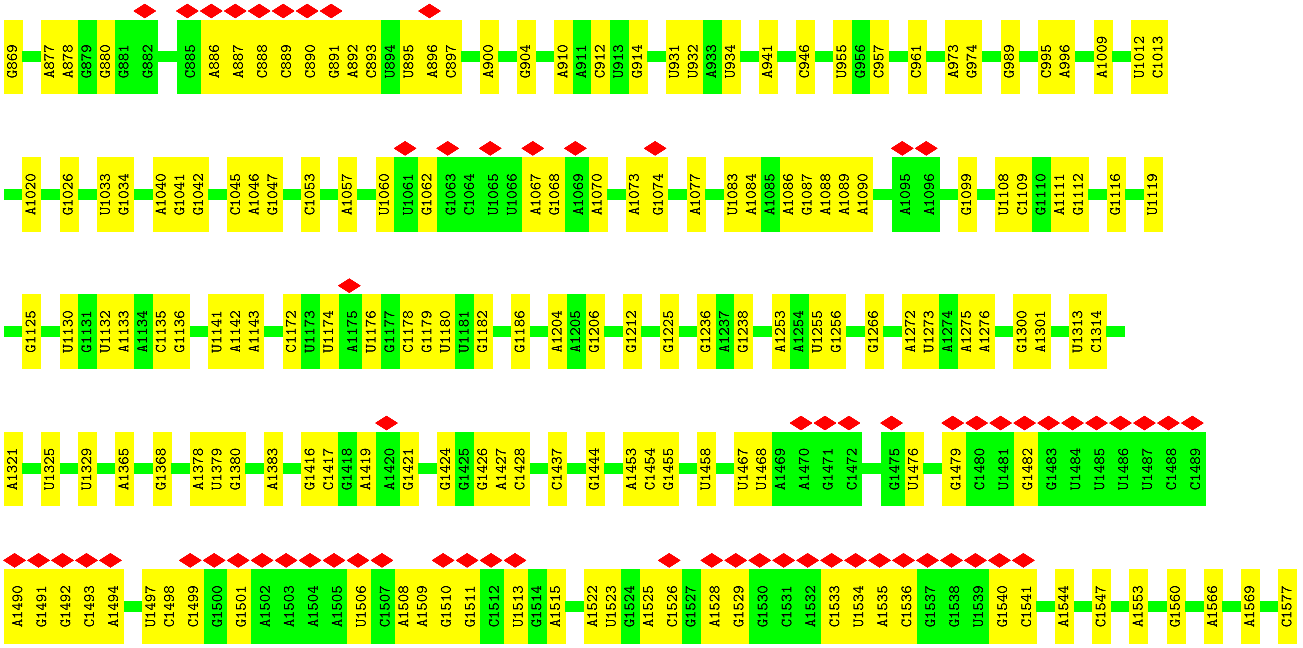
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
62	f	1	1	1	0

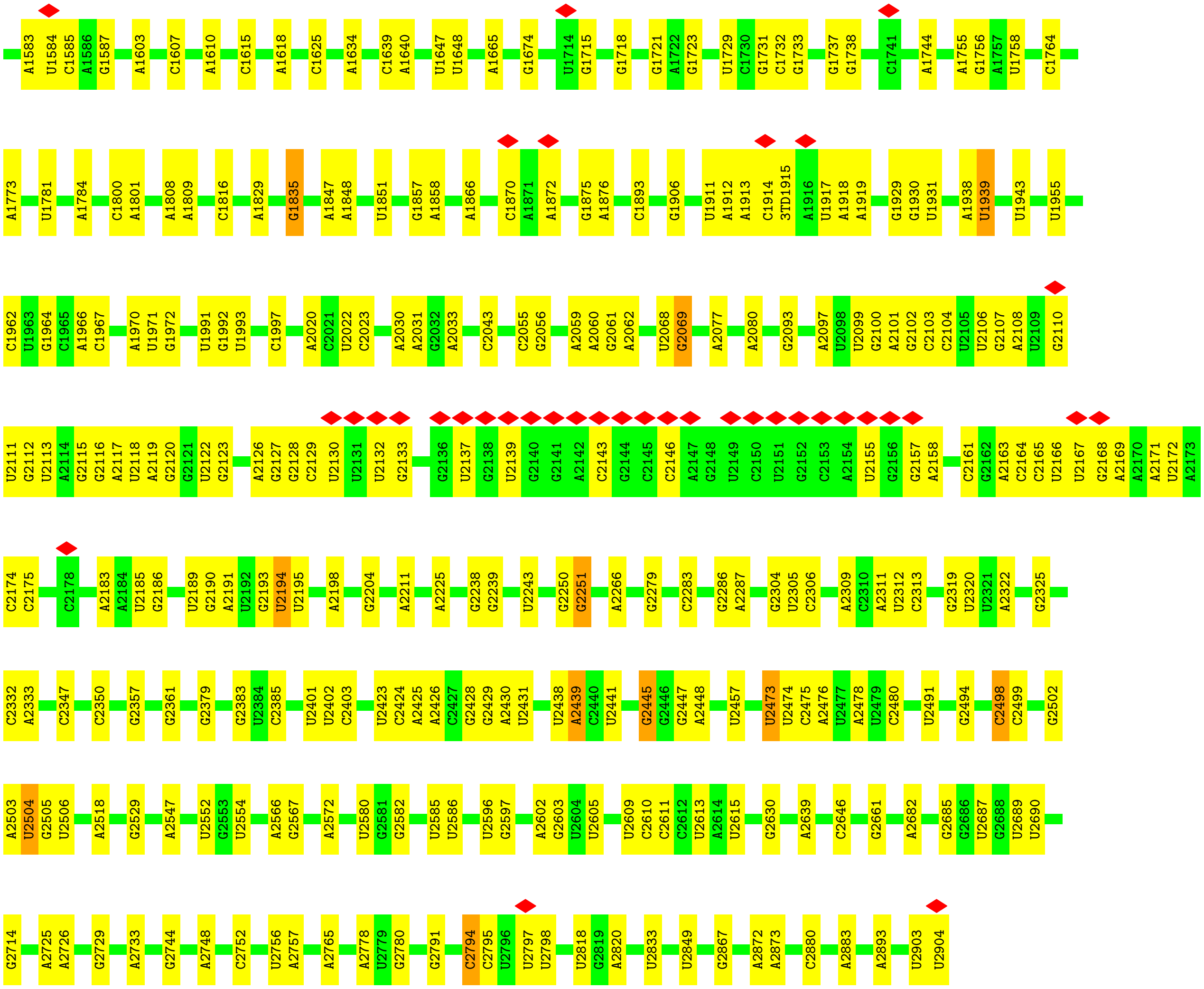
3 Residue-property plots ⓘ

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: 23S ribosomal RNA

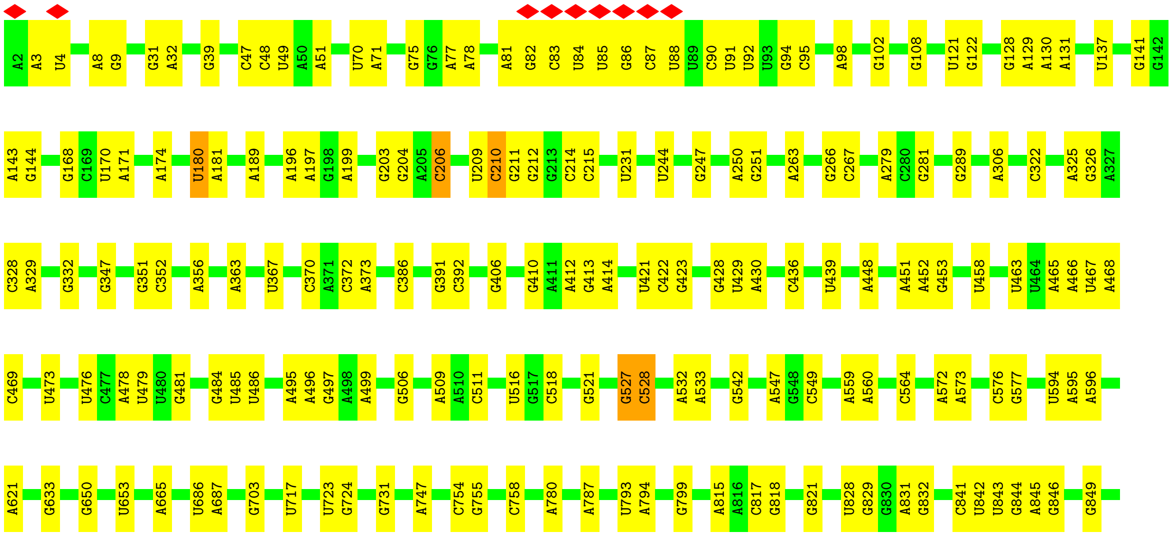
Chain 1:

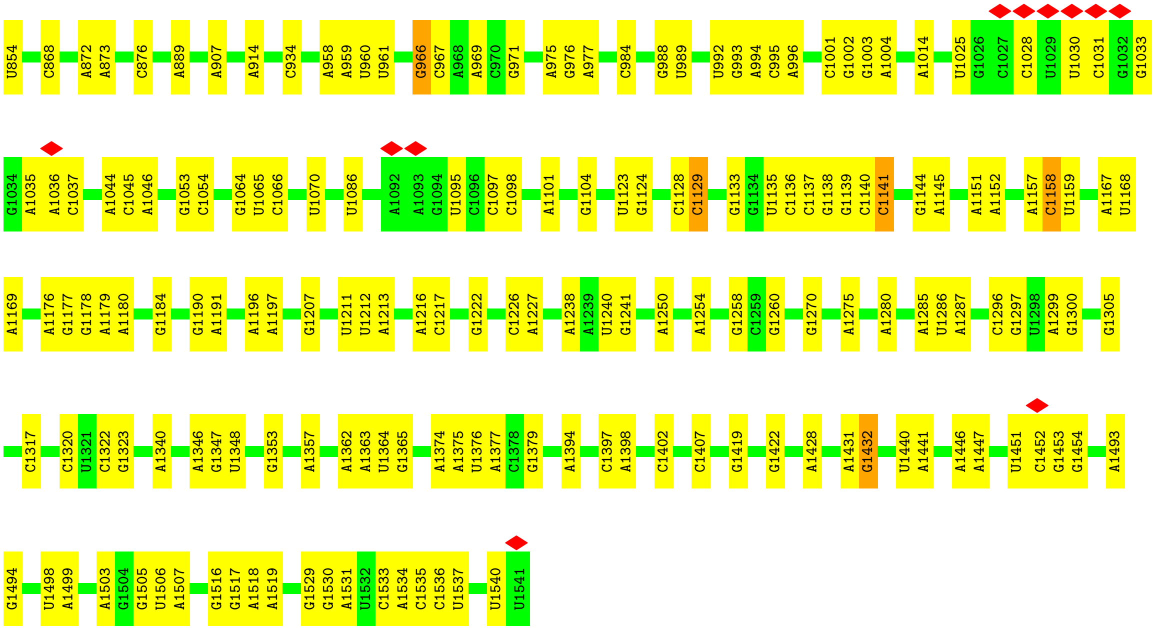




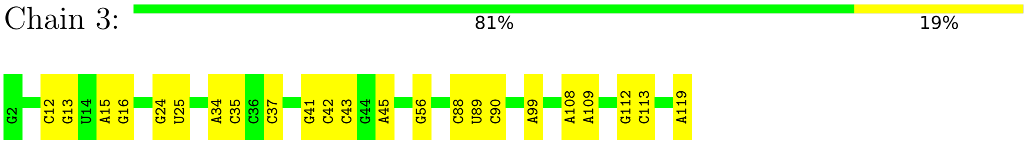
- Molecule 2: 16S ribosomal RNA

Chain 2:

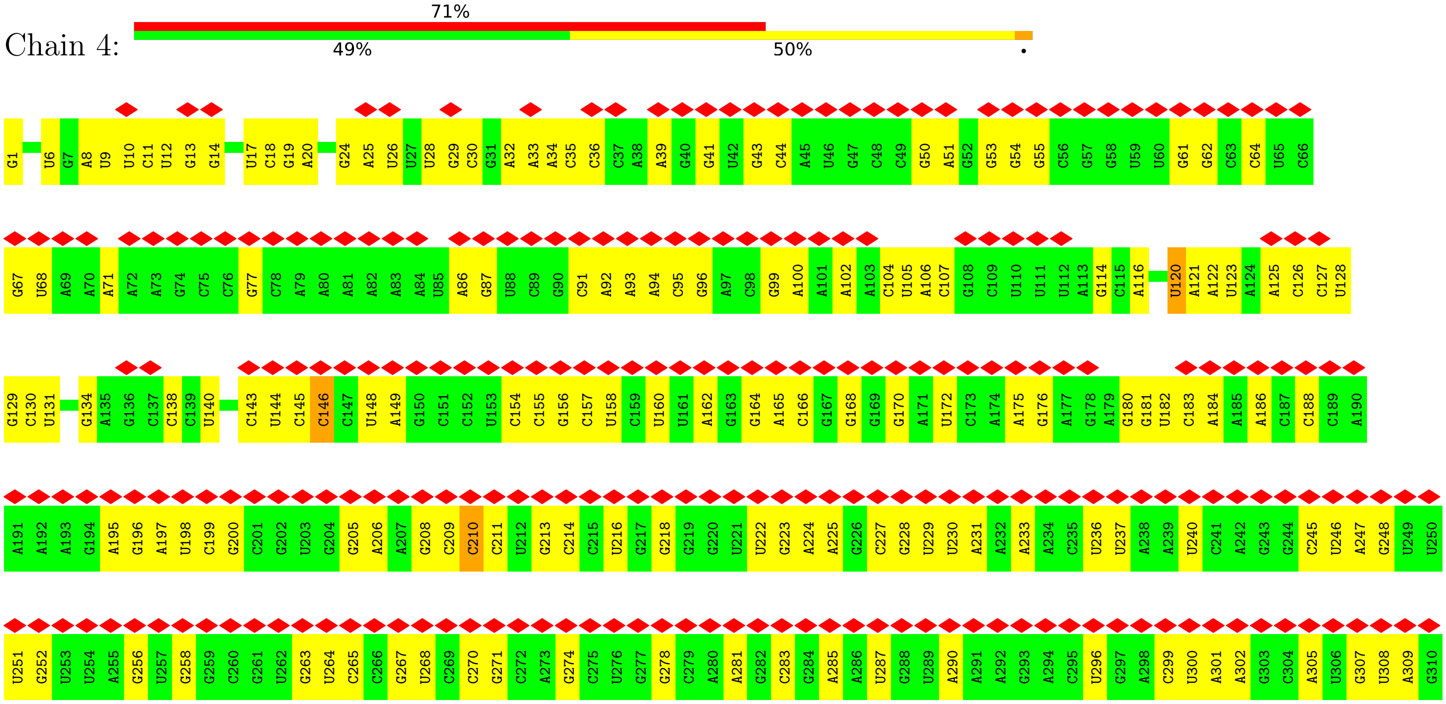




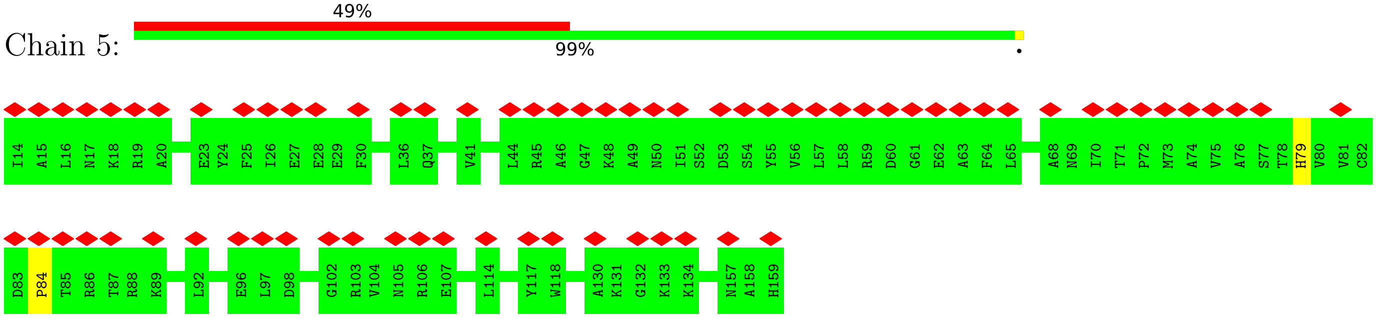
- Molecule 3: 5S ribosomal RNA



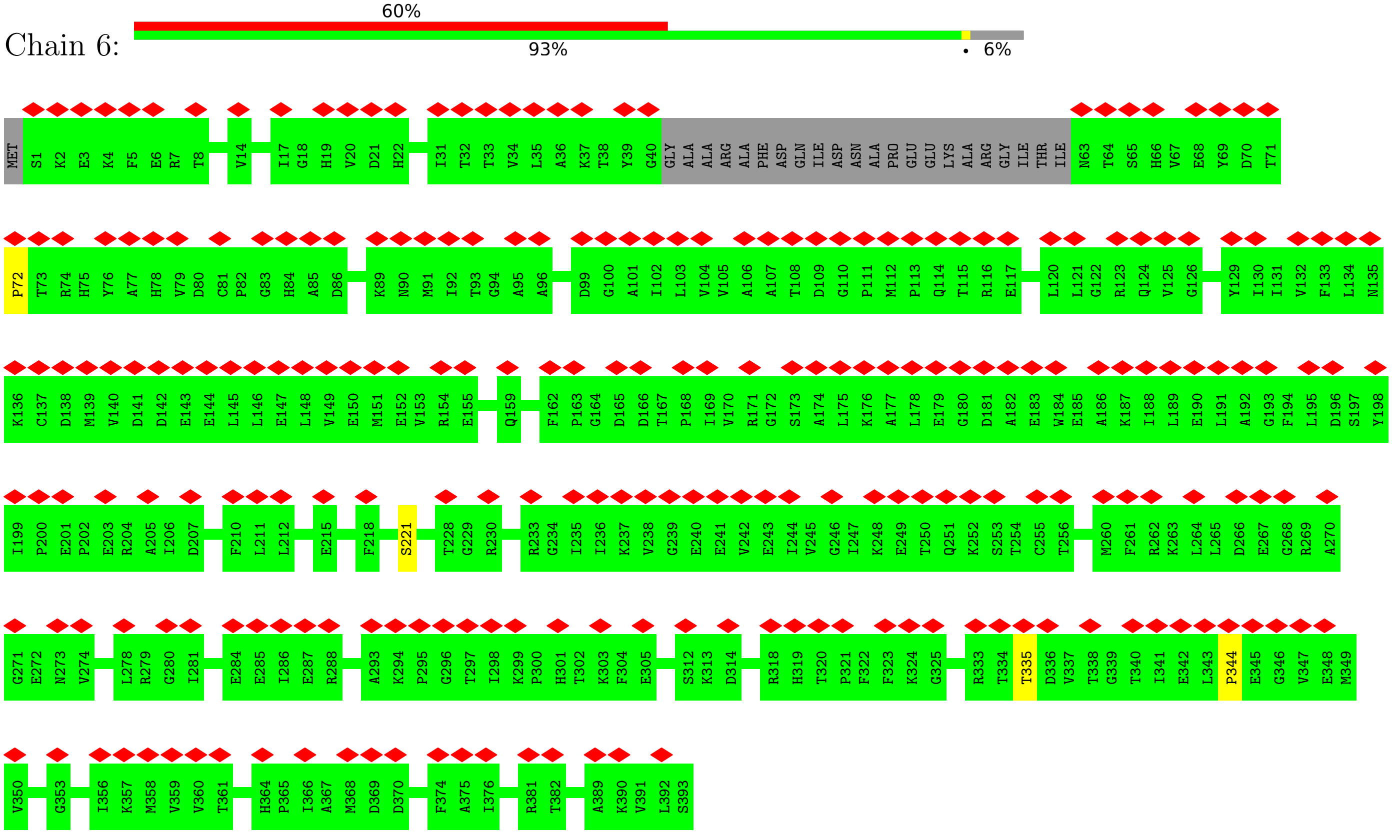
- Molecule 4: transfer-messenger RNA (tmRNA)



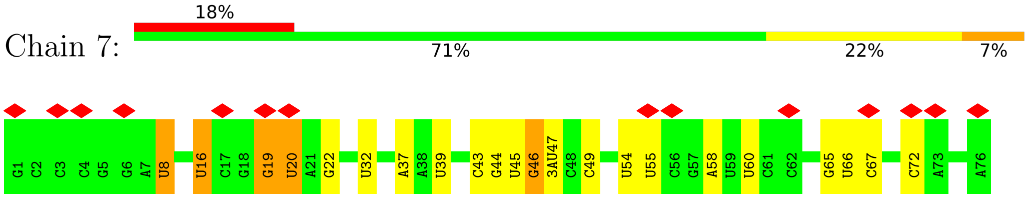
- Molecule 5: SsrA-binding protein



- Molecule 6: Elongation factor Tu 2

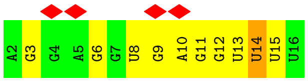


- Molecule 7: tRNA-Phe



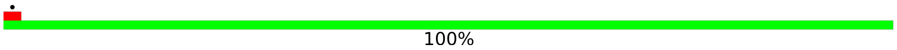
- Molecule 8: mRNA

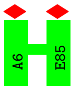
Chain 8:



- Molecule 9: 50S ribosomal protein L27

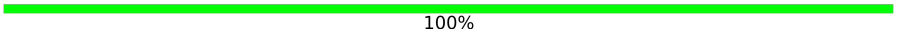
Chain A:





- Molecule 10: 50S ribosomal protein L2

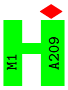
Chain B:



There are no outlier residues recorded for this chain.

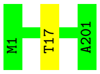
- Molecule 11: 50S ribosomal protein L3

Chain C:



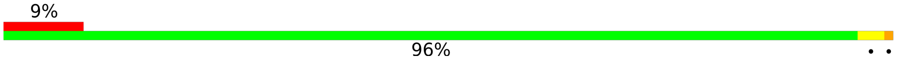
- Molecule 12: 50S ribosomal protein L4

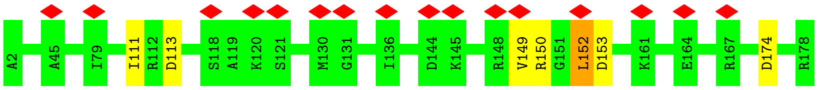
Chain D:



- Molecule 13: 50S ribosomal protein L5

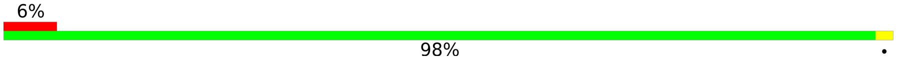
Chain E:

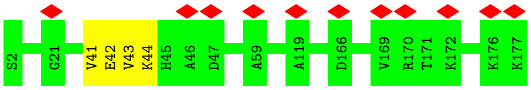




- Molecule 14: 50S ribosomal protein L6

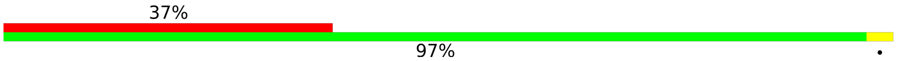
Chain F:

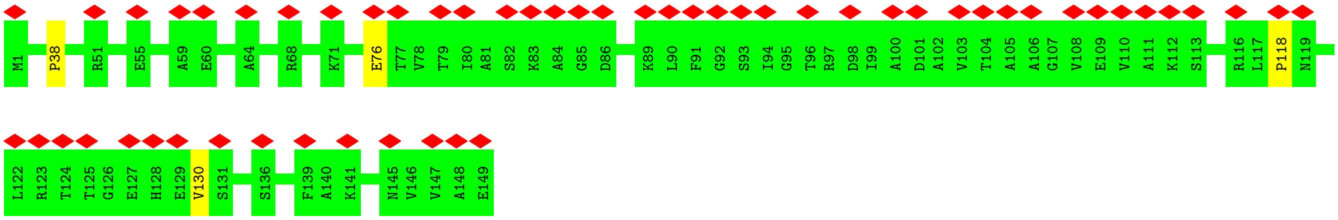




- Molecule 15: 50S ribosomal protein L9

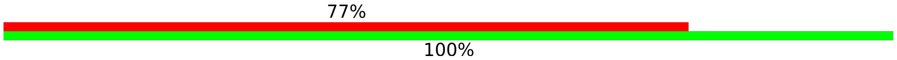
Chain G:

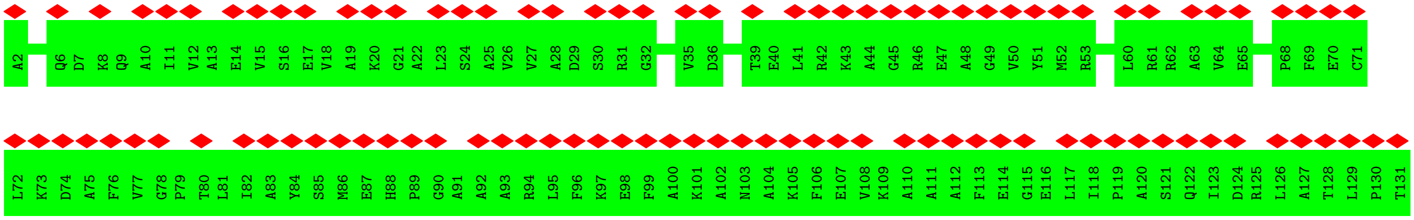




- Molecule 16: 50S ribosomal protein L10

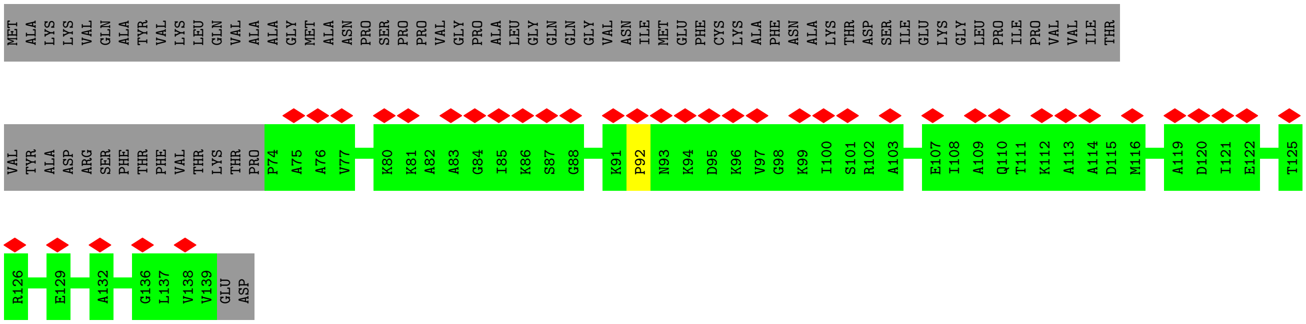
Chain H:





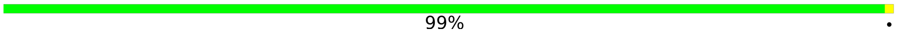
- Molecule 17: 50S ribosomal protein L11

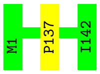
Chain I:



- Molecule 18: 50S ribosomal protein L13

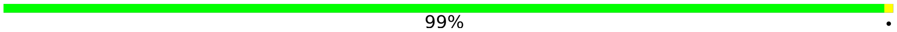
Chain J:

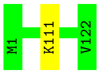




- Molecule 19: 50S ribosomal protein L14

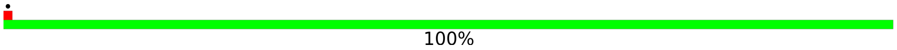
Chain K:

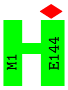




- Molecule 20: 50S ribosomal protein L15

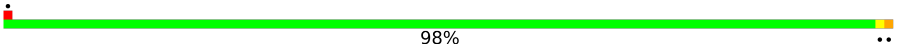
Chain L:

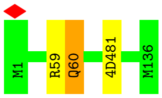




- Molecule 21: 50S ribosomal protein L16

Chain M:





- Molecule 22: 50S ribosomal protein L17

Chain N:

There are no outlier residues recorded for this chain.

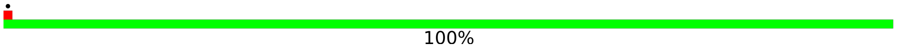
- Molecule 23: 50S ribosomal protein L18

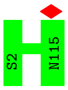
Chain O:

There are no outlier residues recorded for this chain.

- Molecule 24: 50S ribosomal protein L19

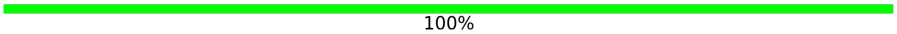
Chain P:





- Molecule 25: 50S ribosomal protein L20

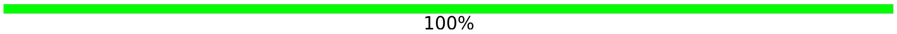
Chain Q:



There are no outlier residues recorded for this chain.

- Molecule 26: 50S ribosomal protein L21

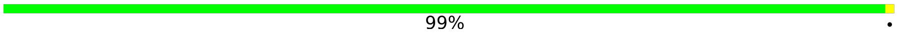
Chain R:

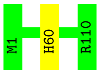


There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L22

Chain S:





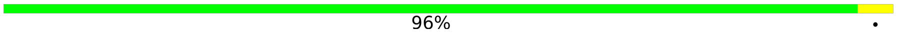
- Molecule 28: 50S ribosomal protein L23

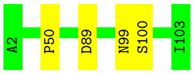
Chain T:

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L24

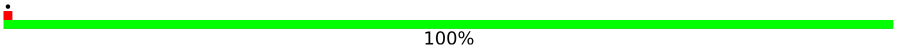
Chain U:

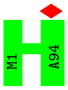




- Molecule 30: 50S ribosomal protein L25

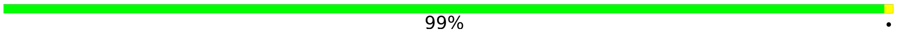
Chain V:

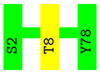




- Molecule 31: 50S ribosomal protein L28

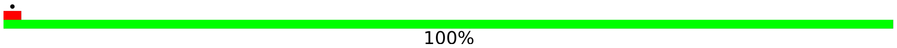
Chain X:

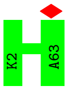




- Molecule 32: 50S ribosomal protein L29

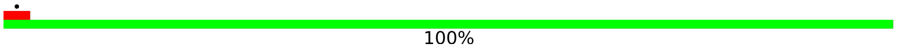
Chain Y:

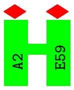




- Molecule 33: 50S ribosomal protein L30

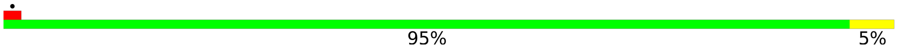
Chain Z:

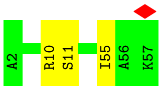




- Molecule 34: 50S ribosomal protein L32

Chain b:





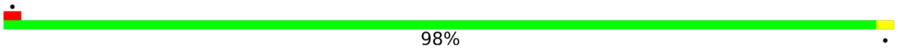
- Molecule 35: 50S ribosomal protein L33

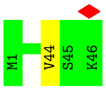
Chain c:

There are no outlier residues recorded for this chain.

- Molecule 36: 50S ribosomal protein L34

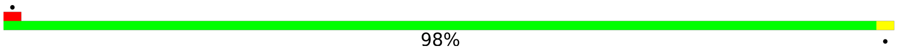
Chain d:

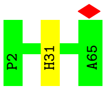




- Molecule 37: 50S ribosomal protein L35

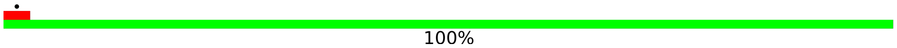
Chain e:

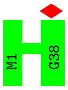




- Molecule 38: 50S ribosomal protein L36

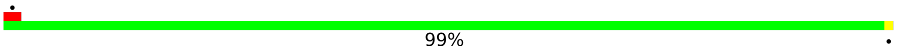
Chain f:

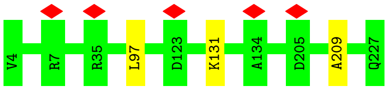




- Molecule 39: 30S ribosomal protein S2

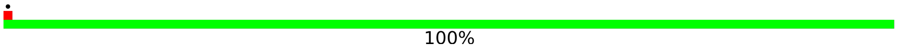
Chain g:

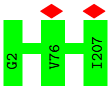




- Molecule 40: 30S ribosomal protein S3

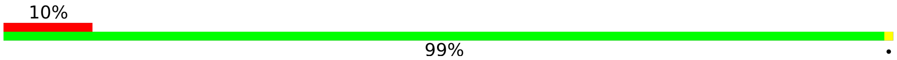
Chain h:

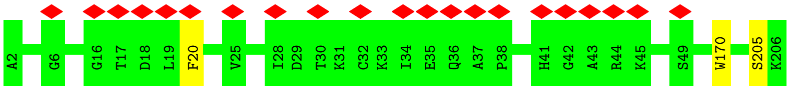




- Molecule 41: 30S ribosomal protein S4

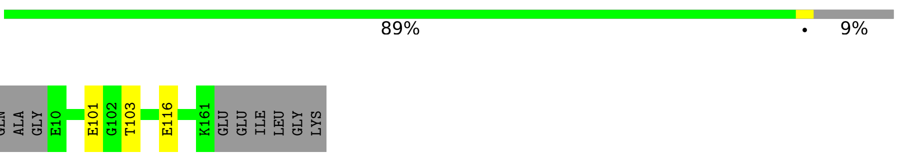
Chain i:





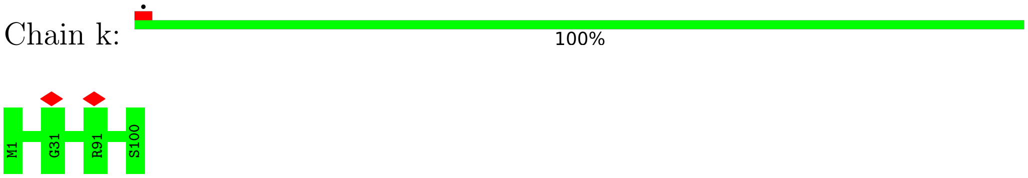
- Molecule 42: 30S ribosomal protein S5

Chain j:



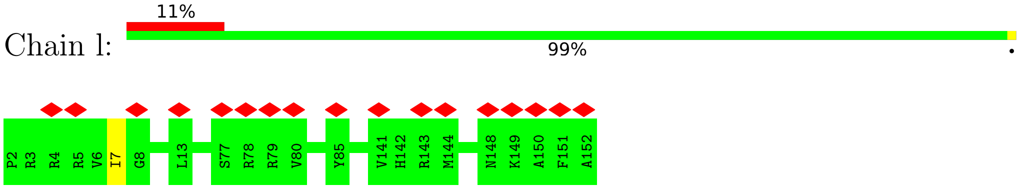
- Molecule 43: 30S ribosomal protein S6

Chain k:



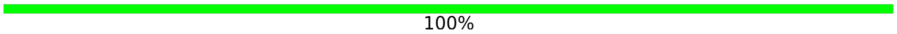
- Molecule 44: 30S ribosomal protein S7

Chain l:



- Molecule 45: 30S ribosomal protein S8

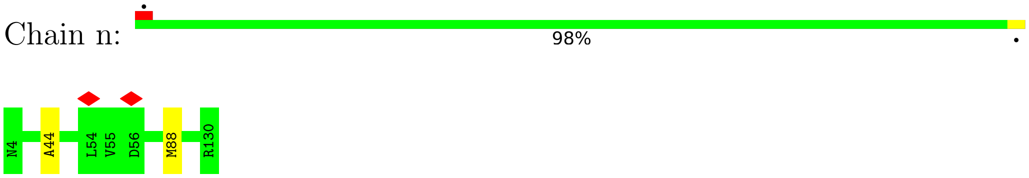
Chain m:



There are no outlier residues recorded for this chain.

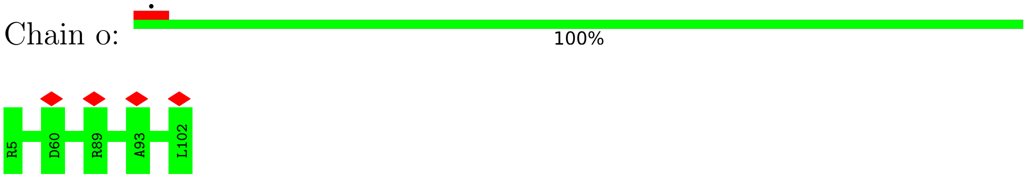
- Molecule 46: 30S ribosomal protein S9

Chain n:



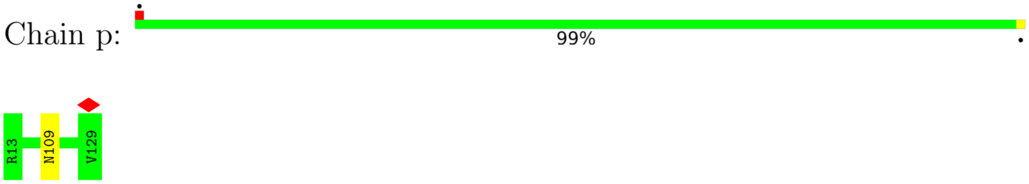
- Molecule 47: 30S ribosomal protein S10

Chain o:



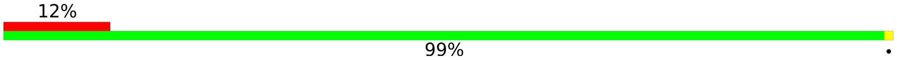
- Molecule 48: 30S ribosomal protein S11

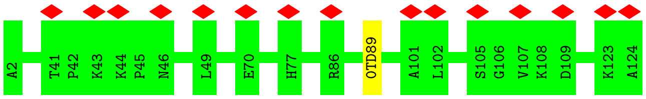
Chain p:



- Molecule 49: 30S ribosomal protein S12

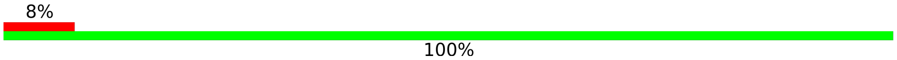
Chain q:

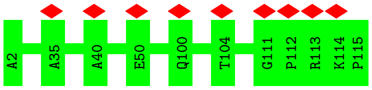




- Molecule 50: 30S ribosomal protein S13

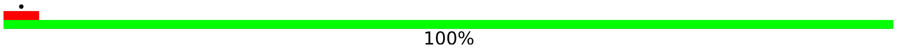
Chain r:

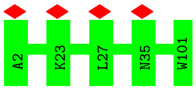




- Molecule 51: 30S ribosomal protein S14

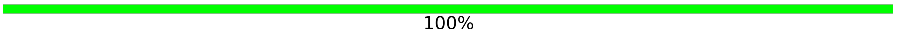
Chain s:





- Molecule 52: 30S ribosomal protein S15

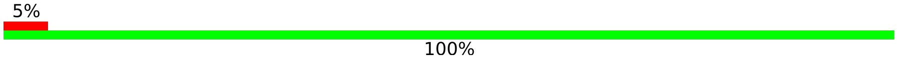
Chain t:

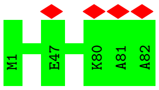


There are no outlier residues recorded for this chain.

- Molecule 53: 30S ribosomal protein S16

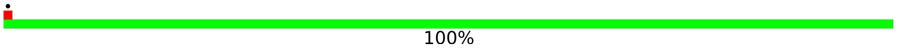
Chain u:

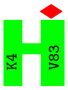




- Molecule 54: 30S ribosomal protein S17

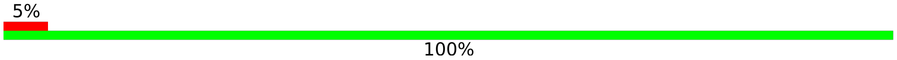
Chain v:

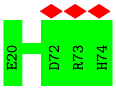




- Molecule 55: 30S ribosomal protein S18

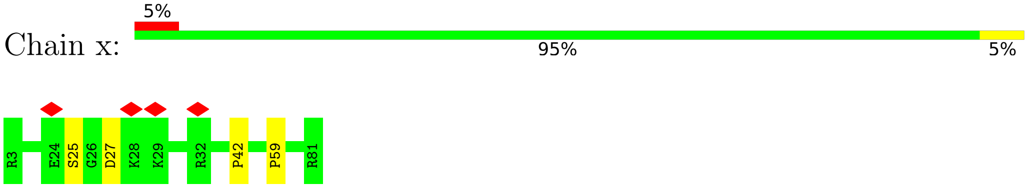
Chain w:





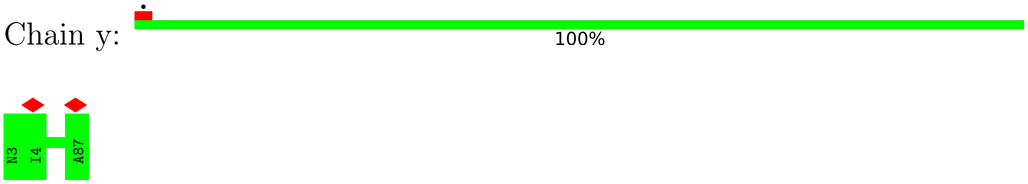
- Molecule 56: 30S ribosomal protein S19

Chain x:



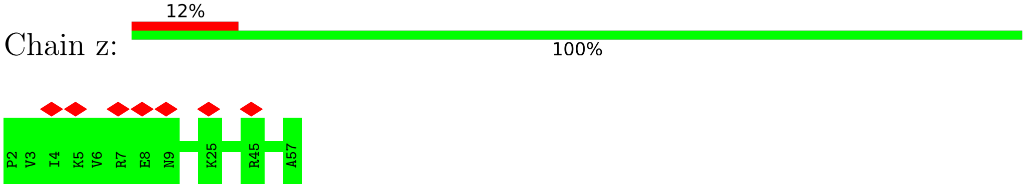
- Molecule 57: 30S ribosomal protein S20

Chain y:



- Molecule 58: 30S ribosomal protein S21

Chain z:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18452	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	35	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	19.820	Depositor
Minimum map value	-6.531	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	446.784, 446.784, 446.784	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	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: KIR, ZN, 2MG, MG, 4D4, 5MC, MA6, G7M, MIA, UR3, 3TD, OMU, 4SU, 6MZ, OMC, 2MA, 4OC, OMG, PSU, 5MU, GDP, 3AU, 0TD, 1MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	1	0.18	1/69307 (0.0%)	0.78	42/108118 (0.0%)
2	2	0.19	0/36722	0.78	20/57280 (0.0%)
3	3	0.15	0/2828	0.74	0/4410
4	4	0.22	1/8616 (0.0%)	0.81	19/13430 (0.1%)
5	5	0.33	1/1203 (0.1%)	0.61	1/1616 (0.1%)
6	6	0.34	2/2924 (0.1%)	0.59	2/3955 (0.1%)
7	7	1.10	14/1624 (0.9%)	1.01	11/2527 (0.4%)
8	8	0.25	0/366	0.95	1/570 (0.2%)
9	A	0.24	0/608	0.42	0/804
10	B	0.23	0/2121	0.46	0/2852
11	C	0.24	0/1586	0.45	0/2134
12	D	0.23	0/1571	0.44	1/2113 (0.0%)
13	E	0.30	0/1434	0.60	1/1926 (0.1%)
14	F	0.26	0/1342	0.59	1/1816 (0.1%)
15	G	0.42	2/1122 (0.2%)	0.61	1/1515 (0.1%)
16	H	0.25	0/993	0.51	0/1340
17	I	0.25	0/471	0.53	0/627
18	J	0.46	1/1152 (0.1%)	0.52	2/1551 (0.1%)
19	K	0.27	0/947	0.56	1/1268 (0.1%)
20	L	0.24	0/1062	0.49	0/1413
21	M	0.24	0/1081	0.51	2/1443 (0.1%)
22	N	0.23	0/973	0.41	0/1301
23	O	0.23	0/902	0.40	0/1209
24	P	0.24	0/929	0.51	0/1242
25	Q	0.24	0/960	0.41	0/1278
26	R	0.27	0/829	0.50	0/1107
27	S	0.24	0/864	0.49	1/1156 (0.1%)
28	T	0.22	0/745	0.42	0/994
29	U	0.48	1/788 (0.1%)	0.65	3/1051 (0.3%)
30	V	0.23	0/766	0.41	0/1025
31	X	0.26	0/635	0.52	1/848 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Y	0.22	0/502	0.36	0/667
33	Z	0.22	0/453	0.47	0/605
34	b	0.58	2/450 (0.4%)	0.69	0/599
35	c	0.23	0/416	0.47	0/554
36	d	0.23	0/380	0.41	0/498
37	e	0.32	0/513	0.60	1/676 (0.1%)
38	f	0.22	0/303	0.41	0/397
39	g	0.26	0/1784	0.58	3/2403 (0.1%)
40	h	0.23	0/1652	0.45	0/2225
41	i	0.27	0/1665	0.62	3/2227 (0.1%)
42	j	0.29	0/1131	0.60	1/1520 (0.1%)
43	k	0.23	0/835	0.49	0/1128
44	l	0.25	0/1196	0.53	0/1602
45	m	0.23	0/989	0.44	0/1326
46	n	0.25	0/1034	0.64	2/1375 (0.1%)
47	o	0.25	0/797	0.53	0/1077
48	p	0.24	0/892	0.50	1/1205 (0.1%)
49	q	0.23	0/959	0.49	0/1286
50	r	0.24	0/892	0.54	0/1193
51	s	0.22	0/817	0.38	0/1088
52	t	0.22	0/722	0.44	0/964
53	u	0.23	0/659	0.44	0/884
54	v	0.24	0/658	0.57	0/881
55	w	0.22	0/463	0.38	0/621
56	x	0.71	2/653 (0.3%)	0.74	2/877 (0.2%)
57	y	0.23	0/671	0.40	0/888
58	z	0.23	0/473	0.36	0/627
All	All	0.24	27/169430 (0.0%)	0.72	123/253312 (0.0%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	20	U	C5-C6	17.59	1.50	1.34
7	7	16	U	C5-C6	17.51	1.50	1.34
7	7	20	U	C2-N3	15.76	1.48	1.37
7	7	16	U	C2-N3	15.68	1.48	1.37
56	x	59	PRO	N-CD	14.86	1.68	1.47

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2195	U	O5'-P-OP2	-29.62	75.16	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2195	U	OP1-P-OP2	-27.22	78.78	119.60
1	1	2195	U	O5'-P-OP1	17.37	131.55	110.70
1	1	2194	U	OP2-P-O3'	13.99	135.97	105.20
1	1	2194	U	OP1-P-O3'	-13.66	75.15	105.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
5	5	144/146 (99%)	127 (88%)	17 (12%)	0	100	100
6	6	367/394 (93%)	343 (94%)	24 (6%)	0	100	100
9	A	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
10	B	269/271 (99%)	257 (96%)	12 (4%)	0	100	100
11	C	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
12	D	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
13	E	175/177 (99%)	149 (85%)	23 (13%)	3 (2%)	9	40
14	F	174/176 (99%)	161 (92%)	11 (6%)	2 (1%)	14	50
15	G	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
16	H	128/130 (98%)	105 (82%)	23 (18%)	0	100	100
17	I	64/142 (45%)	55 (86%)	8 (12%)	1 (2%)	9	42
18	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	K	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
20	L	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
21	M	133/136 (98%)	127 (96%)	5 (4%)	1 (1%)	19	57
22	N	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
23	O	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
24	P	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
25	Q	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
26	R	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
27	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
28	T	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
29	U	100/102 (98%)	88 (88%)	10 (10%)	2 (2%)	7	36
30	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
31	X	75/77 (97%)	75 (100%)	0	0	100	100
32	Y	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
33	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
34	b	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	3	21
35	c	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
36	d	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	6	33
37	e	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
38	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
39	g	222/224 (99%)	201 (90%)	20 (9%)	1 (0%)	29	66
40	h	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
41	i	203/205 (99%)	185 (91%)	17 (8%)	1 (0%)	29	66
42	j	150/167 (90%)	129 (86%)	20 (13%)	1 (1%)	22	60
43	k	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
44	l	149/151 (99%)	143 (96%)	5 (3%)	1 (1%)	22	60
45	m	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
46	n	125/127 (98%)	114 (91%)	11 (9%)	0	100	100
47	o	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
48	p	115/117 (98%)	98 (85%)	17 (15%)	0	100	100
49	q	120/123 (98%)	114 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	r	112/114 (98%)	100 (89%)	12 (11%)	0	100	100
51	s	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
52	t	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
53	u	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
54	v	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
55	w	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
56	x	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
57	y	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
58	z	54/56 (96%)	54 (100%)	0	0	100	100
All	All	6203/6425 (96%)	5787 (93%)	400 (6%)	16 (0%)	44	74

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	F	42	GLU
42	j	103	THR
21	M	60	GLN
29	U	99	ASN
34	b	11	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	5	122/122 (100%)	122 (100%)	0	100	100
6	6	310/327 (95%)	310 (100%)	0	100	100
9	A	59/59 (100%)	59 (100%)	0	100	100
10	B	216/216 (100%)	216 (100%)	0	100	100
11	C	164/164 (100%)	164 (100%)	0	100	100
12	D	165/165 (100%)	165 (100%)	0	100	100
13	E	148/148 (100%)	144 (97%)	4 (3%)	44	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	F	137/137 (100%)	136 (99%)	1 (1%)	84	93
15	G	114/114 (100%)	113 (99%)	1 (1%)	78	90
16	H	99/99 (100%)	99 (100%)	0	100	100
17	I	48/110 (44%)	48 (100%)	0	100	100
18	J	116/116 (100%)	116 (100%)	0	100	100
19	K	103/103 (100%)	103 (100%)	0	100	100
20	L	103/103 (100%)	103 (100%)	0	100	100
21	M	108/108 (100%)	108 (100%)	0	100	100
22	N	100/100 (100%)	100 (100%)	0	100	100
23	O	86/86 (100%)	86 (100%)	0	100	100
24	P	99/99 (100%)	99 (100%)	0	100	100
25	Q	89/89 (100%)	89 (100%)	0	100	100
26	R	84/84 (100%)	84 (100%)	0	100	100
27	S	93/93 (100%)	93 (100%)	0	100	100
28	T	80/80 (100%)	80 (100%)	0	100	100
29	U	83/83 (100%)	83 (100%)	0	100	100
30	V	78/78 (100%)	78 (100%)	0	100	100
31	X	67/67 (100%)	67 (100%)	0	100	100
32	Y	54/54 (100%)	54 (100%)	0	100	100
33	Z	48/48 (100%)	48 (100%)	0	100	100
34	b	47/47 (100%)	47 (100%)	0	100	100
35	c	45/45 (100%)	45 (100%)	0	100	100
36	d	38/38 (100%)	38 (100%)	0	100	100
37	e	51/51 (100%)	51 (100%)	0	100	100
38	f	34/34 (100%)	34 (100%)	0	100	100
39	g	186/186 (100%)	186 (100%)	0	100	100
40	h	170/170 (100%)	170 (100%)	0	100	100
41	i	172/172 (100%)	172 (100%)	0	100	100
42	j	114/126 (90%)	113 (99%)	1 (1%)	78	90
43	k	87/87 (100%)	87 (100%)	0	100	100
44	l	124/124 (100%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	m	104/104 (100%)	104 (100%)	0	100	100
46	n	105/105 (100%)	105 (100%)	0	100	100
47	o	86/86 (100%)	86 (100%)	0	100	100
48	p	90/90 (100%)	90 (100%)	0	100	100
49	q	102/102 (100%)	102 (100%)	0	100	100
50	r	92/92 (100%)	92 (100%)	0	100	100
51	s	83/83 (100%)	83 (100%)	0	100	100
52	t	76/76 (100%)	76 (100%)	0	100	100
53	u	65/65 (100%)	65 (100%)	0	100	100
54	v	74/74 (100%)	74 (100%)	0	100	100
55	w	48/48 (100%)	48 (100%)	0	100	100
56	x	70/70 (100%)	68 (97%)	2 (3%)	42	72
57	y	65/65 (100%)	65 (100%)	0	100	100
58	z	48/48 (100%)	48 (100%)	0	100	100
All	All	5149/5240 (98%)	5140 (100%)	9 (0%)	93	97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	x	25	SER
56	x	27	ASP
13	E	153	ASP
14	F	41	VAL
15	G	130	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
43	k	3	HIS
47	o	58	ASN
45	m	18	GLN
48	p	101	ASN
24	P	56	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2899/2904 (99%)	559 (19%)	24 (0%)
2	2	1536/1540 (99%)	335 (21%)	14 (0%)
3	3	117/118 (99%)	22 (18%)	3 (2%)
4	4	362/363 (99%)	175 (48%)	10 (2%)
7	7	73/76 (96%)	13 (17%)	3 (4%)
8	8	14/15 (93%)	10 (71%)	1 (7%)
All	All	5001/5016 (99%)	1114 (22%)	55 (1%)

5 of 1114 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	G
1	1	10	A
1	1	15	G
1	1	27	G
1	1	28	A

5 of 55 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	391	G
2	2	1346	A
8	8	14	U
4	4	334	A
2	2	429	U

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

46 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	$\#\|Z\| > 2$
1	5MU	1	1939	1	19,22,23	5.27	5 (26%)	28,32,35	3.60	9 (32%)
1	2MG	1	1835	1	18,26,27	2.73	6 (33%)	16,38,41	1.47	3 (18%)
2	4OC	2	1402	2	20,23,24	3.21	8 (40%)	26,32,35	0.88	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	4D4	M	81	21	9,11,12	2.03	2 (22%)	8,13,15	1.86	3 (37%)
2	5MC	2	967	2	18,22,23	3.75	7 (38%)	26,32,35	0.98	1 (3%)
1	3TD	1	1915	1	18,22,23	4.22	6 (33%)	22,32,35	1.65	3 (13%)
2	UR3	2	1498	2	19,22,23	3.01	8 (42%)	26,32,35	1.29	2 (7%)
2	2MG	2	1516	2	18,26,27	2.72	6 (33%)	16,38,41	1.42	4 (25%)
1	6MZ	1	1618	1	18,25,26	2.00	3 (16%)	16,36,39	2.08	4 (25%)
7	3AU	7	47	7	24,28,29	2.40	8 (33%)	33,40,43	1.23	2 (6%)
2	MA6	2	1518	2	18,26,27	1.45	3 (16%)	19,38,41	4.25	3 (15%)
2	5MC	2	1407	2	18,22,23	3.76	7 (38%)	26,32,35	0.99	2 (7%)
49	0TD	q	89	49	7,9,10	1.47	0	6,11,13	2.02	2 (33%)
1	PSU	1	2605	1	18,21,22	1.11	1 (5%)	22,30,33	1.75	4 (18%)
1	6MZ	1	2030	1	18,25,26	1.99	3 (16%)	16,36,39	2.18	4 (25%)
1	OMG	1	2251	7,1	18,26,27	2.90	7 (38%)	19,38,41	1.50	4 (21%)
7	4SU	7	8	7	18,21,22	3.83	7 (38%)	26,30,33	2.23	4 (15%)
7	MIA	7	37	7	24,31,32	2.49	3 (12%)	26,44,47	3.52	8 (30%)
1	OMC	1	2498	1,59	19,22,23	3.40	8 (42%)	26,31,34	0.75	0
1	5MU	1	747	1	19,22,23	5.26	5 (26%)	28,32,35	3.60	9 (32%)
1	2MA	1	2503	1,59	17,25,26	2.56	5 (29%)	17,37,40	1.36	2 (11%)
1	PSU	1	746	1,59	18,21,22	1.07	1 (5%)	22,30,33	1.71	5 (22%)
1	PSU	1	2457	1	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
2	MA6	2	1519	2	18,26,27	1.46	3 (16%)	19,38,41	4.25	3 (15%)
4	PSU	4	342	4	18,21,22	1.12	1 (5%)	22,30,33	1.76	4 (18%)
1	1MG	1	745	1	18,26,27	2.59	5 (27%)	19,39,42	1.42	3 (15%)
7	PSU	7	55	7	18,21,22	1.10	1 (5%)	22,30,33	1.74	4 (18%)
2	G7M	2	527	2	20,26,27	2.49	7 (35%)	17,39,42	1.14	1 (5%)
7	5MU	7	54	7	19,22,23	5.19	5 (26%)	28,32,35	3.51	9 (32%)
1	PSU	1	2504	1	18,21,22	1.09	1 (5%)	22,30,33	1.76	4 (18%)
1	PSU	1	1917	1	18,21,22	1.14	2 (11%)	22,30,33	1.84	5 (22%)
1	PSU	1	955	1	18,21,22	1.10	1 (5%)	22,30,33	1.74	4 (18%)
2	PSU	2	516	2	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)
2	2MG	2	966	2	18,26,27	2.73	6 (33%)	16,38,41	1.47	3 (18%)
1	2MG	1	2445	1	18,26,27	2.68	6 (33%)	16,38,41	1.41	3 (18%)
4	5MU	4	341	4	19,22,23	5.27	5 (26%)	28,32,35	3.52	9 (32%)
1	PSU	1	1911	1	18,21,22	1.08	1 (5%)	22,30,33	1.76	4 (18%)
2	2MG	2	1207	2	18,26,27	2.74	6 (33%)	16,38,41	1.43	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	G7M	1	2069	1	20,26,27	2.47	7 (35%)	17,39,42	1.14	1 (5%)
7	PSU	7	39	7	18,21,22	1.10	1 (5%)	22,30,33	1.73	4 (18%)
7	G7M	7	46	7	20,26,27	4.49	9 (45%)	17,39,42	1.04	1 (5%)
7	PSU	7	32	7	18,21,22	1.10	1 (5%)	22,30,33	1.69	5 (22%)
1	5MC	1	1962	1	18,22,23	3.74	7 (38%)	26,32,35	1.04	2 (7%)
4	PSU	4	347	4	18,21,22	1.10	1 (5%)	22,30,33	1.82	5 (22%)
1	OMU	1	2552	1	19,22,23	2.99	8 (42%)	26,31,34	1.70	5 (19%)
1	PSU	1	2580	1	18,21,22	1.05	1 (5%)	22,30,33	1.86	5 (22%)

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
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2
1	2MG	1	1835	1	-	0/5/27/28	0/3/3/3
2	4OC	2	1402	2	-	0/9/29/30	0/2/2/2
21	4D4	M	81	21	-	4/11/12/14	-
2	5MC	2	967	2	-	0/7/25/26	0/2/2/2
1	3TD	1	1915	1	-	4/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	2/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	6MZ	1	1618	1	-	2/5/27/28	0/3/3/3
7	3AU	7	47	7	-	1/16/34/35	0/2/2/2
2	MA6	2	1518	2	-	2/7/29/30	0/3/3/3
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
49	0TD	q	89	49	-	5/7/12/14	-
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	6MZ	1	2030	1	-	4/5/27/28	0/3/3/3
1	OMG	1	2251	7,1	-	3/5/27/28	0/3/3/3
7	4SU	7	8	7	-	1/7/25/26	0/2/2/2
7	MIA	7	37	7	-	2/11/33/34	0/3/3/3
1	OMC	1	2498	1,59	-	2/9/27/28	0/2/2/2
1	5MU	1	747	1	-	1/7/25/26	0/2/2/2
1	2MA	1	2503	1,59	-	3/3/25/26	0/3/3/3
1	PSU	1	746	1,59	-	2/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MA6	2	1519	2	-	2/7/29/30	0/3/3/3
4	PSU	4	342	4	-	2/7/25/26	0/2/2/2
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
7	PSU	7	55	7	-	0/7/25/26	0/2/2/2
2	G7M	2	527	2	-	2/3/25/26	0/3/3/3
7	5MU	7	54	7	-	0/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
2	PSU	2	516	2	-	0/7/25/26	0/2/2/2
2	2MG	2	966	2	-	2/5/27/28	0/3/3/3
1	2MG	1	2445	1	-	3/5/27/28	0/3/3/3
4	5MU	4	341	4	-	2/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
1	G7M	1	2069	1	-	1/3/25/26	0/3/3/3
7	PSU	7	39	7	-	0/7/25/26	0/2/2/2
7	G7M	7	46	7	-	2/3/25/26	0/3/3/3
7	PSU	7	32	7	-	0/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	0/7/25/26	0/2/2/2
4	PSU	4	347	4	-	0/7/25/26	0/2/2/2
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
1	PSU	1	2580	1	-	0/7/25/26	0/2/2/2

The worst 5 of 196 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	341	5MU	C6-N1	12.75	1.59	1.38
1	1	1939	5MU	C6-N1	12.71	1.59	1.38
1	1	747	5MU	C6-N1	12.70	1.59	1.38
7	7	54	5MU	C6-N1	12.64	1.59	1.38
1	1	1915	3TD	C6-C5	12.36	1.49	1.35

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1519	MA6	N1-C6-N6	-15.63	100.61	117.06
2	2	1518	MA6	N1-C6-N6	-15.48	100.76	117.06
1	1	747	5MU	C5-C4-N3	11.99	125.55	115.31
1	1	1939	5MU	C5-C4-N3	11.99	125.55	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	7	54	5MU	C5-C4-N3	11.83	125.41	115.31

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	M	81	4D4	C-CA-CB-OB
21	M	81	4D4	C-CA-CB-CG
21	M	81	4D4	N-CA-CB-OB
21	M	81	4D4	N-CA-CB-CG
49	q	89	0TD	CG-CB-SB-CSB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 195 ligands modelled in this entry, 193 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	$\#\|Z\| > 2$
61	GDP	6	402	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
60	KIR	6	401	-	56,59,59	1.08	4 (7%)	62,84,84	1.09	4 (6%)

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
61	GDP	6	402	-	-	1/12/32/32	0/3/3/3
60	KIR	6	401	-	-	22/54/98/98	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	6	401	KIR	C37-C36	-4.13	1.32	1.44
60	6	401	KIR	C23-C22	-3.55	1.32	1.43
60	6	401	KIR	C2-N1	3.39	1.38	1.33
61	6	402	GDP	C6-N1	-2.43	1.34	1.37
60	6	401	KIR	C8-C7	-2.26	1.42	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	6	401	KIR	C11-C10-C9	3.73	131.10	123.47
61	6	402	GDP	PA-O3A-PB	-3.49	120.84	132.83
60	6	401	KIR	C20-C21-C22	3.44	122.41	119.13
61	6	402	GDP	C3'-C2'-C1'	3.11	105.66	100.98
60	6	401	KIR	C6-N1-C2	2.96	123.52	116.43

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

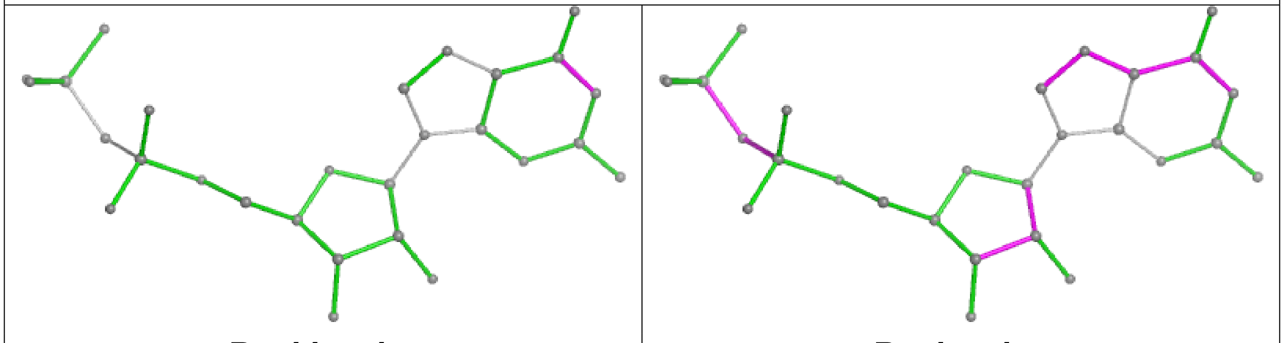
Mol	Chain	Res	Type	Atoms
60	6	401	KIR	C17-C19-C20-O20
60	6	401	KIR	C20-C21-C22-C23
60	6	401	KIR	C44-C21-C22-C23
60	6	401	KIR	C22-C23-C24-C25
60	6	401	KIR	C9-C10-C11-C12

There are no ring outliers.

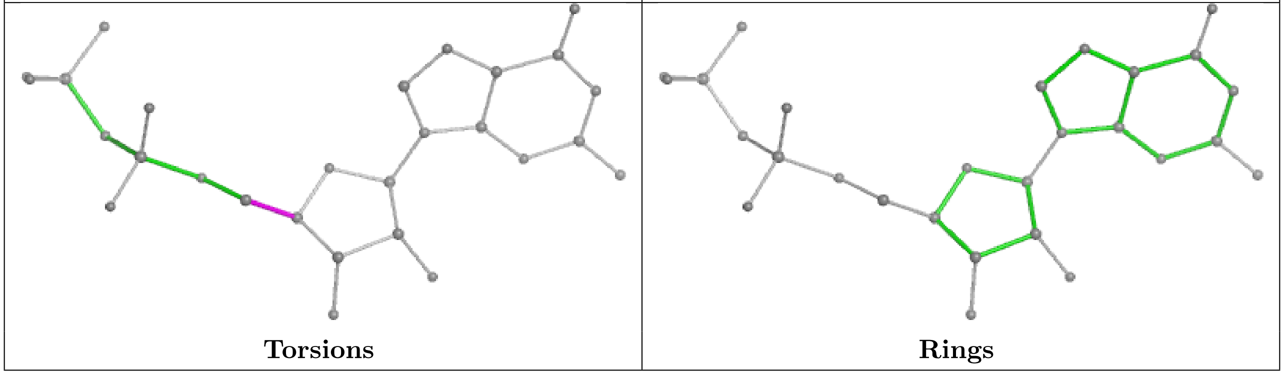
No monomer is involved in short contacts.

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 GDP 6 402

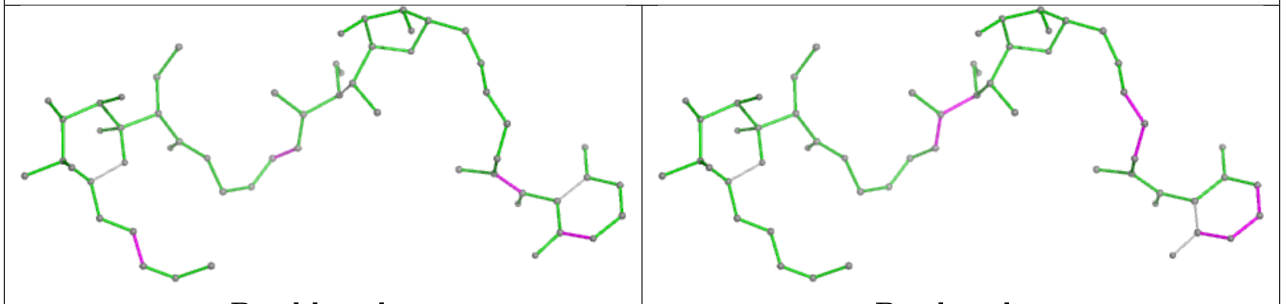


Bond lengths **Bond angles**

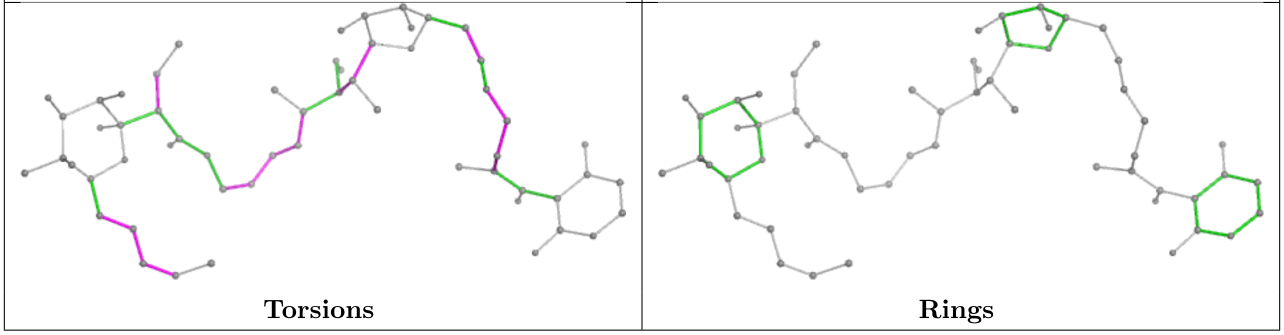


Torsions **Rings**

Ligand KIR 6 401



Bond lengths **Bond angles**



Torsions **Rings**

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

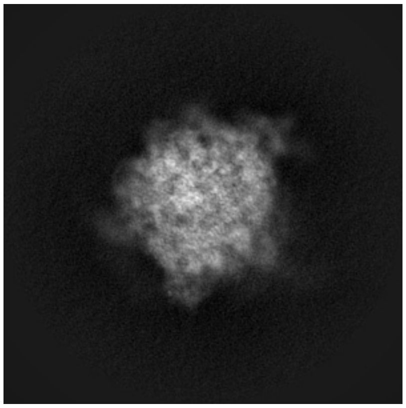
6 Map visualisation

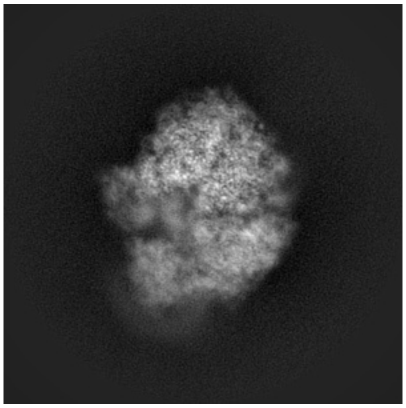
This section contains visualisations of the EMDB entry EMD-11710. These allow visual inspection of the internal detail of the map and identification of artifacts.

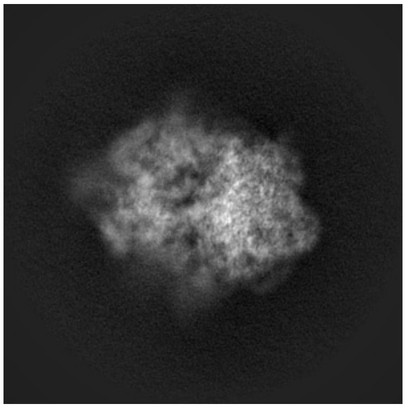
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

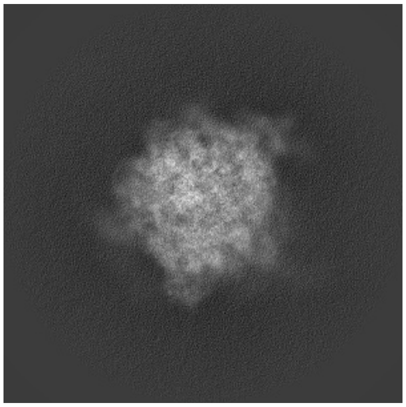
6.1.1 Primary map

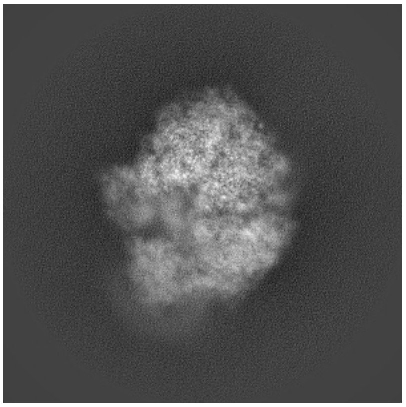

X

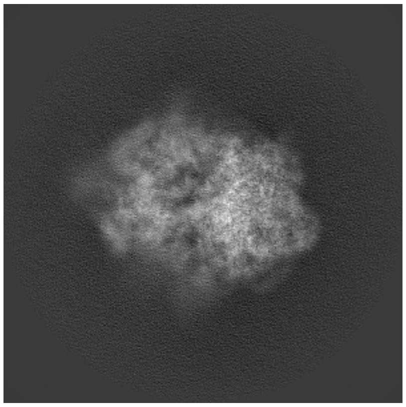

Y


Z

6.1.2 Raw map


X

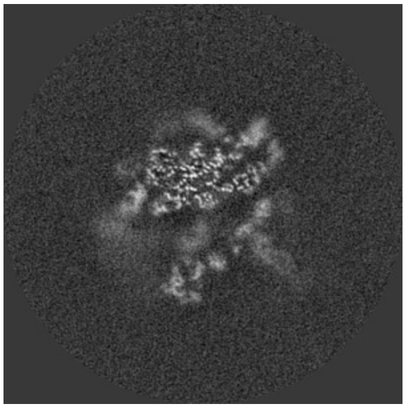

Y

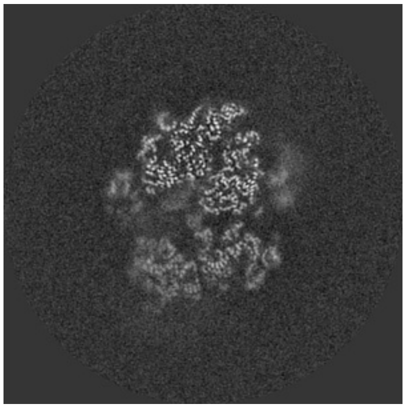

Z

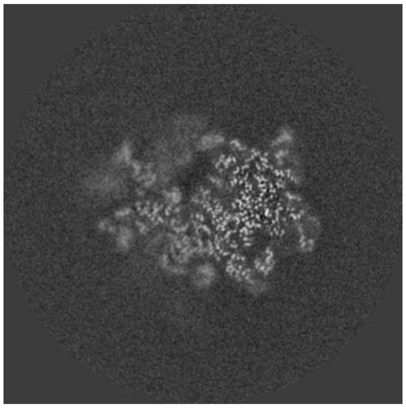
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

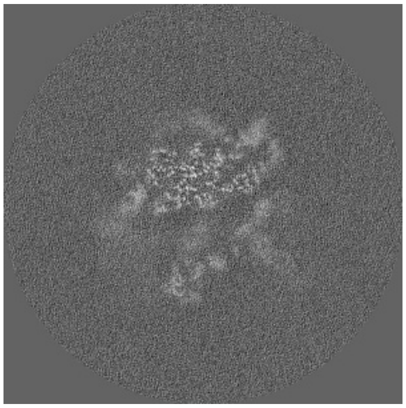
6.2.1 Primary map

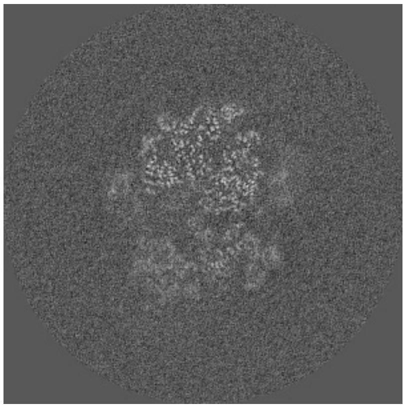

X Index: 208

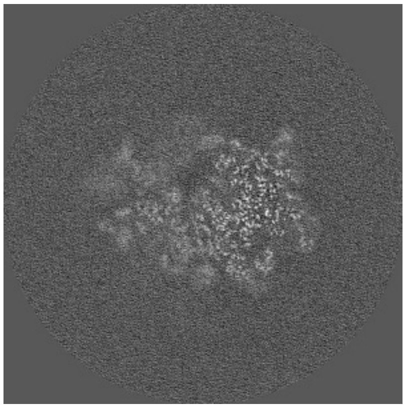

Y Index: 208


Z Index: 208

6.2.2 Raw map


X Index: 208

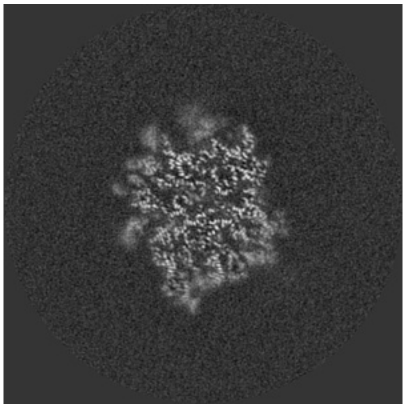

Y Index: 208

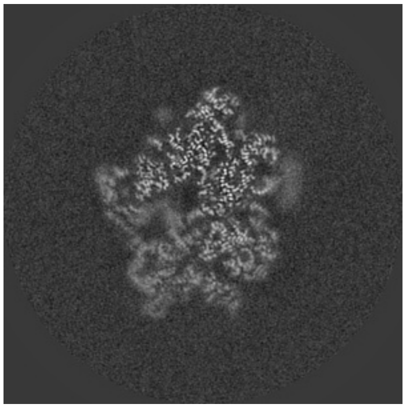

Z Index: 208

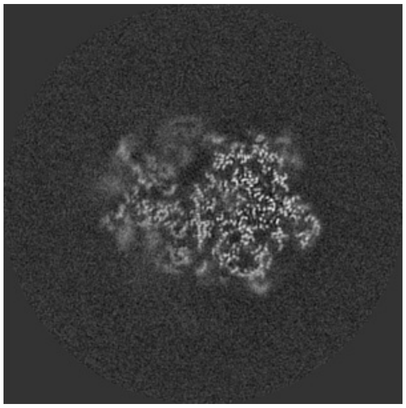
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

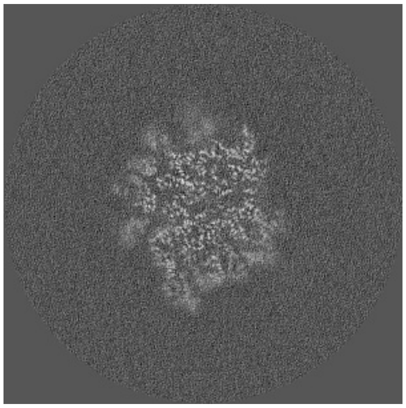
6.3.1 Primary map

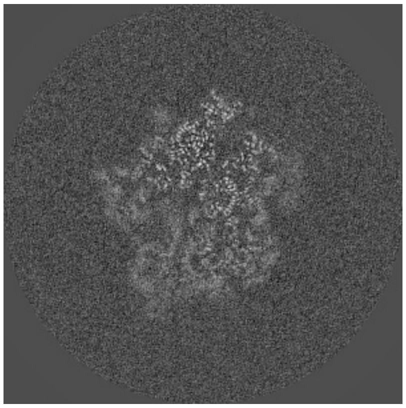

X Index: 236

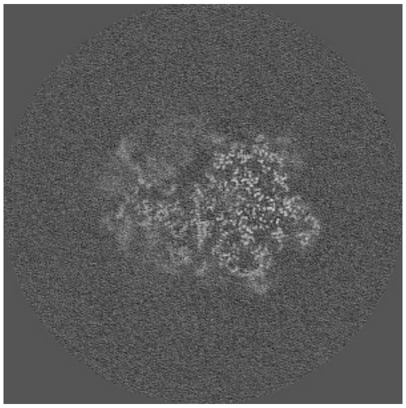

Y Index: 194


Z Index: 213

6.3.2 Raw map


X Index: 235

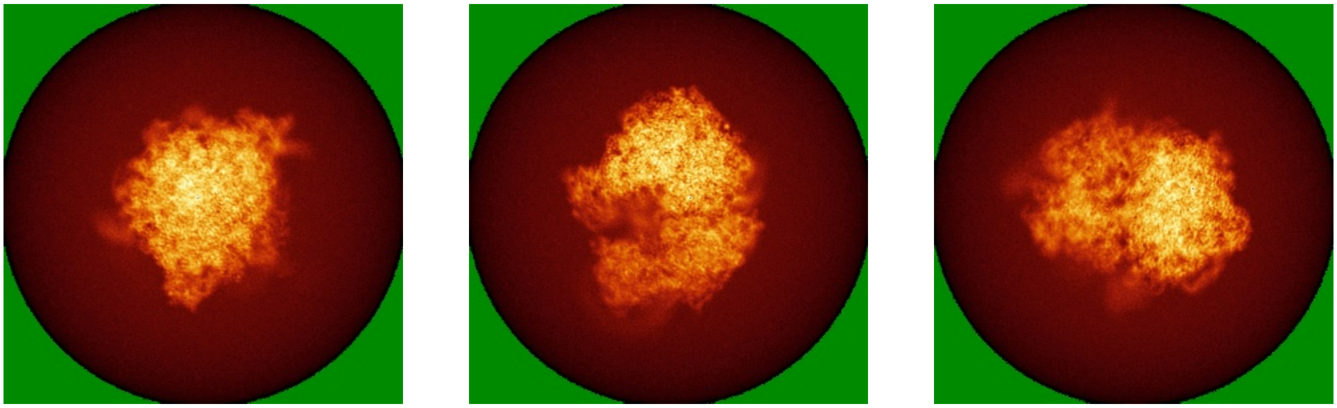

Y Index: 199


Z Index: 213

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

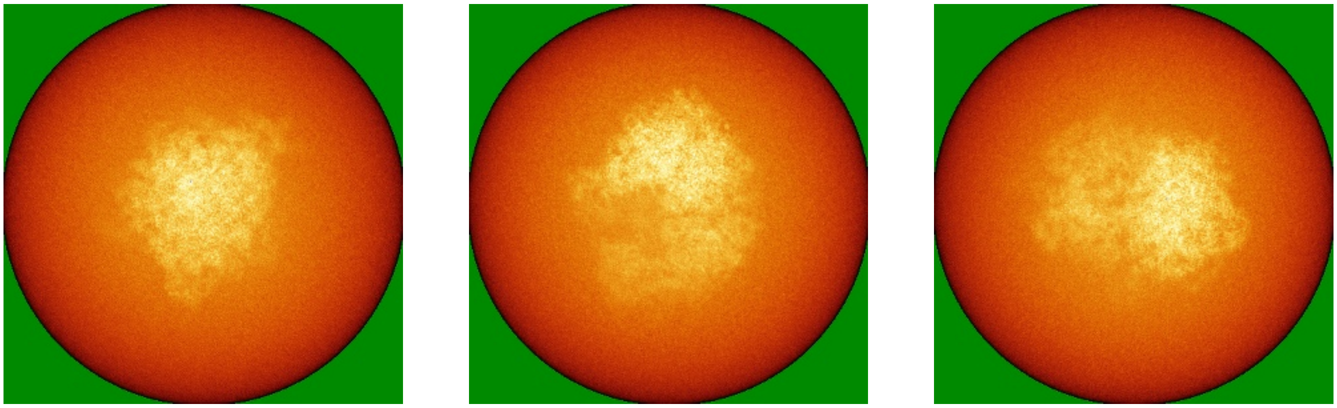
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map

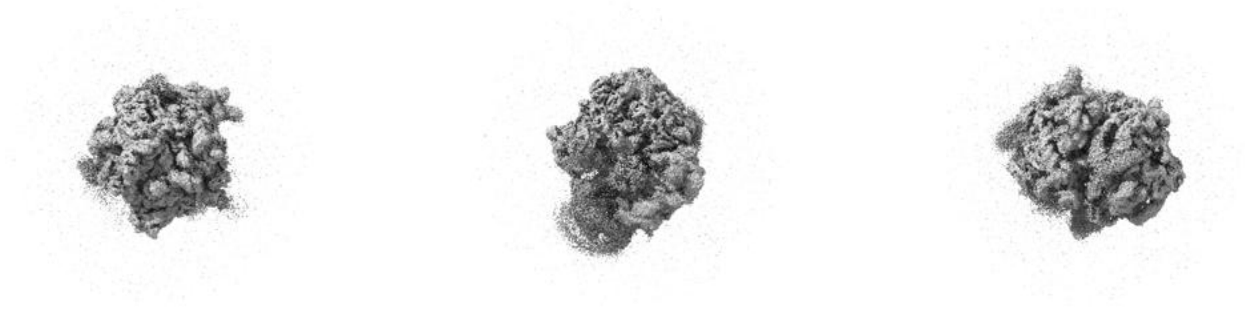


X Y Z

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 ⓘ

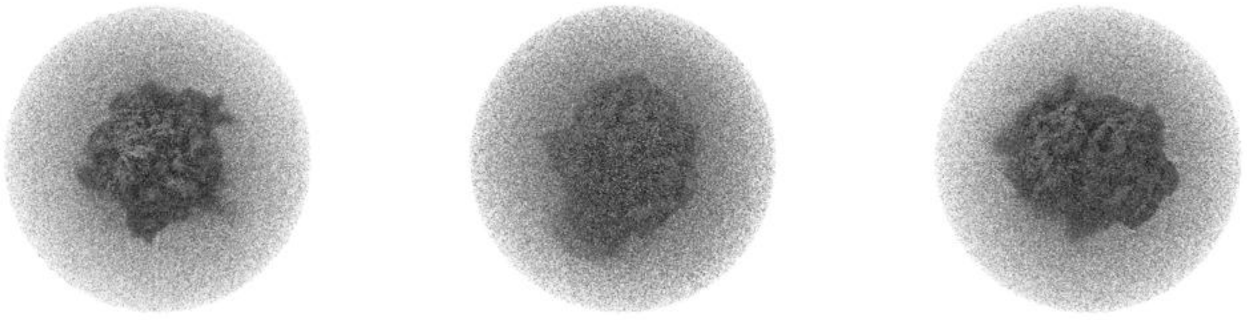
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. 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.

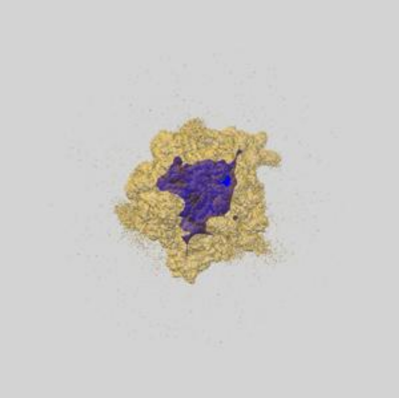
6.6 Mask visualisation ⓘ

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

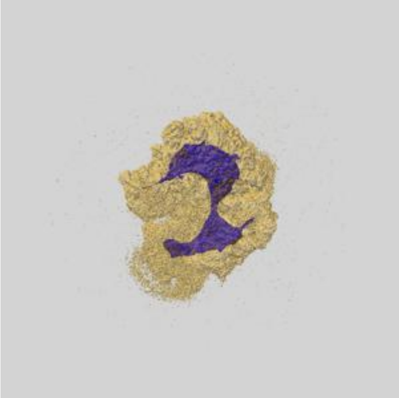
A mask typically either:

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

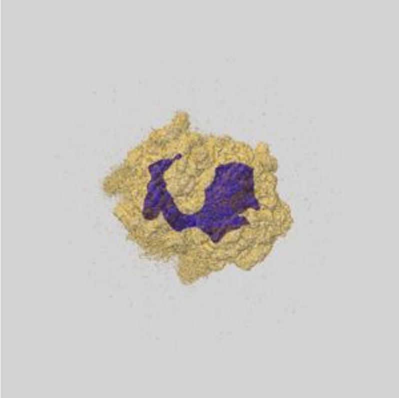
6.6.1 emd_11710_msk_1.map ⓘ



X



Y

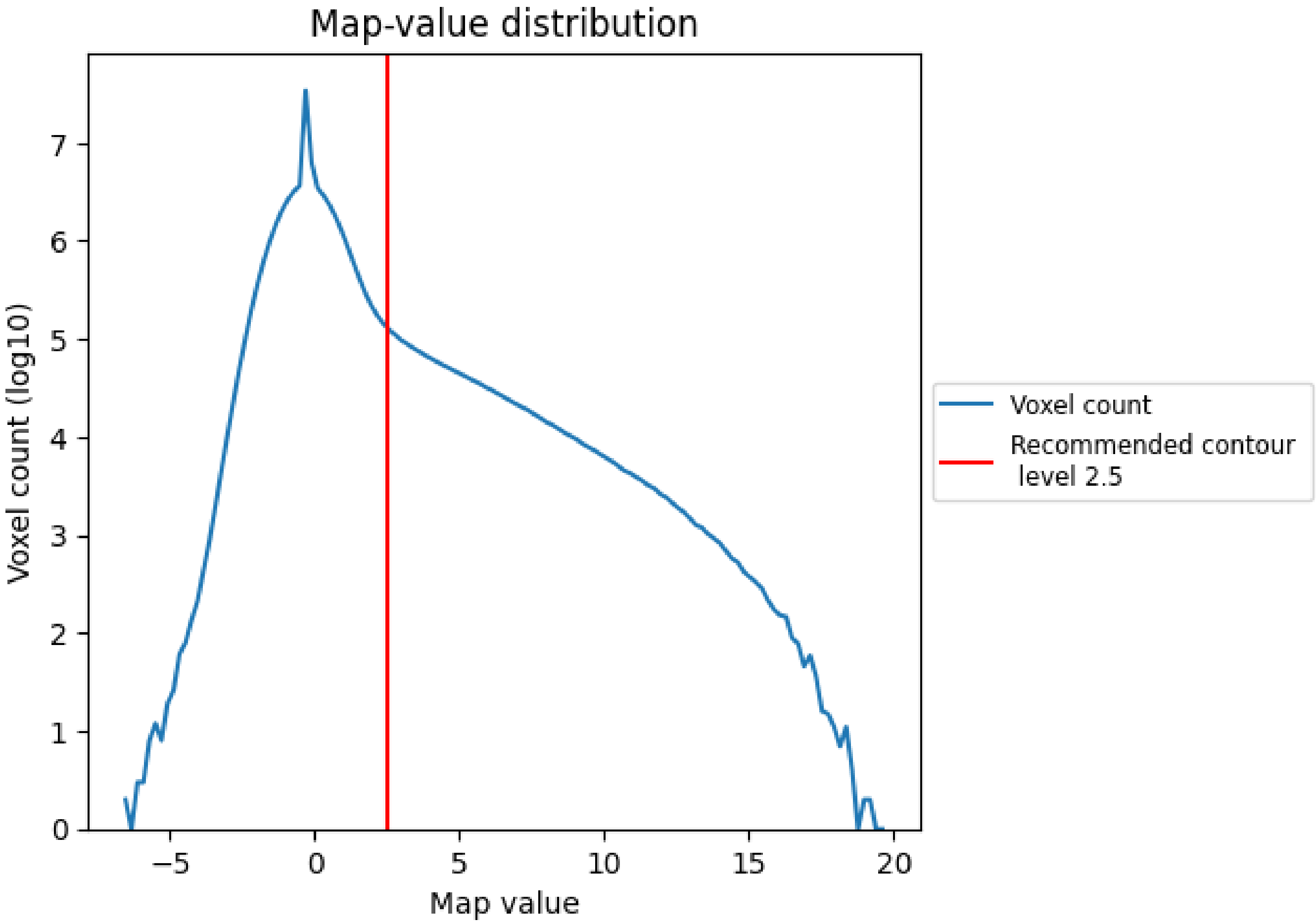


Z

7 Map analysis ⓘ

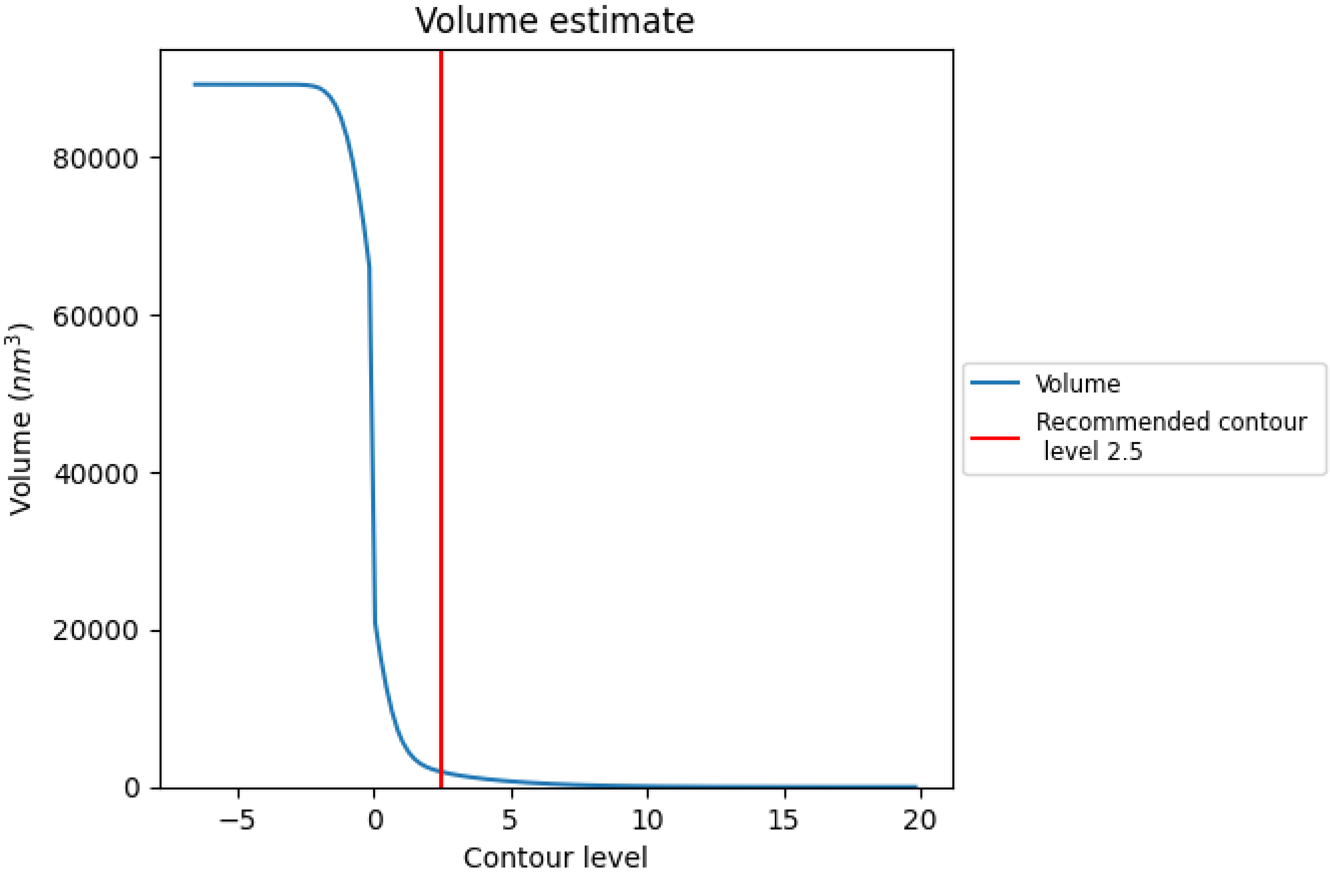
This section contains the results of statistical analysis of the map.

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.

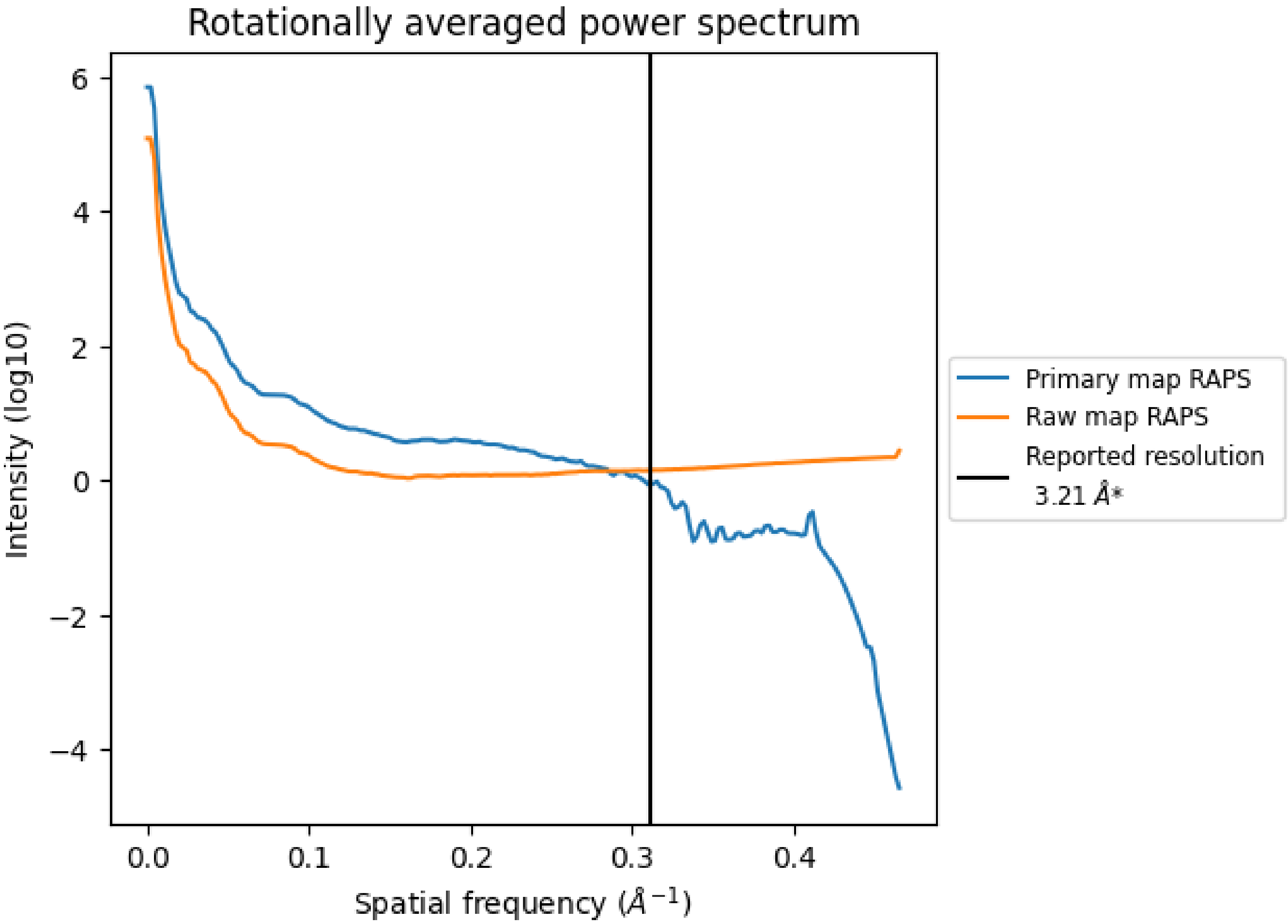
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1895 nm^3; this corresponds to an approximate mass of 1712 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

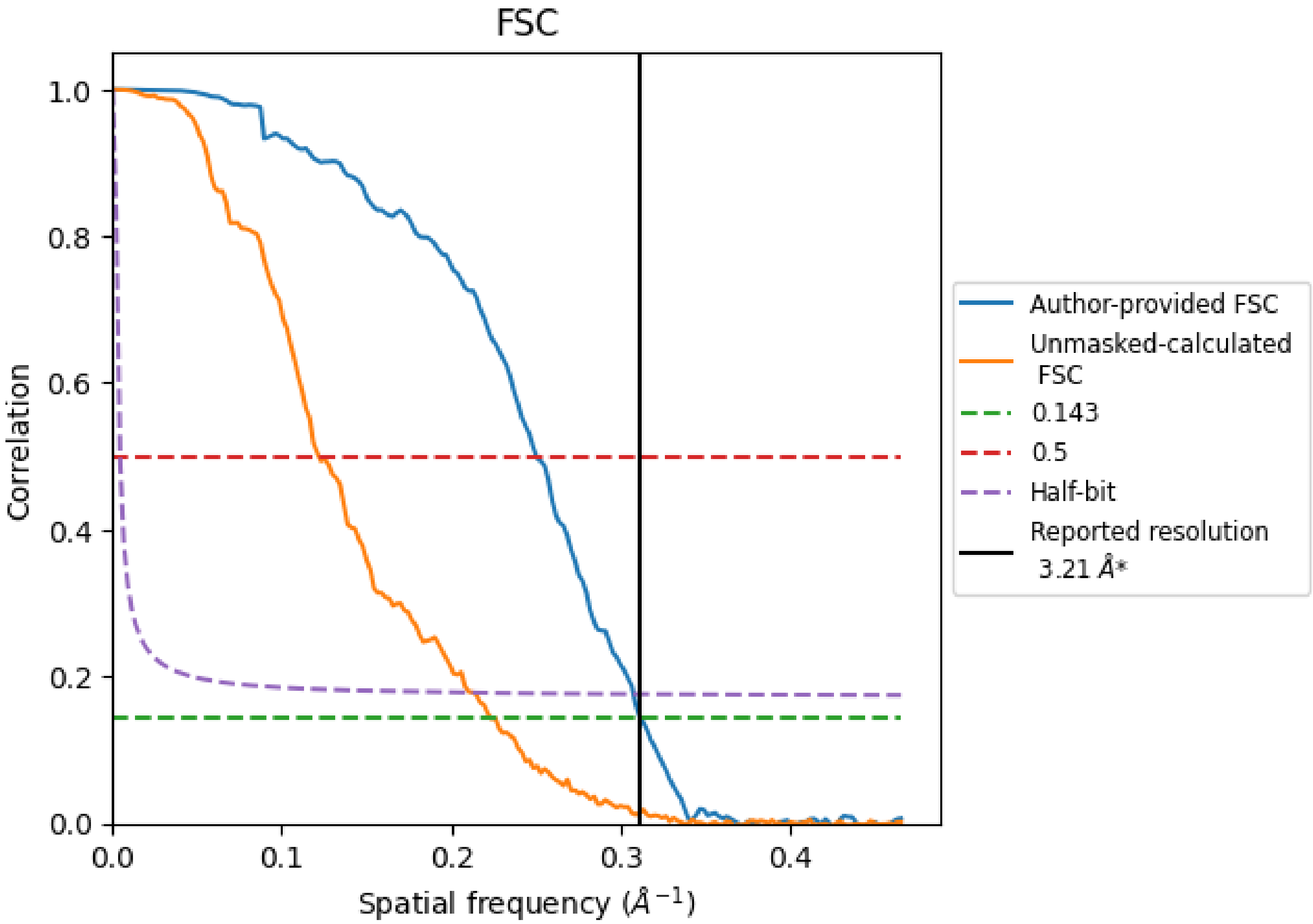


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

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 0.312 Å^{-1}

8.2 Resolution estimates

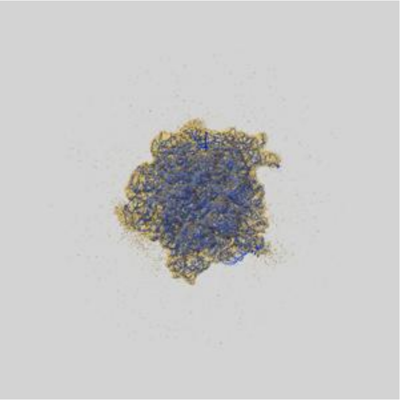
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	4.00	3.25
Unmasked-calculated*	4.47	8.21	4.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.47 differs from the reported value 3.21 by more than 10 %

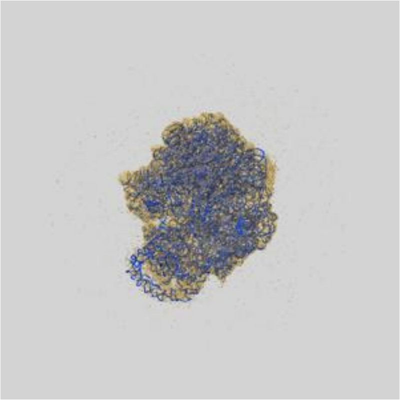
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11710 and PDB model 7ABZ. Per-residue inclusion information can be found in section 3 on page 16.

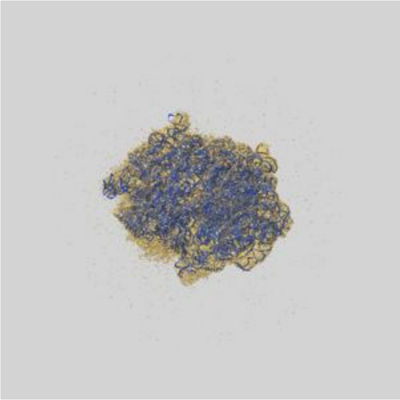
9.1 Map-model overlay



X



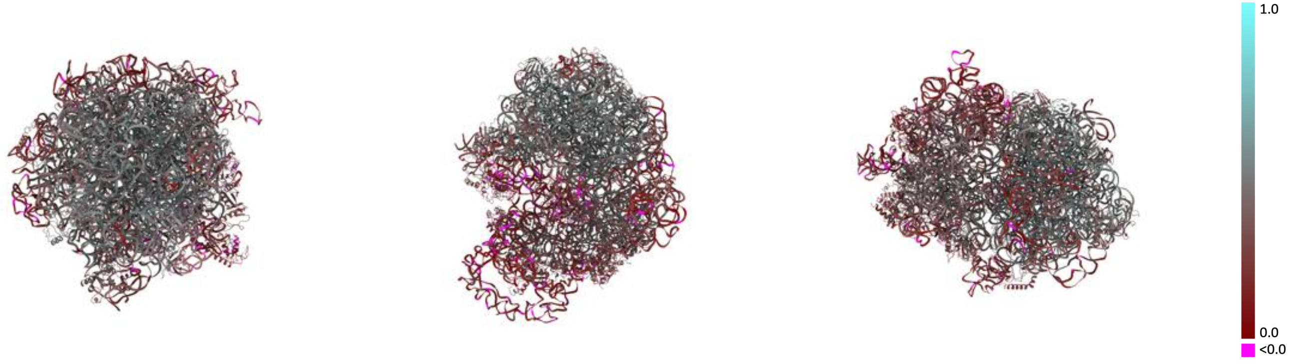
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 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.

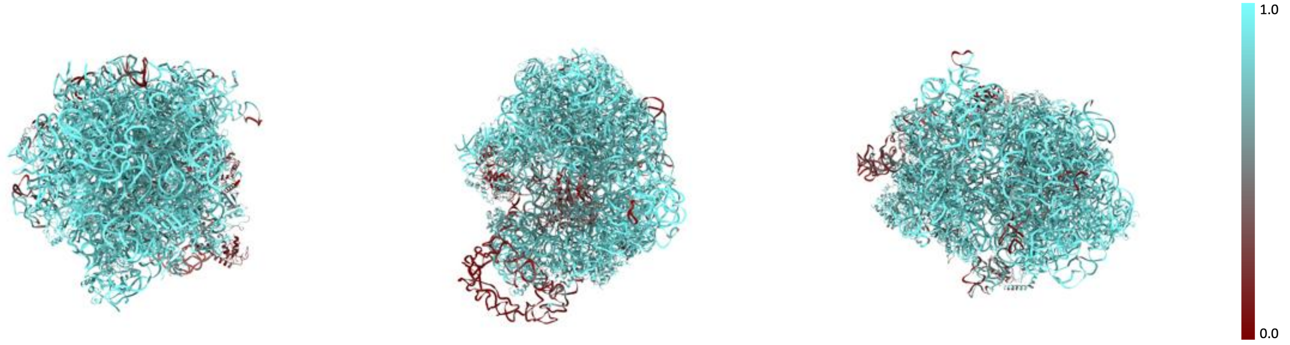
9.2 Q-score mapped to coordinate model ⓘ



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.

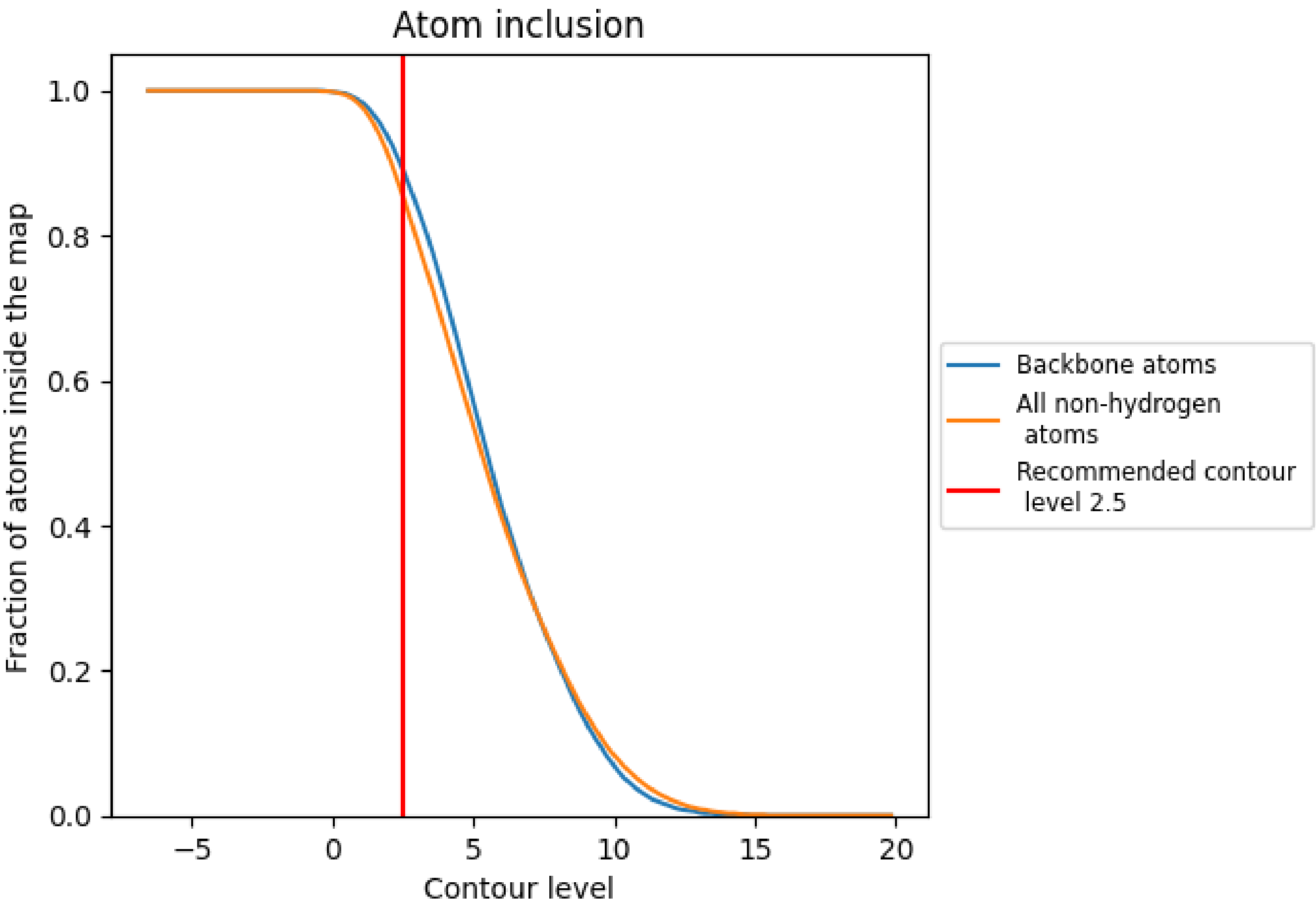
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (2.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8550	0.3590
1	0.9320	0.4120
2	0.9490	0.3250
3	0.9780	0.3560
4	0.2840	0.1290
5	0.4340	0.1850
6	0.3330	0.2090
7	0.6880	0.1980
8	0.6420	0.1550
A	0.8840	0.4690
B	0.9180	0.4830
C	0.9080	0.4870
D	0.9000	0.4620
E	0.7550	0.2140
F	0.7370	0.3160
G	0.5450	0.2720
H	0.2320	0.1770
I	0.3430	0.1790
J	0.9280	0.4840
K	0.8760	0.4660
L	0.9030	0.4760
M	0.8840	0.4680
N	0.9180	0.4750
O	0.9040	0.3780
P	0.8720	0.4560
Q	0.9260	0.4920
R	0.9060	0.4780
S	0.8890	0.4670
T	0.8930	0.4460
U	0.9090	0.4360
V	0.8830	0.4260
X	0.8920	0.4420
Y	0.8510	0.3830
Z	0.9020	0.4770
b	0.9040	0.4680

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	0.9030	0.4520
d	0.9180	0.5090
e	0.9060	0.5070
f	0.8160	0.4060
g	0.7820	0.2890
h	0.8310	0.3320
i	0.7490	0.2570
j	0.8690	0.3970
k	0.8420	0.3170
l	0.7070	0.2120
m	0.8780	0.3910
n	0.8210	0.2320
o	0.7940	0.2700
p	0.8500	0.3360
q	0.7540	0.3250
r	0.7600	0.2110
s	0.8130	0.2840
t	0.8750	0.3510
u	0.8520	0.3320
v	0.8750	0.3700
w	0.8380	0.3370
x	0.7810	0.2120
y	0.8030	0.2710
z	0.6650	0.3150