wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 11:09 am BST

PDB ID	:	7O1C
EMDB ID	:	EMD-12695
Title	:	Cryo-EM structure of an Escherichia coli TnaC(R23F)-ribosome-RF2 complex stalled in response to L-tryptophan
Authors	:	van der Stel, A.X.; Gordon, E.R.; Sengupta, A.; Martinez, A.K.; Klepacki, D.; Perry, T.N.; Herrero del Valle, A.; Vazquez-Laslop, N.; Sachs, M.S.; Cruz-Vera, L.R.; Innis, C.A.
Deposited on	:	2021-03-29
Resolution	:	2.60 Å(reported)
Based on initial model	:	6TBV

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

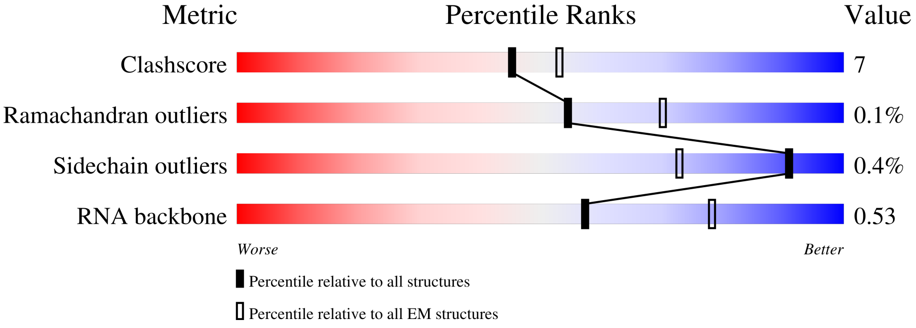
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.60 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)
Clashscore	158937	4297
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	AA	1534	
2	AB	241	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	

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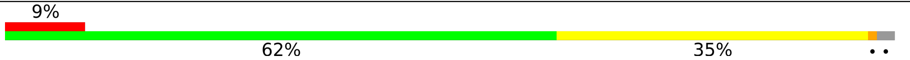
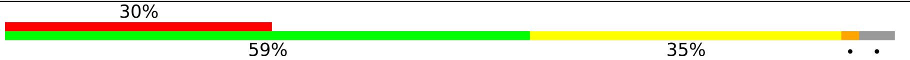
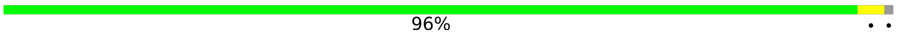
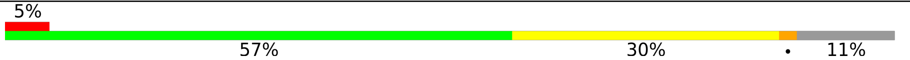
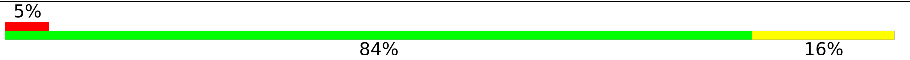
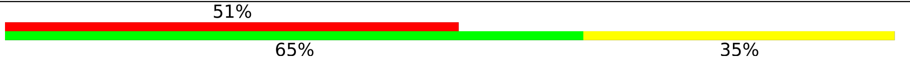
Mol	Chain	Length	Quality of chain
8	AH	130	 75% 23%
9	AI	130	 9% 62% 35%
10	AJ	103	 30% 59% 35%
11	AK	129	 64% 27% 9%
12	AL	124	 75% 23%
13	AM	118	 69% 28%
14	AN	102	 70% 28%
15	AO	89	 96%
16	AP	82	 80% 20%
17	AQ	84	 74% 21% 5%
18	AR	75	 55% 19% 27%
19	AS	92	 5% 57% 30% 11%
20	AT	87	 87% 11%
21	AU	71	 56% 21% 21%
22	BA	2897	 48% 37% 13%
23	BB	120	 61% 28% 10%
24	BC	273	 80% 18%
25	BD	209	 82% 17%
26	BE	201	 5% 84% 16%
27	BF	179	 72% 27%
28	BG	177	 82% 16%
29	BH	149	 51% 65% 35%
30	BI	70	 34% 53% 40% 6%
31	BJ	142	 84% 15%
32	BK	123	 87% 13%

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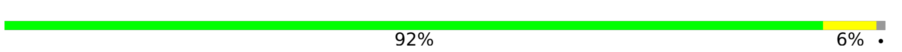
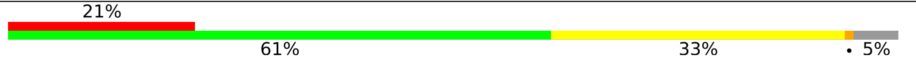
Mol	Chain	Length	Quality of chain
33	BL	144	
34	BM	136	
35	BN	127	
36	BO	117	
37	BP	115	
38	BQ	118	
39	BR	103	
40	BS	110	
41	BT	100	
42	BU	104	
43	BV	94	
44	BW	85	
45	BX	78	
46	BY	63	
47	BZ	59	
48	B0	57	
49	B1	55	
50	B2	46	
51	B3	65	
52	B4	38	
53	B5	17	
54	B7	10	
55	B8	77	
56	B9	365	

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 148175 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 Ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1534	32930	14694	6041	10661	1534	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AC	206	1624	1028	305	288	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	155	1144	711	216	211	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	AF	106	862	545	156	154	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AG	151	1181	735	227	215	4	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AJ	99	795	498	152	144	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AK	117	877	540	174	160	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AL	123	957	591	196	165	5	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	AN	101	799	498	165	133	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	35	ALA	-	insertion	UNP P0AG59

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AQ	80	648	411	121	113	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	AR	55	455	288	86	81	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	AS	82	656	419	125	110	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	AT	86	670	414	138	115	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	AU	56	465	290	96	78	1	0	0

- Molecule 22 is a RNA chain called Ribosomal RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	BA	2897	62209	27759	11446	20107	2897	0	0

- Molecule 23 is a RNA chain called Ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	BB	120	2569	1144	468	837	120	0	0

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	BD	209	1566	980	288	294	4	0	0

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BG	176	1323	832	243	246	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	BH	149	1110	699	197	213	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	BI	66	522	323	99	94	6	0	0

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	BK	123	946	593	181	166	6	0	0

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	BN	118	945	585	194	161	5	0	0

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	BO	117	900	557	179	163	1	0	0

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BT	93	Total 738	C 466	N 139	O 131	S 2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	BU	102	Total 779	C 492	N 146	O 141	0	0

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BW	76	Total 580	C 359	N 117	O 103	S 1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	B1	51	Total	C	N	O	0	0
			414	266	76	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called TnaC-(R23F) - Tryptophanase leader peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B5	17	Total	C	N	O	0	0
			146	97	24	25		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B7	10	Total	C	N	O	P	0	0
			211	94	36	71	10		

- Molecule 55 is a RNA chain called P-site tRNA-Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B8	77	Total 1646	C 733	N 295	O 541	P 77	0	0

- Molecule 56 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B9	348	Total 2768	C 1705	N 482	O 571	S 10	0	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	AA	87	Total 87	Mg 87	0
57	BA	243	Total 243	Mg 243	0
57	BB	1	Total 1	Mg 1	0
57	BC	1	Total 1	Mg 1	0
57	BD	2	Total 2	Mg 2	0
57	BL	3	Total 3	Mg 3	0
57	B8	2	Total 2	Mg 2	0

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	AA	38	Total 38	K 38	0
58	AM	1	Total 1	K 1	0
58	BA	104	Total 104	K 104	0
58	BB	1	Total 1	K 1	0
58	BC	1	Total 1	K 1	0
58	BD	1	Total 1	K 1	0

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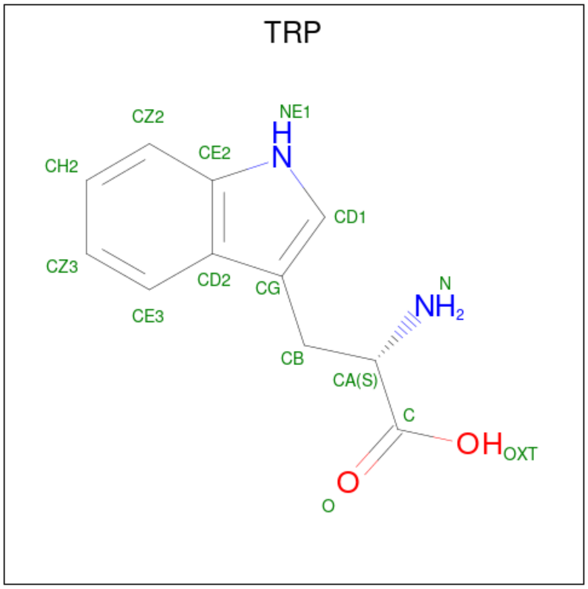
Mol	Chain	Residues	Atoms	AltConf
58	BM	1	Total K 1 1	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
59	AB	1	Total Zn 1 1	0
59	BI	1	Total Zn 1 1	0
59	B4	1	Total Zn 1 1	0

- Molecule 60 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms	AltConf
60	BA	1	Total C N O 15 11 2 2	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	AltConf
61	AA	167	Total O 167 167	0
61	AK	1	Total O 1 1	0

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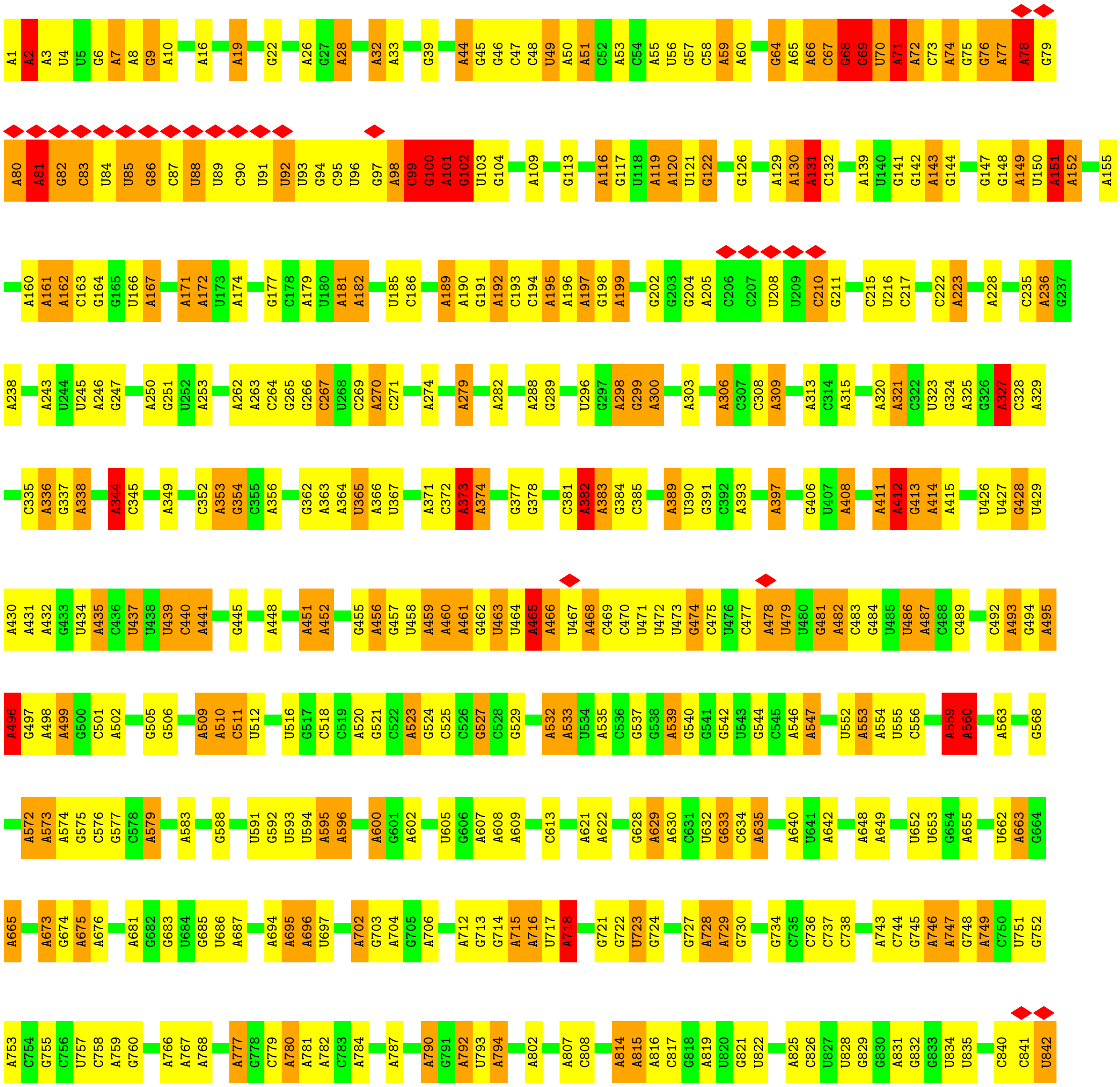
Mol	Chain	Residues	Atoms	AltConf
61	AM	1	Total O 1 1	0
61	AN	3	Total O 3 3	0
61	BA	617	Total O 617 617	0
61	BC	6	Total O 6 6	0
61	BD	2	Total O 2 2	0
61	BN	3	Total O 3 3	0

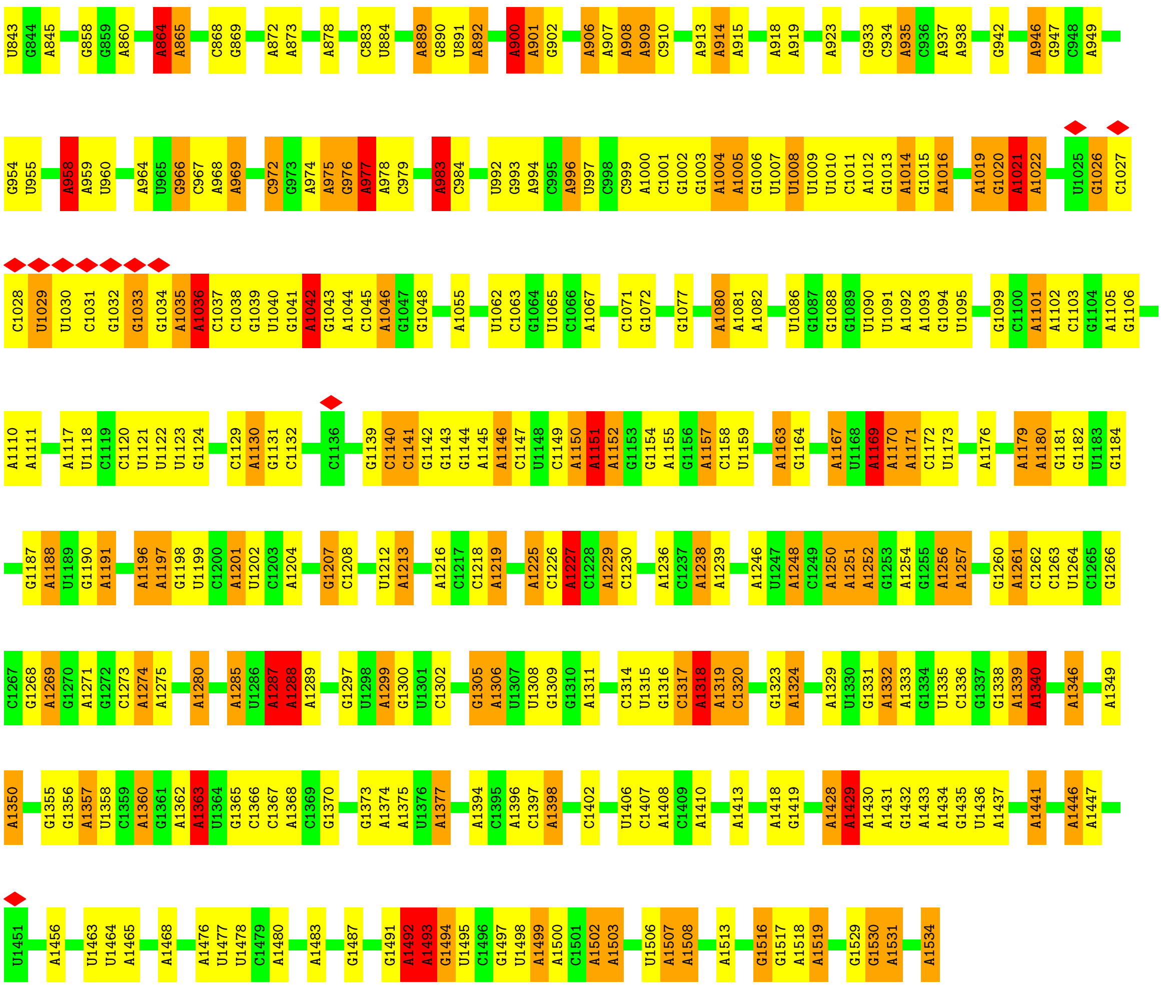
3 Residue-property plots ⓘ

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: Ribosomal RNA 16S

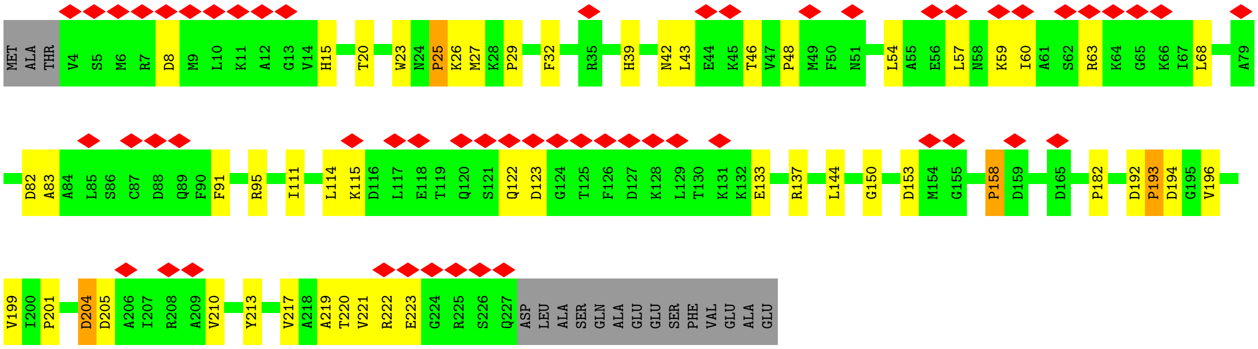
Chain AA:





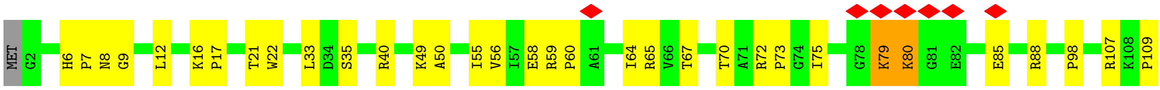
- Molecule 2: 30S ribosomal protein S2

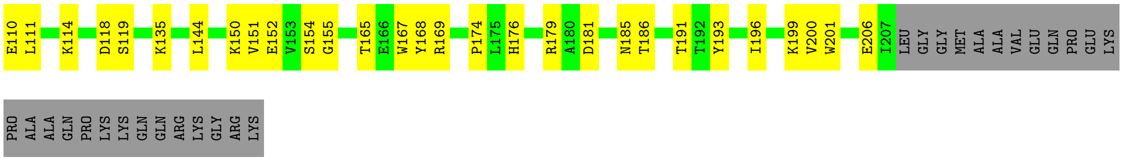
Chain AB:



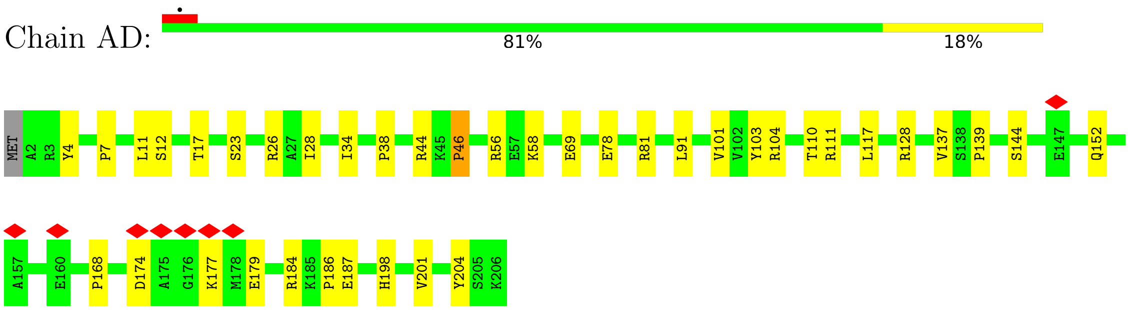
- Molecule 3: 30S ribosomal protein S3

Chain AC:

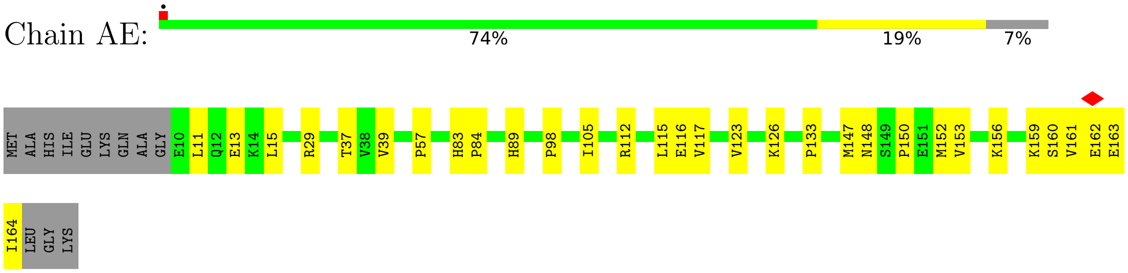




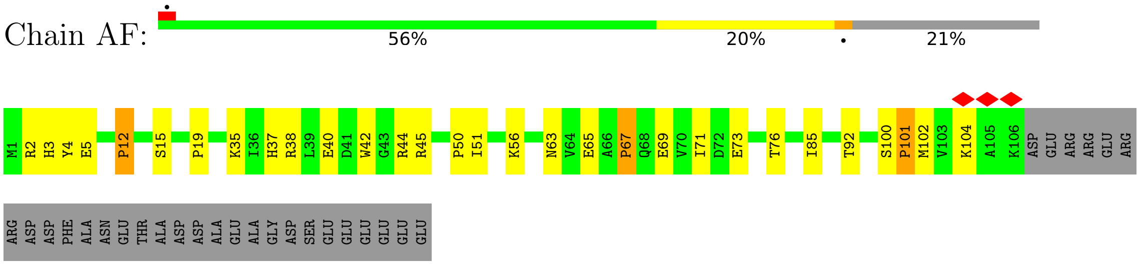
- Molecule 4: 30S ribosomal protein S4



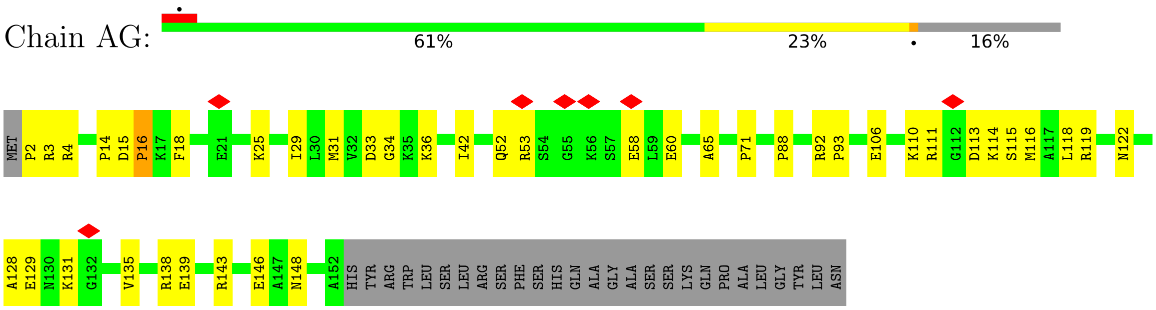
- Molecule 5: 30S ribosomal protein S5



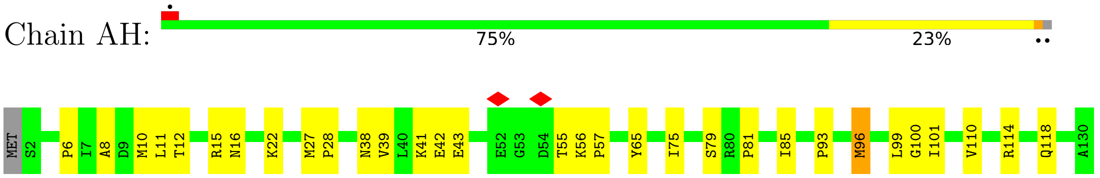
- Molecule 6: 30S ribosomal protein S6



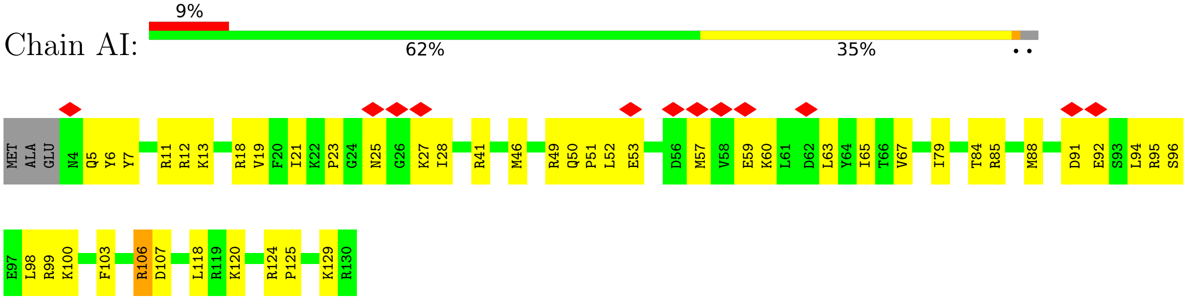
- Molecule 7: 30S ribosomal protein S7



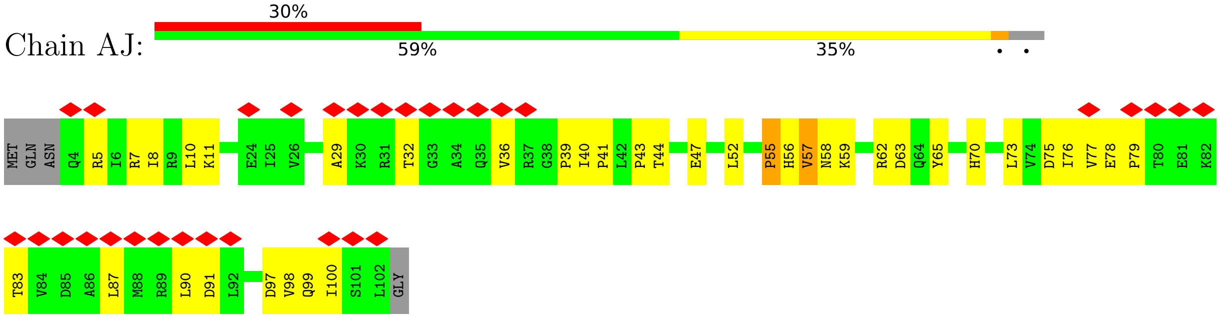
- Molecule 8: 30S ribosomal protein S8



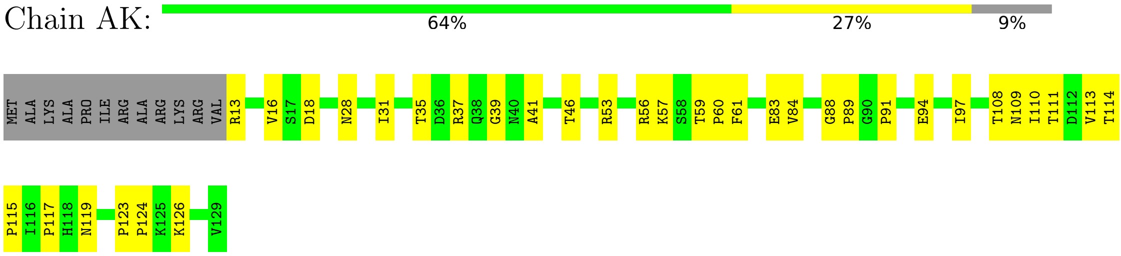
• Molecule 9: 30S ribosomal protein S9



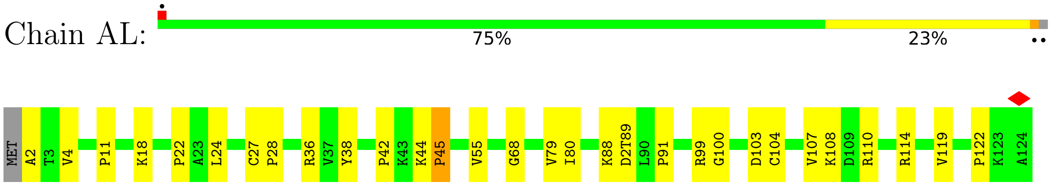
• Molecule 10: 30S ribosomal protein S10



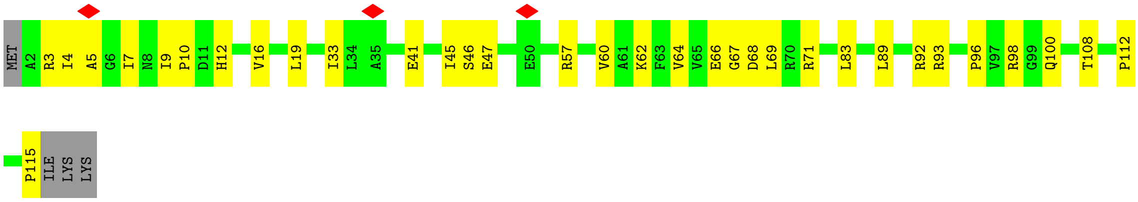
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12

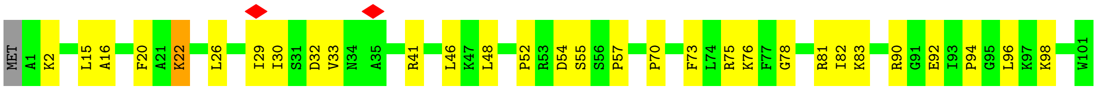


• Molecule 13: 30S ribosomal protein S13



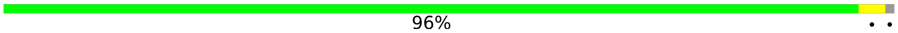
- Molecule 14: 30S ribosomal protein S14

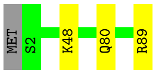
Chain AN:



- Molecule 15: 30S ribosomal protein S15

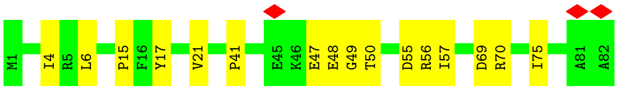
Chain AO:





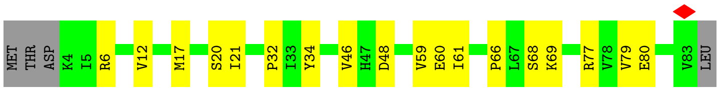
- Molecule 16: 30S ribosomal protein S16

Chain AP:



- Molecule 17: 30S ribosomal protein S17

Chain AQ:

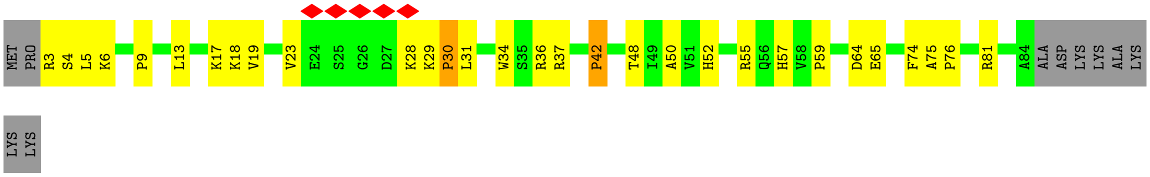


- Molecule 18: 30S ribosomal protein S18

Chain AR:

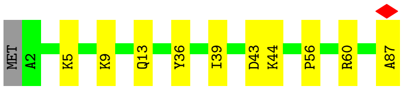
- Molecule 19: 30S ribosomal protein S19

Chain AS:



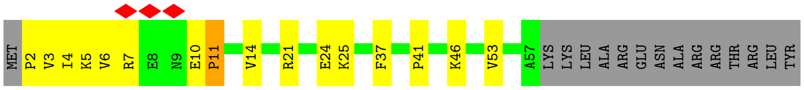
- Molecule 20: 30S ribosomal protein S20

Chain AT:

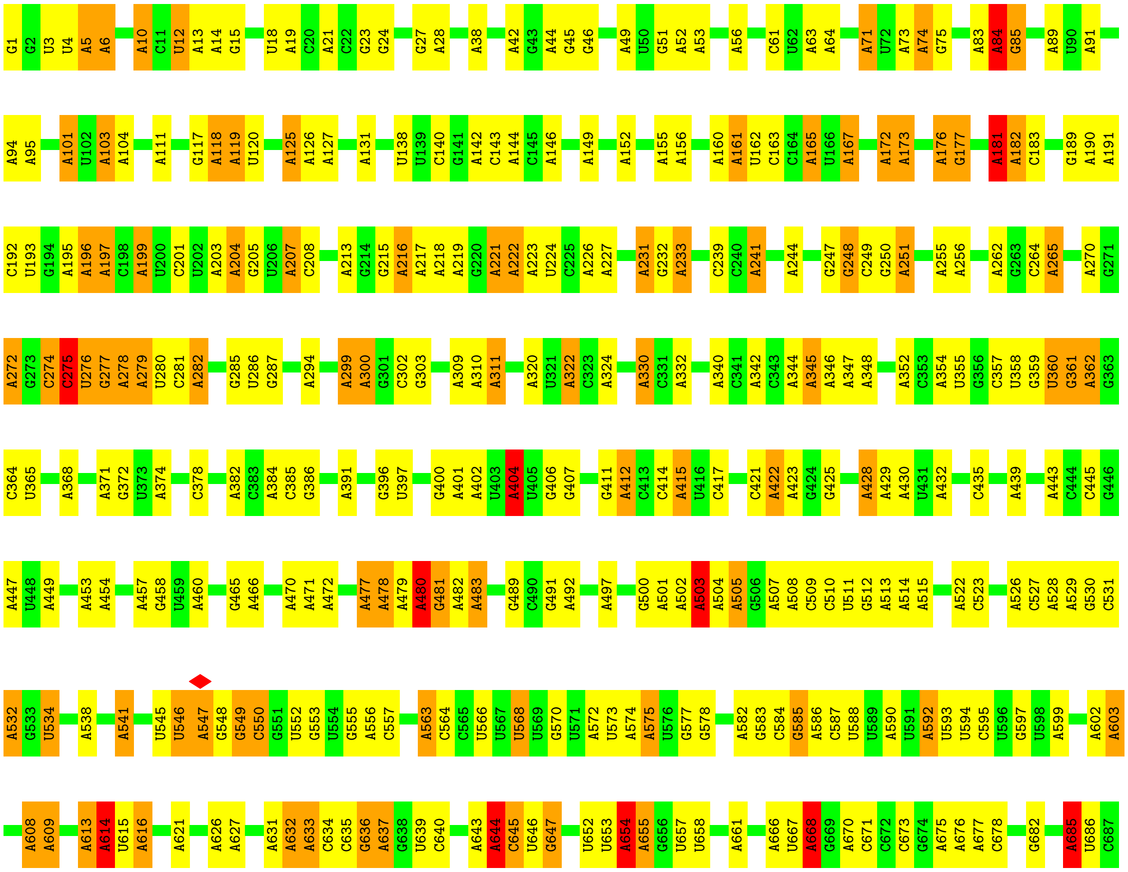
- Molecule 21: 30S ribosomal protein S21

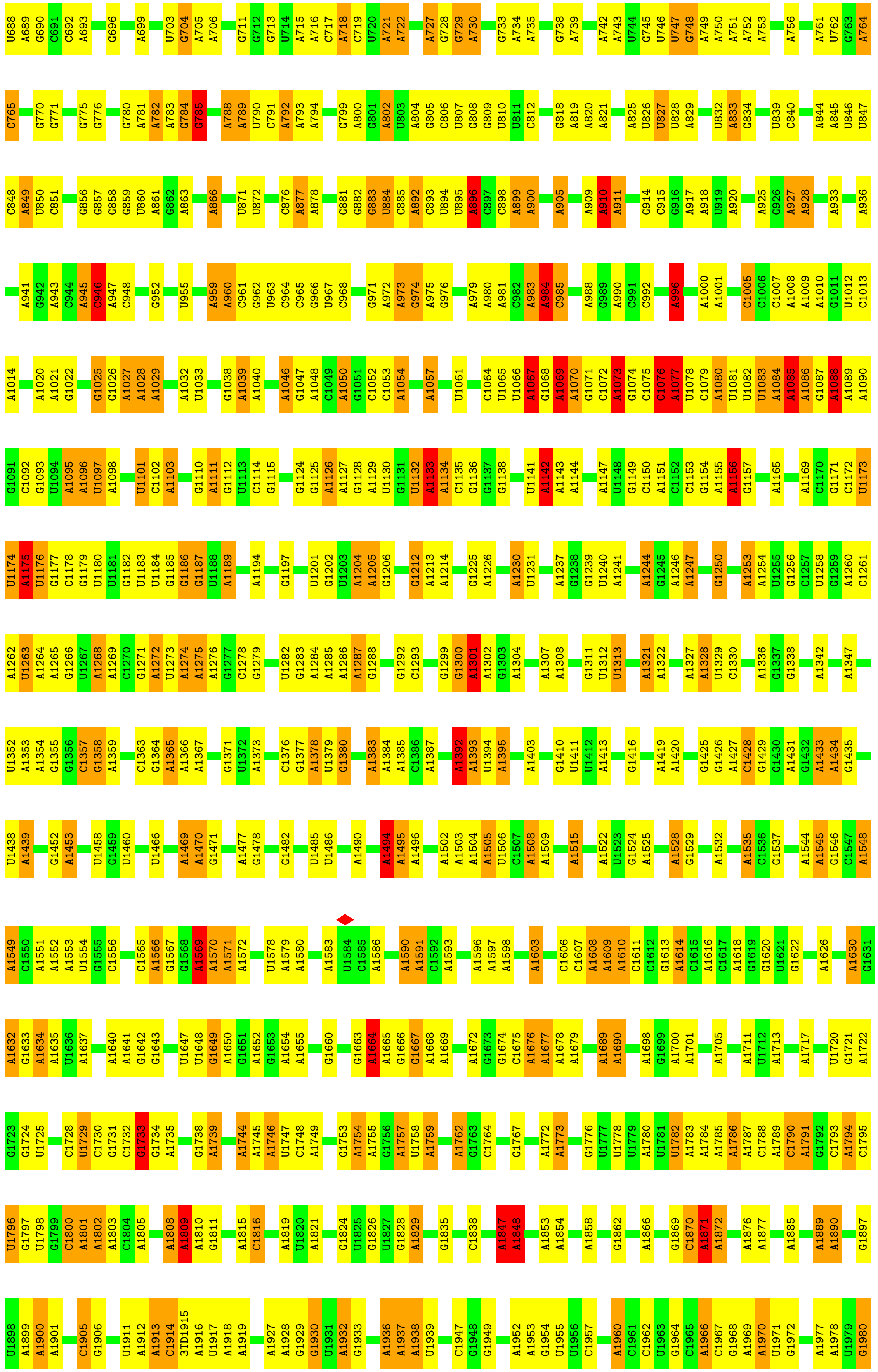
Chain AU:

- Molecule 22: Ribosomal RNA 23S

Chain BA: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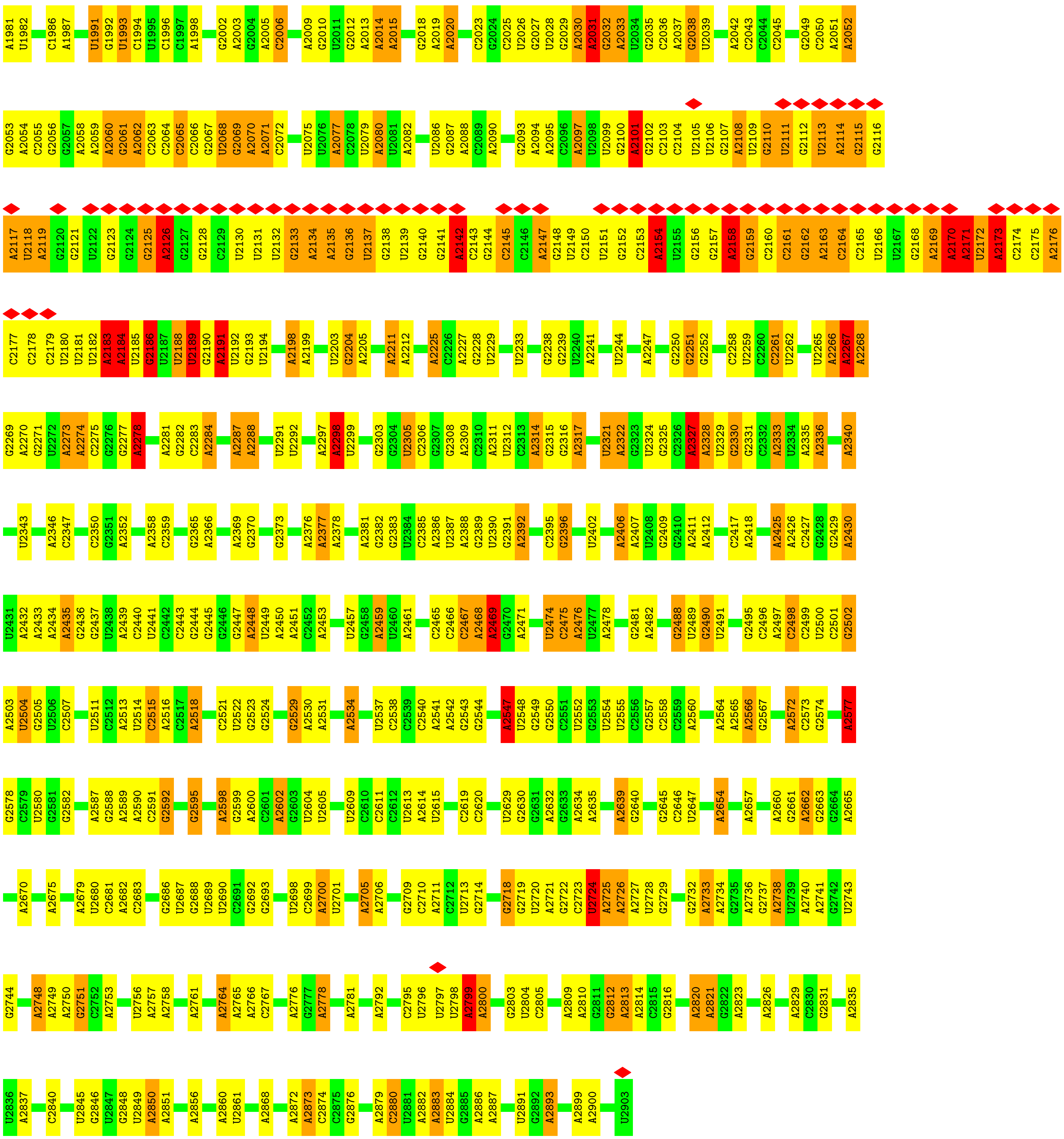
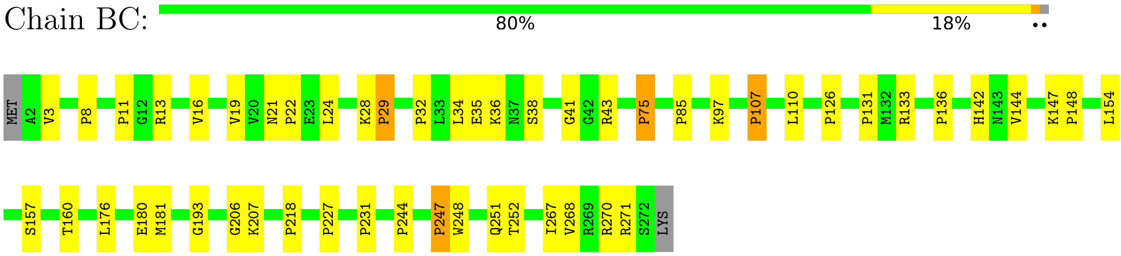


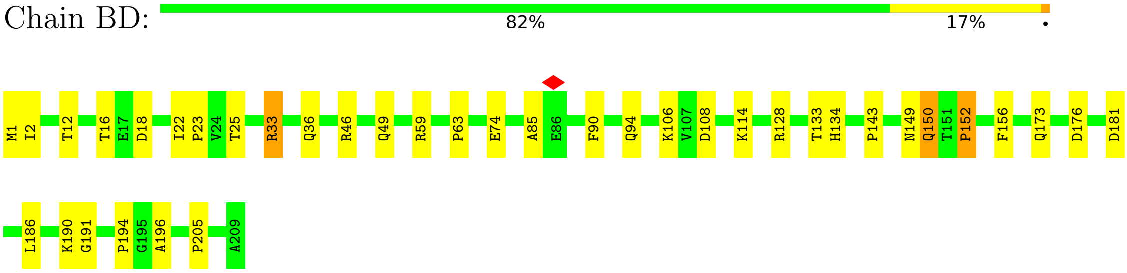
- Molecule 23: Ribosomal RNA 5S

Chain BB:

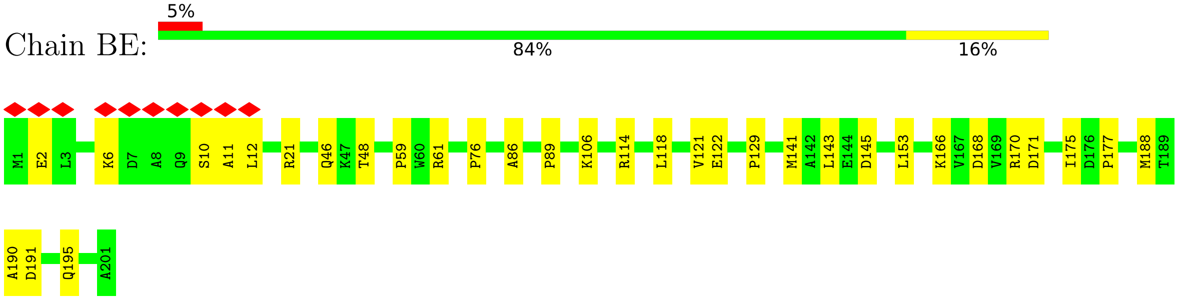
- Molecule 24: 50S ribosomal protein L2



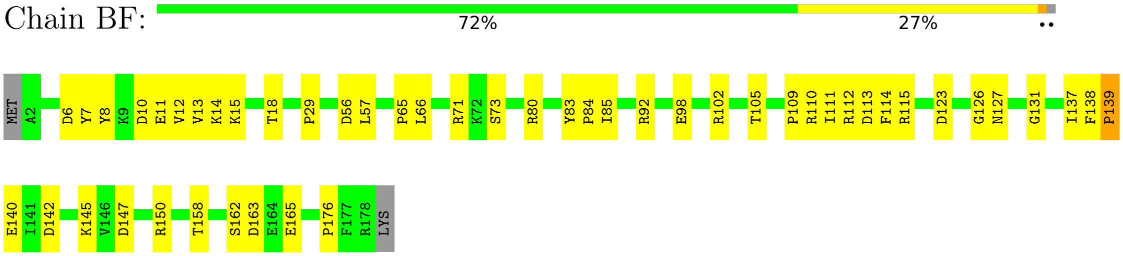
- Molecule 25: 50S ribosomal protein L3



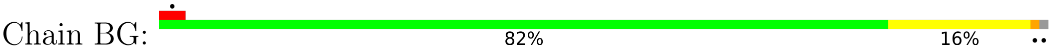
- Molecule 26: 50S ribosomal protein L4

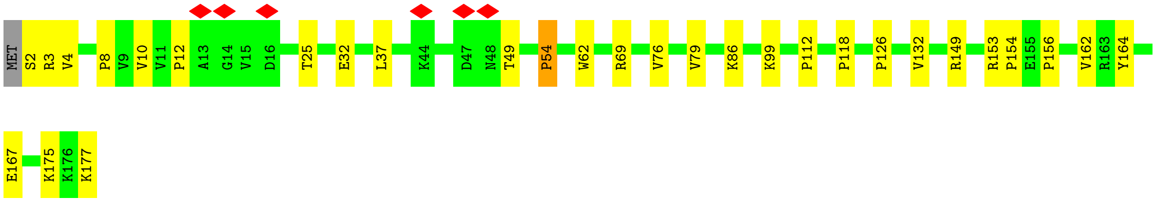


- Molecule 27: 50S ribosomal protein L5



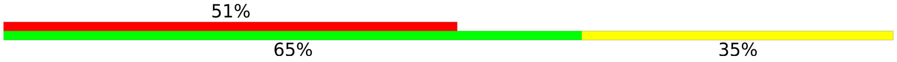
- Molecule 28: 50S ribosomal protein L6

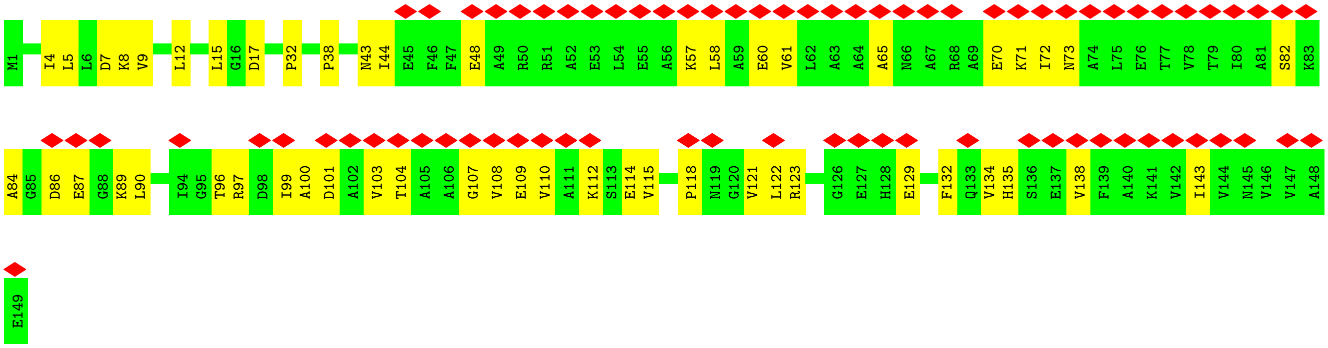




- Molecule 29: 50S ribosomal protein L9

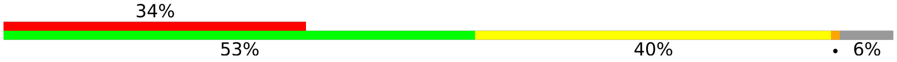
Chain BH:

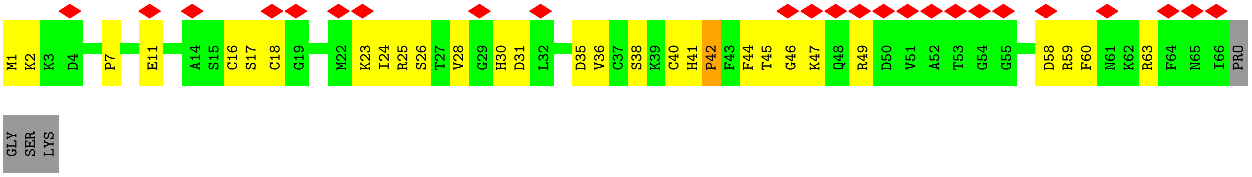




- Molecule 30: 50S ribosomal protein L31

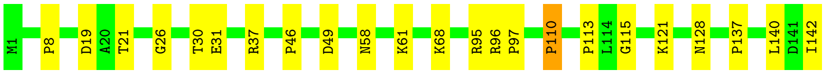
Chain BI:





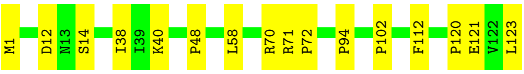
- Molecule 31: 50S ribosomal protein L13

Chain BJ:



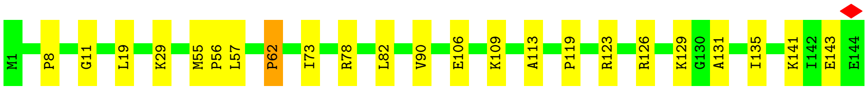
- Molecule 32: 50S ribosomal protein L14

Chain BK:



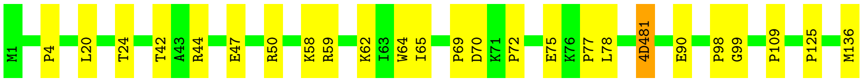
- Molecule 33: 50S ribosomal protein L15

Chain BL:



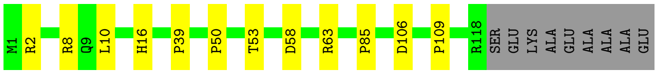
- Molecule 34: 50S ribosomal protein L16

Chain BM:



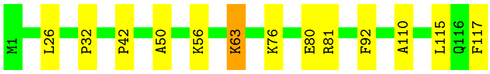
- Molecule 35: 50S ribosomal protein L17

Chain BN:



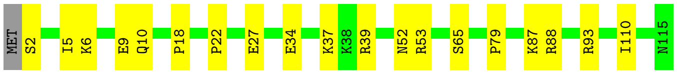
- Molecule 36: 50S ribosomal protein L18

Chain BO:



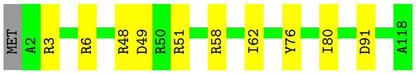
- Molecule 37: 50S ribosomal protein L19

Chain BP:



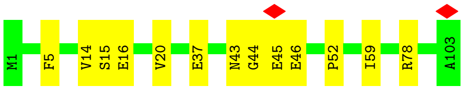
- Molecule 38: 50S ribosomal protein L20

Chain BQ:



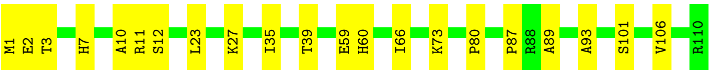
- Molecule 39: 50S ribosomal protein L21

Chain BR:



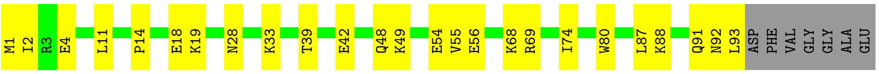
- Molecule 40: 50S ribosomal protein L22

Chain BS:



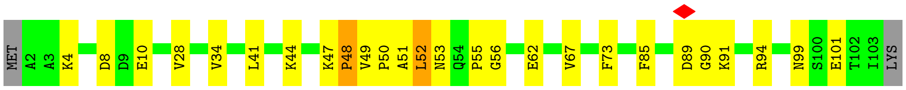
• Molecule 41: 50S ribosomal protein L23

Chain BT:



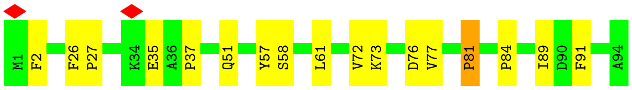
• Molecule 42: 50S ribosomal protein L24

Chain BU:



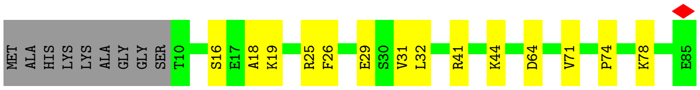
• Molecule 43: 50S ribosomal protein L25

Chain BV:



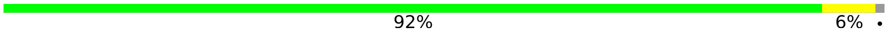
• Molecule 44: 50S ribosomal protein L27

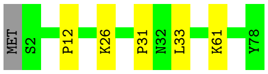
Chain BW:



• Molecule 45: 50S ribosomal protein L28

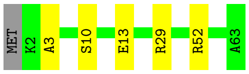
Chain BX:





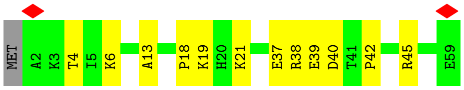
• Molecule 46: 50S ribosomal protein L29

Chain BY:



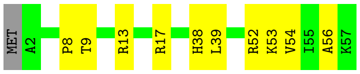
• Molecule 47: 50S ribosomal protein L30

Chain BZ:



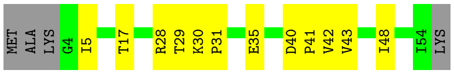
- Molecule 48: 50S ribosomal protein L32

Chain B0:



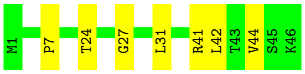
- Molecule 49: 50S ribosomal protein L33

Chain B1:



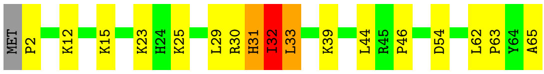
- Molecule 50: 50S ribosomal protein L34

Chain B2:



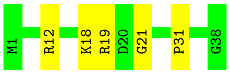
- Molecule 51: 50S ribosomal protein L35

Chain B3:



- Molecule 52: 50S ribosomal protein L36

Chain B4:

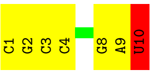


- Molecule 53: TnaC-(R23F) - Tryptophanase leader peptide

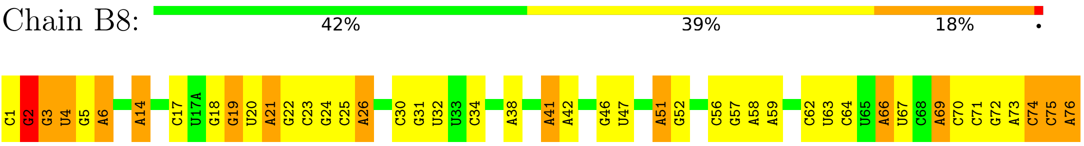
Chain B5:

- Molecule 54: mRNA

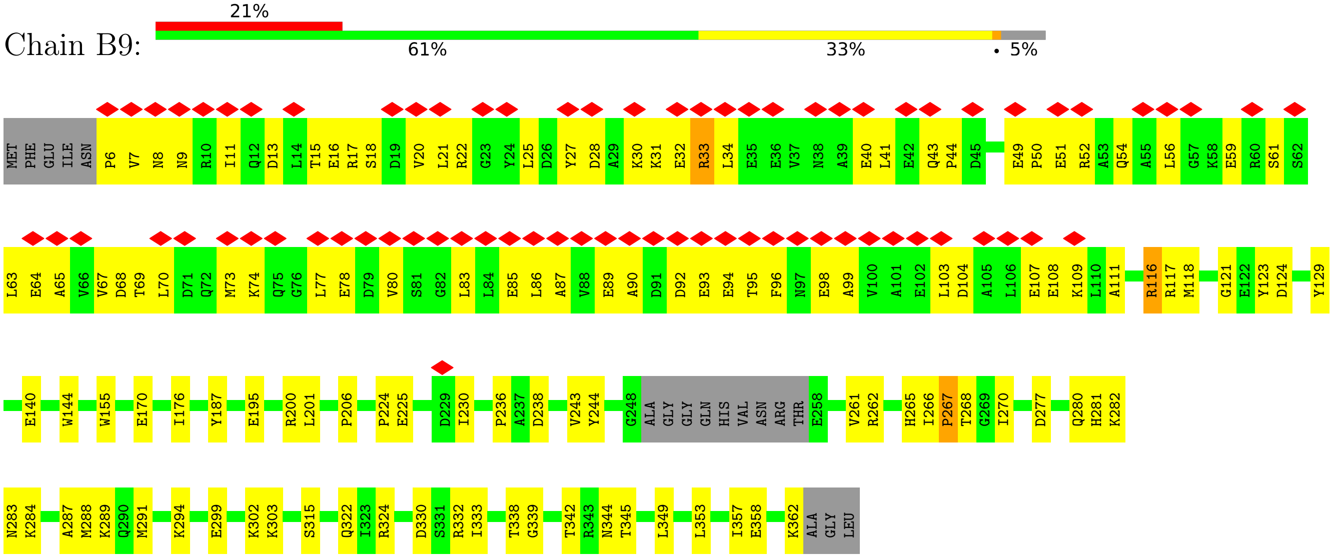
Chain B7:



- Molecule 55: P-site tRNA-Pro



- Molecule 56: Peptide chain release factor RF2



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	113840	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA, FEI TITAN KRIOS	Depositor
Voltage (kV)	200, 300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40, 44	Depositor
Minimum defocus (nm)	-1000, -400	Depositor
Maximum defocus (nm)	-2000, -1600	Depositor
Magnification	55127, 59880	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	370.056, 370.056, 370.056	wwPDB
Map dimensions	408, 408, 408	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.907, 0.907, 0.907	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: G7M, 5MU, K, 6MZ, 3TD, D2T, MEQ, 2MG, MA6, 4OC, 2MA, 5MC, MG, 1MG, OMC, OMG, ZN, OMU, PSU, 4D4, UR3

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	AA	1.65	964/36593 (2.6%)	3.44	4347/57081 (7.6%)
2	AB	0.82	7/1784 (0.4%)	0.56	1/2403 (0.0%)
3	AC	0.86	7/1651 (0.4%)	0.62	2/2225 (0.1%)
4	AD	0.81	6/1665 (0.4%)	0.51	0/2227
5	AE	0.90	5/1157 (0.4%)	0.60	0/1557
6	AF	1.01	5/881 (0.6%)	0.56	0/1189
7	AG	0.96	7/1195 (0.6%)	0.54	0/1602
8	AH	0.94	5/989 (0.5%)	0.62	1/1326 (0.1%)
9	AI	0.76	3/1034 (0.3%)	0.56	0/1375
10	AJ	1.05	6/805 (0.7%)	0.59	0/1089
11	AK	1.11	7/893 (0.8%)	0.62	0/1205
12	AL	1.18	8/960 (0.8%)	0.65	0/1286
13	AM	0.93	5/892 (0.6%)	0.58	0/1193
14	AN	0.89	4/811 (0.5%)	0.55	0/1081
15	AO	0.44	0/722	0.48	0/964
16	AP	0.76	2/659 (0.3%)	0.60	0/884
17	AQ	0.83	2/657 (0.3%)	0.55	0/881
18	AR	0.97	2/462 (0.4%)	0.58	0/621
19	AS	1.09	5/672 (0.7%)	0.65	0/904
20	AT	0.60	1/676 (0.1%)	0.46	0/895
21	AU	1.09	4/472 (0.8%)	0.53	0/627
22	BA	2.12	2046/69120 (3.0%)	3.57	8225/107824 (7.6%)
23	BB	1.74	59/2872 (2.1%)	3.03	258/4478 (5.8%)
24	BC	1.29	23/2121 (1.1%)	0.68	0/2852
25	BD	1.05	11/1576 (0.7%)	0.64	0/2119
26	BE	0.91	6/1571 (0.4%)	0.60	0/2113
27	BF	0.89	6/1434 (0.4%)	0.56	0/1926
28	BG	1.03	8/1343 (0.6%)	0.60	0/1816
29	BH	0.73	3/1121 (0.3%)	0.54	0/1515
30	BI	0.82	2/531 (0.4%)	0.55	0/709
31	BJ	1.09	7/1152 (0.6%)	0.62	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	BK	1.08	5/955 (0.5%)	0.68	0/1279
33	BL	0.95	5/1062 (0.5%)	0.67	0/1413
34	BM	1.16	8/1081 (0.7%)	0.66	0/1443
35	BN	1.07	5/958 (0.5%)	0.68	0/1281
36	BO	0.81	2/910 (0.2%)	0.57	1/1219 (0.1%)
37	BP	0.99	3/929 (0.3%)	0.62	0/1242
38	BQ	0.93	0/960	0.58	0/1278
39	BR	0.91	2/829 (0.2%)	0.64	0/1107
40	BS	0.84	3/864 (0.3%)	0.60	0/1156
41	BT	0.79	1/744 (0.1%)	0.63	0/994
42	BU	0.96	3/787 (0.4%)	0.68	1/1051 (0.1%)
43	BV	1.06	4/766 (0.5%)	0.61	0/1025
44	BW	0.91	1/587 (0.2%)	0.63	0/776
45	BX	0.96	3/635 (0.5%)	0.66	1/848 (0.1%)
46	BY	0.55	0/502	0.56	0/667
47	BZ	0.97	2/453 (0.4%)	0.64	0/605
48	B0	0.89	2/450 (0.4%)	0.61	0/599
49	B1	1.09	2/421 (0.5%)	0.64	0/561
50	B2	0.97	1/380 (0.3%)	0.64	0/498
51	B3	1.21	4/513 (0.8%)	0.82	1/676 (0.1%)
52	B4	1.02	1/303 (0.3%)	0.67	0/397
53	B5	1.33	2/151 (1.3%)	0.81	0/205
54	B7	1.47	3/233 (1.3%)	2.72	14/358 (3.9%)
55	B8	1.87	57/1839 (3.1%)	2.96	169/2866 (5.9%)
56	B9	0.73	8/2806 (0.3%)	0.55	0/3778
All	All	1.72	3353/158589 (2.1%)	3.01	13021/236840 (5.5%)

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
5	AE	0	1
51	B3	0	1
All	All	0	2

The worst 5 of 3353 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	C2'-C1'	-22.33	1.28	1.53
22	BA	2449	U	C5-C6	18.12	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	O4'-C1'	16.77	1.63	1.41
55	B8	59	A	C6-N6	16.71	1.47	1.33
55	B8	58	A	C6-N6	16.69	1.47	1.33

The worst 5 of 13021 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	752	A	N1-C6-N6	-27.47	102.12	118.60
22	BA	2872	A	N1-C6-N6	-24.44	103.94	118.60
22	BA	1668	A	N1-C6-N6	-24.16	104.11	118.60
22	BA	2062	A	N1-C2-N3	-23.43	117.58	129.30
22	BA	1668	A	N1-C2-N3	-23.24	117.68	129.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	89	HIS	Peptide
51	B3	31	HIS	Peptide

5.2 Too-close contacts ⓘ

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	AA	32930	0	16583	454	0
2	AB	1753	0	1780	34	0
3	AC	1624	0	1696	33	0
4	AD	1643	0	1707	20	0
5	AE	1144	0	1185	18	0
6	AF	862	0	864	21	0
7	AG	1181	0	1238	28	0
8	AH	979	0	1031	18	0
9	AI	1022	0	1070	39	0
10	AJ	795	0	836	25	0
11	AK	877	0	887	19	0
12	AL	957	0	1017	19	0
13	AM	883	0	941	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	AN	799	0	841	23	0
15	AO	714	0	734	2	0
16	AP	649	0	666	9	0
17	AQ	648	0	691	10	0
18	AR	455	0	478	10	0
19	AS	656	0	680	24	0
20	AT	670	0	719	7	0
21	AU	465	0	491	11	0
22	BA	62209	0	31287	446	0
23	BB	2569	0	1301	19	0
24	BC	2082	0	2154	26	0
25	BD	1566	0	1618	18	0
26	BE	1552	0	1619	18	0
27	BF	1410	0	1444	38	0
28	BG	1323	0	1371	14	0
29	BH	1110	0	1148	31	0
30	BI	522	0	520	23	0
31	BJ	1129	0	1162	14	0
32	BK	946	0	1023	8	0
33	BL	1053	0	1128	15	0
34	BM	1075	0	1155	13	0
35	BN	945	0	989	7	0
36	BO	900	0	935	7	0
37	BP	917	0	962	12	0
38	BQ	947	0	1019	11	0
39	BR	816	0	839	7	0
40	BS	857	0	922	12	0
41	BT	738	0	807	17	0
42	BU	779	0	831	18	0
43	BV	753	0	780	10	0
44	BW	580	0	594	11	0
45	BX	625	0	652	2	0
46	BY	501	0	531	4	0
47	BZ	449	0	488	8	0
48	B0	444	0	458	7	0
49	B1	414	0	442	6	0
50	B2	377	0	418	3	0
51	B3	504	0	572	16	0
52	B4	302	0	340	3	0
53	B5	146	0	139	5	0
54	B7	211	0	110	5	0
55	B8	1646	0	831	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B9	2768	0	2666	86	0
57	AA	87	0	0	0	0
57	B8	2	0	0	0	0
57	BA	243	0	0	0	0
57	BB	1	0	0	0	0
57	BC	1	0	0	0	0
57	BD	2	0	0	0	0
57	BL	3	0	0	0	0
58	AA	38	0	0	0	0
58	AM	1	0	0	0	0
58	BA	104	0	0	0	0
58	BB	1	0	0	0	0
58	BC	1	0	0	0	0
58	BD	1	0	0	0	0
58	BM	1	0	0	0	0
59	AB	1	0	0	0	0
59	B4	1	0	0	0	0
59	BI	1	0	0	0	0
60	BA	15	0	9	0	0
61	AA	167	0	0	0	0
61	AK	1	0	0	0	0
61	AM	1	0	0	0	0
61	AN	3	0	0	0	0
61	BA	617	0	0	3	0
61	BC	6	0	0	0	0
61	BD	2	0	0	0	0
61	BN	3	0	0	0	0
All	All	148175	0	99399	1626	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 7.

The worst 5 of 1626 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)
55:B8:1:C:H5’	56:B9:282:LYS:NZ	1.70	1.05
22:BA:2185:U:C4	22:BA:2186:G:O6	2.13	1.00
1:AA:1088:G:N2	1:AA:1167:A:H61	1.59	1.00
1:AA:1026:G:C6	1:AA:1035:A:N6	2.32	0.98
22:BA:884:U:O4	22:BA:892:A:C5	2.21	0.93

There are no symmetry-related clashes.

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	
2	AB	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
3	AC	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
4	AD	203/206 (98%)	195 (96%)	8 (4%)	0	100	100
5	AE	153/167 (92%)	144 (94%)	9 (6%)	0	100	100
6	AF	104/135 (77%)	101 (97%)	3 (3%)	0	100	100
7	AG	149/179 (83%)	135 (91%)	14 (9%)	0	100	100
8	AH	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	AI	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
10	AJ	97/103 (94%)	89 (92%)	6 (6%)	2 (2%)	7	13
11	AK	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
12	AL	120/124 (97%)	109 (91%)	11 (9%)	0	100	100
13	AM	112/118 (95%)	98 (88%)	14 (12%)	0	100	100
14	AN	99/102 (97%)	84 (85%)	15 (15%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
17	AQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	80/92 (87%)	75 (94%)	5 (6%)	0	100	100
20	AT	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	AU	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
24	BC	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
25	BD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BE	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	BF	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
28	BG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
29	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
30	BI	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
31	BJ	140/142 (99%)	140 (100%)	0	0	100	100
32	BK	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
33	BL	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
34	BM	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
35	BN	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
36	BO	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
37	BP	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	BS	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	BT	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
42	BU	100/104 (96%)	89 (89%)	10 (10%)	1 (1%)	15	32
43	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
44	BW	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	BX	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
46	BY	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
47	BZ	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	B0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
49	B1	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
50	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	B3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4	6
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	B5	15/17 (88%)	13 (87%)	2 (13%)	0	100	100
56	B9	344/365 (94%)	325 (94%)	19 (6%)	0	100	100
All	All	5934/6296 (94%)	5626 (95%)	302 (5%)	6 (0%)	54	75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	BD	149	ASN
51	B3	32	ILE
51	B3	33	LEU
10	AJ	57	VAL
10	AJ	58	ASN

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	
2	AB	186/199 (94%)	186 (100%)	0	100	100
3	AC	170/190 (90%)	168 (99%)	2 (1%)	71	87
4	AD	172/173 (99%)	171 (99%)	1 (1%)	86	95
5	AE	118/126 (94%)	118 (100%)	0	100	100
6	AF	92/116 (79%)	92 (100%)	0	100	100
7	AG	124/147 (84%)	124 (100%)	0	100	100
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	104 (99%)	1 (1%)	76	90
10	AJ	87/90 (97%)	87 (100%)	0	100	100
11	AK	90/99 (91%)	89 (99%)	1 (1%)	73	88
12	AL	102/103 (99%)	102 (100%)	0	100	100
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	78 (99%)	1 (1%)	69	86
15	AO	76/77 (99%)	75 (99%)	1 (1%)	69	86
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	47 (98%)	1 (2%)	53	77
19	AS	71/79 (90%)	70 (99%)	1 (1%)	67	85
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	48/61 (79%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	BC	216/218 (99%)	216 (100%)	0	100	100
25	BD	163/163 (100%)	161 (99%)	2 (1%)	71	87
26	BE	165/165 (100%)	165 (100%)	0	100	100
27	BF	148/150 (99%)	148 (100%)	0	100	100
28	BG	137/138 (99%)	137 (100%)	0	100	100
29	BH	114/114 (100%)	114 (100%)	0	100	100
30	BI	59/62 (95%)	59 (100%)	0	100	100
31	BJ	116/116 (100%)	115 (99%)	1 (1%)	78	91
32	BK	104/104 (100%)	104 (100%)	0	100	100
33	BL	103/103 (100%)	103 (100%)	0	100	100
34	BM	108/108 (100%)	108 (100%)	0	100	100
35	BN	98/103 (95%)	98 (100%)	0	100	100
36	BO	87/87 (100%)	86 (99%)	1 (1%)	73	88
37	BP	99/100 (99%)	98 (99%)	1 (1%)	76	90
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	84 (100%)	0	100	100
40	BS	93/93 (100%)	93 (100%)	0	100	100
41	BT	80/84 (95%)	80 (100%)	0	100	100
42	BU	83/85 (98%)	83 (100%)	0	100	100
43	BV	78/78 (100%)	78 (100%)	0	100	100
44	BW	57/63 (90%)	57 (100%)	0	100	100
45	BX	67/68 (98%)	67 (100%)	0	100	100
46	BY	54/55 (98%)	54 (100%)	0	100	100
47	BZ	48/49 (98%)	48 (100%)	0	100	100
48	B0	47/48 (98%)	47 (100%)	0	100	100
49	B1	45/49 (92%)	45 (100%)	0	100	100
50	B2	38/38 (100%)	37 (97%)	1 (3%)	46	72
51	B3	51/52 (98%)	51 (100%)	0	100	100
52	B4	34/34 (100%)	34 (100%)	0	100	100
53	B5	17/17 (100%)	16 (94%)	1 (6%)	19	39
56	B9	298/311 (96%)	296 (99%)	2 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4948/5155 (96%)	4930 (100%)	18 (0%)	91	97

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	B2	41	ARG
56	B9	116	ARG
56	B9	33	ARG
19	AS	81	ARG
37	BP	37	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
56	B9	281	HIS
41	BT	48	GLN
11	AK	119	ASN
8	AH	118	GLN
26	BE	97	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	241 (15%)	8 (0%)
22	BA	2890/2897 (99%)	438 (15%)	24 (0%)
23	BB	119/120 (99%)	15 (12%)	1 (0%)
54	B7	8/10 (80%)	2 (25%)	0
55	B8	76/77 (98%)	12 (15%)	2 (2%)
All	All	4623/4638 (99%)	708 (15%)	35 (0%)

5 of 708 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	4	U
1	AA	7	A
1	AA	9	G
1	AA	19	A

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2474	U
22	BA	2518	A
23	BB	66	A
22	BA	685	A
22	BA	276	U

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

37 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	$\#\|Z\| > 2$
22	6MZ	BA	1618	22	18,25,26	2.84	5 (27%)	16,36,39	2.95	4 (25%)
1	5MC	AA	967	1	18,22,23	3.36	7 (38%)	26,32,35	1.12	1 (3%)
22	5MU	BA	747	40,22	19,22,23	0.76	0	28,32,35	1.13	2 (7%)
22	3TD	BA	1915	56,22	18,22,23	4.04	7 (38%)	22,32,35	1.75	3 (13%)
22	PSU	BA	2604	22	18,21,22	3.40	6 (33%)	22,30,33	2.74	6 (27%)
22	G7M	BA	2069	58,22	20,26,27	1.98	5 (25%)	17,39,42	1.22	2 (11%)
22	PSU	BA	1917	22	18,21,22	3.88	6 (33%)	22,30,33	1.96	5 (22%)
22	OMG	BA	2251	55,58,22	18,26,27	2.14	5 (27%)	19,38,41	1.50	5 (26%)
22	2MA	BA	2503	58,22,57	17,25,26	2.15	5 (29%)	17,37,40	1.56	4 (23%)
22	5MU	BA	1939	58,22	19,22,23	1.05	3 (15%)	28,32,35	1.32	4 (14%)
1	4OC	AA	1402	1,57	20,23,24	2.76	8 (40%)	26,32,35	0.96	2 (7%)
22	PSU	BA	2605	22	18,21,22	3.54	8 (44%)	22,30,33	2.06	4 (18%)
1	MA6	AA	1518	1	18,26,27	1.44	5 (27%)	19,38,41	3.33	2 (10%)
22	6MZ	BA	2030	22	18,25,26	2.87	6 (33%)	16,36,39	2.91	4 (25%)
1	PSU	AA	516	1,57	18,21,22	4.01	7 (38%)	22,30,33	1.98	6 (27%)
22	PSU	BA	2580	22	18,21,22	3.58	7 (38%)	22,30,33	1.97	4 (18%)
22	OMU	BA	2552	22,57	19,22,23	2.56	7 (36%)	26,31,34	2.05	6 (23%)
22	PSU	BA	2504	58,22	18,21,22	3.52	6 (33%)	22,30,33	1.74	4 (18%)
1	2MG	AA	966	1	18,26,27	2.37	7 (38%)	16,38,41	1.41	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	2MG	AA	1207	58,1	18,26,27	2.37	7 (38%)	16,38,41	1.43	3 (18%)
1	2MG	AA	1516	1	18,26,27	2.21	6 (33%)	16,38,41	1.81	4 (25%)
12	D2T	AL	89	12	7,9,10	1.02	0	6,11,13	2.65	3 (50%)
22	5MC	BA	1962	58,22	18,22,23	2.90	7 (38%)	26,32,35	1.10	2 (7%)
1	5MC	AA	1407	1	18,22,23	3.14	7 (38%)	26,32,35	1.22	2 (7%)
22	PSU	BA	2457	22	18,21,22	3.44	7 (38%)	22,30,33	2.45	5 (22%)
22	PSU	BA	1911	22	18,21,22	3.98	7 (38%)	22,30,33	2.22	5 (22%)
22	OMC	BA	2498	22,57	19,22,23	2.45	7 (36%)	26,31,34	0.97	2 (7%)
22	1MG	BA	745	22	18,26,27	2.41	5 (27%)	19,39,42	1.52	3 (15%)
22	2MG	BA	1835	22	18,26,27	2.05	5 (27%)	16,38,41	1.78	4 (25%)
34	4D4	BM	81	34	9,11,12	2.44	4 (44%)	8,13,15	1.26	1 (12%)
1	G7M	AA	527	58,1	20,26,27	2.31	6 (30%)	17,39,42	1.26	1 (5%)
22	PSU	BA	955	22	18,21,22	3.56	6 (33%)	22,30,33	2.31	5 (22%)
22	2MG	BA	2445	22	18,26,27	2.12	5 (27%)	16,38,41	2.12	4 (25%)
22	PSU	BA	746	22,57	18,21,22	3.95	8 (44%)	22,30,33	1.73	6 (27%)
25	MEQ	BD	150	25	8,9,10	1.43	2 (25%)	5,10,12	1.50	1 (20%)
1	UR3	AA	1498	1	19,22,23	2.91	8 (42%)	26,32,35	1.43	2 (7%)
1	MA6	AA	1519	1	18,26,27	1.39	3 (16%)	19,38,41	3.70	2 (10%)

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
22	6MZ	BA	1618	22	-	0/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
22	5MU	BA	747	40,22	-	3/7/25/26	0/2/2/2
22	3TD	BA	1915	56,22	-	2/7/25/26	0/2/2/2
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
22	G7M	BA	2069	58,22	-	2/3/25/26	0/3/3/3
22	PSU	BA	1917	22	-	1/7/25/26	0/2/2/2
22	OMG	BA	2251	55,58,22	-	2/5/27/28	0/3/3/3
22	2MA	BA	2503	58,22,57	-	2/3/25/26	0/3/3/3
22	5MU	BA	1939	58,22	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1,57	-	2/9/29/30	0/2/2/2
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
22	6MZ	BA	2030	22	-	2/5/27/28	0/3/3/3
1	PSU	AA	516	1,57	-	1/7/25/26	0/2/2/2
22	PSU	BA	2580	22	-	2/7/25/26	0/2/2/2
22	OMU	BA	2552	22,57	-	0/9/27/28	0/2/2/2
22	PSU	BA	2504	58,22	-	2/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	2MG	AA	1207	58,1	-	0/5/27/28	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
22	5MC	BA	1962	58,22	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	1911	22	-	0/7/25/26	0/2/2/2
22	OMC	BA	2498	22,57	-	0/9/27/28	0/2/2/2
22	1MG	BA	745	22	-	0/3/25/26	0/3/3/3
22	2MG	BA	1835	22	-	0/5/27/28	0/3/3/3
34	4D4	BM	81	34	-	2/11/12/14	-
1	G7M	AA	527	58,1	-	2/3/25/26	0/3/3/3
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
22	2MG	BA	2445	22	-	2/5/27/28	0/3/3/3
22	PSU	BA	746	22,57	-	3/7/25/26	0/2/2/2
25	MEQ	BD	150	25	-	4/8/9/11	-
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3

The worst 5 of 210 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C6-C5	11.61	1.48	1.35
22	BA	1911	PSU	C6-C5	10.71	1.47	1.35
22	BA	1917	PSU	C6-C5	10.44	1.47	1.35
1	AA	516	PSU	C6-C5	10.41	1.47	1.35
22	BA	2030	6MZ	C6-N6	10.36	1.52	1.35

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1519	MA6	N1-C6-N6	-14.58	101.71	117.06
1	AA	1518	MA6	N1-C6-N6	-13.26	103.10	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2030	6MZ	C9-N6-C6	-8.27	115.75	122.87
22	BA	1618	6MZ	C9-N6-C6	-7.09	116.76	122.87
22	BA	1618	6MZ	N3-C2-N1	-6.64	118.29	128.68

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
25	BD	150	MEQ	O-C-CA-CB
22	BA	746	PSU	C2'-C1'-C5-C4
22	BA	747	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	BA	2251	OMG	1	0
22	BA	2030	6MZ	2	0
1	AA	1207	2MG	1	0
1	AA	1516	2MG	1	0
22	BA	2498	OMC	1	0
34	BM	81	4D4	1	0
25	BD	150	MEQ	1	0
1	AA	1519	MA6	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 490 ligands modelled in this entry, 489 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	TRP	BA	3001	-	14,16,16	0.84	1 (7%)	16,22,22	1.04	1 (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
60	TRP	BA	3001	-	-	0/7/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	3001	TRP	OXT-C	-2.11	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	BA	3001	TRP	OXT-C-O	-2.32	118.81	124.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	BA	2
54	B7	1

All chain breaks are listed below:

Model	**Chain**	**Residue-1**	**Atom-1**	**Residue-2**	**Atom-2**	**Distance (Å)**
1	BA	885:C	O3’	892:A	P	13.97
1	BA	2099:U	O3’	2100:G	P	3.25
1	B7	7:U	O3’	8:G	P	2.92

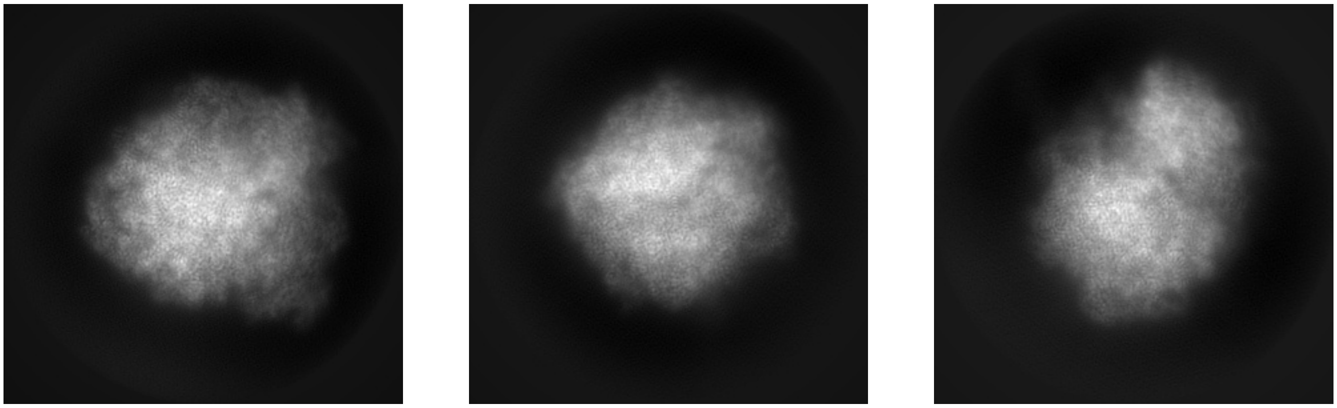
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-12695. 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.

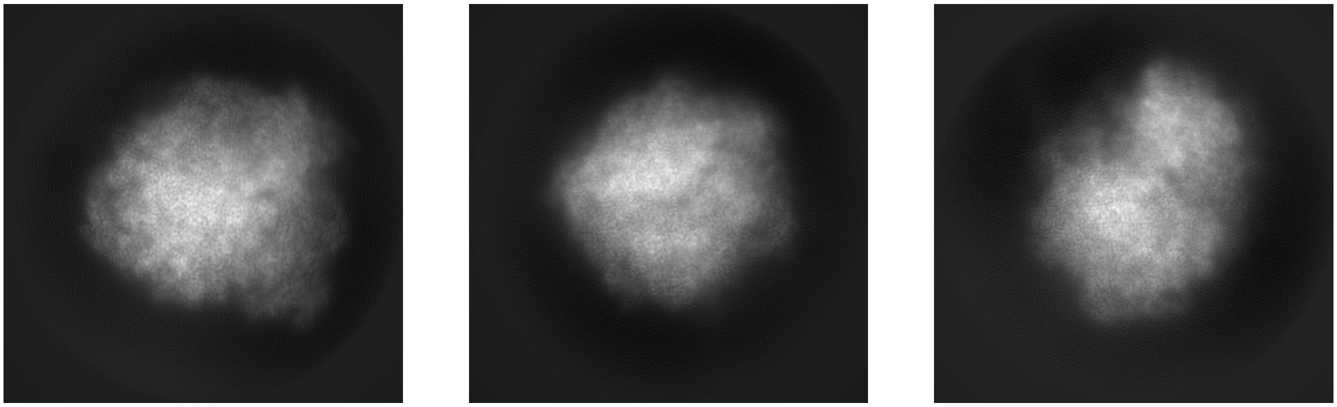
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

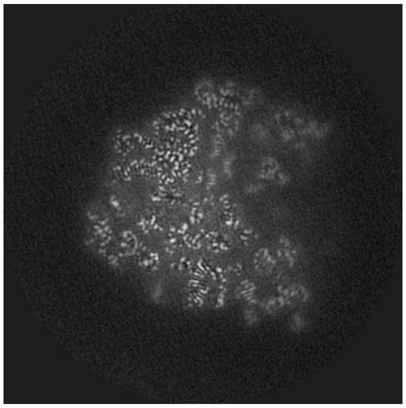


X Y Z

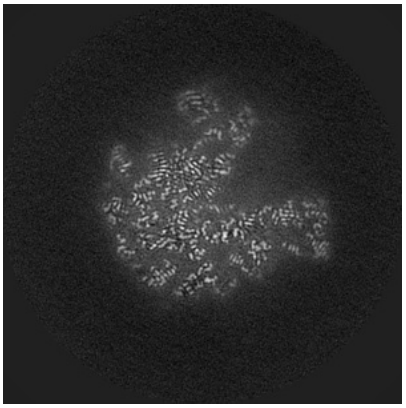
The images above show the map projected in three orthogonal directions.

6.2 Central slices

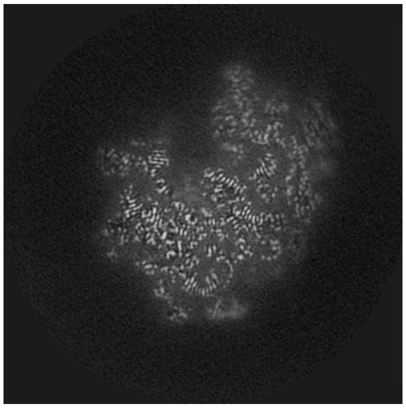
6.2.1 Primary map



X Index: 204

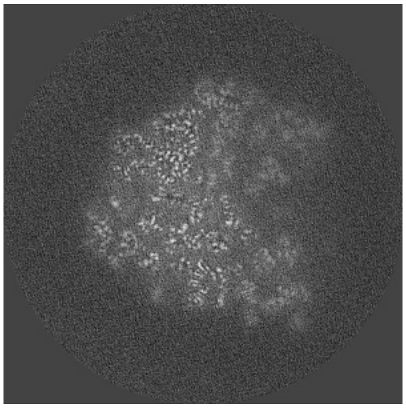


Y Index: 204

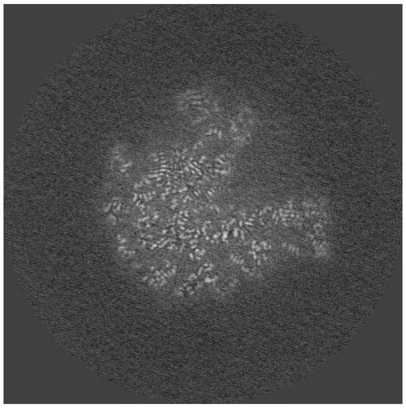


Z Index: 204

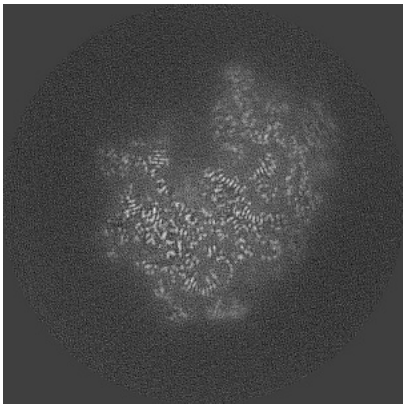
6.2.2 Raw map



X Index: 204



Y Index: 204

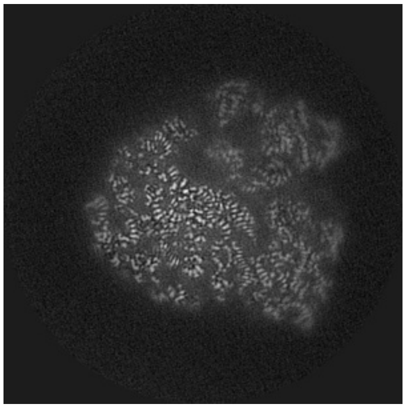


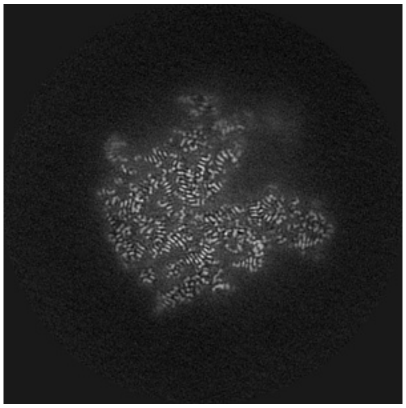
Z Index: 204

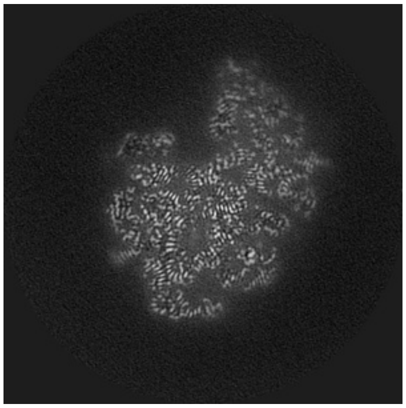
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

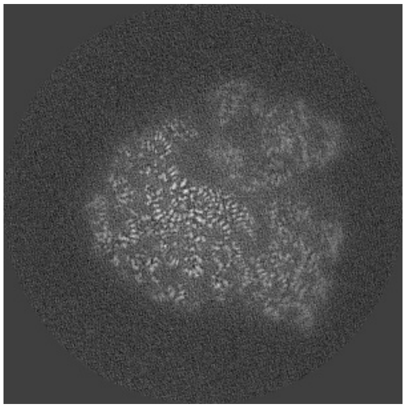
6.3.1 Primary map

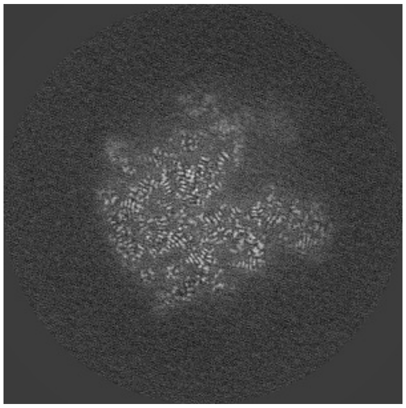

X Index: 219

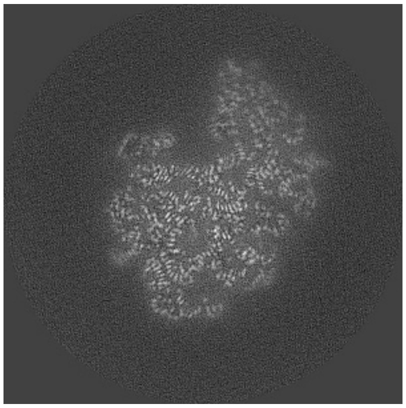

Y Index: 195


Z Index: 188

6.3.2 Raw map


X Index: 219

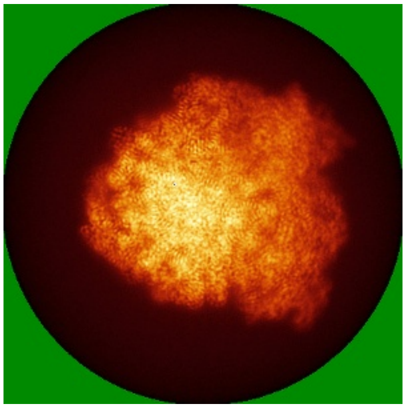

Y Index: 196


Z Index: 187

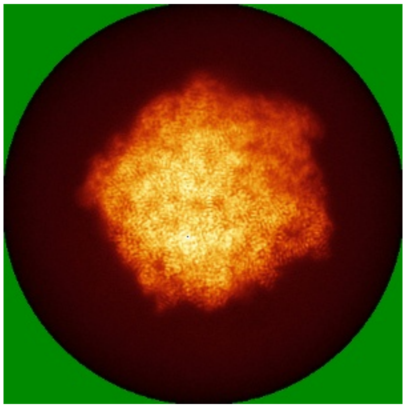
The images above show the largest variance slices of the map in three orthogonal directions.

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

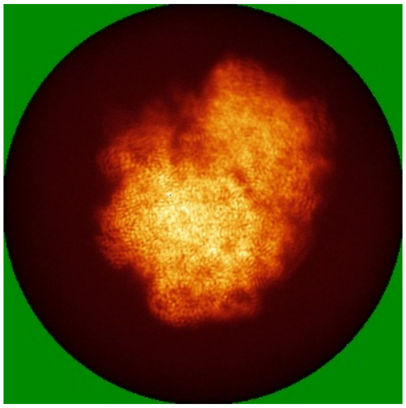
6.4.1 Primary map



X

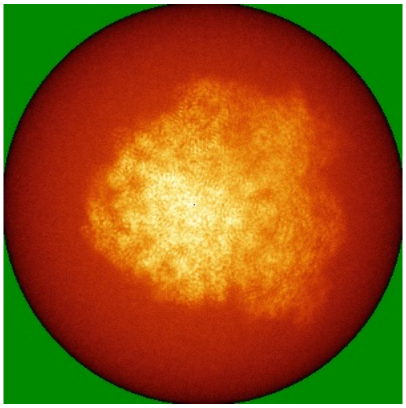


Y

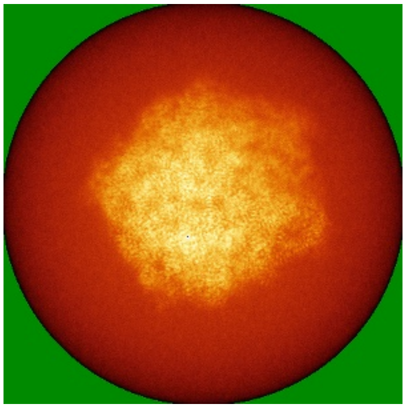


Z

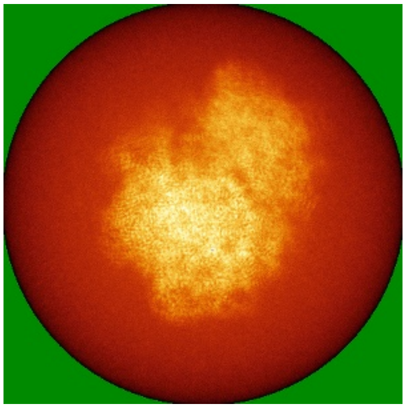
6.4.2 Raw map



X



Y

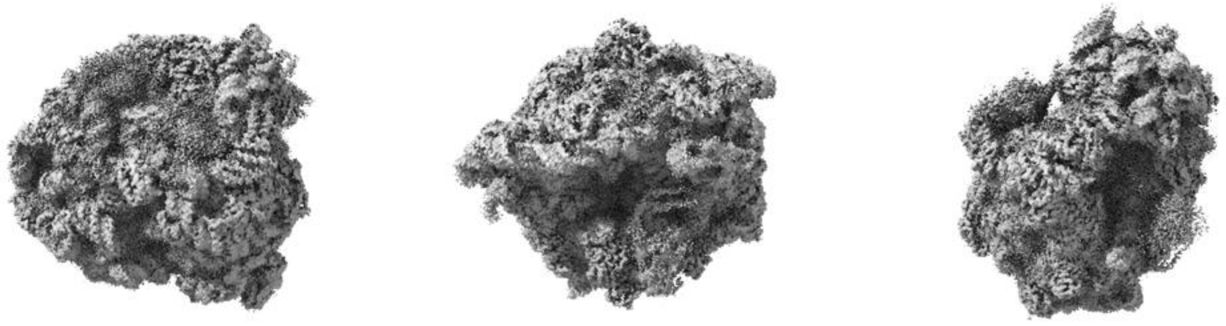


Z

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

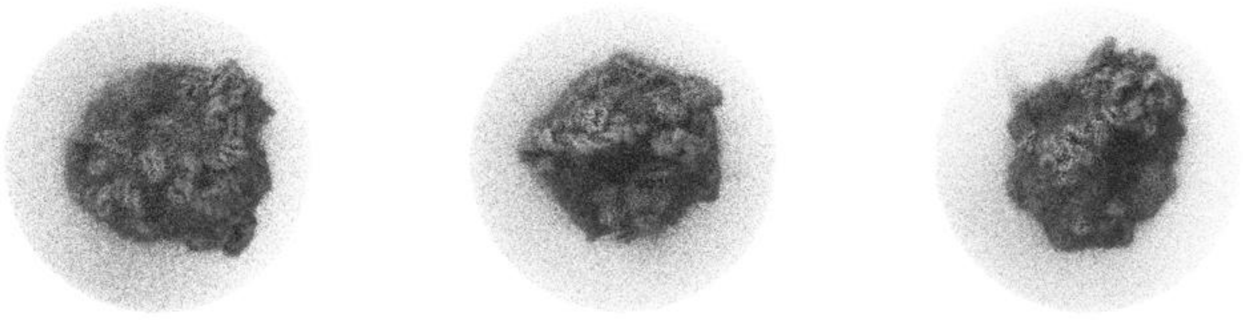
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

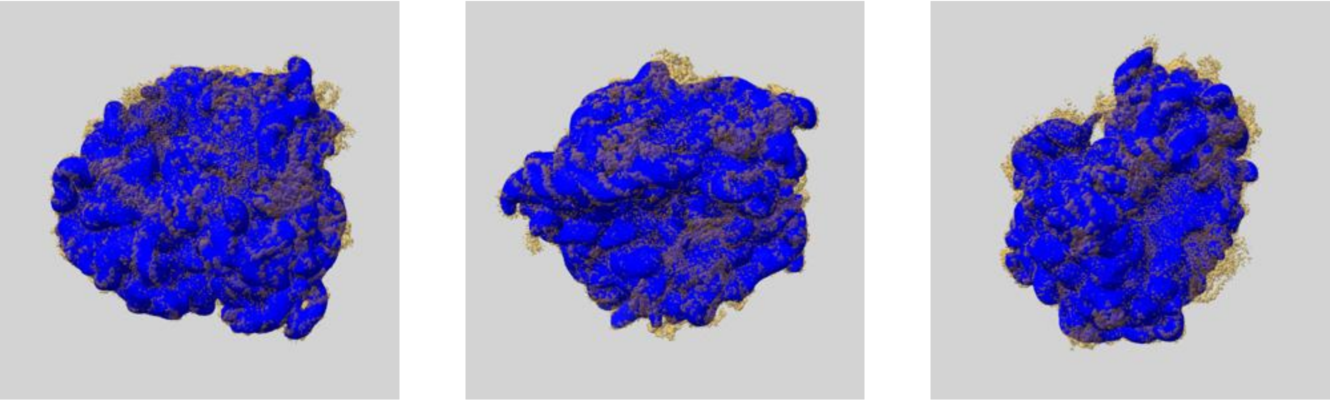
6.6 Mask visualisation ⓘ

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_12695_msk_1.map ⓘ

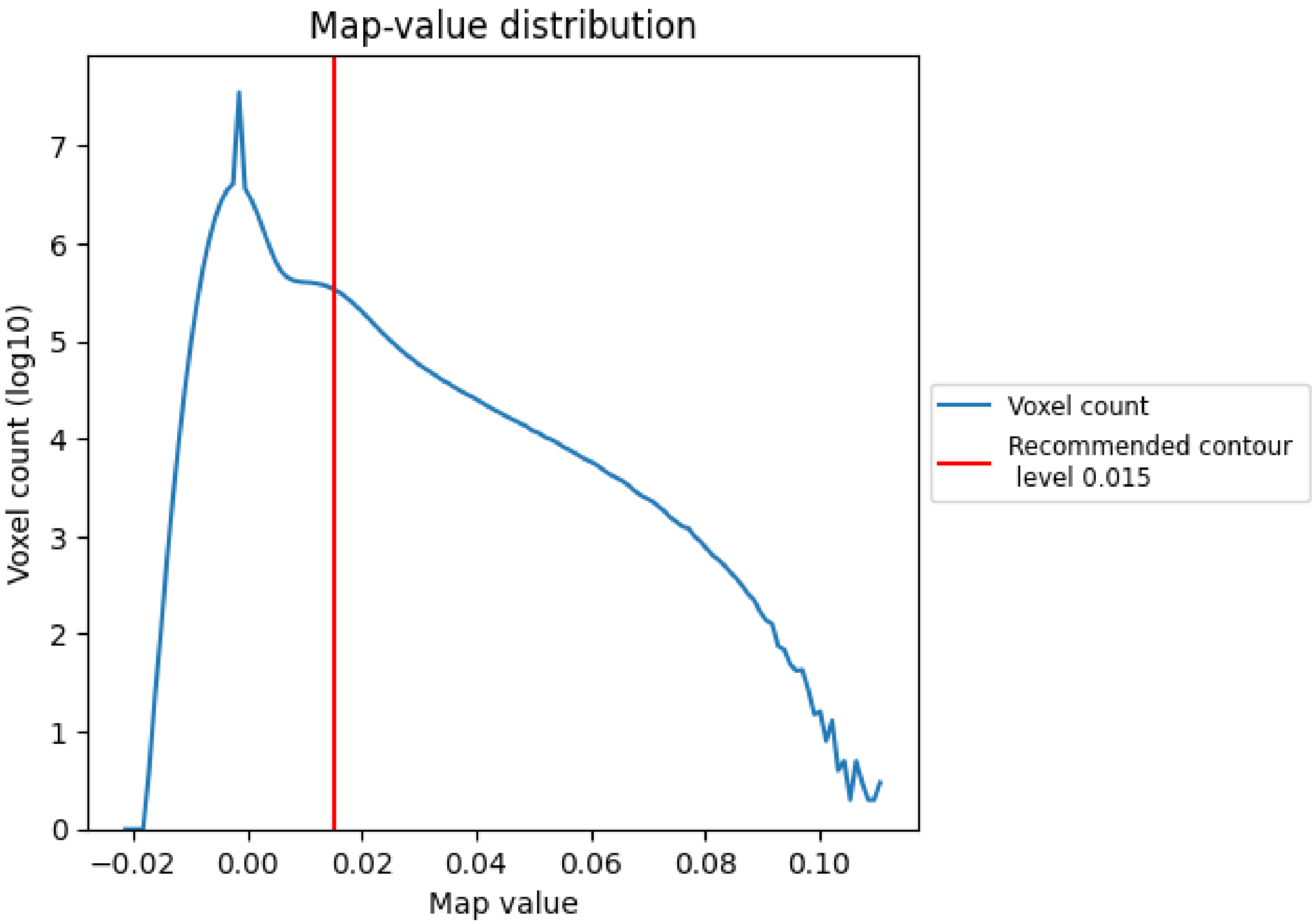


X Y Z

7 Map analysis ⓘ

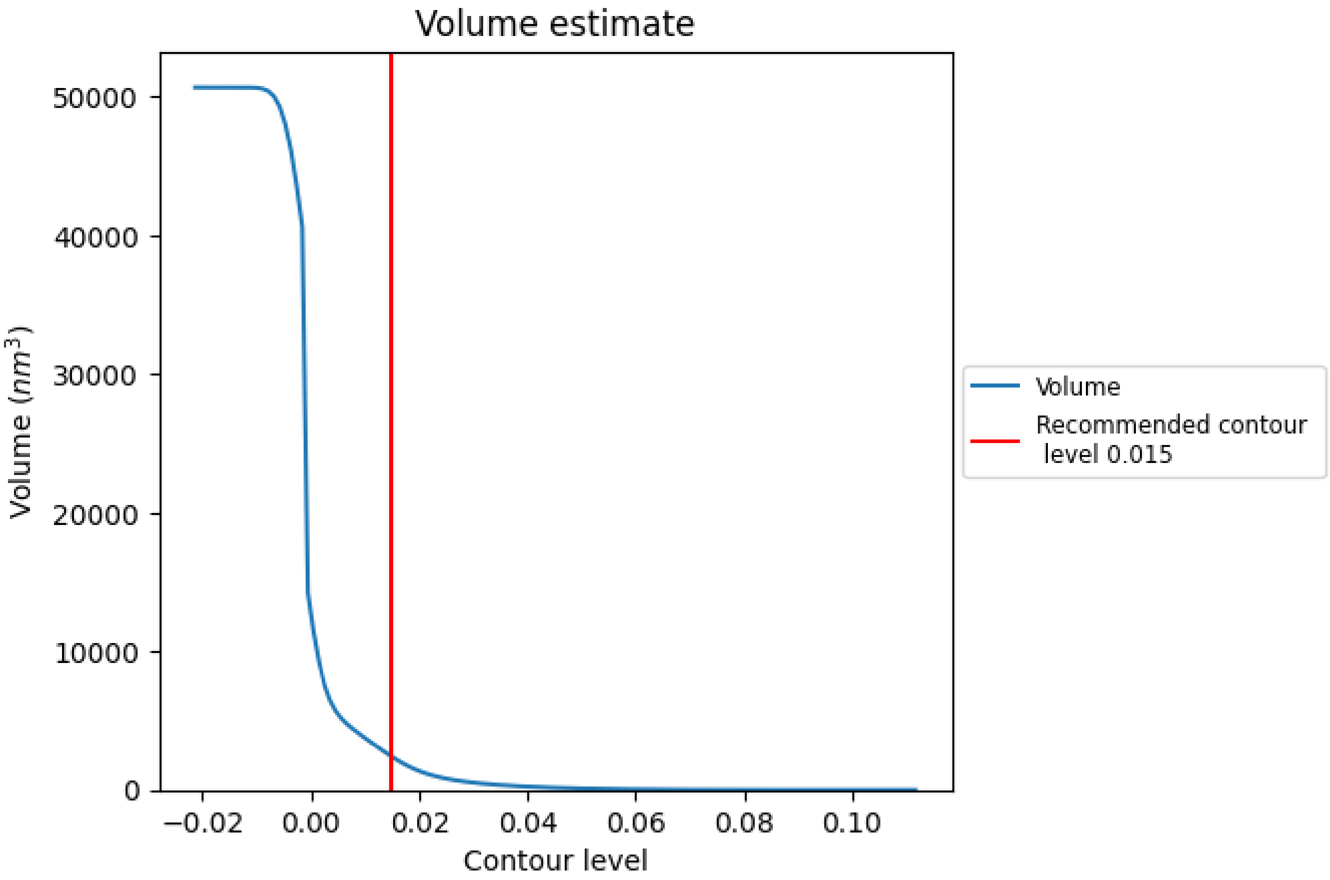
This section contains the results of statistical analysis of the map.

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.

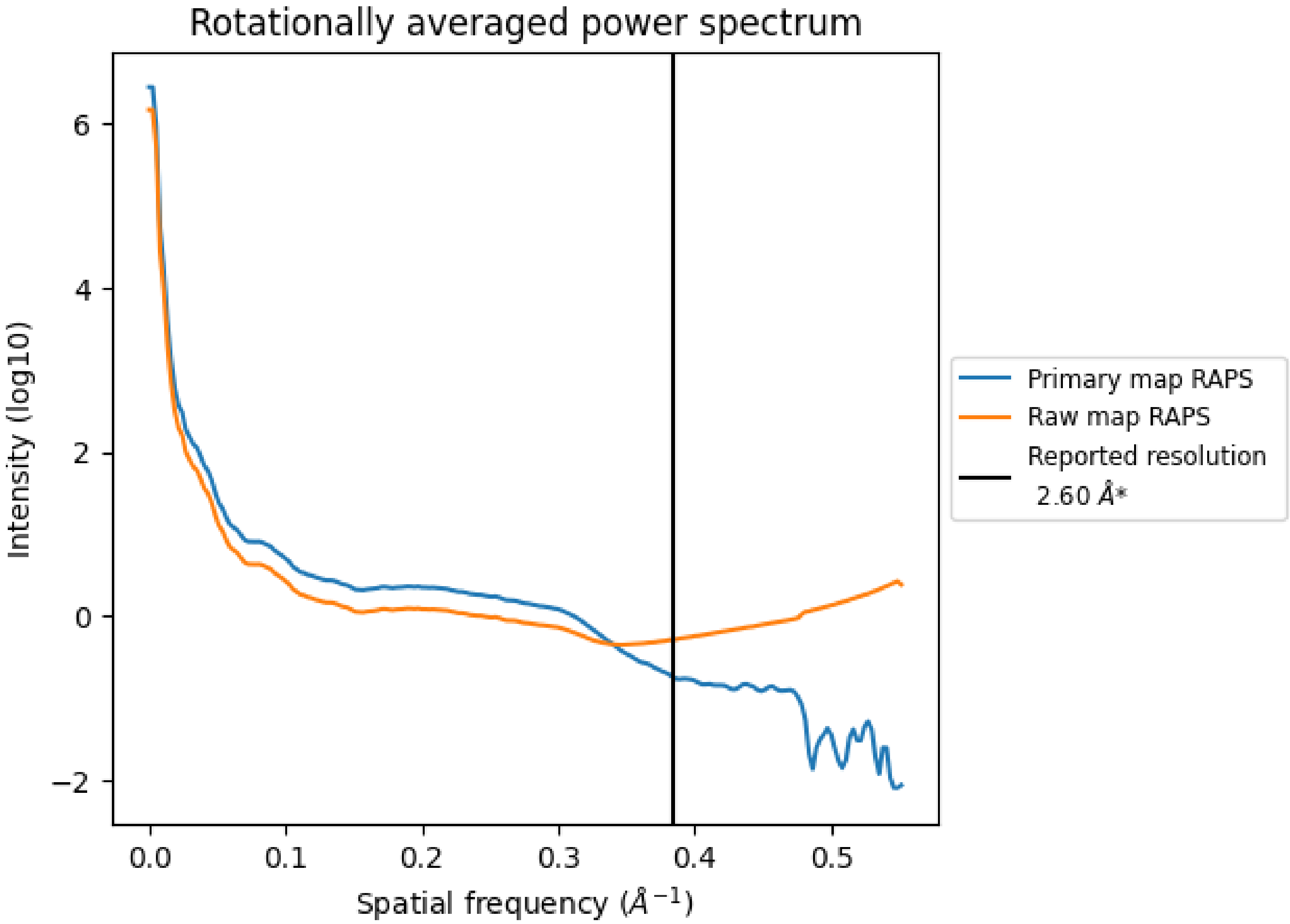
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2396 nm^3; this corresponds to an approximate mass of 2165 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 ⓘ

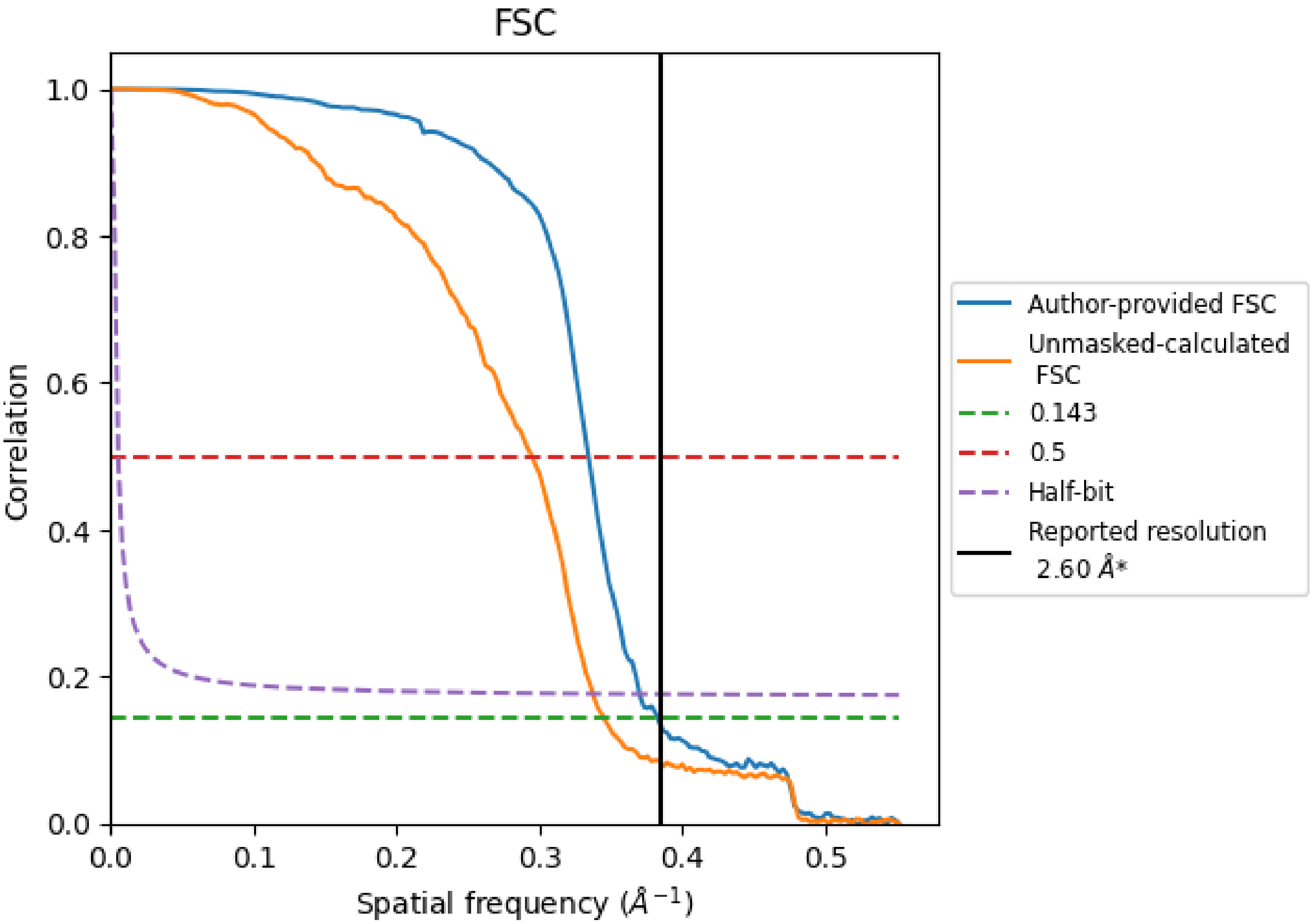


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates ⓘ

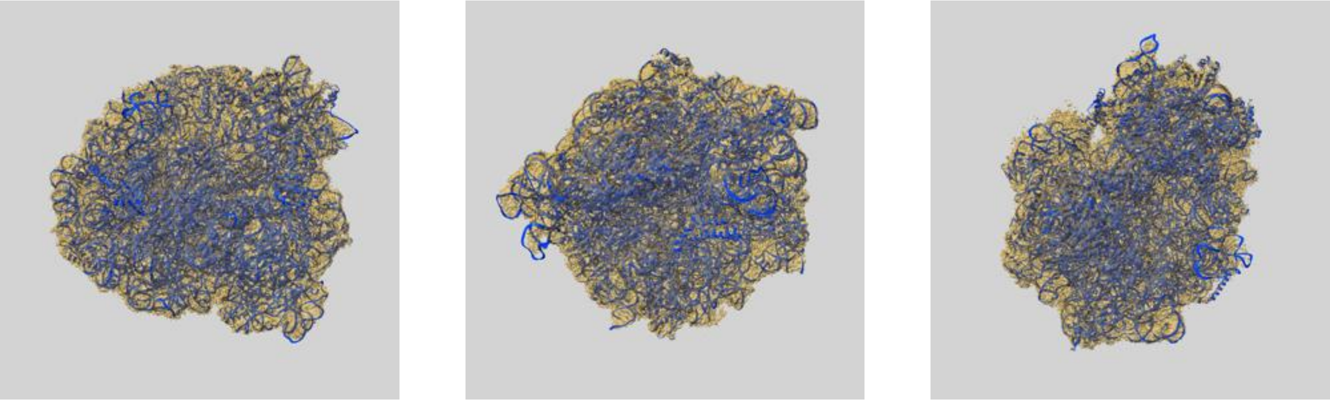
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	2.99	2.70
Unmasked-calculated*	2.90	3.39	2.96

*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 2.90 differs from the reported value 2.6 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12695 and PDB model 7O1C. Per-residue inclusion information can be found in section 3 on page 16.

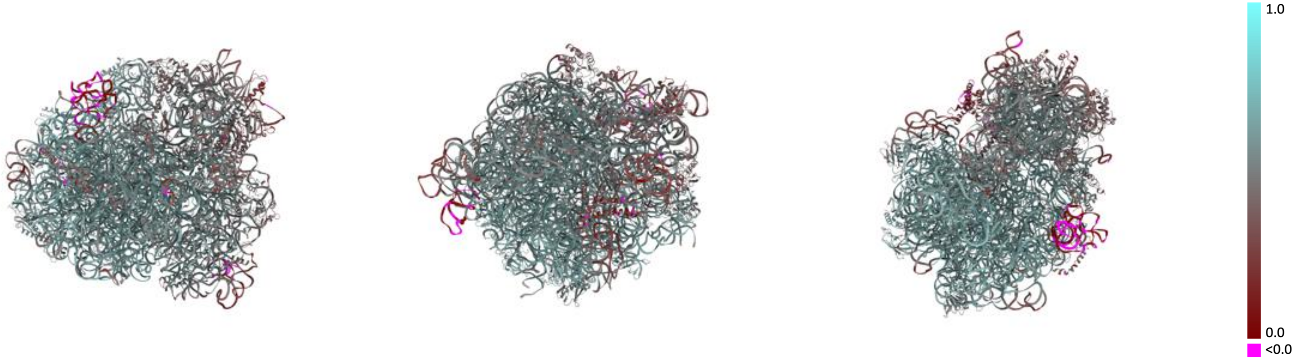
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

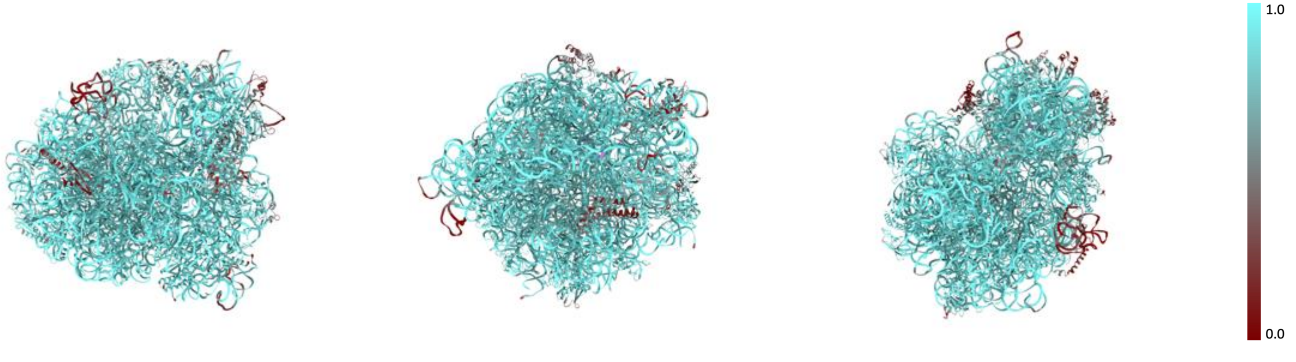
9.2 Q-score mapped to coordinate model ⓘ



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.

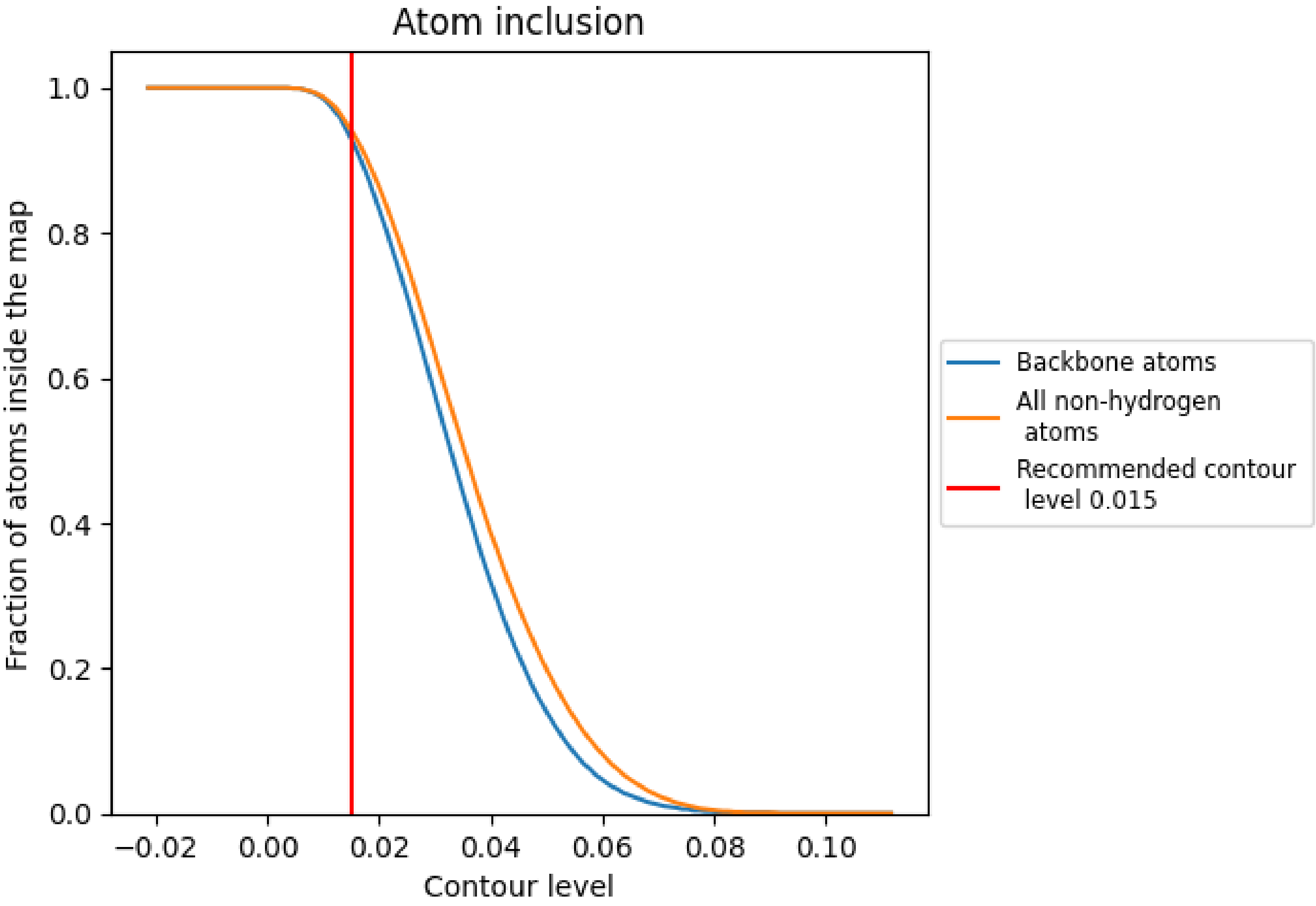
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9410	0.5550
AA	0.9590	0.5270
AB	0.5960	0.3870
AC	0.8500	0.4360
AD	0.8410	0.4500
AE	0.9450	0.5100
AF	0.8810	0.4910
AG	0.8140	0.4290
AH	0.9090	0.5090
AI	0.7840	0.4280
AJ	0.6360	0.3580
AK	0.9530	0.5230
AL	0.9760	0.5520
AM	0.8510	0.4580
AN	0.9040	0.4500
AO	0.9360	0.5230
AP	0.9120	0.4960
AQ	0.9450	0.5040
AR	0.9540	0.5240
AS	0.8330	0.4340
AT	0.9340	0.5270
AU	0.8760	0.4540
B0	0.9740	0.6090
B1	0.9800	0.5780
B2	1.0000	0.6340
B3	1.0000	0.6300
B4	0.9930	0.6200
B5	1.0000	0.5670
B7	1.0000	0.5200
B8	0.9990	0.4730
B9	0.7580	0.3640
BA	0.9710	0.5970
BB	0.9840	0.5930
BC	0.9970	0.6310
BD	0.9730	0.6200

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Chain	Atom inclusion	Q-score
BE	0.8800	0.5710
BF	0.9070	0.4950
BG	0.8610	0.5360
BH	0.4520	0.3840
BI	0.5510	0.3810
BJ	0.9810	0.6150
BK	0.9910	0.6060
BL	0.9570	0.5940
BM	0.9950	0.6130
BN	0.9910	0.6310
BO	0.9280	0.5730
BP	0.9720	0.6060
BQ	0.9880	0.6250
BR	0.9250	0.5830
BS	0.9800	0.6040
BT	0.9650	0.5770
BU	0.9200	0.5460
BV	0.9210	0.5930
BW	0.9810	0.6060
BX	0.9870	0.6060
BY	0.9180	0.5440
BZ	0.9430	0.5870