wwPDB EM Validation Summary Report

Jan 7, 2025 – 07:35 pm GMT

PDB ID	:	9FNY
EMDB ID	:	EMD-50611
Title	:	PF30S-PF30S dimer mediated by aRDF from P. furiosus (Structure I)
Authors	:	Hassan, A.H.; Demo, G.
Deposited on	:	2024-06-11
Resolution	:	3.20 Å(reported)
Based on initial models	:	4V6U, ., 7ZHG

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:

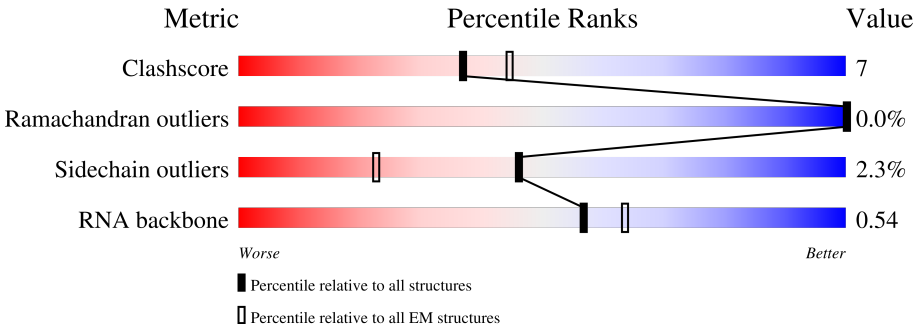
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A1	60	5% 75% 25%
1	B1	60	12% 90% 10%
2	A2	37	62% 32% 5%
2	B2	37	84% 11% 5%
3	A3	306	75% 22%
3	A4	306	76% 19% 5%
3	B3	306	77% 19%

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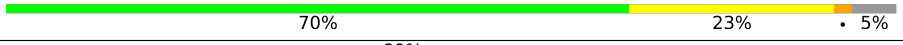
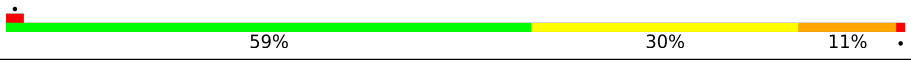
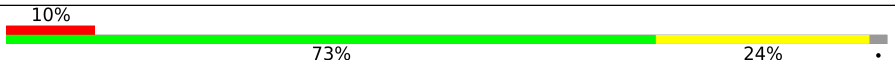
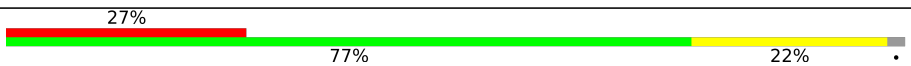
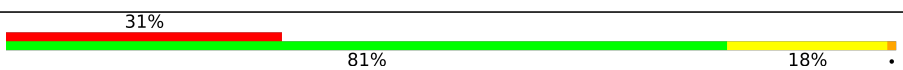
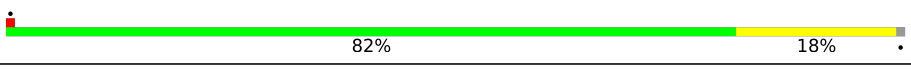
Mol	Chain	Length	Quality of chain
3	B4	306	
4	A5	123	
4	B5	123	
5	AA	1495	
5	BA	1495	
6	AB	202	
6	BB	202	
7	AC	210	
7	BC	210	
8	AD	198	
8	BD	198	
9	AE	180	
9	BE	180	
10	AF	243	
10	BF	243	
11	AG	236	
11	BG	236	
12	AH	125	
12	BH	125	
13	AI	215	
13	BI	215	
14	AJ	130	
14	BJ	130	
15	AK	127	
15	BK	127	

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Mol	Chain	Length	Quality of chain
16	AL	135	76% 19% 5%
16	BL	135	14% 73% 21% 5%
17	AM	102	23% 71% 28%
17	BM	102	24% 76% 24%
18	AN	137	75% 18% 7%
18	BN	137	71% 21% 7%
19	AO	147	72% 25%
19	BO	147	71% 25%
20	AP	148	8% 64% 24% 11%
20	BP	148	59% 65% 23% 11%
21	AQ	56	64% 21% 11%
21	BQ	56	7% 61% 25% 11%
22	AR	158	80% 18%
22	BR	158	80% 18%
23	AS	113	69% 27%
23	BS	113	82% 14%
24	AT	67	81% 13% 6%
24	BT	67	13% 79% 15% 6%
25	AU	132	20% 66% 21% 13%
25	BU	132	63% 72% 15% 13%
26	AV	150	81% 17%
26	BV	150	19% 80% 19%
27	AW	99	69% 23% 6%
27	BW	99	78% 15% 6%
28	AX	50	42% 68% 22% 10%

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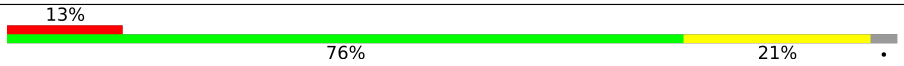
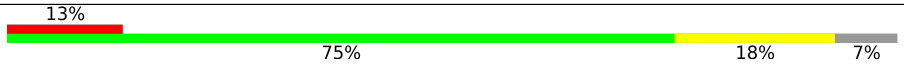
Mol	Chain	Length	Quality of chain
28	BX	50	
29	AY	63	
29	BY	63	
30	AZ	71	
30	BZ	71	

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 130968 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	60	Total	C	N	O	S	0	0
			471	295	83	83	10		
1	B1	60	Total	C	N	O	S	0	0
			471	295	83	83	10		

- Molecule 2 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	35	Total	C	N	O	S	0	0
			335	212	83	38	2		
2	B2	35	Total	C	N	O	S	0	0
			335	212	83	38	2		

- Molecule 3 is a protein called Archaeal Ribosome Dimerizing Factor (aRDF).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A3	298	Total	C	N	O	S	0	0
			2372	1535	395	438	4		
3	A4	292	Total	C	N	O	S	0	0
			2329	1509	388	428	4		
3	B3	295	Total	C	N	O	S	0	0
			2353	1524	391	434	4		
3	B4	290	Total	C	N	O	S	0	0
			2312	1497	385	426	4		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	301	HIS	-	expression tag	UNP Q8U3B0
A3	302	HIS	-	expression tag	UNP Q8U3B0
A3	303	HIS	-	expression tag	UNP Q8U3B0
A3	304	HIS	-	expression tag	UNP Q8U3B0
A3	305	HIS	-	expression tag	UNP Q8U3B0

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Chain	Residue	Modelled	Actual	Comment	Reference
A3	306	HIS	-	expression tag	UNP Q8U3B0
A4	301	HIS	-	expression tag	UNP Q8U3B0
A4	302	HIS	-	expression tag	UNP Q8U3B0
A4	303	HIS	-	expression tag	UNP Q8U3B0
A4	304	HIS	-	expression tag	UNP Q8U3B0
A4	305	HIS	-	expression tag	UNP Q8U3B0
A4	306	HIS	-	expression tag	UNP Q8U3B0
B3	301	HIS	-	expression tag	UNP Q8U3B0
B3	302	HIS	-	expression tag	UNP Q8U3B0
B3	303	HIS	-	expression tag	UNP Q8U3B0
B3	304	HIS	-	expression tag	UNP Q8U3B0
B3	305	HIS	-	expression tag	UNP Q8U3B0
B3	306	HIS	-	expression tag	UNP Q8U3B0
B4	301	HIS	-	expression tag	UNP Q8U3B0
B4	302	HIS	-	expression tag	UNP Q8U3B0
B4	303	HIS	-	expression tag	UNP Q8U3B0
B4	304	HIS	-	expression tag	UNP Q8U3B0
B4	305	HIS	-	expression tag	UNP Q8U3B0
B4	306	HIS	-	expression tag	UNP Q8U3B0

- Molecule 4 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A5	123	Total	C	N	O	S	0	0
			939	599	155	181	4		
4	B5	123	Total	C	N	O	S	0	0
			939	599	155	181	4		

- Molecule 5 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AA	1495	Total	C	N	O	P	0	0
			32135	14297	5954	10389	1495		
5	BA	1495	Total	C	N	O	P	0	0
			32135	14297	5954	10389	1495		

- Molecule 6 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AB	197	Total	C	N	O	S	0	0
			1579	1022	271	282	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	BB	197	Total 1579	C 1022	N 271	O 282	S 4	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AC	195	Total 1532	C 980	N 283	O 266	S 3	0	0
7	BC	195	Total 1532	C 980	N 283	O 266	S 3	0	0

- Molecule 8 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AD	184	Total 1511	C 978	N 263	O 265	S 5	0	0
8	BD	184	Total 1511	C 978	N 263	O 265	S 5	0	0

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AE	173	Total 1455	C 915	N 282	O 254	S 4	0	0
9	BE	173	Total 1455	C 915	N 282	O 254	S 4	0	0

- Molecule 10 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AF	242	Total 1981	C 1280	N 356	O 340	S 5	0	0
10	BF	242	Total 1981	C 1280	N 356	O 340	S 5	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AG	227	Total 1794	C 1134	N 335	O 318	S 7	0	0
11	BG	227	Total 1794	C 1134	N 335	O 318	S 7	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AH	123	Total	C	N	O	S	0	0
			971	615	178	177	1		
12	BH	123	Total	C	N	O	S	0	0
			971	615	178	177	1		

- Molecule 13 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AI	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		
13	BI	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AJ	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		
14	BJ	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		

- Molecule 15 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	AK	124	Total	C	N	O	0	0
			977	607	204	166		
15	BK	124	Total	C	N	O	0	0
			977	607	204	166		

- Molecule 16 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	128	Total	C	N	O	S	0	0
			1006	630	191	180	5		
16	BL	128	Total	C	N	O	S	0	0
			1006	630	191	180	5		

- Molecule 17 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AM	102	Total	C	N	O	S	0	0
			822	507	159	152	4		
17	BM	102	Total	C	N	O	S	0	0
			822	507	159	152	4		

- Molecule 18 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AN	127	Total	C	N	O	S	0	0
			954	591	190	171	2		
18	BN	127	Total	C	N	O	S	0	0
			954	591	190	171	2		

- Molecule 19 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AO	143	Total	C	N	O	S	0	0
			1118	710	215	190	3		
19	BO	143	Total	C	N	O	S	0	0
			1118	710	215	190	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AP	131	Total	C	N	O	S	0	0
			1052	663	206	178	5		
20	BP	131	Total	C	N	O	S	0	0
			1052	663	206	178	5		

- Molecule 21 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AQ	50	Total	C	N	O	S	0	0
			417	266	88	58	5		
21	BQ	50	Total	C	N	O	S	0	0
			417	266	88	58	5		

- Molecule 22 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	155	Total	C	N	O	S	0	0
			1283	818	244	217	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
22	BR	155	Total	C	N	O	S	0	0
			1283	818	244	217	4		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	110	Total	C	N	O	S	0	0
			903	575	168	156	4		
23	BS	110	Total	C	N	O	S	0	0
			903	575	168	156	4		

- Molecule 24 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AT	63	Total	C	N	O	S	0	0
			522	330	100	90	2		
24	BT	63	Total	C	N	O	S	0	0
			522	330	100	90	2		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AU	115	Total	C	N	O	S	0	0
			948	609	177	156	6		
25	BU	115	Total	C	N	O	S	0	0
			948	609	177	156	6		

- Molecule 26 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	AV	148	Total	C	N	O	0	0
			1209	781	218	210		
26	BV	148	Total	C	N	O	0	0
			1209	781	218	210		

- Molecule 27 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AW	93	Total	C	N	O	S	0	0
			774	503	126	143	2		
27	BW	93	Total	C	N	O	S	0	0
			774	503	126	143	2		

- Molecule 28 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AX	45	Total	C	N	O	S	0	0
			369	238	67	59	5		
28	BX	45	Total	C	N	O	S	0	0
			369	238	67	59	5		

- Molecule 29 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AY	61	Total	C	N	O	S	0	0
			465	298	83	79	5		
29	BY	61	Total	C	N	O	S	0	0
			465	298	83	79	5		

- Molecule 30 is a protein called Small ribosomal subunit protein eS28.

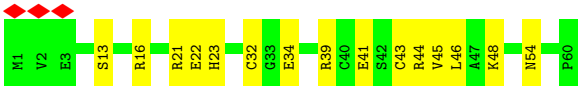
Mol	Chain	Residues	Atoms				AltConf	Trace
30	AZ	66	Total	C	N	O	0	0
			523	320	104	99		
30	BZ	66	Total	C	N	O	0	0
			523	320	104	99		

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.

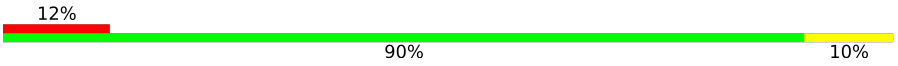
• Molecule 1: RNA-binding protein

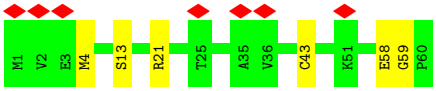
Chain A1:



• Molecule 1: RNA-binding protein

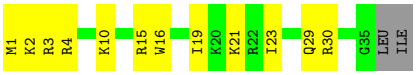
Chain B1:





• Molecule 2: Small ribosomal subunit protein eS32

Chain A2:

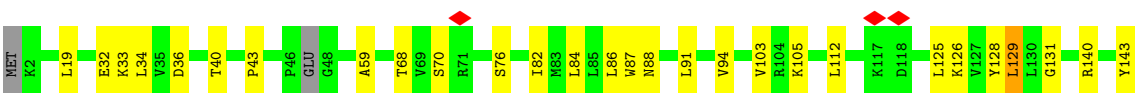


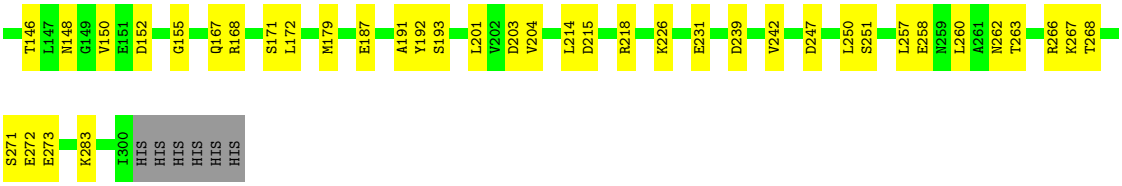
• Molecule 2: Small ribosomal subunit protein eS32

Chain B2:

• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

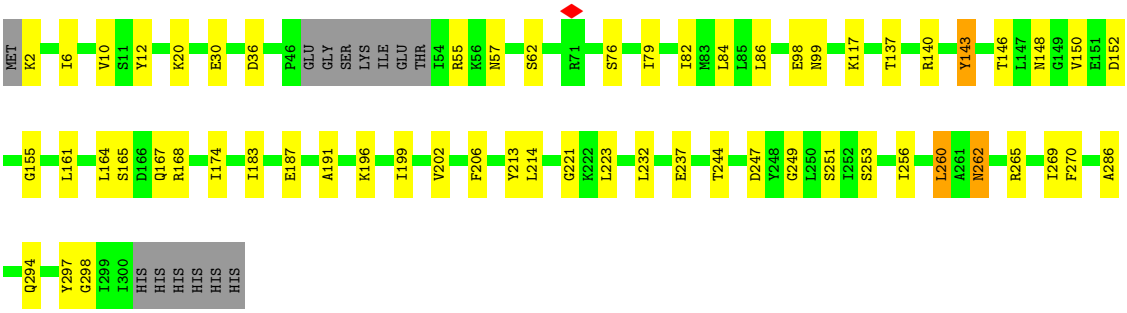
Chain A3:





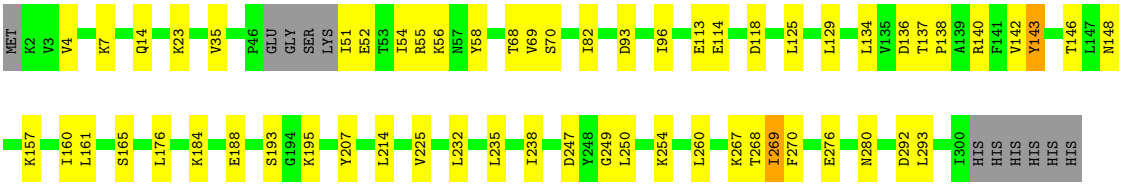
• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

Chain A4:



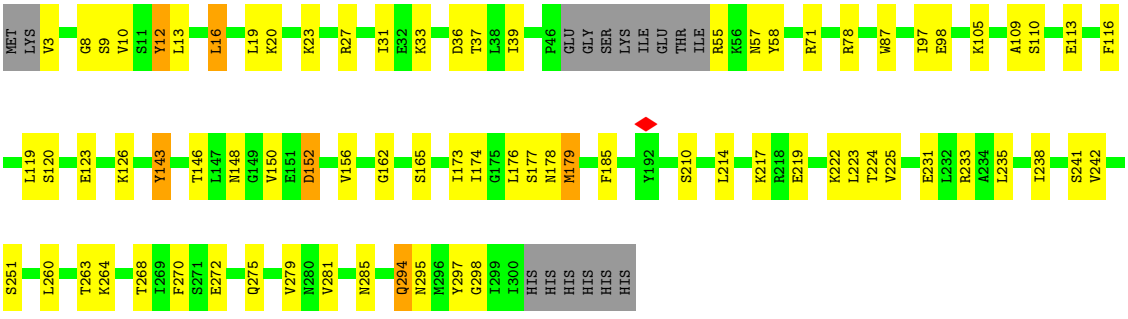
• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

Chain B3:



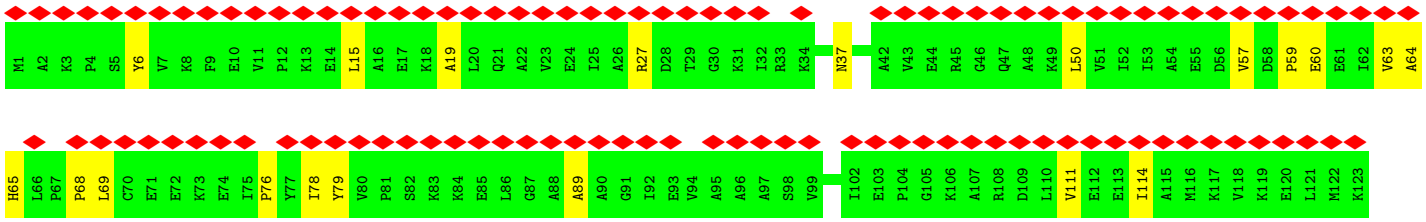
• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

Chain B4:



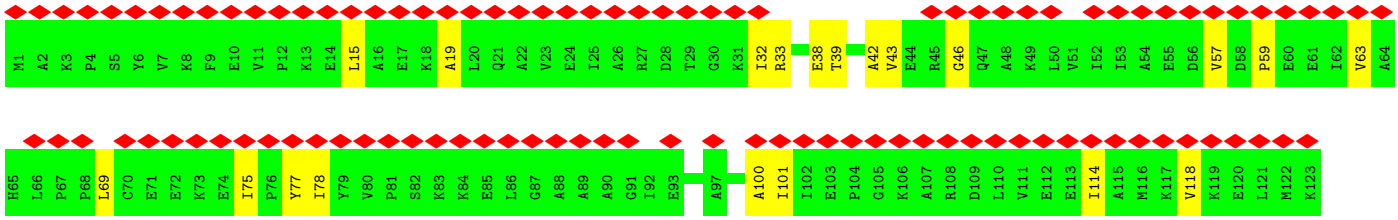
• Molecule 4: Large ribosomal subunit protein eL8

Chain A5:



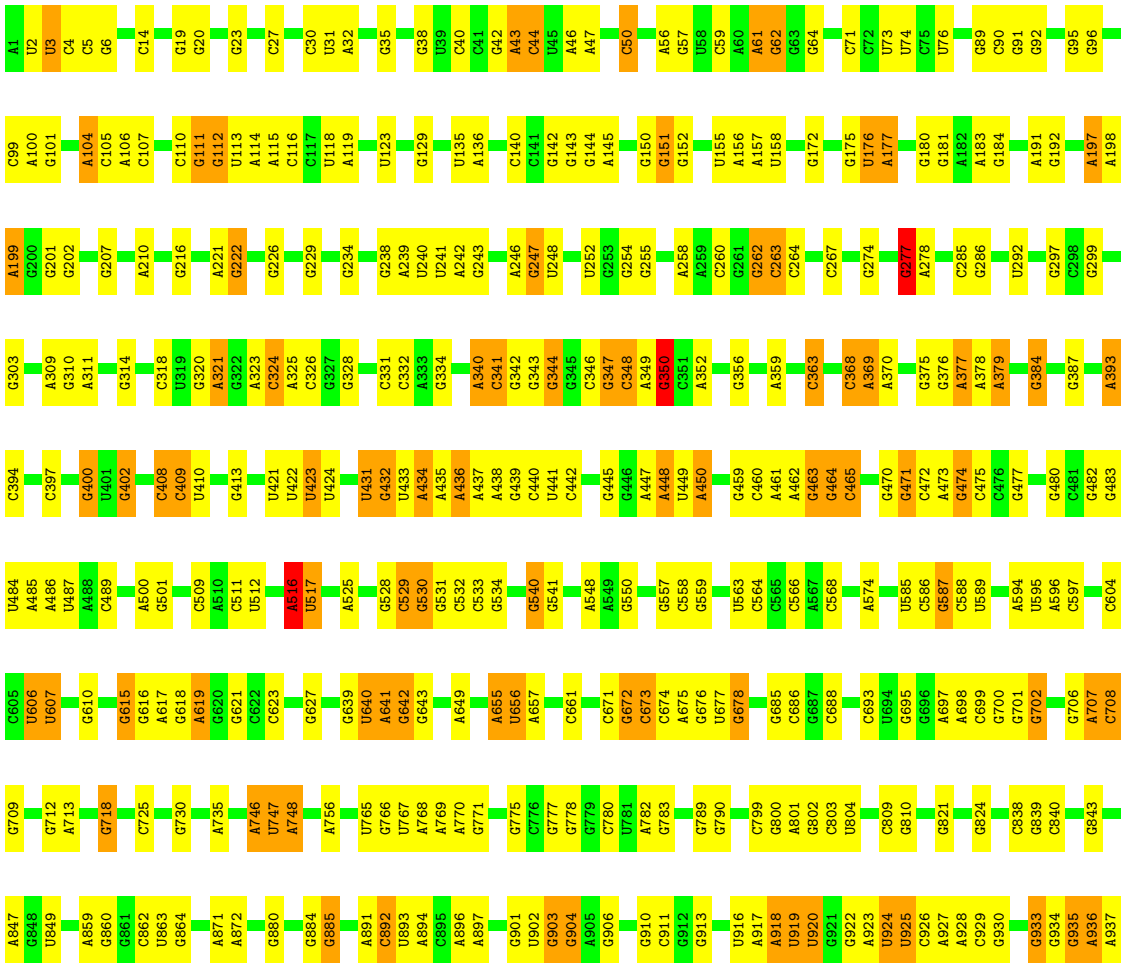
• Molecule 4: Large ribosomal subunit protein eL8

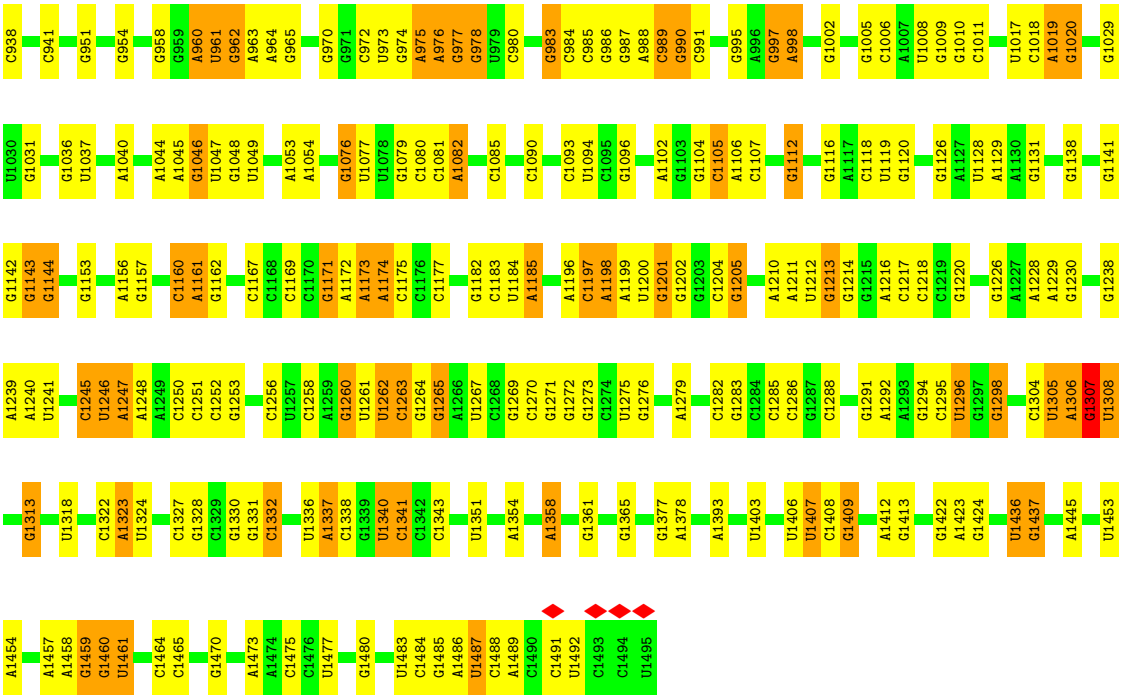
Chain B5:



• Molecule 5: 16S rRNA

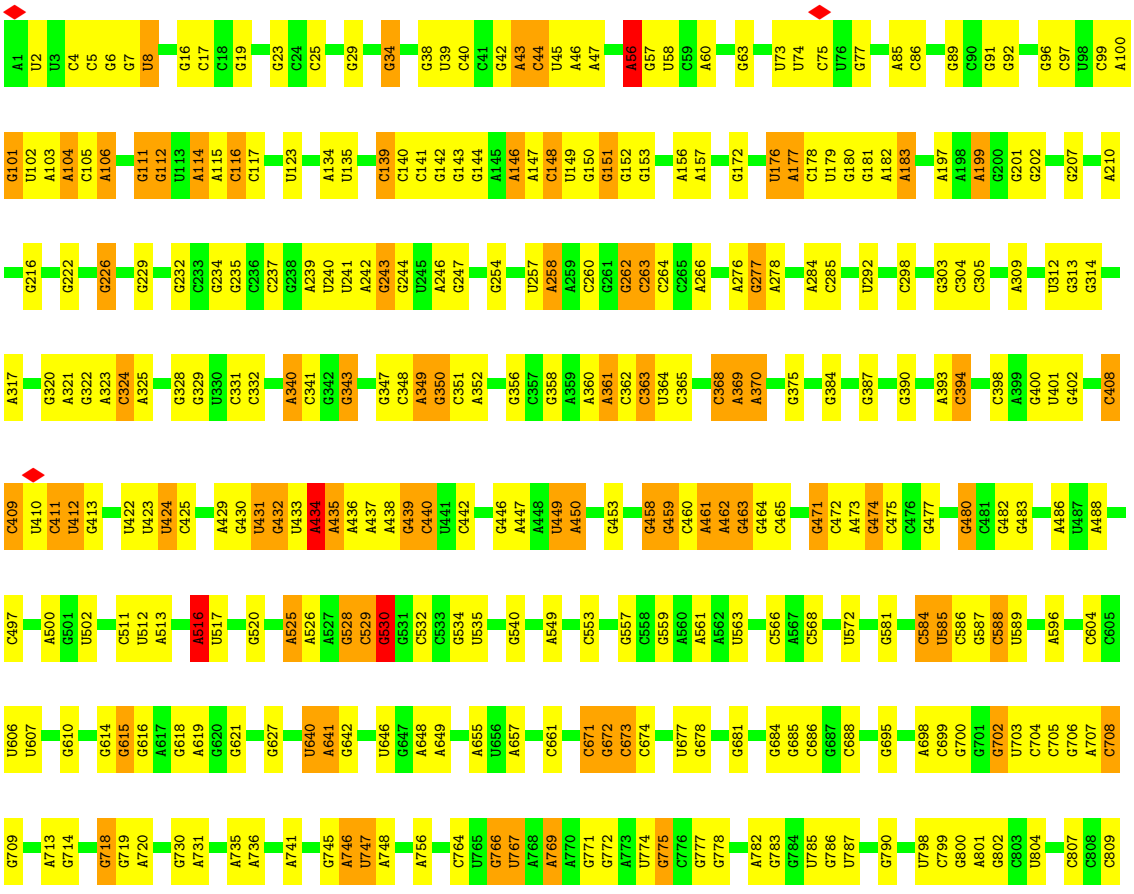
Chain AA:

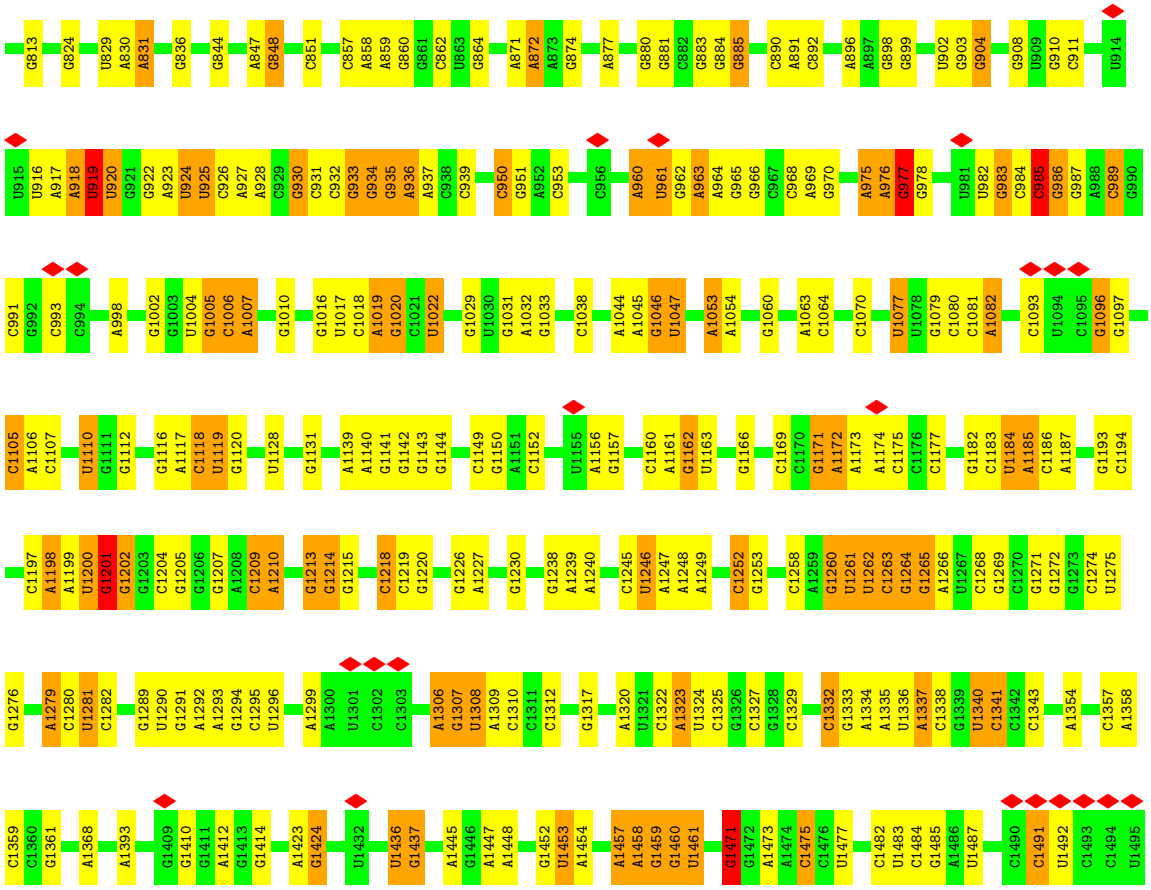




• Molecule 5: 16S rRNA

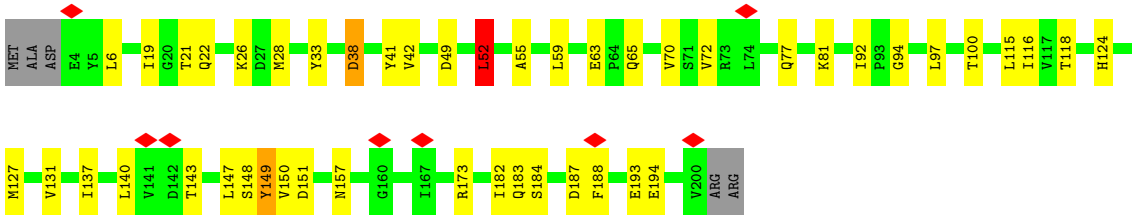
Chain BA:





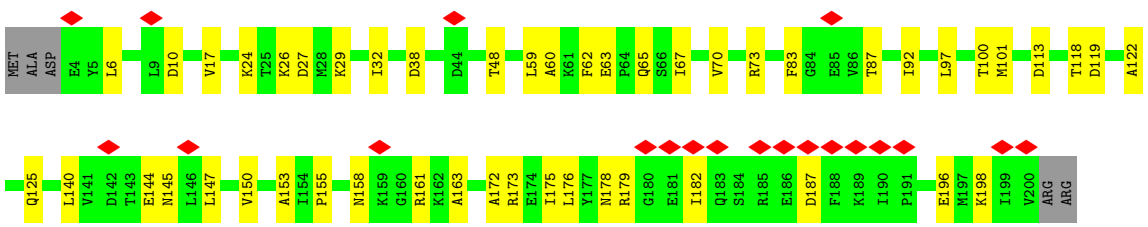
• Molecule 6: Small ribosomal subunit protein uS2

Chain AB:



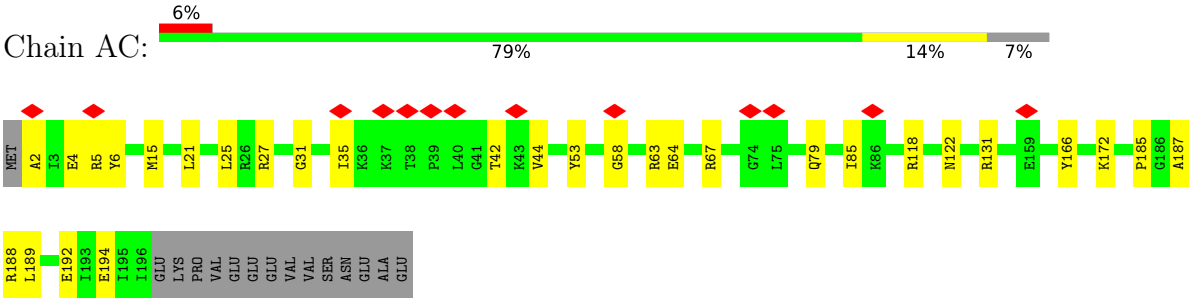
• Molecule 6: Small ribosomal subunit protein uS2

Chain BB:



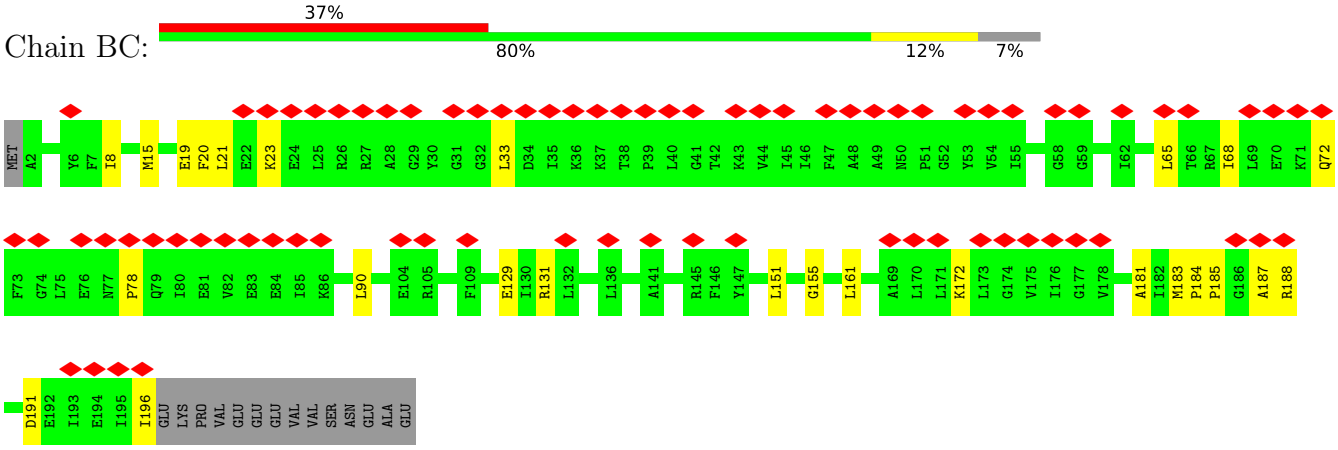
• Molecule 7: Small ribosomal subunit protein uS3

Chain AC:



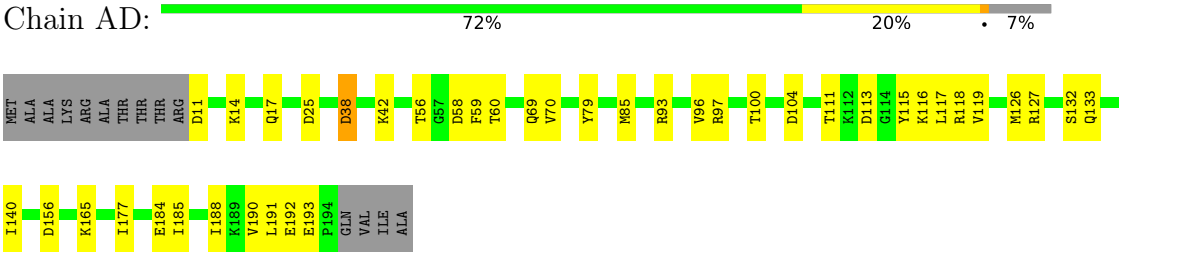
• Molecule 7: Small ribosomal subunit protein uS3

Chain BC:



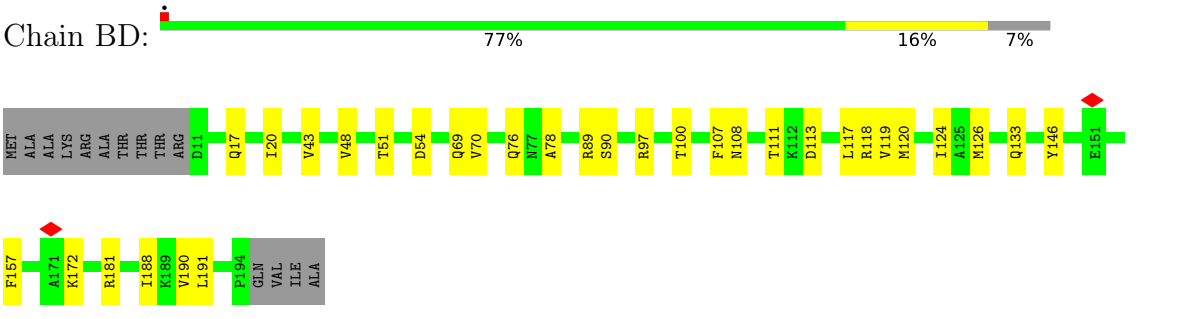
• Molecule 8: Small ribosomal subunit protein eS1

Chain AD:



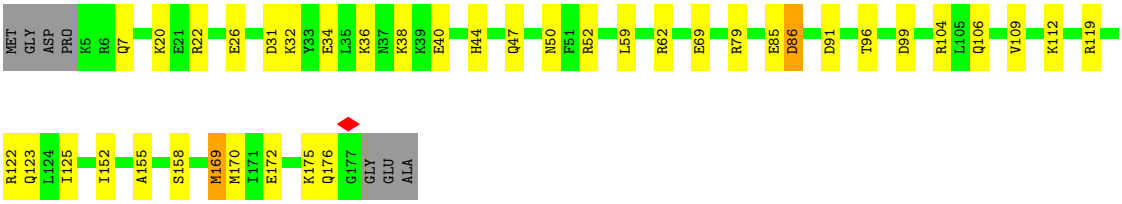
• Molecule 8: Small ribosomal subunit protein eS1

Chain BD:



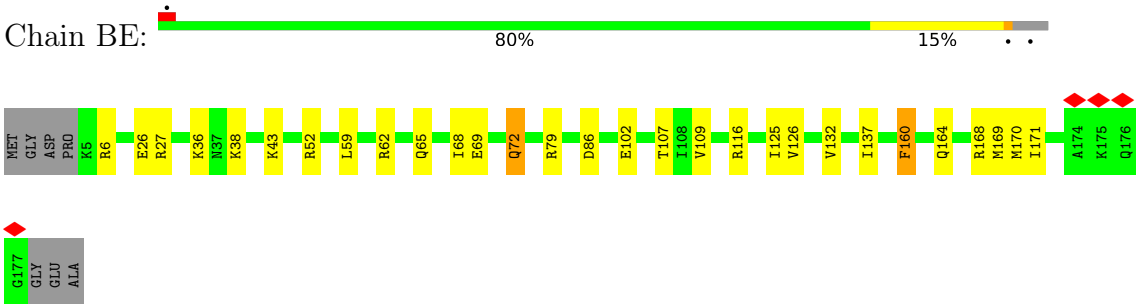
• Molecule 9: Small ribosomal subunit protein uS4

Chain AE:



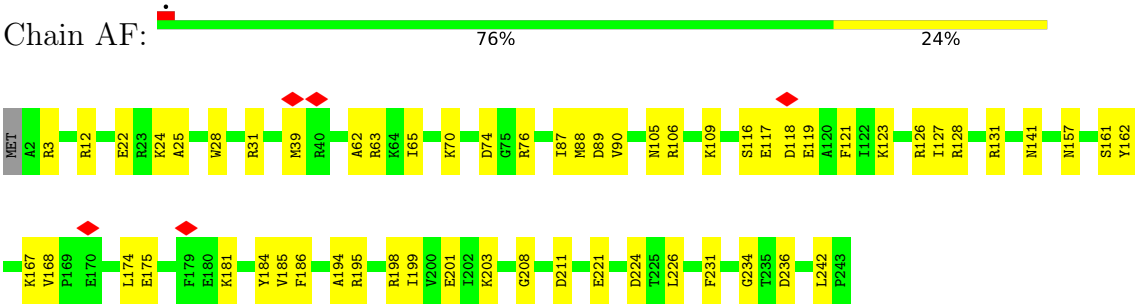
• Molecule 9: Small ribosomal subunit protein uS4

Chain BE:



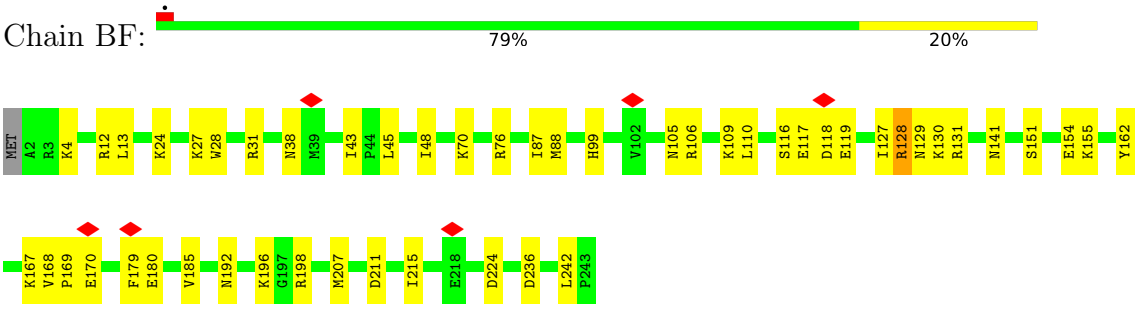
• Molecule 10: Small ribosomal subunit protein eS4

Chain AF:



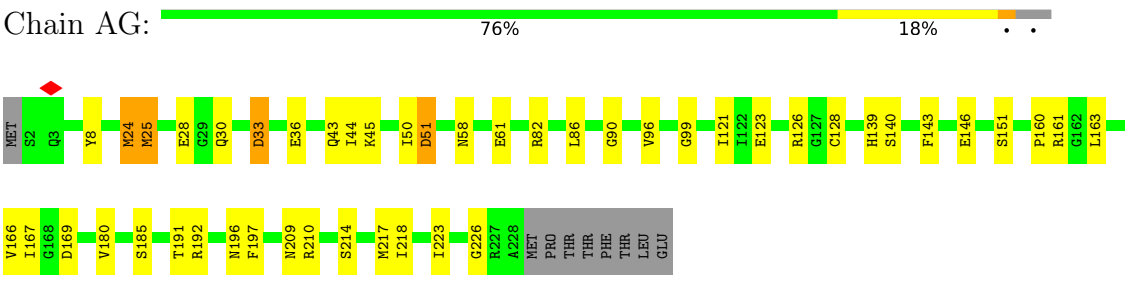
• Molecule 10: Small ribosomal subunit protein eS4

Chain BF:



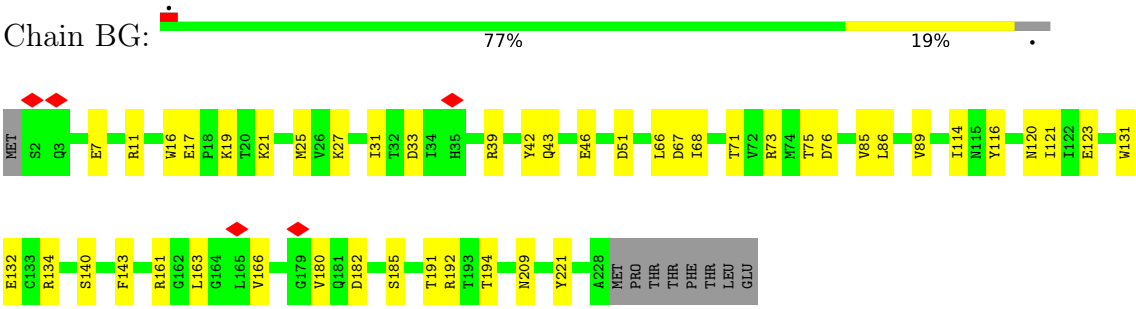
• Molecule 11: Small ribosomal subunit protein uS5

Chain AG:



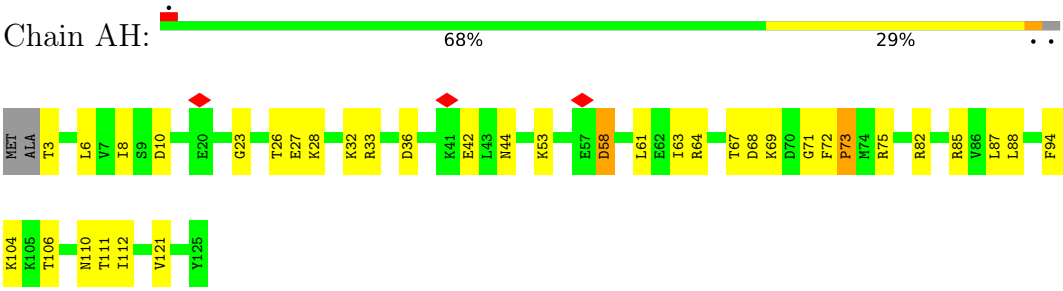
• Molecule 11: Small ribosomal subunit protein uS5

Chain BG:



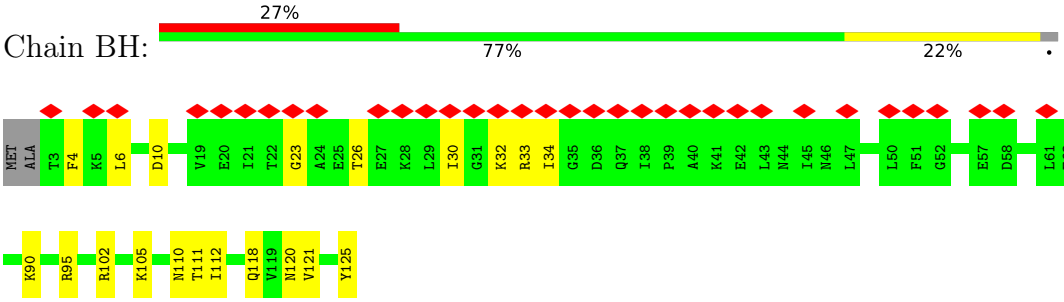
• Molecule 12: Small ribosomal subunit protein eS6

Chain AH:



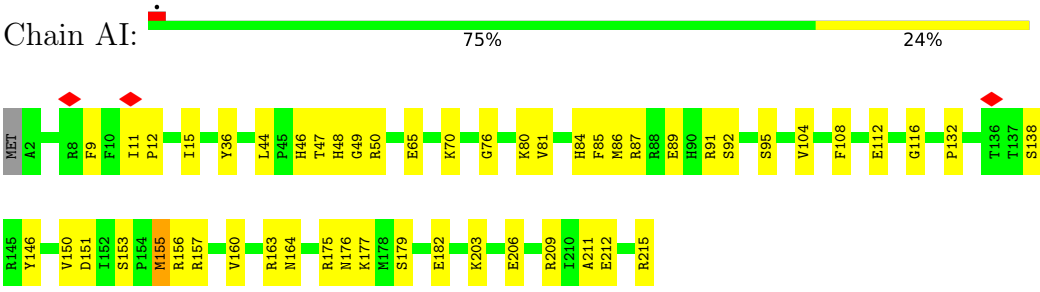
• Molecule 12: Small ribosomal subunit protein eS6

Chain BH:



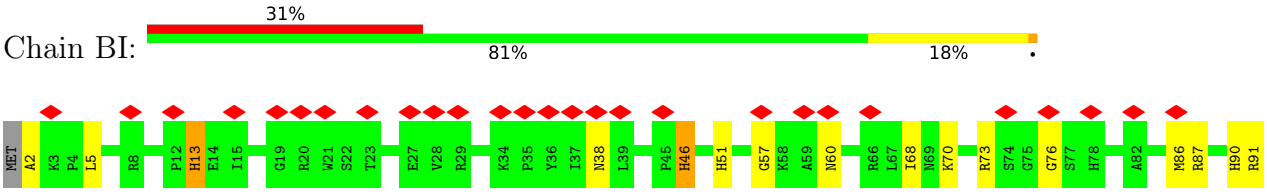
• Molecule 13: Small ribosomal subunit protein uS7

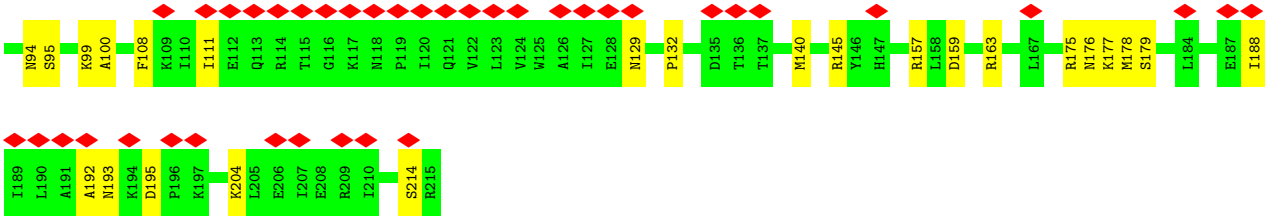
Chain AI:



• Molecule 13: Small ribosomal subunit protein uS7

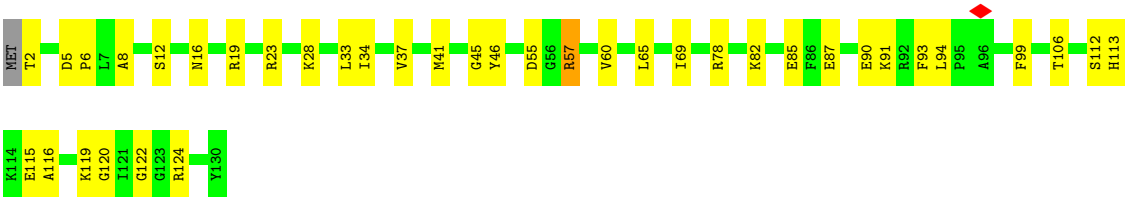
Chain BI:





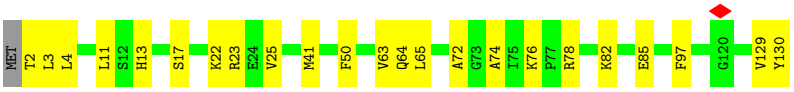
• Molecule 14: Small ribosomal subunit protein uS8

Chain AJ:



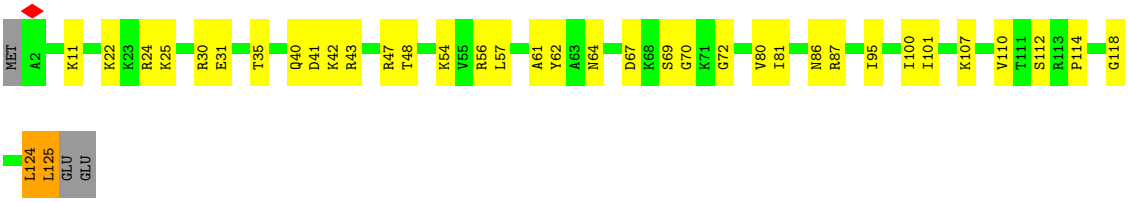
• Molecule 14: Small ribosomal subunit protein uS8

Chain BJ:



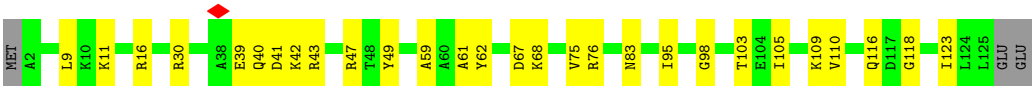
• Molecule 15: Small ribosomal subunit protein eS8

Chain AK:



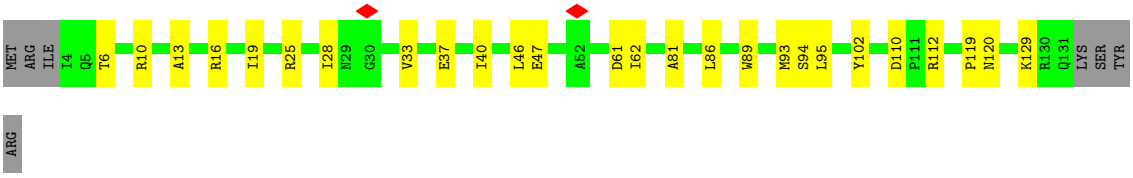
• Molecule 15: Small ribosomal subunit protein eS8

Chain BK:

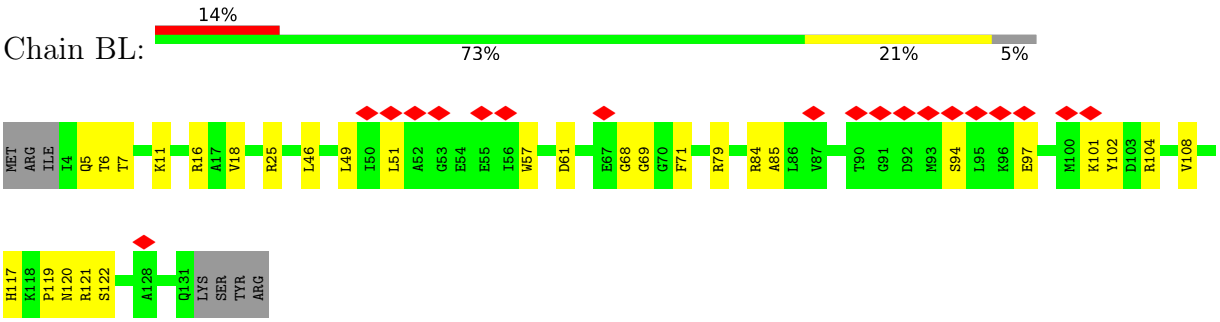


• Molecule 16: Small ribosomal subunit protein uS9

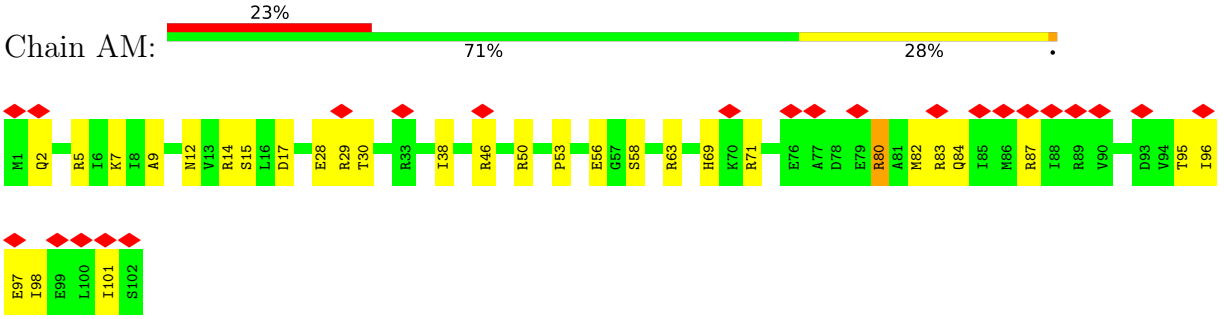
Chain AL:



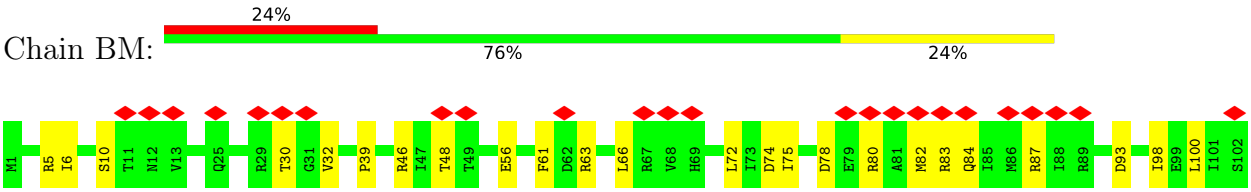
• Molecule 16: Small ribosomal subunit protein uS9



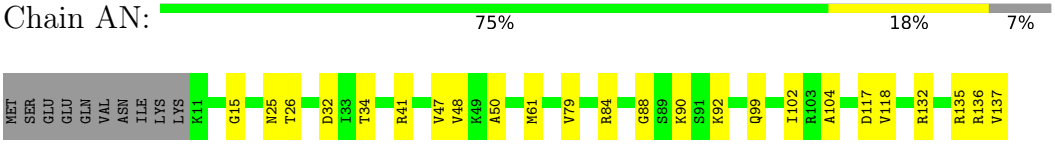
• Molecule 17: Small ribosomal subunit protein uS10



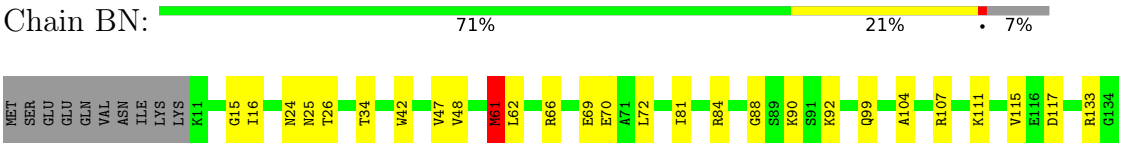
• Molecule 17: Small ribosomal subunit protein uS10



• Molecule 18: Small ribosomal subunit protein uS11

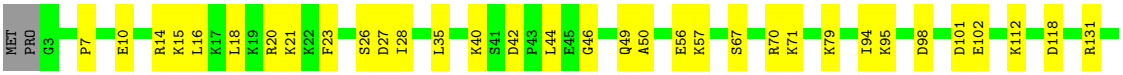


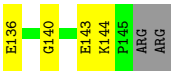
• Molecule 18: Small ribosomal subunit protein uS11



• Molecule 19: Small ribosomal subunit protein uS12

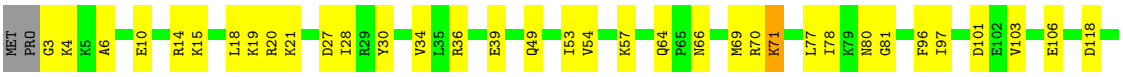
Chain AO:

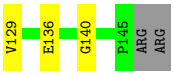




• Molecule 19: Small ribosomal subunit protein uS12

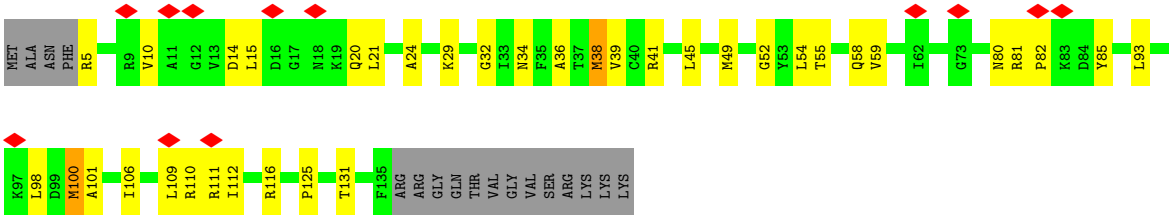
Chain BO:





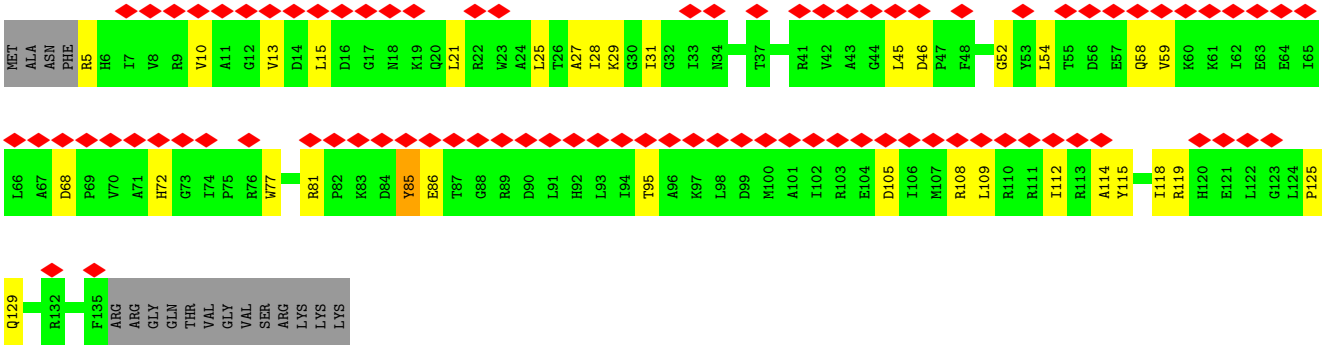
• Molecule 20: Small ribosomal subunit protein uS13

Chain AP:



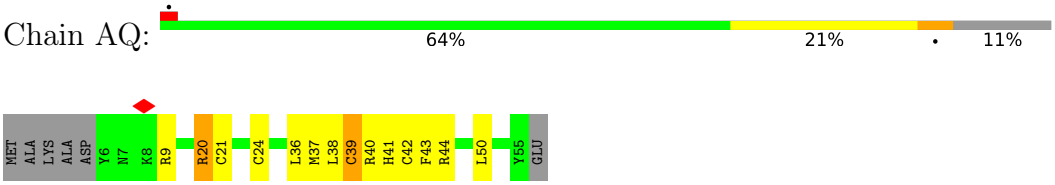
• Molecule 20: Small ribosomal subunit protein uS13

Chain BP:



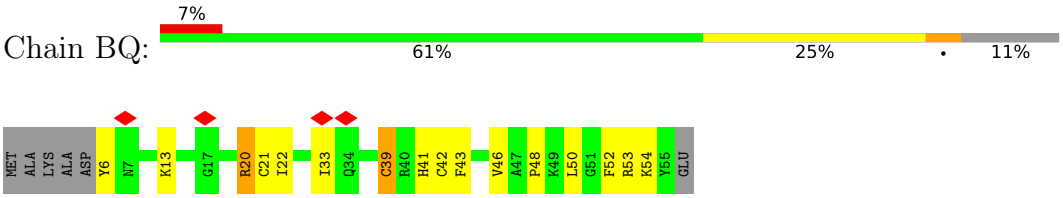
• Molecule 21: Small ribosomal subunit protein uS14

Chain AQ:



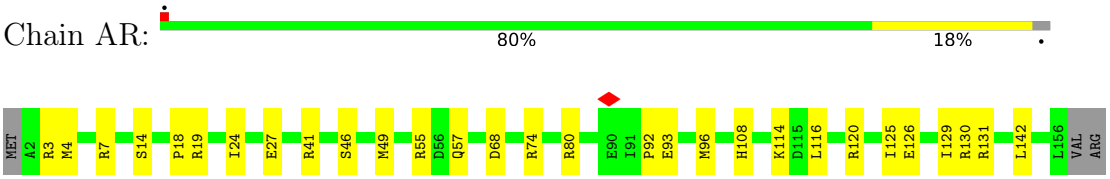
• Molecule 21: Small ribosomal subunit protein uS14

Chain BQ:



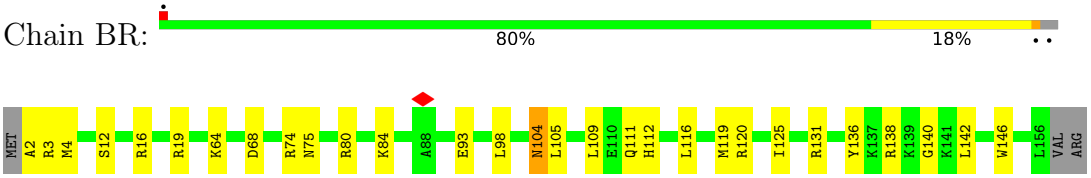
• Molecule 22: Small ribosomal subunit protein uS15

Chain AR:



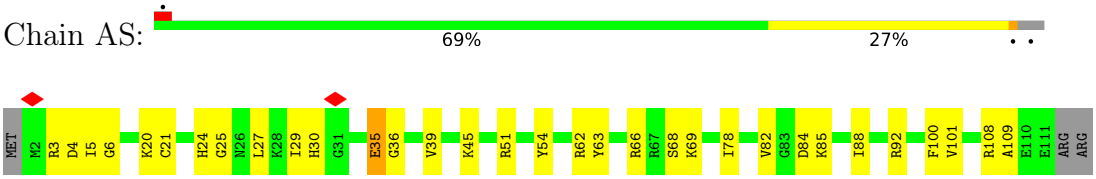
• Molecule 22: Small ribosomal subunit protein uS15

Chain BR:



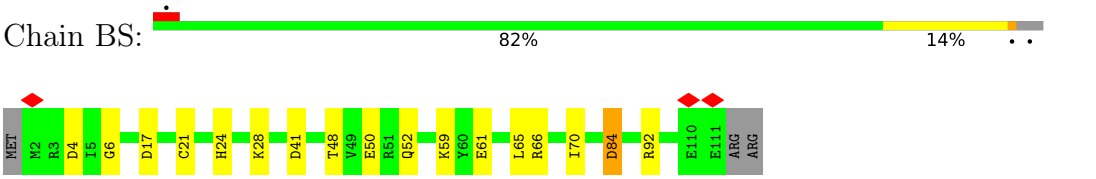
• Molecule 23: Small ribosomal subunit protein uS17

Chain AS:



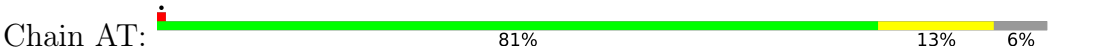
• Molecule 23: Small ribosomal subunit protein uS17

Chain BS:



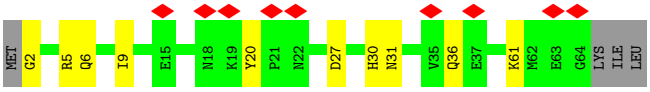
• Molecule 24: Small ribosomal subunit protein eS17

Chain AT:



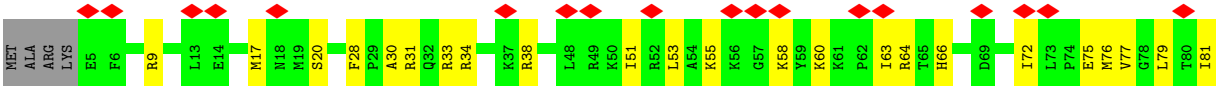
• Molecule 24: Small ribosomal subunit protein eS17

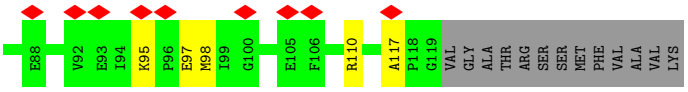
Chain BT:



• Molecule 25: Small ribosomal subunit protein uS19

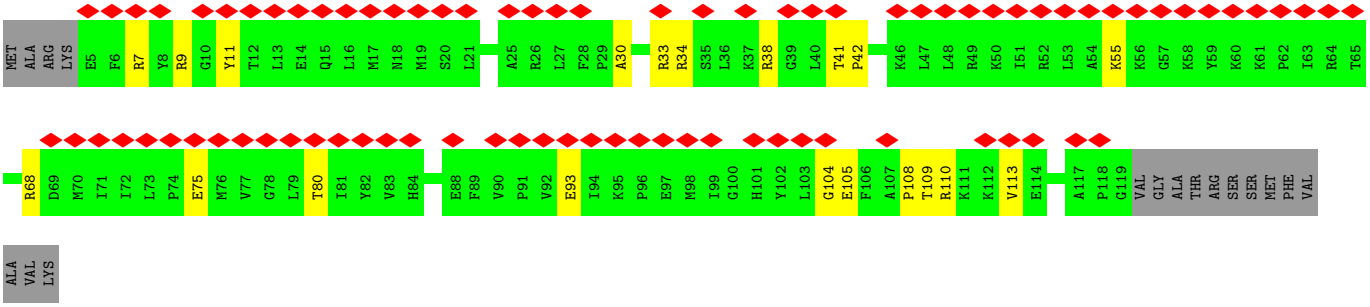
Chain AU:





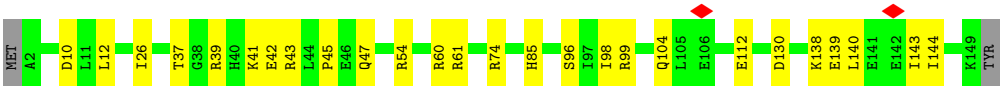
• Molecule 25: Small ribosomal subunit protein uS19

Chain BU:



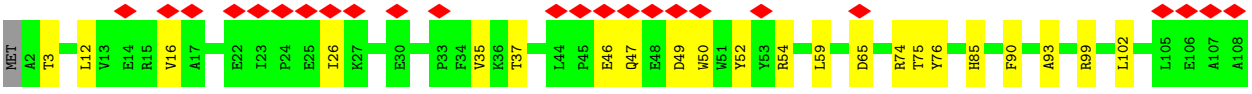
• Molecule 26: Small ribosomal subunit protein eS19

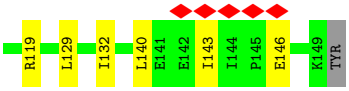
Chain AV:



• Molecule 26: Small ribosomal subunit protein eS19

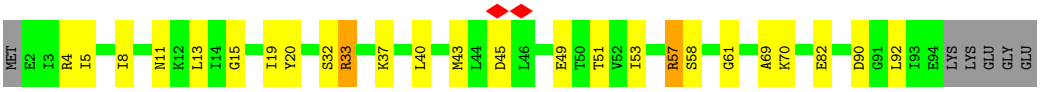
Chain BV:





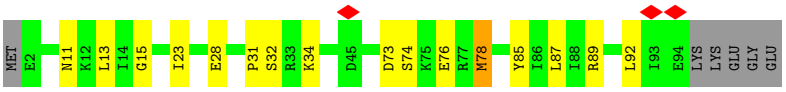
• Molecule 27: Small ribosomal subunit protein eS24

Chain AW:



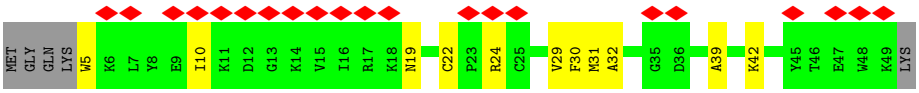
• Molecule 27: Small ribosomal subunit protein eS24

Chain BW:



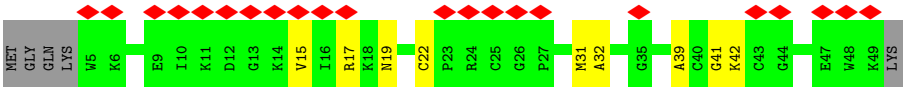
• Molecule 28: Small ribosomal subunit protein eS31

Chain AX:



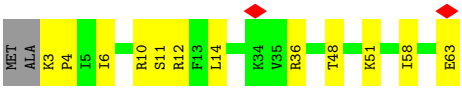
• Molecule 28: Small ribosomal subunit protein eS31

Chain BX:



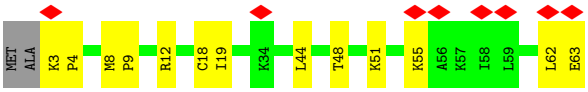
• Molecule 29: Small ribosomal subunit protein eS27

Chain AY:



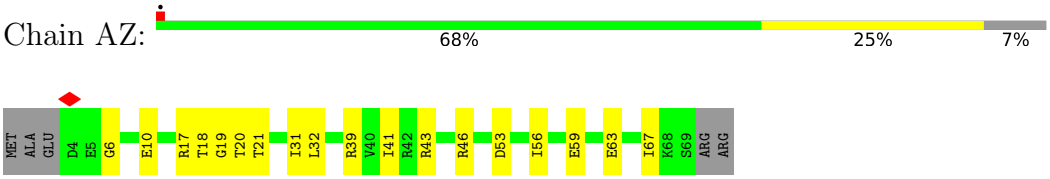
• Molecule 29: Small ribosomal subunit protein eS27

Chain BY:



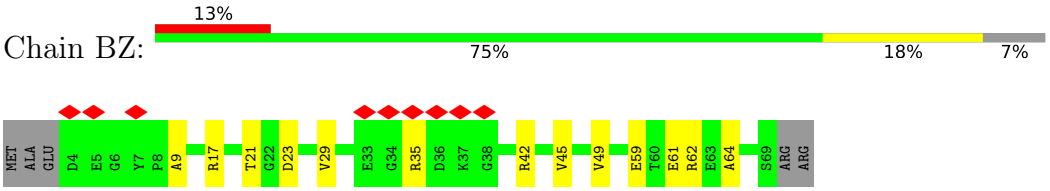
• Molecule 30: Small ribosomal subunit protein eS28

Chain AZ:



• Molecule 30: Small ribosomal subunit protein eS28

Chain BZ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	113596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	19.071	Depositor
Minimum map value	-6.271	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.802	Depositor
Recommended contour level	3	Depositor
Map size (Å)	480.384, 480.384, 480.384	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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	A1	0.34	0/485	0.60	0/656
1	B1	0.31	0/485	0.58	0/656
2	A2	0.47	0/341	0.83	0/440
2	B2	0.39	0/341	0.86	0/440
3	A3	0.36	0/2404	0.60	1/3229 (0.0%)
3	A4	0.35	0/2361	0.59	1/3172 (0.0%)
3	B3	0.32	0/2385	0.57	0/3205
3	B4	0.33	0/2344	0.59	0/3150
4	A5	0.28	0/951	0.53	0/1281
4	B5	0.28	0/951	0.50	0/1281
5	AA	0.64	0/35966	0.91	18/56138 (0.0%)
5	BA	0.55	0/35966	0.91	37/56138 (0.1%)
6	AB	0.31	0/1610	0.59	1/2177 (0.0%)
6	BB	0.31	0/1610	0.61	0/2177
7	AC	0.29	0/1554	0.61	0/2087
7	BC	0.30	0/1554	0.64	0/2087
8	AD	0.32	0/1537	0.61	0/2060
8	BD	0.32	0/1537	0.60	0/2060
9	AE	0.33	0/1478	0.64	0/1980
9	BE	0.29	0/1478	0.63	0/1980
10	AF	0.32	0/2030	0.61	0/2739
10	BF	0.30	0/2030	0.60	0/2739
11	AG	0.34	0/1824	0.62	0/2457
11	BG	0.30	0/1824	0.63	0/2457
12	AH	0.31	0/986	0.65	1/1320 (0.1%)
12	BH	0.32	0/986	0.63	0/1320
13	AI	0.30	0/1765	0.62	0/2371
13	BI	0.29	0/1765	0.60	0/2371
14	AJ	0.36	0/1049	0.63	0/1408
14	BJ	0.34	0/1049	0.63	0/1408
15	AK	0.29	0/986	0.65	0/1315
15	BK	0.29	0/986	0.67	0/1315
16	AL	0.27	0/1021	0.67	0/1369
16	BL	0.31	0/1021	0.68	0/1369

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AM	0.29	0/830	0.73	0/1113
17	BM	0.27	0/830	0.68	0/1113
18	AN	0.33	0/972	0.68	0/1309
18	BN	0.33	0/972	0.68	1/1309 (0.1%)
19	AO	0.36	0/1134	0.66	0/1508
19	BO	0.33	0/1134	0.63	0/1508
20	AP	0.28	0/1070	0.69	1/1440 (0.1%)
20	BP	0.30	0/1070	0.67	0/1440
21	AQ	0.31	0/426	0.73	0/562
21	BQ	0.32	0/426	0.75	0/562
22	AR	0.32	0/1311	0.66	0/1763
22	BR	0.32	0/1311	0.63	0/1763
23	AS	0.36	0/925	0.63	0/1249
23	BS	0.35	0/925	0.61	0/1249
24	AT	0.29	0/528	0.60	0/701
24	BT	0.28	0/528	0.61	0/701
25	AU	0.28	0/968	0.65	0/1293
25	BU	0.31	0/968	0.65	2/1293 (0.2%)
26	AV	0.27	0/1238	0.55	0/1668
26	BV	0.27	0/1238	0.57	0/1668
27	AW	0.32	0/790	0.58	0/1061
27	BW	0.32	0/790	0.65	0/1061
28	AX	0.29	0/381	0.62	0/509
28	BX	0.27	0/381	0.58	0/509
29	AY	0.31	0/472	0.63	0/634
29	BY	0.31	0/472	0.62	0/634
30	AZ	0.29	0/525	0.70	0/703
30	BZ	0.27	0/525	0.69	0/703
All	All	0.48	0/139800	0.79	63/203378 (0.0%)

There are no bond length outliers.

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AA	71	C	N3-C2-O2	-9.71	115.10	121.90
5	BA	140	C	N3-C2-O2	-9.11	115.53	121.90
5	BA	449	U	C2-N1-C1'	8.81	128.27	117.70
5	BA	985	C	N3-C2-O2	-8.45	115.99	121.90
5	BA	1118	C	C2-N1-C1'	8.34	127.98	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	471	0	457	8	0
1	B1	471	0	457	3	0
2	A2	335	0	396	11	0
2	B2	335	0	396	4	0
3	A3	2372	0	2526	42	0
3	A4	2329	0	2481	38	0
3	B3	2353	0	2505	35	0
3	B4	2312	0	2457	48	0
4	A5	939	0	994	15	0
4	B5	939	0	994	13	0
5	AA	32135	0	16231	381	0
5	BA	32135	0	16231	384	0
6	AB	1579	0	1638	28	0
6	BB	1579	0	1638	29	0
7	AC	1532	0	1622	21	0
7	BC	1532	0	1622	15	0
8	AD	1511	0	1595	29	0
8	BD	1511	0	1595	20	0
9	AE	1455	0	1531	28	0
9	BE	1455	0	1531	21	0
10	AF	1981	0	2051	35	0
10	BF	1981	0	2051	30	0
11	AG	1794	0	1850	29	0
11	BG	1794	0	1850	29	0
12	AH	971	0	1027	27	0
12	BH	971	0	1027	20	0
13	AI	1728	0	1775	32	0
13	BI	1728	0	1775	33	0
14	AJ	1028	0	1065	29	0
14	BJ	1028	0	1065	18	0
15	AK	977	0	1064	27	0
15	BK	977	0	1064	17	0
16	AL	1006	0	1052	17	0
16	BL	1006	0	1052	21	0
17	AM	822	0	870	19	0
17	BM	822	0	870	14	0
18	AN	954	0	981	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	BN	954	0	981	22	0
19	AO	1118	0	1214	25	0
19	BO	1118	0	1214	27	0
20	AP	1052	0	1094	25	0
20	BP	1052	0	1094	22	0
21	AQ	417	0	445	11	0
21	BQ	417	0	445	11	0
22	AR	1283	0	1358	23	0
22	BR	1283	0	1358	23	0
23	AS	903	0	922	28	0
23	BS	903	0	922	15	0
24	AT	522	0	557	6	0
24	BT	522	0	557	7	0
25	AU	948	0	1007	25	0
25	BU	948	0	1007	18	0
26	AV	1209	0	1254	22	0
26	BV	1209	0	1254	19	0
27	AW	774	0	794	17	0
27	BW	774	0	794	11	0
28	AX	369	0	361	9	0
28	BX	369	0	361	7	0
29	AY	465	0	507	10	0
29	BY	465	0	507	7	0
30	AZ	523	0	551	13	0
30	BZ	523	0	551	10	0
All	All	130968	0	102495	1633	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 1633 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)
5:BA:777:G:HO2'	14:BJ:2:THR:N	1.53	1.04
5:AA:777:G:HO2'	14:AJ:2:THR:N	1.65	0.94
5:BA:1264:G:H21	5:BA:1293:A:N6	1.65	0.93
5:BA:1264:G:H21	5:BA:1293:A:H62	1.10	0.91
5:AA:516:A:OP2	19:AO:20:ARG:NH1	2.07	0.88

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
1	B1	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
2	A2	33/37 (89%)	33 (100%)	0	0	100	100
2	B2	33/37 (89%)	31 (94%)	2 (6%)	0	100	100
3	A3	294/306 (96%)	268 (91%)	26 (9%)	0	100	100
3	A4	288/306 (94%)	265 (92%)	23 (8%)	0	100	100
3	B3	291/306 (95%)	265 (91%)	25 (9%)	1 (0%)	37	69
3	B4	286/306 (94%)	263 (92%)	23 (8%)	0	100	100
4	A5	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
4	B5	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
6	AB	195/202 (96%)	182 (93%)	13 (7%)	0	100	100
6	BB	195/202 (96%)	188 (96%)	7 (4%)	0	100	100
7	AC	193/210 (92%)	186 (96%)	7 (4%)	0	100	100
7	BC	193/210 (92%)	188 (97%)	4 (2%)	1 (0%)	25	60
8	AD	182/198 (92%)	181 (100%)	1 (0%)	0	100	100
8	BD	182/198 (92%)	180 (99%)	2 (1%)	0	100	100
9	AE	171/180 (95%)	168 (98%)	3 (2%)	0	100	100
9	BE	171/180 (95%)	167 (98%)	4 (2%)	0	100	100
10	AF	240/243 (99%)	226 (94%)	14 (6%)	0	100	100
10	BF	240/243 (99%)	232 (97%)	8 (3%)	0	100	100
11	AG	225/236 (95%)	217 (96%)	8 (4%)	0	100	100
11	BG	225/236 (95%)	215 (96%)	10 (4%)	0	100	100
12	AH	121/125 (97%)	114 (94%)	7 (6%)	0	100	100
12	BH	121/125 (97%)	117 (97%)	4 (3%)	0	100	100
13	AI	212/215 (99%)	193 (91%)	18 (8%)	1 (0%)	25	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	BI	212/215 (99%)	192 (91%)	20 (9%)	0	100	100
14	AJ	127/130 (98%)	113 (89%)	14 (11%)	0	100	100
14	BJ	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
15	AK	122/127 (96%)	116 (95%)	6 (5%)	0	100	100
15	BK	122/127 (96%)	118 (97%)	4 (3%)	0	100	100
16	AL	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
16	BL	126/135 (93%)	120 (95%)	5 (4%)	1 (1%)	16	51
17	AM	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
17	BM	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
18	AN	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
18	BN	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
19	AO	141/147 (96%)	131 (93%)	10 (7%)	0	100	100
19	BO	141/147 (96%)	139 (99%)	2 (1%)	0	100	100
20	AP	129/148 (87%)	124 (96%)	5 (4%)	0	100	100
20	BP	129/148 (87%)	123 (95%)	6 (5%)	0	100	100
21	AQ	48/56 (86%)	42 (88%)	6 (12%)	0	100	100
21	BQ	48/56 (86%)	44 (92%)	4 (8%)	0	100	100
22	AR	153/158 (97%)	146 (95%)	7 (5%)	0	100	100
22	BR	153/158 (97%)	149 (97%)	4 (3%)	0	100	100
23	AS	108/113 (96%)	102 (94%)	6 (6%)	0	100	100
23	BS	108/113 (96%)	102 (94%)	6 (6%)	0	100	100
24	AT	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
24	BT	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
25	AU	113/132 (86%)	110 (97%)	3 (3%)	0	100	100
25	BU	113/132 (86%)	108 (96%)	5 (4%)	0	100	100
26	AV	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
26	BV	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
27	AW	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
27	BW	91/99 (92%)	85 (93%)	6 (7%)	0	100	100
28	AX	43/50 (86%)	41 (95%)	2 (5%)	0	100	100
28	BX	43/50 (86%)	41 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	AY	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
29	BY	59/63 (94%)	55 (93%)	4 (7%)	0	100	100
30	AZ	64/71 (90%)	61 (95%)	3 (5%)	0	100	100
30	BZ	64/71 (90%)	63 (98%)	1 (2%)	0	100	100
All	All	8173/8652 (94%)	7767 (95%)	402 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B3	269	ILE
13	AI	15	ILE
16	BL	119	PRO
7	BC	78	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	53/53 (100%)	52 (98%)	1 (2%)	52	76
1	B1	53/53 (100%)	52 (98%)	1 (2%)	52	76
2	A2	33/35 (94%)	33 (100%)	0	100	100
2	B2	33/35 (94%)	33 (100%)	0	100	100
3	A3	265/273 (97%)	260 (98%)	5 (2%)	52	76
3	A4	260/273 (95%)	254 (98%)	6 (2%)	45	72
3	B3	263/273 (96%)	259 (98%)	4 (2%)	60	81
3	B4	258/273 (94%)	246 (95%)	12 (5%)	22	55
4	A5	99/99 (100%)	99 (100%)	0	100	100
4	B5	99/99 (100%)	98 (99%)	1 (1%)	73	87
6	AB	169/173 (98%)	163 (96%)	6 (4%)	30	62
6	BB	169/173 (98%)	168 (99%)	1 (1%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	AC	153/167 (92%)	150 (98%)	3 (2%)	50 75
7	BC	153/167 (92%)	151 (99%)	2 (1%)	65 83
8	AD	161/171 (94%)	156 (97%)	5 (3%)	35 66
8	BD	161/171 (94%)	157 (98%)	4 (2%)	42 71
9	AE	156/160 (98%)	154 (99%)	2 (1%)	65 83
9	BE	156/160 (98%)	153 (98%)	3 (2%)	52 76
10	AF	212/213 (100%)	205 (97%)	7 (3%)	33 64
10	BF	212/213 (100%)	208 (98%)	4 (2%)	52 76
11	AG	188/197 (95%)	179 (95%)	9 (5%)	21 55
11	BG	188/197 (95%)	185 (98%)	3 (2%)	58 79
12	AH	107/108 (99%)	104 (97%)	3 (3%)	38 68
12	BH	107/108 (99%)	106 (99%)	1 (1%)	75 89
13	AI	183/184 (100%)	175 (96%)	8 (4%)	24 57
13	BI	183/184 (100%)	181 (99%)	2 (1%)	70 86
14	AJ	107/108 (99%)	105 (98%)	2 (2%)	52 76
14	BJ	107/108 (99%)	106 (99%)	1 (1%)	75 89
15	AK	100/103 (97%)	96 (96%)	4 (4%)	27 59
15	BK	100/103 (97%)	98 (98%)	2 (2%)	50 75
16	AL	104/111 (94%)	104 (100%)	0	100 100
16	BL	104/111 (94%)	100 (96%)	4 (4%)	28 60
17	AM	91/91 (100%)	87 (96%)	4 (4%)	24 57
17	BM	91/91 (100%)	87 (96%)	4 (4%)	24 57
18	AN	94/104 (90%)	94 (100%)	0	100 100
18	BN	94/104 (90%)	92 (98%)	2 (2%)	48 74
19	AO	117/121 (97%)	117 (100%)	0	100 100
19	BO	117/121 (97%)	114 (97%)	3 (3%)	41 70
20	AP	108/122 (88%)	105 (97%)	3 (3%)	38 68
20	BP	108/122 (88%)	106 (98%)	2 (2%)	52 76
21	AQ	42/46 (91%)	38 (90%)	4 (10%)	7 28
21	BQ	42/46 (91%)	39 (93%)	3 (7%)	12 42
22	AR	140/143 (98%)	138 (99%)	2 (1%)	62 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	BR	140/143 (98%)	139 (99%)	1 (1%)	81 92
23	AS	99/102 (97%)	97 (98%)	2 (2%)	50 75
23	BS	99/102 (97%)	98 (99%)	1 (1%)	73 87
24	AT	57/61 (93%)	57 (100%)	0	100 100
24	BT	57/61 (93%)	55 (96%)	2 (4%)	31 63
25	AU	101/114 (89%)	96 (95%)	5 (5%)	20 54
25	BU	101/114 (89%)	100 (99%)	1 (1%)	73 87
26	AV	125/127 (98%)	123 (98%)	2 (2%)	58 79
26	BV	125/127 (98%)	120 (96%)	5 (4%)	27 59
27	AW	84/89 (94%)	79 (94%)	5 (6%)	16 48
27	BW	84/89 (94%)	82 (98%)	2 (2%)	44 71
28	AX	37/41 (90%)	36 (97%)	1 (3%)	40 69
28	BX	37/41 (90%)	37 (100%)	0	100 100
29	AY	53/54 (98%)	52 (98%)	1 (2%)	52 76
29	BY	53/54 (98%)	52 (98%)	1 (2%)	52 76
30	AZ	56/60 (93%)	56 (100%)	0	100 100
30	BZ	56/60 (93%)	56 (100%)	0	100 100
All	All	7104/7406 (96%)	6942 (98%)	162 (2%)	46 72

5 of 162 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	BE	72	GLN
19	BO	96	PHE
10	BF	128	ARG
15	BK	83	ASN
23	BS	84	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
7	BC	77	ASN
13	BI	94	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	AA	1494/1495 (99%)	295 (19%)	43 (2%)
5	BA	1494/1495 (99%)	290 (19%)	46 (3%)
All	All	2988/2990 (99%)	585 (19%)	89 (2%)

5 of 585 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	AA	2	U
5	AA	3	U
5	AA	4	C
5	AA	20	G
5	AA	32	A

5 of 89 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	BA	431	U
5	BA	924	U
5	BA	458	G
5	BA	672	G
5	BA	1019	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

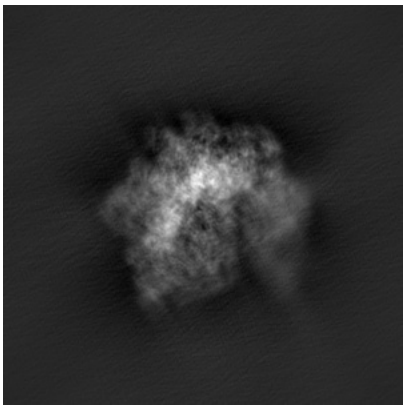
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50611. These allow visual inspection of the internal detail of the map and identification of artifacts.

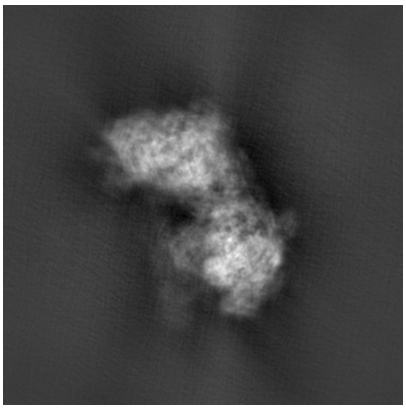
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

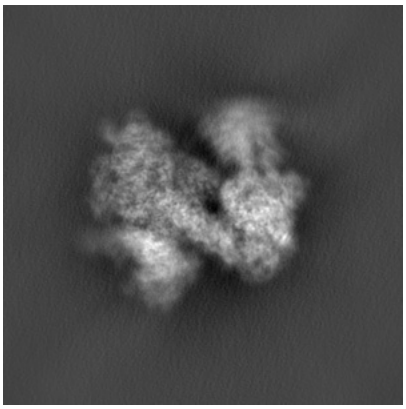
6.1.1 Primary map



X

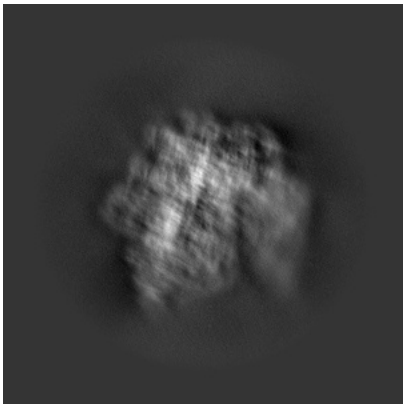


Y

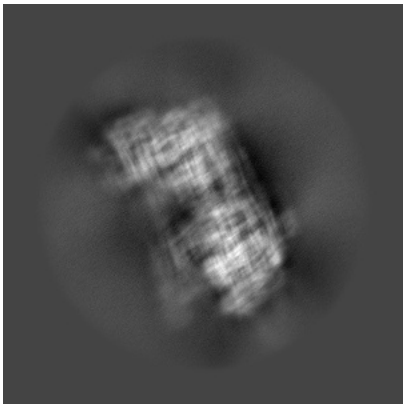


Z

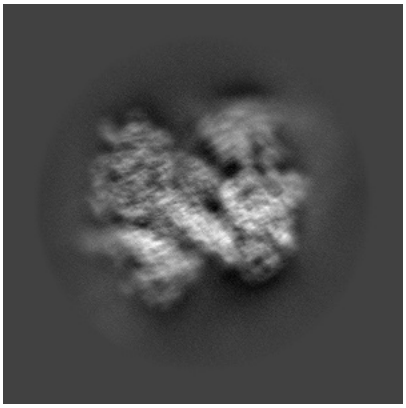
6.1.2 Raw map



X



Y

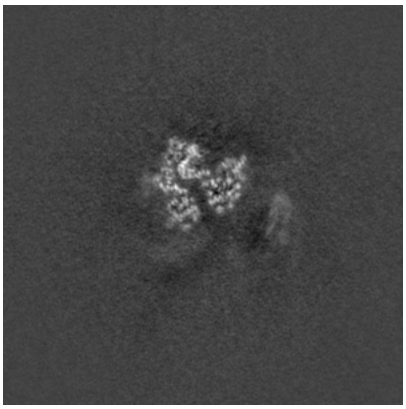


Z

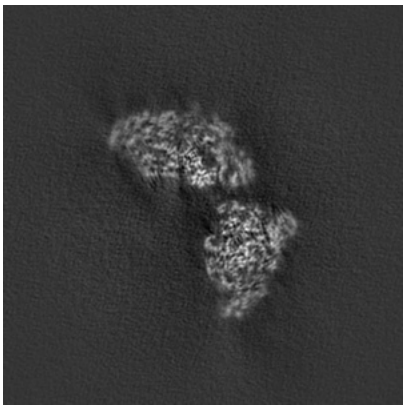
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

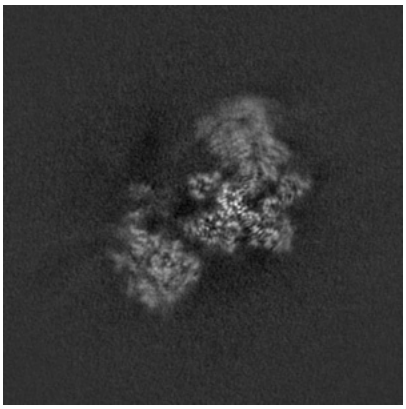
6.2.1 Primary map



X Index: 288

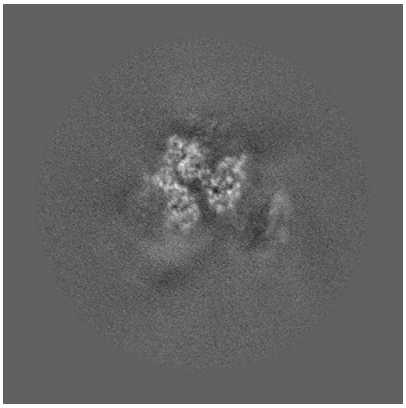


Y Index: 288

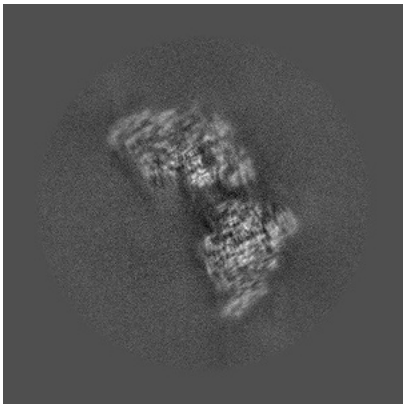


Z Index: 288

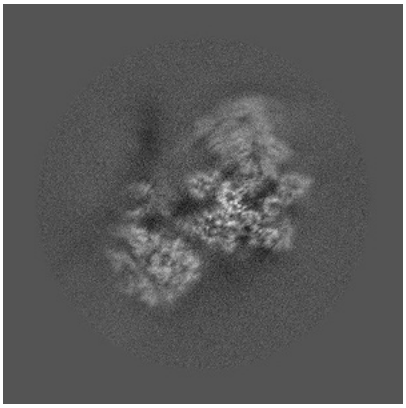
6.2.2 Raw map



X Index: 288



Y Index: 288

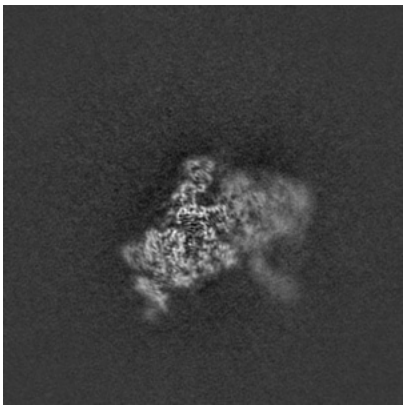


Z Index: 288

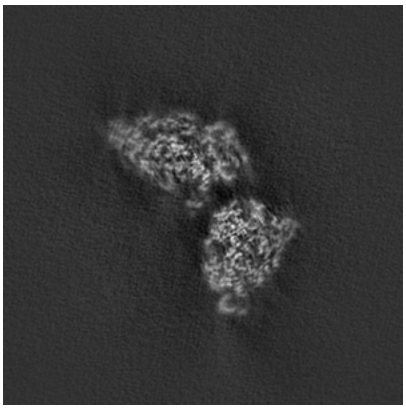
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

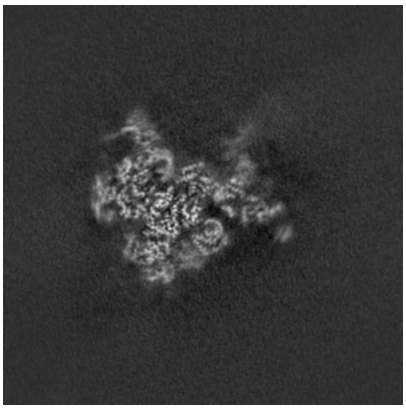
6.3.1 Primary map



X Index: 354

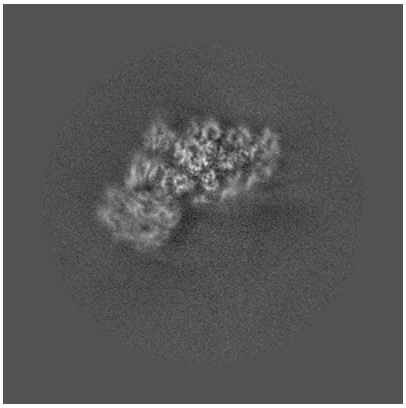


Y Index: 278

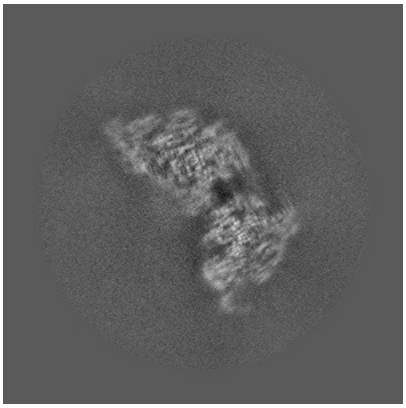


Z Index: 324

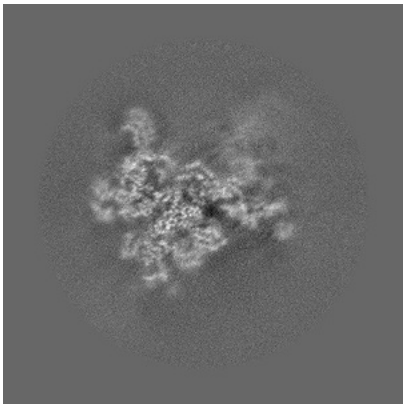
6.3.2 Raw map



X Index: 231



Y Index: 273

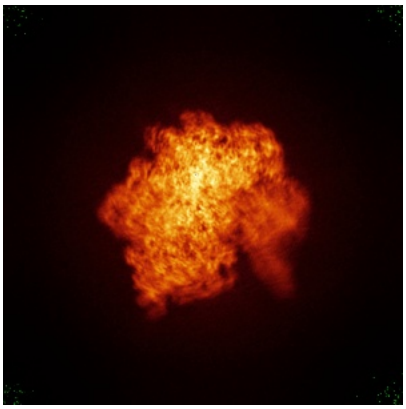


Z Index: 319

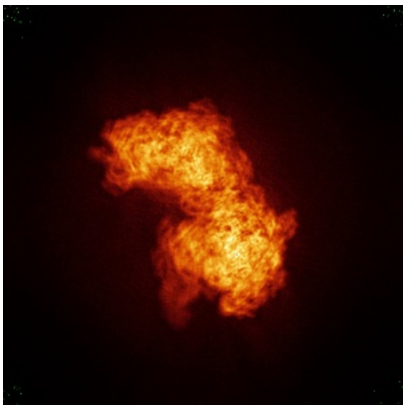
The images above show the largest variance slices of the map in three orthogonal directions.

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

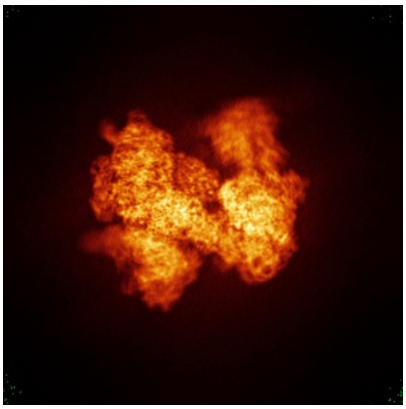
6.4.1 Primary map



X

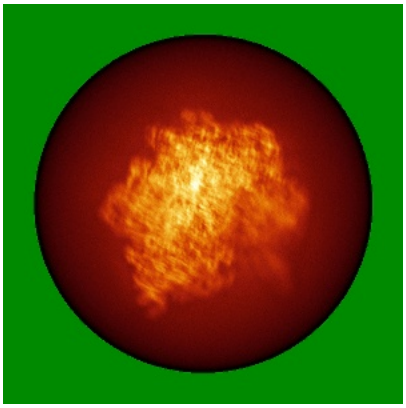


Y

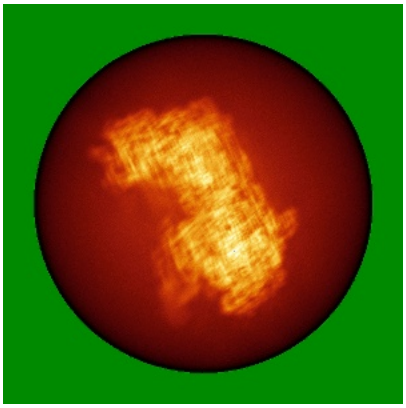


Z

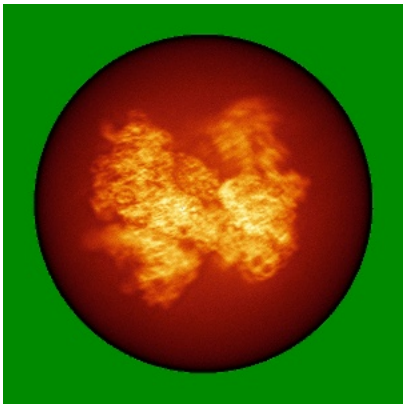
6.4.2 Raw map



X



Y

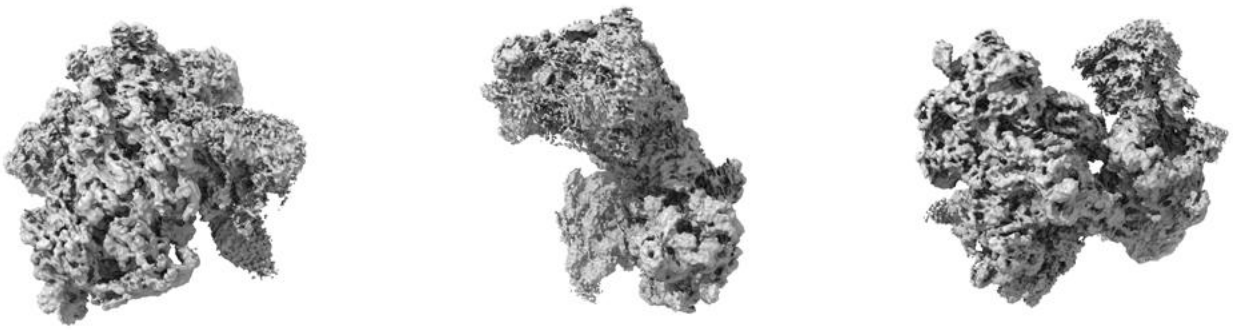


Z

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

6.5 Orthogonal surface views (i)

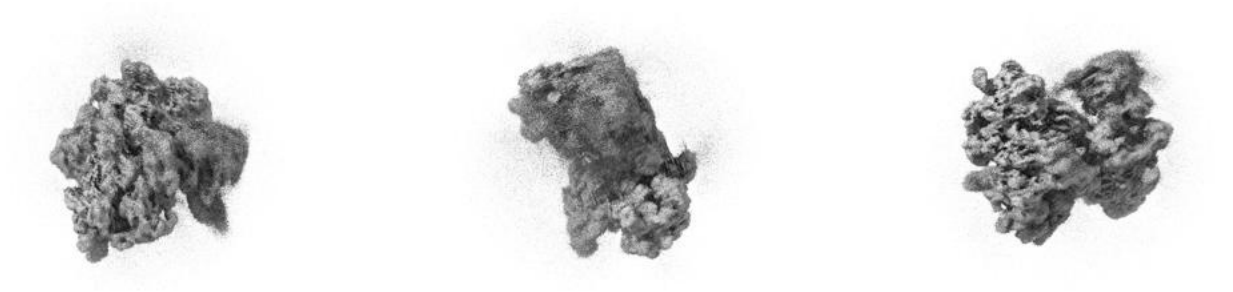
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

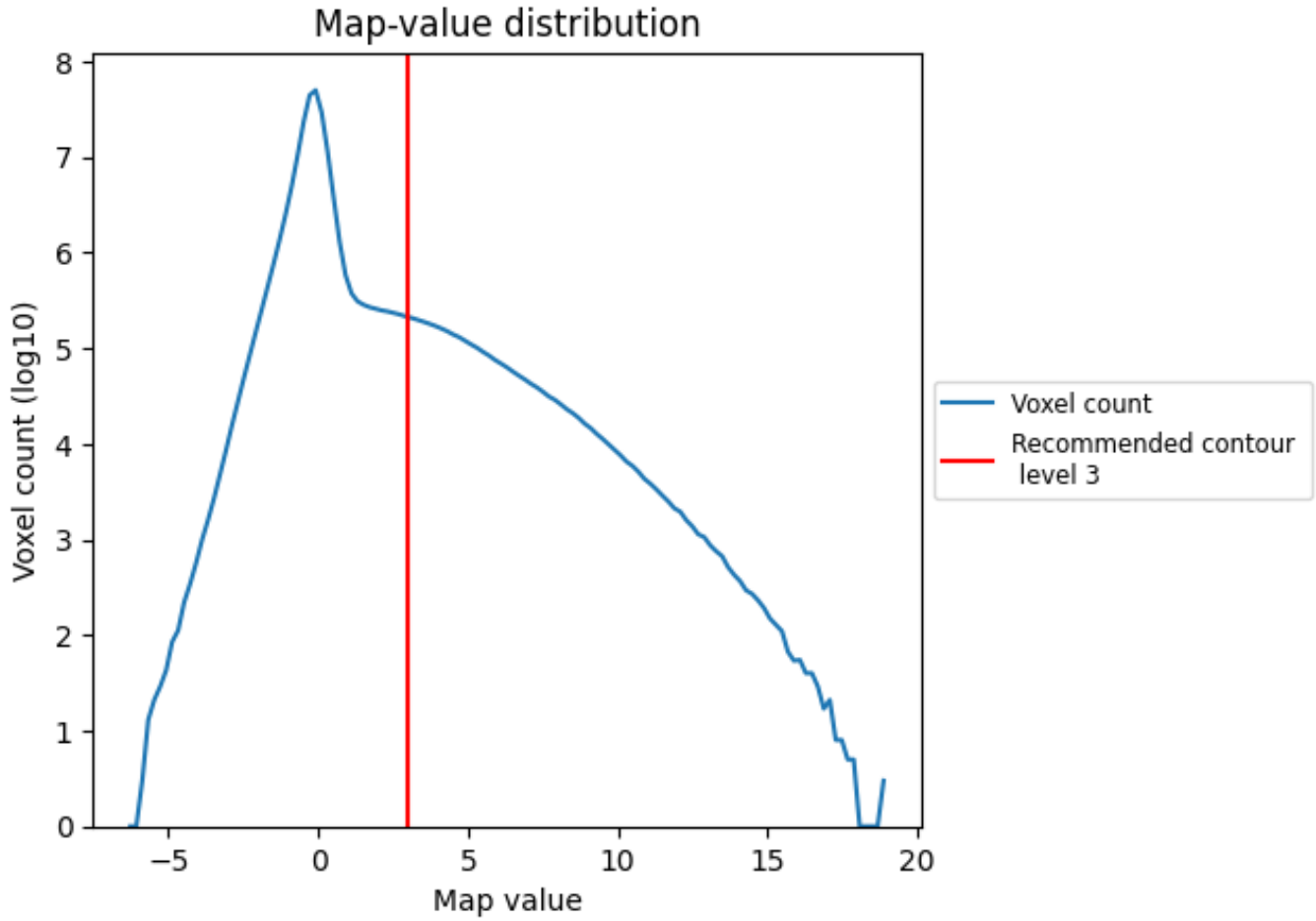
6.6 Mask visualisation (i)

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

7 Map analysis

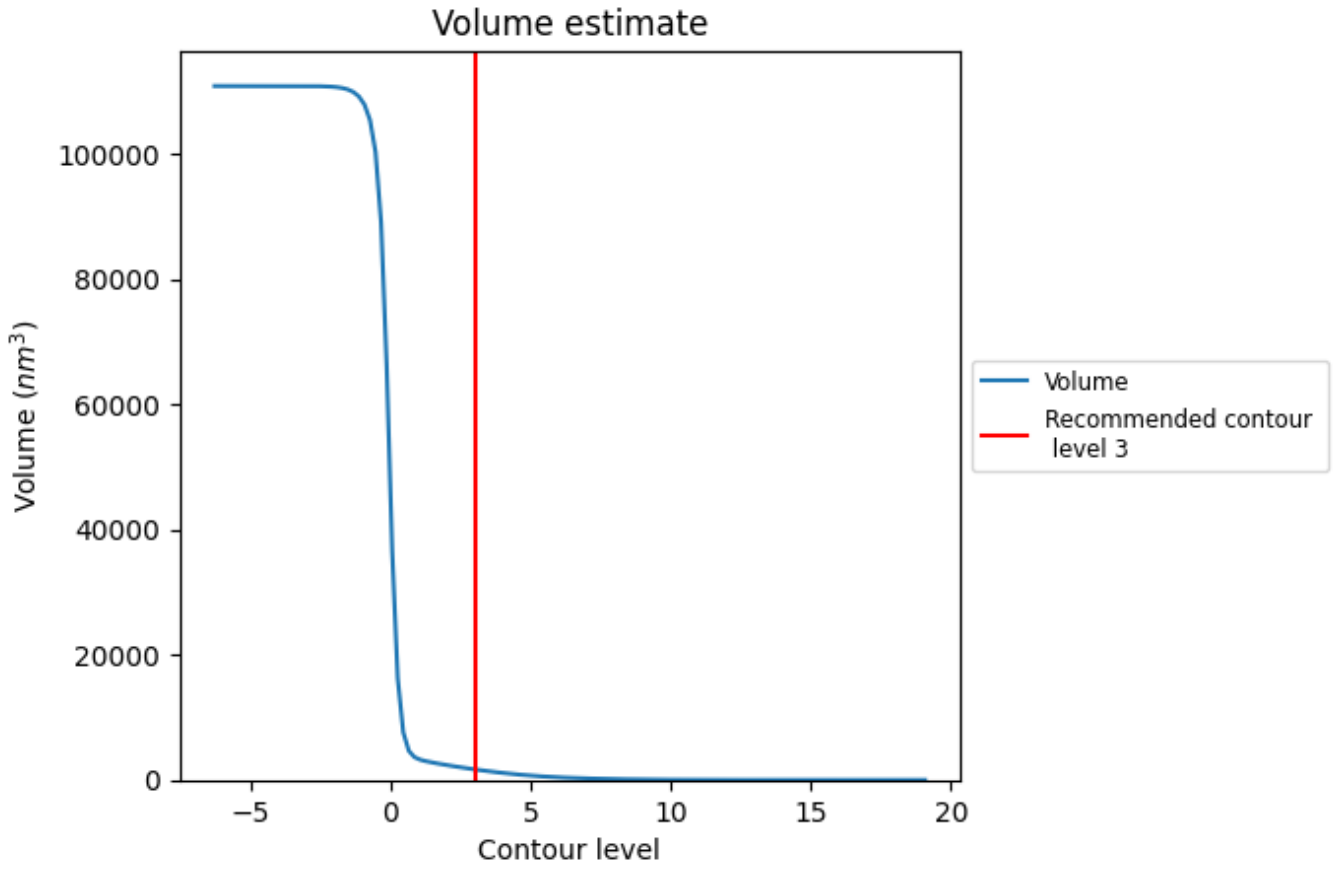
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

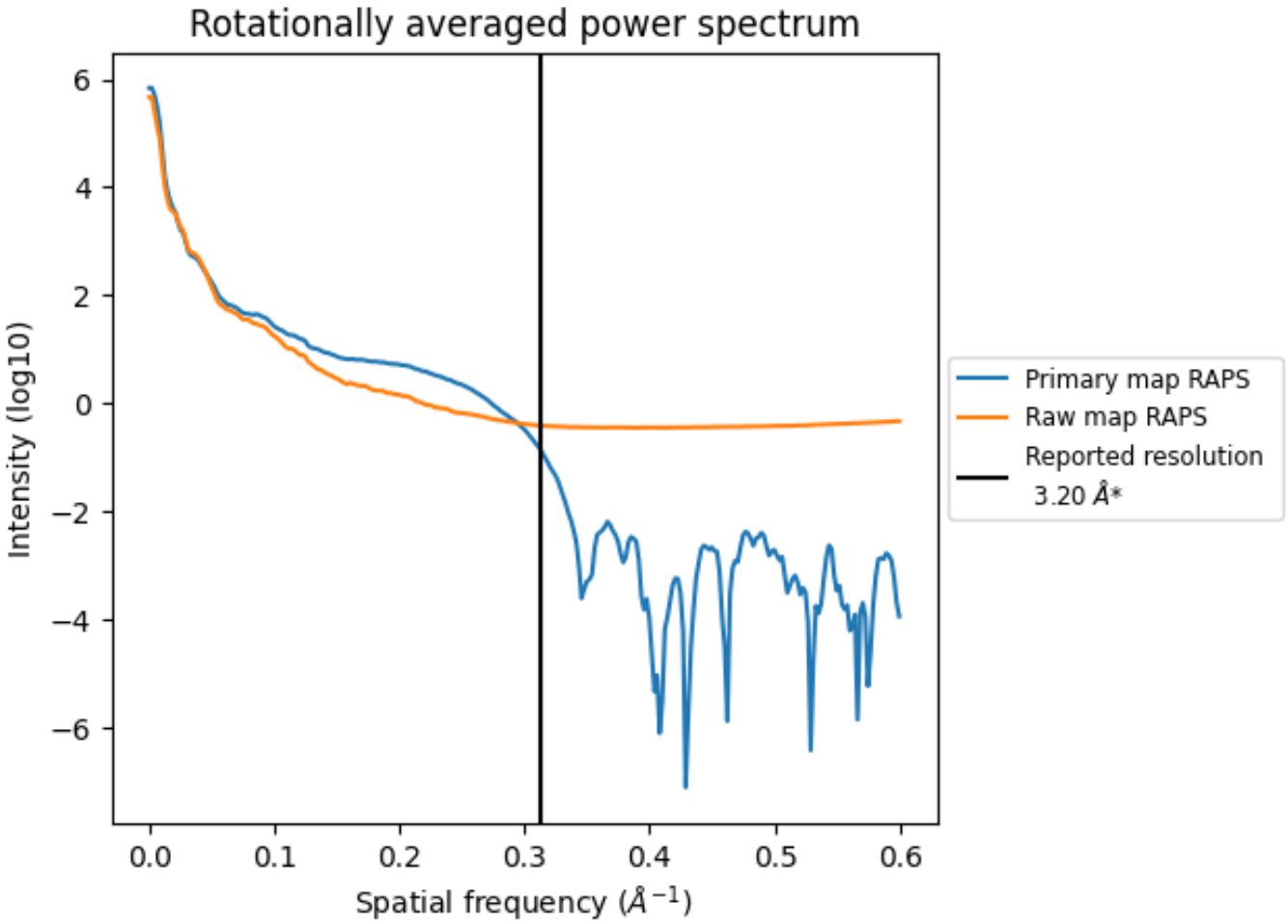
7.2 Volume estimate (i)



The volume at the recommended contour level is 1689 nm^3; this corresponds to an approximate mass of 1525 kDa.

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

7.3 Rotationally averaged power spectrum (i)

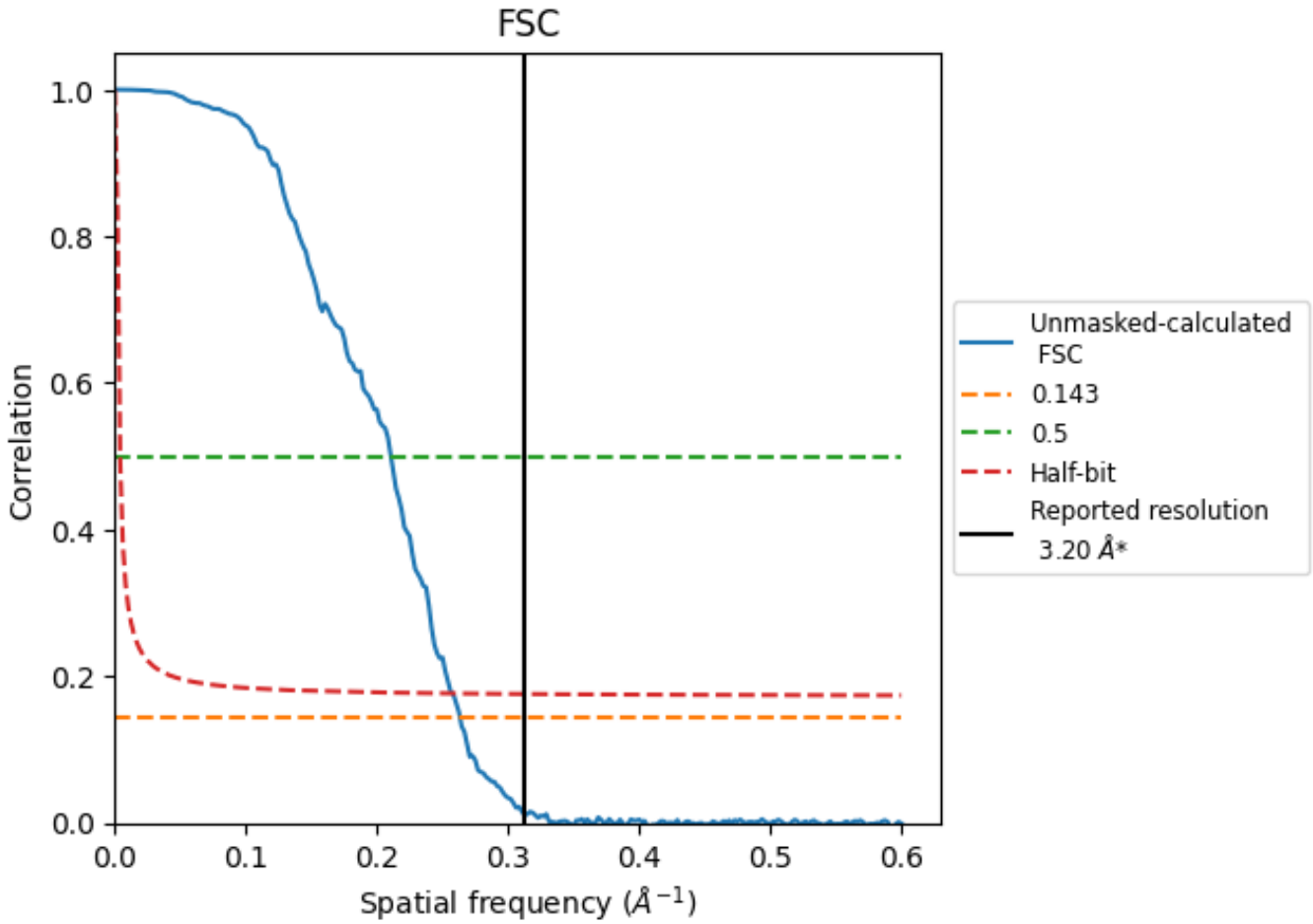


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 (i)

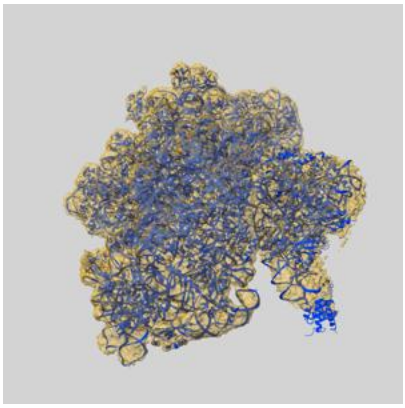
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	4.75	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 3.2 by more than 10 %

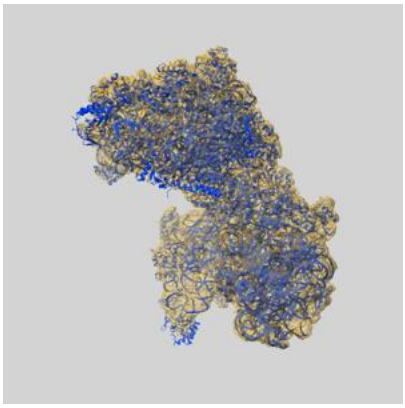
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50611 and PDB model 9FNY. Per-residue inclusion information can be found in section 3 on page 13.

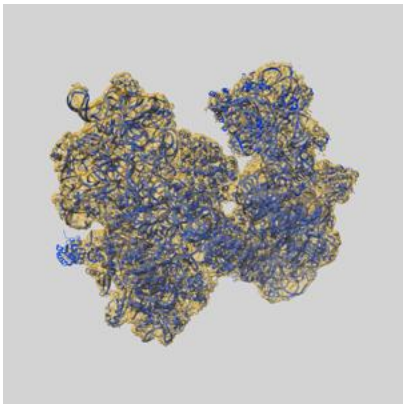
9.1 Map-model overlay



X



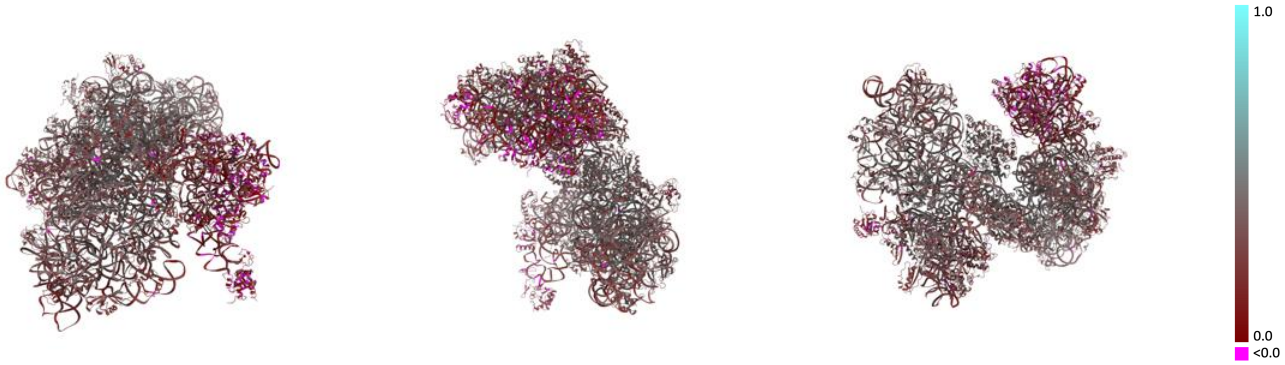
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

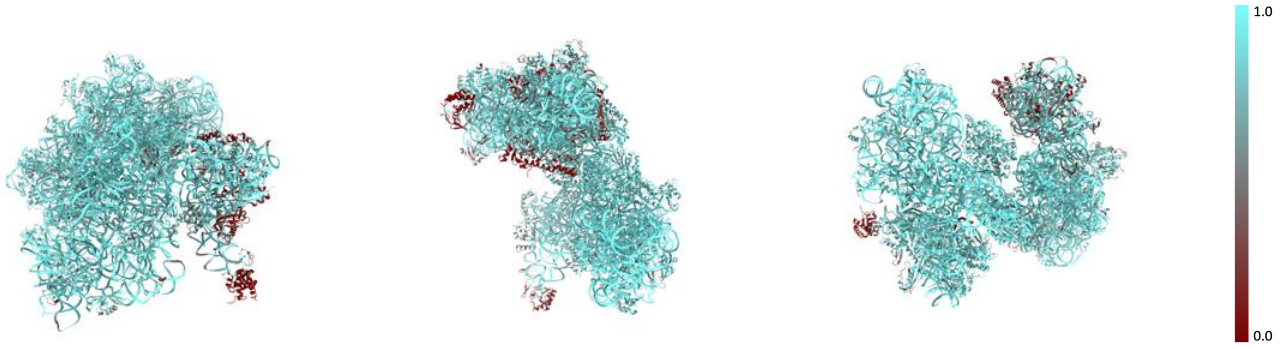
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

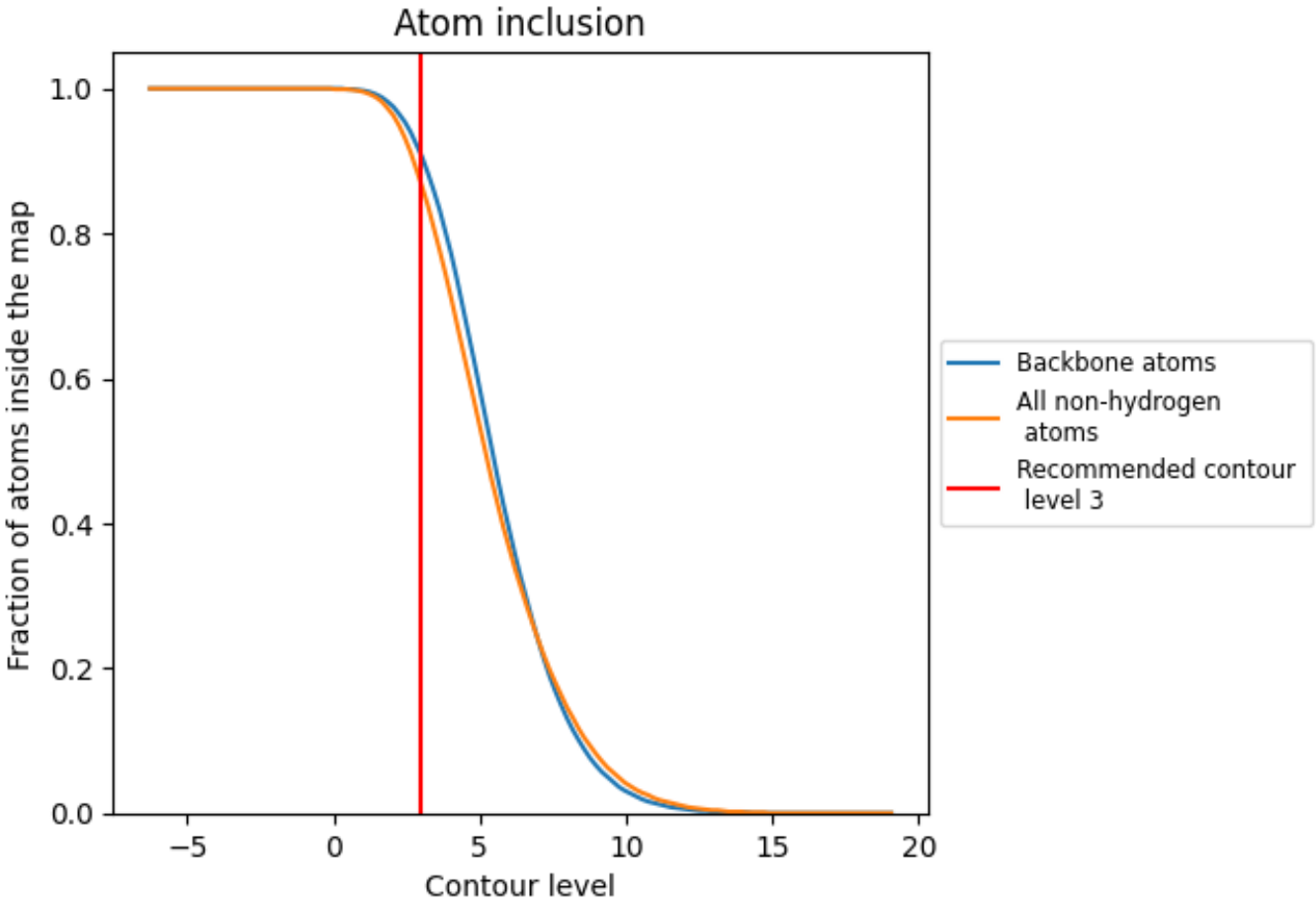
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8690	0.3130
A1	0.8700	0.3900
A2	0.9580	0.4570
A3	0.8810	0.3920
A4	0.8820	0.3870
A5	0.1450	0.1510
AA	0.9750	0.3500
AB	0.8250	0.3460
AC	0.7740	0.3160
AD	0.9250	0.3460
AE	0.8940	0.3740
AF	0.8420	0.3770
AG	0.8630	0.4060
AH	0.8250	0.3020
AI	0.8680	0.2500
AJ	0.9050	0.3920
AK	0.9240	0.3720
AL	0.9070	0.2910
AM	0.6750	0.2800
AN	0.9700	0.4050
AO	0.9300	0.3960
AP	0.7720	0.1890
AQ	0.8910	0.3140
AR	0.8730	0.3390
AS	0.8840	0.3630
AT	0.9000	0.3190
AU	0.6120	0.1680
AV	0.8690	0.2130
AW	0.8180	0.3480
AX	0.4970	0.1410
AY	0.8560	0.2790
AZ	0.9300	0.3010
B1	0.7800	0.3050
B2	0.8810	0.4250
B3	0.8520	0.3770

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B4	0.8620	0.3840
B5	0.1230	0.1200
BA	0.9310	0.2920
BB	0.7250	0.2830
BC	0.5020	0.1980
BD	0.8500	0.3290
BE	0.8560	0.3110
BF	0.8240	0.3400
BG	0.8400	0.3500
BH	0.6420	0.2590
BI	0.5970	0.1750
BJ	0.8580	0.3690
BK	0.8820	0.3410
BL	0.7530	0.1740
BM	0.6560	0.1500
BN	0.9460	0.3670
BO	0.9170	0.3500
BP	0.3020	0.1240
BQ	0.8430	0.1720
BR	0.8670	0.3220
BS	0.8840	0.3840
BT	0.7280	0.2000
BU	0.2350	0.0990
BV	0.6890	0.1210
BW	0.7660	0.2770
BX	0.4470	0.1250
BY	0.7590	0.2620
BZ	0.7720	0.2160