



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 11:32 PM UTC

PDB ID : 8P8W / pdb_00008p8w
EMDB ID : EMD-17145
Title : Mycoplasma pneumoniae di-ribosome in chloramphenicol-treated cells (following 70S)
Authors : Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.
Deposited on : 2023-06-02
Resolution : 8.70 Å (reported)
Based on initial models : 7OOC, 7OOD

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:

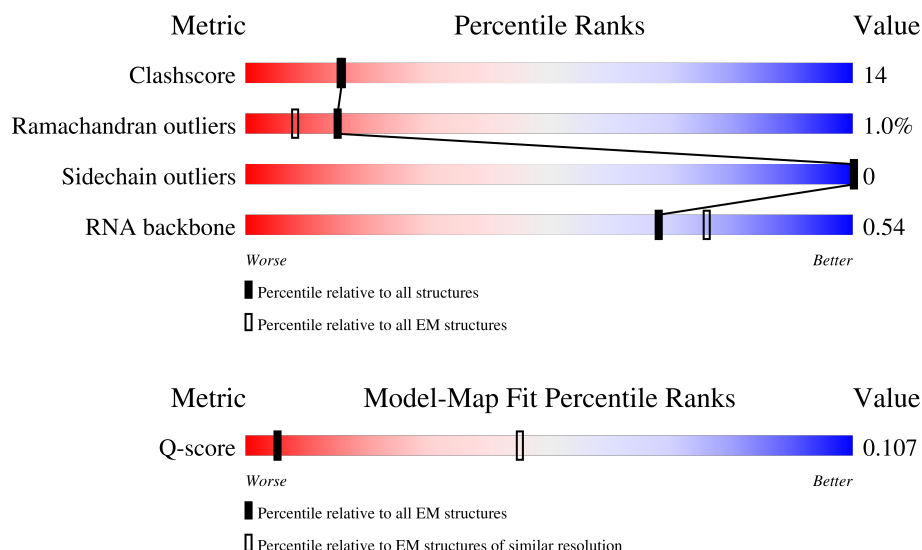
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 8.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	282 (8.20 - 9.20)

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 $\leq 5\%$. 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	0	48	
2	1	59	
3	2	37	

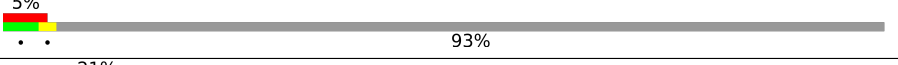
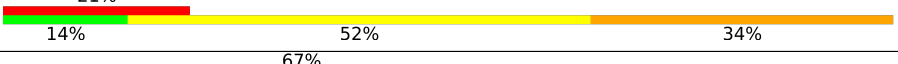
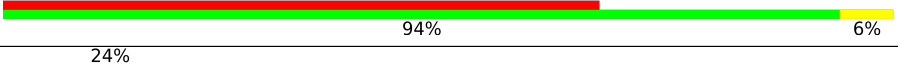
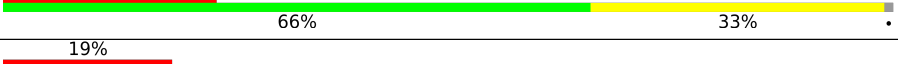
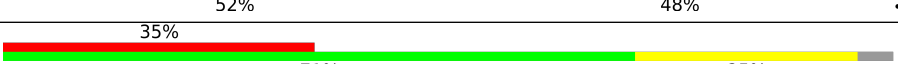
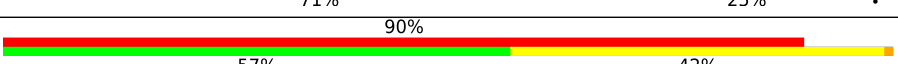
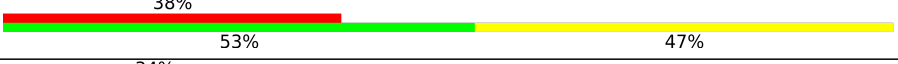
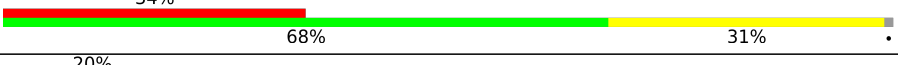
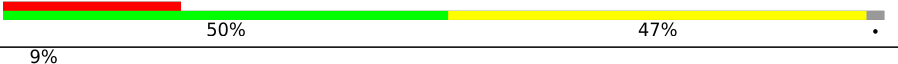
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Mol	Chain	Length	Quality of chain
4	3	2907	
5	4	108	
6	5	1520	
7	6	76	
8	7	75	
9	A	294	
10	B	273	
11	C	205	
11	U	205	
12	D	219	
13	E	215	
14	F	155	
15	G	142	
16	H	132	
17	I	108	
18	J	121	
19	K	139	
20	L	124	
21	M	61	
22	N	86	
23	O	94	
24	P	85	
25	Q	104	
26	R	87	
27	S	87	

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Mol	Chain	Length	Quality of chain
28	T	60	
29	X	444	
30	Y	29	
31	Z	36	
32	a	287	
33	b	287	
34	c	212	
35	d	180	
36	e	184	
37	f	149	
38	g	161	
39	h	137	
40	i	146	
41	j	122	
42	k	151	
43	l	139	
44	m	124	
45	n	116	
46	o	119	
47	p	127	
48	q	100	
49	r	159	
50	s	237	
51	t	111	
52	u	104	

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Mol	Chain	Length	Quality of chain
53	v	65	25% 49% 48% • •
54	w	111	50% 75% 24% •
55	x	97	61% 54% 37% • 8%
56	y	57	19% 53% 44% • •
57	z	53	40% 68% 26% 6%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 151559 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 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	47	Total	C	N	O	S	0	0
			380	236	81	61	2		

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			477	300	99	77	1		

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	37	Total	C	N	O	S	0	0
			304	189	65	46	4		

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	2893	Total	C	N	O	P	0	0
			61995	27704	11293	20105	2893		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	108	Total	C	N	O	P	0	0
			2305	1030	415	752	108		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	1507	Total	C	N	O	P	0	0
			32258	14420	5847	10484	1507		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1003	A	G	conflict	GB 26117688

- Molecule 7 is a RNA chain called tRNA-Ala (E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	76	Total	C	N	O	P	0	0
			1620	723	287	534	76		

- Molecule 8 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	75	Total	C	N	O	P	0	0
			1599	712	279	533	75		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	17	G	-	insertion	GB 26117688
7	55	C	U	conflict	GB 26117688

- Molecule 9 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	268	Total	C	N	O	S	0	0
			2152	1368	379	396	9		

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	225	Total	C	N	O	S	0	0
			1773	1121	328	319	5		

- Molecule 11 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	204	Total	C	N	O	S	0	0
			1669	1057	316	292	4		
11	U	204	Total	C	N	O	S	0	0
			1669	1057	316	292	4		

- Molecule 12 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	173	Total	C	N	O	S	0	0
			1346	846	265	232	3		

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	167	Total	C	N	O	S	0	0
			1362	857	240	263	2		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	155	Total	C	N	O	S	0	0
			1254	790	240	217	7		

- Molecule 15 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	142	Total	C	N	O	S	0	0
			1118	728	194	193	3		

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	129	Total	C	N	O	S	0	0
			1040	661	195	183	1		

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	104	Total	C	N	O	S	0	0
			832	536	147	148	1		

- Molecule 18 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	114	Total	C	N	O	S	0	0
			829	514	153	156	6		

- Molecule 19 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	135	Total	C	N	O	S	0	0
			1071	677	212	180	2		

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	121	Total	C	N	O	S	0	0
			975	609	197	169			

- Molecule 21 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	60	Total	C	N	O	S	0	0
			474	302	96	72	4		

- Molecule 22 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	86	Total	C	N	O	S	0	0
			697	441	131	124	1		

- Molecule 23 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	87	Total	C	N	O	S	0	0
			705	453	130	118	4		

- Molecule 24 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	85	Total	C	N	O	S	0	0
			693	436	138	118	1		

- Molecule 25 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	78	Total	C	N	O	S	0	0
			651	417	129	100	5		

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	86	Total	C	N	O	S	0	0
			700	444	132	122	2		

- Molecule 27 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	79	Total	C	N	O		0	0
			643	391	138	114			

- Molecule 28 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	59	Total	C	N	O	S	0	0
			519	326	111	80	2		

- Molecule 29 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	30	Total	C	N	O	S	0	0
			242	155	43	43	1		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	29	Total	C	N	O	P	0	0
			623	280	120	194	29		

- Molecule 31 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Z	36	Total	C	N	O	0	0
			187	112	37	38		

- Molecule 32 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	285	Total	C	N	O	S	0	0
			2225	1385	437	397	6		

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	231	Total	C	N	O	S	0	0
			1778	1129	320	322	7		

- Molecule 34 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	211	Total	C	N	O	S	0	0
			1654	1053	299	299	3		

- Molecule 35 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	179	Total	C	N	O	S	0	0
			1416	910	251	251	4		

- Molecule 36 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	176	Total	C	N	O		0	0
			1396	899	247	250			

- Molecule 37 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	149	Total	C	N	O	S	0	0
			1210	780	212	215	3		

- Molecule 38 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	125	Total	C	N	O	S	0	0
			951	606	165	177	3		

- Molecule 39 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	128	Total	C	N	O	S	0	0
			959	616	160	177	6		

- Molecule 40 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	144	Total	C	N	O	S	0	0
			1164	737	213	209	5		

- Molecule 41 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	122	Total	C	N	O	S	0	0
			944	595	178	167	4		

- Molecule 42 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	150	Total	C	N	O	S	0	0
			1170	741	228	200	1		

- Molecule 43 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	136	Total	C	N	O	S	0	0
			1079	694	196	182	7		

- Molecule 44 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	119	Total	C	N	O	S	0	0
			958	609	175	171	3		

- Molecule 45 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	116	Total	C	N	O	S	0	0
			918	573	181	162	2		

- Molecule 46 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	118	Total	C	N	O	S	0	0
			966	609	186	170	1		

- Molecule 47 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	118	Total	C	N	O	S	0	0
			981	624	194	161	2		

- Molecule 48 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	99	Total	C	N	O	S	0	0
			811	525	148	134	4		

- Molecule 49 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	142	Total	C	N	O	S	0	0
			1091	677	212	195	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	95	Total	C	N	O	S	0	0
			740	486	125	128	1		

- Molecule 51 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	111	Total	C	N	O	S	0	0
			871	550	166	152	3		

- Molecule 52 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	101	Total	C	N	O	S	0	0
			786	498	148	139	1		

- Molecule 53 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	64	Total	C	N	O	S	0	0
			520	320	109	90	1		

- Molecule 54 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	w	110	Total	C	N	O	0	0
			906	576	168	162		

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	x	89	Total	C	N	O	S	0	0
			708	449	124	131	4		

- Molecule 56 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

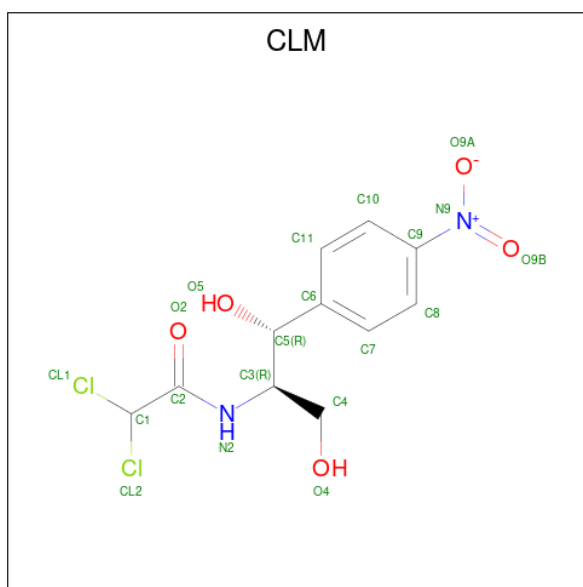
- Molecule 57 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	2	1	Total	Zn	0
			1	1	
58	M	1	Total	Zn	0
			1	1	
58	Q	1	Total	Zn	0
			1	1	
58	x	1	Total	Zn	0
			1	1	
58	y	1	Total	Zn	0
			1	1	
58	z	1	Total	Zn	0
			1	1	

- Molecule 59 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
59	3	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
60	3	1	Total	K	0
			1	1	

- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
61	3	206	Total	Mg	0
			206	206	
61	4	1	Total	Mg	0
			1	1	
61	5	90	Total	Mg	0
			90	90	
61	6	1	Total	Mg	0
			1	1	
61	K	1	Total	Mg	0
			1	1	
61	P	1	Total	Mg	0
			1	1	
61	Y	1	Total	Mg	0
			1	1	

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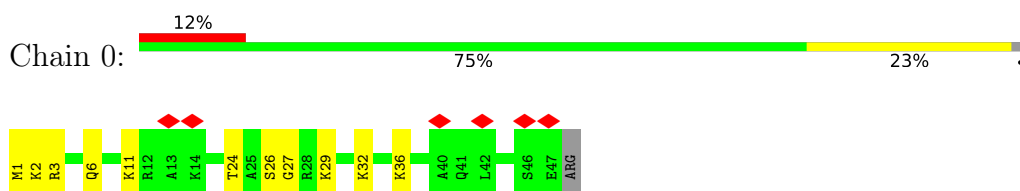
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Mol	Chain	Residues	Atoms		AltConf
61	b	2	Total 2	Mg 2	0
61	i	1	Total 1	Mg 1	0
61	k	2	Total 2	Mg 2	0
61	y	2	Total 2	Mg 2	0

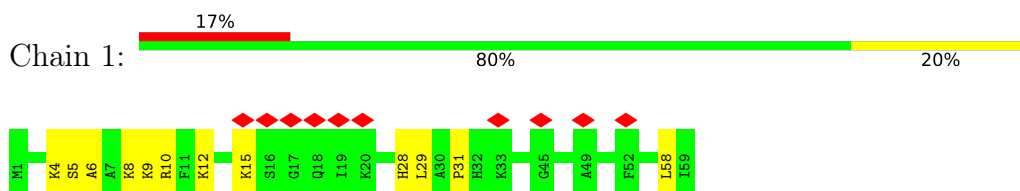
3 Residue-property plots

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.

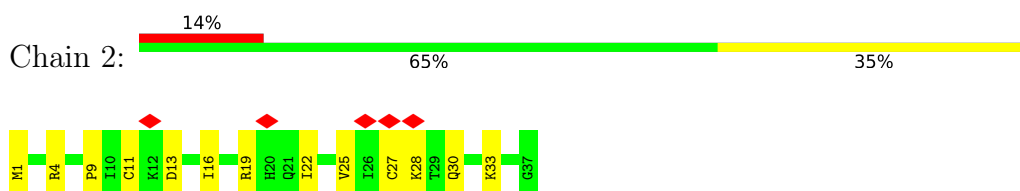
- Molecule 1: 50S ribosomal protein L34



- Molecule 2: 50S ribosomal protein L35

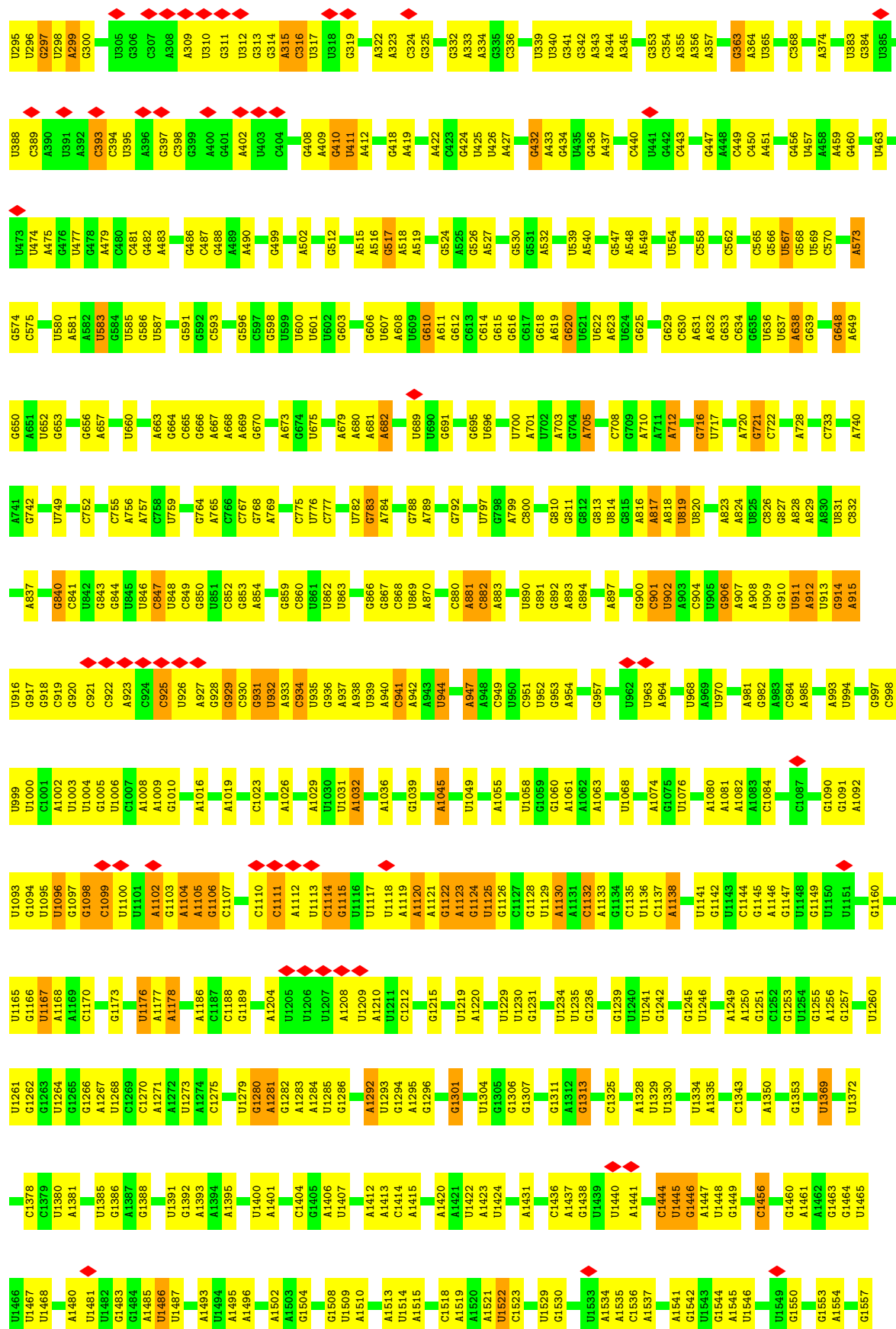


- Molecule 3: 50S ribosomal protein L36



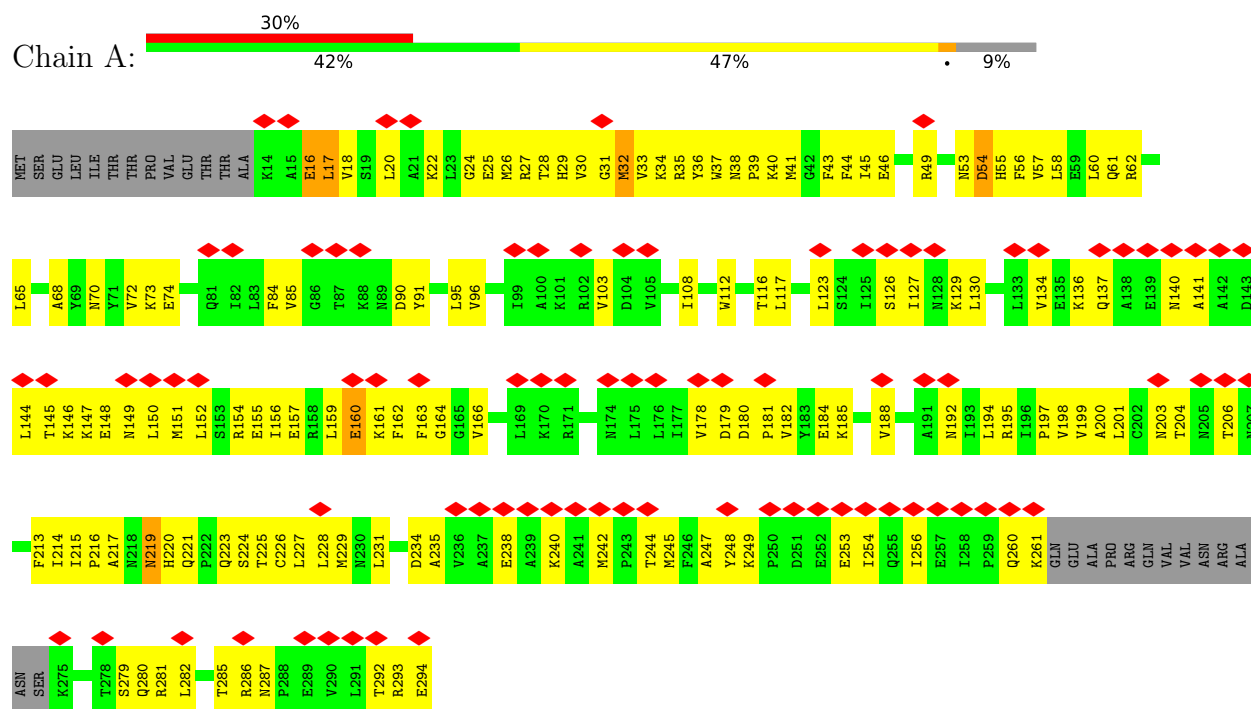
- Molecule 4: 23S ribosomal RNA



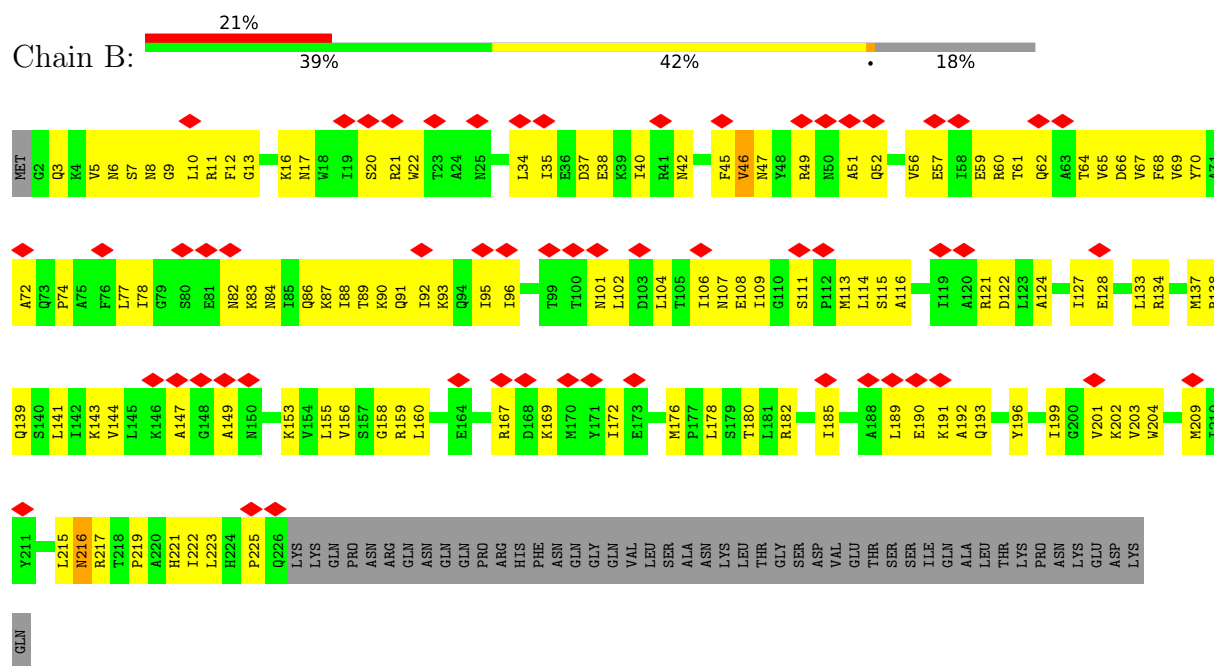




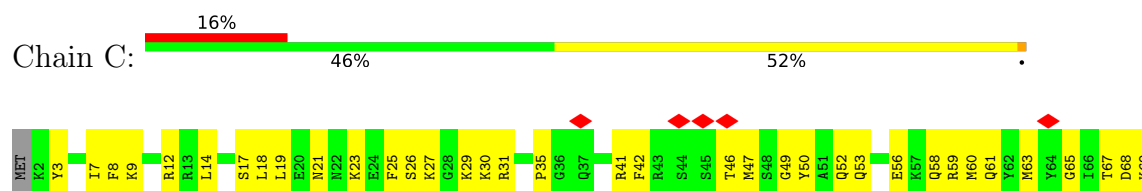
WORLDWIDE
PDB
PROTEIN DATA BANK

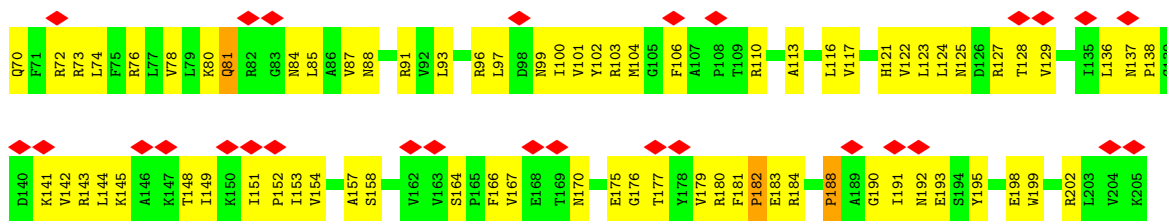


• Molecule 10: 30S ribosomal protein S3

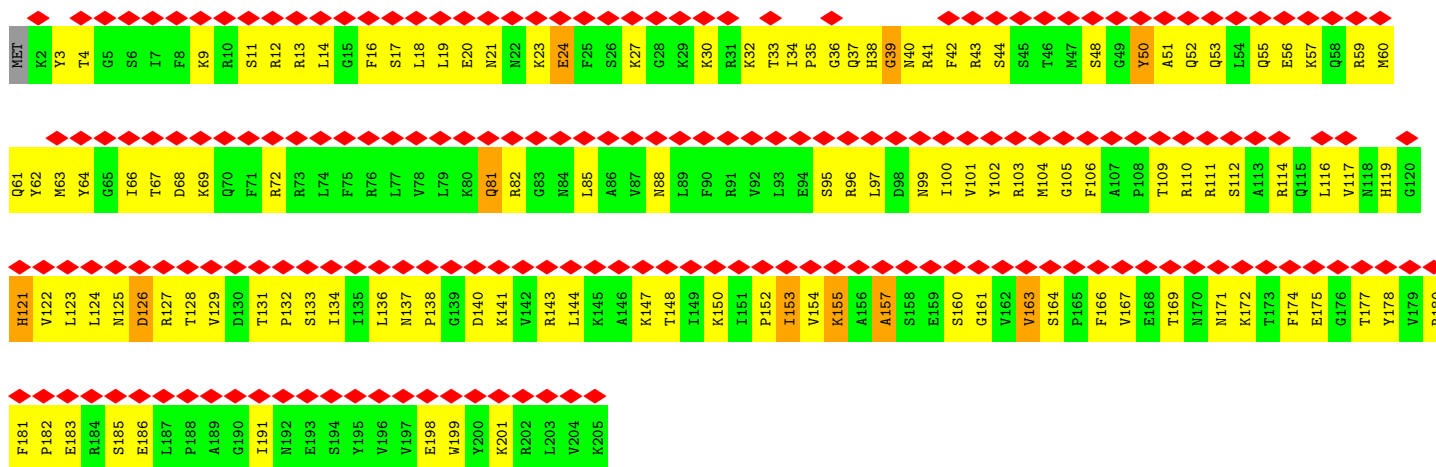
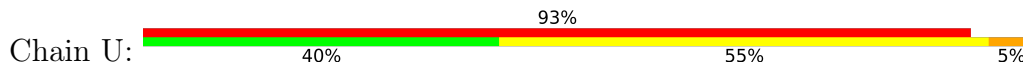


• Molecule 11: 30S ribosomal protein S4

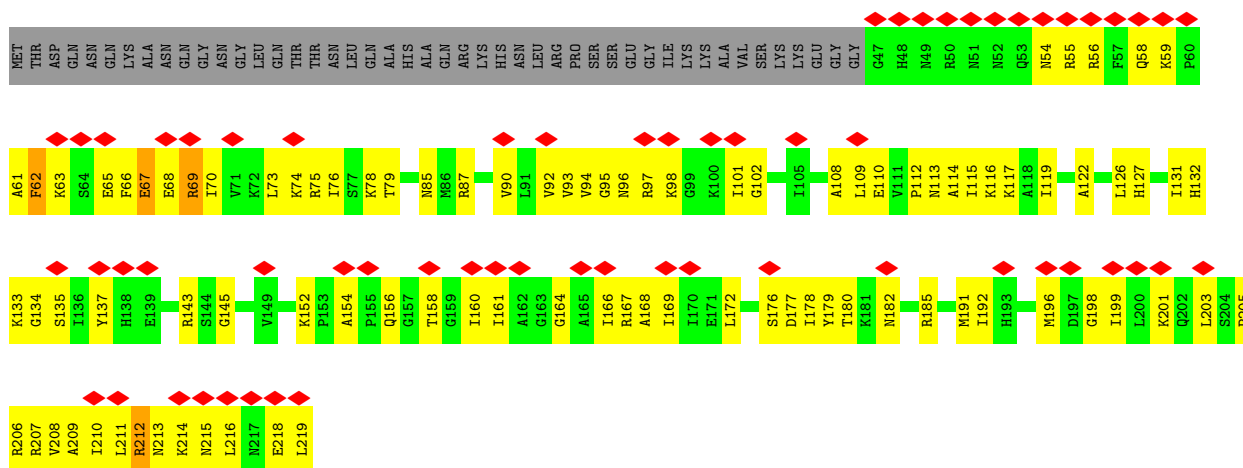




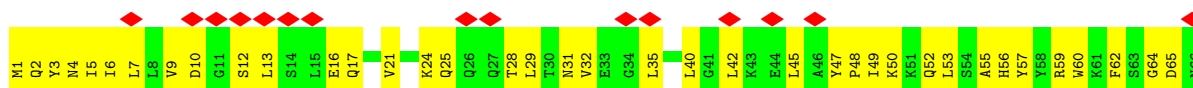
• Molecule 11: 30S ribosomal protein S4

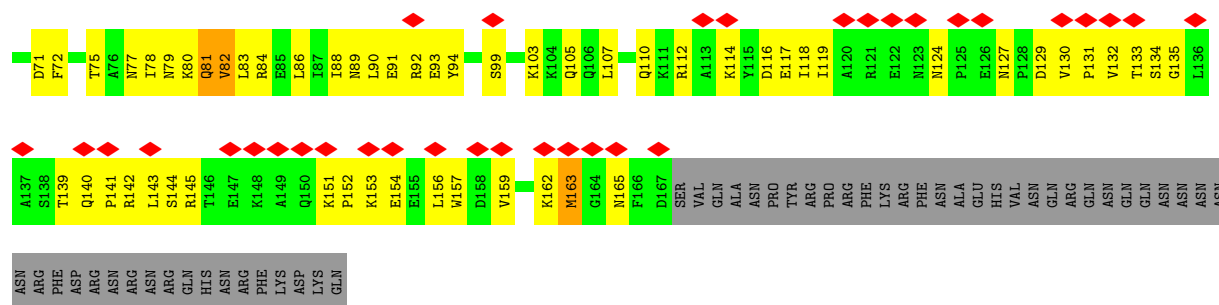


• Molecule 12: 30S ribosomal protein S5

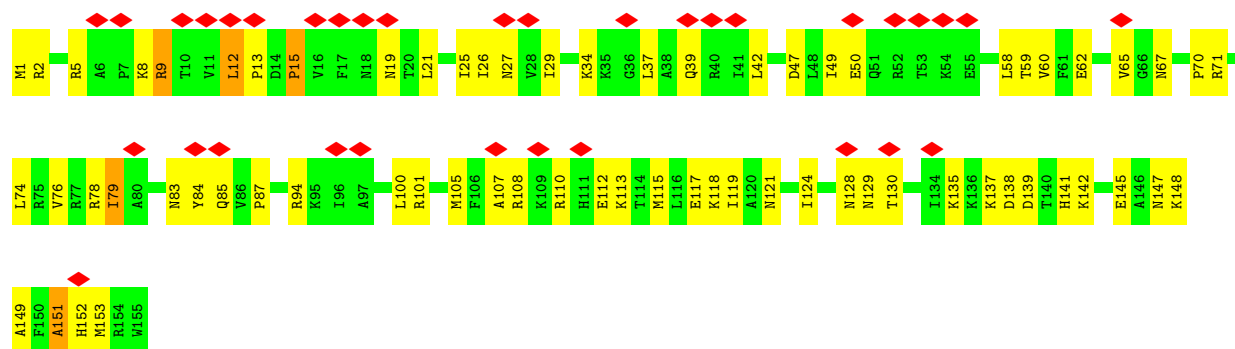


• Molecule 13: 30S ribosomal protein S6

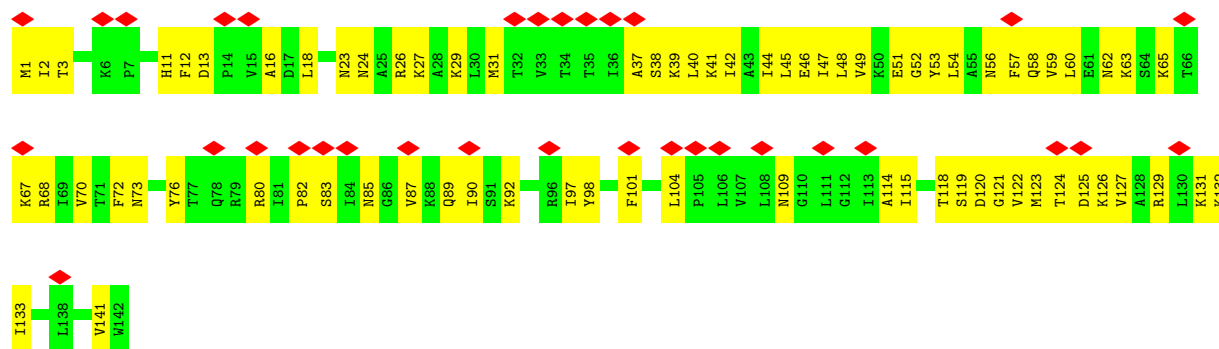




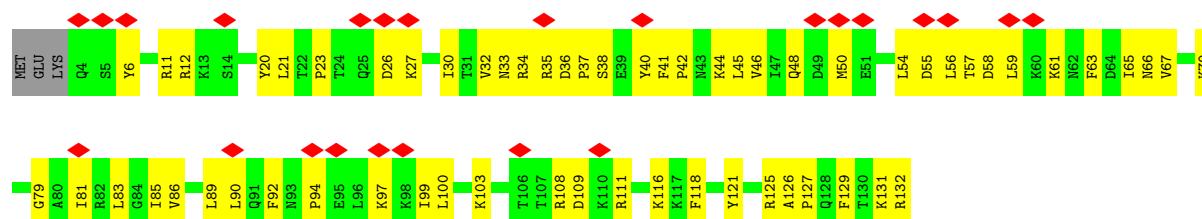
• Molecule 14: 30S ribosomal protein S7

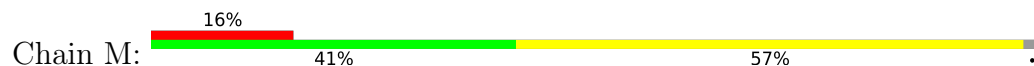


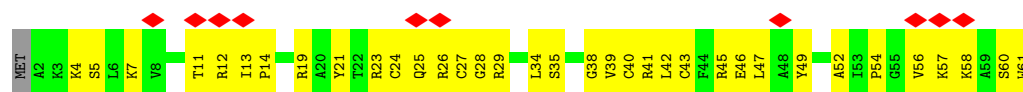
• Molecule 15: 30S ribosomal protein S8



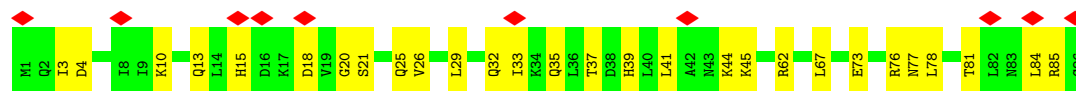
• Molecule 16: 30S ribosomal protein S9



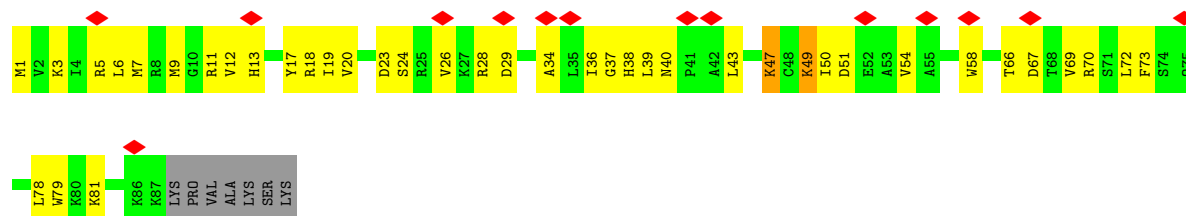




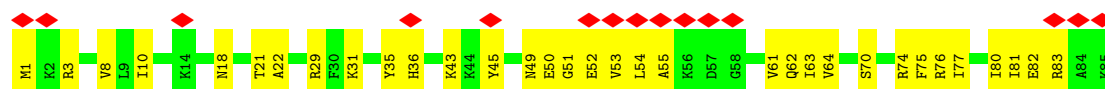
- Molecule 22: 30S ribosomal protein S15



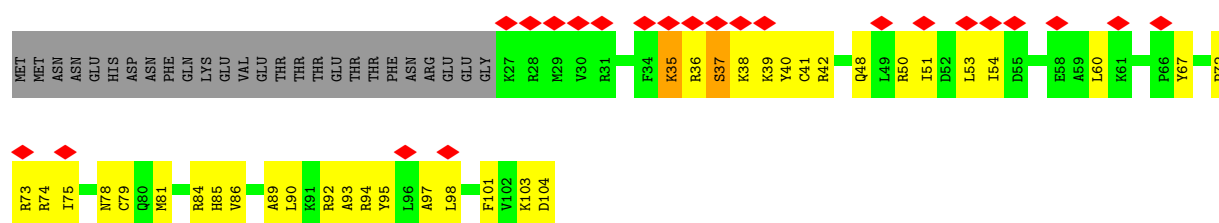
- Molecule 23: 30S ribosomal protein S16



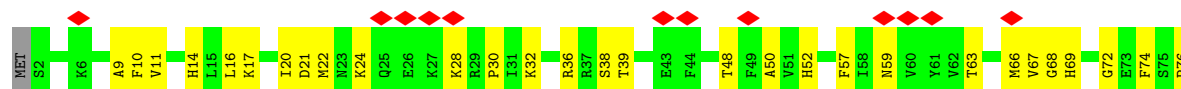
- Molecule 24: 30S ribosomal protein S17



- Molecule 25: 30S ribosomal protein S18

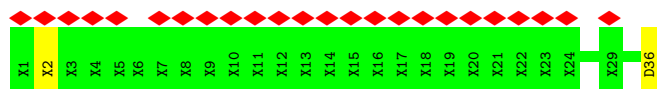


- Molecule 26: 30S ribosomal protein S19

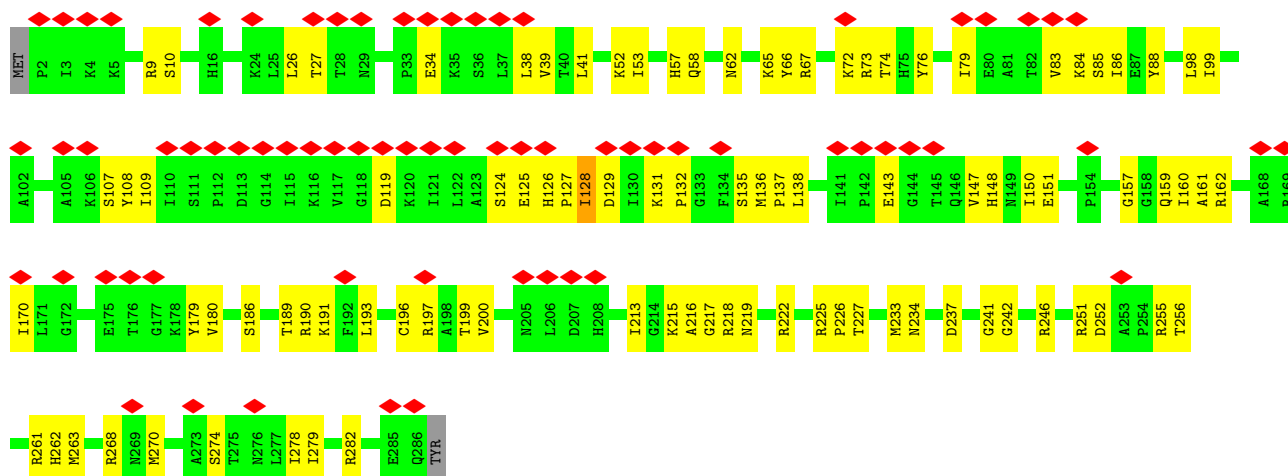




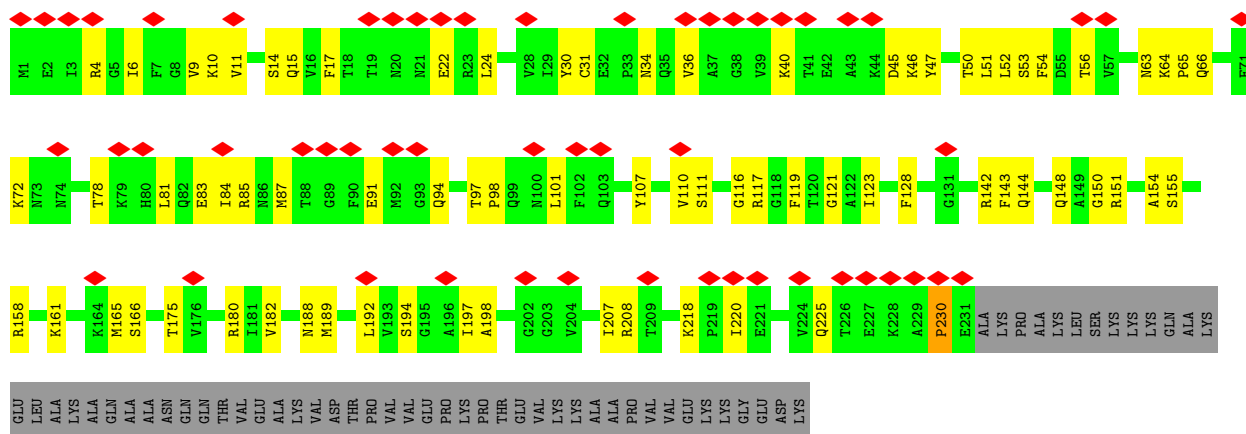
- Molecule 31: Nascent chain



- Molecule 32: 50S ribosomal protein L2

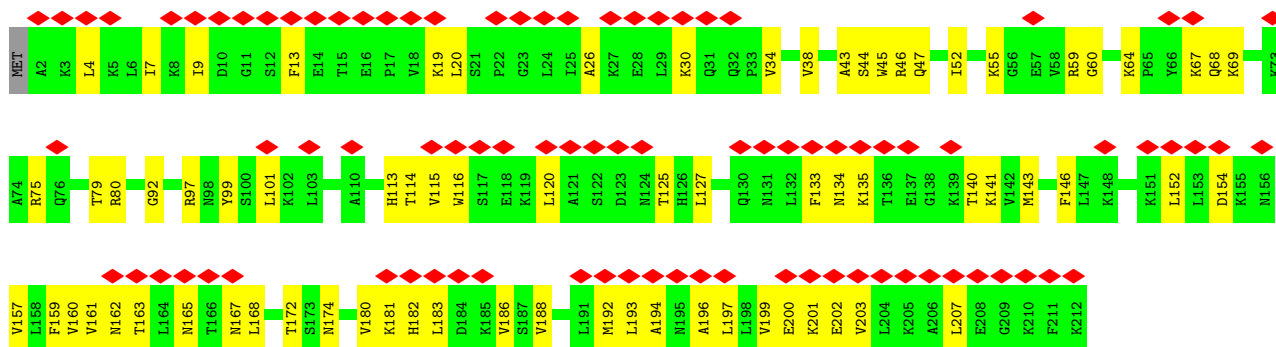


- Molecule 33: 50S ribosomal protein L3

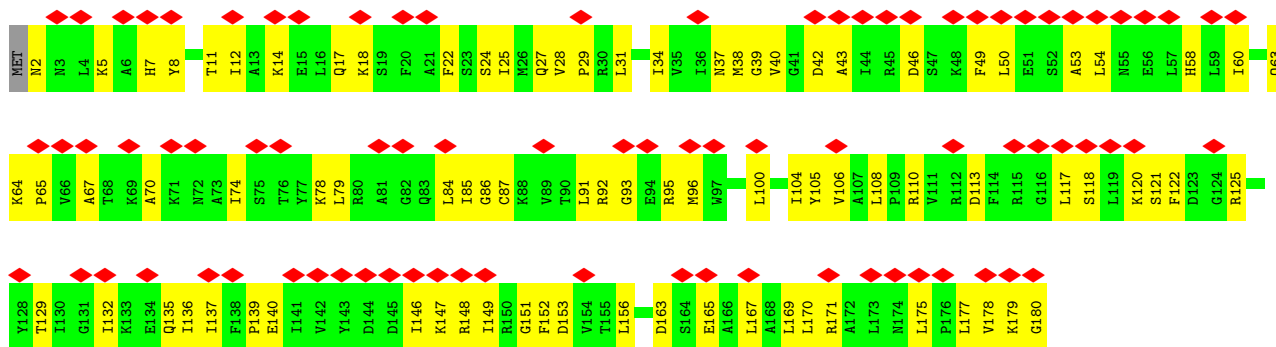


- Molecule 34: 50S ribosomal protein L4

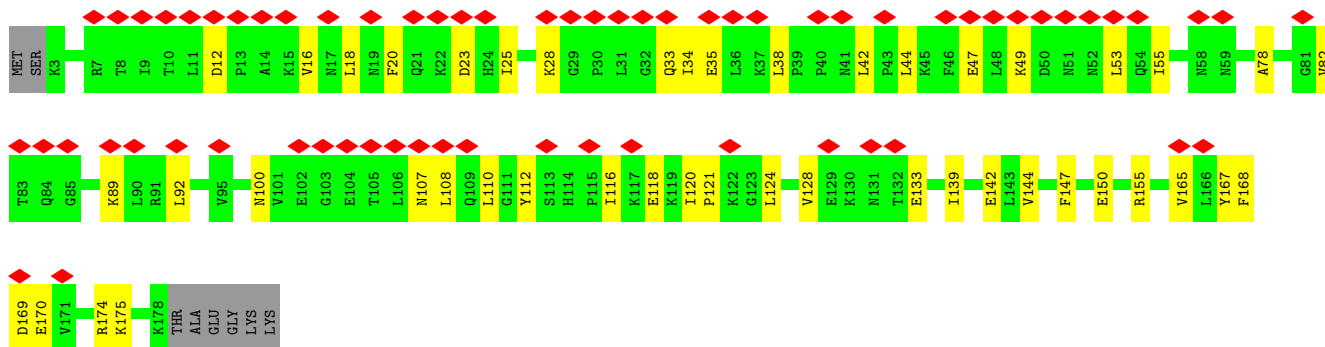




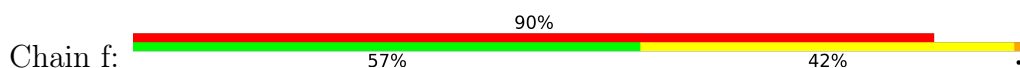
• Molecule 35: 50S ribosomal protein L5

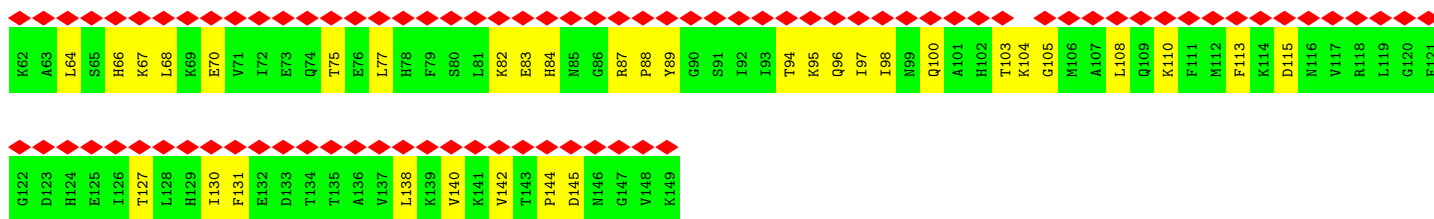


• Molecule 36: 50S ribosomal protein L6

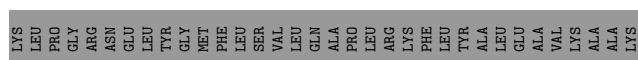
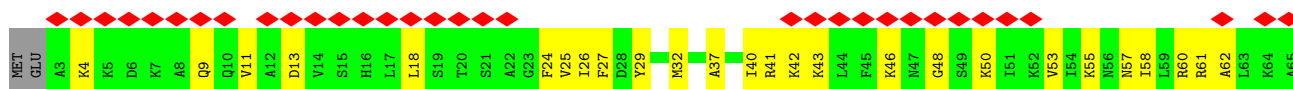
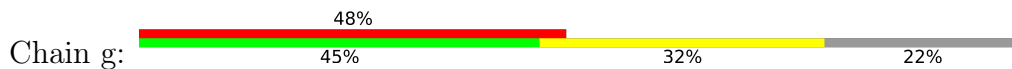


• Molecule 37: 50S ribosomal protein L9

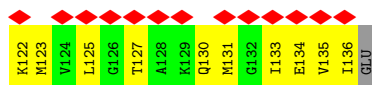
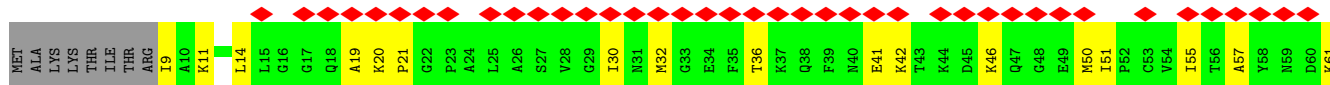
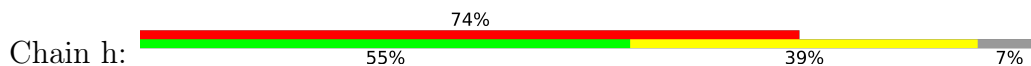




• Molecule 38: 50S ribosomal protein L10



• Molecule 39: 50S ribosomal protein L11

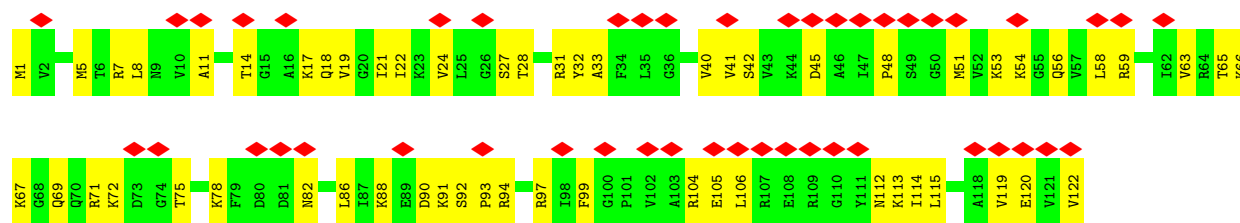


• Molecule 40: 50S ribosomal protein L13

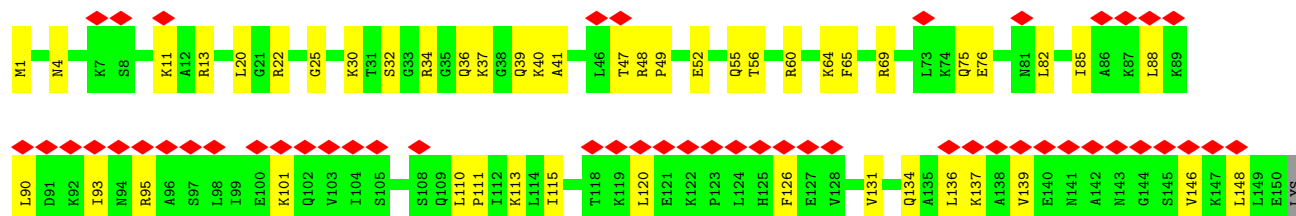


• Molecule 41: 50S ribosomal protein L14

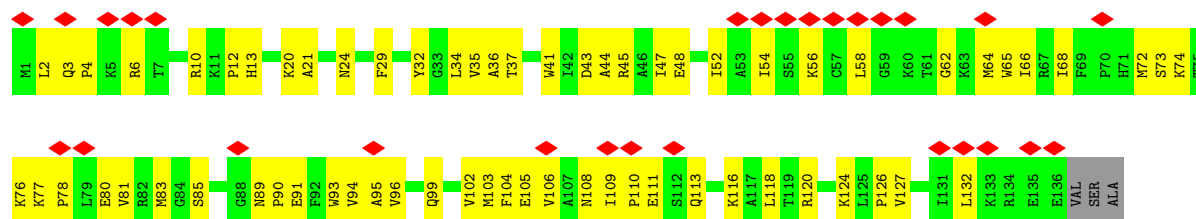




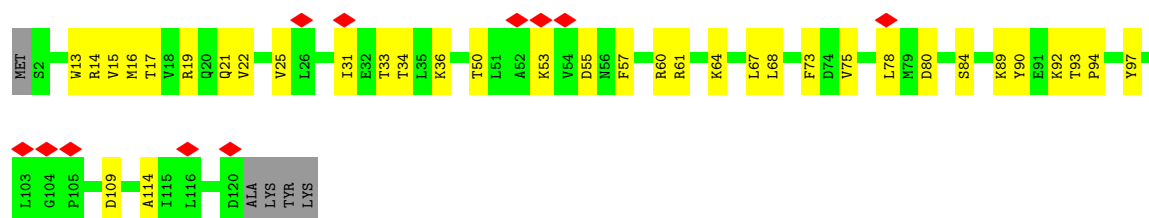
• Molecule 42: 50S ribosomal protein L15



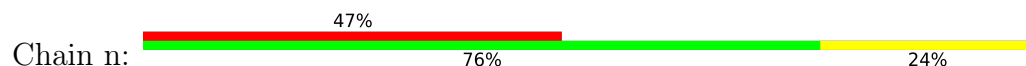
• Molecule 43: 50S ribosomal protein L16

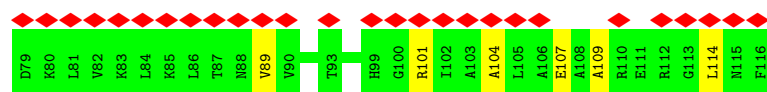


• Molecule 44: 50S ribosomal protein L17

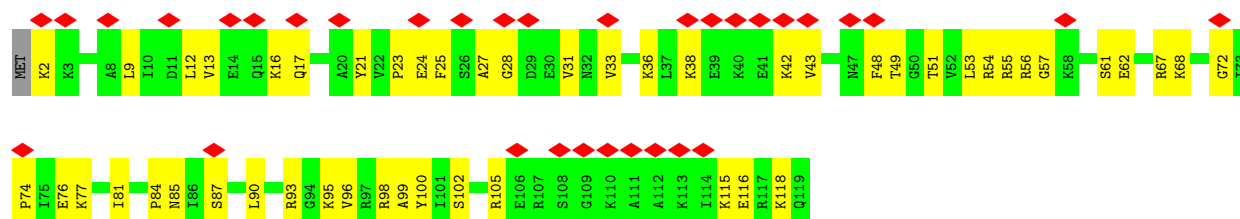


• Molecule 45: 50S ribosomal protein L18

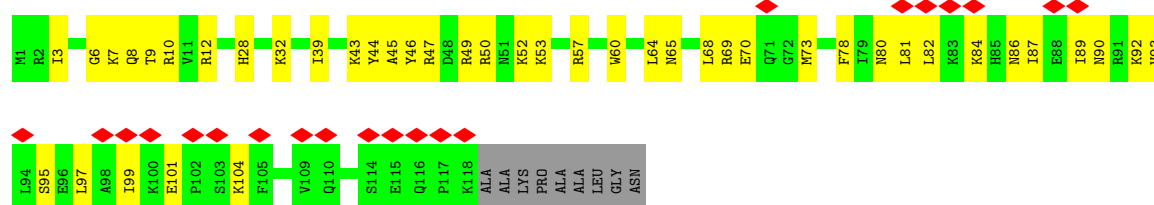




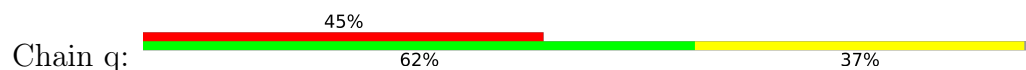
• Molecule 46: 50S ribosomal protein L19



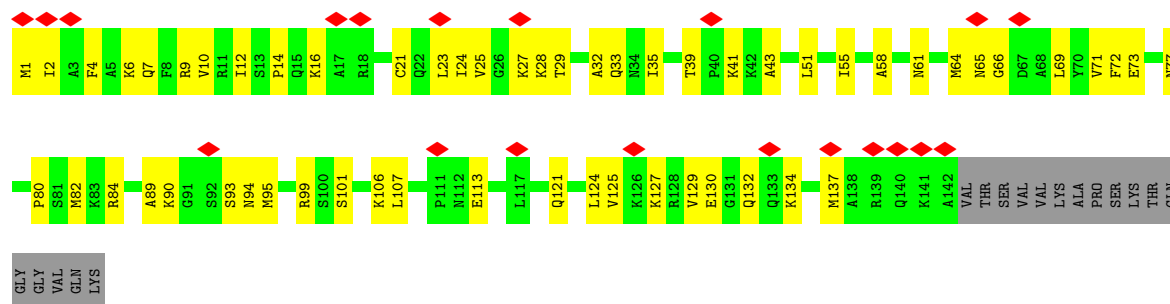
• Molecule 47: 50S ribosomal protein L20



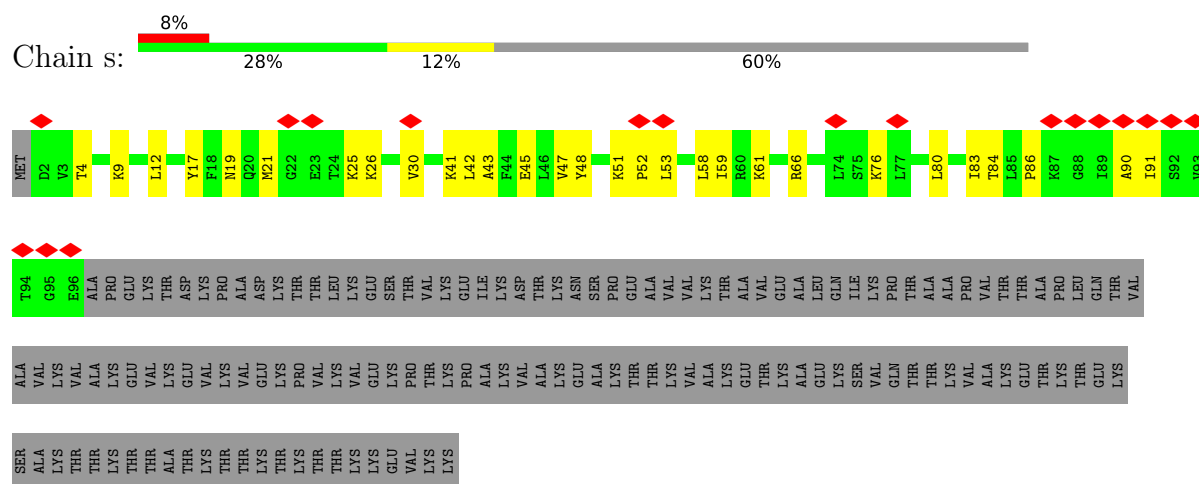
• Molecule 48: 50S ribosomal protein L21



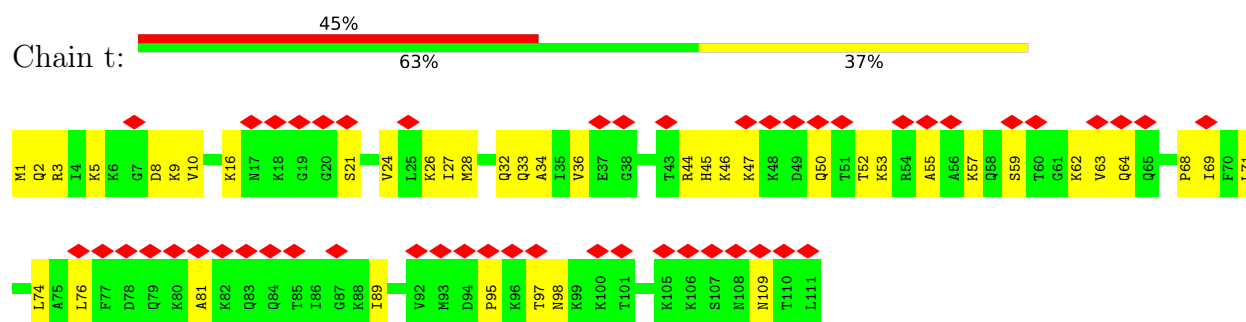
• Molecule 49: 50S ribosomal protein L22



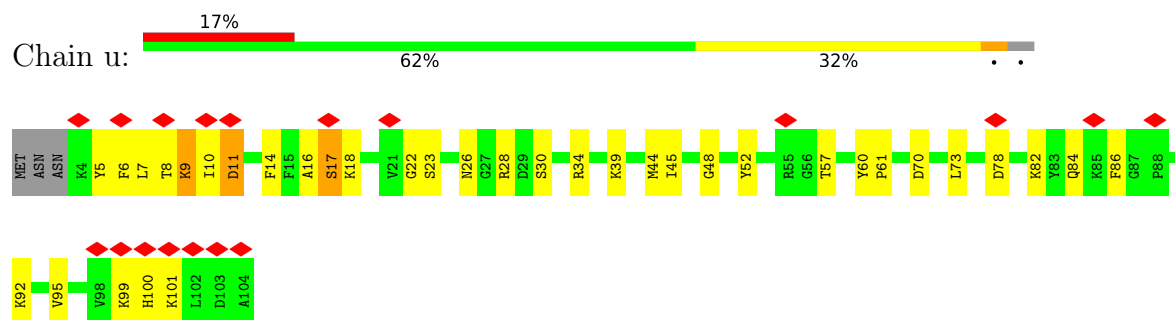
- Molecule 50: 50S ribosomal protein L23



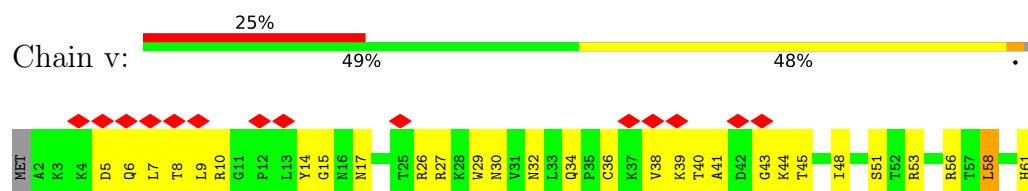
- Molecule 51: 50S ribosomal protein L24



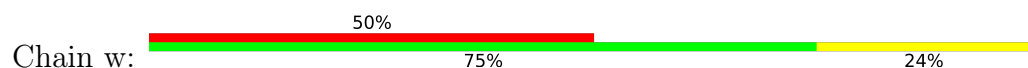
- Molecule 52: 50S ribosomal protein L27

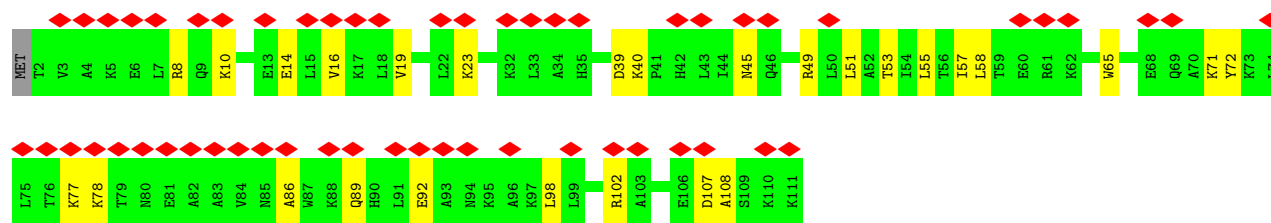


- Molecule 53: 50S ribosomal protein L28

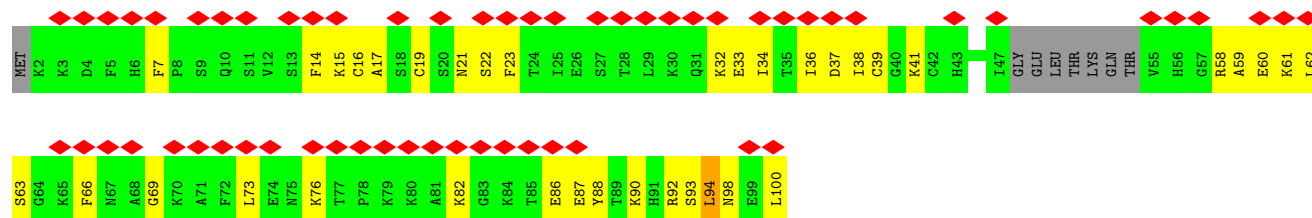


- Molecule 54: 50S ribosomal protein L29

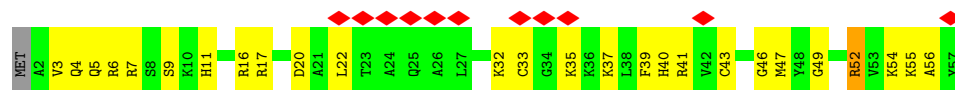




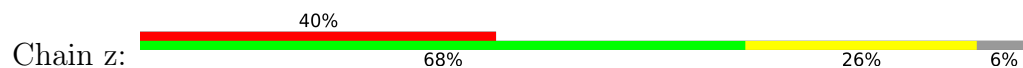
• Molecule 55: 50S ribosomal protein L31



• Molecule 56: 50S ribosomal protein L32



• Molecule 57: 50S ribosomal protein L33 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	963	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.477	Depositor
Minimum map value	-2.425	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.237	Depositor
Recommended contour level	1.2	Depositor
Map size (Å)	793.6, 793.6, 793.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.1, 3.1, 3.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, 5MC, 7MG, 1MG, OMG, B8T, MG, ZN, 2MA, CLM, MA6

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	0	0.14	0/383	0.42	0/504
2	1	0.10	0/484	0.30	0/637
3	2	0.17	0/306	0.54	0/401
4	3	0.10	1/69363 (0.0%)	0.24	1/108161 (0.0%)
5	4	0.08	0/2578	0.20	0/4016
6	5	0.11	0/35992	0.23	1/56111 (0.0%)
7	6	0.16	0/1810	0.47	1/2817 (0.0%)
8	7	0.23	1/1785 (0.1%)	0.31	0/2779
9	A	0.22	0/2186	0.66	2/2952 (0.1%)
10	B	0.18	0/1800	0.53	0/2433
11	C	0.25	0/1700	0.71	0/2278
11	U	0.27	0/1700	0.82	0/2278
12	D	0.23	0/1365	0.61	0/1827
13	E	0.23	0/1384	0.68	0/1867
14	F	0.21	0/1274	0.62	0/1710
15	G	0.22	0/1134	0.62	1/1527 (0.1%)
16	H	0.20	0/1056	0.55	1/1409 (0.1%)
17	I	0.24	0/843	0.64	0/1132
18	J	0.16	0/844	0.48	0/1136
19	K	0.18	0/1089	0.52	0/1461
20	L	0.20	0/986	0.50	0/1321
21	M	0.24	0/483	0.54	0/643
22	N	0.17	0/703	0.50	0/936
23	O	0.24	0/718	0.72	0/962
24	P	0.14	0/702	0.44	0/934
25	Q	0.19	0/663	0.59	0/883
26	R	0.19	0/716	0.56	1/958 (0.1%)
27	S	0.13	0/645	0.38	0/857
28	T	0.23	0/524	0.68	0/685
29	X	0.18	0/245	0.65	0/325
30	Y	0.19	0/699	0.48	0/1087
31	Z	0.89	0/26	1.70	0/33

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	a	0.14	0/2267	0.44	0/3044
33	b	0.21	0/1812	0.55	0/2436
34	c	0.14	0/1681	0.46	0/2257
35	d	0.18	0/1437	0.50	0/1931
36	e	0.17	0/1420	0.47	0/1912
37	f	0.19	0/1233	0.53	0/1653
38	g	0.18	0/960	0.47	0/1284
39	h	0.16	0/968	0.46	0/1298
40	i	0.17	0/1186	0.46	0/1592
41	j	0.19	0/953	0.56	0/1275
42	k	0.15	0/1187	0.50	0/1581
43	l	0.21	0/1104	0.55	0/1481
44	m	0.15	0/973	0.42	0/1309
45	n	0.13	0/927	0.41	0/1239
46	o	0.19	0/976	0.53	0/1296
47	p	0.14	0/996	0.43	0/1325
48	q	0.21	0/828	0.55	0/1111
49	r	0.18	0/1100	0.59	0/1471
50	s	0.12	0/752	0.39	0/1015
51	t	0.23	0/878	0.65	2/1165 (0.2%)
52	u	0.15	0/798	0.52	0/1063
53	v	0.23	0/526	0.69	1/703 (0.1%)
54	w	0.11	0/916	0.34	0/1222
55	x	0.21	0/722	0.76	2/959 (0.2%)
56	y	0.19	0/457	0.62	1/601 (0.2%)
57	z	0.16	0/412	0.48	0/547
All	All	0.14	2/163655 (0.0%)	0.36	14/243830 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	U	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	72	G	O3'-P	-6.41	1.51	1.61
4	3	783	1MG	O3'-P	5.29	1.61	1.56

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1434	C	P-O3'-C3'	-8.27	107.79	120.20
55	x	94	LEU	CA-C-N	7.24	135.37	121.54
55	x	94	LEU	C-N-CA	7.24	135.37	121.54
51	t	95	PRO	CA-N-CD	-6.39	103.05	112.00
26	R	76	PRO	CA-N-CD	-6.21	103.30	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	U	121	HIS	Peptide
11	U	153	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	380	0	429	10	0
2	1	477	0	530	10	0
3	2	304	0	348	11	0
4	3	61995	0	31115	937	0
5	4	2305	0	1164	23	0
6	5	32258	0	16205	508	0
7	6	1620	0	818	26	0
8	7	1599	0	805	24	0
9	A	2152	0	2222	125	0
10	B	1773	0	1841	107	0
11	C	1669	0	1729	116	0
11	U	1669	0	1729	140	0
12	D	1346	0	1433	107	0
13	E	1362	0	1377	88	0
14	F	1254	0	1320	66	0
15	G	1118	0	1238	87	0
16	H	1040	0	1107	59	0
17	I	832	0	918	84	0
18	J	829	0	855	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	1071	0	1165	64	0
20	L	975	0	1043	37	0
21	M	474	0	505	42	0
22	N	697	0	758	22	0
23	O	705	0	755	50	0
24	P	693	0	753	27	0
25	Q	651	0	700	38	0
26	R	700	0	709	42	0
27	S	643	0	694	26	0
28	T	519	0	578	40	0
29	X	242	0	263	8	0
30	Y	623	0	315	25	0
31	Z	187	0	68	2	0
32	a	2225	0	2301	83	0
33	b	1778	0	1821	76	0
34	c	1654	0	1744	61	0
35	d	1416	0	1500	74	0
36	e	1396	0	1481	37	0
37	f	1210	0	1259	56	0
38	g	951	0	1001	42	0
39	h	959	0	1039	41	0
40	i	1164	0	1192	38	0
41	j	944	0	1019	61	0
42	k	1170	0	1274	44	0
43	l	1079	0	1134	68	0
44	m	958	0	1011	29	0
45	n	918	0	979	22	0
46	o	966	0	1042	55	0
47	p	981	0	1062	46	0
48	q	811	0	858	33	0
49	r	1091	0	1178	46	0
50	s	740	0	819	23	0
51	t	871	0	972	35	0
52	u	786	0	823	31	0
53	v	520	0	565	46	0
54	w	906	0	981	15	0
55	x	708	0	710	40	0
56	y	452	0	471	32	0
57	z	408	0	436	11	0
58	2	1	0	0	0	0
58	M	1	0	0	0	0
58	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	x	1	0	0	0	0
58	y	1	0	0	0	0
58	z	1	0	0	0	0
59	3	20	0	11	1	0
60	3	1	0	0	0	0
61	3	206	0	0	0	0
61	4	1	0	0	0	0
61	5	90	0	0	0	0
61	6	1	0	0	0	0
61	K	1	0	0	0	0
61	P	1	0	0	0	0
61	Y	1	0	0	0	0
61	b	2	0	0	0	0
61	i	1	0	0	0	0
61	k	2	0	0	0	0
61	y	2	0	0	0	0
All	All	151559	0	104172	3524	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 14.

The worst 5 of 3524 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)
12:D:211:LEU:HD21	15:G:83:SER:OG	1.53	1.05
22:N:21:SER:O	22:N:25:GLN:NE2	1.91	1.04
11:C:193:GLU:HG3	11:C:195:TYR:HD1	1.23	1.03
12:D:212:ARG:NH1	15:G:53:TYR:CE1	2.29	1.01
12:D:212:ARG:NH1	15:G:53:TYR:CD1	2.31	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	45/48 (94%)	45 (100%)	0	0	100	100
2	1	57/59 (97%)	57 (100%)	0	0	100	100
3	2	35/37 (95%)	35 (100%)	0	0	100	100
9	A	264/294 (90%)	233 (88%)	25 (10%)	6 (2%)	5	28
10	B	223/273 (82%)	197 (88%)	24 (11%)	2 (1%)	14	51
11	C	202/205 (98%)	166 (82%)	33 (16%)	3 (2%)	8	40
11	U	202/205 (98%)	148 (73%)	41 (20%)	13 (6%)	1	12
12	D	171/219 (78%)	141 (82%)	25 (15%)	5 (3%)	3	23
13	E	165/215 (77%)	142 (86%)	18 (11%)	5 (3%)	3	23
14	F	153/155 (99%)	132 (86%)	15 (10%)	6 (4%)	2	19
15	G	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
16	H	127/132 (96%)	115 (91%)	12 (9%)	0	100	100
17	I	102/108 (94%)	88 (86%)	13 (13%)	1 (1%)	12	49
18	J	112/121 (93%)	105 (94%)	7 (6%)	0	100	100
19	K	133/139 (96%)	113 (85%)	15 (11%)	5 (4%)	2	19
20	L	119/124 (96%)	112 (94%)	7 (6%)	0	100	100
21	M	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
22	N	84/86 (98%)	77 (92%)	6 (7%)	1 (1%)	10	44
23	O	85/94 (90%)	78 (92%)	5 (6%)	2 (2%)	4	27
24	P	83/85 (98%)	71 (86%)	11 (13%)	1 (1%)	10	44
25	Q	76/104 (73%)	65 (86%)	9 (12%)	2 (3%)	4	25
26	R	84/87 (97%)	79 (94%)	5 (6%)	0	100	100
27	S	77/87 (88%)	74 (96%)	2 (3%)	1 (1%)	9	42
28	T	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	X	28/444 (6%)	24 (86%)	4 (14%)	0	100	100
31	Z	3/36 (8%)	3 (100%)	0	0	100	100
32	a	283/287 (99%)	267 (94%)	15 (5%)	1 (0%)	30	67
33	b	229/287 (80%)	219 (96%)	9 (4%)	1 (0%)	30	67
34	c	209/212 (99%)	198 (95%)	11 (5%)	0	100	100
35	d	177/180 (98%)	169 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	e	174/184 (95%)	162 (93%)	12 (7%)	0	100	100
37	f	147/149 (99%)	131 (89%)	15 (10%)	1 (1%)	18	56
38	g	123/161 (76%)	117 (95%)	6 (5%)	0	100	100
39	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
40	i	142/146 (97%)	133 (94%)	9 (6%)	0	100	100
41	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
42	k	148/151 (98%)	138 (93%)	10 (7%)	0	100	100
43	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
44	m	117/124 (94%)	112 (96%)	5 (4%)	0	100	100
45	n	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
46	o	116/119 (98%)	108 (93%)	8 (7%)	0	100	100
47	p	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
48	q	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
49	r	140/159 (88%)	137 (98%)	3 (2%)	0	100	100
50	s	93/237 (39%)	89 (96%)	4 (4%)	0	100	100
51	t	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
52	u	99/104 (95%)	86 (87%)	9 (9%)	4 (4%)	2	18
53	v	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
54	w	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
55	x	85/97 (88%)	64 (75%)	21 (25%)	0	100	100
56	y	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
57	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	6255/7355 (85%)	5717 (91%)	478 (8%)	60 (1%)	15	49

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	D	67	GLU
12	D	69	ARG
12	D	212	ARG
12	D	216	LEU
13	E	81	GLN

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	
1	0	40/41 (98%)	40 (100%)	0	100	100
2	1	51/51 (100%)	51 (100%)	0	100	100
3	2	35/35 (100%)	35 (100%)	0	100	100
9	A	239/262 (91%)	239 (100%)	0	100	100
10	B	188/232 (81%)	188 (100%)	0	100	100
11	C	182/183 (100%)	182 (100%)	0	100	100
11	U	182/183 (100%)	182 (100%)	0	100	100
12	D	141/178 (79%)	141 (100%)	0	100	100
13	E	150/196 (76%)	150 (100%)	0	100	100
14	F	132/132 (100%)	132 (100%)	0	100	100
15	G	124/124 (100%)	124 (100%)	0	100	100
16	H	112/115 (97%)	112 (100%)	0	100	100
17	I	97/99 (98%)	97 (100%)	0	100	100
18	J	91/97 (94%)	91 (100%)	0	100	100
19	K	117/120 (98%)	117 (100%)	0	100	100
20	L	102/105 (97%)	102 (100%)	0	100	100
21	M	47/48 (98%)	47 (100%)	0	100	100
22	N	78/78 (100%)	78 (100%)	0	100	100
23	O	76/82 (93%)	76 (100%)	0	100	100
24	P	75/75 (100%)	75 (100%)	0	100	100
25	Q	69/94 (73%)	69 (100%)	0	100	100
26	R	76/77 (99%)	76 (100%)	0	100	100
27	S	71/77 (92%)	71 (100%)	0	100	100
28	T	55/56 (98%)	55 (100%)	0	100	100
29	X	27/406 (7%)	27 (100%)	0	100	100
31	Z	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	a	241/243 (99%)	241 (100%)	0	100	100
33	b	188/233 (81%)	188 (100%)	0	100	100
34	c	183/184 (100%)	183 (100%)	0	100	100
35	d	153/154 (99%)	153 (100%)	0	100	100
36	e	153/159 (96%)	153 (100%)	0	100	100
37	f	134/134 (100%)	134 (100%)	0	100	100
38	g	100/129 (78%)	100 (100%)	0	100	100
39	h	102/110 (93%)	102 (100%)	0	100	100
40	i	126/128 (98%)	126 (100%)	0	100	100
41	j	103/103 (100%)	103 (100%)	0	100	100
42	k	125/126 (99%)	125 (100%)	0	100	100
43	l	113/115 (98%)	113 (100%)	0	100	100
44	m	105/109 (96%)	105 (100%)	0	100	100
45	n	99/99 (100%)	99 (100%)	0	100	100
46	o	104/105 (99%)	104 (100%)	0	100	100
47	p	104/108 (96%)	104 (100%)	0	100	100
48	q	90/91 (99%)	90 (100%)	0	100	100
49	r	118/132 (89%)	118 (100%)	0	100	100
50	s	84/208 (40%)	84 (100%)	0	100	100
51	t	96/96 (100%)	96 (100%)	0	100	100
52	u	82/85 (96%)	82 (100%)	0	100	100
53	v	59/60 (98%)	59 (100%)	0	100	100
54	w	97/98 (99%)	97 (100%)	0	100	100
55	x	79/86 (92%)	79 (100%)	0	100	100
56	y	48/49 (98%)	48 (100%)	0	100	100
57	z	47/50 (94%)	47 (100%)	0	100	100
All	All	5492/6342 (87%)	5492 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
40	i	80	HIS
47	p	106	ASN
41	j	18	GLN
44	m	81	HIS
49	r	120	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	Y	28/29 (96%)	16 (57%)	4 (14%)
4	3	2892/2907 (99%)	536 (18%)	18 (0%)
5	4	107/108 (99%)	29 (27%)	0
6	5	1506/1520 (99%)	258 (17%)	10 (0%)
7	6	76/76 (100%)	23 (30%)	5 (6%)
8	7	74/75 (98%)	20 (27%)	2 (2%)
All	All	4683/4715 (99%)	882 (18%)	39 (0%)

5 of 882 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	3	11	U
4	3	12	A
4	3	13	C
4	3	14	U
4	3	28	G

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	6	1	G
30	Y	34	A
7	6	15	A
7	6	74	C
30	Y	49	U

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

8 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
6	B8T	5	1377	6	19,22,23	4.76	13 (68%)	25,31,34	0.98	1 (4%)
6	MA6	5	1494	6	23,26,27	1.40	3 (13%)	33,38,41	3.24	14 (42%)
6	7MG	5	525	6	23,26,27	3.63	11 (47%)	27,39,42	2.17	9 (33%)
4	1MG	3	783	4	23,26,27	0.59	0	33,39,42	0.73	1 (3%)
6	MA6	5	1493	6	23,26,27	1.41	3 (13%)	33,38,41	3.20	14 (42%)
4	2MA	3	2511	4,61	22,25,26	5.06	15 (68%)	32,37,40	3.73	12 (37%)
4	OMG	3	2259	4,8	23,26,27	0.33	0	32,38,41	0.43	0
6	5MC	5	1375	6	19,22,23	0.82	1 (5%)	26,32,35	0.69	1 (3%)

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
6	B8T	5	1377	6	-	0/7/27/28	0/2/2/2
6	MA6	5	1494	6	-	2/11/29/30	0/3/3/3
6	7MG	5	525	6	-	2/7/37/38	0/3/3/3
4	1MG	3	783	4	-	0/7/25/26	0/3/3/3
6	MA6	5	1493	6	-	0/11/29/30	0/3/3/3
4	2MA	3	2511	4,61	-	2/7/25/26	0/3/3/3
4	OMG	3	2259	4,8	-	3/9/27/28	0/3/3/3
6	5MC	5	1375	6	-	0/7/25/26	0/2/2/2

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	2511	2MA	C4-N3	12.12	1.50	1.34
6	5	1377	B8T	O4'-C1'	9.11	1.63	1.42
4	3	2511	2MA	O4'-C1'	8.88	1.62	1.42
6	5	525	7MG	C8-N9	8.67	1.51	1.45
4	3	2511	2MA	C2-N3	8.16	1.48	1.34

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	2511	2MA	C1'-N9-C8	-13.21	97.79	127.09
4	3	2511	2MA	C4-N9-C1'	11.51	153.55	126.63
6	5	1494	MA6	N1-C6-N6	-10.41	104.18	116.86
6	5	1493	MA6	N1-C6-N6	-10.08	104.57	116.86
6	5	1494	MA6	C5-C6-N6	6.77	136.05	125.33

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	3	2259	OMG	C1'-C2'-O2'-CM2
6	5	525	7MG	O4'-C4'-C5'-O5'
6	5	1494	MA6	O4'-C4'-C5'-O5'
6	5	525	7MG	C3'-C4'-C5'-O5'
6	5	1494	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	783	1MG	3	0
6	5	1493	MA6	1	0
4	3	2259	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 316 ligands modelled in this entry, 315 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
59	CLM	3	3001	-	20,20,20	2.09	2 (10%)	23,27,27	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	CLM	3	3001	-	-	2/20/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	3	3001	CLM	C2-N2	7.45	1.50	1.34
59	3	3001	CLM	O9B-N9	-2.61	1.18	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	3	3001	CLM	C5-C3-C4-O4
59	3	3001	CLM	N2-C3-C4-O4

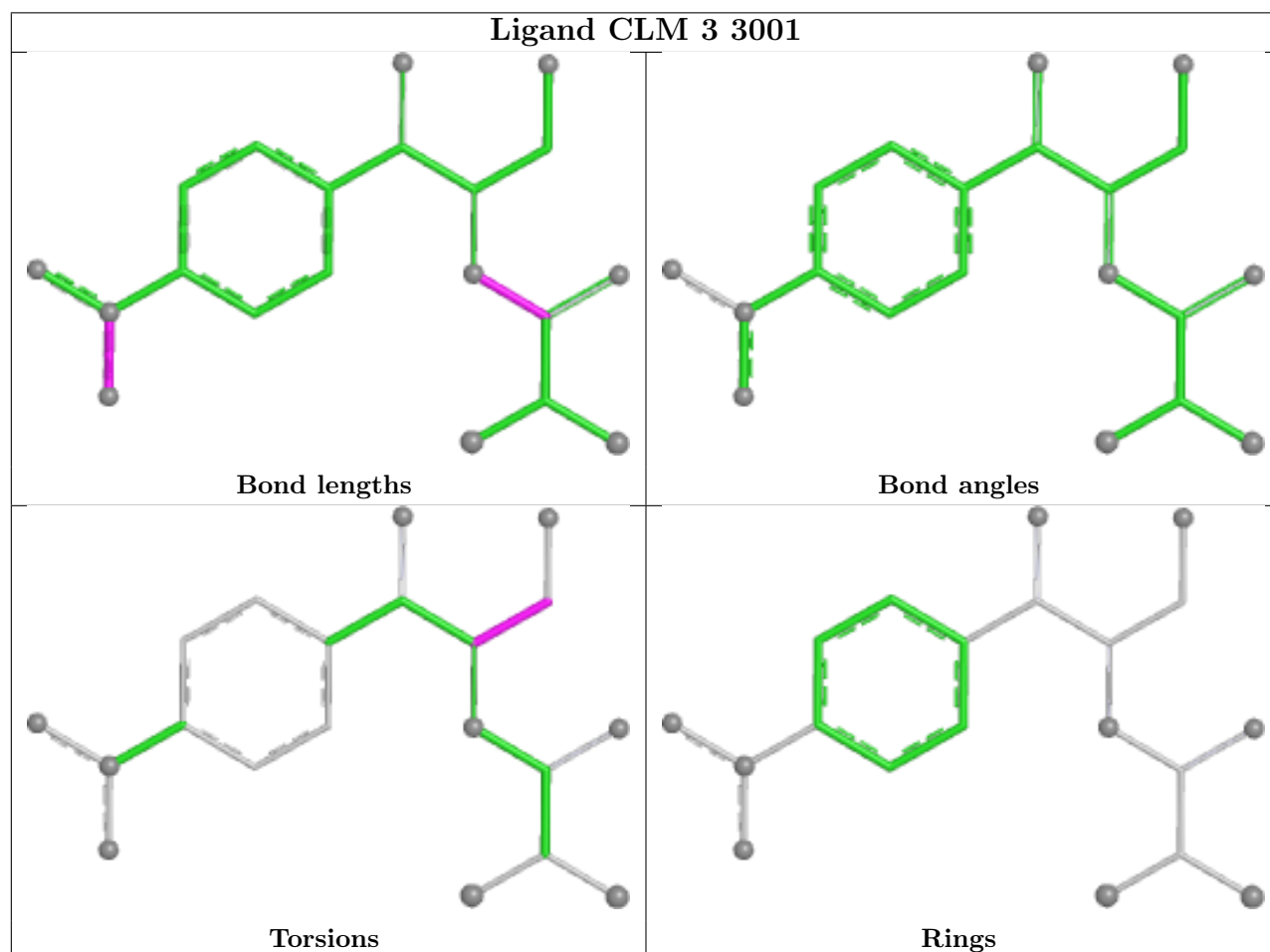
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	3	3001	CLM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

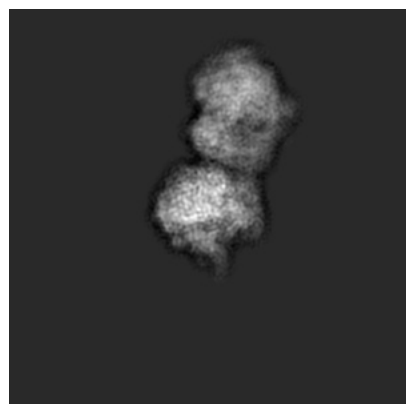
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17145. These allow visual inspection of the internal detail of the map and identification of artifacts.

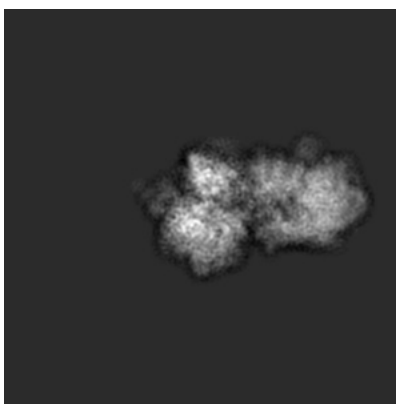
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

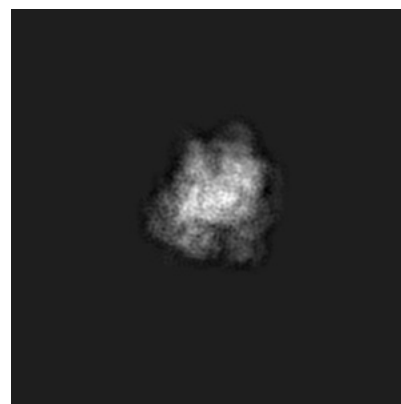
6.1.1 Primary map



X

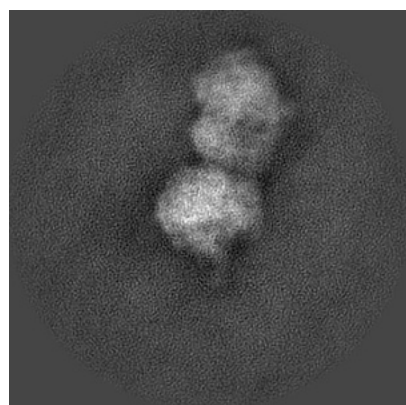


Y

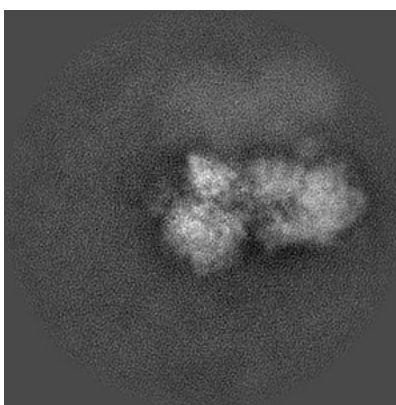


Z

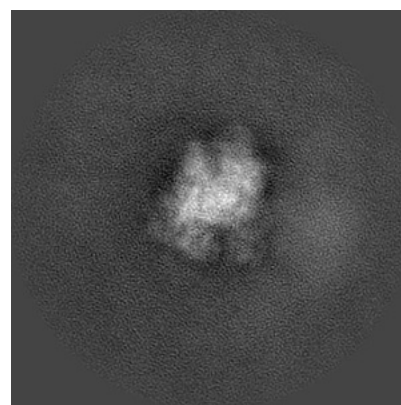
6.1.2 Raw map



X



Y

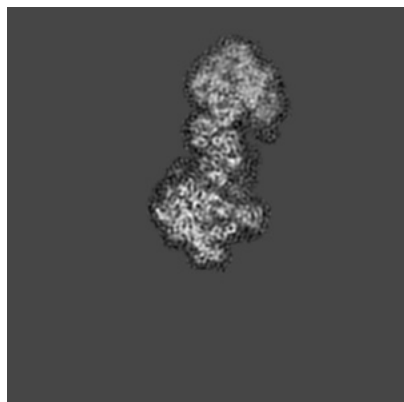


Z

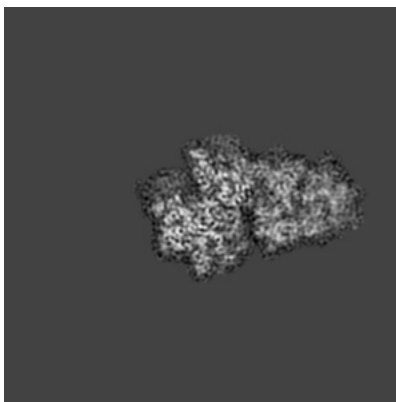
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

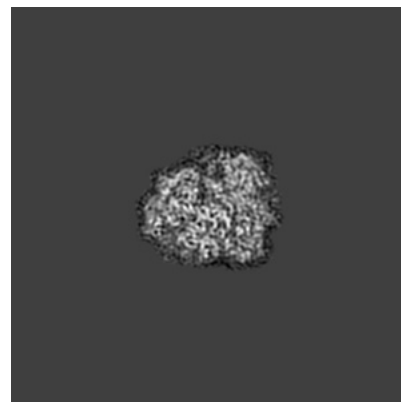
6.2.1 Primary map



X Index: 128

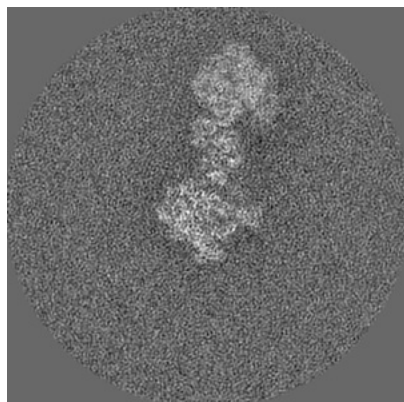


Y Index: 128

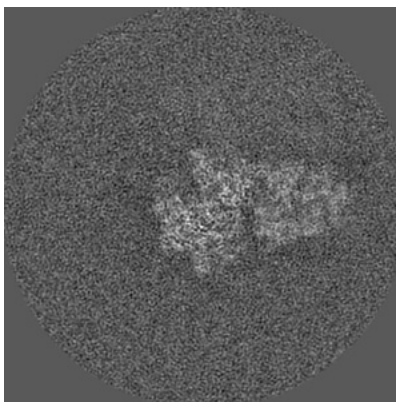


Z Index: 128

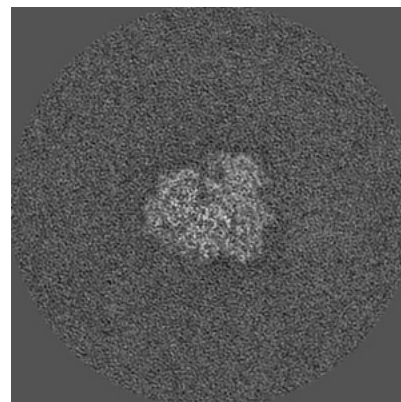
6.2.2 Raw map



X Index: 128



Y Index: 128

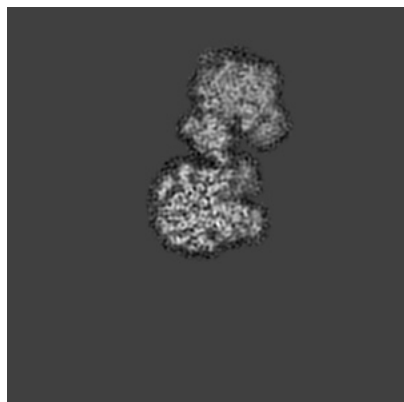


Z Index: 128

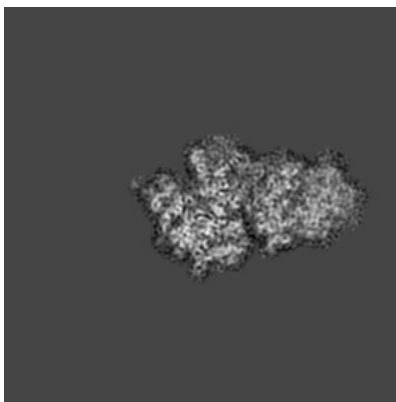
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

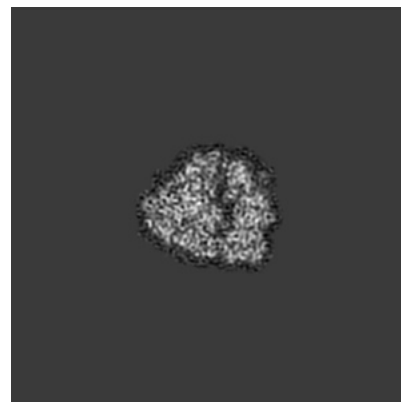
6.3.1 Primary map



X Index: 117

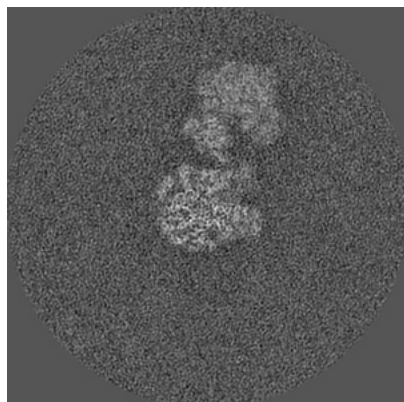


Y Index: 131

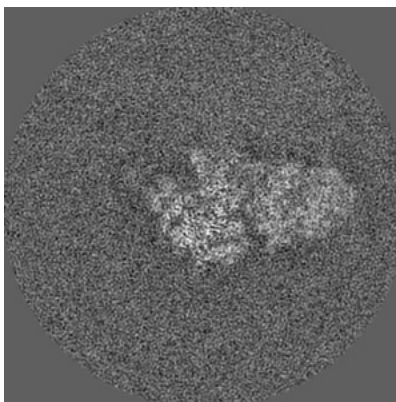


Z Index: 124

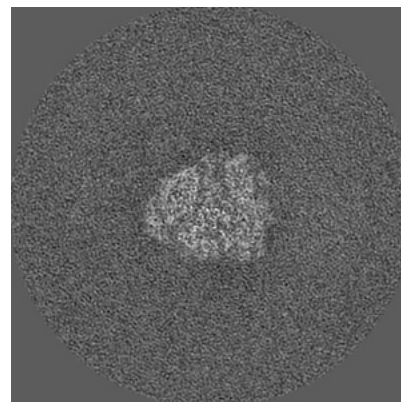
6.3.2 Raw map



X Index: 117



Y Index: 131

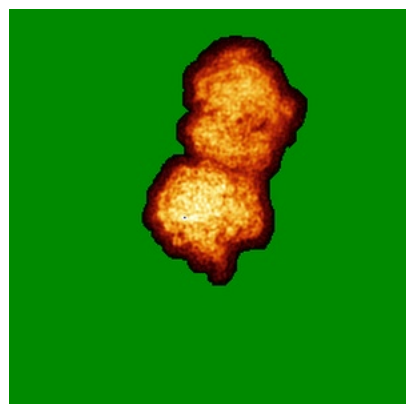


Z Index: 127

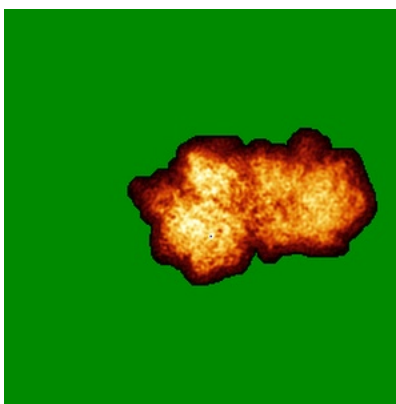
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

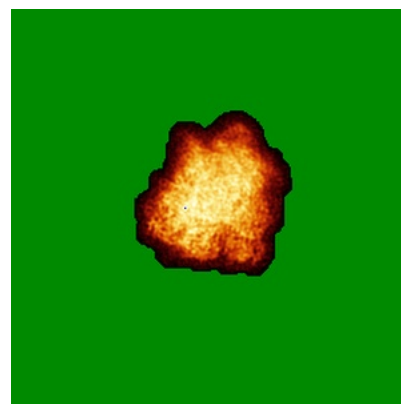
6.4.1 Primary map



X

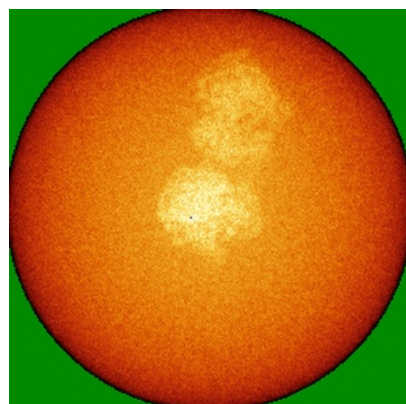


Y

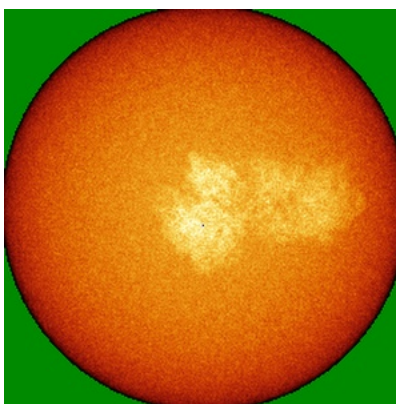


Z

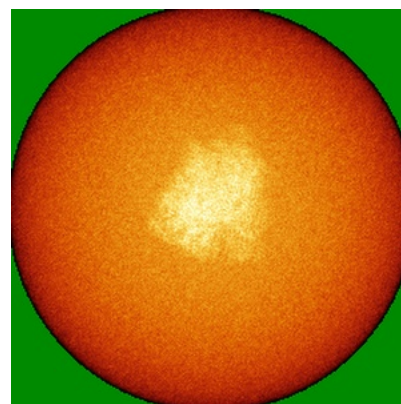
6.4.2 Raw map



X



Y



Z

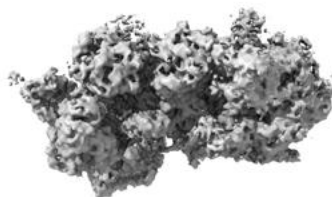
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

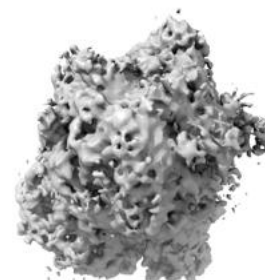
6.5.1 Primary map



X



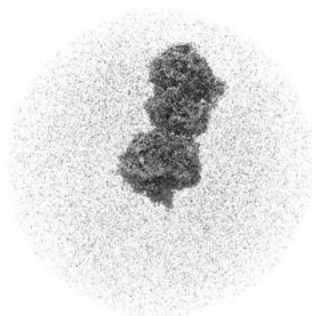
Y



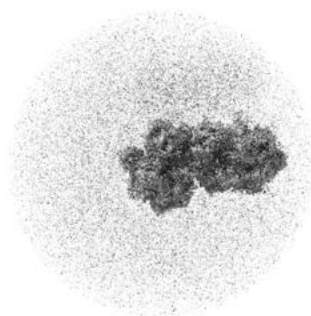
Z

The images above show the 3D surface view of the map at the recommended contour level 1.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

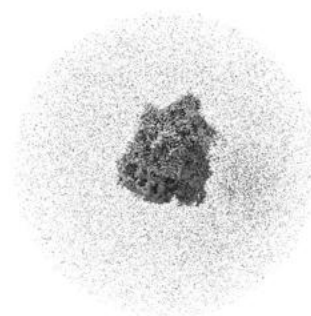
6.5.2 Raw map



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.

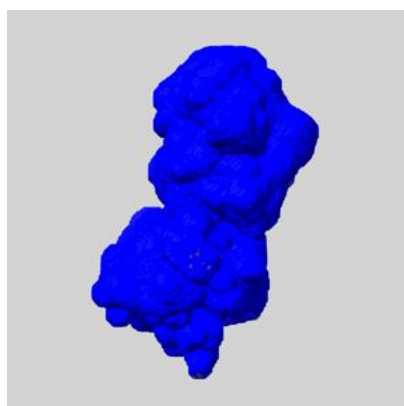
6.6 Mask visualisation [i](#)

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

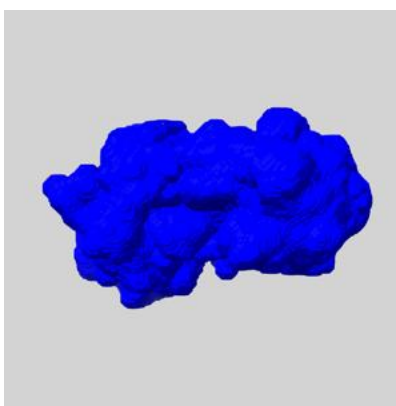
A mask typically either:

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

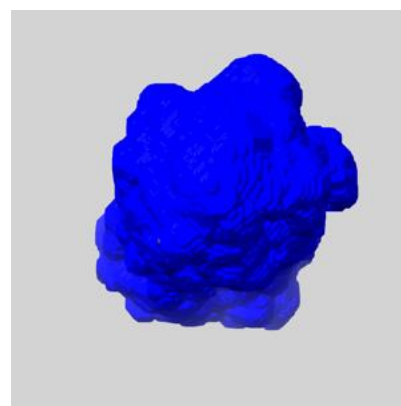
6.6.1 emd_17145_msk_1.map [i](#)



X



Y

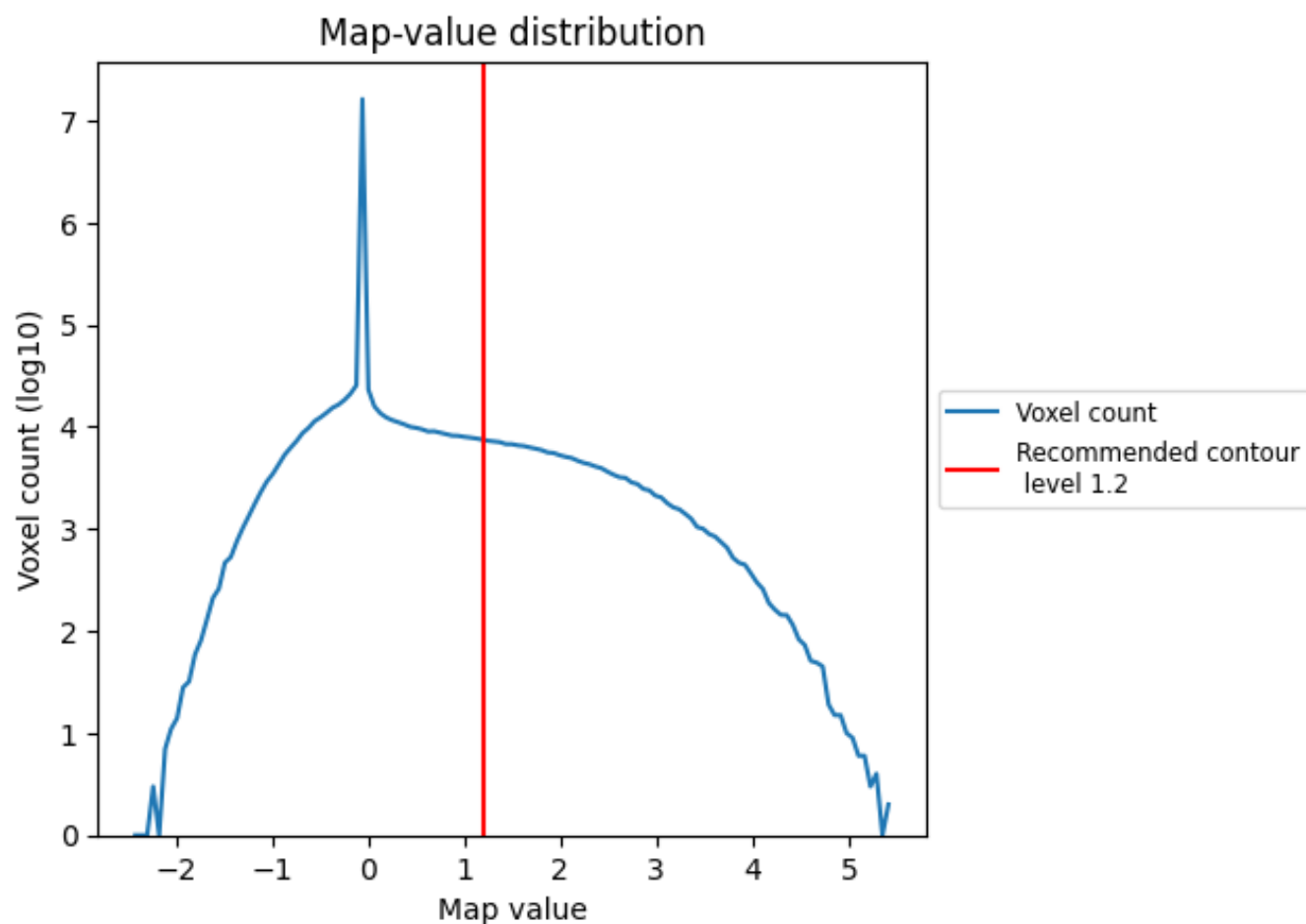


Z

7 Map analysis [i](#)

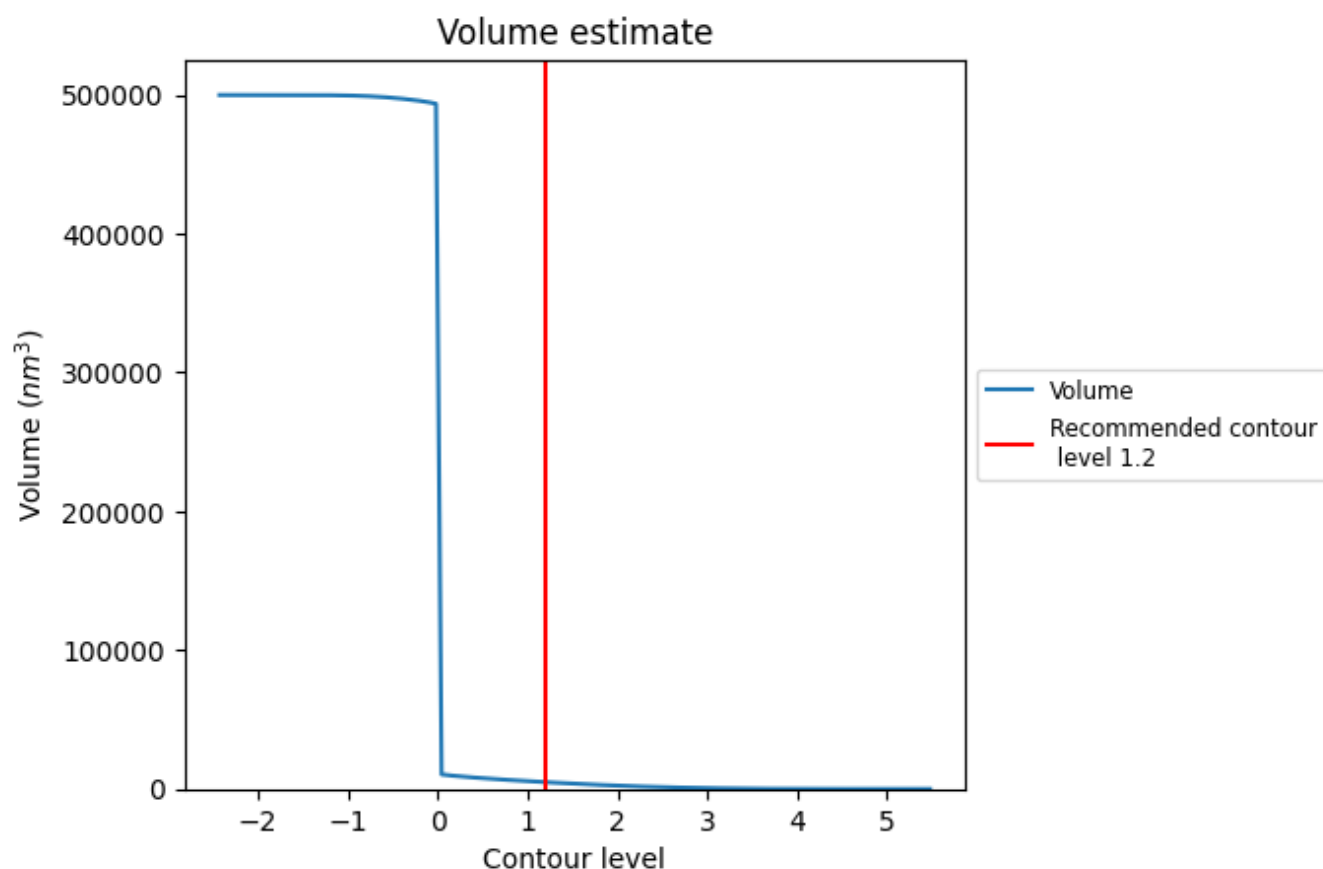
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

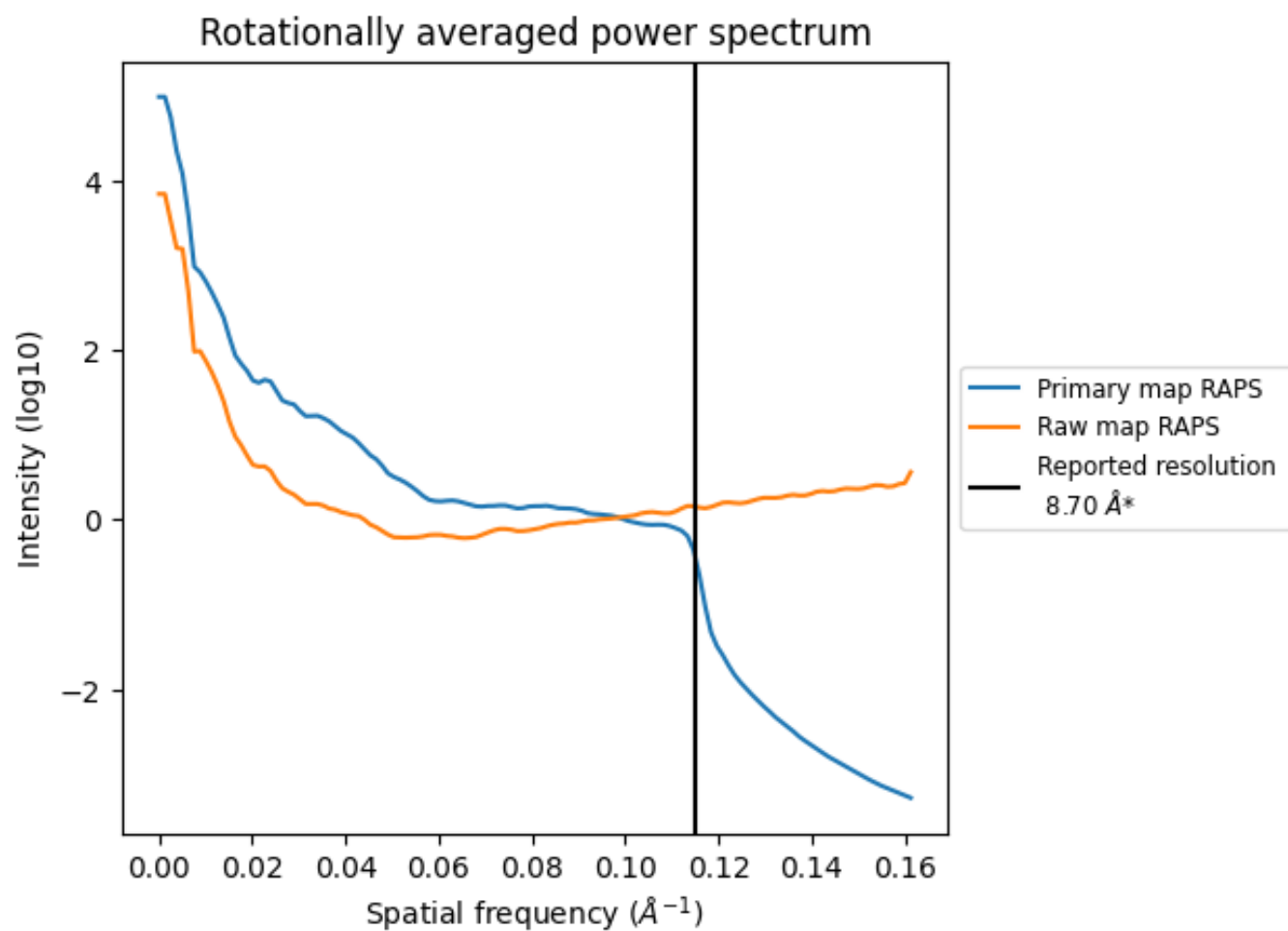
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4893 nm^3 ; this corresponds to an approximate mass of 4420 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 ⓘ

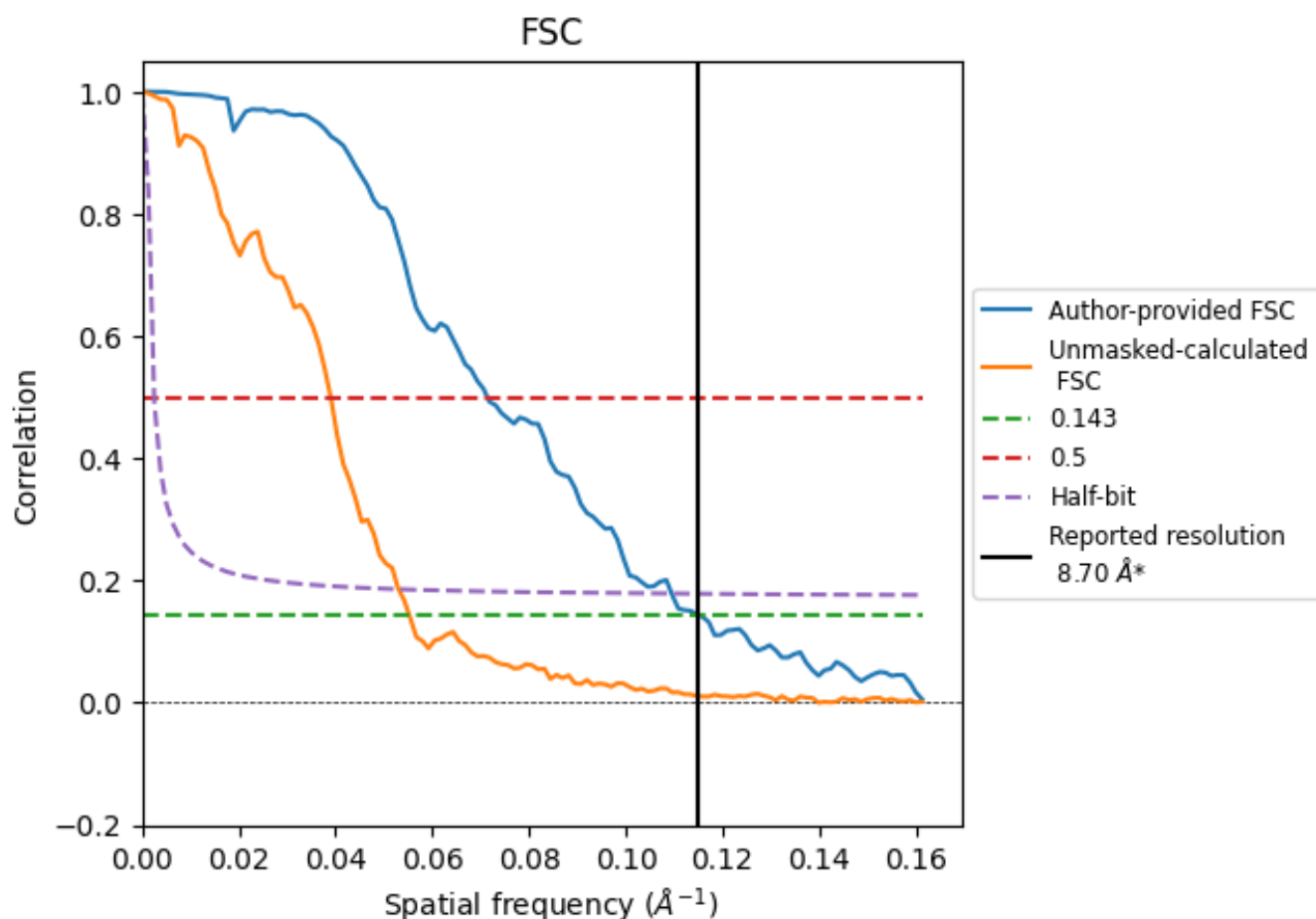


*Reported resolution corresponds to spatial frequency of 0.115 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.115 Å⁻¹

8.2 Resolution estimates [i](#)

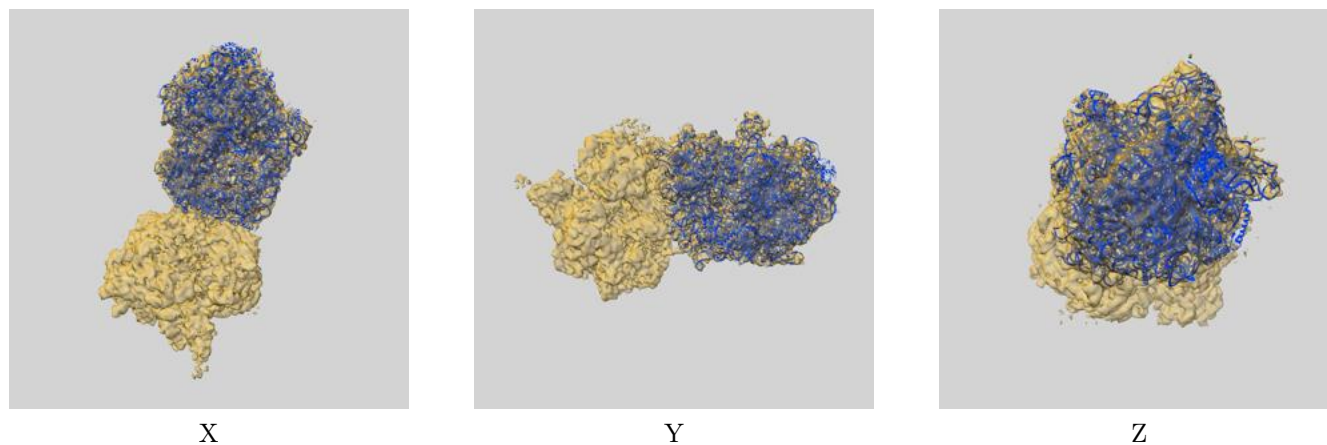
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.70	-	-
Author-provided FSC curve	8.68	14.01	9.13
Unmasked-calculated*	18.08	25.71	18.83

*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 18.08 differs from the reported value 8.7 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17145 and PDB model 8P8W. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



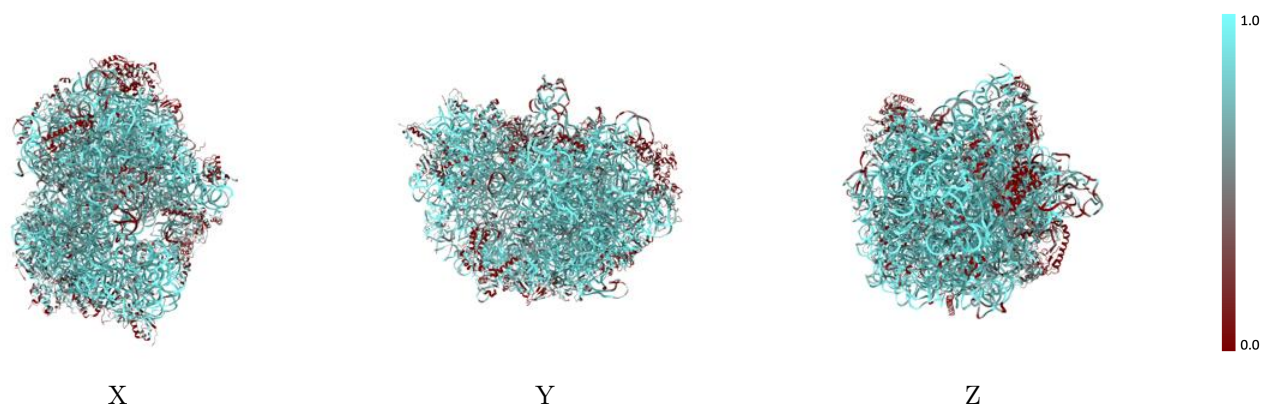
The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



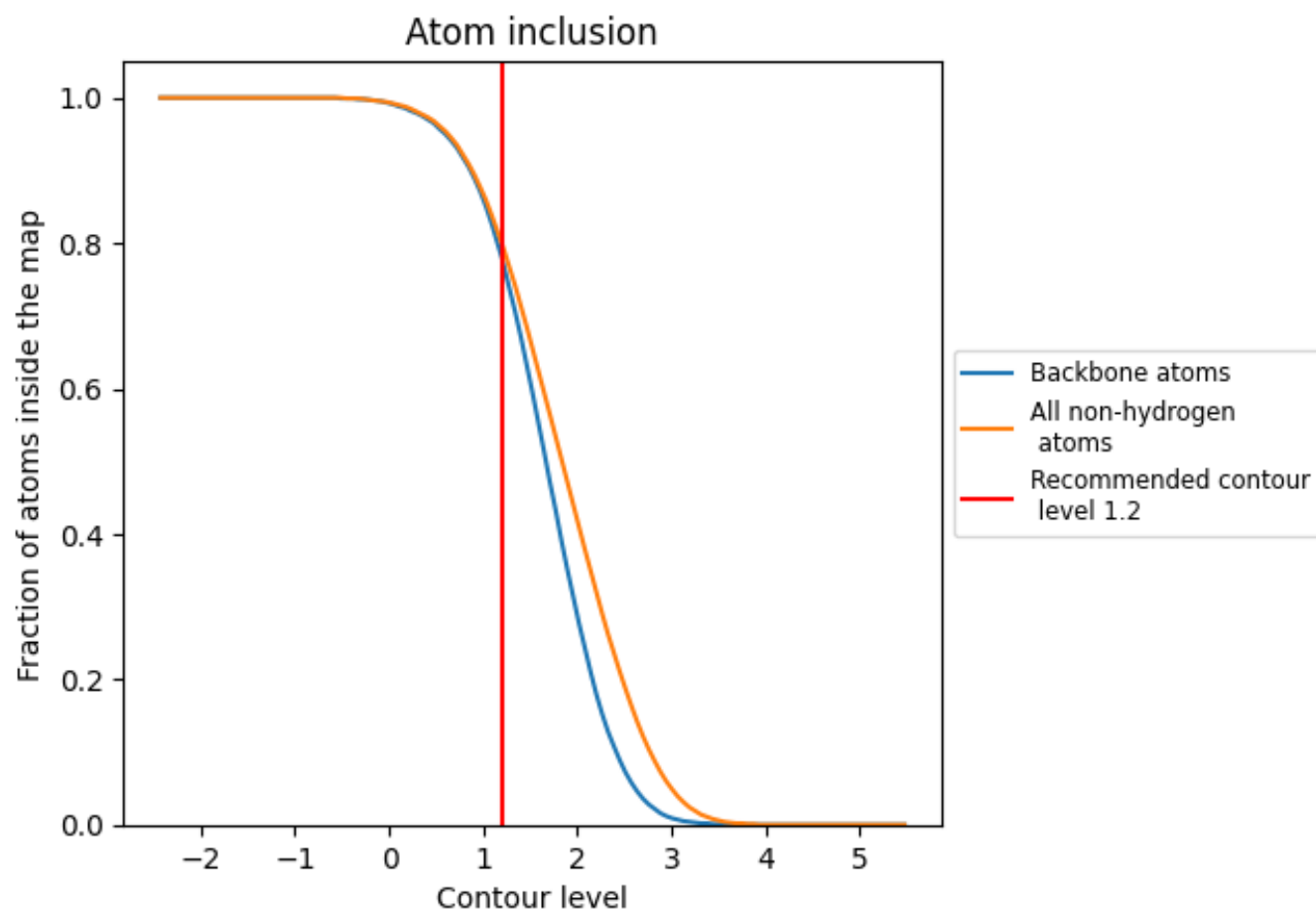
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (1.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 80% 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 (1.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8000	 0.1070
0	 0.7730	 0.0600
1	 0.7720	 0.0250
2	 0.8280	 0.0470
3	 0.9090	 0.1110
4	 0.8440	 0.0940
5	 0.9450	 0.1390
6	 0.3120	 0.0370
7	 0.8440	 0.1400
A	 0.5340	 0.1330
B	 0.5980	 0.1260
C	 0.6970	 0.1340
D	 0.5490	 0.1380
E	 0.5910	 0.1420
F	 0.6460	 0.1170
G	 0.6170	 0.1040
H	 0.6700	 0.0840
I	 0.5560	 0.0880
J	 0.7060	 0.1090
K	 0.6840	 0.1020
L	 0.6610	 0.0890
M	 0.7590	 0.0890
N	 0.7240	 0.1390
O	 0.7320	 0.0820
P	 0.6770	 0.1220
Q	 0.6270	 0.1190
R	 0.6910	 0.0810
S	 0.8540	 0.1100
T	 0.6430	 0.1400
U	 0.0650	 0.0250
X	 0.2090	 0.0830
Y	 0.6830	 0.1210
Z	 0.3740	 0.0170
a	 0.6680	 0.0610
b	 0.6670	 0.0530



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Chain	Atom inclusion	Q-score
c	 0.5230	 0.0460
d	 0.4860	 0.0750
e	 0.5300	 0.0720
f	 0.0820	 0.0390
g	 0.3180	 0.0540
h	 0.1740	 0.0270
i	 0.7780	 0.0780
j	 0.5340	 0.0690
k	 0.5770	 0.0380
l	 0.7390	 0.0670
m	 0.8010	 0.0970
n	 0.4970	 0.0520
o	 0.6210	 0.1010
p	 0.7690	 0.0620
q	 0.5270	 0.0470
r	 0.7510	 0.1020
s	 0.7340	 0.0600
t	 0.5020	 0.0800
u	 0.7590	 0.0310
v	 0.6990	 0.0830
w	 0.3980	 0.0770
x	 0.3170	 0.0920
y	 0.8010	 0.0860
z	 0.5130	 0.0190