



wwPDB EM Validation Summary Report ⓘ

Aug 18, 2026 – 12:58 pm BST

PDB ID : 5NCO / pdb_00005nco
EMDB ID : EMD-3617
Title : Quaternary complex between SRP, SR, and SecYEG bound to the translating ribosome
Authors : Jomaa, A.; Hwang Fu, Y.; Boerhinger, D.; Leibundgut, M.; Shan, S.O.; Ban, N.
Deposited on : 2017-03-06
Resolution : 4.80 Å(reported)

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:

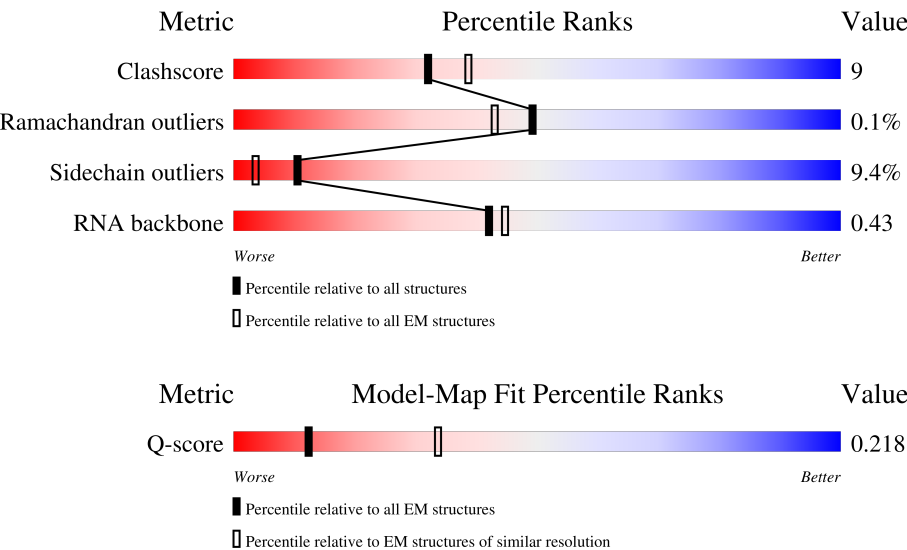
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.80 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.



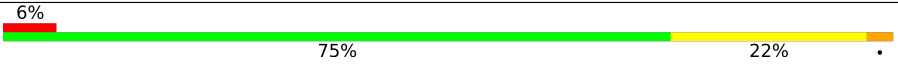
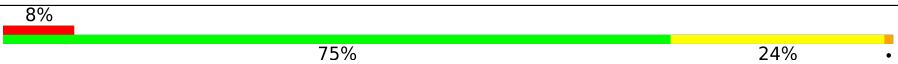
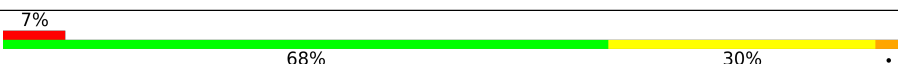
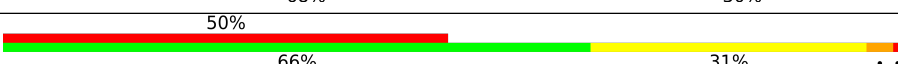
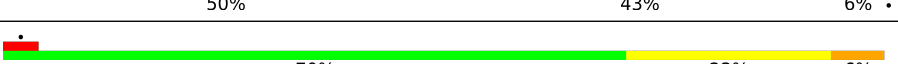
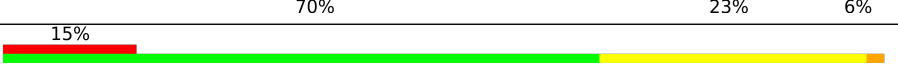
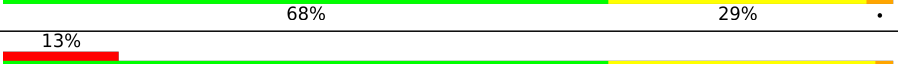
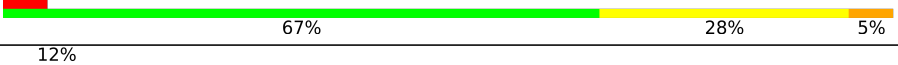
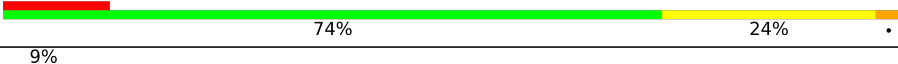
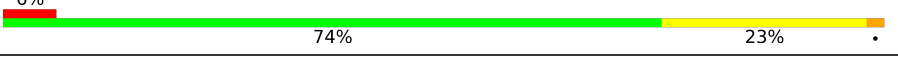
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1575 (4.30 - 5.30)

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	1	104	
2	2	3	
3	A	2903	

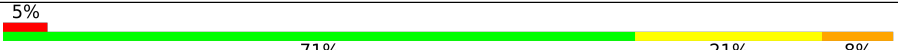
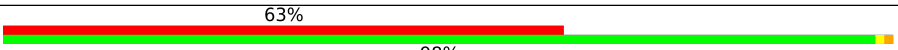
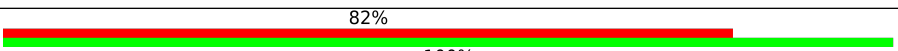
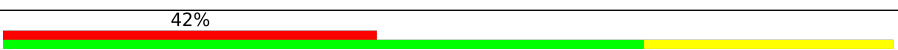
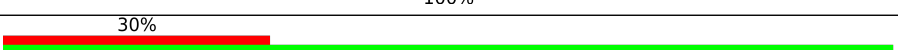
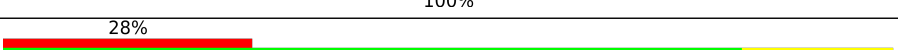
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Mol	Chain	Length	Quality of chain
4	B	120	
5	C	271	
6	D	209	
7	E	201	
8	F	177	
9	G	176	
10	H	149	
11	I	125	
12	J	134	
13	K	142	
14	L	123	
15	M	144	
16	N	136	
17	O	125	
18	P	117	
19	Q	114	
20	R	117	
21	S	103	
22	T	110	
23	U	95	
24	V	102	
25	W	94	
26	X	76	
27	Y	77	
28	Z	62	

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Mol	Chain	Length	Quality of chain
29	a	58	
30	b	56	
31	c	51	
32	d	46	
33	e	64	
34	f	38	
35	g	416	
36	h	56	
37	i	450	
38	j	71	
39	k	23	
40	l	271	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
42	ALF	i	1001	-	-	X	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 101694 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 4.5S SRP RNA (Ffs).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	104	Total	C	N	O	P	0	0
			2224	991	401	728	104		

- Molecule 2 is a RNA chain called P-site tRNA-CCA end.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2883	Total	C	N	O	P	0	0
			61902	27613	11397	20009	2883		

- Molecule 4 is a RNA chain called 5S rRNA.

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

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	125	Total	C	N	O	S	0	0
			946	598	169	175	4		

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

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

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

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

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

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

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	g	416	Total	C	N	O	0	0
			1664	832	416	416		

- Molecule 36 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	h	56	Total	C	N	O	0	0
			224	112	56	56		

- Molecule 37 is a protein called Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	450	Total	C	N	O	S	0	0
			3384	2129	609	628	18		

- Molecule 38 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	j	71	Total	C	N	O	0	0
			284	142	71	71		

- Molecule 39 is a protein called Signal sequence (1A9L).

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	23	Total	C	N	O	0	0
			159	107	25	27		

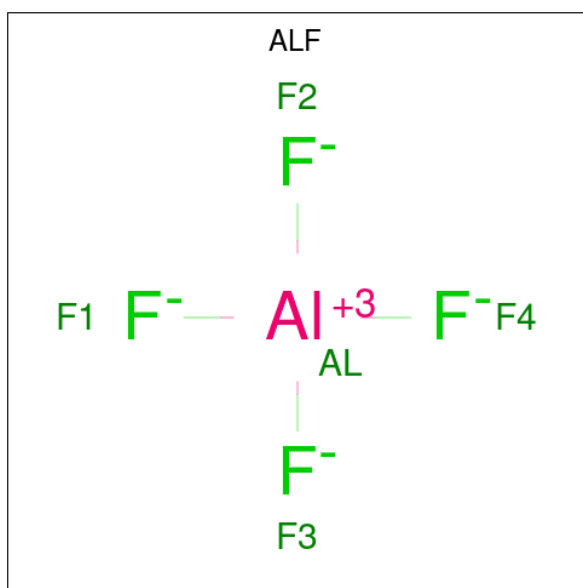
- Molecule 40 is a protein called Signal recognition particle receptor FtsY.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	271	Total	C	N	O	S	0	0
			2067	1306	356	399	6		

- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 42 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).

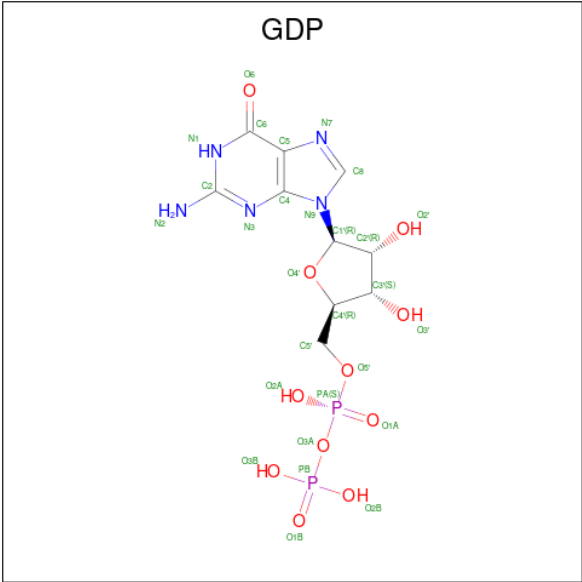


Mol	Chain	Residues	Atoms			AltConf
42	i	1	Total	Al	F	0
			5	1	4	
42	1	1	Total	Al	F	0
			5	1	4	

- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
43	i	1	Total	Mg	0
			1	1	
43	1	1	Total	Mg	0
			1	1	

- Molecule 44 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).

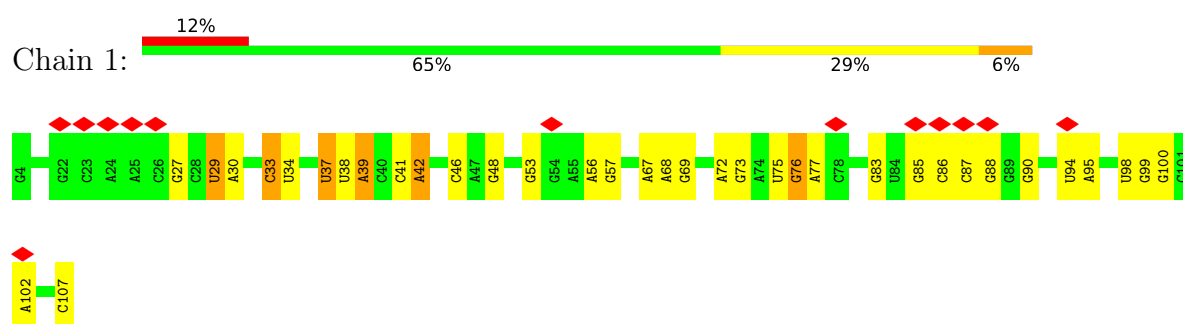


Mol	Chain	Residues	Atoms					AltConf
44	i	1	Total	C	N	O	P	0
			28	10	5	11	2	
44	1	1	Total	C	N	O	P	0
			28	10	5	11	2	

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.

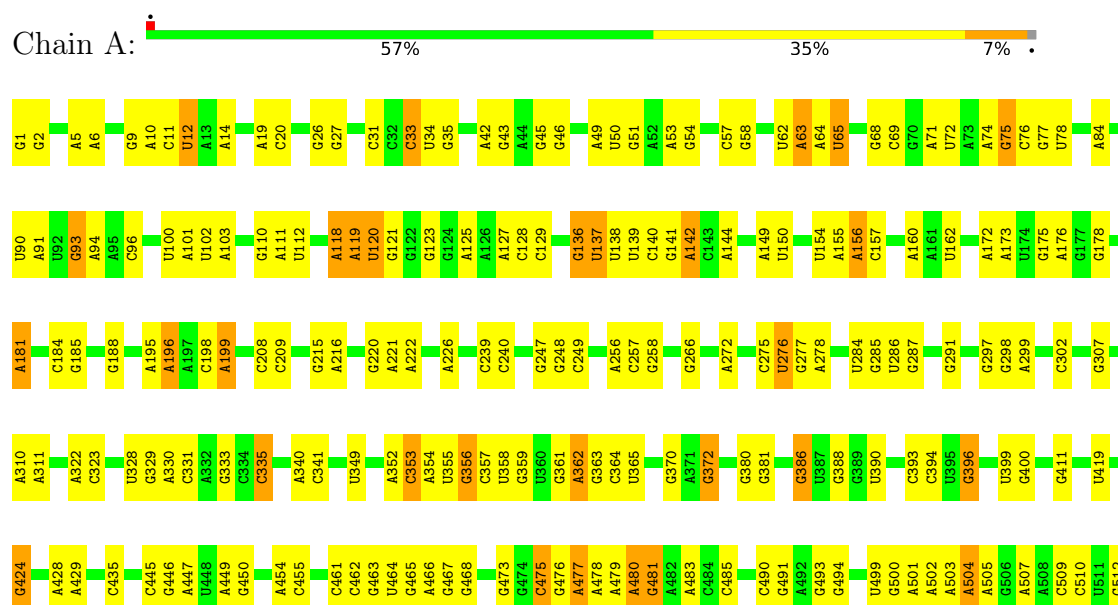
- Molecule 1: 4.5S SRP RNA (Ffs)



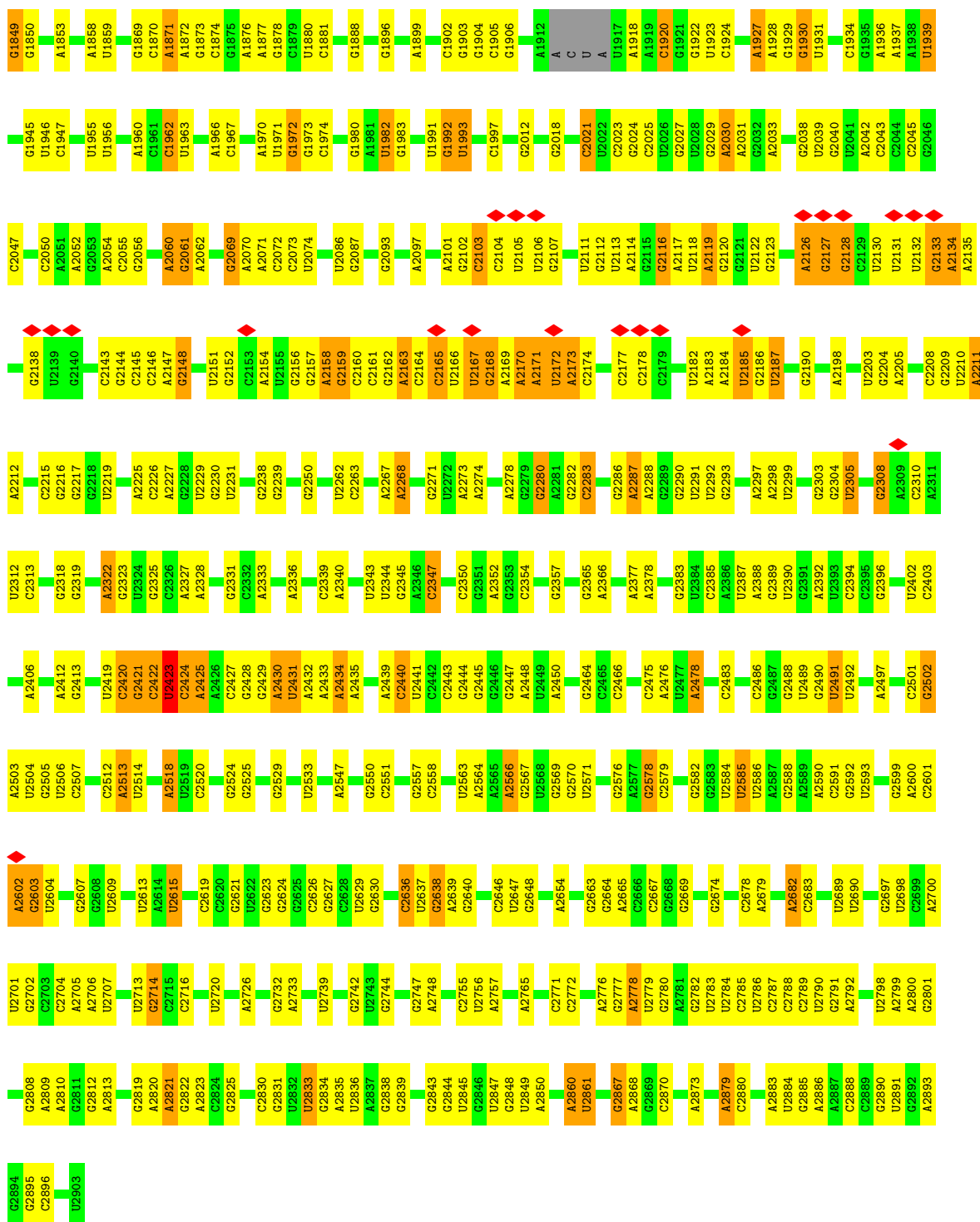
- Molecule 2: P-site tRNA-CCA end



- Molecule 3: 23S rRNA

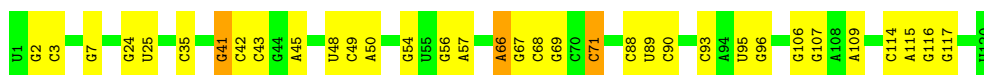




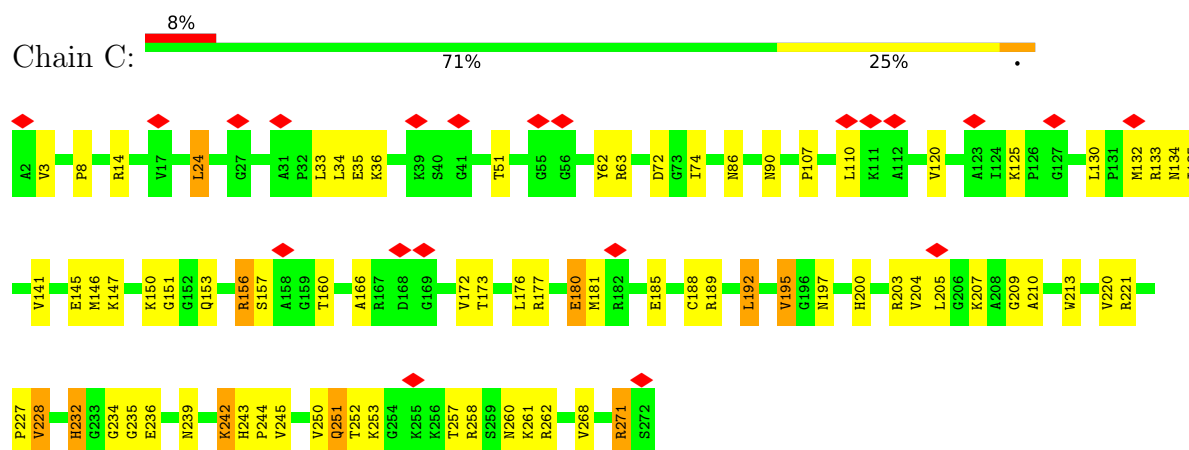


- Molecule 4: 5S rRNA

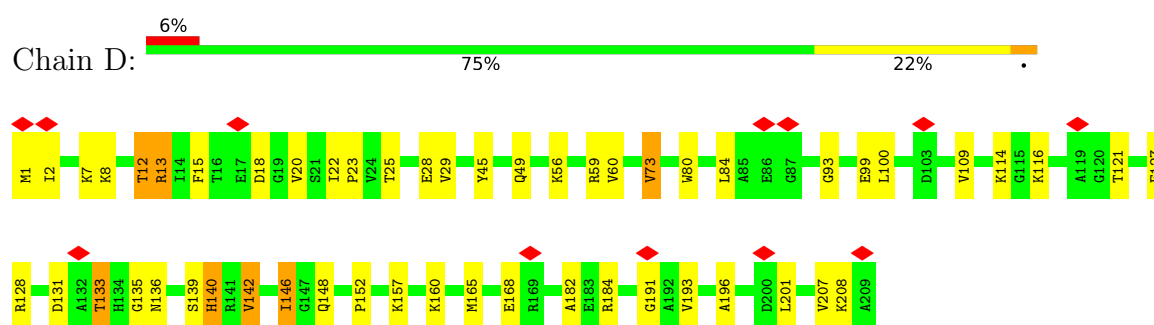
Chain B: 72% 26%



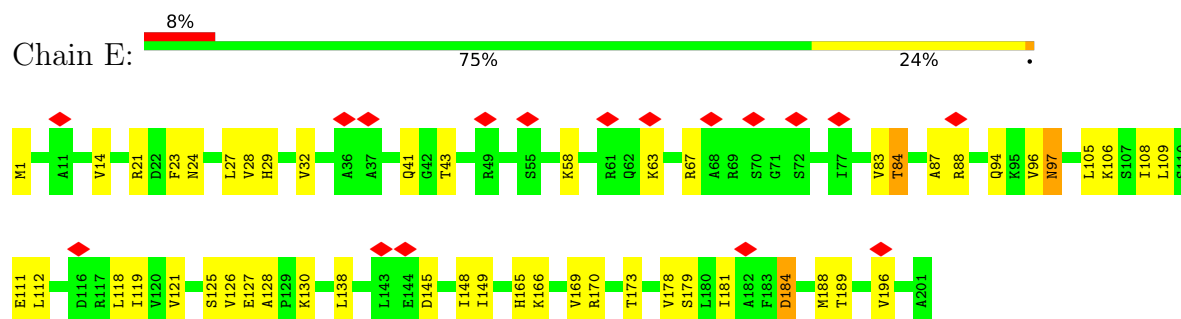
- Molecule 5: 50S ribosomal protein L2



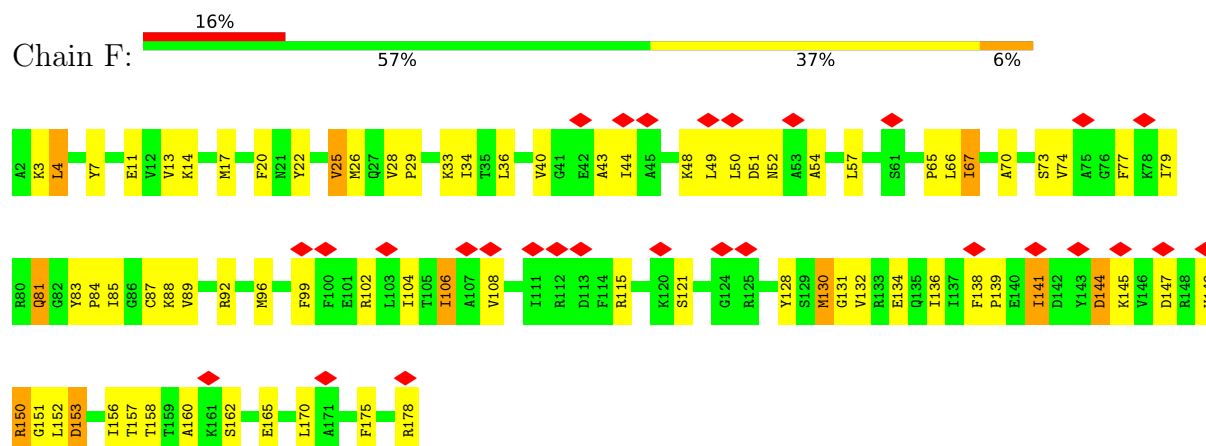
• Molecule 6: 50S ribosomal protein L3



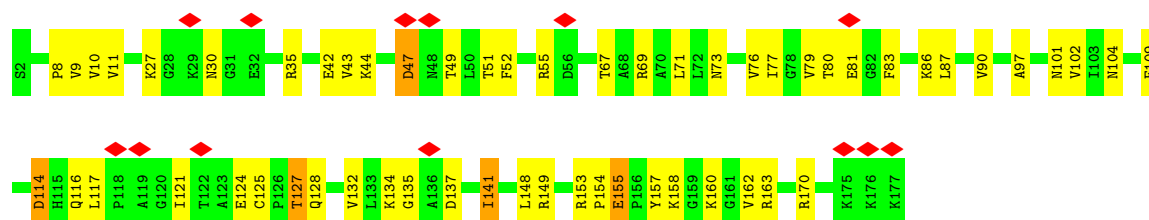
• Molecule 7: 50S ribosomal protein L4



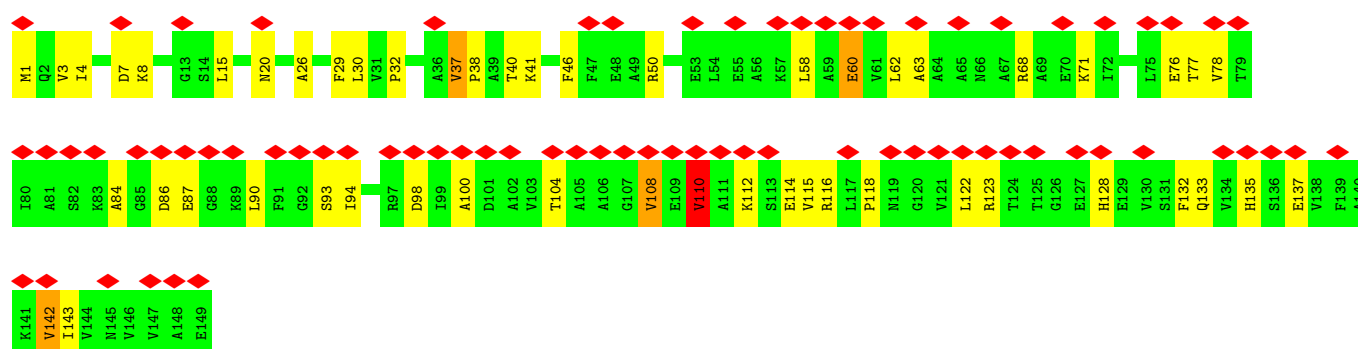
• Molecule 8: 50S ribosomal protein L5



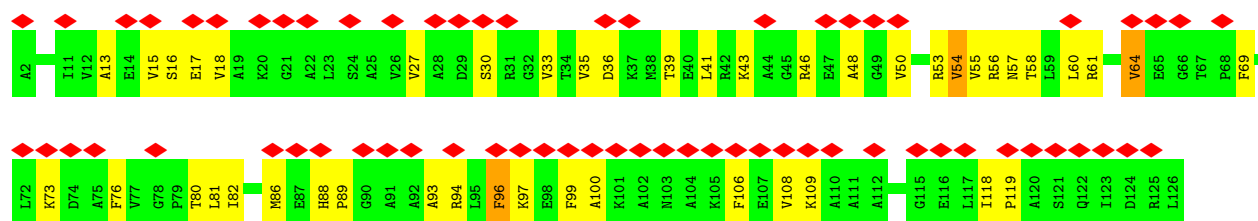
- Molecule 9: 50S ribosomal protein L6



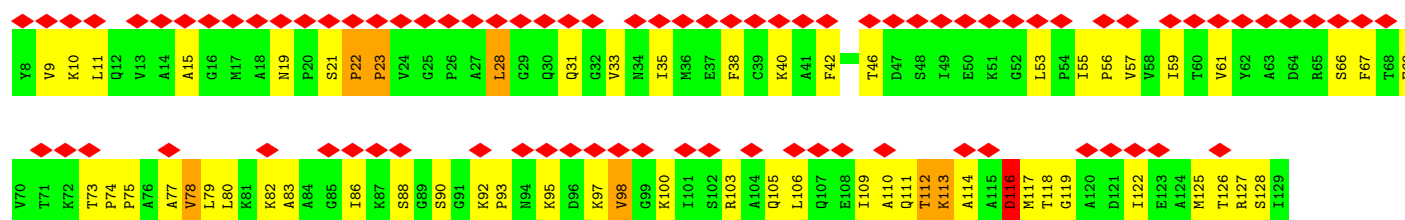
- Molecule 10: 50S ribosomal protein L9

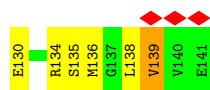


- Molecule 11: 50S ribosomal protein L10



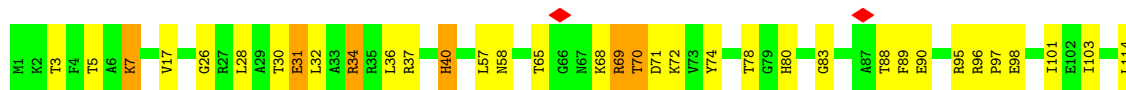
- Molecule 12: 50S ribosomal protein L11





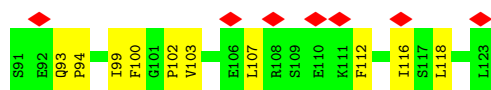
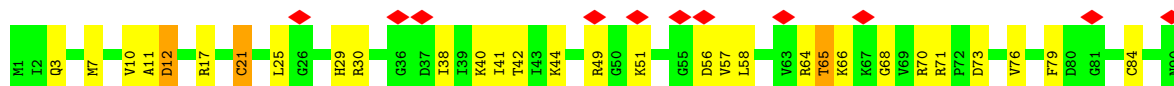
- Molecule 13: 50S ribosomal protein L13

Chain K: 70% 23% 6%



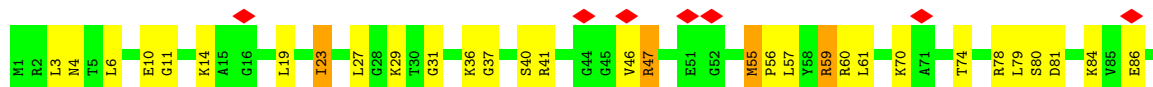
- Molecule 14: 50S ribosomal protein L14

Chain L: 15% 67% 30%



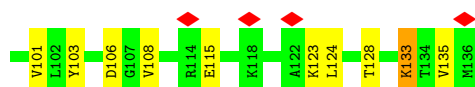
- Molecule 15: 50S ribosomal protein L15

Chain M: 8% 72% 25%

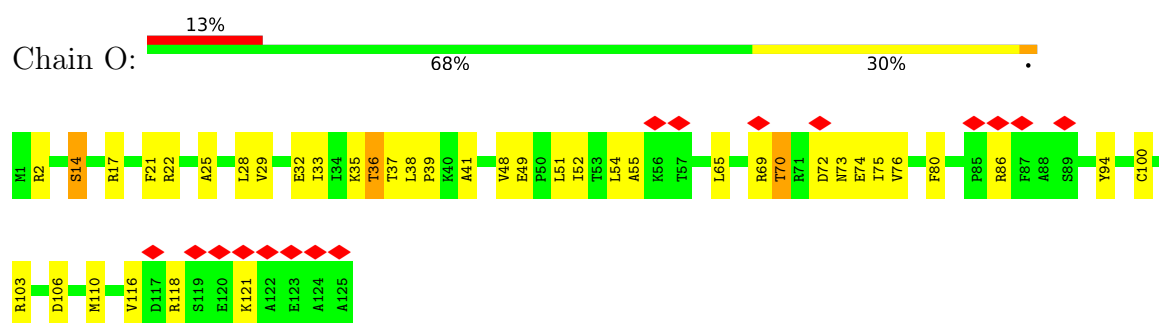


- Molecule 16: 50S ribosomal protein L16

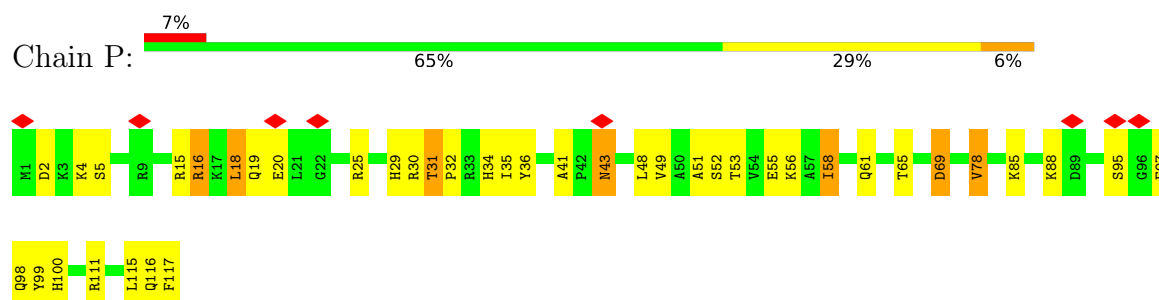
Chain N: 6% 68% 29%



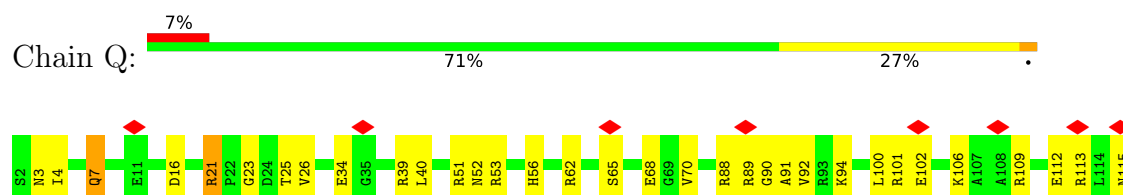
- Molecule 17: 50S ribosomal protein L17



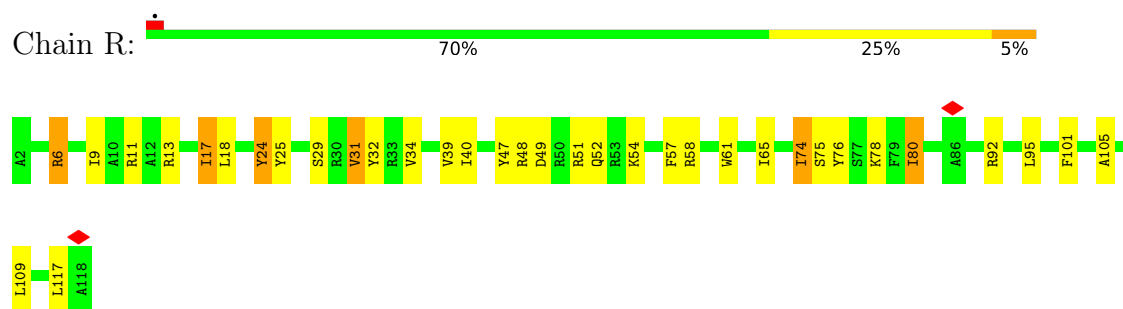
- Molecule 18: 50S ribosomal protein L18



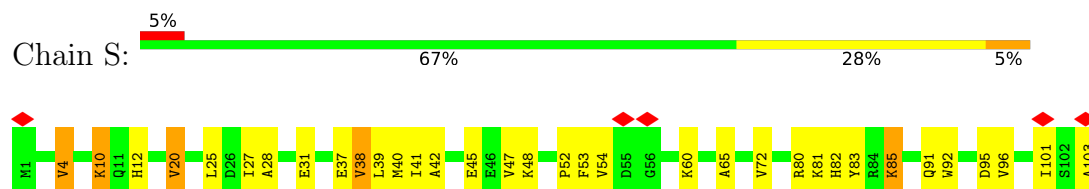
- Molecule 19: 50S ribosomal protein L19



- Molecule 20: 50S ribosomal protein L20

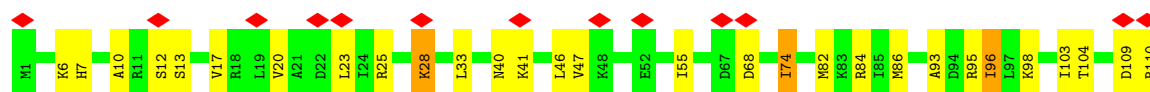


- Molecule 21: 50S ribosomal protein L21

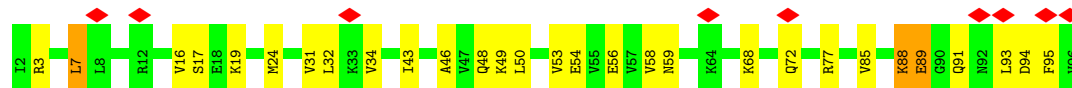


- Molecule 22: 50S ribosomal protein L22

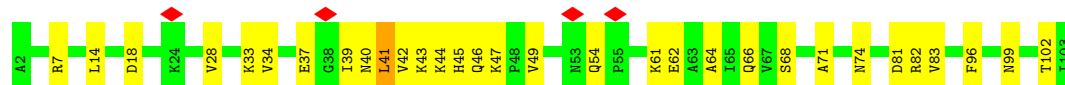




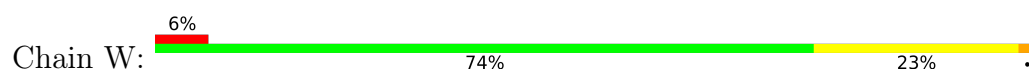
- Molecule 23: 50S ribosomal protein L23



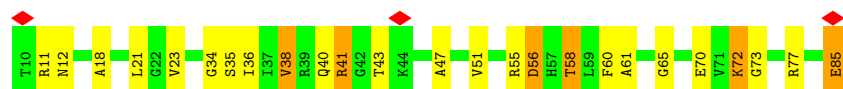
- Molecule 24: 50S ribosomal protein L24



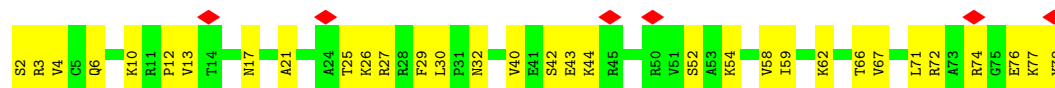
- Molecule 25: 50S ribosomal protein L25



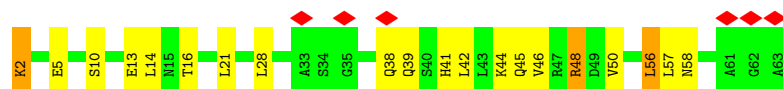
- Molecule 26: 50S ribosomal protein L27



- Molecule 27: 50S ribosomal protein L28



- Molecule 28: 50S ribosomal protein L29



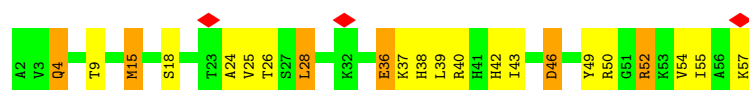
- Molecule 29: 50S ribosomal protein L30

Chain a:  71% 28% .



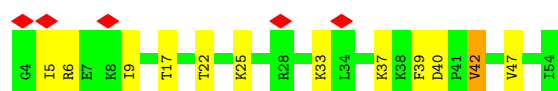
- Molecule 30: 50S ribosomal protein L32

Chain b:  5% 61% 29% 11%



- Molecule 31: 50S ribosomal protein L33

Chain c:  10% 76% 22% .



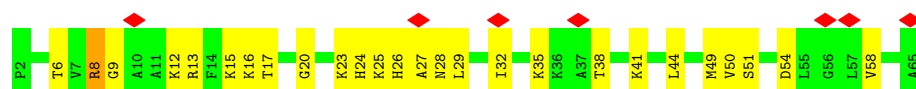
- Molecule 32: 50S ribosomal protein L34

Chain d:  7% 70% 26% .



- Molecule 33: 50S ribosomal protein L35

Chain e:  11% 59% 39% .

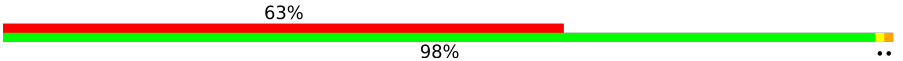


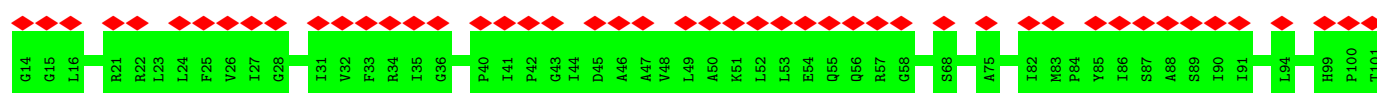
- Molecule 34: 50S ribosomal protein L36

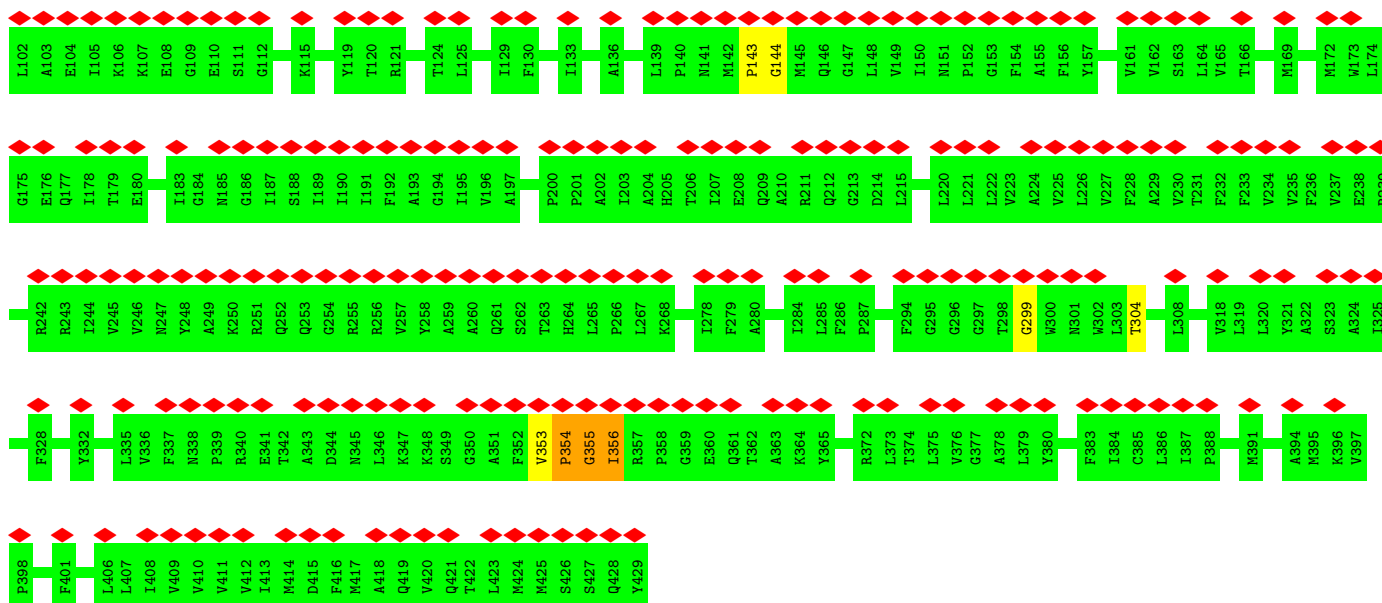
Chain f:  5% 71% 21% 8%



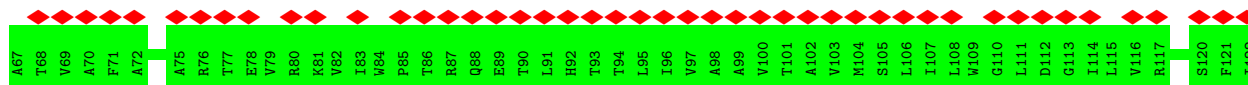
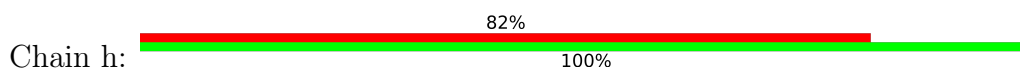
- Molecule 35: Protein translocase subunit SecY

Chain g:  63% 98% ..

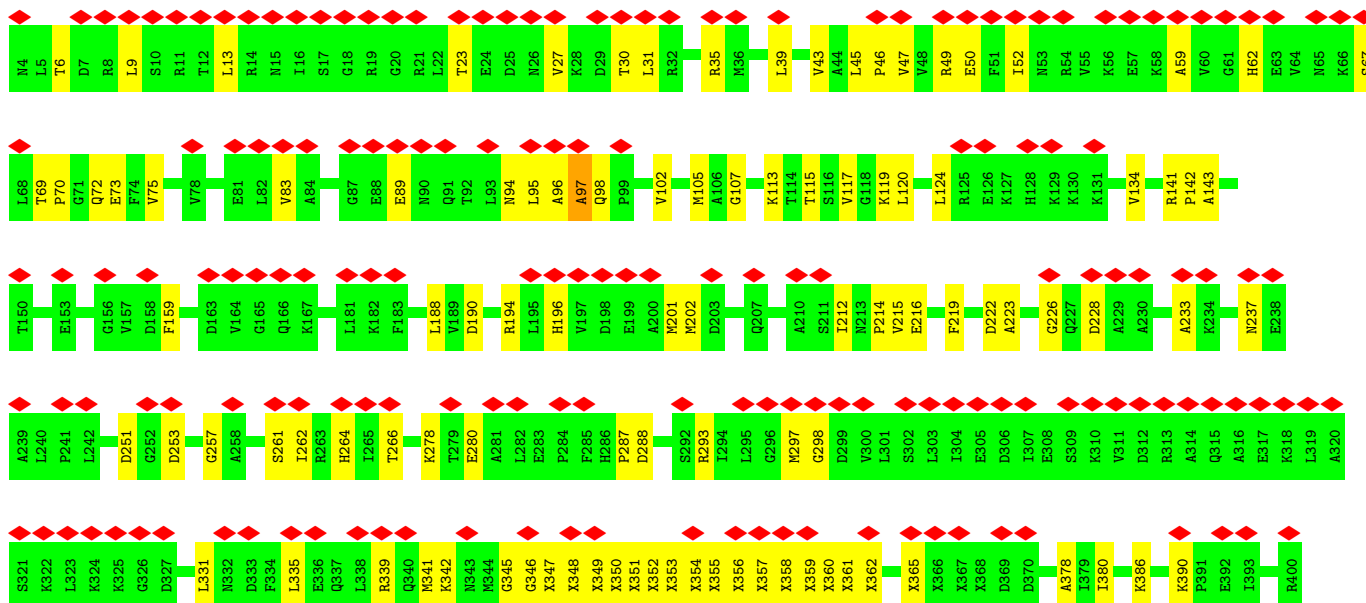
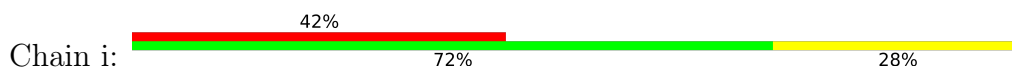


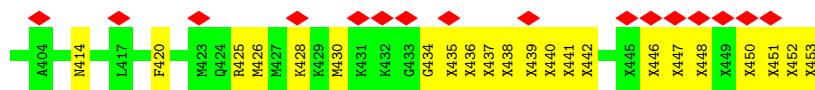


• Molecule 36: Protein translocase subunit SecE

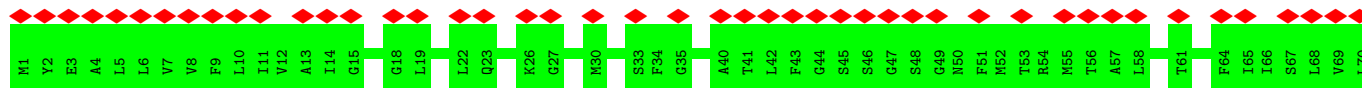


• Molecule 37: Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein,Signal recognition particle protein

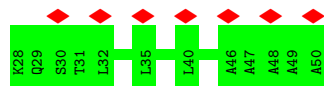




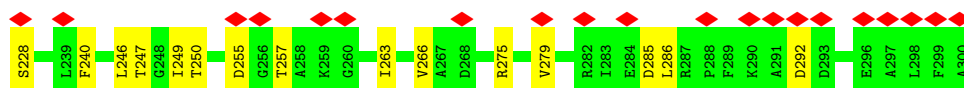
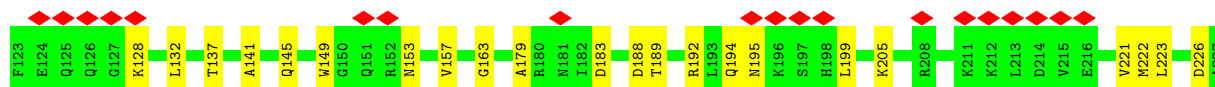
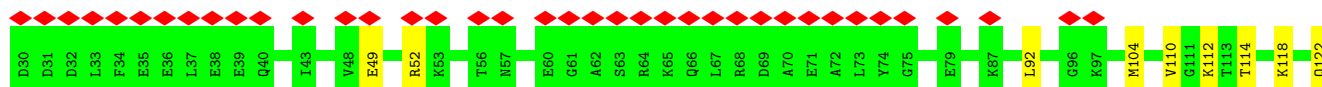
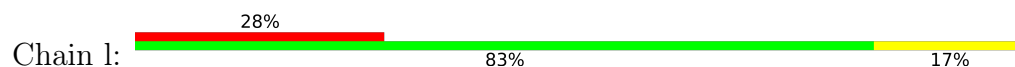
- Molecule 38: Protein-export membrane protein SecG



- Molecule 39: Signal sequence (1A9L)



- Molecule 40: Signal recognition particle receptor FtsY



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; After 3D reconstruction 3D maps were sharpened	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.210	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, MG, ZN, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.07	0/2486	0.14	0/3874
2	2	0.35	0/68	0.51	0/103
3	A	0.35	0/69329	0.48	1/108152 (0.0%)
4	B	0.28	0/2872	0.40	0/4478
5	C	0.61	0/2122	0.96	0/2852
6	D	0.60	0/1586	0.95	5/2134 (0.2%)
7	E	0.57	0/1571	0.91	0/2113
8	F	0.52	1/1435 (0.1%)	0.93	5/1926 (0.3%)
9	G	0.51	0/1343	0.97	3/1816 (0.2%)
10	H	0.59	0/1121	0.90	1/1515 (0.1%)
11	I	0.72	0/958	0.95	0/1290
12	J	0.94	1/993 (0.1%)	1.13	8/1341 (0.6%)
13	K	0.58	0/1152	0.88	2/1551 (0.1%)
14	L	0.57	0/955	0.97	2/1279 (0.2%)
15	M	0.57	0/1062	0.97	3/1413 (0.2%)
16	N	0.59	0/1093	0.96	6/1460 (0.4%)
17	O	0.61	0/1006	0.95	1/1345 (0.1%)
18	P	0.50	0/910	0.93	0/1219
19	Q	0.54	0/929	0.94	2/1242 (0.2%)
20	R	0.73	0/960	0.91	1/1278 (0.1%)
21	S	0.57	0/829	0.95	0/1107
22	T	0.66	0/864	1.05	2/1156 (0.2%)
23	U	0.63	1/763 (0.1%)	0.99	2/1021 (0.2%)
24	V	0.45	0/788	0.88	2/1051 (0.2%)
25	W	0.47	0/766	0.92	0/1025
26	X	0.59	0/587	0.98	2/776 (0.3%)
27	Y	0.61	0/635	0.92	0/848
28	Z	0.51	0/502	0.90	0/667
29	a	0.53	0/453	0.87	0/605
30	b	0.55	0/450	0.89	0/599
31	c	0.55	0/421	1.01	2/561 (0.4%)
32	d	0.66	0/380	0.95	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.62	0/513	0.97	0/676
34	f	0.61	0/303	0.99	0/397
35	g	0.45	1/1663 (0.1%)	1.07	7/2077 (0.3%)
36	h	0.30	0/223	0.83	0/277
37	i	0.27	0/3170	0.73	2/4255 (0.0%)
38	j	0.30	0/283	0.81	0/352
39	k	0.35	0/159	0.76	0/218
40	l	0.26	0/2091	0.68	0/2822
All	All	0.42	4/109794 (0.0%)	0.63	59/163369 (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
5	C	0	1
9	G	0	1
12	J	0	1
35	g	0	1
37	i	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	g	355	GLY	C-N	6.39	1.42	1.33
12	J	22	PRO	CA-C	5.66	1.57	1.52
8	F	108	VAL	CA-CB	5.42	1.57	1.53
23	U	94	ASP	N-CA	5.24	1.52	1.46

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	155	GLU	CA-C-N	9.35	128.98	119.82
9	G	155	GLU	C-N-CA	9.35	128.98	119.82
35	g	354	PRO	CA-C-N	-9.12	103.53	121.41
35	g	354	PRO	C-N-CA	-9.12	103.53	121.41
12	J	116	ASP	N-CA-C	8.01	123.26	113.17

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide
35	g	354	PRO	Peptide
37	i	293	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2224	0	1124	16	0
2	2	62	0	34	1	0
3	A	61902	0	31134	740	0
4	B	2569	0	1301	20	0
5	C	2083	0	2154	51	0
6	D	1565	0	1616	34	0
7	E	1552	0	1619	30	0
8	F	1411	0	1444	45	0
9	G	1323	0	1371	34	0
10	H	1110	0	1148	24	0
11	I	946	0	976	30	0
12	J	979	0	1028	42	0
13	K	1129	0	1162	24	0
14	L	946	0	1023	22	0
15	M	1053	0	1129	29	0
16	N	1074	0	1157	26	0
17	O	993	0	1034	26	0
18	P	900	0	935	22	0
19	Q	917	0	962	20	0
20	R	947	0	1019	26	0
21	S	816	0	839	23	0
22	T	857	0	922	16	0
23	U	756	0	817	21	0
24	V	780	0	831	16	0
25	W	753	0	780	16	0
26	X	580	0	594	16	0
27	Y	625	0	652	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Z	501	0	531	13	0
29	a	449	0	488	9	0
30	b	444	0	458	16	0
31	c	414	0	442	5	0
32	d	377	0	418	7	0
33	e	504	0	572	14	0
34	f	302	0	340	12	0
35	g	1664	0	476	13	0
36	h	224	0	58	0	0
37	i	3384	0	3512	150	0
38	j	284	0	95	0	0
39	k	159	0	189	0	0
40	l	2067	0	2114	32	0
41	f	1	0	0	0	0
42	i	5	0	0	2	0
42	l	5	0	0	1	0
43	i	1	0	0	0	0
43	l	1	0	0	0	0
44	i	28	0	12	3	0
44	l	28	0	12	1	0
All	All	101694	0	68522	1449	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 9.

The worst 5 of 1449 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)
3:A:1283:G:OP1	37:i:428:LYS:NZ	1.79	1.14
37:i:357:UNK:O	37:i:361:UNK:HG3	1.56	1.05
37:i:349:UNK:O	37:i:352:UNK:HG3	1.60	1.00
37:i:434:GLY:O	37:i:438:UNK:HG3	1.62	0.98
3:A:490:C:H41	37:i:425:ARG:CZ	1.80	0.95

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	269/271 (99%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
9	G	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	18	55
11	I	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	16	52
12	J	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
20	R	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
23	U	93/95 (98%)	89 (96%)	3 (3%)	1 (1%)	11	45
24	V	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
28	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
29	a	56/58 (97%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	b	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
31	c	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	g	414/416 (100%)	402 (97%)	12 (3%)	0	100	100
36	h	54/56 (96%)	54 (100%)	0	0	100	100
37	i	408/450 (91%)	397 (97%)	10 (2%)	1 (0%)	43	78
38	j	69/71 (97%)	67 (97%)	2 (3%)	0	100	100
39	k	21/23 (91%)	18 (86%)	3 (14%)	0	100	100
40	l	269/271 (99%)	265 (98%)	4 (2%)	0	100	100
All	All	4667/4779 (98%)	4520 (97%)	143 (3%)	4 (0%)	49	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	i	97	ALA
23	U	89	GLU
10	H	118	PRO
11	I	108	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	216/216 (100%)	190 (88%)	26 (12%)	5	18
6	D	164/164 (100%)	148 (90%)	16 (10%)	7	24
7	E	165/165 (100%)	149 (90%)	16 (10%)	8	25
8	F	148/148 (100%)	127 (86%)	21 (14%)	3	14
9	G	137/137 (100%)	126 (92%)	11 (8%)	11	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	H	114/114 (100%)	100 (88%)	14 (12%)	4	18
11	I	95/95 (100%)	86 (90%)	9 (10%)	8	25
12	J	104/104 (100%)	88 (85%)	16 (15%)	2	13
13	K	116/116 (100%)	99 (85%)	17 (15%)	3	14
14	L	104/104 (100%)	96 (92%)	8 (8%)	12	32
15	M	103/103 (100%)	92 (89%)	11 (11%)	6	22
16	N	109/109 (100%)	99 (91%)	10 (9%)	8	27
17	O	102/102 (100%)	95 (93%)	7 (7%)	14	36
18	P	87/87 (100%)	70 (80%)	17 (20%)	1	8
19	Q	99/99 (100%)	88 (89%)	11 (11%)	6	20
20	R	89/89 (100%)	79 (89%)	10 (11%)	6	20
21	S	84/84 (100%)	73 (87%)	11 (13%)	4	16
22	T	93/93 (100%)	84 (90%)	9 (10%)	8	25
23	U	82/82 (100%)	77 (94%)	5 (6%)	17	39
24	V	83/83 (100%)	75 (90%)	8 (10%)	8	25
25	W	78/78 (100%)	72 (92%)	6 (8%)	12	32
26	X	57/58 (98%)	47 (82%)	10 (18%)	2	11
27	Y	67/67 (100%)	59 (88%)	8 (12%)	5	19
28	Z	54/54 (100%)	47 (87%)	7 (13%)	4	16
29	a	48/48 (100%)	45 (94%)	3 (6%)	16	38
30	b	47/47 (100%)	36 (77%)	11 (23%)	1	5
31	c	45/46 (98%)	40 (89%)	5 (11%)	6	20
32	d	38/38 (100%)	31 (82%)	7 (18%)	1	10
33	e	51/51 (100%)	47 (92%)	4 (8%)	11	32
34	f	34/34 (100%)	31 (91%)	3 (9%)	9	29
37	i	336/338 (99%)	334 (99%)	2 (1%)	78	81
39	k	16/16 (100%)	16 (100%)	0	100	100
40	l	217/217 (100%)	217 (100%)	0	100	100
All	All	3382/3386 (100%)	3063 (91%)	319 (9%)	10	26

5 of 319 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	T	12	SER
29	a	56	LYS
22	T	96	ILE
26	X	12	ASN
31	c	22	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
20	R	37	GLN
23	U	92	ASN
20	R	81	ASN
22	T	102	HIS
26	X	46	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	103/104 (99%)	22 (21%)	0
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	518 (17%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3102/3130 (99%)	554 (17%)	19 (0%)

5 of 554 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	27	G
1	1	29	U
1	1	30	A
1	1	33	C
1	1	34	U

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	2422	C
3	A	2602	A
3	A	2756	U
3	A	2430	A
3	A	1344	U

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](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z > 2$
44	GDP	i	1003	43,42	28,30,30	1.13	3 (10%)	44,47,47	1.87	8 (18%)
42	ALF	i	1001	44	0,4,4	-	-	-	-	-
44	GDP	l	1003	43,42	28,30,30	1.14	3 (10%)	44,47,47	1.85	8 (18%)
42	ALF	l	1001	44	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	GDP	i	1003	43,42	-	4/16/32/32	0/3/3/3
44	GDP	l	1003	43,42	-	7/16/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	i	1003	GDP	C5-C4	3.12	1.47	1.38
44	l	1003	GDP	C5-C4	3.10	1.47	1.38
44	l	1003	GDP	C6-N1	-2.48	1.34	1.38
44	i	1003	GDP	C6-N1	-2.40	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	l	1003	GDP	C5-N7	-2.14	1.34	1.39

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	i	1003	GDP	C5-C4-N3	-6.16	118.46	128.46
44	l	1003	GDP	C5-C4-N3	-6.08	118.59	128.46
44	i	1003	GDP	C2-N3-C4	4.96	121.14	112.30
44	l	1003	GDP	C2-N3-C4	4.93	121.09	112.30
44	i	1003	GDP	N9-C4-N3	4.59	135.15	125.94

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

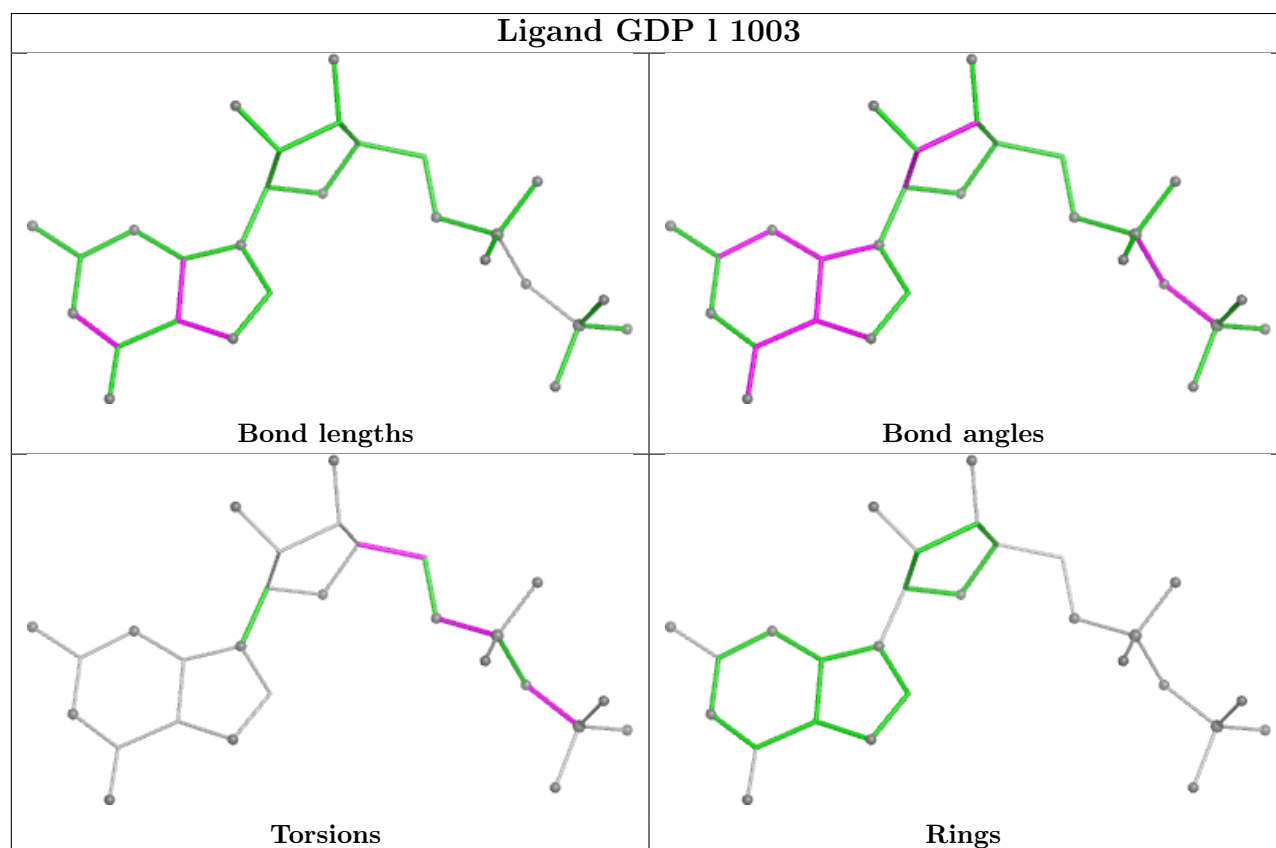
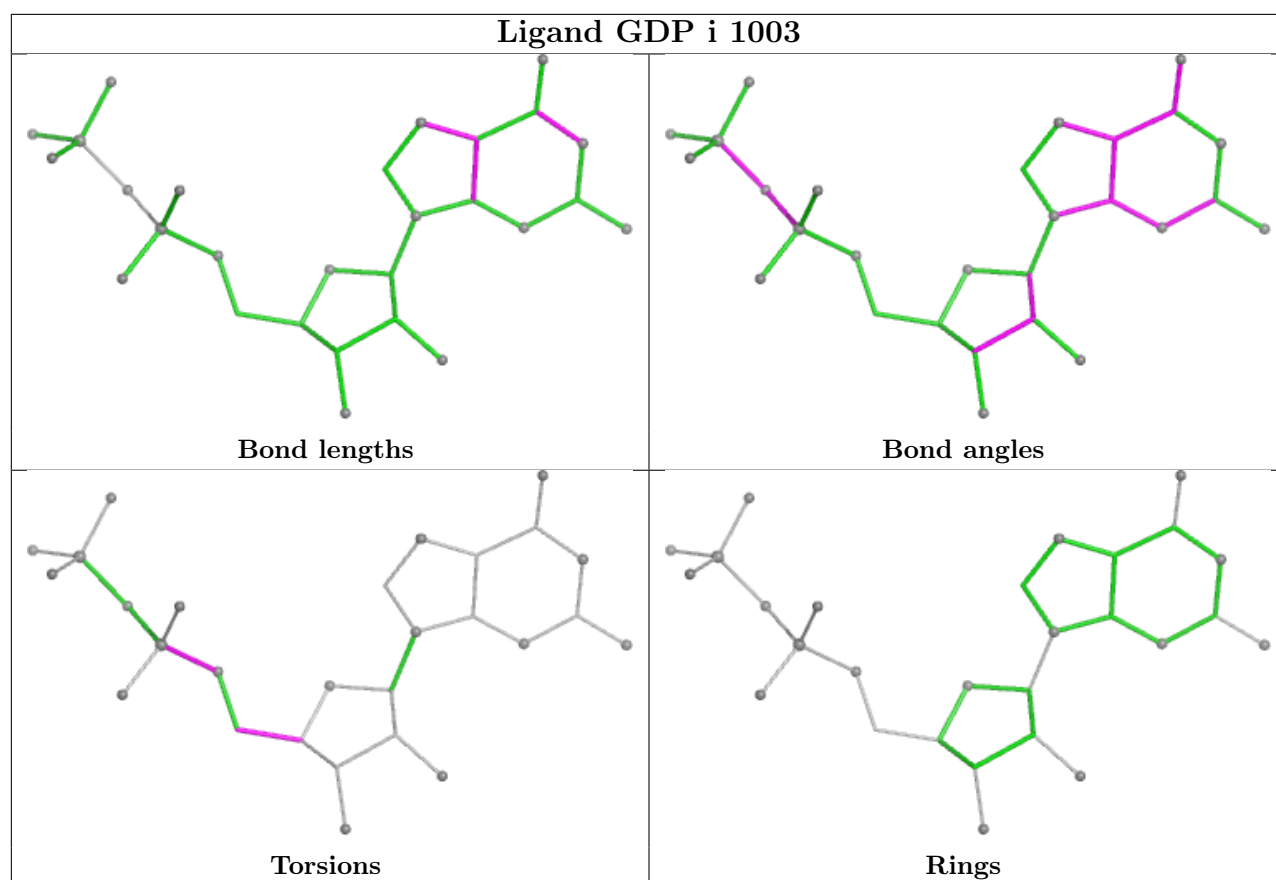
Mol	Chain	Res	Type	Atoms
44	i	1003	GDP	C5'-O5'-PA-O3A
44	i	1003	GDP	O4'-C4'-C5'-O5'
44	i	1003	GDP	C3'-C4'-C5'-O5'
44	l	1003	GDP	PA-O3A-PB-O2B
44	l	1003	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	i	1003	GDP	3	0
42	i	1001	ALF	2	0
44	l	1003	GDP	1	0
42	l	1001	ALF	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.

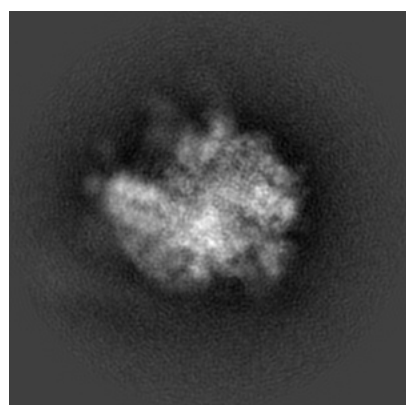
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3617. These allow visual inspection of the internal detail of the map and identification of artifacts.

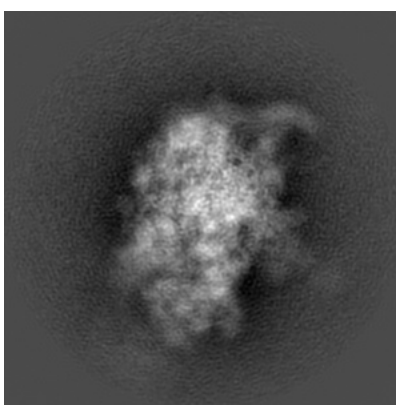
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

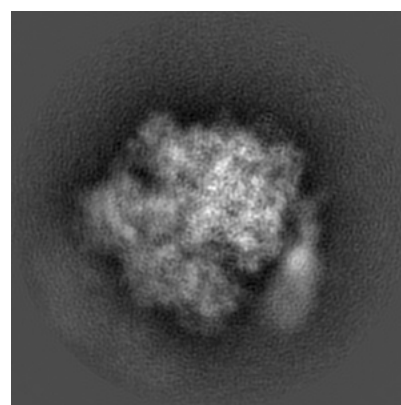
6.1.1 Primary map



X



Y

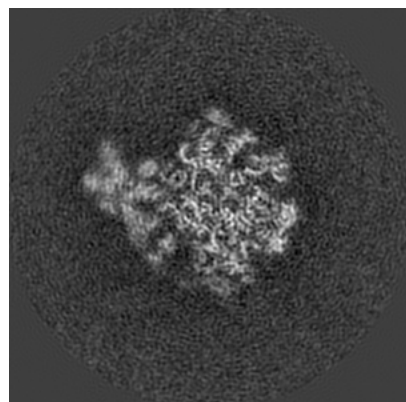


Z

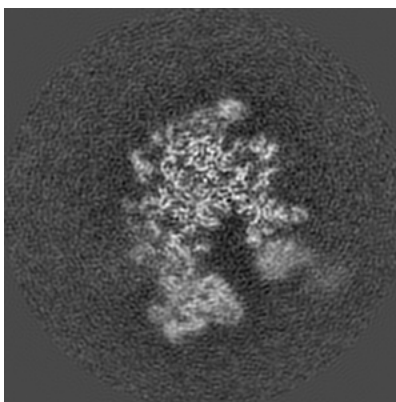
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

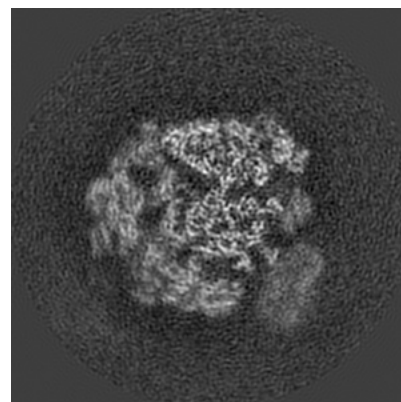
6.2.1 Primary map



X Index: 160



Y Index: 160

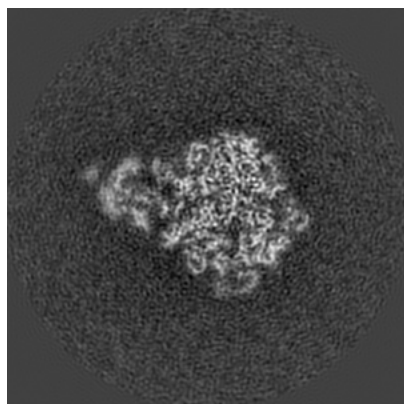


Z Index: 160

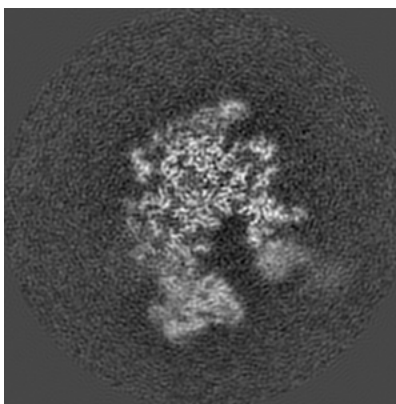
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

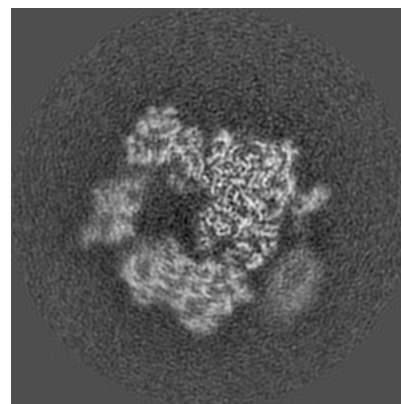
6.3.1 Primary map



X Index: 170



Y Index: 159

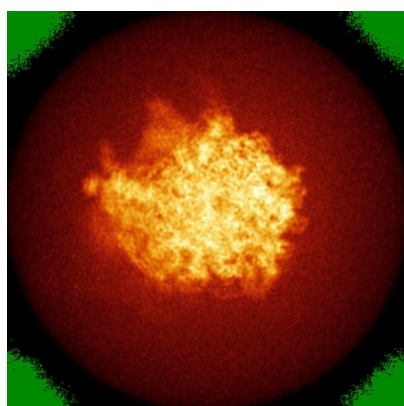


Z Index: 175

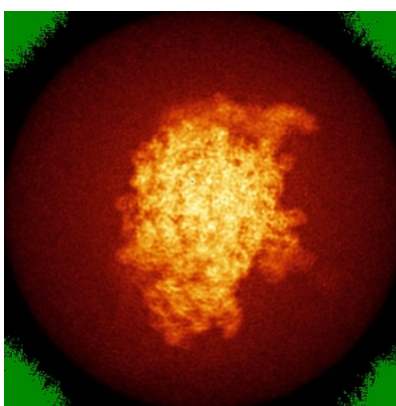
The images above show the largest variance slices of the map in three orthogonal directions.

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

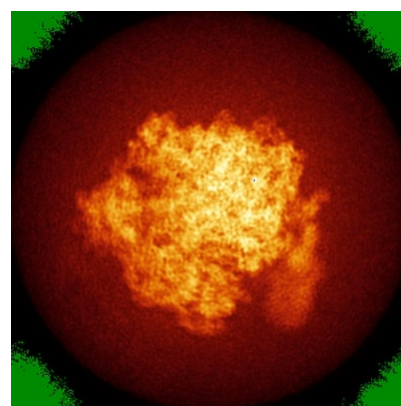
6.4.1 Primary map



X



Y



Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

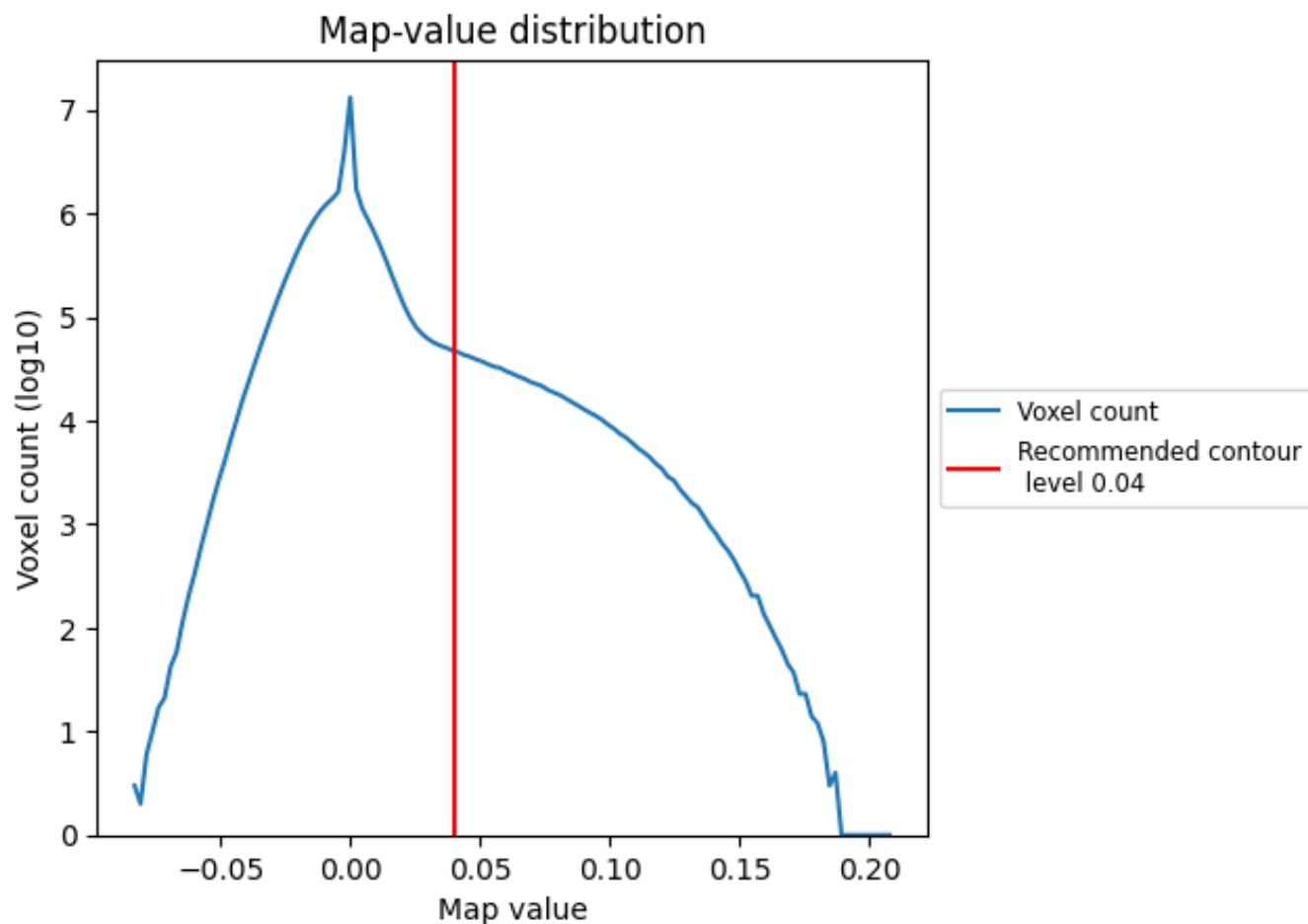
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

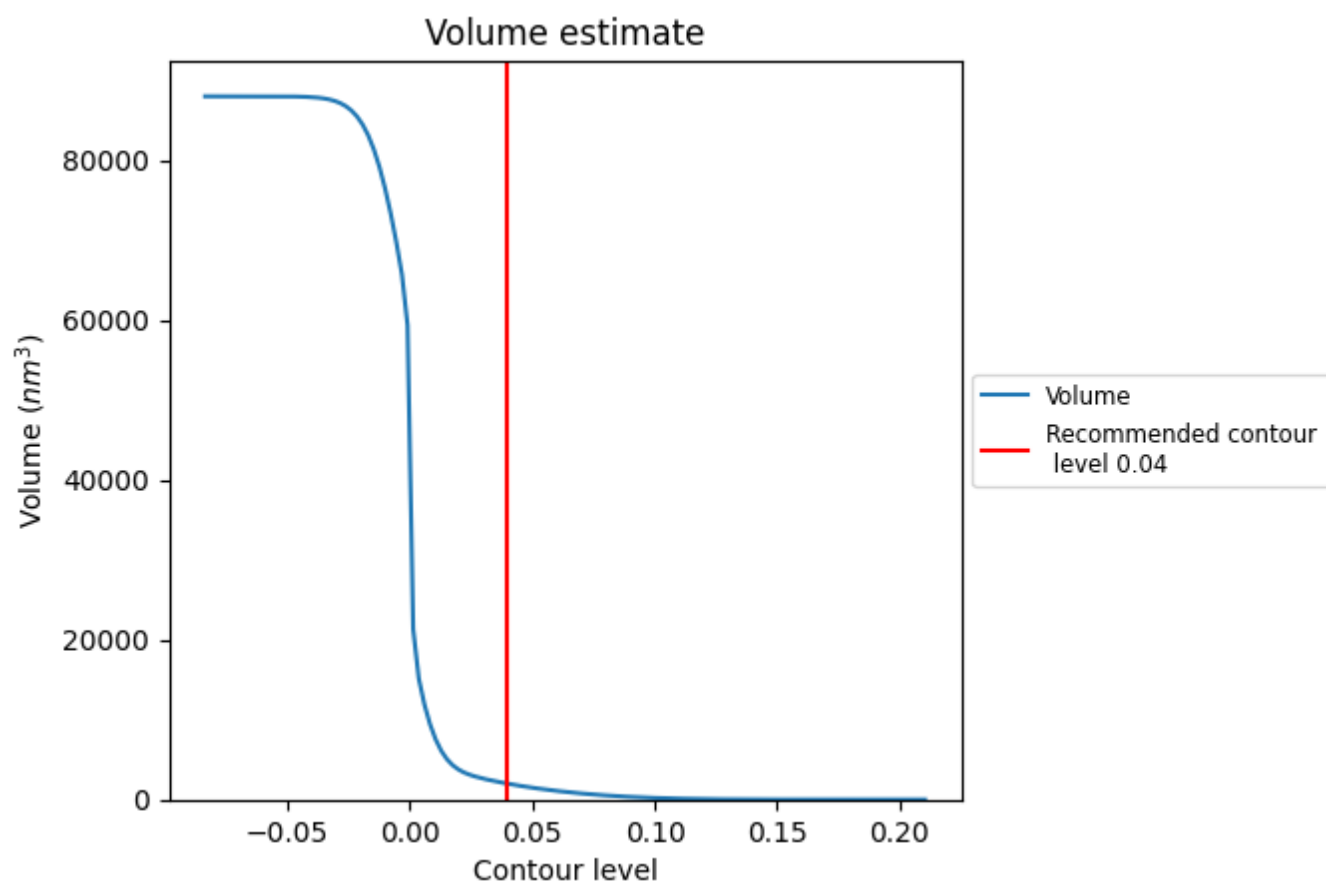
This section contains the results of statistical analysis of the map.

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.

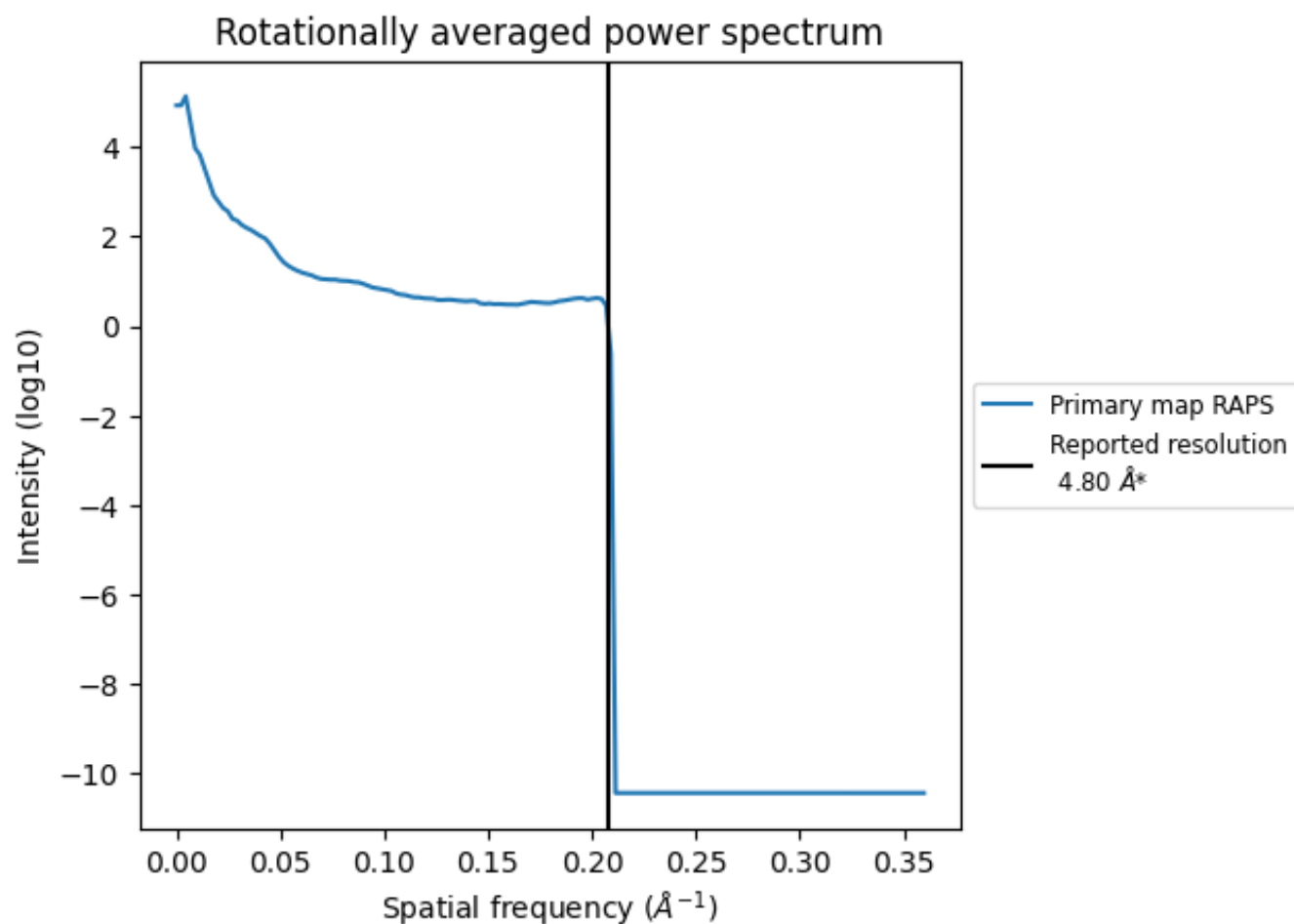
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1992 nm³; this corresponds to an approximate mass of 1799 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 0.208 Å⁻¹

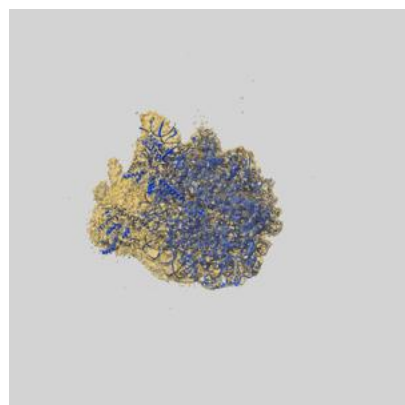
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

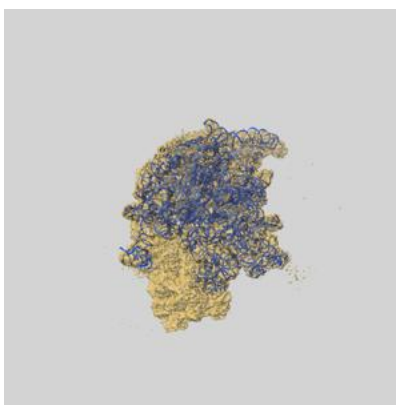
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3617 and PDB model 5NCO. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

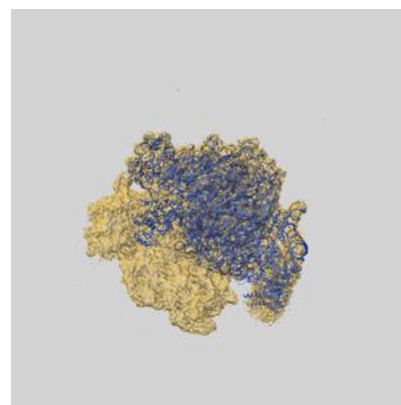
9.1 Map-model overlay [i](#)



X



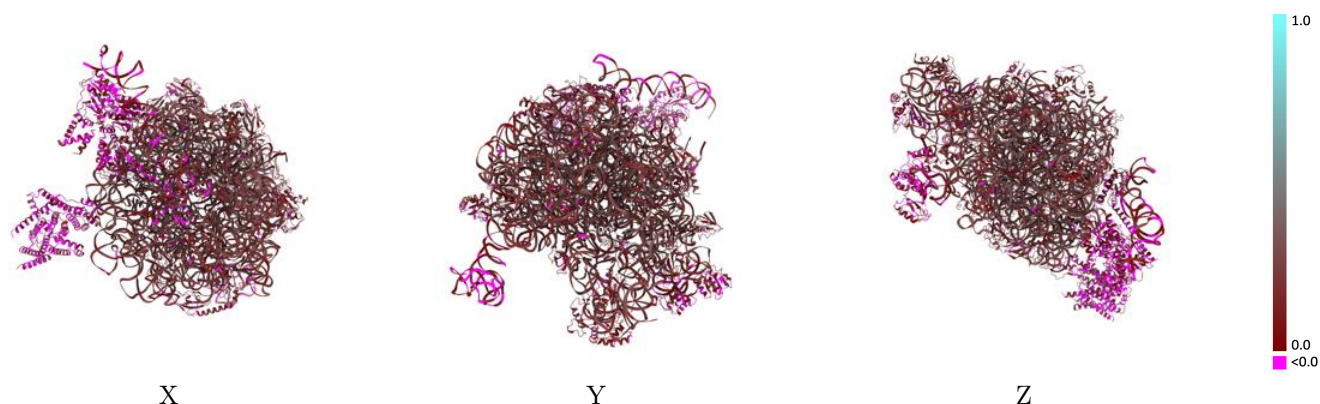
Y



Z

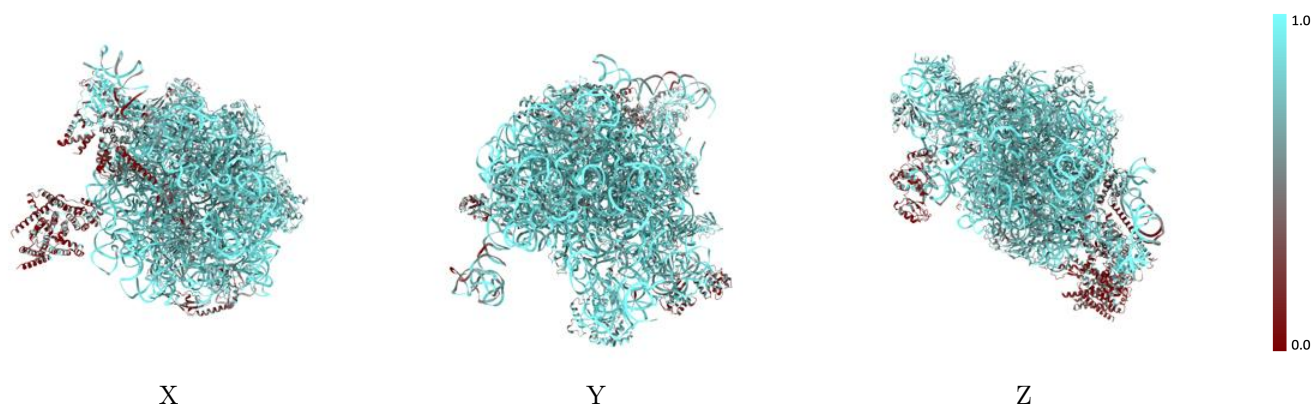
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



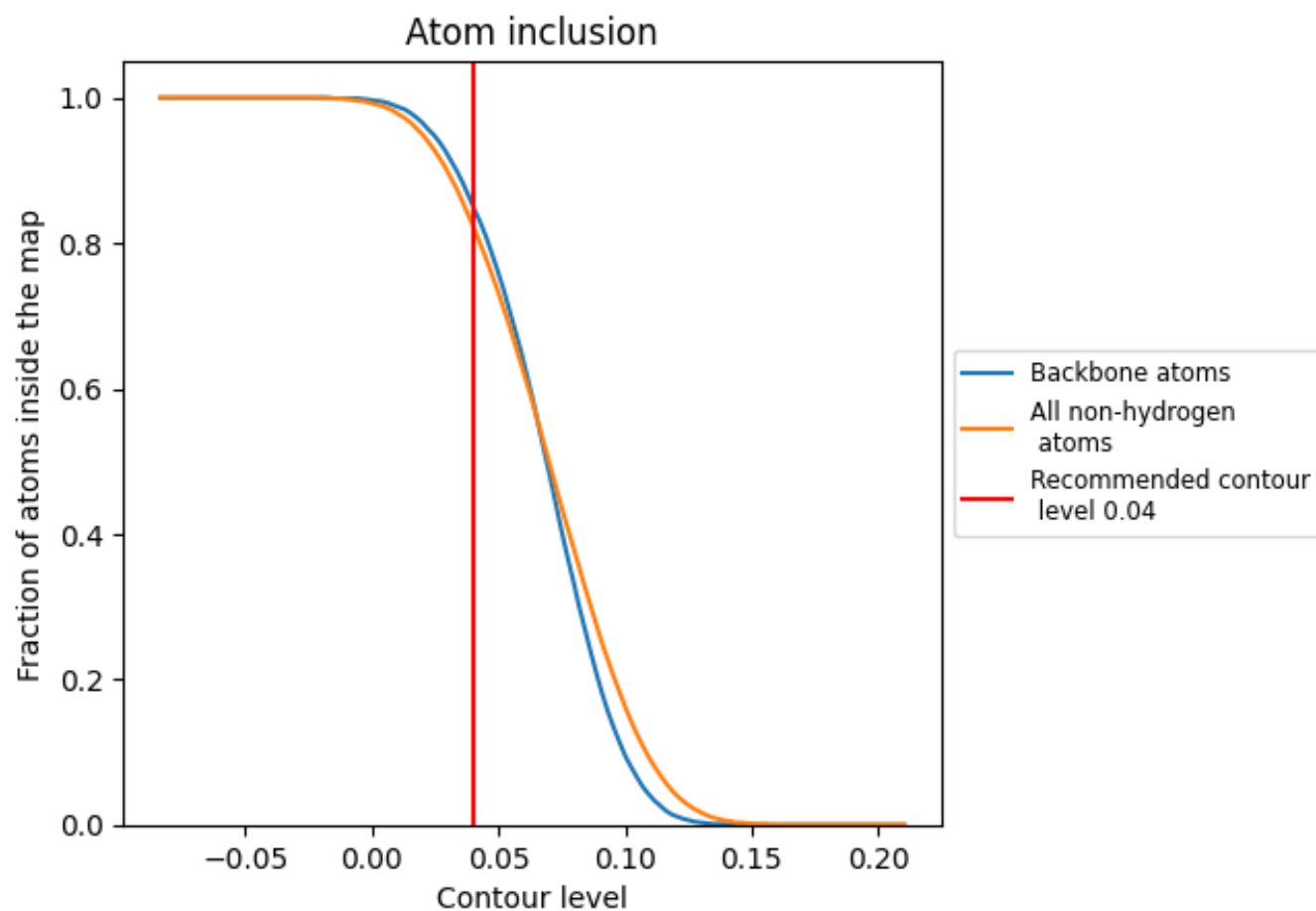
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.2180
1	 0.7470	 0.0820
2	 0.9030	 0.2780
A	 0.9270	 0.2540
B	 0.9510	 0.2450
C	 0.7000	 0.2090
D	 0.7160	 0.2310
E	 0.7210	 0.2080
F	 0.6910	 0.1350
G	 0.7310	 0.2130
H	 0.4340	 0.1410
I	 0.4080	 0.0570
J	 0.3230	 0.0500
K	 0.7270	 0.2280
L	 0.6250	 0.2120
M	 0.7440	 0.2090
N	 0.7420	 0.2390
O	 0.6560	 0.2170
P	 0.7800	 0.1880
Q	 0.6840	 0.2320
R	 0.7880	 0.2280
S	 0.7340	 0.2260
T	 0.6670	 0.2230
U	 0.6860	 0.2060
V	 0.7080	 0.2070
W	 0.7130	 0.2120
X	 0.7500	 0.1850
Y	 0.7010	 0.2080
Z	 0.6910	 0.1640
a	 0.7730	 0.2340
b	 0.7240	 0.2260
c	 0.6670	 0.1380
d	 0.7160	 0.2070
e	 0.6930	 0.2100
f	 0.7750	 0.1990



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Chain	Atom inclusion	Q-score
g	 0.2910	 0.0050
h	 0.1560	 -0.0410
i	 0.5010	 0.0590
j	 0.2820	 0.0170
k	 0.6670	 0.1140
l	 0.6440	 0.0390