wwPDB EM Validation Summary Report (i)

Sep 16, 2026 – 06:55 PM EDT

PDB ID	:	5KCS / pdb_00005kcs
EMDB ID	:	EMD-8238
Title	:	Cryo-EM structure of the Escherichia coli 70S ribosome in complex with antibiotic Evernimycin, mRNA, TetM and P-site tRNA at 3.9A resolution
Authors	:	Arenz, S.; Juette, M.F.; Graf, M.; Nguyen, F.; Huter, P.; Polikanov, Y.S.; Blanchard, S.C.; Wilson, D.N.
Deposited on	:	2016-06-06
Resolution	:	3.90 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 (i) 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 (i)) were used in the production of this report:

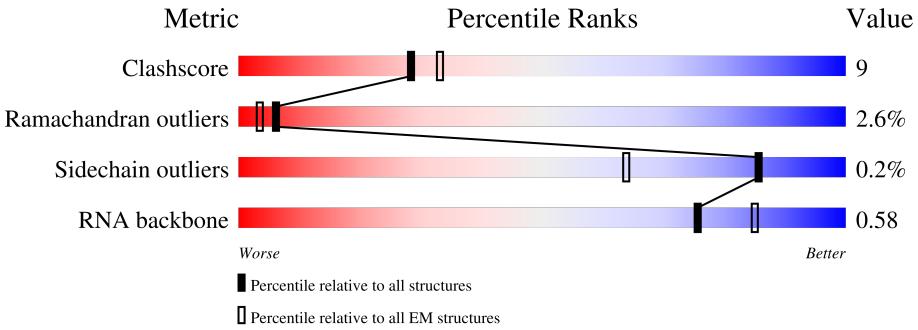
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

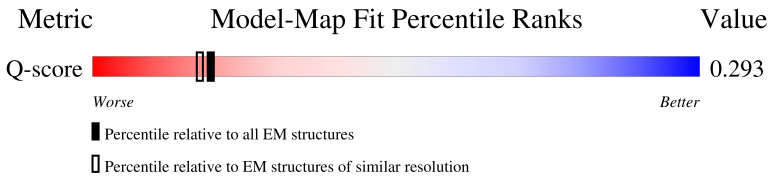
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2904	9% 54% 39% 7%
2	1B	120	8% 65% 29% 6%
3	1D	273	15% 65% 34% .

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Mol	Chain	Length	Quality of chain
4	1E	209	25% 72% 28%
5	1F	201	37% 73% 27%
6	1G	179	61% 70% 27%
7	1H	177	46% 85% 15%
8	1L	121	56% 57% 43%
9	1I	149	92% 77% 21%
10	1J	165	78% 53% 25% 21%
11	1K	142	97% 74% 25%
12	1N	142	21% 76% 23%
13	1O	123	27% 72% 24%
14	1P	144	37% 64% 34%
15	1Q	136	10% 65% 34%
16	1R	127	17% 69% 24% 6%
17	1S	117	52% 86% 13%
18	1T	115	31% 83% 15%
19	1U	118	15% 79% 20%
20	1V	103	36% 76% 24%
21	1W	110	21% 77% 22%
22	1X	100	29% 73% 19% 7%
23	1Y	104	47% 71% 26%
24	1Z	94	38% 73% 27%
25	10	85	18% 62% 26% 12%
26	11	78	27% 77% 22%
27	12	63	44% 76% 24%
28	13	59	20% 73% 25%

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Mol	Chain	Length	Quality of chain
29	14	70	81% 70% 23% 6%
30	15	57	23% 70% 26%
31	16	55	91% 69% 22% 9%
32	17	46	13% 61% 39%
33	18	65	22% 52% 45%
34	19	38	13% 68% 32%
35	1a	1539	15% 57% 39%
36	1b	241	78% 66% 24% 10%
37	1c	233	46% 64% 24% 12%
38	1d	206	73% 66% 33%
39	1e	167	40% 63% 30% 6%
40	1f	135	31% 55% 16% 26%
41	1g	179	54% 61% 23% 16%
42	1h	130	31% 73% 25%
43	1i	130	68% 58% 39%
44	1j	103	71% 59% 35% 5%
45	1k	129	49% 49% 40% 10%
46	1l	124	64% 65% 31%
47	1m	118	49% 81% 14%
48	1n	101	43% 77% 20%
49	1o	89	36% 81% 17%
50	1p	82	50% 66% 33%
51	1q	84	48% 71% 23% 5%
52	1r	75	32% 68% 17% 13%
53	1s	92	36% 58% 28% 14%

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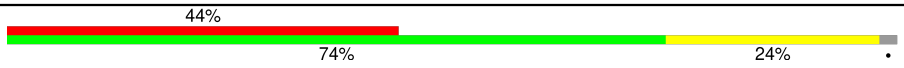
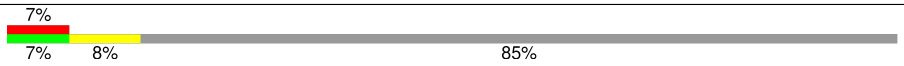
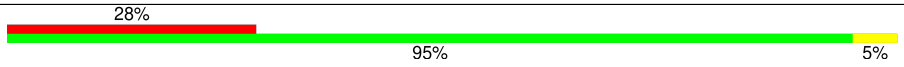
Mol	Chain	Length	Quality of chain
54	1t	87	
55	1u	71	
56	1v	60	
57	1w	639	
58	1x	77	

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 148945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1A	2900	62276	27788	11459	20129	2900	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1847	G	A	conflict	GB 802133627

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1B	120	2570	1144	468	838	120	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1D	271	2082	1288	423	364	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1E	209	1565	979	288	294	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1F	201	1552	974	283	290	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1G	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	1L	69	Total	C	N	O	0	0
			276	138	69	69		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1N	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1O	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1P	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1Q	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1R	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	1S	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1T	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	1U	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1V	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1W	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1X	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1Y	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Z	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	10	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	11	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	12	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	13	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	14	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	15	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	16	50	Total	C	N	O	0	0
			409	263	75	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	17	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	18	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	19	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	1r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	1v	9	Total	C	N	O	P	0	0
			192	86	35	62	9		

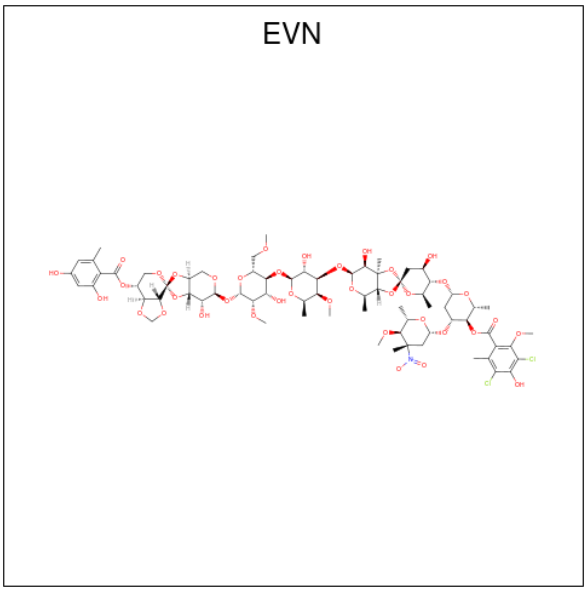
- Molecule 57 is a protein called Tetracycline resistance protein TetM from transposon Tn916.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	1w	639	Total	C	N	O	0	0
			2590	1308	640	642		

- Molecule 58 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	1x	73	Total	C	N	O	P	0	0
			1567	699	285	510	73		

- Molecule 59 is (2R,3R,4R,6S)-6-{[(2R,3aR,4R,4'R,5'S,6S,6'R,7S,7aR)-6-{[(2S,3R,4R,5S,6R)-2-{[(2R,3S,4S,5S,6S)-6-({(2R,3aS,3a'R,6S,7R,7' R,7aS,7a'S)-7'-[(2,4-dihydroxy-6-methyl benzoyl)oxy]-7-hydroxyoctahydro-4H-2,4'-spirobi[[1,3]dioxolo[4,5-c]pyran]-6-yl}ox y)-4-hydroxy-5-methoxy-2-(methoxymethyl)tetrahydro-2H-pyran-3-yl]oxy}-3-hydroxy-5-methoxy -6-methyltetrahydro-2H-pyran-4- yl]oxy}-4',7-dihydroxy-4,6',7a-trimethyloctahydro-4H-spiro[1,3-dioxolo[4,5-c]pyran-2,2'-pyran]-5'-yl]oxy}-4-{[(2R,4S,5R, 6S)-5-methoxy-4,6-dimethyl-4-nitrotetrahydro-2H-pyran-2-yl]oxy}-2-methyltetrahydro-2H-pyran-3-yl 3,5-dichloro-4-hydroxy-2-methoxy-6-methylbenzoate (non-preferred name) (CCD ID: EVN) (formula: $C_{70}H_{97}Cl_2NO_{38}$).



Mol	Chain	Residues	Atoms					AltConf
59	1A	1	Total	C	Cl	N	O	0
			111	70	2	1	38	

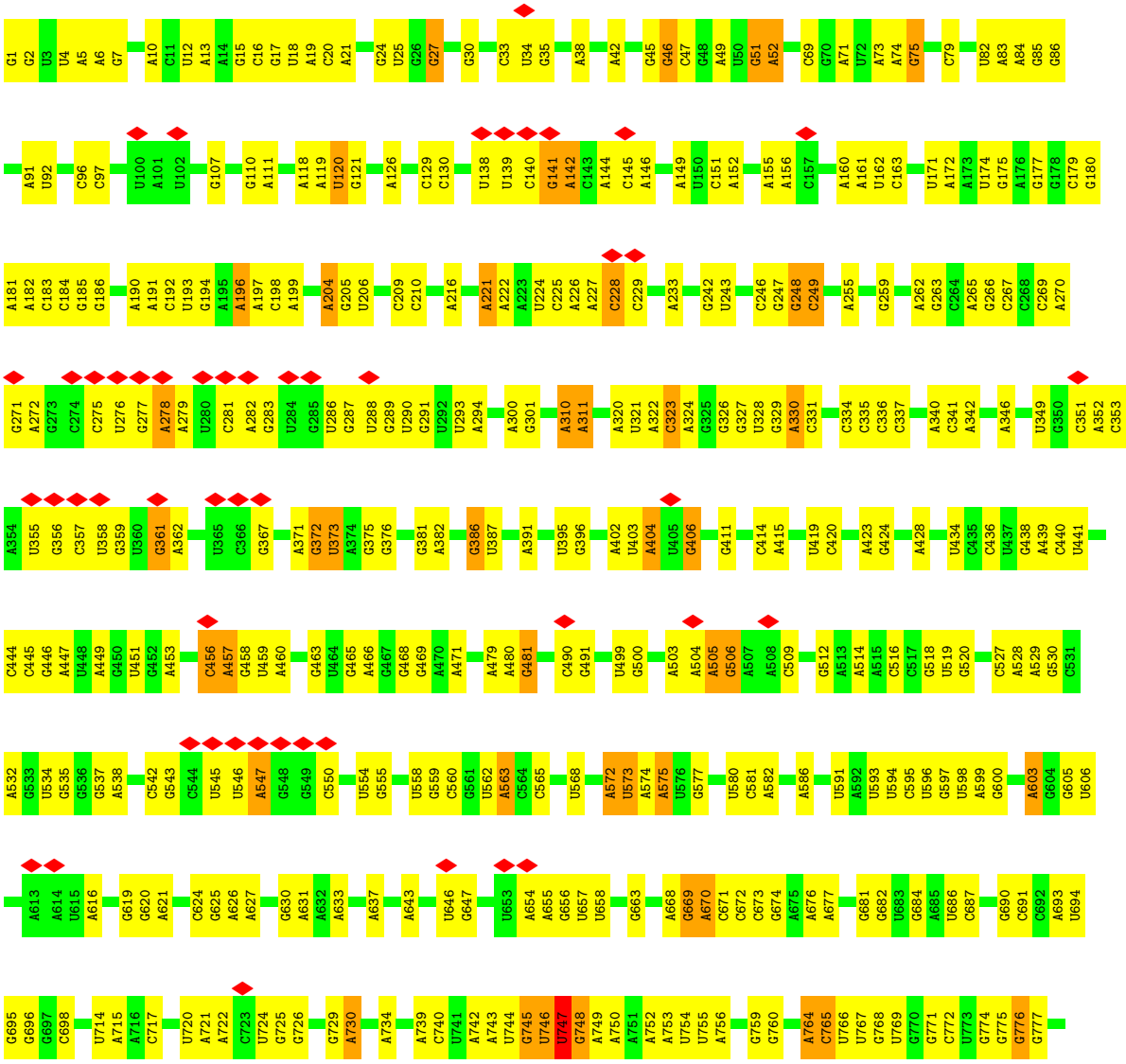
3 Residue-property plots (i)

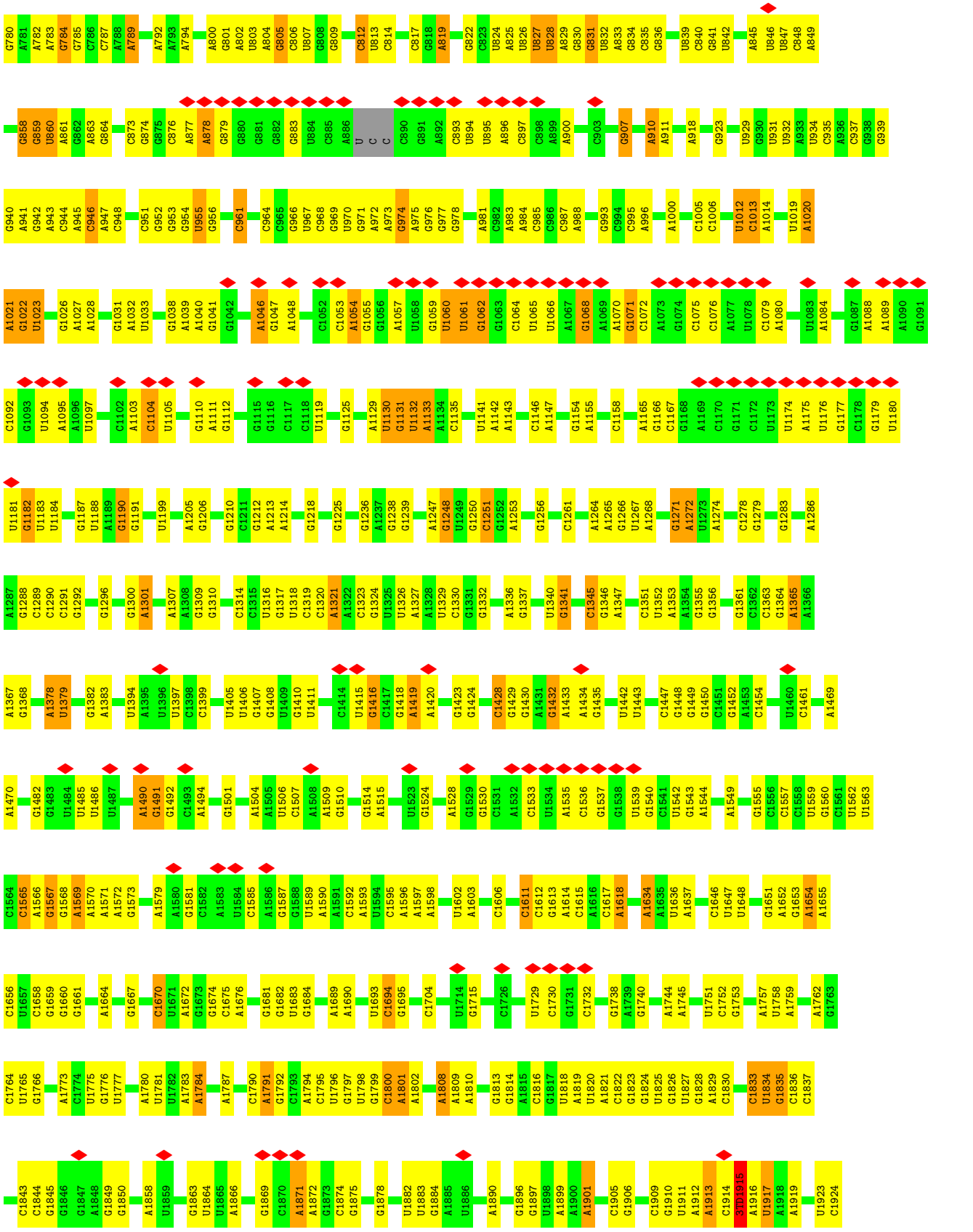
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S Ribosomal RNA

Chain 1A:



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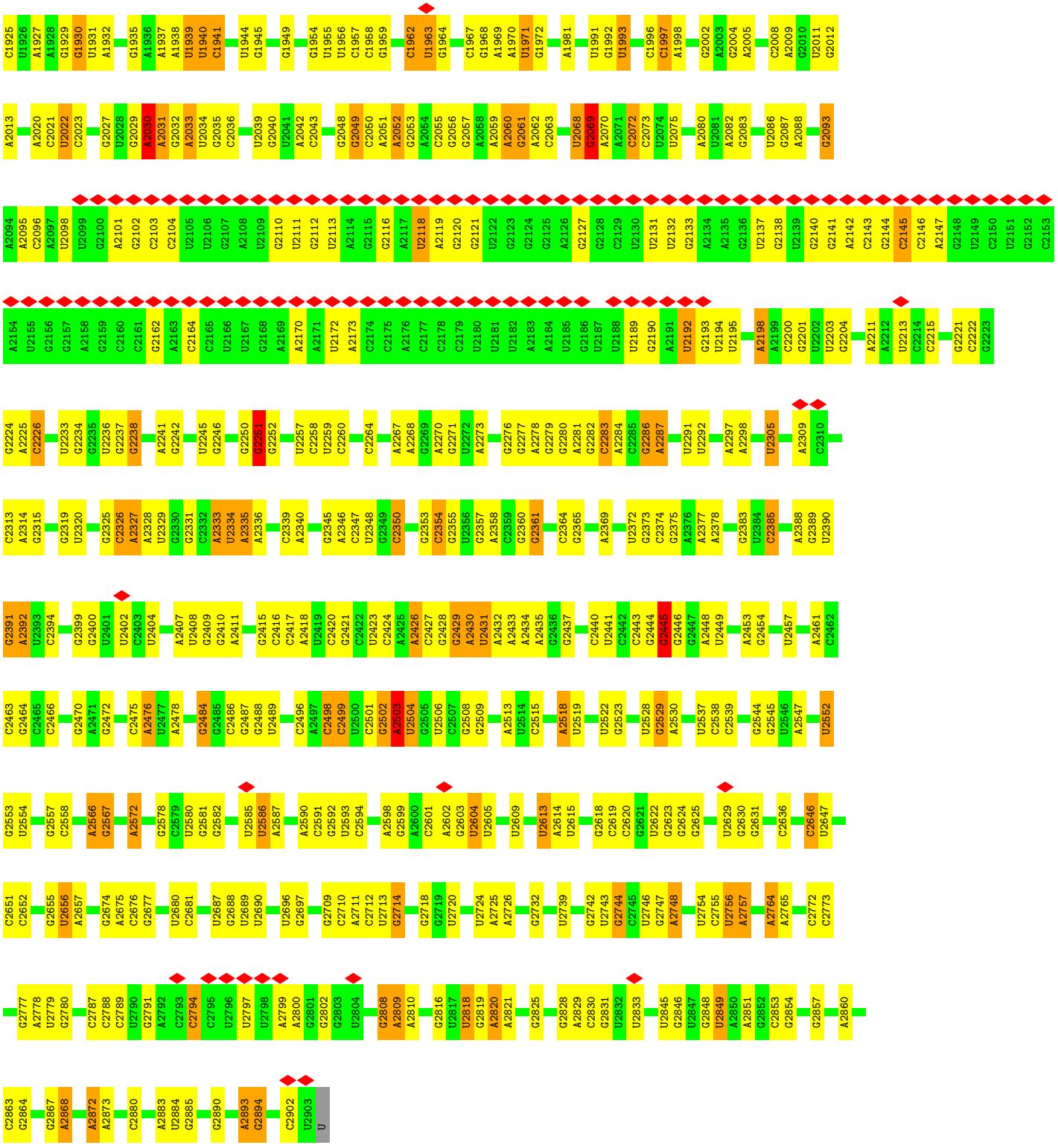


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

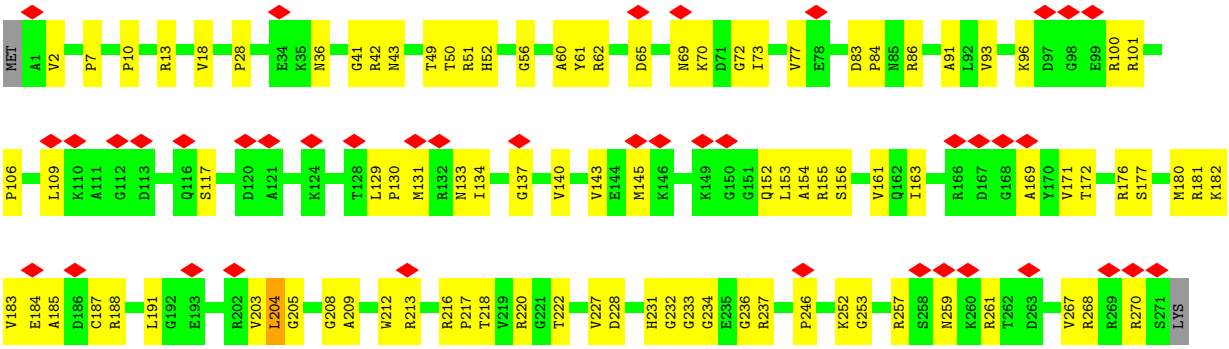




• Molecule 3: 50S ribosomal protein L2

Chain 1D:

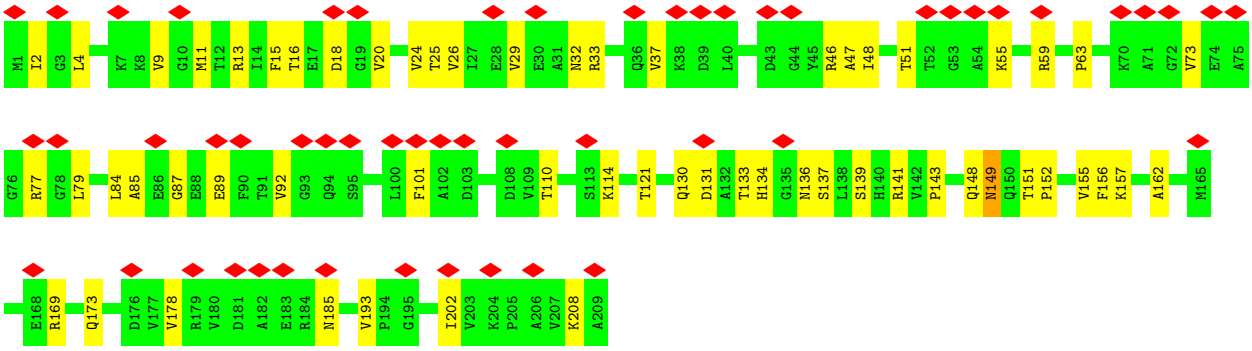




• Molecule 4: 50S ribosomal protein L3

Chain 1E:

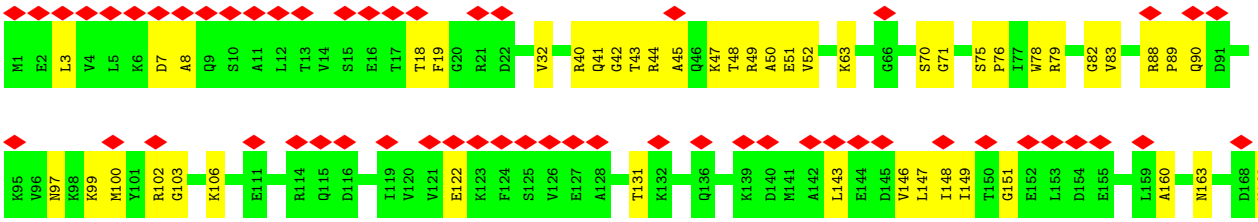


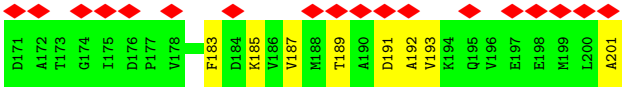


• Molecule 5: 50S ribosomal protein L4

Chain 1F:



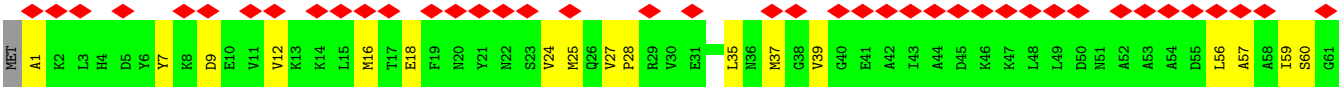




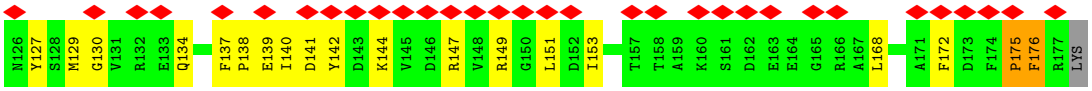
• Molecule 6: 50S ribosomal protein L5

Chain 1G:





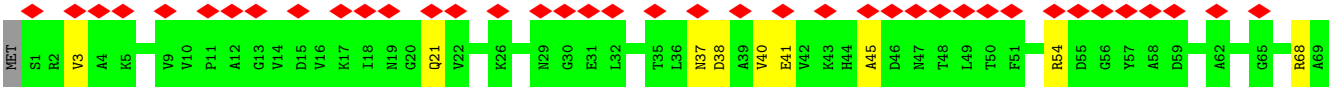


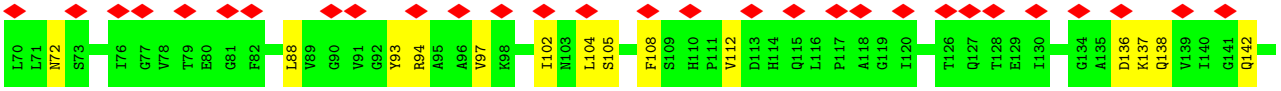


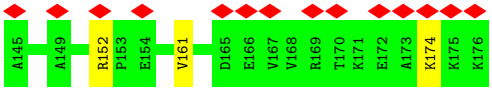
• Molecule 7: 50S ribosomal protein L6

Chain 1H:





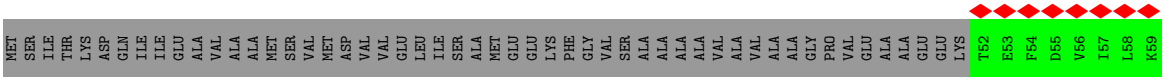


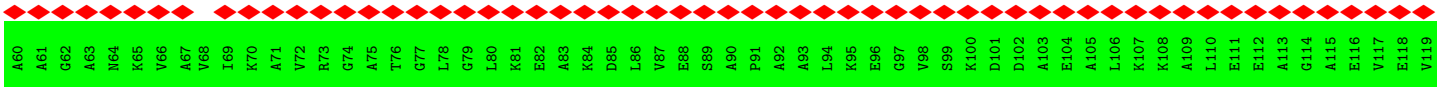


• Molecule 8: 50S ribosomal protein L7/L12

Chain 1L:



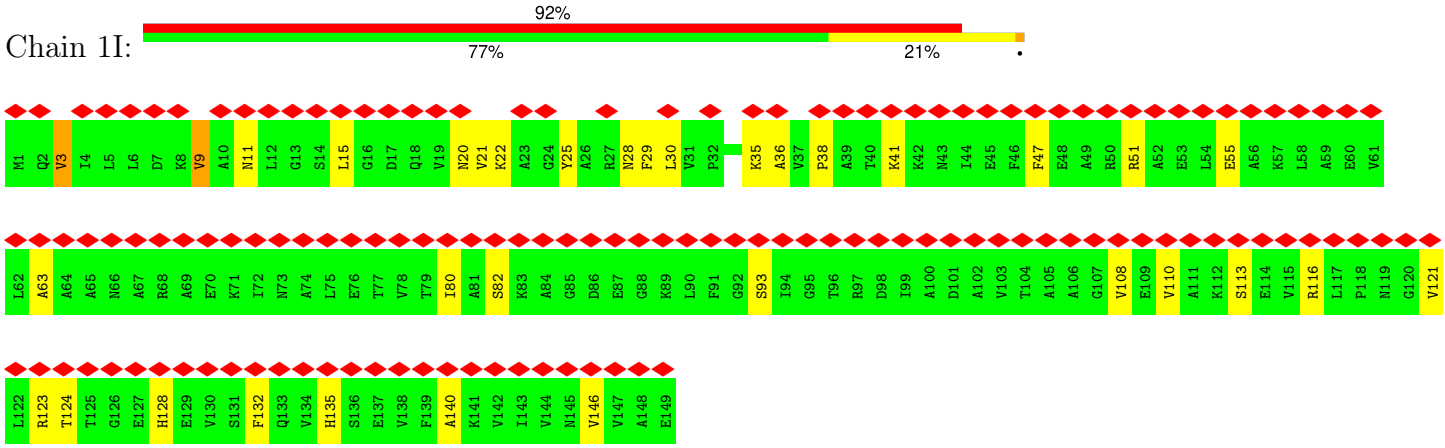






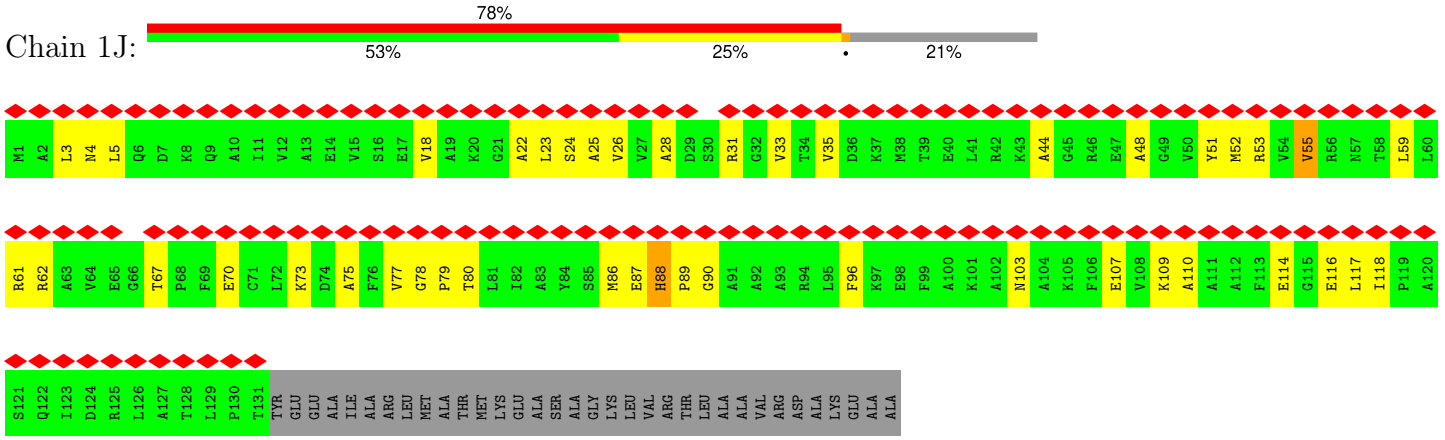
• Molecule 9: 50S ribosomal protein L9

Chain 1I:



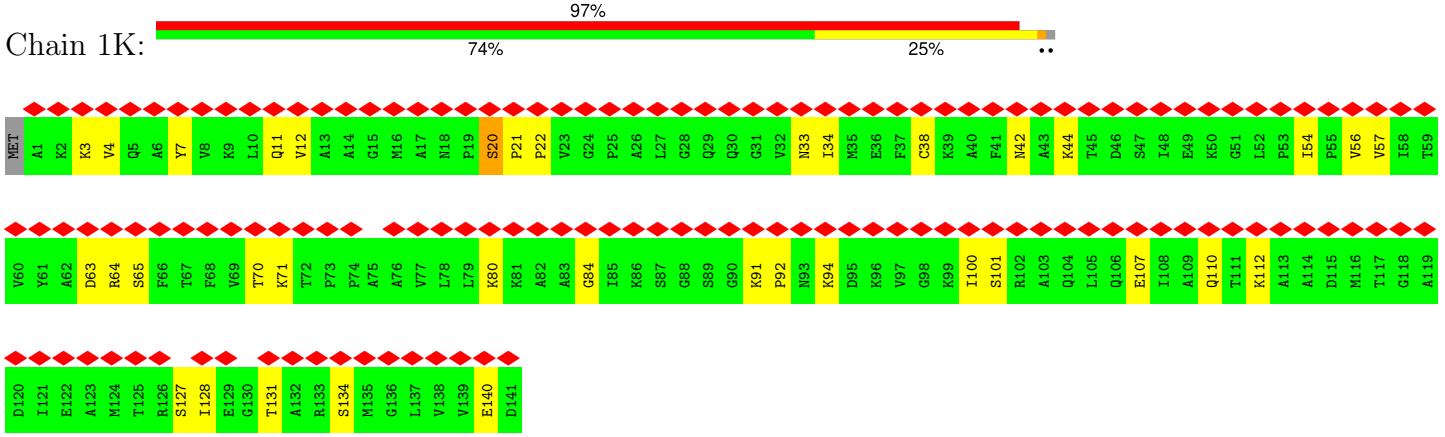
• Molecule 10: 50S ribosomal protein L10

Chain 1J:



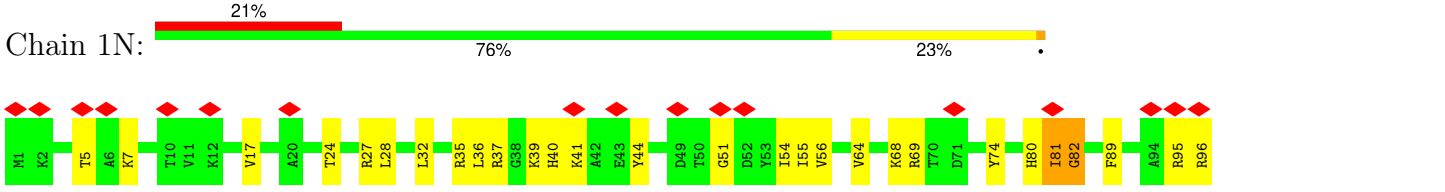
• Molecule 11: 50S ribosomal protein L11

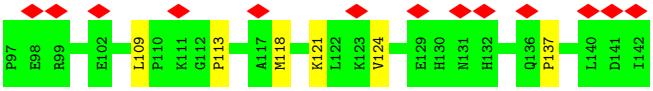
Chain 1K:



• Molecule 12: 50S ribosomal protein L13

Chain 1N:





• Molecule 13: 50S ribosomal protein L14

Chain 1O:



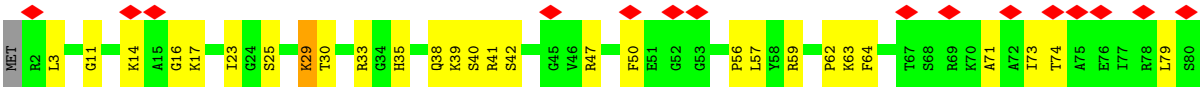




• Molecule 14: 50S ribosomal protein L15

Chain 1P:





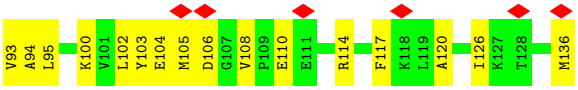


• Molecule 15: 50S ribosomal protein L16

Chain 1Q:



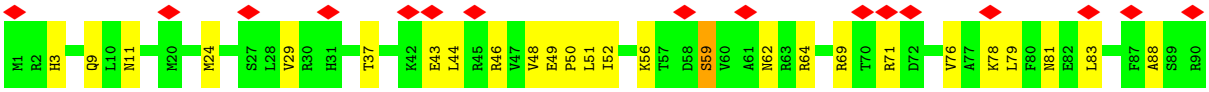


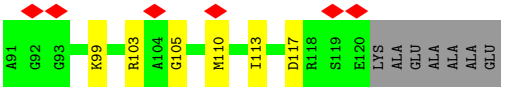


• Molecule 16: 50S ribosomal protein L17

Chain 1R:

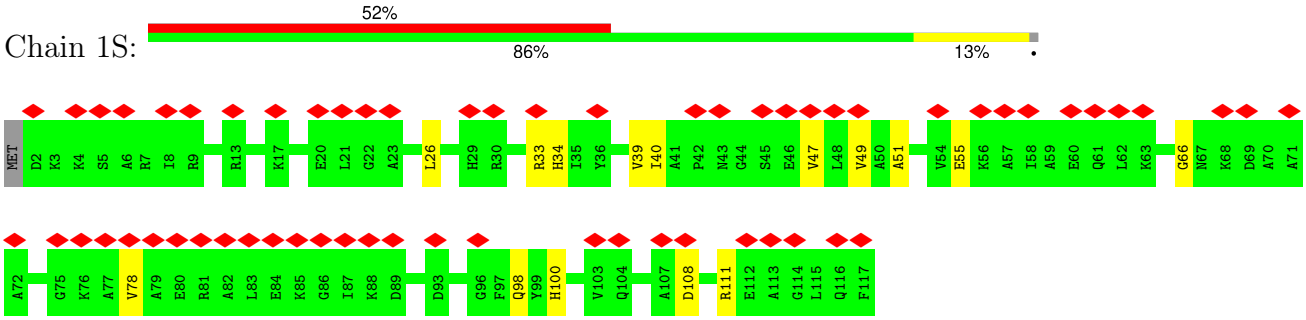






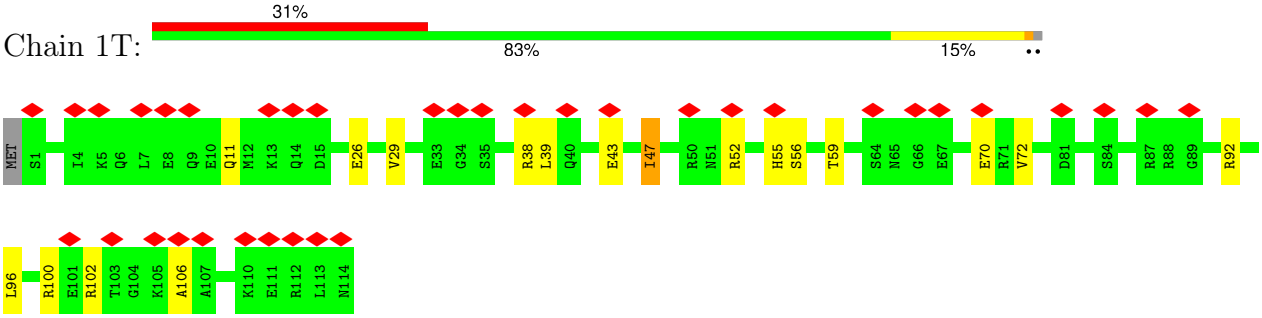
• Molecule 17: 50S ribosomal protein L18

Chain 1S:



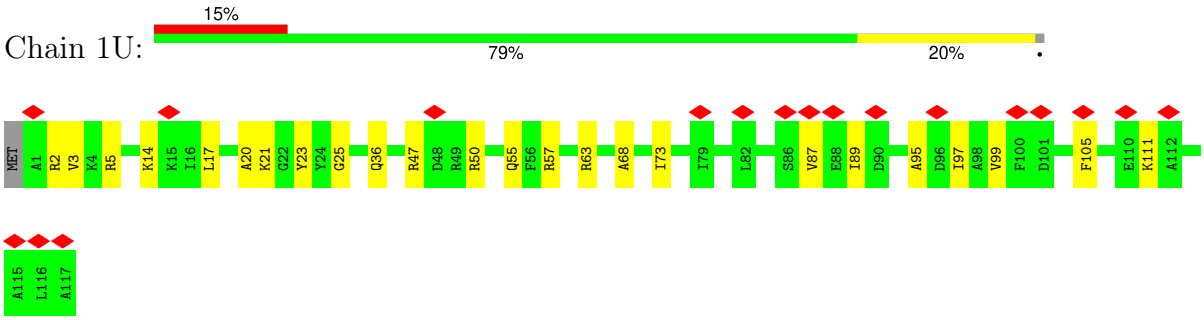
• Molecule 18: 50S ribosomal protein L19

Chain 1T:



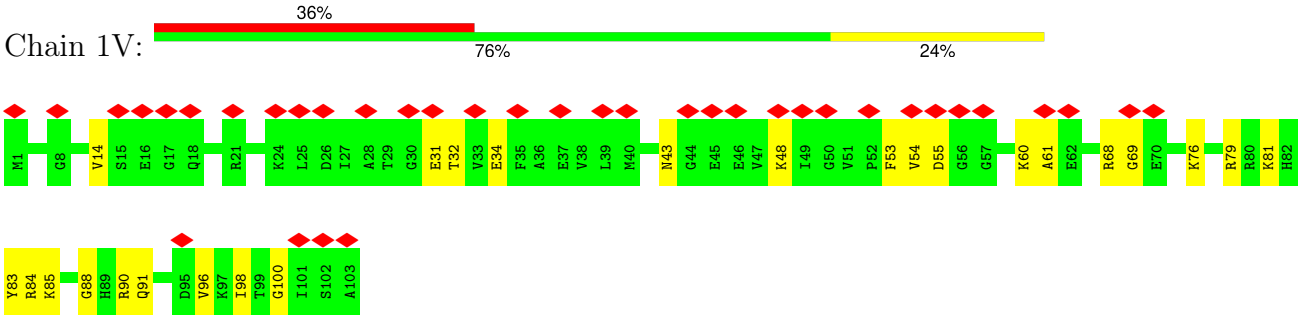
• Molecule 19: 50S ribosomal protein L20

Chain 1U:



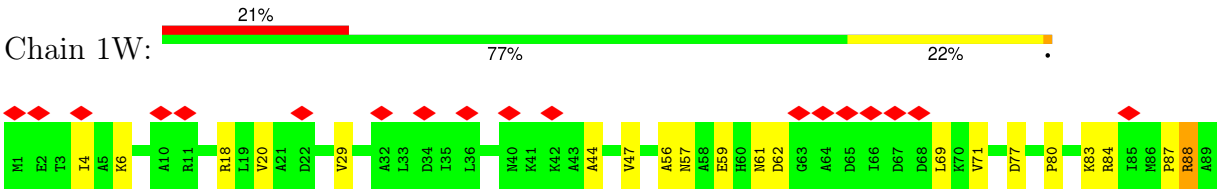
• Molecule 20: 50S ribosomal protein L21

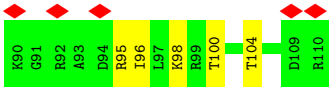
Chain 1V:



• Molecule 21: 50S ribosomal protein L22

Chain 1W:

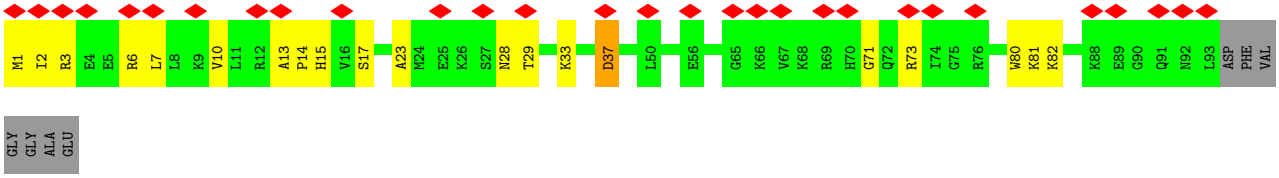




• Molecule 22: 50S ribosomal protein L23

Chain 1X:

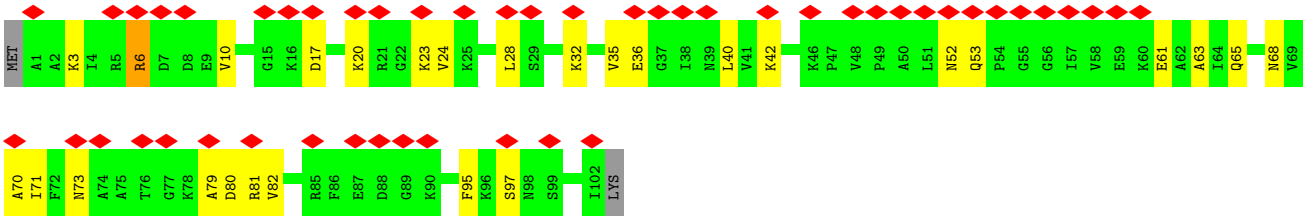




• Molecule 23: 50S ribosomal protein L24

Chain 1Y:

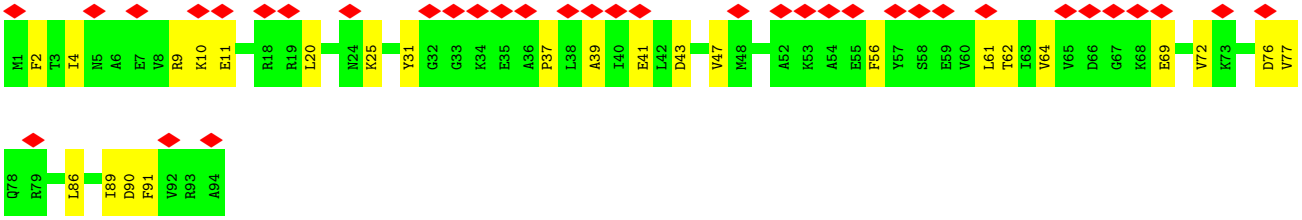




• Molecule 24: 50S ribosomal protein L25

Chain 1Z:

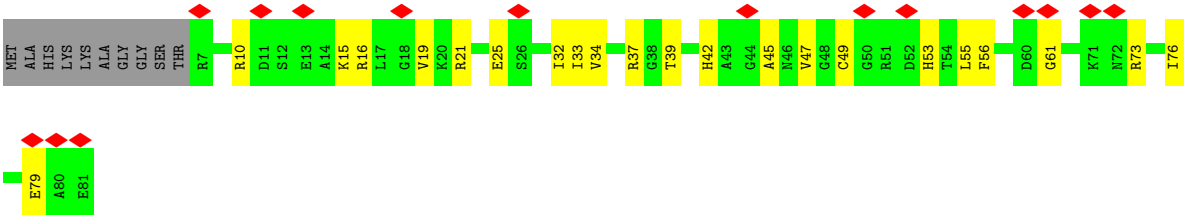




• Molecule 25: 50S ribosomal protein L27

Chain 10:

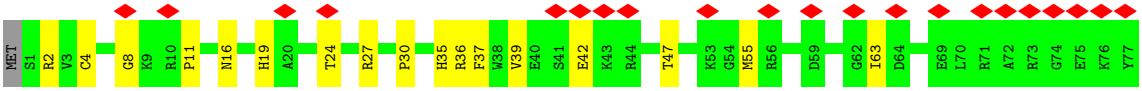




• Molecule 26: 50S ribosomal protein L28

Chain 11:

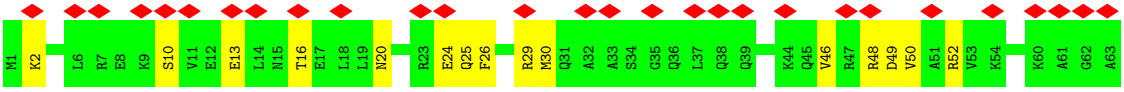




• Molecule 27: 50S ribosomal protein L29

Chain 12:

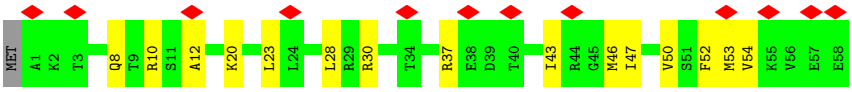




• Molecule 28: 50S ribosomal protein L30

Chain 13:

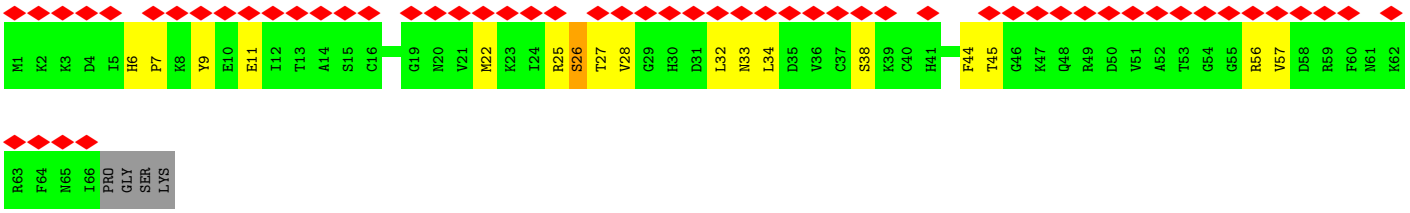




• Molecule 29: 50S ribosomal protein L31

Chain 14:

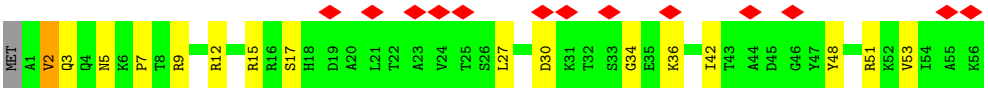




• Molecule 30: 50S ribosomal protein L32

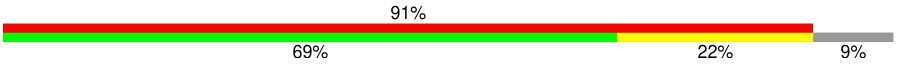
Chain 15:

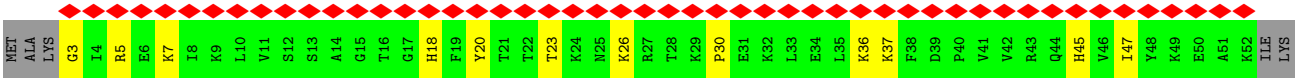




• Molecule 31: 50S ribosomal protein L33

Chain 16:

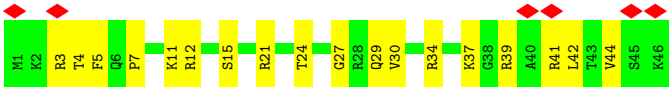




• Molecule 32: 50S ribosomal protein L34

Chain 17:

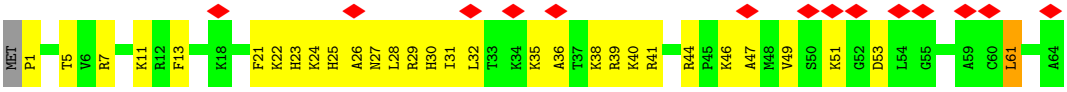




• Molecule 33: 50S ribosomal protein L35

Chain 18:

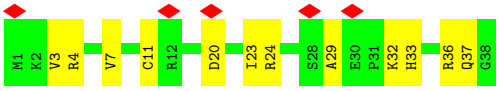




• Molecule 34: 50S ribosomal protein L36

Chain 19:

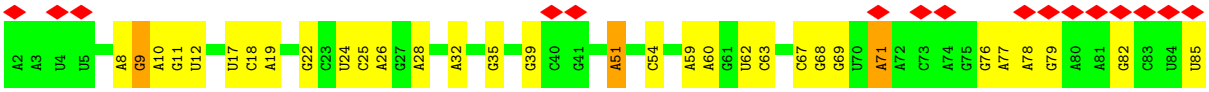


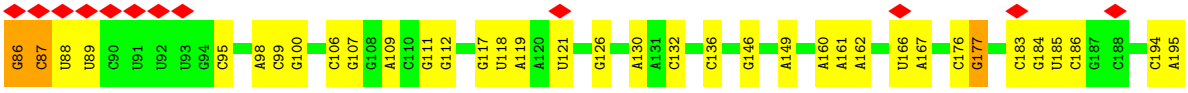


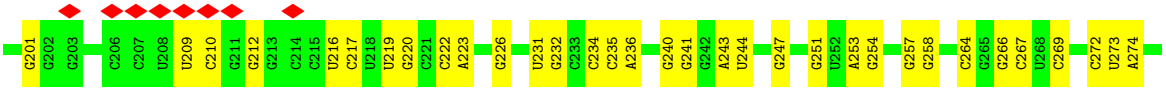
• Molecule 35: 16S Ribosomal RNA

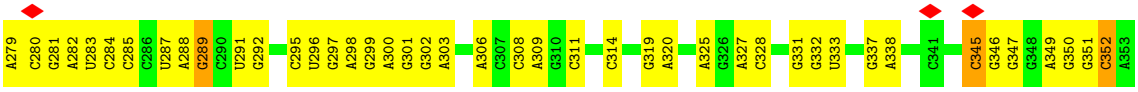
Chain 1a:

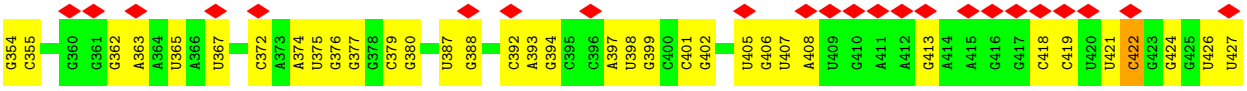


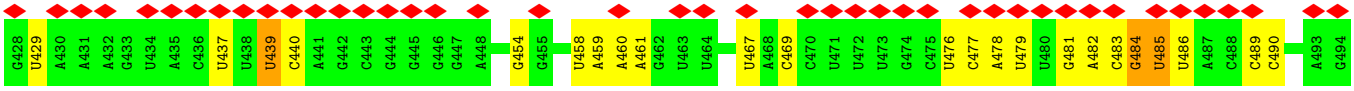


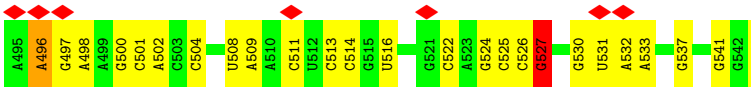


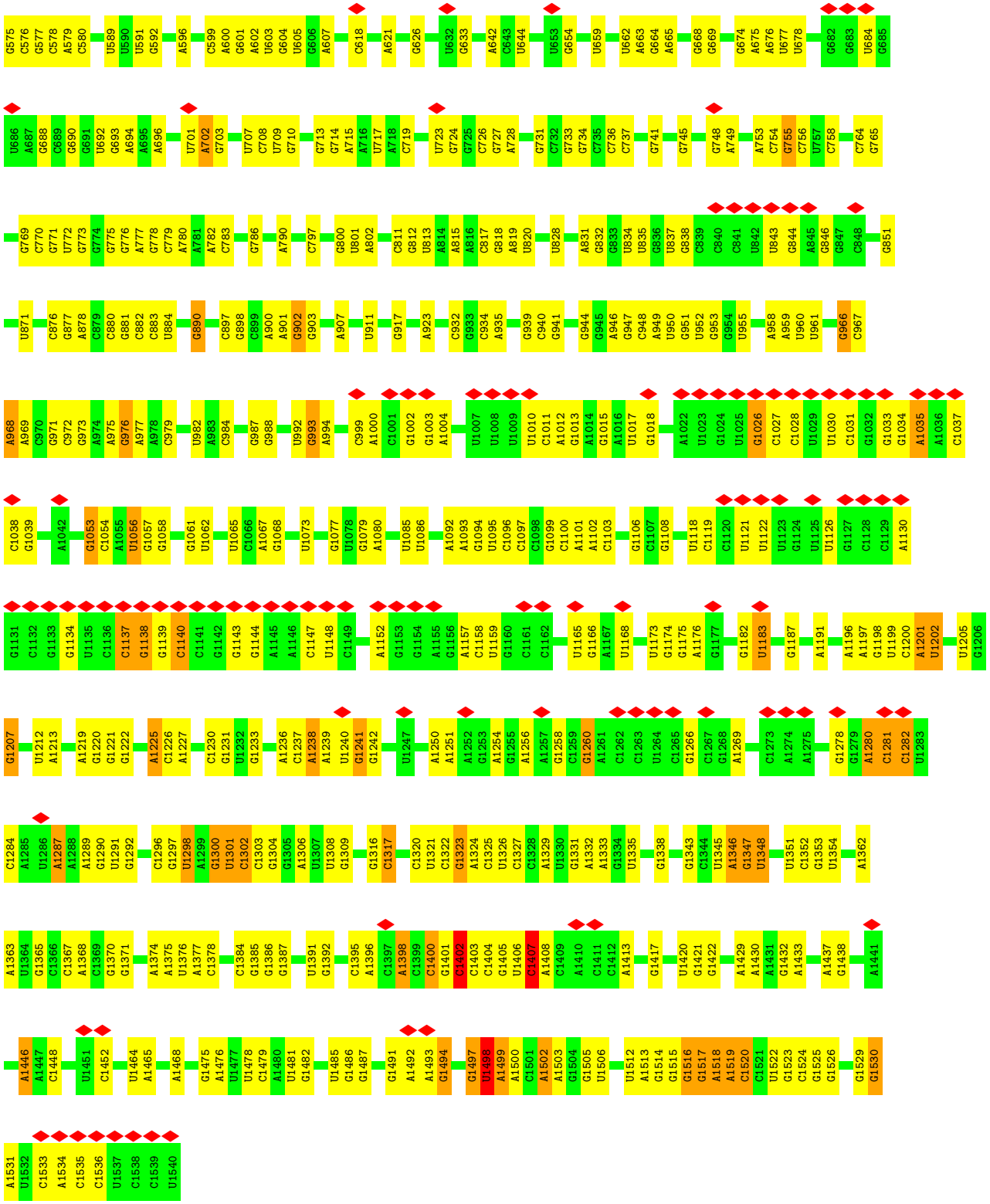








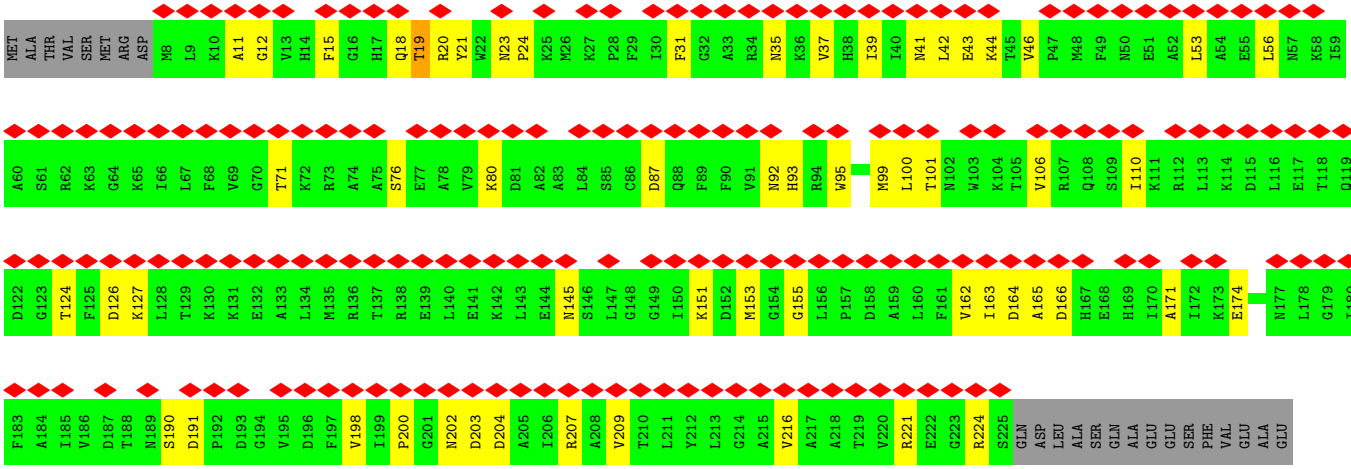




• Molecule 36: 30S ribosomal protein S2

Chain 1b:

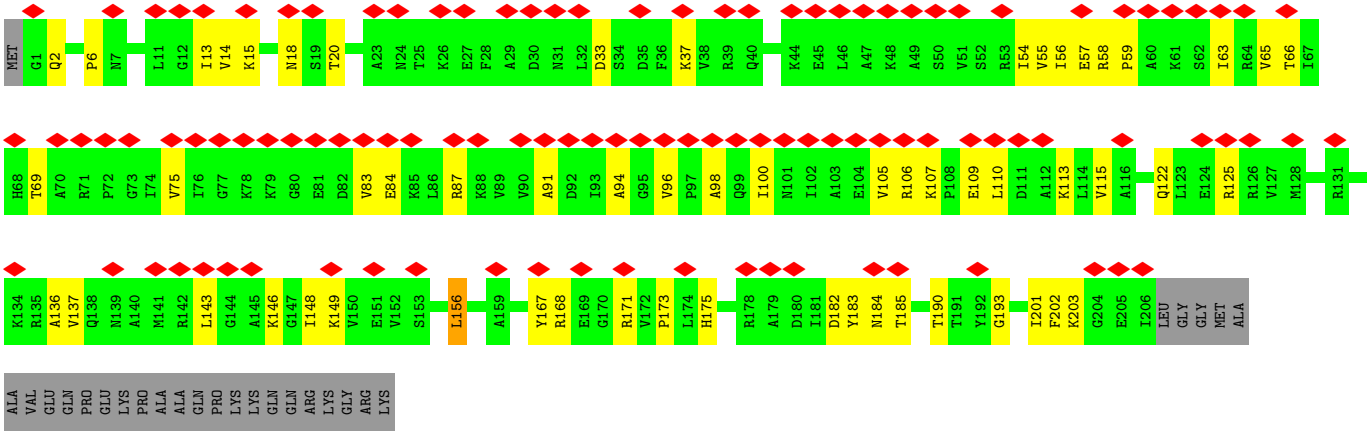




• Molecule 37: 30S ribosomal protein S3

Chain 1c:





• Molecule 38: 30S ribosomal protein S4

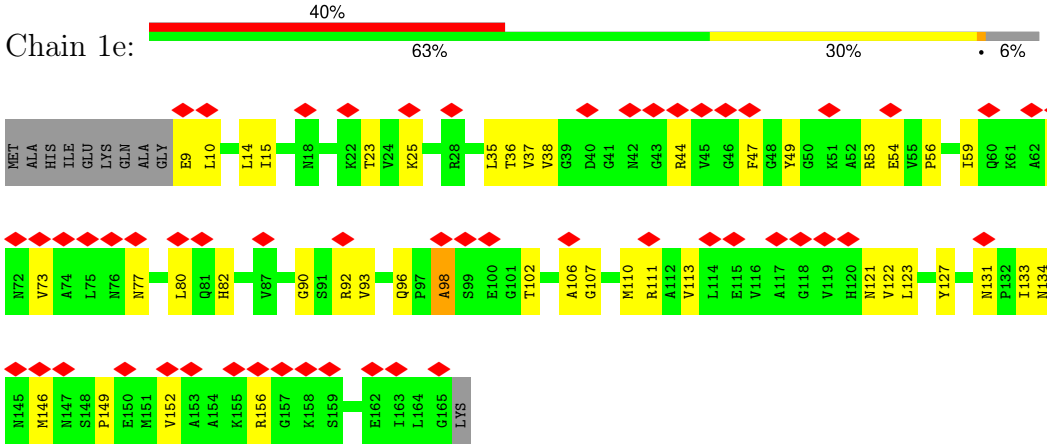
Chain 1d:





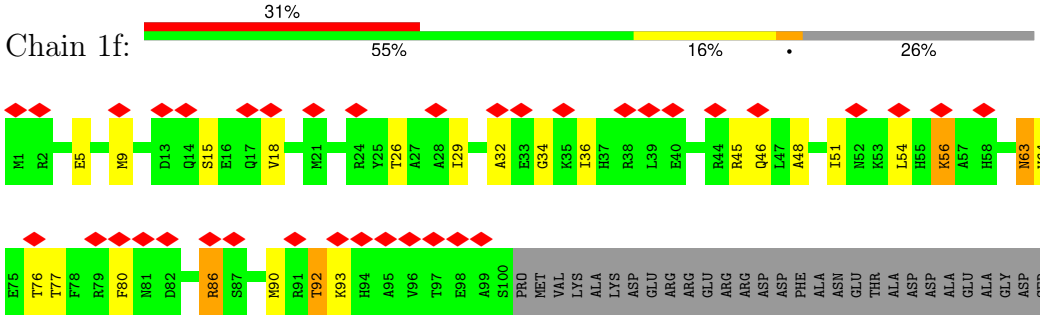
• Molecule 39: 30S ribosomal protein S5

Chain 1e:



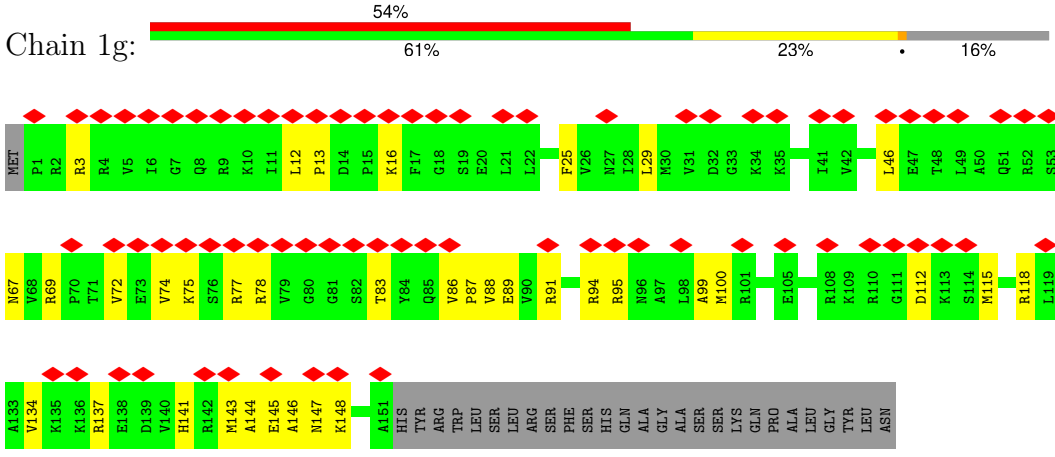
• Molecule 40: 30S ribosomal protein S6

Chain 1f:



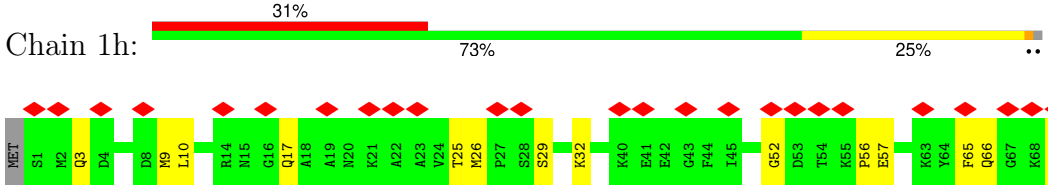
• Molecule 41: 30S ribosomal protein S7

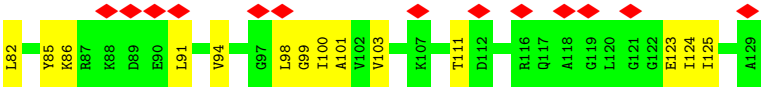
Chain 1g:



• Molecule 42: 30S ribosomal protein S8

Chain 1h:

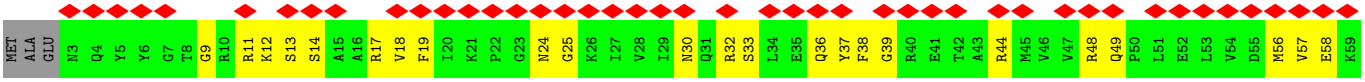


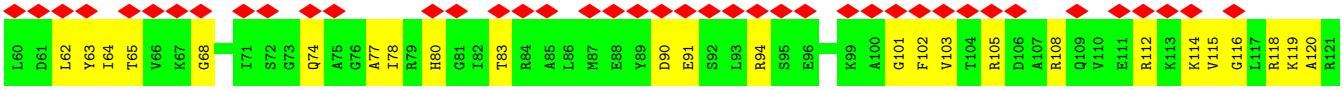


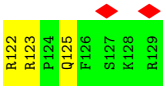
• Molecule 43: 30S ribosomal protein S9

Chain 1i:





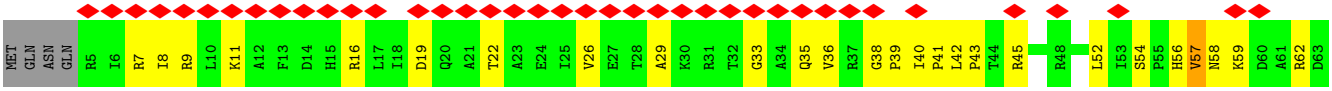


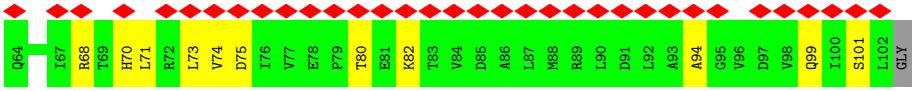


• Molecule 44: 30S ribosomal protein S10

Chain 1j:



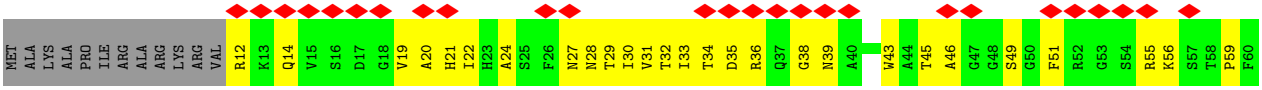


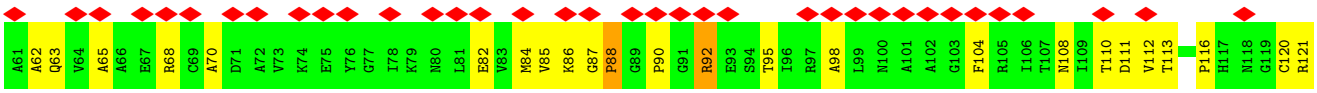


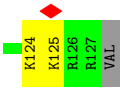
• Molecule 45: 30S ribosomal protein S11

Chain 1k:





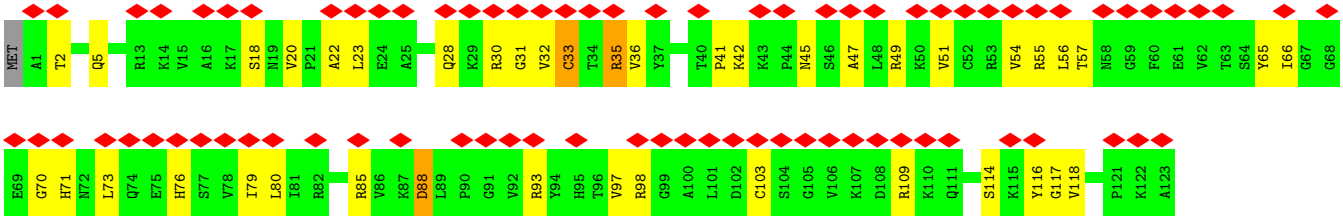




• Molecule 46: 30S ribosomal protein S12

Chain 1l:

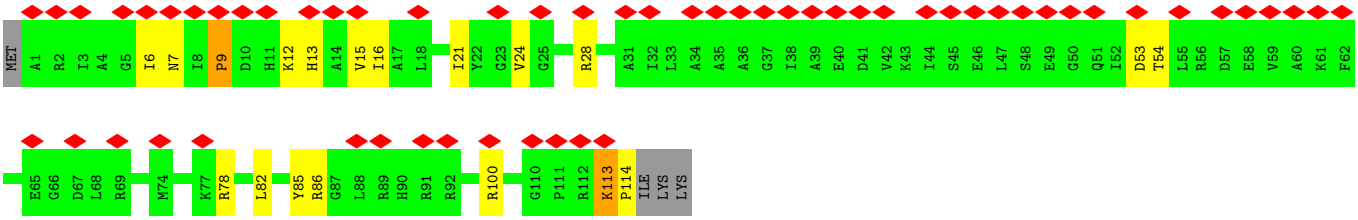




• Molecule 47: 30S ribosomal protein S13

Chain 1m:

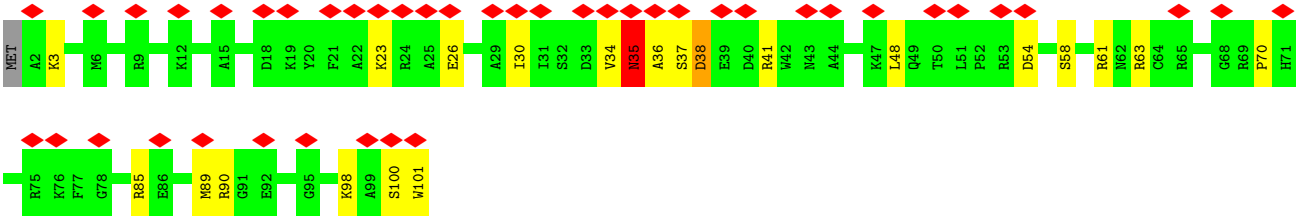




• Molecule 48: 30S ribosomal protein S14

Chain 1n:

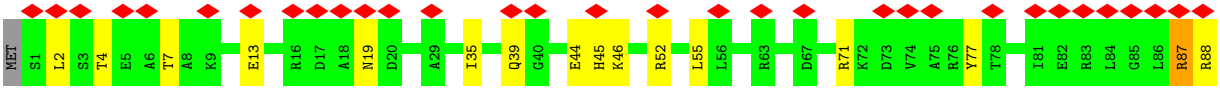




• Molecule 49: 30S ribosomal protein S15

Chain 1o:

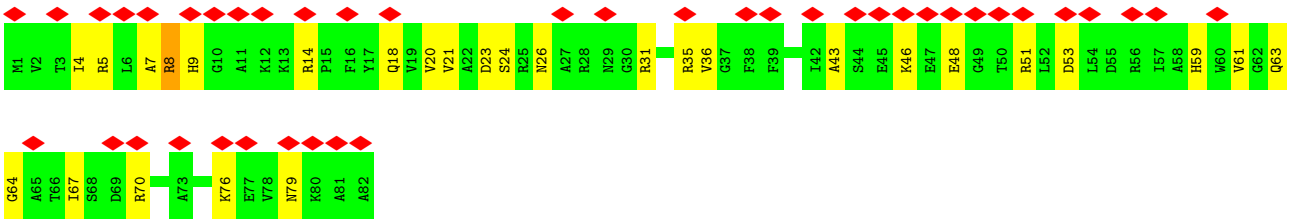




• Molecule 50: 30S ribosomal protein S16

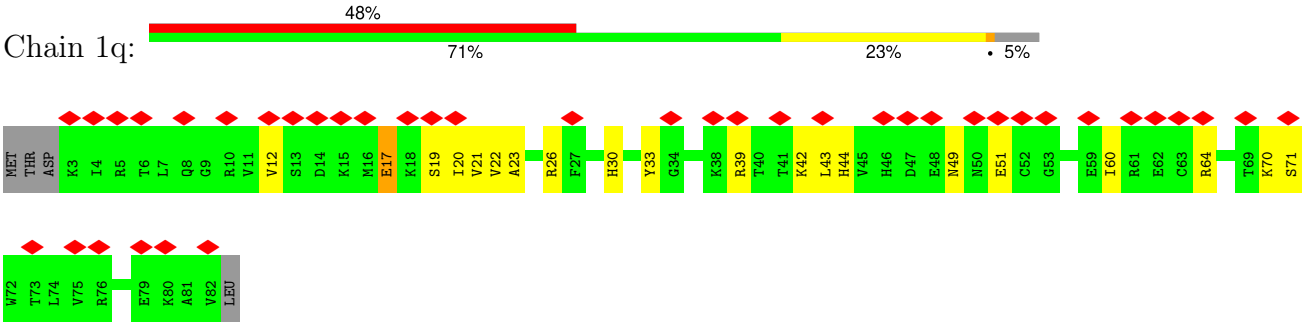
Chain 1p:





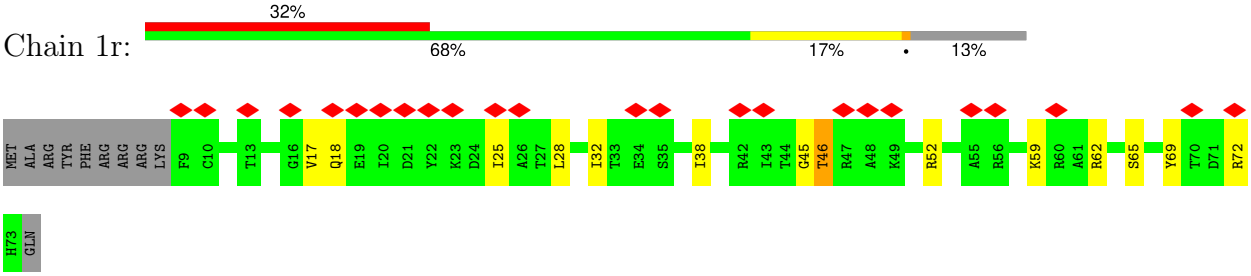
• Molecule 51: 30S ribosomal protein S17

Chain 1q:



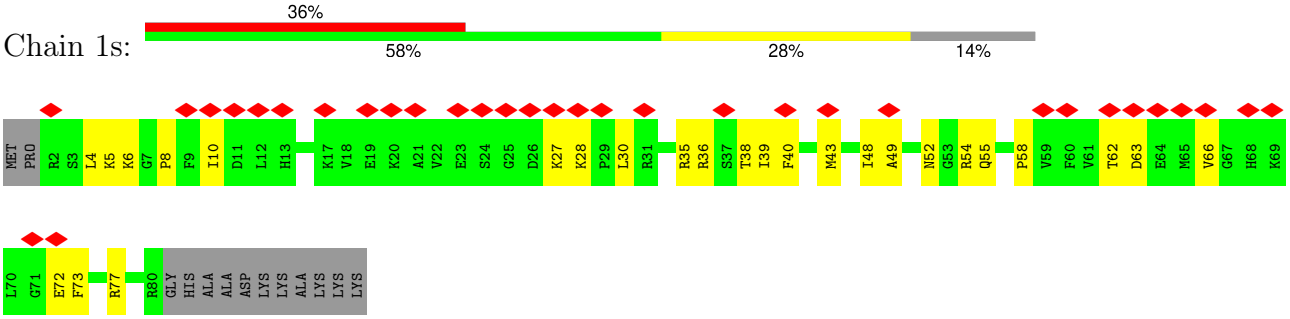
• Molecule 52: 30S ribosomal protein S18

Chain 1r:



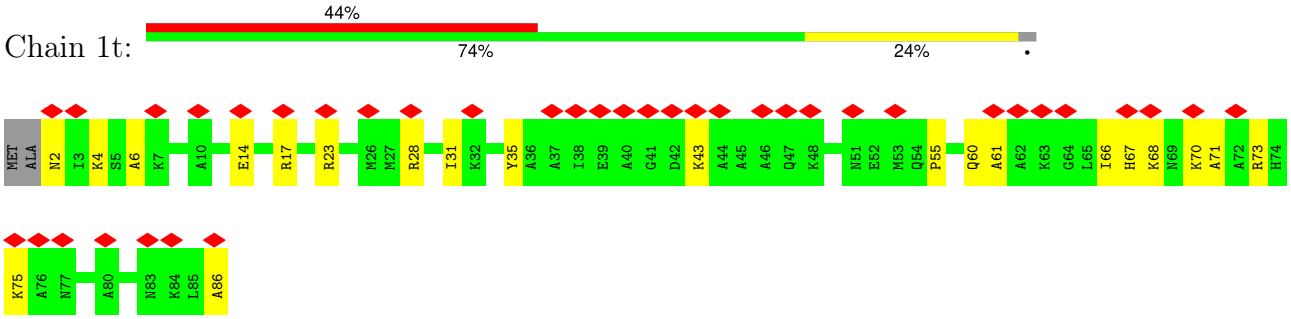
• Molecule 53: 30S ribosomal protein S19

Chain 1s:



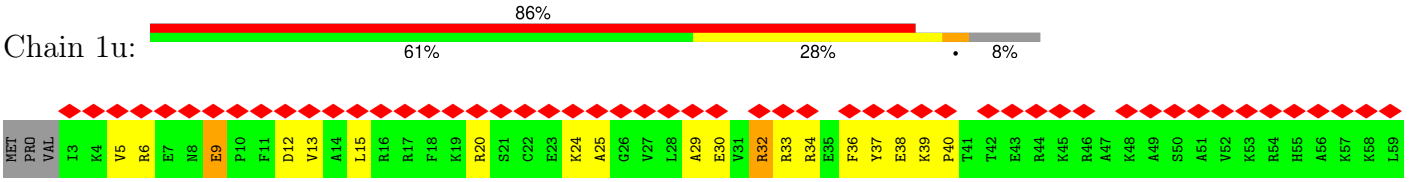
• Molecule 54: 30S ribosomal protein S20

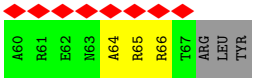
Chain 1t:



• Molecule 55: 30S ribosomal protein S21

Chain 1u:

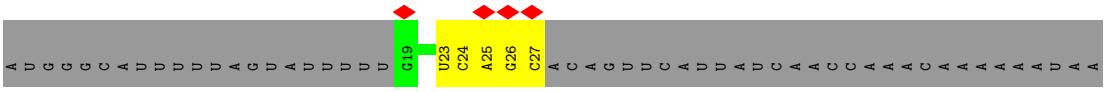




• Molecule 56: mRNA

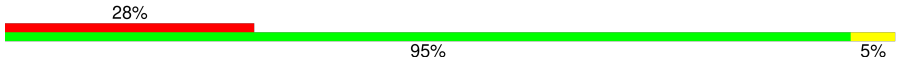
Chain 1v:

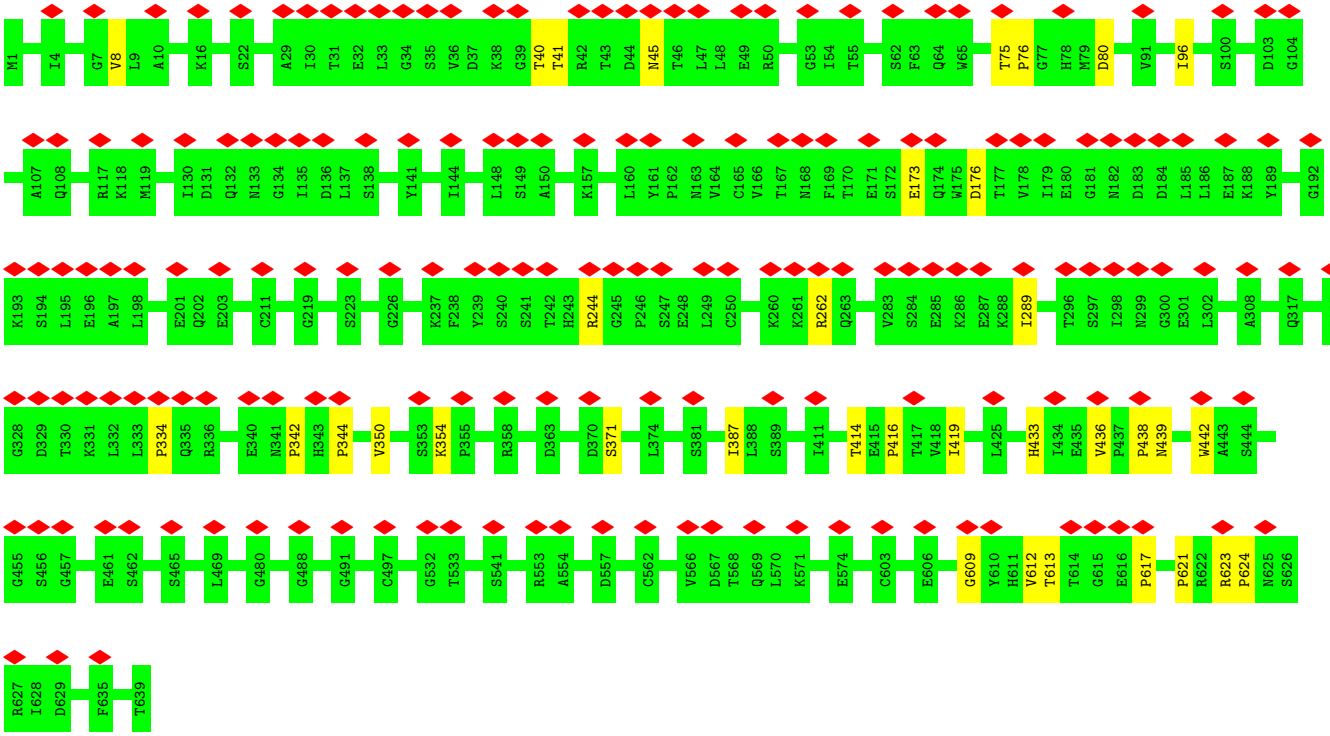




• Molecule 57: Tetracycline resistance protein TetM from transposon Tn916

Chain 1w:

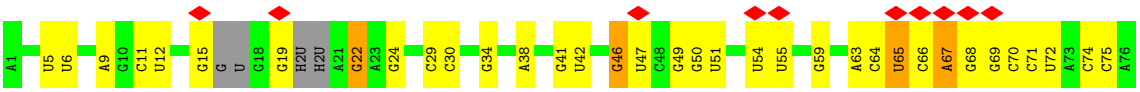




• Molecule 58: P-site tRNA

Chain 1x:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78186	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.018	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00307	Depositor
Map size (Å)	407.74402, 407.74402, 407.74402	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, OMG, OMU, 3TD, OMC, EVN, MA6, 5MC, UR3, 2MG, 4OC, G7M, 5MU, 1MG, H2U, 7MG, 2MA, PSU

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	1A	0.10	0/69174	0.20	0/107910
2	1B	0.09	0/2873	0.19	0/4478
3	1D	0.21	0/2121	0.38	0/2852
4	1E	0.15	0/1586	0.32	0/2134
5	1F	0.14	0/1571	0.30	0/2113
6	1G	0.15	0/1434	0.34	0/1926
7	1H	0.15	0/1343	0.31	0/1816
8	1L	0.15	0/275	0.27	0/342
9	1I	0.16	0/1122	0.31	0/1515
10	1J	0.24	0/1001	0.45	0/1350
11	1K	0.17	0/1046	0.32	0/1410
12	1N	0.15	0/1152	0.33	0/1551
13	1O	0.16	0/947	0.38	0/1268
14	1P	0.16	0/1054	0.37	0/1403
15	1Q	0.21	0/1093	0.45	0/1460
16	1R	0.16	0/973	0.36	0/1301
17	1S	0.15	0/902	0.31	0/1209
18	1T	0.17	0/929	0.37	0/1242
19	1U	0.13	0/960	0.31	0/1278
20	1V	0.17	0/829	0.32	0/1107
21	1W	0.16	0/864	0.34	0/1156
22	1X	0.15	0/744	0.33	0/994
23	1Y	0.16	0/787	0.33	0/1051
24	1Z	0.18	0/766	0.37	0/1025
25	10	0.15	0/582	0.33	0/769
26	11	0.15	0/635	0.34	0/848
27	12	0.11	0/510	0.30	0/677
28	13	0.15	0/453	0.33	0/605
29	14	0.17	0/531	0.34	0/709
30	15	0.14	0/450	0.34	0/599
31	16	0.15	0/416	0.32	0/554

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	17	0.14	0/380	0.37	0/498
33	18	0.15	0/513	0.35	0/676
34	19	0.14	0/303	0.35	0/397
35	1a	0.10	1/36701 (0.0%)	0.19	0/57246
36	1b	0.15	0/1735	0.33	0/2338
37	1c	0.18	0/1651	0.36	0/2225
38	1d	0.24	1/1665 (0.1%)	0.37	0/2227
39	1e	0.15	0/1154	0.37	0/1554
40	1f	0.14	0/835	0.37	0/1128
41	1g	0.15	0/1195	0.38	0/1602
42	1h	0.17	0/989	0.34	0/1326
43	1i	0.17	0/1034	0.41	0/1375
44	1j	0.18	0/796	0.41	0/1077
45	1k	0.16	0/885	0.36	0/1195
46	1l	0.18	0/969	0.40	0/1300
47	1m	0.16	0/892	0.37	0/1193
48	1n	0.16	0/806	0.39	0/1074
49	1o	0.14	0/722	0.31	0/964
50	1p	0.16	0/659	0.32	0/884
51	1q	0.21	0/657	0.41	0/881
52	1r	0.16	0/511	0.36	0/689
53	1s	0.13	0/652	0.31	0/877
54	1t	0.14	0/671	0.32	0/888
55	1u	0.31	1/500 (0.2%)	0.42	0/668
56	1v	0.23	0/214	0.36	0/331
57	1w	0.17	0/2594	0.39	6/3251 (0.2%)
58	1x	0.14	0/1656	0.20	0/2575
All	All	0.13	3/160462 (0.0%)	0.25	6/239091 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1d	16	THR	CA-C	7.44	1.55	1.52
35	1a	1498	UR3	O3'-P	5.36	1.61	1.56
55	1u	9	GLU	C-N	5.04	1.45	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1w	439	ASN	CA-C-N	6.45	126.40	119.76
57	1w	439	ASN	C-N-CA	6.45	126.40	119.76
57	1w	623	ARG	CA-C-N	5.24	126.39	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1w	623	ARG	C-N-CA	5.24	126.39	119.84
57	1w	436	VAL	CA-C-N	5.01	125.54	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	62276	0	31344	881	0
2	1B	2570	0	1301	25	0
3	1D	2082	0	2157	77	0
4	1E	1565	0	1616	47	0
5	1F	1552	0	1619	38	0
6	1G	1410	0	1447	39	0
7	1H	1323	0	1374	17	0
8	1L	276	0	79	0	0
9	1I	1111	0	1148	20	0
10	1J	988	0	1025	25	0
11	1K	1032	0	1088	18	0
12	1N	1129	0	1162	26	0
13	1O	938	0	1012	22	0
14	1P	1045	0	1117	40	0
15	1Q	1074	0	1157	38	0
16	1R	960	0	1000	24	0
17	1S	892	0	923	9	0
18	1T	917	0	965	15	0
19	1U	947	0	1022	19	0
20	1V	816	0	839	17	0
21	1W	857	0	922	21	0
22	1X	738	0	807	12	0
23	1Y	779	0	834	19	0
24	1Z	753	0	780	16	0
25	10	575	0	592	19	0
26	11	625	0	655	15	0
27	12	509	0	543	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	13	449	0	491	9	0
29	14	522	0	522	15	0
30	15	444	0	461	12	0
31	16	409	0	440	9	0
32	17	377	0	418	22	0
33	18	504	0	574	25	0
34	19	302	0	343	9	0
35	1a	33029	0	16644	463	0
36	1b	1704	0	1732	34	0
37	1c	1624	0	1699	40	0
38	1d	1643	0	1710	47	0
39	1e	1141	0	1170	30	0
40	1f	817	0	808	17	0
41	1g	1181	0	1240	27	0
42	1h	979	0	1034	21	0
43	1i	1022	0	1070	37	0
44	1j	786	0	828	23	0
45	1k	869	0	878	44	0
46	1l	955	0	1019	33	0
47	1m	883	0	944	14	0
48	1n	794	0	833	12	0
49	1o	714	0	737	10	0
50	1p	649	0	666	25	0
51	1q	648	0	691	13	0
52	1r	504	0	502	10	0
53	1s	637	0	665	19	0
54	1t	665	0	714	17	0
55	1u	495	0	486	10	0
56	1v	192	0	98	6	0
57	1w	2590	0	731	4	0
58	1x	1567	0	798	24	0
59	1A	111	0	0	0	0
All	All	148945	0	99474	2238	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 2238 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)
1:1A:827:U:H2'	1:1A:2068:U:O2	1.20	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:827:U:C2'	1:1A:2068:U:O2	1.98	1.12
1:1A:827:U:H2'	1:1A:2068:U:C2	1.97	1.00
1:1A:776:G:H22	1:1A:2072:C:H5'	1.35	0.89
6:1G:140:ILE:HG22	6:1G:142:TYR:H	1.43	0.84

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
3	1D	269/273 (98%)	242 (90%)	23 (9%)	4 (2%)	8 37
4	1E	207/209 (99%)	187 (90%)	19 (9%)	1 (0%)	24 59
5	1F	199/201 (99%)	185 (93%)	11 (6%)	3 (2%)	8 37
6	1G	175/179 (98%)	153 (87%)	19 (11%)	3 (2%)	7 35
7	1H	174/177 (98%)	154 (88%)	18 (10%)	2 (1%)	11 43
8	1L	67/121 (55%)	64 (96%)	3 (4%)	0	100 100
9	1I	147/149 (99%)	130 (88%)	13 (9%)	4 (3%)	4 28
10	1J	129/165 (78%)	101 (78%)	23 (18%)	5 (4%)	2 21
11	1K	139/142 (98%)	118 (85%)	14 (10%)	7 (5%)	1 18
12	1N	140/142 (99%)	132 (94%)	6 (4%)	2 (1%)	9 38
13	1O	120/123 (98%)	106 (88%)	11 (9%)	3 (2%)	4 29
14	1P	141/144 (98%)	120 (85%)	16 (11%)	5 (4%)	3 23
15	1Q	134/136 (98%)	120 (90%)	9 (7%)	5 (4%)	2 22
16	1R	118/127 (93%)	103 (87%)	13 (11%)	2 (2%)	7 35
17	1S	114/117 (97%)	103 (90%)	9 (8%)	2 (2%)	6 34
18	1T	112/115 (97%)	105 (94%)	7 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1U	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
20	1V	101/103 (98%)	89 (88%)	8 (8%)	4 (4%)	2	21
21	1W	108/110 (98%)	96 (89%)	12 (11%)	0	100	100
22	1X	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	5	31
23	1Y	100/104 (96%)	86 (86%)	12 (12%)	2 (2%)	6	32
24	1Z	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
25	10	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
26	11	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
27	12	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
28	13	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
29	14	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	7	36
30	15	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	6	33
31	16	48/55 (87%)	42 (88%)	5 (10%)	1 (2%)	5	31
32	17	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
33	18	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
34	19	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	4	27
36	1b	216/241 (90%)	187 (87%)	24 (11%)	5 (2%)	5	30
37	1c	204/233 (88%)	190 (93%)	12 (6%)	2 (1%)	12	45
38	1d	203/206 (98%)	179 (88%)	20 (10%)	4 (2%)	6	32
39	1e	155/167 (93%)	136 (88%)	11 (7%)	8 (5%)	1	17
40	1f	98/135 (73%)	87 (89%)	6 (6%)	5 (5%)	1	17
41	1g	149/179 (83%)	129 (87%)	15 (10%)	5 (3%)	3	24
42	1h	127/130 (98%)	115 (91%)	11 (9%)	1 (1%)	16	50
43	1i	125/130 (96%)	107 (86%)	12 (10%)	6 (5%)	2	18
44	1j	96/103 (93%)	80 (83%)	10 (10%)	6 (6%)	1	15
45	1k	114/129 (88%)	98 (86%)	14 (12%)	2 (2%)	6	34
46	1l	121/124 (98%)	100 (83%)	14 (12%)	7 (6%)	1	16
47	1m	112/118 (95%)	102 (91%)	7 (6%)	3 (3%)	4	28
48	1n	98/101 (97%)	83 (85%)	9 (9%)	6 (6%)	1	15
49	1o	86/89 (97%)	76 (88%)	6 (7%)	4 (5%)	2	19
50	1p	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	1q	78/84 (93%)	65 (83%)	10 (13%)	3 (4%)	2 21
52	1r	63/75 (84%)	57 (90%)	3 (5%)	3 (5%)	2 18
53	1s	77/92 (84%)	70 (91%)	6 (8%)	1 (1%)	9 40
54	1t	83/87 (95%)	78 (94%)	5 (6%)	0	100 100
55	1u	63/71 (89%)	45 (71%)	11 (18%)	7 (11%)	0 6
57	1w	637/639 (100%)	548 (86%)	58 (9%)	31 (5%)	1 18
All	All	6550/6980 (94%)	5803 (89%)	577 (9%)	170 (3%)	6 28

5 of 170 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	18	GLU
7	1H	108	PHE
11	1K	22	PRO
11	1K	92	PRO
12	1N	81	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	216/218 (99%)	216 (100%)	0	100 100
4	1E	164/164 (100%)	164 (100%)	0	100 100
5	1F	165/165 (100%)	164 (99%)	1 (1%)	78 80
6	1G	148/150 (99%)	148 (100%)	0	100 100
7	1H	137/138 (99%)	137 (100%)	0	100 100
9	1I	114/114 (100%)	114 (100%)	0	100 100
10	1J	100/123 (81%)	100 (100%)	0	100 100
11	1K	109/110 (99%)	109 (100%)	0	100 100
12	1N	116/116 (100%)	116 (100%)	0	100 100
13	1O	103/104 (99%)	101 (98%)	2 (2%)	50 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	1P	102/103 (99%)	102 (100%)	0	100	100
15	1Q	109/109 (100%)	109 (100%)	0	100	100
16	1R	100/103 (97%)	100 (100%)	0	100	100
17	1S	86/87 (99%)	86 (100%)	0	100	100
18	1T	99/100 (99%)	98 (99%)	1 (1%)	68	75
19	1U	89/90 (99%)	89 (100%)	0	100	100
20	1V	84/84 (100%)	84 (100%)	0	100	100
21	1W	93/93 (100%)	92 (99%)	1 (1%)	65	74
22	1X	80/84 (95%)	80 (100%)	0	100	100
23	1Y	83/85 (98%)	83 (100%)	0	100	100
24	1Z	78/78 (100%)	78 (100%)	0	100	100
25	10	57/63 (90%)	57 (100%)	0	100	100
26	11	67/68 (98%)	67 (100%)	0	100	100
27	12	55/55 (100%)	55 (100%)	0	100	100
28	13	48/49 (98%)	48 (100%)	0	100	100
29	14	59/62 (95%)	59 (100%)	0	100	100
30	15	47/48 (98%)	47 (100%)	0	100	100
31	16	45/49 (92%)	45 (100%)	0	100	100
32	17	38/38 (100%)	38 (100%)	0	100	100
33	18	51/52 (98%)	50 (98%)	1 (2%)	48	65
34	19	34/34 (100%)	34 (100%)	0	100	100
36	1b	180/199 (90%)	180 (100%)	0	100	100
37	1c	170/190 (90%)	169 (99%)	1 (1%)	78	80
38	1d	172/173 (99%)	172 (100%)	0	100	100
39	1e	114/126 (90%)	114 (100%)	0	100	100
40	1f	87/116 (75%)	87 (100%)	0	100	100
41	1g	124/147 (84%)	124 (100%)	0	100	100
42	1h	104/105 (99%)	104 (100%)	0	100	100
43	1i	105/107 (98%)	105 (100%)	0	100	100
44	1j	86/90 (96%)	86 (100%)	0	100	100
45	1k	89/99 (90%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	1l	103/104 (99%)	103 (100%)	0	100 100
47	1m	92/96 (96%)	92 (100%)	0	100 100
48	1n	79/84 (94%)	77 (98%)	2 (2%)	42 62
49	1o	76/77 (99%)	76 (100%)	0	100 100
50	1p	65/65 (100%)	65 (100%)	0	100 100
51	1q	74/78 (95%)	74 (100%)	0	100 100
52	1r	48/65 (74%)	48 (100%)	0	100 100
53	1s	70/79 (89%)	70 (100%)	0	100 100
54	1t	65/66 (98%)	65 (100%)	0	100 100
55	1u	44/61 (72%)	44 (100%)	0	100 100
57	1w	6/576 (1%)	6 (100%)	0	100 100
All	All	4829/5639 (86%)	4820 (100%)	9 (0%)	85 87

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

Mol	Chain	Res	Type
48	1n	34	VAL
48	1n	35	ASN
18	1T	47	ILE
21	1W	88	ARG
33	18	61	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
41	1g	141	HIS
51	1q	44	HIS
42	1h	3	GLN
49	1o	45	HIS
53	1s	68	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2898/2904 (99%)	427 (14%)	33 (1%)
2	1B	119/120 (99%)	14 (11%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	1a	1538/1539 (99%)	181 (11%)	0
56	1v	8/60 (13%)	0	0
58	1x	70/77 (90%)	5 (7%)	0
All	All	4633/4700 (98%)	627 (13%)	35 (0%)

5 of 627 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	A
1	1A	12	U
1	1A	27	G
1	1A	34	U
1	1A	35	G

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2391	G
1	1A	2566	A
1	1A	2808	G
1	1A	1020	A
1	1A	859	G

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

39 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	$\#\|Z\| > 2$
35	2MG	1a	1516	35	23,26,27	1.28	2 (8%)	33,38,41	2.04	6 (18%)
1	PSU	1A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.14	3 (14%)
35	7MG	1a	527	35	23,26,27	1.55	3 (13%)	27,39,42	2.63	8 (29%)
1	PSU	1A	746	1	18,21,22	1.48	3 (16%)	21,30,33	2.11	4 (19%)
35	MA6	1a	1519	35	23,26,27	1.52	4 (17%)	33,38,41	2.40	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	1MG	1A	745	1	23,26,27	1.25	2 (8%)	33,39,42	1.82	5 (15%)
1	PSU	1A	2457	1	18,21,22	1.37	2 (11%)	21,30,33	2.29	4 (19%)
1	PSU	1A	2605	1	18,21,22	1.40	2 (11%)	21,30,33	2.13	3 (14%)
58	PSU	1x	55	58	18,21,22	1.39	2 (11%)	21,30,33	2.10	5 (23%)
1	PSU	1A	955	1	18,21,22	1.42	2 (11%)	21,30,33	2.21	3 (14%)
35	2MG	1a	1207	35	23,26,27	1.25	4 (17%)	33,38,41	2.18	5 (15%)
1	5MU	1A	747	1	19,22,23	1.50	5 (26%)	27,32,35	2.51	8 (29%)
1	PSU	1A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.21	3 (14%)
1	6MZ	1A	1618	1	22,25,26	1.48	5 (22%)	29,36,39	2.17	10 (34%)
35	5MC	1a	1407	35	19,22,23	1.54	3 (15%)	26,32,35	1.11	2 (7%)
1	5MC	1A	1962	1	19,22,23	1.65	3 (15%)	26,32,35	1.34	4 (15%)
58	PSU	1x	65	58	18,21,22	1.38	3 (16%)	21,30,33	2.14	4 (19%)
1	OMC	1A	2498	1	19,22,23	0.81	0	25,31,34	0.94	1 (4%)
58	5MU	1x	54	58	19,22,23	1.40	6 (31%)	27,32,35	2.16	8 (29%)
1	PSU	1A	2580	1	18,21,22	1.38	2 (11%)	21,30,33	2.23	3 (14%)
1	PSU	1A	2504	1	18,21,22	1.41	2 (11%)	21,30,33	2.19	4 (19%)
35	2MG	1a	966	35	23,26,27	1.30	4 (17%)	33,38,41	2.09	5 (15%)
35	PSU	1a	516	35	18,21,22	1.40	2 (11%)	21,30,33	2.20	3 (14%)
35	MA6	1a	1518	35	23,26,27	1.57	4 (17%)	33,38,41	2.42	12 (36%)
1	H2U	1A	2449	1	18,21,22	1.12	2 (11%)	19,30,33	1.37	2 (10%)
1	2MA	1A	2503	1	22,25,26	1.55	5 (22%)	32,37,40	2.49	9 (28%)
1	G7M	1A	2069	1	23,26,27	1.58	3 (13%)	34,39,42	1.85	6 (17%)
35	5MC	1a	967	35	19,22,23	1.77	3 (15%)	26,32,35	1.40	4 (15%)
1	2MG	1A	2445	1	23,26,27	1.23	3 (13%)	33,38,41	2.14	7 (21%)
1	OMG	1A	2251	58,1	23,26,27	1.17	3 (13%)	32,38,41	2.00	6 (18%)
35	4OC	1a	1402	35	20,23,24	0.88	0	25,32,35	1.46	4 (16%)
1	OMU	1A	2552	1	19,22,23	1.28	3 (15%)	25,31,34	1.92	6 (24%)
1	3TD	1A	1915	1	19,22,23	1.51	5 (26%)	23,32,35	2.30	6 (26%)
1	2MG	1A	1835	1	23,26,27	1.29	4 (17%)	33,38,41	2.16	5 (15%)
35	UR3	1a	1498	35	19,22,23	1.07	2 (10%)	26,32,35	1.82	6 (23%)
1	PSU	1A	2604	1	18,21,22	1.40	2 (11%)	21,30,33	2.19	3 (14%)
1	6MZ	1A	2030	1	22,25,26	1.55	4 (18%)	29,36,39	2.39	10 (34%)
58	7MG	1x	46	58	23,26,27	1.29	2 (8%)	27,39,42	2.77	7 (25%)
1	5MU	1A	1939	1	19,22,23	1.46	6 (31%)	27,32,35	2.22	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	2MG	1a	1516	35	-	0/9/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
35	7MG	1a	527	35	-	3/7/37/38	0/3/3/3
1	PSU	1A	746	1	-	2/7/25/26	0/2/2/2
35	MA6	1a	1519	35	-	1/11/29/30	0/3/3/3
1	1MG	1A	745	1	-	0/7/25/26	0/3/3/3
1	PSU	1A	2457	1	-	2/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
58	PSU	1x	55	58	-	2/7/25/26	0/2/2/2
1	PSU	1A	955	1	-	0/7/25/26	0/2/2/2
35	2MG	1a	1207	35	-	2/9/27/28	0/3/3/3
1	5MU	1A	747	1	-	4/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	6MZ	1A	1618	1	-	2/9/27/28	0/3/3/3
35	5MC	1a	1407	35	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	4/7/25/26	0/2/2/2
58	PSU	1x	65	58	-	0/7/25/26	0/2/2/2
1	OMC	1A	2498	1	-	0/9/27/28	0/2/2/2
58	5MU	1x	54	58	-	0/7/25/26	0/2/2/2
1	PSU	1A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2504	1	-	2/7/25/26	0/2/2/2
35	2MG	1a	966	35	-	3/9/27/28	0/3/3/3
35	PSU	1a	516	35	-	0/7/25/26	0/2/2/2
35	MA6	1a	1518	35	-	2/11/29/30	0/3/3/3
1	H2U	1A	2449	1	-	0/7/38/39	0/2/2/2
1	2MA	1A	2503	1	-	3/7/25/26	0/3/3/3
1	G7M	1A	2069	1	-	2/7/25/26	0/3/3/3
35	5MC	1a	967	35	-	0/7/25/26	0/2/2/2
1	2MG	1A	2445	1	-	1/9/27/28	0/3/3/3
1	OMG	1A	2251	58,1	-	4/9/27/28	0/3/3/3
35	4OC	1a	1402	35	-	3/9/29/30	0/2/2/2
1	OMU	1A	2552	1	-	3/9/27/28	0/2/2/2
1	3TD	1A	1915	1	-	3/7/25/26	0/2/2/2
1	2MG	1A	1835	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	UR3	1a	1498	35	-	2/7/25/26	0/2/2/2
1	PSU	1A	2604	1	-	0/7/25/26	0/2/2/2
1	6MZ	1A	2030	1	-	2/9/27/28	0/3/3/3
58	7MG	1x	46	58	-	2/7/37/38	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	1a	967	5MC	C5-C4	6.47	1.49	1.44
1	1A	1962	5MC	C5-C4	6.04	1.48	1.44
35	1a	1407	5MC	C5-C4	5.55	1.48	1.44
1	1A	2069	G7M	C5-N7	-5.10	1.33	1.39
1	1A	2030	6MZ	C5-C4	5.00	1.48	1.39

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1x	46	7MG	N9-C4-N3	9.74	139.74	125.46
1	1A	2503	2MA	C5-C4-N3	-8.41	118.32	127.18
35	1a	527	7MG	N9-C4-N3	8.39	137.76	125.46
1	1A	1915	3TD	N1-C2-N3	8.09	122.01	116.13
1	1A	2457	PSU	N1-C2-N3	6.96	122.51	115.17

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	746	PSU	O4'-C4'-C5'-O5'
1	1A	747	5MU	C2'-C1'-N1-C2
1	1A	747	5MU	C2'-C1'-N1-C6
1	1A	1618	6MZ	C5-C6-N6-C9
1	1A	1618	6MZ	N1-C6-N6-C9

There are no ring outliers.

24 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	1a	1516	2MG	2	0
1	1A	1917	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	1a	527	7MG	1	0
35	1a	1519	MA6	1	0
1	1A	745	1MG	1	0
1	1A	955	PSU	1	0
1	1A	747	5MU	1	0
1	1A	1618	6MZ	1	0
35	1a	1407	5MC	1	0
58	1x	65	PSU	4	0
1	1A	2498	OMC	1	0
35	1a	1518	MA6	3	0
1	1A	2503	2MA	2	0
1	1A	2069	G7M	2	0
1	1A	2445	2MG	2	0
1	1A	2251	OMG	2	0
35	1a	1402	4OC	1	0
1	1A	1915	3TD	1	0
1	1A	1835	2MG	1	0
35	1a	1498	UR3	3	0
1	1A	2604	PSU	1	0
1	1A	2030	6MZ	2	0
58	1x	46	7MG	1	0
1	1A	1939	5MU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
59	EVN	1A	3001	1	117,123,123	1.97	20 (17%)	155,191,191	1.89	34 (21%)

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	EVN	1A	3001	1	-	23/50/234/234	1/13/13/13

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	3001	EVN	ODS-NDQ	10.70	1.45	1.22
59	1A	3001	EVN	CDN-CAC	-6.77	1.38	1.51
59	1A	3001	EVN	CEG-CDI	-6.09	1.39	1.51
59	1A	3001	EVN	OCW-CCQ	5.84	1.45	1.40
59	1A	3001	EVN	CDD-CDB	-4.60	1.39	1.50

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	1A	3001	EVN	OCX-CCS-CCT	-9.11	99.01	106.63
59	1A	3001	EVN	OCZ-CCT-CCS	-6.12	98.47	106.41
59	1A	3001	EVN	CAE-CAF-CLAG	5.99	128.17	118.95
59	1A	3001	EVN	OCR-CCL-CCK	-5.49	94.64	103.54
59	1A	3001	EVN	CAF-CAA-CAB	5.05	123.19	117.78

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	3001	EVN	C2-C1-O1-CCI
59	1A	3001	EVN	CAW-CAX-ODT-CDU
59	1A	3001	EVN	OAK-CAJ-OAL-CAM
59	1A	3001	EVN	CAD-CAJ-OAL-CAM
59	1A	3001	EVN	CAF-CAE-ODL-CDM

All (1) ring outliers are listed below:

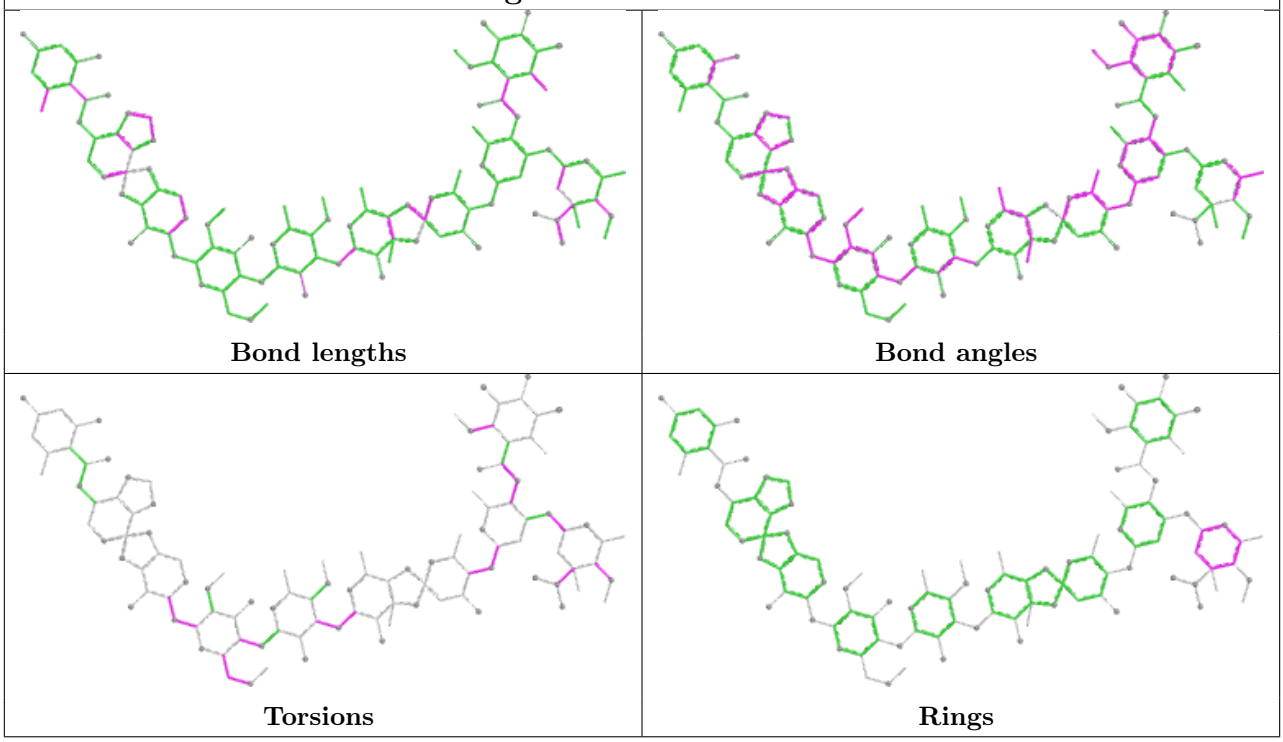
Mol	Chain	Res	Type	Atoms
59	1A	3001	EVN	CAU-CAW-CAX-CAY-CAZ-OAV

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand EVN 1A 3001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

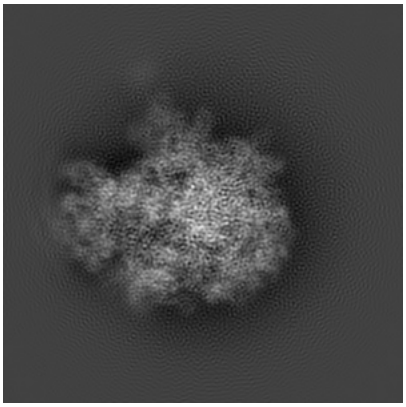
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8238. These allow visual inspection of the internal detail of the map and identification of artifacts.

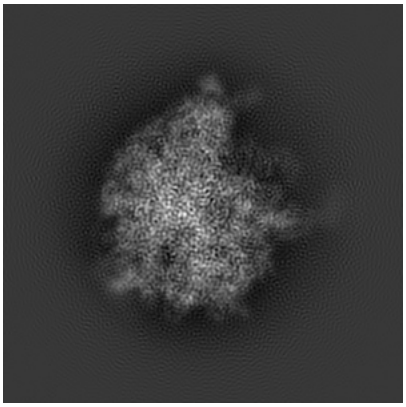
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

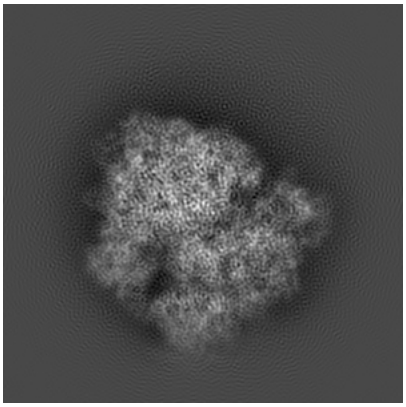
6.1.1 Primary map



X



Y

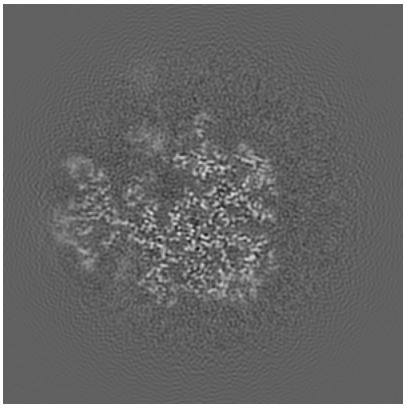


Z

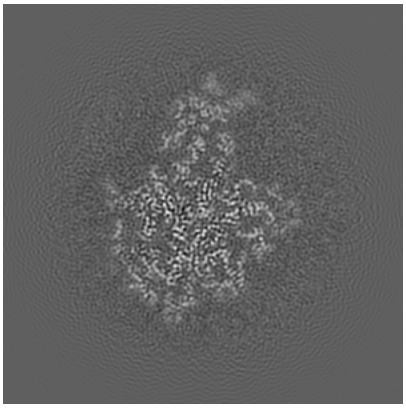
The images above show the map projected in three orthogonal directions.

6.2 Central slices

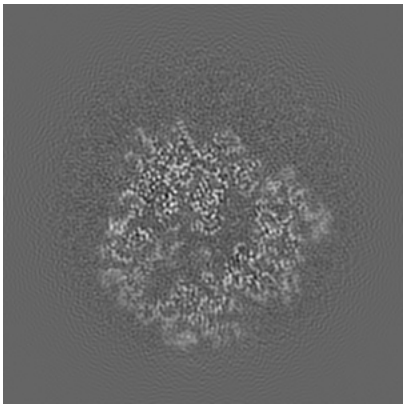
6.2.1 Primary map



X Index: 184



Y Index: 184

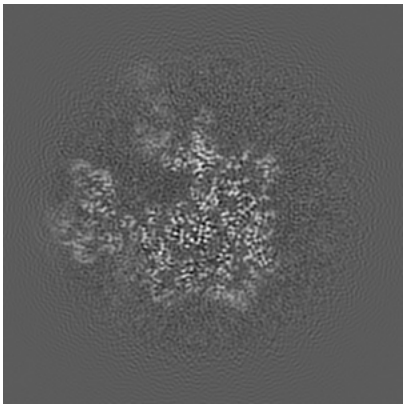


Z Index: 184

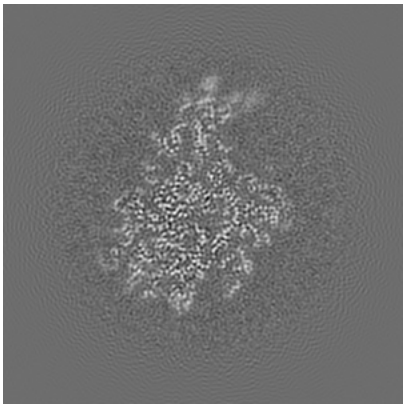
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

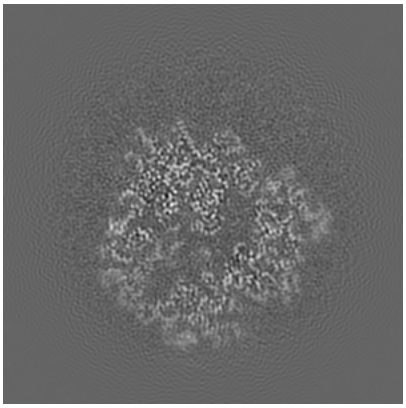
6.3.1 Primary map



X Index: 179



Y Index: 177

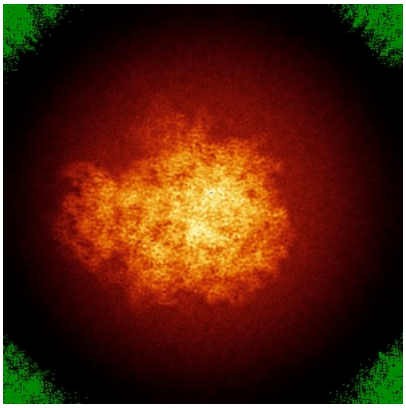


Z Index: 184

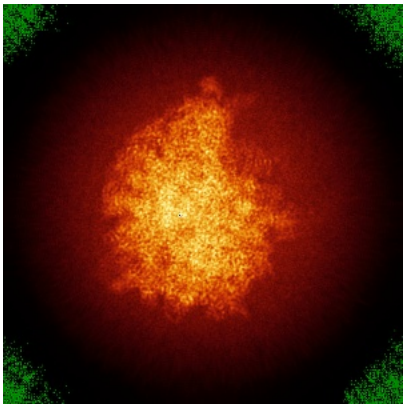
The images above show the largest variance slices of the map in three orthogonal directions.

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

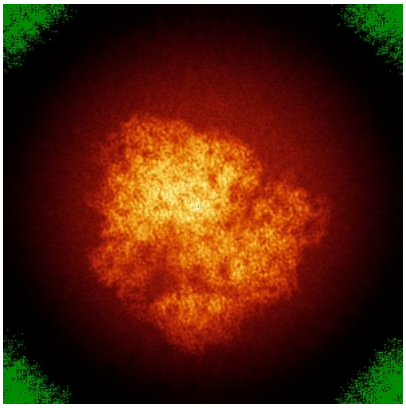
6.4.1 Primary map



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 0.00307. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

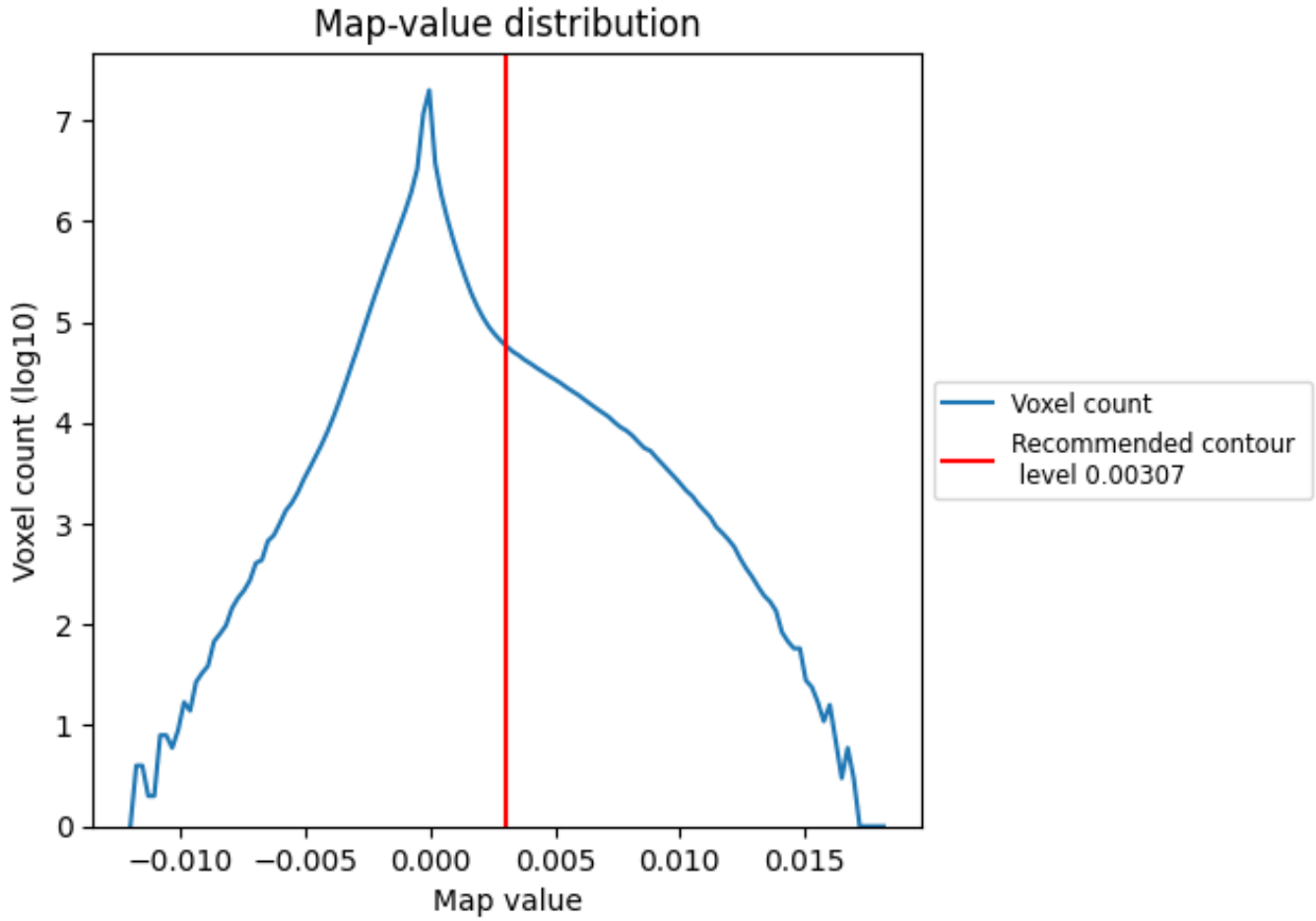
6.6 Mask visualisation (i)

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

7 Map analysis

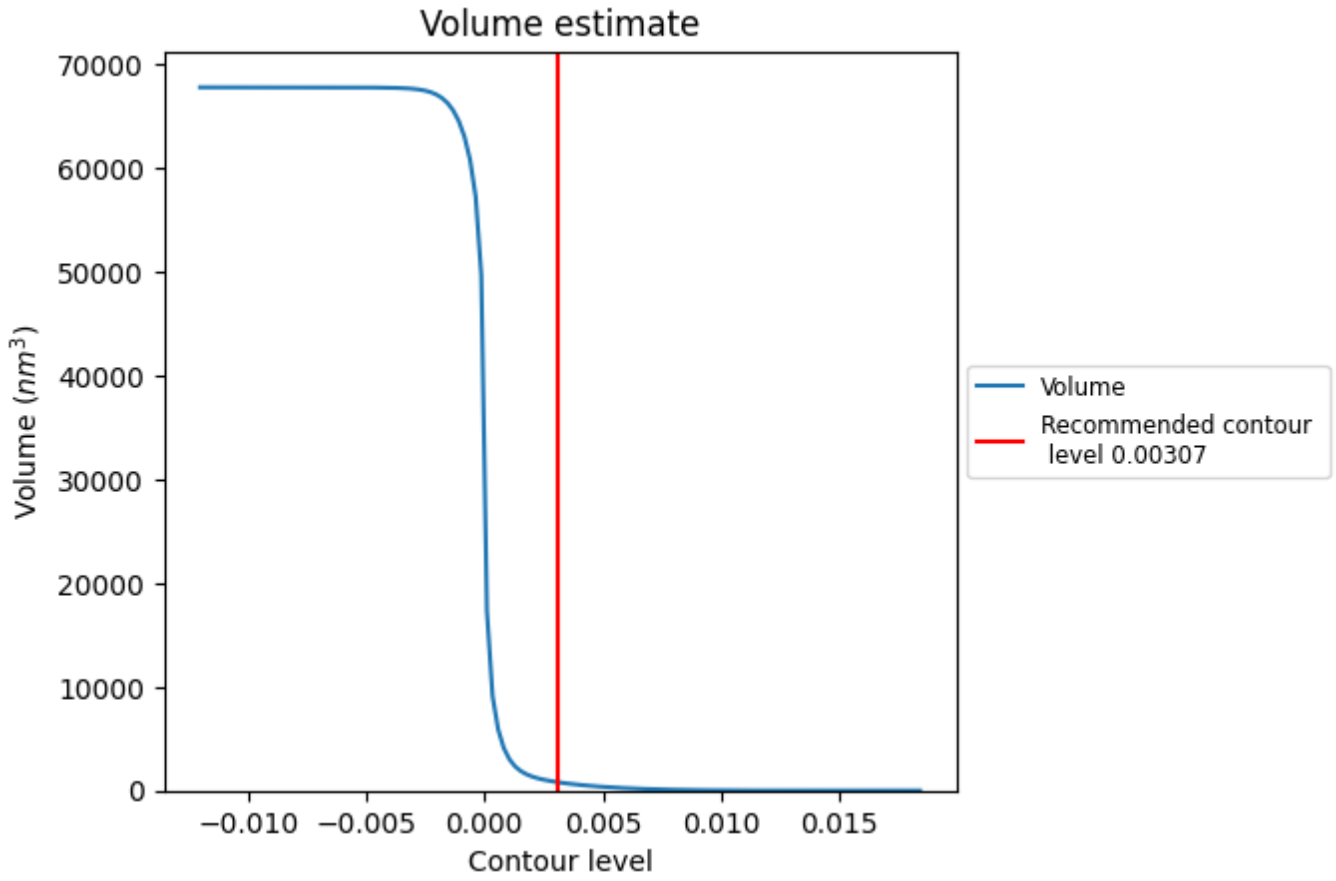
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

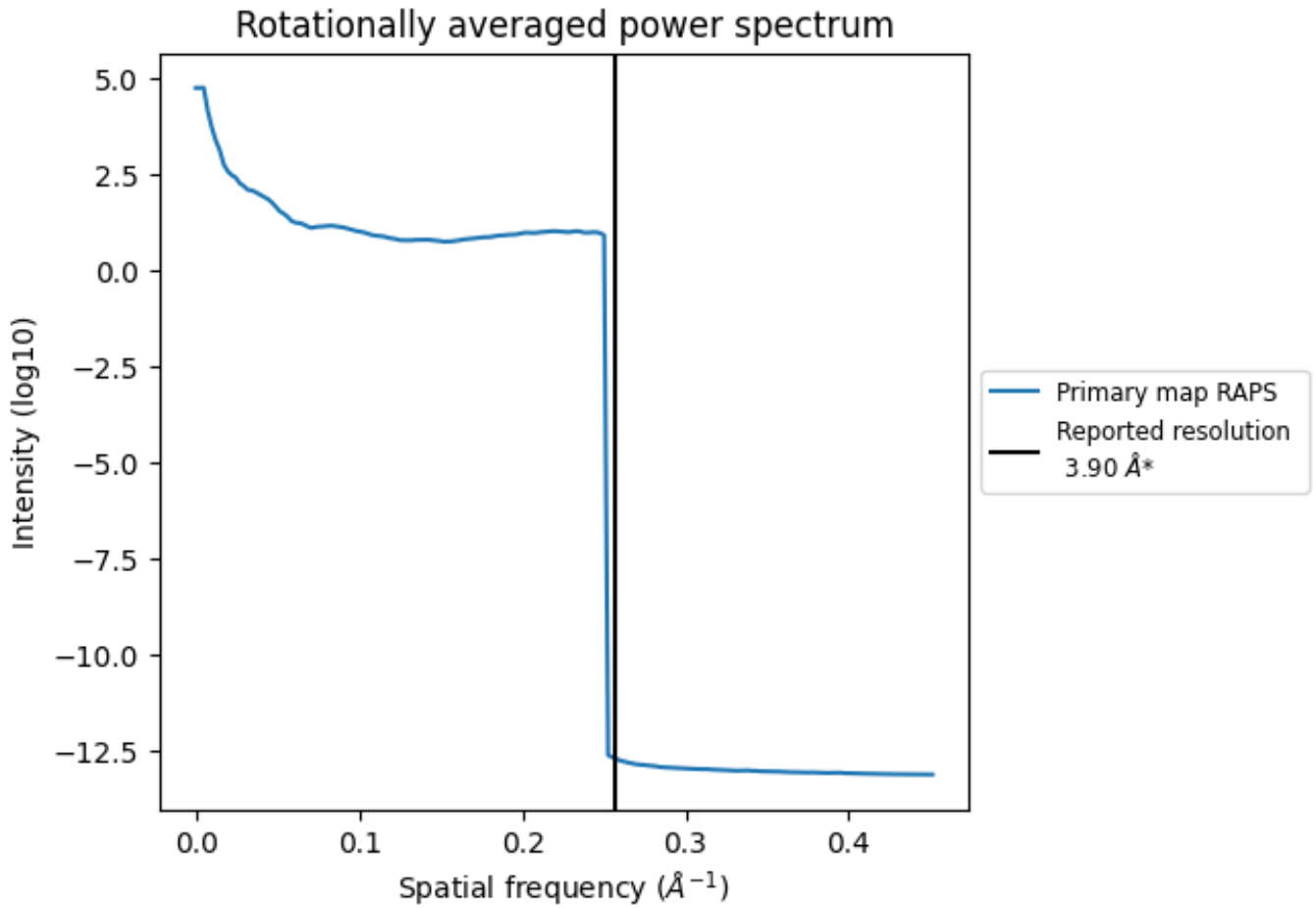
7.2 Volume estimate (i)



The volume at the recommended contour level is 816 nm^3; this corresponds to an approximate mass of 737 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.256 $Å^{-1}$

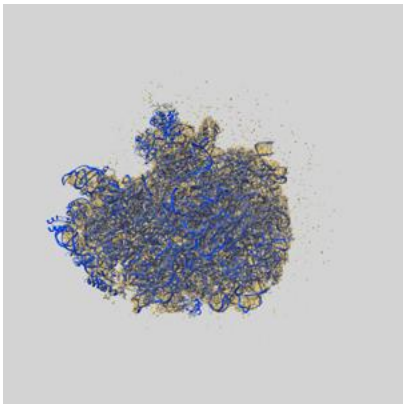
8 Fourier-Shell correlation (i)

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

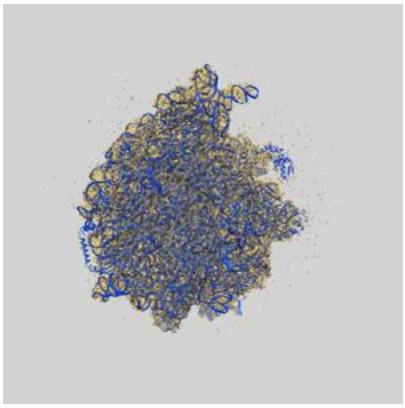
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8238 and PDB model 5KCS. Per-residue inclusion information can be found in section 3 on page 16.

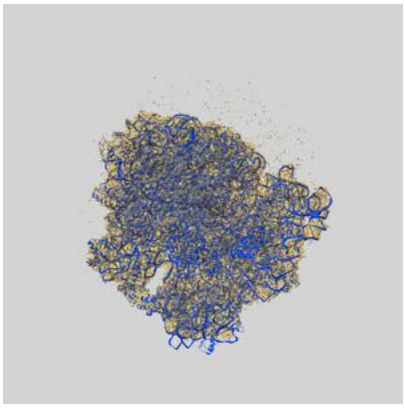
9.1 Map-model overlay



X



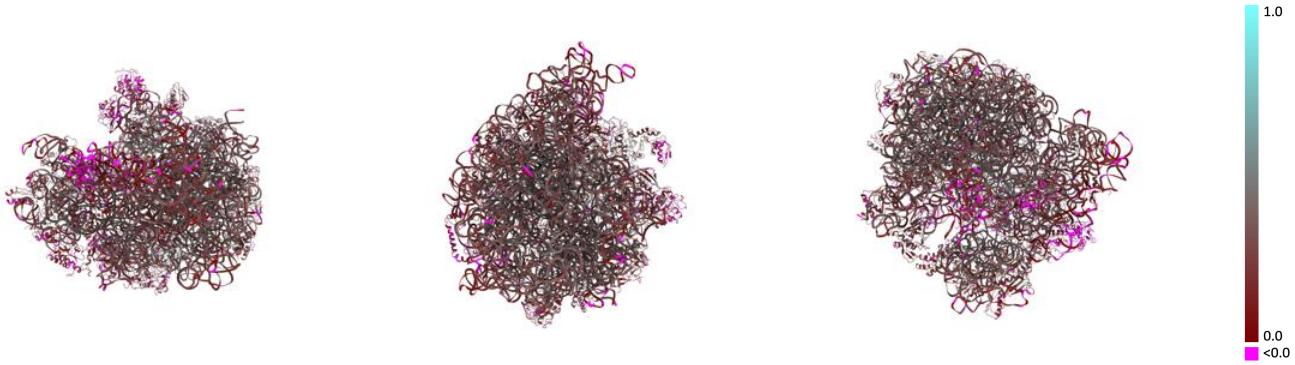
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00307 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

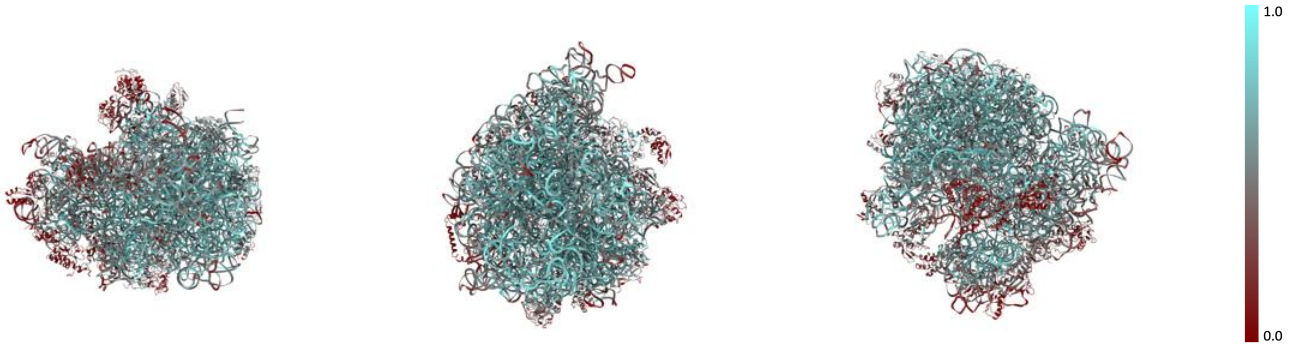
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

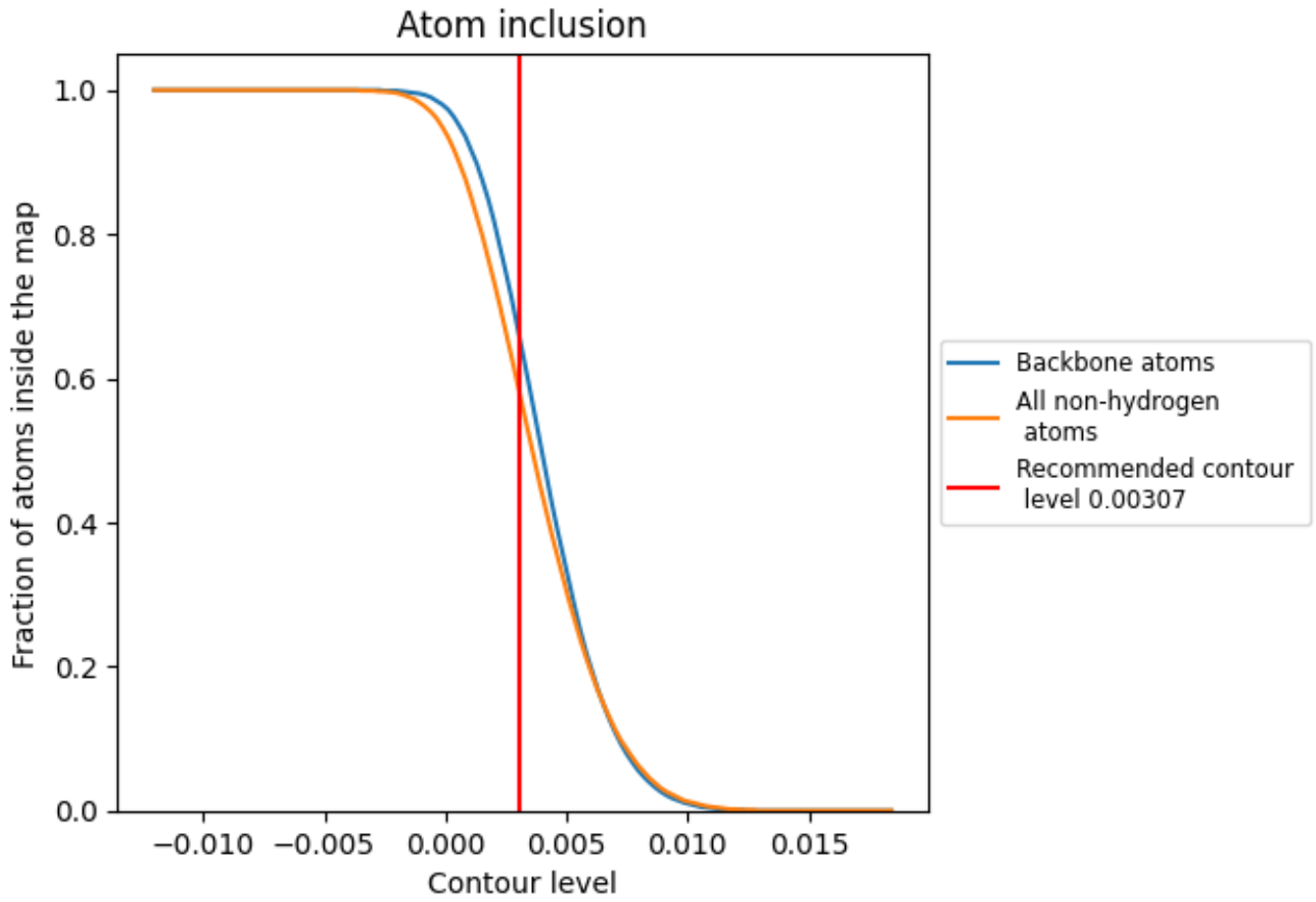
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00307).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 58% 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 (0.00307) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5780	0.2930
10	0.5780	0.3400
11	0.5290	0.3340
12	0.4330	0.2550
13	0.5260	0.3310
14	0.2110	0.1720
15	0.5420	0.3270
16	0.0920	0.1900
17	0.6250	0.3430
18	0.5800	0.3540
19	0.5890	0.3360
1A	0.6810	0.3250
1B	0.6480	0.2900
1D	0.5860	0.3510
1E	0.5360	0.3240
1F	0.4670	0.2970
1G	0.3680	0.2320
1H	0.4030	0.2420
1I	0.0970	0.1240
1J	0.0640	0.0470
1K	0.0760	0.0790
1L	0.0510	0.0670
1N	0.5650	0.3080
1O	0.5170	0.3210
1P	0.4830	0.2900
1Q	0.5860	0.3890
1R	0.5660	0.3360
1S	0.4010	0.2380
1T	0.5100	0.2950
1U	0.6190	0.3520
1V	0.4920	0.2850
1W	0.5480	0.3350
1X	0.4830	0.2990
1Y	0.4200	0.2820
1Z	0.4730	0.2870



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Chain	Atom inclusion	Q-score
1a	0.6150	0.2830
1b	0.1880	0.1630
1c	0.3860	0.2920
1d	0.2750	0.0620
1e	0.4270	0.2330
1f	0.4120	0.2290
1g	0.3210	0.2650
1h	0.4760	0.2870
1i	0.2630	0.2500
1j	0.2180	0.2390
1k	0.3800	0.1990
1l	0.3050	0.0930
1m	0.3770	0.2740
1n	0.4360	0.3030
1o	0.4940	0.2860
1p	0.4240	0.1710
1q	0.4210	0.2330
1r	0.4890	0.3050
1s	0.4410	0.2780
1t	0.4520	0.2520
1u	0.1510	0.1390
1v	0.4640	0.2870
1w	0.5510	0.3290
1x	0.5840	0.3020