Full wwPDB EM Validation Report ⓘ

Jul 11, 2023 – 11:52 AM EDT

PDB ID	:	8FKZ
EMDB ID	:	EMD-29262
Title	:	Human nucleolar pre-60S ribosomal subunit (State G)
Authors	:	Vanden Broeck, A.; Klinge, S.
Deposited on	:	2022-12-21
Resolution	:	3.04 Å(reported)

This is a Full wwPDB EM Validation 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:

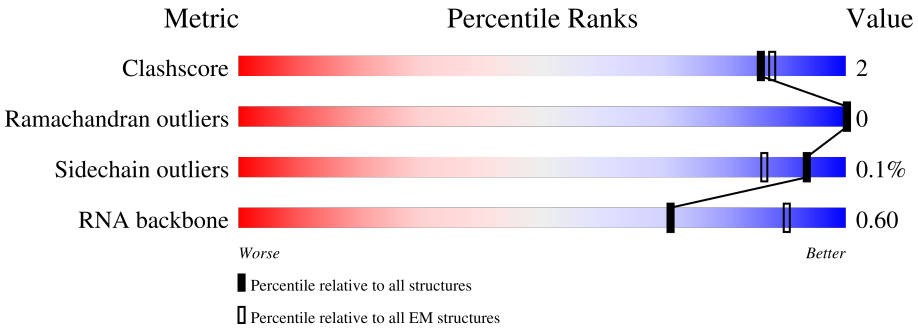
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance

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

The reported resolution of this entry is 3.04 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	BA	165	88% 92% 5%
2	L1	157	7% 81% 17%
3	L2	1167	5% 94%
4	L3	5070	13% 45% 10% 44%
5	L6	211	20% 80% 10% 9%
6	L7	203	6% 93% 6%
7	L8	215	56% 7% 37%

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Mol	Chain	Length	Quality of chain
8	L9	204	81% 9% 10%
9	LA	184	7% 75% 8% 17%
10	LB	188	71% 10% 20%
11	LC	176	7% 92% 8%
12	LD	196	15% 61% 35%
13	LE	160	52% 66% 34%
14	LF	128	8% 79% 20%
15	LG	140	25% 86% 9%
16	LH	156	13% 82% 10% 8%
17	LI	145	10% 83% 10% 8%
18	LJ	136	12% 83% 16%
19	LK	148	11% 69% 27%
20	LL	137	7% 88% 9%
21	LN	403	8% 83% 6% 11%
22	LO	115	18% 77% 6% 17%
23	LP	125	11% 84% 15%
24	LQ	135	91% 5%
25	LR	117	5% 89% 7%
26	LS	123	8% 94% 5%
27	LT	110	97%
28	LU	105	33% 92% 5%
29	LW	97	72% 7% 21%
30	LX	92	34% 77% 18%
31	LY	70	33% 84% 14%
32	LZ	51	86% 12%

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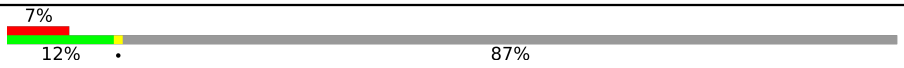
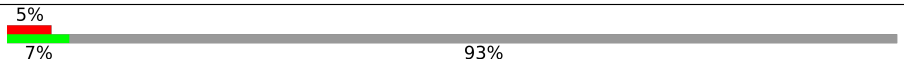
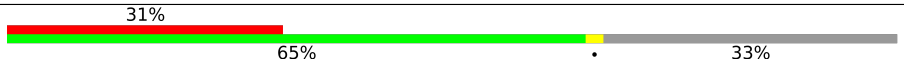
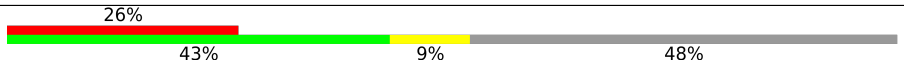
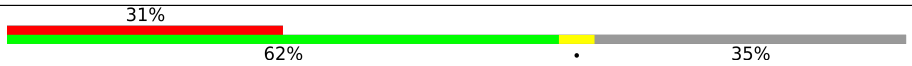
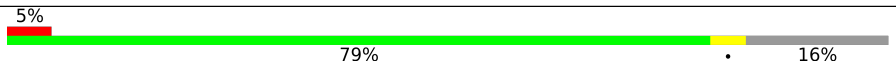
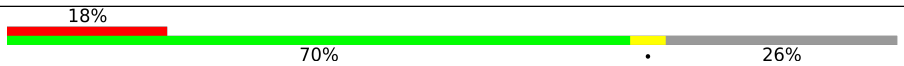
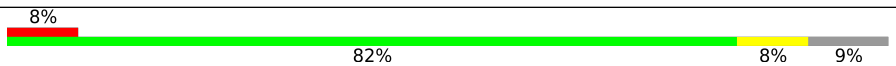
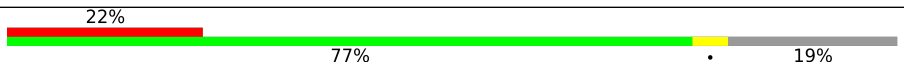
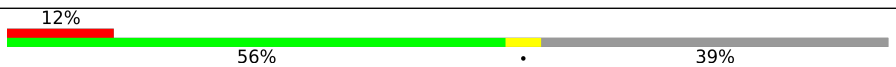
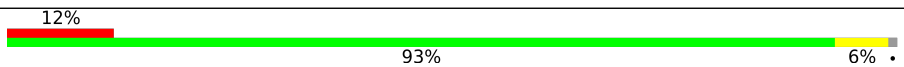
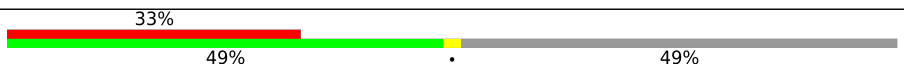
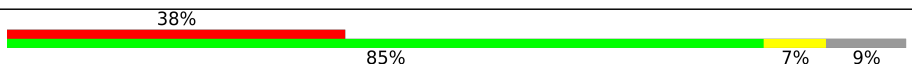
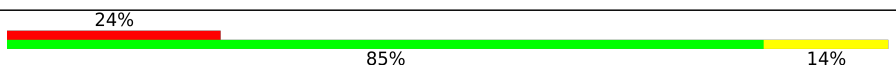
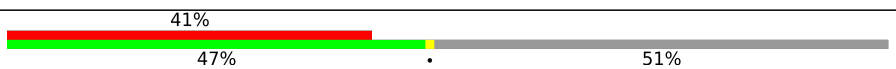
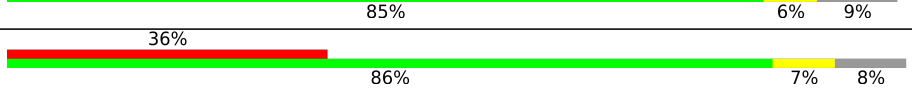
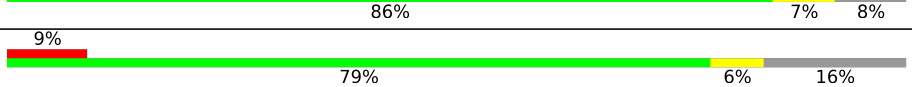
Mol	Chain	Length	Quality of chain
33	NB	549	
34	NC	731	
35	NF	260	
36	NK	129	
37	NL	478	
38	SA	427	
39	SC	288	
40	SD	248	
41	SE	266	
42	SF	257	
43	SG	192	
44	SH	293	
45	SI	255	
46	SK	245	
47	SL	490	
48	SM	588	
49	SQ	239	
50	SR	634	
51	SV	163	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 130011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BA	160	954	570	188	193	3	0	0

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L1	154	3277	1462	581	1080	154	0	0

- Molecule 3 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L2	68	1445	643	258	476	68	0	0

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L3	2833	60779	27048	11149	19749	2833	0	0

- Molecule 5 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L6	191	1539	961	318	257	3	0	0

- Molecule 6 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L7	201	1650	1063	321	261	5	0	0

- Molecule 7 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L8	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 8 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L9	183	Total	C	N	O	S	0	0
			1546	974	325	243	4		

- Molecule 9 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LA	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 10 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LB	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 11 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LC	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 12 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LD	127	Total	C	N	O	S	0	0
			1078	681	224	167	6		

- Molecule 13 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	LE	106	Total	C	N	O	0	0
			690	422	134	134		

- Molecule 14 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LF	103	Total	C	N	O	S	0	0
			842	538	148	154	2		

- Molecule 15 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	127	Total	C	N	O	S	0	0
			934	589	172	168	5		

- Molecule 16 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	143	Total	C	N	O	S	0	0
			1156	740	220	195	1		

- Molecule 17 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 18 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LJ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 19 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LK	108	Total	C	N	O	S	0	0
			852	542	166	141	3		

- Molecule 20 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 21 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LN	358	Total	C	N	O	S	0	0
			2877	1830	528	506	13		

- Molecule 22 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LO	95	Total	C	N	O	S	0	0
			738	468	131	133	6		

- Molecule 23 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LP	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 24 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LQ	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 25 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LR	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 26 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LS	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 27 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LT	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 28 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LU	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 29 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LW	77	Total	C	N	O	S	0	0
			642	395	144	98	5		

- Molecule 30 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LX	75	Total	C	N	O	S	0	0
			585	367	110	101	7		

- Molecule 31 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LY	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 32 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LZ	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 33 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	NB	71	Total	C	N	O	S	0	0
			603	376	125	99	3		

- Molecule 34 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	NC	54	Total	C	N	O	0	0
			350	216	67	67		

- Molecule 35 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	NF	175	Total	C	N	O	S	0	0
			1136	694	233	206	3		

- Molecule 36 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NK	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 37 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NL	312	Total	C	N	O	S	0	0
			2574	1601	506	465	2		

- Molecule 38 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SA	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 39 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SC	214	Total	C	N	O	S	0	0
			1684	1082	321	277	4		

- Molecule 40 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SD	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 41 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SE	215	Total	C	N	O	S	0	0
			1741	1108	336	293	4		

- Molecule 42 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SF	156	Total	C	N	O	S	0	0
			1184	746	228	206	4		

- Molecule 43 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SG	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 44 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SH	150	Total	C	N	O	S	0	0
			1120	716	198	203	3		

- Molecule 45 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SI	233	Total	C	N	O	S	0	0
			1919	1239	361	315	4		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SK	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 47 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SL	238	Total	C	N	O	S	0	0
			1520	945	287	286	2		

- Molecule 48 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SM	399	Total	C	N	O	S	0	0
			3278	2120	576	571	11		

- Molecule 49 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SQ	217	Total	C	N	O	S	0	0
			1771	1129	311	320	11		

- Molecule 50 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SR	586	Total	C	N	O	S	0	0
			4808	3031	868	883	26		

- Molecule 51 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SV	137	Total	C	N	O	S	0	0
			1171	745	227	189	10		

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	L1	5	Total	Mg	0
			5	5	
52	L3	50	Total	Mg	0
			50	50	
52	L9	1	Total	Mg	0
			1	1	
52	LQ	1	Total	Mg	0
			1	1	
52	LR	1	Total	Mg	0
			1	1	
52	LT	1	Total	Mg	0
			1	1	
52	NF	1	Total	Mg	0
			1	1	
52	SA	3	Total	Mg	0
			3	3	
52	SR	1	Total	Mg	0
			1	1	

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	LR	1	Total	Zn	0
			1	1	

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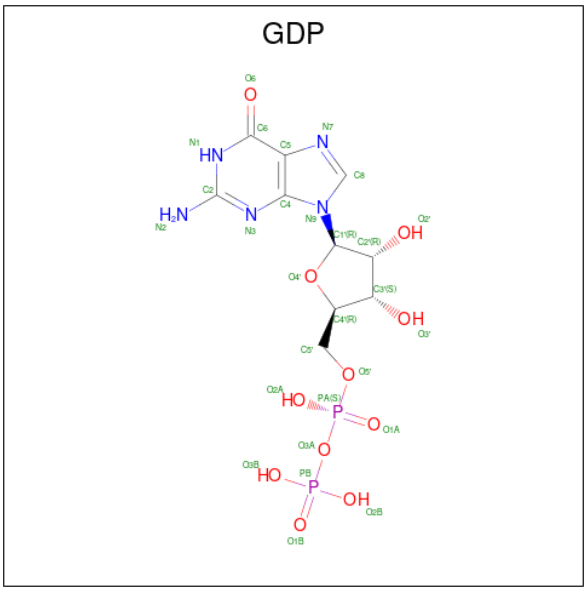
Mol	Chain	Residues	Atoms	AltConf
53	LW	1	Total Zn 1 1	0
53	LX	1	Total Zn 1 1	0
53	SV	1	Total Zn 1 1	0

- Molecule 54 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 55 is POTASSIUM ION (three-letter code: K) (formula: K).

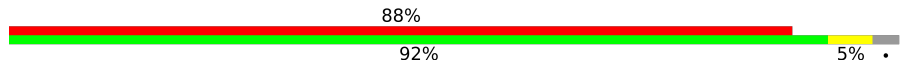
Mol	Chain	Residues	Atoms	AltConf
55	SR	1	Total K 1 1	0

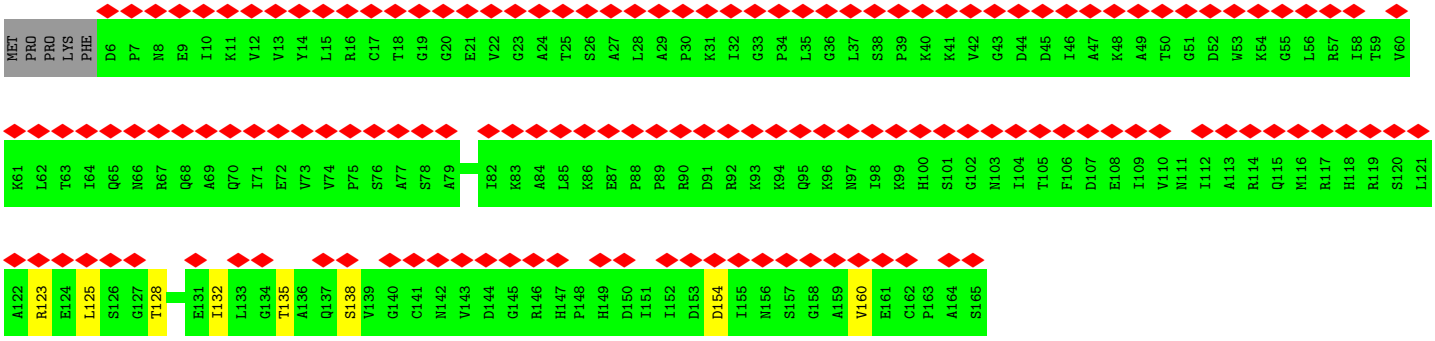
3 Residue-property plots (i)

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: 60S ribosomal protein L12

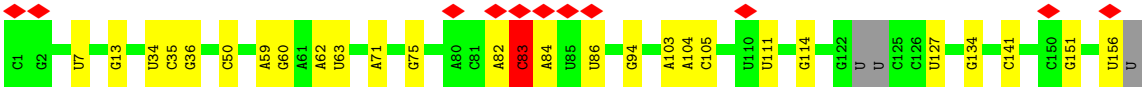
Chain BA:





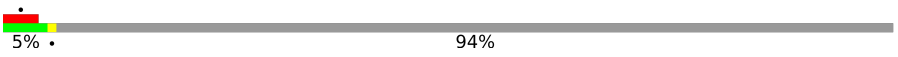
- Molecule 2: 5.8S rRNA

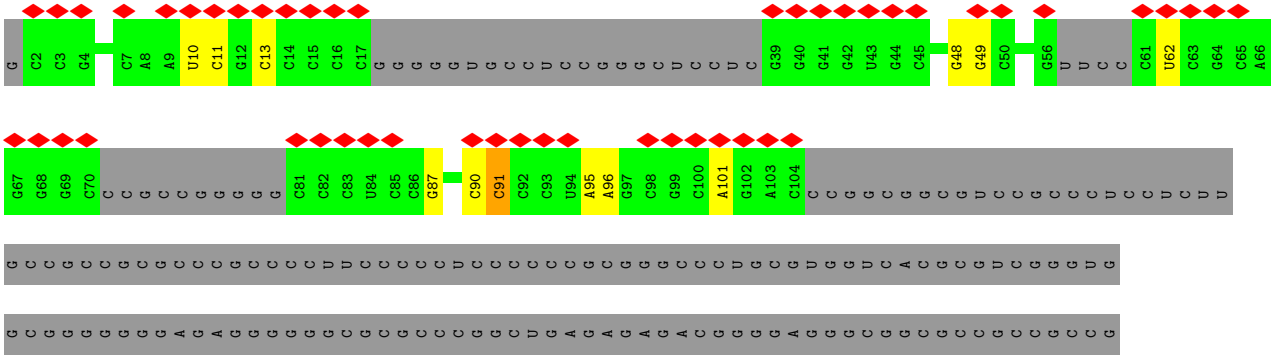
Chain L1:

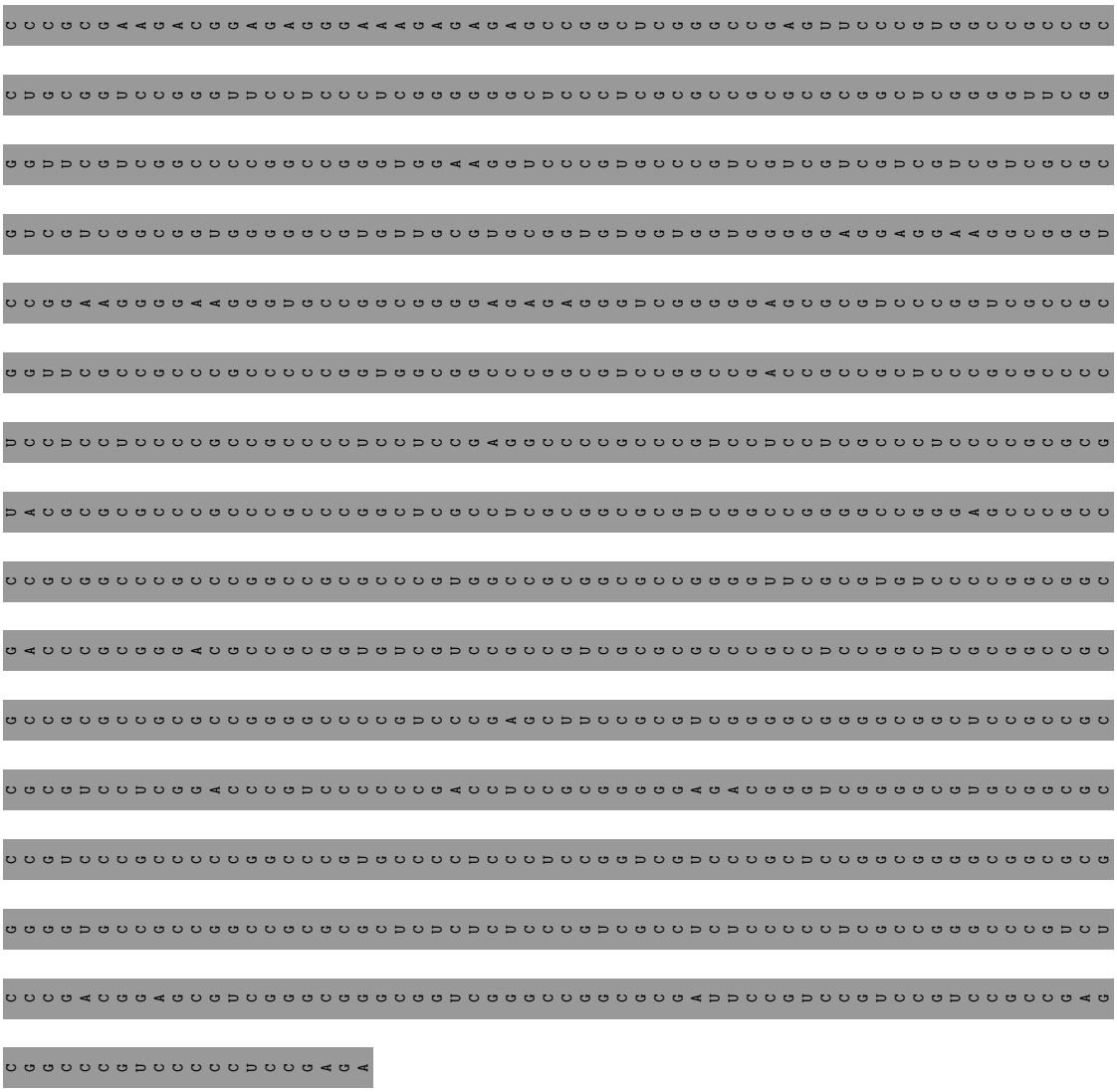


- Molecule 3: ITS2 rRNA

Chain L2:

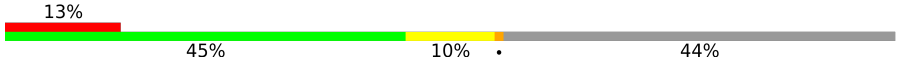


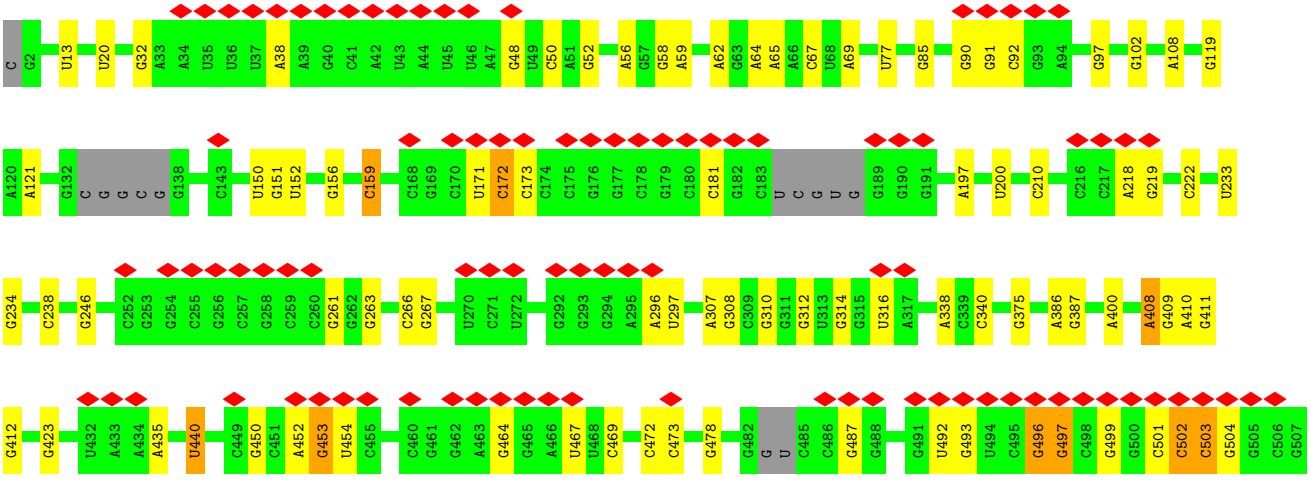


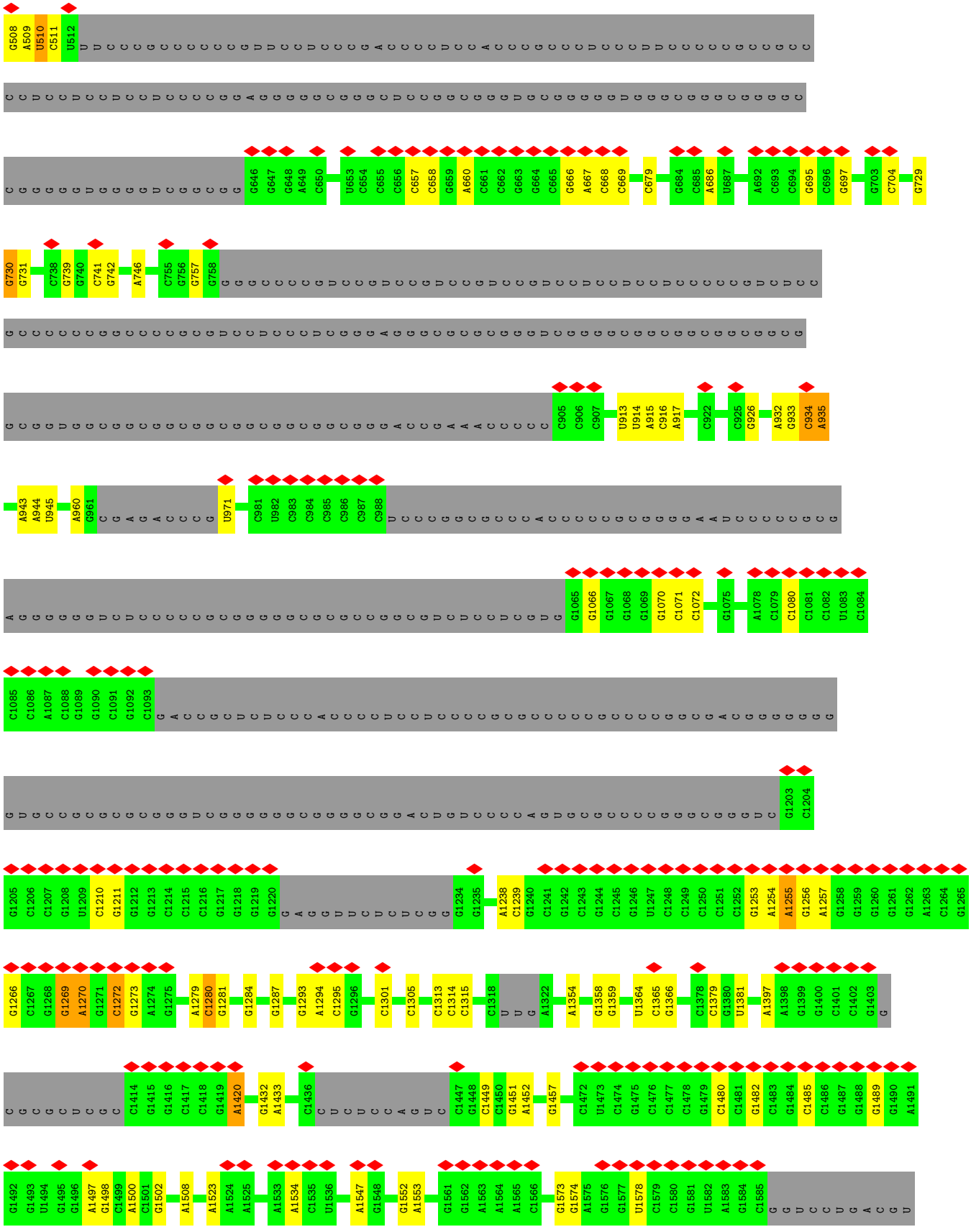


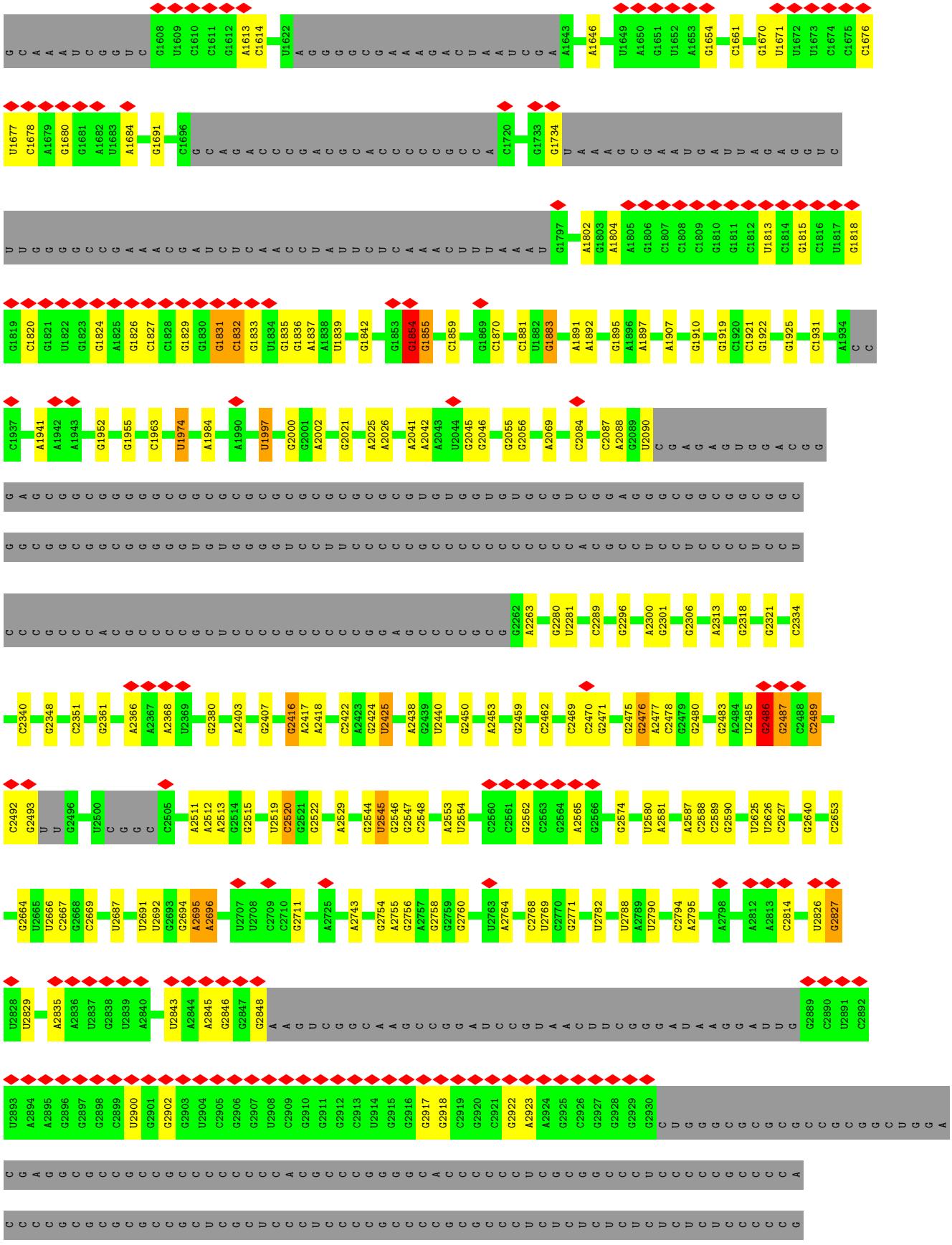
• Molecule 4: 28S rRNA

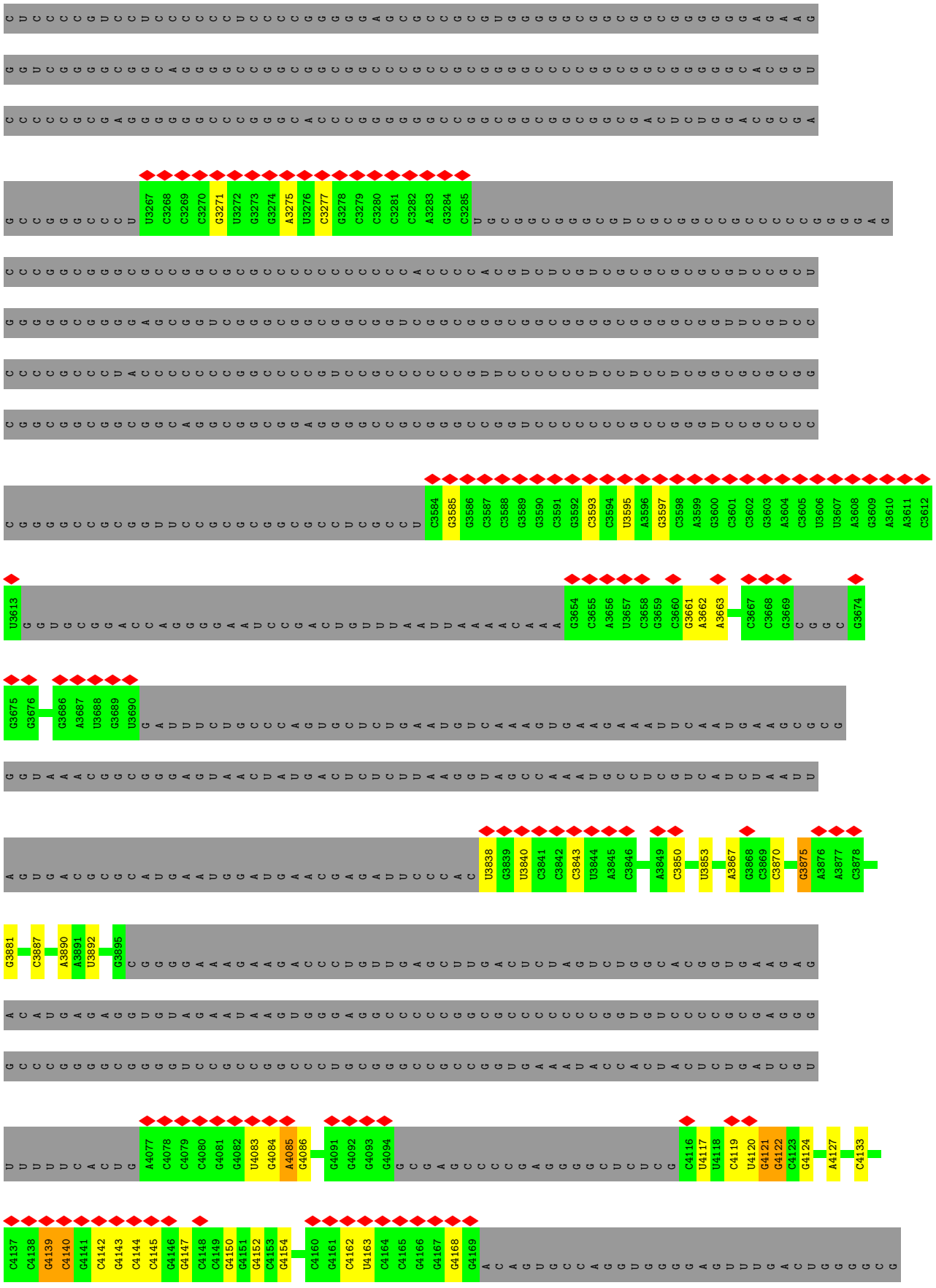
Chain L3:

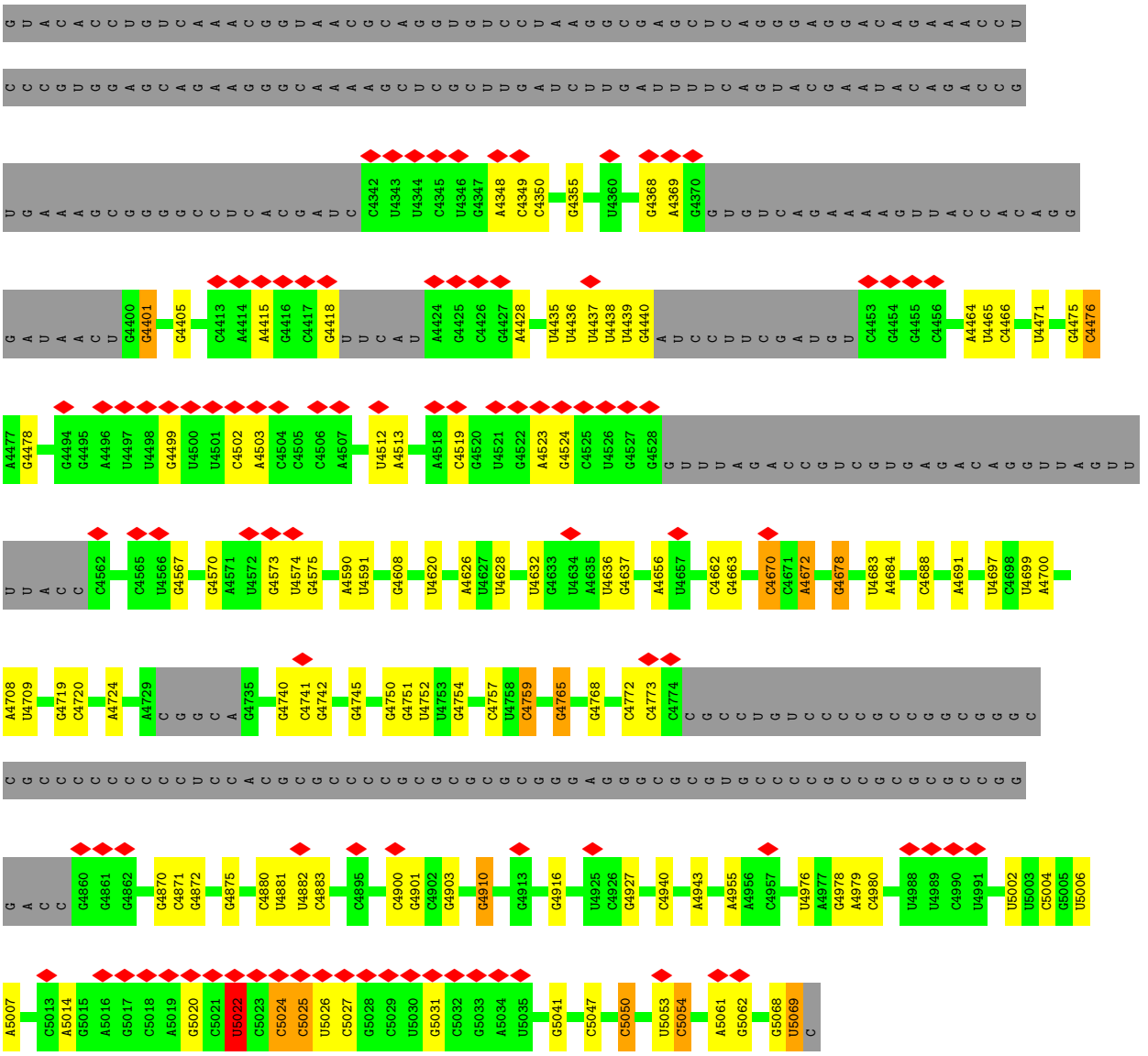






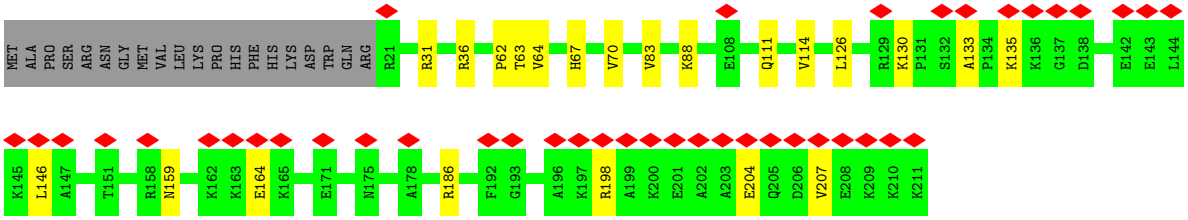






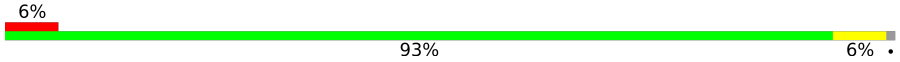
• Molecule 5: 60S ribosomal protein L13

Chain L6:



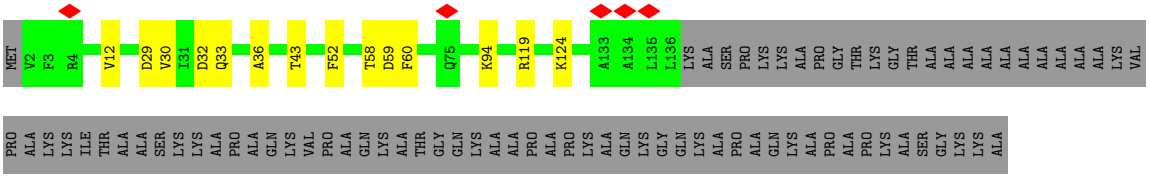
• Molecule 6: 60S ribosomal protein L13a

Chain L7:



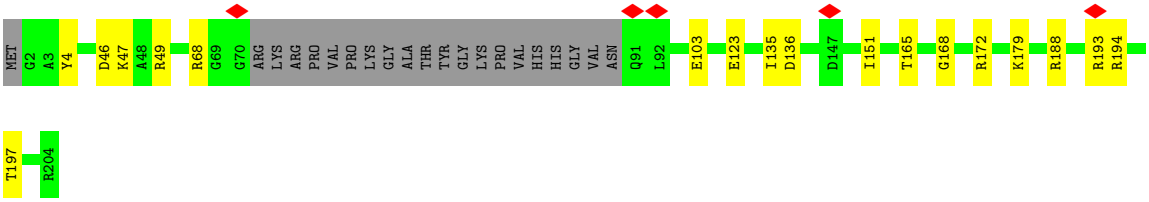
• Molecule 7: 60S ribosomal protein L14

Chain L8:



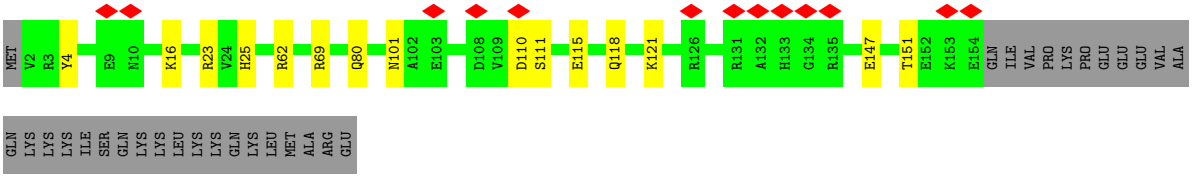
• Molecule 8: 60S ribosomal protein L15

Chain L9:



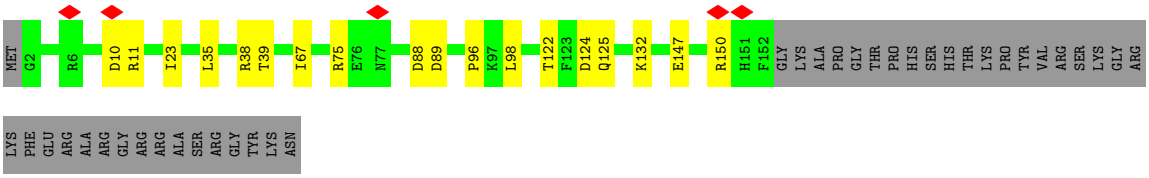
• Molecule 9: 60S ribosomal protein L17

Chain LA:



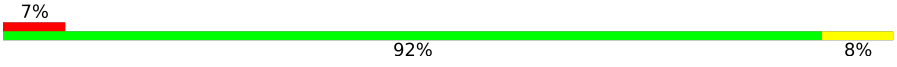
• Molecule 10: 60S ribosomal protein L18

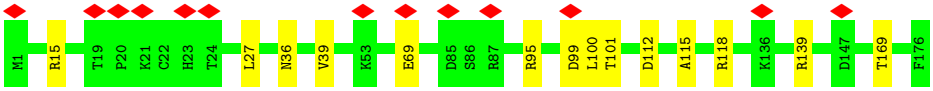
Chain LB:



• Molecule 11: 60S ribosomal protein L18a

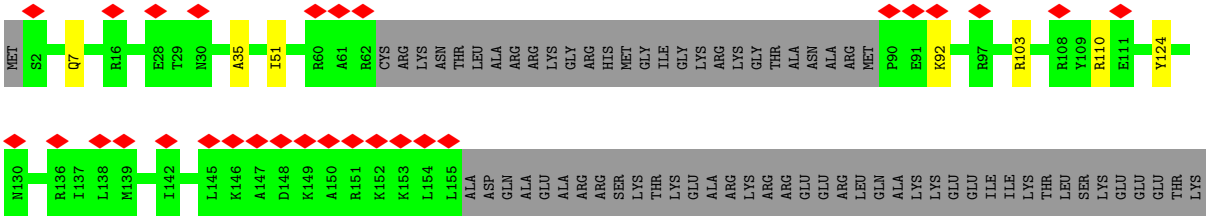
Chain LC:





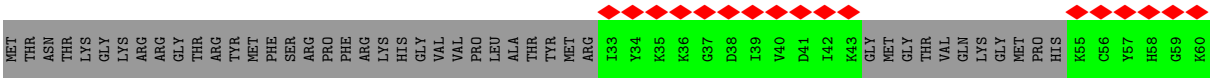
• Molecule 12: 60S ribosomal protein L19

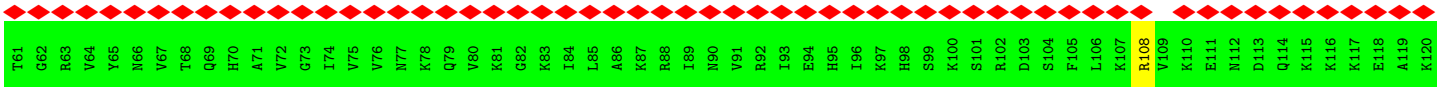
Chain LD:

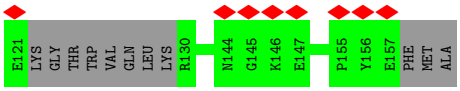


• Molecule 13: 60S ribosomal protein L21

Chain LE:

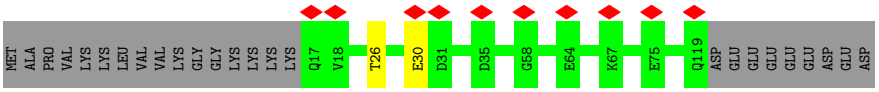






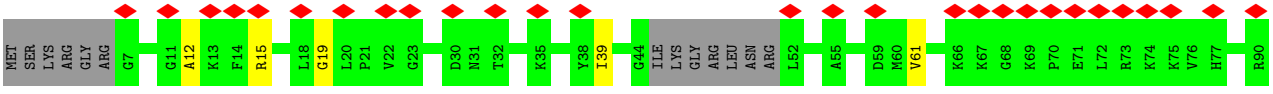
• Molecule 14: 60S ribosomal protein L22

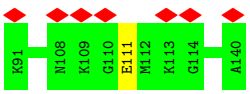
Chain LF:



• Molecule 15: 60S ribosomal protein L23

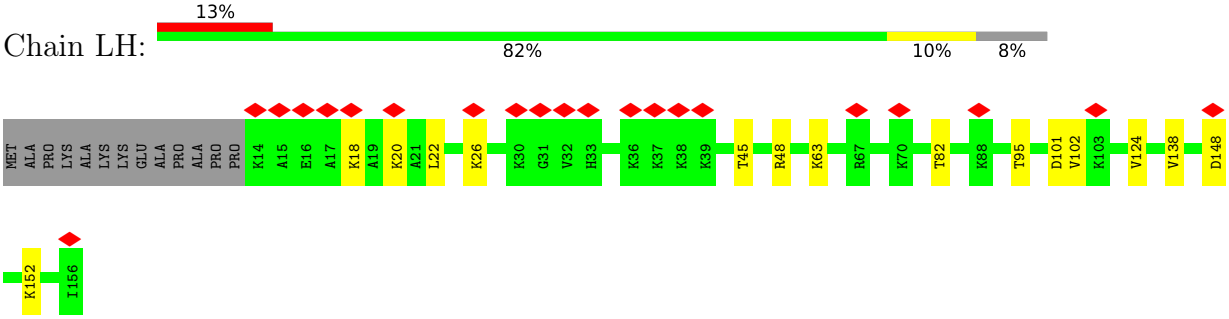
Chain LG:





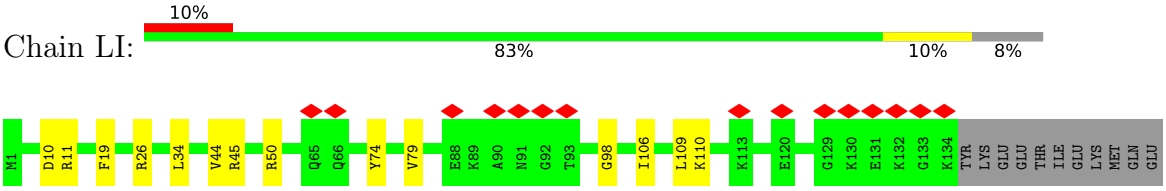
• Molecule 16: 60S ribosomal protein L23a

Chain LH:



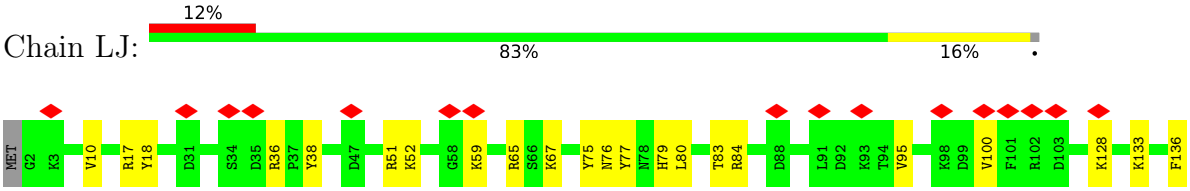
• Molecule 17: 60S ribosomal protein L26

Chain LI:



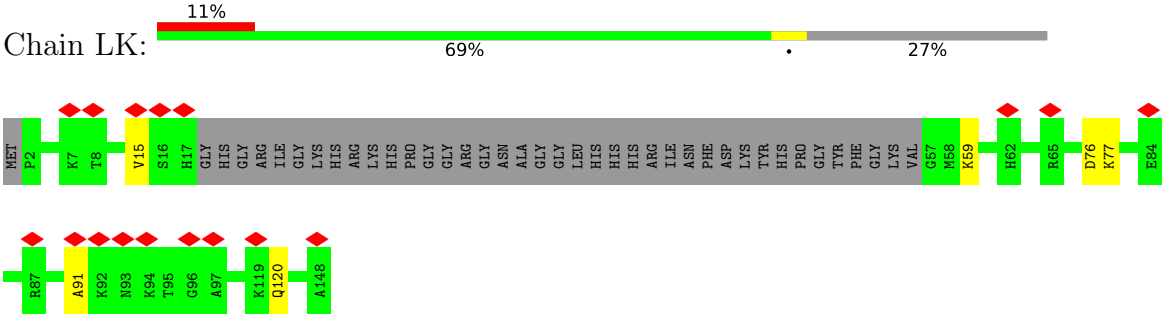
• Molecule 18: 60S ribosomal protein L27

Chain LJ:



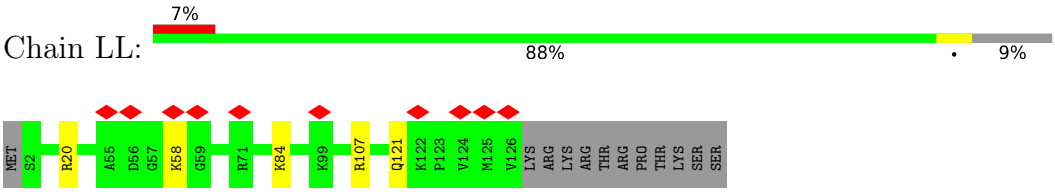
• Molecule 19: 60S ribosomal protein L27a

Chain LK:



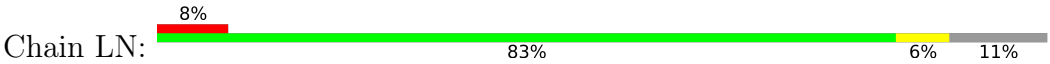
• Molecule 20: 60S ribosomal protein L28

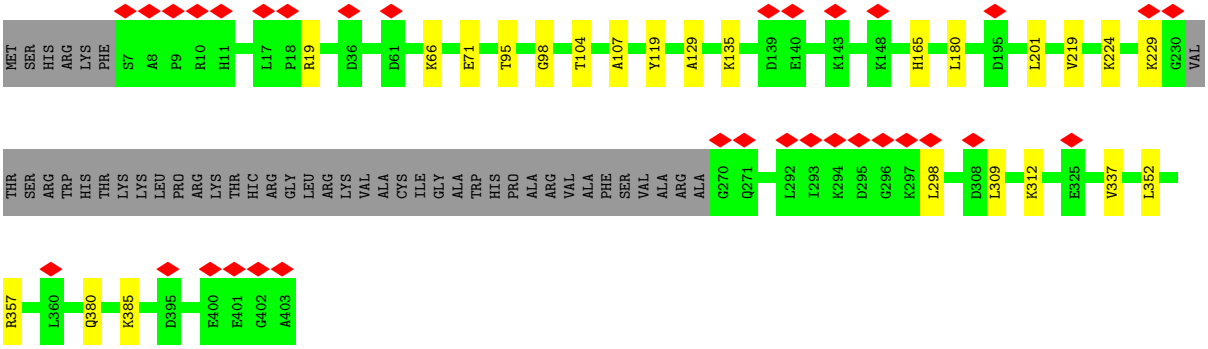
Chain LL:



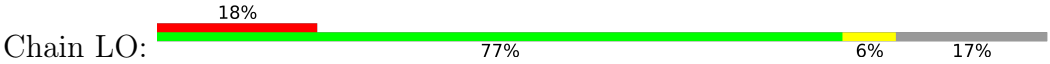
• Molecule 21: 60S ribosomal protein L3

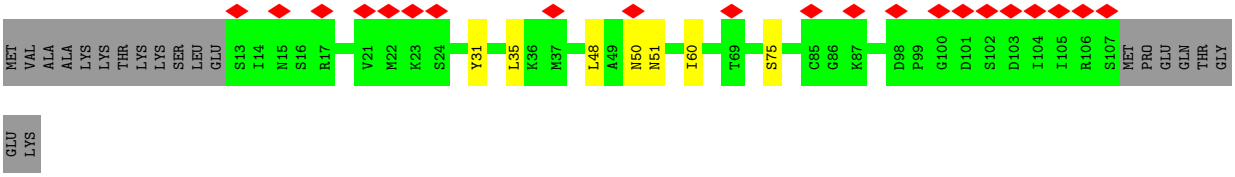
Chain LN:



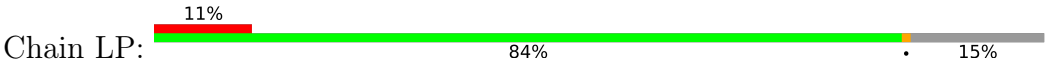


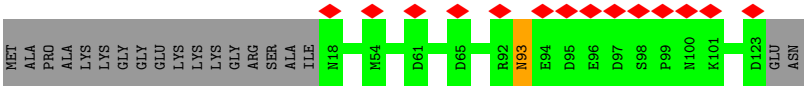
• Molecule 22: 60S ribosomal protein L30



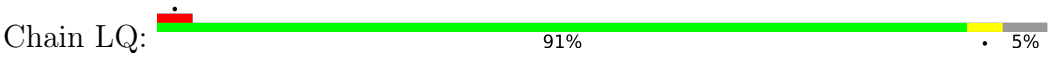


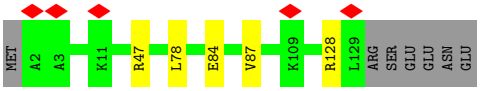
• Molecule 23: 60S ribosomal protein L31



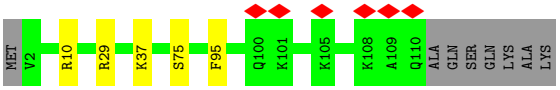


• Molecule 24: 60S ribosomal protein L32

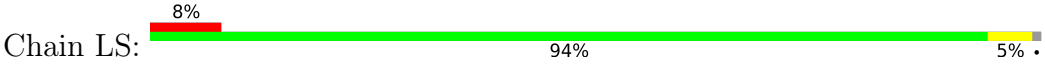


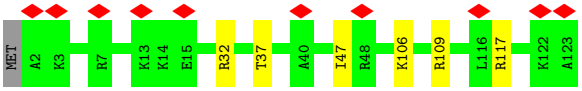


• Molecule 25: 60S ribosomal protein L34

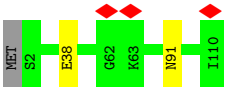


• Molecule 26: 60S ribosomal protein L35

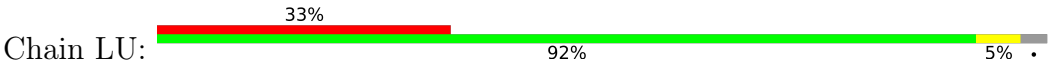


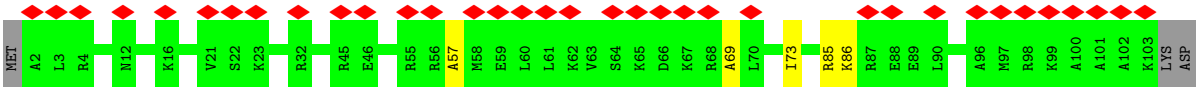


• Molecule 27: 60S ribosomal protein L35a

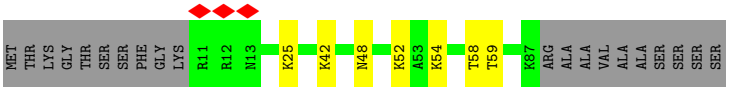


• Molecule 28: 60S ribosomal protein L36

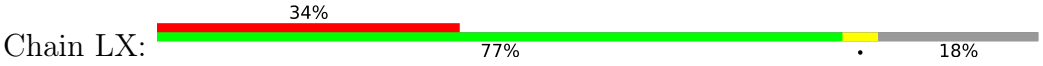


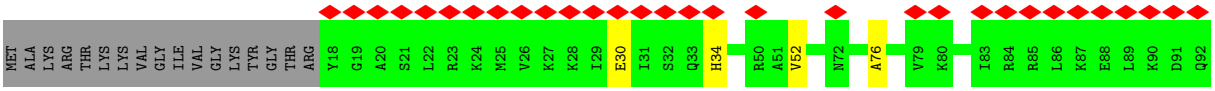


• Molecule 29: 60S ribosomal protein L37

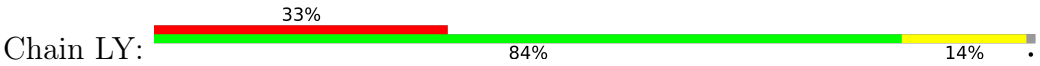


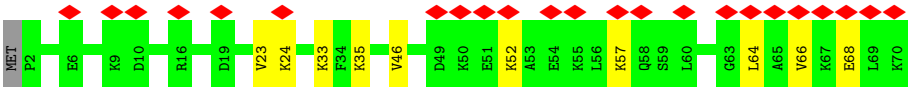
• Molecule 30: 60S ribosomal protein L37a



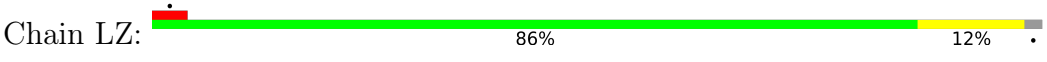


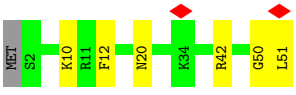
• Molecule 31: 60S ribosomal protein L38





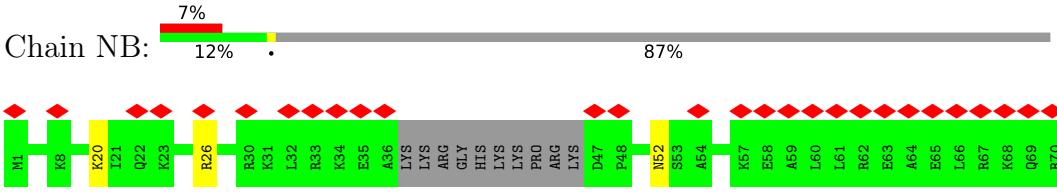
• Molecule 32: 60S ribosomal protein L39





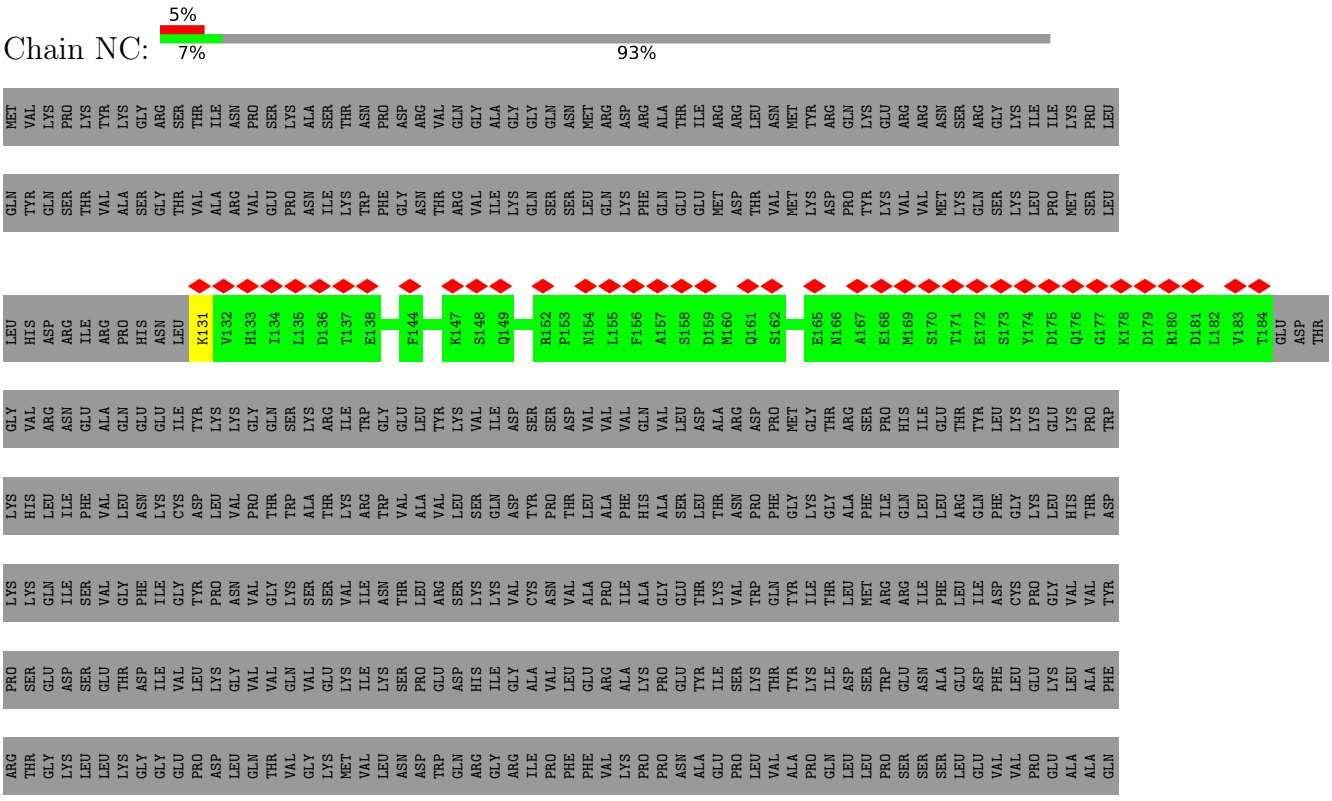
• Molecule 33: Guanine nucleotide-binding protein-like 3

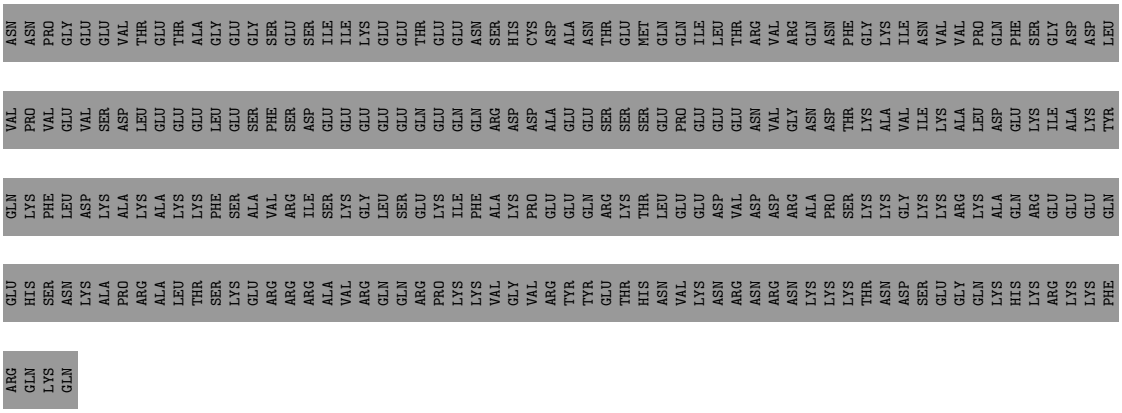
Chain NB:



- Molecule 34: Nucleolar GTP-binding protein 2

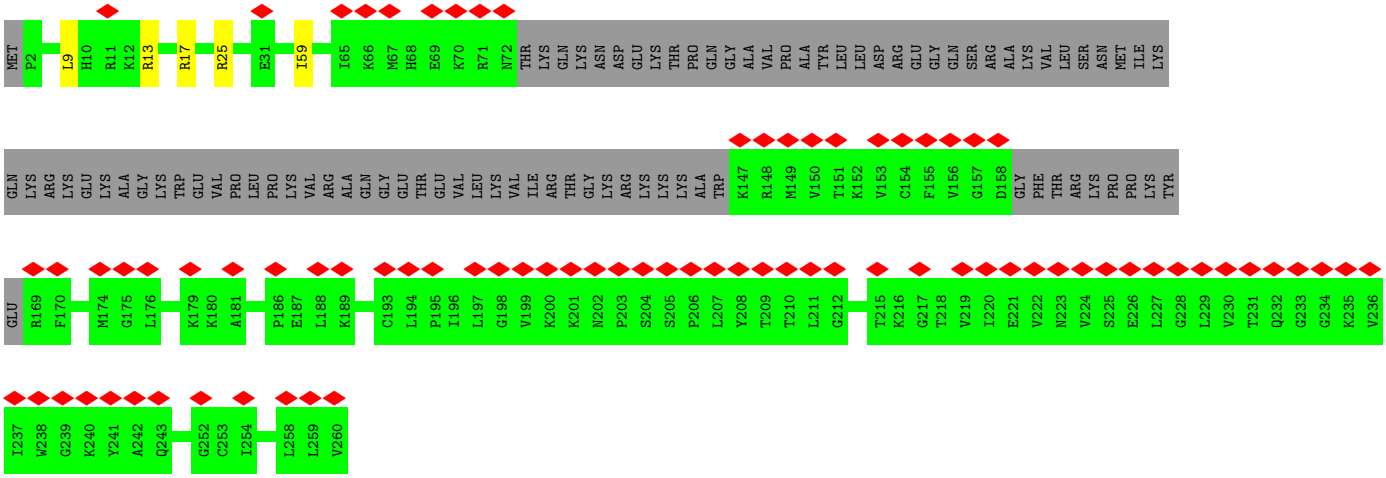
Chain NC:





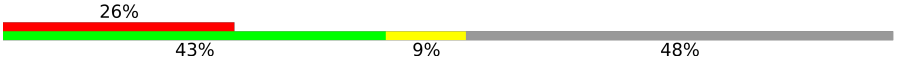
• Molecule 35: Ribosome biogenesis protein NSA2 homolog

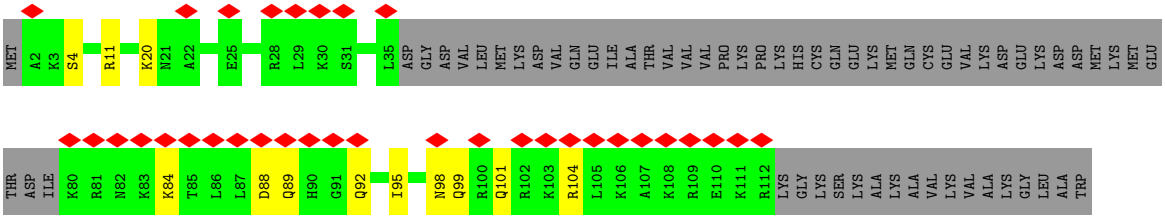
Chain NF:



• Molecule 36: Protein LLP homolog

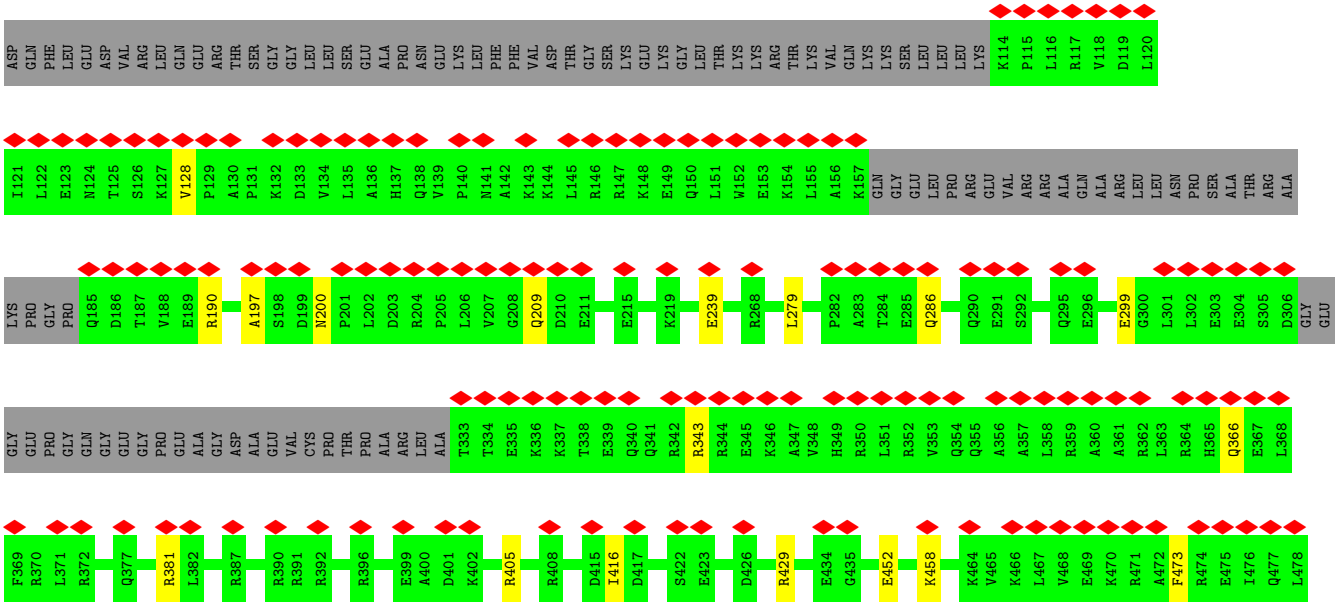
Chain NK:





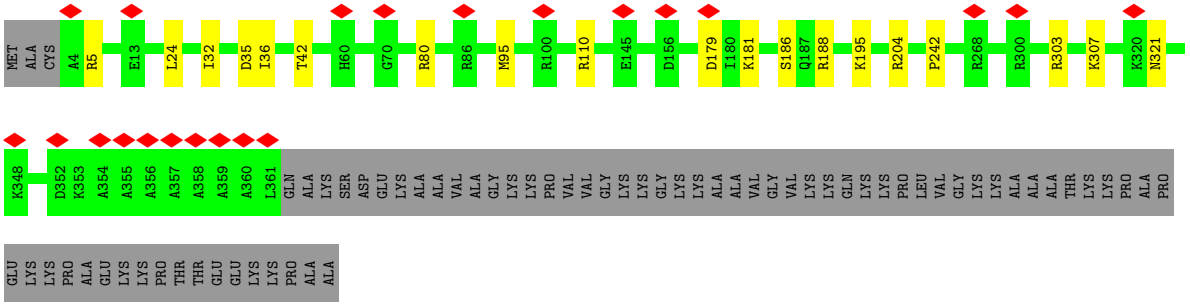
• Molecule 37: Ribosome biogenesis protein NOP53

Chain NL:



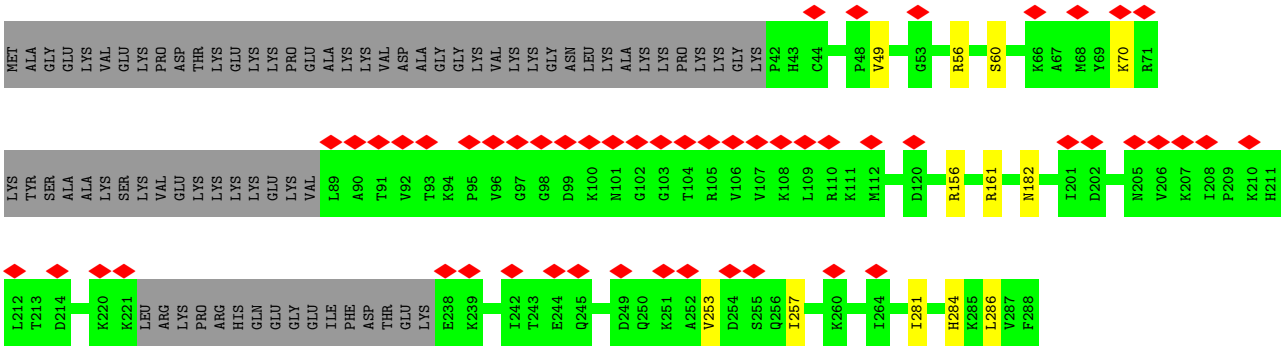
• Molecule 38: 60S ribosomal protein L4

Chain SA:



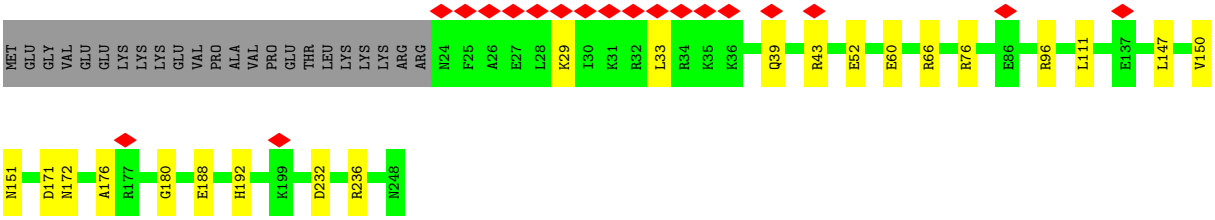
• Molecule 39: 60S ribosomal protein L6

Chain SC:



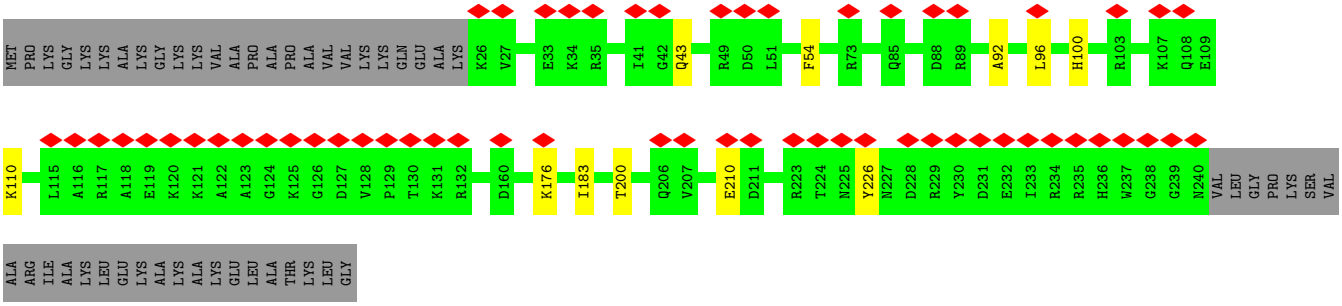
• Molecule 40: 60S ribosomal protein L7

Chain SD:



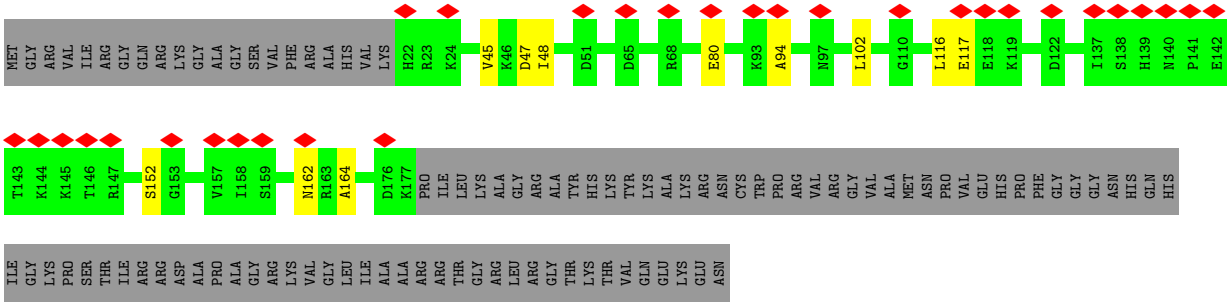
• Molecule 41: 60S ribosomal protein L7a

Chain SE:



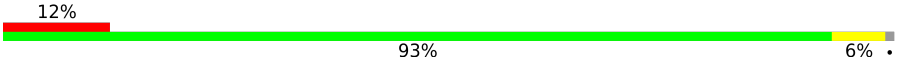
• Molecule 42: 60S ribosomal protein L8

Chain SF:



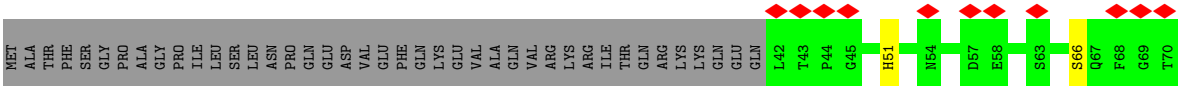
• Molecule 43: 60S ribosomal protein L9

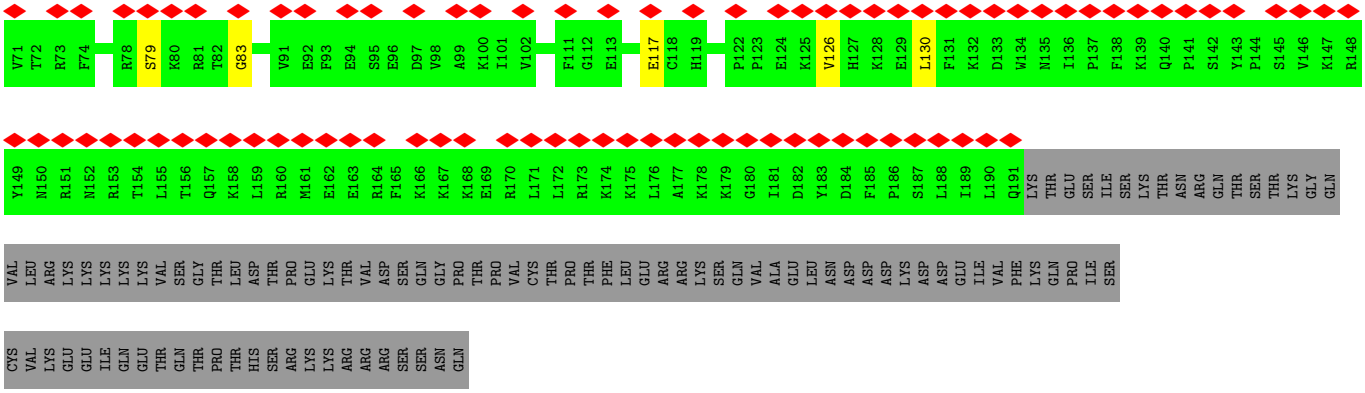
Chain SG:



• Molecule 44: MKI67 FHA domain-interacting nucleolar phosphoprotein

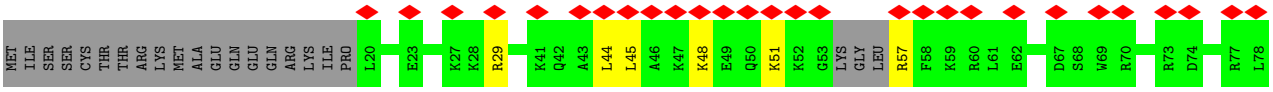
Chain SH:

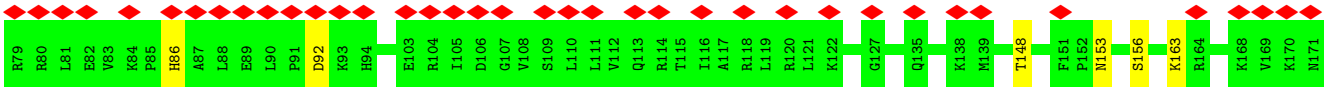


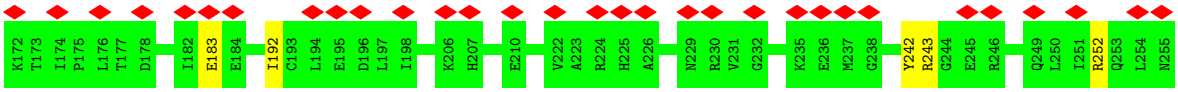


• Molecule 45: 60S ribosomal protein L7-like 1

Chain SI:

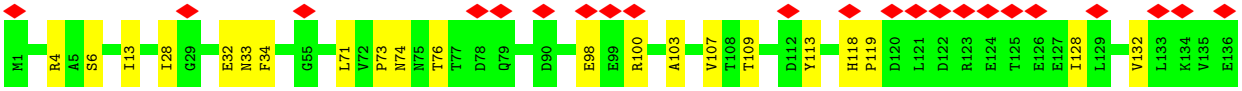


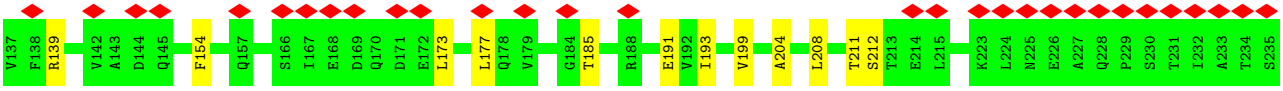


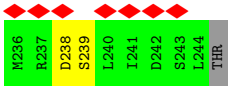


• Molecule 46: Eukaryotic translation initiation factor 6

Chain SK:

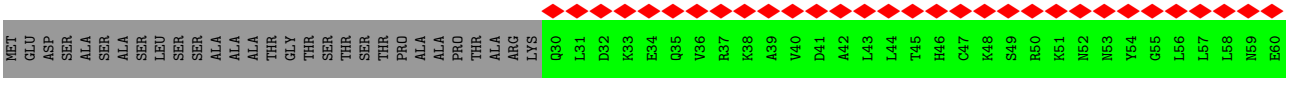


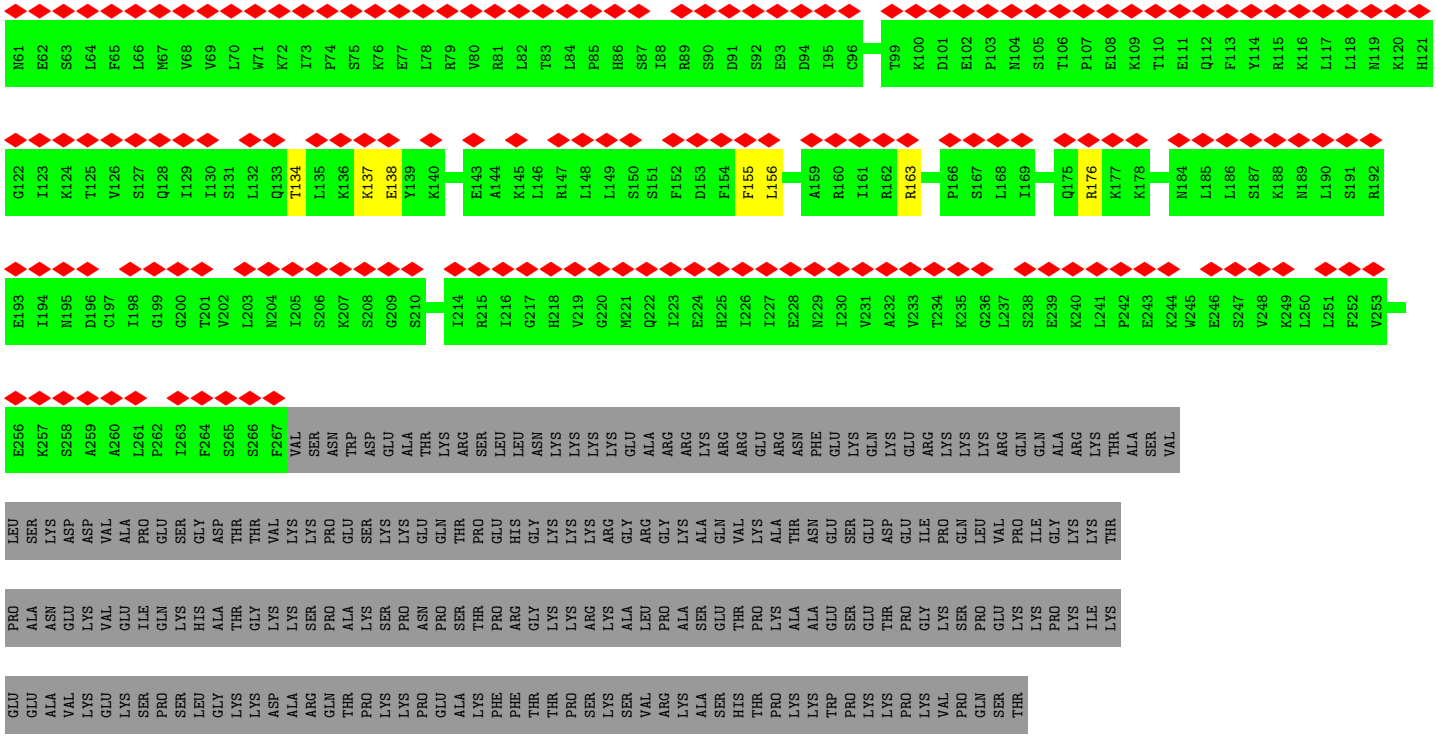




• Molecule 47: Ribosomal L1 domain-containing protein 1

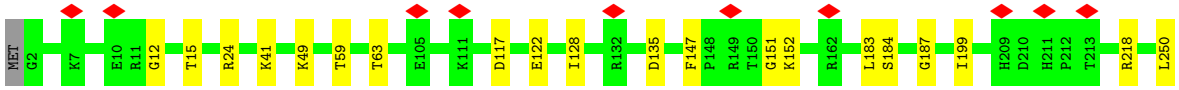
Chain SL:

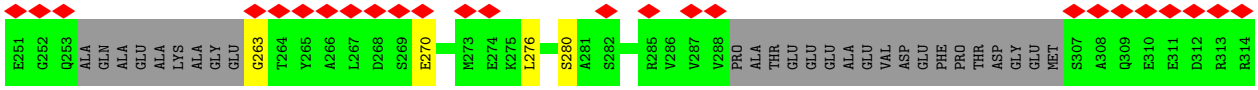


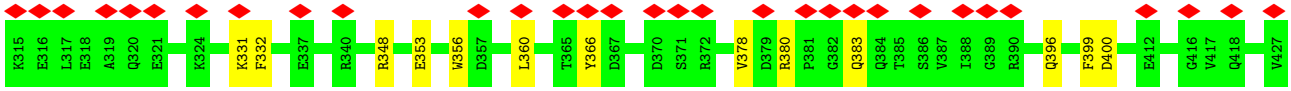


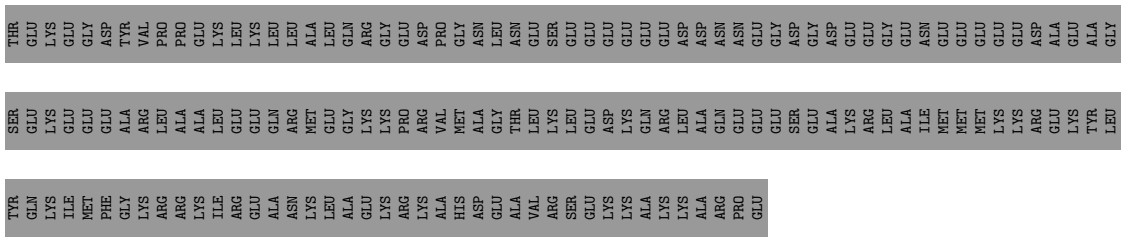
• Molecule 48: Pescadillo homolog

Chain SM:



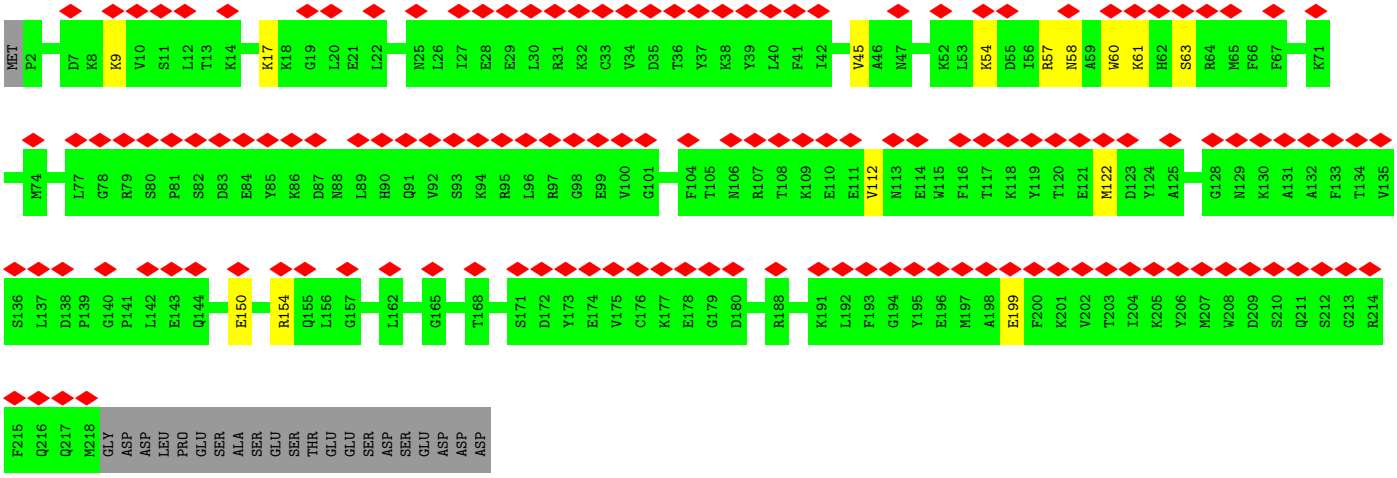






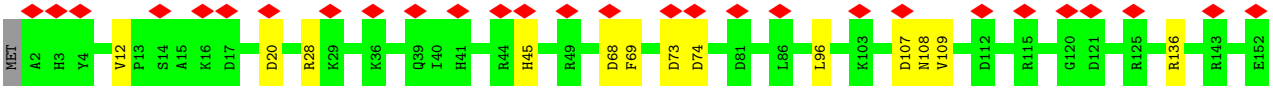
• Molecule 49: mRNA turnover protein 4 homolog

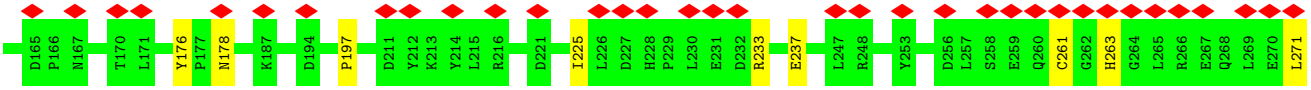
Chain SQ:

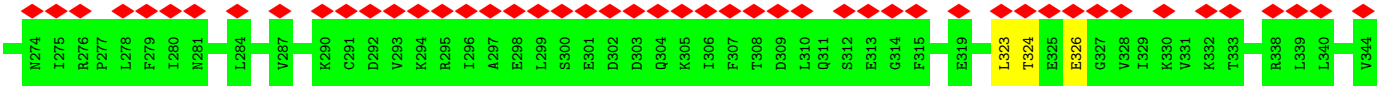


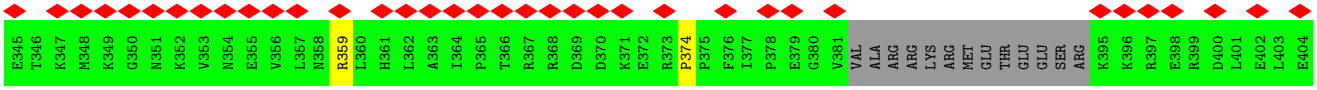
• Molecule 50: GTP-binding protein 4

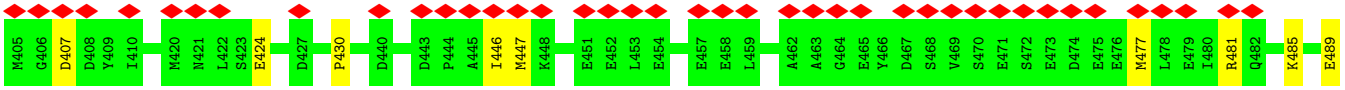
Chain SR:

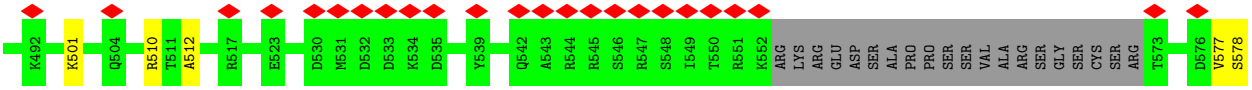


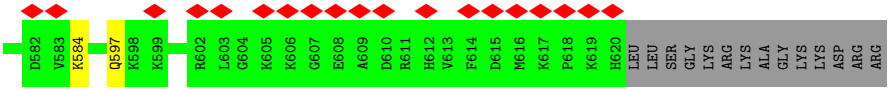






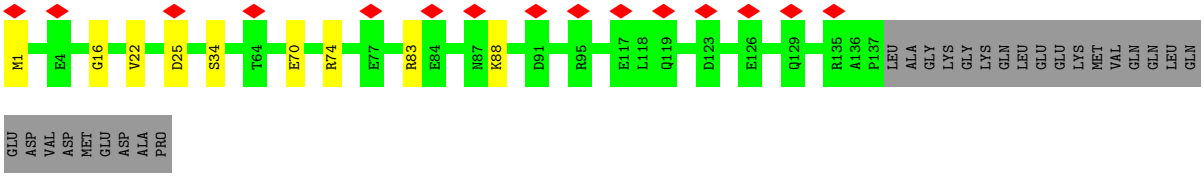






• Molecule 51: Probable ribosome biogenesis protein RLP24

Chain SV:


M1
E4
G16
V22
D25
S34
T64
E70
R74
E77
R83
E84
N87
K88
D91
R95
E117
L118
Q119
D123
E126
Q129
R135
A136
P137
LEU
ALA
GLY
LYS
GLY
LYS
GLN
LEU
GLU
GLU
LYS
MET
VAL
GLN
GLN
LEU
GLN
GLU
ASP
VAL
ASP
MET
GLU
ASP
ALA
PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26472	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.686	Depositor
Minimum map value	-0.534	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, 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	BA	0.24	0/959	0.49	0/1312
2	L1	0.32	0/3659	0.74	1/5698 (0.0%)
3	L2	0.21	0/1608	0.80	0/2497
4	L3	0.29	0/67960	0.78	8/105967 (0.0%)
5	L6	0.27	0/1563	0.61	0/2087
6	L7	0.26	0/1682	0.55	0/2250
7	L8	0.26	0/1133	0.53	0/1516
8	L9	0.27	0/1584	0.62	0/2117
9	LA	0.26	0/1268	0.54	0/1701
10	LB	0.26	0/1239	0.62	0/1658
11	LC	0.28	0/1501	0.57	0/2013
12	LD	0.25	0/1092	0.58	0/1447
13	LE	0.25	0/697	0.50	0/944
14	LF	0.28	0/856	0.53	0/1149
15	LG	0.26	0/947	0.52	0/1270
16	LH	0.25	0/1175	0.53	0/1572
17	LI	0.27	0/1132	0.58	0/1504
18	LJ	0.28	0/1130	0.57	0/1507
19	LK	0.26	0/867	0.53	0/1158
20	LL	0.25	0/1017	0.59	0/1364
21	LN	0.27	0/2932	0.53	0/3919
22	LO	0.27	0/748	0.51	0/1004
23	LP	0.25	0/894	0.57	0/1204
24	LQ	0.25	0/1071	0.56	0/1429
25	LR	0.27	0/878	0.63	0/1170
26	LS	0.25	0/1023	0.56	0/1351
27	LT	0.27	0/895	0.60	0/1198
28	LU	0.26	0/843	0.60	0/1115
29	LW	0.28	0/656	0.69	0/868
30	LX	0.25	0/594	0.51	0/790
31	LY	0.26	0/575	0.53	0/761
32	LZ	0.25	0/454	0.62	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	NB	0.26	0/610	0.56	0/802
34	NC	0.23	0/354	0.44	0/482
35	NF	0.25	0/1145	0.51	0/1536
36	NK	0.25	0/587	0.64	0/767
37	NL	0.25	0/2612	0.56	0/3500
38	SA	0.26	0/2907	0.57	0/3905
39	SC	0.26	0/1716	0.56	0/2303
40	SD	0.26	0/1905	0.55	0/2539
41	SE	0.26	0/1773	0.55	0/2390
42	SF	0.26	0/1205	0.57	0/1618
43	SG	0.26	0/1537	0.55	1/2066 (0.0%)
44	SH	0.26	0/1147	0.49	0/1558
45	SI	0.24	0/1956	0.50	0/2622
46	SK	0.24	0/1877	0.51	0/2554
47	SL	0.25	0/1533	0.48	0/2090
48	SM	0.27	0/3357	0.50	0/4529
49	SQ	0.25	0/1806	0.50	0/2420
50	SR	0.25	0/4890	0.50	0/6569
51	SV	0.27	0/1194	0.55	0/1582
All	All	0.27	0/138743	0.69	10/201971 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L3	2469	C	C2-N1-C1'	6.92	126.42	118.80
4	L3	2486	G	N1-C6-O6	-6.79	115.82	119.90
4	L3	5022	U	O4'-C1'-N1	6.30	113.24	108.20
4	L3	1854	G	O4'-C1'-N9	6.20	113.16	108.20
4	L3	2486	G	C5-C6-O6	5.87	132.12	128.60
43	SG	37	ASP	CB-CG-OD2	5.66	123.40	118.30
4	L3	453	G	C4-N9-C1'	5.44	133.58	126.50
4	L3	971	U	C2-N1-C1'	5.34	124.11	117.70
2	L1	83	C	C2-N1-C1'	5.32	124.65	118.80
4	L3	2469	C	C6-N1-C1'	-5.14	114.63	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	954	0	690	7	0
2	L1	3277	0	1663	12	0
3	L2	1445	0	744	4	0
4	L3	60779	0	30746	210	0
5	L6	1539	0	1659	19	0
6	L7	1650	0	1794	9	0
7	L8	1111	0	1174	9	0
8	L9	1546	0	1585	12	0
9	LA	1242	0	1269	12	0
10	LB	1223	0	1330	12	0
11	LC	1461	0	1502	9	0
12	LD	1078	0	1194	6	0
13	LE	690	0	535	1	0
14	LF	842	0	864	1	0
15	LG	934	0	979	7	0
16	LH	1156	0	1268	12	0
17	LI	1115	0	1205	9	0
18	LJ	1107	0	1182	16	0
19	LK	852	0	916	4	0
20	LL	1002	0	1068	5	0
21	LN	2877	0	2993	21	0
22	LO	738	0	774	4	0
23	LP	879	0	924	1	0
24	LQ	1053	0	1147	5	0
25	LR	868	0	959	5	0
26	LS	1015	0	1148	7	0
27	LT	876	0	912	2	0
28	LU	832	0	917	4	0
29	LW	642	0	672	6	0
30	LX	585	0	612	3	0
31	LY	569	0	637	8	0
32	LZ	444	0	483	5	0
33	NB	603	0	661	3	0
34	NC	350	0	274	0	0
35	NF	1136	0	887	4	0
36	NK	581	0	656	9	0
37	NL	2574	0	2664	15	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	SA	2853	0	3028	14	0
39	SC	1684	0	1781	9	0
40	SD	1870	0	1996	15	0
41	SE	1741	0	1857	10	0
42	SF	1184	0	1239	7	0
43	SG	1518	0	1601	8	0
44	SH	1120	0	988	4	0
45	SI	1919	0	2052	14	0
46	SK	1852	0	1828	23	0
47	SL	1520	0	1207	6	0
48	SM	3278	0	3332	25	0
49	SQ	1771	0	1810	10	0
50	SR	4808	0	4924	34	0
51	SV	1171	0	1232	10	0
52	L1	5	0	0	0	0
52	L3	50	0	0	0	0
52	L9	1	0	0	0	0
52	LQ	1	0	0	0	0
52	LR	1	0	0	0	0
52	LT	1	0	0	0	0
52	NF	1	0	0	0	0
52	SA	3	0	0	0	0
52	SR	1	0	0	0	0
53	LR	1	0	0	0	0
53	LW	1	0	0	0	0
53	LX	1	0	0	0	0
53	SV	1	0	0	0	0
54	SR	28	0	12	0	0
55	SR	1	0	0	0	0
All	All	130011	0	99574	481	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 2.

All (481) 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)
4:L3:1293:G:N2	4:L3:1293:G:OP2	2.10	0.84
40:SD:232:ASP:OD1	40:SD:236:ARG:NH2	2.11	0.83
10:LB:35:LEU:O	10:LB:39:THR:OG1	1.96	0.82
4:L3:695:G:O2'	4:L3:697:G:OP2	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:123:ARG:NH1	4:L3:1997:U:OP2	2.12	0.82
4:L3:2520:C:O2	4:L3:2640:G:N2	2.12	0.81
4:L3:1670:G:N2	4:L3:1670:G:OP2	2.13	0.81
4:L3:62:A:N3	4:L3:77:U:O2'	2.13	0.81
2:L1:75:G:OP2	17:LI:74:TYR:OH	1.99	0.81
10:LB:122:THR:OG1	10:LB:124:ASP:OD1	1.97	0.81
2:L1:50:C:O2'	50:SR:578:SER:OG	1.99	0.80
45:SI:153:ASN:ND2	48:SM:263:GLY:O	2.15	0.80
4:L3:2263:A:OP1	20:LL:107:ARG:NH2	2.14	0.80
36:NK:88:ASP:OD2	36:NK:89:GLN:N	2.16	0.79
29:LW:25:LYS:NZ	32:LZ:50:GLY:O	2.12	0.79
11:LC:95:ARG:NH2	11:LC:112:ASP:OD2	2.15	0.79
4:L3:1480:C:O2'	4:L3:1482:G:OP2	2.00	0.79
4:L3:3892:U:O2'	9:LA:80:GLN:NE2	2.16	0.79
46:SK:119:PRO:O	46:SK:139:ARG:NH2	2.16	0.78
4:L3:308:G:N2	4:L3:308:G:OP2	2.16	0.78
4:L3:219:G:O6	38:SA:181:LYS:NZ	2.13	0.78
4:L3:1859:C:OP1	33:NB:26:ARG:NH1	2.18	0.76
4:L3:408:A:O2'	4:L3:411:G:OP2	2.02	0.75
4:L3:4591:U:OP1	36:NK:4:SER:OG	2.04	0.75
4:L3:5022:U:O2'	4:L3:5025:C:N4	2.19	0.75
4:L3:4670:C:O2'	4:L3:4672:A:OP2	2.05	0.75
4:L3:2476:G:N7	16:LH:48:ARG:NH2	2.35	0.74
50:SR:424:GLU:OE1	51:SV:83:ARG:NE	2.20	0.74
7:L8:12:VAL:O	7:L8:58:THR:OG1	2.06	0.73
18:LJ:36:ARG:NH1	18:LJ:38:TYR:OH	2.21	0.73
4:L3:4663:G:OP1	51:SV:34:SER:OG	2.06	0.73
8:L9:46:ASP:OD1	8:L9:47:LYS:N	2.22	0.72
4:L3:4122:G:O2'	18:LJ:136:PHE:OXT	2.06	0.72
4:L3:4620:U:OP2	4:L3:4670:C:N4	2.22	0.72
45:SI:163:LYS:NZ	48:SM:147:PHE:O	2.22	0.72
4:L3:4117:U:O4'	41:SE:43:GLN:NE2	2.22	0.72
2:L1:134:G:OP1	16:LH:63:LYS:NZ	2.20	0.72
4:L3:2848:G:O2'	4:L3:3838:U:O4	2.04	0.72
4:L3:2922:G:O2'	4:L3:3275:A:N6	2.22	0.72
4:L3:5024:C:OP2	4:L3:5025:C:N4	2.22	0.72
4:L3:1071:C:O2	39:SC:70:LYS:NZ	2.22	0.71
4:L3:1963:C:OP1	49:SQ:17:LYS:NZ	2.22	0.71
46:SK:113:TYR:OH	50:SR:374:PRO:O	2.07	0.71
4:L3:1280:C:O2'	38:SA:321:ASN:OD1	2.02	0.71
4:L3:2553:A:OP2	4:L3:2574:G:O2'	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:502:C:O2'	4:L3:503:C:OP1	2.05	0.70
2:L1:71:A:OP2	2:L1:83:C:N4	2.24	0.70
11:LC:69:GLU:HG3	11:LC:101:THR:HG23	1.74	0.70
4:L3:2407:G:N2	4:L3:2407:G:OP2	2.23	0.70
4:L3:4120:U:O2'	4:L3:4121:G:OP1	2.10	0.69
4:L3:2754:G:OP2	18:LJ:133:LYS:NZ	2.25	0.69
45:SI:92:ASP:OD2	45:SI:242:TYR:OH	2.10	0.69
9:LA:118:GLN:NE2	9:LA:147:GLU:OE2	2.26	0.69
4:L3:2626:U:OP2	50:SR:501:LYS:NZ	2.26	0.69
4:L3:52:G:OP2	29:LW:48:ASN:ND2	2.26	0.68
2:L1:50:C:HO2'	50:SR:578:SER:HG	1.41	0.68
4:L3:151:G:OP2	8:L9:4:TYR:OH	2.10	0.67
4:L3:1485:C:N3	5:L6:198:ARG:NH2	2.42	0.67
38:SA:35:ASP:OD1	38:SA:36:ILE:N	2.28	0.67
16:LH:26:LYS:NZ	37:NL:473:PHE:O	2.26	0.67
3:L2:10:U:OP2	47:SL:163:ARG:NH2	2.27	0.67
4:L3:4626:A:OP2	21:LN:224:LYS:NZ	2.27	0.67
4:L3:1420:A:O2'	4:L3:1500:A:O2'	2.04	0.67
40:SD:39:GLN:OE1	40:SD:43:ARG:NH2	2.27	0.66
4:L3:375:G:OP2	29:LW:52:LYS:NZ	2.24	0.66
4:L3:1952:G:OP1	11:LC:139:ARG:NE	2.28	0.66
39:SC:161:ARG:O	39:SC:182:ASN:ND2	2.29	0.66
4:L3:1883:G:OP1	24:LQ:47:ARG:NH1	2.29	0.66
50:SR:233:ARG:NE	50:SR:237:GLU:OE2	2.29	0.66
5:L6:204:GLU:O	5:L6:207:VAL:HG22	1.95	0.65
2:L1:141:C:O2'	8:L9:136:ASP:OD2	2.08	0.65
4:L3:4978:G:O2'	4:L3:4980:C:OP2	2.10	0.65
29:LW:54:LYS:O	29:LW:58:THR:OG1	2.09	0.65
37:NL:416:ILE:O	45:SI:29:ARG:NH2	2.30	0.65
4:L3:5068:G:N2	4:L3:5069:U:O4	2.24	0.65
7:L8:29:ASP:OD2	7:L8:30:VAL:N	2.29	0.65
3:L2:91:C:OP2	47:SL:176:ARG:NH2	2.30	0.65
15:LG:111:GLU:N	15:LG:111:GLU:OE1	2.30	0.65
4:L3:2574:G:OP2	18:LJ:67:LYS:NZ	2.22	0.65
16:LH:124:VAL:HG22	16:LH:138:VAL:HG12	1.79	0.65
9:LA:115:GLU:OE2	9:LA:151:THR:OG1	2.11	0.64
4:L3:2695:A:OP1	31:LY:35:LYS:NZ	2.26	0.64
48:SM:332:PHE:O	48:SM:366:TYR:OH	2.15	0.64
50:SR:178:ASN:ND2	50:SR:197:PRO:O	2.30	0.64
7:L8:32:ASP:OD2	7:L8:33:GLN:N	2.28	0.64
4:L3:310:G:O3'	28:LU:85:ARG:NH1	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:2588:C:OP1	4:L3:2768:C:O2'	2.12	0.64
48:SM:184:SER:OG	48:SM:187:GLY:O	2.15	0.64
50:SR:176:TYR:CE1	50:SR:271:LEU:HD22	2.33	0.64
4:L3:4691:A:OP1	43:SG:75:SER:OG	2.07	0.64
1:BA:135:THR:HG22	4:L3:1974:U:O4	1.97	0.64
1:BA:128:THR:O	1:BA:132:ILE:HD12	1.98	0.63
4:L3:67:C:OP2	4:L3:312:G:N2	2.30	0.63
4:L3:4678:G:N7	36:NK:11:ARG:NH2	2.46	0.63
18:LJ:84:ARG:NH1	37:NL:299:GLU:O	2.31	0.63
50:SR:261:CYS:SG	50:SR:263:HIS:ND1	2.66	0.63
4:L3:4083:U:O2'	4:L3:4086:G:OP1	2.16	0.63
4:L3:1955:G:OP2	33:NB:52:ASN:ND2	2.31	0.62
49:SQ:58:ASN:O	49:SQ:61:LYS:NZ	2.28	0.62
4:L3:1802:A:O2'	13:LE:108:ARG:NH2	2.32	0.62
4:L3:4567:G:OP1	21:LN:19:ARG:N	2.33	0.62
44:SH:51:HIS:ND1	44:SH:117:GLU:OE1	2.32	0.62
3:L2:13:C:OP1	45:SI:86:HIS:NE2	2.29	0.62
20:LL:20:ARG:NH1	24:LQ:78:LEU:O	2.33	0.61
46:SK:33:ASN:OD1	46:SK:34:PHE:N	2.33	0.61
4:L3:150:U:OP2	41:SE:200:THR:OG1	2.19	0.61
36:NK:101:GLN:OE1	36:NK:104:ARG:NH1	2.33	0.61
4:L3:1646:A:OP2	38:SA:80:ARG:NH2	2.33	0.61
10:LB:88:ASP:OD2	10:LB:89:ASP:N	2.34	0.61
4:L3:5002:U:OP2	21:LN:385:LYS:NZ	2.30	0.61
11:LC:69:GLU:CG	11:LC:101:THR:HG23	2.31	0.60
46:SK:238:ASP:OD1	46:SK:239:SER:N	2.35	0.60
4:L3:1272:C:O2	40:SD:33:LEU:HD23	2.02	0.60
4:L3:2835:A:O2'	21:LN:229:LYS:O	2.13	0.60
4:L3:156:G:OP1	26:LS:109:ARG:NH2	2.35	0.60
9:LA:110:ASP:OD1	9:LA:111:SER:N	2.35	0.60
4:L3:2846:G:O2'	15:LG:19:GLY:O	2.14	0.59
21:LN:95:THR:OG1	21:LN:98:GLY:O	2.16	0.59
4:L3:2845:A:H61	4:L3:3843:C:H42	1.51	0.59
4:L3:90:G:OP2	4:L3:92:C:N4	2.36	0.59
46:SK:107:VAL:HG13	46:SK:118:HIS:HB2	1.83	0.59
4:L3:4880:C:OP1	7:L8:124:LYS:NZ	2.36	0.58
22:LO:50:ASN:OD1	22:LO:51:ASN:N	2.36	0.58
23:LP:93:ASN:ND2	23:LP:93:ASN:O	2.36	0.58
4:L3:4476:C:O2'	4:L3:4478:G:OP2	2.22	0.58
37:NL:128:VAL:HG21	41:SE:176:LYS:NZ	2.18	0.58
3:L2:90:C:OP2	47:SL:176:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:SK:191:GLU:O	46:SK:193:ILE:HD12	2.03	0.58
4:L3:4765:G:OP1	43:SG:23:ARG:NE	2.37	0.58
5:L6:70:VAL:HG12	5:L6:159:ASN:OD1	2.04	0.57
5:L6:126:LEU:HD21	26:LS:117:ARG:CZ	2.34	0.57
1:BA:125:LEU:O	1:BA:128:THR:OG1	2.20	0.57
4:L3:2758:G:OP1	37:NL:405:ARG:NH1	2.37	0.57
5:L6:133:ALA:O	5:L6:135:LYS:NZ	2.37	0.57
4:L3:440:U:O2'	27:LT:91:ASN:O	2.18	0.57
38:SA:179:ASP:OD2	38:SA:204:ARG:NH2	2.38	0.57
21:LN:357:ARG:NH1	50:SR:407:ASP:OD1	2.36	0.57
46:SK:185:THR:OG1	50:SR:359:ARG:NH2	2.37	0.57
8:L9:103:GLU:OE1	8:L9:165:THR:HG21	2.04	0.57
37:NL:209:GLN:OE1	37:NL:209:GLN:N	2.38	0.57
4:L3:102:G:O2'	4:L3:1381:U:O2'	2.22	0.56
4:L3:2562:G:O2'	4:L3:2565:A:N6	2.38	0.56
4:L3:1818:G:O2'	4:L3:1820:C:OP2	2.16	0.56
16:LH:82:THR:HG21	26:LS:37:THR:HG22	1.87	0.56
41:SE:96:LEU:O	41:SE:100:HIS:ND1	2.34	0.56
2:L1:104:A:OP1	29:LW:42:LYS:NZ	2.39	0.56
4:L3:2923:A:O2'	31:LY:52:LYS:NZ	2.24	0.56
4:L3:3277:C:O4'	37:NL:366:GLN:NE2	2.38	0.56
4:L3:4465:U:OP1	50:SR:28:ARG:NH1	2.38	0.56
4:L3:4872:G:OP2	7:L8:94:LYS:NZ	2.37	0.56
17:LI:19:PHE:O	17:LI:26:ARG:NH2	2.39	0.56
41:SE:183:ILE:HD12	41:SE:226:TYR:OH	2.05	0.56
4:L3:2000:G:O6	49:SQ:54:LYS:NZ	2.29	0.56
9:LA:16:LYS:O	9:LA:101:ASN:ND2	2.38	0.56
4:L3:4724:A:O2'	21:LN:104:THR:HG22	2.06	0.56
4:L3:4688:C:HO2'	43:SG:155:SER:HG	1.54	0.56
4:L3:2318:G:N2	4:L3:2321:G:OP2	2.29	0.55
28:LU:69:ALA:O	28:LU:73:ILE:HD12	2.06	0.55
8:L9:193:ARG:O	8:L9:197:THR:HG23	2.07	0.55
4:L3:2366:A:N3	4:L3:3850:C:O2'	2.36	0.55
4:L3:679:C:OP1	20:LL:84:LYS:NZ	2.33	0.55
4:L3:85:G:O2'	4:L3:97:G:O6	2.15	0.55
4:L3:197:A:N3	4:L3:222:C:O2'	2.37	0.54
4:L3:1997:U:O3'	49:SQ:57:ARG:NH2	2.39	0.54
35:NF:17:ARG:NH1	43:SG:180:TYR:OH	2.40	0.54
2:L1:83:C:H42	17:LI:50:ARG:NH1	2.05	0.54
4:L3:2696:A:H62	31:LY:35:LYS:HZ2	1.54	0.54
16:LH:20:LYS:NZ	44:SH:66:SER:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L3:4697:U:OP1	35:NF:25:ARG:NH2	2.40	0.54
2:L1:7:U:O2'	4:L3:1305:C:OP1	2.26	0.54
4:L3:172:C:OP1	5:L6:130:LYS:NZ	2.37	0.54
49:SQ:60:TRP:CH2	49:SQ:112:VAL:HG12	2.43	0.54
4:L3:4471:U:OP1	43:SG:168:LYS:NZ	2.31	0.54
51:SV:70:GLU:N	51:SV:70:GLU:OE1	2.40	0.54
4:L3:152:U:OP2	8:L9:49:ARG:NH2	2.41	0.53
40:SD:171:ASP:OD1	40:SD:172:ASN:N	2.41	0.53
4:L3:2416:G:N2	50:SR:597:GLN:OE1	2.36	0.53
36:NK:98:ASN:OD1	36:NK:99:GLN:N	2.41	0.53
4:L3:307:A:OP1	28:LU:86:LYS:NZ	2.38	0.53
4:L3:2438:A:O2'	4:L3:2440:U:OP2	2.25	0.53
37:NL:190:ARG:NH2	48:SM:117:ASP:OD1	2.41	0.53
40:SD:60:GLU:OE2	40:SD:192:HIS:NE2	2.35	0.53
4:L3:2666:U:OP2	12:LD:124:TYR:OH	2.18	0.53
8:L9:135:ILE:HD12	8:L9:151:ILE:HD13	1.91	0.53
37:NL:197:ALA:O	37:NL:200:ASN:ND2	2.42	0.53
48:SM:356:TRP:HB2	48:SM:360:LEU:HD23	1.91	0.53
10:LB:10:ASP:OD1	10:LB:11:ARG:N	2.42	0.53
4:L3:4979:A:OP2	21:LN:229:LYS:N	2.36	0.53
4:L3:423:G:OP1	9:LA:62:ARG:NH1	2.42	0.52
4:L3:1255:A:OP1	4:L3:1257:A:N6	2.42	0.52
4:L3:238:C:OP2	17:LI:45:ARG:NH2	2.41	0.52
4:L3:2090:U:OP2	38:SA:307:LYS:NZ	2.42	0.52
43:SG:12:ILE:CD1	43:SG:18:ILE:HD12	2.40	0.52
4:L3:4759:C:O2	6:L7:165:LYS:NZ	2.32	0.52
17:LI:34:LEU:HD22	17:LI:44:VAL:HG13	1.92	0.52
46:SK:32:GLU:OE2	46:SK:32:GLU:N	2.42	0.52
7:L8:59:ASP:OD1	7:L8:60:PHE:N	2.42	0.52
50:SR:323:LEU:HD23	50:SR:324:THR:HG23	1.91	0.52
20:LL:20:ARG:NH2	24:LQ:84:GLU:OE1	2.38	0.52
50:SR:485:LYS:NZ	50:SR:489:GLU:OE2	2.39	0.52
49:SQ:60:TRP:HE3	49:SQ:63:SER:HG	1.59	0.51
18:LJ:10:VAL:O	18:LJ:83:THR:OG1	2.18	0.51
45:SI:252:ARG:NH1	48:SM:270:GLU:OE1	2.44	0.51
49:SQ:45:VAL:HG23	49:SQ:45:VAL:O	2.11	0.51
4:L3:2835:A:N6	4:L3:3853:U:O4'	2.43	0.51
21:LN:119:TYR:OH	21:LN:129:ALA:N	2.43	0.51
4:L3:4435:U:O2'	50:SR:136:ARG:NH2	2.43	0.51
4:L3:4502:C:O2	50:SR:45:HIS:NE2	2.44	0.51
5:L6:164:GLU:N	5:L6:164:GLU:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:132:ILE:O	1:BA:135:THR:OG1	2.28	0.51
4:L3:121:A:OP1	41:SE:110:LYS:NZ	2.43	0.51
21:LN:312:LYS:NZ	21:LN:380:GLN:OE1	2.43	0.51
30:LX:30:GLU:OE2	30:LX:34:HIS:ND1	2.41	0.51
46:SK:109:THR:HG22	46:SK:154:PHE:CE1	2.46	0.51
16:LH:95:THR:OG1	16:LH:138:VAL:O	2.24	0.51
18:LJ:95:VAL:O	18:LJ:100:VAL:HG21	2.11	0.51
36:NK:88:ASP:OD1	36:NK:92:GLN:NE2	2.42	0.50
1:BA:135:THR:O	1:BA:138:SER:OG	2.17	0.50
38:SA:5:ARG:NH1	38:SA:24:LEU:O	2.42	0.50
41:SE:210:GLU:HG2	47:SL:137:LYS:HG3	1.92	0.50
4:L3:4085:A:OP2	16:LH:45:THR:HG22	2.12	0.50
15:LG:39:ILE:HD12	15:LG:61:VAL:HG21	1.93	0.50
45:SI:192:ILE:HD11	48:SM:380:ARG:HE	1.77	0.50
26:LS:32:ARG:HH12	26:LS:47:ILE:HG23	1.75	0.50
18:LJ:76:ASN:OD1	18:LJ:77:TYR:N	2.45	0.50
4:L3:2580:U:HO2'	18:LJ:79:HIS:CE1	2.29	0.50
4:L3:3661:G:N7	42:SF:152:SER:OG	2.29	0.50
4:L3:4927:G:OP2	4:L3:4927:G:N2	2.38	0.50
11:LC:115:ALA:O	11:LC:118:ARG:NH1	2.45	0.50
4:L3:297:U:O2'	8:L9:179:LYS:O	2.30	0.50
21:LN:309:LEU:HD11	50:SR:430:PRO:HB3	1.94	0.50
48:SM:280:SER:O	48:SM:348:ARG:NH1	2.44	0.50
4:L3:2361:G:O6	9:LA:25:HIS:ND1	2.45	0.50
4:L3:32:G:O2'	4:L3:50:C:N4	2.45	0.49
4:L3:2087:C:OP1	38:SA:303:ARG:NH1	2.44	0.49
4:L3:4401:G:O4'	33:NB:20:LYS:NZ	2.42	0.49
22:LO:31:TYR:CE1	22:LO:35:LEU:HD21	2.47	0.49
2:L1:13:G:O2'	9:LA:121:LYS:O	2.30	0.49
4:L3:2487:G:OP2	48:SM:152:LYS:NZ	2.45	0.49
5:L6:83:VAL:HG21	5:L6:114:VAL:HG11	1.94	0.49
22:LO:50:ASN:ND2	22:LO:75:SER:O	2.46	0.49
4:L3:400:A:OP1	9:LA:4:TYR:OH	2.25	0.49
4:L3:5022:U:HO2'	4:L3:5025:C:N4	2.08	0.49
24:LQ:84:GLU:O	24:LQ:87:VAL:HG22	2.12	0.49
43:SG:18:ILE:HD11	43:SG:81:ILE:HD11	1.95	0.49
48:SM:135:ASP:OD1	48:SM:199:ILE:HG23	2.13	0.49
50:SR:446:ILE:HG23	50:SR:447:MET:SD	2.53	0.49
4:L3:159:C:O2	5:L6:88:LYS:NZ	2.32	0.49
4:L3:1552:G:O2'	4:L3:1574:G:N2	2.44	0.49
4:L3:4745:G:H22	4:L3:4955:A:H2	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LB:67:ILE:HD12	10:LB:96:PRO:HD2	1.95	0.49
45:SI:148:THR:OG1	45:SI:243:ARG:NE	2.46	0.49
50:SR:73:ASP:OD1	50:SR:74:ASP:N	2.46	0.49
4:L3:1364:U:OP2	5:L6:36:ARG:NH2	2.45	0.48
4:L3:4672:A:OP1	15:LG:15:ARG:NH2	2.44	0.48
8:L9:165:THR:HG23	8:L9:168:GLY:H	1.78	0.48
37:NL:239:GLU:OE1	37:NL:239:GLU:N	2.43	0.48
4:L3:943:A:N6	40:SD:188:GLU:OE2	2.43	0.48
14:LF:26:THR:O	14:LF:30:GLU:OE1	2.32	0.48
50:SR:68:ASP:OD1	50:SR:69:PHE:N	2.46	0.48
48:SM:41:LYS:NZ	48:SM:122:GLU:OE1	2.47	0.48
4:L3:1238:A:O2'	40:SD:52:GLU:OE2	2.31	0.48
4:L3:2483:G:O6	48:SM:24:ARG:NE	2.45	0.48
21:LN:219:VAL:HG11	21:LN:337:VAL:CG2	2.44	0.48
4:L3:2590:G:O2'	4:L3:2755:A:N6	2.45	0.48
41:SE:92:ALA:O	41:SE:96:LEU:HD23	2.13	0.48
6:L7:23:VAL:HG13	6:L7:33:VAL:HG11	1.96	0.48
21:LN:107:ALA:HB2	21:LN:201:LEU:HG	1.95	0.48
42:SF:94:ALA:HB3	42:SF:102:LEU:CD2	2.44	0.48
4:L3:1432:G:O2'	4:L3:1452:A:N6	2.46	0.48
4:L3:2340:C:H4'	38:SA:42:THR:HG23	1.95	0.48
18:LJ:59:LYS:HE2	37:NL:279:LEU:HD13	1.96	0.48
21:LN:352:LEU:HD23	21:LN:352:LEU:H	1.78	0.48
4:L3:423:G:N2	9:LA:118:GLN:OE1	2.39	0.47
4:L3:2843:U:O2'	4:L3:4632:U:OP1	2.30	0.47
8:L9:68:ARG:NH1	8:L9:123:GLU:OE1	2.47	0.47
4:L3:1279:A:O2'	4:L3:1281:G:N7	2.40	0.47
4:L3:4440:G:C2	50:SR:96:LEU:HD13	2.49	0.47
16:LH:101:ASP:OD1	16:LH:102:VAL:N	2.47	0.47
30:LX:76:ALA:HB2	42:SF:80:GLU:HG2	1.96	0.47
18:LJ:83:THR:HG22	25:LR:95:PHE:CZ	2.49	0.47
27:LT:38:GLU:OE2	39:SC:284:HIS:NE2	2.44	0.47
39:SC:253:VAL:HG12	39:SC:257:ILE:HD12	1.96	0.47
4:L3:496:G:O2'	4:L3:497:G:OP1	2.25	0.47
31:LY:23:VAL:CG2	31:LY:64:LEU:HD21	2.45	0.47
16:LH:82:THR:HG21	26:LS:37:THR:CG2	2.44	0.47
18:LJ:52:LYS:O	18:LJ:65:ARG:NE	2.41	0.47
48:SM:183:LEU:HD11	48:SM:399:PHE:CE1	2.50	0.47
4:L3:1895:G:OP1	40:SD:96:ARG:NH2	2.47	0.47
4:L3:2485:U:HO2'	4:L3:2486:G:H8	1.63	0.47
4:L3:4124:G:N2	41:SE:43:GLN:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L6:64:VAL:O	5:L6:67:HIS:ND1	2.48	0.47
17:LI:79:VAL:HG21	17:LI:98:GLY:HA3	1.97	0.47
31:LY:66:VAL:HG23	31:LY:66:VAL:O	2.15	0.47
12:LD:7:GLN:NE2	12:LD:35:ALA:O	2.43	0.47
18:LJ:52:LYS:HE2	18:LJ:52:LYS:HA	1.97	0.47
10:LB:124:ASP:OD1	10:LB:125:GLN:N	2.48	0.47
48:SM:331:LYS:NZ	48:SM:353:GLU:OE1	2.28	0.47
4:L3:1210:C:H41	40:SD:66:ARG:CZ	2.29	0.46
38:SA:186:SER:O	38:SA:188:ARG:NH1	2.43	0.46
21:LN:219:VAL:HG11	21:LN:337:VAL:HG21	1.97	0.46
46:SK:107:VAL:HG13	46:SK:118:HIS:CB	2.45	0.46
1:BA:154:ASP:HB3	1:BA:160:VAL:HG23	1.98	0.46
45:SI:156:SER:OG	45:SI:252:ARG:NH2	2.48	0.46
4:L3:2045:G:O6	4:L3:3870:C:O2'	2.32	0.46
4:L3:3890:A:N6	4:L3:4570:G:O2'	2.46	0.46
17:LI:50:ARG:HE	17:LI:110:LYS:HD3	1.80	0.46
37:NL:452:GLU:OE1	48:SM:63:THR:HG21	2.15	0.46
4:L3:1573:G:OP1	12:LD:92:LYS:NZ	2.42	0.46
10:LB:23:ILE:HD11	38:SA:32:ILE:O	2.15	0.46
4:L3:1839:U:O2'	40:SD:111:LEU:O	2.33	0.46
4:L3:1895:G:O2'	4:L3:1907:A:N3	2.44	0.46
4:L3:2368:A:N6	4:L3:2827:G:O2'	2.49	0.46
4:L3:4980:C:N3	9:LA:69:ARG:NH2	2.62	0.46
11:LC:15:ARG:HB3	11:LC:27:LEU:HD23	1.98	0.46
40:SD:176:ALA:O	40:SD:180:GLY:N	2.49	0.46
42:SF:47:ASP:OD1	42:SF:48:ILE:N	2.49	0.46
4:L3:314:G:O2'	4:L3:4355:G:OP1	2.33	0.46
4:L3:2522:G:OP2	25:LR:29:ARG:NH2	2.49	0.46
6:L7:3:GLU:OE1	6:L7:31:ARG:NH2	2.49	0.46
6:L7:54:TYR:OH	6:L7:73:PHE:O	2.34	0.46
4:L3:730:G:OP2	40:SD:76:ARG:NE	2.47	0.46
4:L3:1892:A:OP2	4:L3:3875:G:N1	2.45	0.45
4:L3:4435:U:OP2	4:L3:4436:U:O2'	2.24	0.45
4:L3:4940:C:OP1	39:SC:156:ARG:NH2	2.48	0.45
4:L3:4768:G:OP1	6:L7:168:TYR:OH	2.31	0.45
4:L3:2489:C:OP1	48:SM:151:GLY:N	2.49	0.45
4:L3:5047:C:O2'	4:L3:5050:C:OP2	2.27	0.45
37:NL:286:GLN:OE1	37:NL:286:GLN:N	2.49	0.45
39:SC:49:VAL:O	39:SC:49:VAL:HG23	2.17	0.45
4:L3:1269:G:O2'	4:L3:1270:A:N3	2.49	0.45
4:L3:2296:G:O2'	38:SA:242:PRO:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:SK:98:GLU:OE2	51:SV:74:ARG:NH2	2.49	0.45
5:L6:126:LEU:HD21	26:LS:117:ARG:NH1	2.31	0.45
10:LB:147:GLU:OE2	10:LB:150:ARG:NH2	2.49	0.45
36:NK:20:LYS:NZ	50:SR:407:ASP:OD2	2.37	0.45
4:L3:2515:G:OP1	25:LR:37:LYS:NZ	2.48	0.45
31:LY:24:LYS:N	31:LY:35:LYS:O	2.50	0.45
46:SK:71:LEU:HD21	46:SK:132:VAL:HG21	1.99	0.45
4:L3:2664:G:OP1	12:LD:110:ARG:NH1	2.50	0.45
4:L3:4910:G:N2	6:L7:106:ASP:O	2.50	0.45
15:LG:39:ILE:HG23	15:LG:61:VAL:CG2	2.47	0.45
39:SC:281:ILE:HG23	39:SC:286:LEU:HD11	1.98	0.45
50:SR:108:ASN:OD1	50:SR:109:VAL:N	2.49	0.45
4:L3:4903:G:H3'	36:NK:84:LYS:HZ3	1.81	0.45
48:SM:128:ILE:HD12	48:SM:128:ILE:H	1.81	0.45
2:L1:36:G:N2	4:L3:20:U:OP2	2.50	0.44
8:L9:172:ARG:O	8:L9:188:ARG:NH1	2.50	0.44
46:SK:128:ILE:O	46:SK:132:VAL:HG22	2.17	0.44
49:SQ:150:GLU:OE2	49:SQ:154:ARG:NE	2.45	0.44
4:L3:934:C:HO2'	4:L3:935:A:P	2.40	0.44
4:L3:943:A:H62	40:SD:151:ASN:HD21	1.65	0.44
5:L6:63:THR:HG22	5:L6:64:VAL:N	2.33	0.44
44:SH:79:SER:O	44:SH:83:GLY:N	2.47	0.44
4:L3:2380:G:N2	4:L3:2425:U:OP1	2.45	0.44
7:L8:36:ALA:HB2	7:L8:52:PHE:CZ	2.52	0.44
4:L3:1433:A:N6	4:L3:1451:G:O2'	2.50	0.44
4:L3:2403:A:OP1	25:LR:10:ARG:NH1	2.49	0.44
16:LH:18:LYS:O	16:LH:22:LEU:N	2.43	0.44
4:L3:338:A:OP1	5:L6:31:ARG:NH2	2.51	0.44
4:L3:2667:C:OP2	12:LD:103:ARG:NH1	2.47	0.44
5:L6:62:PRO:O	5:L6:63:THR:OG1	2.27	0.44
16:LH:148:ASP:OD1	16:LH:152:LYS:NZ	2.39	0.44
32:LZ:12:PHE:CD2	32:LZ:51:LEU:HD22	2.53	0.44
22:LO:48:LEU:HD11	22:LO:60:ILE:HG21	1.99	0.44
4:L3:2546:G:OP1	48:SM:49:LYS:NZ	2.50	0.44
4:L3:2845:A:H61	4:L3:3843:C:N4	2.14	0.44
45:SI:44:LEU:O	45:SI:48:LYS:N	2.51	0.44
46:SK:100:ARG:NH1	51:SV:25:ASP:O	2.51	0.44
4:L3:2088:A:OP2	10:LB:38:ARG:NH1	2.49	0.44
17:LI:106:ILE:HG21	17:LI:109:LEU:HD23	1.99	0.44
31:LY:33:LYS:HG2	31:LY:46:VAL:HG12	1.99	0.44
50:SR:12:VAL:HG23	50:SR:12:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L1:156:U:O2	45:SI:57:ARG:NH2	2.51	0.43
4:L3:2900:U:OP1	37:NL:343:ARG:NH1	2.51	0.43
25:LR:75:SER:O	25:LR:75:SER:OG	2.34	0.43
47:SL:134:THR:HG23	47:SL:138:GLU:OE2	2.19	0.43
15:LG:12:ALA:O	21:LN:66:LYS:NZ	2.41	0.43
44:SH:126:VAL:HG23	44:SH:130:LEU:HD22	1.99	0.43
46:SK:103:ALA:O	46:SK:107:VAL:HG23	2.19	0.43
51:SV:22:VAL:O	51:SV:22:VAL:HG13	2.19	0.43
4:L3:2794:C:HO2'	4:L3:2795:A:H8	1.65	0.43
4:L3:4752:U:H4'	6:L7:4:VAL:HG11	1.99	0.43
4:L3:508:G:O2'	4:L3:510:U:OP2	2.25	0.43
4:L3:1364:U:OP2	5:L6:36:ARG:NH1	2.50	0.43
6:L7:193:THR:OG1	7:L8:119:ARG:NH1	2.52	0.43
4:L3:1449:C:OP1	10:LB:132:LYS:NZ	2.52	0.43
4:L3:1892:A:OP2	4:L3:3875:G:N2	2.51	0.43
37:NL:429:ARG:NH1	45:SI:183:GLU:OE1	2.51	0.43
4:L3:2580:U:HO2'	4:L3:2581:A:H5'	1.82	0.43
6:L7:84:VAL:HG11	6:L7:102:LEU:HD22	2.00	0.43
43:SG:43:VAL:HG21	43:SG:73:ILE:HD13	2.00	0.43
4:L3:1831:G:O2'	4:L3:1832:C:OP1	2.28	0.43
4:L3:3663:A:N6	4:L3:4168:G:O2'	2.52	0.43
17:LI:10:ASP:OD2	17:LI:11:ARG:N	2.52	0.43
29:LW:58:THR:HG22	29:LW:59:THR:N	2.34	0.43
4:L3:4662:C:O2'	4:L3:5004:C:OP1	2.35	0.43
45:SI:45:LEU:HD12	45:SI:48:LYS:HD2	2.01	0.43
4:L3:2545:U:O2'	4:L3:2547:G:N7	2.41	0.42
15:LG:39:ILE:HD12	15:LG:61:VAL:CG2	2.49	0.42
21:LN:71:GLU:OE2	51:SV:1:MET:N	2.39	0.42
46:SK:4:ARG:HB3	46:SK:208:LEU:HD23	2.01	0.42
49:SQ:60:TRP:HH2	49:SQ:112:VAL:HG12	1.82	0.42
4:L3:934:C:O2'	4:L3:935:A:P	2.78	0.42
4:L3:4628:U:O2'	51:SV:16:GLY:O	2.28	0.42
4:L3:2334:C:OP2	38:SA:195:LYS:NZ	2.48	0.42
4:L3:4405:G:N2	50:SR:20:ASP:OD1	2.48	0.42
4:L3:4910:G:H4'	21:LN:95:THR:HG22	2.01	0.42
30:LX:52:VAL:HG13	30:LX:52:VAL:O	2.19	0.42
49:SQ:122:MET:HE2	49:SQ:199:GLU:HA	2.01	0.42
19:LK:15:VAL:HG22	19:LK:15:VAL:O	2.20	0.42
48:SM:396:GLN:NE2	48:SM:400:ASP:OD2	2.48	0.42
50:SR:225:ILE:HG13	50:SR:271:LEU:HD21	2.02	0.42
19:LK:76:ASP:OD2	19:LK:77:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:SD:147:LEU:O	40:SD:150:VAL:HG22	2.19	0.42
46:SK:28:ILE:HG23	46:SK:28:ILE:O	2.18	0.42
47:SL:155:PHE:C	47:SL:156:LEU:HD12	2.40	0.42
4:L3:2625:U:OP2	50:SR:510:ARG:NH1	2.49	0.42
10:LB:67:ILE:HD13	10:LB:98:LEU:HD11	2.02	0.42
11:LC:99:ASP:OD2	11:LC:100:LEU:N	2.51	0.42
19:LK:91:ALA:N	19:LK:120:GLN:OE1	2.53	0.42
4:L3:2459:G:N2	4:L3:2462:C:OP2	2.48	0.42
4:L3:2756:G:C2	48:SM:59:THR:HG21	2.55	0.42
31:LY:57:LYS:NZ	31:LY:68:GLU:OE2	2.52	0.42
48:SM:12:GLY:O	48:SM:15:THR:HG22	2.19	0.42
4:L3:1239:C:H5	39:SC:60:SER:HG	1.68	0.42
5:L6:111:GLN:HA	5:L6:114:VAL:HG22	2.01	0.42
21:LN:135:LYS:HD3	36:NK:95:ILE:HD12	2.02	0.42
32:LZ:12:PHE:HD2	32:LZ:51:LEU:HD22	1.85	0.42
46:SK:199:VAL:HG23	46:SK:204:ALA:HB2	2.01	0.42
4:L3:2280:G:HO2'	4:L3:2281:U:H6	1.67	0.41
4:L3:2691:U:C2	4:L3:2692:U:C5	3.08	0.41
21:LN:298:LEU:HD23	21:LN:298:LEU:H	1.86	0.41
4:L3:92:C:H42	19:LK:59:LYS:NZ	2.19	0.41
8:L9:194:ARG:O	8:L9:197:THR:OG1	2.38	0.41
46:SK:73:PRO:O	46:SK:76:THR:HG22	2.20	0.41
4:L3:1457:G:O2'	10:LB:75:ARG:NH2	2.47	0.41
32:LZ:20:ASN:ND2	32:LZ:42:ARG:O	2.47	0.41
46:SK:74:ASN:OD1	51:SV:74:ARG:NH1	2.49	0.41
50:SR:477:MET:O	50:SR:481:ARG:HG3	2.20	0.41
4:L3:156:G:OP2	26:LS:106:LYS:NZ	2.54	0.41
4:L3:1508:A:OP1	38:SA:110:ARG:NH2	2.54	0.41
4:L3:1854:G:O2'	4:L3:1855:G:P	2.78	0.41
4:L3:4875:G:H2'	11:LC:169:THR:HG22	2.01	0.41
5:L6:146:LEU:HD12	5:L6:146:LEU:O	2.21	0.41
20:LL:58:LYS:O	20:LL:121:GLN:NE2	2.52	0.41
42:SF:117:GLU:O	42:SF:162:ASN:ND2	2.53	0.41
4:L3:2782:U:OP2	32:LZ:10:LYS:NZ	2.49	0.41
40:SD:29:LYS:O	40:SD:33:LEU:HD13	2.21	0.41
42:SF:116:LEU:HD12	42:SF:164:ALA:HB2	2.02	0.41
35:NF:9:LEU:HD21	35:NF:13:ARG:HH21	1.84	0.41
46:SK:211:THR:HG22	46:SK:212:SER:N	2.36	0.41
4:L3:2306:G:OP1	24:LQ:128:ARG:NH1	2.54	0.41
4:L3:4139:G:HO2'	4:L3:4140:C:H5	1.64	0.41
7:L8:43:THR:HG22	7:L8:43:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:SM:250:LEU:HD21	48:SM:276:LEU:HG	2.02	0.41
50:SR:447:MET:CE	51:SV:88:LYS:HG3	2.51	0.41
50:SR:577:VAL:O	50:SR:577:VAL:HG12	2.21	0.41
4:L3:2756:G:N3	48:SM:59:THR:HG21	2.36	0.41
4:L3:5022:U:HO2'	4:L3:5025:C:H42	1.51	0.41
11:LC:36:ASN:OD1	11:LC:39:VAL:HG23	2.21	0.41
12:LD:51:ILE:HD13	50:SR:512:ALA:HB1	2.03	0.41
45:SI:48:LYS:HA	45:SI:51:LYS:HD2	2.02	0.41
50:SR:324:THR:O	50:SR:326:GLU:N	2.54	0.41
4:L3:4428:A:H2	35:NF:59:ILE:HD13	1.85	0.41
46:SK:6:SER:HA	46:SK:13:ILE:HD11	2.03	0.40
4:L3:2418:A:OP1	9:LA:23:ARG:NH1	2.54	0.40
4:L3:4085:A:H2'	41:SE:54:PHE:O	2.22	0.40
18:LJ:17:ARG:NH1	18:LJ:18:TYR:OH	2.55	0.40
21:LN:165:HIS:HB3	21:LN:180:LEU:HD23	2.02	0.40
50:SR:107:ASP:OD1	50:SR:108:ASN:N	2.54	0.40
4:L3:1552:G:O2'	4:L3:1553:A:OP2	2.35	0.40
4:L3:2755:A:OP2	18:LJ:51:ARG:NH1	2.55	0.40
4:L3:5053:U:O2'	4:L3:5054:C:OP2	2.30	0.40
5:L6:186:ARG:HG2	5:L6:186:ARG:HH11	1.86	0.40
28:LU:57:ALA:HB1	28:LU:73:ILE:HD11	2.02	0.40
48:SM:378:VAL:HG11	48:SM:383:GLN:HG2	2.03	0.40
42:SF:45:VAL:HG13	42:SF:45:VAL:O	2.21	0.40
46:SK:173:LEU:O	46:SK:177:LEU:HD23	2.21	0.40
18:LJ:75:TYR:CB	18:LJ:80:LEU:HD21	2.51	0.40
39:SC:281:ILE:CG2	39:SC:286:LEU:HD11	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	158/165 (96%)	158 (100%)	0	0	100	100
5	L6	189/211 (90%)	185 (98%)	4 (2%)	0	100	100
6	L7	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
7	L8	133/215 (62%)	129 (97%)	4 (3%)	0	100	100
8	L9	179/204 (88%)	178 (99%)	1 (1%)	0	100	100
9	LA	151/184 (82%)	150 (99%)	1 (1%)	0	100	100
10	LB	149/188 (79%)	149 (100%)	0	0	100	100
11	LC	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
12	LD	123/196 (63%)	122 (99%)	1 (1%)	0	100	100
13	LE	100/160 (62%)	99 (99%)	1 (1%)	0	100	100
14	LF	101/128 (79%)	100 (99%)	1 (1%)	0	100	100
15	LG	123/140 (88%)	122 (99%)	1 (1%)	0	100	100
16	LH	141/156 (90%)	140 (99%)	1 (1%)	0	100	100
17	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
18	LJ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
19	LK	104/148 (70%)	102 (98%)	2 (2%)	0	100	100
20	LL	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
21	LN	354/403 (88%)	349 (99%)	5 (1%)	0	100	100
22	LO	93/115 (81%)	93 (100%)	0	0	100	100
23	LP	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
24	LQ	126/135 (93%)	126 (100%)	0	0	100	100
25	LR	107/117 (92%)	107 (100%)	0	0	100	100
26	LS	120/123 (98%)	120 (100%)	0	0	100	100
27	LT	107/110 (97%)	107 (100%)	0	0	100	100
28	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
29	LW	75/97 (77%)	73 (97%)	2 (3%)	0	100	100
30	LX	73/92 (79%)	72 (99%)	1 (1%)	0	100	100
31	LY	67/70 (96%)	67 (100%)	0	0	100	100
32	LZ	48/51 (94%)	48 (100%)	0	0	100	100
33	NB	67/549 (12%)	66 (98%)	1 (2%)	0	100	100
34	NC	52/731 (7%)	52 (100%)	0	0	100	100
35	NF	169/260 (65%)	167 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	NK	63/129 (49%)	63 (100%)	0	0	100	100
37	NL	306/478 (64%)	304 (99%)	2 (1%)	0	100	100
38	SA	356/427 (83%)	350 (98%)	6 (2%)	0	100	100
39	SC	208/288 (72%)	206 (99%)	2 (1%)	0	100	100
40	SD	223/248 (90%)	219 (98%)	4 (2%)	0	100	100
41	SE	213/266 (80%)	212 (100%)	1 (0%)	0	100	100
42	SF	154/257 (60%)	152 (99%)	2 (1%)	0	100	100
43	SG	188/192 (98%)	188 (100%)	0	0	100	100
44	SH	148/293 (50%)	146 (99%)	2 (1%)	0	100	100
45	SI	229/255 (90%)	225 (98%)	4 (2%)	0	100	100
46	SK	242/245 (99%)	238 (98%)	4 (2%)	0	100	100
47	SL	236/490 (48%)	232 (98%)	4 (2%)	0	100	100
48	SM	393/588 (67%)	392 (100%)	1 (0%)	0	100	100
49	SQ	215/239 (90%)	214 (100%)	1 (0%)	0	100	100
50	SR	580/634 (92%)	572 (99%)	8 (1%)	0	100	100
51	SV	135/163 (83%)	135 (100%)	0	0	100	100
All	All	7963/11167 (71%)	7884 (99%)	79 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	53/137 (39%)	53 (100%)	0	100	100
5	L6	159/177 (90%)	159 (100%)	0	100	100
6	L7	173/174 (99%)	173 (100%)	0	100	100
7	L8	115/161 (71%)	115 (100%)	0	100	100
8	L9	155/172 (90%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	LA	134/163 (82%)	134 (100%)	0	100	100
10	LB	136/165 (82%)	136 (100%)	0	100	100
11	LC	157/157 (100%)	157 (100%)	0	100	100
12	LD	118/175 (67%)	118 (100%)	0	100	100
13	LE	45/140 (32%)	45 (100%)	0	100	100
14	LF	93/115 (81%)	93 (100%)	0	100	100
15	LG	96/107 (90%)	96 (100%)	0	100	100
16	LH	124/133 (93%)	124 (100%)	0	100	100
17	LI	124/135 (92%)	124 (100%)	0	100	100
18	LJ	117/118 (99%)	116 (99%)	1 (1%)	78	91
19	LK	92/121 (76%)	92 (100%)	0	100	100
20	LL	109/121 (90%)	109 (100%)	0	100	100
21	LN	312/348 (90%)	312 (100%)	0	100	100
22	LO	80/97 (82%)	80 (100%)	0	100	100
23	LP	97/110 (88%)	96 (99%)	1 (1%)	76	91
24	LQ	114/121 (94%)	114 (100%)	0	100	100
25	LR	94/100 (94%)	94 (100%)	0	100	100
26	LS	109/110 (99%)	109 (100%)	0	100	100
27	LT	88/89 (99%)	88 (100%)	0	100	100
28	LU	86/89 (97%)	86 (100%)	0	100	100
29	LW	66/80 (82%)	66 (100%)	0	100	100
30	LX	62/75 (83%)	62 (100%)	0	100	100
31	LY	64/65 (98%)	64 (100%)	0	100	100
32	LZ	47/48 (98%)	47 (100%)	0	100	100
33	NB	65/485 (13%)	65 (100%)	0	100	100
34	NC	24/654 (4%)	23 (96%)	1 (4%)	30	64
35	NF	65/228 (28%)	65 (100%)	0	100	100
36	NK	61/115 (53%)	61 (100%)	0	100	100
37	NL	272/402 (68%)	270 (99%)	2 (1%)	84	93
38	SA	298/348 (86%)	297 (100%)	1 (0%)	92	97
39	SC	177/252 (70%)	176 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	SD	194/215 (90%)	194 (100%)	0	100 100
41	SE	186/223 (83%)	186 (100%)	0	100 100
42	SF	122/199 (61%)	122 (100%)	0	100 100
43	SG	169/171 (99%)	169 (100%)	0	100 100
44	SH	102/274 (37%)	102 (100%)	0	100 100
45	SI	208/228 (91%)	208 (100%)	0	100 100
46	SK	212/213 (100%)	212 (100%)	0	100 100
47	SL	101/437 (23%)	101 (100%)	0	100 100
48	SM	354/509 (70%)	353 (100%)	1 (0%)	92 97
49	SQ	194/214 (91%)	193 (100%)	1 (0%)	88 95
50	SR	533/574 (93%)	532 (100%)	1 (0%)	93 98
51	SV	127/149 (85%)	127 (100%)	0	100 100
All	All	6683/9693 (69%)	6673 (100%)	10 (0%)	93 98

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	LJ	128	LYS
23	LP	93	ASN
34	NC	131	LYS
37	NL	381	ARG
37	NL	458	LYS
38	SA	95	MET
39	SC	56	ARG
48	SM	218	ARG
49	SQ	9	LYS
50	SR	584	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
9	LA	80	GLN
11	LC	91	HIS
28	LU	15	HIS
29	LW	76	HIS
34	NC	133	HIS
37	NL	366	GLN

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Mol	Chain	Res	Type
39	SC	136	HIS
39	SC	190	HIS
46	SK	83	HIS
48	SM	211	HIS
48	SM	245	HIS
50	SR	157	HIS
50	SR	209	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	17 (11%)	0
3	L2	64/1167 (5%)	9 (14%)	0
4	L3	2797/5070 (55%)	346 (12%)	9 (0%)
All	All	3013/6394 (47%)	372 (12%)	9 (0%)

All (372) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	34	U
2	L1	35	C
2	L1	59	A
2	L1	60	G
2	L1	62	A
2	L1	63	U
2	L1	82	A
2	L1	83	C
2	L1	84	A
2	L1	86	U
2	L1	94	G
2	L1	103	A
2	L1	105	C
2	L1	111	U
2	L1	114	G
2	L1	127	U
2	L1	151	G
3	L2	11	C
3	L2	48	G
3	L2	49	G
3	L2	62	U
3	L2	87	G

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Mol	Chain	Res	Type
3	L2	91	C
3	L2	95	A
3	L2	96	A
3	L2	101	A
4	L3	13	U
4	L3	38	A
4	L3	48	G
4	L3	56	A
4	L3	58	G
4	L3	59	A
4	L3	64	A
4	L3	65	A
4	L3	69	A
4	L3	91	G
4	L3	108	A
4	L3	119	G
4	L3	159	C
4	L3	171	U
4	L3	172	C
4	L3	173	C
4	L3	181	C
4	L3	200	U
4	L3	210	C
4	L3	218	A
4	L3	233	U
4	L3	234	G
4	L3	246	G
4	L3	261	G
4	L3	263	G
4	L3	266	C
4	L3	267	G
4	L3	296	A
4	L3	316	U
4	L3	340	C
4	L3	386	A
4	L3	387	G
4	L3	409	G
4	L3	410	A
4	L3	412	G
4	L3	435	A
4	L3	440	U
4	L3	450	G

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Mol	Chain	Res	Type
4	L3	452	A
4	L3	453	G
4	L3	454	U
4	L3	464	G
4	L3	467	U
4	L3	469	C
4	L3	472	C
4	L3	473	C
4	L3	478	G
4	L3	487	G
4	L3	492	U
4	L3	493	G
4	L3	496	G
4	L3	497	G
4	L3	499	G
4	L3	501	C
4	L3	502	C
4	L3	503	C
4	L3	504	G
4	L3	509	A
4	L3	510	U
4	L3	511	C
4	L3	657	C
4	L3	658	C
4	L3	660	A
4	L3	666	G
4	L3	667	A
4	L3	668	C
4	L3	669	C
4	L3	686	A
4	L3	704	C
4	L3	729	G
4	L3	730	G
4	L3	731	G
4	L3	739	G
4	L3	741	C
4	L3	742	G
4	L3	746	A
4	L3	757	G
4	L3	913	U
4	L3	914	U
4	L3	915	A

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Mol	Chain	Res	Type
4	L3	916	C
4	L3	917	A
4	L3	926	G
4	L3	932	A
4	L3	933	G
4	L3	935	A
4	L3	944	A
4	L3	945	U
4	L3	960	A
4	L3	1066	G
4	L3	1070	G
4	L3	1072	C
4	L3	1080	C
4	L3	1211	G
4	L3	1253	G
4	L3	1254	A
4	L3	1255	A
4	L3	1256	G
4	L3	1266	G
4	L3	1269	G
4	L3	1270	A
4	L3	1272	C
4	L3	1273	G
4	L3	1280	C
4	L3	1284	G
4	L3	1287	G
4	L3	1294	A
4	L3	1295	C
4	L3	1301	C
4	L3	1313	C
4	L3	1314	C
4	L3	1315	C
4	L3	1354	A
4	L3	1358	G
4	L3	1359	G
4	L3	1365	C
4	L3	1366	G
4	L3	1379	C
4	L3	1397	A
4	L3	1420	A
4	L3	1489	G
4	L3	1497	A

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Mol	Chain	Res	Type
4	L3	1498	G
4	L3	1502	G
4	L3	1523	A
4	L3	1534	A
4	L3	1547	A
4	L3	1578	U
4	L3	1613	A
4	L3	1614	C
4	L3	1654	G
4	L3	1661	C
4	L3	1671	U
4	L3	1676	C
4	L3	1677	U
4	L3	1678	C
4	L3	1680	G
4	L3	1684	A
4	L3	1691	G
4	L3	1734	G
4	L3	1804	A
4	L3	1813	U
4	L3	1815	G
4	L3	1824	G
4	L3	1826	G
4	L3	1827	C
4	L3	1829	G
4	L3	1832	C
4	L3	1833	G
4	L3	1835	G
4	L3	1836	G
4	L3	1837	A
4	L3	1842	G
4	L3	1854	G
4	L3	1855	G
4	L3	1870	C
4	L3	1881	C
4	L3	1883	G
4	L3	1891	A
4	L3	1897	A
4	L3	1910	G
4	L3	1919	G
4	L3	1921	C
4	L3	1922	G

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Mol	Chain	Res	Type
4	L3	1925	G
4	L3	1931	C
4	L3	1941	A
4	L3	1974	U
4	L3	1984	A
4	L3	1997	U
4	L3	2002	A
4	L3	2021	G
4	L3	2025	A
4	L3	2026	A
4	L3	2041	A
4	L3	2042	A
4	L3	2046	G
4	L3	2055	G
4	L3	2056	G
4	L3	2069	A
4	L3	2084	C
4	L3	2289	C
4	L3	2300	A
4	L3	2301	G
4	L3	2313	A
4	L3	2348	G
4	L3	2351	C
4	L3	2416	G
4	L3	2417	A
4	L3	2422	C
4	L3	2424	G
4	L3	2425	U
4	L3	2450	G
4	L3	2453	A
4	L3	2470	C
4	L3	2471	G
4	L3	2475	G
4	L3	2476	G
4	L3	2477	A
4	L3	2478	C
4	L3	2480	G
4	L3	2487	G
4	L3	2489	C
4	L3	2492	C
4	L3	2493	G
4	L3	2511	A

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Mol	Chain	Res	Type
4	L3	2512	A
4	L3	2513	A
4	L3	2519	U
4	L3	2520	C
4	L3	2529	A
4	L3	2544	G
4	L3	2545	U
4	L3	2548	C
4	L3	2554	U
4	L3	2587	A
4	L3	2589	C
4	L3	2627	C
4	L3	2653	C
4	L3	2669	C
4	L3	2687	U
4	L3	2694	G
4	L3	2695	A
4	L3	2696	A
4	L3	2711	G
4	L3	2743	A
4	L3	2760	G
4	L3	2764	A
4	L3	2769	U
4	L3	2771	G
4	L3	2788	U
4	L3	2790	U
4	L3	2814	C
4	L3	2826	U
4	L3	2827	G
4	L3	2829	U
4	L3	2902	G
4	L3	2917	G
4	L3	2918	G
4	L3	3271	G
4	L3	3585	G
4	L3	3593	C
4	L3	3595	U
4	L3	3597	G
4	L3	3662	A
4	L3	3840	U
4	L3	3867	A
4	L3	3875	G

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Mol	Chain	Res	Type
4	L3	3881	G
4	L3	3887	C
4	L3	4084	G
4	L3	4085	A
4	L3	4119	C
4	L3	4121	G
4	L3	4122	G
4	L3	4127	A
4	L3	4133	C
4	L3	4139	G
4	L3	4140	C
4	L3	4142	C
4	L3	4143	G
4	L3	4144	C
4	L3	4145	C
4	L3	4147	G
4	L3	4150	G
4	L3	4152	G
4	L3	4154	G
4	L3	4162	C
4	L3	4163	U
4	L3	4348	A
4	L3	4349	C
4	L3	4350	C
4	L3	4368	G
4	L3	4369	A
4	L3	4401	G
4	L3	4415	A
4	L3	4418	G
4	L3	4437	U
4	L3	4438	U
4	L3	4439	U
4	L3	4464	A
4	L3	4466	C
4	L3	4475	G
4	L3	4476	C
4	L3	4499	G
4	L3	4503	A
4	L3	4512	U
4	L3	4513	A
4	L3	4519	C
4	L3	4523	A

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Mol	Chain	Res	Type
4	L3	4524	G
4	L3	4573	G
4	L3	4574	U
4	L3	4575	G
4	L3	4590	A
4	L3	4608	G
4	L3	4636	U
4	L3	4637	G
4	L3	4656	A
4	L3	4670	C
4	L3	4672	A
4	L3	4678	G
4	L3	4683	U
4	L3	4684	A
4	L3	4700	A
4	L3	4708	A
4	L3	4709	U
4	L3	4719	G
4	L3	4720	C
4	L3	4740	G
4	L3	4741	C
4	L3	4742	G
4	L3	4750	G
4	L3	4751	G
4	L3	4754	G
4	L3	4757	C
4	L3	4759	C
4	L3	4765	G
4	L3	4772	C
4	L3	4773	C
4	L3	4870	G
4	L3	4871	C
4	L3	4882	U
4	L3	4883	C
4	L3	4900	C
4	L3	4901	G
4	L3	4910	G
4	L3	4916	G
4	L3	4943	A
4	L3	4976	U
4	L3	5006	U
4	L3	5007	A

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Mol	Chain	Res	Type
4	L3	5014	A
4	L3	5020	G
4	L3	5022	U
4	L3	5024	C
4	L3	5025	C
4	L3	5026	U
4	L3	5027	C
4	L3	5031	G
4	L3	5041	G
4	L3	5050	C
4	L3	5054	C
4	L3	5061	A
4	L3	5062	G
4	L3	5069	U

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L3	408	A
4	L3	496	G
4	L3	502	C
4	L3	503	C
4	L3	934	C
4	L3	1831	G
4	L3	2486	G
4	L3	4699	U
4	L3	4881	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 70 ligands modelled in this entry, 69 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	GDP	SR	1001	55,52	24,30,30	2.56	8 (33%)	30,47,47	1.75	9 (30%)

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
54	GDP	SR	1001	55,52	-	2/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	SR	1001	GDP	O6-C6	8.36	1.40	1.23
54	SR	1001	GDP	C2-N2	4.71	1.45	1.34
54	SR	1001	GDP	O4'-C1'	4.39	1.47	1.41
54	SR	1001	GDP	C2'-C1'	-2.36	1.50	1.53
54	SR	1001	GDP	C5-C4	2.32	1.49	1.43
54	SR	1001	GDP	PB-O3B	-2.21	1.46	1.54
54	SR	1001	GDP	PB-O2B	-2.21	1.46	1.54
54	SR	1001	GDP	C2'-C3'	-2.06	1.47	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	SR	1001	GDP	C3'-C2'-C1'	4.04	107.06	100.98
54	SR	1001	GDP	C5-C6-N1	3.33	119.83	113.95
54	SR	1001	GDP	O3B-PB-O3A	2.97	114.60	104.64
54	SR	1001	GDP	PA-O3A-PB	-2.86	123.00	132.83
54	SR	1001	GDP	C2-N1-C6	-2.86	119.83	125.10
54	SR	1001	GDP	O2B-PB-O3A	2.78	113.96	104.64
54	SR	1001	GDP	C2'-C3'-C4'	2.63	107.76	102.64
54	SR	1001	GDP	O6-C6-C5	-2.23	120.03	124.37
54	SR	1001	GDP	O2A-PA-O1A	-2.16	101.58	112.24

There are no chirality outliers.

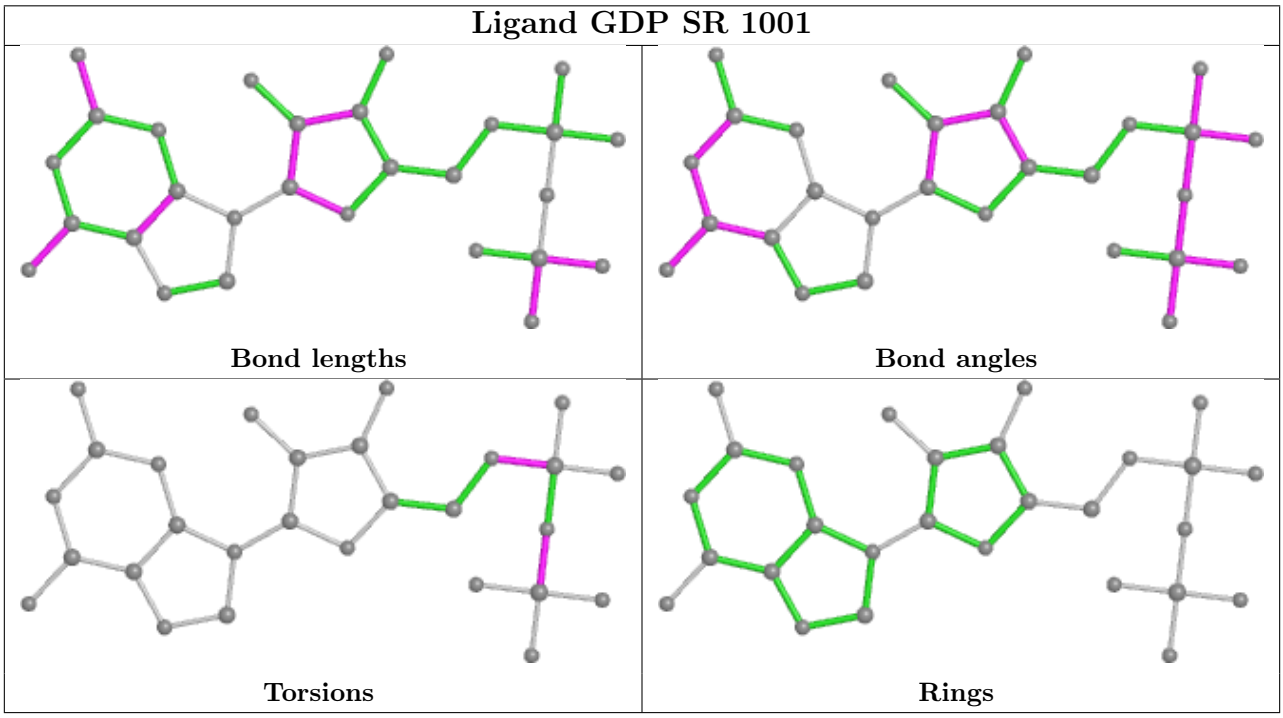
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	SR	1001	GDP	PA-O3A-PB-O1B
54	SR	1001	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

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.



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.

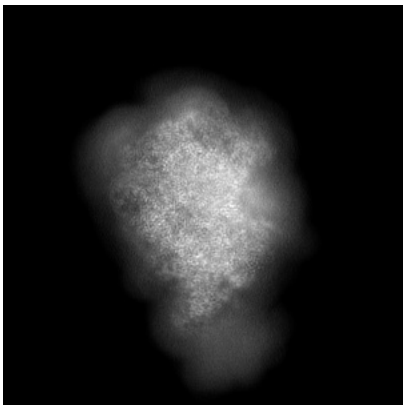
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29262. These allow visual inspection of the internal detail of the map and identification of artifacts.

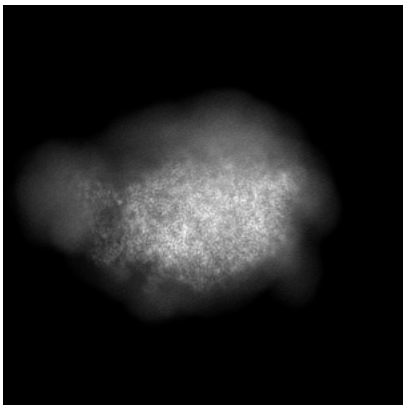
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

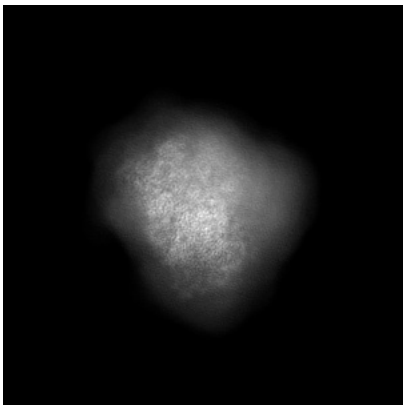
6.1.1 Primary map



X

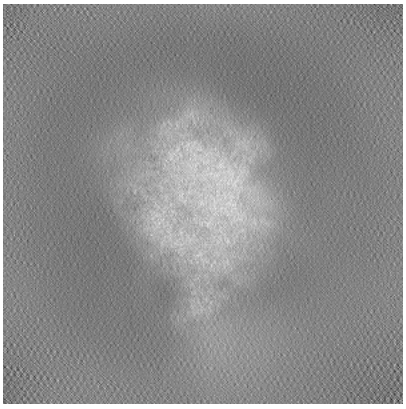


Y

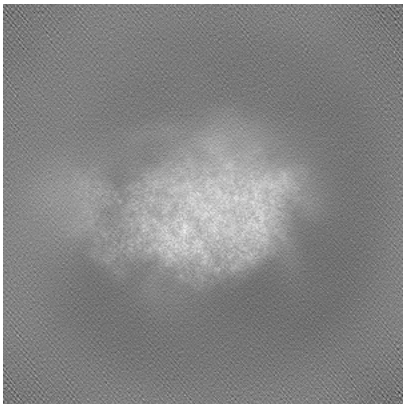


Z

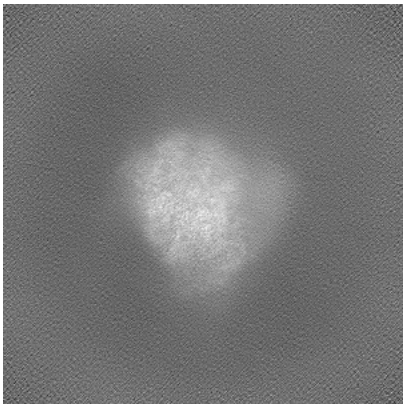
6.1.2 Raw map



X



Y

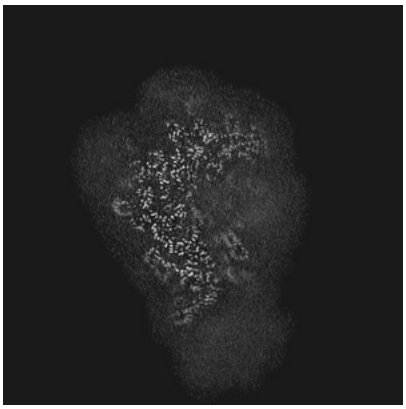


Z

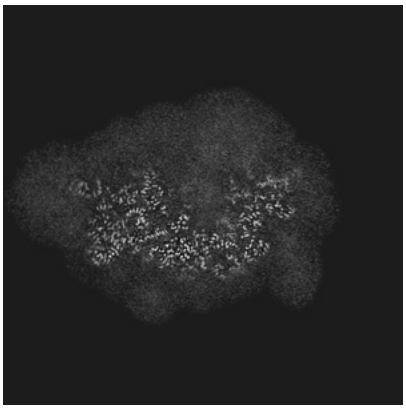
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

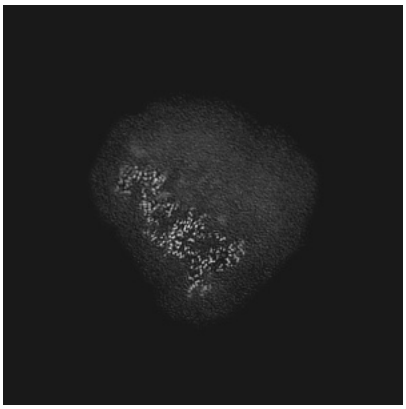
6.2.1 Primary map



X Index: 240

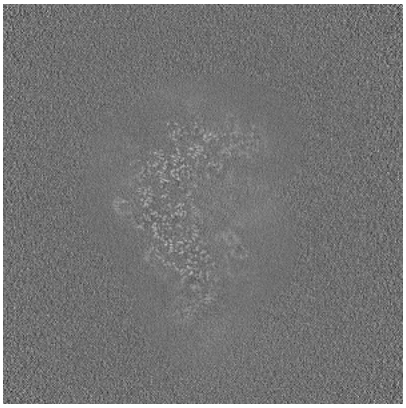


Y Index: 240

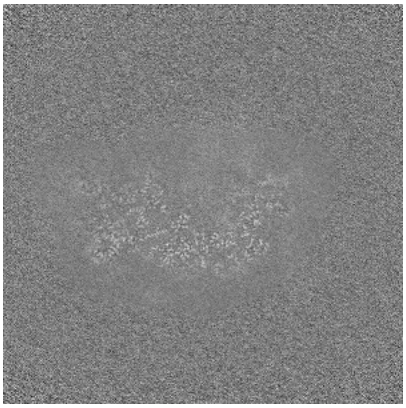


Z Index: 240

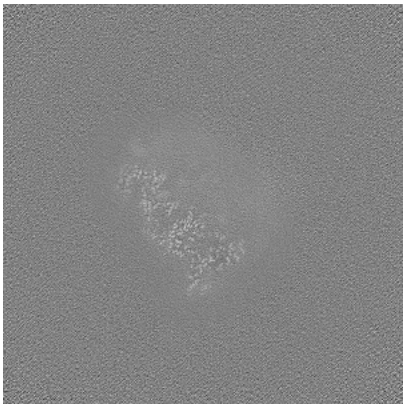
6.2.2 Raw map



X Index: 240



Y Index: 240

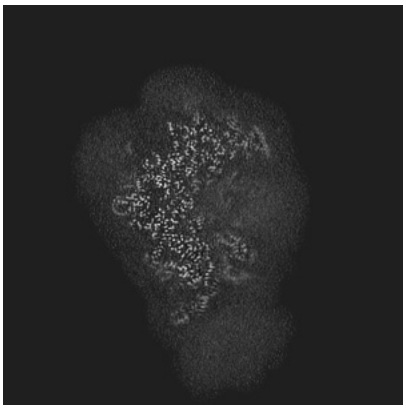


Z Index: 240

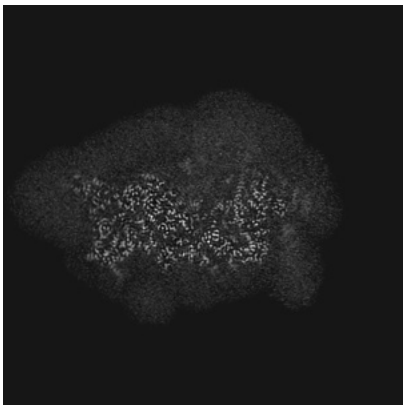
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

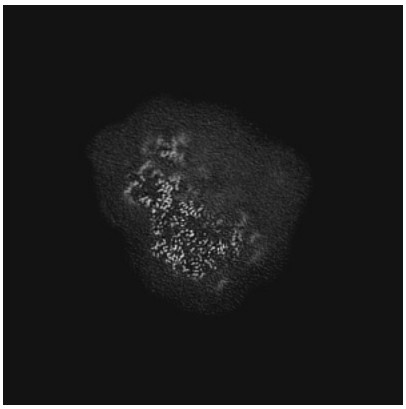
6.3.1 Primary map



X Index: 237

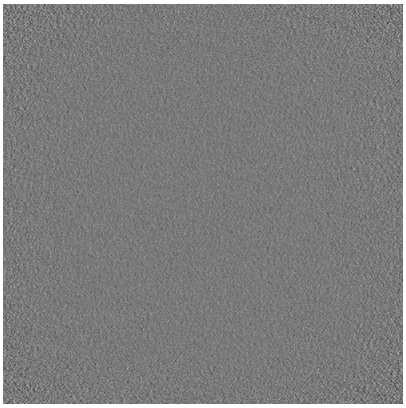


Y Index: 231

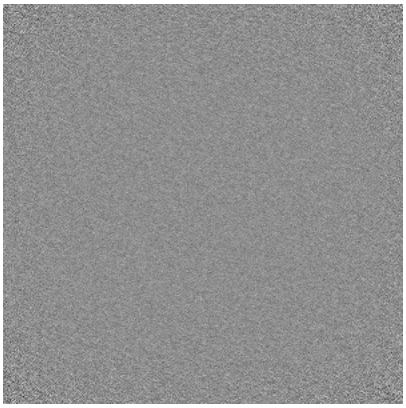


Z Index: 217

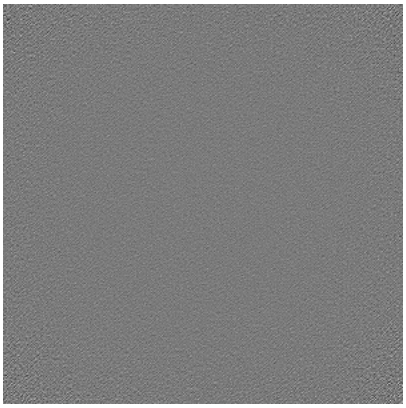
6.3.2 Raw map



X Index: 0



Y Index: 0

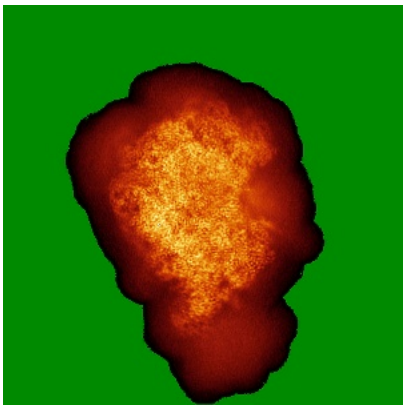


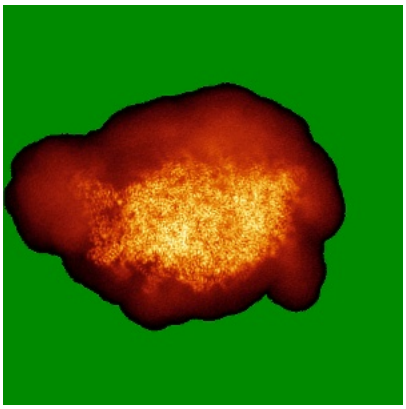
Z Index: 0

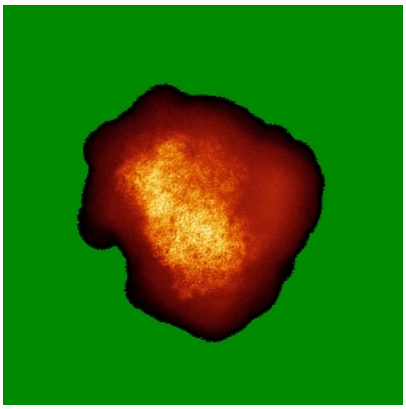
The images above show the largest variance slices of the map in three orthogonal directions.

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

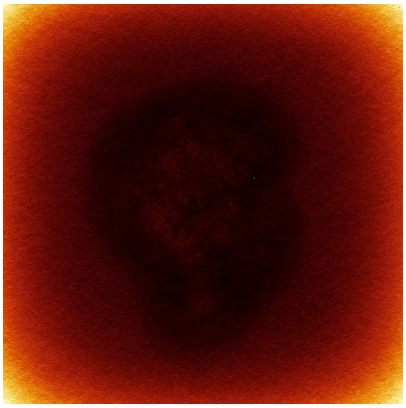
6.4.1 Primary map

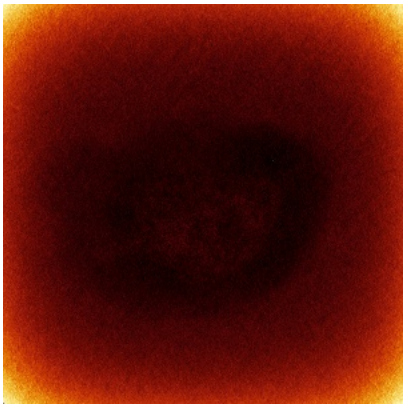

X

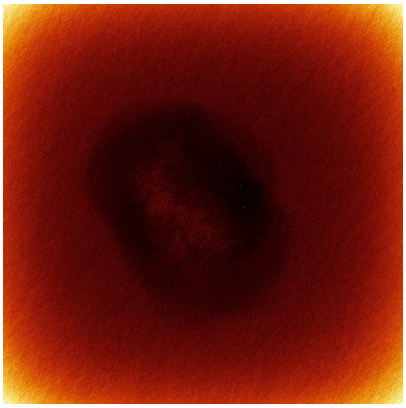

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

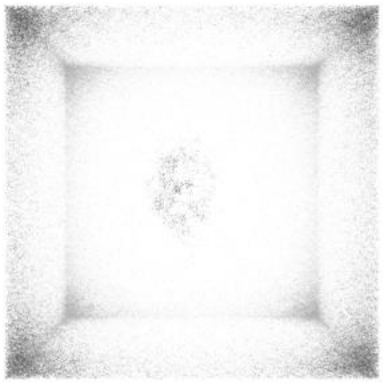
X

Y

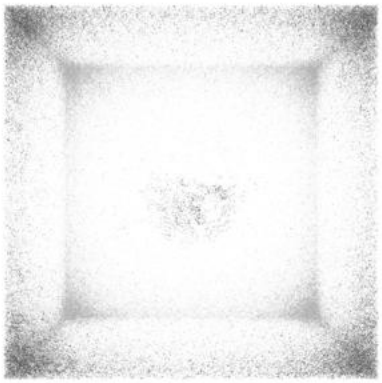
Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y

Z

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

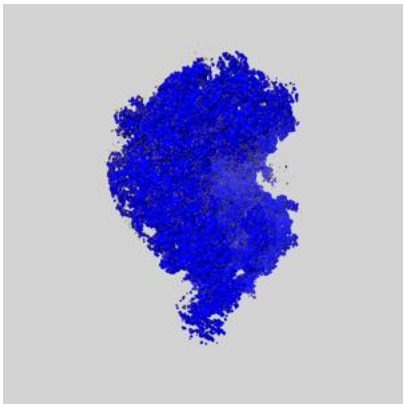
6.6 Mask visualisation (i)

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

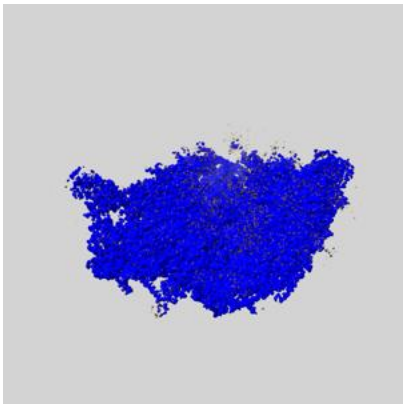
A mask typically either:

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

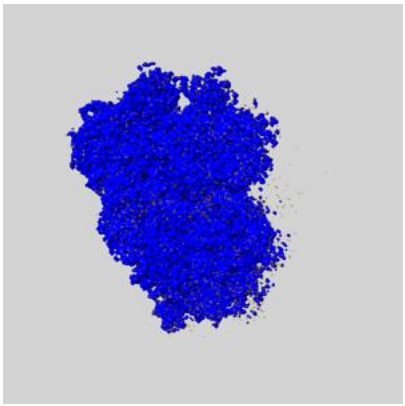
6.6.1 emd_29262_msk_1.map (i)



X



Y

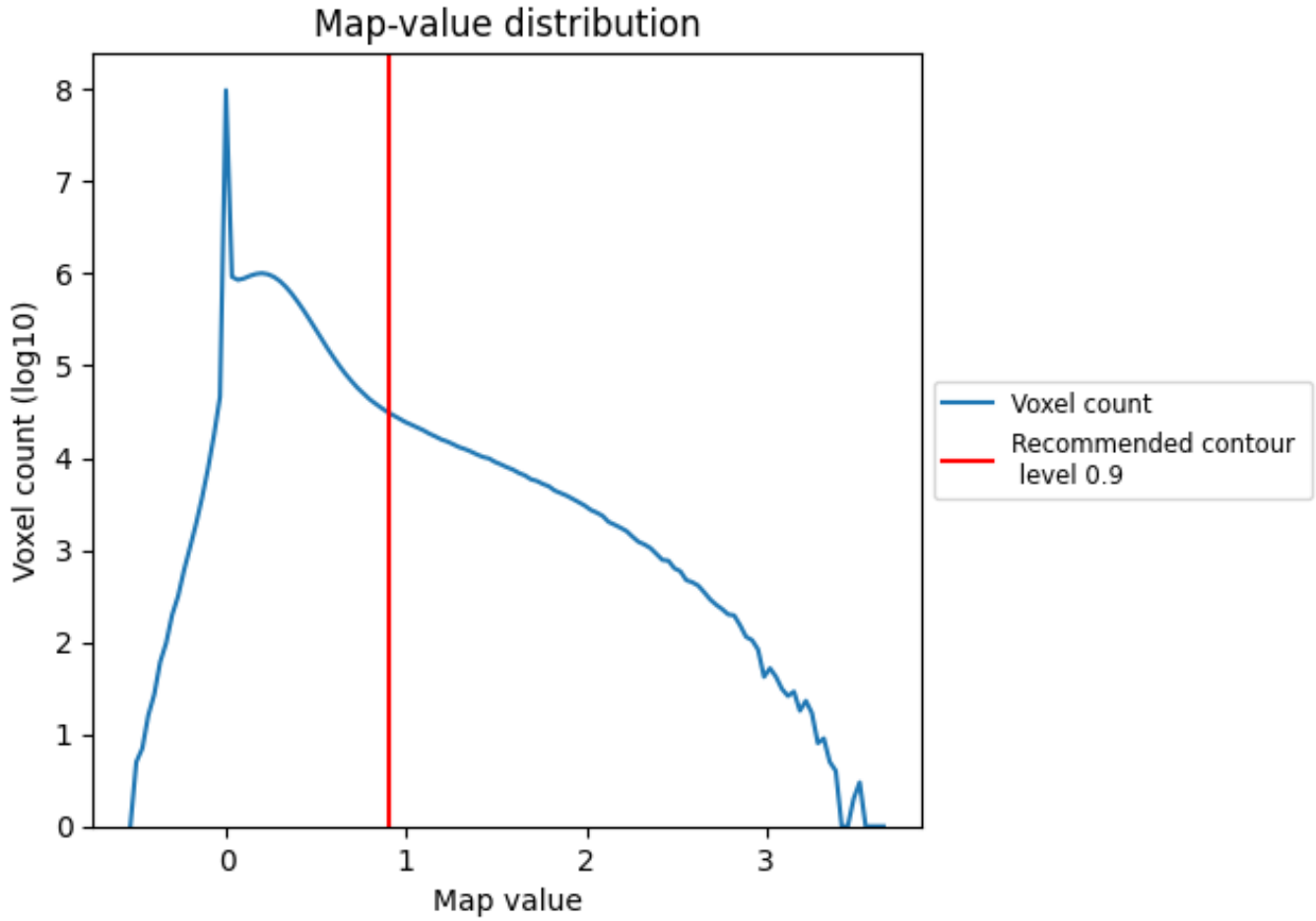


Z

7 Map analysis

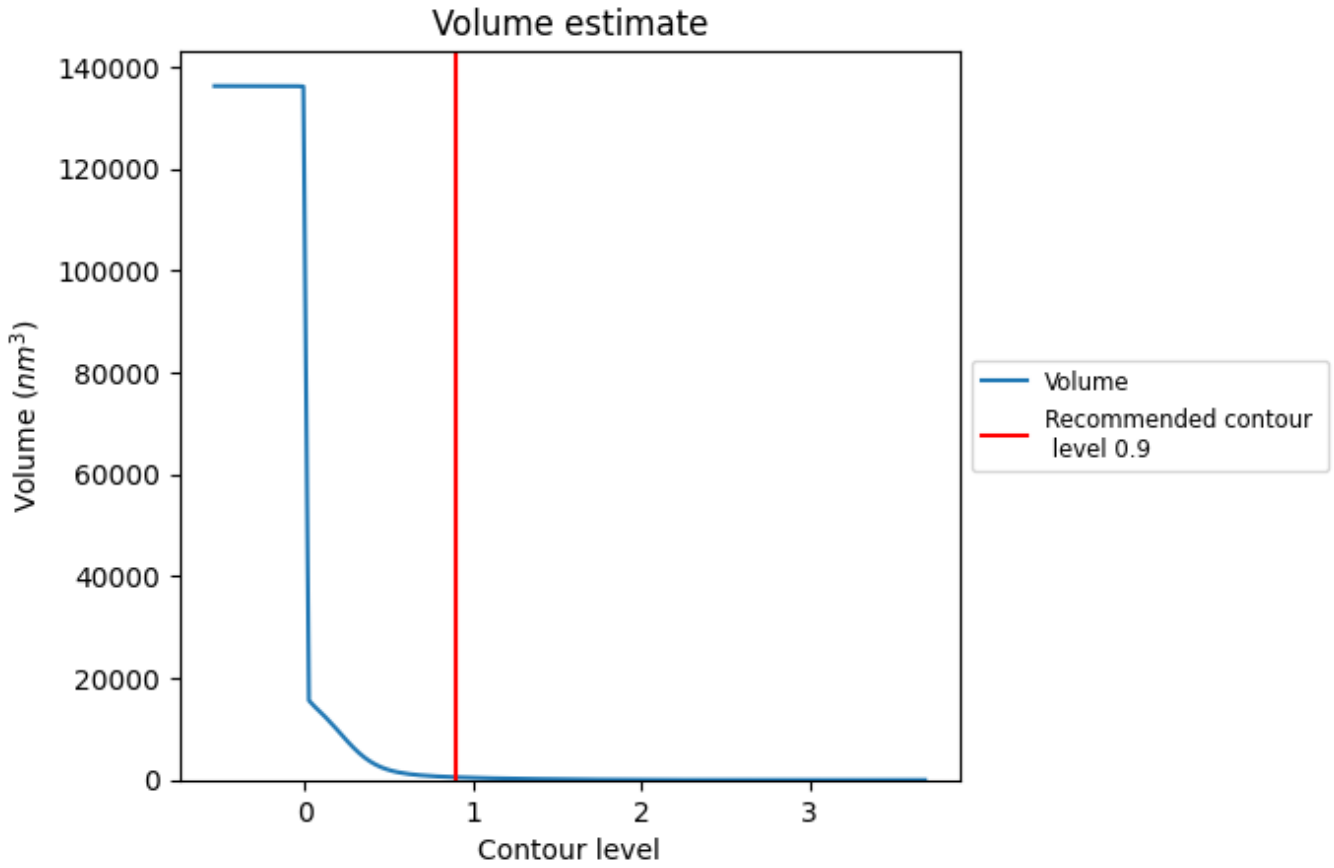
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

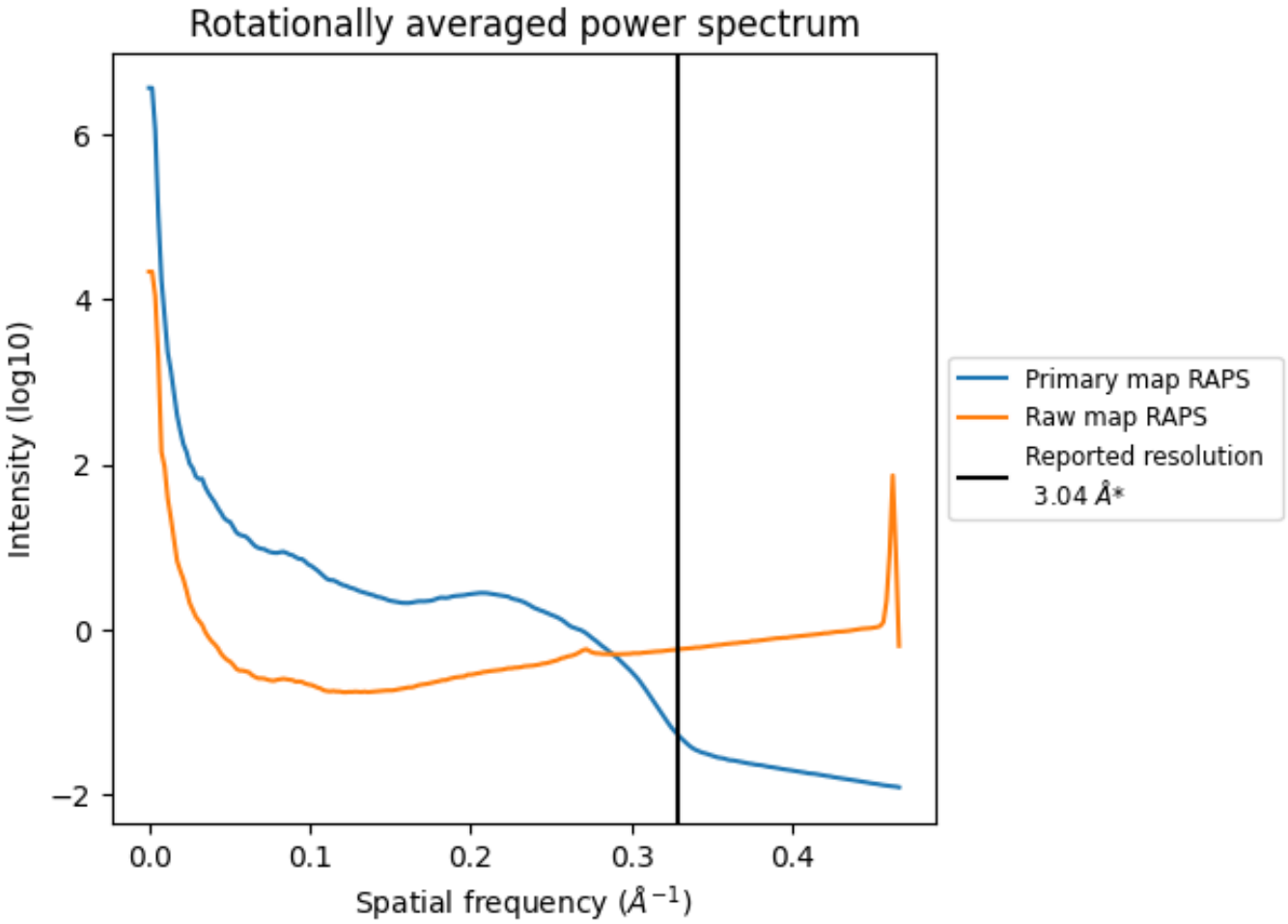
7.2 Volume estimate



The volume at the recommended contour level is 538 nm^3; this corresponds to an approximate mass of 486 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)

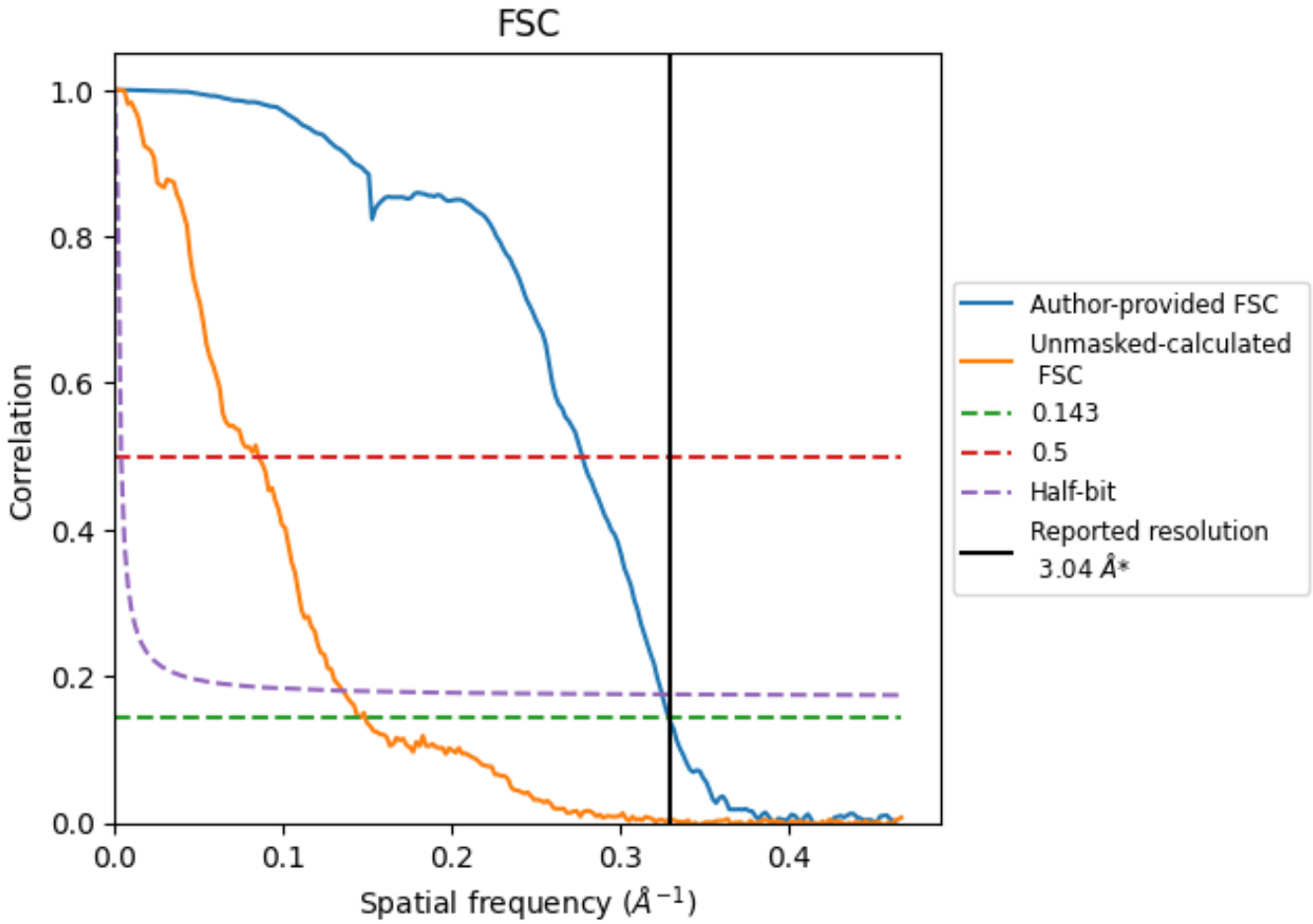


*Reported resolution corresponds to spatial frequency of 0.329 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.329 Å^{-1}

8.2 Resolution estimates (i)

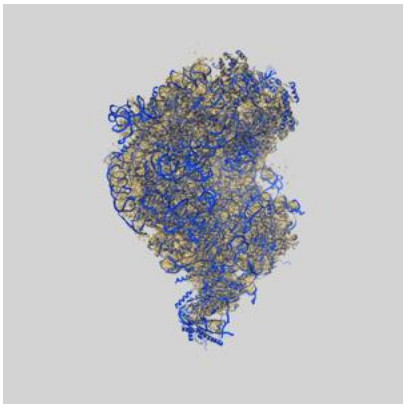
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.61	3.08
Unmasked-calculated*	6.72	11.74	7.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.72 differs from the reported value 3.04 by more than 10 %

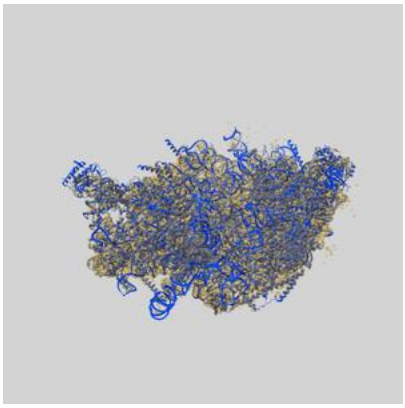
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29262 and PDB model 8FKZ. Per-residue inclusion information can be found in section 3 on page 14.

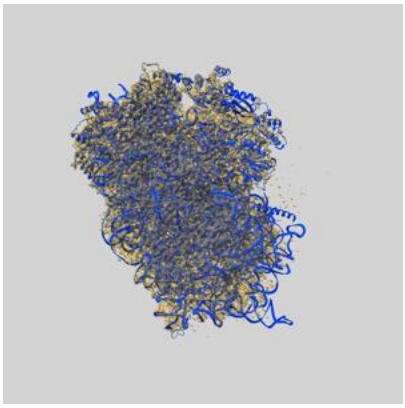
9.1 Map-model overlay



X



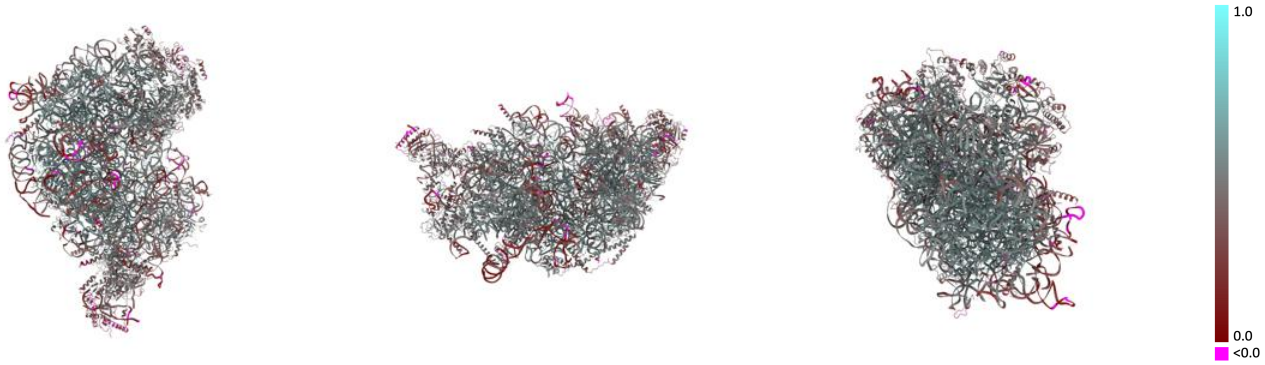
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

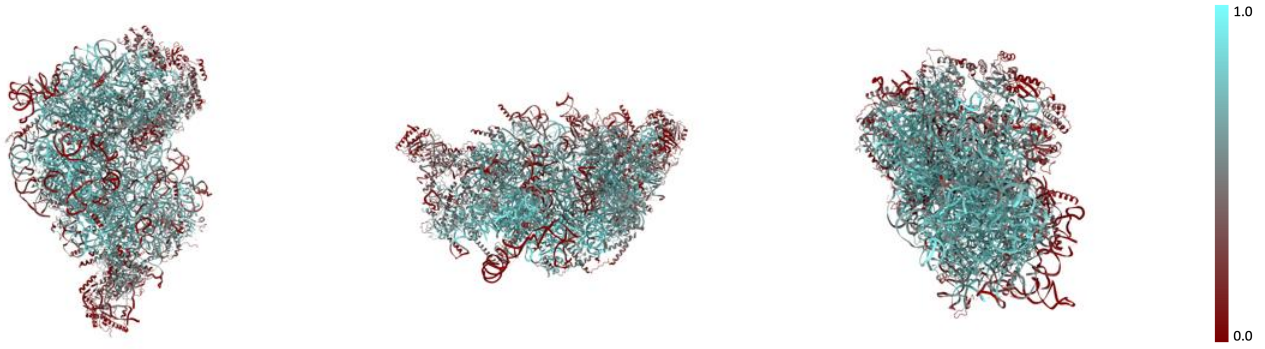
9.2 Q-score mapped to coordinate model



X Y Z

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

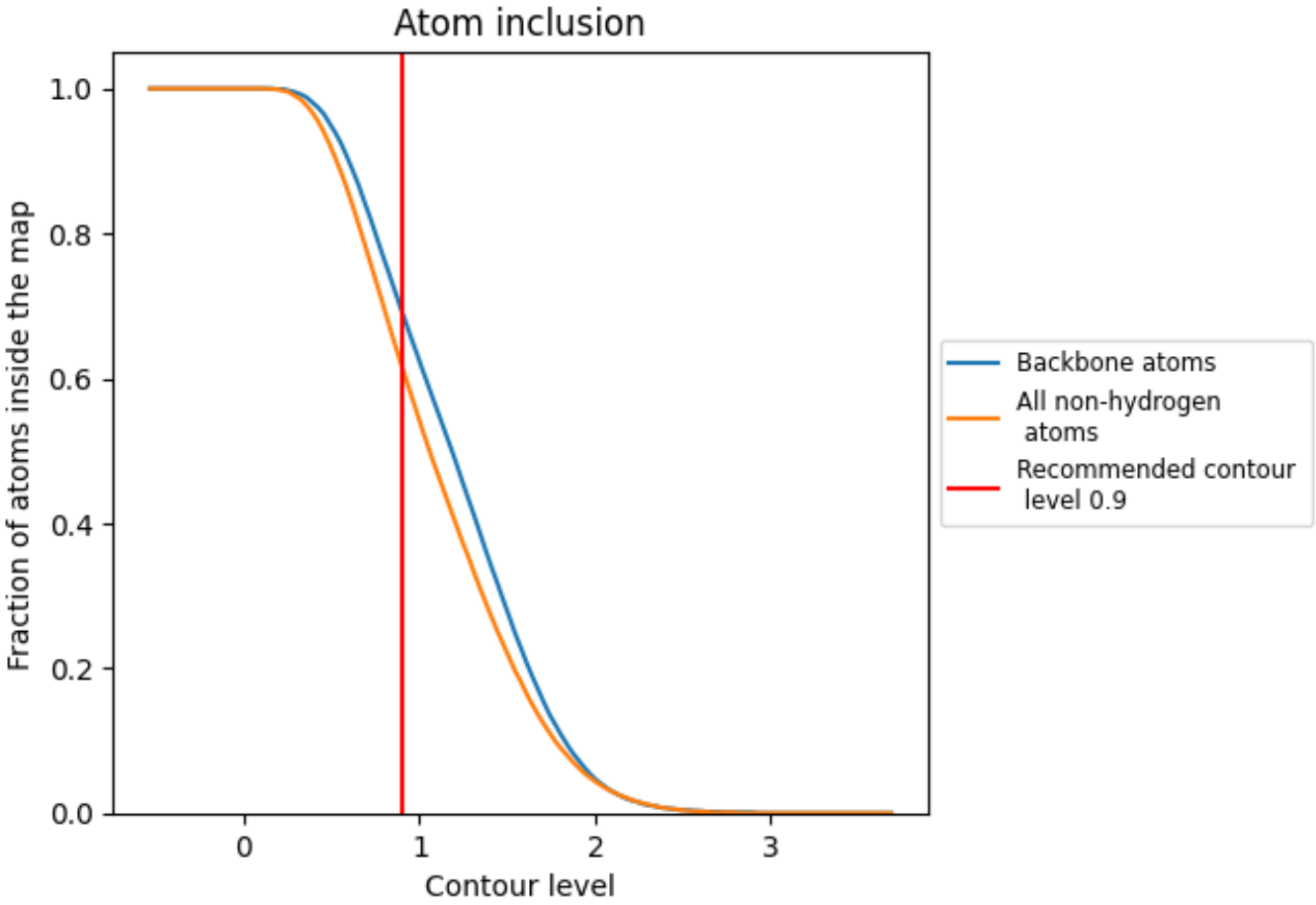
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 62% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6160	0.4700
BA	0.1360	0.3060
L1	0.8390	0.5320
L2	0.2590	0.3420
L3	0.6610	0.4500
L6	0.5850	0.4790
L7	0.7130	0.5450
L8	0.7260	0.5420
L9	0.7790	0.5570
LA	0.6830	0.5320
LB	0.7220	0.5660
LC	0.7030	0.5410
LD	0.5910	0.4850
LE	0.2430	0.3650
LF	0.6420	0.5010
LG	0.5090	0.4720
LH	0.6310	0.4990
LI	0.6850	0.5420
LJ	0.6680	0.4920
LK	0.6180	0.5400
LL	0.7240	0.5520
LN	0.6820	0.5310
LO	0.5550	0.4900
LP	0.6690	0.5210
LQ	0.7350	0.5670
LR	0.7160	0.5470
LS	0.6590	0.5250
LT	0.8040	0.5760
LU	0.5090	0.4450
LW	0.7540	0.5570
LX	0.4360	0.4180
LY	0.5240	0.4940
LZ	0.7330	0.5630
NB	0.3650	0.4410
NC	0.2800	0.4270

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Chain	Atom inclusion	Q-score
NF	0.4720	0.4720
NK	0.3990	0.4640
NL	0.4270	0.4390
SA	0.7220	0.5580
SC	0.5680	0.5130
SD	0.6960	0.5350
SE	0.5280	0.4290
SF	0.5600	0.4970
SG	0.6250	0.5220
SH	0.3020	0.3510
SI	0.4370	0.4230
SK	0.5290	0.4560
SL	0.1930	0.3450
SM	0.6100	0.4720
SQ	0.3150	0.4100
SR	0.4490	0.4500
SV	0.6440	0.4960