Full wwPDB EM Validation Report ⓘ

Jul 13, 2023 – 08:04 PM EDT

PDB ID	:	8FKT
EMDB ID	:	EMD-29256
Title	:	Human nucleolar pre-60S ribosomal subunit (State C1)
Authors	:	Vanden Broeck, A.; Klinge, S.
Deposited on	:	2022-12-21
Resolution	:	2.81 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:

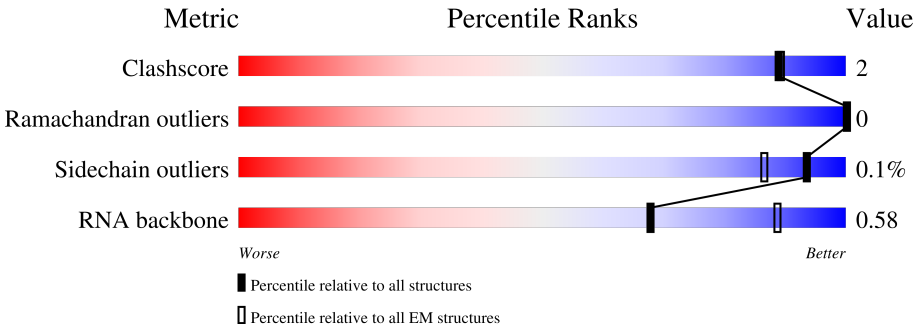
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.81 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	61%, 90%, 7%
2	BB	217	74%, 98%
3	L1	157	15%, 82%, 13%
4	L2	1167	94%
5	L3	5070	6%, 34%, 7%, 58%
6	L6	211	52%, 5%, 43%
7	L7	203	95%

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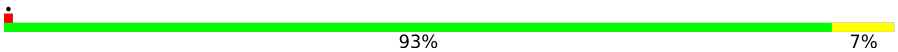
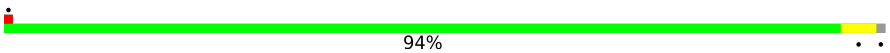
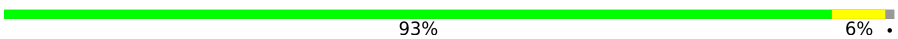
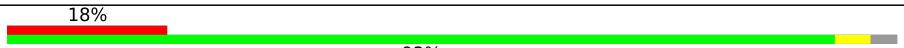
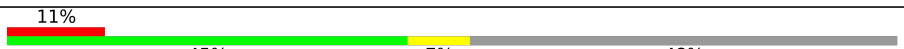
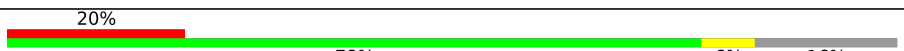
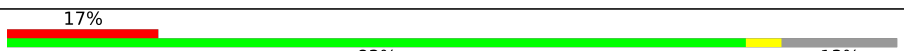
Mol	Chain	Length	Quality of chain
8	L8	215	
9	L9	204	
10	LA	184	
11	LB	188	
12	LC	176	
13	LE	160	
14	LG	140	
15	LH	156	
16	LI	145	
17	LK	148	
18	LN	403	
19	LQ	135	
20	LS	123	
21	LT	110	
22	LU	105	
23	LW	97	
24	NB	549	
25	NF	260	
26	NH	180	
27	NI	881	
28	NK	129	
29	NM	300	
30	NO	461	
31	NQ	385	
32	NS	349	

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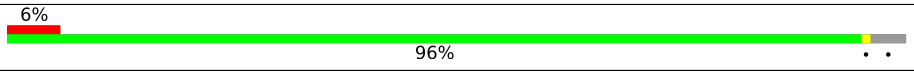
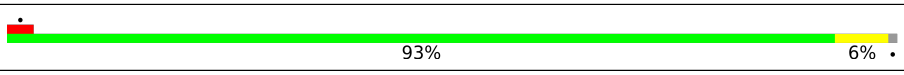
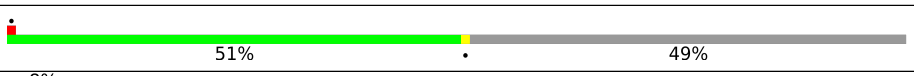
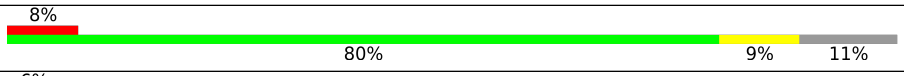
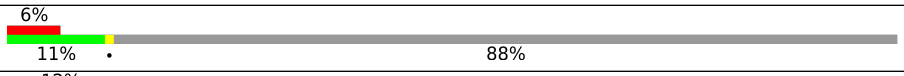
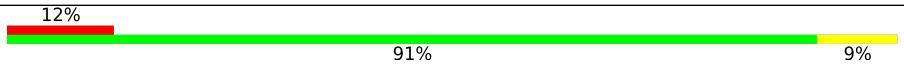
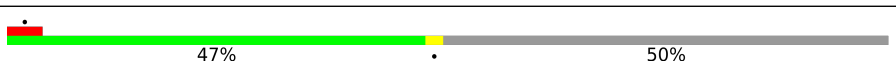
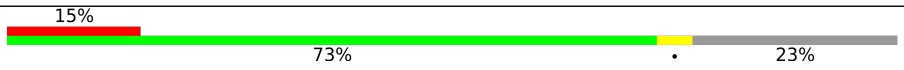
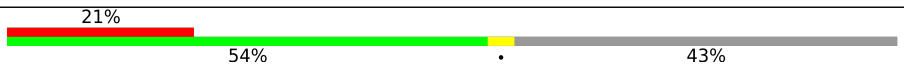
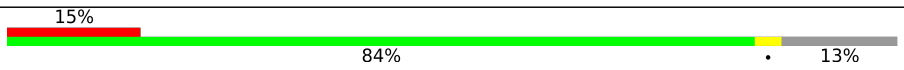
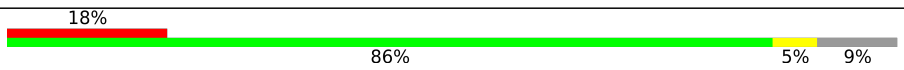
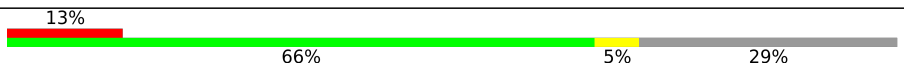
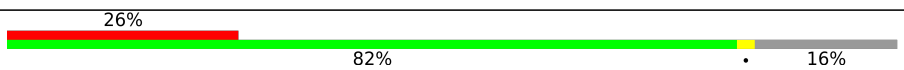
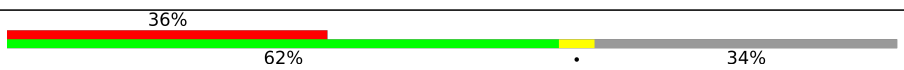
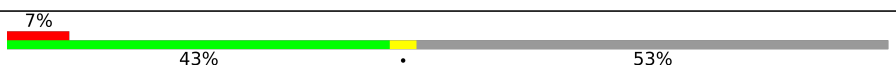
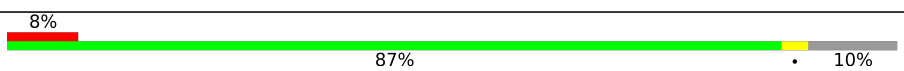
Mol	Chain	Length	Quality of chain
33	SA	427	
34	SC	288	
35	SD	248	
36	SE	266	
37	SG	192	
38	SH	293	
39	SI	255	
40	SJ	847	
41	SK	245	
42	SL	490	
43	SM	588	
44	SN	306	
45	SO	353	
46	SQ	239	
47	SR	634	
48	SS	746	
49	ST	365	
50	SV	163	
51	SW	670	
52	SY	812	
53	SZ	178	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 134945 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	1208	749	226	229	4	0	0

- Molecule 2 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	BB	213	1057	631	213	213	0	0

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L1	152	3234	1443	571	1068	152	0	0

- Molecule 4 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L2	69	1468	653	263	483	69	0	0

- Molecule 5 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	L3	2125	45561	20291	8341	14804	2125	0	0

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L6	120	998	625	218	154	1	0	0

- Molecule 7 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L7	199	Total	C	N	O	S	0	0
			1634	1053	319	257	5		

- Molecule 8 is a protein called 60S ribosomal protein L14.

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

- Molecule 9 is a protein called 60S ribosomal protein L15.

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

- Molecule 10 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LA	160	Total	C	N	O	S	0	0
			1286	809	240	229	8		

- Molecule 11 is a protein called 60S ribosomal protein L18.

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

- Molecule 12 is a protein called 60S ribosomal protein L18a.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	113	Total	C	N	O	S	0	0
			747	461	143	142	1		

- Molecule 14 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG	134	Total	C	N	O	S	0	0
			993	625	187	176	5		

- Molecule 15 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	LH	133	Total	C	N	O	0	0
			813	499	172	142		

- Molecule 16 is a protein called 60S ribosomal protein L26.

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

- Molecule 17 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LK	108	Total	C	N	O	S	0	0
			642	388	137	115	2		

- Molecule 18 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LN	358	Total	C	N	O	S	0	0
			2884	1834	531	506	13		

- Molecule 19 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	133	Total	C	N	O	S	0	0
			1096	690	225	176	5		

- Molecule 20 is a protein called 60S ribosomal protein L35.

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

- Molecule 21 is a protein called 60S ribosomal protein L35a.

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

- Molecule 22 is a protein called 60S ribosomal protein L36.

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

- Molecule 23 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LW	74	Total	C	N	O	S	0	0
			612	379	134	94	5		

- Molecule 24 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	NB	387	Total	C	N	O	S	0	0
			2424	1493	475	450	6		

- Molecule 25 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	NF	203	Total	C	N	O	S	0	0
			1661	1058	316	278	9		

- Molecule 26 is a protein called 60S ribosome subunit biogenesis protein NIP7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	NH	180	Total	C	N	O	S	0	0
			1441	925	245	263	8		

- Molecule 27 is a protein called ATP-dependent RNA helicase DDX54.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	NI	598	Total	C	N	O	S	0	0
			3866	2387	736	737	6		

- Molecule 28 is a protein called Protein LLP homolog.

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

- Molecule 29 is a protein called Protein MAK16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	NM	182	Total	C	N	O	S	0	0
			1550	983	286	273	8		

- Molecule 30 is a protein called Ribosomal RNA processing protein 1 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	NO	305	Total	C	N	O	S	0	0
			2487	1577	437	461	12		

- Molecule 31 is a protein called WD repeat-containing protein 74.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	NQ	324	Total	C	N	O	S	0	0
			2502	1559	471	457	15		

- Molecule 32 is a protein called Ribosome production factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	NS	305	Total	C	N	O	S	0	0
			2529	1607	472	444	6		

- Molecule 33 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SA	360	Total	C	N	O	S	0	0
			2864	1803	572	475	14		

- Molecule 34 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SC	199	Total	C	N	O	S	0	0
			1627	1046	305	274	2		

- Molecule 35 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SD	239	Total	C	N	O	S	0	0
			1985	1275	381	320	9		

- Molecule 36 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	SE	185	Total	C	N	O	S	0	0
			1491	946	289	252	4		

- Molecule 37 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SG	190	Total	C	N	O	S	1	0
			1526	961	287	272	6		

- Molecule 38 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SH	150	Total	C	N	O	S	0	0
			1267	819	224	220	4		

- Molecule 39 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SI	228	Total	C	N	O	S	1	0
			1887	1224	352	307	4		

- Molecule 40 is a protein called pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SJ	101	Total	C	N	O	S	0	0
			855	537	165	152	1		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 42 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SL	243	Total	C	N	O	S	0	0
			1960	1254	344	356	6		

- Molecule 43 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SM	453	Total	C	N	O	S	0	0
			3735	2408	667	648	12		

- Molecule 44 is a protein called Probable rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SN	173	Total	C	N	O	S	0	0
			1350	849	251	243	7		

- Molecule 45 is a protein called Ribosome biogenesis protein BRX1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SO	307	Total	C	N	O	S	0	0
			2544	1637	458	434	15		

- Molecule 46 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SQ	217	Total	C	N	O	S	1	0
			1778	1134	313	320	11		

- Molecule 47 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SR	449	Total	C	N	O	S	0	0
			3695	2352	651	675	17		

- Molecule 48 is a protein called Ribosome biogenesis protein BOP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	SS	256	Total	C	N	O	P	S	0	0
			2116	1337	375	394	2	8		

- Molecule 49 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	ST	116	Total	C	N	O	S	0	0
			787	489	152	144	2		

- Molecule 50 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 51 is a protein called ATP-dependent RNA helicase DDX18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SW	444	Total	C	N	O	S	0	0
			3549	2282	605	645	17		

- Molecule 52 is a protein called Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SY	378	Total	C	N	O	S	0	0
			2985	1887	533	550	15		

- Molecule 53 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SZ	160	Total	C	N	O	S	0	0
			1338	835	260	238	5		

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	L1	5	Total	Mg	0
			5	5	
54	L2	1	Total	Mg	0
			1	1	
54	L3	52	Total	Mg	0
			52	52	
54	L9	1	Total	Mg	0
			1	1	
54	LQ	1	Total	Mg	0
			1	1	
54	LT	1	Total	Mg	0
			1	1	

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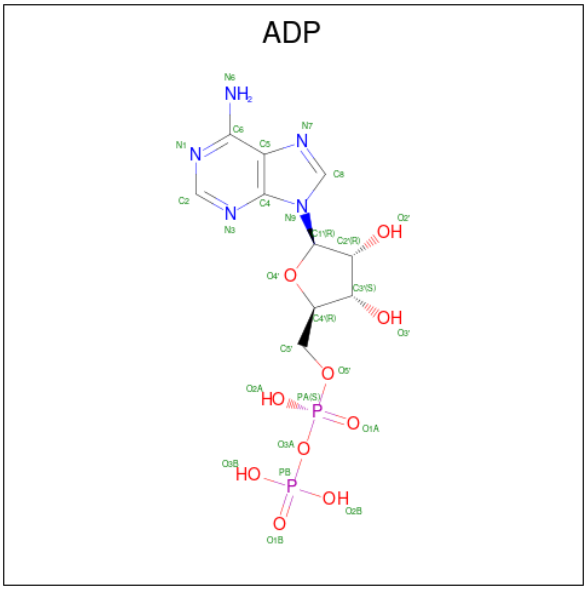
Mol	Chain	Residues	Atoms	AltConf
54	NI	1	Total Mg 1 1	0
54	SA	1	Total Mg 1 1	0
54	SR	1	Total Mg 1 1	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

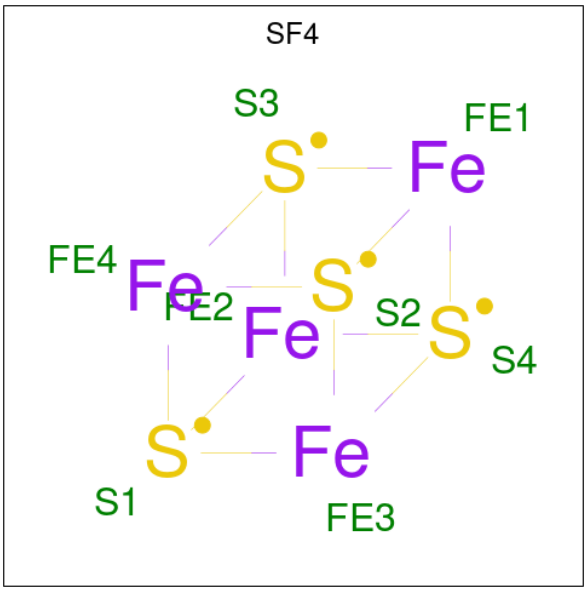
Mol	Chain	Residues	Atoms	AltConf
55	LW	1	Total Zn 1 1	0
55	SV	1	Total Zn 1 1	0

- Molecule 56 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



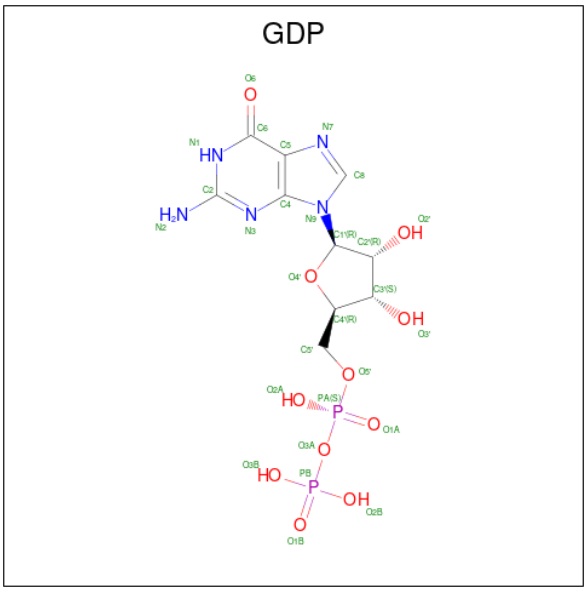
Mol	Chain	Residues	Atoms	AltConf
56	NI	1	Total C N O P 27 10 5 10 2	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
57	NM	1	Total	Fe	S	0
			8	4	4	

- Molecule 58 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

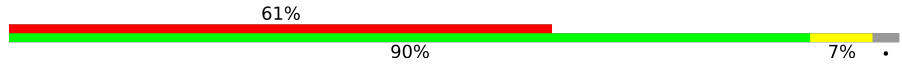
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
59	SR	1	1	1	0

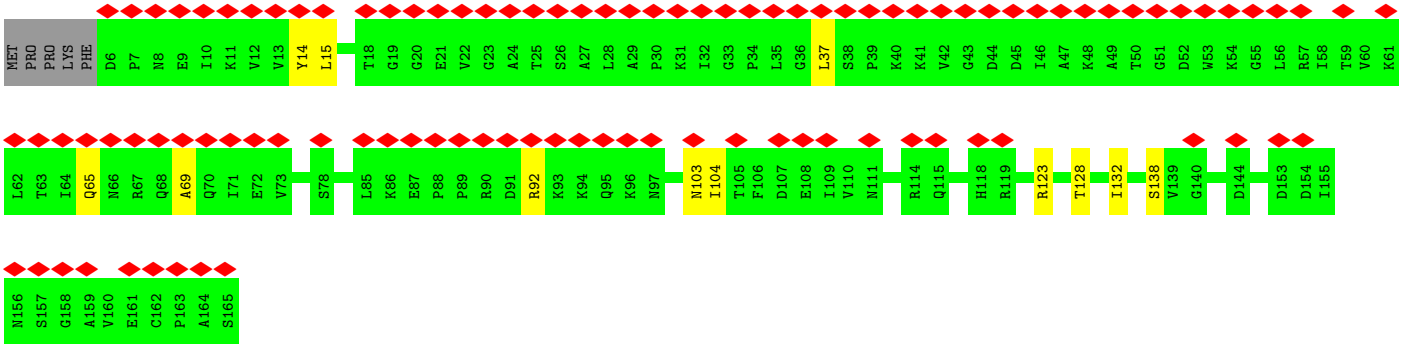
3 Residue-property plots (i)

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

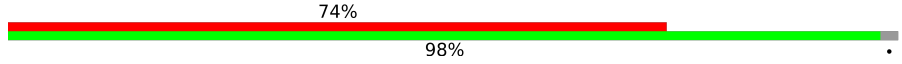
Chain BA:

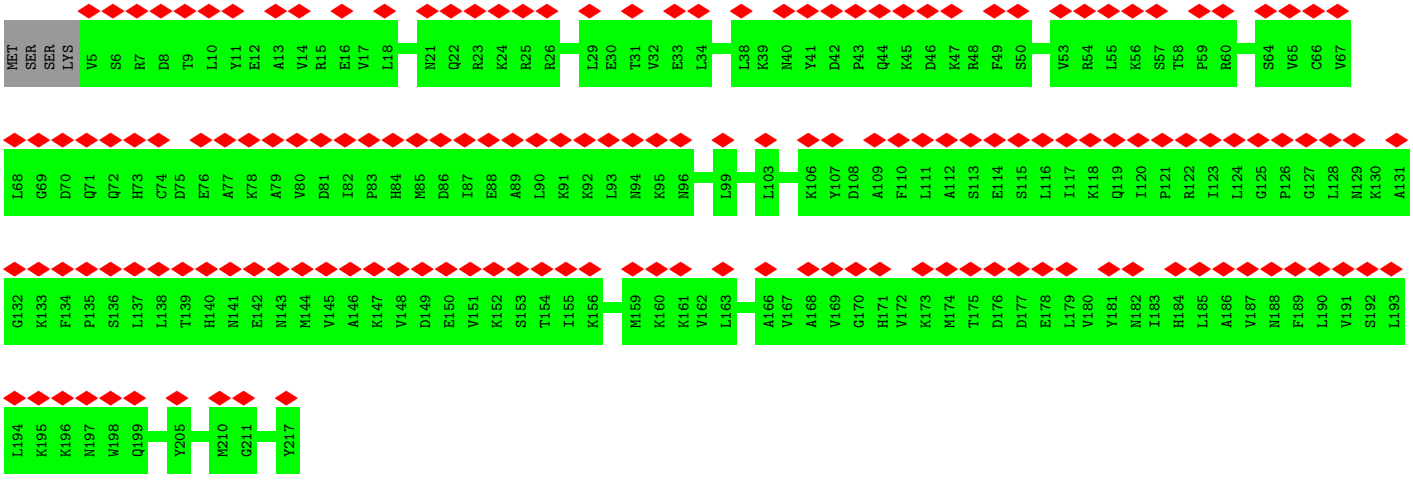




• Molecule 2: 60S ribosomal protein L10a

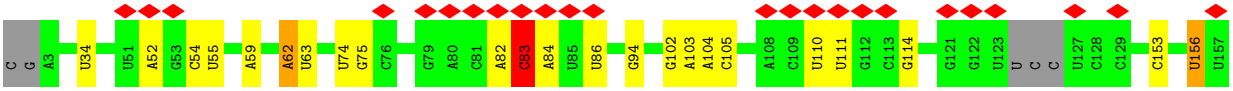
Chain BB:





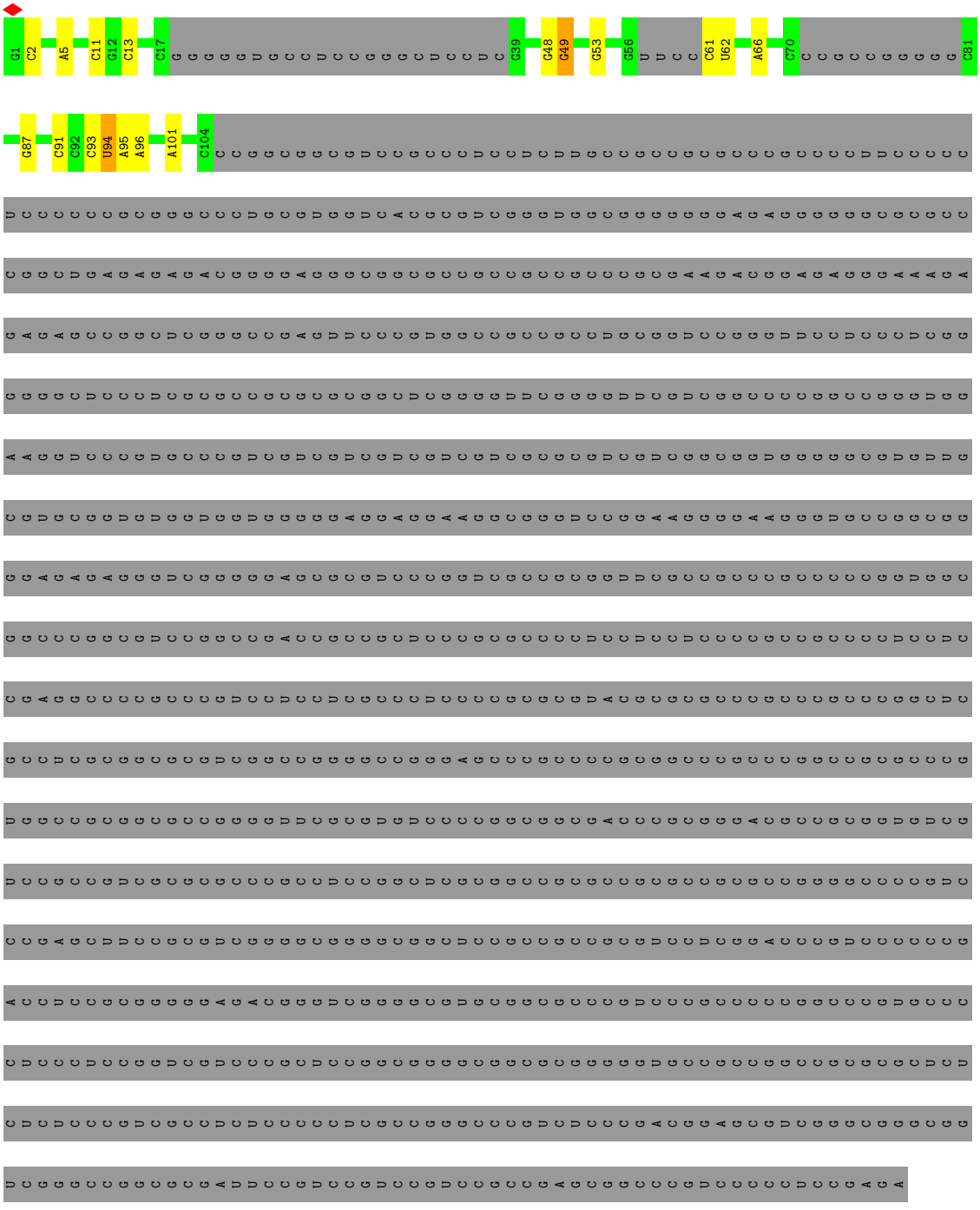
• Molecule 3: 5.8S rRNA

Chain L1:



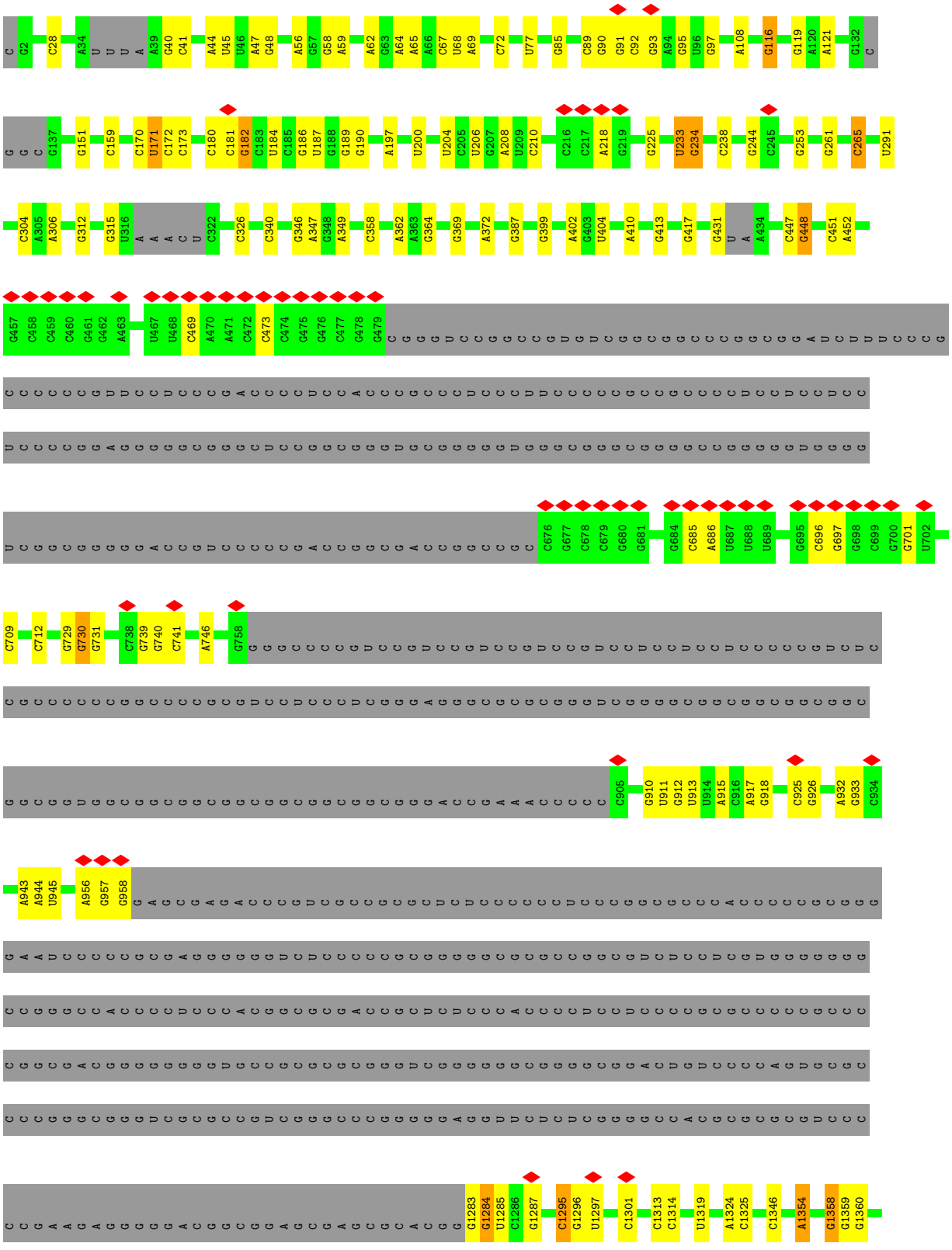
• Molecule 4: ITS2 rRNA

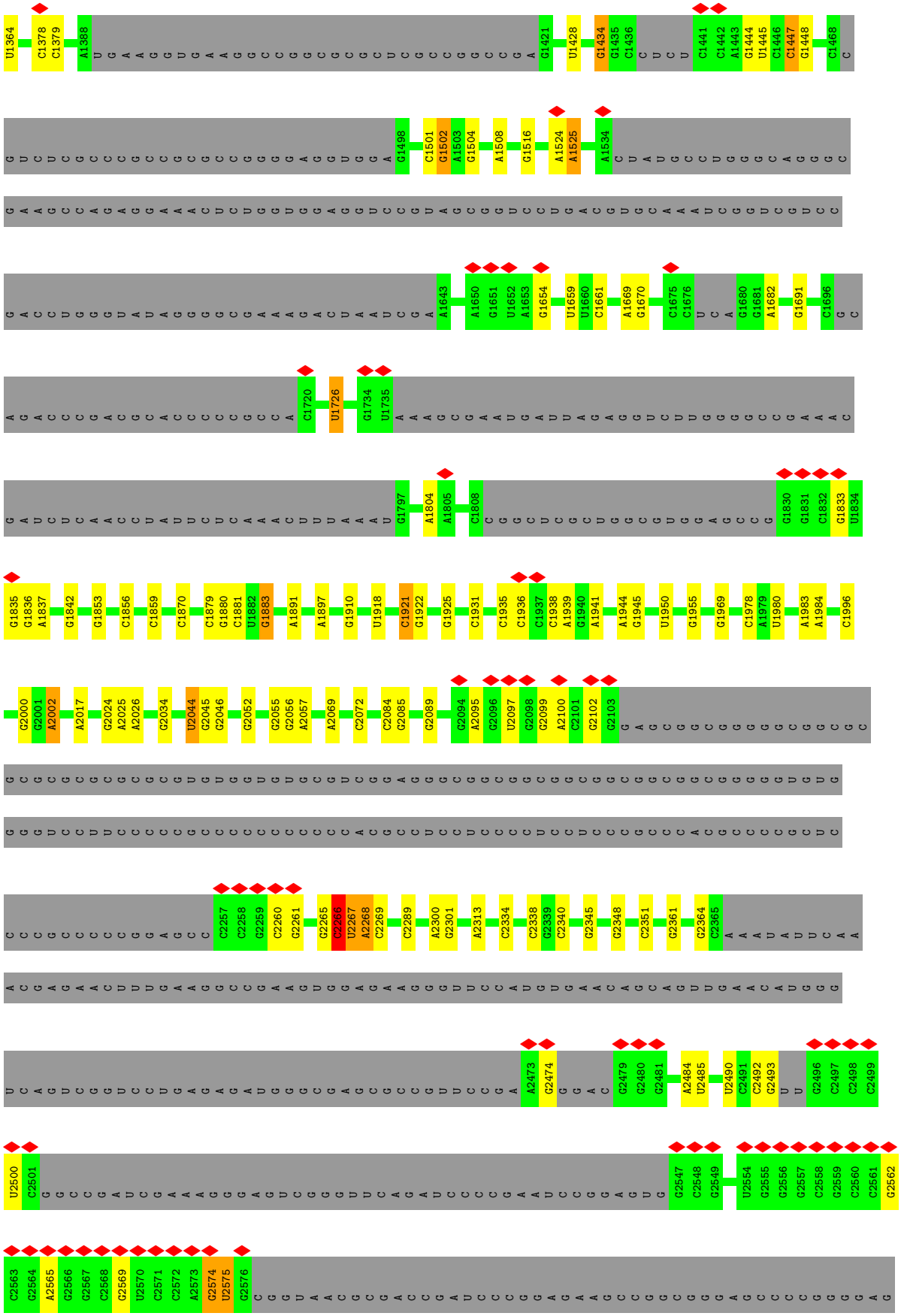
Chain L2: 94%

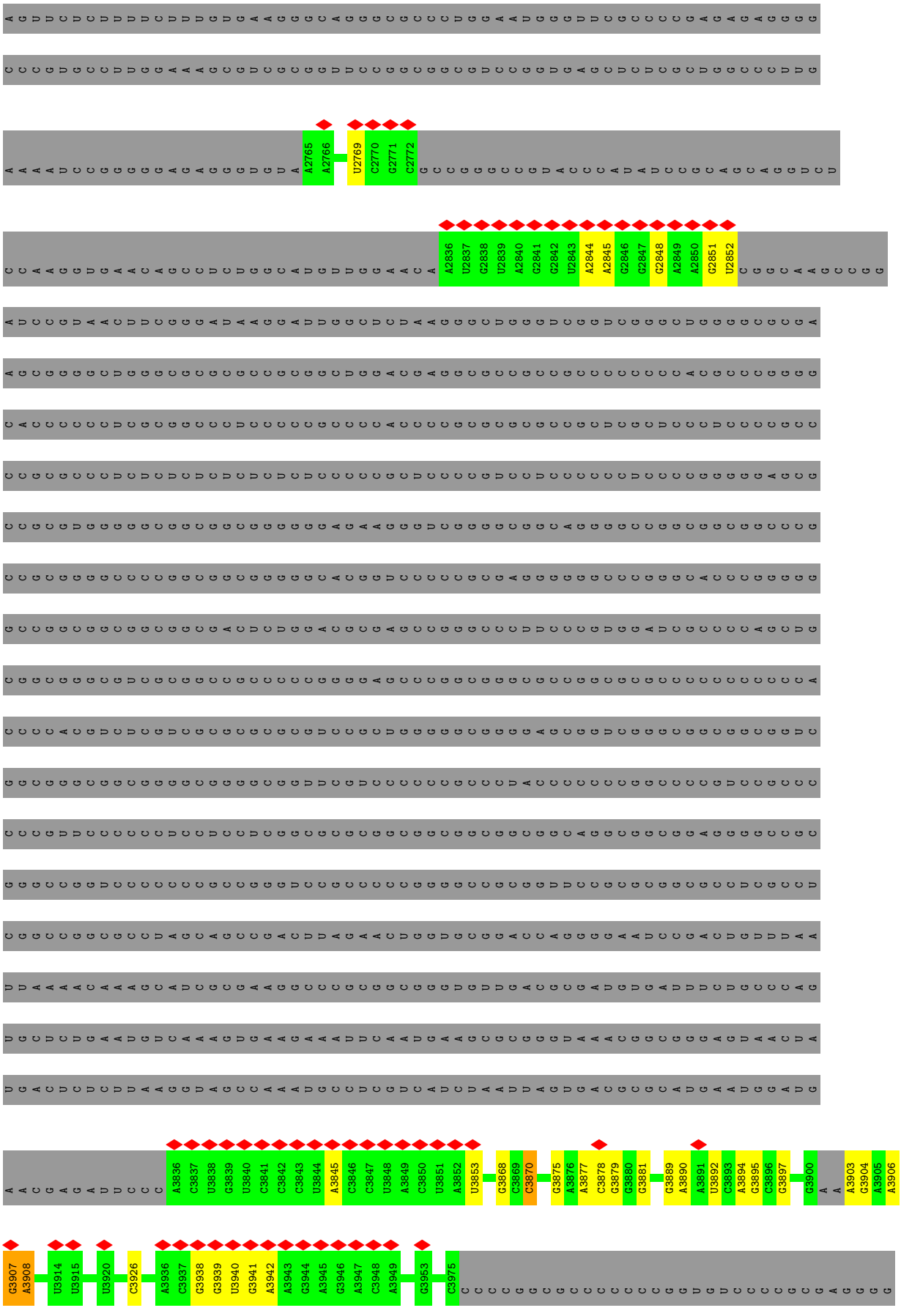


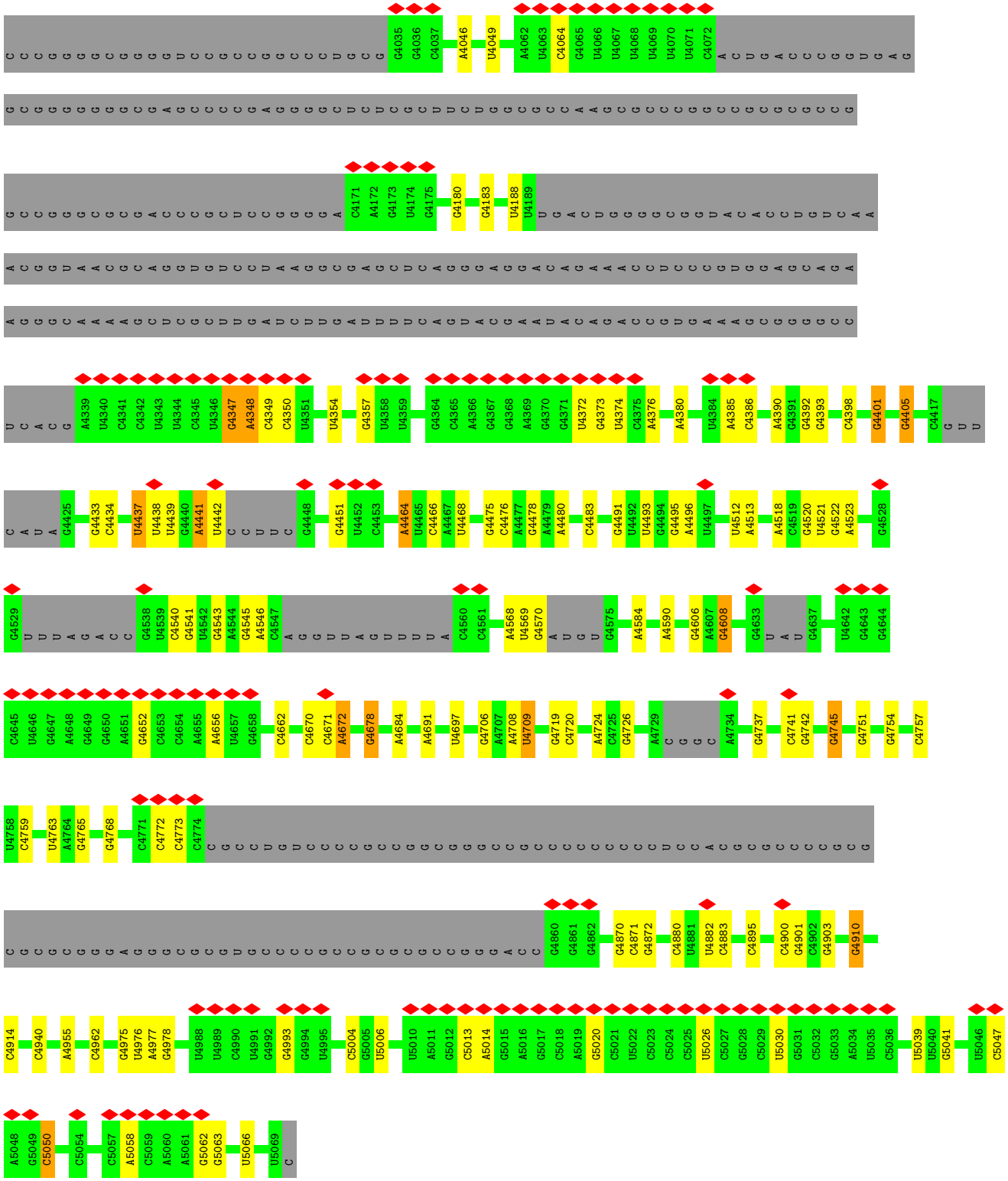
• Molecule 5: 28S rRNA

Chain L3:



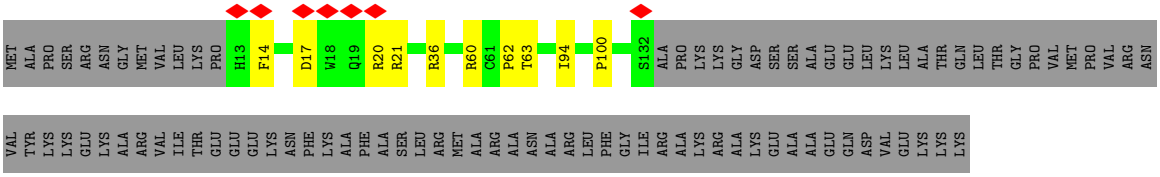






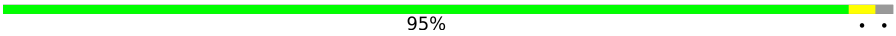
• Molecule 6: 60S ribosomal protein L13

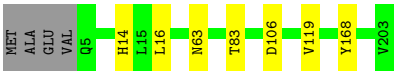
Chain L6:



• Molecule 7: 60S ribosomal protein L13a

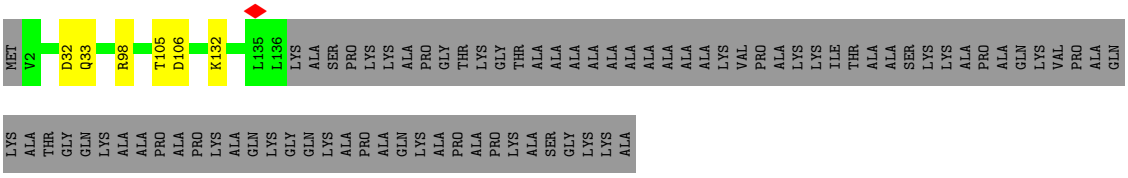
Chain L7:





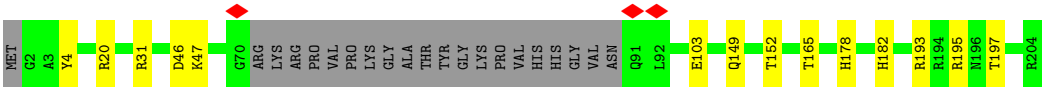
• Molecule 8: 60S ribosomal protein L14

Chain L8:



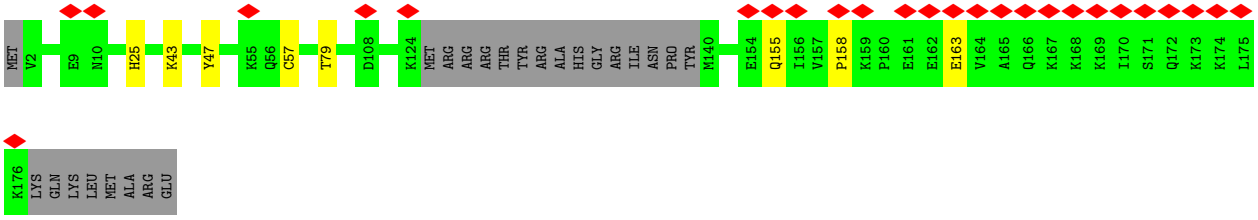
• Molecule 9: 60S ribosomal protein L15

Chain L9:



• Molecule 10: 60S ribosomal protein L17

Chain LA:

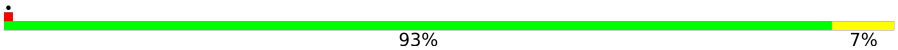


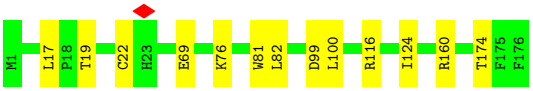
• Molecule 11: 60S ribosomal protein L18

Chain LB:

• Molecule 12: 60S ribosomal protein L18a

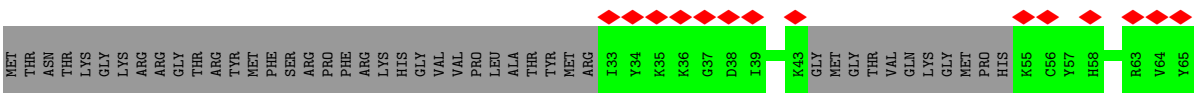
Chain LC:

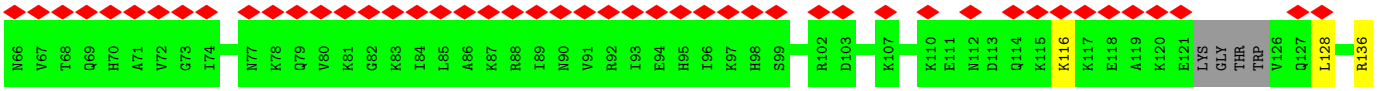


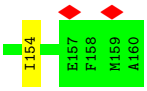


• Molecule 13: 60S ribosomal protein L21

Chain LE:

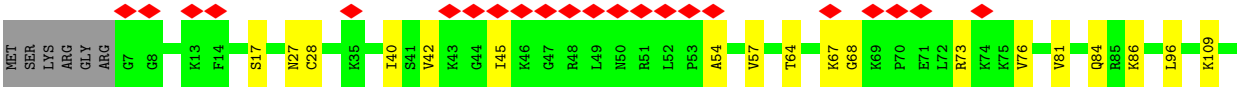






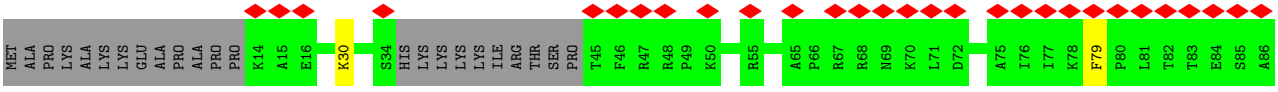
• Molecule 14: 60S ribosomal protein L23

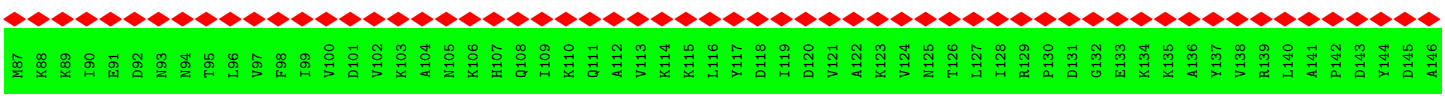
Chain LG:

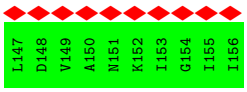


• Molecule 15: 60S ribosomal protein L23a

Chain LH:

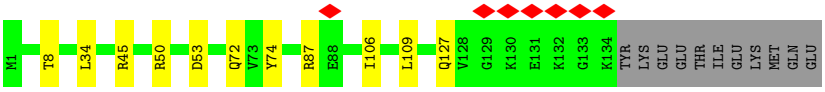






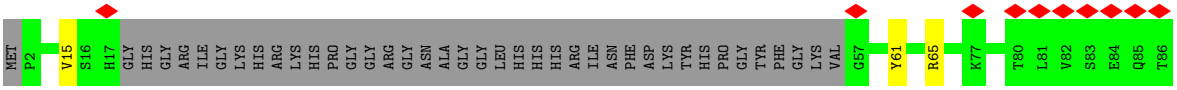
• Molecule 16: 60S ribosomal protein L26

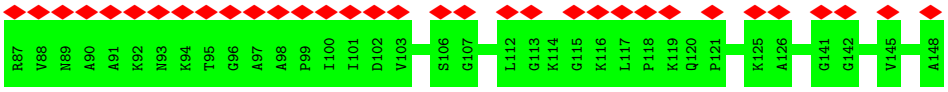
Chain LI:



• Molecule 17: 60S ribosomal protein L27a

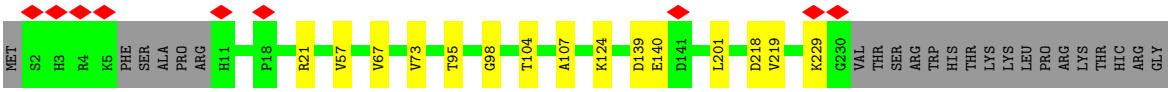
Chain LK:

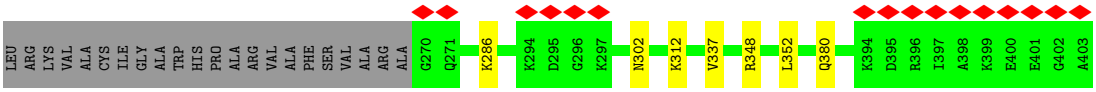




• Molecule 18: 60S ribosomal protein L3

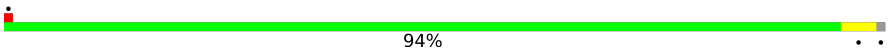
Chain LN:





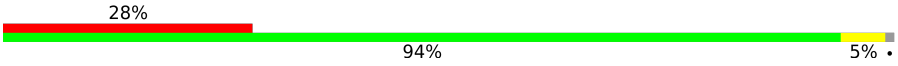
• Molecule 19: 60S ribosomal protein L32

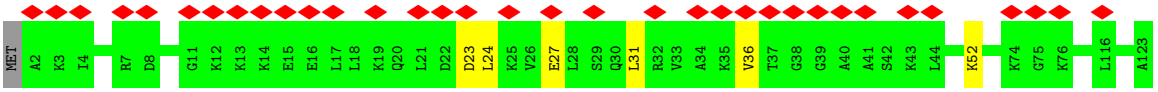
Chain LQ:



• Molecule 20: 60S ribosomal protein L35

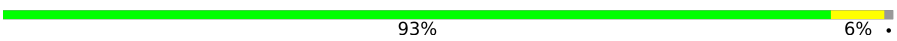
Chain LS:

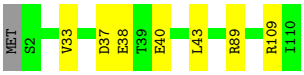




• Molecule 21: 60S ribosomal protein L35a

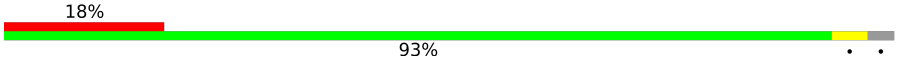
Chain LT:

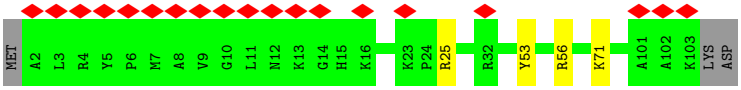




• Molecule 22: 60S ribosomal protein L36

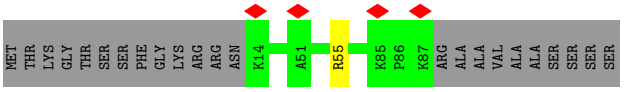
Chain LU:





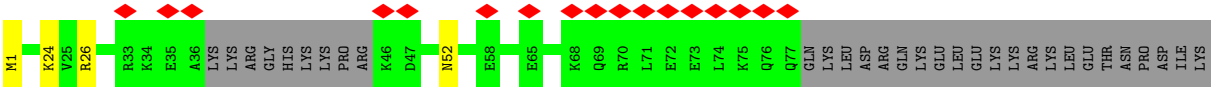
• Molecule 23: 60S ribosomal protein L37

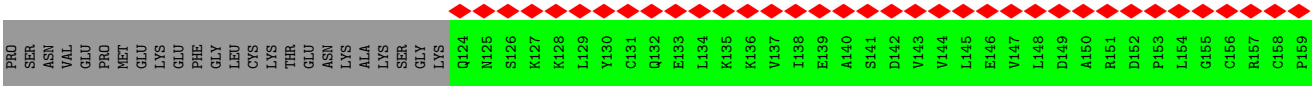
Chain LW:

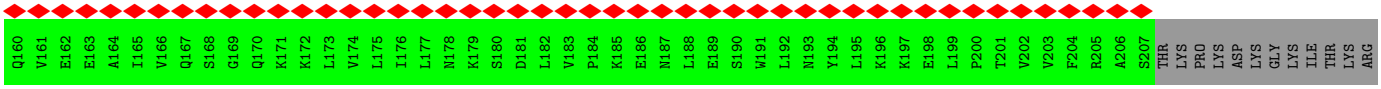


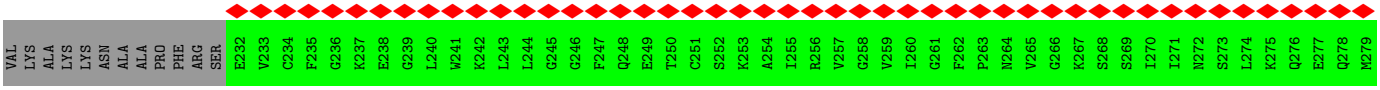
• Molecule 24: Guanine nucleotide-binding protein-like 3

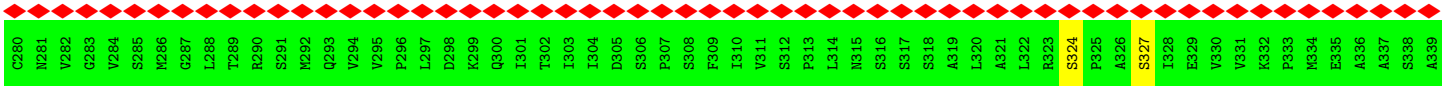
Chain NB:

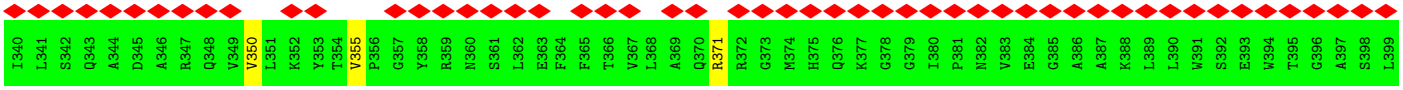


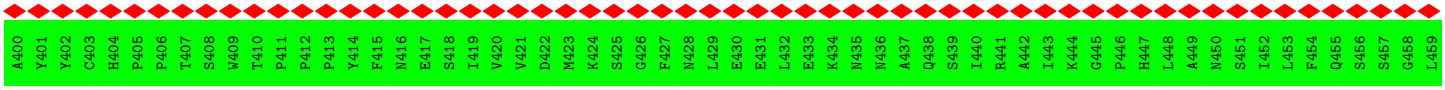


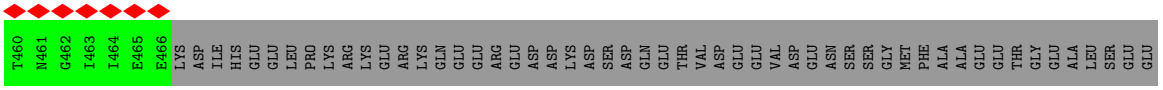






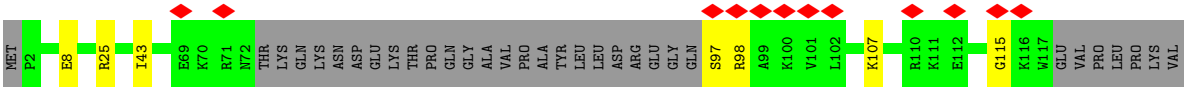


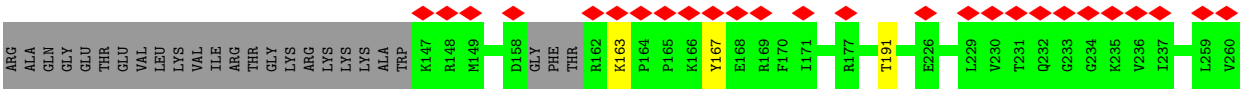




• Molecule 25: Ribosome biogenesis protein NSA2 homolog

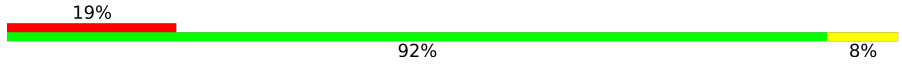
Chain NF:

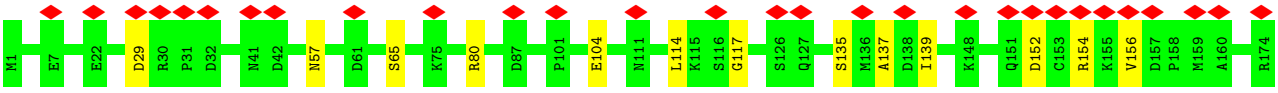


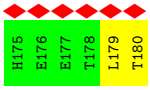


• Molecule 26: 60S ribosome subunit biogenesis protein NIP7 homolog

Chain NH:

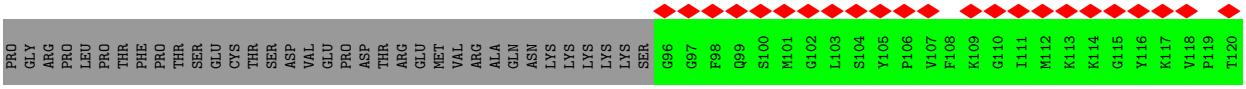


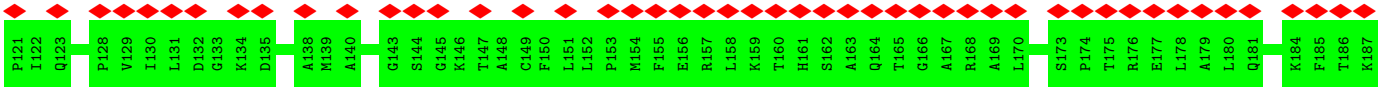


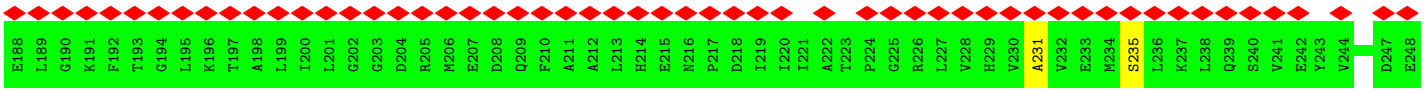


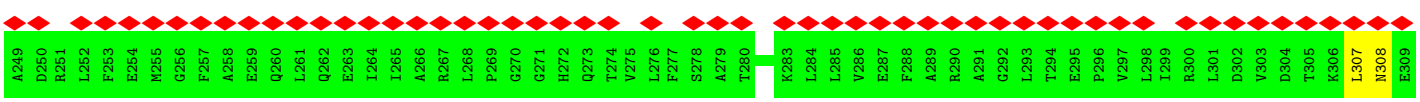
• Molecule 27: ATP-dependent RNA helicase DDX54

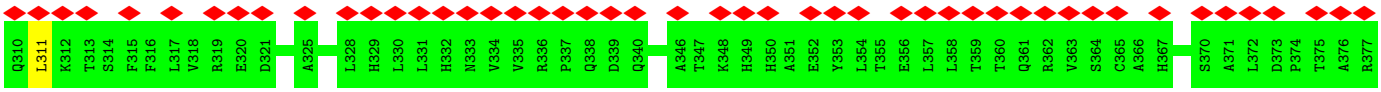
Chain NI:

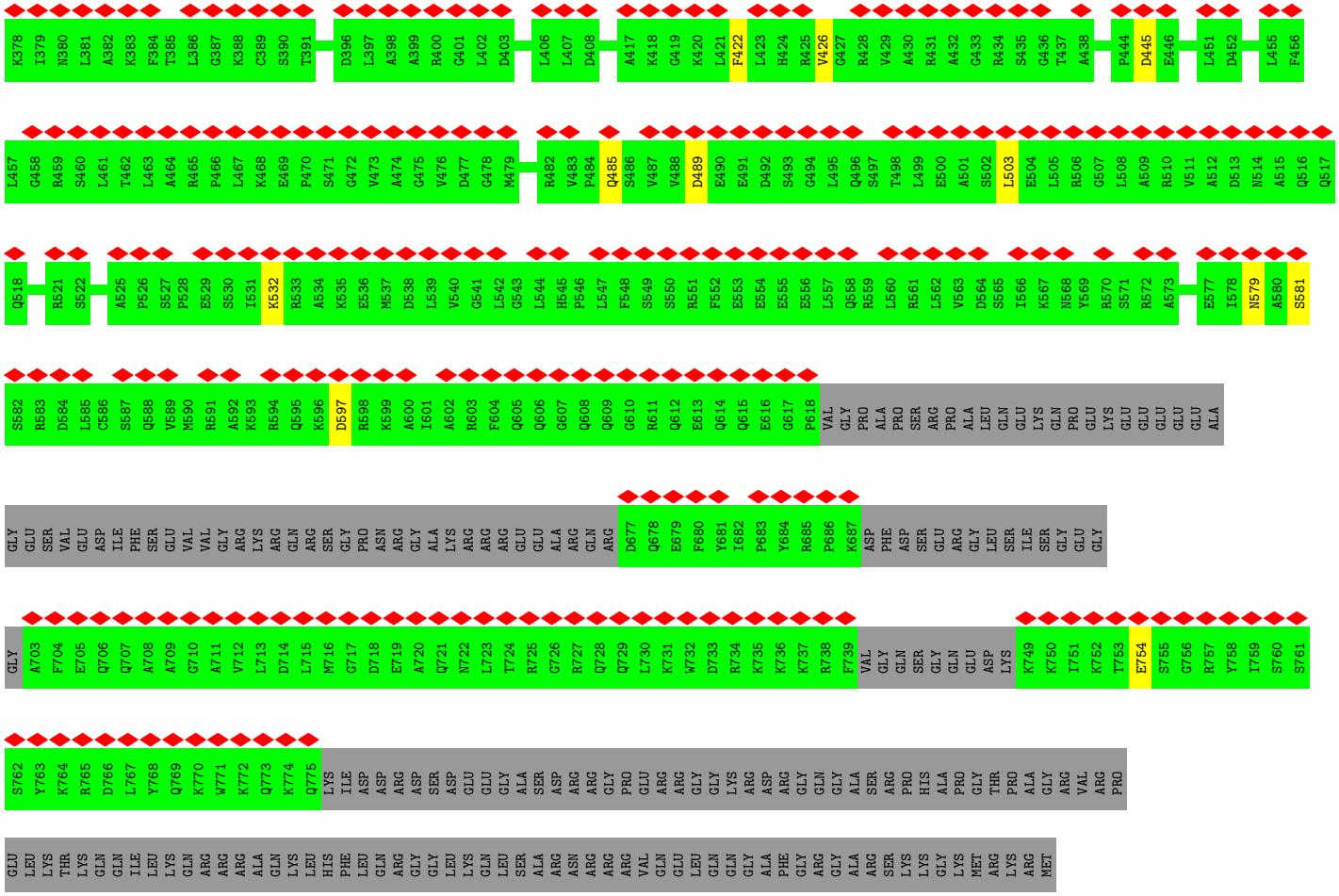






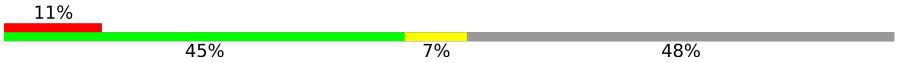


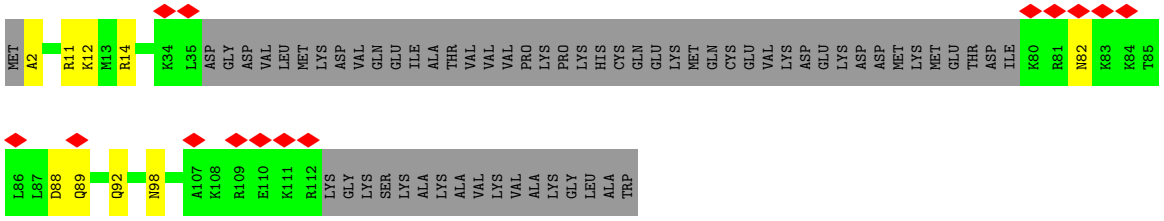




• Molecule 28: Protein LLP homolog

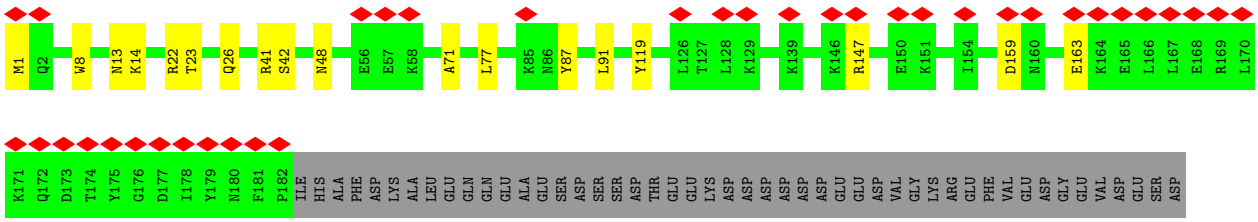
Chain NK:

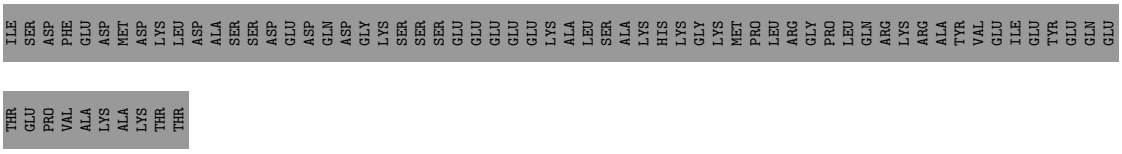




• Molecule 29: Protein MAK16 homolog

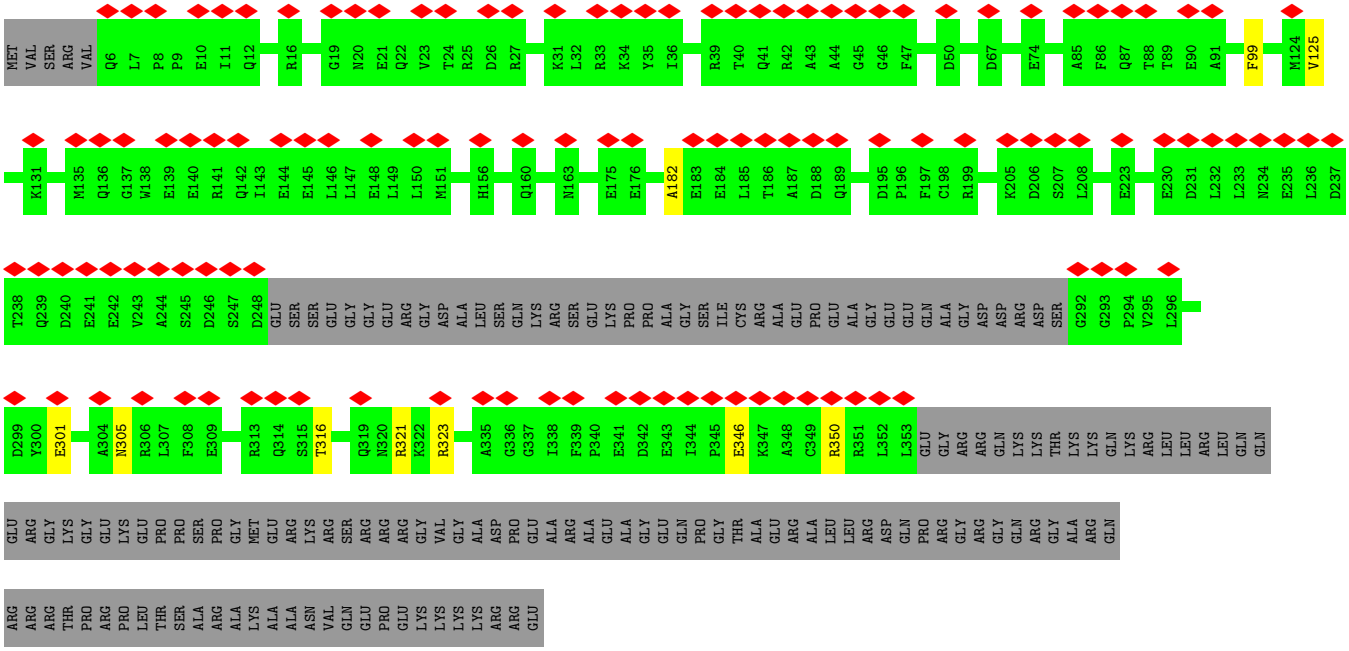
Chain NM:





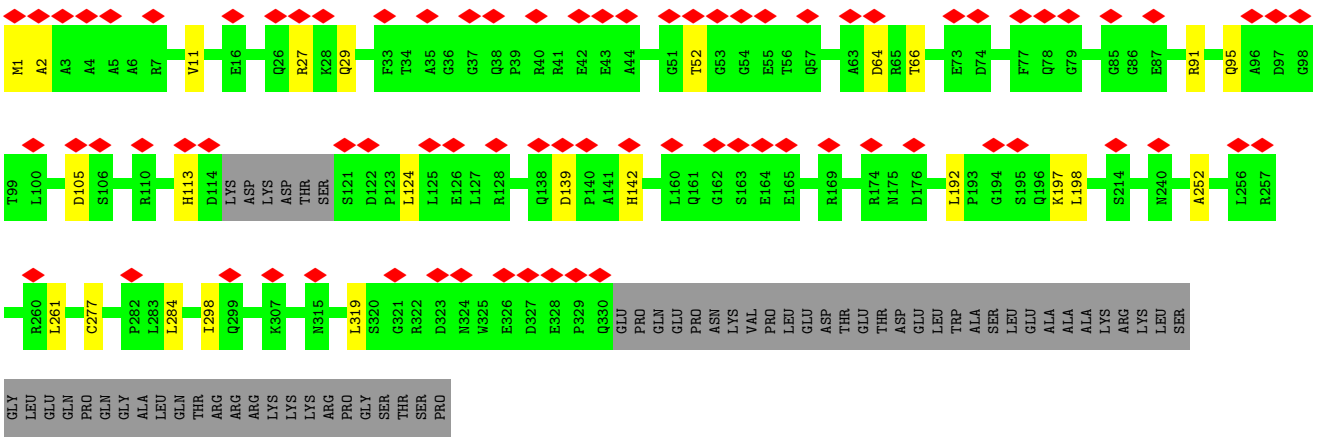
• Molecule 30: Ribosomal RNA processing protein 1 homolog A

Chain NO:



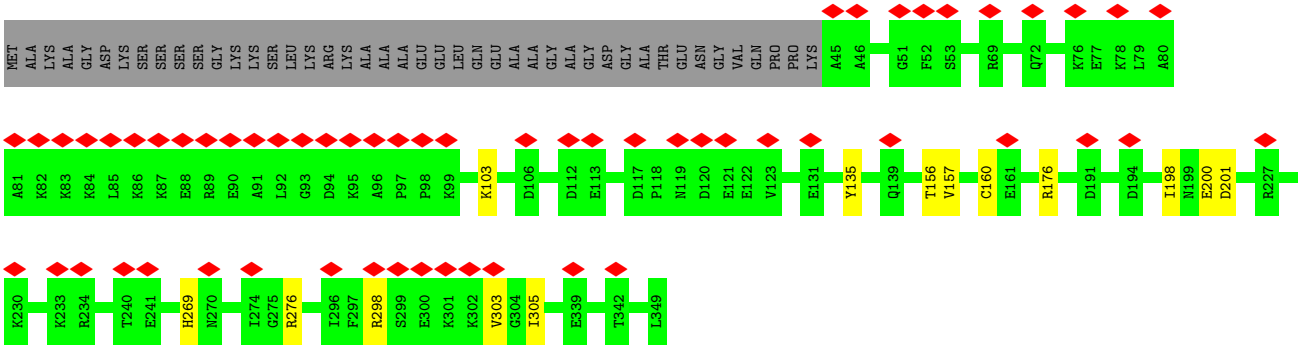
• Molecule 31: WD repeat-containing protein 74

Chain NQ:



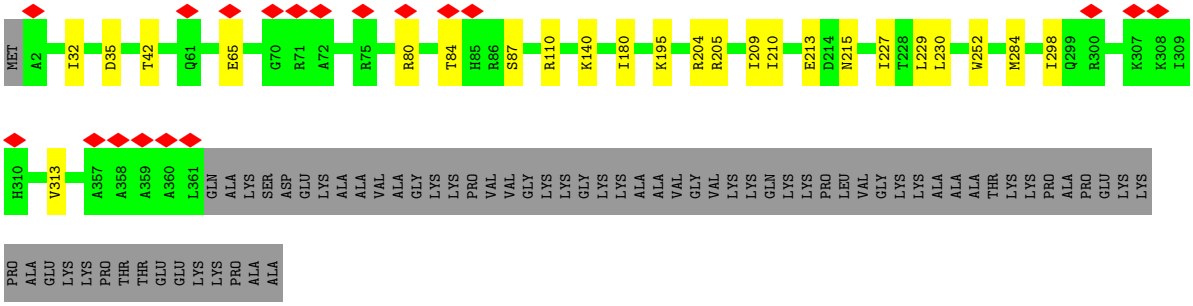
• Molecule 32: Ribosome production factor 1

Chain NS:



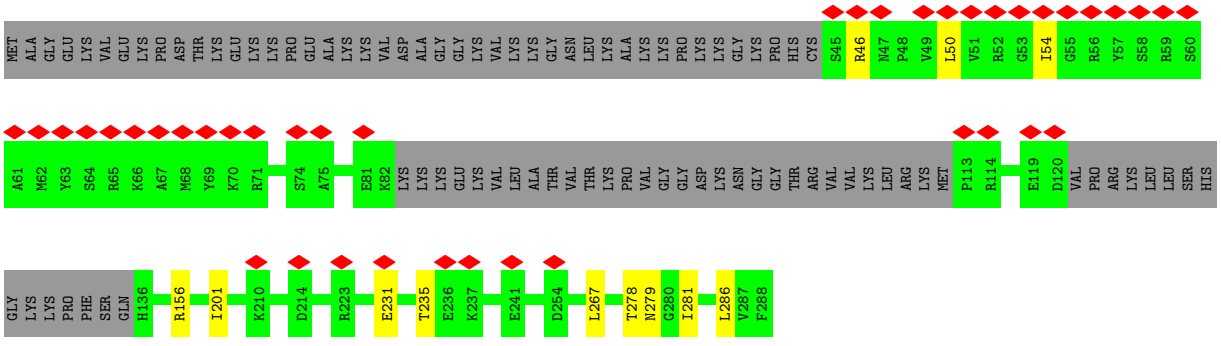
• Molecule 33: 60S ribosomal protein L4

Chain SA:



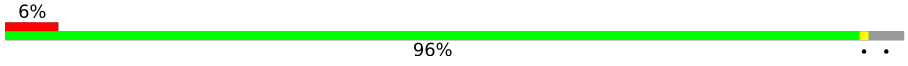
• Molecule 34: 60S ribosomal protein L6

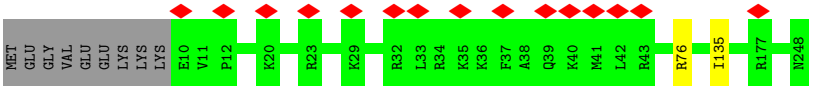
Chain SC:



• Molecule 35: 60S ribosomal protein L7

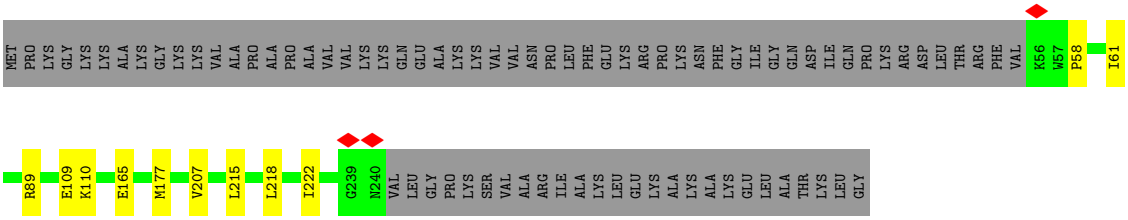
Chain SD:



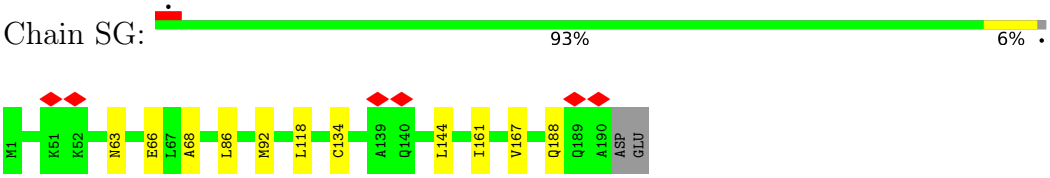


• Molecule 36: 60S ribosomal protein L7a

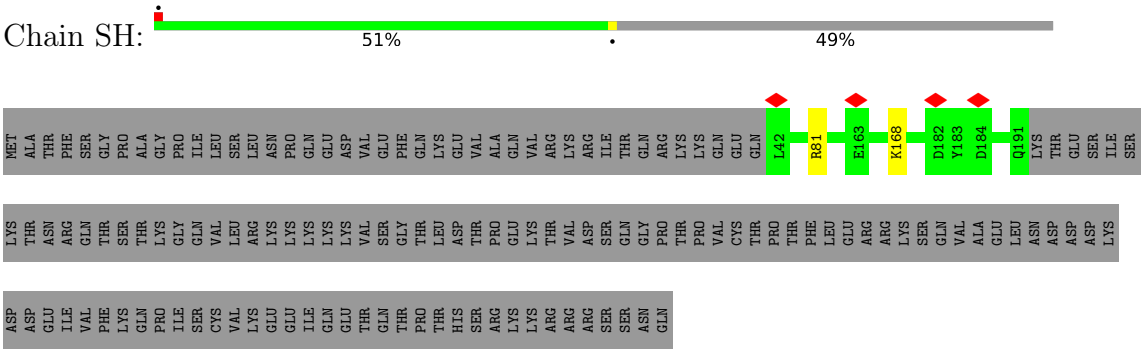
Chain SE:



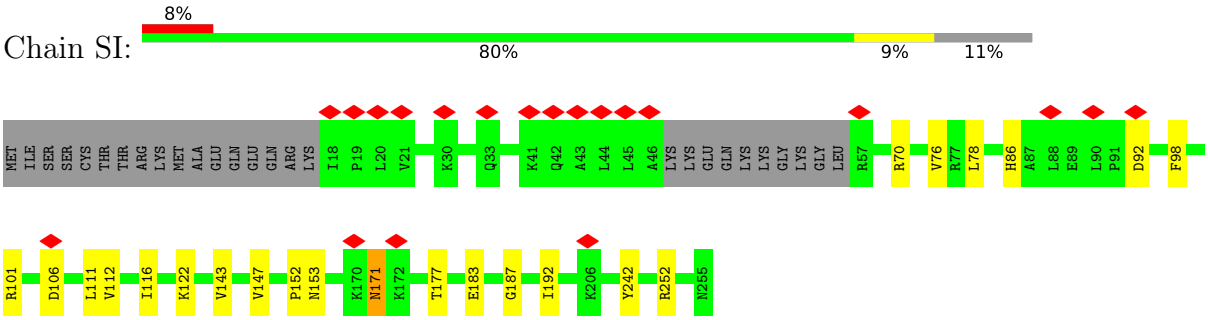
• Molecule 37: 60S ribosomal protein L9



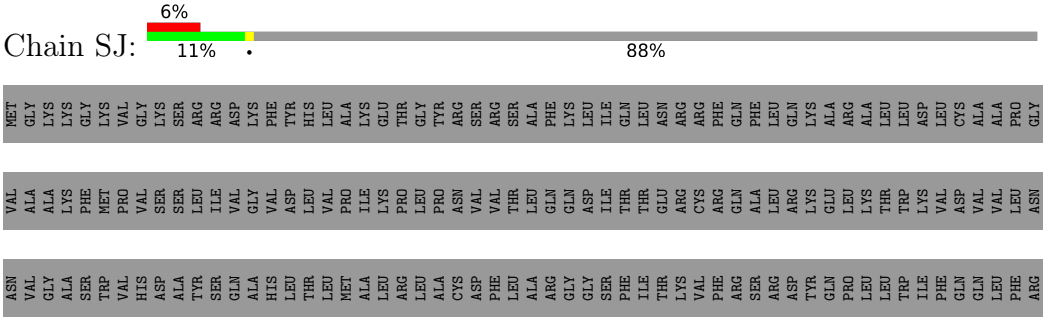
• Molecule 38: MKI67 FHA domain-interacting nucleolar phosphoprotein

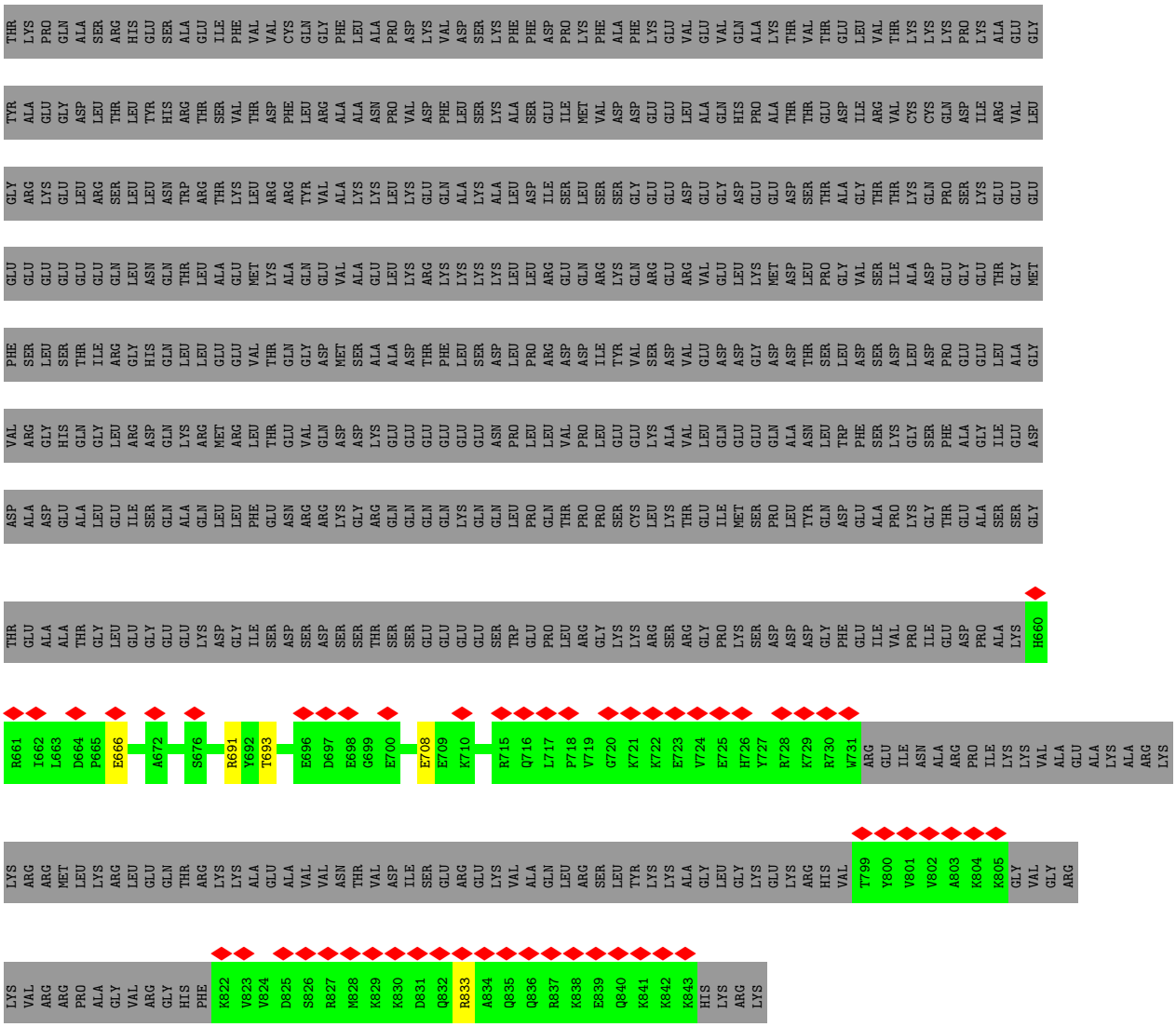


• Molecule 39: 60S ribosomal protein L7-like 1



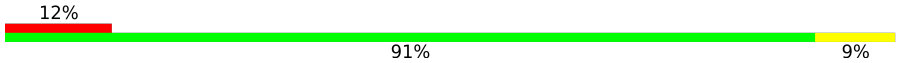
• Molecule 40: pre-rRNA 2'-O-ribose RNA methyltransferase FTSJ3

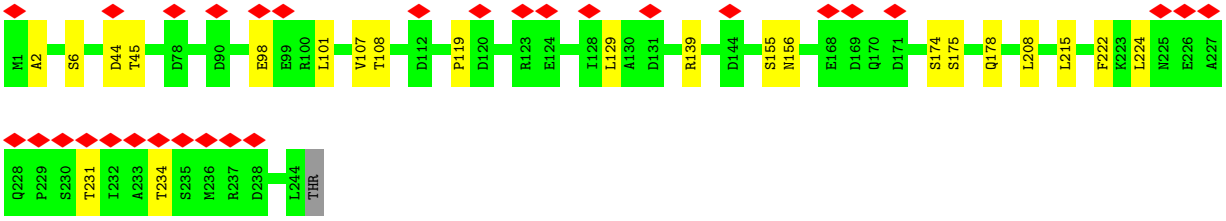




• Molecule 41: Eukaryotic translation initiation factor 6

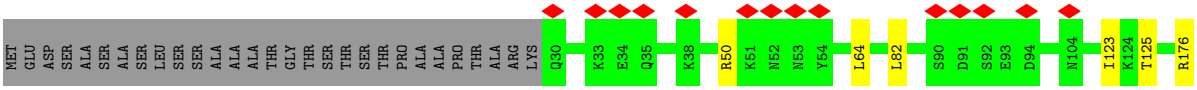
Chain SK:

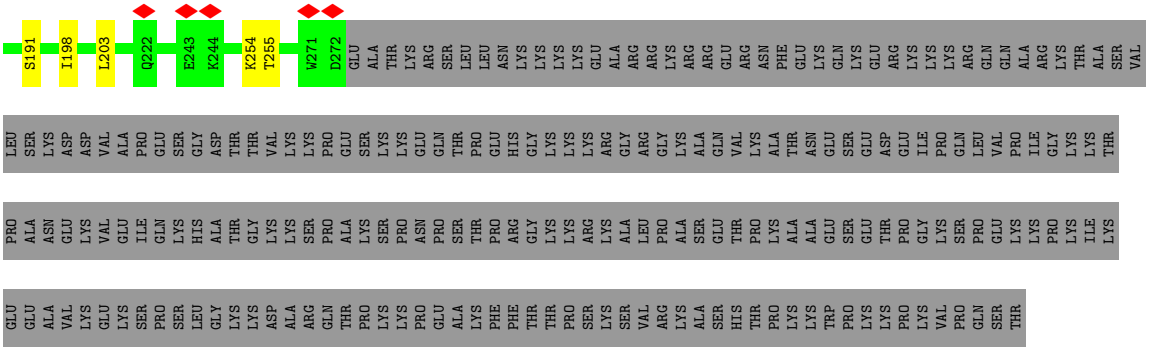




• Molecule 42: Ribosomal L1 domain-containing protein 1

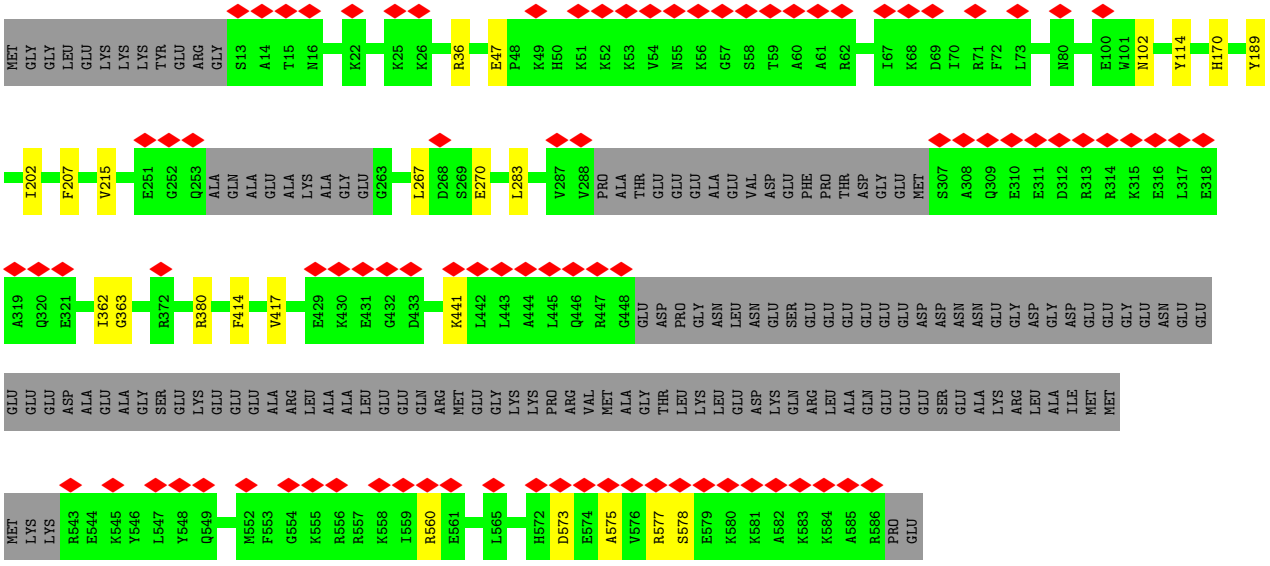
Chain SL:





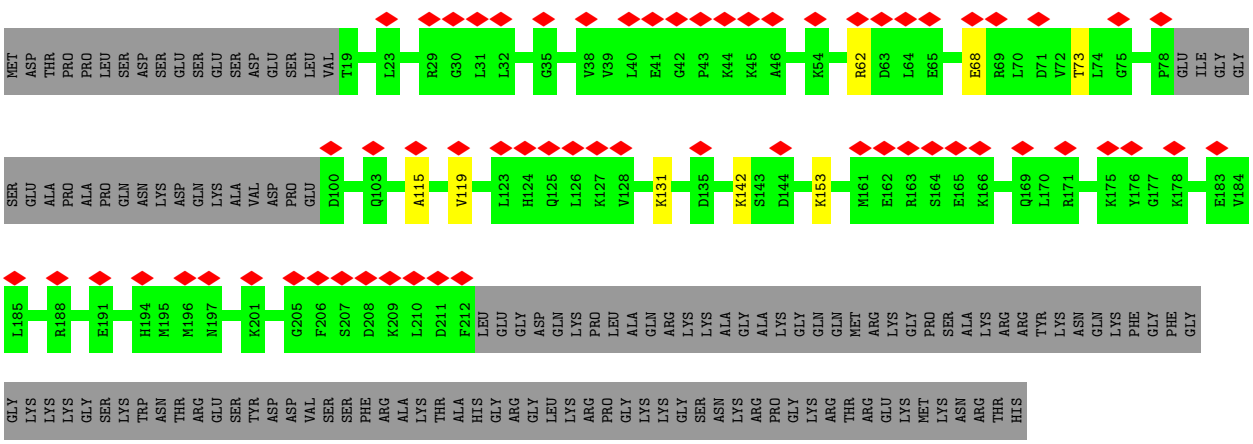
• Molecule 43: Pescadillo homolog

Chain SM:



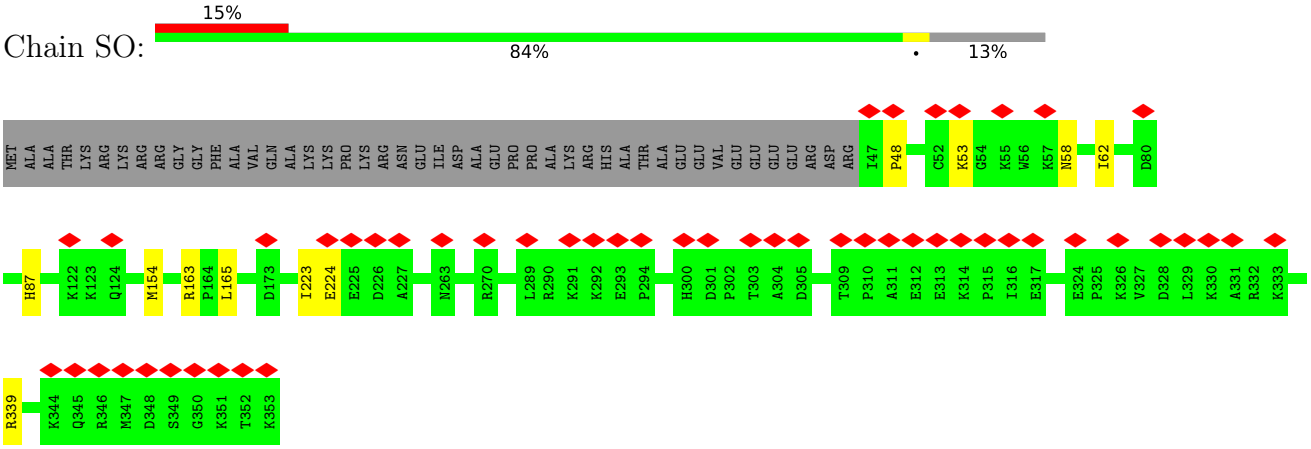
• Molecule 44: Probable rRNA-processing protein EBP2

Chain SN:



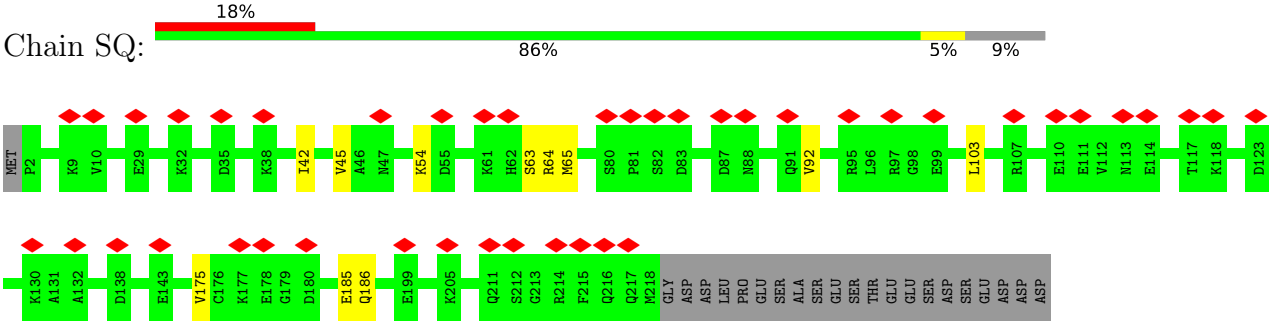
• Molecule 45: Ribosome biogenesis protein BRX1 homolog

Chain SO:



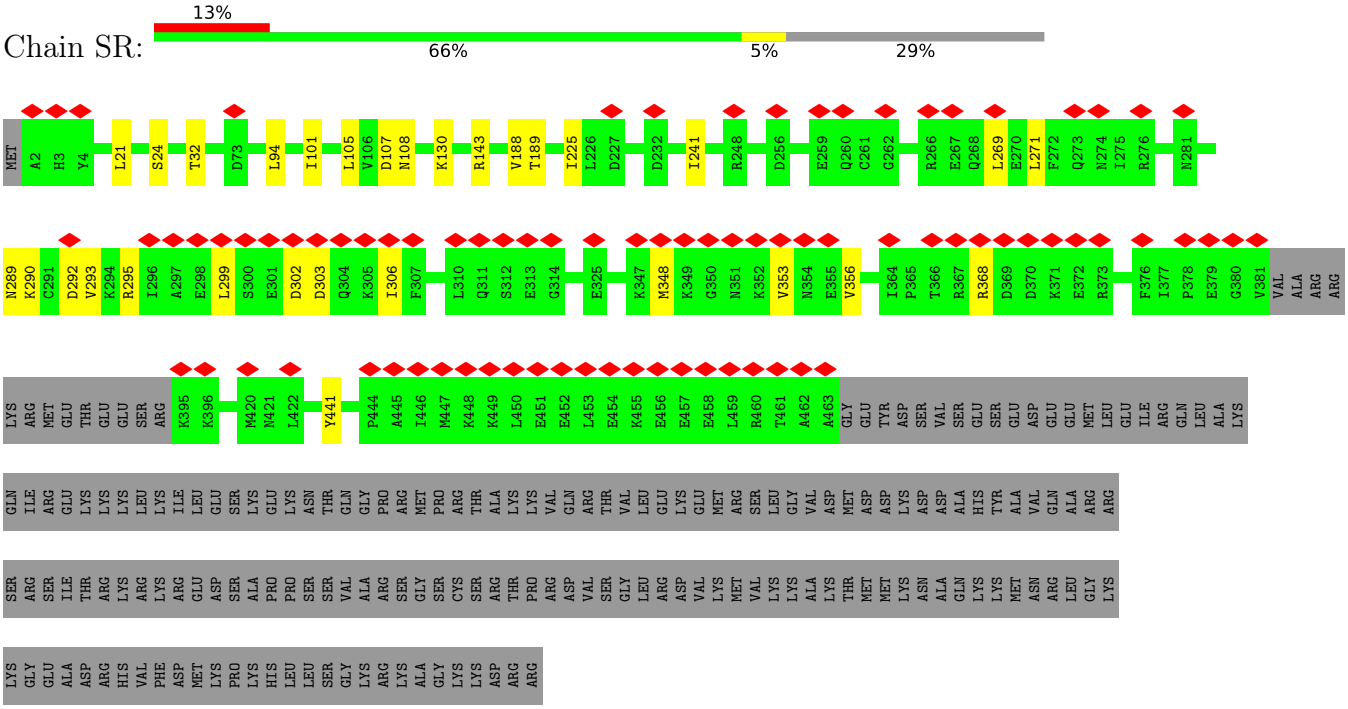
• Molecule 46: mRNA turnover protein 4 homolog

Chain SQ:



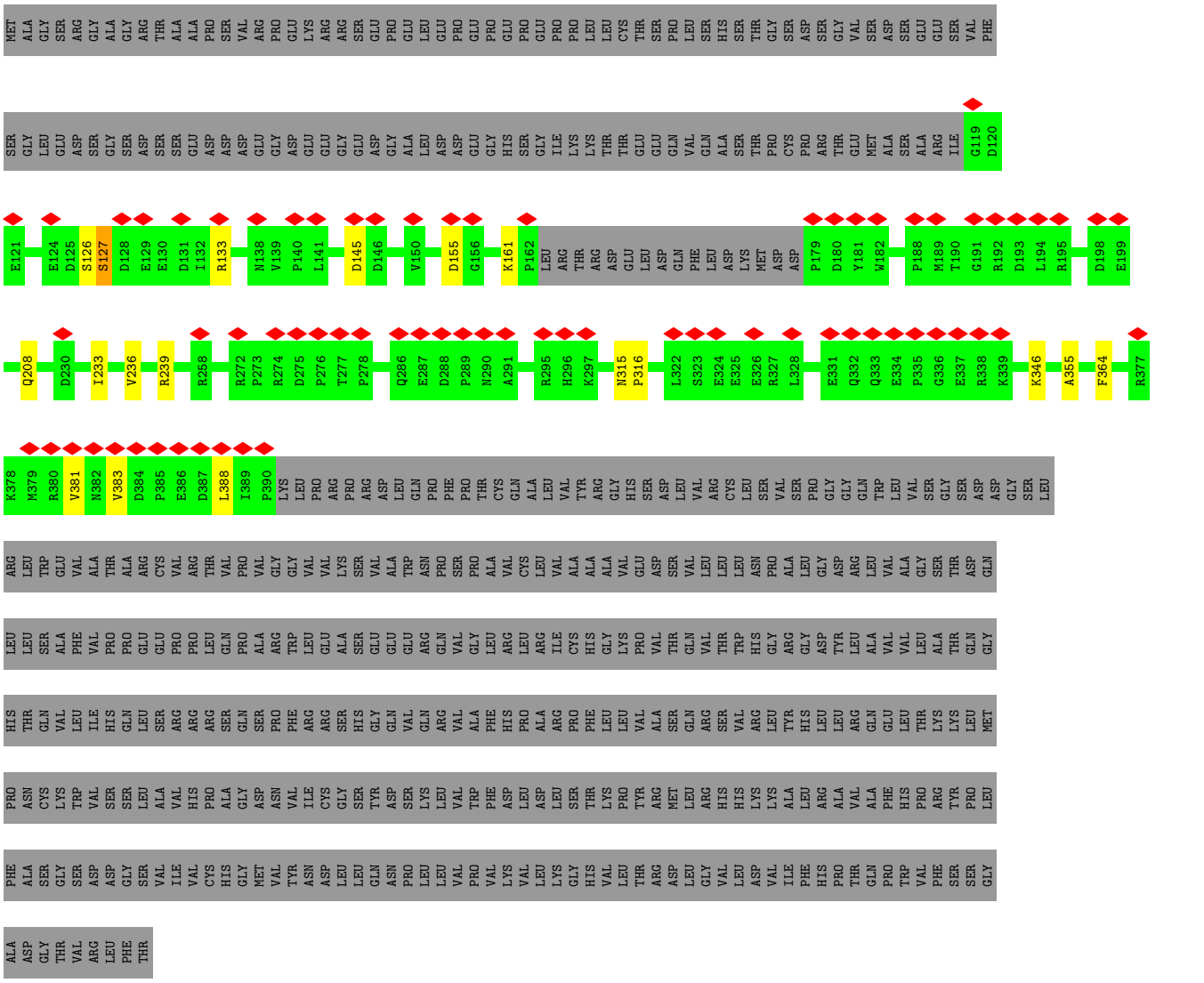
• Molecule 47: GTP-binding protein 4

Chain SR:

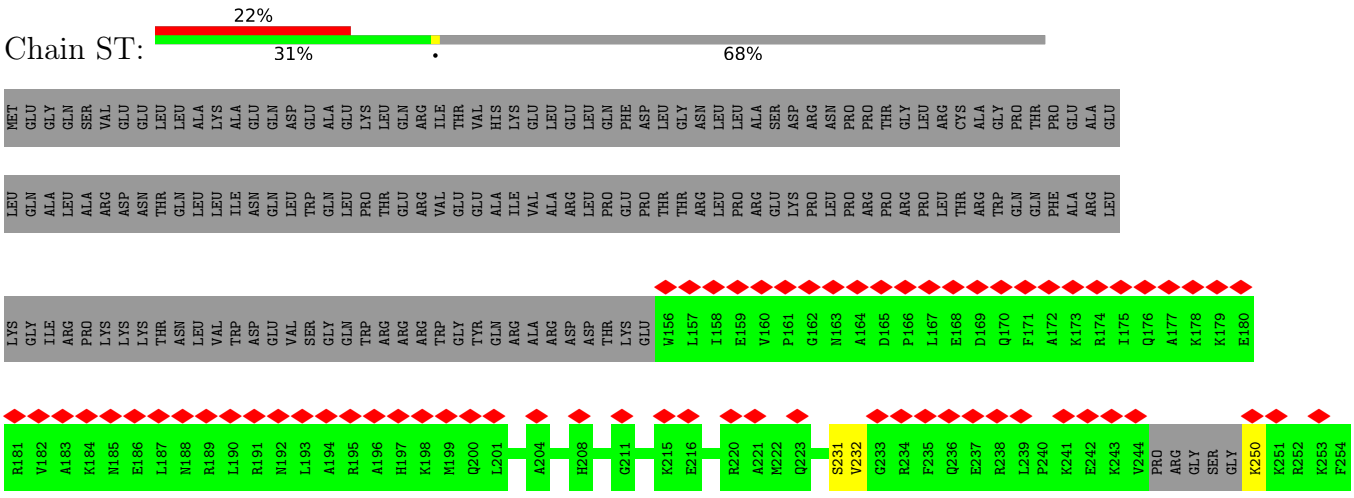


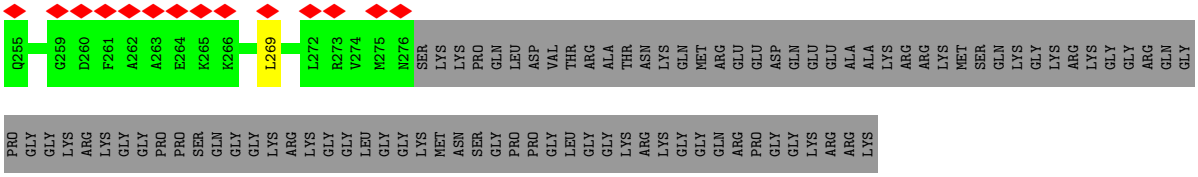
• Molecule 48: Ribosome biogenesis protein BOP1

Chain SS:

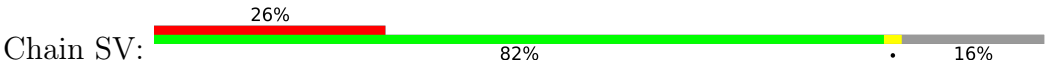


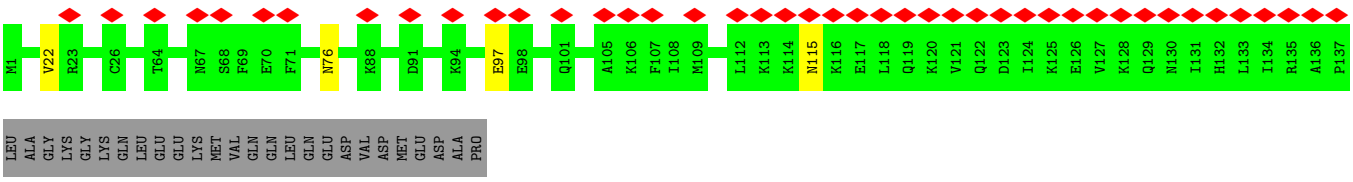
• Molecule 49: Ribosome biogenesis regulatory protein homolog



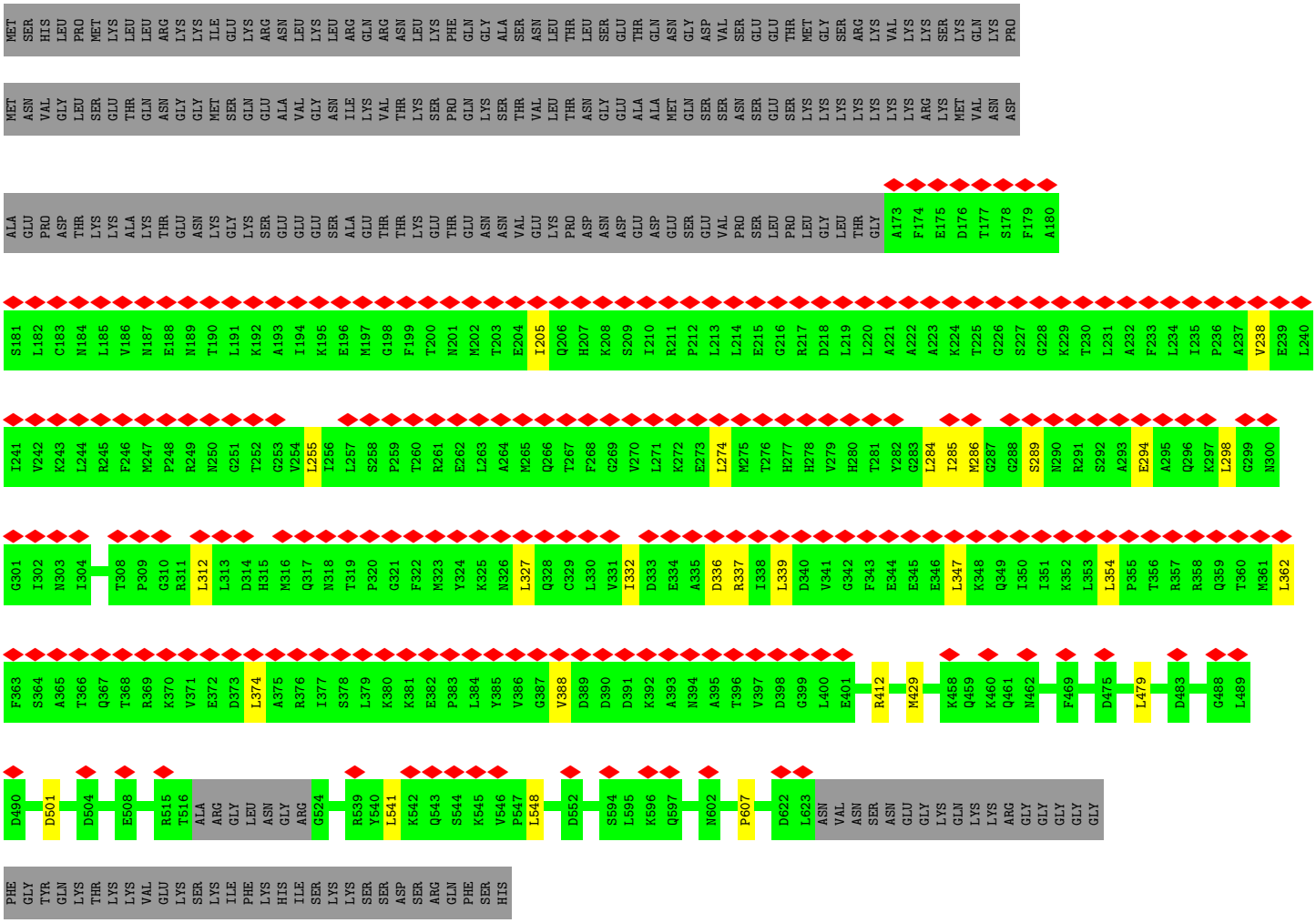


• Molecule 50: Probable ribosome biogenesis protein RLP24



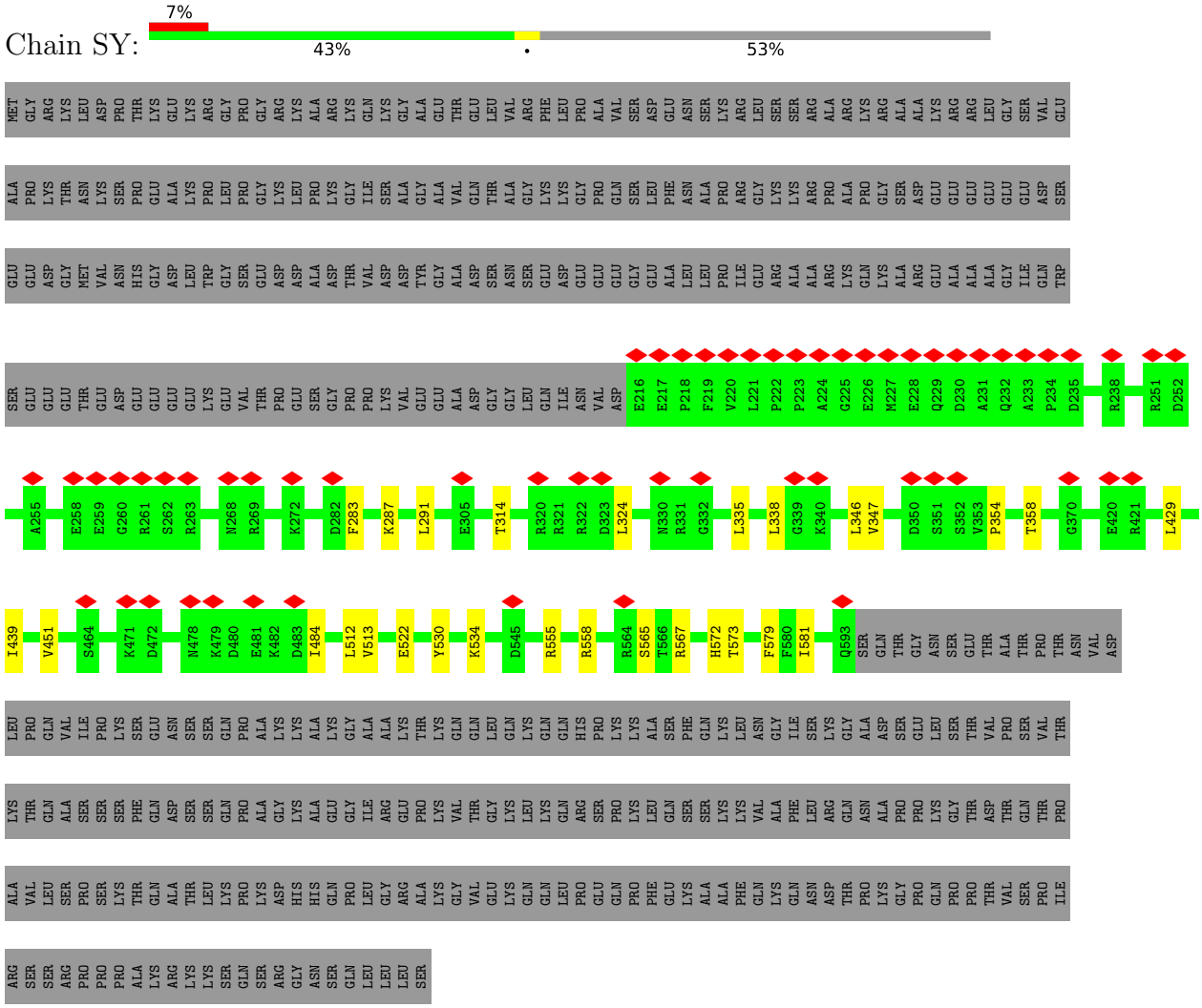


• Molecule 51: ATP-dependent RNA helicase DDX18



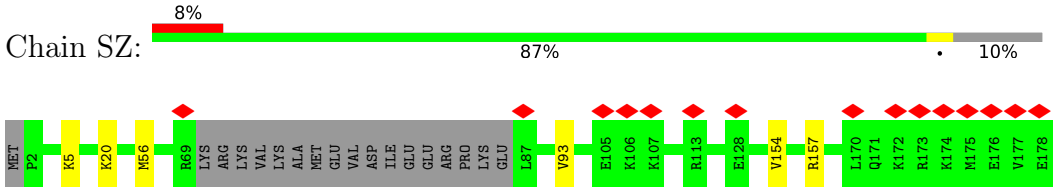
• Molecule 52: Probable 28S rRNA (cytosine(4447)-C(5))-methyltransferase

Chain SY:



• Molecule 53: Nucleolar protein 16

Chain SZ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45396	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	6.688	Depositor
Minimum map value	-0.123	Depositor
Average map value	0.047	Depositor
Map value standard deviation	0.170	Depositor
Recommended contour level	1.0	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: K, AME, MG, GDP, SEP, SF4, ADP, ZN

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	0.26	0/1224	0.53	0/1651
2	BB	0.24	0/1056	0.46	0/1472
3	L1	0.47	0/3611	0.76	1/5623 (0.0%)
4	L2	0.45	0/1634	0.80	0/2538
5	L3	0.49	0/50941	0.79	7/79394 (0.0%)
6	L6	0.31	0/1020	0.66	0/1367
7	L7	0.33	0/1666	0.58	0/2228
8	L8	0.33	0/1133	0.56	0/1516
9	L9	0.32	0/1584	0.64	0/2117
10	LA	0.28	0/1309	0.49	0/1752
11	LB	0.29	0/1239	0.63	0/1658
12	LC	0.34	0/1501	0.59	0/2013
13	LE	0.28	0/755	0.51	0/1021
14	LG	0.30	0/1007	0.56	0/1350
15	LH	0.24	0/818	0.53	0/1111
16	LI	0.33	0/1132	0.63	1/1504 (0.1%)
17	LK	0.25	0/648	0.53	0/880
18	LN	0.31	0/2938	0.54	0/3923
19	LQ	0.31	0/1114	0.60	0/1486
20	LS	0.28	0/1023	0.56	0/1351
21	LT	0.35	0/895	0.62	0/1198
22	LU	0.30	0/843	0.62	0/1115
23	LW	0.30	0/626	0.64	0/829
24	NB	0.25	0/2449	0.46	0/3335
25	NF	0.29	0/1690	0.53	0/2247
26	NH	0.30	0/1473	0.53	0/1988
27	NI	0.24	0/3906	0.48	0/5329
28	NK	0.26	0/587	0.60	0/767
29	NM	0.30	0/1566	0.57	0/2097
30	NO	0.27	0/2530	0.50	0/3412
31	NQ	0.26	0/2556	0.55	0/3466
32	NS	0.27	0/2592	0.54	0/3487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	SA	0.30	0/2918	0.59	0/3920
34	SC	0.27	0/1657	0.54	0/2219
35	SD	0.32	0/2022	0.57	0/2696
36	SE	0.29	0/1517	0.56	0/2046
37	SG	0.30	0/1548	0.56	0/2081
38	SH	0.32	0/1298	0.52	0/1742
39	SI	0.29	0/1930	0.53	0/2595
40	SJ	0.26	0/868	0.52	0/1153
41	SK	0.27	0/1877	0.53	0/2554
42	SL	0.29	0/1994	0.53	0/2684
43	SM	0.30	0/3819	0.51	0/5139
44	SN	0.26	0/1368	0.50	0/1830
45	SO	0.27	0/2608	0.51	0/3506
46	SQ	0.27	0/1817	0.52	0/2435
47	SR	0.28	0/3768	0.51	0/5086
48	SS	0.31	0/2159	0.55	0/2932
49	ST	0.27	0/795	0.49	0/1072
50	SV	0.30	0/1194	0.56	0/1582
51	SW	0.28	0/3620	0.49	0/4886
52	SY	0.30	0/3046	0.54	0/4117
53	SZ	0.28	0/1364	0.55	0/1826
All	All	0.38	0/142253	0.66	9/203326 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L3	2266	C	N1-C2-O2	6.70	122.92	118.90
5	L3	2266	C	C2-N1-C1'	6.68	126.15	118.80
5	L3	2266	C	N3-C2-O2	-6.13	117.61	121.90
5	L3	2266	C	C6-N1-C2	-5.87	117.95	120.30
5	L3	4709	U	C2-N1-C1'	5.48	124.27	117.70
3	L1	83	C	C2-N1-C1'	5.34	124.67	118.80
5	L3	417	G	O4'-C1'-N9	5.29	112.44	108.20
5	L3	4975	G	O4'-C1'-N9	5.23	112.39	108.20
16	LI	53	ASP	CB-CG-OD1	5.22	123.00	118.30

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	1208	0	1257	8	0
2	BB	1057	0	464	0	0
3	L1	3234	0	1639	6	0
4	L2	1468	0	755	10	0
5	L3	45561	0	23045	141	0
6	L6	998	0	1067	9	0
7	L7	1634	0	1779	5	0
8	L8	1111	0	1174	4	0
9	L9	1546	0	1585	10	0
10	LA	1286	0	1338	7	0
11	LB	1223	0	1330	13	0
12	LC	1461	0	1502	11	0
13	LE	747	0	599	3	0
14	LG	993	0	1050	15	0
15	LH	813	0	640	2	0
16	LI	1115	0	1205	9	0
17	LK	642	0	455	3	0
18	LN	2884	0	3000	16	0
19	LQ	1096	0	1183	7	0
20	LS	1015	0	1148	4	0
21	LT	876	0	912	6	0
22	LU	832	0	917	3	0
23	LW	612	0	640	1	0
24	NB	2424	0	1868	8	0
25	NF	1661	0	1776	9	0
26	NH	1441	0	1448	11	0
27	NI	3866	0	3171	13	0
28	NK	581	0	656	8	0
29	NM	1550	0	1599	14	0
30	NO	2487	0	2506	6	0
31	NQ	2502	0	2481	13	0
32	NS	2529	0	2563	13	0
33	SA	2864	0	3038	18	0
34	SC	1627	0	1751	8	0
35	SD	1985	0	2128	2	0
36	SE	1491	0	1592	9	0
37	SG	1526	0	1614	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	SH	1267	0	1291	2	0
39	SI	1887	0	2011	18	0
40	SJ	855	0	876	5	0
41	SK	1852	0	1828	13	0
42	SL	1960	0	2052	8	0
43	SM	3735	0	3830	15	0
44	SN	1350	0	1345	8	0
45	SO	2544	0	2631	11	0
46	SQ	1778	0	1817	9	0
47	SR	3695	0	3755	23	0
48	SS	2116	0	2028	16	0
49	ST	787	0	698	3	0
50	SV	1171	0	1232	4	0
51	SW	3549	0	3628	17	0
52	SY	2985	0	3004	19	0
53	SZ	1338	0	1352	5	0
54	L1	5	0	0	0	0
54	L2	1	0	0	0	0
54	L3	52	0	0	0	0
54	L9	1	0	0	0	0
54	LQ	1	0	0	0	0
54	LT	1	0	0	0	0
54	NI	1	0	0	0	0
54	SA	1	0	0	0	0
54	SR	1	0	0	0	0
55	LW	1	0	0	0	0
55	SV	1	0	0	0	0
56	NI	27	0	12	0	0
57	NM	8	0	0	0	0
58	SR	28	0	12	0	0
59	SR	1	0	0	0	0
All	All	134945	0	110277	437	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 (437) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:712:C:O2	5:L3:1284:G:N2	2.01	0.92
14:LG:40:ILE:HD11	14:LG:64:THR:HG23	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:712:C:N3	5:L3:1284:G:N1	2.22	0.85
5:L3:184:U:O2'	5:L3:189:G:OP2	1.95	0.85
51:SW:238:VAL:HG21	51:SW:274:LEU:HD22	1.63	0.81
4:L2:53:G:OP2	38:SH:81:ARG:NH1	2.15	0.80
36:SE:109:GLU:OE2	43:SM:102:ASN:ND2	2.14	0.79
30:NO:346:GLU:OE1	30:NO:350:ARG:NH2	2.15	0.79
46:SQ:64:ARG:NH1	46:SQ:65:MET:O	2.16	0.78
5:L3:1319:U:O2	5:L3:1324:A:N6	2.17	0.78
5:L3:3890:A:OP2	5:L3:4570:G:N2	2.17	0.78
5:L3:1444:G:HO2'	5:L3:1448:G:HO2'	1.30	0.77
5:L3:1524:A:O2'	5:L3:1525:A:O5'	2.01	0.76
25:NF:163:LYS:NZ	25:NF:167:TYR:O	2.18	0.76
5:L3:2045:G:O6	5:L3:3870:C:O2'	2.02	0.76
5:L3:1501:C:O2'	11:LB:68:ARG:NH1	2.20	0.75
9:L9:20:ARG:NH2	40:SJ:693:THR:O	2.19	0.75
32:NS:156:THR:OG1	32:NS:200:GLU:OE1	2.01	0.74
3:L1:75:G:OP2	16:LI:74:TYR:OH	2.06	0.74
25:NF:8:GLU:OE2	27:NI:581:SER:OG	2.05	0.74
5:L3:1508:A:OP1	33:SA:110:ARG:NH2	2.19	0.74
5:L3:62:A:N3	5:L3:77:U:O2'	2.21	0.73
5:L3:2574:G:O2'	5:L3:2575:U:OP1	2.06	0.73
5:L3:306:A:OP1	22:LU:53:TYR:OH	2.06	0.72
5:L3:2338:C:OP1	29:NM:22:ARG:NH1	2.23	0.72
5:L3:4354:U:OP1	52:SY:530:TYR:OH	2.05	0.72
5:L3:1983:A:N1	27:NI:579:ASN:ND2	2.37	0.72
51:SW:289:SER:OG	51:SW:294:GLU:OE2	2.07	0.71
5:L3:4678:G:OP1	28:NK:14:ARG:NH1	2.22	0.71
5:L3:2361:G:O6	10:LA:25:HIS:ND1	2.23	0.71
39:SI:92:ASP:OD2	39:SI:242:TYR:OH	2.09	0.71
5:L3:4468:U:HO2'	28:NK:2:ALA:N	1.89	0.70
5:L3:1883:G:OP1	19:LQ:47:ARG:NH1	2.25	0.70
5:L3:304:C:OP2	40:SJ:691:ARG:NH2	2.24	0.70
18:LN:107:ALA:HB2	18:LN:201:LEU:HD22	1.73	0.70
5:L3:1833:G:N2	5:L3:1835:G:O4'	2.25	0.69
41:SK:119:PRO:O	41:SK:139:ARG:NH2	2.24	0.69
1:BA:138:SER:OG	5:L3:2002:A:N6	2.25	0.69
5:L3:4662:C:O2'	5:L3:5004:C:OP1	2.07	0.69
5:L3:5063:G:O6	18:LN:124:LYS:NZ	2.26	0.69
18:LN:286:LYS:NZ	18:LN:302:ASN:O	2.23	0.69
45:SO:224:GLU:OE2	49:ST:250:LYS:NZ	2.23	0.69
5:L3:4441:A:N6	27:NI:445:ASP:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:3907:G:O2'	5:L3:3908:A:OP1	2.11	0.67
5:L3:5039:U:O3'	50:SV:115:ASN:ND2	2.27	0.67
24:NB:324:SER:OG	24:NB:327:SER:OG	1.98	0.67
19:LQ:84:GLU:O	19:LQ:87:VAL:HG22	1.94	0.67
5:L3:116:G:O2'	48:SS:239:ARG:NH1	2.27	0.67
26:NH:104:GLU:OE2	26:NH:135:SER:OG	2.10	0.66
33:SA:213:GLU:OE1	33:SA:215:ASN:ND2	2.29	0.66
45:SO:48:PRO:O	48:SS:133:ARG:NH1	2.29	0.66
5:L3:238:C:OP2	16:LI:45:ARG:NH2	2.29	0.65
3:L1:62:A:OP1	20:LS:52:LYS:NZ	2.29	0.65
39:SI:70:ARG:NH1	39:SI:106:ASP:O	2.29	0.65
4:L2:61:C:N3	42:SL:50:ARG:NH1	2.45	0.65
11:LB:88:ASP:OD1	11:LB:89:ASP:N	2.30	0.65
41:SK:98:GLU:OE2	50:SV:76:ASN:ND2	2.29	0.65
39:SI:177:THR:CG2	48:SS:355:ALA:HB3	2.27	0.65
52:SY:555:ARG:O	52:SY:558:ARG:NH1	2.30	0.64
16:LI:34:LEU:HD21	16:LI:109:LEU:HD21	1.78	0.64
4:L2:13:C:OP1	39:SI:86:HIS:NE2	2.27	0.64
5:L3:4940:C:OP1	34:SC:156:ARG:NH1	2.30	0.64
1:BA:92:ARG:NH2	5:L3:1980:U:OP2	2.30	0.64
30:NO:301:GLU:OE2	30:NO:305:ASN:ND2	2.32	0.63
4:L2:91:C:OP2	42:SL:176:ARG:NH2	2.32	0.63
11:LB:35:LEU:HD21	33:SA:298:ILE:HD11	1.80	0.63
18:LN:57:VAL:HG12	18:LN:73:VAL:HG22	1.81	0.63
5:L3:121:A:OP1	36:SE:110:LYS:NZ	2.32	0.62
3:L1:156:U:OP2	36:SE:89:ARG:NH2	2.32	0.62
39:SI:252:ARG:NH1	43:SM:270:GLU:OE1	2.32	0.62
4:L2:5:A:N6	4:L2:95:A:O2'	2.32	0.62
5:L3:1444:G:O2'	5:L3:1448:G:O2'	2.11	0.62
5:L3:2072:C:OP1	11:LB:2:GLY:N	2.32	0.62
10:LA:158:PRO:O	32:NS:276:ARG:NH2	2.32	0.62
5:L3:1524:A:HO2'	5:L3:1525:A:P	2.22	0.62
6:L6:62:PRO:O	6:L6:63:THR:OG1	2.15	0.62
5:L3:4543:G:N3	26:NH:80:ARG:NH2	2.48	0.62
11:LB:39:THR:HG22	11:LB:41:SER:H	1.65	0.62
12:LC:17:LEU:HD21	13:LE:136:ARG:HH11	1.65	0.61
47:SR:302:ASP:OD2	47:SR:303:ASP:N	2.33	0.61
5:L3:1921:C:O2'	12:LC:160:ARG:NH2	2.33	0.61
11:LB:124:ASP:OD1	11:LB:125:GLN:N	2.34	0.61
5:L3:2044:U:N3	7:L7:63:ASN:OD1	2.33	0.61
10:LA:163:GLU:OE1	32:NS:276:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LB:122:THR:OG1	11:LB:124:ASP:OD1	2.16	0.61
39:SI:143:VAL:O	39:SI:147:VAL:HG12	2.00	0.61
5:L3:957:G:N2	5:L3:1283:G:OP2	2.34	0.61
15:LH:79:PHE:CB	20:LS:36:VAL:HG21	2.31	0.60
28:NK:88:ASP:OD1	28:NK:89:GLN:N	2.34	0.60
51:SW:284:LEU:HD21	51:SW:286:MET:HG3	1.82	0.60
12:LC:81:TRP:CZ3	13:LE:154:ILE:HD12	2.37	0.60
43:SM:189:TYR:CZ	43:SM:202:ILE:HD12	2.35	0.60
48:SS:233:ILE:HD11	51:SW:607:PRO:HD3	1.84	0.60
14:LG:27:ASN:OD1	14:LG:28:CYS:N	2.34	0.60
21:LT:40:GLU:OE2	21:LT:109:ARG:NH2	2.35	0.59
39:SI:177:THR:HG23	48:SS:355:ALA:HB3	1.84	0.59
27:NI:307:LEU:HD21	27:NI:311:LEU:HD23	1.85	0.59
47:SR:188:VAL:HG23	47:SR:189:THR:HG23	1.83	0.59
30:NO:182:ALA:O	34:SC:46:ARG:NH1	2.35	0.59
39:SI:101:ARG:NH1	39:SI:122:LYS:O	2.36	0.59
39:SI:112:VAL:O	39:SI:116:ILE:HD12	2.02	0.59
41:SK:6:SER:OG	41:SK:208:LEU:HD13	2.02	0.59
43:SM:170:HIS:HB3	43:SM:283:LEU:HD11	1.85	0.59
14:LG:68:GLY:O	14:LG:73:ARG:NH1	2.36	0.59
14:LG:40:ILE:CD1	14:LG:64:THR:HG23	2.32	0.58
33:SA:84:THR:OG1	33:SA:87:SER:OG	2.07	0.58
51:SW:285:ILE:HD11	51:SW:298:LEU:HD21	1.85	0.58
5:L3:402:A:O2'	32:NS:103:LYS:O	2.21	0.58
14:LG:42:VAL:HG13	14:LG:45:ILE:HG22	1.86	0.58
9:L9:103:GLU:OE2	9:L9:165:THR:HG21	2.04	0.58
5:L3:404:U:O3'	16:LI:87:ARG:NH2	2.37	0.58
21:LT:33:VAL:HG23	21:LT:38:GLU:HB2	1.85	0.58
32:NS:176:ARG:NH2	34:SC:231:GLU:O	2.35	0.58
5:L3:206:U:O2'	5:L3:208:A:N7	2.30	0.58
5:L3:2334:C:OP2	33:SA:195:LYS:NZ	2.33	0.58
5:L3:4763:U:O2'	12:LC:174:THR:OG1	2.19	0.58
29:NM:159:ASP:OD2	32:NS:305:ILE:HD11	2.04	0.58
14:LG:64:THR:HG22	14:LG:76:VAL:HG22	1.86	0.58
5:L3:4437:U:OP2	25:NF:107:LYS:NZ	2.28	0.57
19:LQ:131:SER:N	32:NS:201:ASP:OD2	2.37	0.57
5:L3:1659:U:H2'	17:LK:15:VAL:HG23	1.87	0.57
5:L3:4706:G:OP1	28:NK:12:LYS:NZ	2.37	0.56
19:LQ:118:LEU:HD12	29:NM:119:TYR:HE1	1.69	0.56
5:L3:2851:G:N2	27:NI:754:GLU:O	2.38	0.56
40:SJ:666:GLU:OE1	48:SS:208:GLN:NE2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:SO:53:LYS:NZ	48:SS:155:ASP:OD2	2.37	0.56
5:L3:1950:U:O2'	12:LC:116:ARG:NH1	2.38	0.56
5:L3:4763:U:HO2'	12:LC:174:THR:HG1	1.48	0.56
43:SM:207:PHE:CD2	48:SS:355:ALA:HB2	2.41	0.56
53:SZ:56:MET:HG2	53:SZ:93:VAL:HG21	1.87	0.56
47:SR:269:LEU:HD12	47:SR:306:ILE:HG23	1.88	0.56
41:SK:2:ALA:HB3	41:SK:215:LEU:HD11	1.87	0.56
43:SM:47:GLU:OE1	43:SM:47:GLU:N	2.38	0.56
26:NH:154:ARG:O	26:NH:154:ARG:NH1	2.39	0.56
29:NM:163:GLU:OE1	32:NS:303:VAL:HG13	2.05	0.56
19:LQ:118:LEU:HD12	29:NM:119:TYR:CE1	2.40	0.55
8:L8:32:ASP:OD2	8:L8:33:GLN:N	2.36	0.55
1:BA:128:THR:O	1:BA:132:ILE:HD12	2.05	0.55
1:BA:138:SER:HG	5:L3:2002:A:N6	2.04	0.55
3:L1:74:U:O4	16:LI:72:GLN:NE2	2.37	0.55
6:L6:21:ARG:NH1	9:L9:197:THR:OG1	2.40	0.55
41:SK:101:LEU:HB3	41:SK:107:VAL:HG21	1.88	0.55
25:NF:115:GLY:O	27:NI:532:LYS:NZ	2.39	0.55
48:SS:383:VAL:HG21	48:SS:388:LEU:HD11	1.88	0.55
5:L3:4478:G:N2	5:L3:4608:G:O2'	2.40	0.55
9:L9:46:ASP:OD1	9:L9:47:LYS:N	2.40	0.54
24:NB:1:MET:HE3	25:NF:43:ILE:HD12	1.88	0.54
10:LA:155:GLN:OE1	32:NS:298:ARG:NH1	2.41	0.54
33:SA:204:ARG:NH1	33:SA:205:ARG:O	2.40	0.54
37:SG:86:LEU:HD22	37:SG:188:GLN:O	2.07	0.54
5:L3:4437:U:O2'	47:SR:143:ARG:NH2	2.41	0.54
51:SW:412:ARG:NH2	51:SW:501:ASP:OD1	2.40	0.54
34:SC:201:ILE:HD11	34:SC:267:LEU:HD21	1.90	0.53
51:SW:284:LEU:HD23	51:SW:285:ILE:N	2.23	0.53
5:L3:2562:G:O2'	5:L3:2565:A:N6	2.40	0.53
5:L3:4672:A:OP1	14:LG:17:SER:OG	2.11	0.53
44:SN:119:VAL:HG21	45:SO:165:LEU:HD13	1.89	0.53
5:L3:2269:C:O2'	29:NM:13:ASN:ND2	2.42	0.53
24:NB:1:MET:CE	25:NF:43:ILE:HD12	2.38	0.53
26:NH:57:ASN:HD22	52:SY:451:VAL:HG12	1.72	0.53
43:SM:575:ALA:O	43:SM:578:SER:OG	2.23	0.53
5:L3:364:G:O6	23:LW:55:ARG:NH2	2.41	0.53
18:LN:139:ASP:OD1	18:LN:140:GLU:N	2.42	0.53
31:NQ:91:ARG:NE	31:NQ:105:ASP:OD2	2.41	0.53
52:SY:429:LEU:HD12	52:SY:439:ILE:HD11	1.91	0.53
12:LC:76:LYS:NZ	12:LC:100:LEU:O	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L3:1354:A:HO2'	17:LK:61:TYR:HH	1.56	0.53
33:SA:84:THR:HG1	33:SA:87:SER:HG	1.45	0.53
12:LC:82:LEU:HD12	12:LC:124:ILE:HG23	1.91	0.53
18:LN:218:ASP:OD2	18:LN:348:ARG:NH2	2.40	0.52
47:SR:441:TYR:OH	50:SV:97:GLU:OE2	2.21	0.52
47:SR:348:MET:HA	47:SR:348:MET:HE3	1.91	0.52
36:SE:218:LEU:O	36:SE:222:ILE:HD12	2.09	0.52
52:SY:579:PHE:HE2	52:SY:581:ILE:HD11	1.73	0.52
5:L3:1447:C:O5'	30:NO:323:ARG:NH2	2.42	0.52
33:SA:180:ILE:HD11	33:SA:227:ILE:HD11	1.92	0.52
31:NQ:52:THR:OG1	31:NQ:95:GLN:OE1	2.23	0.52
39:SI:171:ASN:O	39:SI:171:ASN:ND2	2.35	0.52
46:SQ:45:VAL:HG23	46:SQ:45:VAL:O	2.09	0.52
47:SR:107:ASP:OD1	47:SR:108:ASN:N	2.42	0.52
18:LN:95:THR:OG1	18:LN:98:GLY:O	2.16	0.52
5:L3:1859:C:OP1	24:NB:26:ARG:NH1	2.43	0.51
5:L3:4962:C:O2	28:NK:92:GLN:NE2	2.43	0.51
5:L3:1516:G:O2'	6:L6:17:ASP:OD1	2.21	0.51
5:L3:4872:G:O6	8:L8:98:ARG:NH1	2.44	0.51
41:SK:174:SER:O	41:SK:178:GLN:N	2.42	0.51
34:SC:50:LEU:O	34:SC:54:ILE:N	2.44	0.51
37:SG:92:MET:HE1	37:SG:161:ILE:HD12	1.93	0.51
31:NQ:1:MET:SD	31:NQ:2:ALA:N	2.83	0.51
1:BA:123:ARG:NH2	46:SQ:63:SER:O	2.44	0.51
9:L9:149:GLN:O	9:L9:152:THR:OG1	2.26	0.51
20:LS:23:ASP:OD1	20:LS:24:LEU:N	2.44	0.51
31:NQ:27:ARG:O	31:NQ:29:GLN:NE2	2.44	0.50
5:L3:72:C:N3	6:L6:60:ARG:NH2	2.60	0.50
5:L3:2267:U:OP1	29:NM:41:ARG:N	2.45	0.50
31:NQ:64:ASP:O	31:NQ:66:THR:N	2.45	0.50
26:NH:114:LEU:O	26:NH:117:GLY:N	2.44	0.50
51:SW:205:ILE:HD13	51:SW:388:VAL:HG21	1.93	0.50
44:SN:73:THR:HG23	44:SN:73:THR:O	2.12	0.50
52:SY:287:LYS:NZ	52:SY:522:GLU:OE1	2.26	0.50
52:SY:314:THR:HG22	52:SY:324:LEU:HD23	1.94	0.50
7:L7:14:HIS:CE1	7:L7:119:VAL:HG23	2.47	0.50
33:SA:209:ILE:HB	33:SA:229:LEU:HD13	1.93	0.50
52:SY:338:LEU:HD13	52:SY:347:VAL:HG22	1.94	0.50
5:L3:1283:G:H5'	33:SA:313:VAL:HG13	1.92	0.49
16:LI:106:ILE:HG21	16:LI:109:LEU:HD23	1.93	0.49
27:NI:597:ASP:OD2	47:SR:94:LEU:HD22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:SR:356:VAL:HG12	47:SR:356:VAL:O	2.11	0.49
51:SW:327:LEU:HD23	51:SW:354:LEU:HD23	1.94	0.49
10:LA:47:TYR:OH	10:LA:57:CYS:O	2.26	0.49
5:L3:709:C:OP1	21:LT:89:ARG:NH2	2.46	0.49
5:L3:4895:C:O3'	8:L8:132:LYS:NZ	2.46	0.49
22:LU:71:LYS:NZ	48:SS:127:SEP:O3P	2.37	0.49
44:SN:142:LYS:NZ	45:SO:154:MET:O	2.44	0.49
48:SS:315:ASN:OD1	48:SS:346:LYS:NZ	2.23	0.49
4:L2:49:G:H1'	39:SI:76:VAL:HG21	1.95	0.49
29:NM:13:ASN:OD1	29:NM:14:LYS:N	2.45	0.49
20:LS:27:GLU:O	20:LS:31:LEU:HD23	2.13	0.49
43:SM:36:ARG:NH2	43:SM:114:TYR:OH	2.41	0.49
4:L2:93:C:HO2'	4:L2:94:U:P	2.36	0.49
5:L3:233:U:HO2'	5:L3:234:G:H8	1.59	0.49
12:LC:99:ASP:OD1	12:LC:100:LEU:N	2.45	0.49
52:SY:565:SER:O	52:SY:567:ARG:NH1	2.45	0.49
18:LN:219:VAL:HG11	18:LN:337:VAL:CG2	2.43	0.48
41:SK:175:SER:O	47:SR:368:ARG:NH2	2.45	0.48
47:SR:225:ILE:HD11	47:SR:241:ILE:HD11	1.95	0.48
3:L1:83:C:H42	16:LI:50:ARG:CZ	2.26	0.48
5:L3:4678:G:N7	28:NK:11:ARG:NH2	2.60	0.48
5:L3:5047:C:O2'	5:L3:5050:C:OP2	2.25	0.48
37:SG:134:CYS:SG	37:SG:144:LEU:HD11	2.54	0.48
5:L3:369:G:N2	5:L3:372:A:OP2	2.40	0.48
5:L3:1502:G:OP1	11:LB:65:ARG:NH1	2.46	0.48
27:NI:231:ALA:O	27:NI:235:SER:N	2.47	0.48
29:NM:23:THR:OG1	29:NM:26:GLN:O	2.24	0.48
1:BA:37:LEU:HD11	1:BA:69:ALA:HB2	1.96	0.48
5:L3:1434:G:OP1	24:NB:371:ARG:NH1	2.42	0.48
5:L3:5066:U:OP1	10:LA:43:LYS:NZ	2.45	0.48
47:SR:225:ILE:CD1	47:SR:241:ILE:HD11	2.44	0.48
5:L3:4483:C:H5"	47:SR:21:LEU:HD13	1.95	0.48
41:SK:2:ALA:CB	41:SK:215:LEU:HD11	2.44	0.48
30:NO:316:THR:O	30:NO:321:ARG:NH1	2.47	0.48
33:SA:65:GLU:OE1	33:SA:80:ARG:NH1	2.47	0.47
44:SN:131:LYS:NZ	45:SO:223:ILE:O	2.47	0.47
4:L2:93:C:O2'	4:L2:94:U:O5'	2.23	0.47
26:NH:152:ASP:O	26:NH:156:VAL:HG13	2.14	0.47
41:SK:108:THR:HG21	41:SK:129:LEU:HD11	1.95	0.47
5:L3:4910:G:H4'	18:LN:95:THR:HG22	1.96	0.47
25:NF:97:SER:OG	25:NF:98:ARG:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SW:336:ASP:HA	51:SW:339:LEU:HD12	1.95	0.47
52:SY:335:LEU:HD22	52:SY:346:LEU:HB3	1.97	0.47
13:LE:116:LYS:HG3	13:LE:128:LEU:HD11	1.96	0.47
5:L3:1358:G:O2'	5:L3:1360:G:O6	2.30	0.47
12:LC:19:THR:HG23	12:LC:22:CYS:H	1.80	0.47
26:NH:65:SER:OG	52:SY:439:ILE:HD12	2.15	0.47
5:L3:4726:G:OP2	28:NK:98:ASN:ND2	2.48	0.47
1:BA:103:ASN:OD1	1:BA:104:ILE:N	2.48	0.46
5:L3:40:G:OP2	44:SN:153:LYS:NZ	2.48	0.46
5:L3:4401:G:OP1	24:NB:24:LYS:NZ	2.45	0.46
14:LG:57:VAL:HA	14:LG:81:VAL:HG13	1.97	0.46
47:SR:225:ILE:HG23	47:SR:271:LEU:HD21	1.96	0.46
1:BA:14:TYR:C	1:BA:15:LEU:HD12	2.35	0.46
5:L3:47:A:OP2	6:L6:20:ARG:NH1	2.47	0.46
5:L3:2000:G:O2'	5:L3:2017:A:N1	2.44	0.46
5:L3:4434:C:O4'	25:NF:191:THR:HG23	2.14	0.46
5:L3:4724:A:O2'	18:LN:104:THR:HG22	2.15	0.46
15:LH:30:LYS:O	36:SE:89:ARG:NH1	2.47	0.46
5:L3:1726:U:H5'	35:SD:135:ILE:HD11	1.96	0.46
42:SL:123:ILE:HD11	42:SL:191:SER:HA	1.97	0.46
5:L3:4993:G:H22	5:L3:5058:A:H2	1.63	0.46
5:L3:4046:A:N1	52:SY:558:ARG:NH2	2.64	0.46
33:SA:210:ILE:HG21	33:SA:252:TRP:CZ3	2.51	0.46
34:SC:235:THR:O	34:SC:235:THR:HG23	2.15	0.46
5:L3:4910:G:N2	7:L7:106:ASP:O	2.48	0.46
5:L3:4347:G:O2'	5:L3:4348:A:O5'	2.29	0.46
41:SK:222:PHE:O	41:SK:224:LEU:N	2.49	0.46
5:L3:68:U:OP1	9:L9:178:HIS:ND1	2.44	0.46
5:L3:346:G:OP1	16:LI:8:THR:HG23	2.15	0.46
21:LT:43:LEU:O	21:LT:109:ARG:NH1	2.49	0.46
27:NI:422:PHE:O	27:NI:426:VAL:HG22	2.16	0.46
39:SI:183:GLU:O	39:SI:187:GLY:N	2.48	0.46
5:L3:28:C:OP2	9:L9:193:ARG:NH2	2.49	0.46
5:L3:4697:U:OP1	25:NF:25:ARG:NH2	2.49	0.46
44:SN:68:GLU:O	45:SO:163:ARG:NH2	2.49	0.46
48:SS:145:ASP:O	48:SS:161:LYS:NZ	2.49	0.45
43:SM:215:VAL:HG23	48:SS:364:PHE:CG	2.51	0.45
46:SQ:185:GLU:N	46:SQ:185:GLU:OE2	2.49	0.45
21:LT:33:VAL:HG13	21:LT:33:VAL:O	2.16	0.45
43:SM:573:ASP:O	43:SM:577:ARG:NE	2.43	0.45
5:L3:4903:G:OP1	28:NK:82:ASN:ND2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:SN:62:ARG:NH1	45:SO:58:ASN:OD1	2.50	0.45
47:SR:295:ARG:O	47:SR:299:LEU:HD13	2.17	0.45
51:SW:429:MET:SD	51:SW:479:LEU:HD23	2.56	0.45
5:L3:244:G:O6	53:SZ:20:LYS:NZ	2.48	0.45
5:L3:730:G:OP2	35:SD:76:ARG:NE	2.50	0.45
5:L3:2562:G:N2	5:L3:2565:A:OP2	2.49	0.45
4:L2:66:A:OP2	38:SH:168:LYS:NZ	2.40	0.45
52:SY:287:LYS:O	52:SY:291:LEU:HD23	2.16	0.44
5:L3:182:G:N7	45:SO:339:ARG:NH1	2.65	0.44
5:L3:4768:G:OP1	7:L7:168:TYR:OH	2.27	0.44
33:SA:140:LYS:O	33:SA:204:ARG:NH2	2.49	0.44
47:SR:289:ASN:OD1	47:SR:290:LYS:N	2.48	0.44
32:NS:160:CYS:SG	32:NS:198:ILE:HD12	2.57	0.44
29:NM:71:ALA:HA	29:NM:77:LEU:HD13	1.98	0.44
37:SG:63:ASN:ND2	37:SG:66:GLU:OE2	2.51	0.44
5:L3:45:U:O2'	6:L6:14:PHE:O	2.20	0.44
5:L3:171:U:O4	53:SZ:157:ARG:NH1	2.49	0.44
5:L3:1295:C:O2'	32:NS:157:VAL:HG11	2.17	0.44
14:LG:109:LYS:HE3	27:NI:503:LEU:HD22	1.98	0.44
36:SE:58:PRO:HG2	36:SE:61:ILE:HD12	1.98	0.44
5:L3:1346:C:OP1	11:LB:148:VAL:HG12	2.17	0.44
5:L3:1364:U:OP2	6:L6:36:ARG:NH1	2.44	0.44
21:LT:37:ASP:OD1	21:LT:38:GLU:N	2.50	0.44
5:L3:740:G:H2'	5:L3:741:C:N1	2.33	0.44
5:L3:958:G:N2	5:L3:1285:U:OP1	2.33	0.44
5:L3:358:C:O2	53:SZ:5:LYS:NZ	2.51	0.44
5:L3:4745:G:H22	5:L3:4955:A:H2	1.66	0.44
24:NB:350:VAL:HG13	24:NB:355:VAL:O	2.17	0.44
8:L8:105:THR:HG22	8:L8:106:ASP:N	2.33	0.43
11:LB:42:THR:HG22	11:LB:42:THR:O	2.18	0.43
31:NQ:113:HIS:CD2	31:NQ:124:LEU:HD21	2.53	0.43
47:SR:101:ILE:HG22	47:SR:105:LEU:HD13	2.00	0.43
26:NH:29:ASP:OD1	49:ST:269:LEU:HD11	2.18	0.43
5:L3:265:C:N4	53:SZ:154:VAL:HG21	2.32	0.43
18:LN:312:LYS:NZ	18:LN:380:GLN:OE1	2.50	0.43
30:NO:99:PHE:CD2	30:NO:125:VAL:HG11	2.53	0.43
45:SO:62:ILE:HD12	45:SO:87:HIS:NE2	2.33	0.43
34:SC:278:THR:HG22	34:SC:279:ASN:N	2.33	0.43
52:SY:512:LEU:HD23	52:SY:513:VAL:N	2.32	0.43
29:NM:42:SER:O	29:NM:48:ASN:ND2	2.51	0.43
5:L3:4569:U:N3	5:L3:4570:G:O6	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:SK:231:THR:O	41:SK:234:THR:OG1	2.30	0.43
5:L3:1669:A:H2'	5:L3:1670:G:O4'	2.19	0.43
14:LG:96:LEU:HD11	50:SV:22:VAL:HG23	2.01	0.43
33:SA:210:ILE:HD13	33:SA:230:LEU:HB2	1.98	0.43
5:L3:291:U:O2'	9:L9:182:HIS:NE2	2.45	0.43
5:L3:1428:U:OP1	11:LB:42:THR:HG21	2.18	0.43
7:L7:16:LEU:HD21	7:L7:83:THR:HG21	2.00	0.43
46:SQ:65:MET:CG	46:SQ:103:LEU:HD13	2.49	0.43
18:LN:219:VAL:HG11	18:LN:337:VAL:HG21	1.99	0.43
39:SI:153:ASN:ND2	43:SM:267:LEU:HD12	2.34	0.43
5:L3:4180:G:N2	26:NH:57:ASN:OD1	2.52	0.43
18:LN:352:LEU:HD23	18:LN:352:LEU:H	1.83	0.43
19:LQ:131:SER:HG	32:NS:201:ASP:CG	2.22	0.43
27:NI:307:LEU:HD23	27:NI:308:ASN:N	2.33	0.43
44:SN:115:ALA:O	44:SN:119:VAL:HG22	2.19	0.43
46:SQ:42:ILE:HD11	46:SQ:92:VAL:HG13	2.01	0.43
5:L3:911:U:H2'	5:L3:912:G:O4'	2.18	0.42
48:SS:316:PRO:O	48:SS:346:LYS:NZ	2.49	0.42
5:L3:85:G:O2'	5:L3:97:G:O6	2.29	0.42
5:L3:2268:A:OP1	29:NM:8:TRP:NE1	2.44	0.42
51:SW:284:LEU:HD23	51:SW:284:LEU:C	2.39	0.42
41:SK:44:ASP:OD1	41:SK:45:THR:N	2.52	0.42
47:SR:348:MET:CE	47:SR:353:VAL:HG11	2.49	0.42
51:SW:347:LEU:HD23	51:SW:374:LEU:HD11	2.01	0.42
18:LN:67:VAL:O	18:LN:67:VAL:HG12	2.20	0.42
27:NI:485:GLN:NE2	27:NI:489:ASP:OD1	2.52	0.42
31:NQ:192:LEU:HD12	31:NQ:197:LYS:HB2	2.00	0.42
39:SI:98:PHE:HB2	39:SI:152:PRO:HG3	2.00	0.42
43:SM:414:PHE:O	43:SM:417:VAL:HG22	2.18	0.42
5:L3:151:G:OP2	9:L9:4:TYR:OH	2.26	0.42
5:L3:4569:U:H4'	10:LA:79:THR:HG21	2.00	0.42
42:SL:64:LEU:HD23	42:SL:255:THR:HG22	2.02	0.42
51:SW:541:LEU:HD13	51:SW:548:LEU:HD21	2.01	0.42
29:NM:87:TYR:CZ	29:NM:91:LEU:HD11	2.55	0.42
32:NS:135:TYR:O	32:NS:269:HIS:NE2	2.50	0.42
5:L3:4977:A:O2'	18:LN:21:ARG:NH2	2.52	0.42
5:L3:4978:G:H22	18:LN:229:LYS:HE3	1.85	0.42
14:LG:84:GLN:NE2	14:LG:86:LYS:O	2.53	0.42
33:SA:35:ASP:OD1	33:SA:35:ASP:N	2.52	0.42
41:SK:155:SER:OG	41:SK:156:ASN:N	2.53	0.42
5:L3:1955:G:OP2	24:NB:52:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:NH:179:LEU:O	26:NH:180:THR:OG1	2.35	0.42
36:SE:207:VAL:HG21	36:SE:215:LEU:HD22	2.02	0.42
3:L1:102:G:OP2	3:L1:104:A:O2'	2.30	0.41
5:L3:4464:A:N7	47:SR:32:THR:OG1	2.45	0.41
12:LC:69:GLU:OE2	12:LC:76:LYS:NZ	2.51	0.41
19:LQ:114:ARG:NH1	29:NM:119:TYR:OH	2.53	0.41
36:SE:165:GLU:OE2	36:SE:165:GLU:N	2.53	0.41
5:L3:447:C:H2'	5:L3:448:G:O4'	2.20	0.41
5:L3:4354:U:OP1	52:SY:534:LYS:NZ	2.45	0.41
33:SA:284:MET:HB2	33:SA:284:MET:HE2	1.95	0.41
16:LI:127:GLN:HA	16:LI:127:GLN:OE1	2.21	0.41
31:NQ:298:ILE:O	31:NQ:298:ILE:HG22	2.19	0.41
34:SC:281:ILE:HG23	34:SC:286:LEU:HD21	2.01	0.41
51:SW:255:LEU:HD21	51:SW:312:LEU:HD21	2.02	0.41
4:L2:61:C:C2	42:SL:50:ARG:NH1	2.89	0.41
5:L3:44:A:N1	5:L3:90:G:O2'	2.49	0.41
6:L6:94:ILE:O	6:L6:94:ILE:HG22	2.20	0.41
14:LG:45:ILE:HD13	14:LG:54:ALA:HB2	2.02	0.41
36:SE:177:MET:CE	48:SS:236:VAL:HG23	2.50	0.41
14:LG:67:LYS:HA	14:LG:73:ARG:HD3	2.02	0.41
31:NQ:252:ALA:HB1	31:NQ:261:LEU:HD11	2.03	0.41
11:LB:23:ILE:HD11	33:SA:32:ILE:O	2.21	0.41
42:SL:82:LEU:HB2	42:SL:203:LEU:HD13	2.01	0.41
5:L3:4405:G:OP2	47:SR:130:LYS:NZ	2.31	0.41
11:LB:91:ARG:O	17:LK:65:ARG:NH1	2.53	0.41
39:SI:78:LEU:HD13	39:SI:111:LEU:HD23	2.03	0.41
47:SR:292:ASP:OD1	47:SR:293:VAL:N	2.53	0.41
5:L3:2569:G:OP1	43:SM:560:ARG:NH1	2.51	0.41
6:L6:100:PRO:O	22:LU:25:ARG:NH2	2.50	0.41
9:L9:31:ARG:NH1	40:SJ:708:GLU:OE2	2.53	0.41
39:SI:116:ILE:HD12	39:SI:116:ILE:H	1.84	0.41
39:SI:171:ASN:HD22	39:SI:171:ASN:C	2.22	0.41
39:SI:192:ILE:HD11	43:SM:380:ARG:HE	1.86	0.41
46:SQ:175:VAL:O	46:SQ:186:GLN:NE2	2.53	0.41
51:SW:332:ILE:HB	51:SW:362:LEU:HD12	2.02	0.41
5:L3:180:C:N3	45:SO:339:ARG:NH1	2.69	0.41
5:L3:2340:C:H4'	33:SA:42:THR:HG23	2.03	0.41
26:NH:137:ALA:O	26:NH:139:ILE:N	2.54	0.41
31:NQ:11:VAL:HG22	31:NQ:319:LEU:HD12	2.02	0.41
37:SG:118:LEU:HD11	37:SG:167:VAL:HG22	2.03	0.41
42:SL:125:THR:HG21	42:SL:198:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SY:354:PRO:O	52:SY:358:THR:HG23	2.21	0.41
52:SY:572:HIS:CD2	52:SY:573:THR:HG23	2.56	0.41
5:L3:3903:A:H2'	5:L3:3904:G:O4'	2.21	0.41
5:L3:4405:G:O6	47:SR:24:SER:OG	2.38	0.41
47:SR:348:MET:HE3	47:SR:353:VAL:HG11	2.02	0.41
52:SY:335:LEU:HD23	52:SY:347:VAL:O	2.20	0.40
31:NQ:139:ASP:OD2	31:NQ:142:HIS:ND1	2.34	0.40
31:NQ:197:LYS:C	31:NQ:198:LEU:HD12	2.42	0.40
46:SQ:65:MET:HG2	46:SQ:103:LEU:HD13	2.03	0.40
5:L3:1879:C:H2'	5:L3:1880:G:O4'	2.21	0.40
5:L3:4691:A:O2'	37:SG:68:ALA:O	2.36	0.40
31:NQ:277:CYS:SG	31:NQ:284:LEU:HD13	2.62	0.40
42:SL:254:LYS:NZ	42:SL:255:THR:O	2.45	0.40
49:ST:231:SER:O	49:ST:232:VAL:HG12	2.21	0.40
5:L3:1325:C:O2	40:SJ:833:ARG:NH1	2.47	0.40
5:L3:2052:G:O2'	5:L3:2057:A:N1	2.43	0.40
5:L3:2266:C:O2	5:L3:2266:C:H2'	2.21	0.40
43:SM:362:ILE:HG22	43:SM:363:GLY:N	2.36	0.40
5:L3:67:C:OP2	5:L3:312:G:N2	2.49	0.40
5:L3:1996:C:O2	46:SQ:54:LYS:NZ	2.55	0.40
14:LG:45:ILE:HD13	14:LG:54:ALA:CB	2.52	0.40
14:LG:109:LYS:HG3	27:NI:503:LEU:HD22	2.03	0.40
48:SS:381:VAL:HG12	48:SS:383:VAL:HG13	2.04	0.40
51:SW:336:ASP:OD1	51:SW:337:ARG:N	2.55	0.40
52:SY:283:PHE:CZ	52:SY:484:ILE:HD12	2.56	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%)	157 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BB	211/217 (97%)	206 (98%)	5 (2%)	0	100	100
6	L6	118/211 (56%)	116 (98%)	2 (2%)	0	100	100
7	L7	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
8	L8	133/215 (62%)	129 (97%)	4 (3%)	0	100	100
9	L9	179/204 (88%)	179 (100%)	0	0	100	100
10	LA	156/184 (85%)	156 (100%)	0	0	100	100
11	LB	149/188 (79%)	149 (100%)	0	0	100	100
12	LC	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
13	LE	107/160 (67%)	104 (97%)	3 (3%)	0	100	100
14	LG	132/140 (94%)	129 (98%)	3 (2%)	0	100	100
15	LH	129/156 (83%)	126 (98%)	3 (2%)	0	100	100
16	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
17	LK	104/148 (70%)	100 (96%)	4 (4%)	0	100	100
18	LN	352/403 (87%)	347 (99%)	5 (1%)	0	100	100
19	LQ	131/135 (97%)	131 (100%)	0	0	100	100
20	LS	120/123 (98%)	120 (100%)	0	0	100	100
21	LT	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
22	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
23	LW	72/97 (74%)	72 (100%)	0	0	100	100
24	NB	379/549 (69%)	375 (99%)	4 (1%)	0	100	100
25	NF	195/260 (75%)	193 (99%)	2 (1%)	0	100	100
26	NH	178/180 (99%)	176 (99%)	2 (1%)	0	100	100
27	NI	590/881 (67%)	585 (99%)	5 (1%)	0	100	100
28	NK	63/129 (49%)	63 (100%)	0	0	100	100
29	NM	180/300 (60%)	180 (100%)	0	0	100	100
30	NO	301/461 (65%)	300 (100%)	1 (0%)	0	100	100
31	NQ	320/385 (83%)	316 (99%)	4 (1%)	0	100	100
32	NS	303/349 (87%)	297 (98%)	6 (2%)	0	100	100
33	SA	358/427 (84%)	354 (99%)	4 (1%)	0	100	100
34	SC	193/288 (67%)	190 (98%)	3 (2%)	0	100	100
35	SD	237/248 (96%)	233 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	SE	183/266 (69%)	181 (99%)	2 (1%)	0	100	100
37	SG	189/192 (98%)	185 (98%)	4 (2%)	0	100	100
38	SH	148/293 (50%)	146 (99%)	2 (1%)	0	100	100
39	SI	225/255 (88%)	221 (98%)	4 (2%)	0	100	100
40	SJ	95/847 (11%)	95 (100%)	0	0	100	100
41	SK	242/245 (99%)	235 (97%)	7 (3%)	0	100	100
42	SL	241/490 (49%)	233 (97%)	8 (3%)	0	100	100
43	SM	445/588 (76%)	445 (100%)	0	0	100	100
44	SN	169/306 (55%)	169 (100%)	0	0	100	100
45	SO	305/353 (86%)	302 (99%)	3 (1%)	0	100	100
46	SQ	216/239 (90%)	214 (99%)	2 (1%)	0	100	100
47	SR	445/634 (70%)	439 (99%)	6 (1%)	0	100	100
48	SS	250/746 (34%)	241 (96%)	9 (4%)	0	100	100
49	ST	112/365 (31%)	109 (97%)	3 (3%)	0	100	100
50	SV	135/163 (83%)	133 (98%)	2 (2%)	0	100	100
51	SW	440/670 (66%)	433 (98%)	7 (2%)	0	100	100
52	SY	376/812 (46%)	374 (100%)	2 (0%)	0	100	100
53	SZ	156/178 (88%)	154 (99%)	2 (1%)	0	100	100
All	All	10630/15584 (68%)	10496 (99%)	134 (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	132/137 (96%)	131 (99%)	1 (1%)	81	94
6	L6	104/177 (59%)	104 (100%)	0	100	100
7	L7	171/174 (98%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	L8	115/161 (71%)	115 (100%)	0	100 100
9	L9	155/172 (90%)	154 (99%)	1 (1%)	86 95
10	LA	142/163 (87%)	142 (100%)	0	100 100
11	LB	136/165 (82%)	136 (100%)	0	100 100
12	LC	157/157 (100%)	157 (100%)	0	100 100
13	LE	51/140 (36%)	51 (100%)	0	100 100
14	LG	102/107 (95%)	102 (100%)	0	100 100
15	LH	39/133 (29%)	39 (100%)	0	100 100
16	LI	124/135 (92%)	124 (100%)	0	100 100
17	LK	29/121 (24%)	29 (100%)	0	100 100
18	LN	313/348 (90%)	313 (100%)	0	100 100
19	LQ	119/121 (98%)	119 (100%)	0	100 100
20	LS	109/110 (99%)	109 (100%)	0	100 100
21	LT	88/89 (99%)	88 (100%)	0	100 100
22	LU	86/89 (97%)	85 (99%)	1 (1%)	71 91
23	LW	63/80 (79%)	63 (100%)	0	100 100
24	NB	142/485 (29%)	142 (100%)	0	100 100
25	NF	180/228 (79%)	180 (100%)	0	100 100
26	NH	155/155 (100%)	155 (100%)	0	100 100
27	NI	267/730 (37%)	267 (100%)	0	100 100
28	NK	61/115 (53%)	61 (100%)	0	100 100
29	NM	168/272 (62%)	167 (99%)	1 (1%)	86 95
30	NO	269/392 (69%)	269 (100%)	0	100 100
31	NQ	265/318 (83%)	265 (100%)	0	100 100
32	NS	276/305 (90%)	276 (100%)	0	100 100
33	SA	299/348 (86%)	299 (100%)	0	100 100
34	SC	178/252 (71%)	178 (100%)	0	100 100
35	SD	207/215 (96%)	207 (100%)	0	100 100
36	SE	158/223 (71%)	158 (100%)	0	100 100
37	SG	170/171 (99%)	170 (100%)	0	100 100
38	SH	140/274 (51%)	140 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	SI	205/228 (90%)	204 (100%)	1 (0%)	88 96
40	SJ	91/733 (12%)	91 (100%)	0	100 100
41	SK	212/213 (100%)	212 (100%)	0	100 100
42	SL	226/437 (52%)	226 (100%)	0	100 100
43	SM	401/509 (79%)	400 (100%)	1 (0%)	93 98
44	SN	133/260 (51%)	133 (100%)	0	100 100
45	SO	283/319 (89%)	283 (100%)	0	100 100
46	SQ	195/214 (91%)	195 (100%)	0	100 100
47	SR	410/574 (71%)	410 (100%)	0	100 100
48	SS	227/648 (35%)	227 (100%)	0	100 100
49	ST	60/300 (20%)	60 (100%)	0	100 100
50	SV	127/149 (85%)	127 (100%)	0	100 100
51	SW	393/591 (66%)	393 (100%)	0	100 100
52	SY	325/685 (47%)	325 (100%)	0	100 100
53	SZ	141/158 (89%)	141 (100%)	0	100 100
All	All	8599/13280 (65%)	8593 (100%)	6 (0%)	93 98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BA	65	GLN
9	L9	195	ARG
22	LU	56	ARG
29	NM	147	ARG
39	SI	171	ASN
43	SM	441	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
7	L7	90	HIS
16	LI	96	HIS
18	LN	3	HIS
22	LU	26	HIS
31	NQ	113	HIS
32	NS	335	HIS

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Mol	Chain	Res	Type
33	SA	245	HIS
34	SC	136	HIS
34	SC	190	HIS
34	SC	227	HIS
40	SJ	712	HIS
40	SJ	726	HIS
43	SM	154	HIS
47	SR	157	HIS
50	SV	115	ASN
51	SW	187	ASN
51	SW	278	HIS
52	SY	430	HIS
52	SY	574	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L1	150/157 (95%)	19 (12%)	0
4	L2	65/1167 (5%)	9 (13%)	0
5	L3	2089/5070 (41%)	288 (13%)	4 (0%)
All	All	2304/6394 (36%)	316 (13%)	4 (0%)

All (316) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L1	34	U
3	L1	52	A
3	L1	54	C
3	L1	55	U
3	L1	59	A
3	L1	62	A
3	L1	63	U
3	L1	82	A
3	L1	83	C
3	L1	84	A
3	L1	86	U
3	L1	94	G
3	L1	103	A
3	L1	105	C
3	L1	110	U
3	L1	111	U

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Mol	Chain	Res	Type
3	L1	114	G
3	L1	153	C
3	L1	156	U
4	L2	2	C
4	L2	11	C
4	L2	48	G
4	L2	49	G
4	L2	62	U
4	L2	87	G
4	L2	94	U
4	L2	96	A
4	L2	101	A
5	L3	41	C
5	L3	48	G
5	L3	56	A
5	L3	58	G
5	L3	59	A
5	L3	64	A
5	L3	65	A
5	L3	69	A
5	L3	89	C
5	L3	91	G
5	L3	92	C
5	L3	93	G
5	L3	95	G
5	L3	108	A
5	L3	116	G
5	L3	119	G
5	L3	159	C
5	L3	170	C
5	L3	171	U
5	L3	172	C
5	L3	173	C
5	L3	181	C
5	L3	182	G
5	L3	186	G
5	L3	187	U
5	L3	190	G
5	L3	197	A
5	L3	200	U
5	L3	204	U
5	L3	210	C

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Mol	Chain	Res	Type
5	L3	218	A
5	L3	225	G
5	L3	233	U
5	L3	234	G
5	L3	253	G
5	L3	261	G
5	L3	265	C
5	L3	315	G
5	L3	326	C
5	L3	340	C
5	L3	347	A
5	L3	349	A
5	L3	362	A
5	L3	387	G
5	L3	399	G
5	L3	410	A
5	L3	413	G
5	L3	431	G
5	L3	448	G
5	L3	451	C
5	L3	452	A
5	L3	469	C
5	L3	473	C
5	L3	685	C
5	L3	686	A
5	L3	696	C
5	L3	697	G
5	L3	701	G
5	L3	729	G
5	L3	730	G
5	L3	731	G
5	L3	739	G
5	L3	746	A
5	L3	910	G
5	L3	913	U
5	L3	915	A
5	L3	917	A
5	L3	918	G
5	L3	925	C
5	L3	926	G
5	L3	932	A
5	L3	933	G

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Mol	Chain	Res	Type
5	L3	943	A
5	L3	944	A
5	L3	945	U
5	L3	956	A
5	L3	1284	G
5	L3	1287	G
5	L3	1295	C
5	L3	1296	G
5	L3	1297	U
5	L3	1301	C
5	L3	1313	C
5	L3	1314	C
5	L3	1354	A
5	L3	1358	G
5	L3	1359	G
5	L3	1378	C
5	L3	1379	C
5	L3	1434	G
5	L3	1445	U
5	L3	1447	C
5	L3	1502	G
5	L3	1504	G
5	L3	1525	A
5	L3	1654	G
5	L3	1661	C
5	L3	1682	A
5	L3	1691	G
5	L3	1726	U
5	L3	1804	A
5	L3	1836	G
5	L3	1837	A
5	L3	1842	G
5	L3	1853	G
5	L3	1856	C
5	L3	1870	C
5	L3	1881	C
5	L3	1883	G
5	L3	1891	A
5	L3	1897	A
5	L3	1910	G
5	L3	1918	U
5	L3	1921	C

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Mol	Chain	Res	Type
5	L3	1922	G
5	L3	1925	G
5	L3	1931	C
5	L3	1935	C
5	L3	1936	C
5	L3	1938	C
5	L3	1939	A
5	L3	1941	A
5	L3	1944	A
5	L3	1945	G
5	L3	1969	G
5	L3	1978	C
5	L3	1984	A
5	L3	2002	A
5	L3	2024	G
5	L3	2025	A
5	L3	2026	A
5	L3	2034	G
5	L3	2044	U
5	L3	2046	G
5	L3	2055	G
5	L3	2056	G
5	L3	2069	A
5	L3	2084	C
5	L3	2085	G
5	L3	2089	G
5	L3	2095	A
5	L3	2097	U
5	L3	2099	G
5	L3	2100	A
5	L3	2102	G
5	L3	2260	C
5	L3	2261	G
5	L3	2265	G
5	L3	2266	C
5	L3	2267	U
5	L3	2268	A
5	L3	2289	C
5	L3	2300	A
5	L3	2301	G
5	L3	2313	A
5	L3	2345	G

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Mol	Chain	Res	Type
5	L3	2348	G
5	L3	2351	C
5	L3	2364	G
5	L3	2474	G
5	L3	2484	A
5	L3	2485	U
5	L3	2490	U
5	L3	2492	C
5	L3	2493	G
5	L3	2500	U
5	L3	2575	U
5	L3	2769	U
5	L3	2844	A
5	L3	2845	A
5	L3	2848	G
5	L3	2852	U
5	L3	3845	A
5	L3	3853	U
5	L3	3868	G
5	L3	3870	C
5	L3	3875	G
5	L3	3877	A
5	L3	3878	C
5	L3	3879	G
5	L3	3881	G
5	L3	3889	G
5	L3	3892	U
5	L3	3894	A
5	L3	3895	G
5	L3	3897	G
5	L3	3906	A
5	L3	3907	G
5	L3	3908	A
5	L3	3926	C
5	L3	3938	G
5	L3	3939	G
5	L3	3940	U
5	L3	3941	G
5	L3	3942	A
5	L3	4049	U
5	L3	4064	C
5	L3	4183	G

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Mol	Chain	Res	Type
5	L3	4188	U
5	L3	4348	A
5	L3	4349	C
5	L3	4350	C
5	L3	4357	G
5	L3	4372	U
5	L3	4373	G
5	L3	4374	U
5	L3	4376	A
5	L3	4380	A
5	L3	4385	A
5	L3	4386	C
5	L3	4390	A
5	L3	4392	G
5	L3	4393	G
5	L3	4398	C
5	L3	4401	G
5	L3	4405	G
5	L3	4433	G
5	L3	4437	U
5	L3	4438	U
5	L3	4439	U
5	L3	4441	A
5	L3	4442	U
5	L3	4451	G
5	L3	4464	A
5	L3	4466	C
5	L3	4475	G
5	L3	4476	C
5	L3	4480	A
5	L3	4491	G
5	L3	4493	U
5	L3	4495	G
5	L3	4496	A
5	L3	4512	U
5	L3	4513	A
5	L3	4518	A
5	L3	4521	U
5	L3	4522	G
5	L3	4523	A
5	L3	4540	C
5	L3	4541	G

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Mol	Chain	Res	Type
5	L3	4545	G
5	L3	4546	A
5	L3	4568	A
5	L3	4584	A
5	L3	4590	A
5	L3	4606	G
5	L3	4608	G
5	L3	4652	G
5	L3	4656	A
5	L3	4670	C
5	L3	4671	C
5	L3	4672	A
5	L3	4678	G
5	L3	4684	A
5	L3	4708	A
5	L3	4709	U
5	L3	4719	G
5	L3	4720	C
5	L3	4737	G
5	L3	4741	C
5	L3	4742	G
5	L3	4745	G
5	L3	4751	G
5	L3	4754	G
5	L3	4757	C
5	L3	4759	C
5	L3	4765	G
5	L3	4772	C
5	L3	4773	C
5	L3	4870	G
5	L3	4871	C
5	L3	4880	C
5	L3	4882	U
5	L3	4883	C
5	L3	4900	C
5	L3	4901	G
5	L3	4910	G
5	L3	4914	C
5	L3	4976	U
5	L3	5006	U
5	L3	5013	C
5	L3	5014	A

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Mol	Chain	Res	Type
5	L3	5020	G
5	L3	5026	U
5	L3	5030	U
5	L3	5041	G
5	L3	5050	C
5	L3	5062	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L3	2574	G
5	L3	4347	G
5	L3	4520	G
5	L3	5013	C

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	AME	NM	1	29	9,10,11	1.45	2 (22%)	9,11,13	1.49	2 (22%)
48	SEP	SS	127	48	8,9,10	1.50	1 (12%)	8,12,14	1.33	2 (25%)
48	SEP	SS	126	48	8,9,10	1.53	1 (12%)	8,12,14	1.65	2 (25%)

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
29	AME	NM	1	29	-	3/9/10/12	-
48	SEP	SS	127	48	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	SEP	SS	126	48	-	4/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	SS	126	SEP	P-O1P	3.35	1.61	1.50
48	SS	127	SEP	P-O1P	3.29	1.61	1.50
29	NM	1	AME	CT1-N	3.22	1.45	1.34
29	NM	1	AME	OT-CT1	-2.01	1.18	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	SS	126	SEP	OG-CB-CA	3.63	111.67	108.14
29	NM	1	AME	CE-SD-CG	2.55	109.17	100.40
48	SS	127	SEP	P-OG-CB	-2.49	111.44	118.30
29	NM	1	AME	CT2-CT1-N	2.18	119.78	116.10
48	SS	126	SEP	OG-P-O1P	2.09	112.35	106.47
48	SS	127	SEP	OG-CB-CA	2.04	110.13	108.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	NM	1	AME	CA-CB-CG-SD
29	NM	1	AME	C-CA-CB-CG
48	SS	126	SEP	CB-OG-P-O2P
48	SS	126	SEP	CB-OG-P-O3P
48	SS	126	SEP	CB-OG-P-O1P
29	NM	1	AME	N-CA-CB-CG
48	SS	127	SEP	N-CA-CB-OG
48	SS	126	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	SS	127	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 70 ligands modelled in this entry, 67 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
58	GDP	SR	1001	59,54	24,30,30	2.53	8 (33%)	30,47,47	1.71	9 (30%)
57	SF4	NM	401	29	0,12,12	-	-	-		
56	ADP	NI	1001	54	24,29,29	0.93	1 (4%)	29,45,45	1.46	4 (13%)

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
58	GDP	SR	1001	59,54	-	0/12/32/32	0/3/3/3
57	SF4	NM	401	29	-	-	0/6/5/5
56	ADP	NI	1001	54	-	1/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	SR	1001	GDP	O6-C6	8.20	1.40	1.23
58	SR	1001	GDP	C2-N2	4.73	1.45	1.34
58	SR	1001	GDP	O4'-C1'	4.12	1.46	1.41
58	SR	1001	GDP	C2'-C1'	-2.55	1.49	1.53
58	SR	1001	GDP	PB-O3B	-2.32	1.45	1.54
56	NI	1001	ADP	C5-C4	2.30	1.47	1.40
58	SR	1001	GDP	PB-O2B	-2.30	1.46	1.54
58	SR	1001	GDP	C5-C4	2.26	1.48	1.43
58	SR	1001	GDP	C2'-C3'	-2.19	1.47	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	NI	1001	ADP	N3-C2-N1	-3.73	122.84	128.68
58	SR	1001	GDP	C3'-C2'-C1'	3.67	106.50	100.98
58	SR	1001	GDP	C5-C6-N1	3.36	119.89	113.95
56	NI	1001	ADP	PA-O3A-PB	-3.29	121.55	132.83
58	SR	1001	GDP	C2-N1-C6	-2.91	119.73	125.10
58	SR	1001	GDP	O2B-PB-O3A	2.91	114.38	104.64
56	NI	1001	ADP	C3'-C2'-C1'	2.81	105.20	100.98
58	SR	1001	GDP	O3B-PB-O3A	2.77	113.93	104.64
56	NI	1001	ADP	C4-C5-N7	-2.61	106.68	109.40
58	SR	1001	GDP	PA-O3A-PB	-2.55	124.06	132.83
58	SR	1001	GDP	C2'-C3'-C4'	2.53	107.57	102.64
58	SR	1001	GDP	O2A-PA-O1A	-2.16	101.58	112.24
58	SR	1001	GDP	O6-C6-C5	-2.07	120.32	124.37

There are no chirality outliers.

All (1) torsion outliers are listed below:

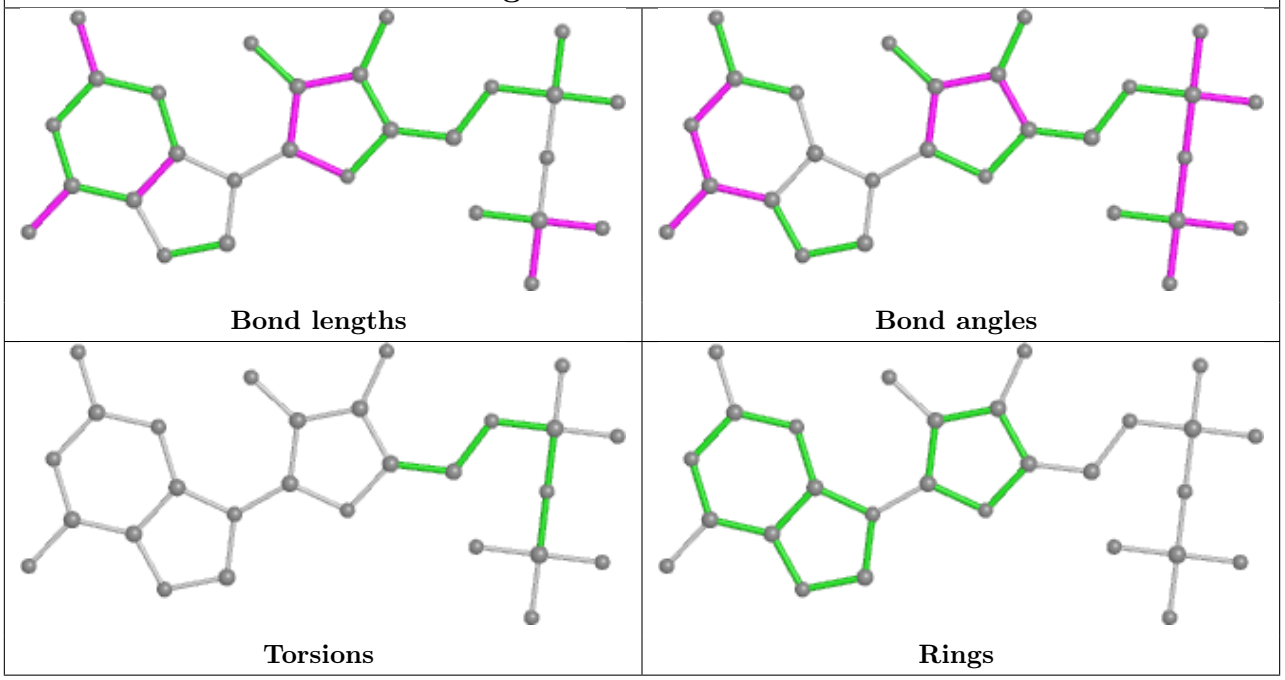
Mol	Chain	Res	Type	Atoms
56	NI	1001	ADP	PA-O3A-PB-O3B

There are no ring outliers.

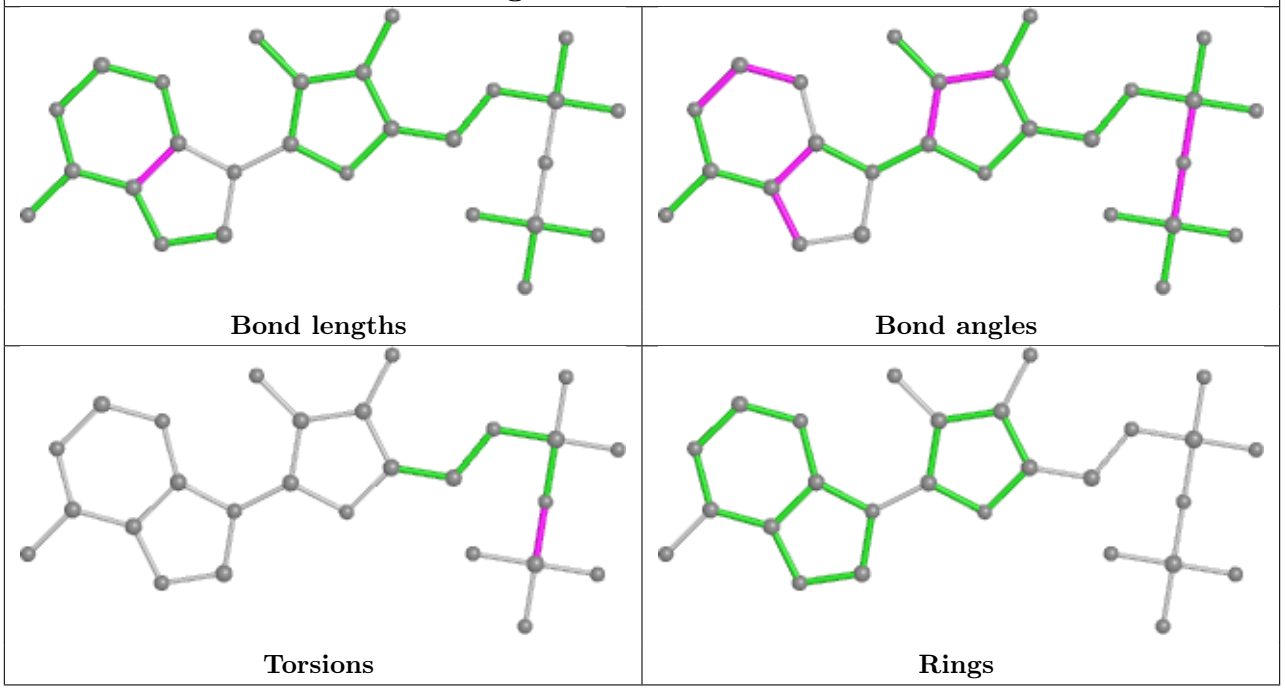
No monomer is involved in short contacts.

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.

Ligand GDP SR 1001



Ligand ADP NI 1001



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.

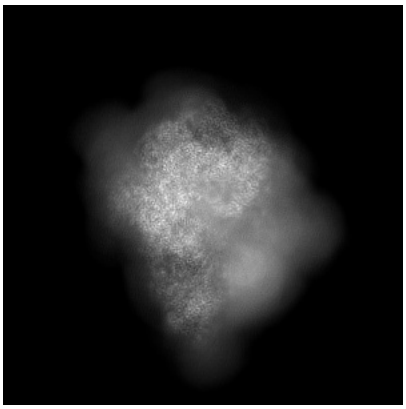
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29256. These allow visual inspection of the internal detail of the map and identification of artifacts.

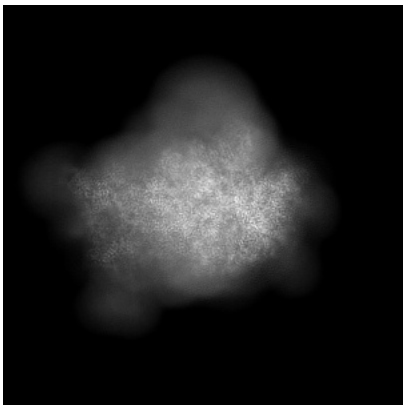
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

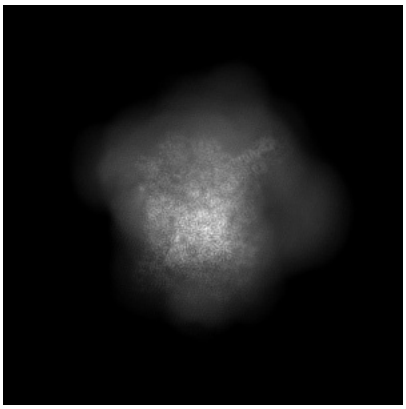
6.1.1 Primary map



X

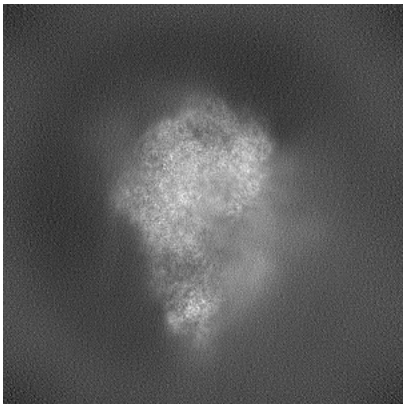


Y

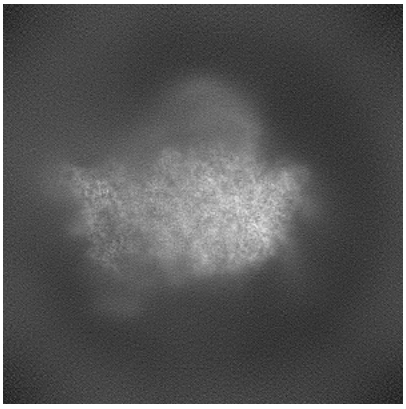


Z

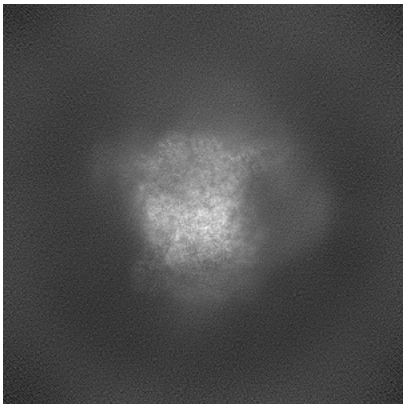
6.1.2 Raw map



X



Y

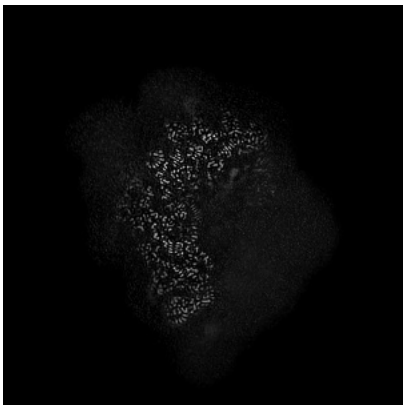


Z

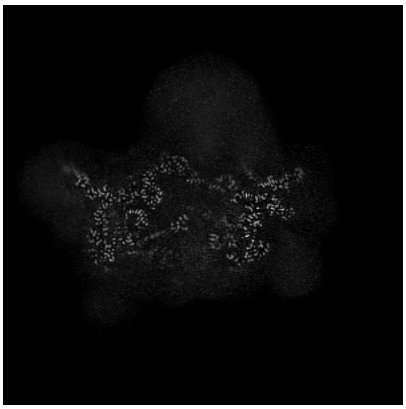
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

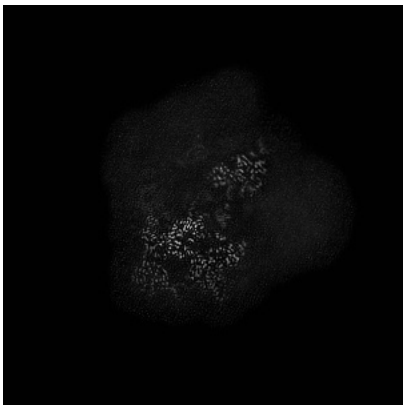
6.2.1 Primary map



X Index: 240

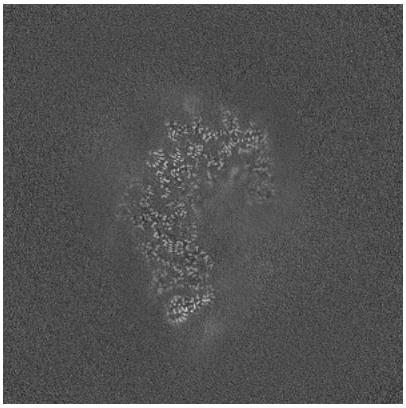


Y Index: 240

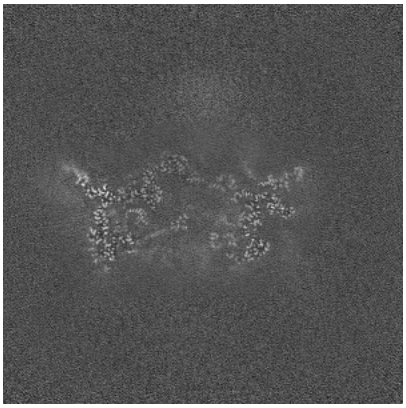


Z Index: 240

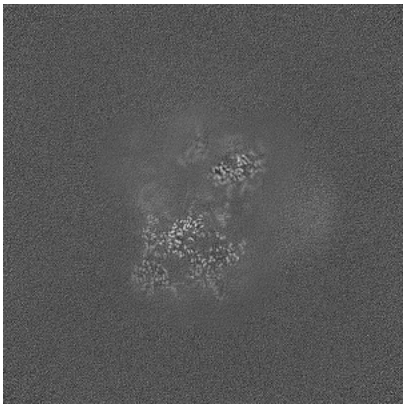
6.2.2 Raw map



X Index: 240



Y Index: 240

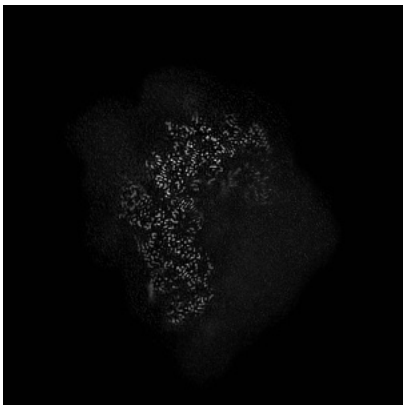


Z Index: 240

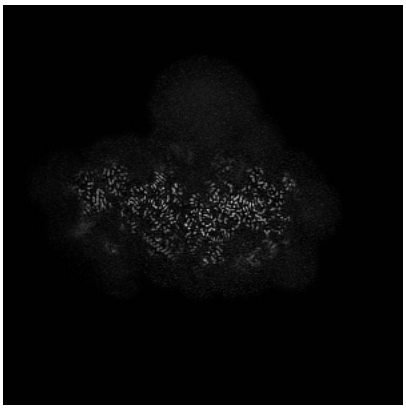
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

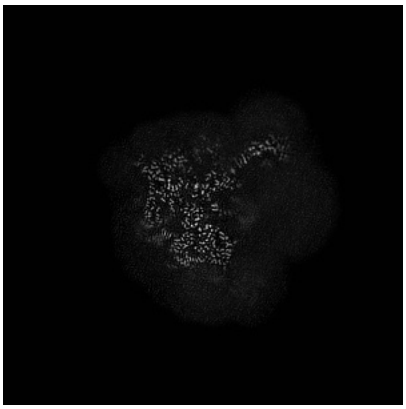
6.3.1 Primary map



X Index: 237

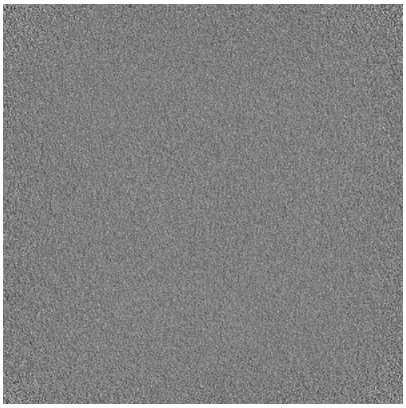


Y Index: 211

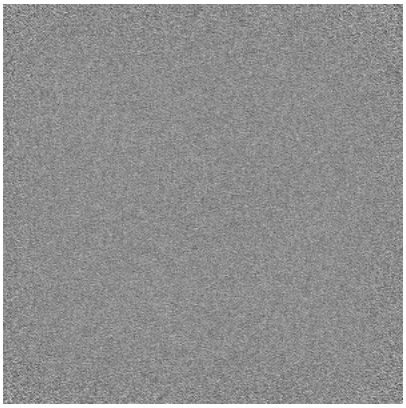


Z Index: 288

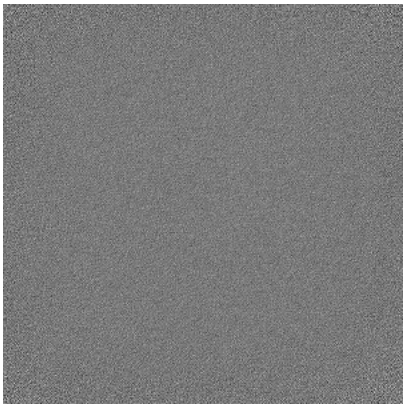
6.3.2 Raw map



X Index: 0



Y Index: 0

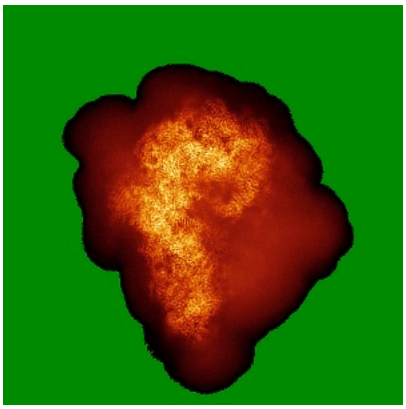


Z Index: 0

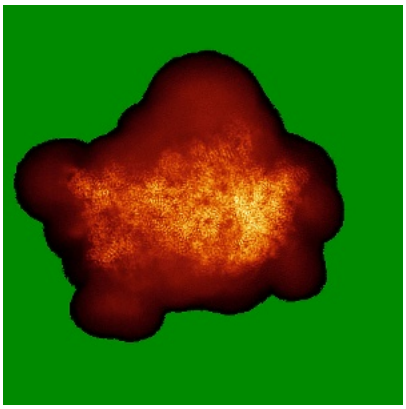
The images above show the largest variance slices of the map in three orthogonal directions.

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

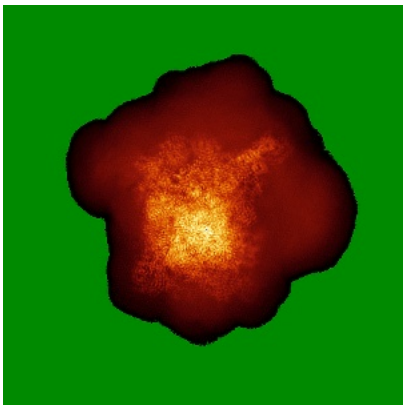
6.4.1 Primary map



X

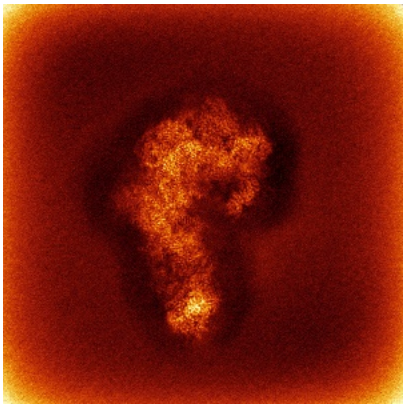


Y

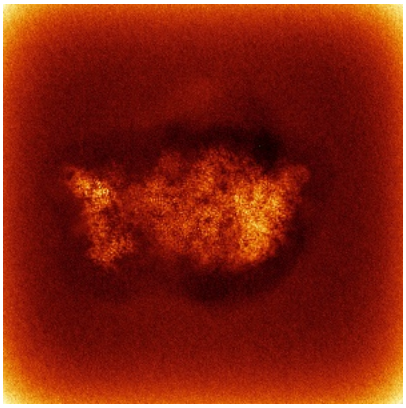


Z

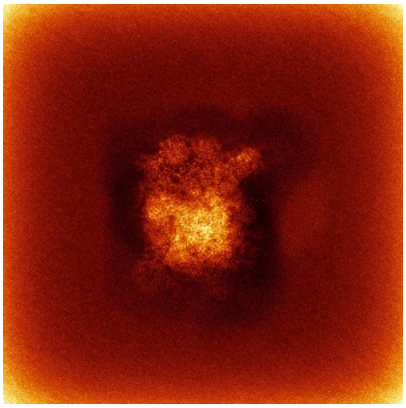
6.4.2 Raw map



X



Y



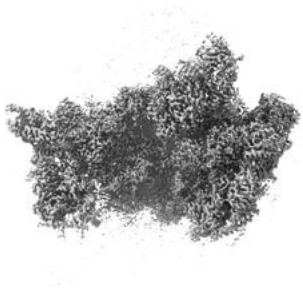
Z

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

6.5.2 Raw map

X

Y

Z

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

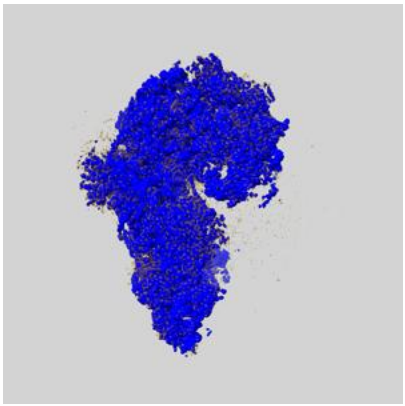
6.6 Mask visualisation

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

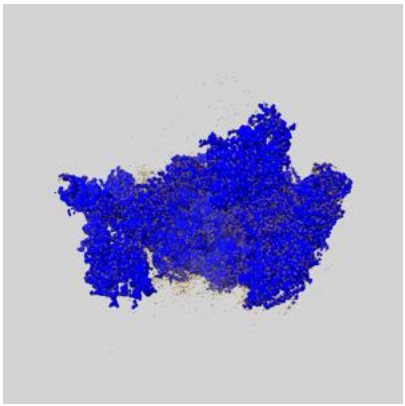
A mask typically either:

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

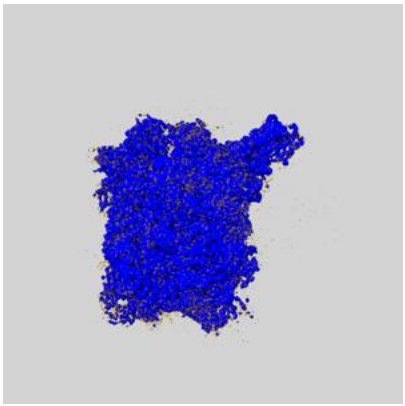
6.6.1 emd_29256_msk_1.map



X



Y

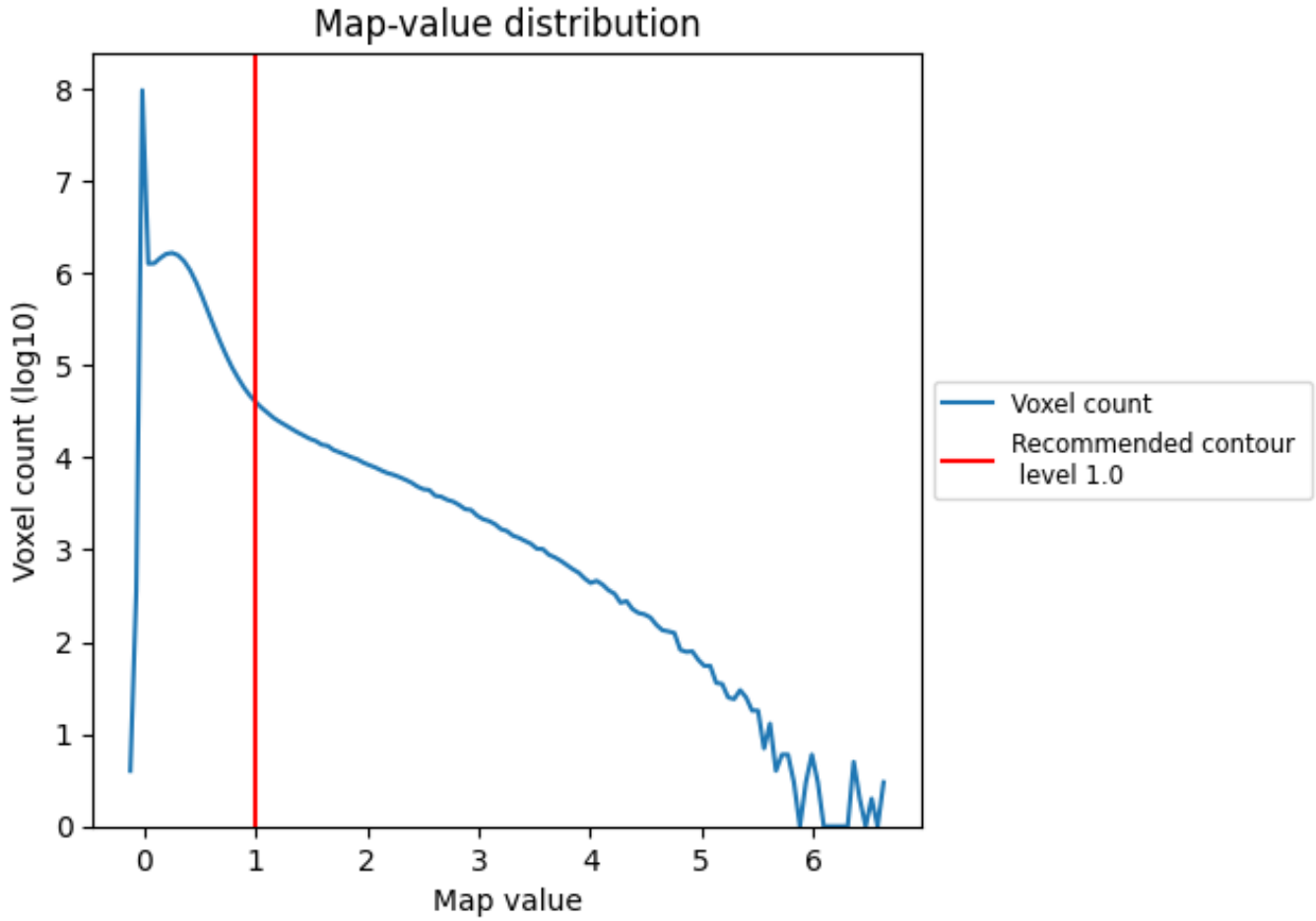


Z

7 Map analysis

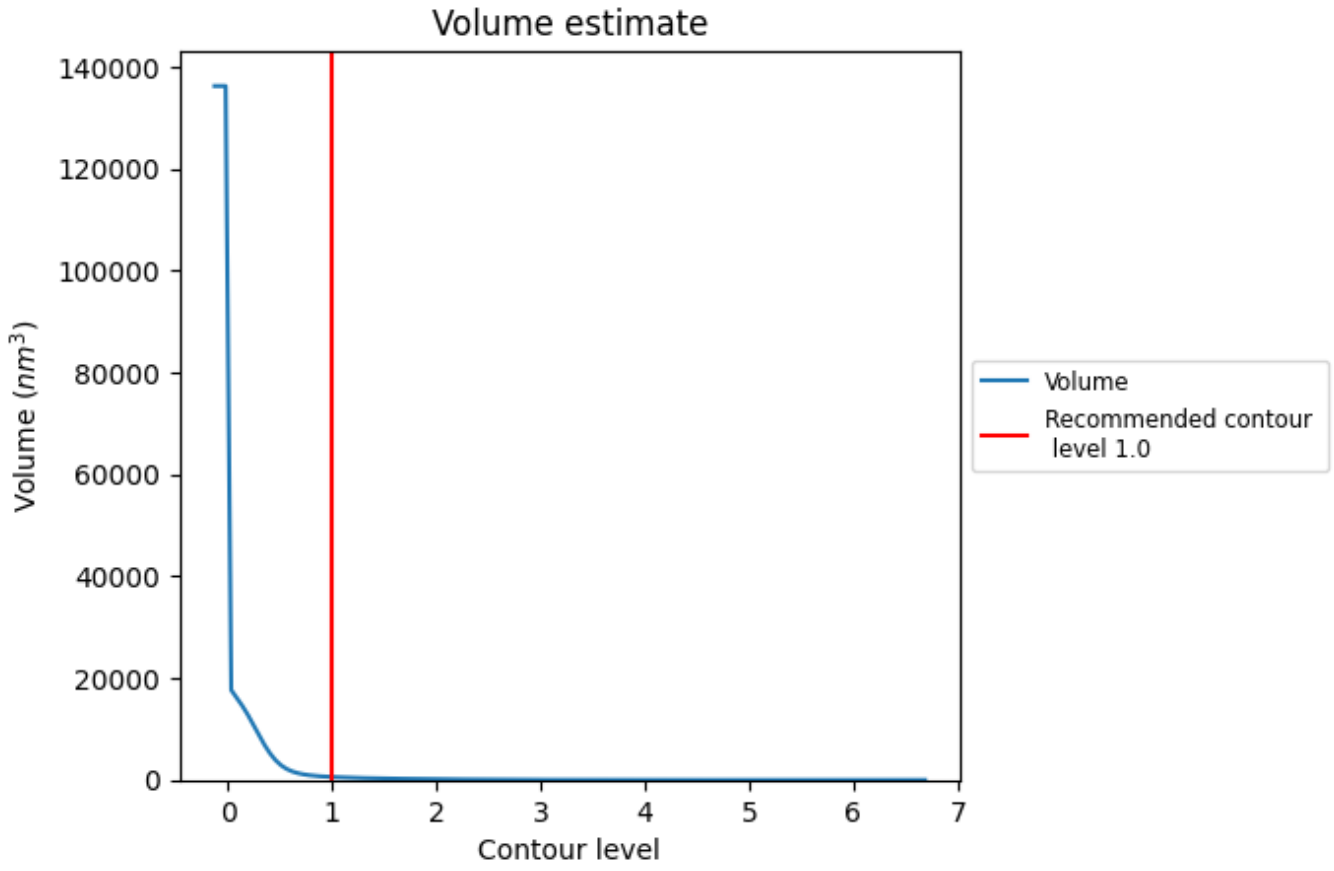
This section contains the results of statistical analysis of the map.

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.

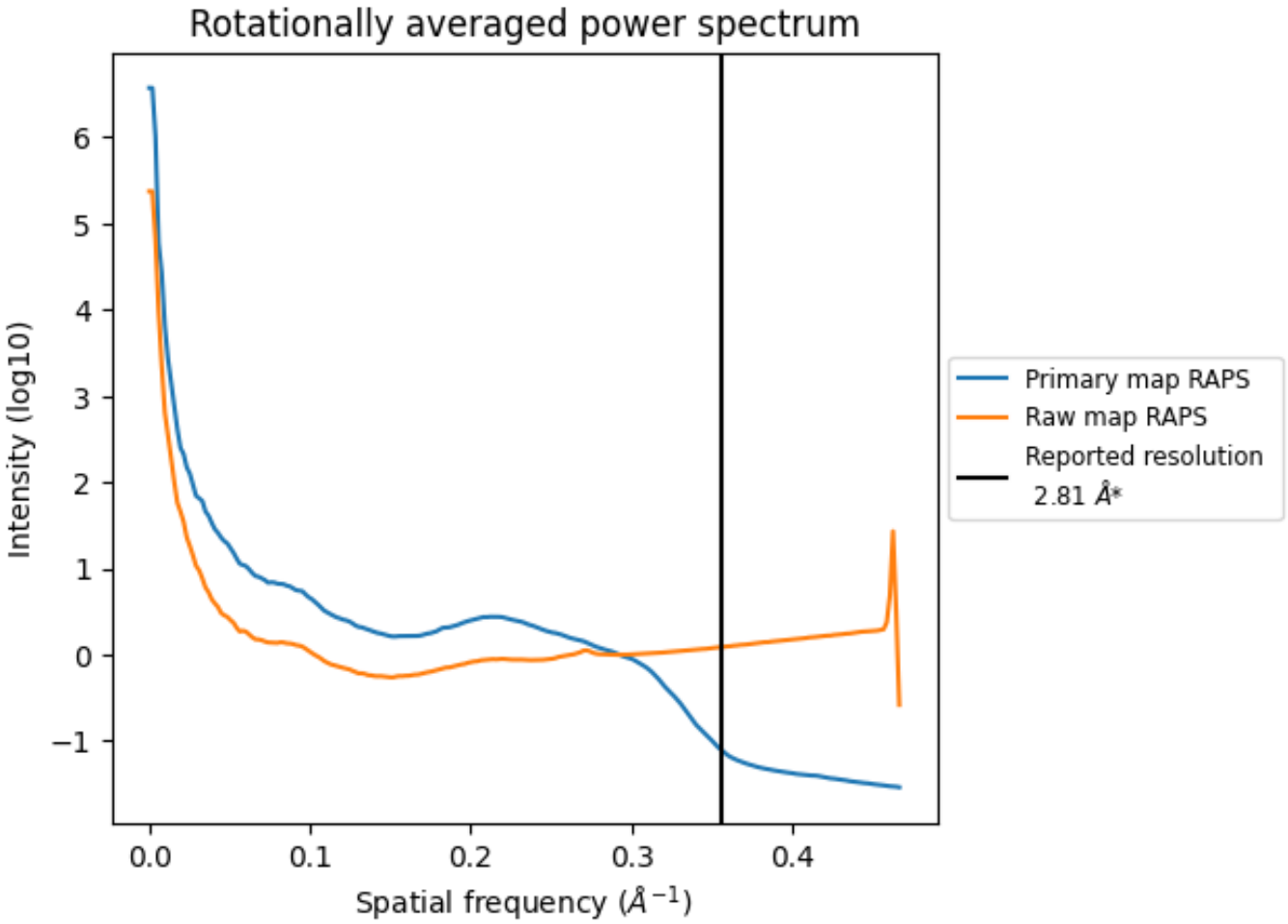
7.2 Volume estimate



The volume at the recommended contour level is 588 nm^3; this corresponds to an approximate mass of 531 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)

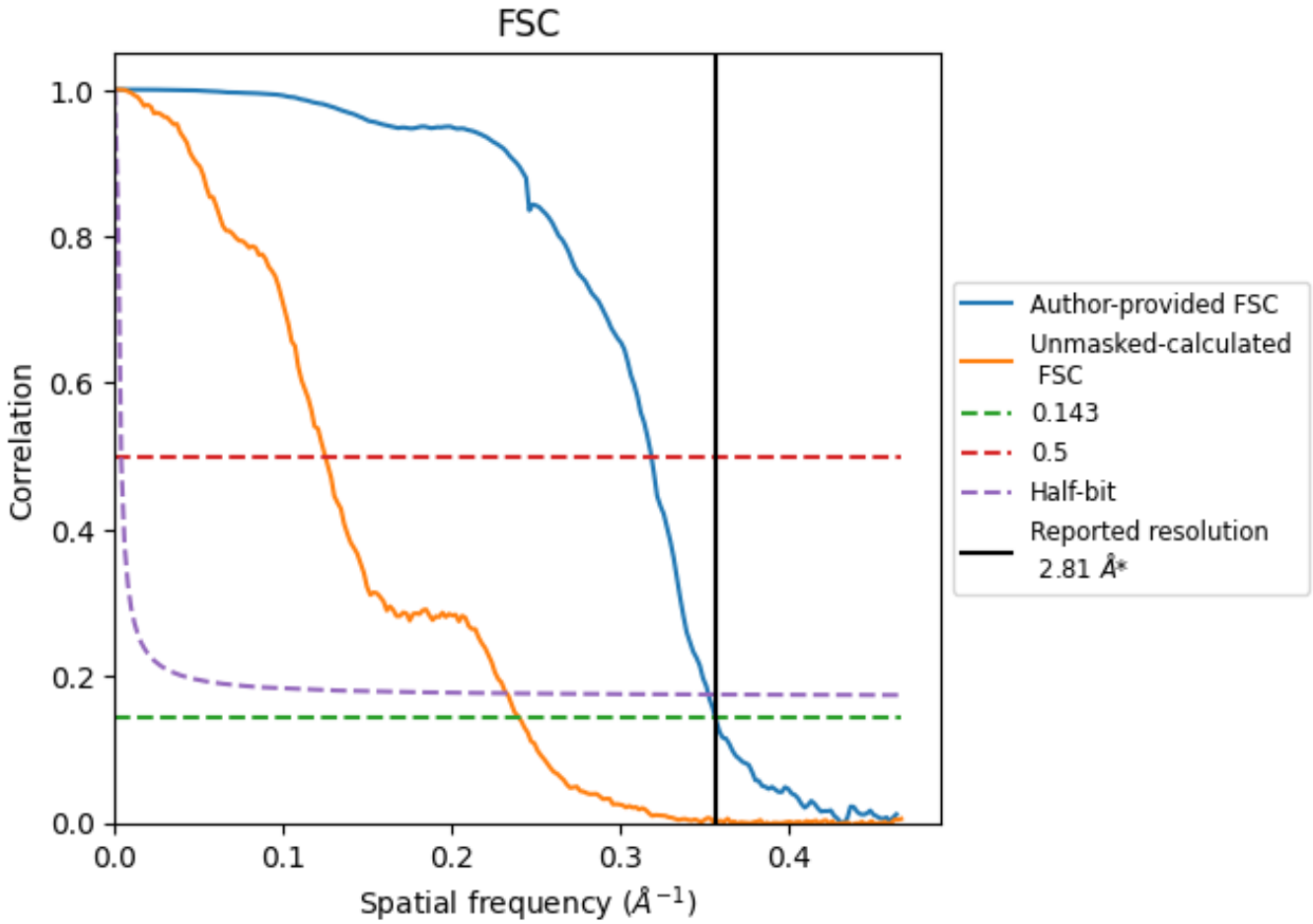


*Reported resolution corresponds to spatial frequency of 0.356 $Å^{-1}$

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 0.356 Å^{-1}

8.2 Resolution estimates (i)

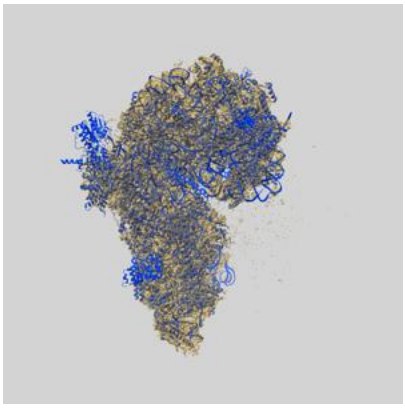
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.14	2.84
Unmasked-calculated*	4.17	8.02	4.30

*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 4.17 differs from the reported value 2.81 by more than 10 %

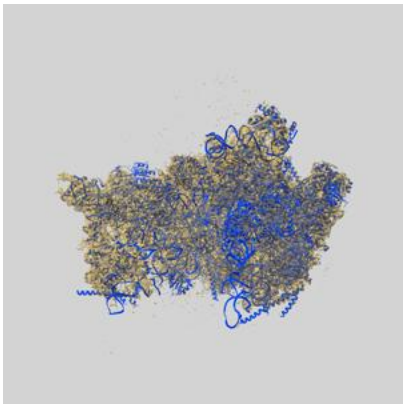
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29256 and PDB model 8FKT. Per-residue inclusion information can be found in section 3 on page 16.

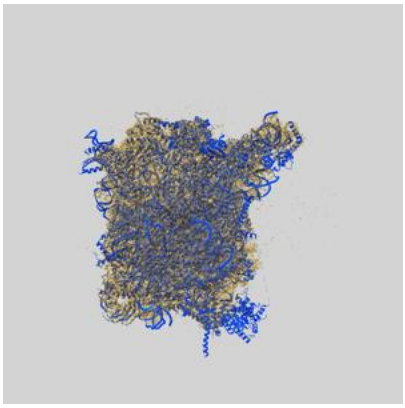
9.1 Map-model overlay



X



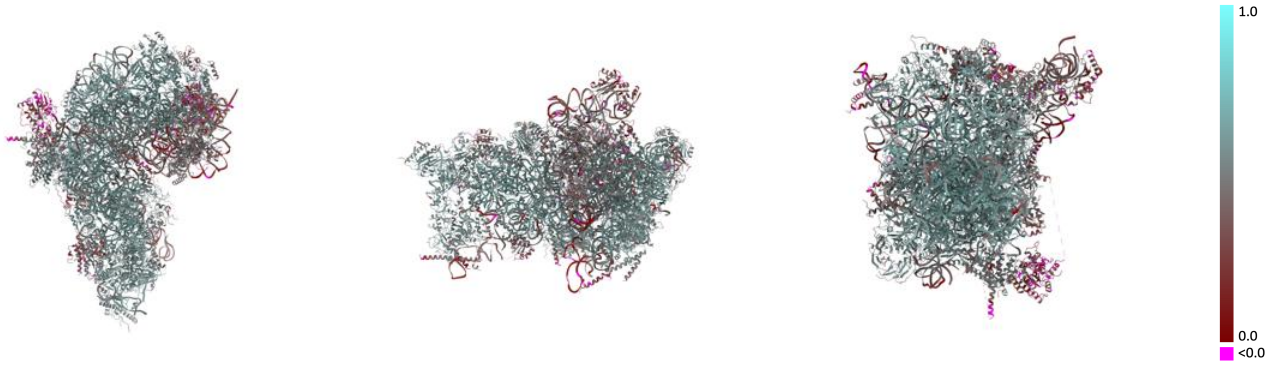
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

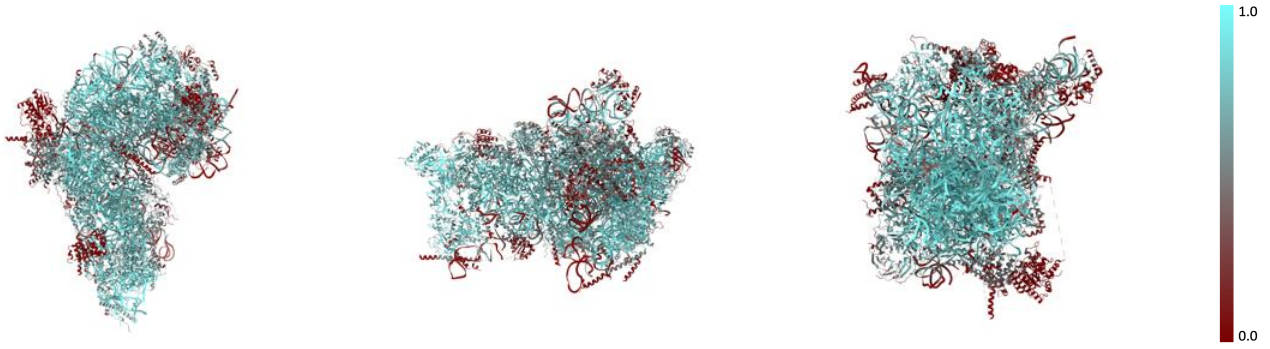
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

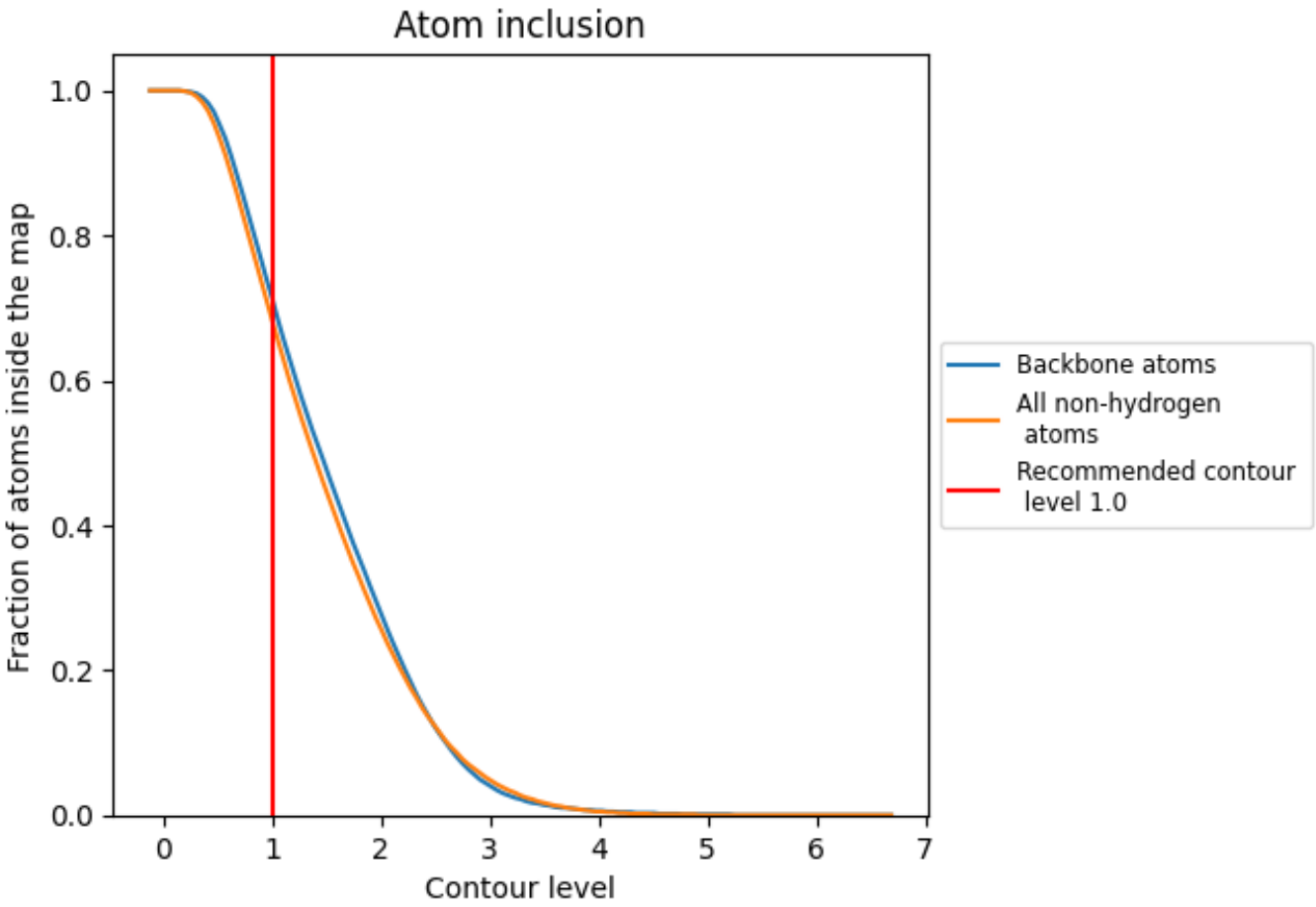
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6820	0.5240
BA	0.3140	0.4180
BB	0.2640	0.2980
L1	0.7680	0.5490
L2	0.8790	0.5500
L3	0.7720	0.5300
L6	0.8190	0.5910
L7	0.8850	0.6130
L8	0.8860	0.6050
L9	0.8760	0.6260
LA	0.6590	0.5360
LB	0.8560	0.6080
LC	0.8930	0.6220
LE	0.4580	0.4600
LG	0.6070	0.5210
LH	0.2840	0.4200
LI	0.8000	0.5950
LK	0.5310	0.4350
LN	0.7950	0.5950
LQ	0.8830	0.6270
LS	0.5890	0.5330
LT	0.9500	0.6420
LU	0.6620	0.5720
LW	0.7860	0.6000
NB	0.1940	0.2960
NF	0.6500	0.5230
NH	0.6120	0.4310
NI	0.2320	0.4010
NK	0.6330	0.5480
NM	0.6490	0.5410
NO	0.4570	0.4810
NQ	0.5600	0.5260
NS	0.6150	0.5430
SA	0.8170	0.5970
SC	0.6810	0.5550

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Chain	Atom inclusion	Q-score
SD	0.8220	0.5940
SE	0.7940	0.5940
SG	0.8130	0.6100
SH	0.7830	0.5660
SI	0.7220	0.5410
SJ	0.3800	0.4620
SK	0.6830	0.5360
SL	0.7330	0.5400
SM	0.6600	0.5120
SN	0.4770	0.4640
SO	0.6360	0.5470
SQ	0.6140	0.5470
SR	0.6770	0.5480
SS	0.5890	0.5140
ST	0.2720	0.3740
SV	0.5630	0.4820
SW	0.4040	0.4480
SY	0.6390	0.4300
SZ	0.7020	0.5550