



# wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 10:33 am GMT

PDB ID : 4V8Z  
EMDB ID : EMD-2422  
Title : Cryo-EM reconstruction of the 80S-eIF5B-Met-itRNAMet Eukaryotic Translation Initiation Complex  
Authors : Fernandez, I.S.; Bai, X.C.; Hussain, T.; Kelley, A.C.; Lorsch, J.R.; Ramakrishnan, V.; Scheres, S.H.W.  
Deposited on : 2013-07-20  
Resolution : 6.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

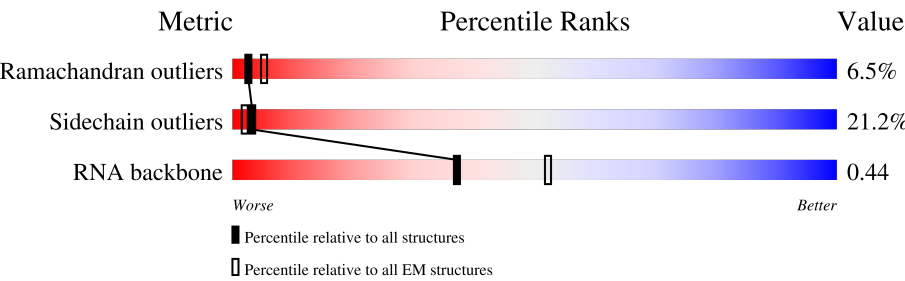
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 6.60 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)
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A0	119	<div><div>51%</div><div>58%18%6%18%</div></div>
2	A1	82	<div><div>48%</div><div>83%15%..</div></div>
3	A2	67	<div><div>82%</div><div>60%34%6%</div></div>
4	A3	56	<div><div>48%</div><div>77%14%.5%</div></div>
5	A4	63	<div><div>52%</div><div>81%13%.5%</div></div>
6	A5	152	<div><div>44%</div><div>33%11%.53%</div></div>
7	A6	319	<div><div>73%</div><div>85%14%. </div></div>
8	A7	273	<div><div>50%</div><div>47%9%.42%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	AA	252	
10	AB	255	
11	AC	254	
12	AD	240	
13	AE	261	
14	AF	225	
15	AG	236	
16	AH	190	
17	AI	200	
18	AJ	197	
19	AK	105	
20	AL	156	
21	AM	143	
22	AN	151	
23	AO	137	
24	AP	142	
25	AQ	143	
26	AR	136	
27	AS	146	
28	AT	144	
29	AU	121	
30	AV	87	
31	AW	130	
32	AX	145	
33	AY	135	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	AZ	108	
35	BA	253	
36	BB	386	
37	BC	361	
38	BD	296	
39	BE	175	
40	BF	243	
41	BG	255	
42	BH	191	
43	BI	220	
44	BJ	173	
45	BK	174	
46	BL	198	
47	BM	137	
48	BN	203	
49	BO	218	
50	BP	183	
51	BQ	185	
52	BR	188	
53	BS	172	
54	BT	159	
55	BU	120	
56	BV	136	
57	BW	155	
58	BX	141	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	BY	126	
60	BZ	135	
61	Ba	148	
62	Bb	58	
63	Bc	104	
64	Bd	112	
65	Be	129	
66	Bf	106	
67	Bg	120	
68	Bh	119	
69	Bi	99	
70	Bj	87	
71	Bk	77	
72	Bl	50	
73	Bm	128	
74	Bn	25	
75	Bo	105	
76	Bq	312	
77	Br	47	
78	Bs	46	
79	B2	1800	
80	B5	3396	
81	B7	121	
82	B8	158	
83	CV	586	

Continued on next page...

Mol	Chain	Length	Quality of chain
84	CW	76	<p>20% 34% 51% 11%</p>
85	CX	3	<p>33% 67%</p>

## 2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 219371 atoms, of which 8407 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 40S RIBOSOMAL PROTEIN S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A3	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A4	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 6 is a protein called UBIQUITIN-40S RIBOSOMAL PROTEIN S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A5	71	Total	C	N	O	S	0	0
			516	328	93	91	4		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A5	82	UNK	LYS	SEE REMARK 999	UNP P05759
A5	83	UNK	LYS	SEE REMARK 999	UNP P05759
A5	84	UNK	VAL	SEE REMARK 999	UNP P05759
A5	85	UNK	TYR	SEE REMARK 999	UNP P05759
A5	86	UNK	THR	SEE REMARK 999	UNP P05759
A5	87	UNK	THR	SEE REMARK 999	UNP P05759
A5	88	UNK	PRO	SEE REMARK 999	UNP P05759
A5	89	UNK	LYS	SEE REMARK 999	UNP P05759
A5	90	UNK	LYS	SEE REMARK 999	UNP P05759
A5	91	UNK	ILE	SEE REMARK 999	UNP P05759
A5	92	UNK	LYS	SEE REMARK 999	UNP P05759
A5	93	UNK	HIS	SEE REMARK 999	UNP P05759
A5	94	UNK	LYS	SEE REMARK 999	UNP P05759
A5	95	UNK	HIS	SEE REMARK 999	UNP P05759
A5	96	UNK	LYS	SEE REMARK 999	UNP P05759
A5	97	UNK	LYS	SEE REMARK 999	UNP P05759
A5	98	UNK	VAL	SEE REMARK 999	UNP P05759
A5	99	UNK	LYS	SEE REMARK 999	UNP P05759
A5	100	UNK	LEU	SEE REMARK 999	UNP P05759
A5	101	UNK	ALA	SEE REMARK 999	UNP P05759

- Molecule 7 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A6	318	Total	C	N	O	S	0	0
			2437	1541	418	470	8		

- Molecule 8 is a protein called SUPPRESSOR PROTEIN STM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	A7	159	Total	C	N	O	0	0
			1105	653	221	231		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A7	9	UNK	GLY	SEE REMARK 999	UNP P39015
A7	10	UNK	ASN	SEE REMARK 999	UNP P39015
A7	11	UNK	ASP	SEE REMARK 999	UNP P39015
A7	12	UNK	VAL	SEE REMARK 999	UNP P39015

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A7	13	UNK	GLU	SEE REMARK 999	UNP P39015
A7	14	UNK	ASP	SEE REMARK 999	UNP P39015
A7	15	UNK	ALA	SEE REMARK 999	UNP P39015
A7	16	UNK	ASP	SEE REMARK 999	UNP P39015
A7	17	UNK	VAL	SEE REMARK 999	UNP P39015
A7	18	UNK	VAL	SEE REMARK 999	UNP P39015
A7	19	UNK	VAL	SEE REMARK 999	UNP P39015
A7	20	UNK	LEU	SEE REMARK 999	UNP P39015
A7	151	UNK	LEU	SEE REMARK 999	UNP P39015
A7	152	UNK	GLN	SEE REMARK 999	UNP P39015
A7	153	UNK	ASP	SEE REMARK 999	UNP P39015
A7	154	UNK	TYR	SEE REMARK 999	UNP P39015
A7	155	UNK	LEU	SEE REMARK 999	UNP P39015
A7	156	UNK	ASN	SEE REMARK 999	UNP P39015
A7	157	UNK	GLN	SEE REMARK 999	UNP P39015
A7	158	UNK	GLN	SEE REMARK 999	UNP P39015
A7	159	UNK	ALA	SEE REMARK 999	UNP P39015
A7	160	UNK	ASN	SEE REMARK 999	UNP P39015
A7	161	UNK	ASN	SEE REMARK 999	UNP P39015
A7	162	UNK	GLN	SEE REMARK 999	UNP P39015
A7	163	UNK	PHE	SEE REMARK 999	UNP P39015
A7	164	UNK	ASN	SEE REMARK 999	UNP P39015
A7	165	UNK	LYS	SEE REMARK 999	UNP P39015
A7	166	UNK	VAL	SEE REMARK 999	UNP P39015
A7	167	UNK	PRO	SEE REMARK 999	UNP P39015
A7	168	UNK	GLU	SEE REMARK 999	UNP P39015
A7	169	UNK	ALA	SEE REMARK 999	UNP P39015
A7	170	UNK	LYS	SEE REMARK 999	UNP P39015
A7	171	UNK	LYS	SEE REMARK 999	UNP P39015
A7	172	UNK	VAL	SEE REMARK 999	UNP P39015
A7	173	UNK	GLU	SEE REMARK 999	UNP P39015
A7	174	UNK	LEU	SEE REMARK 999	UNP P39015
A7	175	UNK	ASP	SEE REMARK 999	UNP P39015

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AA	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AB	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AG	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AH	184	Total	C	N	O		0	0
			1481	951	265	265			

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AK	96	Total	C	N	O	S	0	0
			772	499	126	145	2		

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AL	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AM	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AO	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AP	124	Total	C	N	O	S	0	0
			977	622	182	166	7		

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AQ	141	Total	C	N	O	S	0	0
			1105	708	203	194			

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AR	120	Total	C	N	O	S	0	0
			926	577	177	170	2		

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AT	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 33 is a protein called 40S RIBOSOMAL PROTEIN S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AY	134	Total	C	N	O		0	0
			1073	676	208	189			

- Molecule 34 is a protein called 40S RIBOSOMAL PROTEIN S25-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AZ	70	Total	C	N	O		0	0
			563	360	104	99			

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN L2-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	252	Total	C	N	O	S	0	0
			1912	1190	388	333	1		

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BB	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 38 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BD	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BE	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BF	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		

- Molecule 41 is a protein called 60S RIBOSOMAL PROTEIN L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BG	231	Total	C	N	O	S	0	0
			1763	1130	316	314	3		

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BH	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BI	213	Total	C	N	O	S	0	0
			1722	1094	325	297	6		

- Molecule 44 is a protein called 60S RIBOSOMAL PROTEIN L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BK	153	Total	C	H	N	O	0	3
			1509	450	756	153	150		

- Molecule 46 is a protein called 60S RIBOSOMAL PROTEIN L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	BL	194	Total	C	N	O	0	0
			1548	965	316	267		

- Molecule 47 is a protein called 60S RIBOSOMAL PROTEIN L14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BM	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	89	ALA	GLY	conflict	UNP P38754

- Molecule 48 is a protein called 60S RIBOSOMAL PROTEIN L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 49 is a protein called 60S RIBOSOMAL PROTEIN L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BO	197	Total	C	N	O	S	197	0
			3119	2008	581	528	2		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	3	VAL	SER	microheterogeneity	UNP P26784
BO	4	GLU	GLN	microheterogeneity	UNP P26784
BO	11	GLY	ALA	microheterogeneity	UNP P26784
BO	13	GLY	ASP	microheterogeneity	UNP P26784
BO	16	VAL	LEU	microheterogeneity	UNP P26784
BO	22	VAL	THR	microheterogeneity	UNP P26784
BO	23	VAL	ILE	microheterogeneity	UNP P26784

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
BO	27	LEU	VAL	microheterogeneity	UNP P26784
BO	40	GLU	ALA	microheterogeneity	UNP P26784
BO	80	PHE	LEU	microheterogeneity	UNP P26784
BO	84	LEU	ILE	microheterogeneity	UNP P26784
BO	104	VAL	ILE	microheterogeneity	UNP P26784
BO	158	ALA	ASP	microheterogeneity	UNP P26784
BO	163	SER	ARG	microheterogeneity	UNP P26784
BO	179	ALA	SER	microheterogeneity	UNP P26784
BO	182	ASN	SER	microheterogeneity	UNP P26784
BO	184	THR	ALA	microheterogeneity	UNP P26784
BO	186	ALA	SER	microheterogeneity	UNP P26784
BO	196	ALA	SER	microheterogeneity	UNP P26784
BO	197	LEU	PHE	microheterogeneity	UNP P26784

- Molecule 50 is a protein called 60S RIBOSOMAL PROTEIN L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	BP	155	Total	C	N	O	0	0
			1227	764	238	225		

- Molecule 51 is a protein called 60S RIBOSOMAL PROTEIN L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 52 is a protein called 60S RIBOSOMAL PROTEIN L19-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	BR	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 53 is a protein called 60S RIBOSOMAL PROTEIN L20-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 54 is a protein called 60S RIBOSOMAL PROTEIN L21-A.



Mol	Chain	Residues	Atoms					AltConf	Trace
54	BT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 55 is a protein called 60S RIBOSOMAL PROTEIN L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BU	98	Total	C	N	O		0	0
			778	505	127	146			

- Molecule 56 is a protein called 60S RIBOSOMAL PROTEIN L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 57 is a protein called 60S RIBOSOMAL PROTEIN L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BW	135	Total	C	N	O	S	0	0
			1038	651	206	180	1		

- Molecule 58 is a protein called 60S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BX	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 59 is a protein called 60S RIBOSOMAL PROTEIN L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BY	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 60 is a protein called 60S RIBOSOMAL PROTEIN L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BZ	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 61 is a protein called 60S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Ba	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 62 is a protein called 60S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bb	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 63 is a protein called 60S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bc	100	Total	C	N	O	S	0	0
			767	492	128	146	1		

- Molecule 64 is a protein called 60S RIBOSOMAL PROTEIN L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bd	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 65 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Be	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 66 is a protein called 60S RIBOSOMAL PROTEIN L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bf	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 67 is a protein called 60S RIBOSOMAL PROTEIN L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bg	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 68 is a protein called 60S RIBOSOMAL PROTEIN L35-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bh	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 69 is a protein called 60S RIBOSOMAL PROTEIN L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bi	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 70 is a protein called 60S RIBOSOMAL PROTEIN L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 71 is a protein called 60S RIBOSOMAL PROTEIN L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bk	77	Total	C	N	O		0	0
			608	388	114	106			

- Molecule 72 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bl	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 73 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bm	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 74 is a protein called 60S RIBOSOMAL PROTEIN L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bn	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 75 is a protein called 60S RIBOSOMAL PROTEIN L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bo	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 76 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P0.

Mol	Chain	Residues	Atoms					AltConf	Trace	
76	Bq	145	Total	C	H	N	O	S	0	2
			2185	683	1110	194	195	3		

- Molecule 77 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Br	47	Total	C	H	N	O	0	0
			473	141	237	47	48		

- Molecule 78 is a protein called 60S ACIDIC RIBOSOMAL PROTEIN P2.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bs	46	Total	C	H	N	O	0	0
			463	138	232	46	47		

- Molecule 79 is a RNA chain called 18S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	B2	1781	Total	C	N	O	P	1	0
			37835	16910	6661	12482	1782		

- Molecule 80 is a RNA chain called 25S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	B5	3147	Total	C	H	N	O	P	0	0
			67972	30066	664	12132	21965	3145		

- Molecule 81 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	B7	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 82 is a RNA chain called 5.8S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	B8	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 83 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 5B, PROBABLE TRANSLATION INITIATION FACTOR IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
83	CV	570	Total	C	H	N	O	S	0	2
			9036	2819	4585	766	847	19		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CV	340	ASP	-	linker	UNP P39730
CV	341	LEU	-	linker	UNP P39730
CV	342	THR	-	linker	UNP P39730
CV	343	GLY	-	linker	UNP P39730
CV	344	LEU	-	linker	UNP P39730
CV	345	LEU	-	linker	UNP P39730
CV	346	ASP	-	linker	UNP P39730
CV	347	SER	-	linker	UNP P39730
CV	348	VAL	-	linker	UNP P39730
CV	349	ASP	-	linker	UNP P39730
CV	350	THR	-	linker	UNP P39730

- Molecule 84 is a RNA chain called EUKARYOTIC RIBOSOMAL PI TRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	CW	76	Total	C	H	N	O	P	0	0
			2403	721	789	285	533	75		

- Molecule 85 is a RNA chain called 5'-R(\*AP\*UP\*GP)-3'.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	CX	3	Total	C	H	N	O	P	0	0
			96	29	34	12	19	2		

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	A0	1	Total	Zn	0
			1	1	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
86	A1	1	Total 1	Zn 1	0
86	A3	1	Total 1	Zn 1	0
86	A5	1	Total 1	Zn 1	0
86	Bj	1	Total 1	Zn 1	0
86	Bm	1	Total 1	Zn 1	0

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

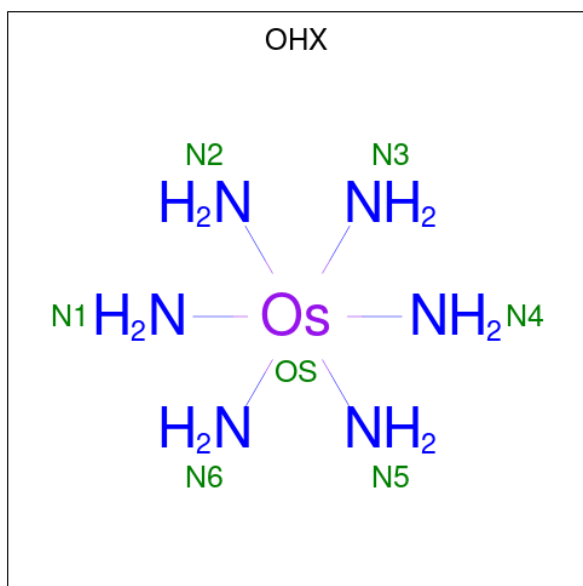
Mol	Chain	Residues	Atoms		AltConf
87	A0	2	Total 2	Mg 2	0
87	A3	3	Total 3	Mg 3	0
87	A5	1	Total 1	Mg 1	0
87	AB	1	Total 1	Mg 1	0
87	AC	2	Total 2	Mg 2	0
87	AE	1	Total 1	Mg 1	0
87	AG	1	Total 1	Mg 1	0
87	AI	1	Total 1	Mg 1	0
87	AJ	1	Total 1	Mg 1	0
87	AL	2	Total 2	Mg 2	0
87	AN	1	Total 1	Mg 1	0
87	AP	1	Total 1	Mg 1	0
87	AS	1	Total 1	Mg 1	0
87	AU	1	Total 1	Mg 1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
87	BD	4	Total	Mg	0
			4	4	
87	BF	1	Total	Mg	0
			1	1	
87	BS	3	Total	Mg	0
			3	3	
87	B2	168	Total	Mg	0
			168	168	
87	B5	3	Total	Mg	0
			3	3	
87	B7	27	Total	Mg	0
			27	27	
87	CW	1	Total	Mg	0
			1	1	

- Molecule 88 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			AltConf
88	A3	1	Total	N	Os	0
			7	6	1	
88	A6	1	Total	N	Os	0
			7	6	1	
88	AC	1	Total	N	Os	0
			7	6	1	
88	AI	1	Total	N	Os	0
			14	12	2	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
88	AI	1	Total 14	N 12	Os 2	0
88	AL	1	Total 7	N 6	Os 1	0
88	AN	1	Total 7	N 6	Os 1	0
88	AP	1	Total 7	N 6	Os 1	0
88	BR	1	Total 7	N 6	Os 1	0
88	Bn	1	Total 7	N 6	Os 1	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0
88	B2	1	Total 1274	N 1092	Os 182	0

*Continued on next page...*



[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B2	1	Total	N	Os	0
			1274	1092	182	
88	B5	1	Total	N	Os	0
			21	18	3	

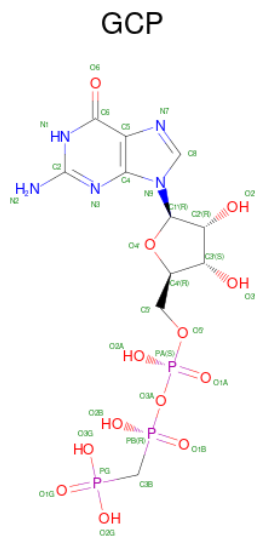
*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
88	B5	1	Total	N	Os	0
			21	18	3	
88	B5	1	Total	N	Os	0
			21	18	3	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	B7	1	Total	N	Os	0
			91	78	13	
88	CV	1	Total	N	Os	0
			7	6	1	
88	CX	1	Total	N	Os	0
			7	6	1	

- Molecule 89 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).

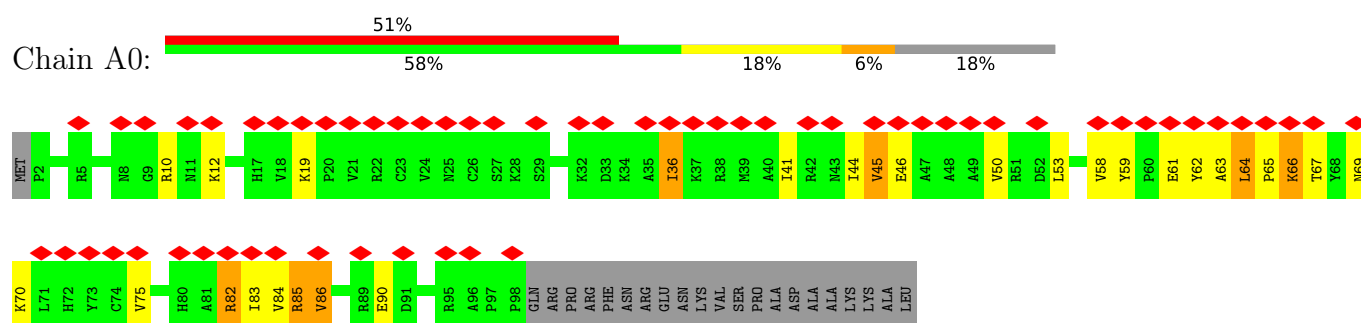


Mol	Chain	Residues	Atoms					AltConf
89	CV	1	Total	C	N	O	P	0
			32	11	5	13	3	

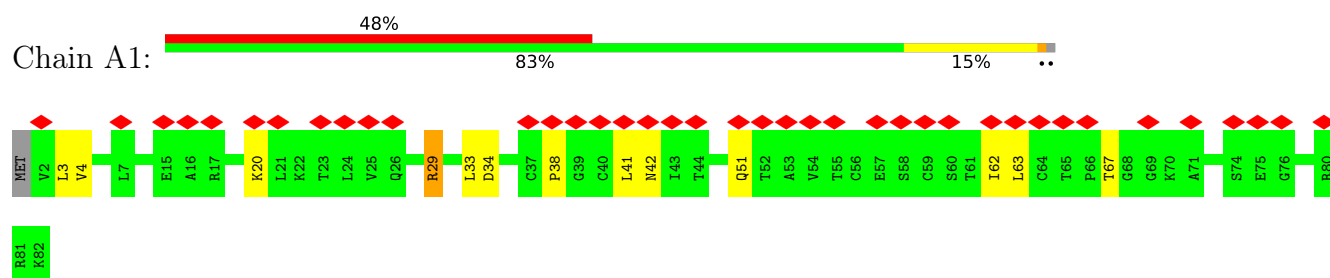
### 3 Residue-property plots [i](#)

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.

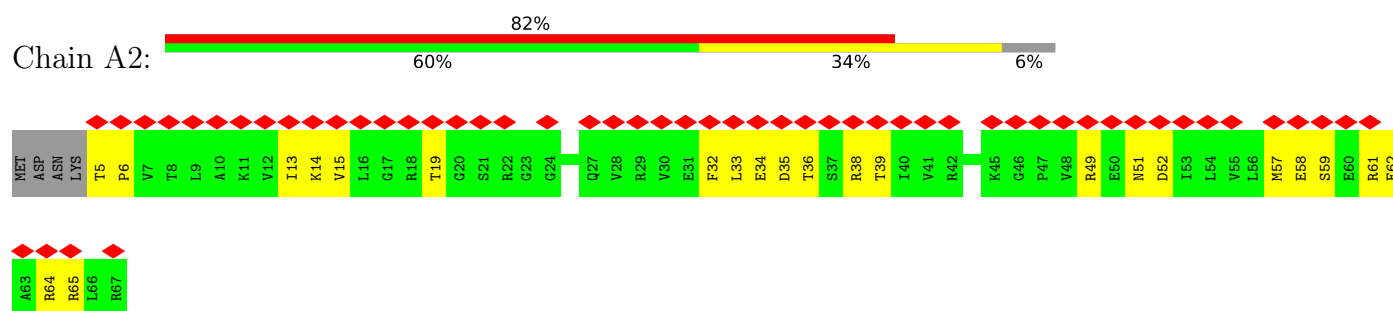
#### • Molecule 1: 40S RIBOSOMAL PROTEIN S26-A



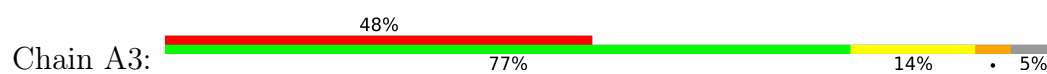
#### • Molecule 2: 40S RIBOSOMAL PROTEIN S27-A



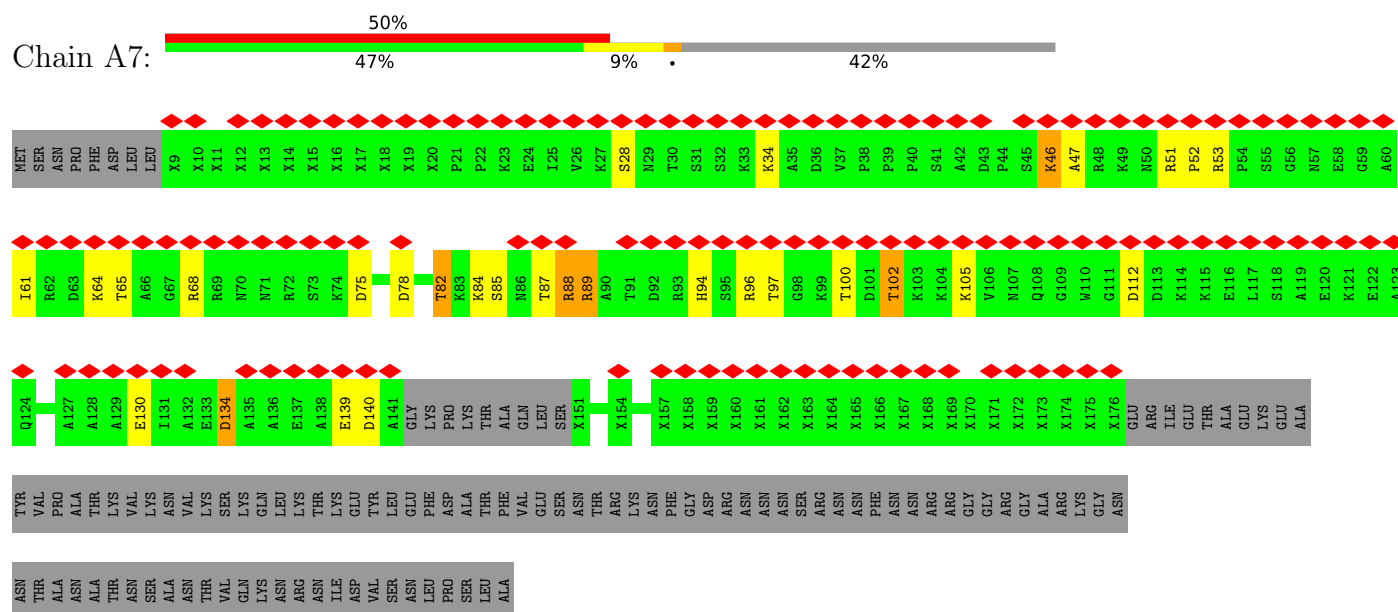
#### • Molecule 3: 40S RIBOSOMAL PROTEIN S28-A

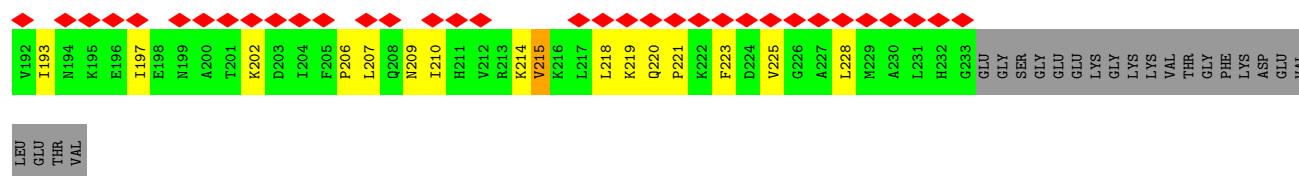


#### • Molecule 4: 40S RIBOSOMAL PROTEIN S29-A



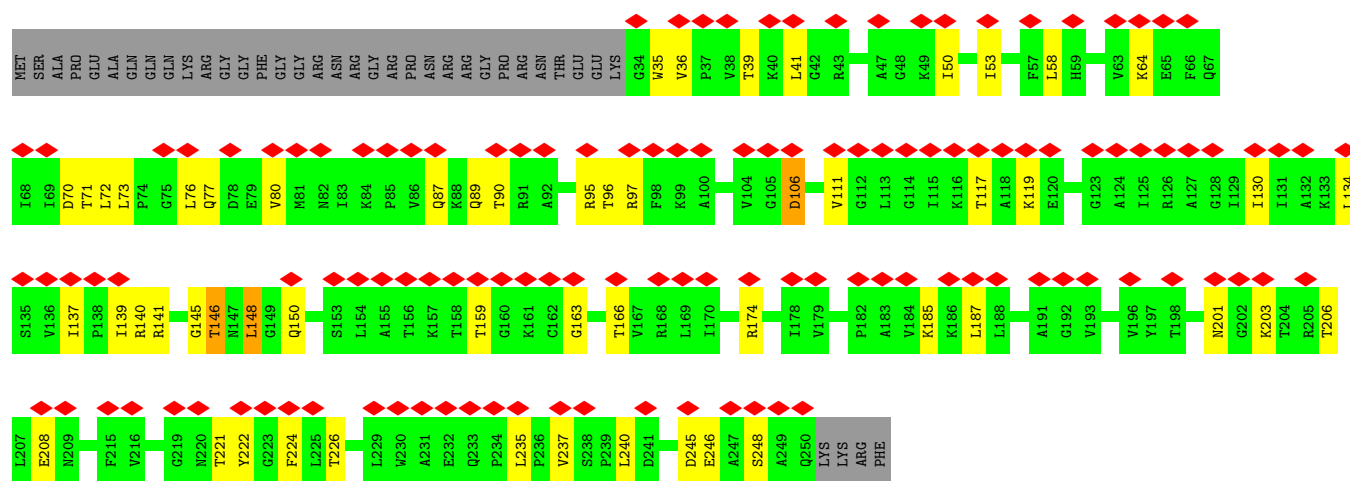






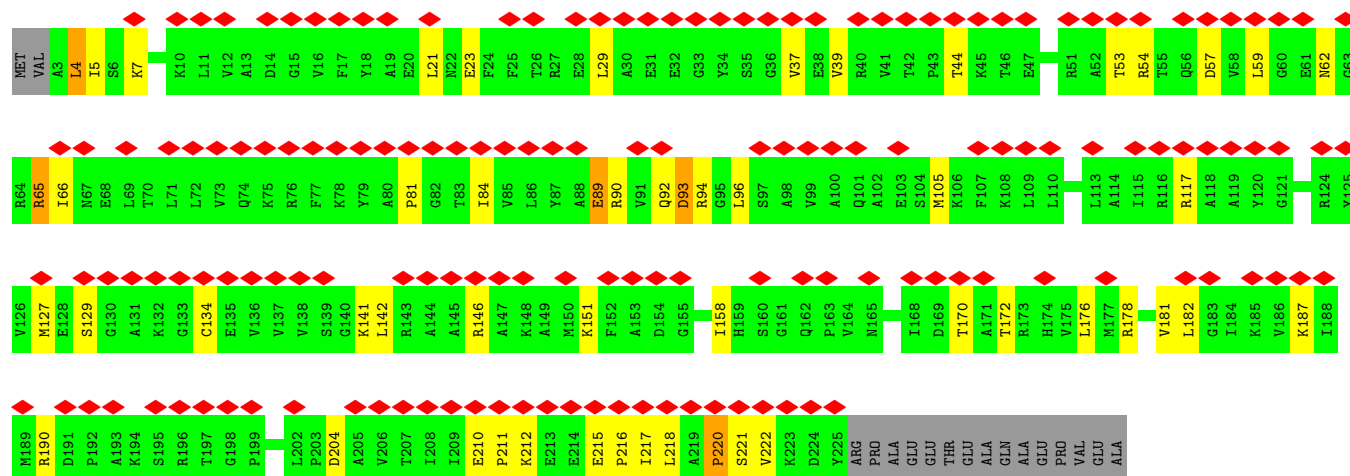
• Molecule 11: 40S RIBOSOMAL PROTEIN S2

Chain AC:



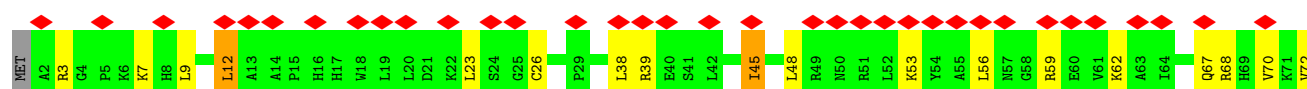
• Molecule 12: 40S RIBOSOMAL PROTEIN S3

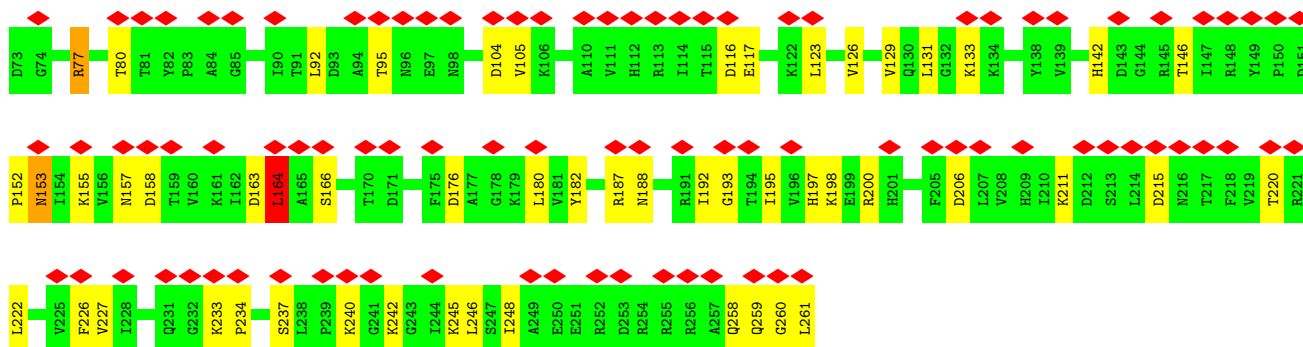
Chain AD:



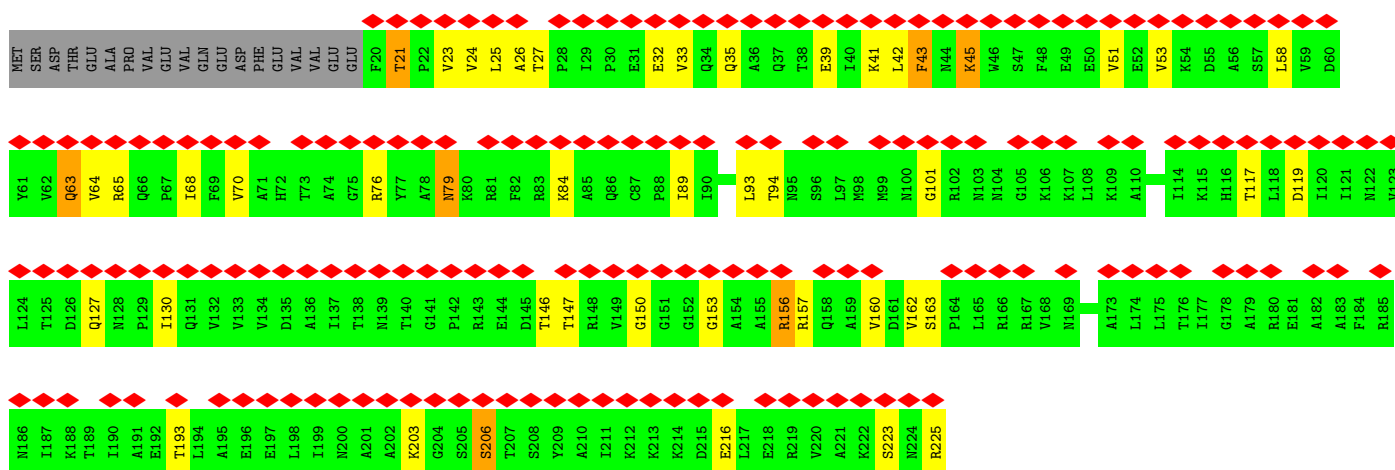
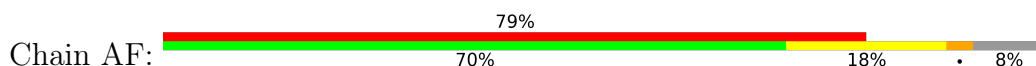
• Molecule 13: 40S RIBOSOMAL PROTEIN S4-A

Chain AE:

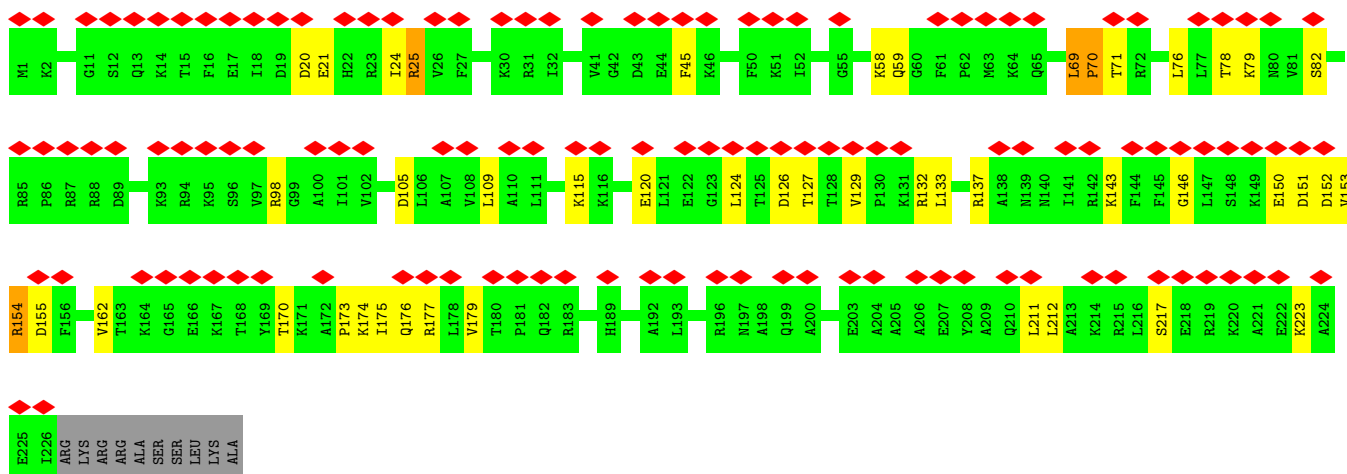
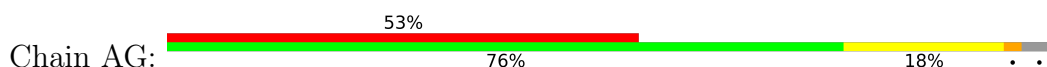




• Molecule 14: 40S RIBOSOMAL PROTEIN S5

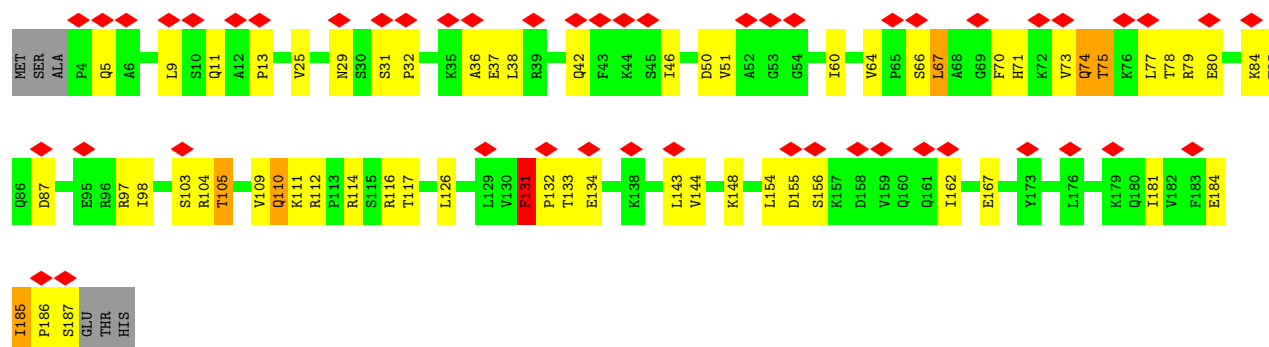


• Molecule 15: 40S RIBOSOMAL PROTEIN S6-A

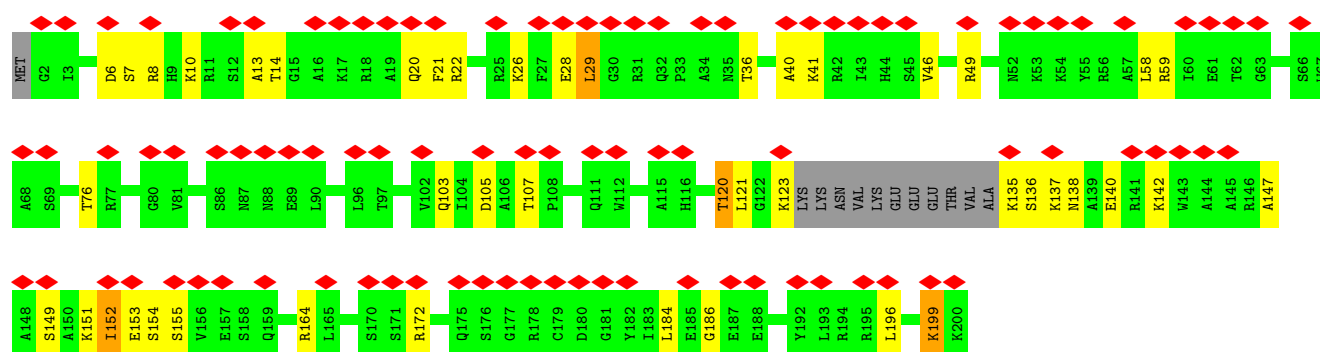


• Molecule 16: 40S RIBOSOMAL PROTEIN S7-A

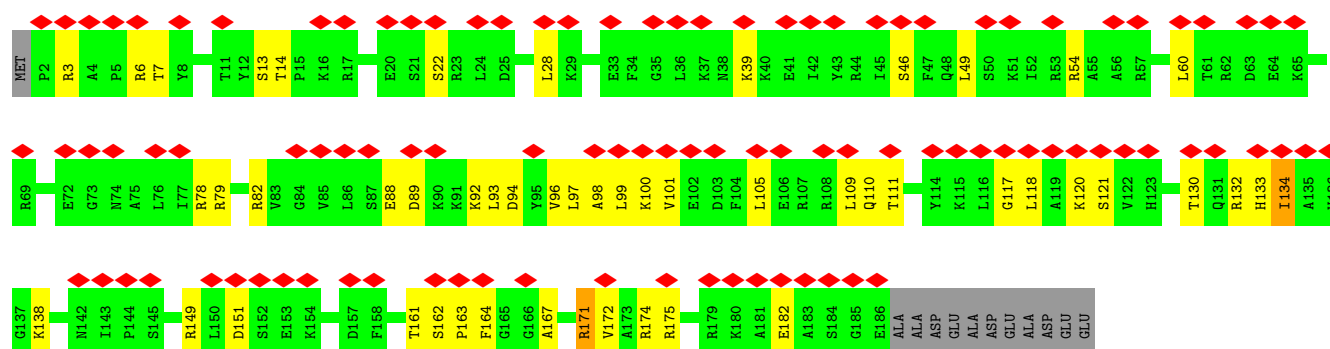




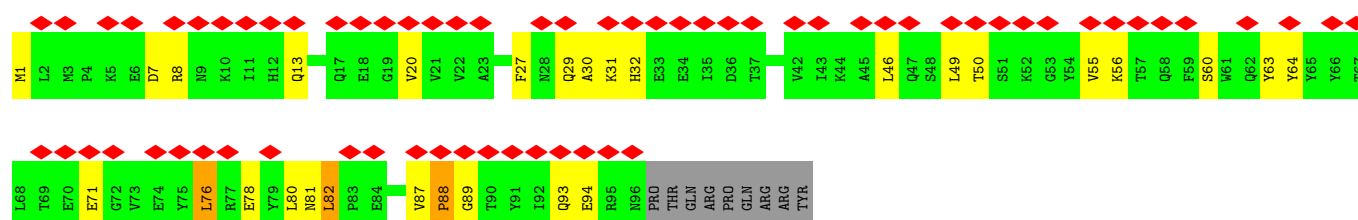
• Molecule 17: 40S RIBOSOMAL PROTEIN S8-A



• Molecule 18: 40S RIBOSOMAL PROTEIN S9-A

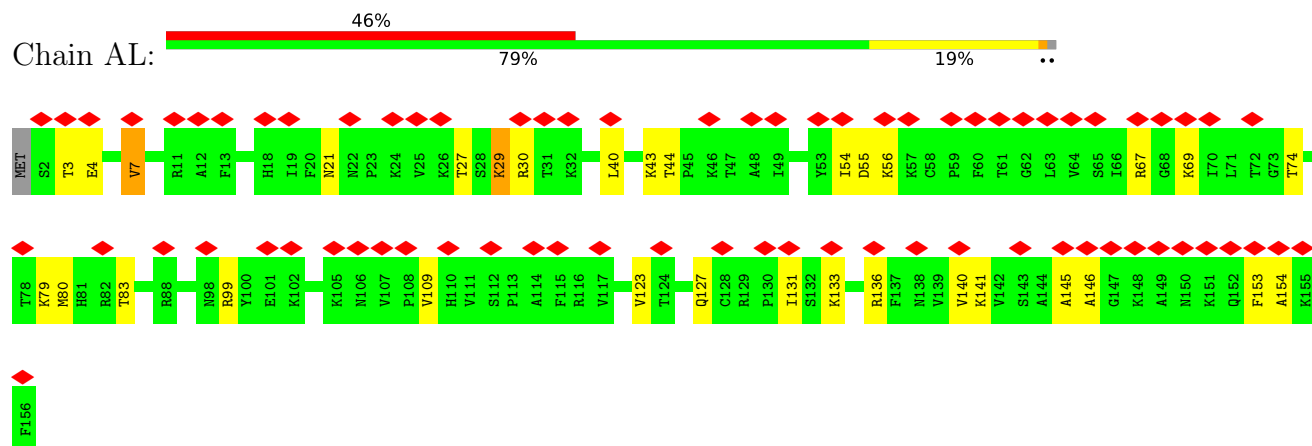


• Molecule 19: 40S RIBOSOMAL PROTEIN S10-A

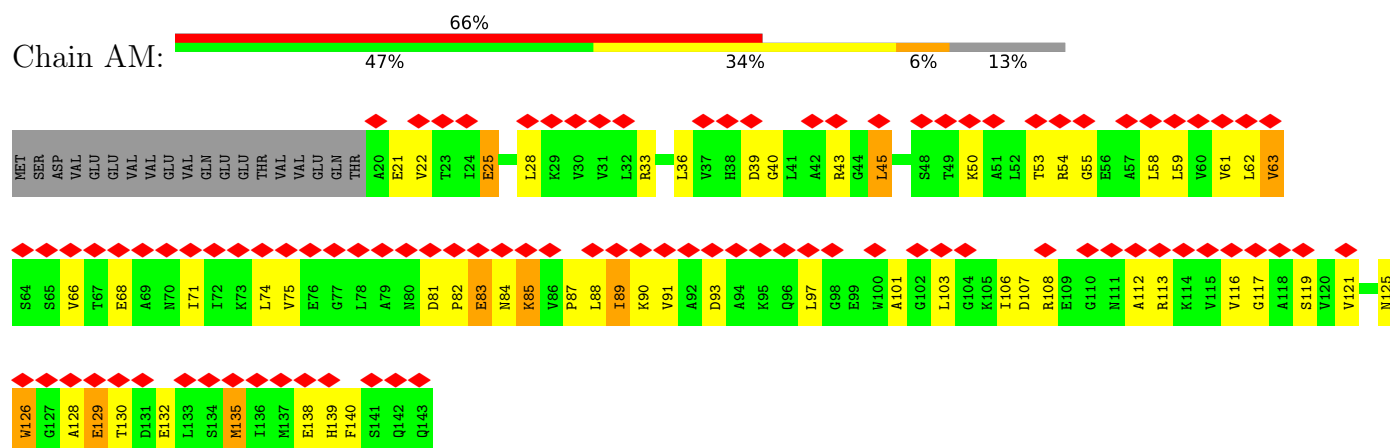




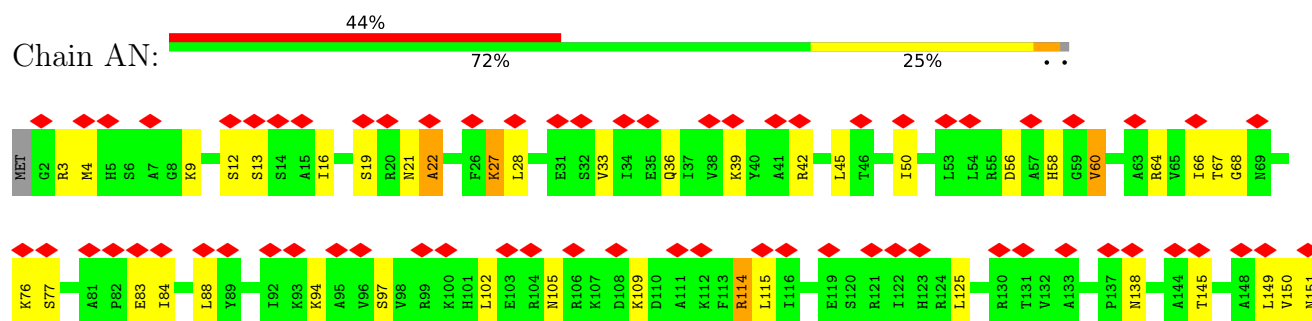
- Molecule 20: 40S RIBOSOMAL PROTEIN S11-A



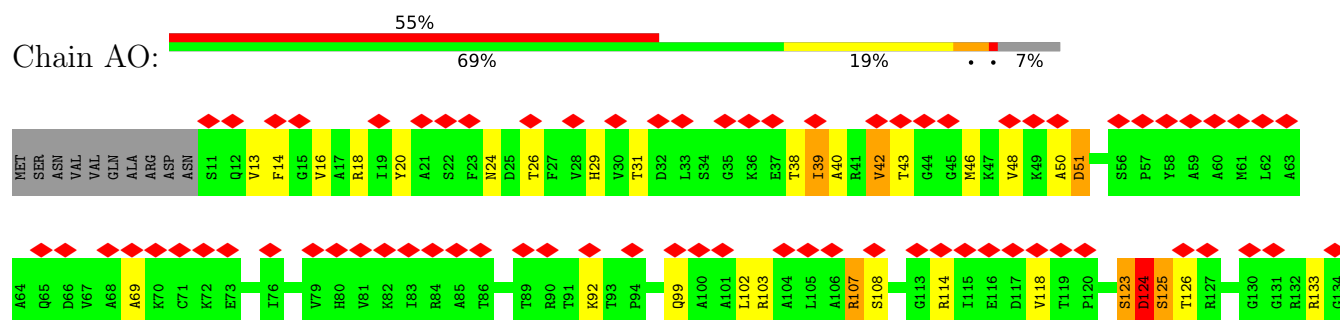
- Molecule 21: 40S RIBOSOMAL PROTEIN S12



- Molecule 22: 40S RIBOSOMAL PROTEIN S13

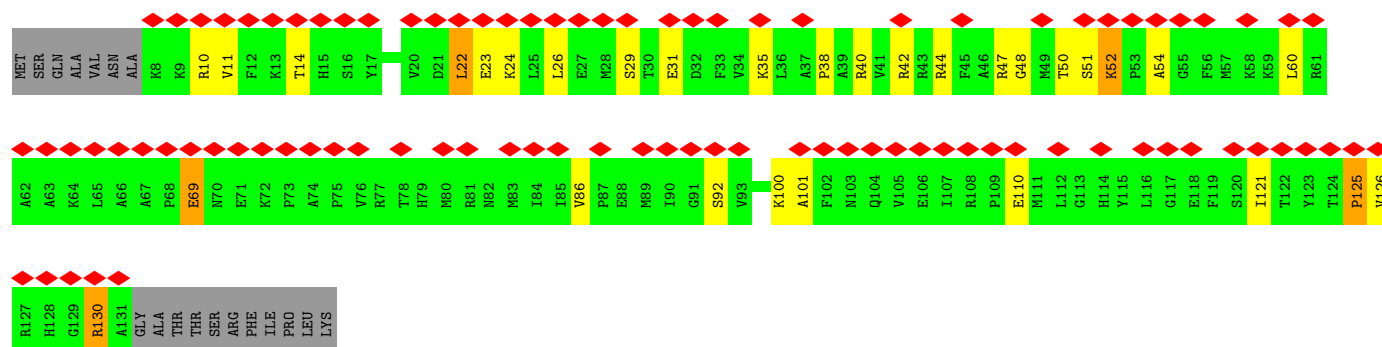


- Molecule 23: 40S RIBOSOMAL PROTEIN S14-A

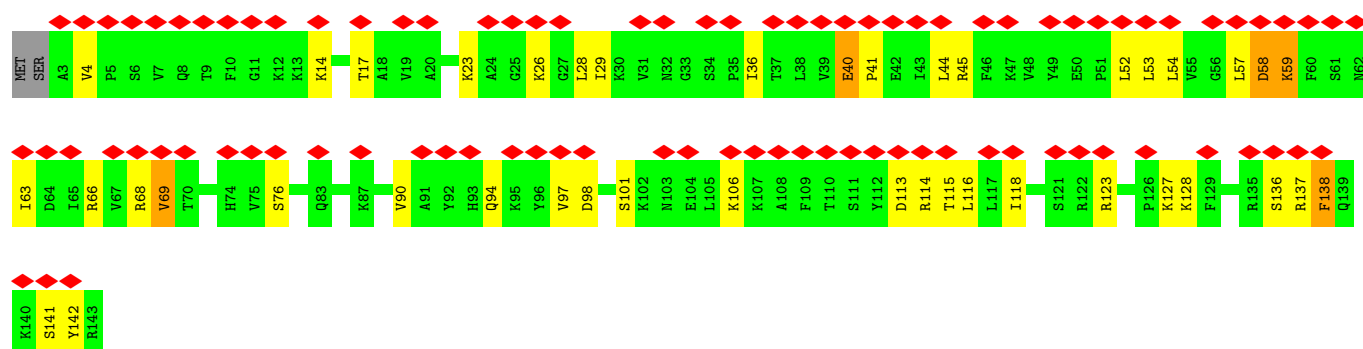
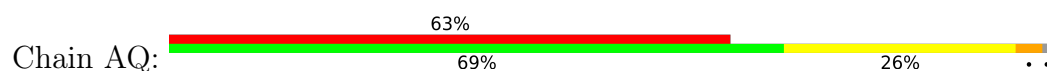




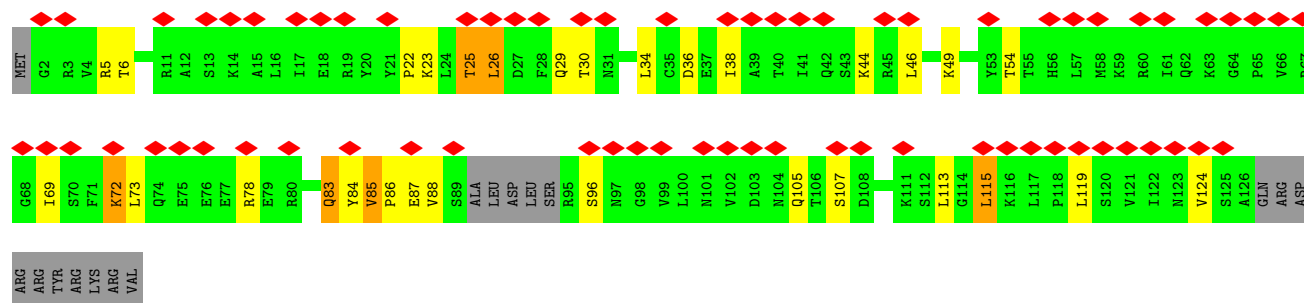
• Molecule 24: 40S RIBOSOMAL PROTEIN S15

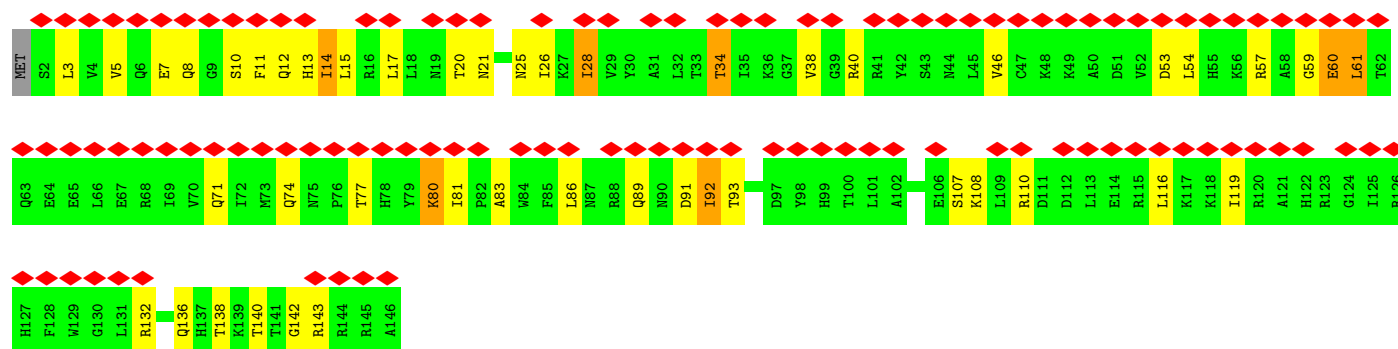


• Molecule 25: 40S RIBOSOMAL PROTEIN S16-A



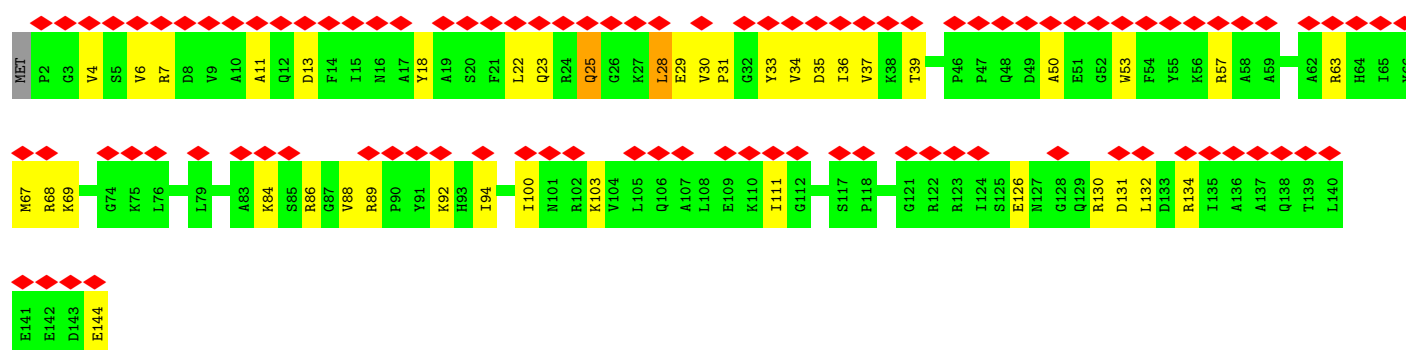
• Molecule 26: 40S RIBOSOMAL PROTEIN S17-A





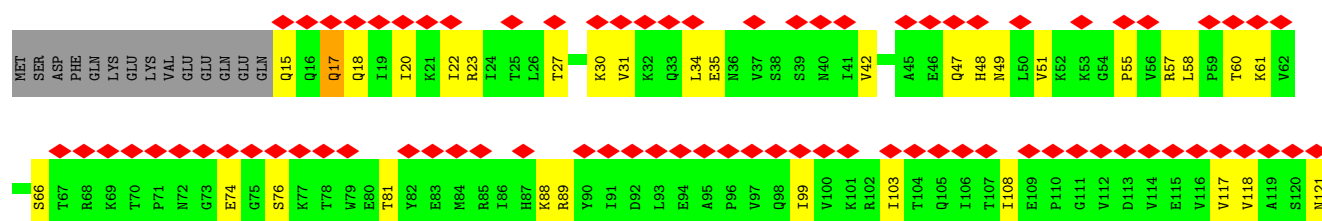
• Molecule 28: 40S RIBOSOMAL PROTEIN S19-A

Chain AT:



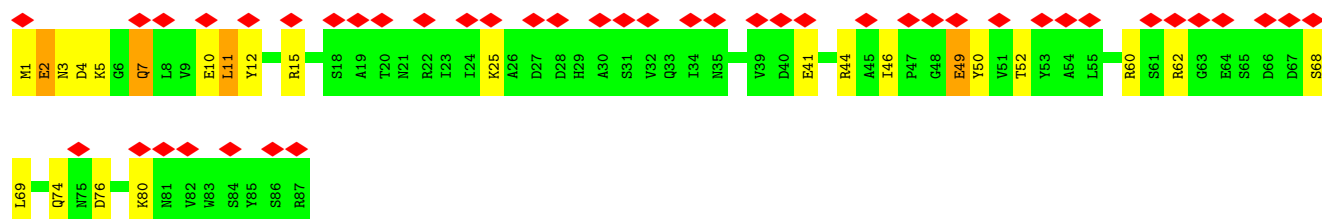
• Molecule 29: 40S RIBOSOMAL PROTEIN S20

Chain AU:




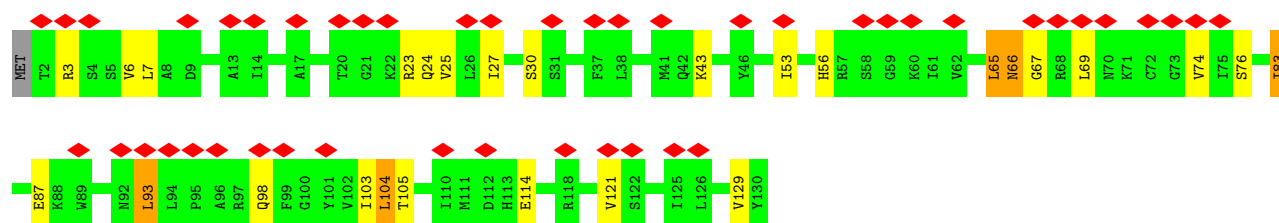
• Molecule 30: 40S RIBOSOMAL PROTEIN S21-A

Chain AV:




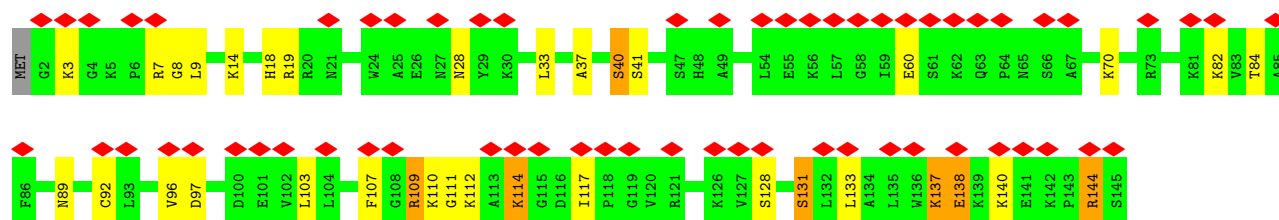
• Molecule 31: 40S RIBOSOMAL PROTEIN S22-A

Chain AW: 

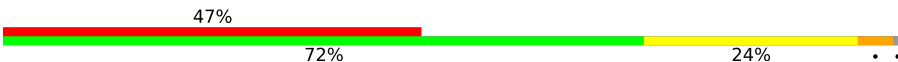


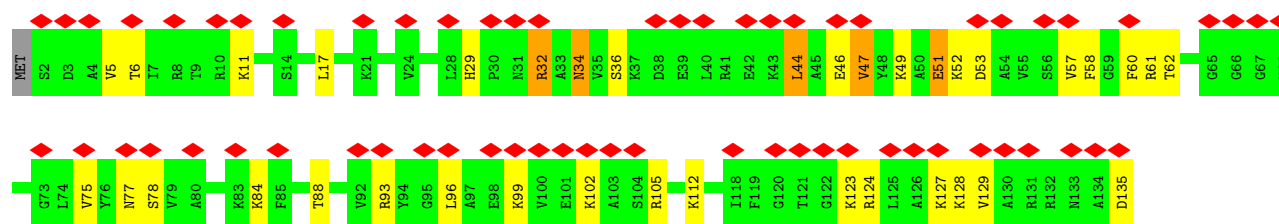
• Molecule 32: 40S RIBOSOMAL PROTEIN S23-A

Chain AX: 



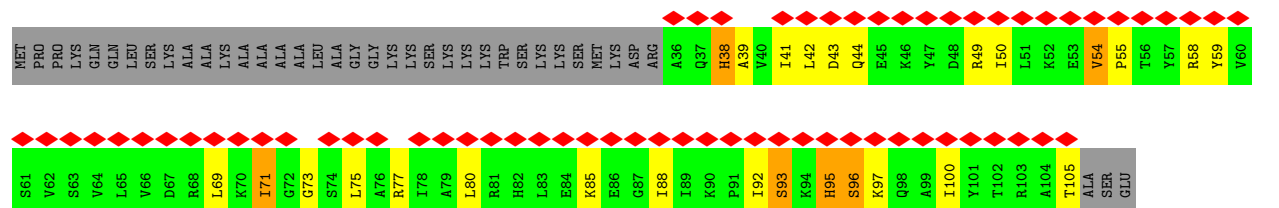
• Molecule 33: 40S RIBOSOMAL PROTEIN S24-A

Chain AY: 

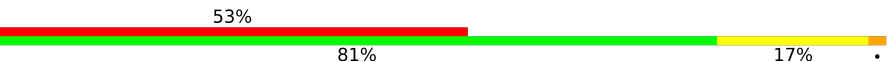


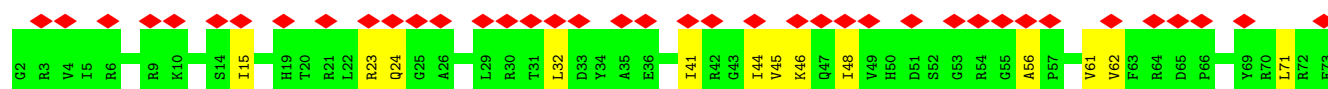
• Molecule 34: 40S RIBOSOMAL PROTEIN S25-A

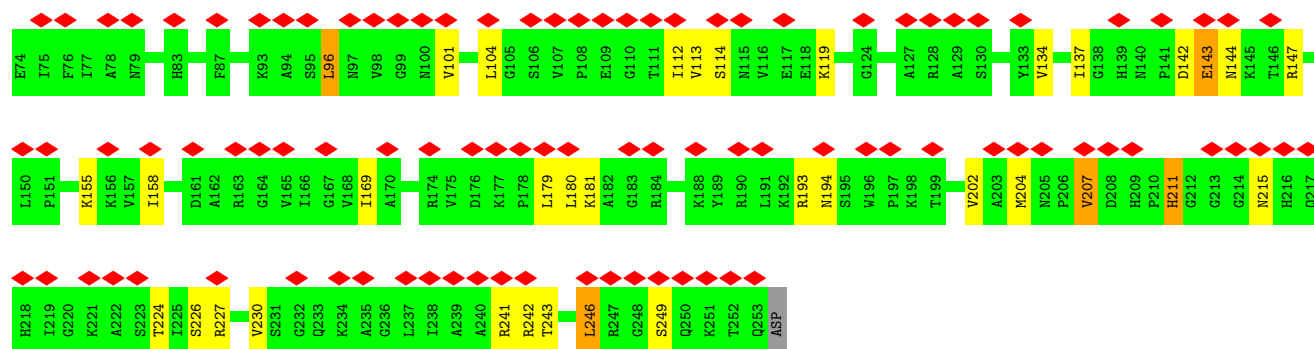
Chain AZ: 



• Molecule 35: 60S RIBOSOMAL PROTEIN L2-B

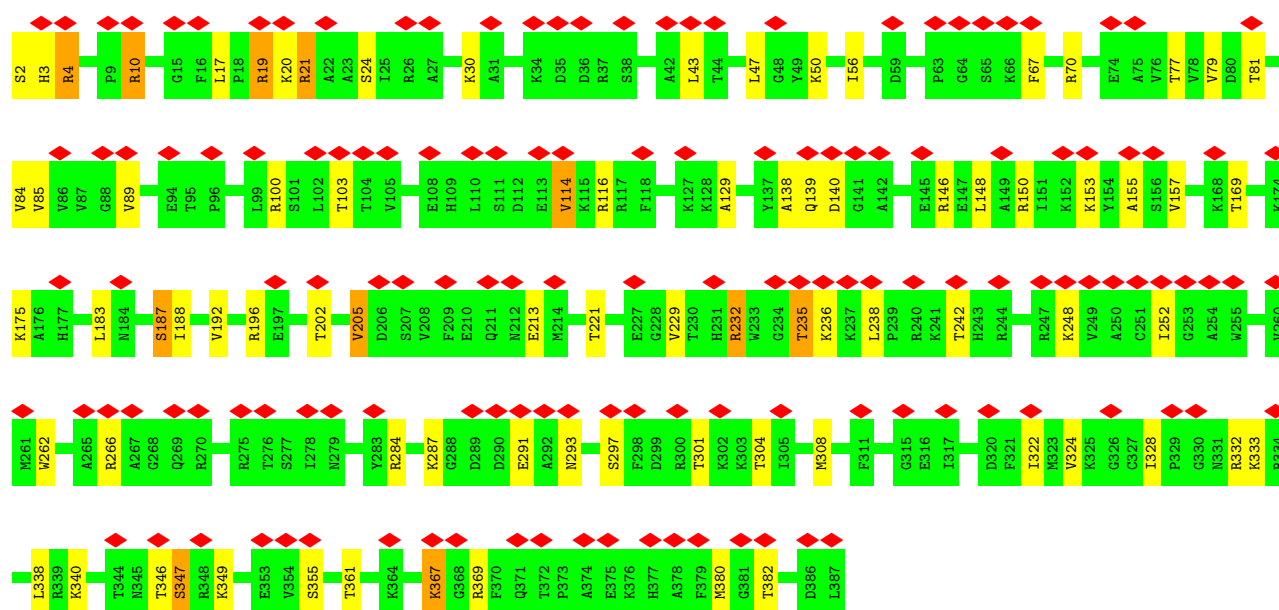
Chain BA: 





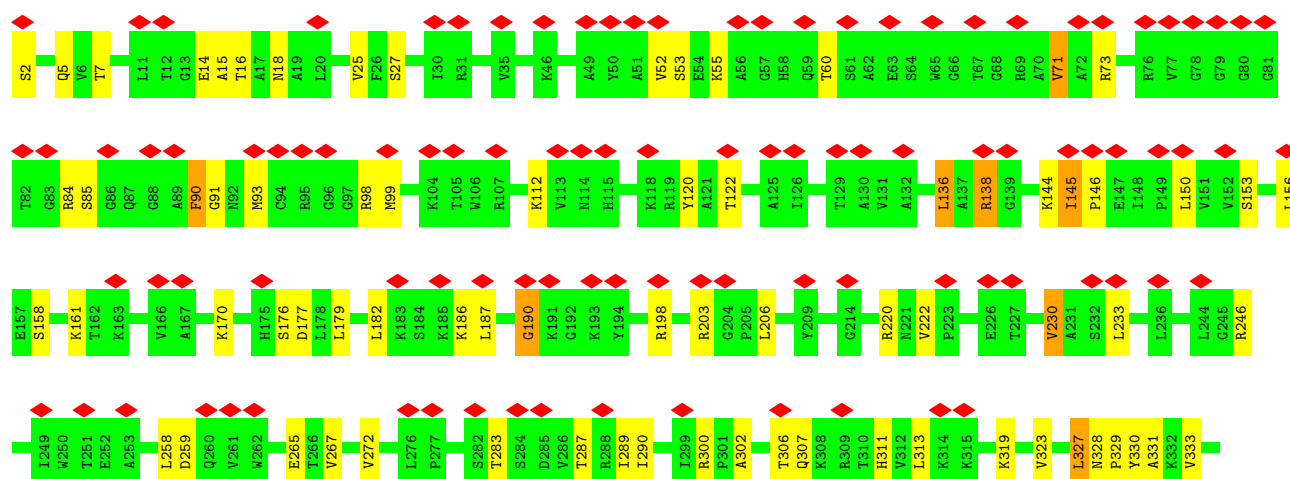
• Molecule 36: 60S RIBOSOMAL PROTEIN L3

Chain BB: 36% 79% 18%

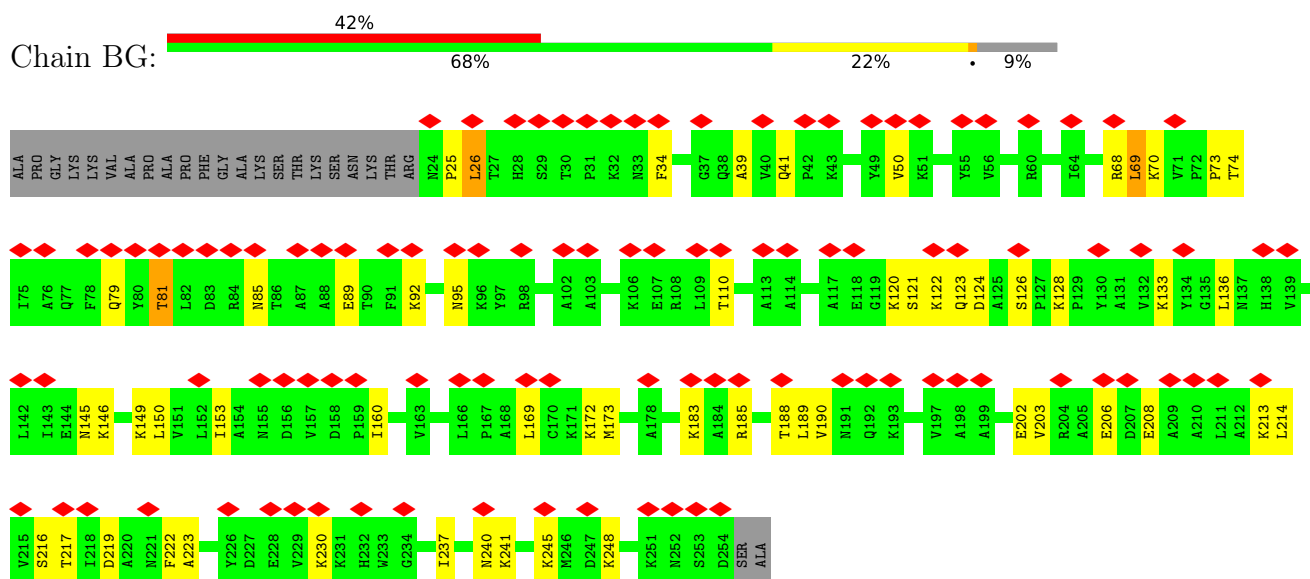


• Molecule 37: 60S RIBOSOMAL PROTEIN L4-A

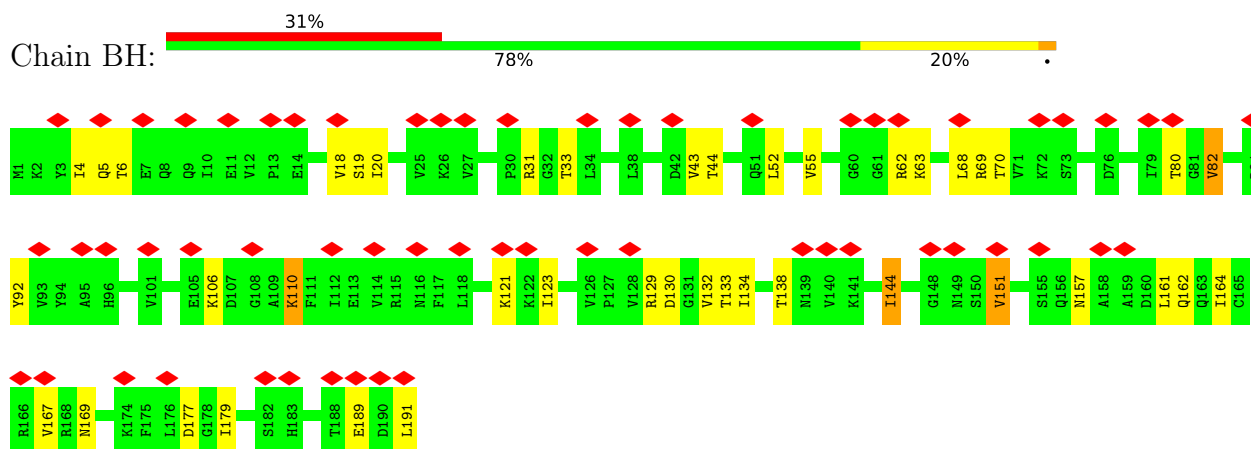
Chain BC: 29% 76% 21%



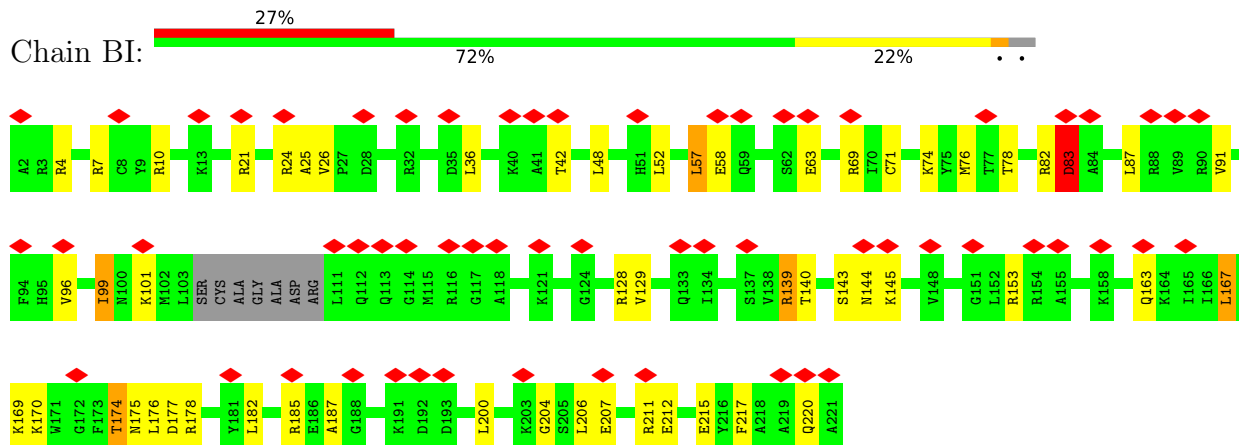




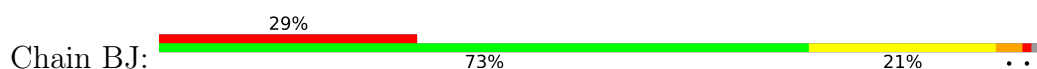
• Molecule 42: 60S RIBOSOMAL PROTEIN L9-A

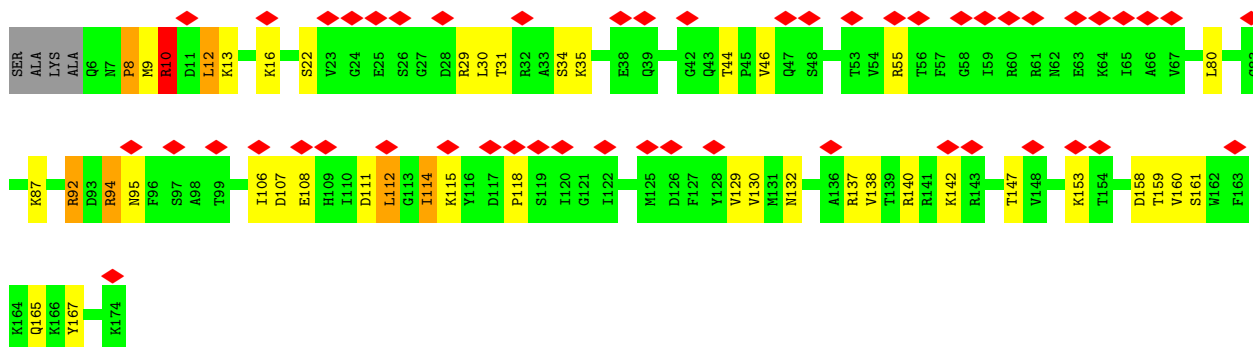


• Molecule 43: 60S RIBOSOMAL PROTEIN L10

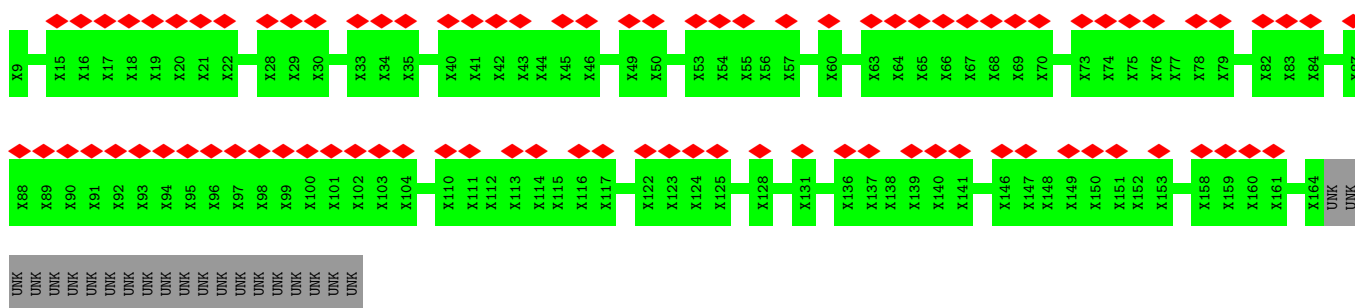


• Molecule 44: 60S RIBOSOMAL PROTEIN L11-A

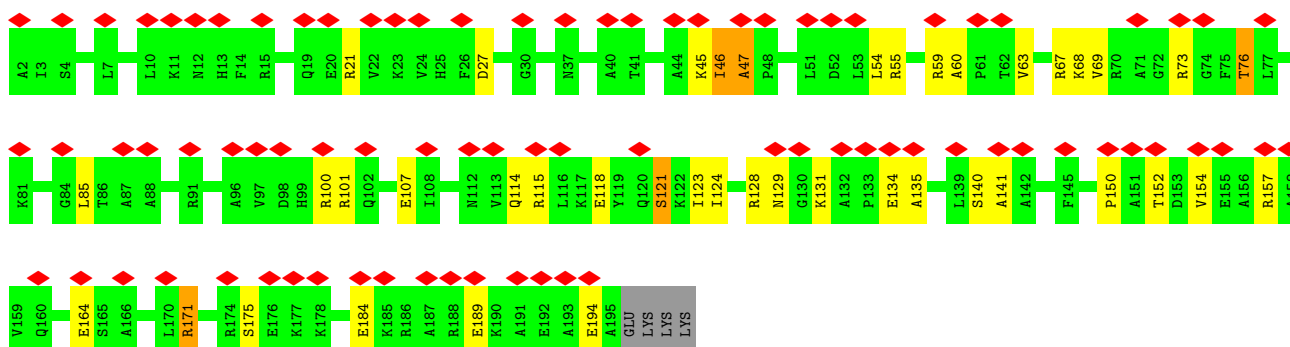
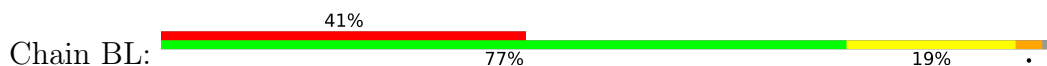




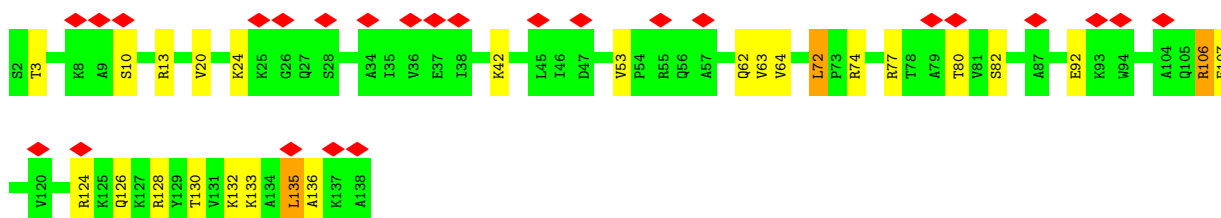
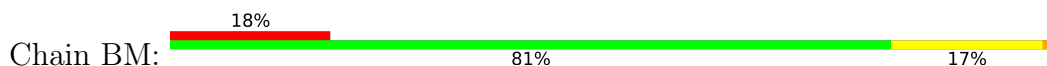
• Molecule 45: 60S RIBOSOMAL PROTEIN L11-A



• Molecule 46: 60S RIBOSOMAL PROTEIN L13-A

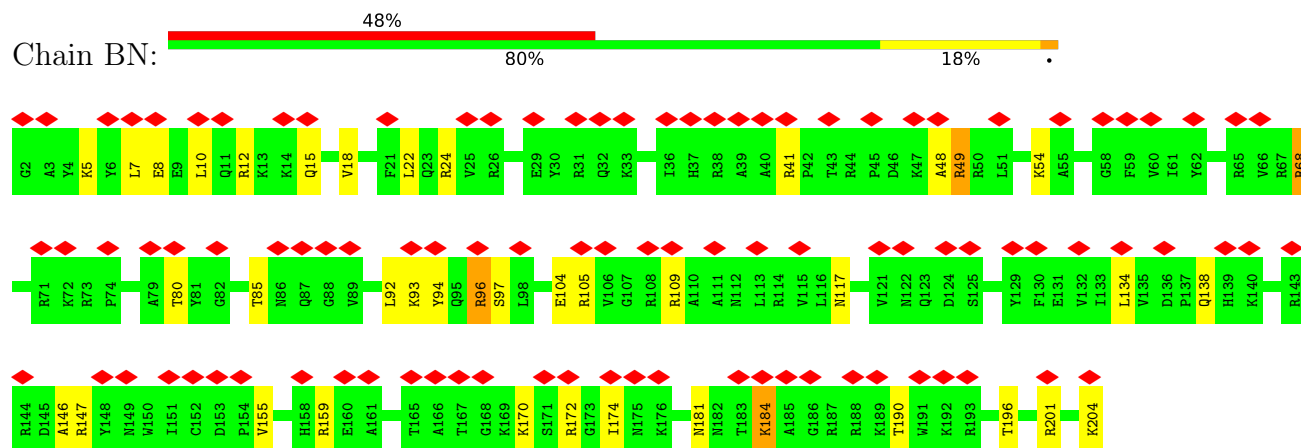


• Molecule 47: 60S RIBOSOMAL PROTEIN L14-B

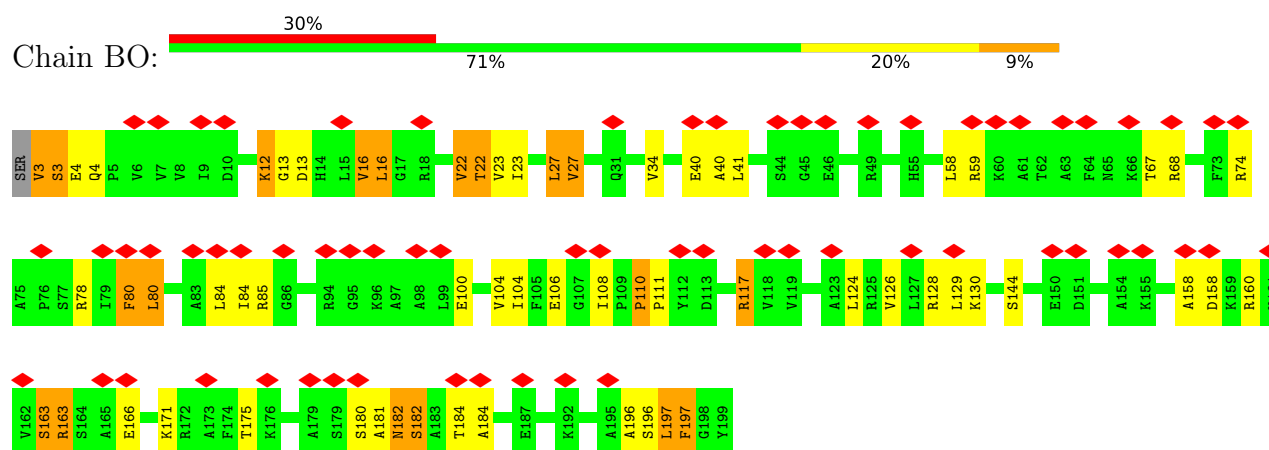




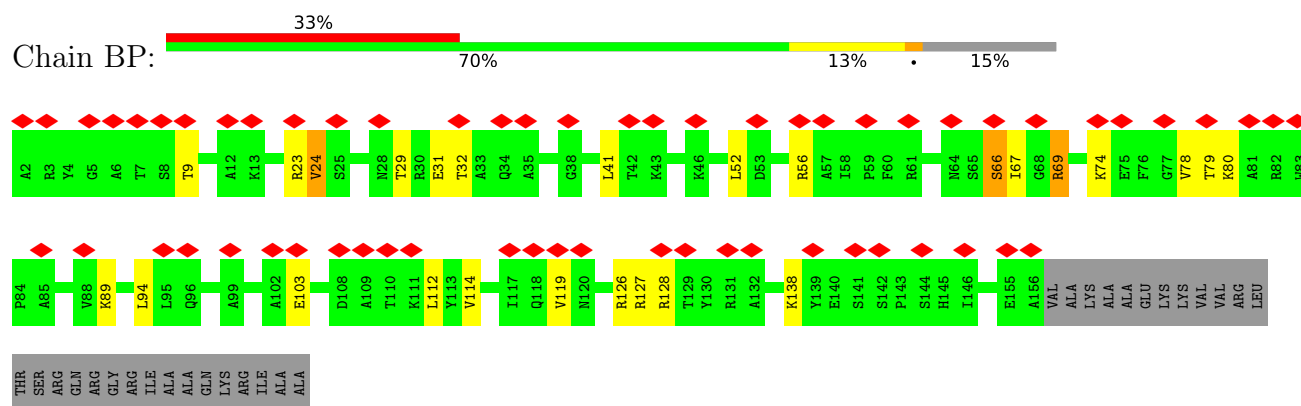
- Molecule 48: 60S RIBOSOMAL PROTEIN L15-A



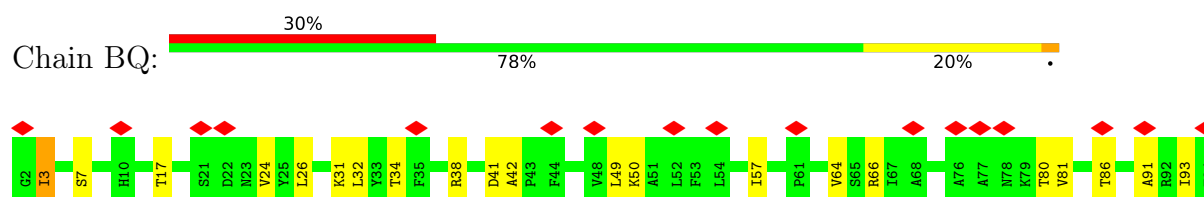
- Molecule 49: 60S RIBOSOMAL PROTEIN L16-A

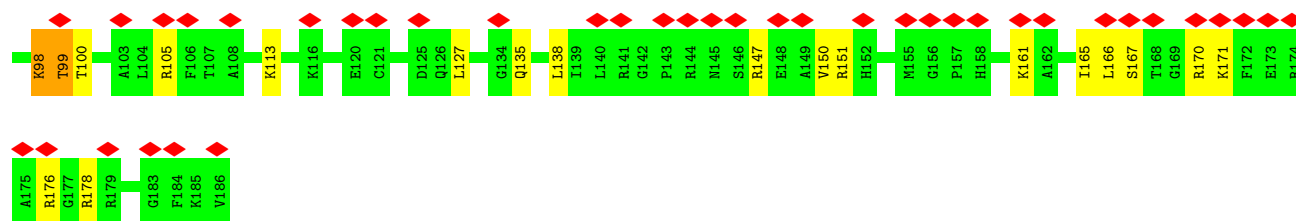


- Molecule 50: 60S RIBOSOMAL PROTEIN L17-A

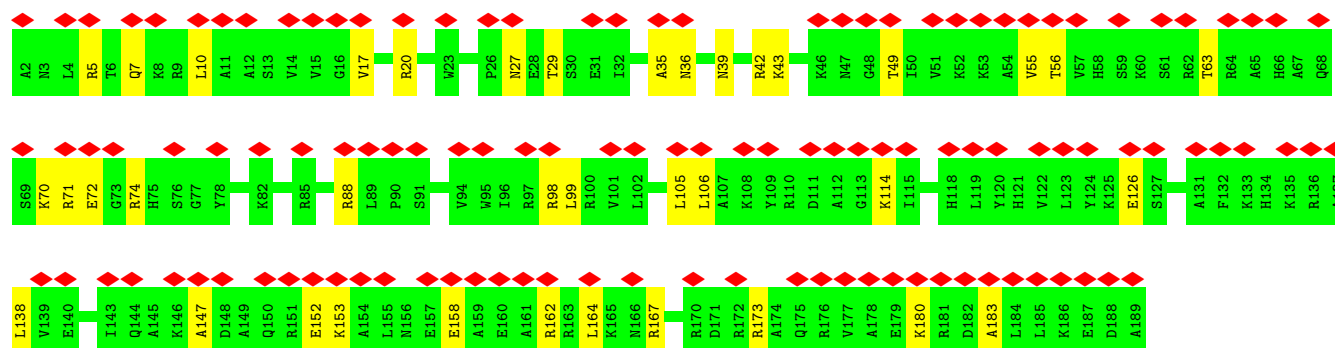


- Molecule 51: 60S RIBOSOMAL PROTEIN L18-A

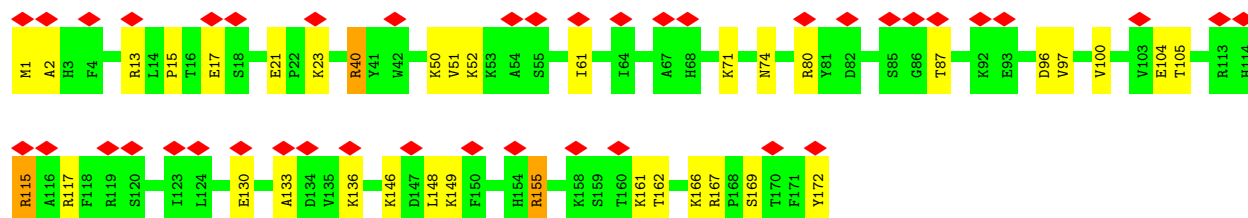
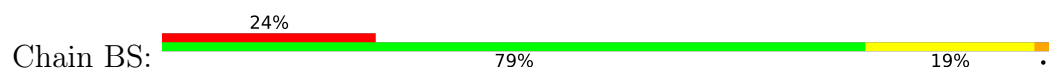




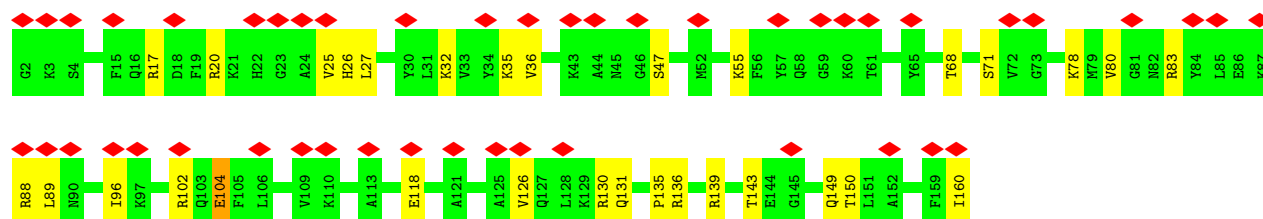
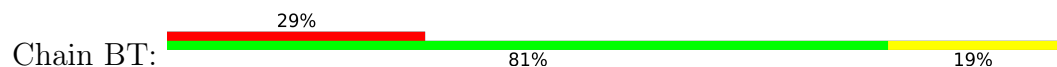
• Molecule 52: 60S RIBOSOMAL PROTEIN L19-B



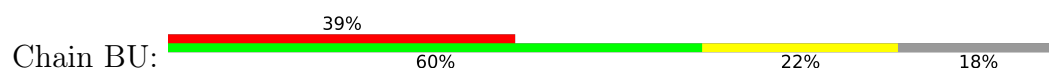
• Molecule 53: 60S RIBOSOMAL PROTEIN L20-B

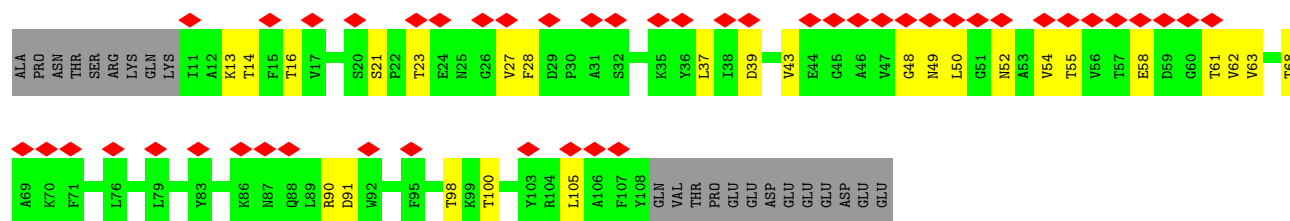


• Molecule 54: 60S RIBOSOMAL PROTEIN L21-A

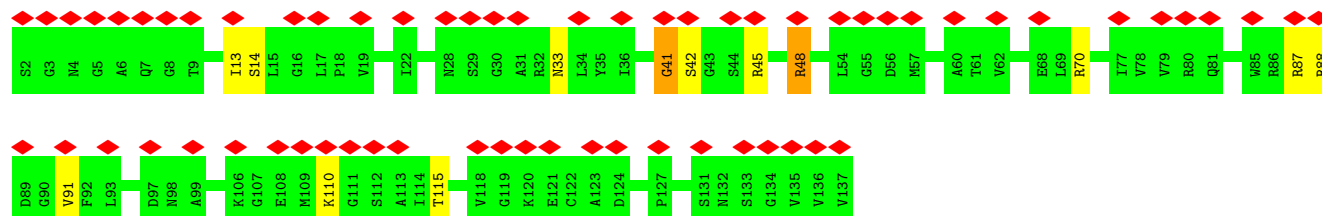


• Molecule 55: 60S RIBOSOMAL PROTEIN L22-A

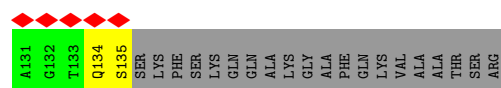
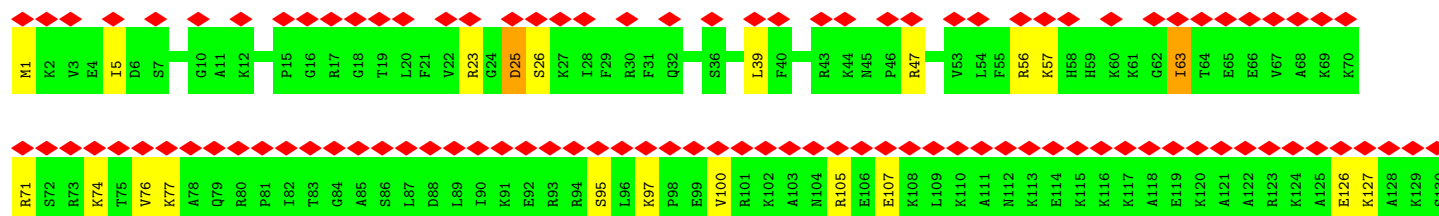
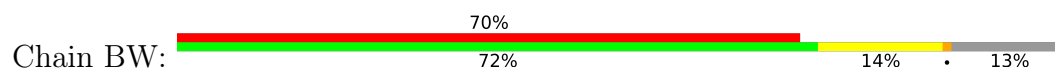




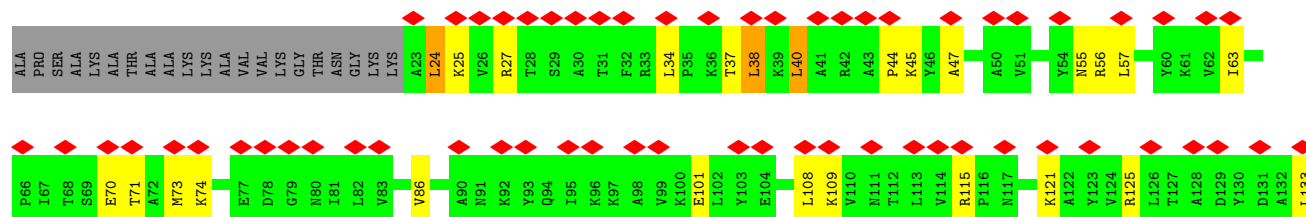
• Molecule 56: 60S RIBOSOMAL PROTEIN L23-A



• Molecule 57: 60S RIBOSOMAL PROTEIN L24-A

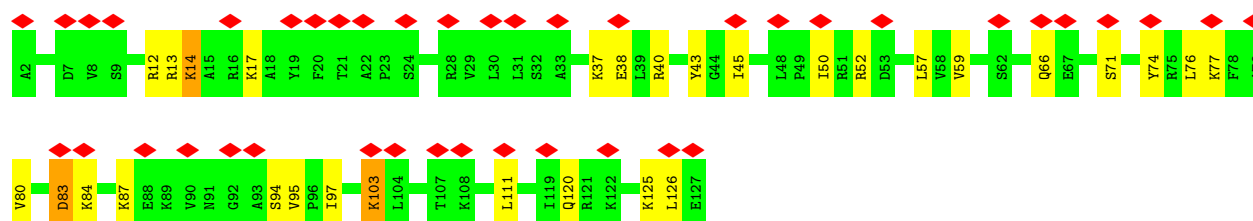
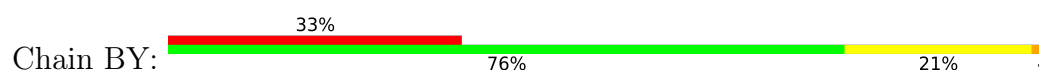


• Molecule 58: 60S RIBOSOMAL PROTEIN L25

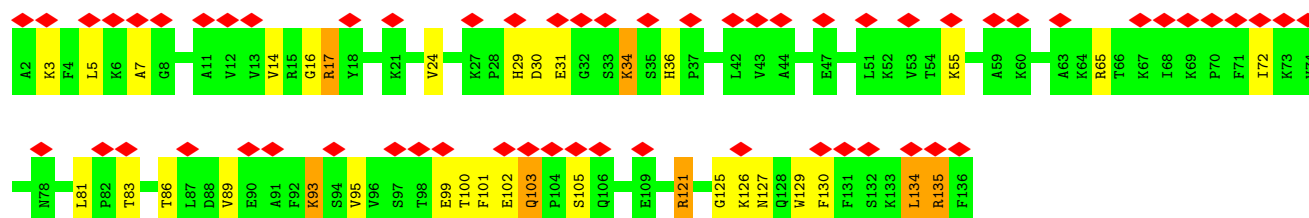
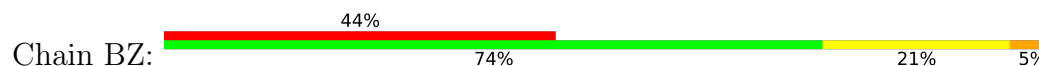


• Molecule 59: 60S RIBOSOMAL PROTEIN L26-A

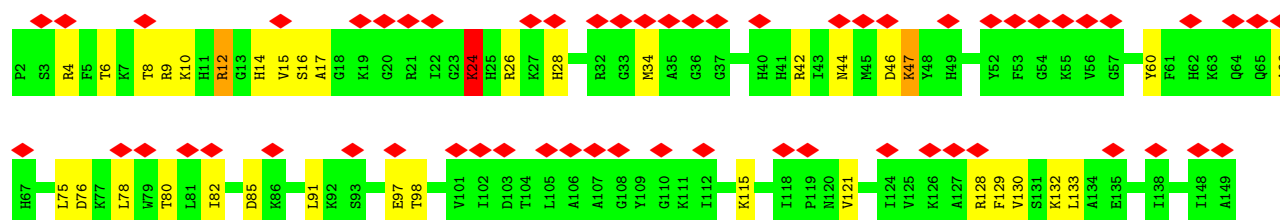
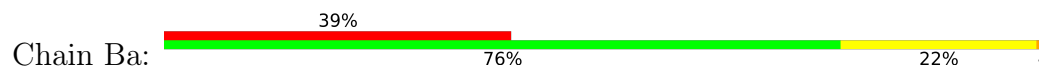




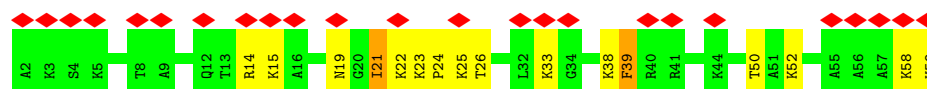
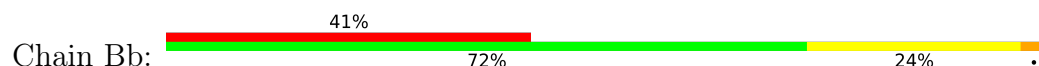
• Molecule 60: 60S RIBOSOMAL PROTEIN L27-A



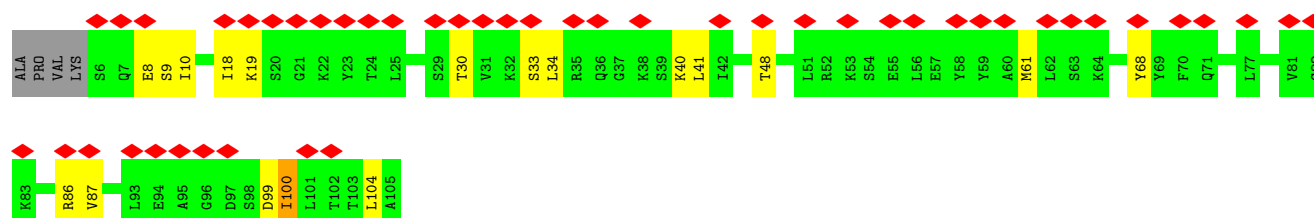
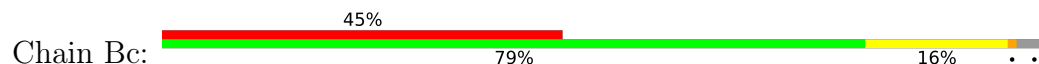
• Molecule 61: 60S RIBOSOMAL PROTEIN L28



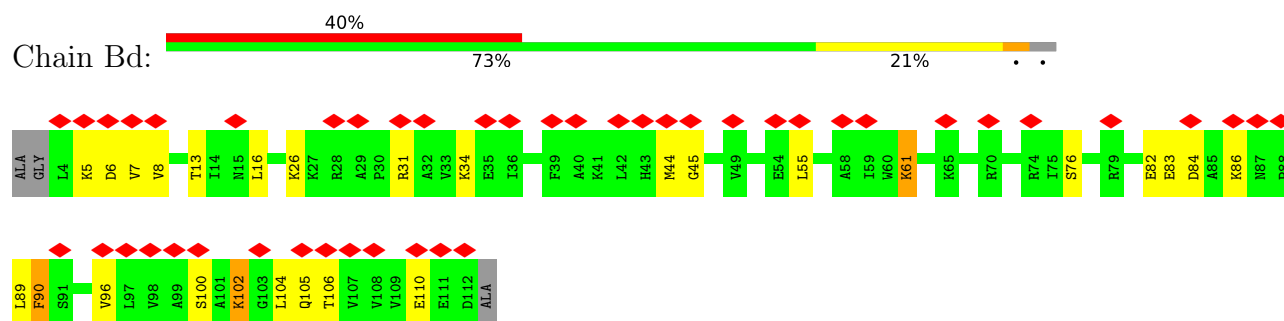
• Molecule 62: 60S RIBOSOMAL PROTEIN L29



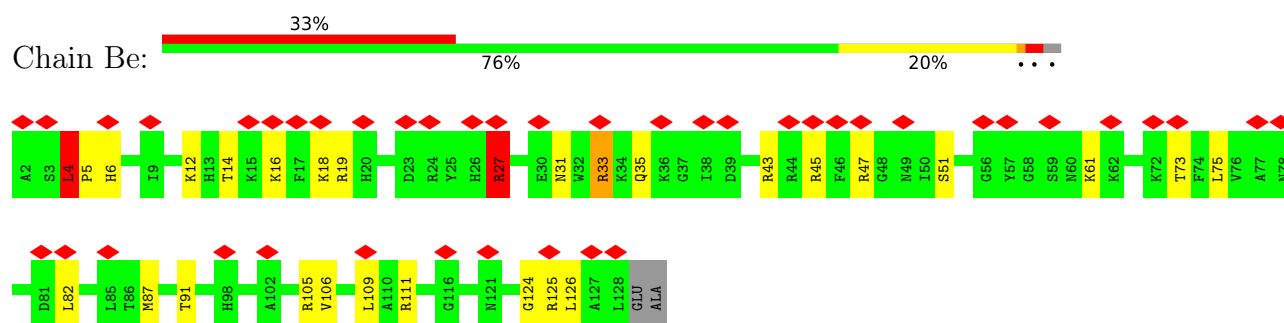
• Molecule 63: 60S RIBOSOMAL PROTEIN L30



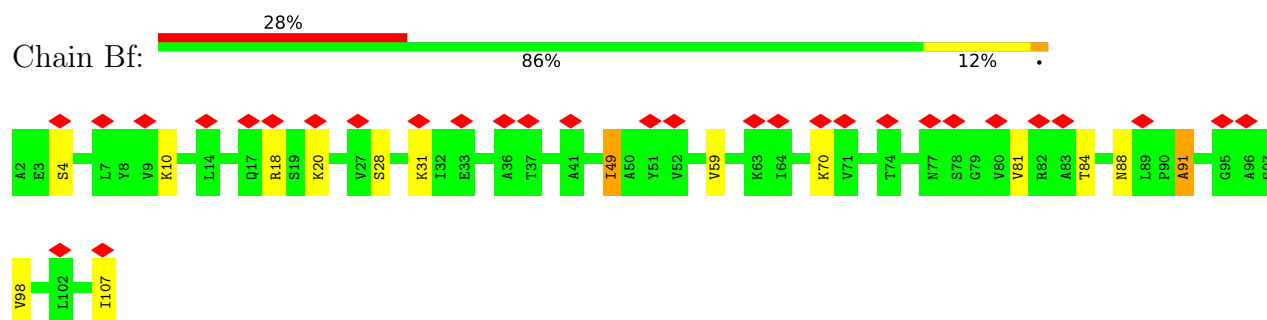
- Molecule 64: 60S RIBOSOMAL PROTEIN L31-A



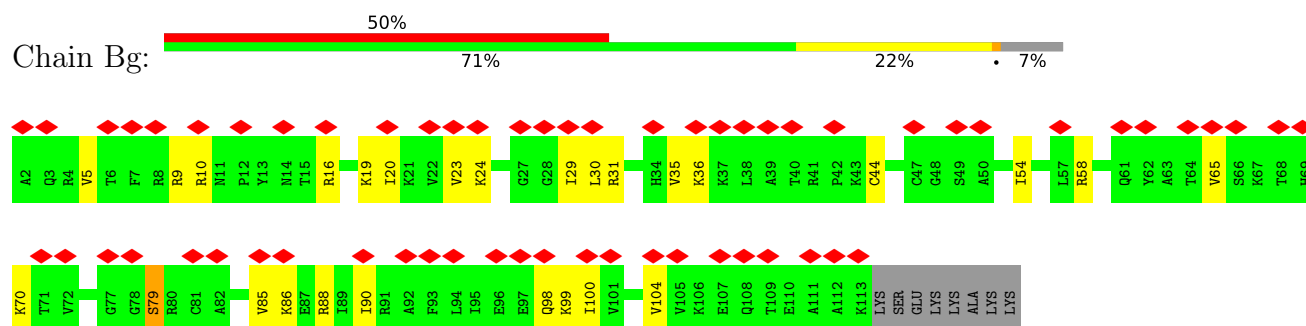
- Molecule 65: 60S RIBOSOMAL PROTEIN L32



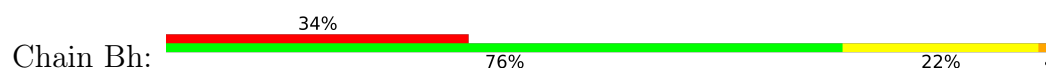
- Molecule 66: 60S RIBOSOMAL PROTEIN L33-A

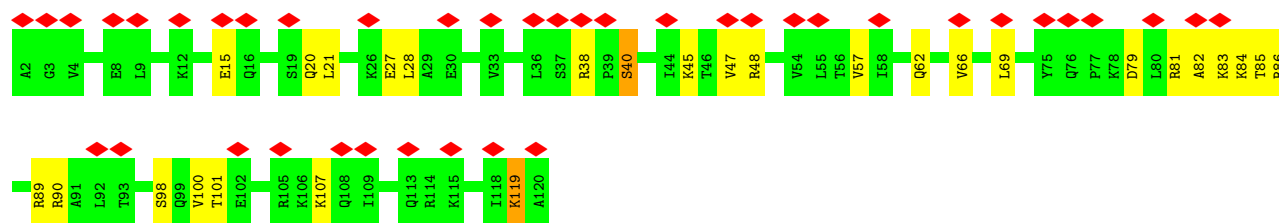


- Molecule 67: 60S RIBOSOMAL PROTEIN L34-A

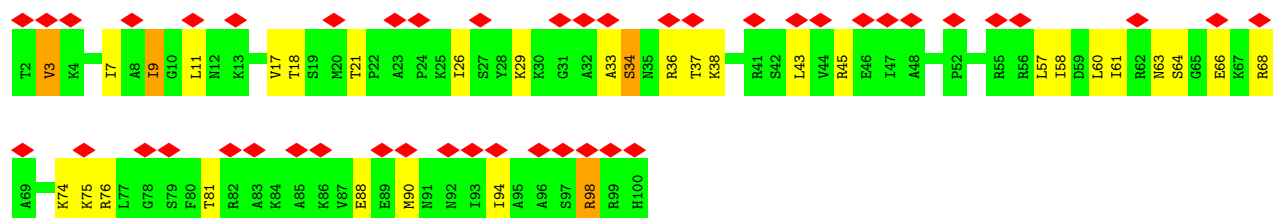


- Molecule 68: 60S RIBOSOMAL PROTEIN L35-B

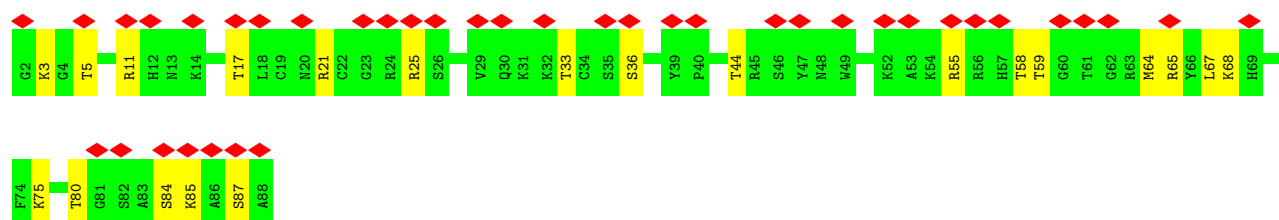
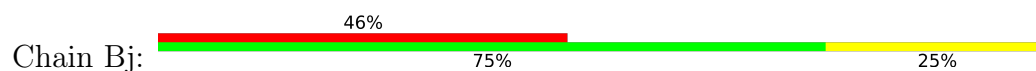




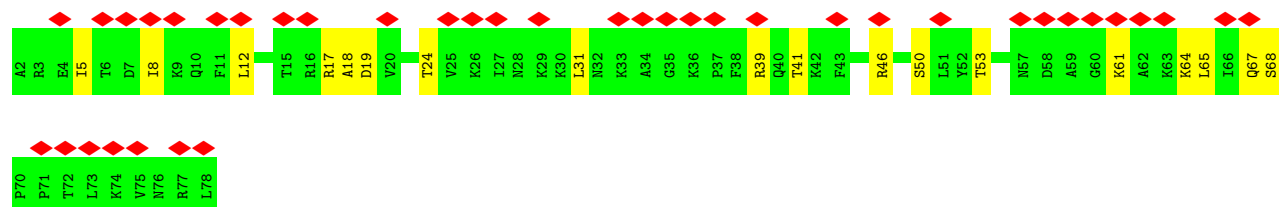
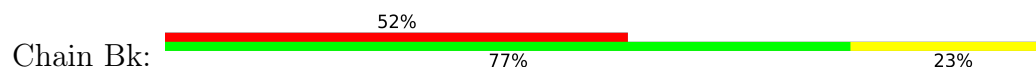
• Molecule 69: 60S RIBOSOMAL PROTEIN L36-A



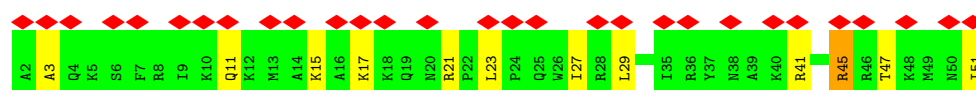
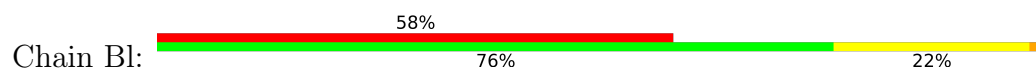
• Molecule 70: 60S RIBOSOMAL PROTEIN L37-A



• Molecule 71: 60S RIBOSOMAL PROTEIN L38

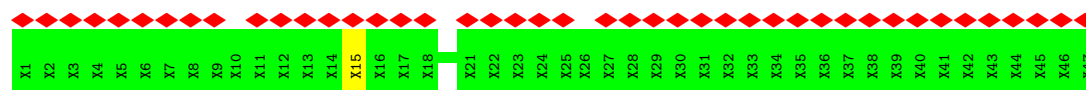


• Molecule 72: 60S RIBOSOMAL PROTEIN L39

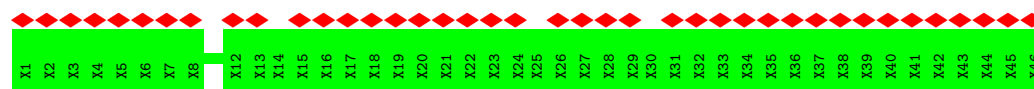


• Molecule 73: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

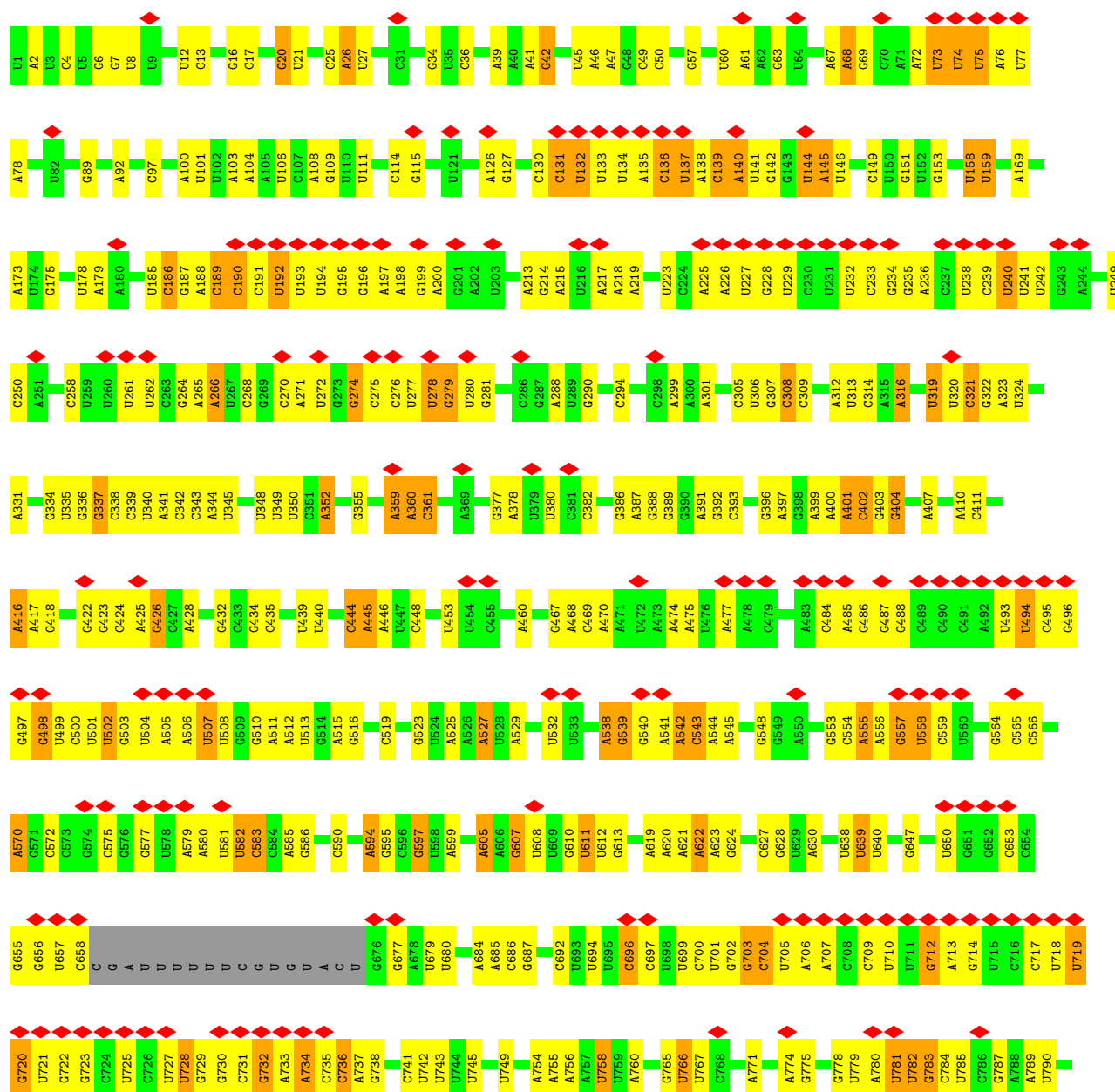




• Molecule 78: 60S ACIDIC RIBOSOMAL PROTEIN P2

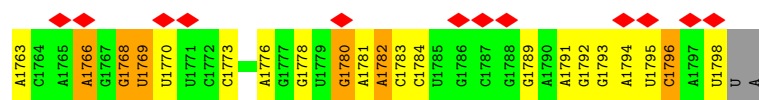


• Molecule 79: 18S RIBOSOMAL RNA

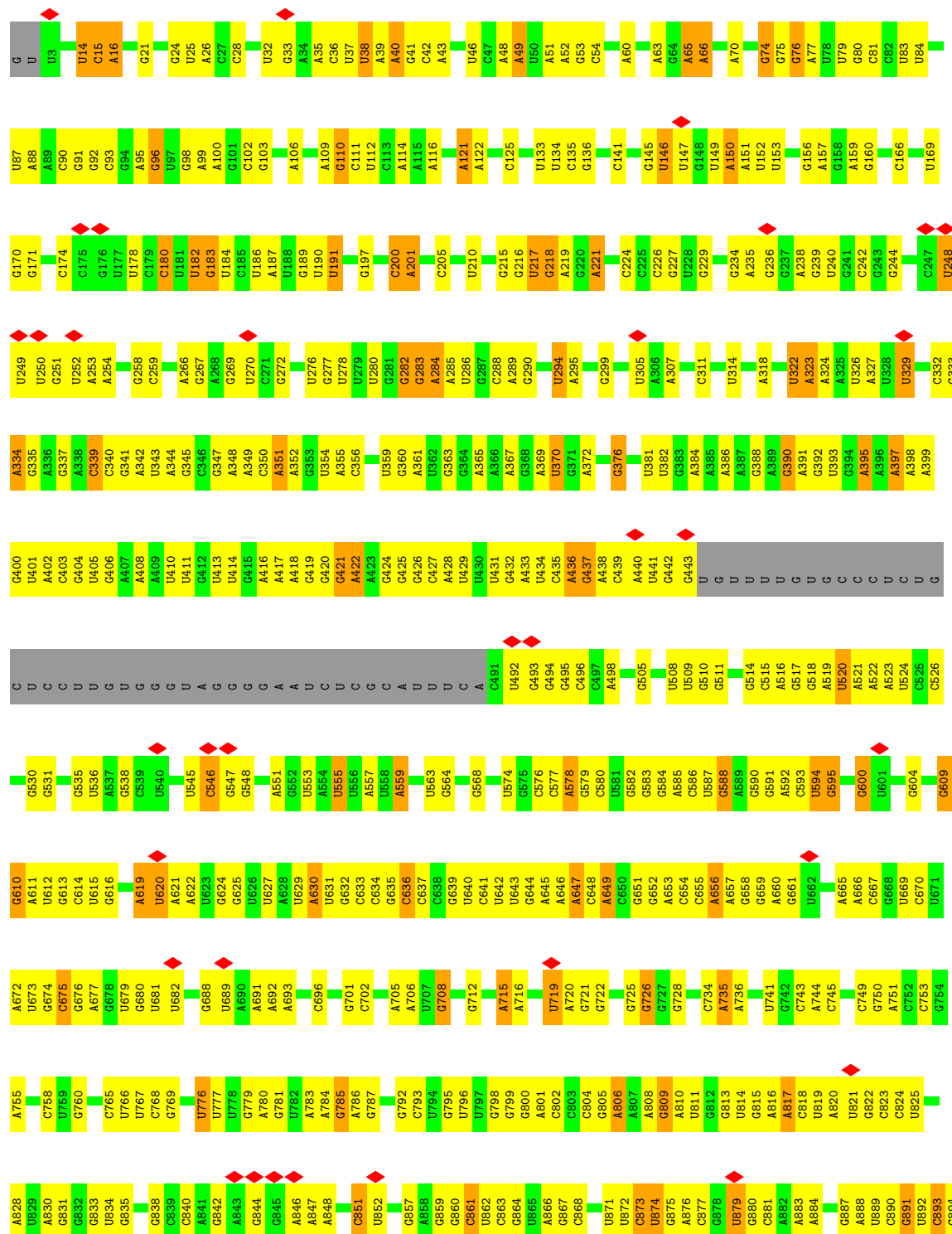


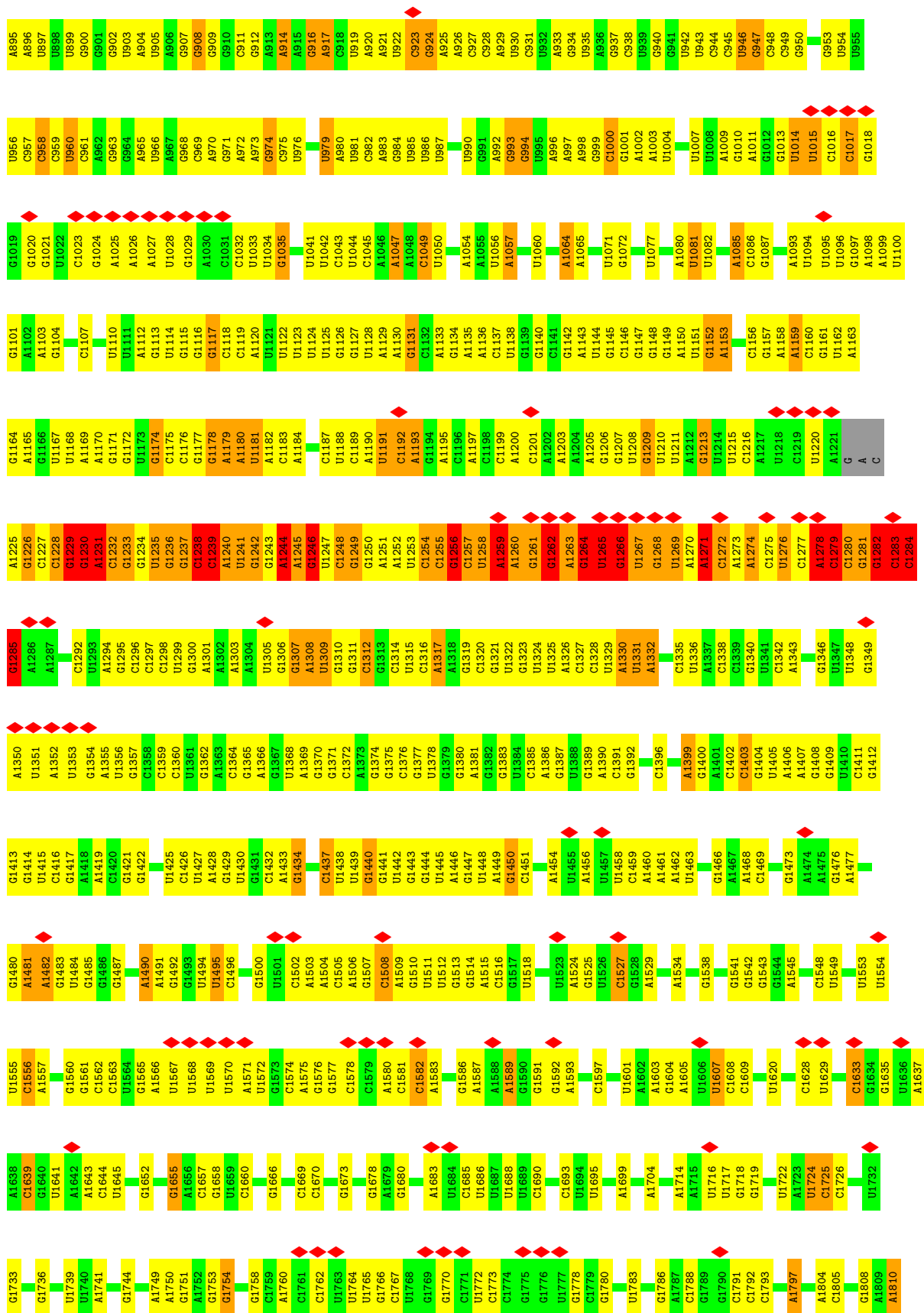






• Molecule 80: 25S RIBOSOMAL RNA













● Molecule 85: 5'-R(\*AP\*UP\*GP)-3'

Chain CX: 33% 67%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5143	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	16	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	79096	Depositor
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	0.643	Depositor
Minimum map value	-0.362	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	424.8, 424.8, 424.8	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.77, 1.77, 1.77	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OHX, ZN, HSO, GCP, MG

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	A0	0.54	0/782	0.77	0/1047
2	A1	0.53	0/620	0.81	1/838 (0.1%)
3	A2	0.43	0/499	0.72	0/670
4	A3	0.70	0/452	0.94	1/600 (0.2%)
5	A4	0.50	0/483	0.71	0/643
6	A5	0.53	0/404	0.99	1/542 (0.2%)
7	A6	0.49	0/2490	0.70	0/3389
8	A7	0.86	2/925 (0.2%)	0.87	2/1240 (0.2%)
9	AA	0.54	0/1617	0.80	0/2215
10	AB	0.45	0/1735	0.81	0/2335
11	AC	0.60	0/1665	0.77	0/2263
12	AD	0.59	0/1759	0.74	0/2368
13	AE	0.57	0/2109	0.86	1/2839 (0.0%)
14	AF	0.49	0/1629	0.72	0/2202
15	AG	0.55	0/1823	0.75	0/2439
16	AH	0.52	0/1506	0.77	0/2028
17	AI	0.68	0/1514	0.89	3/2021 (0.1%)
18	AJ	0.59	0/1519	0.81	0/2035
19	AK	0.55	0/789	0.83	3/1067 (0.3%)
20	AL	0.70	0/1239	0.81	0/1673
21	AM	0.49	0/898	0.76	0/1220
22	AN	0.61	0/1215	0.83	3/1638 (0.2%)
23	AO	0.48	0/901	0.82	1/1217 (0.1%)
24	AP	0.60	0/998	0.86	3/1341 (0.2%)
25	AQ	0.56	0/1125	0.85	3/1510 (0.2%)
26	AR	0.54	0/935	0.81	0/1254
27	AS	0.59	0/1211	0.80	0/1628
28	AT	0.57	0/1130	0.81	0/1517
29	AU	0.55	0/865	0.76	0/1169
30	AV	0.52	0/693	0.75	0/935
31	AW	0.65	0/1038	0.86	3/1395 (0.2%)
32	AX	0.72	0/1139	0.91	2/1518 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	AY	0.56	0/1087	0.77	1/1449 (0.1%)
34	AZ	0.50	0/571	0.85	1/768 (0.1%)
35	BA	0.87	1/1946 (0.1%)	1.05	4/2614 (0.2%)
36	BB	1.02	4/3146 (0.1%)	1.11	13/4228 (0.3%)
37	BC	0.87	0/2800	1.07	11/3790 (0.3%)
38	BD	0.89	1/2408 (0.0%)	0.96	3/3248 (0.1%)
39	BE	0.90	1/1269 (0.1%)	1.00	3/1705 (0.2%)
40	BF	0.99	1/1828 (0.1%)	1.04	6/2461 (0.2%)
41	BG	0.64	0/1795	0.81	1/2429 (0.0%)
42	BH	0.97	2/1539 (0.1%)	1.01	1/2073 (0.0%)
43	BI	0.92	1/1758 (0.1%)	1.08	12/2358 (0.5%)
44	BJ	0.81	1/1374 (0.1%)	0.99	4/1842 (0.2%)
46	BL	0.82	0/1573	1.04	6/2113 (0.3%)
47	BM	0.96	0/1074	1.01	4/1446 (0.3%)
48	BN	0.83	1/1757 (0.1%)	1.00	6/2354 (0.3%)
49	BO	0.98	11/3159 (0.3%)	1.02	25/4205 (0.6%)
50	BP	1.05	1/1250 (0.1%)	1.09	5/1683 (0.3%)
51	BQ	0.89	1/1465 (0.1%)	1.12	9/1965 (0.5%)
52	BR	0.78	1/1538 (0.1%)	0.87	2/2050 (0.1%)
53	BS	1.02	0/1481	1.09	7/1990 (0.4%)
54	BT	1.01	2/1300 (0.2%)	1.01	1/1743 (0.1%)
55	BU	0.56	0/794	0.77	0/1076
56	BV	0.98	0/1018	1.09	4/1369 (0.3%)
57	BW	0.80	0/1052	0.90	2/1398 (0.1%)
58	BX	0.72	0/974	0.86	0/1314
59	BY	0.79	1/1004 (0.1%)	0.98	2/1341 (0.1%)
60	BZ	0.55	0/1118	0.83	2/1497 (0.1%)
61	Ba	0.95	2/1204 (0.2%)	1.14	9/1612 (0.6%)
62	Bb	0.91	0/473	1.14	1/629 (0.2%)
63	Bc	0.61	0/775	0.77	0/1040
64	Bd	0.94	2/897 (0.2%)	0.95	1/1205 (0.1%)
65	Be	1.03	0/1041	1.27	12/1394 (0.9%)
66	Bf	1.12	0/868	1.09	3/1168 (0.3%)
67	Bg	0.72	0/890	0.92	0/1189
68	Bh	0.67	0/974	0.80	0/1297
69	Bi	0.67	0/777	0.85	0/1033
70	Bj	0.87	0/696	1.04	3/923 (0.3%)
71	Bk	0.50	0/614	0.70	0/822
72	Bl	0.90	0/443	1.02	1/588 (0.2%)
73	Bm	1.08	2/423 (0.5%)	1.13	1/562 (0.2%)
74	Bn	0.90	0/234	1.15	1/300 (0.3%)
75	Bo	0.83	0/860	0.89	1/1136 (0.1%)
76	Bq	1.09	0/1090	1.31	4/1474 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
79	B2	0.92	33/42128 (0.1%)	1.49	828/65642 (1.3%)
80	B5	1.49	661/75336 (0.9%)	1.92	3722/117449 (3.2%)
81	B7	1.38	12/2883 (0.4%)	1.80	119/4491 (2.6%)
82	B8	1.16	4/3746 (0.1%)	1.70	128/5832 (2.2%)
83	CV	1.87	8/4407 (0.2%)	1.47	47/5931 (0.8%)
84	CW	2.08	51/1801 (2.8%)	3.23	250/2803 (8.9%)
85	CX	2.12	4/69 (5.8%)	3.20	11/106 (10.4%)
All	All	1.14	811/222414 (0.4%)	1.53	5304/325931 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A1	0	1
6	A5	0	2
8	A7	0	1
10	AB	0	1
16	AH	0	1
20	AL	0	1
23	AO	0	1
26	AR	0	2
34	AZ	0	3
35	BA	0	2
37	BC	0	1
38	BD	0	1
39	BE	0	1
40	BF	0	2
49	BO	0	2
53	BS	0	1
56	BV	0	1
59	BY	0	1
60	BZ	0	1
61	Ba	0	3
62	Bb	0	1
76	Bq	0	7
77	Br	0	1
80	B5	0	35
83	CV	0	18
84	CW	0	32
85	CX	0	2
All	All	0	125

The worst 5 of 811 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	CV	63	GLU	N-CA	69.03	2.84	1.46
83	CV	210	TRP	CD2-CE3	34.76	1.92	1.40
83	CV	210	TRP	CD2-CE2	33.01	1.80	1.41
83	CV	210	TRP	CE2-CZ2	31.95	1.94	1.39
83	CV	210	TRP	CE3-CZ3	26.33	1.83	1.38

The worst 5 of 5304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	CW	36	U	P-O3'-C3'	-59.91	47.81	119.70
80	B5	1152	G	N3-C4-C5	33.59	145.40	128.60
80	B5	1256	G	P-O3'-C3'	32.78	159.04	119.70
80	B5	1152	G	N3-C4-N9	-31.65	107.01	126.00
80	B5	1152	G	N3-C2-N2	-26.89	101.08	119.90

There are no chirality outliers.

5 of 125 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A1	42	ASN	Peptide
6	A5	105	TYR	Peptide
6	A5	138	ARG	Peptide
8	A7	134	ASP	Sidechain
10	AB	131	ASP	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	A0	95/119 (80%)	57 (60%)	21 (22%)	17 (18%)	0	2
2	A1	79/82 (96%)	62 (78%)	13 (16%)	4 (5%)	2	19
3	A2	61/67 (91%)	47 (77%)	9 (15%)	5 (8%)	1	12
4	A3	51/56 (91%)	43 (84%)	6 (12%)	2 (4%)	3	23
5	A4	58/63 (92%)	49 (84%)	7 (12%)	2 (3%)	3	26
6	A5	50/152 (33%)	30 (60%)	9 (18%)	11 (22%)	0	1
7	A6	316/319 (99%)	273 (86%)	30 (10%)	13 (4%)	3	23
8	A7	120/273 (44%)	92 (77%)	17 (14%)	11 (9%)	1	10
9	AA	204/252 (81%)	143 (70%)	35 (17%)	26 (13%)	0	5
10	AB	212/255 (83%)	132 (62%)	42 (20%)	38 (18%)	0	2
11	AC	215/254 (85%)	187 (87%)	16 (7%)	12 (6%)	2	18
12	AD	221/240 (92%)	180 (81%)	27 (12%)	14 (6%)	1	16
13	AE	258/261 (99%)	201 (78%)	36 (14%)	21 (8%)	1	12
14	AF	204/225 (91%)	155 (76%)	30 (15%)	19 (9%)	0	10
15	AG	224/236 (95%)	190 (85%)	23 (10%)	11 (5%)	2	20
16	AH	182/190 (96%)	128 (70%)	27 (15%)	27 (15%)	0	3
17	AI	184/200 (92%)	155 (84%)	14 (8%)	15 (8%)	1	12
18	AJ	183/197 (93%)	153 (84%)	18 (10%)	12 (7%)	1	15
19	AK	94/105 (90%)	66 (70%)	18 (19%)	10 (11%)	0	8
20	AL	153/156 (98%)	125 (82%)	19 (12%)	9 (6%)	1	17
21	AM	122/143 (85%)	66 (54%)	23 (19%)	33 (27%)	0	0
22	AN	148/151 (98%)	125 (84%)	15 (10%)	8 (5%)	2	19
23	AO	125/137 (91%)	94 (75%)	16 (13%)	15 (12%)	0	6
24	AP	122/142 (86%)	92 (75%)	15 (12%)	15 (12%)	0	5
25	AQ	139/143 (97%)	114 (82%)	14 (10%)	11 (8%)	1	13
26	AR	116/136 (85%)	87 (75%)	17 (15%)	12 (10%)	0	8
27	AS	143/146 (98%)	110 (77%)	19 (13%)	14 (10%)	0	9
28	AT	141/144 (98%)	111 (79%)	18 (13%)	12 (8%)	1	11
29	AU	105/121 (87%)	87 (83%)	13 (12%)	5 (5%)	2	21
30	AV	85/87 (98%)	64 (75%)	11 (13%)	10 (12%)	0	6
31	AW	127/130 (98%)	114 (90%)	10 (8%)	3 (2%)	6	33
32	AX	142/145 (98%)	111 (78%)	13 (9%)	18 (13%)	0	5

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	AY	132/135 (98%)	106 (80%)	13 (10%)	13 (10%)	0	9
34	AZ	68/108 (63%)	46 (68%)	11 (16%)	11 (16%)	0	3
35	BA	250/253 (99%)	213 (85%)	30 (12%)	7 (3%)	5	30
36	BB	384/386 (100%)	341 (89%)	34 (9%)	9 (2%)	6	34
37	BC	359/361 (99%)	306 (85%)	32 (9%)	21 (6%)	1	18
38	BD	292/296 (99%)	267 (91%)	19 (6%)	6 (2%)	7	36
39	BE	153/175 (87%)	134 (88%)	15 (10%)	4 (3%)	5	31
40	BF	221/243 (91%)	201 (91%)	16 (7%)	4 (2%)	8	40
41	BG	229/255 (90%)	180 (79%)	28 (12%)	21 (9%)	1	10
42	BH	189/191 (99%)	172 (91%)	13 (7%)	4 (2%)	7	36
43	BI	209/220 (95%)	175 (84%)	22 (10%)	12 (6%)	1	18
44	BJ	167/173 (96%)	135 (81%)	19 (11%)	13 (8%)	1	13
46	BL	192/198 (97%)	161 (84%)	20 (10%)	11 (6%)	1	18
47	BM	135/137 (98%)	124 (92%)	10 (7%)	1 (1%)	22	63
48	BN	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	4	28
49	BO	352/218 (162%)	324 (92%)	18 (5%)	10 (3%)	5	30
50	BP	153/183 (84%)	142 (93%)	9 (6%)	2 (1%)	12	48
51	BQ	183/185 (99%)	168 (92%)	9 (5%)	6 (3%)	4	26
52	BR	186/188 (99%)	167 (90%)	16 (9%)	3 (2%)	9	44
53	BS	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	66
54	BT	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	12	48
55	BU	96/120 (80%)	80 (83%)	13 (14%)	3 (3%)	4	27
56	BV	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	10	46
57	BW	133/155 (86%)	106 (80%)	19 (14%)	8 (6%)	1	17
58	BX	118/141 (84%)	104 (88%)	6 (5%)	8 (7%)	1	15
59	BY	124/126 (98%)	107 (86%)	12 (10%)	5 (4%)	3	23
60	BZ	133/135 (98%)	107 (80%)	13 (10%)	13 (10%)	0	9
61	Ba	146/148 (99%)	123 (84%)	18 (12%)	5 (3%)	3	26
62	Bb	56/58 (97%)	44 (79%)	7 (12%)	5 (9%)	1	11
63	Bc	98/104 (94%)	87 (89%)	8 (8%)	3 (3%)	4	27
64	Bd	107/112 (96%)	88 (82%)	13 (12%)	6 (6%)	2	18

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	Be	125/129 (97%)	110 (88%)	9 (7%)	6 (5%)	2	21
66	Bf	104/106 (98%)	96 (92%)	5 (5%)	3 (3%)	4	29
67	Bg	110/120 (92%)	93 (84%)	13 (12%)	4 (4%)	3	25
68	Bh	117/119 (98%)	99 (85%)	14 (12%)	4 (3%)	3	26
69	Bi	97/99 (98%)	77 (79%)	13 (13%)	7 (7%)	1	14
70	Bj	85/87 (98%)	75 (88%)	8 (9%)	2 (2%)	6	33
71	Bk	75/77 (97%)	61 (81%)	10 (13%)	4 (5%)	2	19
72	Bl	48/50 (96%)	41 (85%)	6 (12%)	1 (2%)	7	36
73	Bm	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	7	38
74	Bn	23/25 (92%)	22 (96%)	0	1 (4%)	2	22
75	Bo	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	8	38
76	Bq	141/312 (45%)	105 (74%)	14 (10%)	22 (16%)	0	3
83	CV	555/586 (95%)	450 (81%)	61 (11%)	44 (8%)	1	13
All	All	11839/12944 (92%)	9833 (83%)	1245 (10%)	761 (6%)	2	16

5 of 761 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A0	19	LYS
1	A0	45	VAL
1	A0	46	GLU
1	A0	62	TYR
1	A0	65	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	83/101 (82%)	65 (78%)	18 (22%)	1	6
2	A1	70/71 (99%)	62 (89%)	8 (11%)	5	21
3	A2	56/60 (93%)	38 (68%)	18 (32%)	0	2

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A3	47/49 (96%)	38 (81%)	9 (19%)	1	8
5	A4	51/54 (94%)	43 (84%)	8 (16%)	2	14
6	A5	43/116 (37%)	32 (74%)	11 (26%)	0	3
7	A6	259/262 (99%)	221 (85%)	38 (15%)	3	15
8	A7	97/195 (50%)	74 (76%)	23 (24%)	1	4
9	AA	164/210 (78%)	122 (74%)	42 (26%)	0	3
10	AB	191/224 (85%)	137 (72%)	54 (28%)	0	2
11	AC	176/205 (86%)	130 (74%)	46 (26%)	0	3
12	AD	182/195 (93%)	138 (76%)	44 (24%)	0	4
13	AE	221/222 (100%)	166 (75%)	55 (25%)	0	3
14	AF	173/191 (91%)	137 (79%)	36 (21%)	1	7
15	AG	188/201 (94%)	149 (79%)	39 (21%)	1	7
16	AH	165/170 (97%)	124 (75%)	41 (25%)	0	3
17	AI	150/161 (93%)	118 (79%)	32 (21%)	1	6
18	AJ	158/166 (95%)	117 (74%)	41 (26%)	0	3
19	AK	77/98 (79%)	58 (75%)	19 (25%)	0	3
20	AL	129/137 (94%)	105 (81%)	24 (19%)	1	9
21	AM	88/119 (74%)	55 (62%)	33 (38%)	0	0
22	AN	127/128 (99%)	91 (72%)	36 (28%)	0	2
23	AO	81/105 (77%)	57 (70%)	24 (30%)	0	2
24	AP	101/118 (86%)	82 (81%)	19 (19%)	1	9
25	AQ	117/119 (98%)	83 (71%)	34 (29%)	0	2
26	AR	94/124 (76%)	70 (74%)	24 (26%)	0	3
27	AS	128/129 (99%)	87 (68%)	41 (32%)	0	2
28	AT	115/116 (99%)	84 (73%)	31 (27%)	0	3
29	AU	100/114 (88%)	71 (71%)	29 (29%)	0	2
30	AV	74/74 (100%)	56 (76%)	18 (24%)	0	4
31	AW	110/111 (99%)	84 (76%)	26 (24%)	1	4
32	AX	119/120 (99%)	97 (82%)	22 (18%)	1	10
33	AY	112/113 (99%)	84 (75%)	28 (25%)	0	3
34	AZ	61/89 (68%)	43 (70%)	18 (30%)	0	2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	BA	192/195 (98%)	153 (80%)	39 (20%)	1	7
36	BB	320/322 (99%)	250 (78%)	70 (22%)	1	6
37	BC	288/288 (100%)	223 (77%)	65 (23%)	1	5
38	BD	243/244 (100%)	196 (81%)	47 (19%)	1	8
39	BE	135/152 (89%)	115 (85%)	20 (15%)	3	15
40	BF	187/204 (92%)	158 (84%)	29 (16%)	2	14
41	BG	177/207 (86%)	138 (78%)	39 (22%)	1	6
42	BH	171/171 (100%)	132 (77%)	39 (23%)	1	5
43	BI	179/186 (96%)	142 (79%)	37 (21%)	1	7
44	BJ	147/149 (99%)	114 (78%)	33 (22%)	1	6
46	BL	154/158 (98%)	124 (80%)	30 (20%)	1	8
47	BM	108/108 (100%)	84 (78%)	24 (22%)	1	6
48	BN	175/175 (100%)	143 (82%)	32 (18%)	1	10
49	BO	323/178 (182%)	267 (83%)	56 (17%)	2	11
50	BP	125/145 (86%)	103 (82%)	22 (18%)	2	11
51	BQ	150/150 (100%)	123 (82%)	27 (18%)	1	10
52	BR	153/153 (100%)	121 (79%)	32 (21%)	1	7
53	BS	156/156 (100%)	123 (79%)	33 (21%)	1	6
54	BT	136/136 (100%)	109 (80%)	27 (20%)	1	8
55	BU	85/106 (80%)	62 (73%)	23 (27%)	0	3
56	BV	104/104 (100%)	96 (92%)	8 (8%)	13	37
57	BW	100/129 (78%)	85 (85%)	15 (15%)	3	15
58	BX	104/117 (89%)	81 (78%)	23 (22%)	1	6
59	BY	109/109 (100%)	85 (78%)	24 (22%)	1	6
60	BZ	115/115 (100%)	89 (77%)	26 (23%)	1	5
61	Ba	118/118 (100%)	95 (80%)	23 (20%)	1	8
62	Bb	46/46 (100%)	35 (76%)	11 (24%)	0	4
63	Bc	84/87 (97%)	68 (81%)	16 (19%)	1	9
64	Bd	94/96 (98%)	73 (78%)	21 (22%)	1	6
65	Be	109/110 (99%)	89 (82%)	20 (18%)	1	10
66	Bf	90/90 (100%)	79 (88%)	11 (12%)	5	20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	Bg	95/102 (93%)	71 (75%)	24 (25%)	0	3
68	Bh	103/104 (99%)	77 (75%)	26 (25%)	0	3
69	Bi	80/81 (99%)	51 (64%)	29 (36%)	0	1
70	Bj	70/70 (100%)	53 (76%)	17 (24%)	0	4
71	Bk	67/68 (98%)	53 (79%)	14 (21%)	1	7
72	Bl	45/45 (100%)	34 (76%)	11 (24%)	0	4
73	Bm	47/116 (40%)	34 (72%)	13 (28%)	0	3
74	Bn	23/23 (100%)	16 (70%)	7 (30%)	0	2
75	Bo	90/90 (100%)	74 (82%)	16 (18%)	2	10
76	Bq	101/254 (40%)	91 (90%)	10 (10%)	8	26
83	CV	481/497 (97%)	450 (94%)	31 (6%)	17	42
All	All	9986/10821 (92%)	7877 (79%)	2109 (21%)	3	6

5 of 2109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
63	Bc	48	THR
66	Bf	81	VAL
63	Bc	40	LYS
83	CV	69	VAL
27	AS	5	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
48	BN	90	ASN
67	Bg	33	GLN
51	BQ	158	HIS
60	BZ	57	HIS
72	Bl	19	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
79	B2	1764/1800 (98%)	545 (30%)	86 (4%)
80	B5	3140/3396 (92%)	741 (23%)	131 (4%)

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
81	B7	120/121 (99%)	18 (15%)	0
82	B8	157/158 (99%)	32 (20%)	3 (1%)
84	CW	74/76 (97%)	23 (31%)	5 (6%)
85	CX	2/3 (66%)	0	0
All	All	5257/5554 (94%)	1359 (25%)	225 (4%)

5 of 1359 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
79	B2	2	A
79	B2	4	C
79	B2	8	U
79	B2	16	G
79	B2	20	G

5 of 225 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
80	B5	908	G
84	CW	20	U
80	B5	1434	G
82	B8	156	U
80	B5	2996	U

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

9 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	$\# Z  > 2$
83	HSO	CV	296	83	6,10,10	2.30	2 (33%)	4,12,12	2.25	2 (50%)
83	HSO	CV	556	83	6,10,10	2.35	2 (33%)	4,12,12	2.02	2 (50%)
83	HSO	CV	541	83	6,10,10	2.66	2 (33%)	4,12,12	1.64	2 (50%)
83	HSO	CV	295	83	6,10,10	2.10	1 (16%)	4,12,12	1.46	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
83	HSO	CV	105	83	6,10,10	2.30	2 (33%)	4,12,12	1.84	2 (50%)
83	HSO	CV	80	83	6,10,10	2.37	2 (33%)	4,12,12	1.35	0
83	HSO	CV	554	83	6,10,10	2.44	2 (33%)	4,12,12	1.50	1 (25%)
83	HSO	CV	229	83	6,10,10	2.01	1 (16%)	4,12,12	1.69	1 (25%)
83	HSO	CV	13	83	6,10,10	2.17	1 (16%)	4,12,12	1.46	1 (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
83	HSO	CV	296	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	556	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	541	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	295	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	105	83	-	3/6/6/6	0/1/1/1
83	HSO	CV	80	83	-	4/6/6/6	0/1/1/1
83	HSO	CV	554	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	229	83	-	2/6/6/6	0/1/1/1
83	HSO	CV	13	83	-	5/6/6/6	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	CV	296	HSO	O-C	-4.65	1.22	1.42
83	CV	556	HSO	O-C	-4.65	1.22	1.42
83	CV	541	HSO	O-C	-4.64	1.22	1.42
83	CV	295	HSO	O-C	-4.63	1.22	1.42
83	CV	13	HSO	O-C	-4.60	1.23	1.42

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	CV	296	HSO	CB-CA-C	-3.71	105.49	112.21
83	CV	556	HSO	CB-CA-C	-2.84	107.07	112.21
83	CV	556	HSO	O-C-CA	2.64	121.97	111.52
83	CV	105	HSO	CB-CA-C	-2.64	107.44	112.21
83	CV	229	HSO	O-C-CA	2.63	121.91	111.52

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	CV	13	HSO	N-CA-CB-CG
83	CV	13	HSO	O-C-CA-CB
83	CV	13	HSO	CA-CB-CG-ND1
83	CV	13	HSO	CA-CB-CG-CD2
83	CV	80	HSO	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 443 ligands modelled in this entry, 232 are monoatomic - leaving 211 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	$\# Z  > 2$
88	OHX	B2	2071	-	0,6,6	-	-	-		
88	OHX	B2	2056	-	0,6,6	-	-	-		
88	OHX	B2	1954	-	0,6,6	-	-	-		
88	OHX	B2	1987	-	0,6,6	-	-	-		
88	OHX	B2	2015	-	0,6,6	-	-	-		
88	OHX	AI	301	-	0,6,6	-	-	-		
88	OHX	B7	219	87	0,6,6	-	-	-		
88	OHX	B2	2001	-	0,6,6	-	-	-		
88	OHX	B2	2080	-	0,6,6	-	-	-		
88	OHX	B7	220	-	0,6,6	-	-	-		
88	OHX	B2	1936	-	0,6,6	-	-	-		
88	OHX	B2	1924	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	B2	1950	-	0,6,6	-	-	-		
88	OHX	B2	2058	-	0,6,6	-	-	-		
88	OHX	B2	1996	-	0,6,6	-	-	-		
89	GCP	CV	602	-	27,34,34	2.12	6 (22%)	34,54,54	2.52	9 (26%)
88	OHX	B2	1923	-	0,6,6	-	-	-		
88	OHX	B2	2039	-	0,6,6	-	-	-		
88	OHX	B2	1971	-	0,6,6	-	-	-		
88	OHX	B2	1914	-	0,6,6	-	-	-		
88	OHX	B2	1990	-	0,6,6	-	-	-		
88	OHX	B2	2025	-	0,6,6	-	-	-		
88	OHX	B2	1926	-	0,6,6	-	-	-		
88	OHX	B2	1945	-	0,6,6	-	-	-		
88	OHX	B2	2053	-	0,6,6	-	-	-		
88	OHX	B2	2074	-	0,6,6	-	-	-		
88	OHX	B2	1974	-	0,6,6	-	-	-		
88	OHX	B2	1927	-	0,6,6	-	-	-		
88	OHX	B2	1938	-	0,6,6	-	-	-		
88	OHX	B2	1977	-	0,6,6	-	-	-		
88	OHX	B2	1952	-	0,6,6	-	-	-		
88	OHX	B2	1913	-	0,6,6	-	-	-		
88	OHX	B2	1928	-	0,6,6	-	-	-		
88	OHX	B2	1998	-	0,6,6	-	-	-		
88	OHX	B2	1917	-	0,6,6	-	-	-		
88	OHX	B2	1972	-	0,6,6	-	-	-		
88	OHX	B7	214	-	0,6,6	-	-	-		
88	OHX	B2	2052	-	0,6,6	-	-	-		
88	OHX	B2	2000	-	0,6,6	-	-	-		
88	OHX	Bn	101	-	0,6,6	-	-	-		
88	OHX	B2	1941	-	0,6,6	-	-	-		
88	OHX	B2	1982	-	0,6,6	-	-	-		
88	OHX	B2	2006	-	0,6,6	-	-	-		
88	OHX	B2	2020	-	0,6,6	-	-	-		
88	OHX	B2	1964	-	0,6,6	-	-	-		
88	OHX	B2	1975	-	0,6,6	-	-	-		
88	OHX	B7	210	-	0,6,6	-	-	-		
88	OHX	B2	2066	-	0,6,6	-	-	-		
88	OHX	B2	1995	-	0,6,6	-	-	-		
88	OHX	B2	2065	-	0,6,6	-	-	-		
88	OHX	B2	2003	-	0,6,6	-	-	-		
88	OHX	B2	1957	-	0,6,6	-	-	-		
88	OHX	B2	2024	-	0,6,6	-	-	-		
88	OHX	B2	2076	-	0,6,6	-	-	-		
88	OHX	B2	1966	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	B2	2007	-	0,6,6	-	-	-		
88	OHX	B2	1956	-	0,6,6	-	-	-		
88	OHX	B2	2059	-	0,6,6	-	-	-		
88	OHX	B2	2069	79	0,6,6	-	-	-		
88	OHX	B2	2032	-	0,6,6	-	-	-		
88	OHX	B2	1953	-	0,6,6	-	-	-		
88	OHX	B2	1919	-	0,6,6	-	-	-		
88	OHX	B2	2057	-	0,6,6	-	-	-		
88	OHX	A3	102	-	0,6,6	-	-	-		
88	OHX	B2	1969	-	0,6,6	-	-	-		
88	OHX	B2	2008	-	0,6,6	-	-	-		
88	OHX	A6	401	-	0,6,6	-	-	-		
88	OHX	B2	2049	-	0,6,6	-	-	-		
88	OHX	B5	3402	-	0,6,6	-	-	-		
88	OHX	B2	1962	-	0,6,6	-	-	-		
88	OHX	B2	1903	-	0,6,6	-	-	-		
88	OHX	B2	1901	-	0,6,6	-	-	-		
88	OHX	B2	1939	-	0,6,6	-	-	-		
88	OHX	B2	2068	-	0,6,6	-	-	-		
88	OHX	B2	1931	-	0,6,6	-	-	-		
88	OHX	B2	1965	-	0,6,6	-	-	-		
88	OHX	B2	2082	-	0,6,6	-	-	-		
88	OHX	B2	1915	-	0,6,6	-	-	-		
88	OHX	B2	1947	-	0,6,6	-	-	-		
88	OHX	B2	2009	-	0,6,6	-	-	-		
88	OHX	B2	2050	-	0,6,6	-	-	-		
88	OHX	B7	206	-	0,6,6	-	-	-		
88	OHX	B2	2060	-	0,6,6	-	-	-		
88	OHX	B2	1993	-	0,6,6	-	-	-		
88	OHX	B2	1904	-	0,6,6	-	-	-		
88	OHX	B2	2062	87,88	0,6,6	-	-	-		
88	OHX	B2	2026	-	0,6,6	-	-	-		
88	OHX	B2	2012	-	0,6,6	-	-	-		
88	OHX	B2	2038	-	0,6,6	-	-	-		
88	OHX	B2	2044	-	0,6,6	-	-	-		
88	OHX	CX	101	-	0,6,6	-	-	-		
88	OHX	B2	1918	88	0,6,6	-	-	-		
88	OHX	B2	1909	88	0,6,6	-	-	-		
88	OHX	B2	2077	-	0,6,6	-	-	-		
88	OHX	AN	201	-	0,6,6	-	-	-		
88	OHX	B2	2043	-	0,6,6	-	-	-		
88	OHX	B2	1906	87	0,6,6	-	-	-		
88	OHX	B2	1970	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	B2	2078	-	0,6,6	-	-	-		
88	OHX	B2	2023	-	0,6,6	-	-	-		
88	OHX	B7	204	-	0,6,6	-	-	-		
88	OHX	B2	2018	-	0,6,6	-	-	-		
88	OHX	B2	1920	-	0,6,6	-	-	-		
88	OHX	B2	1944	-	0,6,6	-	-	-		
88	OHX	B5	3401	-	0,6,6	-	-	-		
88	OHX	B2	1930	-	0,6,6	-	-	-		
88	OHX	B2	1997	-	0,6,6	-	-	-		
88	OHX	B2	1907	-	0,6,6	-	-	-		
88	OHX	B7	212	-	0,6,6	-	-	-		
88	OHX	B2	1916	-	0,6,6	-	-	-		
88	OHX	B2	2048	87	0,6,6	-	-	-		
88	OHX	B2	1992	-	0,6,6	-	-	-		
88	OHX	B7	201	-	0,6,6	-	-	-		
88	OHX	B2	2005	-	0,6,6	-	-	-		
88	OHX	B2	2028	-	0,6,6	-	-	-		
88	OHX	B2	1943	-	0,6,6	-	-	-		
88	OHX	AC	301	-	0,6,6	-	-	-		
88	OHX	B2	1960	-	0,6,6	-	-	-		
88	OHX	B7	205	-	0,6,6	-	-	-		
88	OHX	B2	1999	-	0,6,6	-	-	-		
88	OHX	B7	203	-	0,6,6	-	-	-		
88	OHX	B2	1988	-	0,6,6	-	-	-		
88	OHX	B2	2036	-	0,6,6	-	-	-		
88	OHX	B2	2064	-	0,6,6	-	-	-		
88	OHX	B7	215	-	0,6,6	-	-	-		
88	OHX	B2	1908	-	0,6,6	-	-	-		
88	OHX	B2	1955	-	0,6,6	-	-	-		
88	OHX	B2	1981	-	0,6,6	-	-	-		
88	OHX	B2	1991	-	0,6,6	-	-	-		
88	OHX	B5	3403	-	0,6,6	-	-	-		
88	OHX	B2	1935	-	0,6,6	-	-	-		
88	OHX	B2	2040	-	0,6,6	-	-	-		
88	OHX	B2	1994	-	0,6,6	-	-	-		
88	OHX	B2	1933	-	0,6,6	-	-	-		
88	OHX	B2	1984	-	0,6,6	-	-	-		
88	OHX	B2	2054	-	0,6,6	-	-	-		
88	OHX	B2	2070	-	0,6,6	-	-	-		
88	OHX	B2	2079	-	0,6,6	-	-	-		
88	OHX	B2	2081	-	0,6,6	-	-	-		
88	OHX	B2	1973	-	0,6,6	-	-	-		
88	OHX	B2	2061	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	B2	1980	-	0,6,6	-	-	-		
88	OHX	B2	1967	-	0,6,6	-	-	-		
88	OHX	B2	1986	-	0,6,6	-	-	-		
88	OHX	B2	1946	-	0,6,6	-	-	-		
88	OHX	B2	2035	-	0,6,6	-	-	-		
88	OHX	B2	1949	-	0,6,6	-	-	-		
88	OHX	B2	2072	-	0,6,6	-	-	-		
88	OHX	B2	2047	-	0,6,6	-	-	-		
88	OHX	B2	2073	-	0,6,6	-	-	-		
88	OHX	B2	2030	-	0,6,6	-	-	-		
88	OHX	B2	1932	-	0,6,6	-	-	-		
88	OHX	AP	201	-	0,6,6	-	-	-		
88	OHX	B2	1905	-	0,6,6	-	-	-		
88	OHX	B2	2004	-	0,6,6	-	-	-		
88	OHX	B2	1961	-	0,6,6	-	-	-		
88	OHX	B2	2021	-	0,6,6	-	-	-		
88	OHX	B2	2031	-	0,6,6	-	-	-		
88	OHX	B2	2042	-	0,6,6	-	-	-		
88	OHX	B7	202	-	0,6,6	-	-	-		
88	OHX	B2	1951	-	0,6,6	-	-	-		
88	OHX	B2	2027	-	0,6,6	-	-	-		
88	OHX	B2	1959	-	0,6,6	-	-	-		
88	OHX	B2	2067	-	0,6,6	-	-	-		
88	OHX	B2	1979	-	0,6,6	-	-	-		
88	OHX	CV	601	-	0,6,6	-	-	-		
88	OHX	B2	2063	-	0,6,6	-	-	-		
88	OHX	AL	201	-	0,6,6	-	-	-		
88	OHX	B2	1922	-	0,6,6	-	-	-		
88	OHX	B2	2013	-	0,6,6	-	-	-		
88	OHX	B2	2033	-	0,6,6	-	-	-		
88	OHX	B2	2022	-	0,6,6	-	-	-		
88	OHX	B2	1921	-	0,6,6	-	-	-		
88	OHX	B2	2037	-	0,6,6	-	-	-		
88	OHX	B2	1963	-	0,6,6	-	-	-		
88	OHX	B2	2041	-	0,6,6	-	-	-		
88	OHX	B2	2075	-	0,6,6	-	-	-		
88	OHX	B2	2017	-	0,6,6	-	-	-		
88	OHX	B7	221	-	0,6,6	-	-	-		
88	OHX	B2	1912	-	0,6,6	-	-	-		
88	OHX	B2	2011	-	0,6,6	-	-	-		
88	OHX	B2	2051	-	0,6,6	-	-	-		
88	OHX	B2	1958	-	0,6,6	-	-	-		
88	OHX	B2	2034	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
88	OHX	B2	2019	-	0,6,6	-	-	-		
88	OHX	B2	2014	-	0,6,6	-	-	-		
88	OHX	B2	2046	-	0,6,6	-	-	-		
88	OHX	B2	2055	-	0,6,6	-	-	-		
88	OHX	B2	1985	-	0,6,6	-	-	-		
88	OHX	B2	1910	-	0,6,6	-	-	-		
88	OHX	B2	2045	-	0,6,6	-	-	-		
88	OHX	B2	1989	-	0,6,6	-	-	-		
88	OHX	B2	1968	-	0,6,6	-	-	-		
88	OHX	B2	1978	-	0,6,6	-	-	-		
88	OHX	B2	1902	-	0,6,6	-	-	-		
88	OHX	B2	1983	-	0,6,6	-	-	-		
88	OHX	BR	201	-	0,6,6	-	-	-		
88	OHX	B2	1925	-	0,6,6	-	-	-		
88	OHX	B2	2002	-	0,6,6	-	-	-		
88	OHX	B2	1934	-	0,6,6	-	-	-		
88	OHX	B2	1940	-	0,6,6	-	-	-		
88	OHX	B2	2029	88	0,6,6	-	-	-		
88	OHX	B2	1911	-	0,6,6	-	-	-		
88	OHX	B2	2016	-	0,6,6	-	-	-		
88	OHX	B2	1942	-	0,6,6	-	-	-		
88	OHX	B2	1976	-	0,6,6	-	-	-		
88	OHX	B2	2010	-	0,6,6	-	-	-		
88	OHX	B2	1929	-	0,6,6	-	-	-		
88	OHX	AI	302	-	0,6,6	-	-	-		
88	OHX	B2	1937	-	0,6,6	-	-	-		
88	OHX	B2	1948	-	0,6,6	-	-	-		

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
89	GCP	CV	602	-	-	1/15/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	CV	602	GCP	C2'-C1'	-6.48	1.43	1.53
89	CV	602	GCP	C6-N1	5.32	1.42	1.33
89	CV	602	GCP	C4-N3	2.81	1.40	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	CV	602	GCP	C8-N7	-2.35	1.30	1.34
89	CV	602	GCP	PB-O3A	-2.31	1.55	1.58

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	CV	602	GCP	O3G-PG-C3B	-7.36	88.55	106.40
89	CV	602	GCP	C5-C6-N1	-7.05	113.79	123.43
89	CV	602	GCP	C2-N1-C6	5.19	124.18	115.93
89	CV	602	GCP	N3-C2-N1	-3.57	122.46	127.22
89	CV	602	GCP	C4-C5-C6	-2.97	117.96	120.80

There are no chirality outliers.

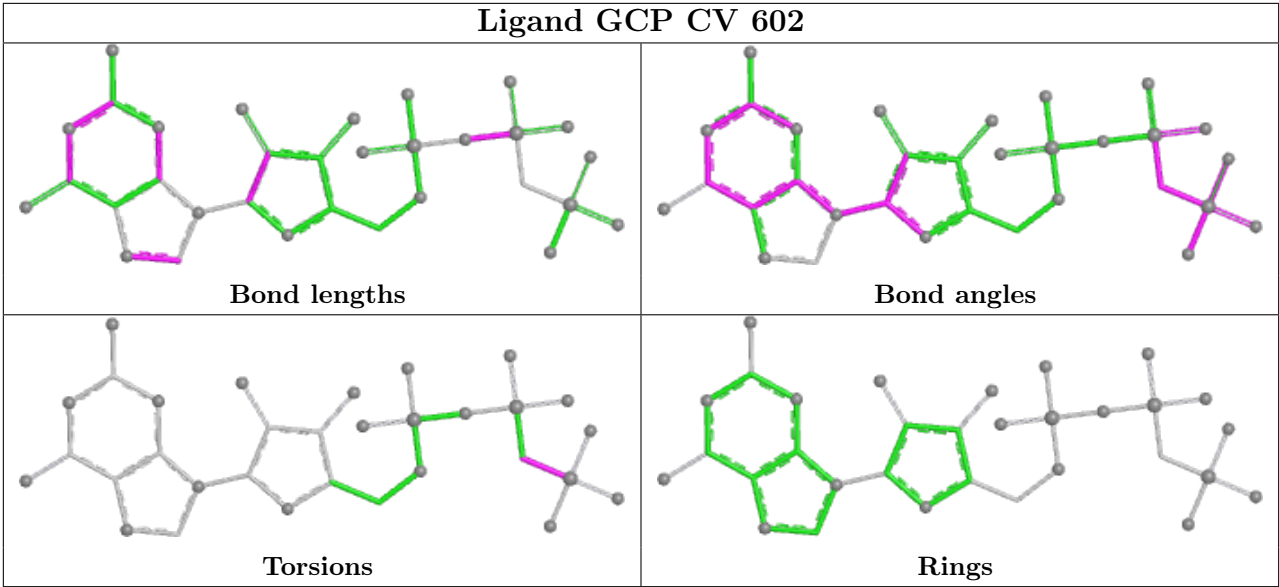
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	CV	602	GCP	PB-C3B-PG-O1G

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
80	B5	1
84	CW	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B5	1285:G	O3'	1286:A	P	6.77
1	CW	33:U	O3'	34:C	P	4.25

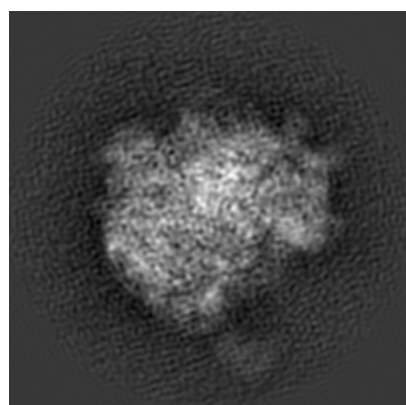
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2422. These allow visual inspection of the internal detail of the map and identification of artifacts.

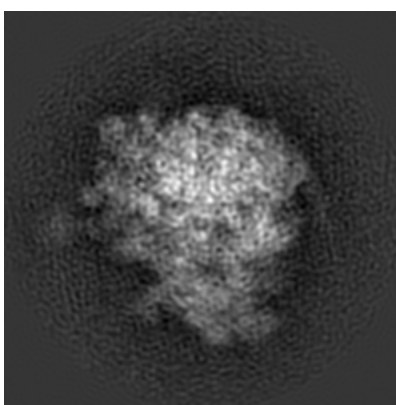
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

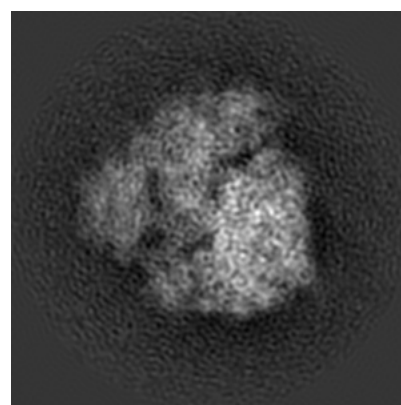
#### 6.1.1 Primary map



X



Y

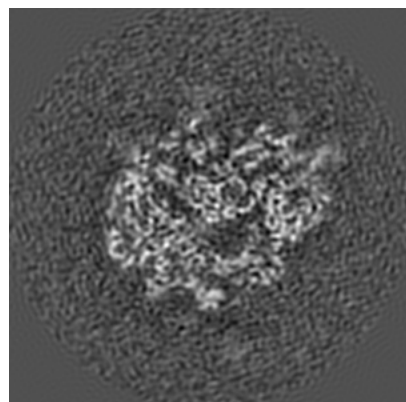


Z

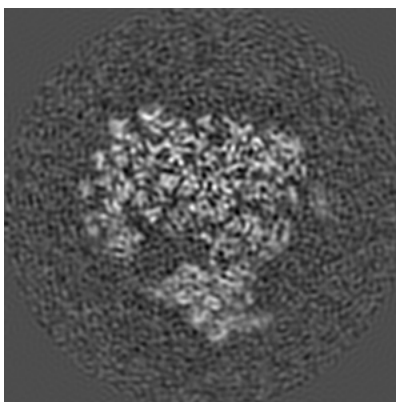
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

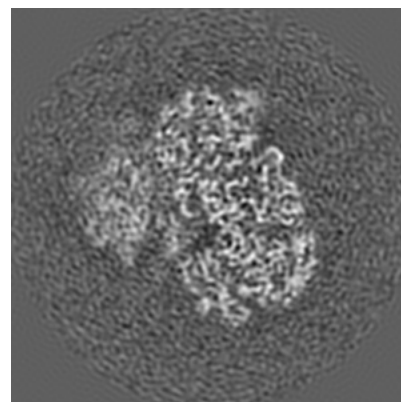
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

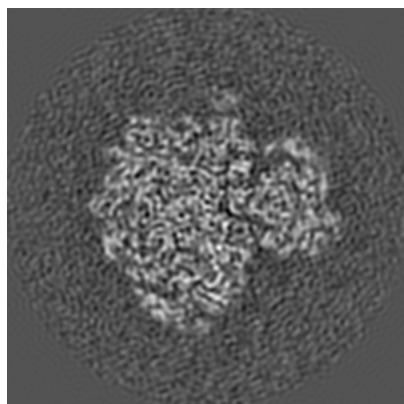


Z Index: 120

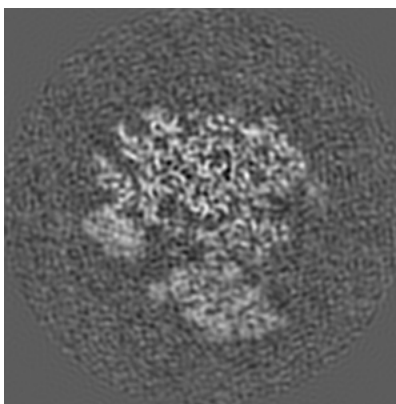
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

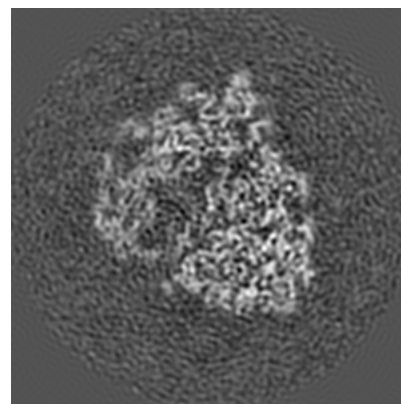
### 6.3.1 Primary map



X Index: 133



Y Index: 124



Z Index: 113

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

## 6.4 Orthogonal surface views [i](#)

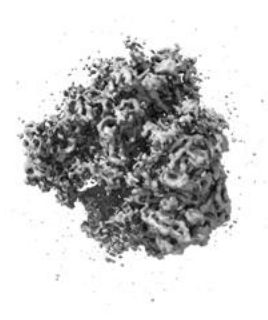
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

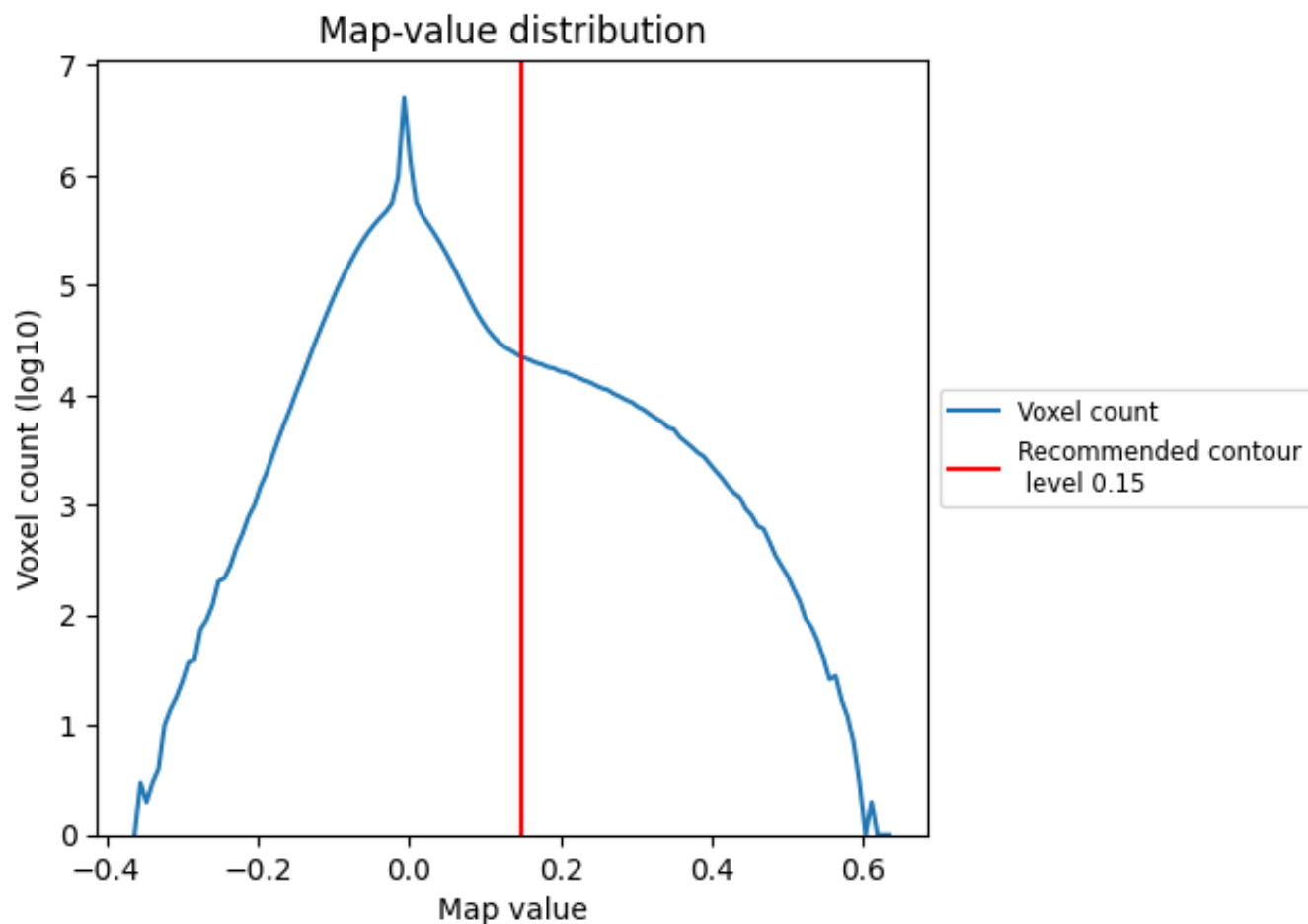
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

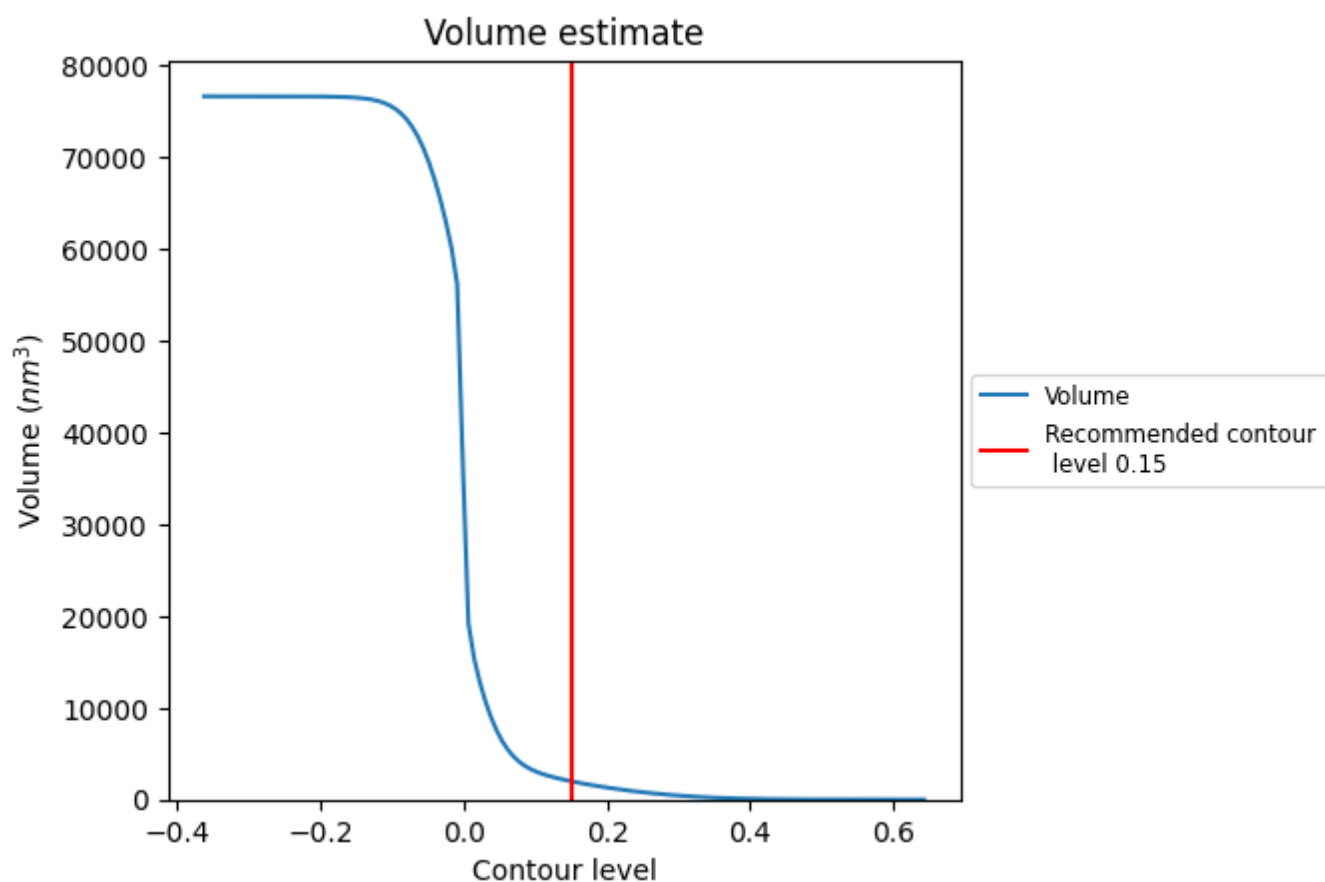
### 7.1 Map-value distribution [i](#)



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



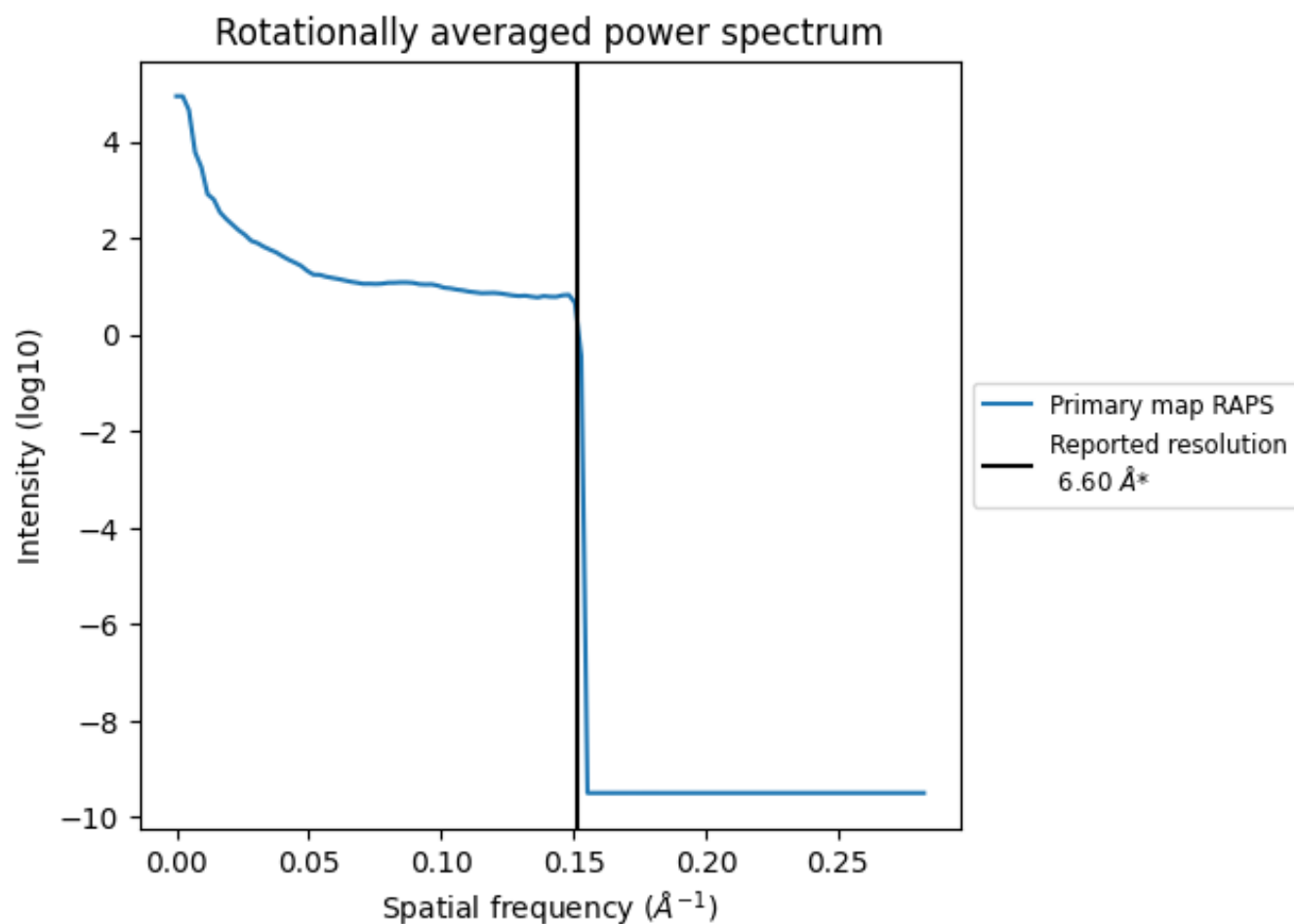
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1997 nm<sup>3</sup>; this corresponds to an approximate mass of 1804 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.152  $\text{\AA}^{-1}$

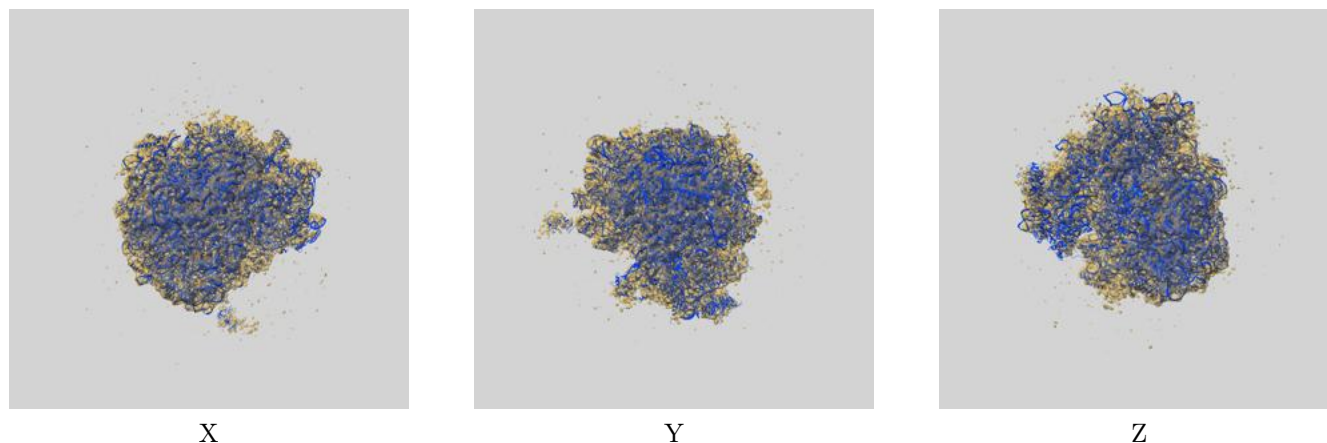
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

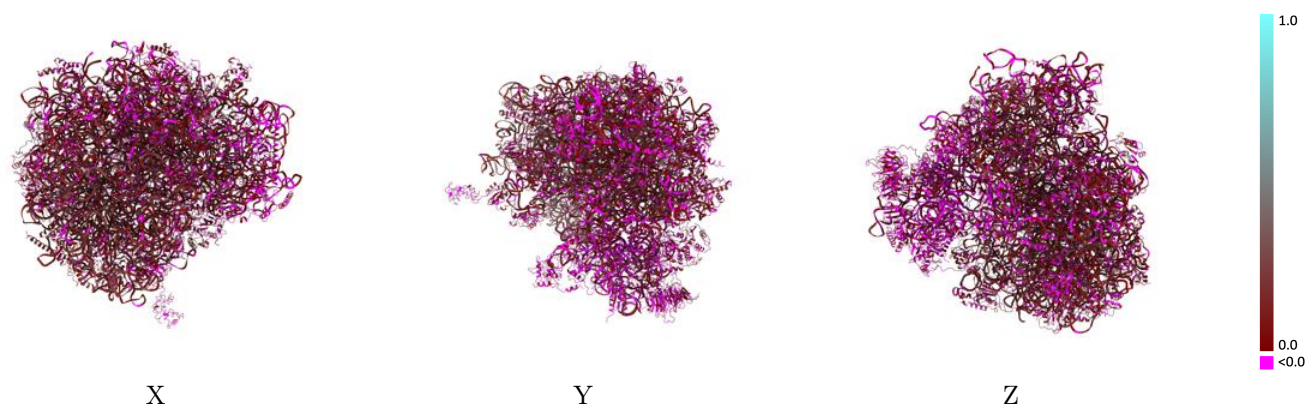
This section contains information regarding the fit between EMDB map EMD-2422 and PDB model 4V8Z. Per-residue inclusion information can be found in section [3](#) on page [35](#).

### 9.1 Map-model overlay [i](#)



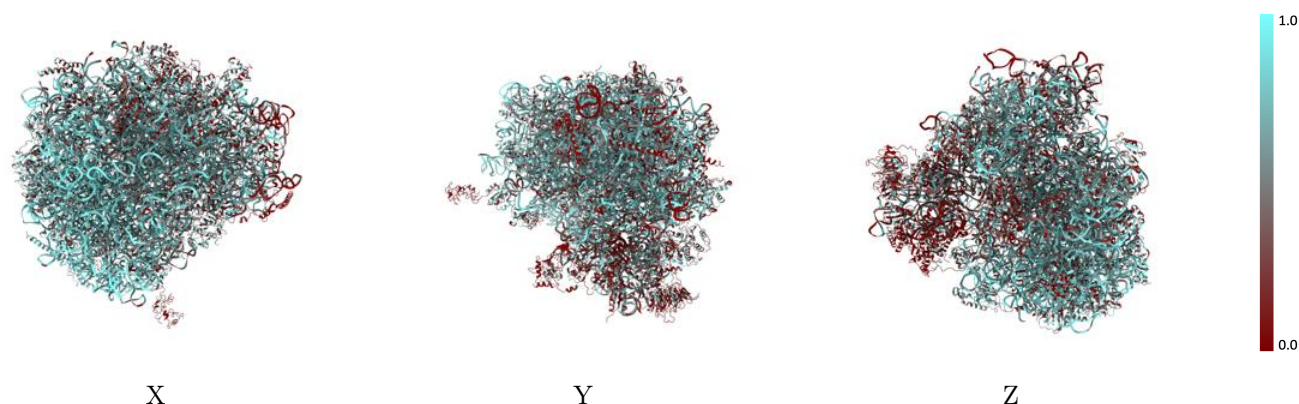
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



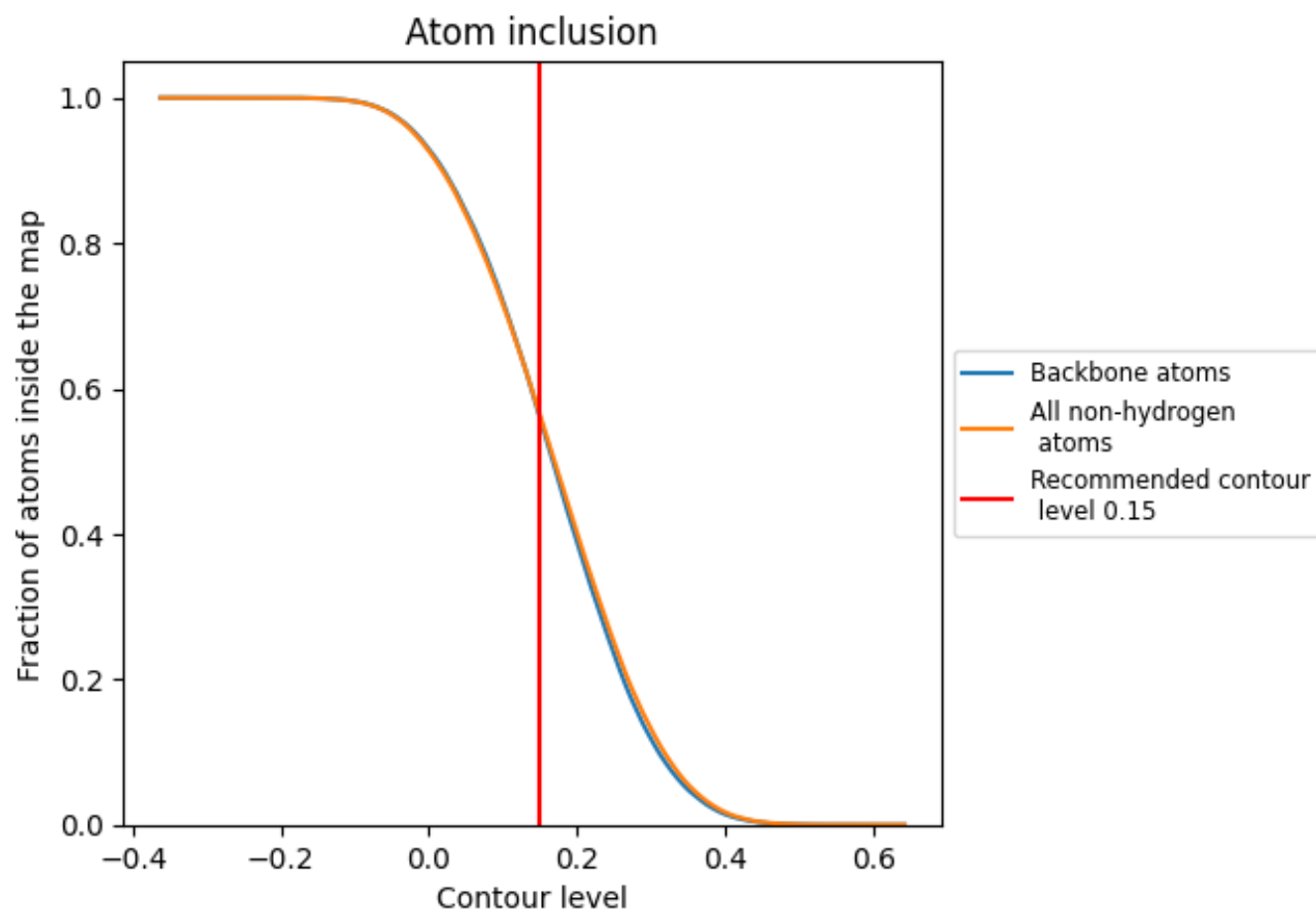
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5647	 0.1080
A0	 0.3315	 -0.0020
A1	 0.4120	 0.0760
A2	 0.1153	 -0.0000
A3	 0.3687	 0.0080
A4	 0.3791	 0.0510
A5	 0.0512	 -0.0100
A6	 0.2510	 0.0200
A7	 0.1377	 0.0190
AA	 0.4135	 0.0530
AB	 0.2238	 0.0100
AC	 0.3921	 0.0420
AD	 0.2866	 -0.0120
AE	 0.4218	 0.0540
AF	 0.1330	 -0.0030
AG	 0.3766	 0.0160
AH	 0.5544	 0.1420
AI	 0.4252	 0.0370
AJ	 0.4317	 0.0580
AK	 0.2863	 -0.0190
AL	 0.4349	 0.0800
AM	 0.2034	 0.0190
AN	 0.4652	 0.1190
AO	 0.3701	 -0.0040
AP	 0.2320	 0.0100
AQ	 0.3114	 0.0080
AR	 0.3944	 0.0960
AS	 0.2199	 0.0110
AT	 0.3006	 0.0260
AU	 0.2414	 0.0090
AV	 0.4277	 0.0470
AW	 0.4880	 0.1130
AX	 0.4388	 0.1160
AY	 0.4467	 0.0390
AZ	 0.0530	 0.0150



*Continued on next page...*



















*Continued from previous page...*

Chain	Atom inclusion	Q-score
B2	 0.5483	 0.0840
B5	 0.7489	 0.1610
B7	 0.8476	 0.1770
B8	 0.7513	 0.1470
BA	 0.3855	 0.0620
BB	 0.4890	 0.1010
BC	 0.5558	 0.1160
BD	 0.5696	 0.1270
BE	 0.5990	 0.1360
BF	 0.5954	 0.1490
BG	 0.4714	 0.0510
BH	 0.5436	 0.1110
BI	 0.5398	 0.1340
BJ	 0.5392	 0.1260
BK	 0.4409	 0.0840
BL	 0.4926	 0.0910
BM	 0.6357	 0.1480
BN	 0.4465	 0.0670
BO	 0.5482	 0.1400
BP	 0.5214	 0.0980
BQ	 0.5333	 0.1170
BR	 0.3288	 0.0290
BS	 0.5673	 0.1260
BT	 0.5298	 0.1380
BU	 0.4254	 0.0610
BV	 0.4433	 0.1270
BW	 0.2184	 0.0370
BX	 0.3938	 0.0650
BY	 0.5559	 0.0940
BZ	 0.4556	 0.0410
Ba	 0.4825	 0.1010
Bb	 0.4934	 0.1510
Bc	 0.4106	 0.0580
Bd	 0.4877	 0.0570
Be	 0.5372	 0.1380
Bf	 0.5505	 0.1240
Bg	 0.4007	 0.0400
Bh	 0.4973	 0.1060
Bi	 0.4664	 0.0640
Bj	 0.4787	 0.0670
Bk	 0.4286	 0.0610
Bl	 0.4169	 0.0610

*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
Bm	 0.4851	 0.1270
Bn	 0.1781	 0.0130
Bo	 0.4662	 0.1040
Bq	 0.4815	 0.1050
Br	 0.1356	 0.0410
Bs	 0.1169	 0.0360
CV	 0.4618	 0.1390
CW	 0.5950	 0.2240
CX	 0.5797	 0.1470