



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:24 PM UTC

PDB ID : 4V7B / pdb_00004v7b
EMDB ID : EMD-5775
Title : Visualization of two tRNAs trapped in transit during EF-G-mediated translocation
Authors : Ramrath, D.J.F.; Lancaster, L.; Sprink, T.; Mielke, T.; Loerke, J.; Noller, H.F.; Spahn, C.M.T.
Deposited on : 2013-10-27
Resolution : 6.80 Å (reported)
Based on initial model : 4KIY

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

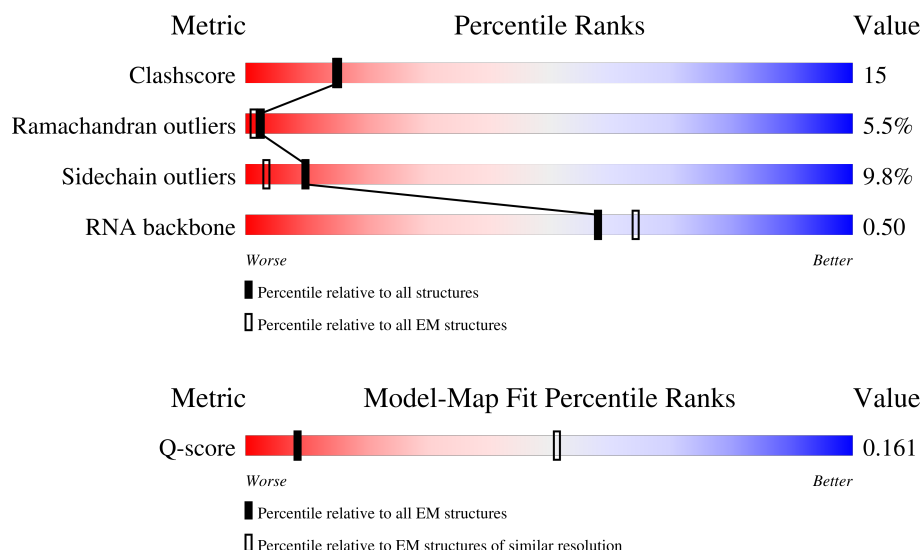
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 6.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	503 (6.30 - 7.30)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	
2	AB	241	

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Mol	Chain	Length	Quality of chain
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	77	
23	AW	77	
24	AX	19	
25	AY	704	
26	BB	120	
27	BC	273	

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Mol	Chain	Length	Quality of chain
28	BA	2904	
29	BD	209	
30	BE	201	
31	BF	179	
32	BG	177	
33	BH	50	
34	BI	142	
35	BJ	142	
36	BK	123	
37	BL	144	
38	BM	136	
39	BN	127	
40	BO	117	
41	BP	115	
42	BQ	118	
43	BR	103	
44	BS	110	
45	BT	100	
46	BU	104	
47	BV	94	
48	BW	85	
49	BX	78	
50	BY	63	
51	BZ	59	
52	B0	57	

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Mol	Chain	Length	Quality of chain
53	B1	55	
54	B2	46	
55	B3	65	
56	B4	38	
57	B5	165	
58	B6	121	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	FUA	AY	801	-	-	X	-
60	GDP	AY	802	-	-	X	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 150958 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1533	Total	C	N	O	P	0	0
			32895	14671	6036	10655	1533		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	102	Total	C	N	O	S	0	0
			832	525	150	150	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called modified formyl-methionine specific initiator transfer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 23 is a RNA chain called formyl-methionine specific initiator transfer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0
			1635	732	291	536	76		

- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	19	Total	C	N	O	P	0	0
			416	187	86	124	19		

- Molecule 25 is a protein called Elongation Factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	671	Total	C	N	O	S	0	0
			5194	3278	895	998	23		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BC	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	2854	Total	C	N	O	P	0	0
			61274	27334	11279	19807	2854		

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BH	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 34 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BO	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BT	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	BU	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

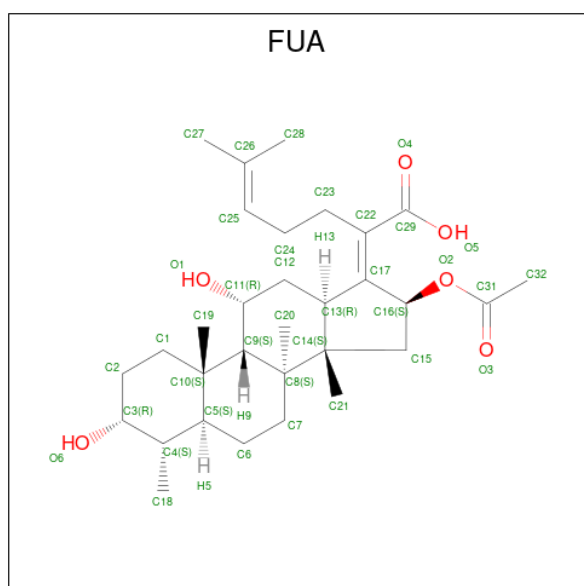
- Molecule 57 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B5	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

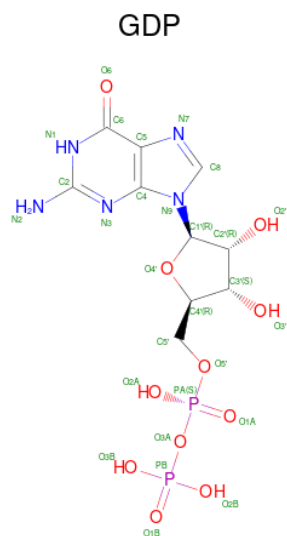
Mol	Chain	Residues	Atoms					AltConf	Trace
58	B6	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 59 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms			AltConf
59	AY	1	Total	C	O	0
			37	31	6	

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

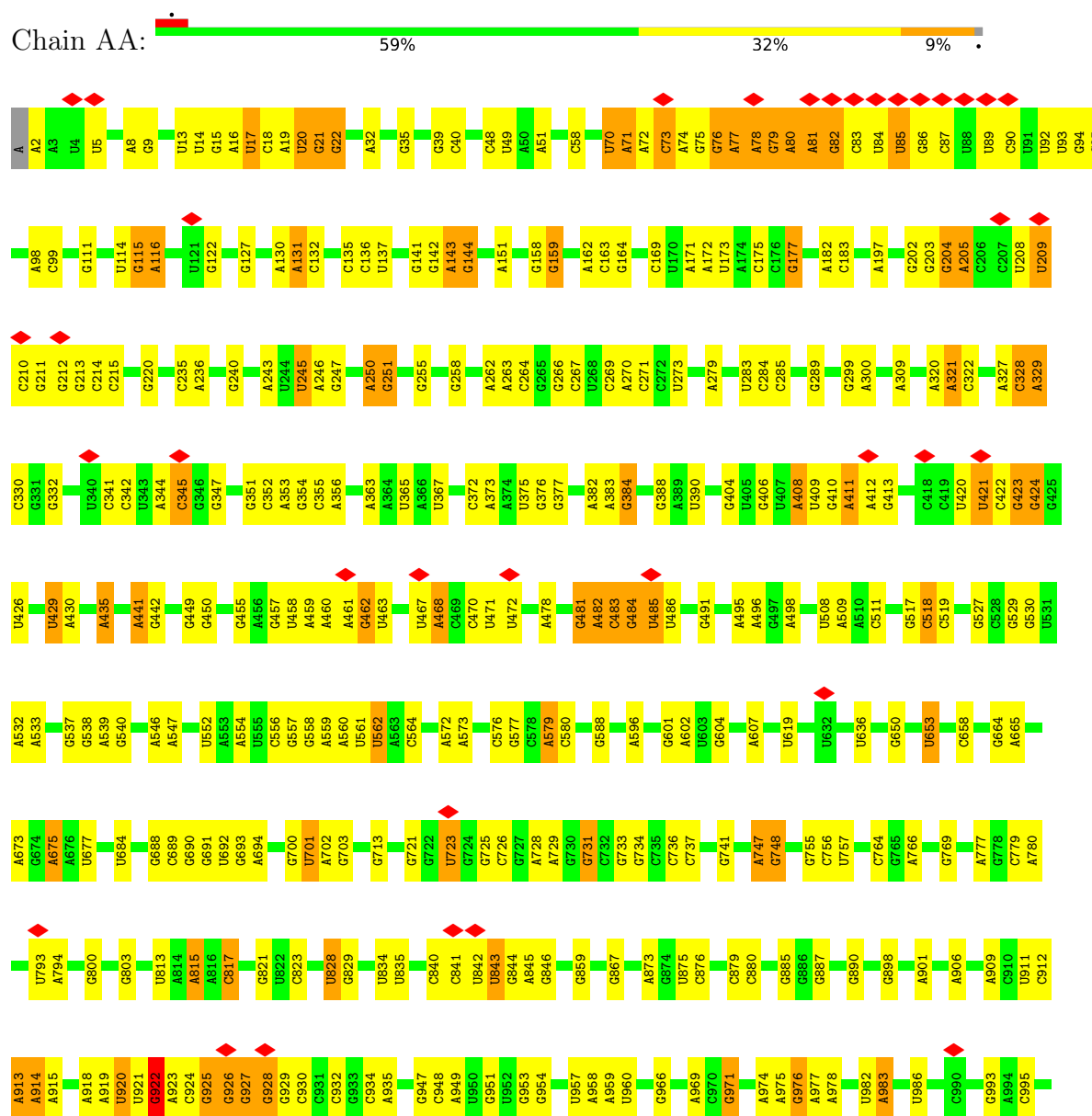


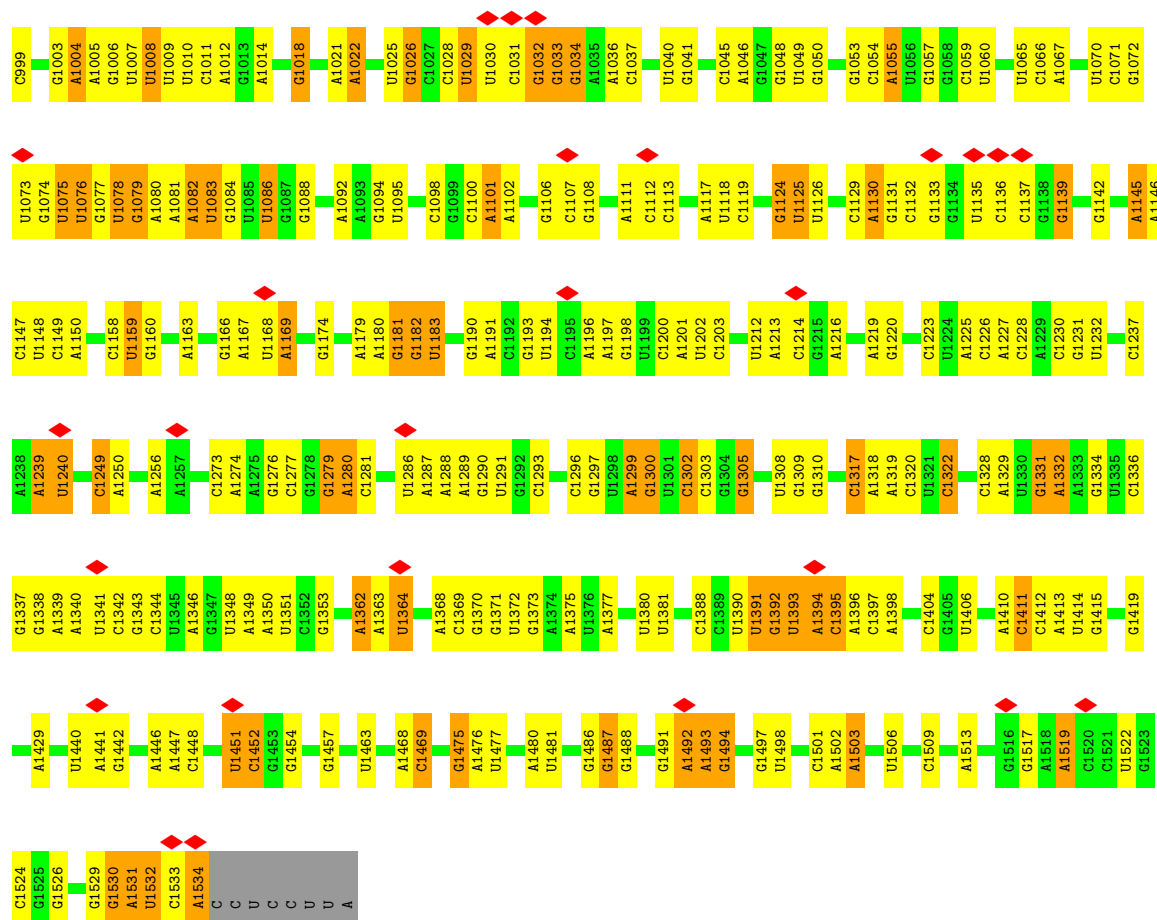
Mol	Chain	Residues	Atoms					AltConf
60	AY	1	Total	C	N	O	P	0
			28	10	5	11	2	

3 Residue-property plots

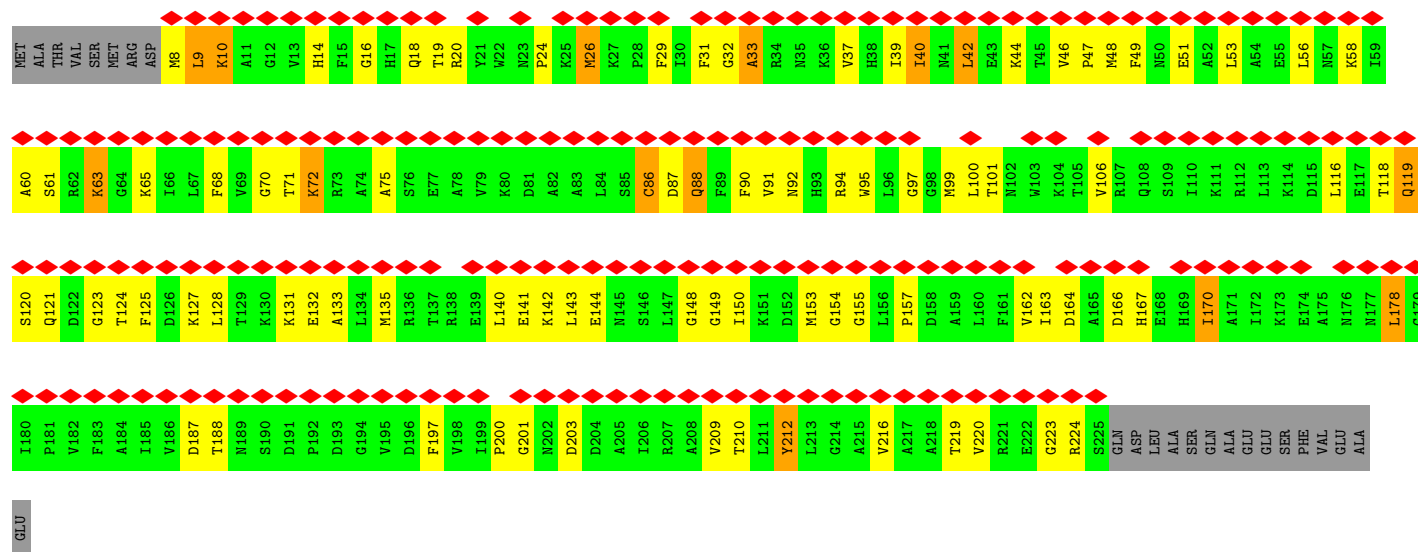
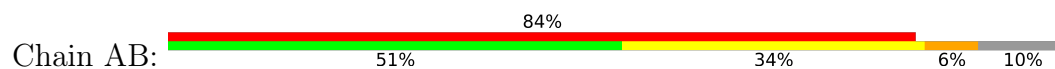
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S ribosomal RNA



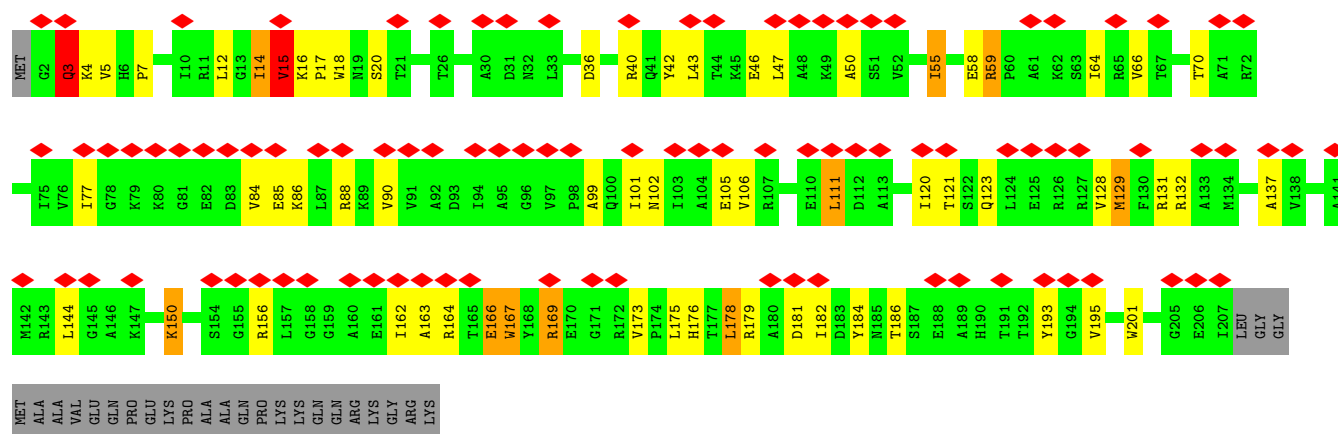


• Molecule 2: 30S ribosomal protein S2



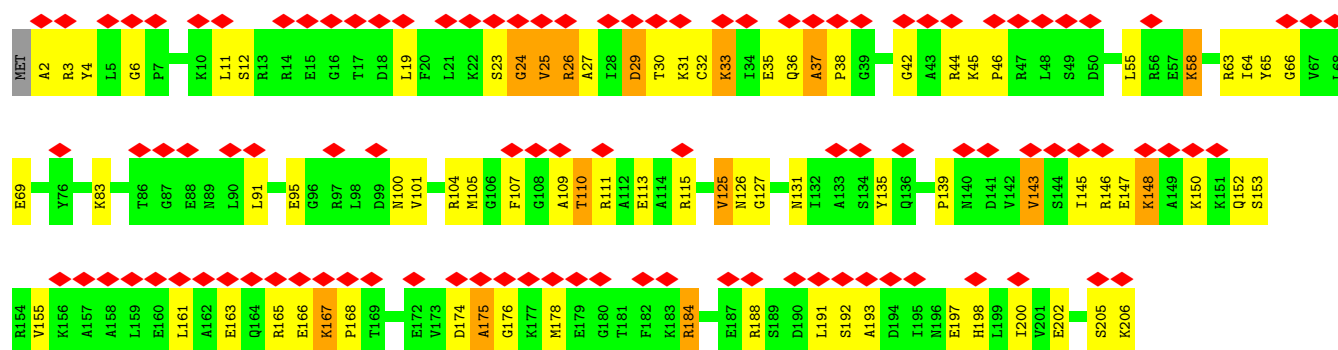
• Molecule 3: 30S ribosomal protein S3

Chain AC: 



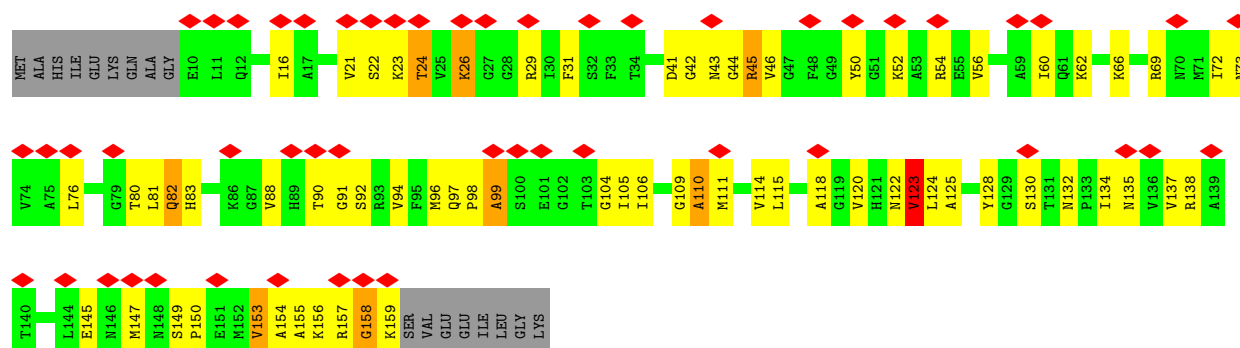
• Molecule 4: 30S ribosomal protein S4

Chain AD: 



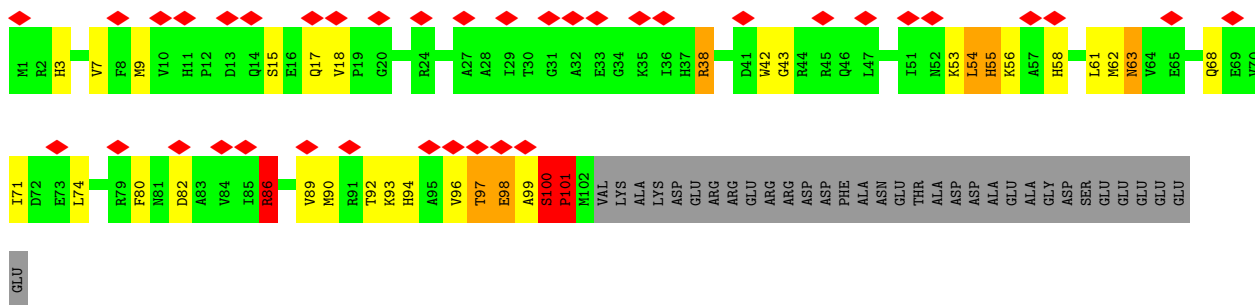
• Molecule 5: 30S ribosomal protein S5

Chain AE: 

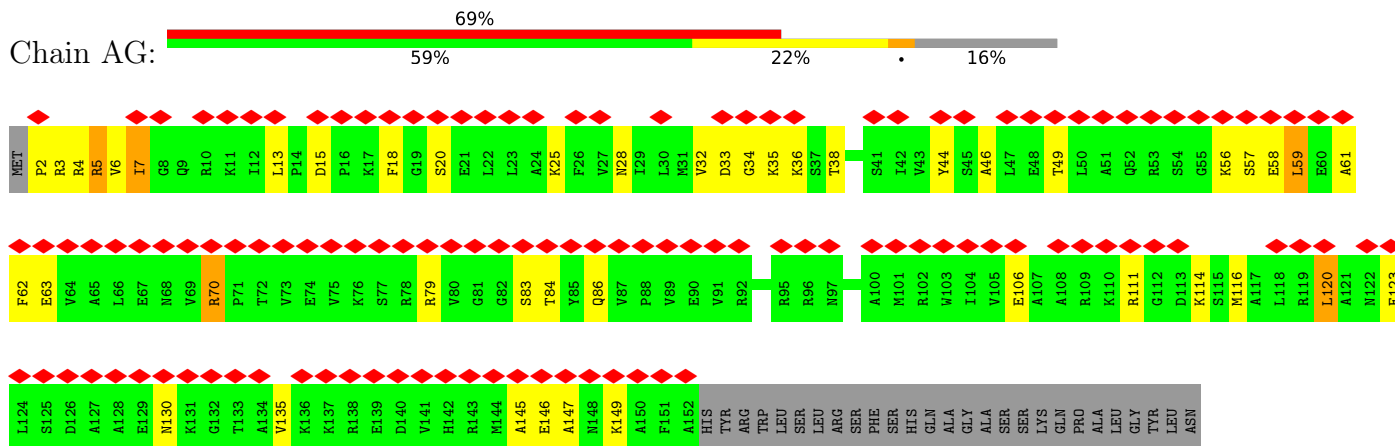


• Molecule 6: 30S ribosomal protein S6

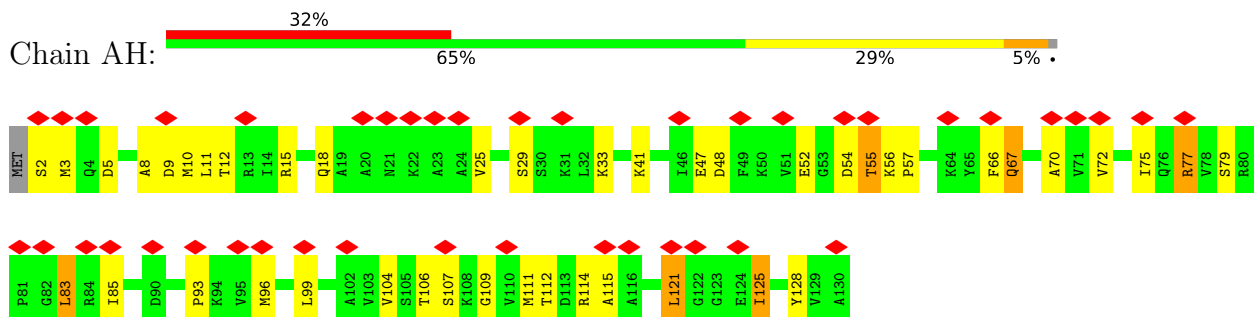
Chain AF: 



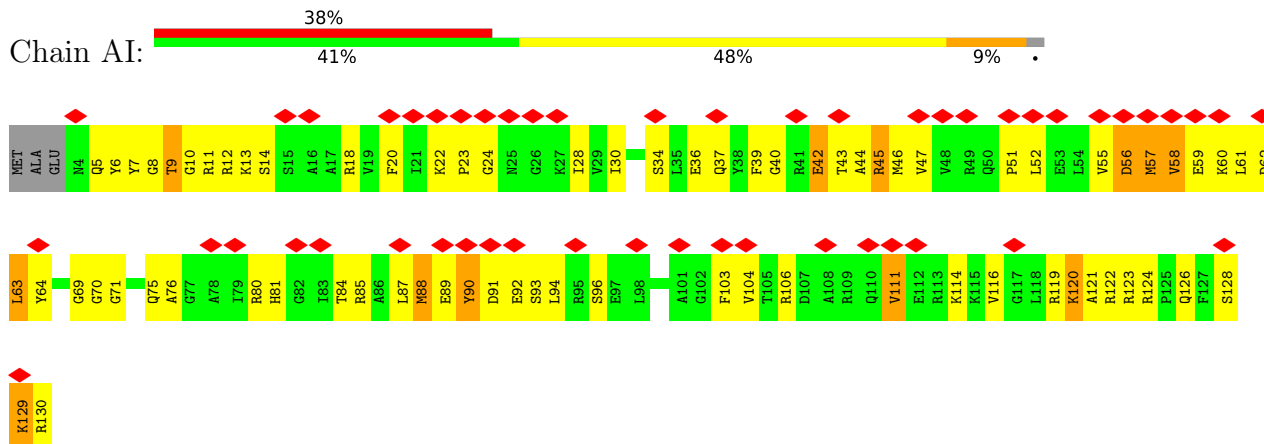
• Molecule 7: 30S ribosomal protein S7



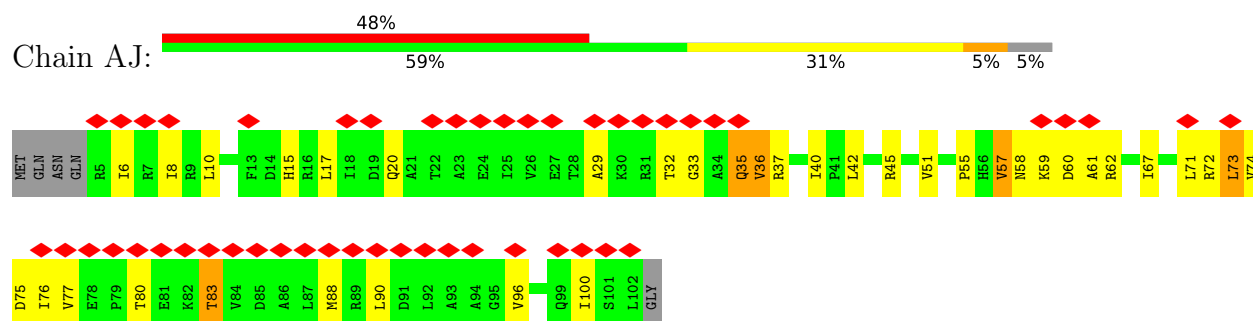
• Molecule 8: 30S ribosomal protein S8



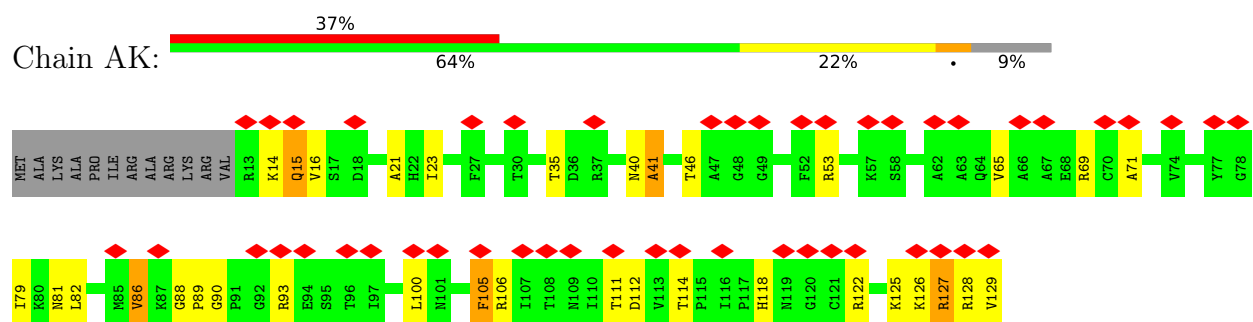
• Molecule 9: 30S ribosomal protein S9



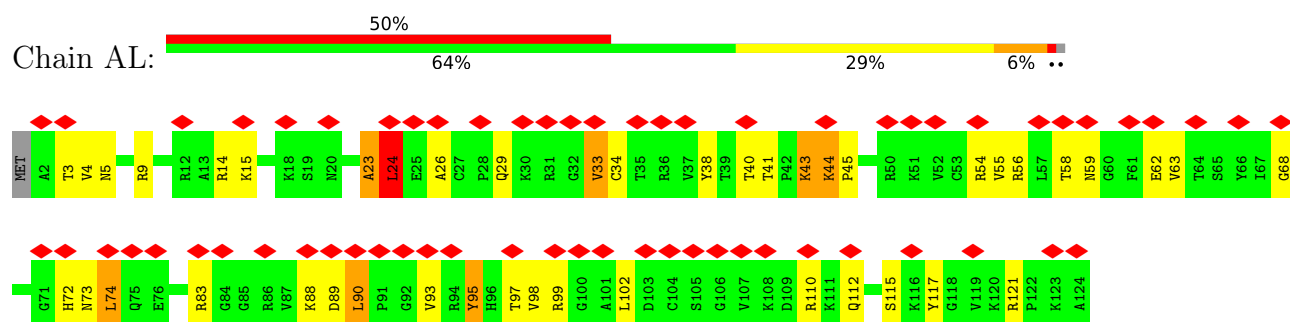
- Molecule 10: 30S ribosomal protein S10



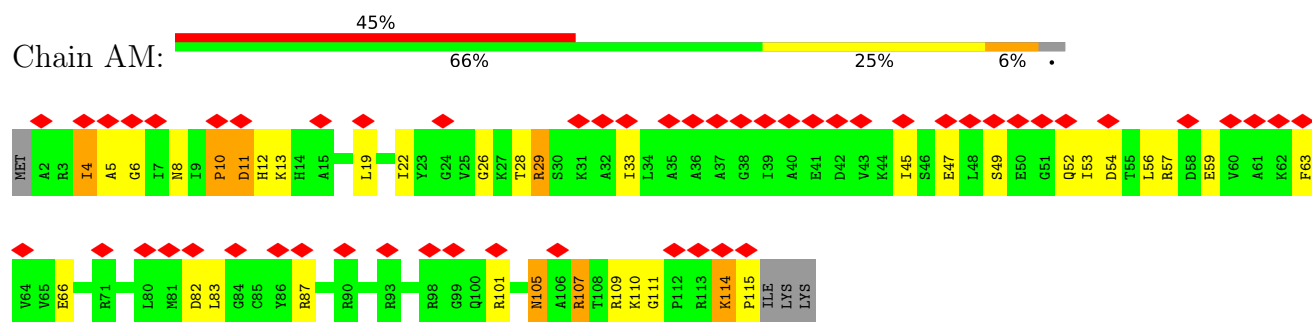
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

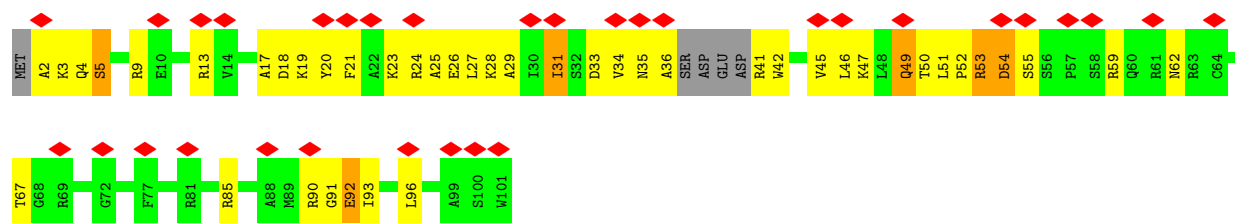


- Molecule 13: 30S ribosomal protein S13

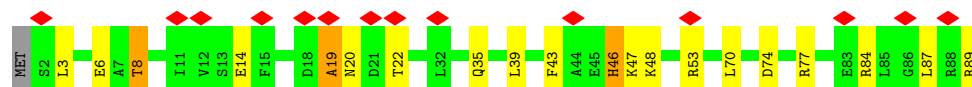
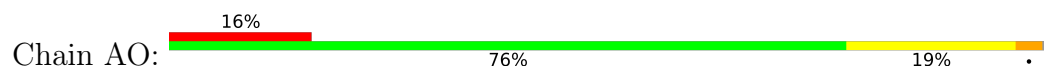


- Molecule 14: 30S ribosomal protein S14

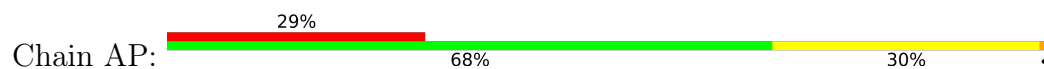




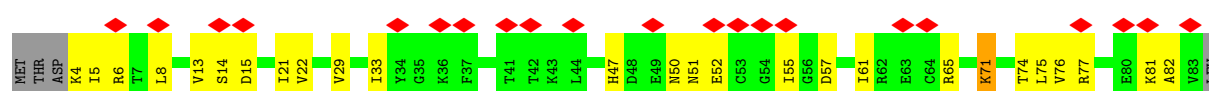
- Molecule 15: 30S ribosomal protein S15



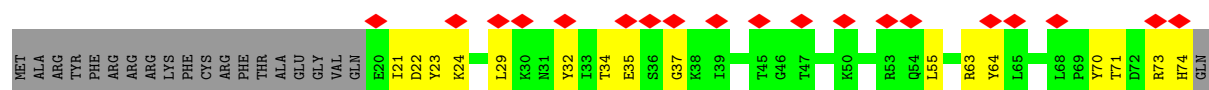
- Molecule 16: 30S ribosomal protein S16



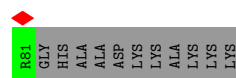
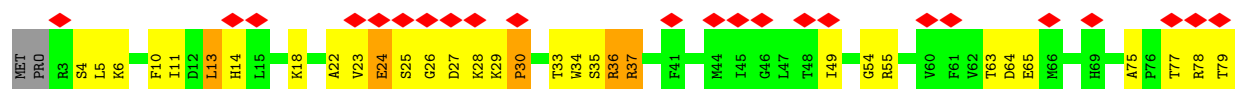
- Molecule 17: 30S ribosomal protein S17



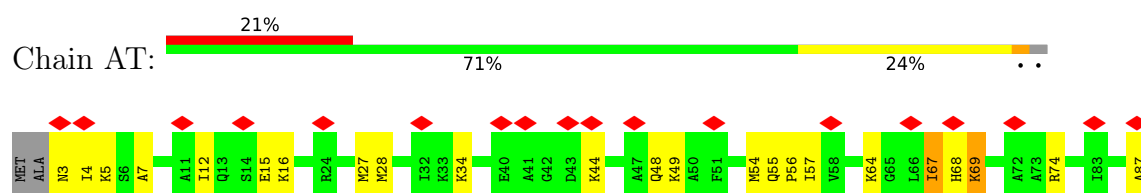
- Molecule 18: 30S ribosomal protein S18



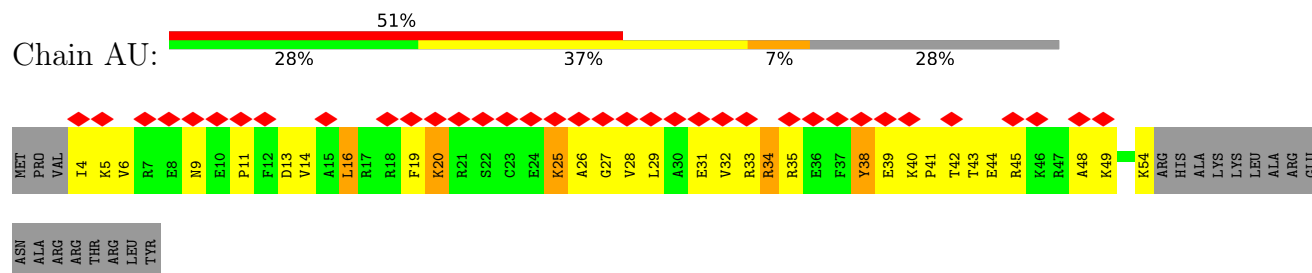
- Molecule 19: 30S ribosomal protein S19



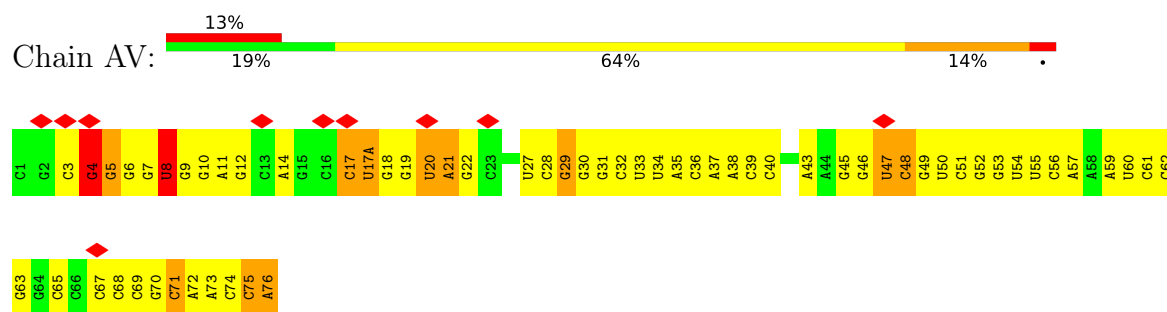
- Molecule 20: 30S ribosomal protein S20



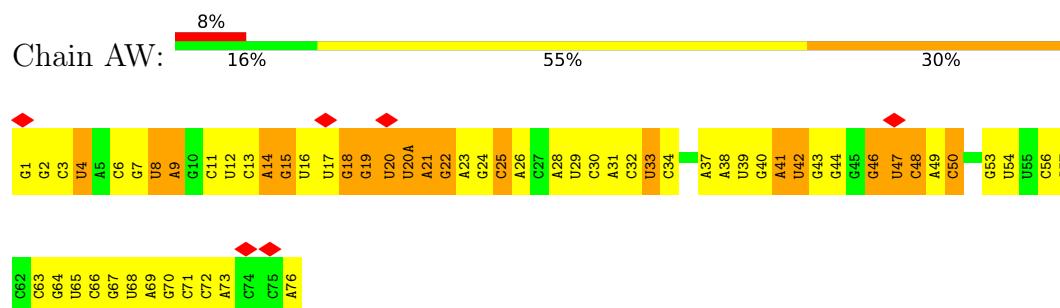
- Molecule 21: 30S ribosomal protein S21



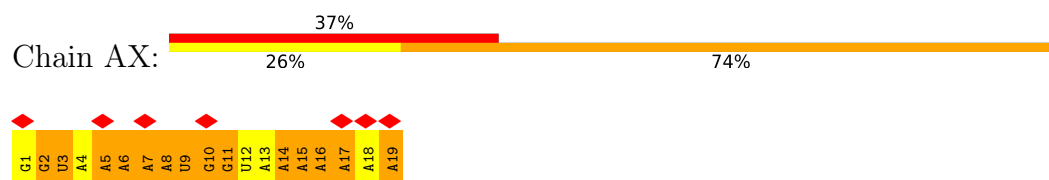
- Molecule 22: modified formyl-methionine specific initiator transfer RNA



- Molecule 23: formyl-methionine specific initiator transfer RNA

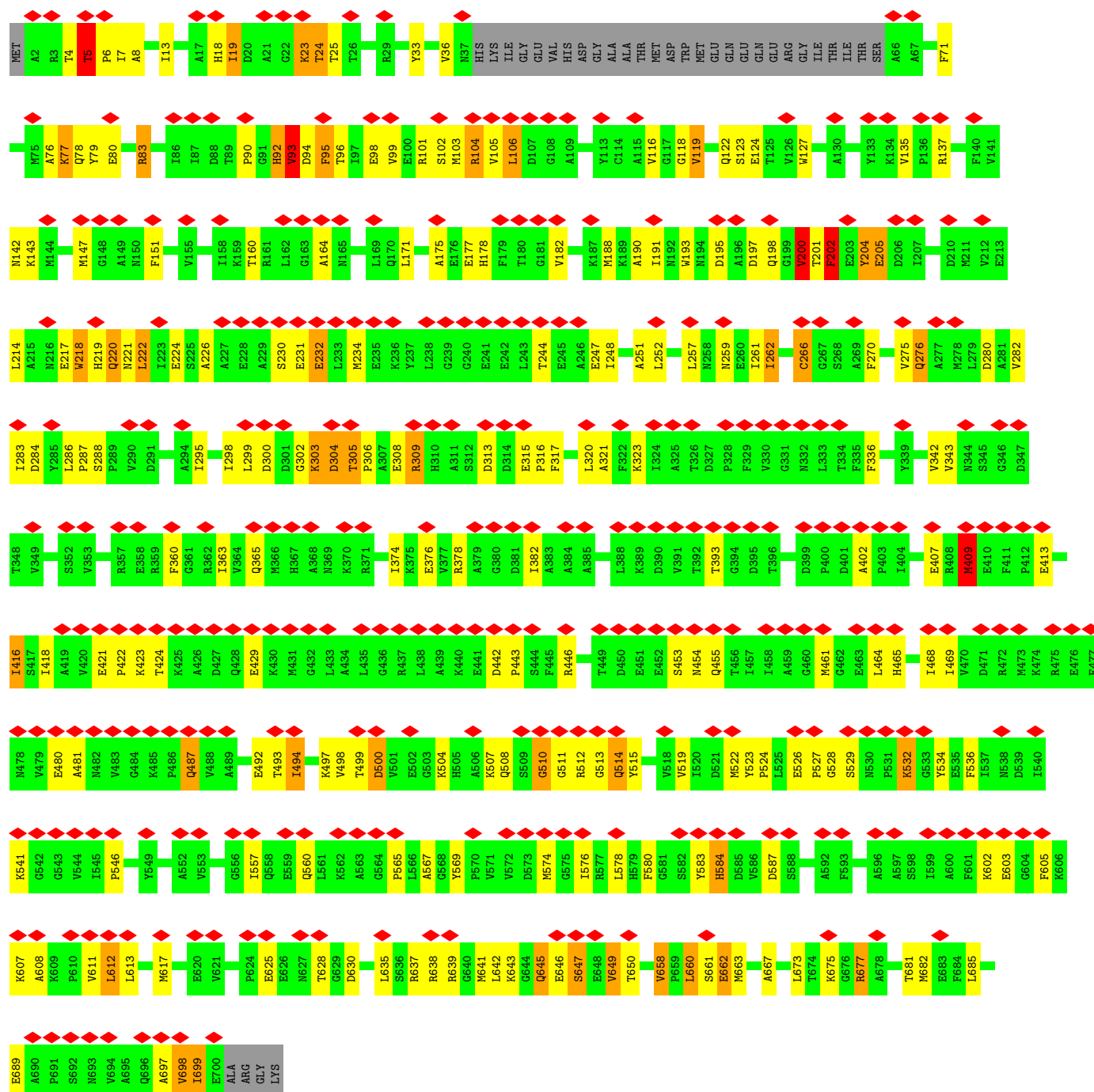


- Molecule 24: messenger RNA



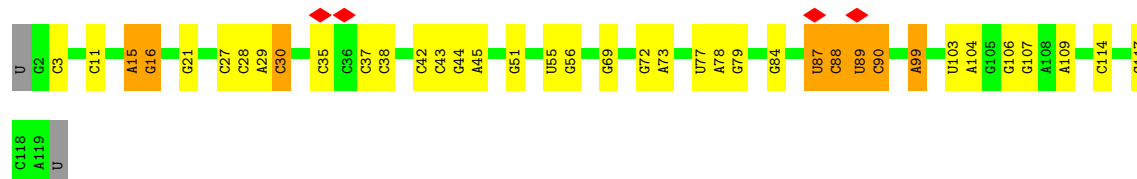
- Molecule 25: Elongation Factor G



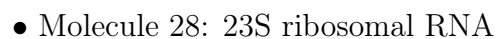


• Molecule 26: 5S ribosomal RNA

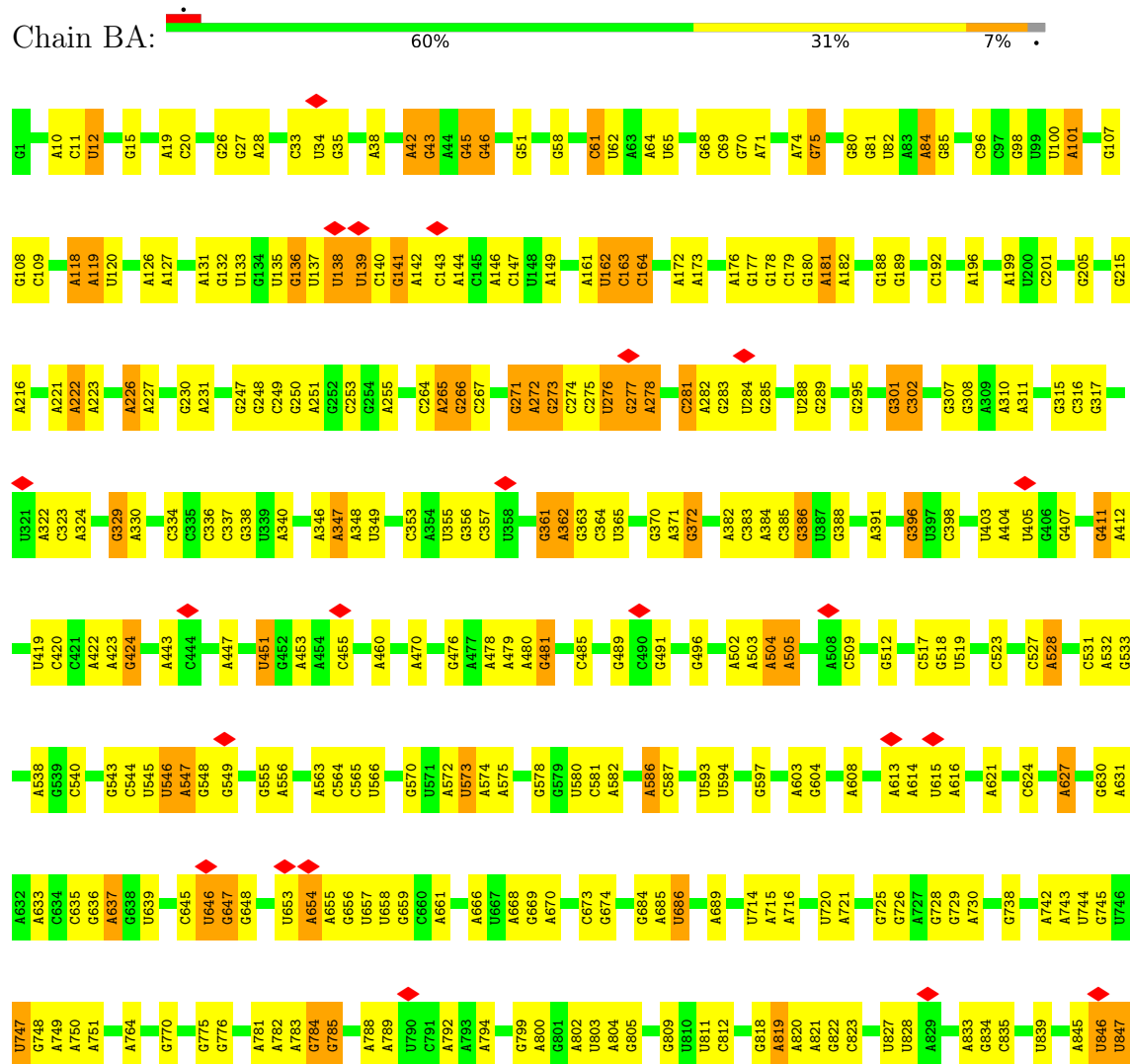
Chain BB: 67% 25% 7% .



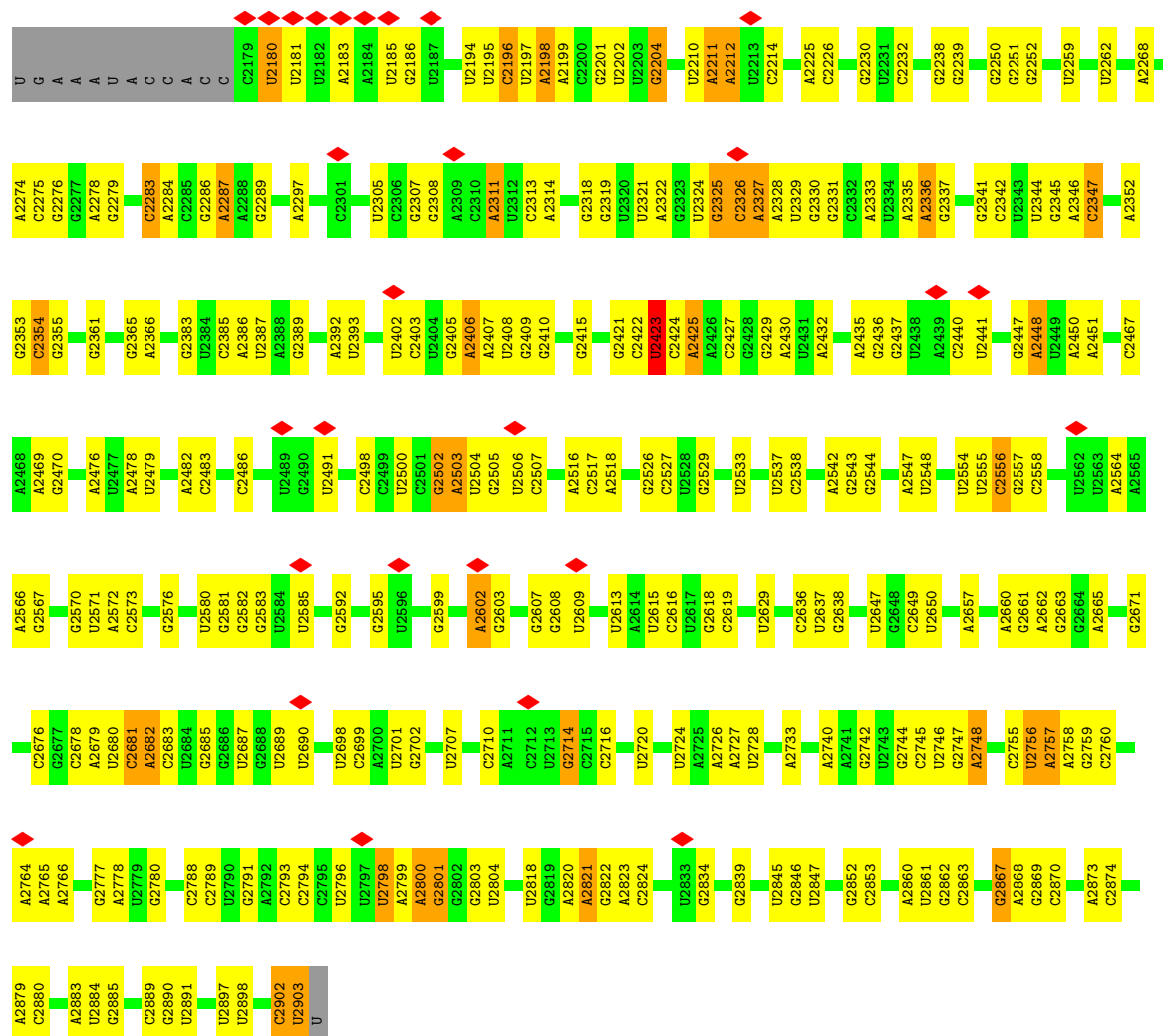
Chain BC:



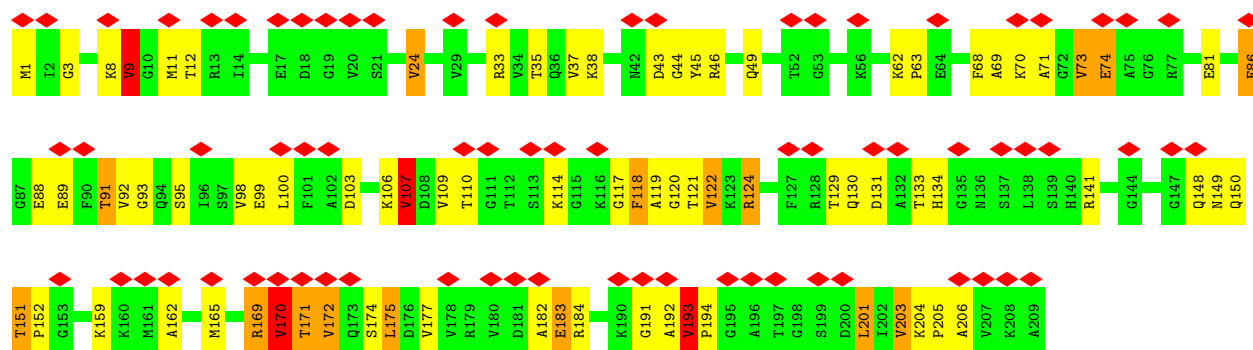
Chain BA:





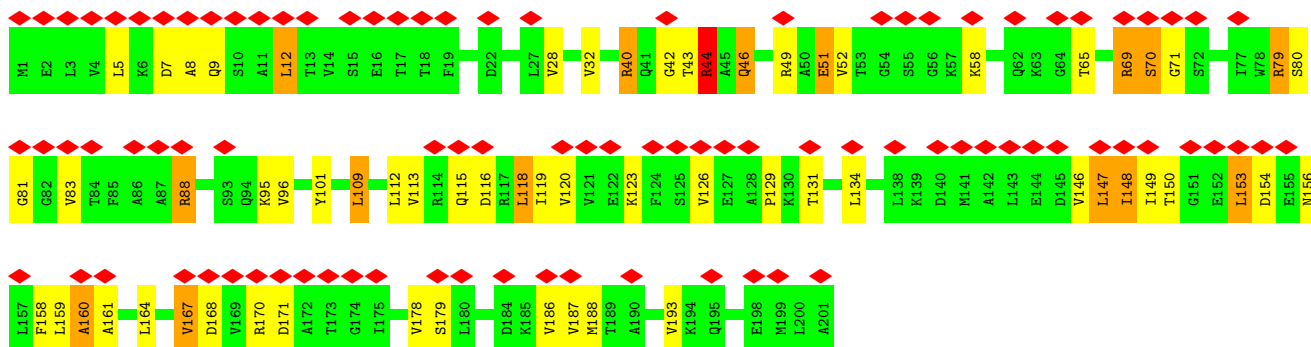


• Molecule 29: 50S ribosomal protein L3

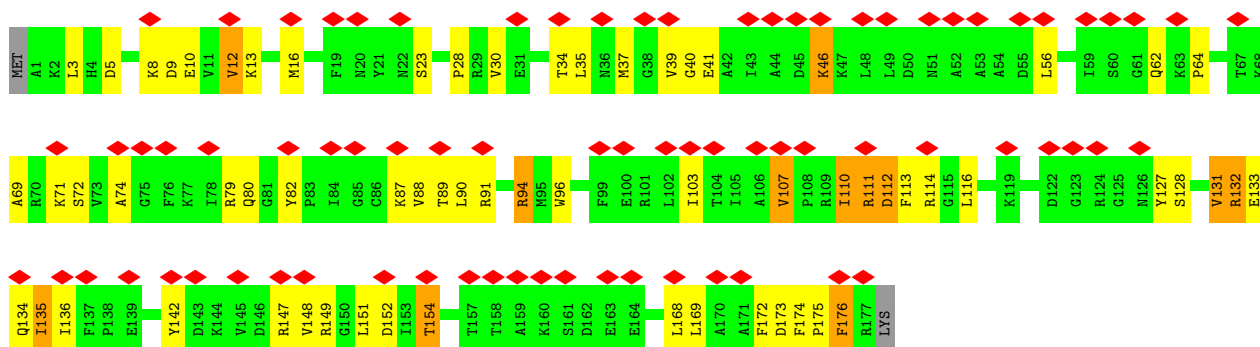
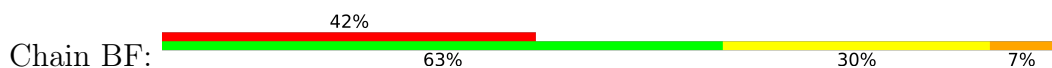


• Molecule 30: 50S ribosomal protein L4

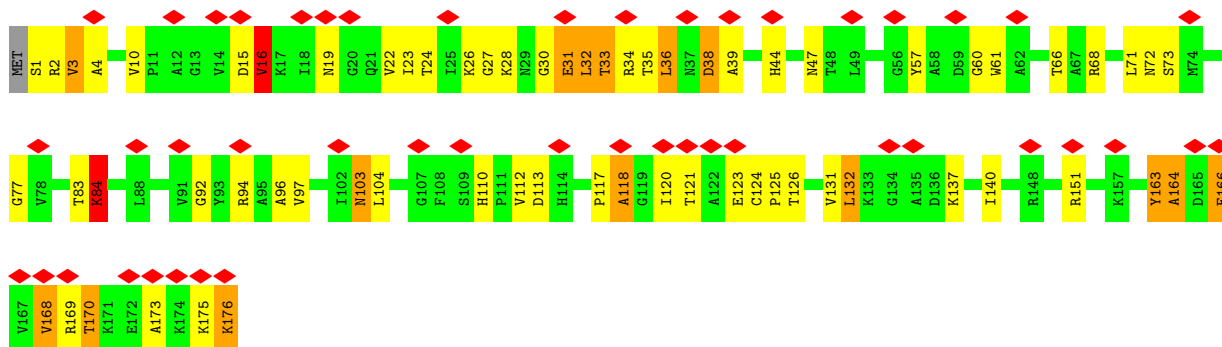




• Molecule 31: 50S ribosomal protein L5



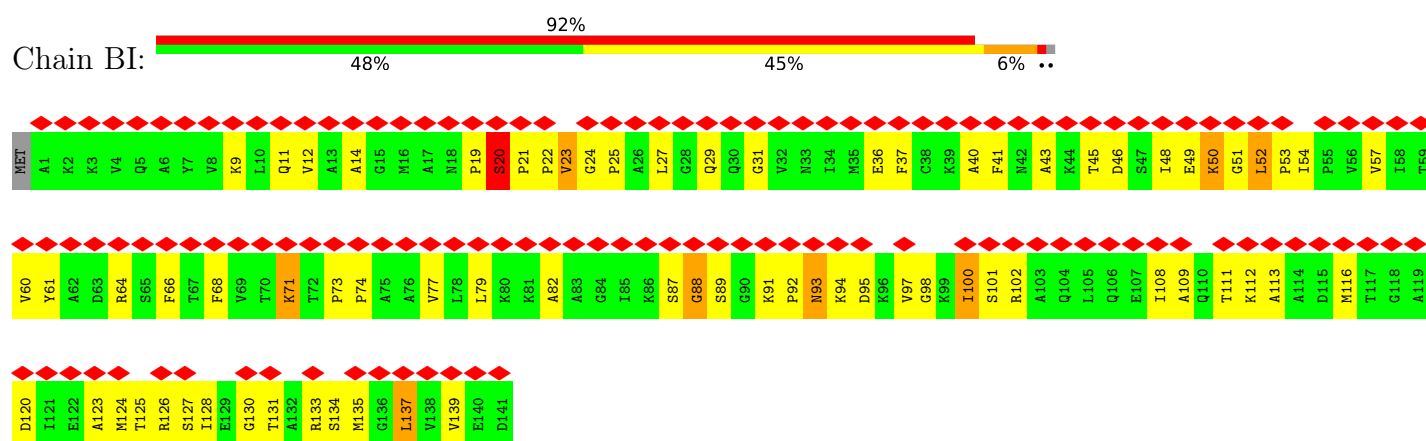
• Molecule 32: 50S ribosomal protein L6



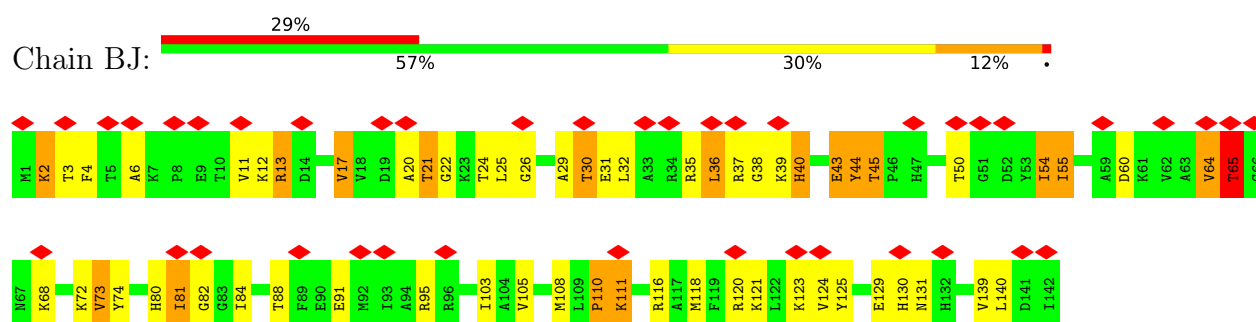
• Molecule 33: 50S ribosomal protein L9



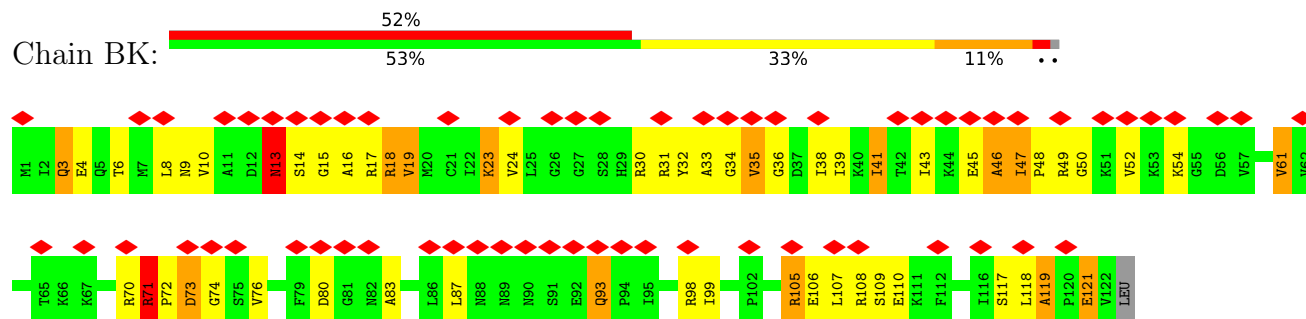
• Molecule 34: 50S ribosomal protein L11



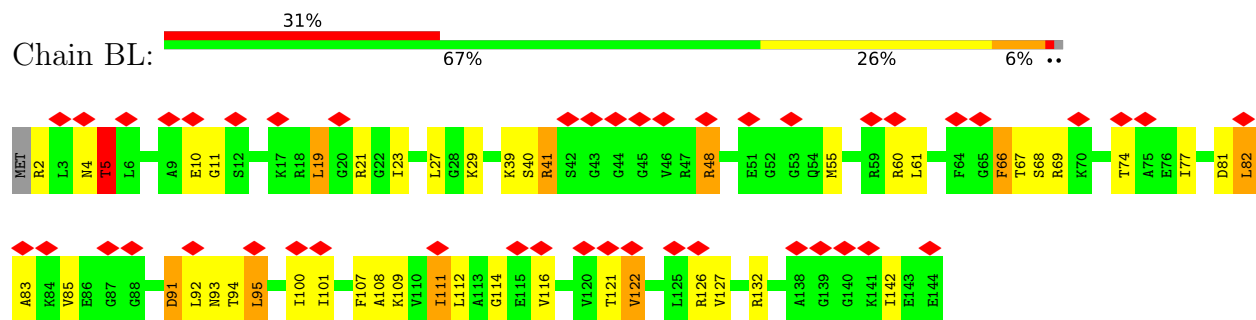
• Molecule 35: 50S ribosomal protein L13



• Molecule 36: 50S ribosomal protein L14

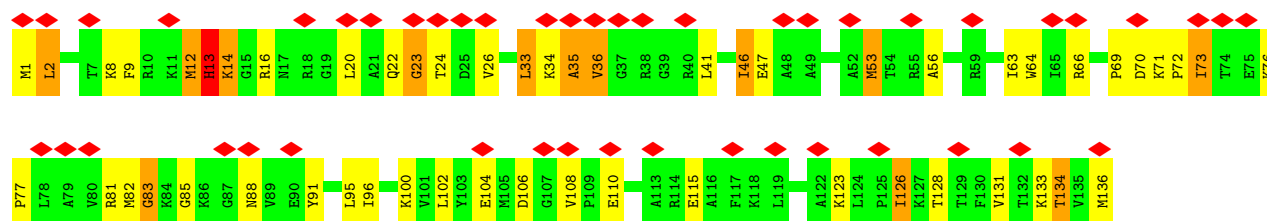


• Molecule 37: 50S ribosomal protein L15

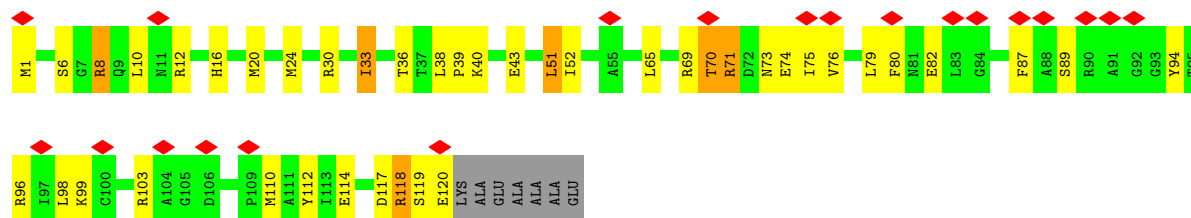


• Molecule 38: 50S ribosomal protein L16

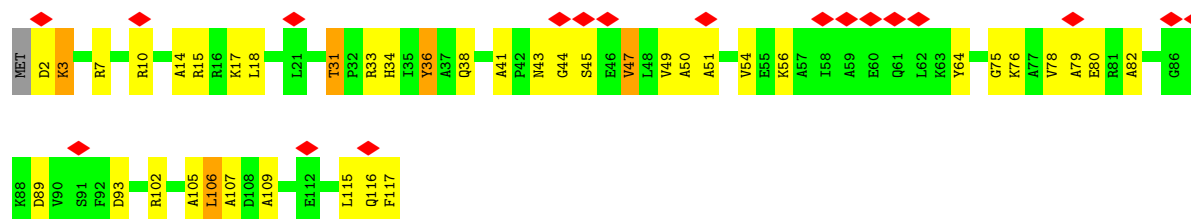




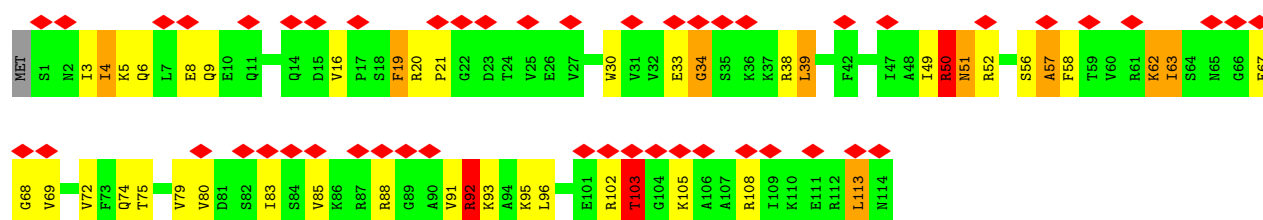
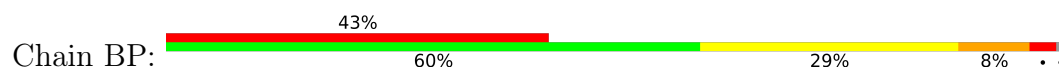
• Molecule 39: 50S ribosomal protein L17



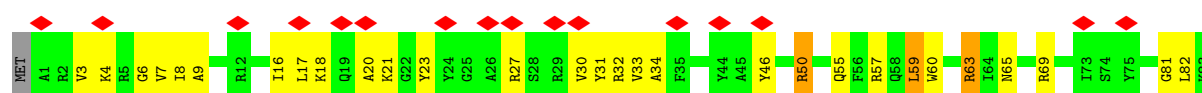
• Molecule 40: 50S ribosomal protein L18

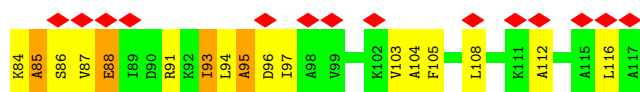


• Molecule 41: 50S ribosomal protein L19

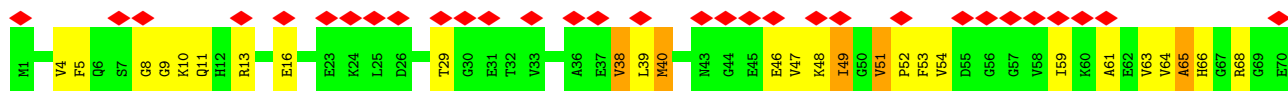


• Molecule 42: 50S ribosomal protein L20

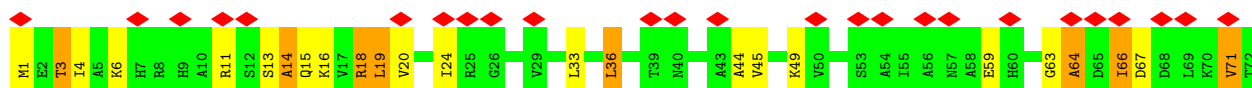




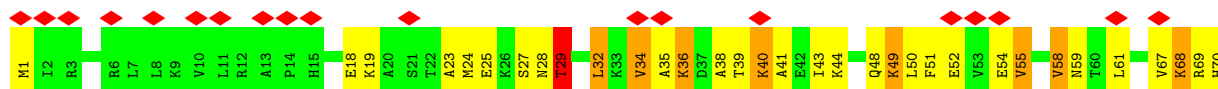
- Molecule 43: 50S ribosomal protein L21



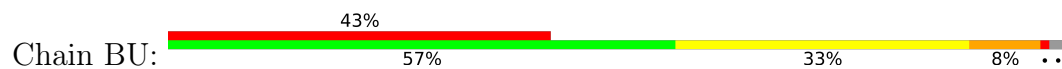
- Molecule 44: 50S ribosomal protein L22



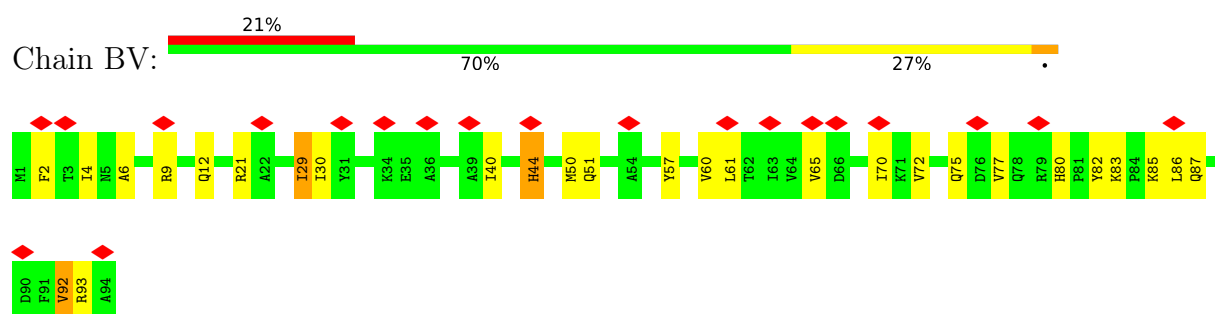
- Molecule 45: 50S ribosomal protein L23



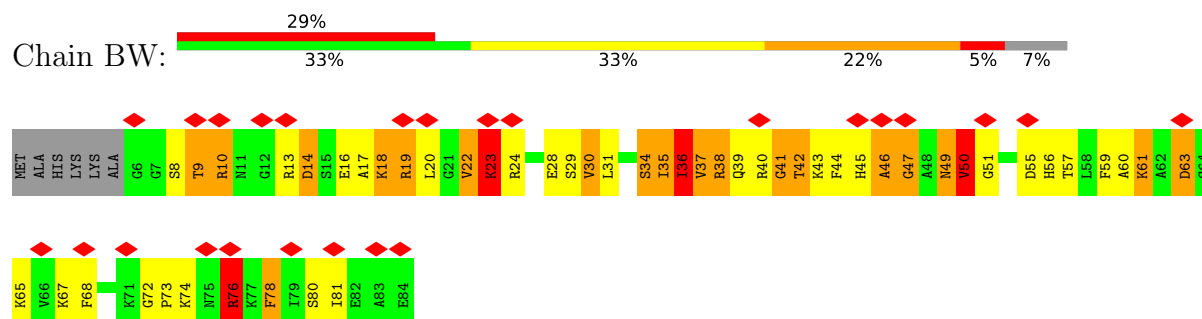
- Molecule 46: 50S ribosomal protein L24



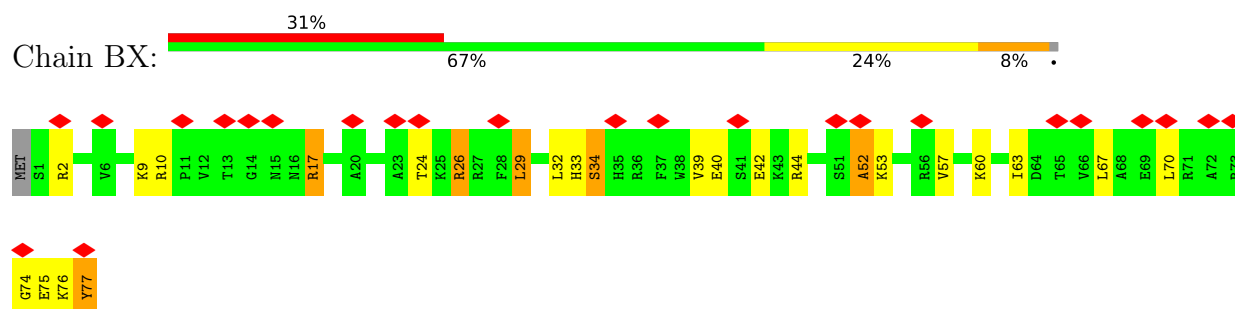
- Molecule 47: 50S ribosomal protein L25



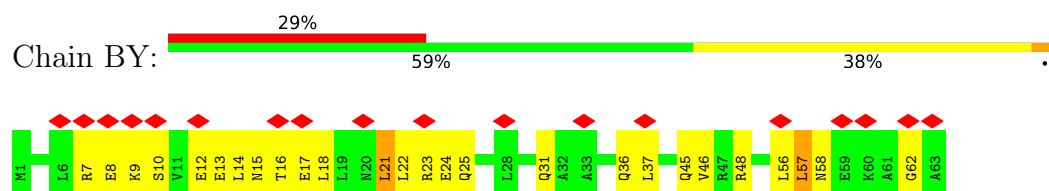
- Molecule 48: 50S ribosomal protein L27



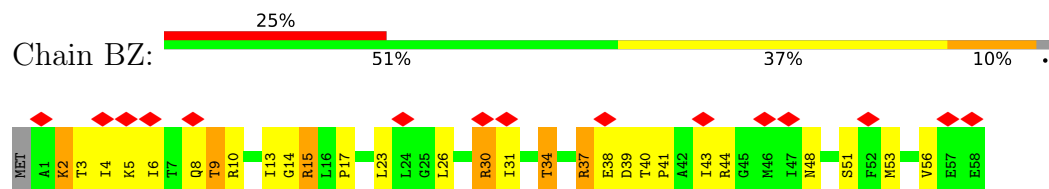
- Molecule 49: 50S ribosomal protein L28



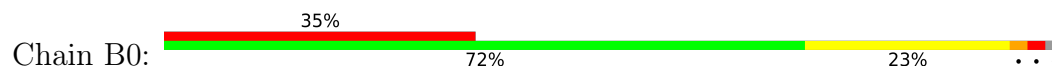
- Molecule 50: 50S ribosomal protein L29



- Molecule 51: 50S ribosomal protein L30

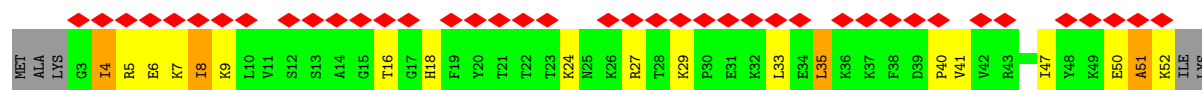
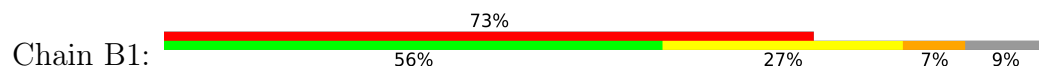


- Molecule 52: 50S ribosomal protein L32

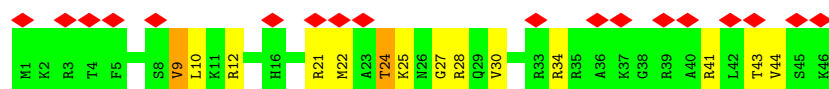
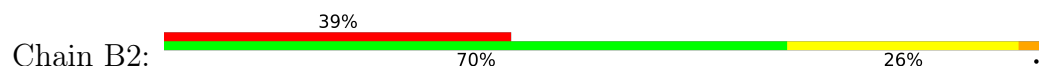




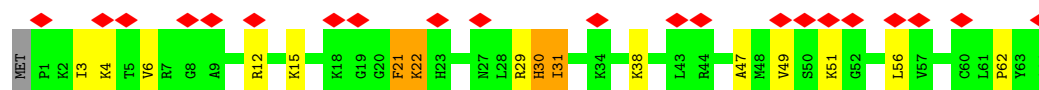
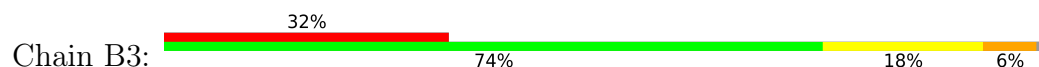
- Molecule 53: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L34



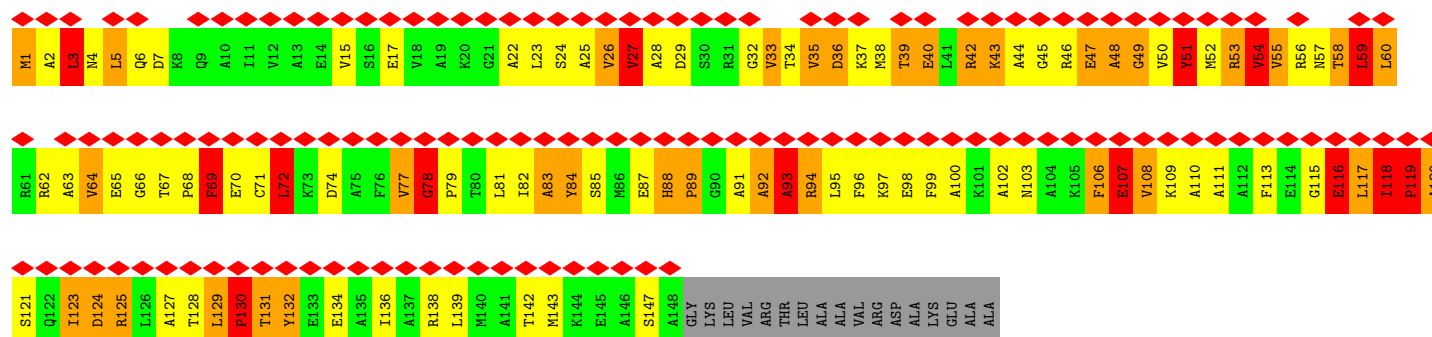
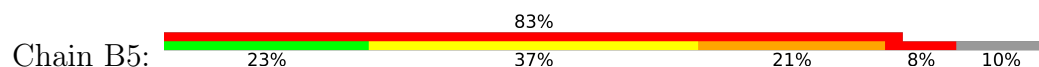
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 57: 50S ribosomal protein L10



- Molecule 58: 50S ribosomal protein L7/L12



MET	S1	I2	T3	K4	D5	Q6	I7	I8	E9	A10	V11	A12	A13	M14	S15	V16	M17	D18	V19	V20	E21	L22	I23	S24	A25	M26	E27	E28	K29	F30	GLY	VAL	SER	ALA	ALA	ALA	ALA	ALA	ALA	VAL	VAL	GLY	PRO	VAL	GLU	ALA	ALA	GLU	GLU	LYS	THR	PHE	ASP	VAL	ILE	LEU	LYS
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ALA	ALA	GLY	ALA	ASN	LYS	VAL	ALA	VAL	ILE	LYS	ALA	VAL	ARG	GLY	ALA	THR	GLY	LEU	GLY	LEU	LYS	GLU	ALA	LYS	ASP	LEU	VAL	GLU	SER	ALA	PRO	ALA	ALA	LEU	LYS	GLU	GLY	VAL	SER	LYS	ASP	ASP	ALA	GLU	ALA	LEU	LYS	LYS	ALA	LEU	GLU	ALA	GLY	ALA	GLU	VAL	VAL
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LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	279309	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	The volumes were CTF-corrected in defocus groups with an average of approximately 906 individual images per group.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20.00	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	12.702	Depositor
Minimum map value	-5.078	Depositor
Average map value	0.197	Depositor
Map value standard deviation	0.875	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	378.0, 378.0, 378.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.26, 1.26, 1.26	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, GDP, FUA

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	AA	0.36	1/36834 (0.0%)	0.58	5/57462 (0.0%)
2	AB	0.62	0/1735	0.98	4/2338 (0.2%)
3	AC	0.58	0/1651	0.96	6/2225 (0.3%)
4	AD	0.66	0/1665	1.08	6/2227 (0.3%)
5	AE	0.66	0/1118	1.07	4/1504 (0.3%)
6	AF	0.64	0/851	0.92	0/1150
7	AG	0.65	0/1195	0.93	0/1602
8	AH	0.62	0/989	0.95	2/1326 (0.2%)
9	AI	0.70	0/1034	1.07	2/1375 (0.1%)
10	AJ	0.72	0/796	1.05	1/1077 (0.1%)
11	AK	0.66	0/893	1.07	2/1205 (0.2%)
12	AL	0.69	0/969	1.08	4/1300 (0.3%)
13	AM	0.62	0/892	1.06	0/1193
14	AN	0.66	0/785	1.02	4/1043 (0.4%)
15	AO	0.59	0/722	0.97	2/964 (0.2%)
16	AP	0.65	0/659	1.01	1/884 (0.1%)
17	AQ	0.61	0/657	1.00	0/881
18	AR	0.55	0/462	0.86	0/621
19	AS	0.59	0/652	1.14	4/877 (0.5%)
20	AT	0.60	0/671	0.88	0/888
21	AU	0.82	0/430	1.12	2/570 (0.4%)
22	AV	0.47	0/1810	0.73	0/2821
23	AW	0.22	0/1827	0.47	0/2845
24	AX	0.39	0/469	0.69	0/730
25	AY	0.58	0/5291	0.94	7/7160 (0.1%)
26	BB	0.37	0/2828	0.55	0/4410
27	BC	0.71	0/2121	1.10	10/2852 (0.4%)
28	BA	0.44	0/68626	0.60	5/107056 (0.0%)
29	BD	0.74	0/1586	1.12	7/2134 (0.3%)
30	BE	0.69	0/1571	1.02	4/2113 (0.2%)
31	BF	0.60	0/1434	1.00	5/1926 (0.3%)
32	BG	0.69	0/1343	0.99	1/1816 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BH	0.68	0/389	1.05	1/523 (0.2%)
34	BI	0.83	0/1046	1.23	12/1410 (0.9%)
35	BJ	0.81	1/1152 (0.1%)	1.07	3/1551 (0.2%)
36	BK	0.83	0/947	1.03	1/1268 (0.1%)
37	BL	0.74	0/1054	1.01	0/1403
38	BM	0.79	0/1093	1.05	3/1460 (0.2%)
39	BN	0.68	0/973	0.91	0/1301
40	BO	0.59	0/902	0.98	1/1209 (0.1%)
41	BP	0.67	0/929	1.03	3/1242 (0.2%)
42	BQ	0.79	0/960	0.96	1/1278 (0.1%)
43	BR	0.71	0/829	1.04	3/1107 (0.3%)
44	BS	0.76	1/864 (0.1%)	0.98	2/1156 (0.2%)
45	BT	0.73	0/744	1.11	3/994 (0.3%)
46	BU	0.69	0/787	1.08	0/1051
47	BV	0.61	0/766	0.92	3/1025 (0.3%)
48	BW	0.95	2/603 (0.3%)	1.32	5/797 (0.6%)
49	BX	0.66	0/635	1.00	1/848 (0.1%)
50	BY	0.55	0/510	0.98	0/677
51	BZ	0.74	0/453	1.08	0/605
52	B0	0.69	0/450	0.91	0/599
53	B1	0.68	0/416	1.01	2/554 (0.4%)
54	B2	0.72	0/380	1.00	0/498
55	B3	0.71	0/513	0.99	1/676 (0.1%)
56	B4	0.85	1/303 (0.3%)	1.19	1/397 (0.3%)
57	B5	0.90	1/1131 (0.1%)	2.04	52/1524 (3.4%)
58	B6	0.79	0/227	0.98	1/304 (0.3%)
All	All	0.51	7/163622 (0.0%)	0.75	187/244032 (0.1%)

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
6	AF	0	1
12	AL	0	1
22	AV	0	3
25	AY	0	1
27	BC	0	1
29	BD	0	1
35	BJ	0	1
36	BK	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
57	B5	0	1
All	All	0	11

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	922	G	O3'-P	7.58	1.72	1.61
48	BW	35	ILE	CA-CB	7.22	1.62	1.54
56	B4	3	VAL	CA-CB	-5.97	1.49	1.55
48	BW	50	VAL	CA-CB	5.58	1.62	1.54
35	BJ	43	GLU	CA-C	-5.27	1.45	1.52

The worst 5 of 187 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BD	151	THR	CA-C-N	-14.34	103.99	119.19
29	BD	151	THR	C-N-CA	-14.34	103.99	119.19
57	B5	131	THR	N-CA-C	-13.39	96.68	111.28
57	B5	92	ALA	CA-C-N	12.65	145.69	121.54
57	B5	92	ALA	C-N-CA	12.65	145.69	121.54

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	AF	101	PRO	Peptide
12	AL	23	ALA	Peptide
22	AV	29	G	Sidechain
22	AV	4	G	Sidechain
22	AV	8	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32895	0	16542	957	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AB	1704	0	1732	92	0
3	AC	1624	0	1696	42	0
4	AD	1643	0	1707	72	0
5	AE	1105	0	1147	144	0
6	AF	832	0	824	27	0
7	AG	1181	0	1236	54	0
8	AH	979	0	1031	29	0
9	AI	1022	0	1067	122	0
10	AJ	786	0	828	23	0
11	AK	877	0	887	33	0
12	AL	955	0	1016	40	0
13	AM	883	0	941	32	0
14	AN	774	0	824	37	0
15	AO	714	0	733	12	0
16	AP	649	0	666	15	0
17	AQ	648	0	691	11	0
18	AR	455	0	478	11	0
19	AS	637	0	665	41	0
20	AT	665	0	714	16	0
21	AU	425	0	449	44	0
22	AV	1640	0	832	136	0
23	AW	1635	0	829	97	0
24	AX	416	0	207	169	0
25	AY	5194	0	5170	228	0
26	BB	2529	0	1281	21	0
27	BC	2082	0	2157	51	0
28	BA	61274	0	30812	871	0
29	BD	1565	0	1616	54	0
30	BE	1552	0	1619	40	0
31	BF	1410	0	1442	62	0
32	BG	1323	0	1374	47	0
33	BH	384	0	405	37	0
34	BI	1032	0	1088	63	0
35	BJ	1129	0	1162	58	0
36	BK	938	0	1012	43	0
37	BL	1045	0	1117	39	0
38	BM	1074	0	1156	53	0
39	BN	960	0	1000	30	0
40	BO	892	0	923	24	0
41	BP	917	0	965	52	0
42	BQ	947	0	1022	53	0
43	BR	816	0	839	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BS	857	0	922	30	0
45	BT	738	0	807	39	0
46	BU	779	0	834	32	0
47	BV	753	0	780	17	0
48	BW	596	0	610	86	0
49	BX	625	0	655	16	0
50	BY	509	0	543	14	0
51	BZ	449	0	491	18	0
52	B0	444	0	461	19	0
53	B1	409	0	440	15	0
54	B2	377	0	418	8	0
55	B3	504	0	574	10	0
56	B4	302	0	340	17	0
57	B5	1117	0	1155	132	0
58	B6	227	0	237	7	0
59	AY	37	0	44	59	0
60	AY	28	0	12	26	0
All	All	150958	0	103225	3717	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 3717 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AY:92:HIS:CE1	59:AY:801:FUA:H283	1.23	1.69
1:AA:1498:U:C5	24:AX:12:U:H5''	1.26	1.64
1:AA:1498:U:C4	24:AX:12:U:H5''	1.32	1.61
24:AX:14:A:H2'	24:AX:15:A:C5'	1.24	1.58
24:AX:14:A:C2'	24:AX:15:A:H5''	1.16	1.57

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/241 (90%)	151 (70%)	51 (24%)	14 (6%)	1	12
3	AC	204/233 (88%)	181 (89%)	18 (9%)	5 (2%)	4	26
4	AD	203/206 (98%)	162 (80%)	30 (15%)	11 (5%)	1	15
5	AE	148/167 (89%)	123 (83%)	18 (12%)	7 (5%)	2	16
6	AF	100/135 (74%)	79 (79%)	15 (15%)	6 (6%)	1	13
7	AG	149/179 (83%)	128 (86%)	20 (13%)	1 (1%)	18	56
8	AH	127/130 (98%)	114 (90%)	12 (9%)	1 (1%)	16	54
9	AI	125/130 (96%)	104 (83%)	15 (12%)	6 (5%)	2	16
10	AJ	96/103 (93%)	69 (72%)	20 (21%)	7 (7%)	1	10
11	AK	115/129 (89%)	97 (84%)	12 (10%)	6 (5%)	1	15
12	AL	121/124 (98%)	101 (84%)	16 (13%)	4 (3%)	3	21
13	AM	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	1	15
14	AN	92/101 (91%)	73 (79%)	13 (14%)	6 (6%)	1	12
15	AO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	5	28
16	AP	80/82 (98%)	60 (75%)	17 (21%)	3 (4%)	2	19
17	AQ	78/84 (93%)	59 (76%)	15 (19%)	4 (5%)	1	15
18	AR	53/75 (71%)	47 (89%)	6 (11%)	0	100	100
19	AS	77/92 (84%)	65 (84%)	11 (14%)	1 (1%)	9	42
20	AT	83/87 (95%)	74 (89%)	7 (8%)	2 (2%)	4	27
21	AU	49/71 (69%)	26 (53%)	20 (41%)	3 (6%)	1	13
25	AY	667/704 (95%)	541 (81%)	92 (14%)	34 (5%)	1	15
27	BC	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	1	14
29	BD	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1	11
30	BE	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	1	16
31	BF	175/179 (98%)	141 (81%)	30 (17%)	4 (2%)	5	28
32	BG	174/177 (98%)	127 (73%)	30 (17%)	17 (10%)	0	7
33	BH	48/50 (96%)	29 (60%)	14 (29%)	5 (10%)	0	6
34	BI	139/142 (98%)	97 (70%)	33 (24%)	9 (6%)	1	12
35	BJ	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	1	12
36	BK	120/123 (98%)	96 (80%)	14 (12%)	10 (8%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BL	141/144 (98%)	104 (74%)	32 (23%)	5 (4%)	3	20
38	BM	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	0	9
39	BN	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	16	54
40	BO	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	14	51
41	BP	112/115 (97%)	86 (77%)	17 (15%)	9 (8%)	1	9
42	BQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	3	20
43	BR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	3	23
44	BS	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	2	17
45	BT	91/100 (91%)	57 (63%)	24 (26%)	10 (11%)	0	5
46	BU	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	0	7
47	BV	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
48	BW	77/85 (91%)	39 (51%)	22 (29%)	16 (21%)	0	2
49	BX	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	2	18
50	BY	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	12
51	BZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	2	20
52	B0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	10
53	B1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	1	13
54	B2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
55	B3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	3	21
56	B4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	0	9
57	B5	146/165 (88%)	77 (53%)	40 (27%)	29 (20%)	0	2
58	B6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	2	20
All	All	6365/6876 (93%)	5040 (79%)	977 (15%)	348 (6%)	2	14

5 of 348 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	33	ALA
2	AB	40	ILE
2	AB	119	GLN
3	AC	101	ILE
4	AD	24	GLY

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	
2	AB	180/199 (90%)	165 (92%)	15 (8%)	10	30
3	AC	170/190 (90%)	153 (90%)	17 (10%)	7	24
4	AD	172/173 (99%)	164 (95%)	8 (5%)	23	45
5	AE	113/126 (90%)	104 (92%)	9 (8%)	11	31
6	AF	89/116 (77%)	80 (90%)	9 (10%)	7	23
7	AG	124/147 (84%)	114 (92%)	10 (8%)	11	31
8	AH	104/105 (99%)	95 (91%)	9 (9%)	9	29
9	AI	105/107 (98%)	93 (89%)	12 (11%)	5	18
10	AJ	86/90 (96%)	83 (96%)	3 (4%)	32	53
11	AK	90/99 (91%)	85 (94%)	5 (6%)	19	40
12	AL	103/104 (99%)	95 (92%)	8 (8%)	11	32
13	AM	92/96 (96%)	86 (94%)	6 (6%)	15	37
14	AN	79/84 (94%)	74 (94%)	5 (6%)	16	37
15	AO	76/77 (99%)	72 (95%)	4 (5%)	20	41
16	AP	65/65 (100%)	61 (94%)	4 (6%)	16	38
17	AQ	74/78 (95%)	66 (89%)	8 (11%)	6	21
18	AR	48/65 (74%)	46 (96%)	2 (4%)	26	48
19	AS	70/79 (89%)	64 (91%)	6 (9%)	10	29
20	AT	65/66 (98%)	58 (89%)	7 (11%)	6	21
21	AU	44/61 (72%)	37 (84%)	7 (16%)	2	11
25	AY	552/578 (96%)	494 (90%)	58 (10%)	6	21
27	BC	216/218 (99%)	199 (92%)	17 (8%)	11	32
29	BD	164/164 (100%)	143 (87%)	21 (13%)	4	15
30	BE	165/165 (100%)	146 (88%)	19 (12%)	5	18
31	BF	148/150 (99%)	135 (91%)	13 (9%)	9	28
32	BG	137/138 (99%)	122 (89%)	15 (11%)	6	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BH	40/40 (100%)	37 (92%)	3 (8%)	12	33
34	BI	109/110 (99%)	106 (97%)	3 (3%)	38	60
35	BJ	116/116 (100%)	97 (84%)	19 (16%)	2	10
36	BK	103/104 (99%)	88 (85%)	15 (15%)	3	13
37	BL	102/103 (99%)	89 (87%)	13 (13%)	4	16
38	BM	109/109 (100%)	93 (85%)	16 (15%)	3	13
39	BN	100/103 (97%)	90 (90%)	10 (10%)	7	24
40	BO	86/87 (99%)	78 (91%)	8 (9%)	8	26
41	BP	99/100 (99%)	86 (87%)	13 (13%)	4	15
42	BQ	89/90 (99%)	80 (90%)	9 (10%)	7	23
43	BR	84/84 (100%)	74 (88%)	10 (12%)	5	18
44	BS	93/93 (100%)	83 (89%)	10 (11%)	6	21
45	BT	80/84 (95%)	75 (94%)	5 (6%)	16	37
46	BU	83/85 (98%)	75 (90%)	8 (10%)	8	25
47	BV	78/78 (100%)	73 (94%)	5 (6%)	16	37
48	BW	59/63 (94%)	50 (85%)	9 (15%)	3	12
49	BX	67/68 (98%)	59 (88%)	8 (12%)	5	18
50	BY	55/55 (100%)	51 (93%)	4 (7%)	13	34
51	BZ	48/49 (98%)	38 (79%)	10 (21%)	1	6
52	B0	47/48 (98%)	46 (98%)	1 (2%)	47	65
53	B1	45/49 (92%)	42 (93%)	3 (7%)	15	36
54	B2	38/38 (100%)	35 (92%)	3 (8%)	11	32
55	B3	51/52 (98%)	45 (88%)	6 (12%)	5	18
56	B4	34/34 (100%)	29 (85%)	5 (15%)	3	13
57	B5	112/123 (91%)	93 (83%)	19 (17%)	2	10
58	B6	26/85 (31%)	21 (81%)	5 (19%)	1	8
All	All	5284/5590 (94%)	4767 (90%)	517 (10%)	10	24

5 of 517 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	BY	21	LEU
53	B1	8	ILE

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Mol	Chain	Res	Type
50	BY	16	THR
25	AY	504	LYS
25	AY	418	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
25	AY	465	HIS
50	BY	41	HIS
29	BD	49	GLN
47	BV	80	HIS
41	BP	55	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1542 (99%)	283 (18%)	18 (1%)
22	AV	76/77 (98%)	15 (19%)	0
23	AW	76/77 (98%)	27 (35%)	2 (2%)
24	AX	18/19 (94%)	14 (77%)	1 (5%)
26	BB	117/120 (97%)	17 (14%)	0
28	BA	2850/2904 (98%)	464 (16%)	41 (1%)
All	All	4669/4739 (98%)	820 (17%)	62 (1%)

5 of 820 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	9	G
1	AA	17	U
1	AA	20	U
1	AA	21	G

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	BA	527	C
28	BA	2211	A
28	BA	931	U
28	BA	2142	A

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Mol	Chain	Res	Type
28	BA	2756	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	5MU	AV	54	22	18,21,23	0.39	0	25,30,35	0.50	0

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
22	5MU	AV	54	22	-	0/7/25/26	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	54	5MU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands 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$
60	GDP	AY	802	-	29,30,30	1.06	1 (3%)	45,47,47	1.72	9 (20%)
59	FUA	AY	801	-	39,40,40	1.71	7 (17%)	50,64,64	1.70	8 (16%)

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
60	GDP	AY	802	-	-	2/16/32/32	0/3/3/3
59	FUA	AY	801	-	-	7/16/92/92	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AY	801	FUA	C23-C22	-4.43	1.39	1.51
59	AY	801	FUA	C23-C24	-4.38	1.39	1.53
59	AY	801	FUA	C29-C22	4.22	1.53	1.47
59	AY	801	FUA	C24-C25	-3.54	1.39	1.50
59	AY	801	FUA	C14-C8	-3.26	1.53	1.59

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AY	802	GDP	C2-N3-C4	5.35	121.52	112.30
59	AY	801	FUA	C24-C23-C22	5.35	124.11	112.72
60	AY	802	GDP	C5-C4-N3	-4.78	120.78	128.39
59	AY	801	FUA	C13-C12-C11	-4.19	105.81	111.90
59	AY	801	FUA	C16-O2-C31	-3.96	111.11	117.00

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

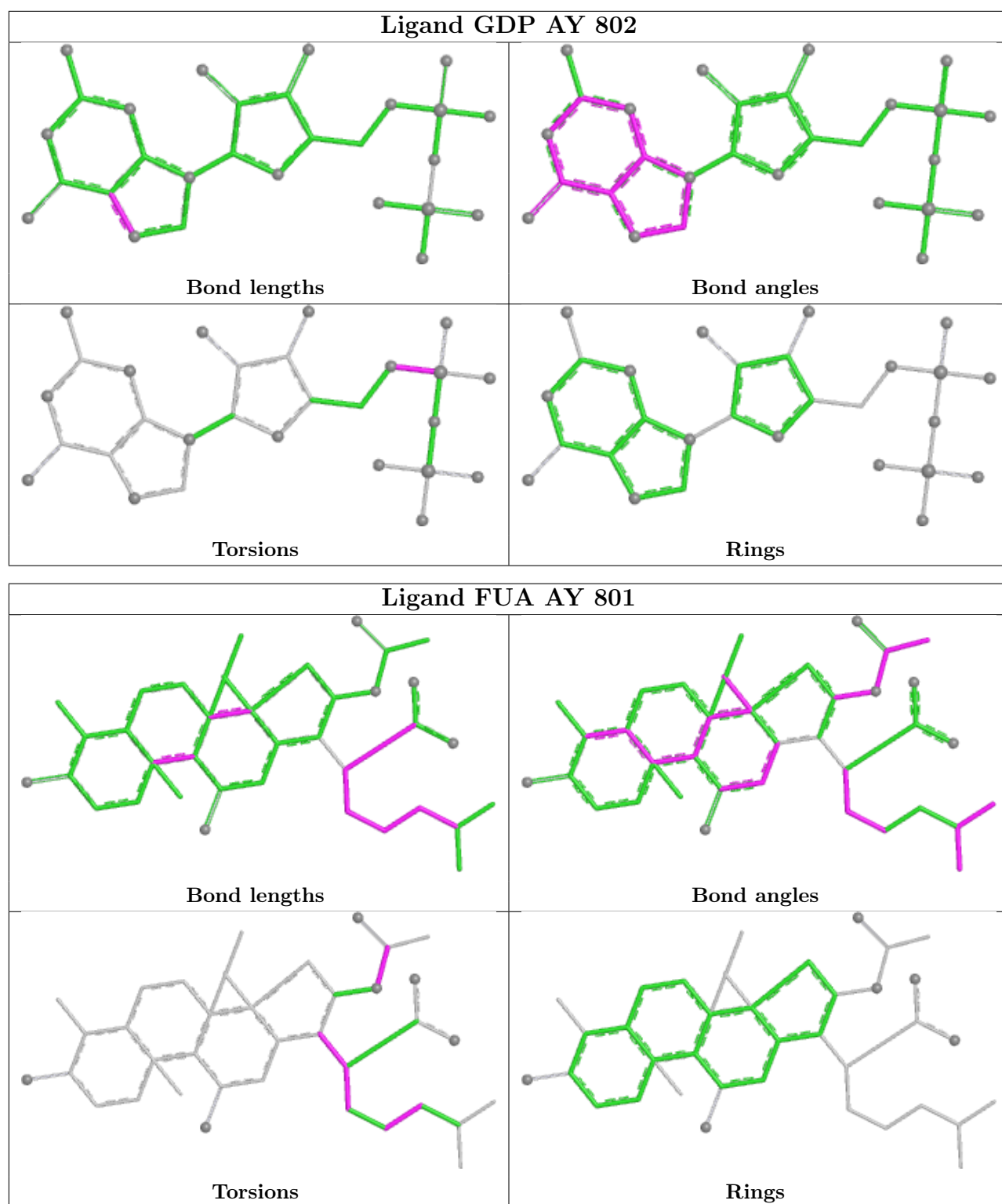
Mol	Chain	Res	Type	Atoms
59	AY	801	FUA	C13-C17-C22-C23
59	AY	801	FUA	C13-C17-C22-C29
60	AY	802	GDP	C5'-O5'-PA-O3A
60	AY	802	GDP	C5'-O5'-PA-O1A
59	AY	801	FUA	C32-C31-O2-C16

There are no ring outliers.

2 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AY	802	GDP	26	0
59	AY	801	FUA	59	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

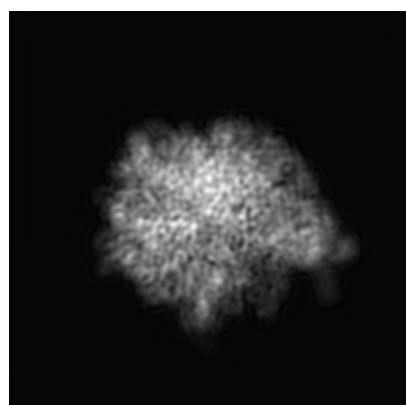
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5775. These allow visual inspection of the internal detail of the map and identification of artifacts.

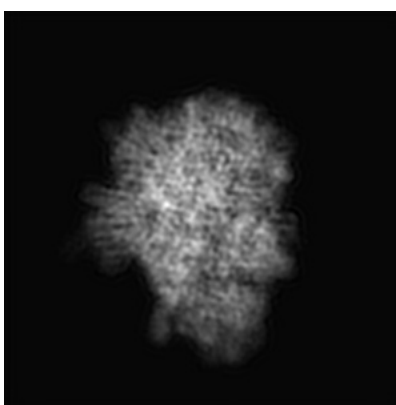
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

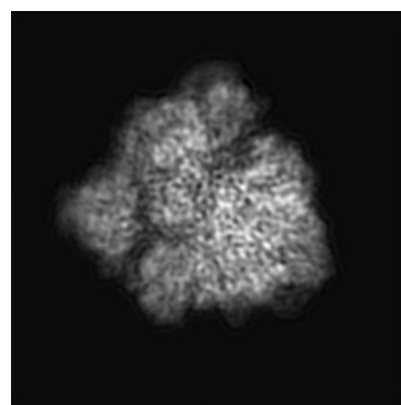
6.1.1 Primary map



X



Y

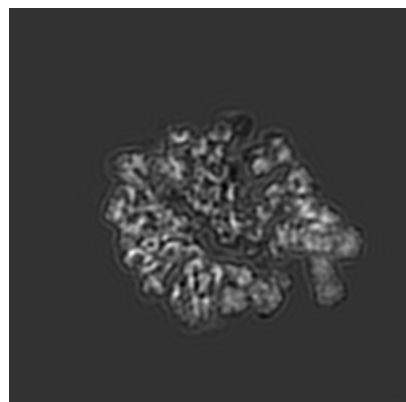


Z

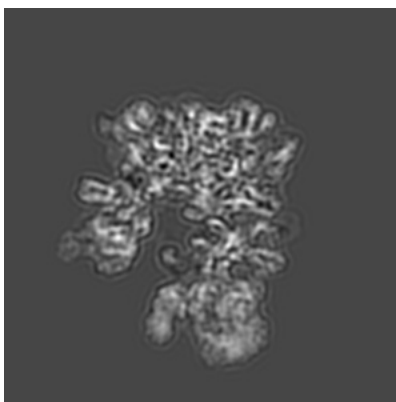
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

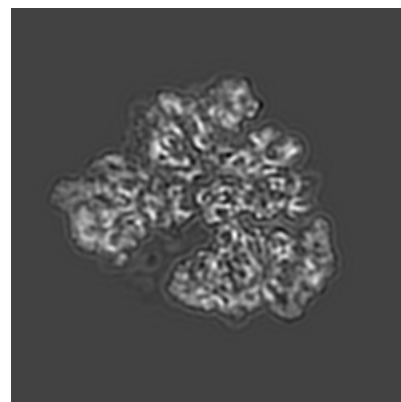
6.2.1 Primary map



X Index: 150



Y Index: 150

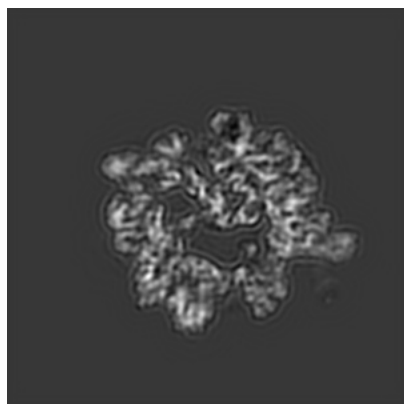


Z Index: 150

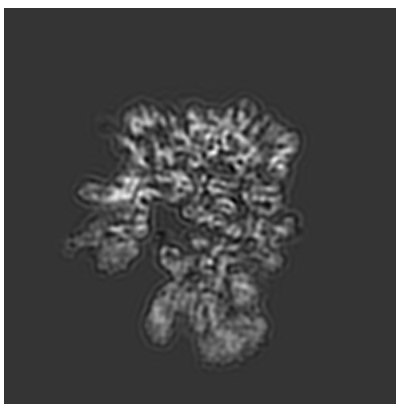
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

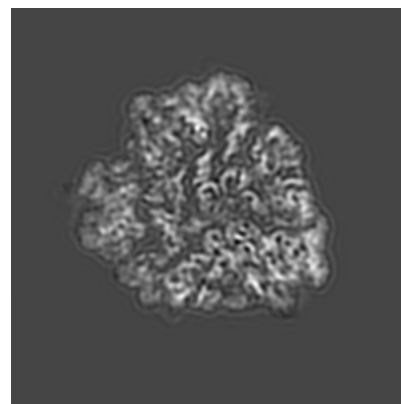
6.3.1 Primary map



X Index: 141



Y Index: 154

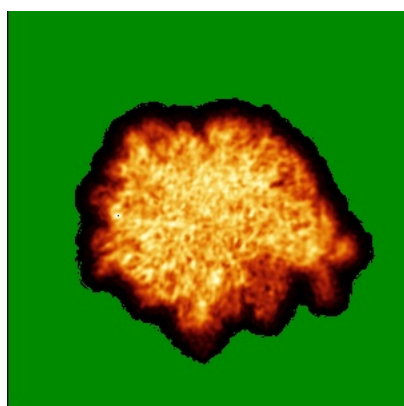


Z Index: 141

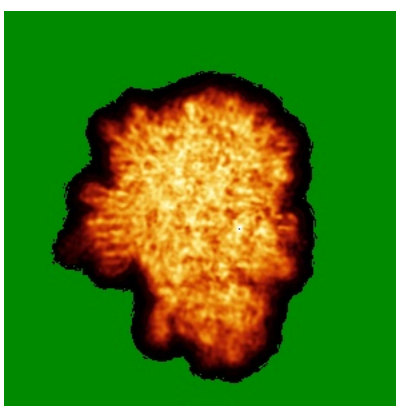
The images above show the largest variance slices of the map in three orthogonal directions.

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

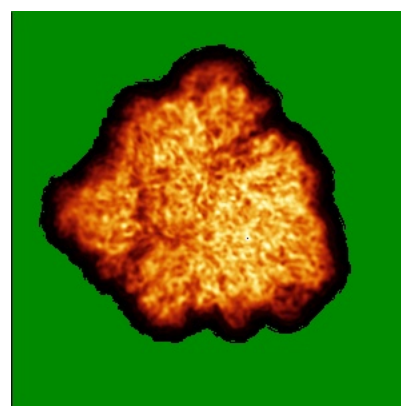
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

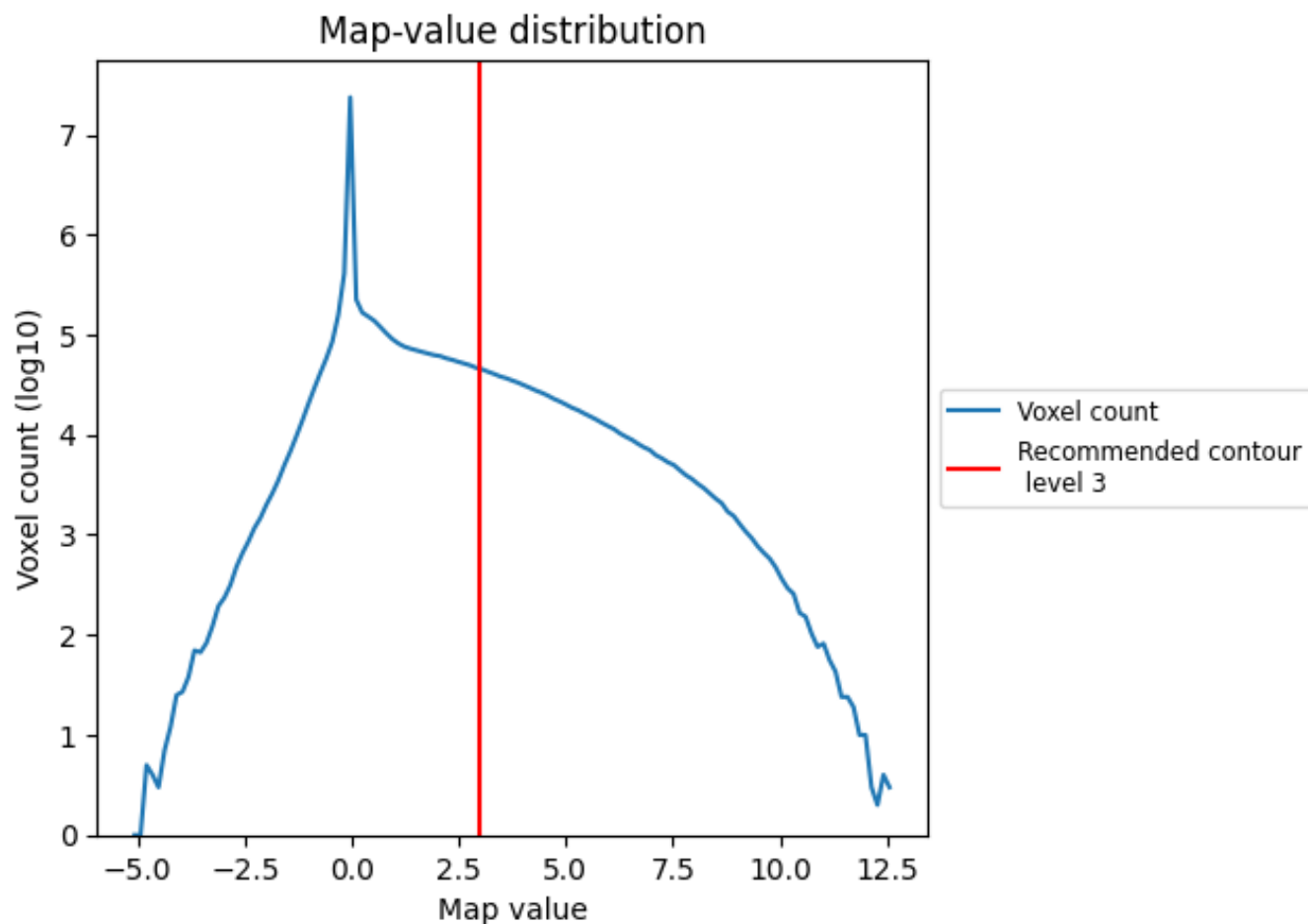
6.6 Mask visualisation

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

7 Map analysis [i](#)

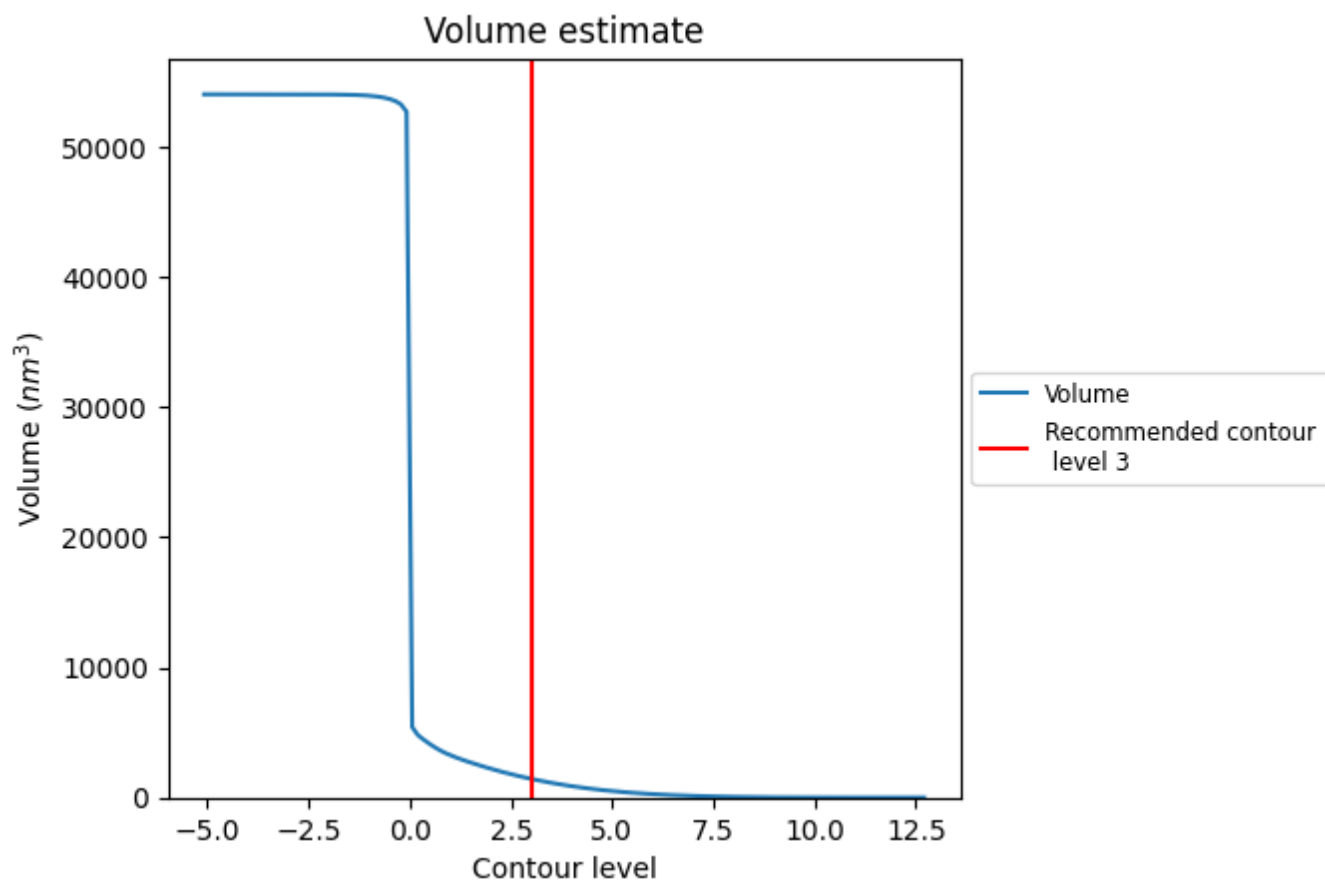
This section contains the results of statistical analysis of the map.

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.

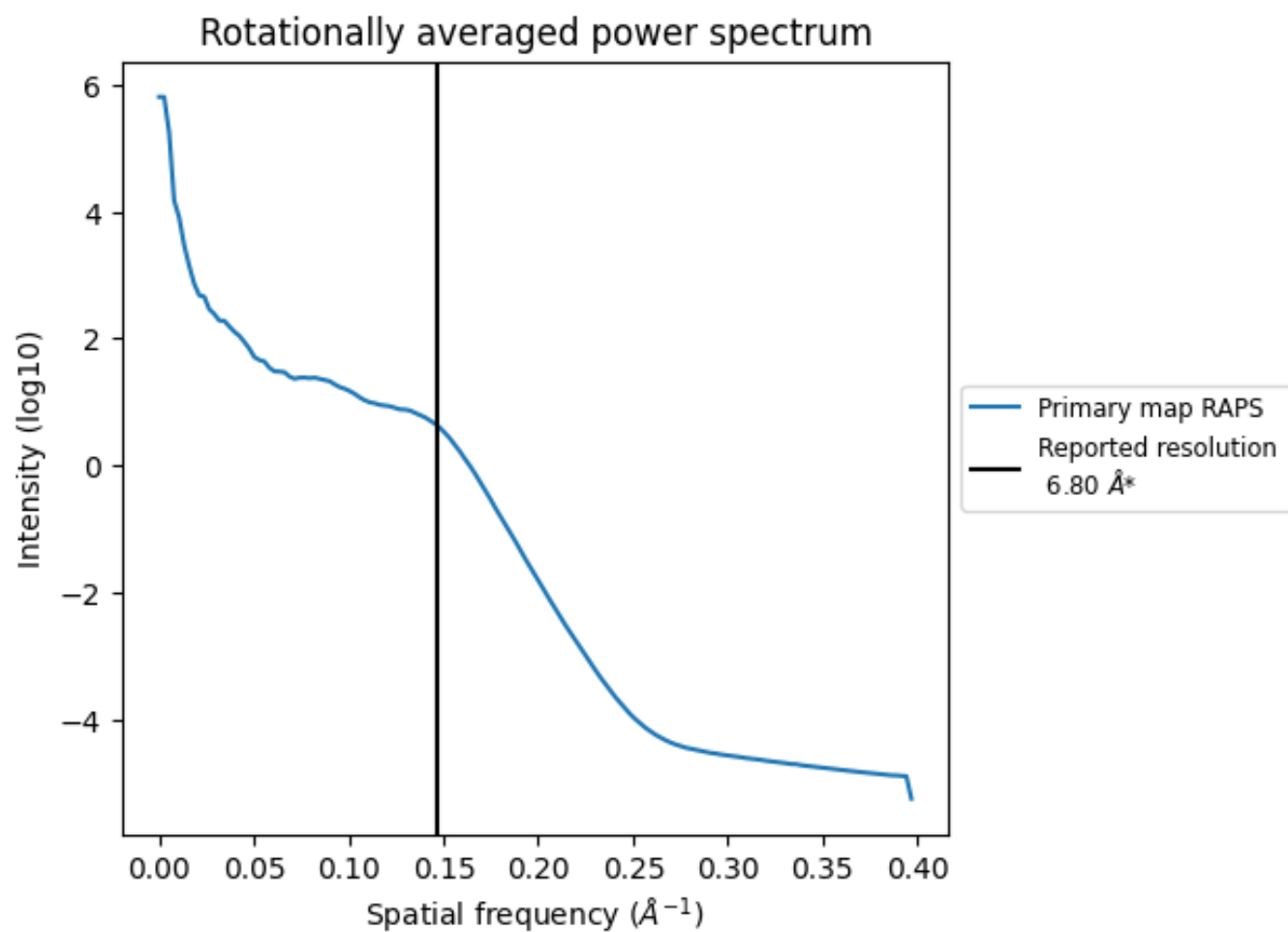
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1436 nm³; this corresponds to an approximate mass of 1297 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 0.147 Å⁻¹

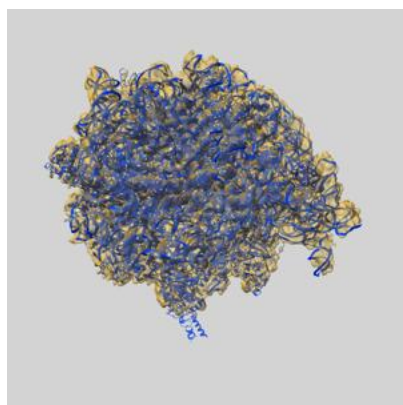
8 Fourier-Shell correlation

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

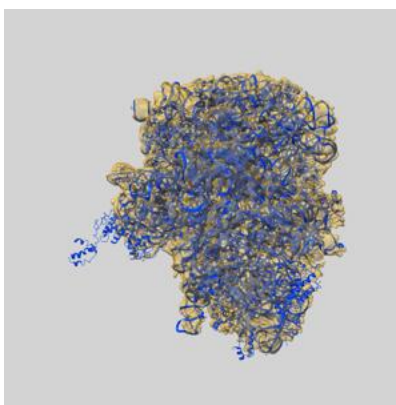
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5775 and PDB model 4V7B. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

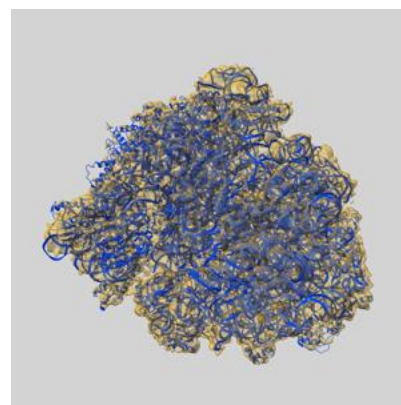
9.1 Map-model overlay [i](#)



X



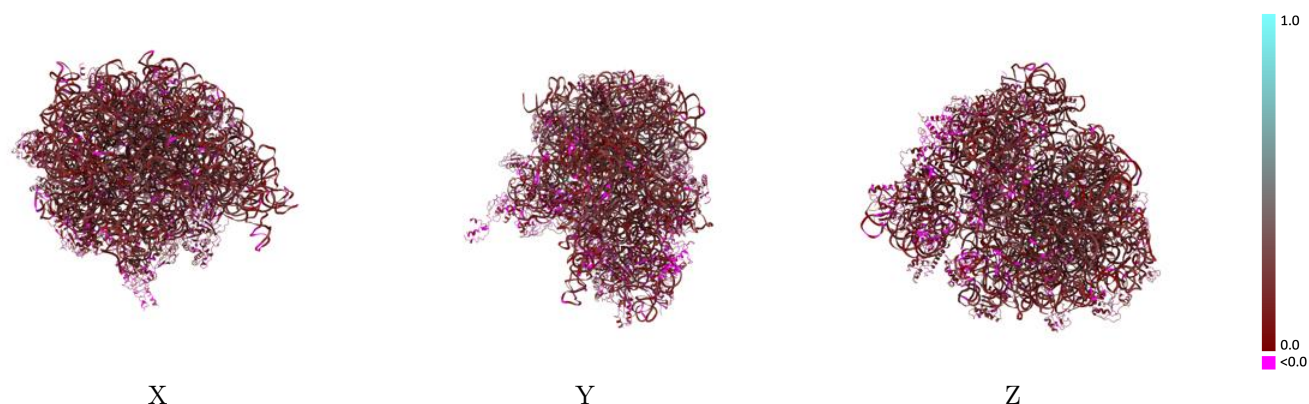
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

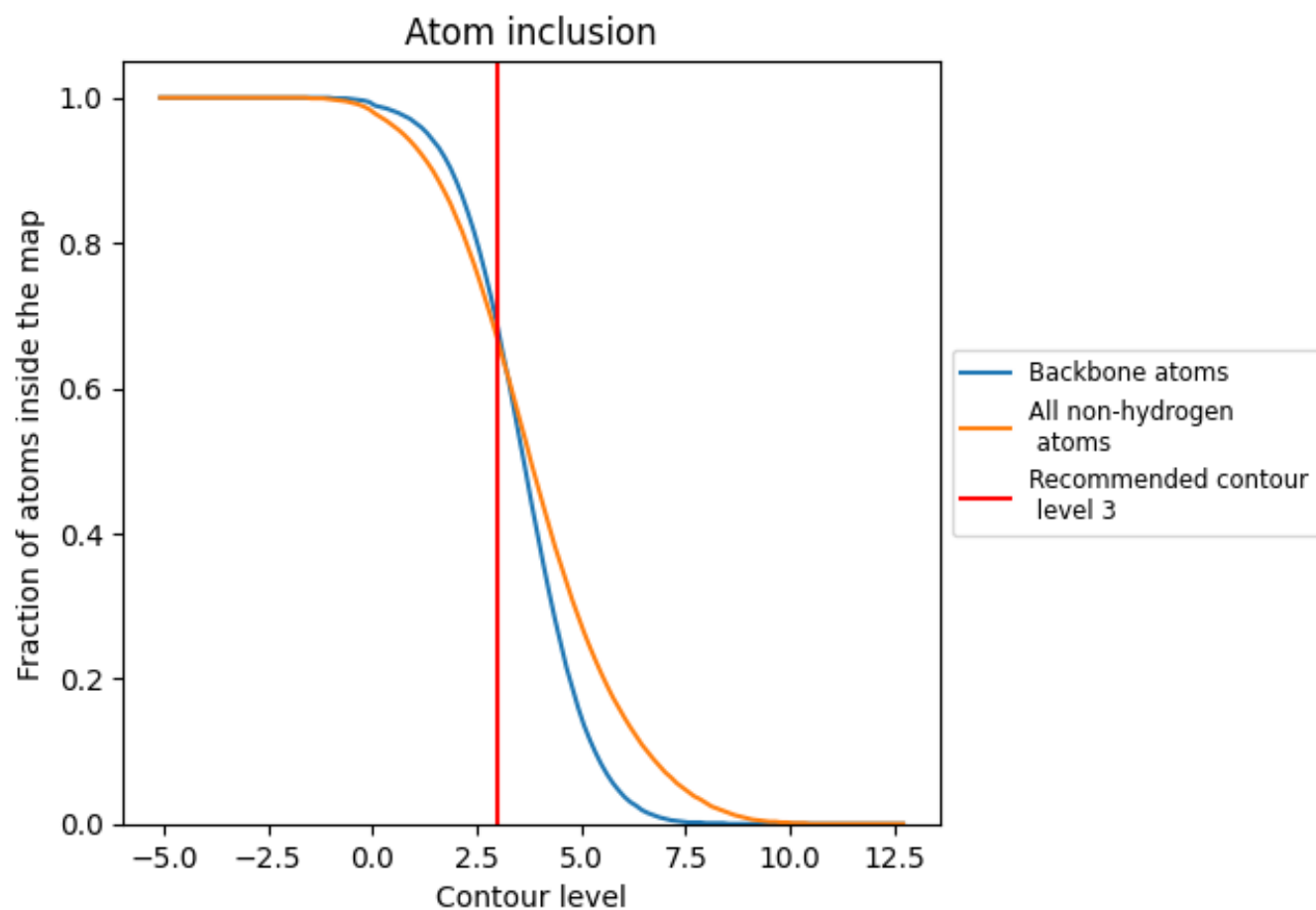


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 67% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6660	 0.1610
AA	 0.7850	 0.1720
AB	 0.0880	 0.0200
AC	 0.4420	 0.1190
AD	 0.4240	 0.1010
AE	 0.5120	 0.1290
AF	 0.4910	 0.0840
AG	 0.1710	 0.0750
AH	 0.5090	 0.1360
AI	 0.5090	 0.1040
AJ	 0.3710	 0.1080
AK	 0.4840	 0.1240
AL	 0.3910	 0.1350
AM	 0.4440	 0.1130
AN	 0.5170	 0.1330
AO	 0.5580	 0.1320
AP	 0.5680	 0.1500
AQ	 0.5250	 0.1240
AR	 0.5300	 0.1380
AS	 0.5200	 0.1130
AT	 0.5800	 0.1490
AU	 0.2640	 0.0750
AV	 0.5900	 0.1730
AW	 0.6870	 0.1750
AX	 0.4660	 0.1420
AY	 0.4010	 0.1200
B0	 0.4880	 0.1490
B1	 0.2170	 0.0820
B2	 0.4540	 0.1290
B3	 0.4850	 0.1390
B4	 0.5650	 0.1340
B5	 0.0610	 0.0430
B6	 0.0000	 -0.0070
BA	 0.7820	 0.1890
BB	 0.8300	 0.1790



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Chain	Atom inclusion	Q-score
BC	 0.4660	 0.1220
BD	 0.4860	 0.1390
BE	 0.4070	 0.1510
BF	 0.4620	 0.0710
BG	 0.5780	 0.1650
BH	 0.1030	 0.0470
BI	 0.1090	 0.0710
BJ	 0.5340	 0.1320
BK	 0.3750	 0.1530
BL	 0.5310	 0.1540
BM	 0.5040	 0.1650
BN	 0.5740	 0.1350
BO	 0.6290	 0.1580
BP	 0.4370	 0.1500
BQ	 0.5610	 0.1150
BR	 0.4970	 0.1460
BS	 0.4900	 0.1310
BT	 0.5000	 0.1400
BU	 0.4470	 0.1040
BV	 0.5810	 0.1310
BW	 0.5240	 0.1290
BX	 0.5060	 0.1570
BY	 0.5390	 0.1350
BZ	 0.5540	 0.1400