



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 09:40 am BST

PDB ID : 6ZTJ / pdb_00006ztj
EMDB ID : EMD-11418
Title : E. coli 70S-RNAP expressome complex in NusG-coupled state (38 nt intervening mRNA)
Authors : Webster, M.W.; Takacs, M.; Weixlbaumer, A.
Deposited on : 2020-07-20
Resolution : 3.40 Å (reported)
Based on initial models : 4YBB, 6ALH

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:

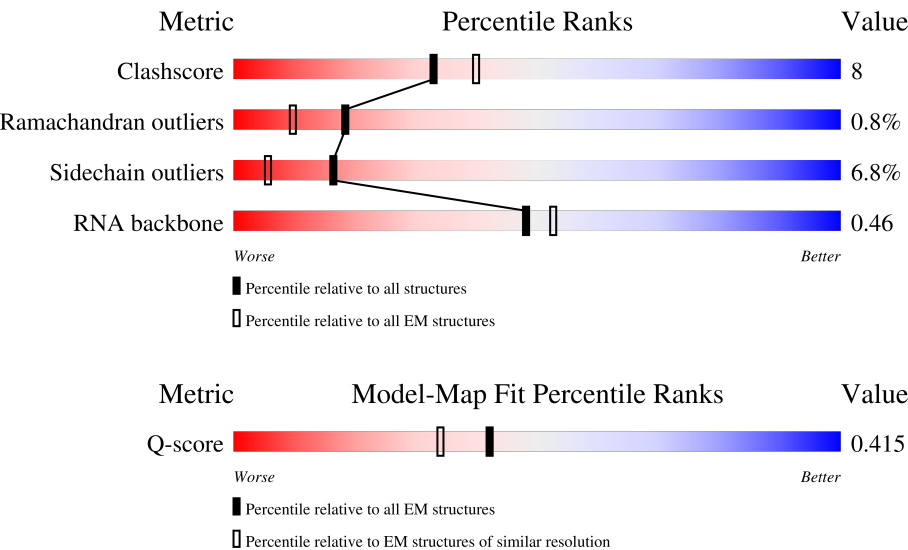
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal 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 i

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	
3	AC	233	

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Mol	Chain	Length	Quality of chain
4	AD	206	
5	AE	167	
6	AF	131	
7	AG	156	
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	53	
23	AW	77	
24	AX	76	
25	AY	557	
26	BA	2904	
27	BB	120	
28	BC	273	

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Mol	Chain	Length	Quality of chain
29	BD	209	
30	BE	201	
31	BF	179	
32	BG	177	
33	BH	149	
34	BI	165	
35	BJ	142	
36	BK	142	
37	BL	123	
38	BM	144	
39	BN	136	
40	BO	127	
41	BP	117	
42	BQ	115	
43	BR	118	
44	BS	103	
45	BT	110	
46	BU	100	
47	BV	104	
48	BW	94	
49	BX	85	
50	BY	78	
51	BZ	63	
52	B1	59	
53	B2	57	

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Mol	Chain	Length	Quality of chain
54	B3	55	
55	B4	46	
56	B5	65	
57	B6	50	
58	B7	70	
59	CN	39	
60	CT	39	
61	CA	329	
61	CB	329	
62	CC	1342	
63	CD	1407	
64	CE	91	
65	CF	181	

2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 176970 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
			32909	14684	6037	10655	1533		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	226	Total	C	N	O	S	0	0
			1765	1116	317	324	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

- 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	156	Total	C	N	O	S	0	0
			1148	715	217	210	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	9	CYS	GLY	conflict	UNP A0A090BZW5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	153	Total	C	N	O	S	0	0
			1203	750	231	218	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	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	101	Total	C	N	O	S	0	0
			808	504	155	148	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	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	100	Total	C	N	O	S	0	0
			805	499	164	139	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	60	Total	C	N	O	0	0
			494	310	93	91		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	40	Total	C	N	O	P	0	0
			849	381	154	274	40		

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	AW	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 24 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0
			1624	724	290	533	76	1		

- Molecule 25 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	AY	89	Total	C	N	O	0	0
			677	423	112	142		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BA	2900	Total	C	N	O	P	0	0
			62270	27786	11456	20128	2900		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BC	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- 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
			1566	980	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	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BG	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

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

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

- Molecule 34 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 35 is a protein called 50S ribosomal protein L11.

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

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	77	VAL	ILE	conflict	UNP P02413

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BP	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BU	96	Total	C	N	O	S	0	0
			764	484	142	136	2		

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	BV	103	Total	C	N	O		
			789	498	148	143	0	0

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BX	76	Total	C	N	O	S		
			582	360	117	104	1	0	0

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B1	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B2	56	Total	C	N	O	S		
			444	269	94	80	1	0	0

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	B3	53	Total	C	N	O	0	0
			436	281	80	75		

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B4	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B6	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 58 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B7	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 59 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CN	30	Total	C	N	O	P	0	0
			618	294	114	180	30		

- Molecule 60 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CT	30	Total	C	N	O	P	0	0
			606	288	105	183	30		

- Molecule 61 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CA	229	Total	C	N	O	S	0	0
			1775	1106	313	350	6		
61	CB	219	Total	C	N	O	S	0	0
			1684	1051	295	332	6		

- Molecule 62 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	CC	1320	Total	C	N	O	S	0	0
			10415	6535	1815	2021	44		

- Molecule 63 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	CD	1333	Total	C	N	O	S	0	0
			10375	6518	1851	1956	50		

- Molecule 64 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	CE	51	Total	C	N	O	S	0	0
			399	246	77	75	1		

- Molecule 65 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	CF	161	Total	C	N	O	S	0	0
			1283	818	221	237	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CF	121	ALA	LYS	conflict	UNP P0AFG1

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

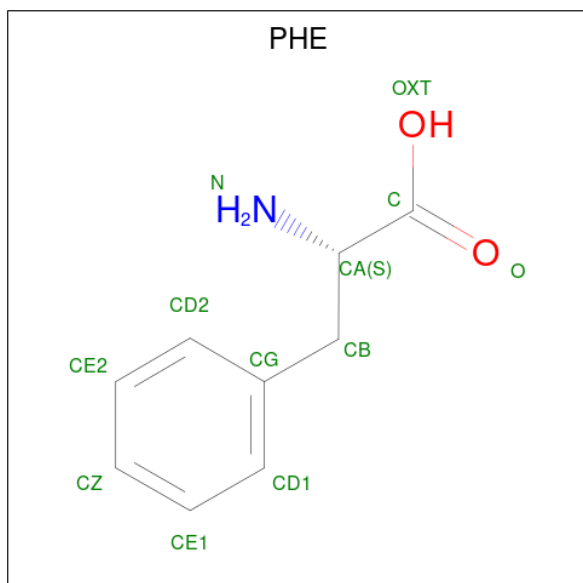
Mol	Chain	Residues	Atoms		AltConf
66	AA	148	Total	Mg	0
			148	148	
66	AI	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
66	AW	1	Total	Mg	0
			1	1	
66	AX	1	Total	Mg	0
			1	1	
66	BA	314	Total	Mg	0
			314	314	
66	BB	6	Total	Mg	0
			6	6	
66	BC	3	Total	Mg	0
			3	3	
66	BD	1	Total	Mg	0
			1	1	
66	BE	1	Total	Mg	0
			1	1	
66	BQ	1	Total	Mg	0
			1	1	
66	BT	1	Total	Mg	0
			1	1	
66	CD	1	Total	Mg	0
			1	1	

- Molecule 67 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
67	AX	1	Total	C	N	O	0
			11	9	1	1	

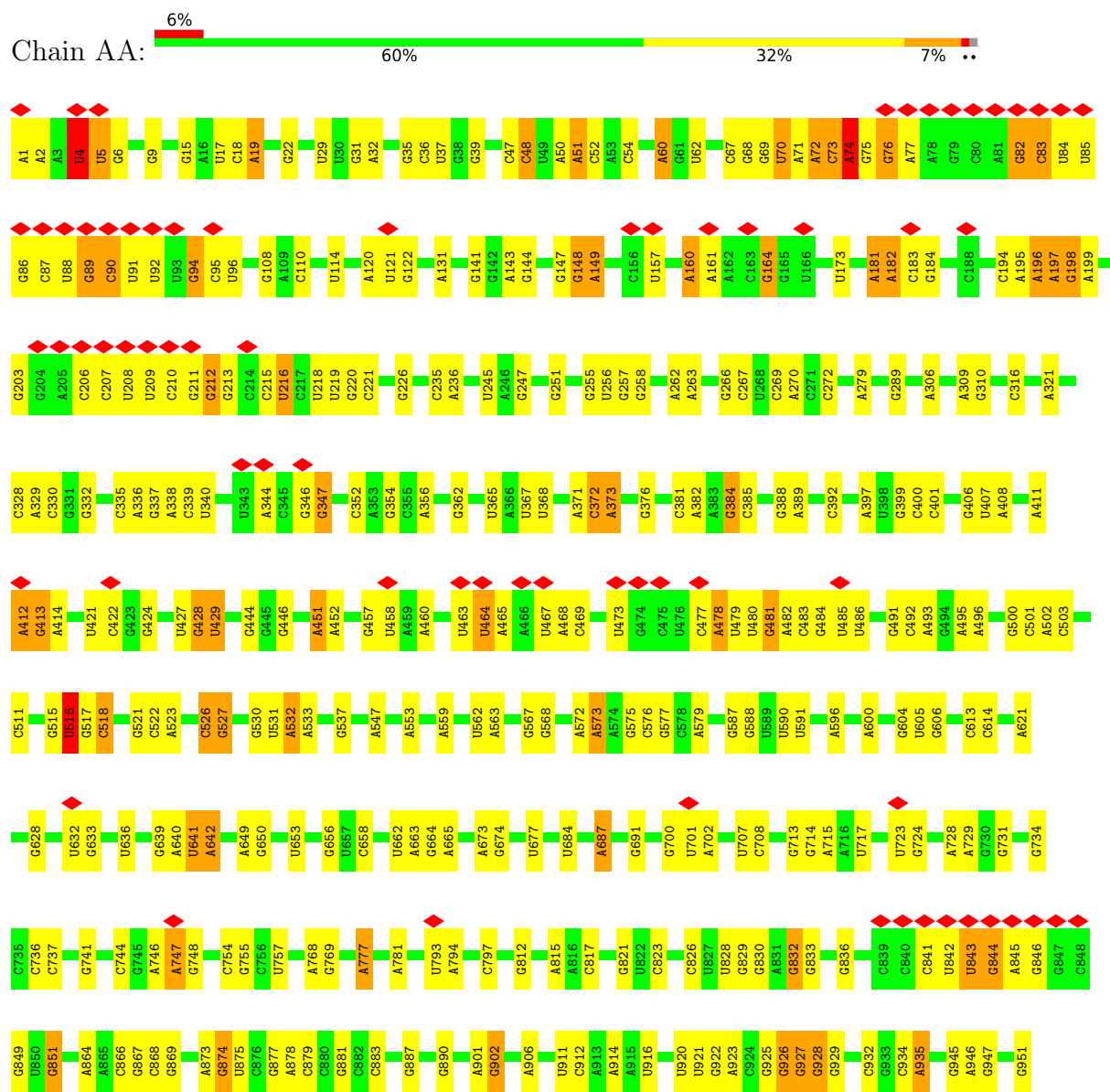
- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

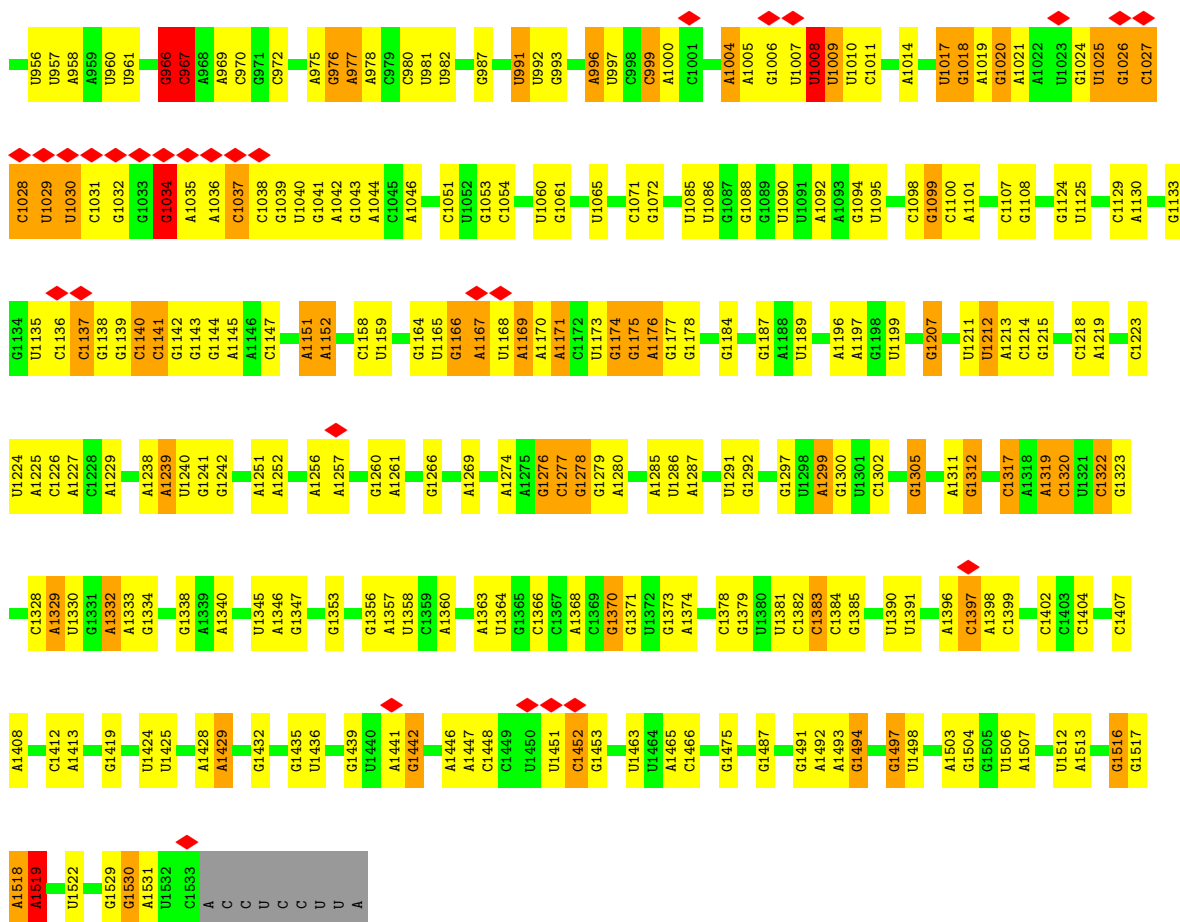
Mol	Chain	Residues	Atoms		AltConf
68	B6	1	Total 1	Zn 1	0
68	B7	1	Total 1	Zn 1	0
68	CD	2	Total 2	Zn 2	0

3 Residue-property plots

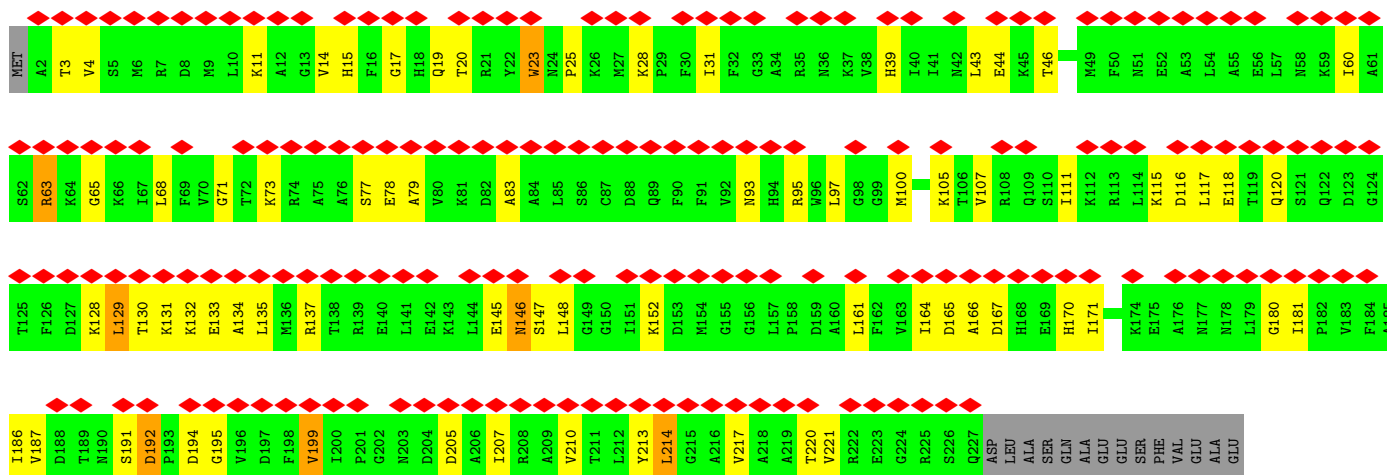
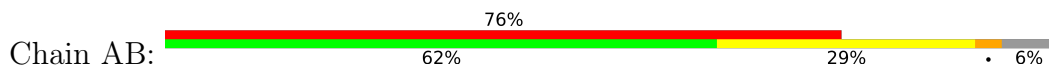
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



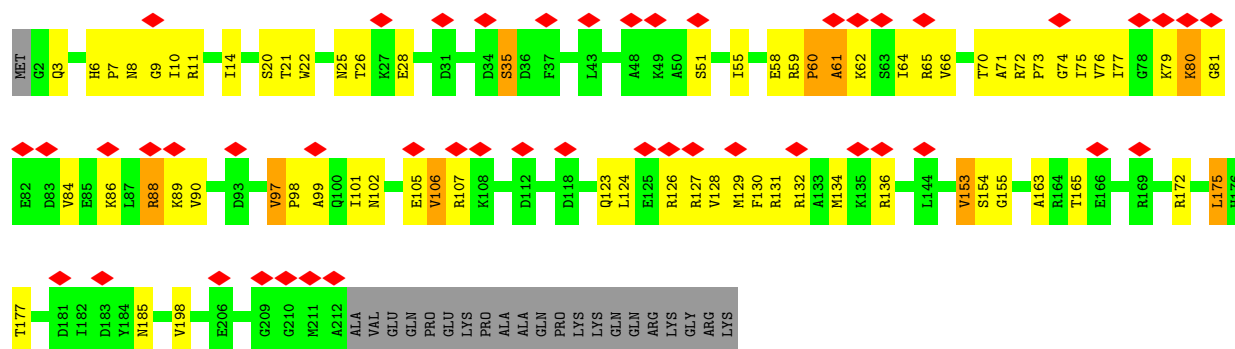


• Molecule 2: 30S ribosomal protein S2

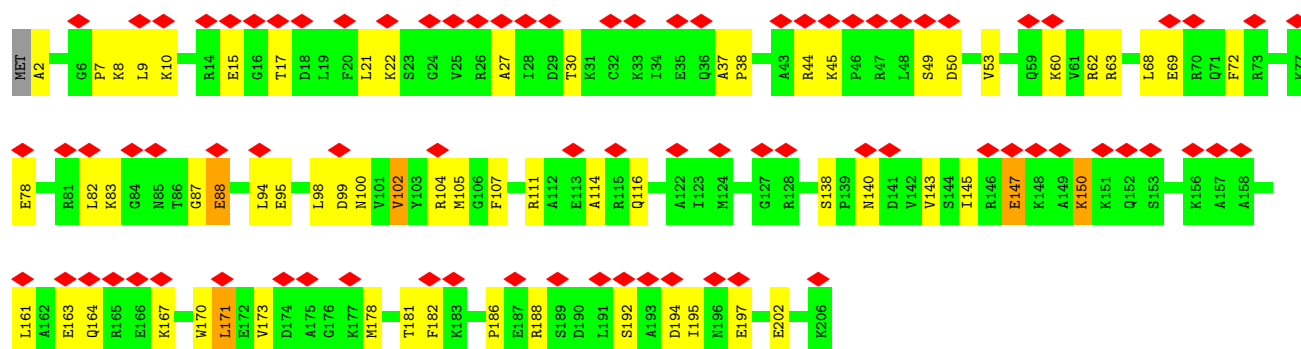


• Molecule 3: 30S ribosomal protein S3

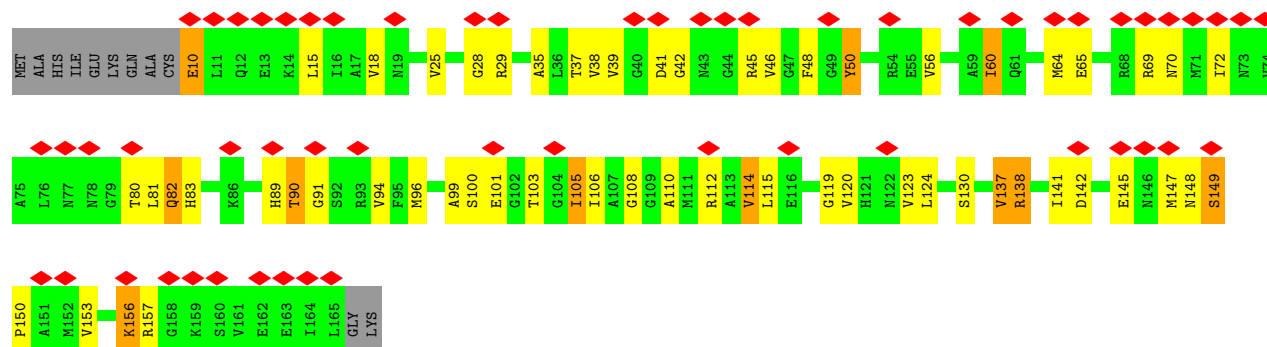




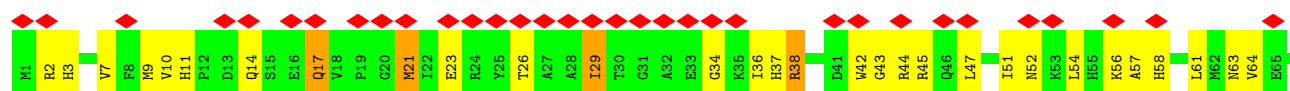
• Molecule 4: 30S ribosomal protein S4

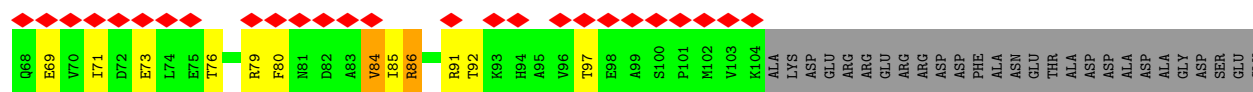


• Molecule 5: 30S ribosomal protein S5

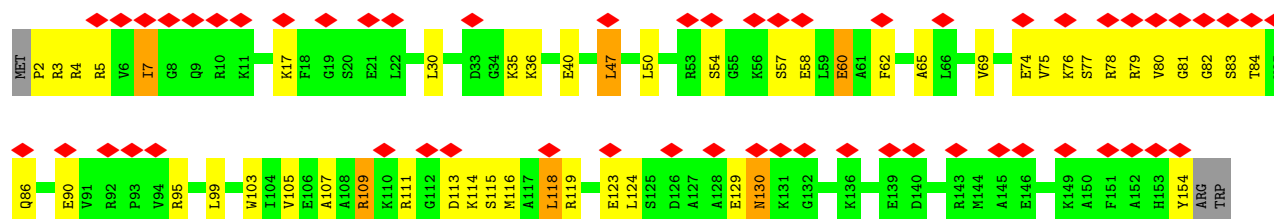
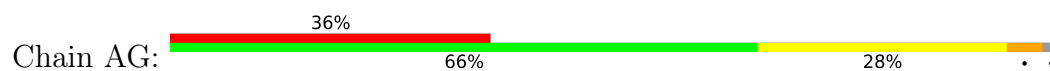


• Molecule 6: 30S ribosomal protein S6

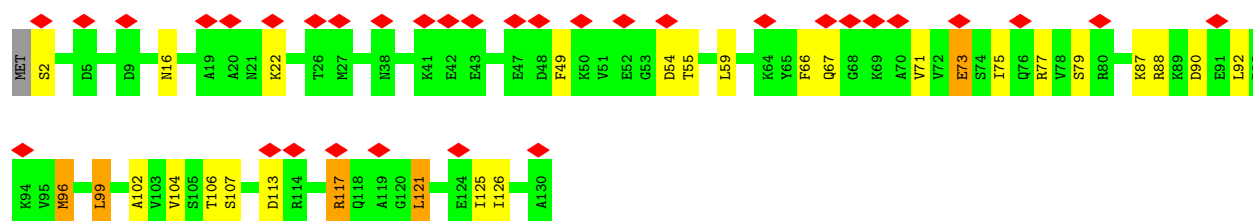
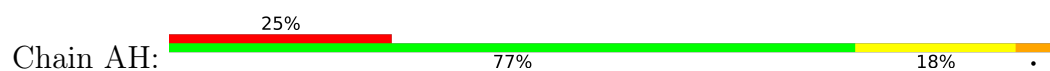




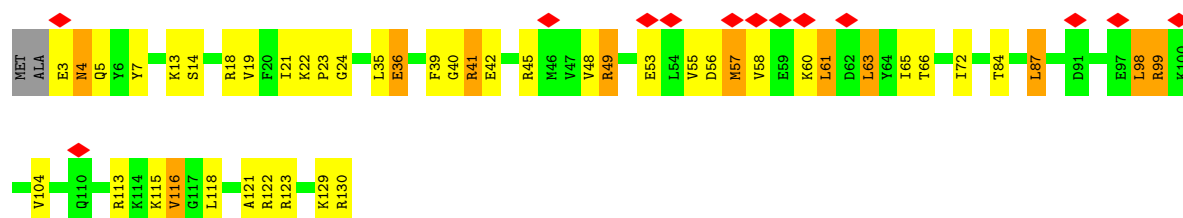
• Molecule 7: 30S ribosomal protein S7



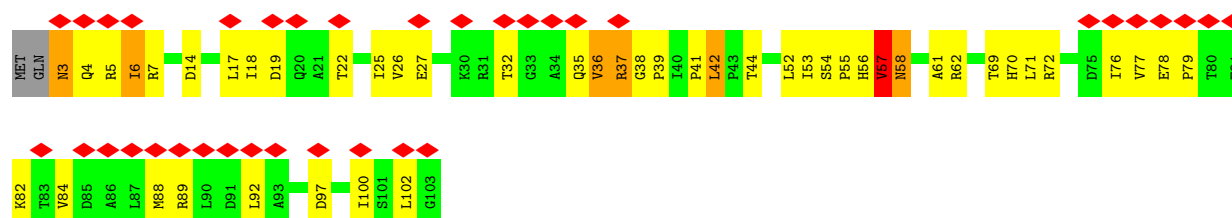
• Molecule 8: 30S ribosomal protein S8



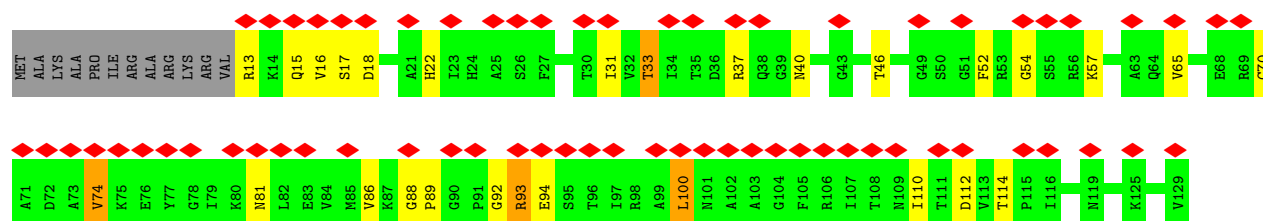
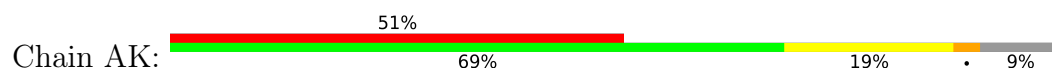
• Molecule 9: 30S ribosomal protein S9



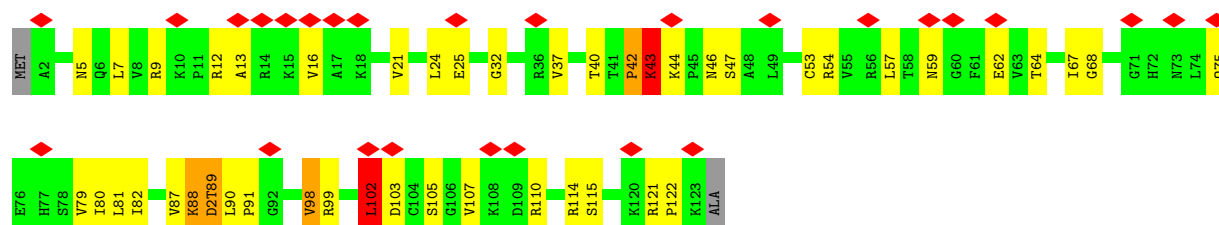
• Molecule 10: 30S ribosomal protein S10



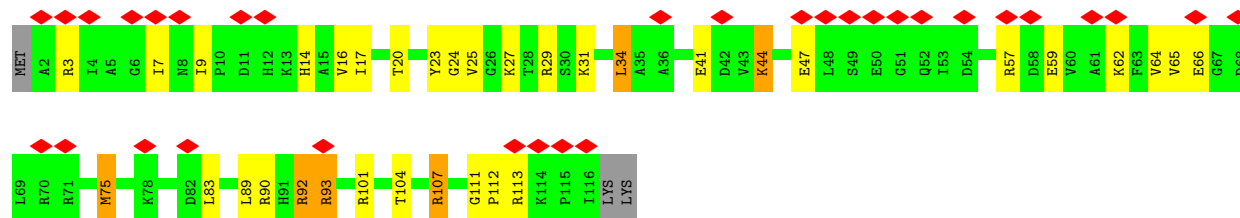
• Molecule 11: 30S ribosomal protein S11



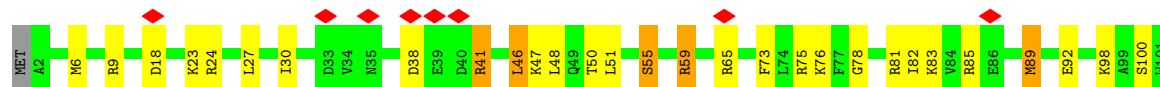
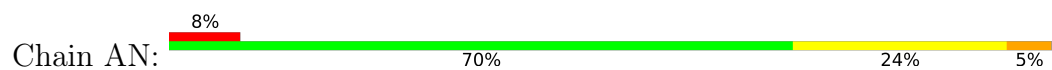
- Molecule 12: 30S ribosomal protein S12



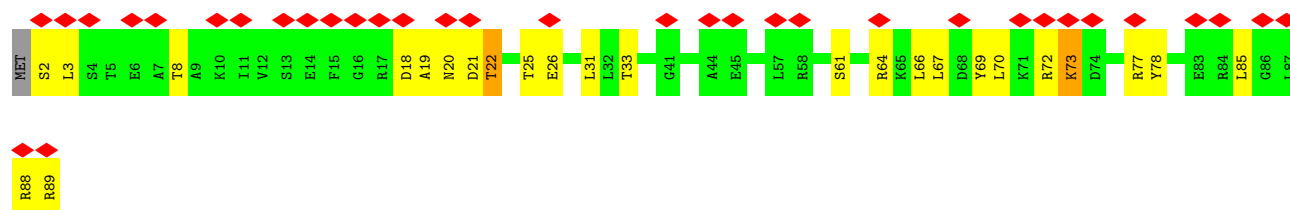
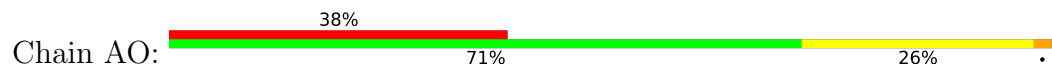
- Molecule 13: 30S ribosomal protein S13



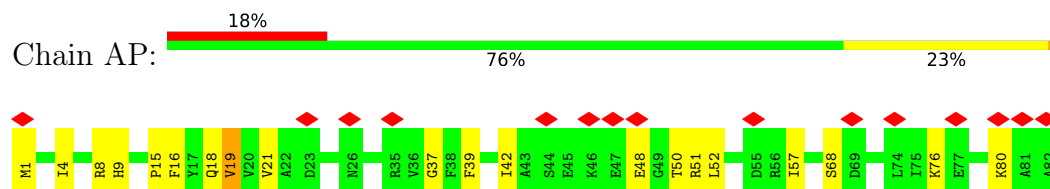
- Molecule 14: 30S ribosomal protein S14



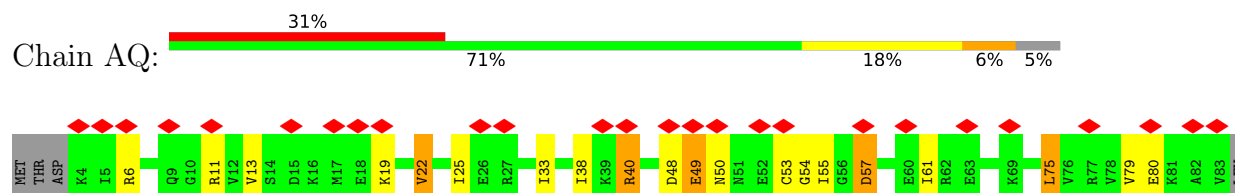
- Molecule 15: 30S ribosomal protein S15



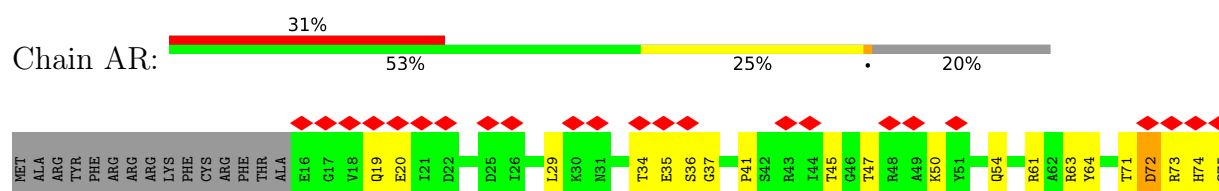
- Molecule 16: 30S ribosomal protein S16



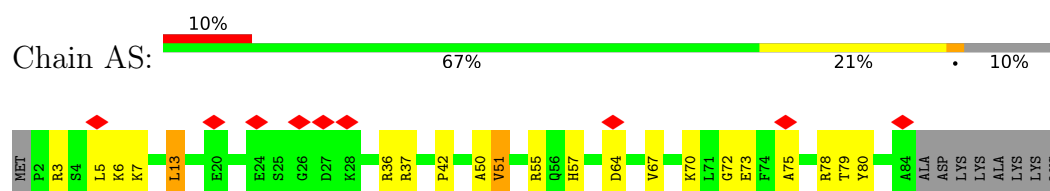
- Molecule 17: 30S ribosomal protein S17



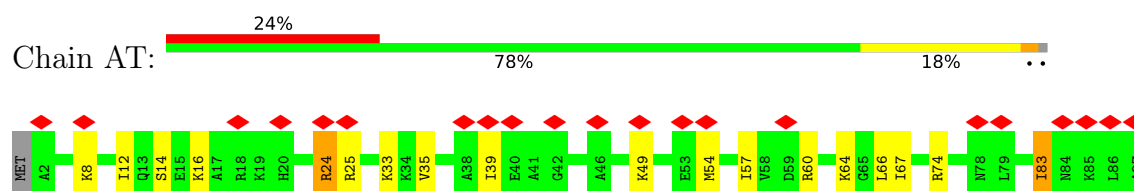
- Molecule 18: 30S ribosomal protein S18



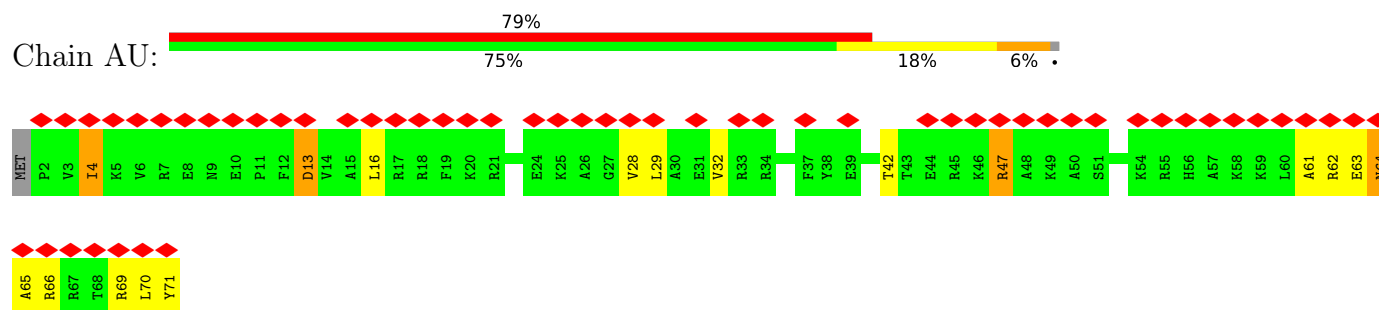
- Molecule 19: 30S ribosomal protein S19



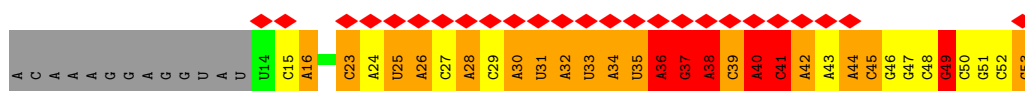
- Molecule 20: 30S ribosomal protein S20



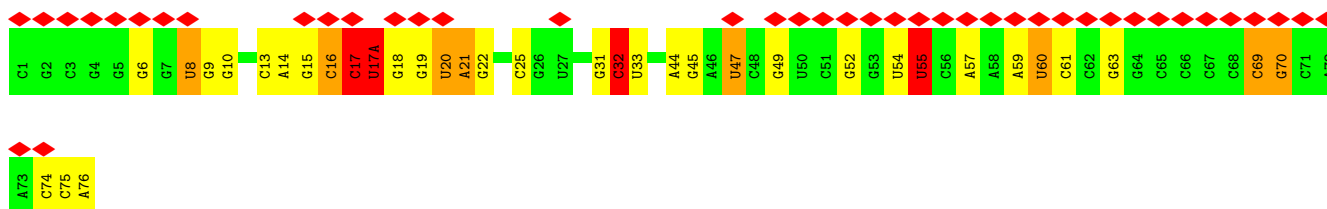
- Molecule 21: 30S ribosomal protein S21



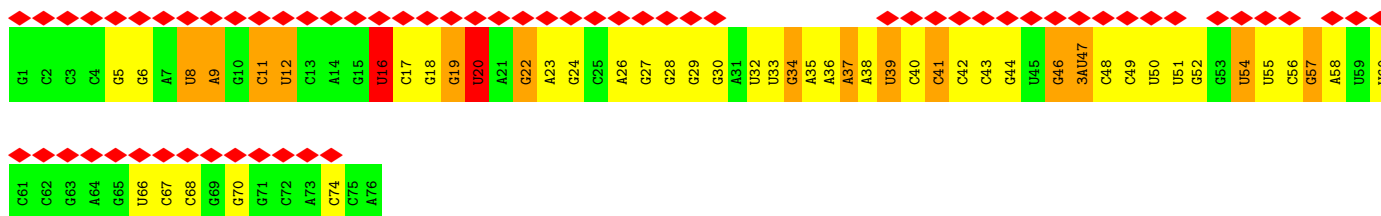
- Molecule 22: mRNA



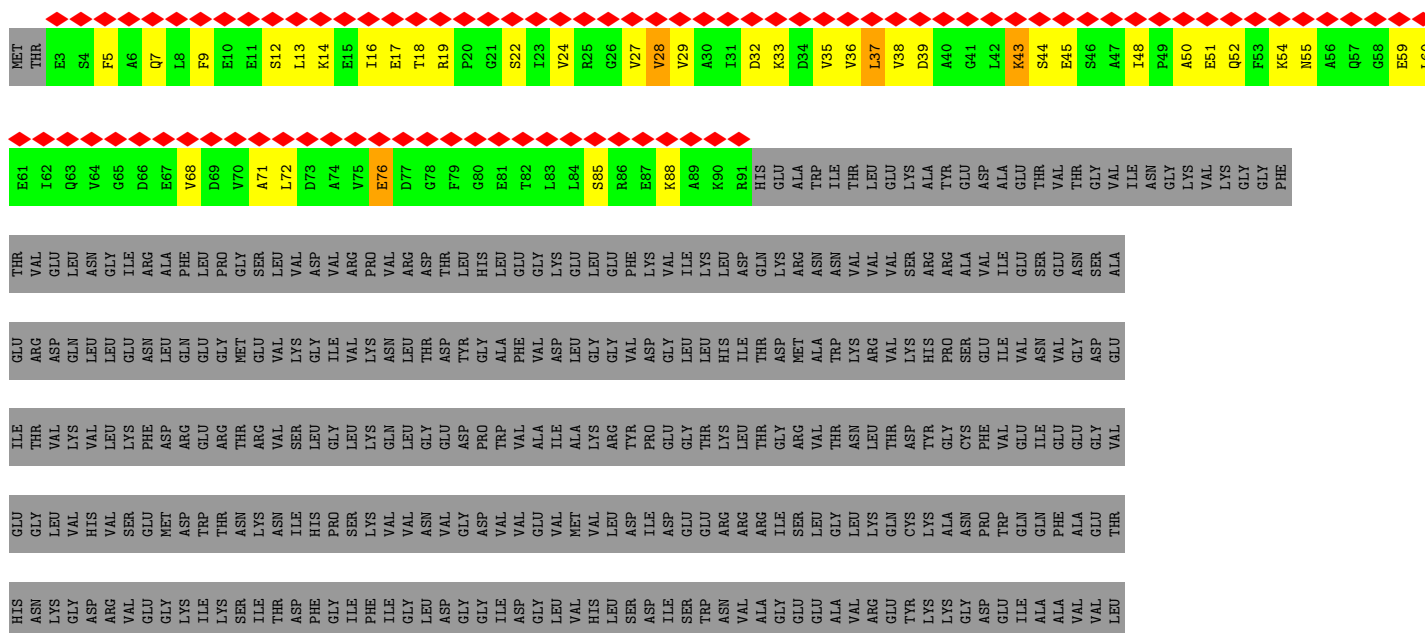
Chain AW:



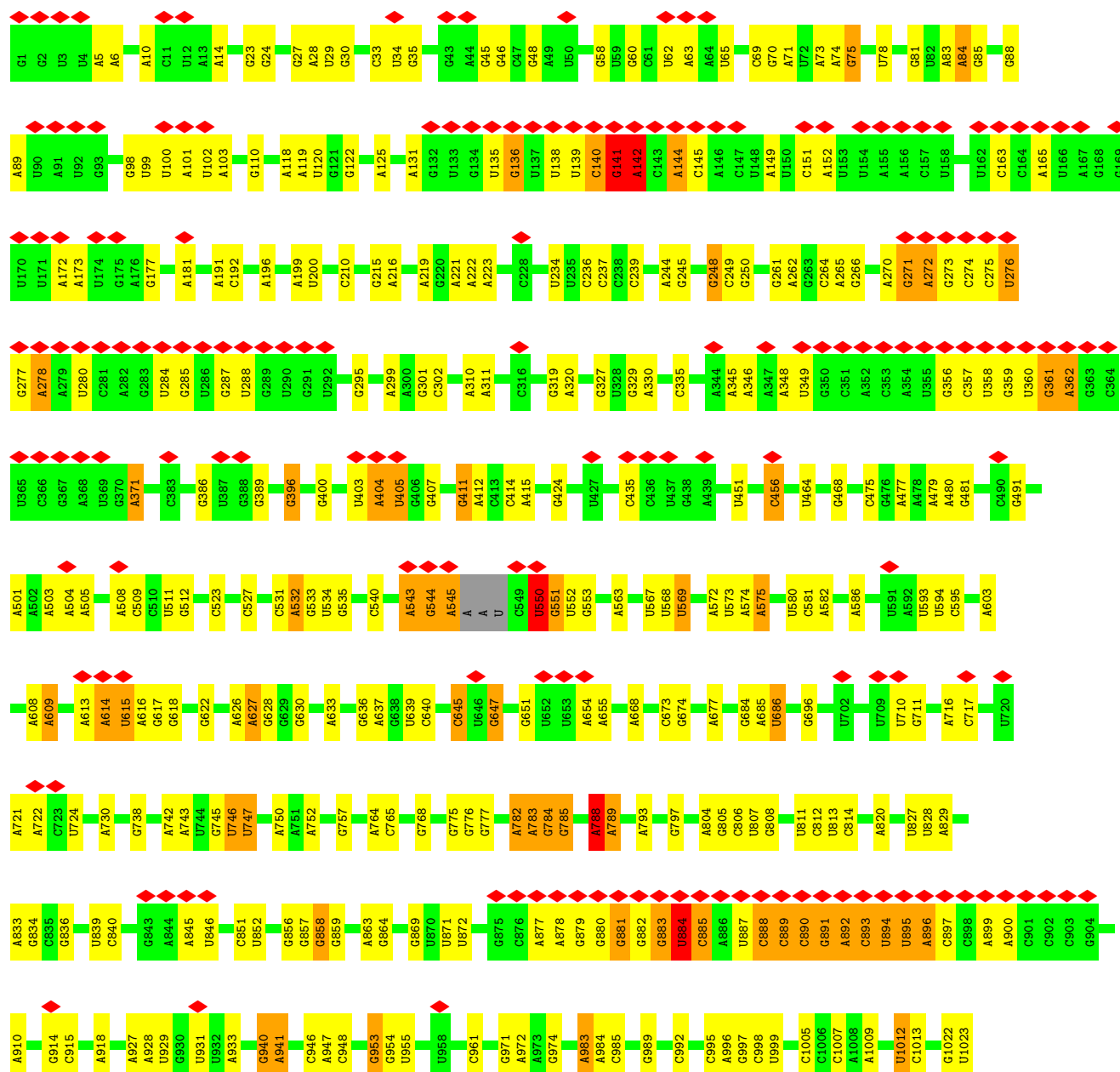
Chain AX:

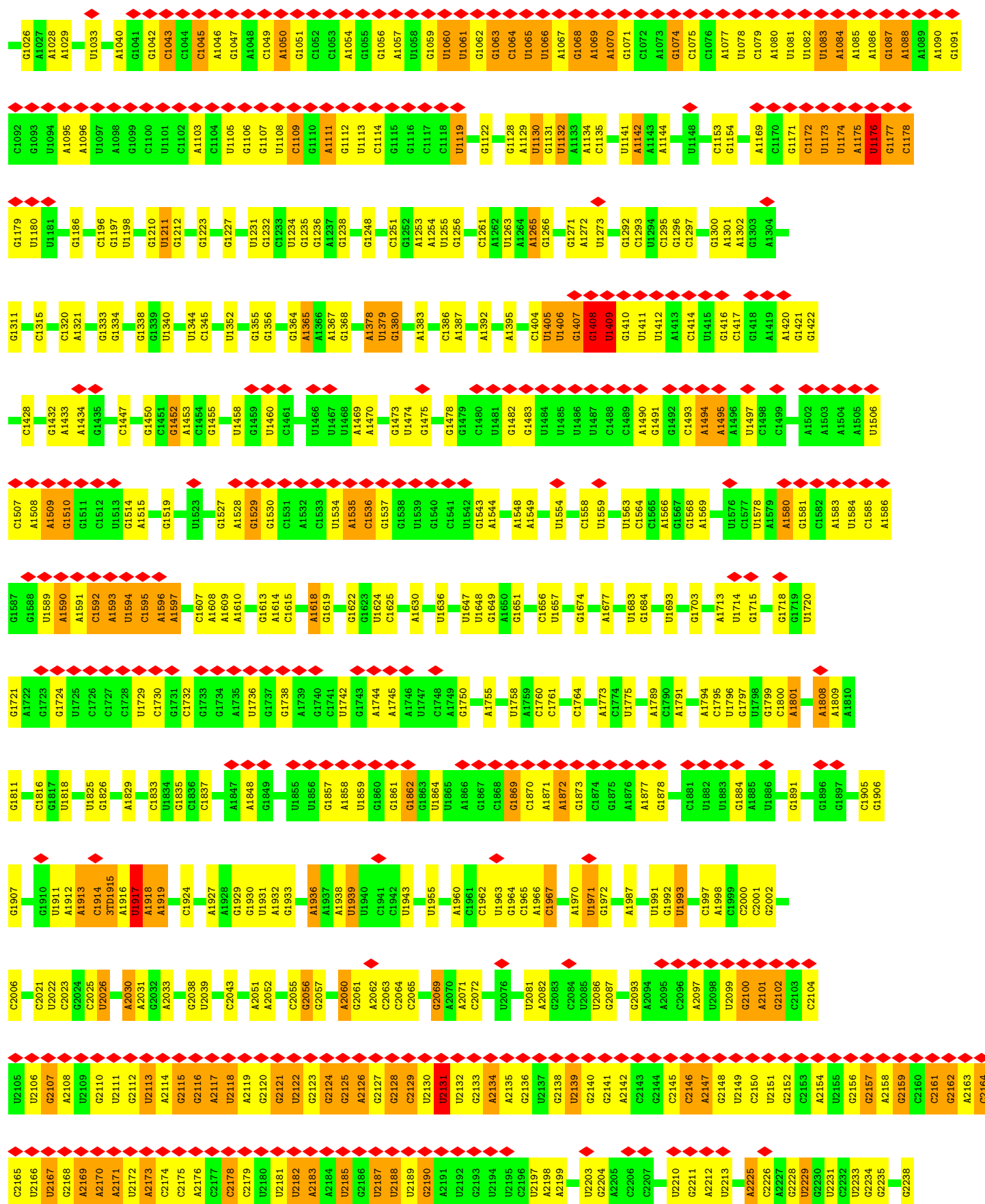


Chain AY:

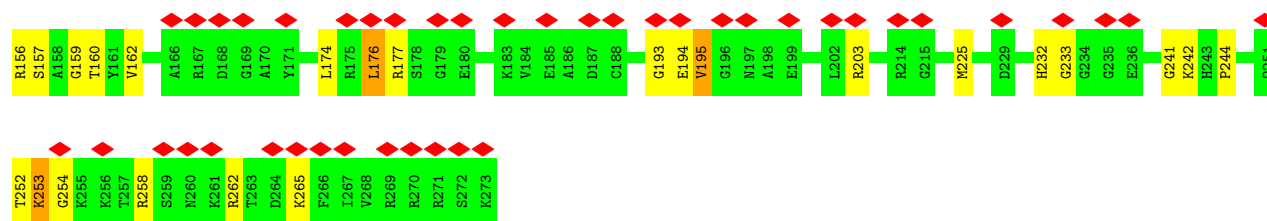


- Molecule 26: 23S ribosomal RNA

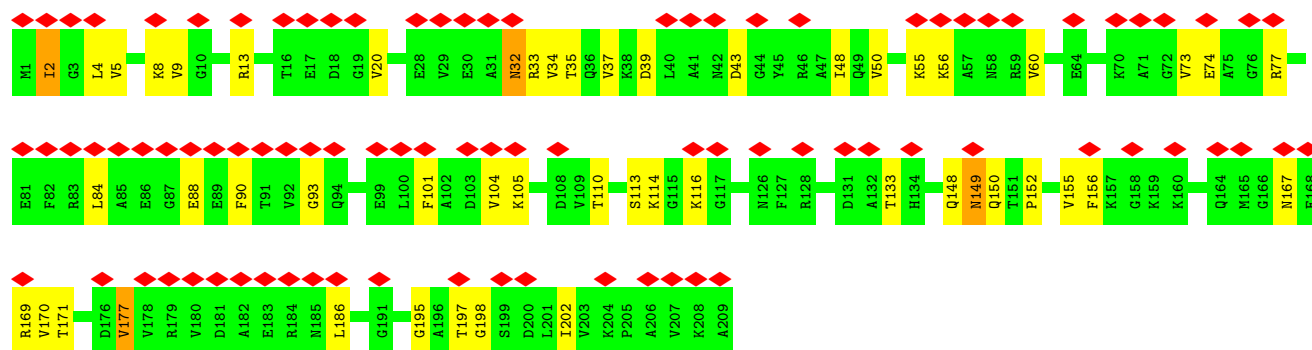
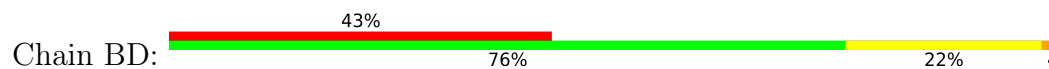




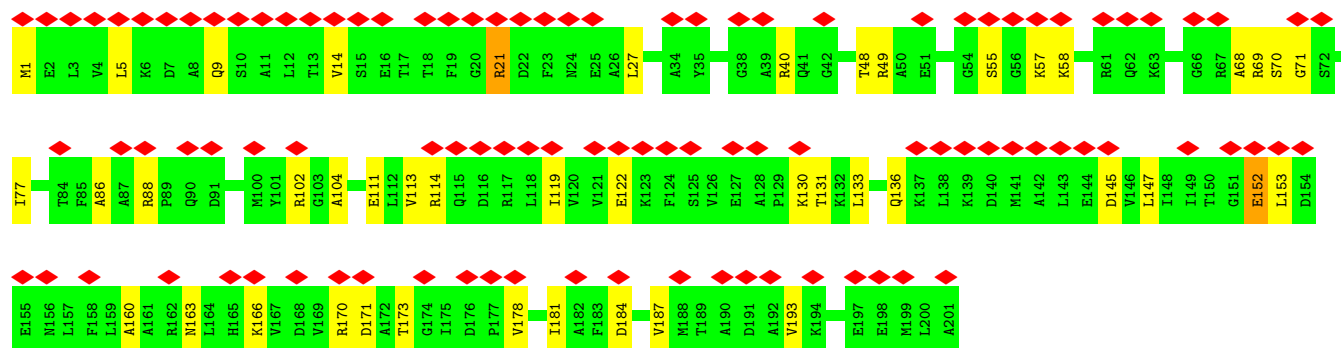
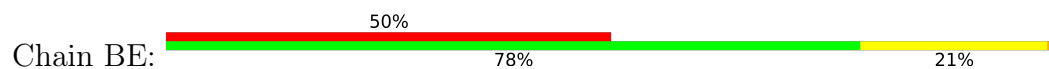




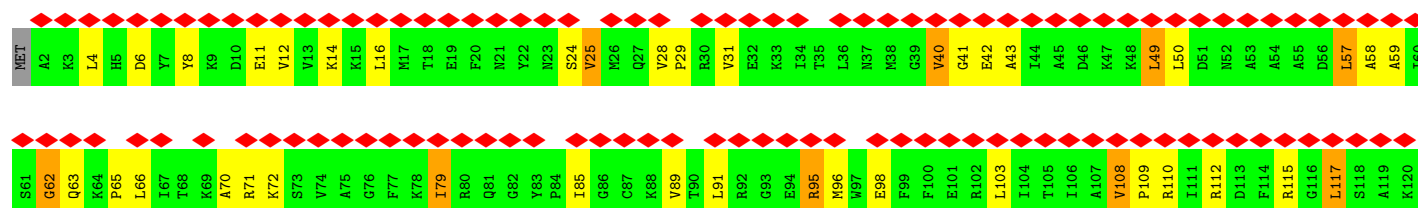
• Molecule 29: 50S ribosomal protein L3

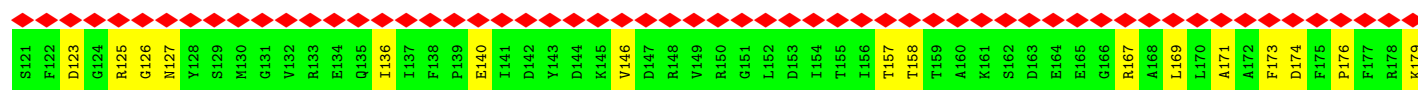


• Molecule 30: 50S ribosomal protein L4

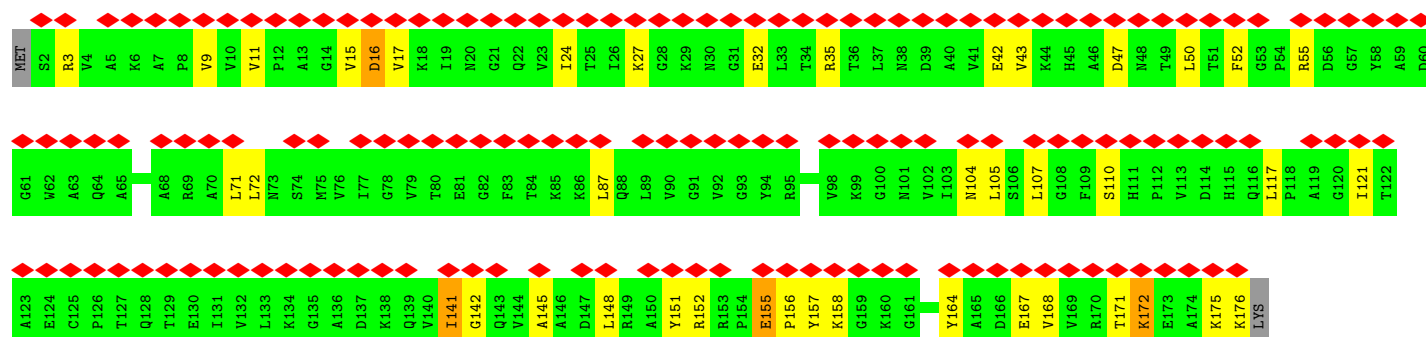
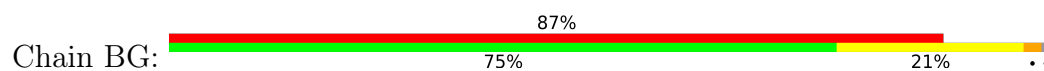


• Molecule 31: 50S ribosomal protein L5

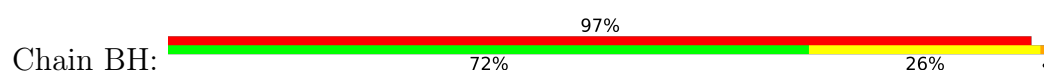




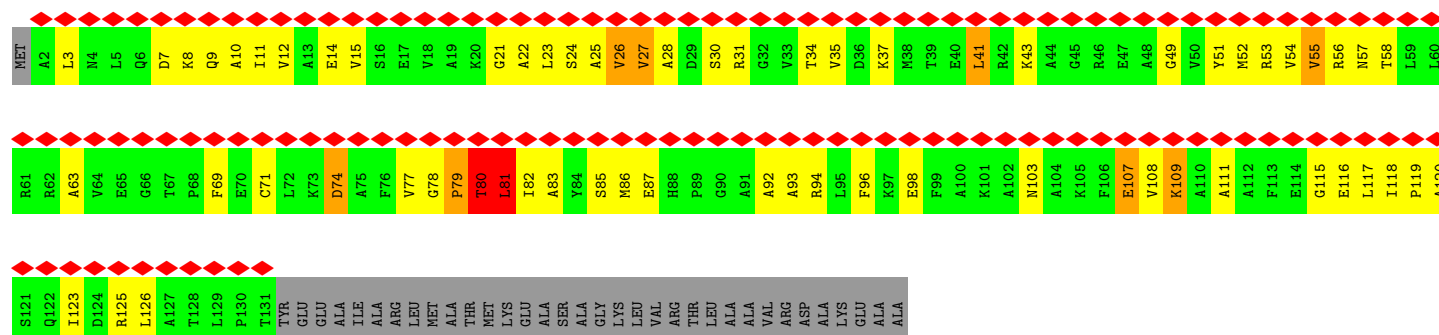
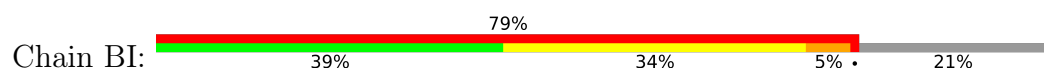
• Molecule 32: 50S ribosomal protein L6



• Molecule 33: 50S ribosomal protein L9



• Molecule 34: 50S ribosomal protein L10

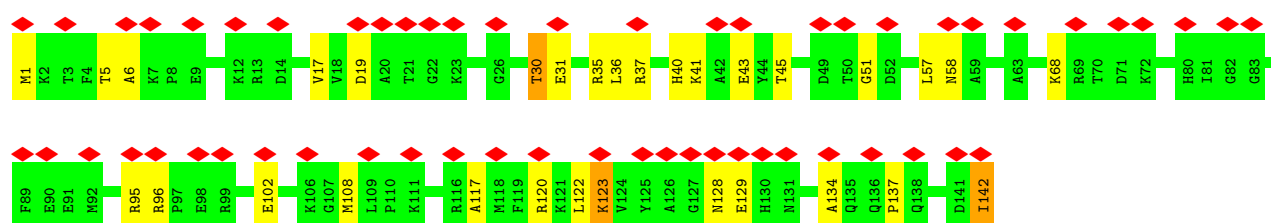
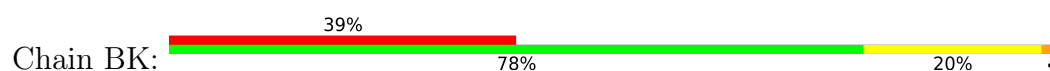


• Molecule 35: 50S ribosomal protein L11

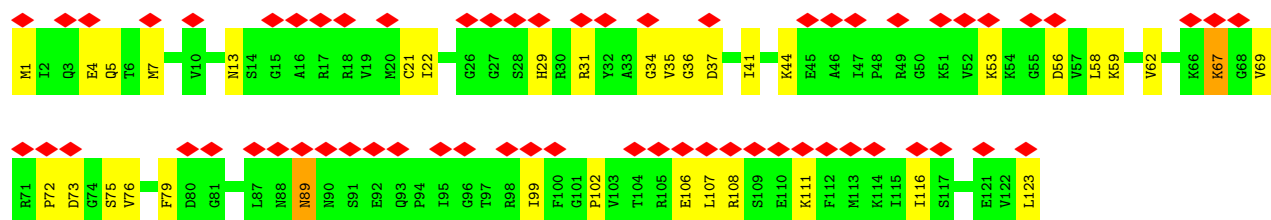
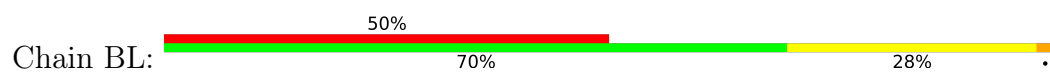




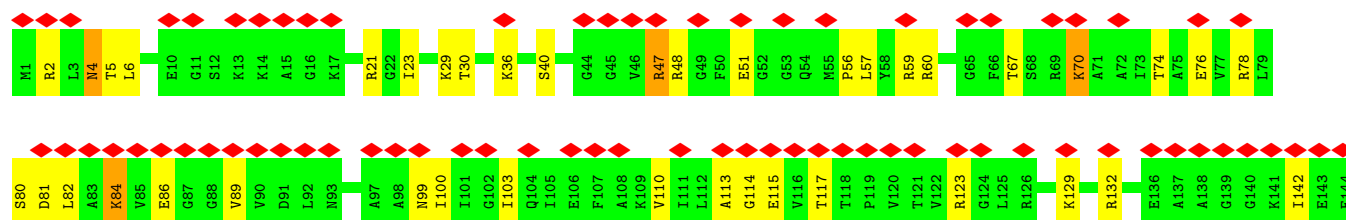
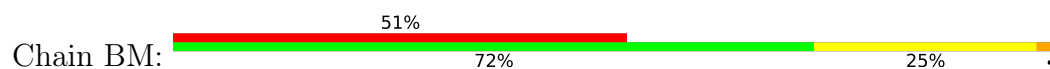
• Molecule 36: 50S ribosomal protein L13



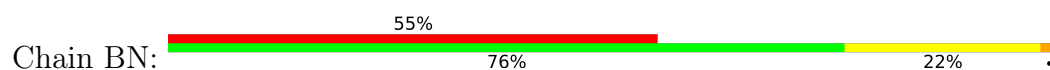
• Molecule 37: 50S ribosomal protein L14

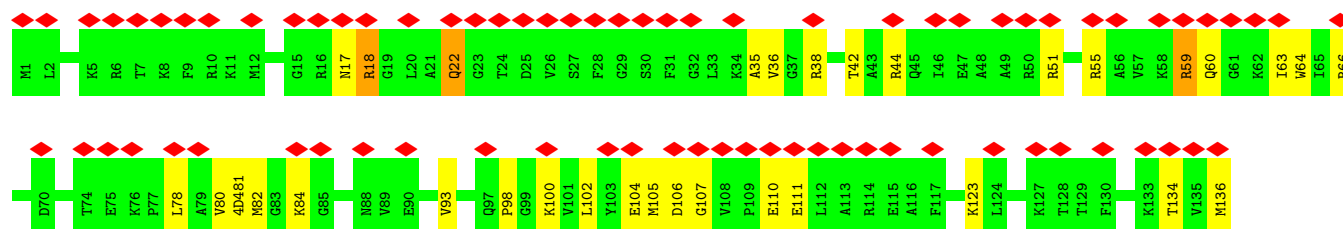


• Molecule 38: 50S ribosomal protein L15

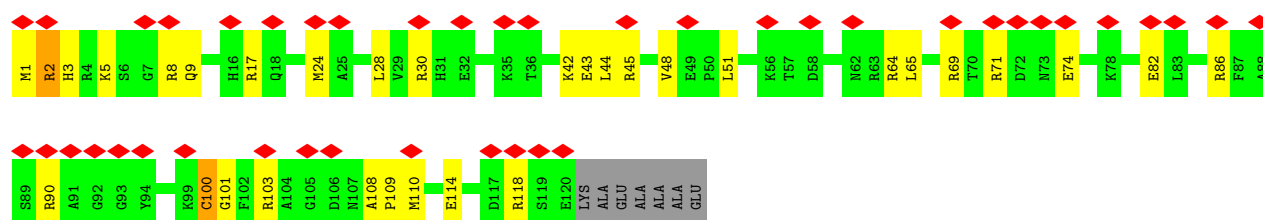


• Molecule 39: 50S ribosomal protein L16

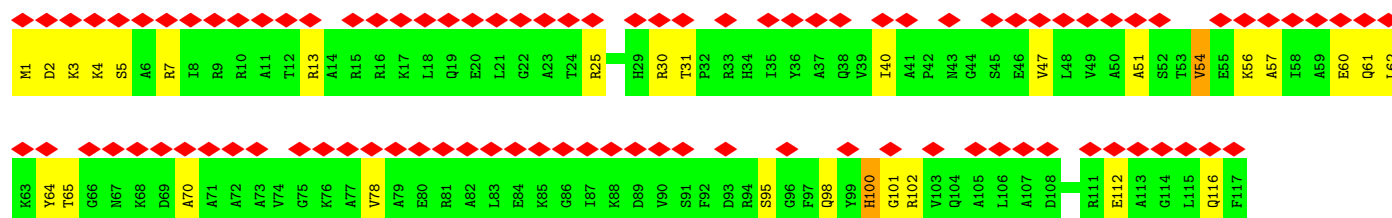
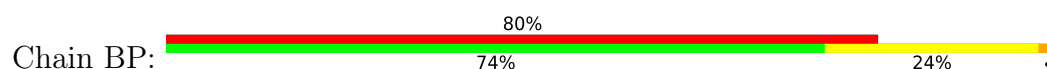




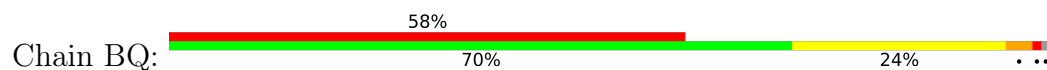
• Molecule 40: 50S ribosomal protein L17



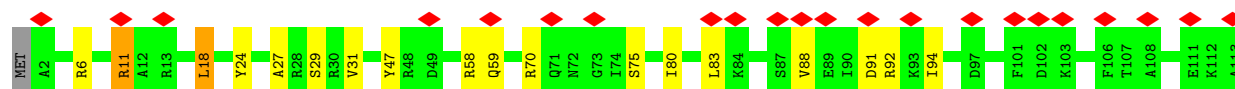
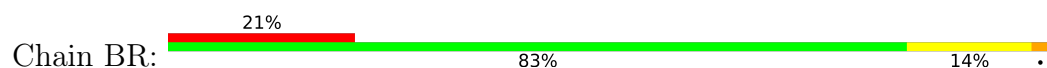
• Molecule 41: 50S ribosomal protein L18



• Molecule 42: 50S ribosomal protein L19

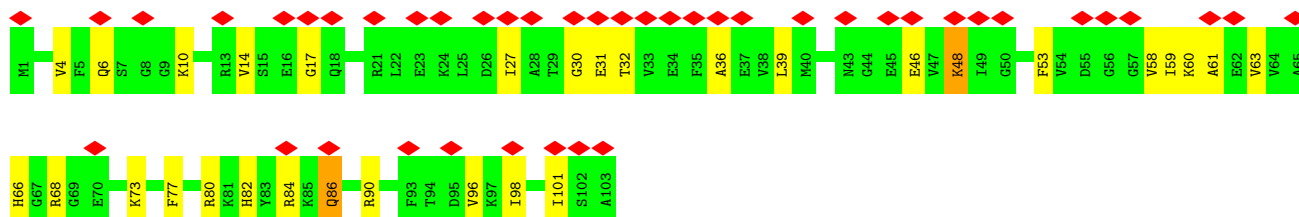
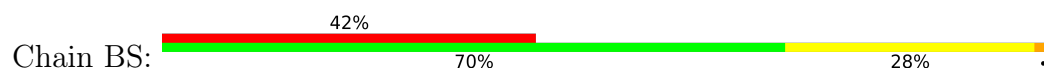


• Molecule 43: 50S ribosomal protein L20

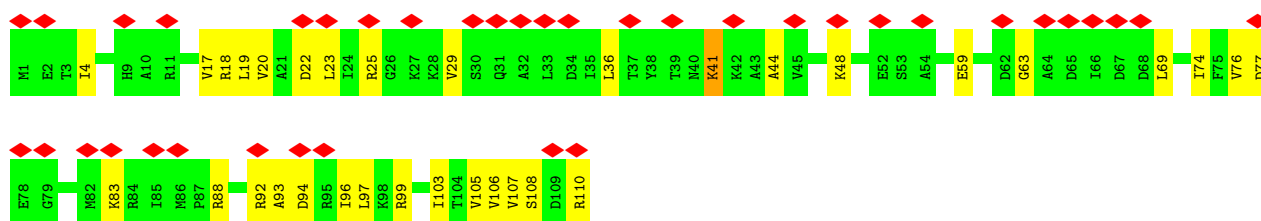
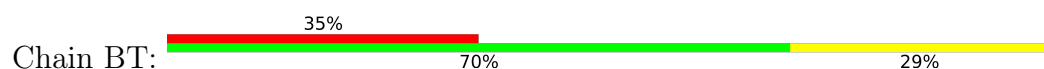




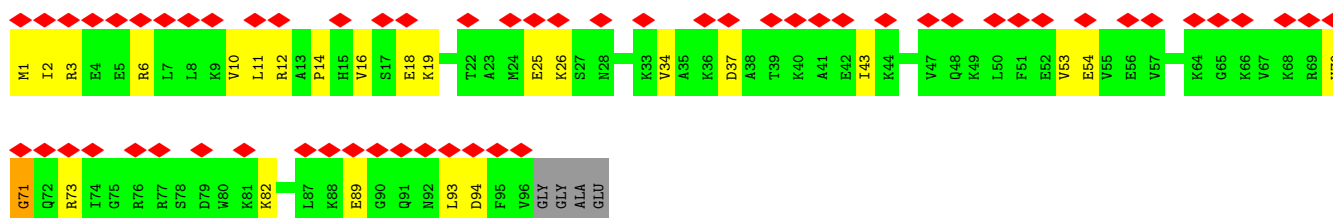
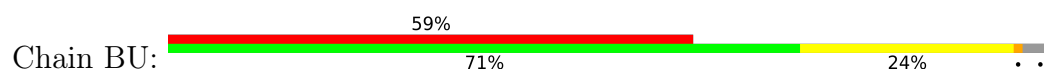
- Molecule 44: 50S ribosomal protein L21



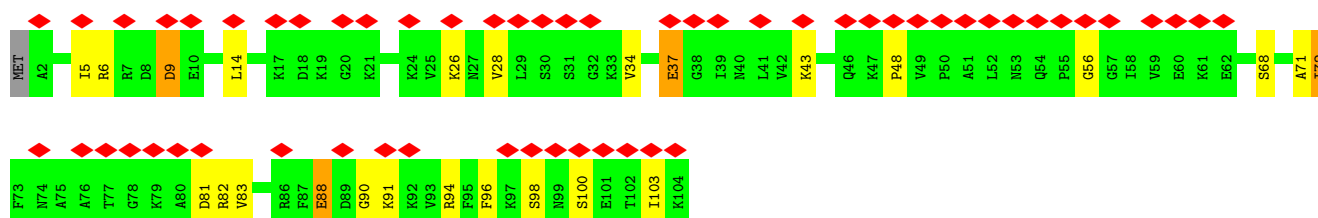
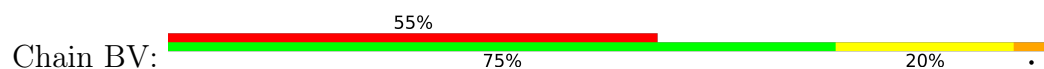
- Molecule 45: 50S ribosomal protein L22



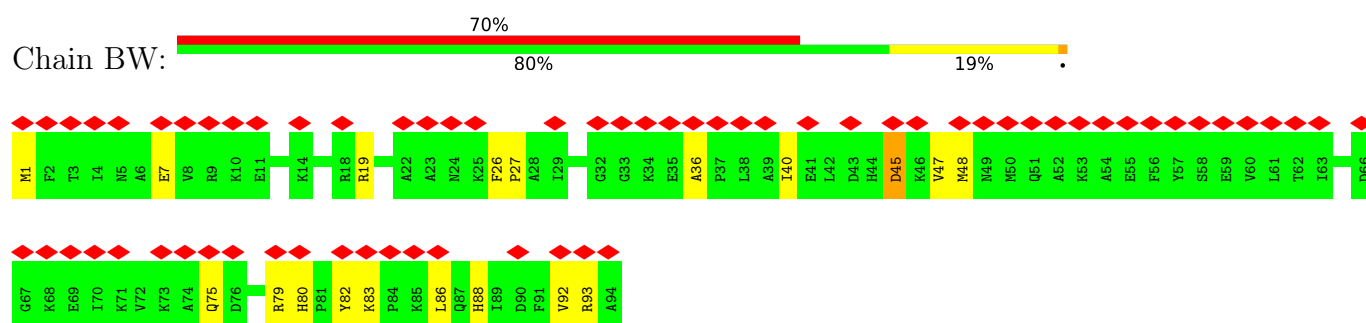
- Molecule 46: 50S ribosomal protein L23



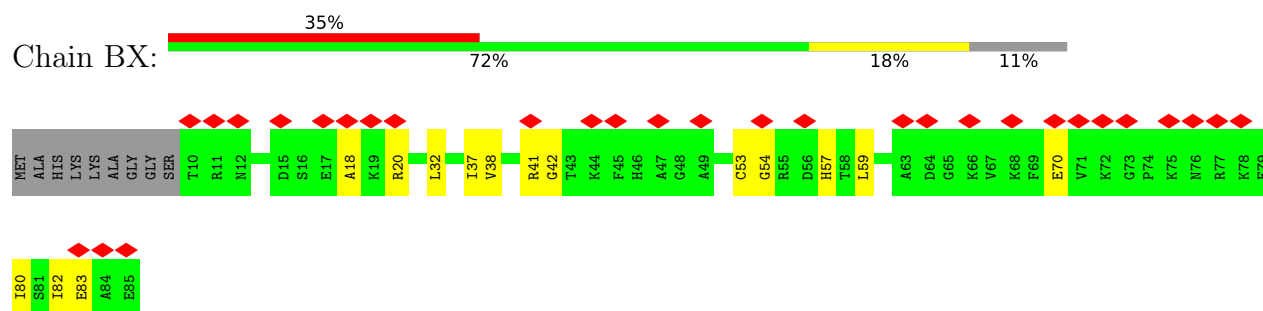
- Molecule 47: 50S ribosomal protein L24



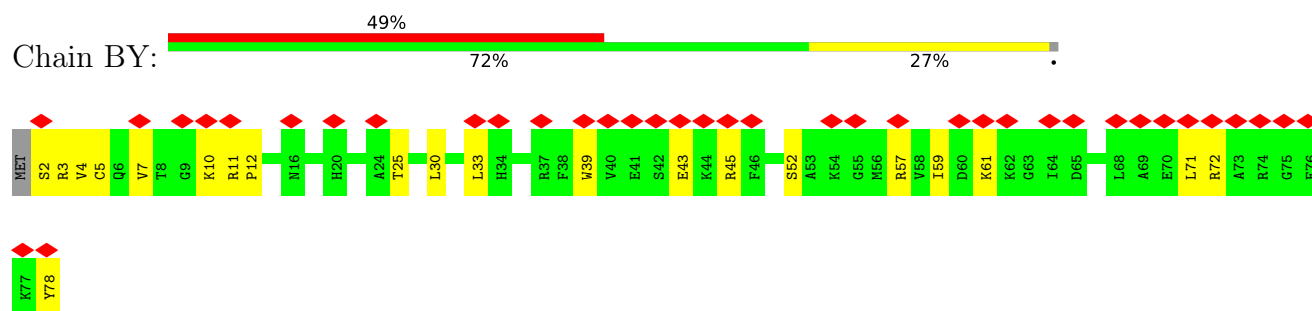
- Molecule 48: 50S ribosomal protein L25



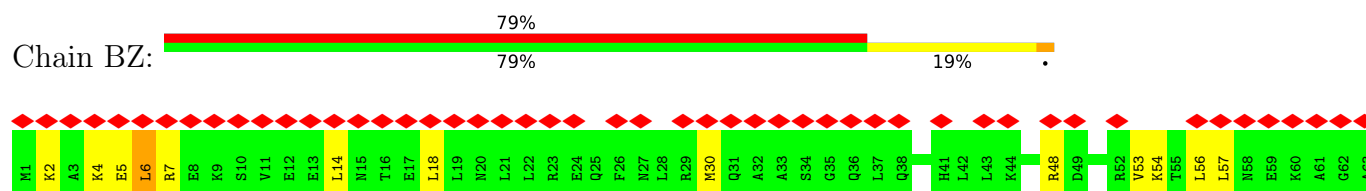
- Molecule 49: 50S ribosomal protein L27



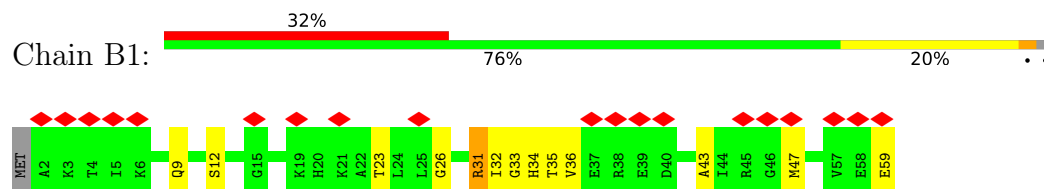
- Molecule 50: 50S ribosomal protein L28



- Molecule 51: 50S ribosomal protein L29

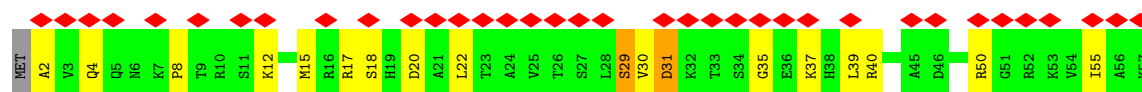


- Molecule 52: 50S ribosomal protein L30

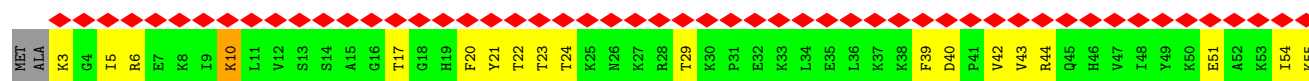


- Molecule 53: 50S ribosomal protein L32

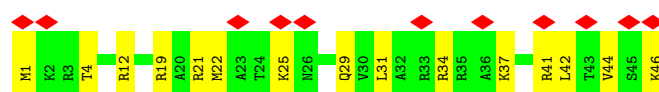




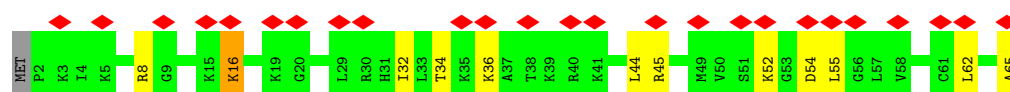
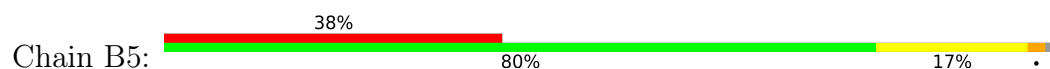
- Molecule 54: 50S ribosomal protein L33



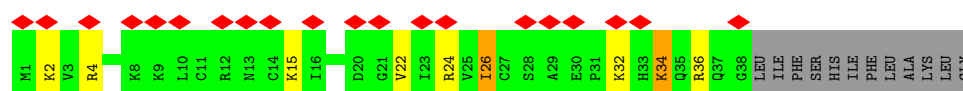
- Molecule 55: 50S ribosomal protein L34



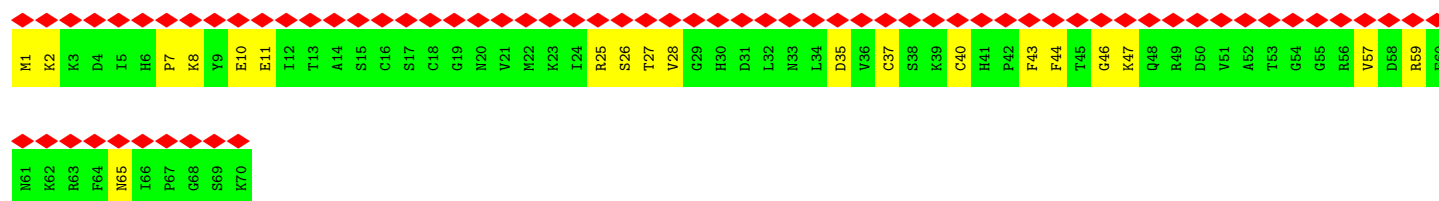
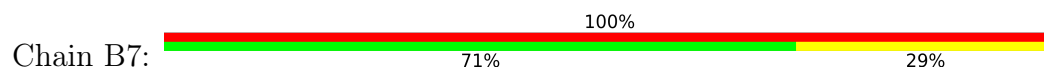
- Molecule 56: 50S ribosomal protein L35



- Molecule 57: 50S ribosomal protein L36



- Molecule 58: 50S ribosomal protein L31

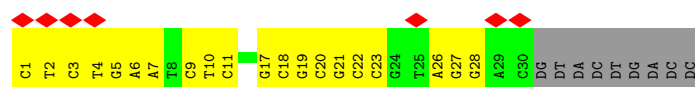


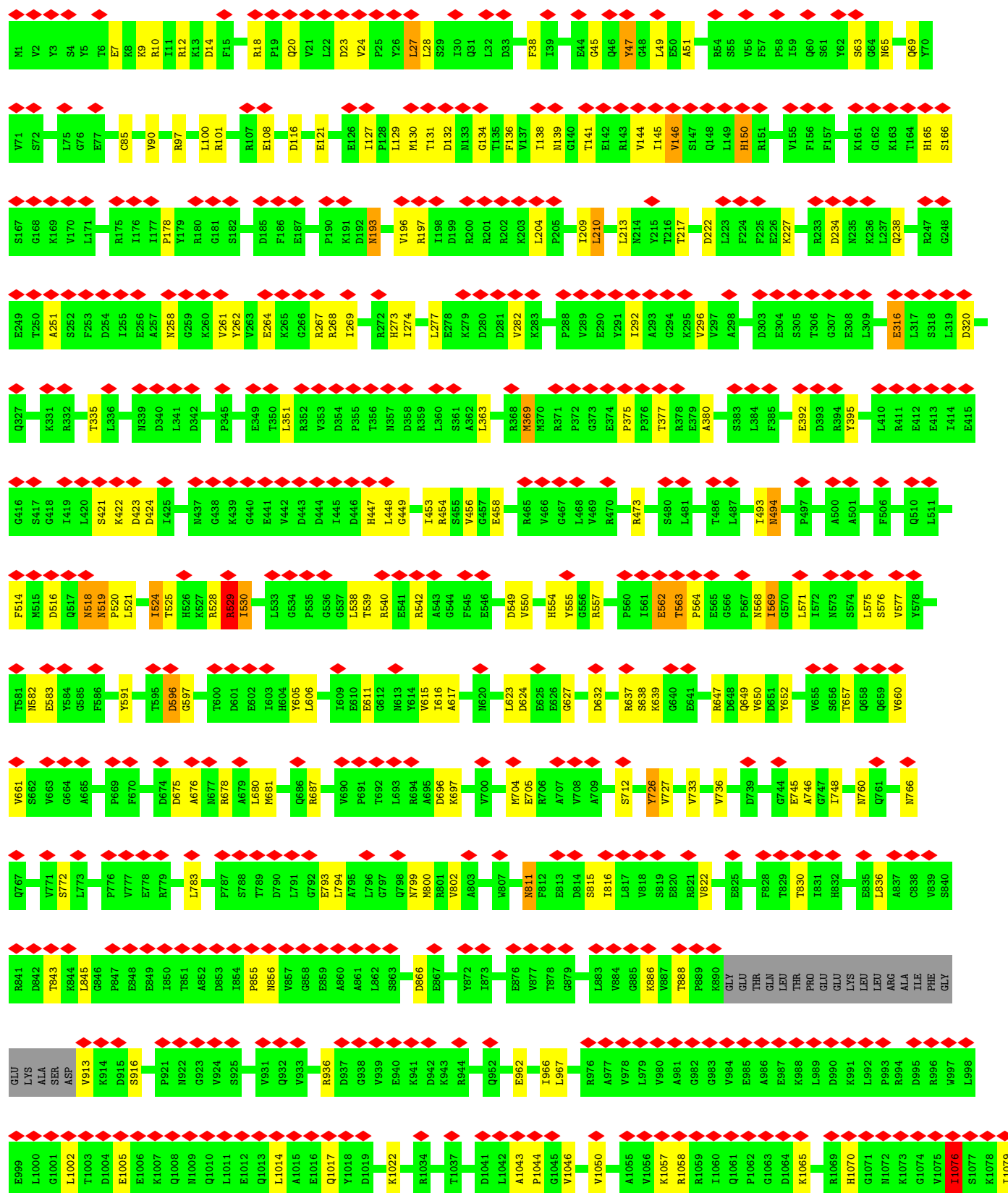
- Molecule 59: Non-template DNA strand

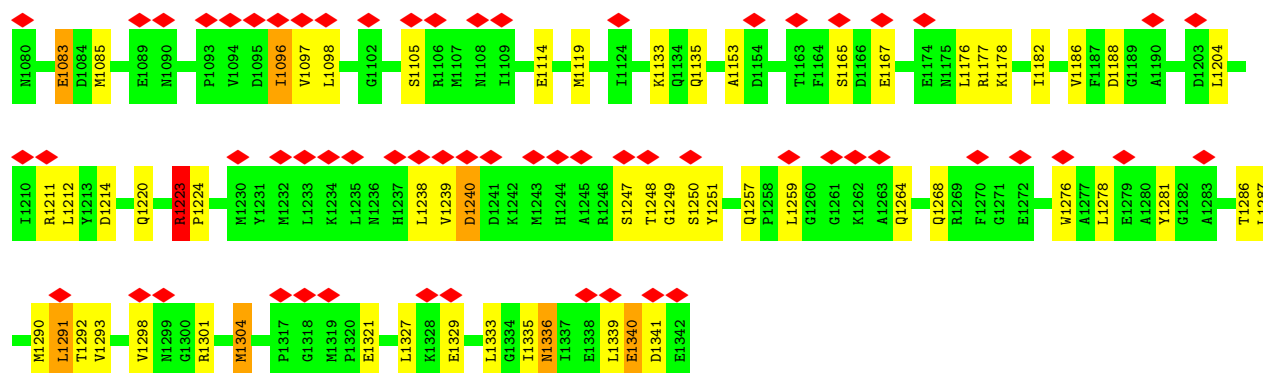




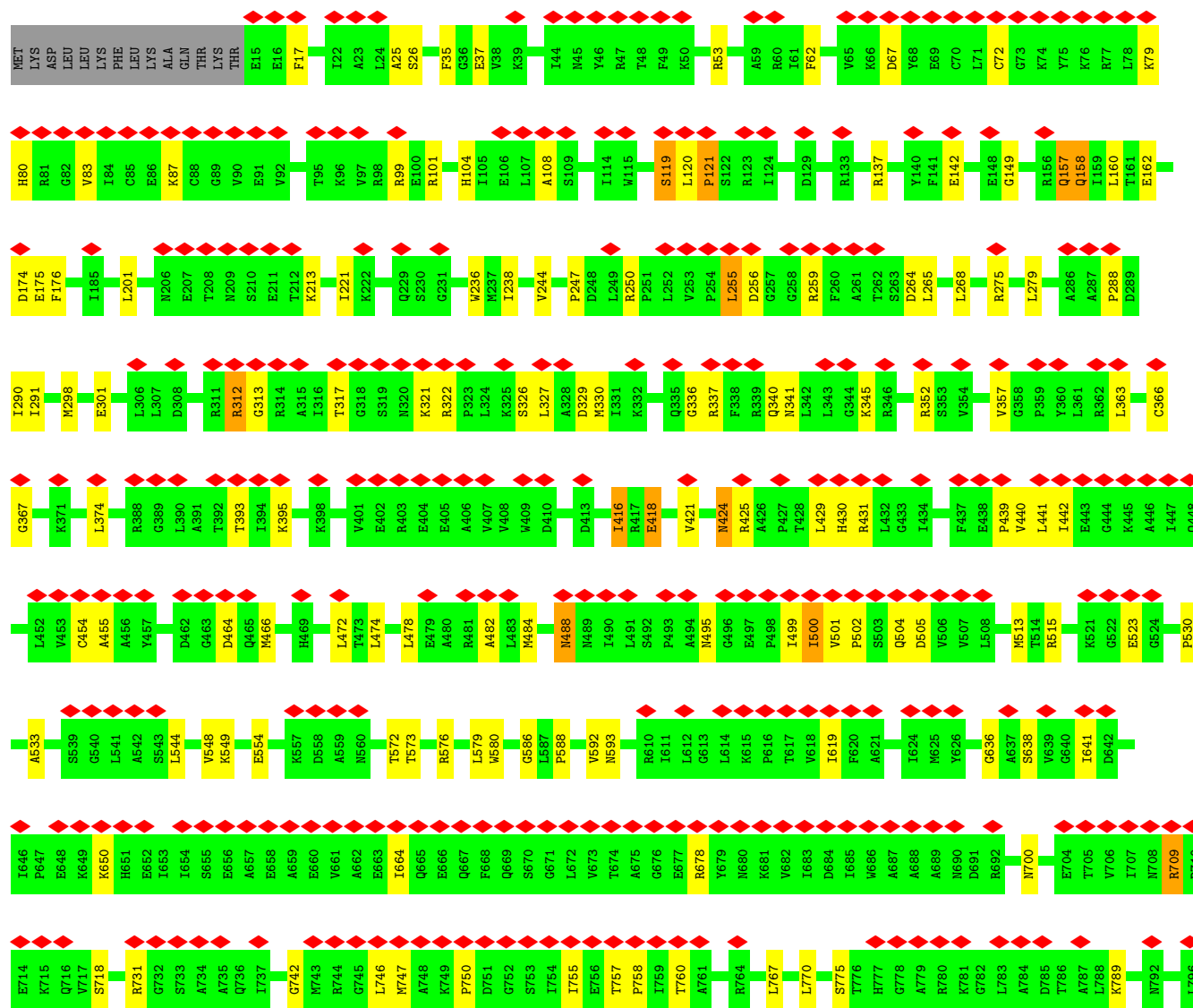
- Molecule 60: Template DNA strand

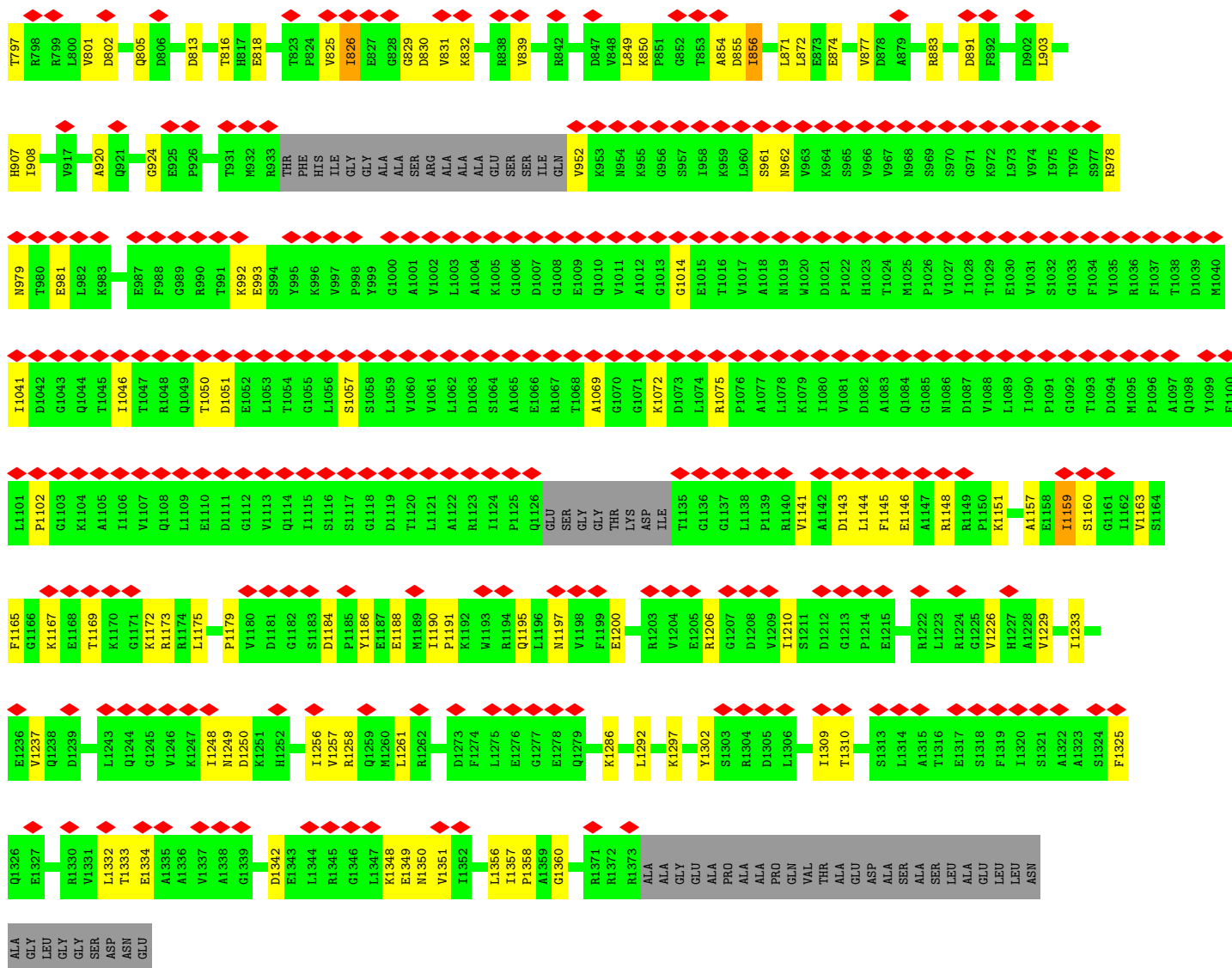






• Molecule 63: DNA-directed RNA polymerase subunit beta'

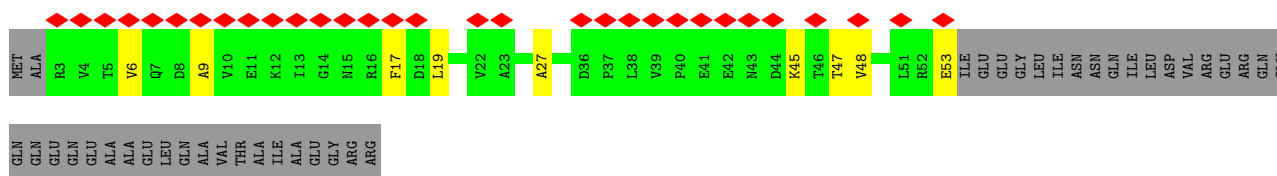




• Molecule 64: DNA-directed RNA polymerase subunit omega



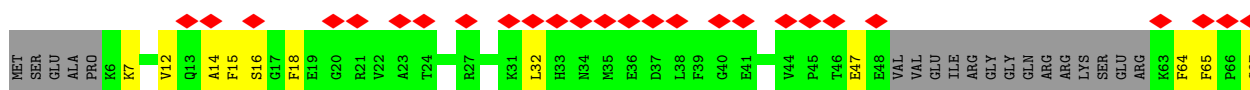
Chain CE:



• Molecule 65: Transcription termination/antitermination protein NusG



Chain CF:



Y68	V69	L70	V71	Q72	M73	V74	M75	N76	D77	A78	S79	W80	H81	S85	V86	P87	R88	V89	M90	G91	F92	I93	G94	G95	T96	S97	D98	R99	P100	I103	S104	D105	K106	E107	V108	D109	A110	I111	M112	N113	R114	L115	Q116	Q117	V118	G119	D120	A121	P122	R123	P124	K125	T126	L127	F128	E129	P130
G131	E132	M133	V134	R135	V136	N137	D138	G139	P140	F141	A142	D143	F144	N145	G146	V147	V148	E149	E150	V151	D152	Y153	E154	K155	S156	R157	L158	K159	V160	S161	V162	S163	I164	F165	G166	R167	A168	T169	P170	V171	E172	L173	D174	F175	S176	Q177	V178	E179	K180	ALA							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15327	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.415	Depositor
Minimum map value	-0.341	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	673.28, 673.28, 673.28	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, 7MG, 6MZ, 5MC, 3TD, D2T, OMC, MG, 4SU, UR3, MEQ, OMU, 5MU, 3AU, 2MA, H2U, PSU, MA6, OMG, ZN, 1MG, 4OC, G7M, 2MG, 4D4

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	0.38	0/36569	0.58	9/57044 (0.0%)
2	AB	0.28	0/1796	0.68	0/2420
3	AC	0.37	0/1680	0.71	2/2263 (0.1%)
4	AD	0.32	0/1665	0.64	0/2227
5	AE	0.33	0/1161	0.77	2/1563 (0.1%)
6	AF	0.32	0/867	0.68	0/1171
7	AG	0.32	0/1219	0.75	0/1635
8	AH	0.30	0/989	0.58	0/1326
9	AI	0.40	0/1043	0.79	0/1387
10	AJ	0.39	0/818	0.85	3/1105 (0.3%)
11	AK	0.27	0/893	0.58	0/1205
12	AL	0.40	0/954	0.94	7/1279 (0.5%)
13	AM	0.35	0/900	0.68	0/1204
14	AN	0.39	0/817	0.61	0/1088
15	AO	0.29	0/722	0.63	0/964
16	AP	0.32	0/659	0.66	0/884
17	AQ	0.32	0/657	0.65	0/881
18	AR	0.29	0/501	0.60	0/672
19	AS	0.40	0/680	0.72	0/915
20	AT	0.31	0/676	0.54	0/895
21	AU	0.30	0/598	0.74	1/792 (0.1%)
22	AV	0.79	0/949	0.93	7/1475 (0.5%)
23	AW	0.33	0/1725	0.61	2/2687 (0.1%)
24	AX	0.22	0/1584	0.32	0/2463
25	AY	0.14	0/682	0.42	0/918
26	BA	0.32	2/69165 (0.0%)	0.56	13/107893 (0.0%)
27	BB	0.27	0/2872	0.49	0/4478
28	BC	0.30	0/2131	0.67	0/2863
29	BD	0.30	0/1576	0.60	0/2119
30	BE	0.26	0/1571	0.55	0/2113
31	BF	0.24	0/1444	0.63	0/1937

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BG	0.23	0/1333	0.60	0/1805
33	BH	0.25	0/1122	0.74	0/1515
34	BI	0.25	0/993	0.98	1/1340 (0.1%)
35	BJ	0.25	0/1046	0.70	1/1410 (0.1%)
36	BK	0.28	0/1152	0.52	0/1551
37	BL	0.31	0/956	0.61	0/1279
38	BM	0.30	0/1061	0.64	0/1412
39	BN	0.28	0/1081	0.52	0/1443
40	BO	0.30	0/973	0.60	0/1301
41	BP	0.25	0/910	0.66	0/1219
42	BQ	0.28	0/929	0.69	0/1242
43	BR	0.37	0/960	0.62	0/1278
44	BS	0.32	0/829	0.76	0/1107
45	BT	0.31	0/864	0.60	0/1156
46	BU	0.24	0/771	0.53	0/1031
47	BV	0.24	0/797	0.66	0/1062
48	BW	0.26	0/766	0.58	0/1025
49	BX	0.29	0/589	0.58	0/779
50	BY	0.26	0/635	0.52	0/848
51	BZ	0.25	0/510	0.67	0/677
52	B1	0.31	0/453	0.68	0/605
53	B2	0.35	0/450	0.85	2/599 (0.3%)
54	B3	0.21	0/443	0.70	0/587
55	B4	0.30	0/380	0.68	0/498
56	B5	0.28	0/513	0.61	0/676
57	B6	0.28	0/302	0.53	0/397
58	B7	0.28	0/559	0.86	1/745 (0.1%)
59	CN	0.79	0/693	0.77	0/1068
60	CT	1.19	0/676	0.84	0/1039
61	CA	1.10	0/1797	0.96	0/2436
61	CB	0.81	0/1703	0.90	0/2308
62	CC	1.34	18/10581 (0.2%)	1.05	2/14275 (0.0%)
63	CD	1.10	6/10532 (0.1%)	0.97	1/14219 (0.0%)
64	CE	0.44	0/401	0.83	0/540
65	CF	0.27	0/1312	0.59	0/1771
All	All	0.54	26/188635 (0.0%)	0.66	54/278109 (0.0%)

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
1	AA	0	3
2	AB	0	1
10	AJ	0	1
12	AL	0	1
13	AM	0	1
22	AV	0	1
26	BA	0	1
28	BC	0	1
31	BF	0	1
34	BI	0	1
40	BO	0	1
49	BX	0	1
58	B7	0	1
All	All	0	15

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	CC	799	ASN	CB-CG	-6.31	1.36	1.52
63	CD	424	ASN	CB-CG	-6.29	1.36	1.52
62	CC	519	ASN	CB-CG	-6.21	1.36	1.52
62	CC	530	ILE	CB-CG2	-6.15	1.32	1.52
63	CD	760	THR	CA-C	-6.09	1.42	1.52

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	1176	U	O4'-C1'-N1	11.17	125.26	108.50
22	AV	38	A	C4'-C3'-O3'	-10.79	93.22	109.40
21	AU	64	ASN	N-CA-C	-9.77	94.72	109.86
34	BI	49	GLY	N-CA-C	9.66	122.74	111.63
5	AE	50	TYR	CA-C-N	8.65	138.36	121.41

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1027	C	Sidechain
1	AA	1034	G	Sidechain
1	AA	60	A	Sidechain
2	AB	17	GLY	Mainchain
10	AJ	42	LEU	Mainchain

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	32909	0	16580	337	0
2	AB	1765	0	1792	50	0
3	AC	1653	0	1727	70	0
4	AD	1643	0	1707	40	0
5	AE	1148	0	1195	48	0
6	AF	848	0	846	24	0
7	AG	1203	0	1254	35	0
8	AH	979	0	1031	18	0
9	AI	1031	0	1076	38	0
10	AJ	808	0	845	43	0
11	AK	877	0	887	21	0
12	AL	951	0	1011	38	0
13	AM	891	0	952	26	0
14	AN	805	0	844	26	0
15	AO	714	0	734	16	0
16	AP	649	0	666	11	0
17	AQ	648	0	691	12	0
18	AR	494	0	512	12	0
19	AS	663	0	688	20	0
20	AT	670	0	719	14	0
21	AU	590	0	629	12	0
22	AV	849	0	433	63	0
23	AW	1645	0	842	12	0
24	AX	1624	0	823	33	0
25	AY	677	0	675	22	0
26	BA	62270	0	31337	604	0
27	BB	2569	0	1301	29	0
28	BC	2092	0	2167	37	0
29	BD	1566	0	1618	34	0
30	BE	1552	0	1618	26	0
31	BF	1420	0	1457	46	0
32	BG	1313	0	1358	23	0
33	BH	1111	0	1148	32	0
34	BI	980	0	1013	57	0
35	BJ	1032	0	1088	35	0
36	BK	1129	0	1162	17	0
37	BL	947	0	1023	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BM	1052	0	1127	24	0
39	BN	1075	0	1154	21	0
40	BO	960	0	1000	21	0
41	BP	900	0	935	18	0
42	BQ	917	0	962	26	0
43	BR	947	0	1019	19	0
44	BS	816	0	839	18	0
45	BT	857	0	922	23	0
46	BU	764	0	829	15	0
47	BV	789	0	844	15	0
48	BW	753	0	780	12	0
49	BX	582	0	599	6	0
50	BY	625	0	652	13	0
51	BZ	509	0	543	11	0
52	B1	449	0	488	7	0
53	B2	444	0	458	14	0
54	B3	436	0	477	12	0
55	B4	377	0	418	14	0
56	B5	504	0	572	9	0
57	B6	301	0	340	6	0
58	B7	549	0	549	15	0
59	CN	618	0	338	59	0
60	CT	606	0	338	38	0
61	CA	1775	0	1800	22	0
61	CB	1684	0	1713	18	0
62	CC	10415	0	10428	216	0
63	CD	10375	0	10595	198	0
64	CE	399	0	417	5	0
65	CF	1283	0	1261	102	0
66	AA	148	0	0	0	0
66	AI	1	0	0	0	0
66	AW	1	0	0	0	0
66	AX	1	0	0	0	0
66	BA	314	0	0	0	0
66	BB	6	0	0	0	0
66	BC	3	0	0	0	0
66	BD	1	0	0	0	0
66	BE	1	0	0	0	0
66	BQ	1	0	0	0	0
66	BT	1	0	0	0	0
66	CD	1	0	0	0	0
67	AX	11	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	B6	1	0	0	0	0
68	B7	1	0	0	0	0
68	CD	2	0	0	0	0
All	All	176970	0	127854	2535	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 8.

The worst 5 of 2535 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)
3:AC:88:ARG:NH2	63:CD:79:LYS:HD3	1.37	1.36
62:CC:375:PRO:CG	65:CF:80:TRP:CH2	2.08	1.35
3:AC:88:ARG:CZ	63:CD:79:LYS:HD3	1.65	1.26
3:AC:102:ASN:HA	22:AV:36:A:N6	1.49	1.26
59:CN:18:DG:N2	65:CF:12:VAL:O	1.76	1.19

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	224/241 (93%)	209 (93%)	14 (6%)	1 (0%)	30	59
3	AC	209/233 (90%)	198 (95%)	6 (3%)	5 (2%)	4	22
4	AD	203/206 (98%)	194 (96%)	8 (4%)	1 (0%)	24	54
5	AE	154/167 (92%)	140 (91%)	12 (8%)	2 (1%)	9	33
6	AF	102/131 (78%)	97 (95%)	5 (5%)	0	100	100
7	AG	151/156 (97%)	139 (92%)	11 (7%)	1 (1%)	18	47
8	AH	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AI	126/130 (97%)	108 (86%)	14 (11%)	4 (3%)	3	17
10	AJ	99/103 (96%)	92 (93%)	3 (3%)	4 (4%)	2	15
11	AK	115/129 (89%)	100 (87%)	14 (12%)	1 (1%)	14	42
12	AL	119/124 (96%)	112 (94%)	5 (4%)	2 (2%)	7	28
13	AM	113/118 (96%)	106 (94%)	6 (5%)	1 (1%)	14	42
14	AN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	10	35
16	AP	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	AQ	78/84 (93%)	72 (92%)	6 (8%)	0	100	100
18	AR	58/75 (77%)	55 (95%)	2 (3%)	1 (2%)	7	28
19	AS	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
20	AT	84/87 (97%)	84 (100%)	0	0	100	100
21	AU	68/71 (96%)	65 (96%)	3 (4%)	0	100	100
25	AY	87/557 (16%)	75 (86%)	12 (14%)	0	100	100
28	BC	270/273 (99%)	248 (92%)	19 (7%)	3 (1%)	11	38
29	BD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24	54
30	BE	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
31	BF	176/179 (98%)	168 (96%)	7 (4%)	1 (1%)	21	50
32	BG	173/177 (98%)	158 (91%)	14 (8%)	1 (1%)	21	50
33	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
34	BI	128/165 (78%)	99 (77%)	24 (19%)	5 (4%)	2	15
35	BJ	139/142 (98%)	111 (80%)	24 (17%)	4 (3%)	3	19
36	BK	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
37	BL	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
38	BM	142/144 (99%)	130 (92%)	10 (7%)	2 (1%)	9	31
39	BN	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
40	BO	118/127 (93%)	107 (91%)	11 (9%)	0	100	100
41	BP	115/117 (98%)	107 (93%)	7 (6%)	1 (1%)	14	42
42	BQ	112/115 (97%)	103 (92%)	8 (7%)	1 (1%)	14	42
43	BR	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
44	BS	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	12	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BT	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
46	BU	94/100 (94%)	87 (93%)	5 (5%)	2 (2%)	5	24
47	BV	101/104 (97%)	95 (94%)	6 (6%)	0	100	100
48	BW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
49	BX	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
50	BY	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
51	BZ	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
52	B1	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
53	B2	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
54	B3	51/55 (93%)	48 (94%)	3 (6%)	0	100	100
55	B4	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
56	B5	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
57	B6	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
58	B7	68/70 (97%)	60 (88%)	8 (12%)	0	100	100
61	CA	227/329 (69%)	217 (96%)	10 (4%)	0	100	100
61	CB	215/329 (65%)	205 (95%)	9 (4%)	1 (0%)	24	54
62	CC	1316/1342 (98%)	1197 (91%)	110 (8%)	9 (1%)	18	47
63	CD	1327/1407 (94%)	1222 (92%)	95 (7%)	10 (1%)	16	44
64	CE	49/91 (54%)	40 (82%)	8 (16%)	1 (2%)	6	25
65	CF	157/181 (87%)	143 (91%)	11 (7%)	3 (2%)	6	26
All	All	9264/10441 (89%)	8585 (93%)	608 (7%)	71 (1%)	18	44

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	80	LYS
5	AE	90	THR
9	AI	56	ASP
11	AK	93	ARG
12	AL	88	LYS

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	187/199 (94%)	171 (91%)	16 (9%)	10	33
3	AC	172/190 (90%)	155 (90%)	17 (10%)	7	26
4	AD	172/173 (99%)	158 (92%)	14 (8%)	11	36
5	AE	118/126 (94%)	102 (86%)	16 (14%)	3	15
6	AF	91/112 (81%)	80 (88%)	11 (12%)	5	19
7	AG	126/129 (98%)	114 (90%)	12 (10%)	8	29
8	AH	104/105 (99%)	93 (89%)	11 (11%)	6	23
9	AI	106/107 (99%)	90 (85%)	16 (15%)	3	11
10	AJ	88/90 (98%)	76 (86%)	12 (14%)	3	15
11	AK	90/99 (91%)	84 (93%)	6 (7%)	15	41
12	AL	102/103 (99%)	93 (91%)	9 (9%)	9	31
13	AM	93/96 (97%)	83 (89%)	10 (11%)	6	22
14	AN	83/84 (99%)	74 (89%)	9 (11%)	6	22
15	AO	76/77 (99%)	72 (95%)	4 (5%)	20	47
16	AP	65/65 (100%)	60 (92%)	5 (8%)	12	37
17	AQ	74/78 (95%)	65 (88%)	9 (12%)	5	19
18	AR	52/65 (80%)	50 (96%)	2 (4%)	29	54
19	AS	72/79 (91%)	69 (96%)	3 (4%)	26	52
20	AT	65/66 (98%)	61 (94%)	4 (6%)	16	43
21	AU	60/61 (98%)	52 (87%)	8 (13%)	4	15
25	AY	73/461 (16%)	61 (84%)	12 (16%)	2	10
28	BC	217/218 (100%)	209 (96%)	8 (4%)	30	55
29	BD	163/163 (100%)	155 (95%)	8 (5%)	22	49
30	BE	165/165 (100%)	153 (93%)	12 (7%)	13	39
31	BF	149/150 (99%)	133 (89%)	16 (11%)	6	23
32	BG	136/138 (99%)	124 (91%)	12 (9%)	9	31
33	BH	114/114 (100%)	108 (95%)	6 (5%)	20	47
34	BI	99/123 (80%)	81 (82%)	18 (18%)	2	7
35	BJ	109/110 (99%)	91 (84%)	18 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BK	116/116 (100%)	107 (92%)	9 (8%)	11	37
37	BL	104/104 (100%)	97 (93%)	7 (7%)	15	41
38	BM	103/103 (100%)	92 (89%)	11 (11%)	6	23
39	BN	108/108 (100%)	100 (93%)	8 (7%)	13	38
40	BO	100/103 (97%)	96 (96%)	4 (4%)	28	53
41	BP	87/87 (100%)	79 (91%)	8 (9%)	8	29
42	BQ	99/100 (99%)	83 (84%)	16 (16%)	2	10
43	BR	89/90 (99%)	84 (94%)	5 (6%)	19	46
44	BS	84/84 (100%)	77 (92%)	7 (8%)	10	35
45	BT	93/93 (100%)	88 (95%)	5 (5%)	20	47
46	BU	83/84 (99%)	78 (94%)	5 (6%)	17	43
47	BV	84/85 (99%)	78 (93%)	6 (7%)	13	39
48	BW	78/78 (100%)	73 (94%)	5 (6%)	16	42
49	BX	58/63 (92%)	54 (93%)	4 (7%)	14	40
50	BY	67/68 (98%)	64 (96%)	3 (4%)	24	51
51	BZ	55/55 (100%)	52 (94%)	3 (6%)	19	46
52	B1	48/49 (98%)	44 (92%)	4 (8%)	10	35
53	B2	47/48 (98%)	44 (94%)	3 (6%)	16	42
54	B3	48/49 (98%)	42 (88%)	6 (12%)	4	18
55	B4	38/38 (100%)	37 (97%)	1 (3%)	40	61
56	B5	51/52 (98%)	48 (94%)	3 (6%)	18	44
57	B6	34/44 (77%)	32 (94%)	2 (6%)	18	44
58	B7	62/62 (100%)	60 (97%)	2 (3%)	34	58
61	CA	197/286 (69%)	193 (98%)	4 (2%)	48	65
61	CB	187/286 (65%)	177 (95%)	10 (5%)	20	47
62	CC	1139/1157 (98%)	1093 (96%)	46 (4%)	28	53
63	CD	1118/1168 (96%)	1094 (98%)	24 (2%)	47	64
64	CE	43/75 (57%)	41 (95%)	2 (5%)	23	50
65	CF	141/157 (90%)	126 (89%)	15 (11%)	6	23
All	All	7782/8638 (90%)	7250 (93%)	532 (7%)	16	40

5 of 532 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
62	CC	657	THR
62	CC	1005	GLU
62	CC	575	LEU
65	CF	132	GLU
25	AY	7	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
62	CC	955	GLN
62	CC	1111	GLN
63	CD	1227	HIS
20	AT	75	HIS
20	AT	61	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1542 (99%)	310 (20%)	33 (2%)
22	AV	39/53 (73%)	27 (69%)	5 (12%)
23	AW	76/77 (98%)	27 (35%)	7 (9%)
24	AX	75/76 (98%)	20 (26%)	1 (1%)
26	BA	2898/2904 (99%)	570 (19%)	71 (2%)
27	BB	119/120 (99%)	14 (11%)	0
All	All	4739/4772 (99%)	968 (20%)	117 (2%)

5 of 968 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	19	A
1	AA	22	G

5 of 117 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	310	A
26	BA	2585	U
26	BA	984	A

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Mol	Chain	Res	Type
26	BA	2573	C
26	BA	2062	A

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

53 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$
24	PSU	AX	55	24	18,21,22	1.10	1 (5%)	22,30,33	1.89	5 (22%)
24	7MG	AX	46	24	20,25,27	3.27	10 (50%)	27,37,42	2.22	8 (29%)
26	1MG	BA	745	26	22,26,27	2.72	5 (22%)	33,39,42	1.82	7 (21%)
1	UR3	AA	1498	1,66	19,22,23	2.59	7 (36%)	26,32,35	1.31	1 (3%)
1	MA6	AA	1518	1	23,26,27	1.54	6 (26%)	34,38,41	3.87	11 (32%)
26	PSU	BA	1911	26	18,21,22	1.07	1 (5%)	22,30,33	1.77	3 (13%)
26	3TD	BA	1915	26	18,22,23	4.47	10 (55%)	22,32,35	1.91	4 (18%)
26	5MU	BA	1939	26	19,22,23	1.42	4 (21%)	28,32,35	2.29	6 (21%)
26	PSU	BA	2604	26	18,21,22	1.01	1 (5%)	22,30,33	1.67	3 (13%)
26	5MC	BA	1962	26	18,22,23	3.97	7 (38%)	26,32,35	1.14	1 (3%)
26	2MG	BA	2445	26	23,26,27	2.77	9 (39%)	32,38,41	2.85	13 (40%)
26	PSU	BA	2605	26	18,21,22	1.04	1 (5%)	22,30,33	1.96	6 (27%)
26	G7M	BA	2069	26	23,26,27	2.60	9 (39%)	35,39,42	2.58	12 (34%)
1	PSU	AA	516	1	18,21,22	1.05	2 (11%)	22,30,33	2.04	7 (31%)
24	MIA	AX	37	24	21,24,32	1.76	4 (19%)	31,35,47	2.03	9 (29%)
26	H2U	BA	2449	26	18,21,22	2.82	5 (27%)	21,30,33	2.13	5 (23%)
26	PSU	BA	2457	26	18,21,22	1.05	1 (5%)	22,30,33	2.00	6 (27%)
24	5MU	AX	54	24	19,22,23	1.34	5 (26%)	28,32,35	2.09	6 (21%)
26	PSU	BA	746	66,26	18,21,22	1.03	1 (5%)	22,30,33	2.12	8 (36%)
1	2MG	AA	1207	1,66	23,26,27	2.82	9 (39%)	32,38,41	2.83	13 (40%)
12	D2T	AL	89	12	7,9,10	1.11	0	6,11,13	2.48	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	AA	1402	1	20,23,24	3.40	9 (45%)	26,32,35	1.01	2 (7%)
23	OMC	AW	32	23	19,22,23	3.03	8 (42%)	26,31,34	0.92	1 (3%)
23	H2U	AW	20	23	18,21,22	3.07	5 (27%)	21,30,33	1.99	5 (23%)
23	PSU	AW	55	23	18,21,22	1.04	1 (5%)	22,30,33	1.98	7 (31%)
26	5MU	BA	747	26	19,22,23	1.41	4 (21%)	28,32,35	2.16	6 (21%)
26	6MZ	BA	1618	26	22,25,26	2.73	4 (18%)	30,36,39	2.30	10 (33%)
24	3AU	AX	47	24	18,21,29	3.40	8 (44%)	26,30,43	1.64	4 (15%)
29	MEQ	BD	150	29	8,9,10	0.86	0	5,10,12	0.92	0
24	PSU	AX	39	24	18,21,22	1.14	1 (5%)	22,30,33	1.78	5 (22%)
1	MA6	AA	1519	1	23,26,27	1.58	6 (26%)	34,38,41	3.88	11 (32%)
24	PSU	AX	32	24,66	18,21,22	1.09	2 (11%)	22,30,33	1.77	4 (18%)
26	OMU	BA	2552	26	19,22,23	3.01	7 (36%)	26,31,34	1.71	5 (19%)
26	2MA	BA	2503	66,26	22,25,26	4.00	10 (45%)	33,37,40	2.59	10 (30%)
26	PSU	BA	2504	26	18,21,22	1.06	3 (16%)	22,30,33	2.05	6 (27%)
26	2MG	BA	1835	26	23,26,27	2.77	9 (39%)	32,38,41	2.90	13 (40%)
1	5MC	AA	1407	1	18,22,23	3.89	7 (38%)	26,32,35	0.97	1 (3%)
39	4D4	BN	81	39	9,11,12	2.41	2 (22%)	8,13,15	0.86	0
26	PSU	BA	955	66,26	18,21,22	1.07	2 (11%)	22,30,33	1.74	4 (18%)
1	G7M	AA	527	1	23,26,27	2.53	9 (39%)	35,39,42	2.61	12 (34%)
24	H2U	AX	16	24	18,21,22	3.05	5 (27%)	21,30,33	2.01	5 (23%)
1	2MG	AA	1516	1	23,26,27	2.73	9 (39%)	32,38,41	2.78	13 (40%)
26	OMG	BA	2251	23,26	23,26,27	2.53	8 (34%)	33,38,41	2.10	11 (33%)
24	4SU	AX	8	24	18,21,22	4.12	8 (44%)	26,30,33	2.26	5 (19%)
1	2MG	AA	966	1	23,26,27	2.82	9 (39%)	32,38,41	2.71	15 (46%)
24	H2U	AX	20	24	18,21,22	3.15	5 (27%)	21,30,33	1.95	4 (19%)
26	6MZ	BA	2030	26	22,25,26	2.63	5 (22%)	30,36,39	2.53	10 (33%)
23	5MU	AW	54	23	19,22,23	1.41	5 (26%)	28,32,35	2.11	6 (21%)
26	OMC	BA	2498	26	19,22,23	2.91	8 (42%)	26,31,34	0.87	1 (3%)
26	PSU	BA	2580	26	18,21,22	1.05	2 (11%)	22,30,33	2.07	6 (27%)
1	5MC	AA	967	1	18,22,23	3.99	7 (38%)	26,32,35	1.03	1 (3%)
26	PSU	BA	1917	26	18,21,22	0.99	1 (5%)	22,30,33	1.80	5 (22%)
23	4SU	AW	8	23	18,21,22	4.16	8 (44%)	26,30,33	2.28	5 (19%)

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
24	PSU	AX	55	24	-	4/7/25/26	0/2/2/2
24	7MG	AX	46	24	-	2/7/34/38	0/3/3/3
26	1MG	BA	745	26	-	0/7/25/26	0/3/3/3
1	UR3	AA	1498	1,66	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	1/11/29/30	0/3/3/3
26	PSU	BA	1911	26	-	1/7/25/26	0/2/2/2
26	3TD	BA	1915	26	-	3/7/25/26	0/2/2/2
26	5MU	BA	1939	26	-	2/7/25/26	0/2/2/2
26	PSU	BA	2604	26	-	0/7/25/26	0/2/2/2
26	5MC	BA	1962	26	-	0/7/25/26	0/2/2/2
26	2MG	BA	2445	26	-	2/9/27/28	0/3/3/3
26	PSU	BA	2605	26	-	0/7/25/26	0/2/2/2
26	G7M	BA	2069	26	-	2/7/25/26	0/3/3/3
1	PSU	AA	516	1	-	2/7/25/26	0/2/2/2
24	MIA	AX	37	24	-	0/7/25/34	0/3/3/3
26	H2U	BA	2449	26	-	2/7/38/39	0/2/2/2
26	PSU	BA	2457	26	-	0/7/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
26	PSU	BA	746	66,26	-	2/7/25/26	0/2/2/2
1	2MG	AA	1207	1,66	-	2/9/27/28	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
23	OMC	AW	32	23	-	3/9/27/28	0/2/2/2
23	H2U	AW	20	23	-	7/7/38/39	0/2/2/2
23	PSU	AW	55	23	-	3/7/25/26	0/2/2/2
26	5MU	BA	747	26	-	0/7/25/26	0/2/2/2
26	6MZ	BA	1618	26	-	4/9/27/28	0/3/3/3
24	3AU	AX	47	24	-	2/7/25/35	0/2/2/2
29	MEQ	BD	150	29	-	4/8/9/11	-
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	3/11/29/30	0/3/3/3
24	PSU	AX	32	24,66	-	2/7/25/26	0/2/2/2
26	OMU	BA	2552	26	-	2/9/27/28	0/2/2/2
26	2MA	BA	2503	66,26	-	2/7/25/26	0/3/3/3
26	PSU	BA	2504	26	-	0/7/25/26	0/2/2/2
26	2MG	BA	1835	26	-	0/9/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	4D4	BN	81	39	-	4/11/12/14	-
26	PSU	BA	955	66,26	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	1/7/25/26	0/3/3/3
24	H2U	AX	16	24	-	4/7/38/39	0/2/2/2
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
26	OMG	BA	2251	23,26	-	0/9/27/28	0/3/3/3
24	4SU	AX	8	24	-	1/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/9/27/28	0/3/3/3
24	H2U	AX	20	24	-	3/7/38/39	0/2/2/2
26	6MZ	BA	2030	26	-	3/9/27/28	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
26	OMC	BA	2498	26	-	2/9/27/28	0/2/2/2
26	PSU	BA	2580	26	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	3/7/25/26	0/2/2/2
26	PSU	BA	1917	26	-	2/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	2/7/25/26	0/2/2/2

The worst 5 of 275 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2503	2MA	C4-N3	12.32	1.49	1.34
26	BA	1915	3TD	C6-C5	11.99	1.49	1.35
26	BA	1618	6MZ	C6-N6	11.41	1.46	1.34
26	BA	2030	6MZ	C6-N6	10.61	1.45	1.34
1	AA	967	5MC	C6-C5	10.01	1.51	1.34

The worst 5 of 331 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	MA6	N1-C6-N6	-16.51	99.03	117.08
1	AA	1519	MA6	N1-C6-N6	-16.20	99.37	117.08
1	AA	1518	MA6	C5-C6-N6	9.15	141.24	125.30
1	AA	1519	MA6	C5-C6-N6	8.73	140.50	125.30
23	AW	8	4SU	C4-N3-C2	-8.08	119.49	127.34

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
24	AX	32	PSU	C2'-C1'-C5-C4
24	AX	46	7MG	O4'-C4'-C5'-O5'

There are no ring outliers.

24 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	1	0
26	BA	1915	3TD	3	0
26	BA	2605	PSU	1	0
1	AA	516	PSU	1	0
24	AX	37	MIA	1	0
26	BA	2449	H2U	1	0
24	AX	54	5MU	1	0
1	AA	1207	2MG	3	0
12	AL	89	D2T	3	0
23	AW	32	OMC	1	0
23	AW	55	PSU	1	0
29	BD	150	MEQ	2	0
24	AX	39	PSU	1	0
1	AA	1519	MA6	1	0
26	BA	2504	PSU	1	0
1	AA	527	G7M	1	0
24	AX	16	H2U	1	0
1	AA	1516	2MG	1	0
26	BA	2251	OMG	2	0
1	AA	966	2MG	2	0
24	AX	20	H2U	3	0
26	BA	2030	6MZ	1	0
1	AA	967	5MC	1	0
26	BA	1917	PSU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 484 ligands modelled in this entry, 483 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
67	PHE	AX	101	24	10,11,12	0.49	0	10,13,15	0.32	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
67	PHE	AX	101	24	-	2/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
67	AX	101	PHE	CA-CB-CG-CD1
67	AX	101	PHE	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
63	CD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	1357:ILE	C	1358:PRO	N	1.15

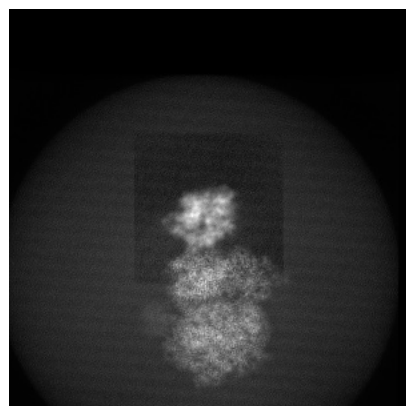
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11418. These allow visual inspection of the internal detail of the map and identification of artifacts.

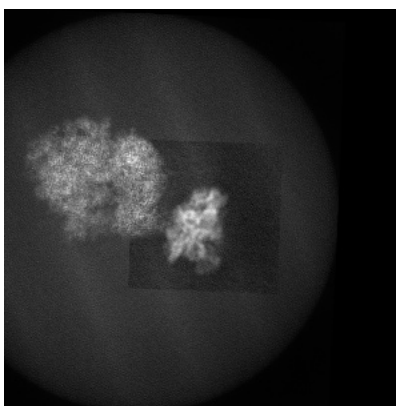
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

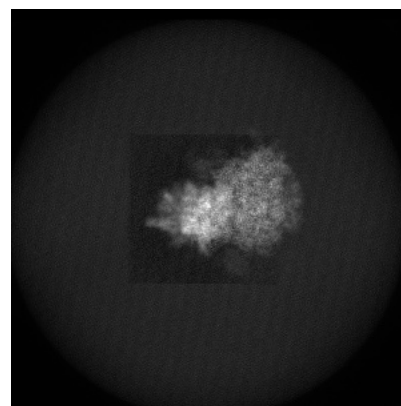
6.1.1 Primary map



X

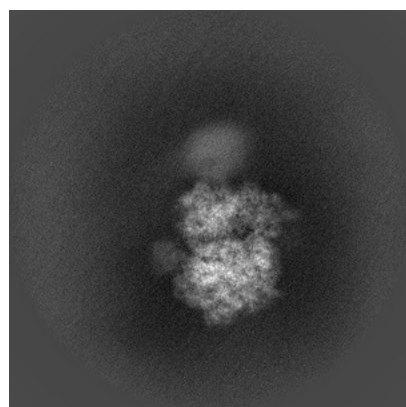


Y

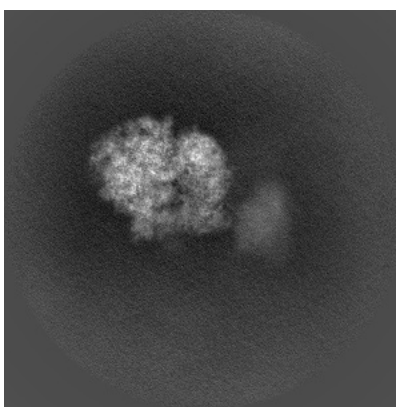


Z

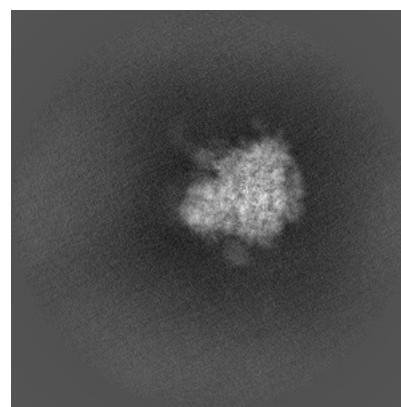
6.1.2 Raw map



X



Y

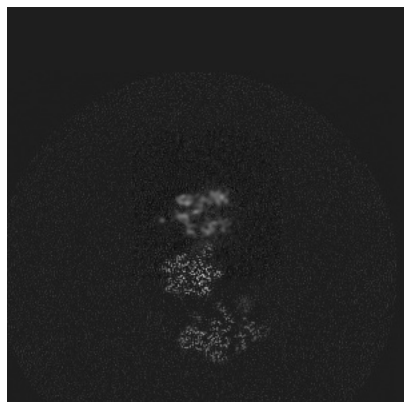


Z

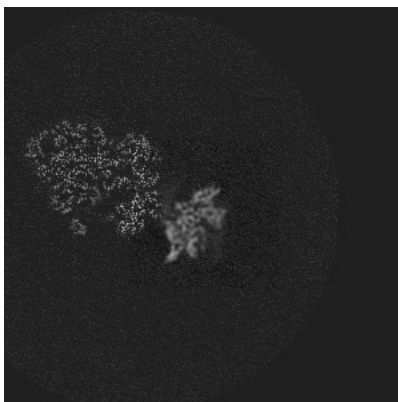
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

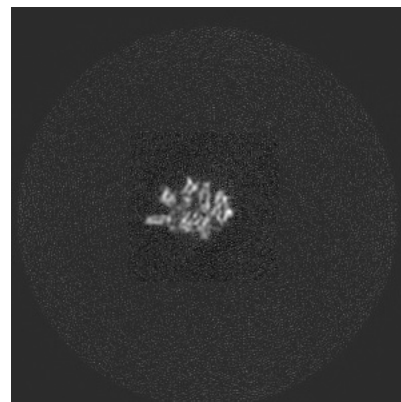
6.2.1 Primary map



X Index: 320

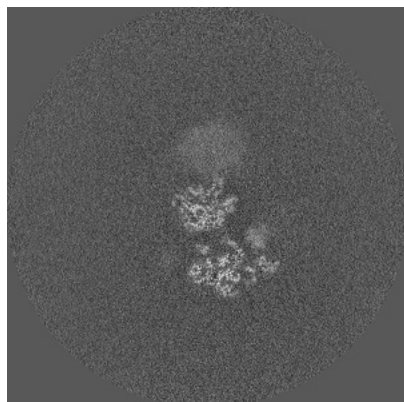


Y Index: 320

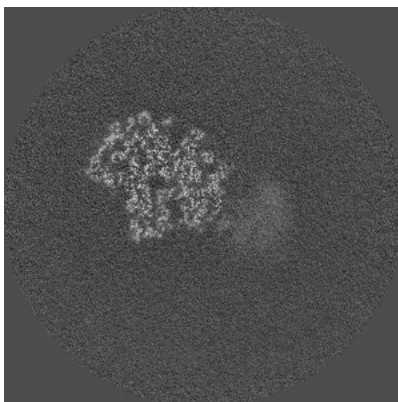


Z Index: 320

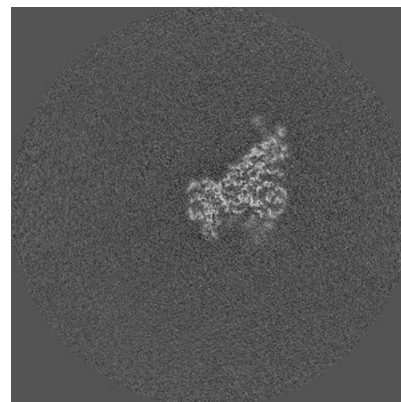
6.2.2 Raw map



X Index: 320



Y Index: 320

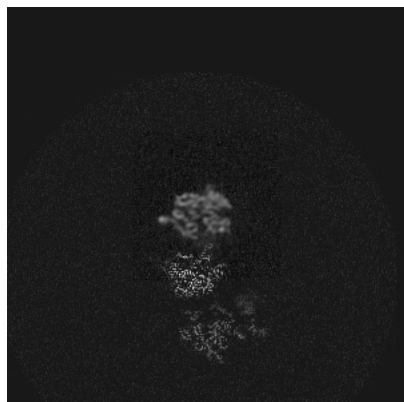


Z Index: 320

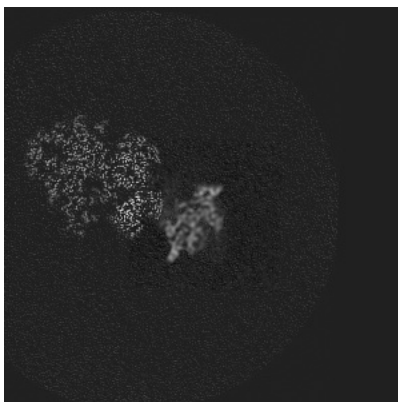
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

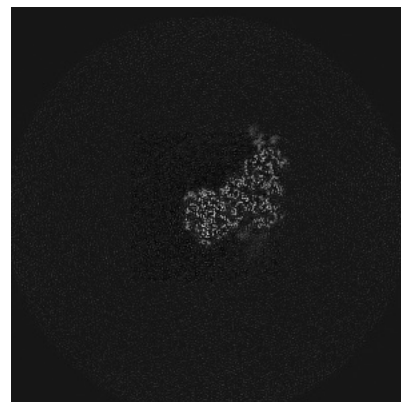
6.3.1 Primary map



X Index: 315

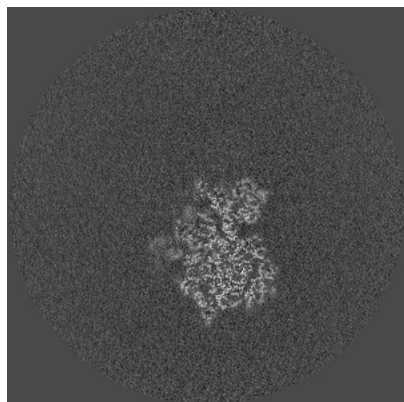


Y Index: 315

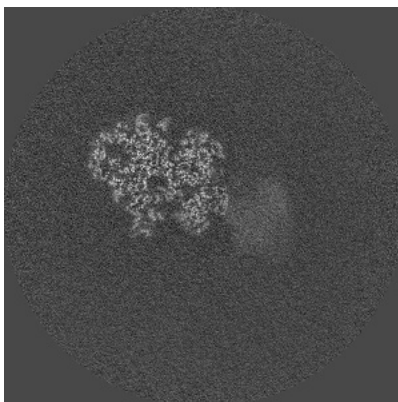


Z Index: 212

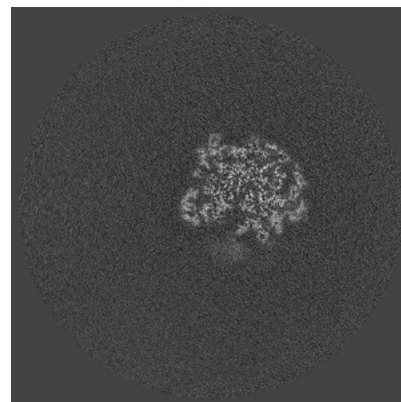
6.3.2 Raw map



X Index: 377



Y Index: 331

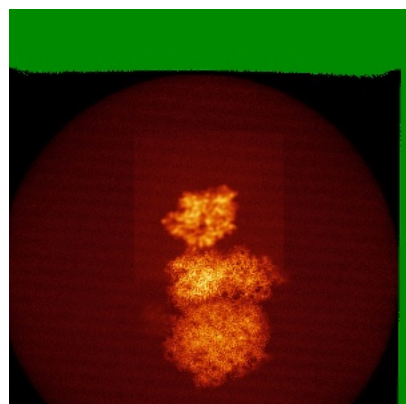


Z Index: 229

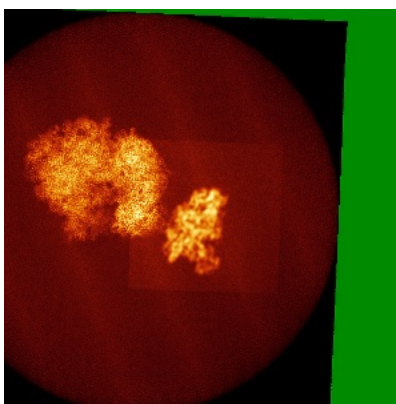
The images above show the largest variance slices of the map in three orthogonal directions.

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

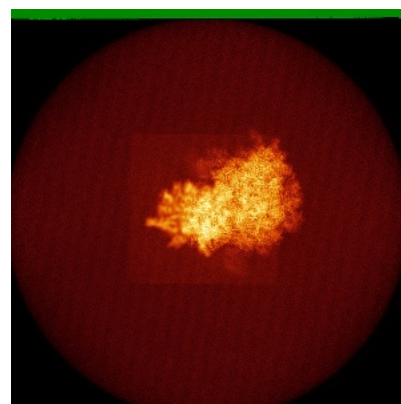
6.4.1 Primary map



X

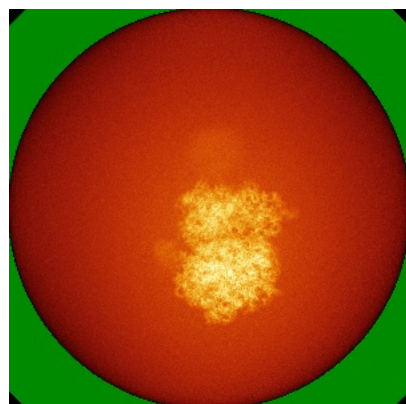


Y

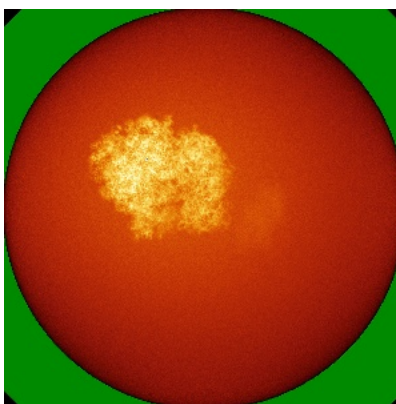


Z

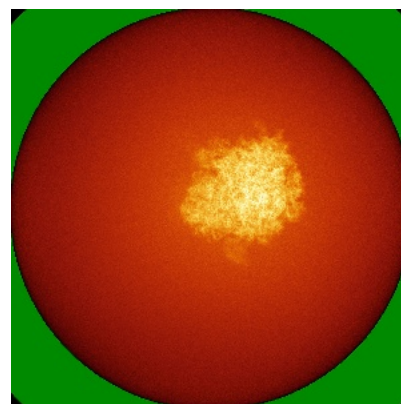
6.4.2 Raw map



X



Y

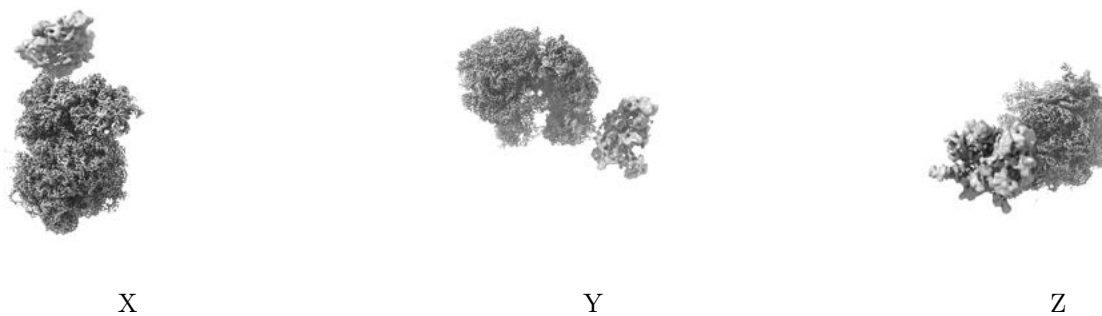


Z

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

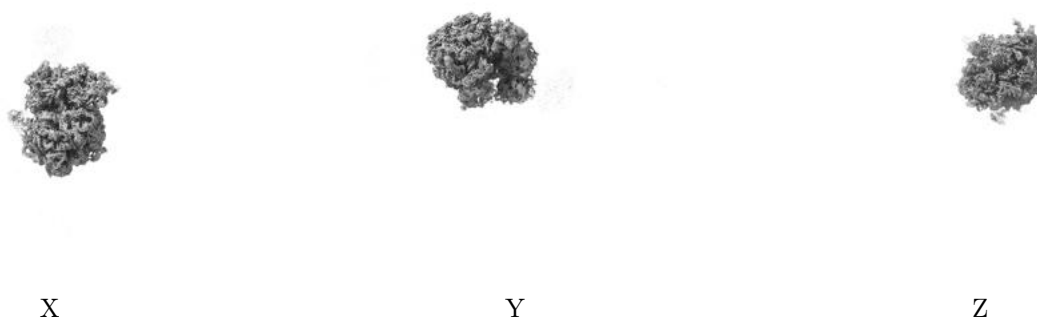
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

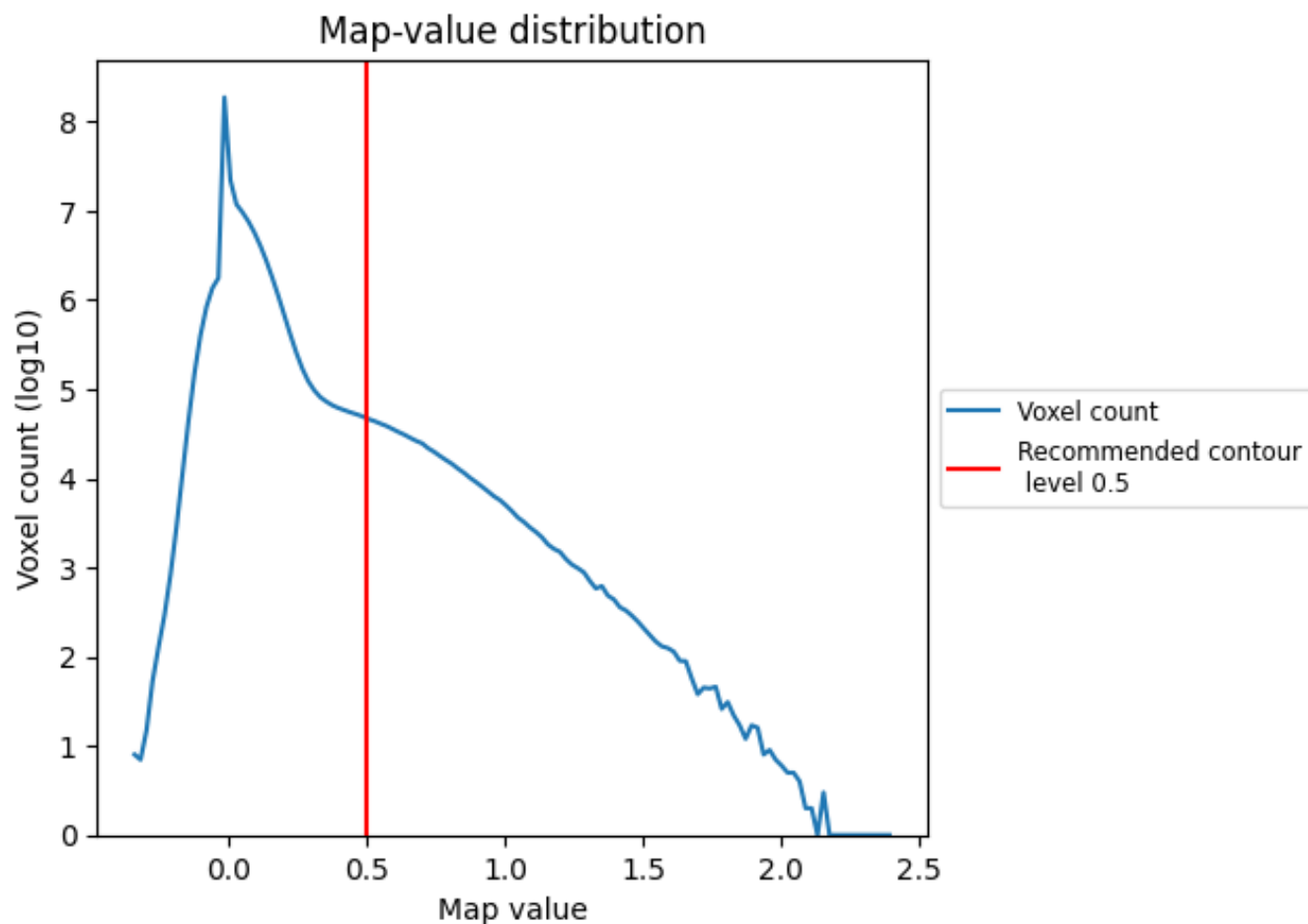
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

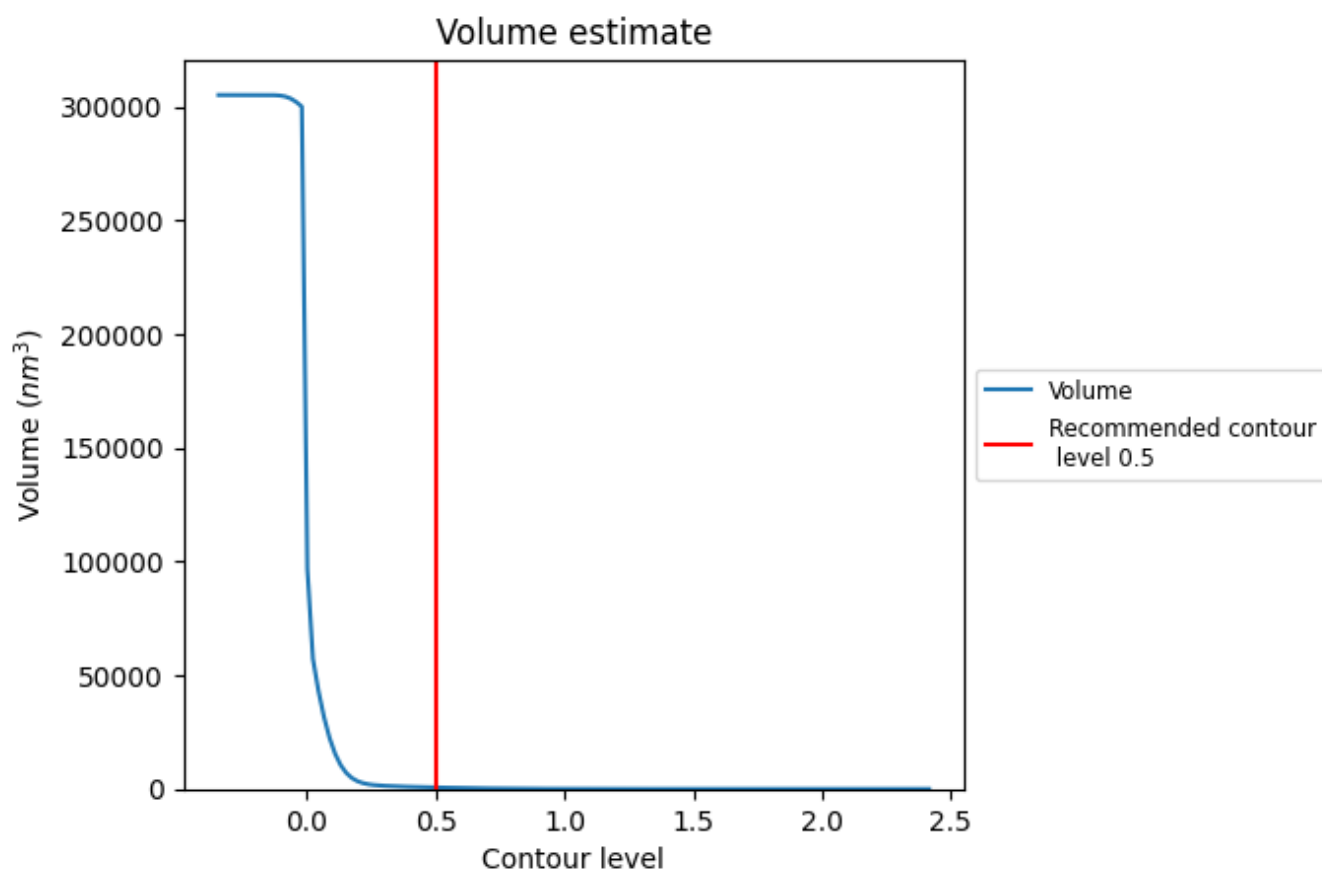
This section contains the results of statistical analysis of the map.

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.

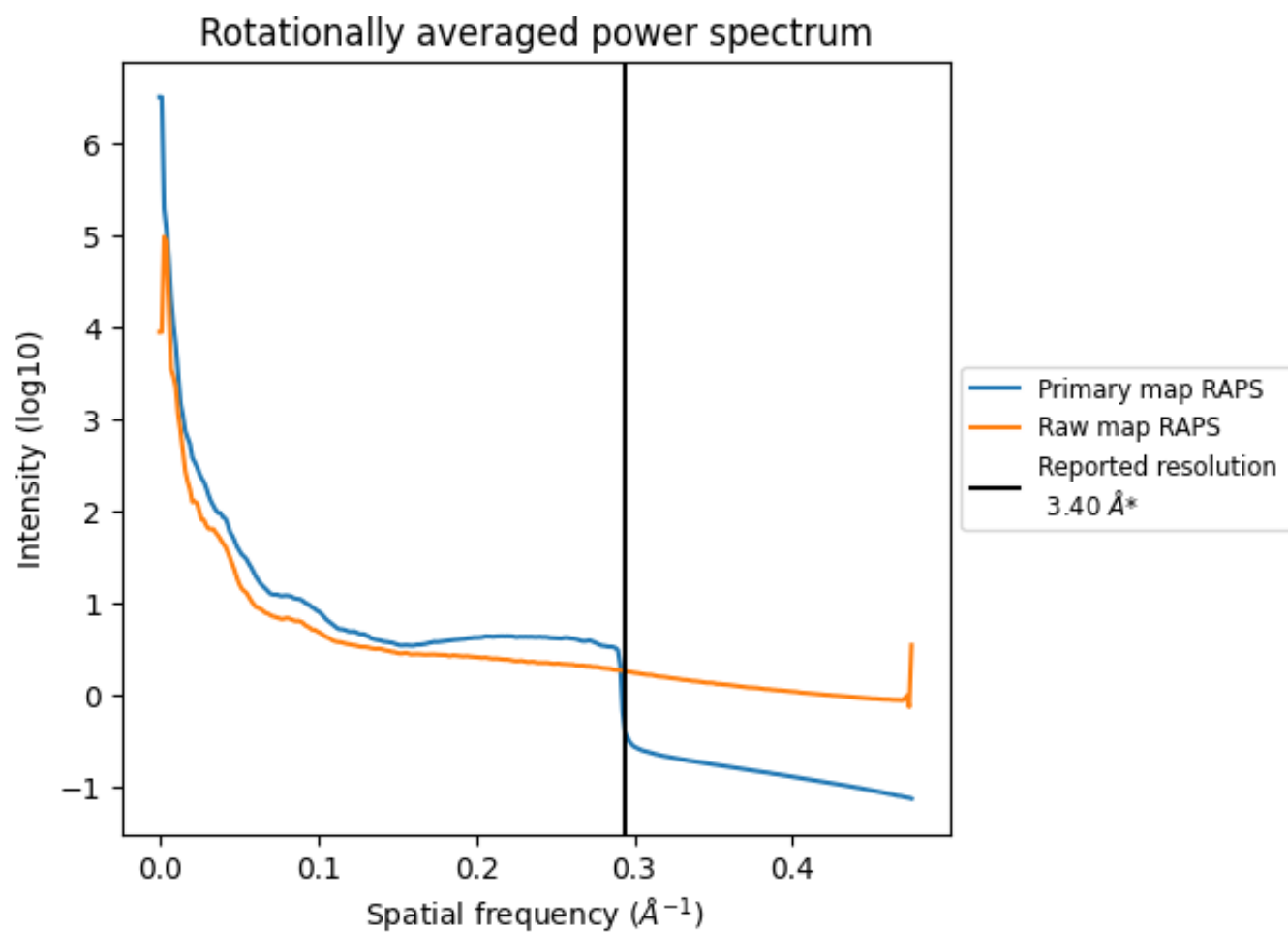
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 654 nm^3 ; this corresponds to an approximate mass of 591 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 ⓘ

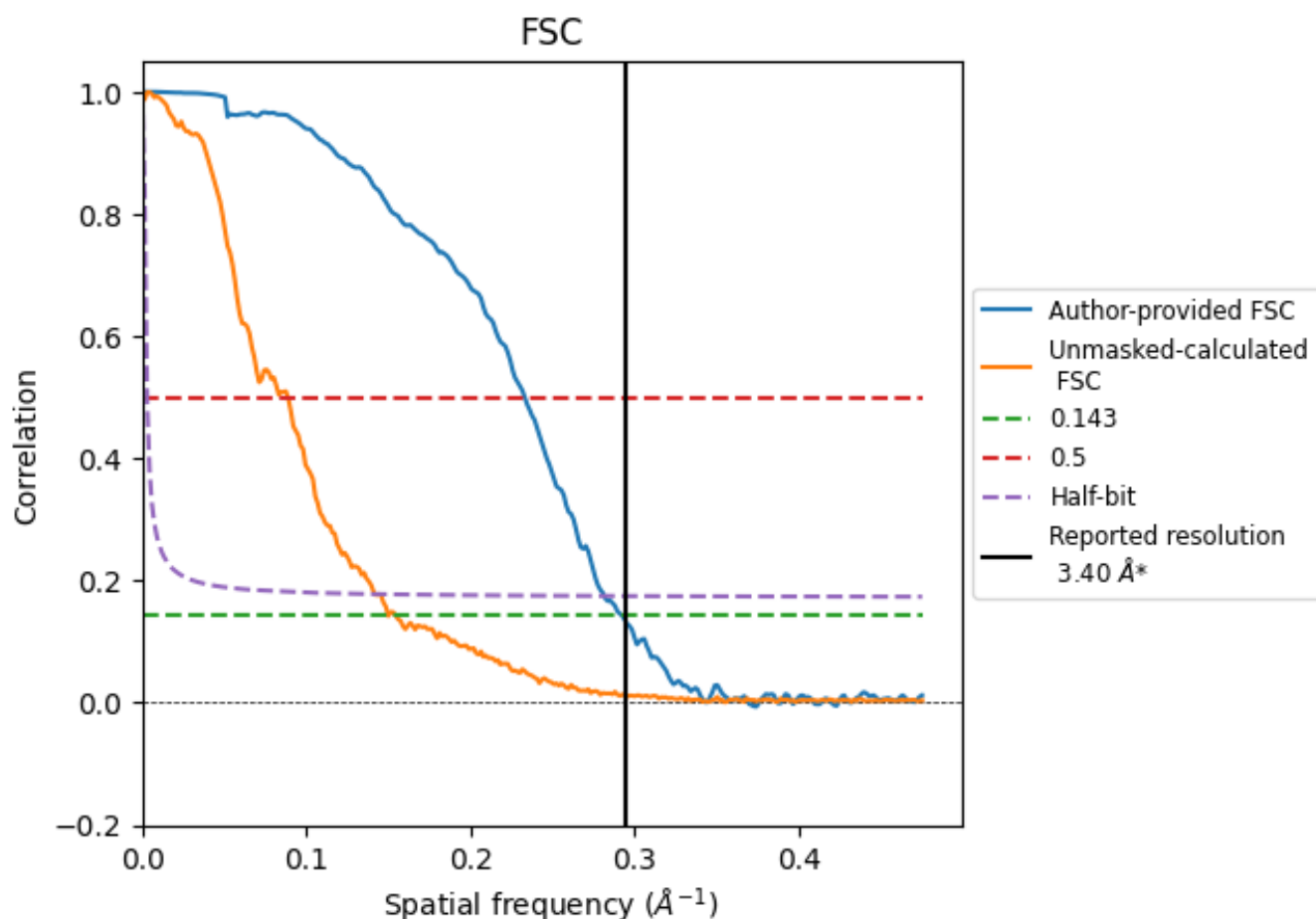


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

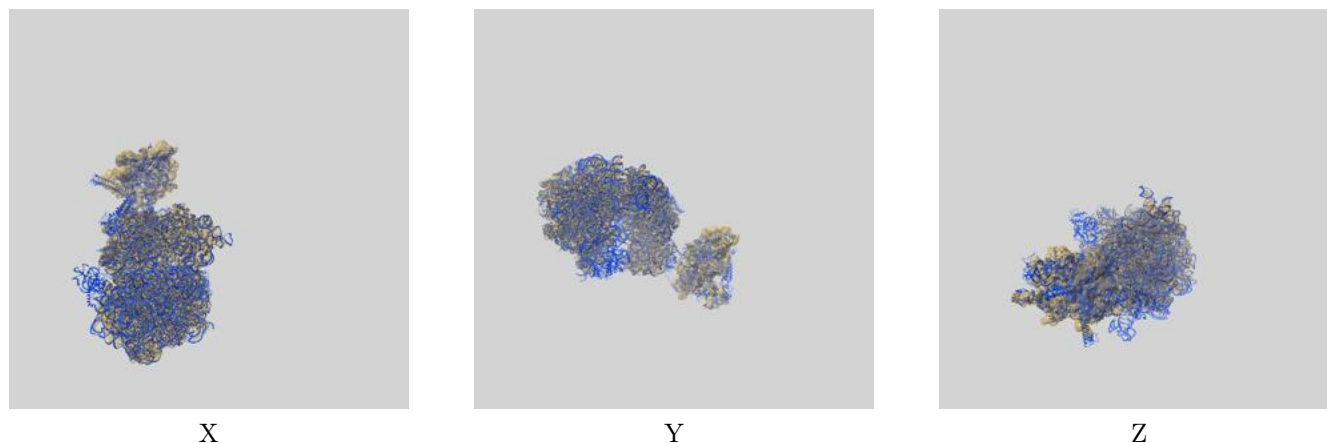
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	4.29	3.55
Unmasked-calculated*	6.67	11.26	7.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.67 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

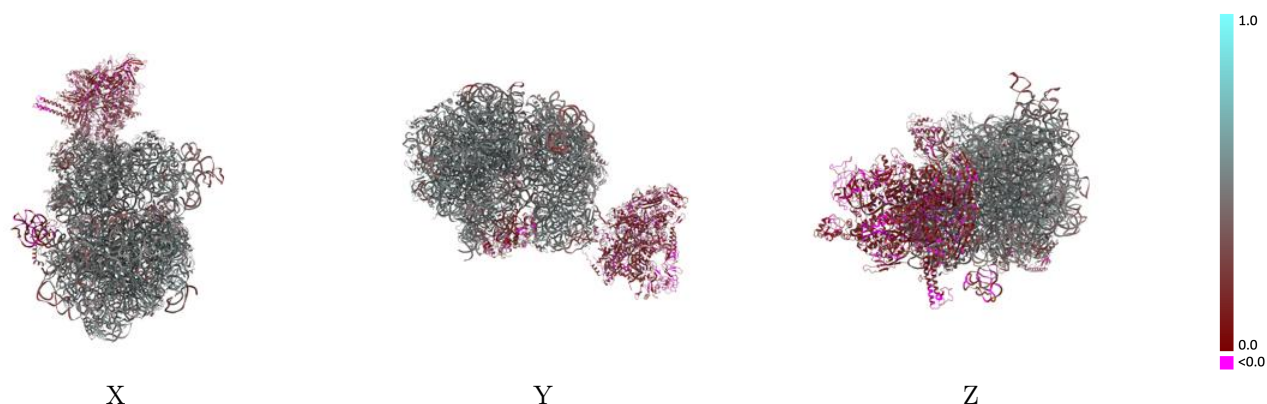
This section contains information regarding the fit between EMDB map EMD-11418 and PDB model 6ZTJ. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



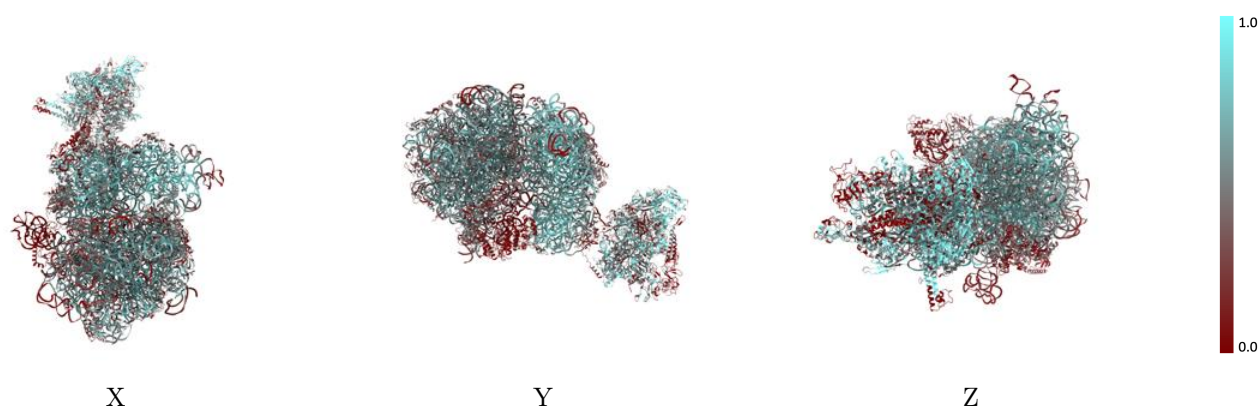
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



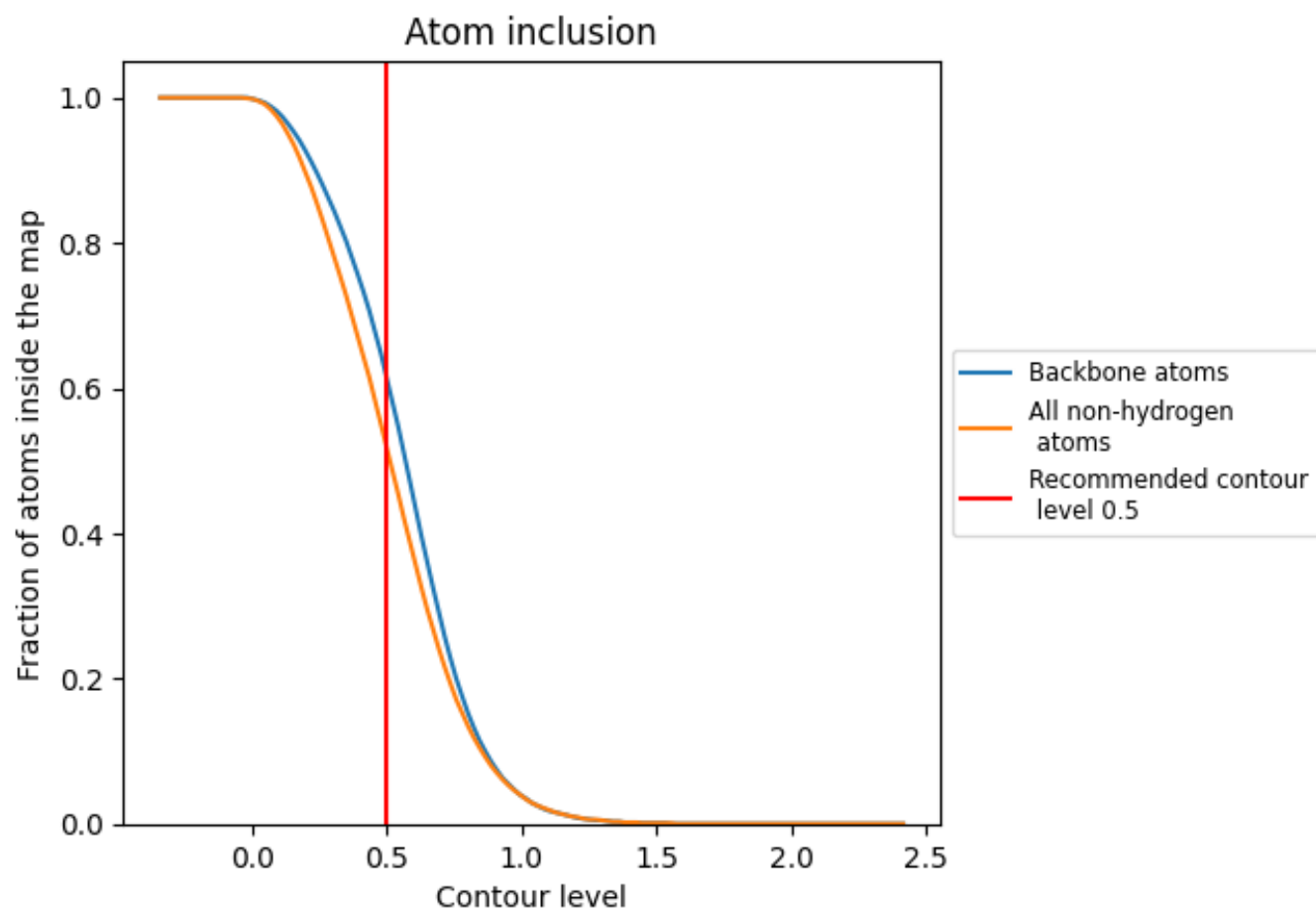
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 61% of all backbone atoms, 52% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5180	 0.4150
AA	 0.7250	 0.4790
AB	 0.2420	 0.4180
AC	 0.5560	 0.4950
AD	 0.4380	 0.4710
AE	 0.4830	 0.4930
AF	 0.3760	 0.4510
AG	 0.4690	 0.4420
AH	 0.5060	 0.4900
AI	 0.6160	 0.4900
AJ	 0.5020	 0.4680
AK	 0.4000	 0.4740
AL	 0.5550	 0.5060
AM	 0.5480	 0.4710
AN	 0.6560	 0.5010
AO	 0.4880	 0.4850
AP	 0.5740	 0.4990
AQ	 0.4870	 0.4810
AR	 0.4250	 0.4720
AS	 0.6600	 0.4980
AT	 0.5270	 0.4910
AU	 0.2450	 0.3910
AV	 0.2890	 0.3010
AW	 0.3570	 0.4410
AX	 0.2030	 0.4340
AY	 0.0020	 0.3590
B1	 0.4440	 0.4930
B2	 0.3480	 0.4970
B3	 0.0210	 0.4460
B4	 0.5150	 0.5320
B5	 0.4520	 0.5190
B6	 0.3900	 0.5070
B7	 0.0130	 0.3290
BA	 0.5490	 0.4720
BB	 0.4510	 0.4660



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Chain	Atom inclusion	Q-score
BC	 0.4470	 0.5170
BD	 0.4280	 0.5090
BE	 0.3860	 0.4830
BF	 0.1270	 0.4160
BG	 0.1860	 0.4270
BH	 0.0360	 0.2540
BI	 0.0000	 0.1480
BJ	 0.0000	 0.1760
BK	 0.4600	 0.5090
BL	 0.3980	 0.4990
BM	 0.4070	 0.5000
BN	 0.3830	 0.5110
BO	 0.4630	 0.5160
BP	 0.2660	 0.4710
BQ	 0.3510	 0.4880
BR	 0.5450	 0.5190
BS	 0.4320	 0.5130
BT	 0.4660	 0.5030
BU	 0.3240	 0.4730
BV	 0.3770	 0.4770
BW	 0.3100	 0.4850
BX	 0.4360	 0.5110
BY	 0.3910	 0.4940
BZ	 0.2660	 0.4410
CA	 0.6040	 0.1270
CB	 0.6620	 0.1250
CC	 0.4760	 0.1230
CD	 0.4330	 0.1080
CE	 0.3200	 0.1200
CF	 0.2340	 0.1990
CN	 0.4140	 0.1560
CT	 0.5740	 0.1830