



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 06:31 AM EST

PDB ID : 4V69
EMDB ID : EMD-5036
Title : Ternary complex-bound E.coli 70S ribosome.
Authors : Villa, E.; Sengupta, J.; Trabuco, L.G.; LeBarron, J.; Baxter, W.T.; Shaikh, T.R.; Grassucci, R.A.; Nissen, P.; Ehrenberg, M.; Schulten, K.; Frank, J.
Deposited on : 2008-12-11
Resolution : 6.70 Å (reported)
Based on initial models : 2J00, 1OB2, 2I2V, 2I2U

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

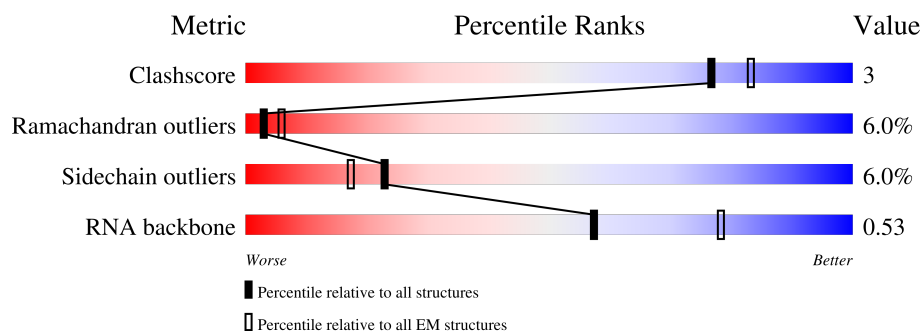
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AJ	98	<div> <div>38%</div> <div>66%</div> <div>26%</div> <div>7%</div> <div>.</div> </div>
2	AK	117	<div> <div>34%</div> <div>69%</div> <div>26%</div> <div>.</div> </div>
3	AL	123	<div> <div>37%</div> <div>67%</div> <div>26%</div> <div>7%</div> <div>.</div> </div>
4	AM	113	<div> <div>22%</div> <div>58%</div> <div>28%</div> <div>13%</div> </div>
5	AN	96	<div> <div>22%</div> <div>58%</div> <div>28%</div> <div>12%</div> <div>.</div> </div>
6	AO	88	<div> <div>13%</div> <div>65%</div> <div>27%</div> <div>6%</div> <div>.</div> </div>
7	AP	80	<div> <div>22%</div> <div>65%</div> <div>29%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
8	AQ	80	
9	AR	55	
10	AS	79	
11	AT	85	
12	AU	51	
13	AB	218	
14	AC	206	
15	AD	205	
16	AE	150	
17	AF	100	
18	AG	150	
19	AH	129	
20	AI	127	
21	AA	1530	
22	AY	76	
23	AW	76	
24	AX	11	
25	AZ	393	
26	AV	77	
27	B5	234	
28	BI	141	
29	BJ	142	
30	BK	121	
31	BL	143	
32	BM	136	

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Mol	Chain	Length	Quality of chain
33	BN	120	
34	BO	116	
35	BP	114	
36	BQ	117	
37	BR	103	
38	BS	110	
39	BT	93	
40	BU	102	
41	BV	94	
42	BW	79	
43	BX	77	
44	BY	63	
45	BC	271	
46	BZ	58	
47	B0	56	
48	B1	50	
49	B2	46	
50	B3	64	
51	B4	38	
52	BD	209	
53	BE	201	
54	BF	178	
55	BG	176	
56	BH	149	
57	BB	2903	

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Mol	Chain	Length	Quality of chain
58	BA	117	<div><div></div><div>38%</div><div>46%</div><div>15%</div></div>

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 152250 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AJ	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 2 is a protein called 30S ribosomal protein S11.

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

- Molecule 3 is a protein called 30S ribosomal protein S12.

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

- Molecule 4 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AM	113	Total	C	N	O	S	0	0
			877	541	177	156	3		

- Molecule 5 is a protein called 30S ribosomal protein S14.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	?	-	SER	deletion	UNP P0AG59
AN	?	-	ASP	deletion	UNP P0AG59
AN	?	-	GLU	deletion	UNP P0AG59

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Chain	Residue	Modelled	Actual	Comment	Reference
AN	?	-	ASP	deletion	UNP P0AG59

- Molecule 6 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AO	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 7 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AP	80	Total	C	N	O	S	0	0
			639	400	126	112	1		

- Molecule 8 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AQ	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 9 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AR	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 10 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AS	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 11 is a protein called 30S ribosomal protein S20.

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

- Molecule 12 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AU	51	Total	C	N	O	S	0	0
			426	265	86	74	1		

- Molecule 13 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AB	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 14 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AC	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 15 is a protein called 30S ribosomal protein S4.

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

- Molecule 16 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AE	150	Total	C	N	O	S	0	0
			1106	687	211	202	6		

- Molecule 17 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AF	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 18 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AG	150	Total	C	N	O	S	0	0
			1175	730	226	215	4		

- Molecule 19 is a protein called 30S ribosomal protein S8.

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

- Molecule 20 is a protein called 30S ribosomal protein S9.

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

- Molecule 21 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AA	1530	Total	C	N	O	P	0	0
			32832	14642	6024	10636	1530		

- Molecule 22 is a RNA chain called A/T-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AY	76	Total	C	N	O	P	0	0
			1622	725	293	529	75		

- Molecule 23 is a RNA chain called P-site tRNA fMet (Unmodified bases except for Thymine 54).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0
			232	106	44	72	10		

- Molecule 25 is a protein called Elongation factor Tu.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AZ	393	Total	C	N	O	S	0	0
			3035	1918	523	581	13		

- Molecule 26 is a RNA chain called E-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AV	77	Total	C	N	O	P	0	0
			1645	733	297	538	77		

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 28 is a protein called 50S ribosomal protein L11.

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

- Molecule 29 is a protein called 50S ribosomal protein L13.

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

- Molecule 30 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BK	121	Total	C	N	O	S	0	0
			931	582	179	165	5		

- Molecule 31 is a protein called 50S ribosomal protein L15.

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

- Molecule 32 is a protein called 50S ribosomal protein L16.

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

- Molecule 33 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BN	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 34 is a protein called 50S ribosomal protein L18.

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

- Molecule 35 is a protein called 50S ribosomal protein L19.

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

- Molecule 36 is a protein called 50S ribosomal protein L20.

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

- Molecule 37 is a protein called 50S ribosomal protein L21.

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

- Molecule 38 is a protein called 50S ribosomal protein L22.

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

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BT	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 40 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BU	102	Total	C	N	O		
			780	492	146	142	0	0

- Molecule 41 is a protein called 50S ribosomal protein L25.

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

- Molecule 42 is a protein called 50S ribosomal protein L27.

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

- Molecule 43 is a protein called 50S ribosomal protein L28.

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

- Molecule 44 is a protein called 50S ribosomal protein L29.

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

- Molecule 45 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BC	271	Total	C	N	O	S		
			2083	1288	423	365	7	0	0

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B1	50	Total	C	N	O	S	0	0
			410	263	75	72			

- Molecule 49 is a protein called 50S ribosomal protein L34.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L36.

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

- Molecule 52 is a protein called 50S ribosomal protein L3.

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

- Molecule 53 is a protein called 50S ribosomal protein L4.

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

- Molecule 54 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 55 is a protein called 50S ribosomal protein L6.

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

- Molecule 56 is a protein called 50S ribosomal protein L9.

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

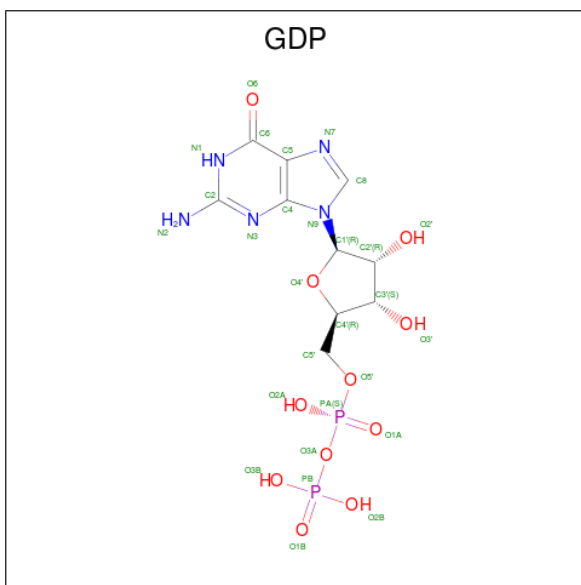
- Molecule 57 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BB	2903	Total	C	N	O	P	0	0
			62321	27801	11467	20150	2903		

- Molecule 58 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BA	117	Total	C	N	O	P	0	0
			2508	1116	459	816	117		

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

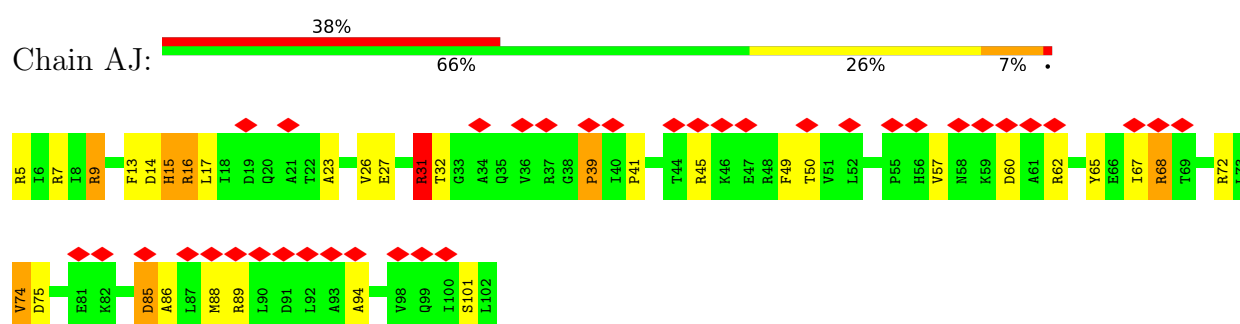


Mol	Chain	Residues	Atoms					AltConf
59	AZ	1	Total	C	N	O	P	0
			28	10	5	11	2	

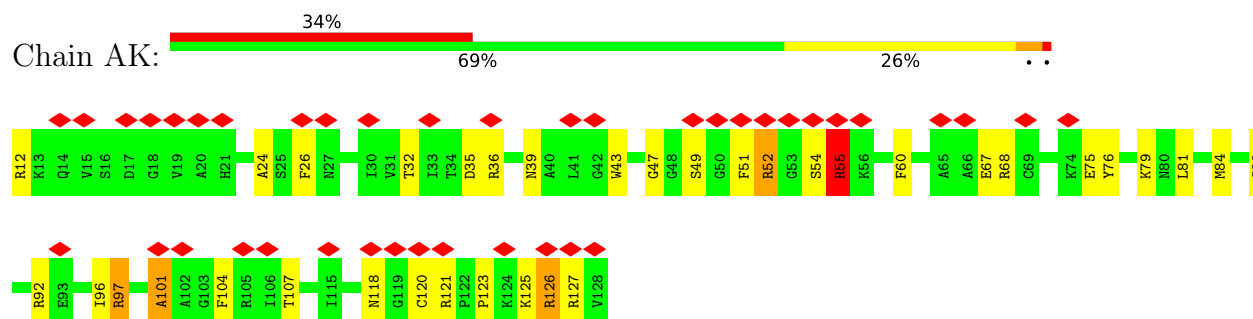
3 Residue-property plots [i](#)

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

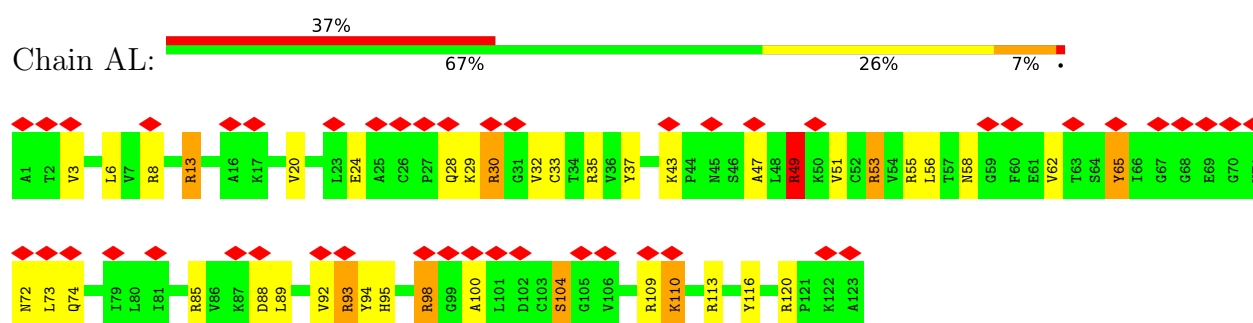
• Molecule 1: 30S ribosomal protein S10



• Molecule 2: 30S ribosomal protein S11

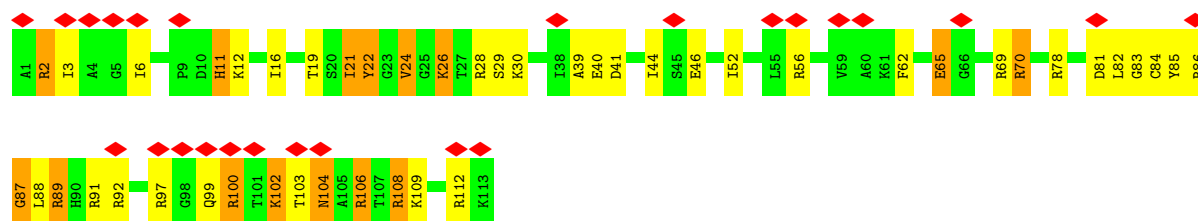


• Molecule 3: 30S ribosomal protein S12



• Molecule 4: 30S ribosomal protein S13

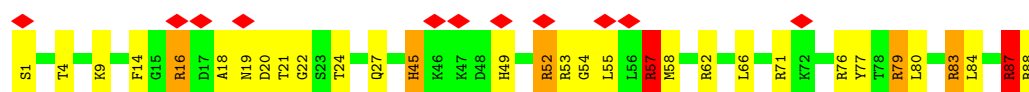




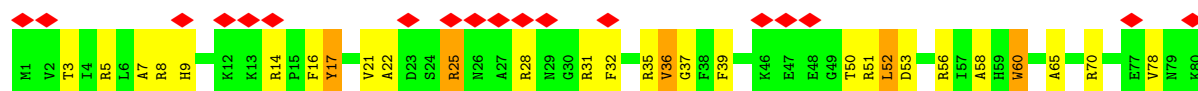
• Molecule 5: 30S ribosomal protein S14



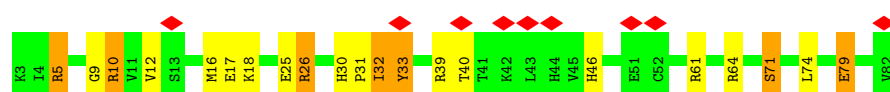
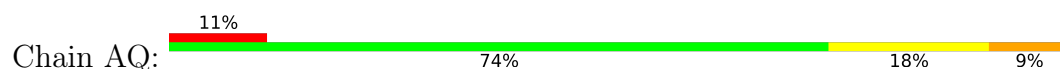
• Molecule 6: 30S ribosomal protein S15



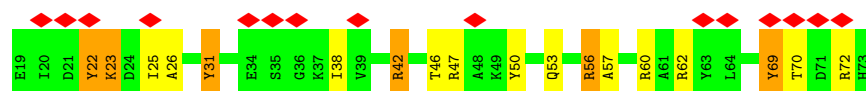
• Molecule 7: 30S ribosomal protein S16



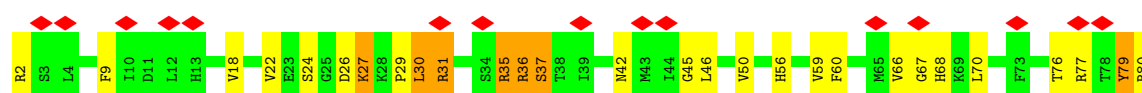
• Molecule 8: 30S ribosomal protein S17



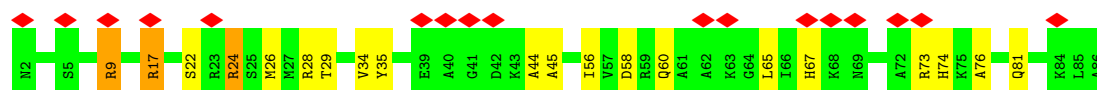
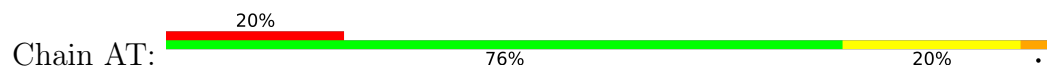
• Molecule 9: 30S ribosomal protein S18



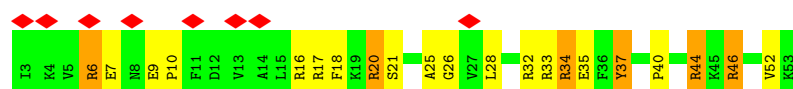
• Molecule 10: 30S ribosomal protein S19



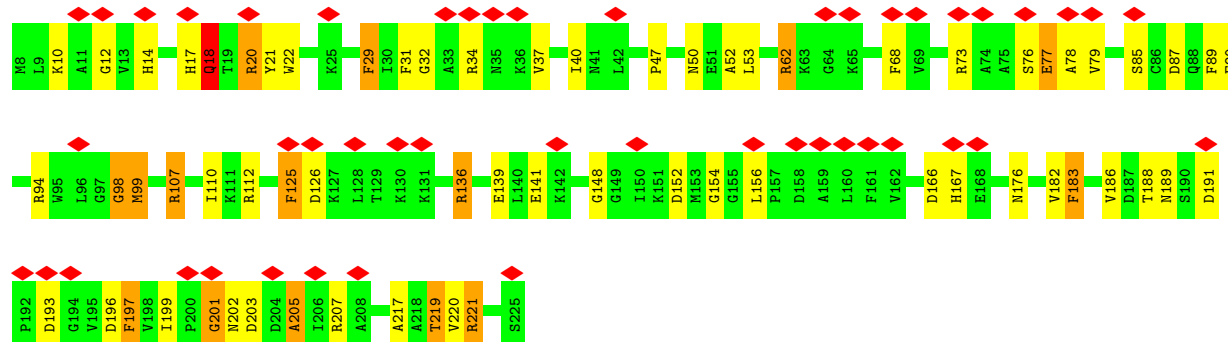
• Molecule 11: 30S ribosomal protein S20



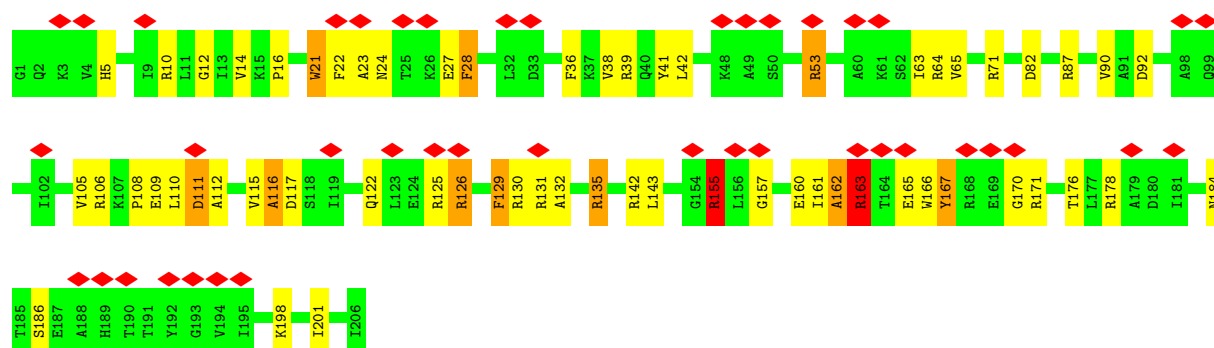
• Molecule 12: 30S ribosomal protein S21



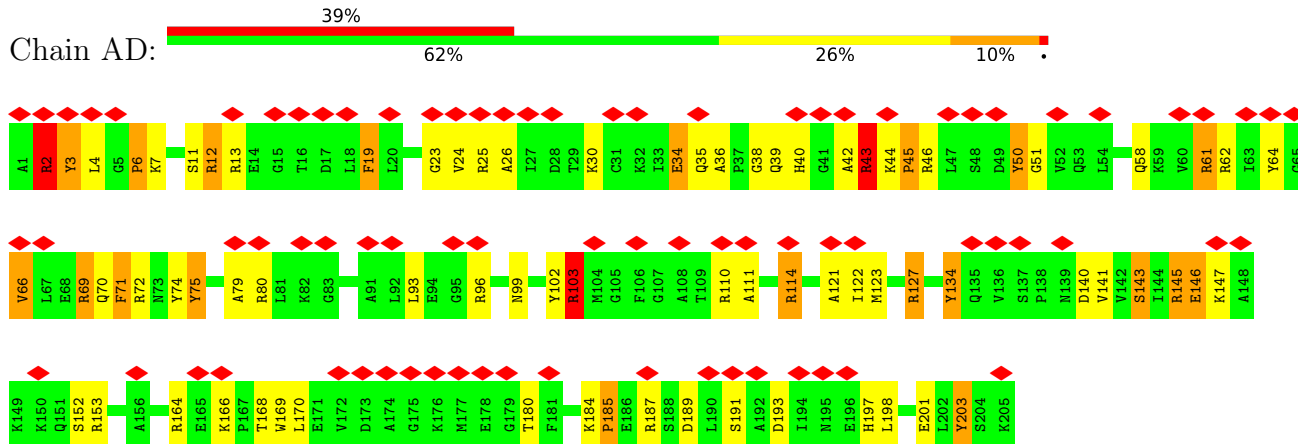
• Molecule 13: 30S ribosomal protein S2

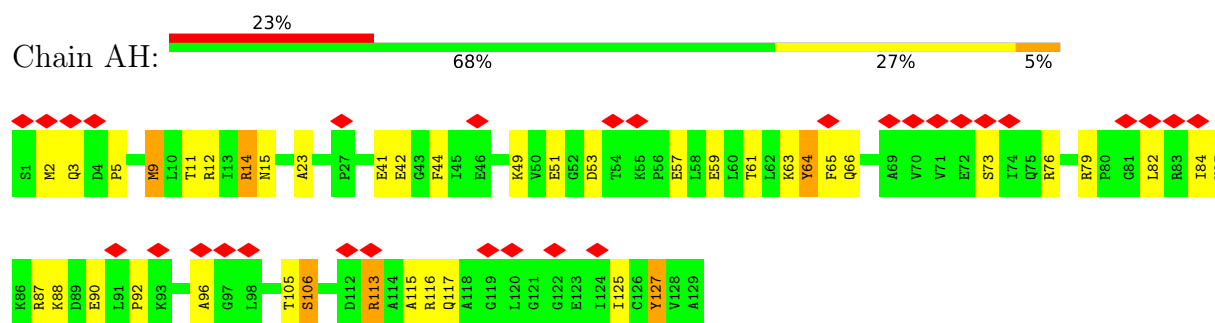


• Molecule 14: 30S ribosomal protein S3

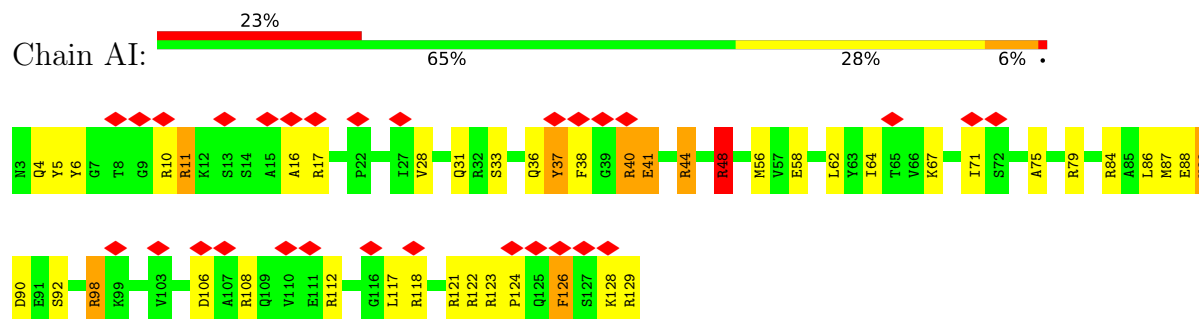


- Molecule 15: 30S ribosomal protein S4

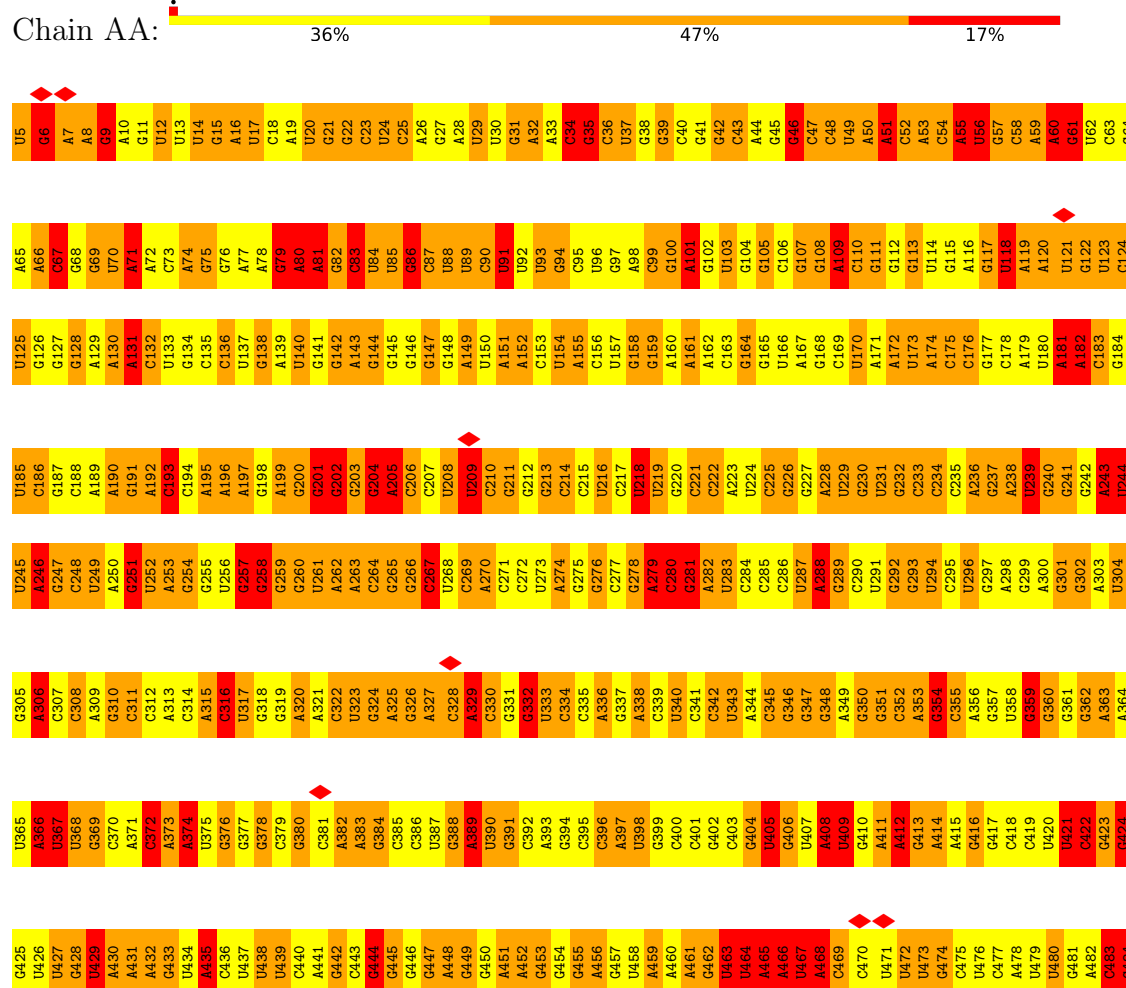




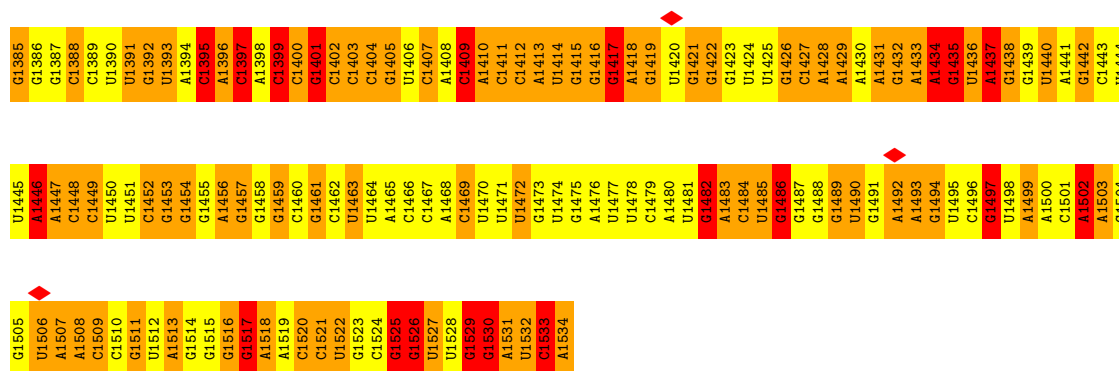
- Molecule 20: 30S ribosomal protein S9



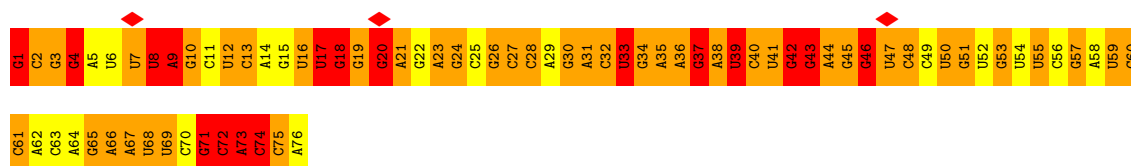
- Molecule 21: 16S rRNA



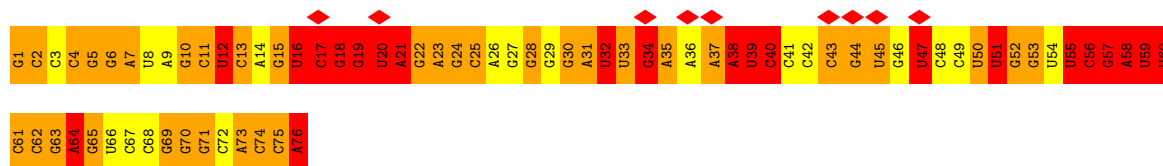
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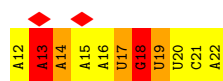
• Molecule 22: A/T-site tRNA Phe



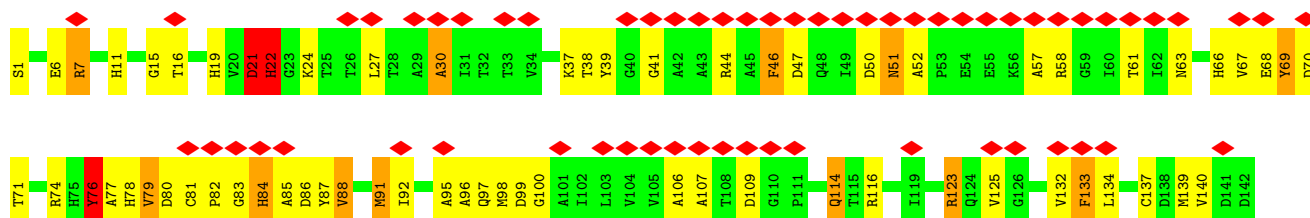
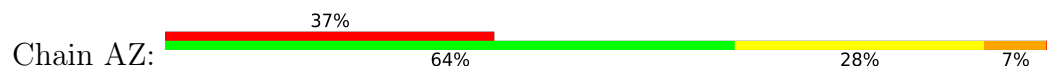
• Molecule 23: P-site tRNA fMet (Unmodified bases except for Thymine 54)

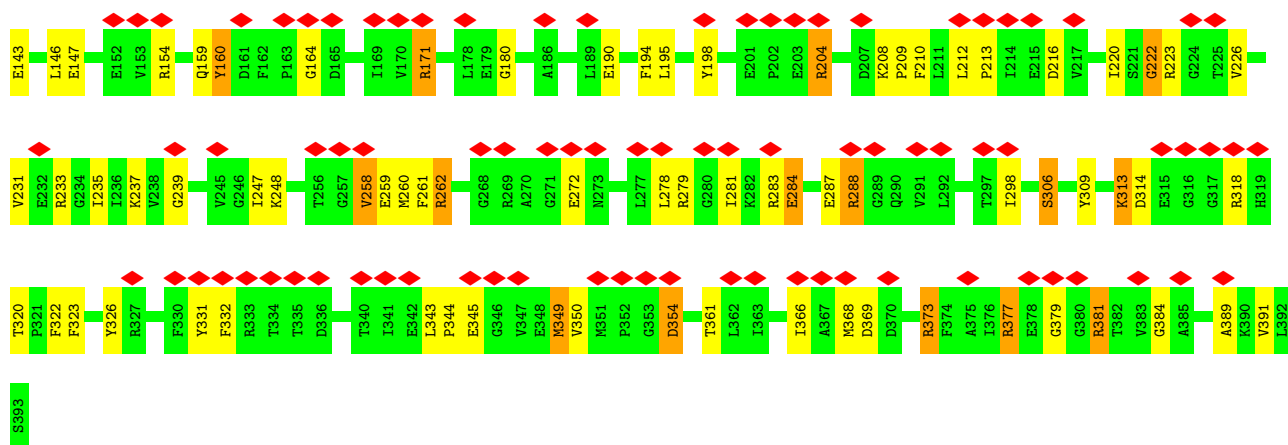


• Molecule 24: mRNA

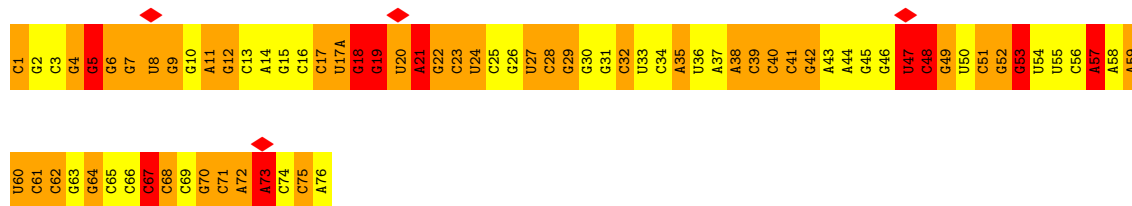


• Molecule 25: Elongation factor Tu

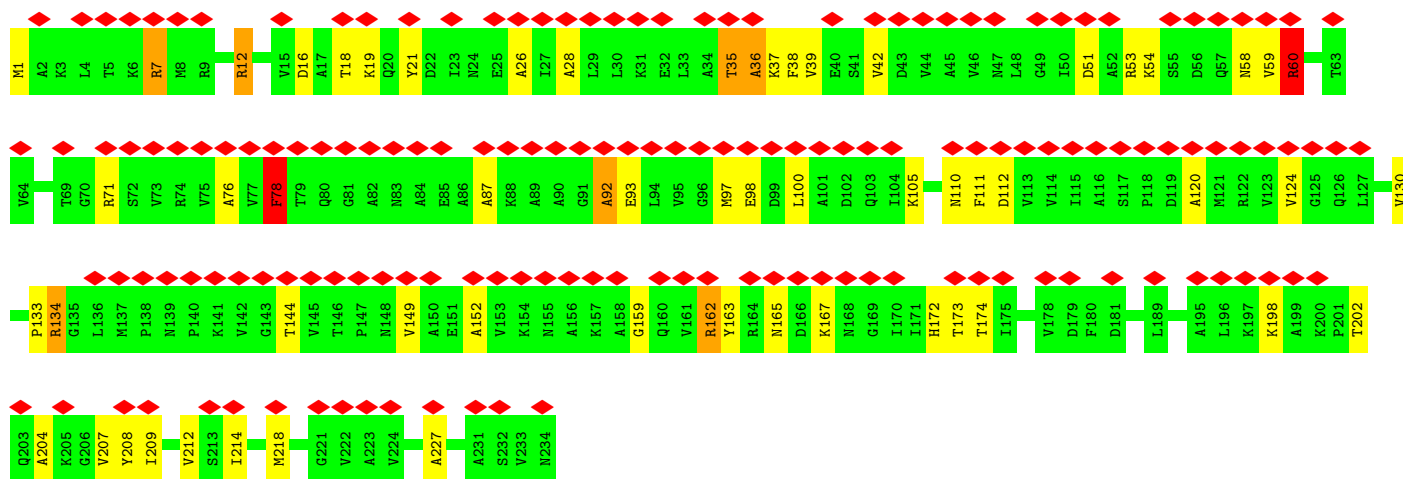
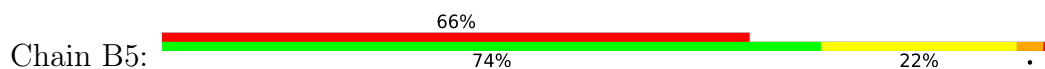




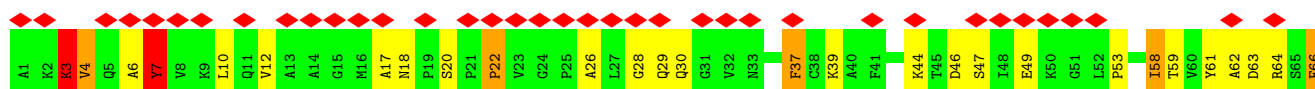
• Molecule 26: E-site tRNA Phe



• Molecule 27: 50S ribosomal protein L1

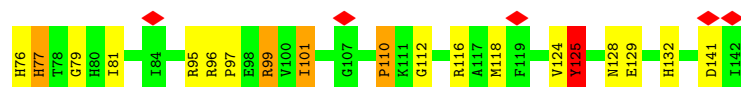
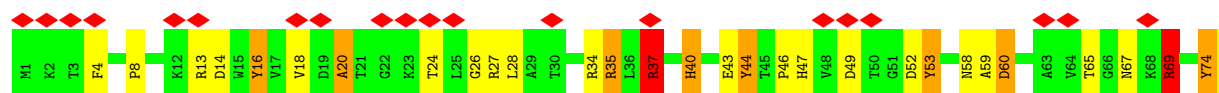


• Molecule 28: 50S ribosomal protein L11

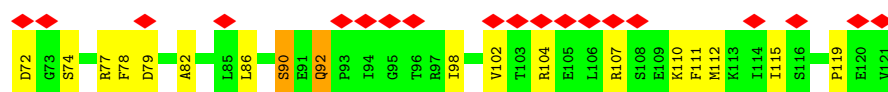




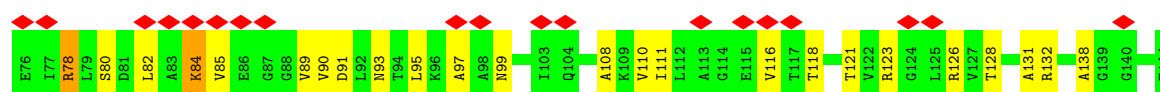
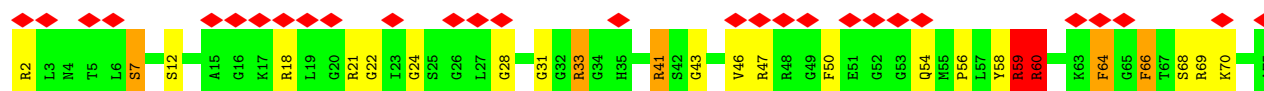
• Molecule 29: 50S ribosomal protein L13



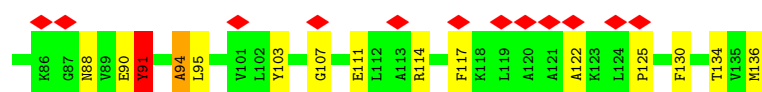
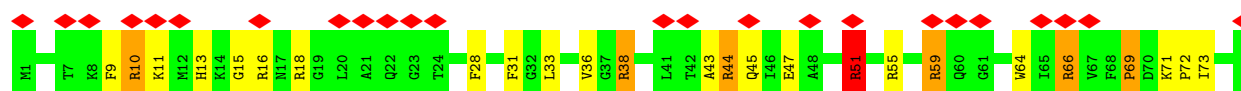
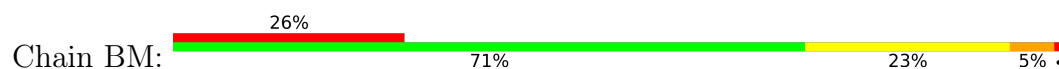
• Molecule 30: 50S ribosomal protein L14



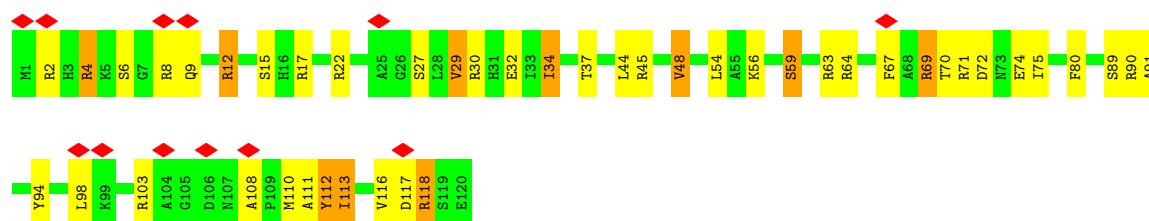
• Molecule 31: 50S ribosomal protein L15



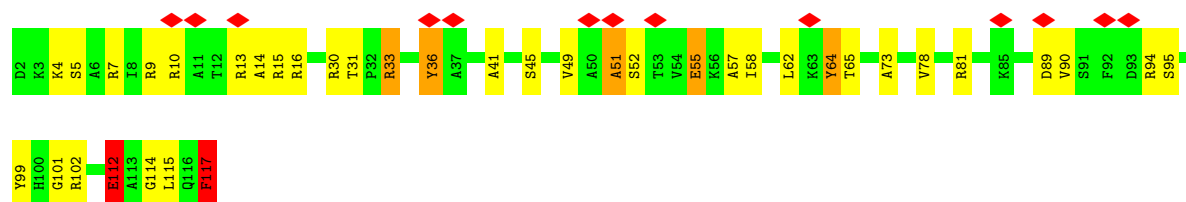
• Molecule 32: 50S ribosomal protein L16



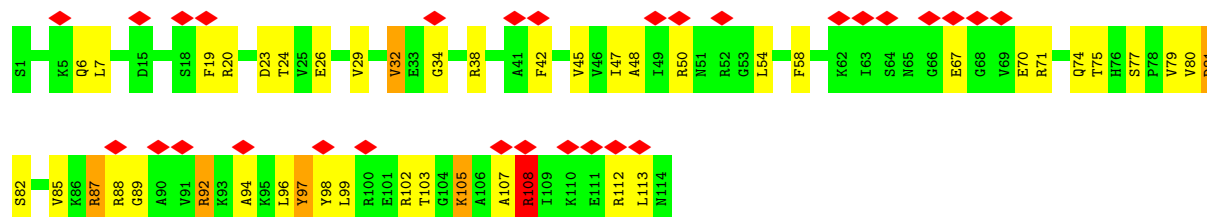
• Molecule 33: 50S ribosomal protein L17



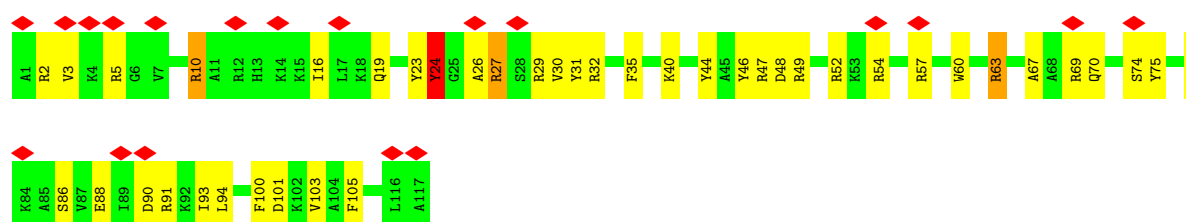
• Molecule 34: 50S ribosomal protein L18



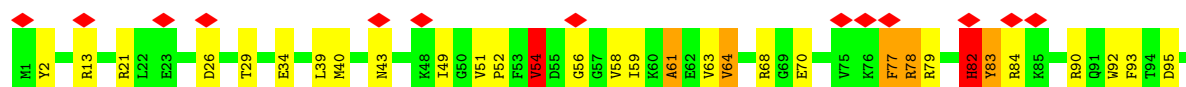
• Molecule 35: 50S ribosomal protein L19

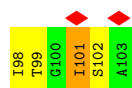


• Molecule 36: 50S ribosomal protein L20

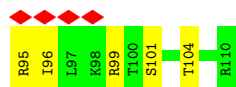
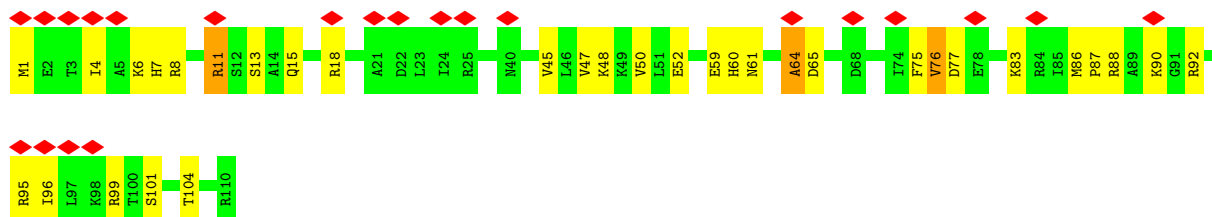
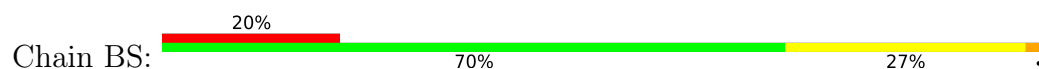


• Molecule 37: 50S ribosomal protein L21

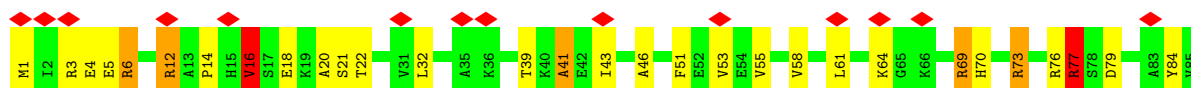




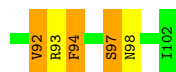
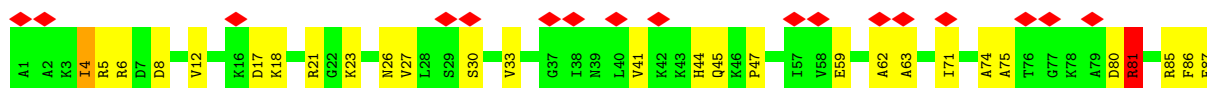
- Molecule 38: 50S ribosomal protein L22



- Molecule 39: 50S ribosomal protein L23



- Molecule 40: 50S ribosomal protein L24

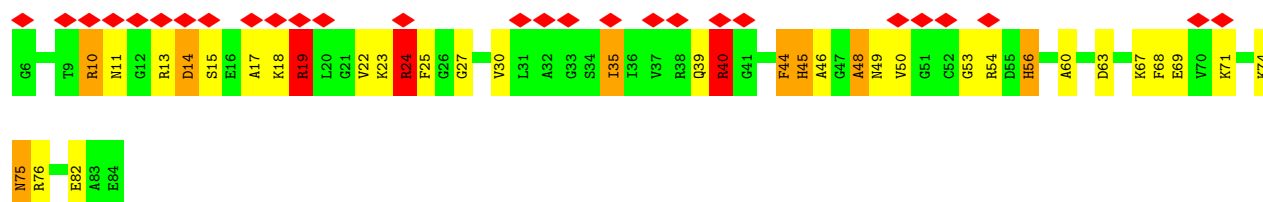


- Molecule 41: 50S ribosomal protein L25



- Molecule 42: 50S ribosomal protein L27

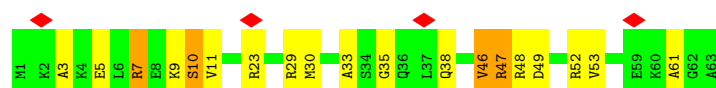




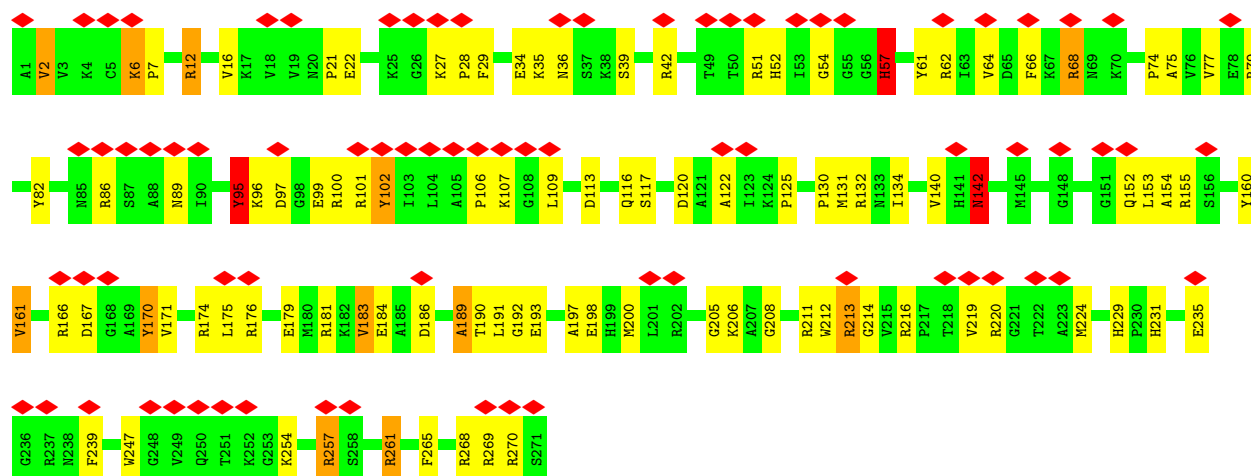
- Molecule 43: 50S ribosomal protein L28



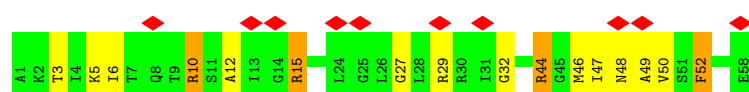
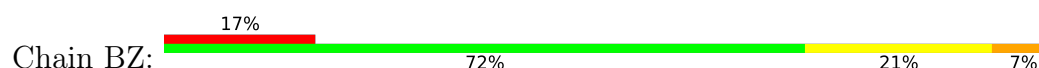
- Molecule 44: 50S ribosomal protein L29



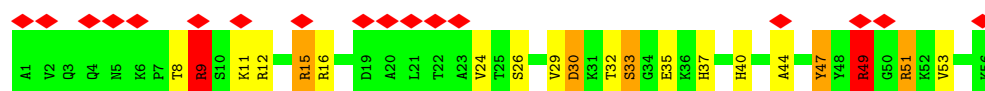
- Molecule 45: 50S ribosomal protein L2



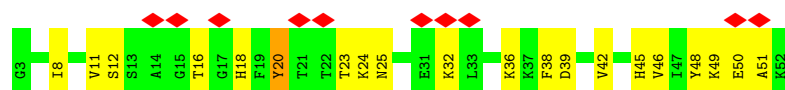
- Molecule 46: 50S ribosomal protein L30



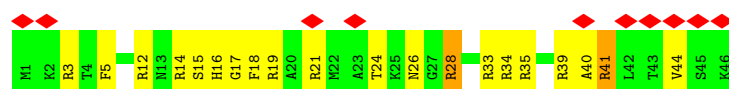
- Molecule 47: 50S ribosomal protein L32



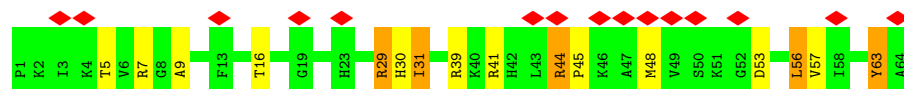
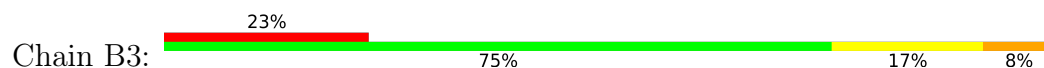
• Molecule 48: 50S ribosomal protein L33



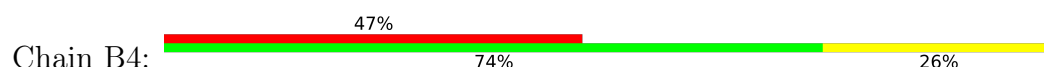
• Molecule 49: 50S ribosomal protein L34



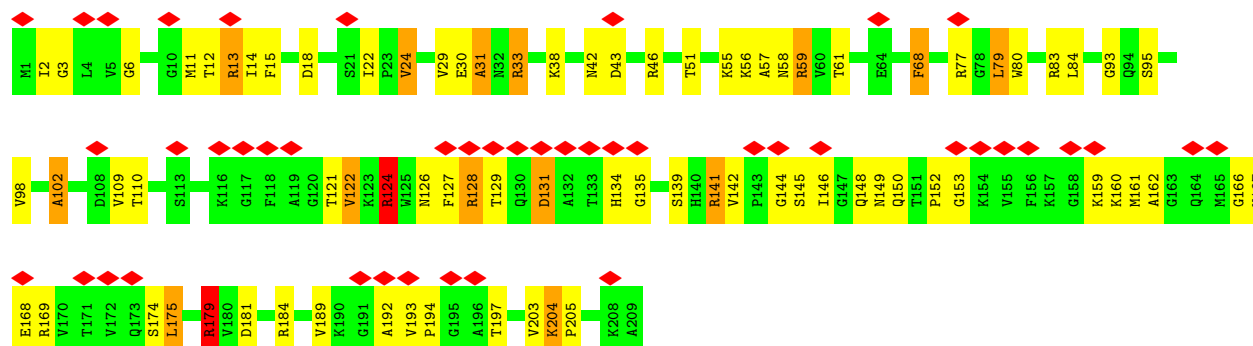
• Molecule 50: 50S ribosomal protein L35



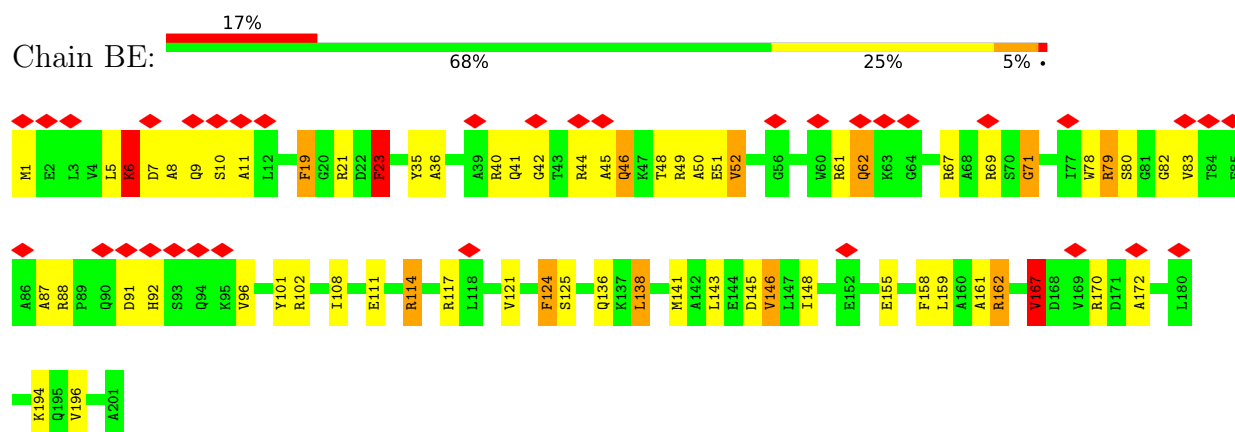
• Molecule 51: 50S ribosomal protein L36



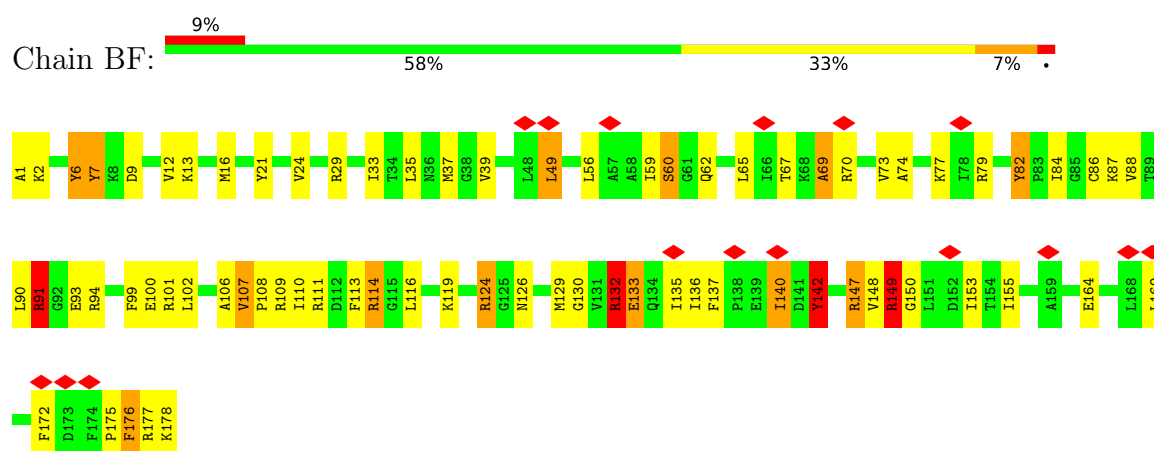
• Molecule 52: 50S ribosomal protein L3



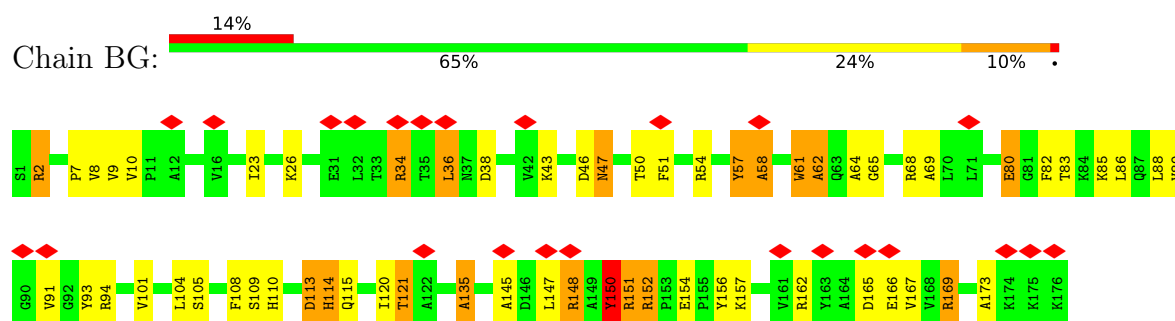
- Molecule 53: 50S ribosomal protein L4



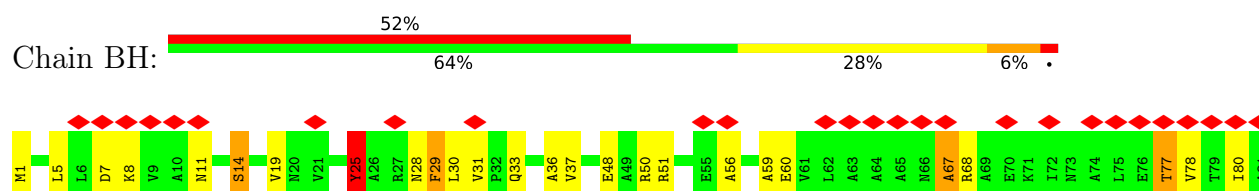
- Molecule 54: 50S ribosomal protein L5

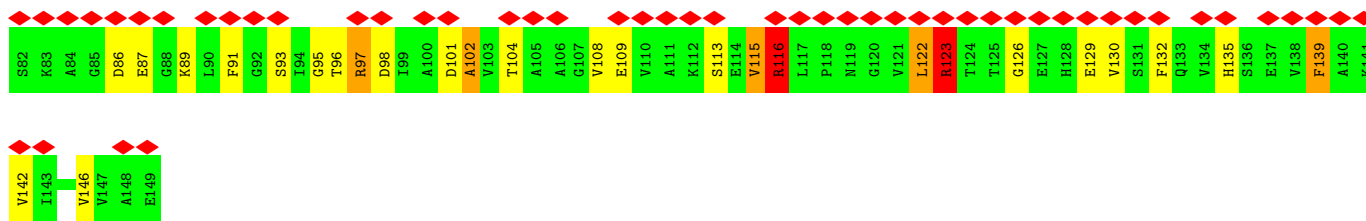


- Molecule 55: 50S ribosomal protein L6



- Molecule 56: 50S ribosomal protein L9





• Molecule 57: 23S ribosomal RNA



G1	G2	G3	G4	G5	G6	G7	G8	G9	G10	G11	G12	G13	G14	G15	G16	G17	G18	G19	G20	G21	G22	G23	G24	G25	G26	G27	G28	G29	G30	G31	G32	G33	G34	G35	G36	G37	G38	G39	G40	G41	G42	G43	G44	G45	G46	G47	G48	G49	G50	G51	G52	G53	G54	G55	G56	G57	G58	G59	G60
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G121	G122	G123	G124	G125	G126	G127	G128	G129	G130	G131	G132	G133	G134	G135	G136	G137	G138	G139	G140	G141	G142	G143	G144	G145	G146	G147	G148	G149	G150	G151	G152	G153	G154	G155	G156	G157	G158	G159	G160	G161	G162	G163	G164	G165	G166	G167	G168	G169	G170	G171	G172	G173	G174	G175	G176	G177	G178	G179	G180
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U2522	C2462	C2342	G2282	G2222	G2162	G2102	A2042	U1982	G1922	G1862	A1802	U1742
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G2527	C2467	G2347	G2287	A2227	U2167	G2107	C2047	A1987	U1927	G1867	G1807	U1747
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A2469	G2349	G2349	G2289	U2229	A2169	U2109	G2049	G1989	G1929	C1869	A1809	G1749
A2530	G2409	G2410	G2290	G2230	A2170	U2110	C2050	C1990	C1870	G1869	A1810	A1750
A2531	A2411	U2291	U2291	U2231	A2171	U2111	A2051	U1991	U1931	A1871	G1811	U1751
G2532	A2412	A2352	U2292	C2232	U2172	G2112	A2052	G1992	A1932	A1872	C1812	C1752
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A2534	G2414	C2354	G2294	G2234	C2174	U2114	A2054	C1994	C1874	A1874	A1814	A1754
G2535	G2415	G2355	C2295	G2235	C2175	G2115	C2055	U1995	G1935	G1875	A1815	A1755
G2536	U2356	U2356	U2296	U2236	C2176	G2116	C2056	C1996	A1936	A1876	G1816	G1756
U2537	G2417	G2357	G2297	G2237	C2177	A2117	G2057	C1997	A1937	A1877	G1817	A1757
C2538	A2418	A2358	A2298	G2238	C2178	U2118	A2058	A1998	G1878	G1878	U1818	U1758
U2539	U2419	C2359	U2299	G2239	C2179	G2119	A2059	C1999	U1939	A1879	A1819	A1759
C2540	G2420	G2360	C2300	U2240	U2180	G2120	A2060	C2000	U1940	U1880	U1820	C1760
A2541	G2421	G2361	C2301	A2241	U2181	G2121	G2061	C2001	C1941	C1881	A1821	C1761
A2542	C2422	C2362	U2302	G2242	U2182	U2122	A2062	G2002	C1942	U1882	C1822	A1762
G2543	G2363	G2363	G2303	U2243	A2183	G2123	C2063	A2003	U1943	G1883	G1823	G1763
G2544	G2364	G2364	G2304	U2244	A2184	G2124	C2064	G2004	U1944	G1884	G1824	C1764
G2545	G2365	G2365	U2305	U2245	U2185	G2125	C2065	A2005	G1945	U1885	U1825	U1765
U2546	A2366	A2366	C2306	G2246	U2186	A2126	C2066	G2006	U1946	U1886	G1826	G1766
A2547	C2427	G2367	G2307	A2247	U2187	G2127	G2067	U2007	C1947	C1887	U1827	G1767
U2548	G2488	C2368	G2308	G2248	U2188	G2128	U2068	C2008	G1948	G1888	G1828	C1768
U2549	U2489	A2369	A2309	U2249	U2189	G2129	G2069	A2009	G1949	A1889	A1829	U1769
G2550	G2490	G2370	C2310	G2250	U2190	G2129	A2070	G2010	G1950	A1890	G1830	G1770
C2551	U2431	G2371	A2311	G2251	A2191	U2130	A2071	U2011	U1951	G1891	G1831	C1771
U2552	U2432	U2372	U2312	G2252	U2192	U2131	C2072	G2012	A1952	C1892	C1832	A1772
G2553	U2493	G2373	C2313	G2253	U2193	U2132	C2073	A2013	G1953	C1893	C1833	A1773
U2554	A2434	C2374	A2314	G2254	U2194	G2133	U2074	A2014	G1954	C1894	U1834	C1774
U2555	A2435	G2375	G2315	G2255	U2195	G2134	U2075	A2015	U1955	C1895	G1835	U1775
C2556	G2436	A2376	C2316	G2256	C2196	A2135	U2076	U2016	U1956	G1896	C1836	G1776
G2557	G2437	A2377	A2317	U2257	U2197	G2136	A2077	U2017	C1957	G1897	C1837	U1777
C2558	U2438	G2378	G2318	U2258	A2198	A2137	C2078	G2018	C1958	U1898	U1778	U1778
C2559	G2379	G2319	G2319	U2259	A2199	G2138	U2079	A2019	G1959	A1899	G1839	U1779
A2560	C2380	U2320	G2200	C2260	G2200	U2139	A2080	A2020	A1960	A1900	G1840	A1780
U2561	C2381	U2321	G2201	G2261	G2201	U2140	U2081	C2021	C1961	A1901	U1841	U1781
U2562	G2382	A2322	U2202	U2262	U2202	G2141	A2082	U2022	C1962	C1902	G1842	U1782
U2563	G2383	G2323	U2203	C2263	G2203	A2142	G2083	C2023	G1963	G1903	C1843	A1783
A2564	U2384	G2324	G2204	C2264	G2204	C2143	C2084	G2024	U1964	G1904	C1844	A1784
A2565	C2385	G2325	U2265	U2265	A2205	G2144	U2085	C2025	G1965	G1905	A1785	A1785
A2566	A2386	C2326	A2266	A2266	C2206	G2145	U2086	U2026	A1966	G1906	G1846	A1786
G2567	U2387	A2327	A2267	A2267	C2207	G2146	G2087	G2027	C1967	G1907	A1847	A1787
U2568	A2388	A2328	A2328	A2268	C2208	A2147	A2088	U2028	G1968	C1908	A1848	C1788
G2569	G2389	U2329	G2209	G2269	G2209	G2148	C2089	G2029	U1969	G1909	A1849	A1789
G2570	U2390	G2330	U2210	A2270	U2210	U2149	A2090	G1910	C1970	C1909	G1850	C1790
U2571	G2391	G2331	A2211	G2271	A2211	C2150	C2091	U1911	A1970	U1911	U1851	A1791
C2572	U2392	C2332	U2212	U2272	A2212	U2151	U2092	G2032	U1971	A1912	U1852	G1792
A2573	G2393	A2333	U2213	A2273	U2213	G2152	G2093	A2033	G1972	A1913	A1853	C1793
G2574	C2394	U2334	A2274	A2274	C2214	C2153	A2094	U2034	C1973	U1914	A1854	A1794
C2575	G2395	A2335	C2275	C2275	C2215	G2154	A2095	G2035	G1974	U1915	U1855	C1795
G2576	G2396	A2336	G2276	G2276	C2216	U2155	C2096	G2036	G1975	A1916	U1856	U1796
U2577	G2397	G2337	G2277	G2277	G2217	G2156	A2097	A2037	U1976	U1917	G1857	G1797
G2578	U2398	G2338	A2278	G2278	G2218	G2157	U2098	G2038	A1977	A1918	U1798	U1798
C2579	G2399	G2339	U2279	G2279	U2219	A2158	U2099	U2039	A1978	A1919	A1858	G1799
U2580	U2400	A2340	G2280	G2280	U2220	G2159	G2100	G2040	U1979	C1920	G1860	C1800
G2581	U2401	G2341	A2281		G2221	C2160	A2101	U2041	A1980	G1921	G1861	A1801

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131599	Depositor
Resolution determination method	Not provided	
CTF correction method	Correction of reconstruction of each defocus group	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	4520	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	58279	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	303.004	Depositor
Minimum map value	-114.578	Depositor
Average map value	6.031	Depositor
Map value standard deviation	29.145	Depositor
Recommended contour level	90.0	Depositor
Map size (\AA)	370.80002, 370.80002, 370.80002	wwPDB
Map dimensions	309, 309, 309	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.2, 1.2, 1.2	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

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	AJ	1.80	12/797 (1.5%)	1.89	19/1077 (1.8%)
2	AK	1.83	17/893 (1.9%)	2.02	24/1205 (2.0%)
3	AL	1.73	7/969 (0.7%)	1.96	24/1300 (1.8%)
4	AM	1.83	12/885 (1.4%)	2.12	35/1181 (3.0%)
5	AN	1.84	13/786 (1.7%)	2.19	27/1046 (2.6%)
6	AO	1.75	9/724 (1.2%)	1.94	16/966 (1.7%)
7	AP	1.90	14/649 (2.2%)	2.07	22/870 (2.5%)
8	AQ	1.80	10/658 (1.5%)	1.95	11/881 (1.2%)
9	AR	1.81	5/463 (1.1%)	2.10	16/621 (2.6%)
10	AS	1.77	6/653 (0.9%)	1.98	15/877 (1.7%)
11	AT	1.70	8/671 (1.2%)	1.88	12/888 (1.4%)
12	AU	1.95	8/431 (1.9%)	2.14	13/570 (2.3%)
13	AB	1.69	20/1736 (1.2%)	2.01	42/2338 (1.8%)
14	AC	1.76	18/1652 (1.1%)	1.95	34/2225 (1.5%)
15	AD	1.79	20/1665 (1.2%)	2.02	46/2227 (2.1%)
16	AE	1.75	12/1119 (1.1%)	2.03	28/1504 (1.9%)
17	AF	1.80	5/836 (0.6%)	1.98	19/1128 (1.7%)
18	AG	1.83	15/1188 (1.3%)	2.09	34/1591 (2.1%)
19	AH	1.72	10/989 (1.0%)	2.00	24/1326 (1.8%)
20	AI	1.77	10/1034 (1.0%)	2.01	29/1375 (2.1%)
21	AA	3.42	4975/36763 (13.5%)	3.74	8350/57350 (14.6%)
22	AY	4.00	354/1814 (19.5%)	4.28	526/2827 (18.6%)
23	AW	5.13	269/1809 (14.9%)	3.87	451/2819 (16.0%)
24	AX	3.54	39/260 (15.0%)	3.68	65/403 (16.1%)
25	AZ	1.79	30/3091 (1.0%)	2.04	97/4182 (2.3%)
26	AV	3.50	261/1814 (14.4%)	3.81	416/2825 (14.7%)
27	B5	1.66	6/1748 (0.3%)	2.01	42/2355 (1.8%)
28	BI	1.69	5/1046 (0.5%)	2.02	30/1410 (2.1%)
29	BJ	1.75	9/1152 (0.8%)	1.97	27/1551 (1.7%)
30	BK	1.76	6/940 (0.6%)	2.06	30/1258 (2.4%)
31	BL	1.85	17/1054 (1.6%)	2.05	30/1403 (2.1%)
32	BM	1.83	16/1093 (1.5%)	2.20	29/1460 (2.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BN	1.87	16/974 (1.6%)	2.12	35/1301 (2.7%)
34	BO	1.87	15/902 (1.7%)	2.04	26/1209 (2.2%)
35	BP	1.78	6/929 (0.6%)	2.00	27/1242 (2.2%)
36	BQ	1.78	14/960 (1.5%)	2.16	38/1278 (3.0%)
37	BR	1.86	14/829 (1.7%)	2.09	25/1107 (2.3%)
38	BS	1.71	14/864 (1.6%)	1.97	19/1156 (1.6%)
39	BT	1.61	3/745 (0.4%)	2.03	23/994 (2.3%)
40	BU	1.72	5/788 (0.6%)	1.96	14/1051 (1.3%)
41	BV	1.70	7/766 (0.9%)	1.99	27/1025 (2.6%)
42	BW	1.85	15/603 (2.5%)	2.15	22/797 (2.8%)
43	BX	1.85	11/635 (1.7%)	1.98	18/848 (2.1%)
44	BY	1.67	5/510 (1.0%)	1.93	14/677 (2.1%)
45	BC	1.78	22/2122 (1.0%)	2.01	50/2852 (1.8%)
46	BZ	1.64	4/453 (0.9%)	1.99	11/605 (1.8%)
47	B0	1.78	2/450 (0.4%)	2.04	14/599 (2.3%)
48	B1	1.75	2/417 (0.5%)	1.91	8/554 (1.4%)
49	B2	1.87	7/380 (1.8%)	2.44	22/498 (4.4%)
50	B3	1.63	5/513 (1.0%)	1.85	10/676 (1.5%)
51	B4	1.88	3/303 (1.0%)	1.98	8/397 (2.0%)
52	BD	1.71	15/1586 (0.9%)	2.02	39/2134 (1.8%)
53	BE	1.71	13/1571 (0.8%)	1.99	42/2113 (2.0%)
54	BF	1.75	12/1444 (0.8%)	2.09	40/1937 (2.1%)
55	BG	1.76	21/1343 (1.6%)	2.07	37/1816 (2.0%)
56	BH	1.65	10/1122 (0.9%)	2.01	37/1515 (2.4%)
57	BB	3.38	9332/69800 (13.4%)	3.73	15942/108892 (14.6%)
58	BA	3.35	371/2804 (13.2%)	3.76	649/4371 (14.8%)
All	All	3.03	16162/165195 (9.8%)	3.37	27780/246683 (11.3%)

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	AJ	0	3
2	AK	0	4
3	AL	0	7
4	AM	0	5
5	AN	0	5
6	AO	0	5
7	AP	0	3
8	AQ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	AR	0	4
10	AS	0	1
11	AT	0	3
12	AU	0	5
13	AB	0	4
14	AC	0	5
15	AD	0	9
16	AE	0	1
17	AF	0	2
18	AG	0	4
19	AH	0	4
20	AI	0	6
21	AA	0	713
22	AY	0	40
23	AW	3	39
24	AX	0	3
25	AZ	0	8
26	AV	0	37
27	B5	1	7
28	BI	0	3
29	BJ	0	9
30	BK	0	1
31	BL	0	8
32	BM	0	4
33	BN	0	3
34	BO	0	4
35	BP	0	2
36	BQ	0	4
37	BR	0	6
38	BS	0	1
39	BT	0	2
40	BU	0	2
41	BV	0	4
42	BW	0	3
43	BX	0	3
44	BY	0	2
45	BC	0	9
46	BZ	0	3
47	B0	0	4
48	B1	0	2
49	B2	0	1
50	B3	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
51	B4	0	1
52	BD	0	5
53	BE	0	7
54	BF	0	9
55	BG	0	5
56	BH	0	3
57	BB	0	1349
58	BA	0	56
All	All	4	2445

The worst 5 of 16162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	63	G	N9-C8	84.56	1.97	1.37
23	AW	63	G	N7-C5	78.06	1.86	1.39
23	AW	63	G	C5-C4	69.51	1.87	1.38
23	AW	63	G	N9-C4	65.35	1.90	1.38
23	AW	63	G	C8-N7	61.20	1.67	1.30

The worst 5 of 27780 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	523	A	N1-C6-N6	27.08	134.85	118.60
57	BB	2097	A	N1-C6-N6	26.55	134.53	118.60
57	BB	725	G	N1-C6-O6	26.46	135.78	119.90
57	BB	2274	A	N1-C6-N6	26.21	134.33	118.60
58	BA	9	G	N1-C6-O6	25.88	135.43	119.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	AW	17	C	C1'
23	AW	47	U	C1'
23	AW	70	G	C3'
27	B5	37	LYS	CA

5 of 2445 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AJ	16	ARG	Sidechain
1	AJ	68	ARG	Sidechain
1	AJ	9	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	AK	26	PHE	Sidechain
2	AK	55	ARG	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	AJ	787	0	828	4	0
2	AK	877	0	887	1	0
3	AL	955	0	1019	9	0
4	AM	877	0	937	8	0
5	AN	774	0	828	9	0
6	AO	716	0	742	8	0
7	AP	639	0	656	2	0
8	AQ	649	0	691	3	0
9	AR	456	0	478	4	0
10	AS	638	0	665	7	0
11	AT	665	0	714	1	0
12	AU	426	0	449	0	0
13	AB	1705	0	1732	9	0
14	AC	1625	0	1699	7	0
15	AD	1643	0	1710	17	0
16	AE	1106	0	1148	6	0
17	AF	818	0	808	6	0
18	AG	1175	0	1230	10	0
19	AH	979	0	1034	4	0
20	AI	1022	0	1070	4	0
21	AA	32832	0	16503	179	0
22	AY	1622	0	812	11	0
23	AW	1619	0	822	22	0
24	AX	232	0	120	2	0
25	AZ	3035	0	3049	17	0
26	AV	1645	0	834	6	0
27	B5	1733	0	1823	10	0
28	BI	1032	0	1088	4	0
29	BJ	1129	0	1162	8	0
30	BK	931	0	1003	5	0
31	BL	1045	0	1117	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BM	1074	0	1157	1	0
33	BN	961	0	1000	5	0
34	BO	892	0	923	2	0
35	BP	917	0	965	5	0
36	BQ	947	0	1022	4	0
37	BR	816	0	839	3	0
38	BS	857	0	922	3	0
39	BT	739	0	807	4	0
40	BU	780	0	834	5	0
41	BV	753	0	780	3	0
42	BW	596	0	610	5	0
43	BX	625	0	655	3	0
44	BY	509	0	543	1	0
45	BC	2083	0	2157	16	0
46	BZ	449	0	491	0	0
47	B0	444	0	461	6	0
48	B1	410	0	440	4	0
49	B2	377	0	418	3	0
50	B3	504	0	574	3	0
51	B4	302	0	343	0	0
52	BD	1565	0	1616	16	0
53	BE	1552	0	1619	7	0
54	BF	1420	0	1460	10	0
55	BG	1323	0	1374	7	0
56	BH	1111	0	1148	4	0
57	BB	62321	0	31298	323	0
58	BA	2508	0	1268	8	0
59	AZ	28	0	12	0	0
All	All	152250	0	103394	772	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 3.

The worst 5 of 772 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)
23:AW:63:G:C5	23:AW:63:G:C4	1.87	1.59
23:AW:63:G:C8	23:AW:63:G:N7	1.67	1.56
23:AW:63:G:C5	23:AW:63:G:N7	1.86	1.43
23:AW:63:G:C4	23:AW:63:G:N9	1.90	1.40
23:AW:63:G:C8	23:AW:63:G:N9	1.97	1.31

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AJ	96/98 (98%)	77 (80%)	11 (12%)	8 (8%)	1	12
2	AK	115/117 (98%)	90 (78%)	18 (16%)	7 (6%)	1	17
3	AL	121/123 (98%)	107 (88%)	11 (9%)	3 (2%)	5	32
4	AM	111/113 (98%)	81 (73%)	20 (18%)	10 (9%)	1	11
5	AN	94/96 (98%)	67 (71%)	18 (19%)	9 (10%)	0	10
6	AO	86/88 (98%)	73 (85%)	8 (9%)	5 (6%)	1	18
7	AP	78/80 (98%)	61 (78%)	14 (18%)	3 (4%)	3	24
8	AQ	78/80 (98%)	62 (80%)	13 (17%)	3 (4%)	3	24
9	AR	53/55 (96%)	43 (81%)	10 (19%)	0	100	100
10	AS	77/79 (98%)	55 (71%)	17 (22%)	5 (6%)	1	16
11	AT	83/85 (98%)	73 (88%)	8 (10%)	2 (2%)	6	33
12	AU	49/51 (96%)	35 (71%)	10 (20%)	4 (8%)	1	12
13	AB	216/218 (99%)	166 (77%)	37 (17%)	13 (6%)	1	17
14	AC	204/206 (99%)	168 (82%)	26 (13%)	10 (5%)	2	20
15	AD	203/205 (99%)	161 (79%)	28 (14%)	14 (7%)	1	15
16	AE	148/150 (99%)	118 (80%)	21 (14%)	9 (6%)	1	17
17	AF	98/100 (98%)	79 (81%)	15 (15%)	4 (4%)	3	22
18	AG	148/150 (99%)	122 (82%)	18 (12%)	8 (5%)	2	19
19	AH	127/129 (98%)	96 (76%)	26 (20%)	5 (4%)	3	23
20	AI	125/127 (98%)	102 (82%)	21 (17%)	2 (2%)	9	44
25	AZ	391/393 (100%)	319 (82%)	52 (13%)	20 (5%)	2	19
27	B5	232/234 (99%)	195 (84%)	31 (13%)	6 (3%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	BI	139/141 (99%)	121 (87%)	11 (8%)	7 (5%)	2	20
29	BJ	140/142 (99%)	116 (83%)	11 (8%)	13 (9%)	0	10
30	BK	119/121 (98%)	96 (81%)	18 (15%)	5 (4%)	3	22
31	BL	141/143 (99%)	118 (84%)	16 (11%)	7 (5%)	2	20
32	BM	134/136 (98%)	101 (75%)	26 (19%)	7 (5%)	2	19
33	BN	118/120 (98%)	97 (82%)	17 (14%)	4 (3%)	3	26
34	BO	114/116 (98%)	100 (88%)	8 (7%)	6 (5%)	2	19
35	BP	112/114 (98%)	87 (78%)	15 (13%)	10 (9%)	1	11
36	BQ	115/117 (98%)	99 (86%)	14 (12%)	2 (2%)	9	42
37	BR	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	2	20
38	BS	108/110 (98%)	85 (79%)	15 (14%)	8 (7%)	1	14
39	BT	91/93 (98%)	64 (70%)	19 (21%)	8 (9%)	1	11
40	BU	100/102 (98%)	79 (79%)	13 (13%)	8 (8%)	1	12
41	BV	92/94 (98%)	76 (83%)	14 (15%)	2 (2%)	6	35
42	BW	77/79 (98%)	56 (73%)	10 (13%)	11 (14%)	0	4
43	BX	75/77 (97%)	60 (80%)	10 (13%)	5 (7%)	1	15
44	BY	61/63 (97%)	47 (77%)	11 (18%)	3 (5%)	2	20
45	BC	269/271 (99%)	201 (75%)	43 (16%)	25 (9%)	0	10
46	BZ	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
47	B0	54/56 (96%)	43 (80%)	9 (17%)	2 (4%)	3	24
48	B1	48/50 (96%)	44 (92%)	2 (4%)	2 (4%)	3	22
49	B2	44/46 (96%)	32 (73%)	11 (25%)	1 (2%)	6	34
50	B3	62/64 (97%)	54 (87%)	5 (8%)	3 (5%)	2	21
51	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	30
52	BD	207/209 (99%)	152 (73%)	39 (19%)	16 (8%)	1	13
53	BE	199/201 (99%)	157 (79%)	29 (15%)	13 (6%)	1	16
54	BF	176/178 (99%)	129 (73%)	28 (16%)	19 (11%)	0	8
55	BG	174/176 (99%)	137 (79%)	23 (13%)	14 (8%)	1	12
56	BH	147/149 (99%)	107 (73%)	23 (16%)	17 (12%)	0	6
All	All	6242/6344 (98%)	4971 (80%)	897 (14%)	374 (6%)	3	17

5 of 374 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AJ	67	ILE
3	AL	24	GLU
4	AM	3	ILE
4	AM	29	SER
4	AM	99	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AJ	86/86 (100%)	82 (95%)	4 (5%)	26	51
2	AK	90/90 (100%)	87 (97%)	3 (3%)	38	61
3	AL	103/103 (100%)	98 (95%)	5 (5%)	25	50
4	AM	91/91 (100%)	85 (93%)	6 (7%)	16	41
5	AN	79/79 (100%)	78 (99%)	1 (1%)	69	82
6	AO	76/76 (100%)	74 (97%)	2 (3%)	46	66
7	AP	65/65 (100%)	63 (97%)	2 (3%)	40	62
8	AQ	74/74 (100%)	67 (90%)	7 (10%)	8	27
9	AR	48/48 (100%)	47 (98%)	1 (2%)	53	72
10	AS	70/70 (100%)	67 (96%)	3 (4%)	29	54
11	AT	65/65 (100%)	65 (100%)	0	100	100
12	AU	44/44 (100%)	42 (96%)	2 (4%)	27	52
13	AB	180/180 (100%)	172 (96%)	8 (4%)	28	53
14	AC	170/170 (100%)	158 (93%)	12 (7%)	14	39
15	AD	172/172 (100%)	163 (95%)	9 (5%)	23	48
16	AE	113/113 (100%)	106 (94%)	7 (6%)	18	43
17	AF	87/87 (100%)	81 (93%)	6 (7%)	15	40
18	AG	123/123 (100%)	115 (94%)	8 (6%)	17	42
19	AH	104/104 (100%)	95 (91%)	9 (9%)	10	31
20	AI	105/105 (100%)	97 (92%)	8 (8%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AZ	325/326 (100%)	303 (93%)	22 (7%)	16	41
27	B5	181/181 (100%)	170 (94%)	11 (6%)	18	44
28	BI	109/109 (100%)	100 (92%)	9 (8%)	11	34
29	BJ	116/116 (100%)	107 (92%)	9 (8%)	12	36
30	BK	102/102 (100%)	94 (92%)	8 (8%)	12	36
31	BL	102/102 (100%)	100 (98%)	2 (2%)	55	74
32	BM	109/109 (100%)	100 (92%)	9 (8%)	11	34
33	BN	100/100 (100%)	97 (97%)	3 (3%)	41	63
34	BO	86/86 (100%)	83 (96%)	3 (4%)	36	59
35	BP	99/99 (100%)	92 (93%)	7 (7%)	14	39
36	BQ	89/89 (100%)	86 (97%)	3 (3%)	37	60
37	BR	84/84 (100%)	78 (93%)	6 (7%)	14	39
38	BS	93/93 (100%)	89 (96%)	4 (4%)	29	54
39	BT	80/80 (100%)	72 (90%)	8 (10%)	7	26
40	BU	83/83 (100%)	72 (87%)	11 (13%)	4	18
41	BV	78/78 (100%)	75 (96%)	3 (4%)	33	57
42	BW	59/59 (100%)	53 (90%)	6 (10%)	7	25
43	BX	67/67 (100%)	60 (90%)	7 (10%)	7	24
44	BY	55/55 (100%)	53 (96%)	2 (4%)	35	59
45	BC	216/216 (100%)	205 (95%)	11 (5%)	24	48
46	BZ	48/48 (100%)	44 (92%)	4 (8%)	11	34
47	B0	47/47 (100%)	42 (89%)	5 (11%)	6	24
48	B1	45/45 (100%)	42 (93%)	3 (7%)	16	41
49	B2	38/38 (100%)	37 (97%)	1 (3%)	46	66
50	B3	51/51 (100%)	49 (96%)	2 (4%)	32	56
51	B4	34/34 (100%)	34 (100%)	0	100	100
52	BD	164/164 (100%)	150 (92%)	14 (8%)	10	33
53	BE	165/165 (100%)	157 (95%)	8 (5%)	25	51
54	BF	149/149 (100%)	139 (93%)	10 (7%)	16	41
55	BG	137/137 (100%)	126 (92%)	11 (8%)	12	35
56	BH	114/114 (100%)	107 (94%)	7 (6%)	18	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	5170/5171 (100%)	4858 (94%)	312 (6%)	23	44

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BX	26	ARG
54	BF	59	ILE
45	BC	36	ASN
50	B3	29	ARG
55	BG	113	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
39	BT	28	ASN
48	B1	45	HIS
41	BV	75	GLN
45	BC	57	HIS
53	BE	97	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1530 (99%)	281 (18%)	42 (2%)
22	AY	75/76 (98%)	20 (26%)	5 (6%)
23	AW	75/76 (98%)	24 (32%)	6 (8%)
24	AX	10/11 (90%)	3 (30%)	0
26	AV	76/77 (98%)	14 (18%)	0
57	BB	2902/2903 (99%)	491 (16%)	63 (2%)
58	BA	116/117 (99%)	19 (16%)	4 (3%)
All	All	4783/4790 (99%)	852 (17%)	120 (2%)

5 of 852 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	14	U

5 of 120 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	BB	548	G
57	BB	2402	U
57	BB	1068	G
57	BB	2336	A
58	BA	66	A

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	$\# Z > 2$
26	5MU	AV	54	26	19,22,23	1.33	4 (21%)	28,32,35	1.19	3 (10%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AV	54	5MU	O2'-C2'	-2.46	1.37	1.43
26	AV	54	5MU	C6-N1	2.43	1.42	1.38
26	AV	54	5MU	O4'-C1'	2.29	1.47	1.42
26	AV	54	5MU	C2-N1	2.22	1.42	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AV	54	5MU	C6-N1-C2	-2.96	118.30	121.30
26	AV	54	5MU	O4'-C1'-N1	2.77	114.70	108.36
26	AV	54	5MU	C1'-N1-C6	2.40	125.13	121.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
59	GDP	AZ	401	-	24,30,30	1.81	6 (25%)	30,47,47	1.80	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GDP	AZ	401	-	-	2/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AZ	401	GDP	O4'-C1'	5.64	1.48	1.41
59	AZ	401	GDP	C5-C4	-2.72	1.36	1.43
59	AZ	401	GDP	C2'-C1'	-2.19	1.50	1.53
59	AZ	401	GDP	O3'-C3'	-2.15	1.37	1.43
59	AZ	401	GDP	C5-C6	-2.12	1.43	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AZ	401	GDP	PA-O3A-PB	7.32	157.95	132.83
59	AZ	401	GDP	O6-C6-N1	2.68	123.81	120.65
59	AZ	401	GDP	O3'-C3'-C2'	2.25	119.11	111.82
59	AZ	401	GDP	C3'-C2'-C1'	2.16	104.23	100.98

There are no chirality outliers.

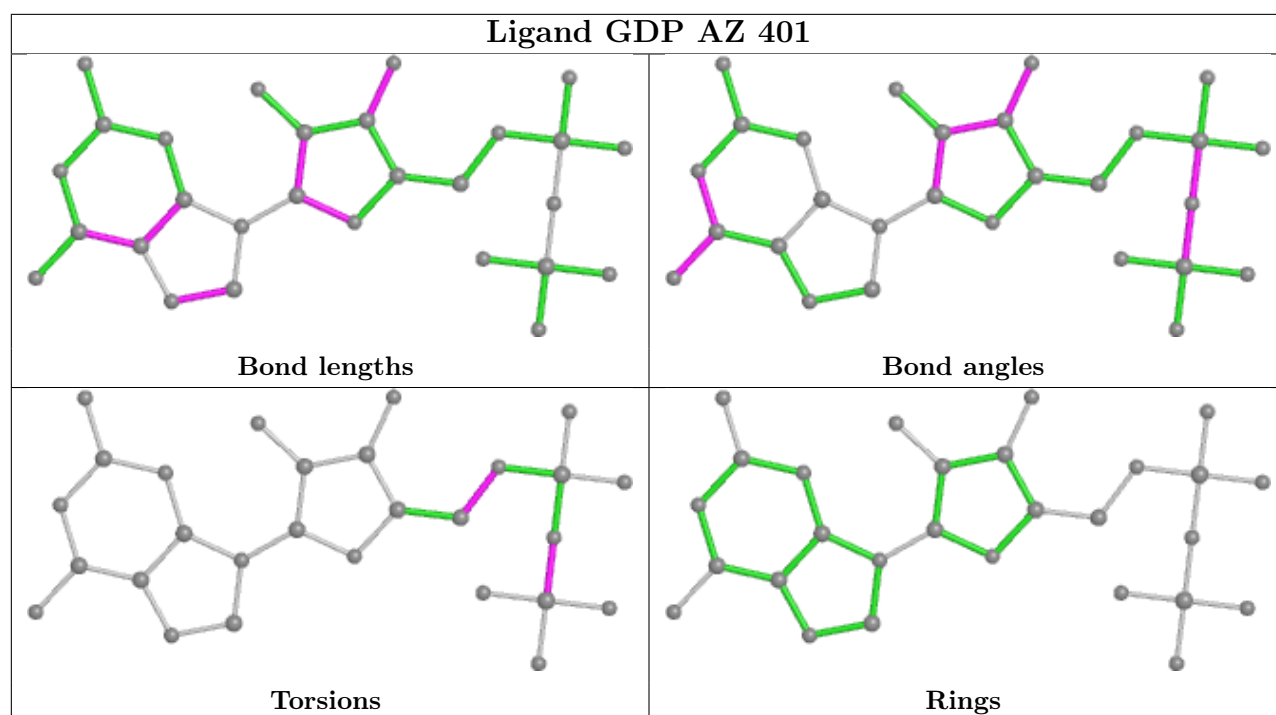
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AZ	401	GDP	PA-O3A-PB-O3B
59	AZ	401	GDP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

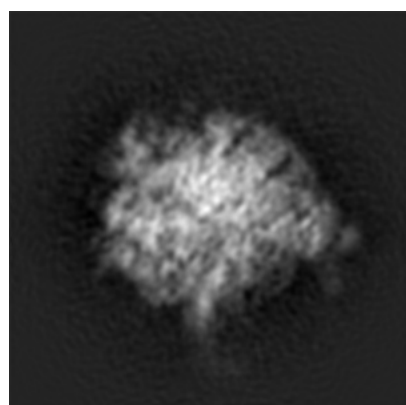
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5036. These allow visual inspection of the internal detail of the map and identification of artifacts.

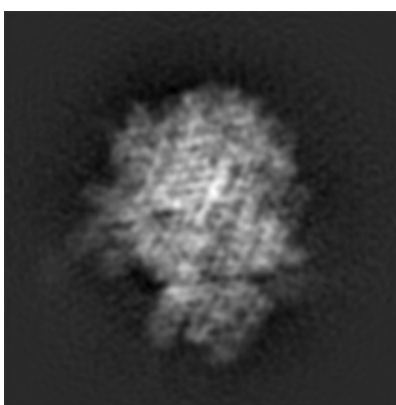
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

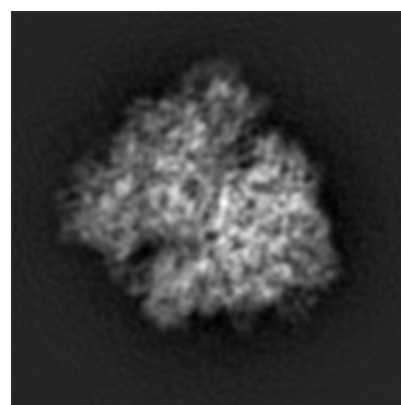
6.1.1 Primary map



X



Y

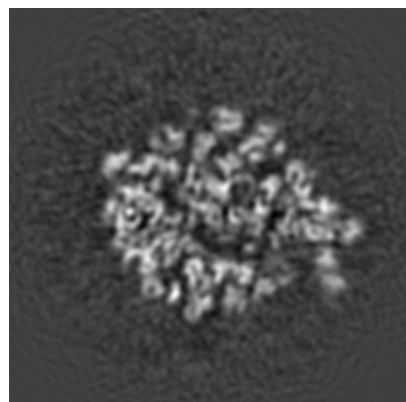


Z

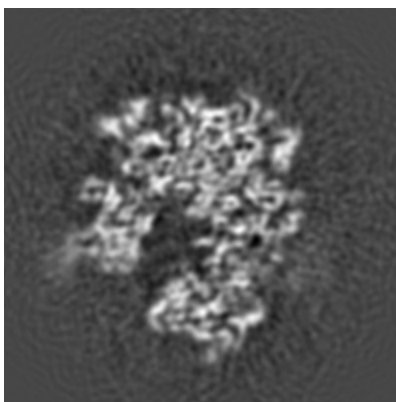
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

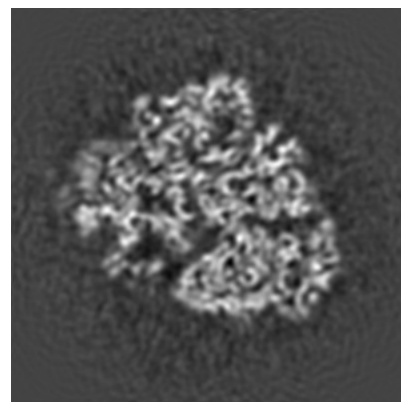
6.2.1 Primary map



X Index: 154



Y Index: 154

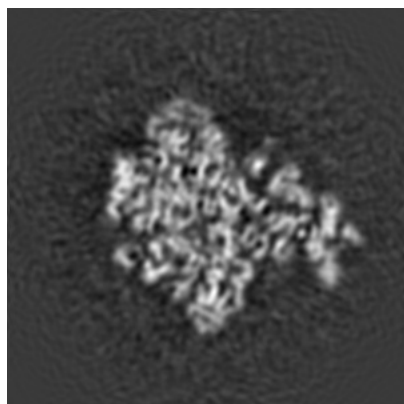


Z Index: 154

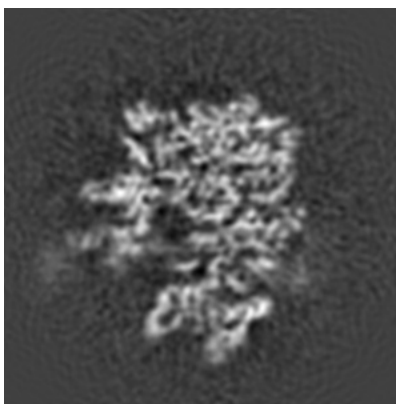
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

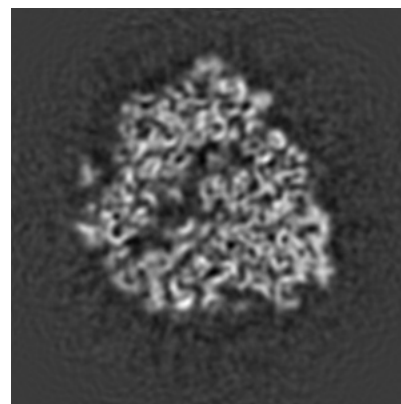
6.3.1 Primary map



X Index: 164



Y Index: 160

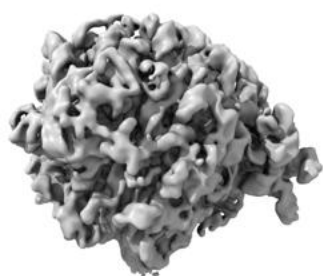


Z Index: 142

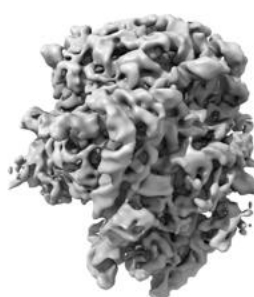
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

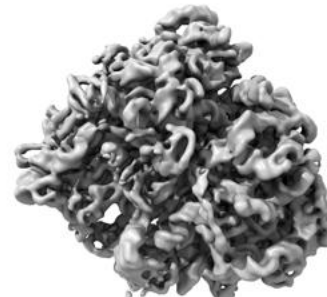
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 90.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

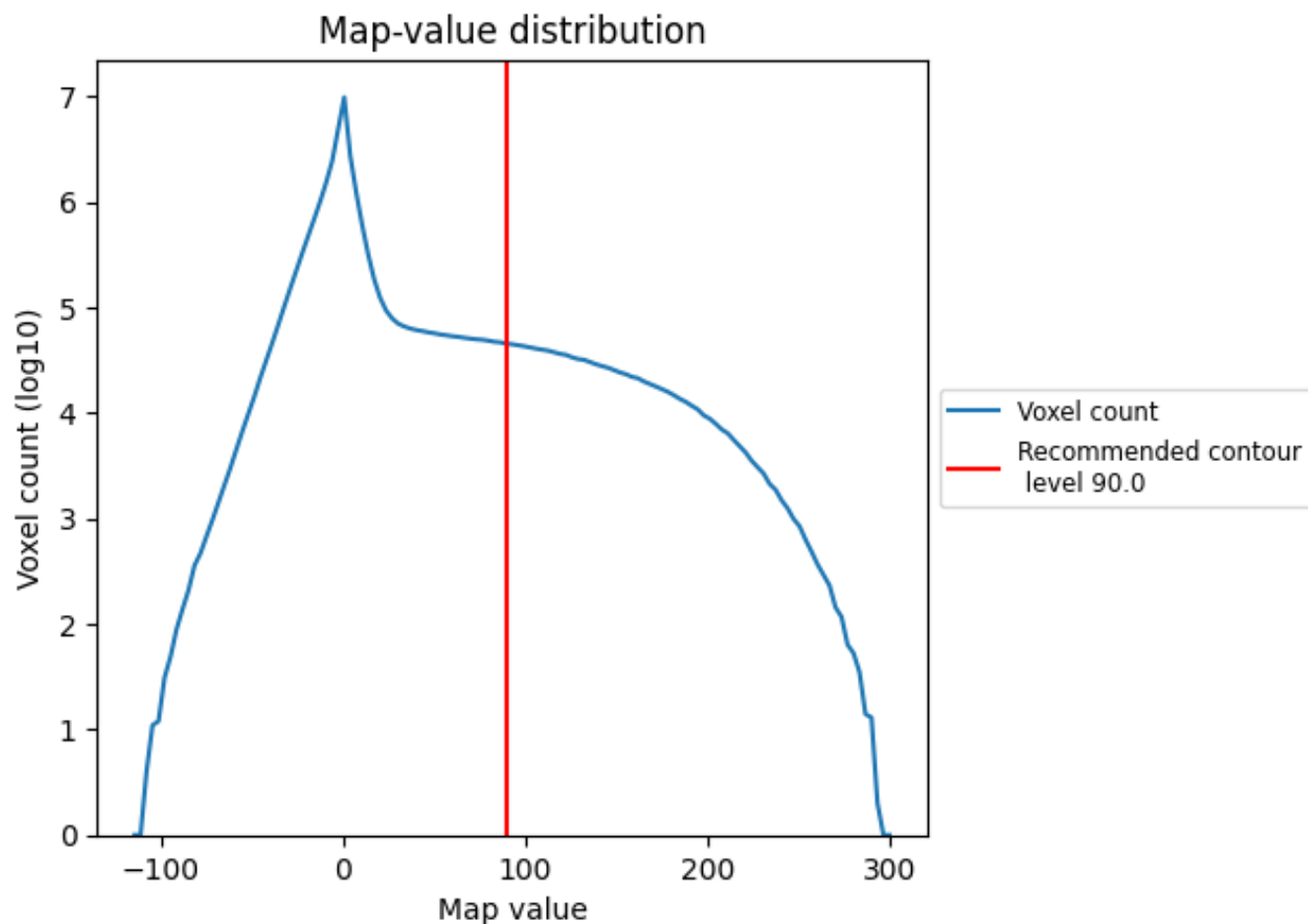
6.5 Mask visualisation

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

7 Map analysis [i](#)

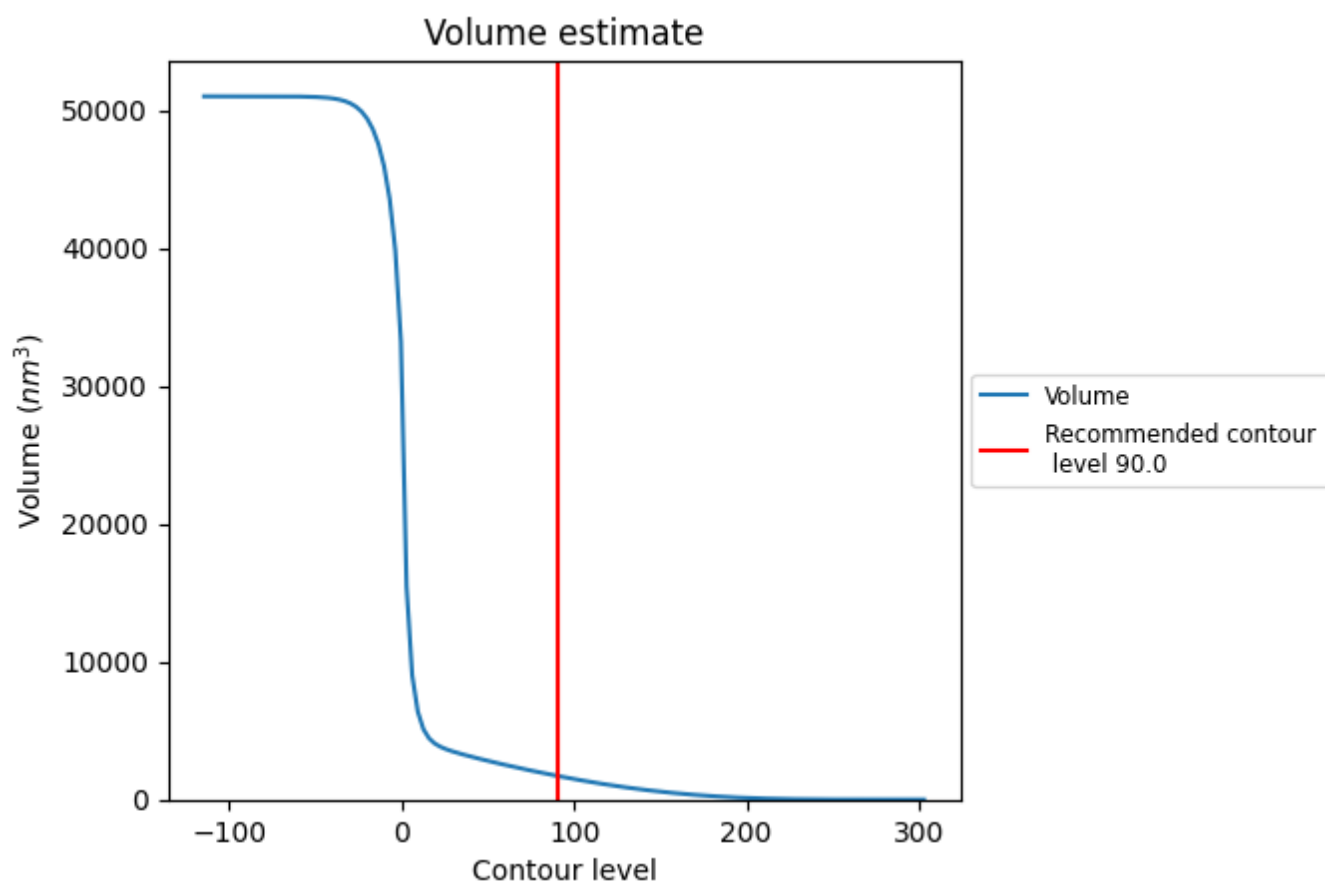
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

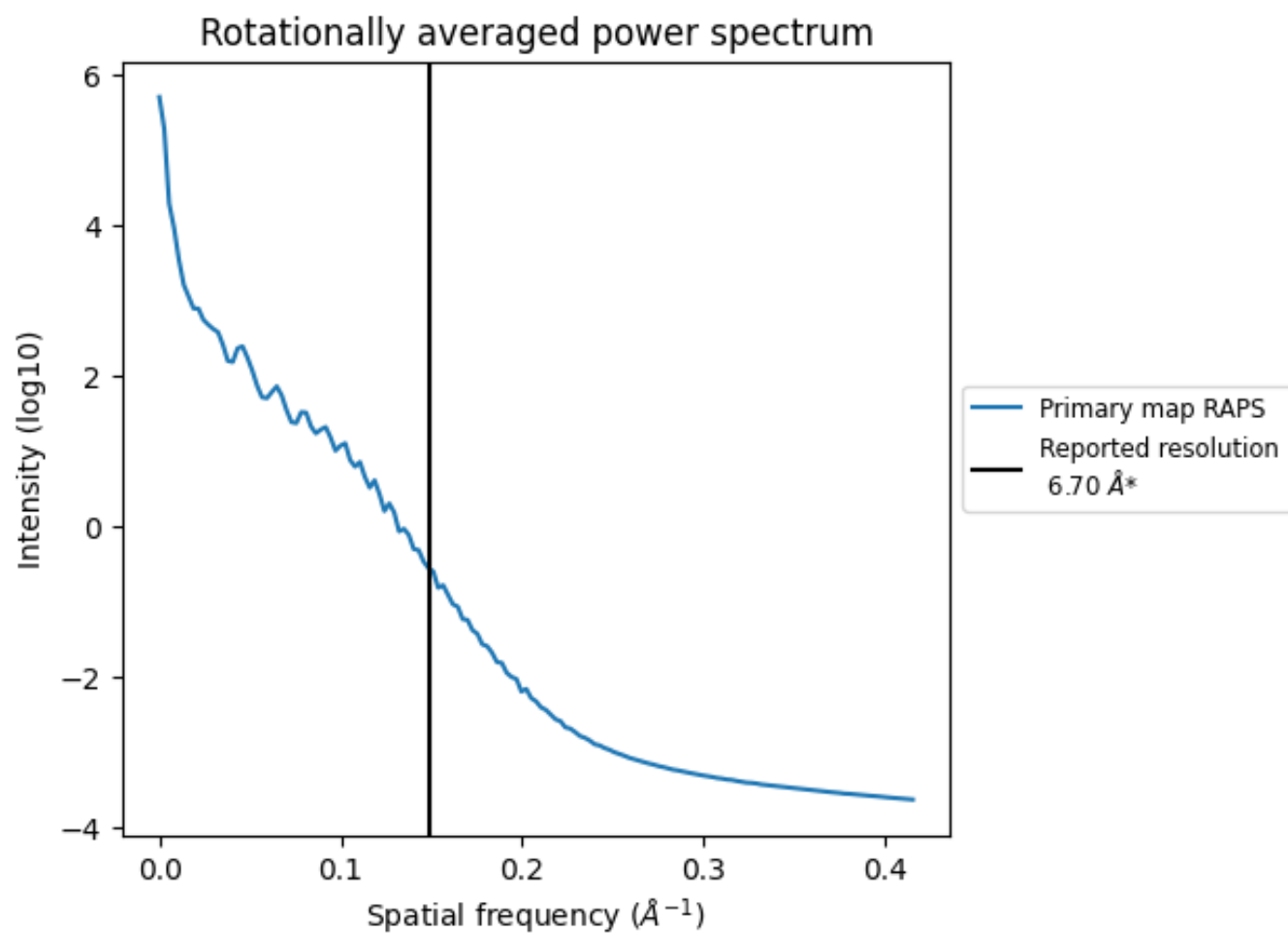
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1724 nm³; this corresponds to an approximate mass of 1557 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 0.149 Å⁻¹

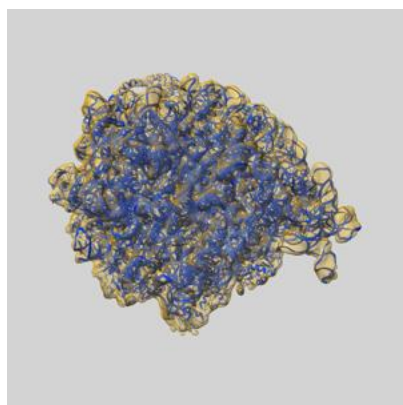
8 Fourier-Shell correlation

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

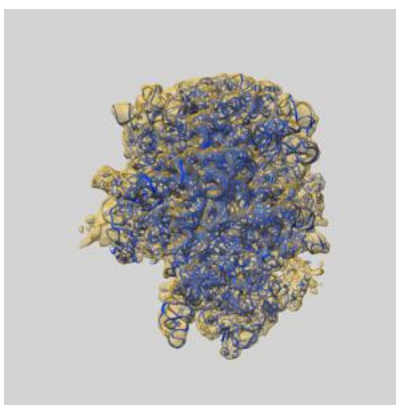
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5036 and PDB model 4V69. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

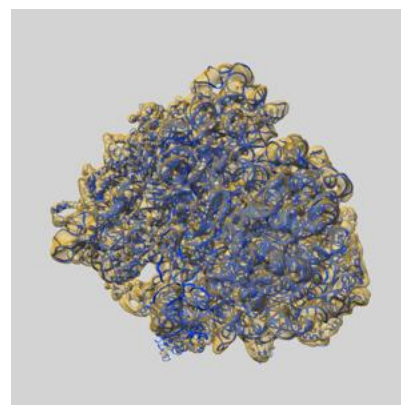
9.1 Map-model overlay [i](#)



X



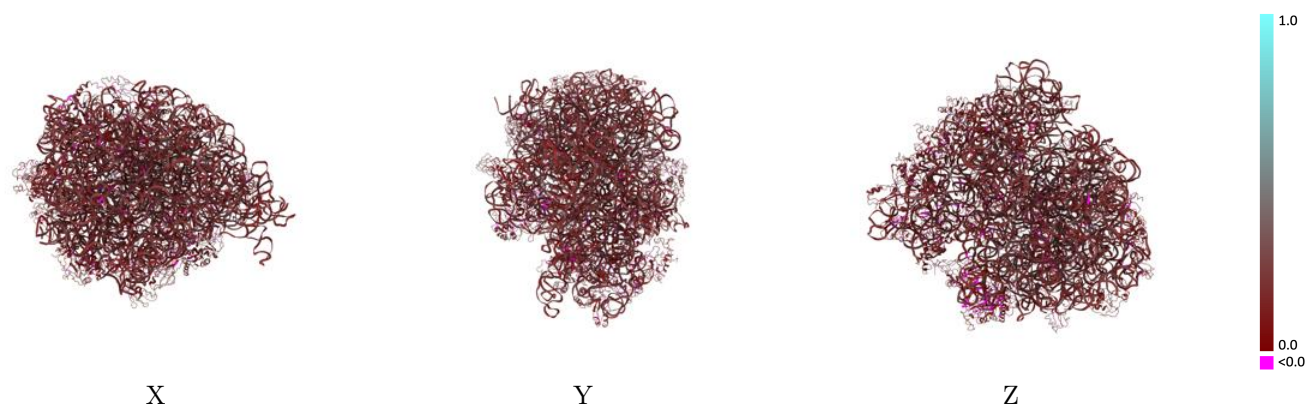
Y



Z

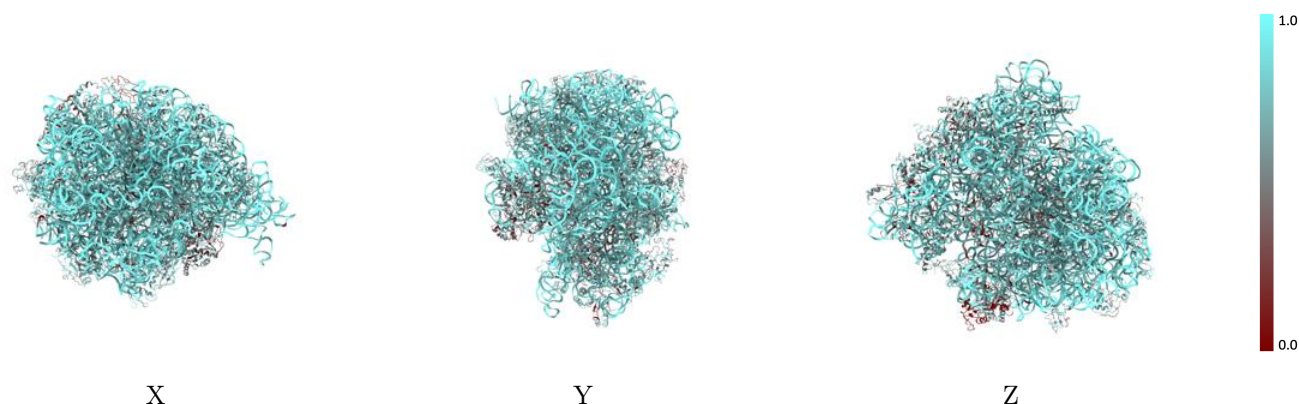
The images above show the 3D surface view of the map at the recommended contour level 90.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



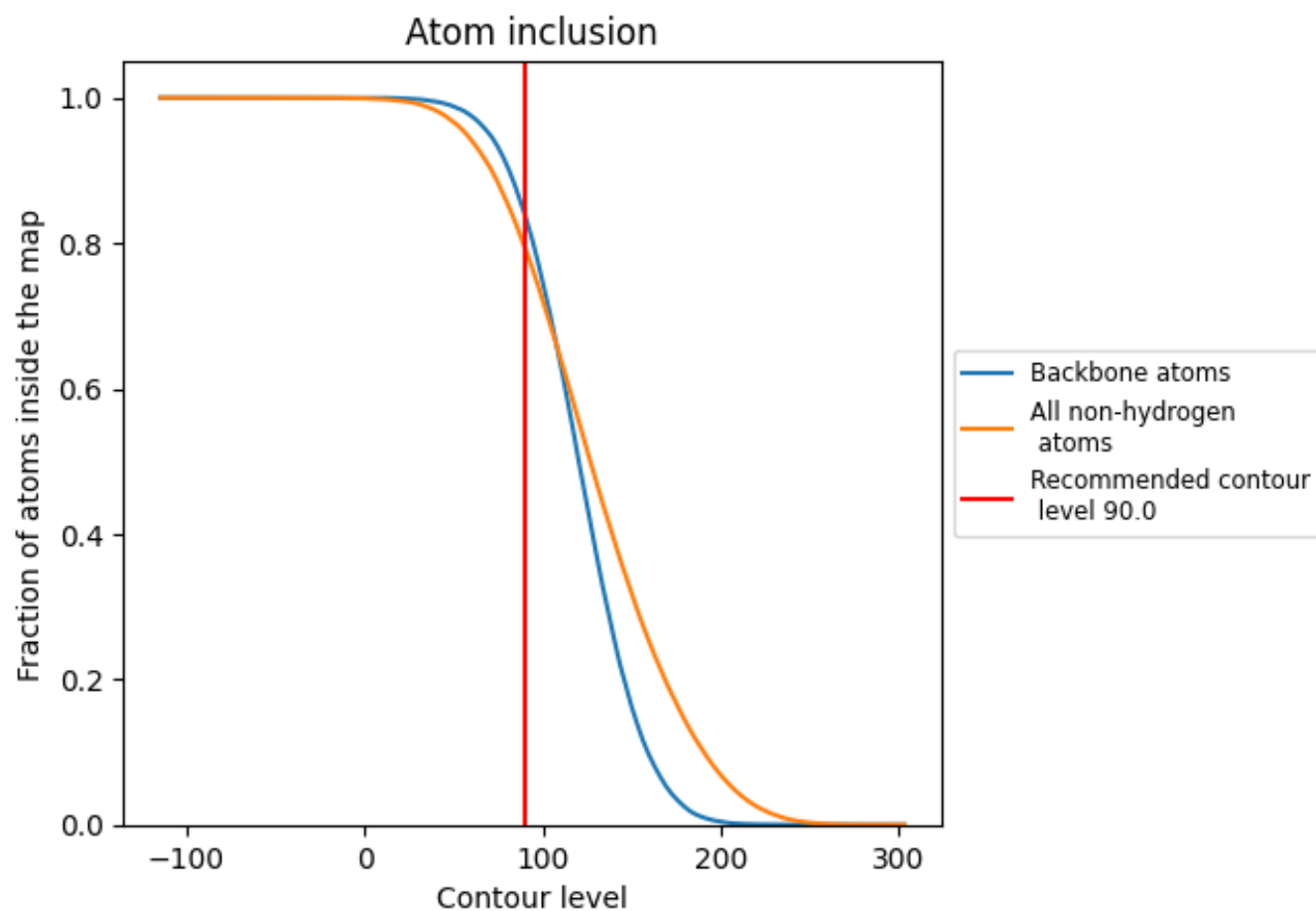
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (90.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (90.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7931	 0.1860
AA	 0.8950	 0.2030
AB	 0.5979	 0.1550
AC	 0.5997	 0.1680
AD	 0.4981	 0.1540
AE	 0.5932	 0.1600
AF	 0.6512	 0.1650
AG	 0.6072	 0.1460
AH	 0.5604	 0.1590
AI	 0.6098	 0.1320
AJ	 0.4580	 0.1330
AK	 0.5100	 0.1580
AL	 0.4788	 0.1550
AM	 0.6189	 0.1590
AN	 0.6057	 0.1390
AO	 0.6232	 0.1520
AP	 0.6143	 0.1330
AQ	 0.6825	 0.1460
AR	 0.5492	 0.1480
AS	 0.6736	 0.1430
AT	 0.6031	 0.1520
AU	 0.7469	 0.2000
AV	 0.7939	 0.1990
AW	 0.7085	 0.1720
AX	 0.7543	 0.2270
AY	 0.7891	 0.1930
AZ	 0.4790	 0.1640
B0	 0.6402	 0.1350
B1	 0.6169	 0.1530
B2	 0.5972	 0.1010
B3	 0.5886	 0.1460
B4	 0.4966	 0.1260
B5	 0.3004	 0.0990
BA	 0.9238	 0.2090
BB	 0.9050	 0.2040



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Chain	Atom inclusion	Q-score
BC	 0.5796	 0.1420
BD	 0.5845	 0.1460
BE	 0.6171	 0.1630
BF	 0.7332	 0.1620
BG	 0.6839	 0.1710
BH	 0.4088	 0.1420
BI	 0.4638	 0.1380
BJ	 0.6027	 0.1590
BK	 0.4084	 0.1560
BL	 0.5305	 0.1450
BM	 0.5422	 0.1470
BN	 0.6652	 0.1340
BO	 0.7219	 0.1530
BP	 0.5631	 0.1700
BQ	 0.6134	 0.1150
BR	 0.6274	 0.1580
BS	 0.5921	 0.1460
BT	 0.6279	 0.1380
BU	 0.6732	 0.1560
BV	 0.7249	 0.1700
BW	 0.5379	 0.0990
BX	 0.5807	 0.1520
BY	 0.7062	 0.1360
BZ	 0.6590	 0.1660