



wwPDB EM Validation Summary Report ⓘ

Feb 22, 2024 – 09:35 PM 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 : 2I2V, 2I2U, 1OB2, 2J00

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:

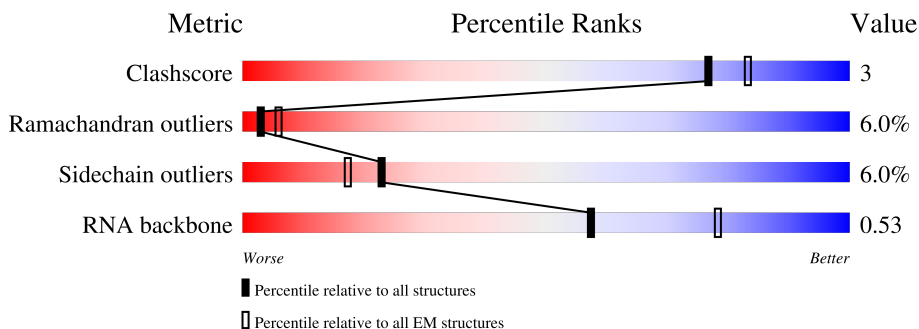
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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	38% 66% 26% 7% .
2	AK	117	34% 69% 26% ..
3	AL	123	37% 67% 26% 7% .
4	AM	113	22% 58% 28% 13%
5	AN	96	22% 58% 28% 12% .
6	AO	88	13% 65% 27% 6% .
7	AP	80	22% 65% 29% 6%

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Mol	Chain	Length	Quality of chain
8	AQ	80	11% 74% 18% 9%
9	AR	55	27% 67% 22% 11%
10	AS	79	19% 65% 27% 9%
11	AT	85	20% 76% 20% .
12	AU	51	16% 59% 29% 12%
13	AB	218	22% 70% 23% 7%
14	AC	206	20% 70% 24% 5% .
15	AD	205	39% 62% 26% 10% .
16	AE	150	28% 68% 29% .
17	AF	100	19% 69% 25% 5% .
18	AG	150	25% 60% 33% 6% .
19	AH	129	23% 68% 27% 5%
20	AI	127	23% 65% 28% 6% .
21	AA	1530	. 36% 47% 17%
22	AY	76	. 24% 54% 22%
23	AW	76	12% 24% 47% 29%
24	AX	11	18% 55% 27% 18%
25	AZ	393	37% 64% 28% 7% .
26	AV	77	5% 39% 48% 13%
27	B5	234	66% 74% 22% . .
28	BI	141	48% 67% 28% . .
29	BJ	142	18% 65% 24% 8% .
30	BK	121	45% 67% 27% 6%
31	BL	143	33% 66% 28% 5% .
32	BM	136	26% 71% 23% 5% .


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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	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left, a larger yellow segment in the middle, and a larger orange segment on the right. The percentages for each segment are 15% (red), 38% (yellow), and 46% (orange).</p>

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
			Total	C	N	O	S		
1	AJ	98	787	493	150	143	1	0	0

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

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

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

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

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

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

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

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

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	
			Total	C	N	O			S
6	AO	88	716	440	146	129	1	0	0

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	P		
26	AV	77	1645	733	297	538	77	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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.

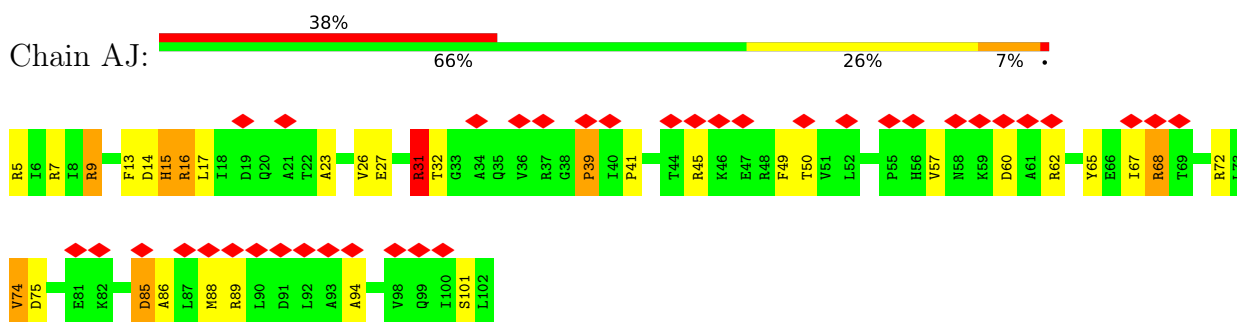
Mol	Chain	Residues	Atoms					AltConf	Trace
58	BA	117	Total	C	N	O	P	0	0
			2508	1116	459	816	117		

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

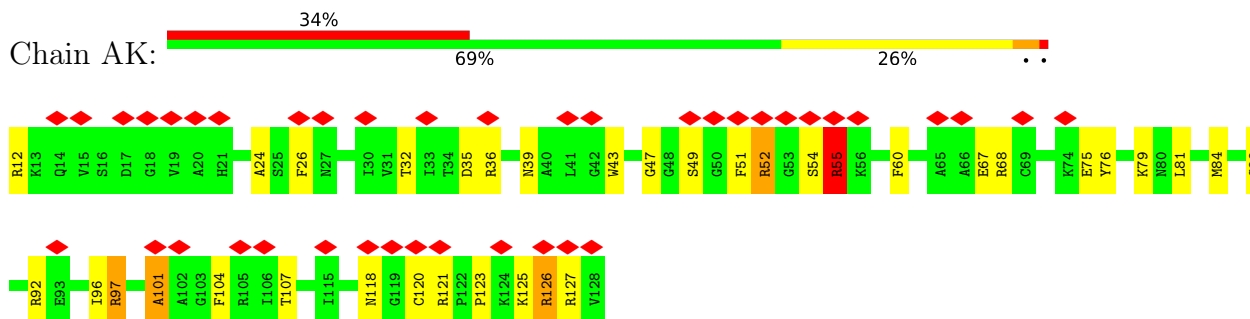
3 Residue-property plots [i](#)

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.

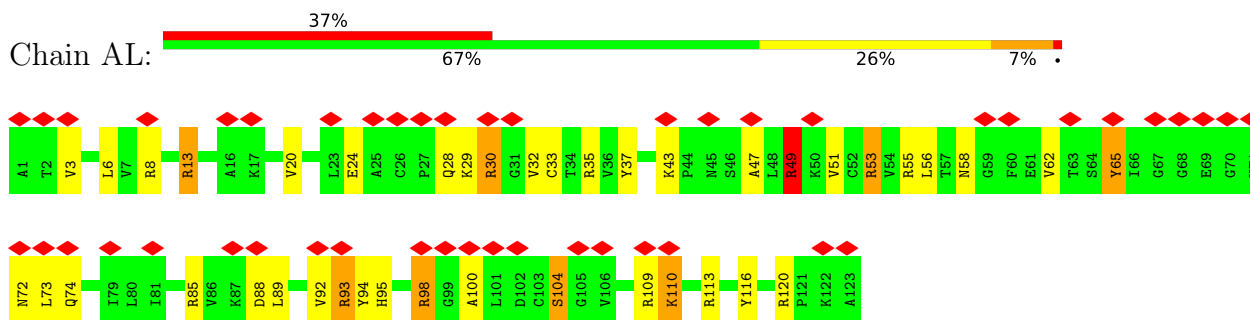
- Molecule 1: 30S ribosomal protein S10



- Molecule 2: 30S ribosomal protein S11

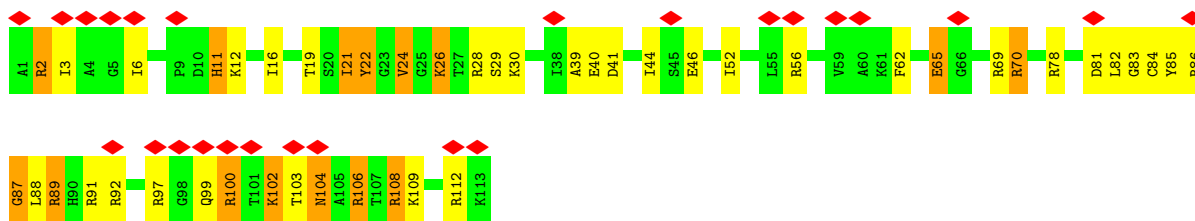


- Molecule 3: 30S ribosomal protein S12

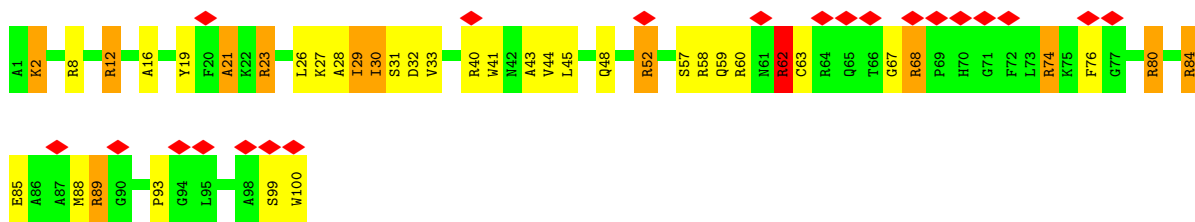


- Molecule 4: 30S ribosomal protein S13

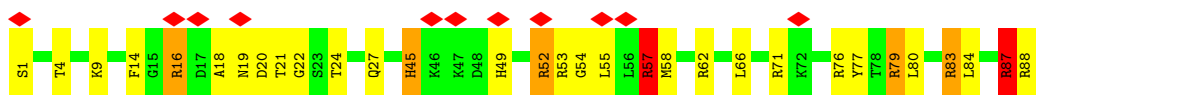




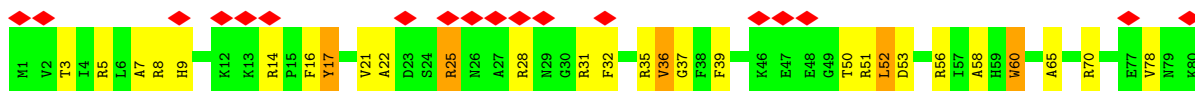
- Molecule 5: 30S ribosomal protein S14



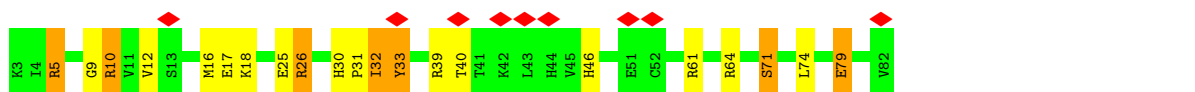
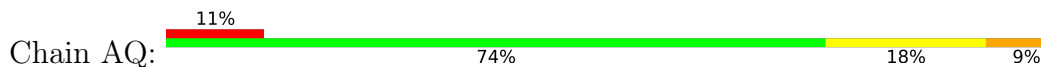
- Molecule 6: 30S ribosomal protein S15



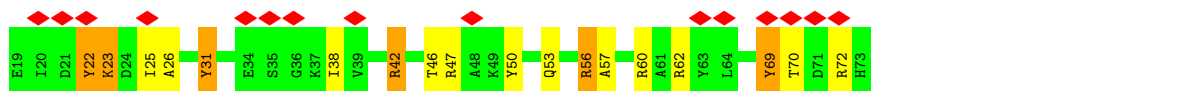
- Molecule 7: 30S ribosomal protein S16



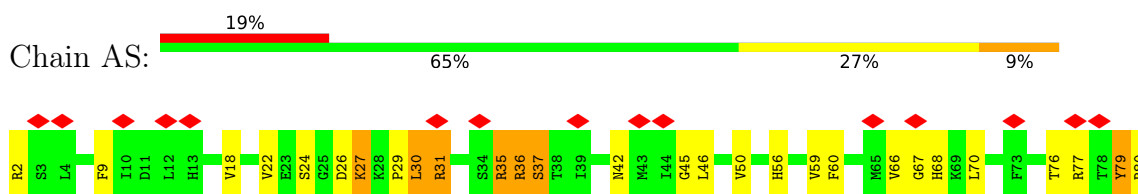
- Molecule 8: 30S ribosomal protein S17



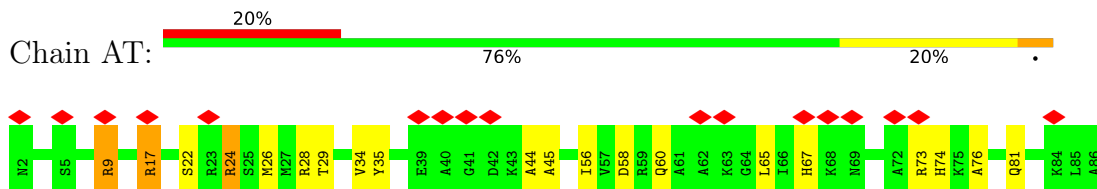
- Molecule 9: 30S ribosomal protein S18



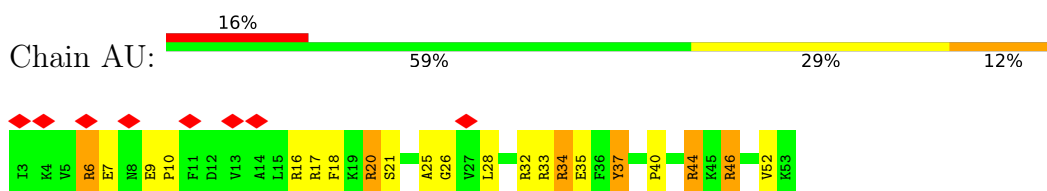
- Molecule 10: 30S ribosomal protein S19



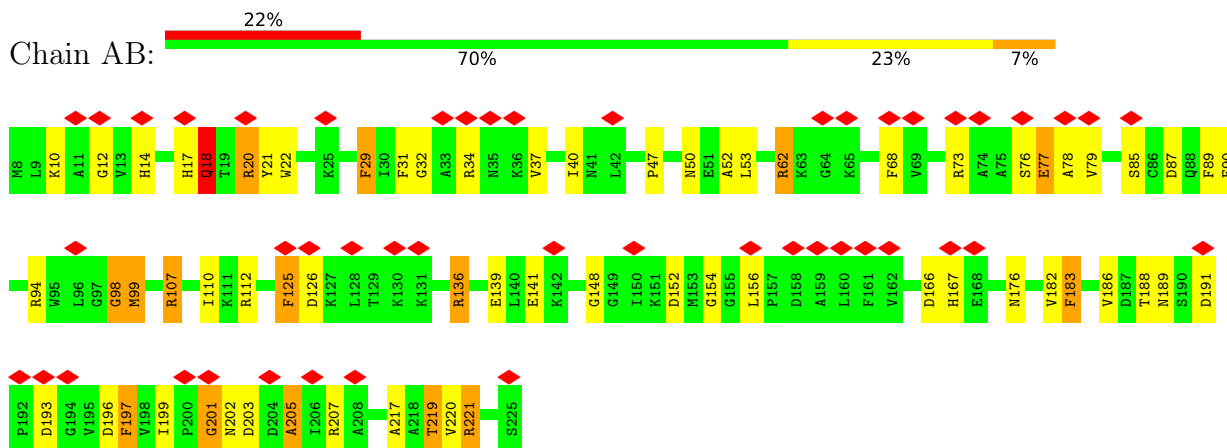
- Molecule 11: 30S ribosomal protein S20



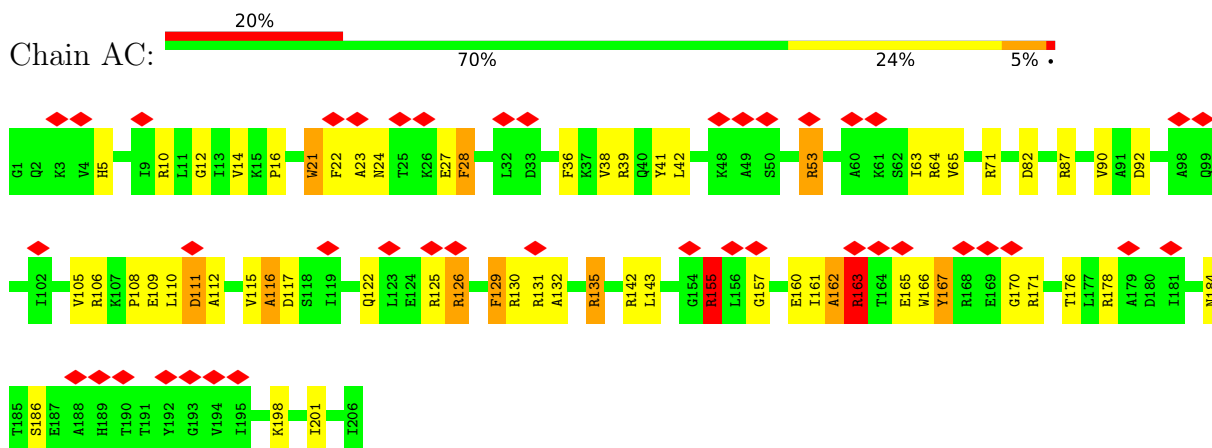
- Molecule 12: 30S ribosomal protein S21



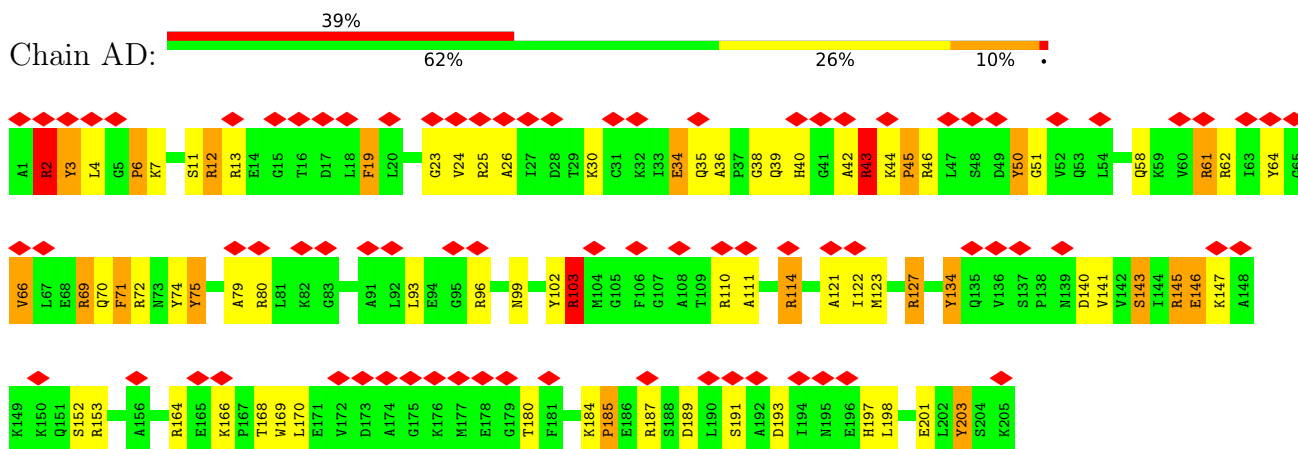
- Molecule 13: 30S ribosomal protein S2



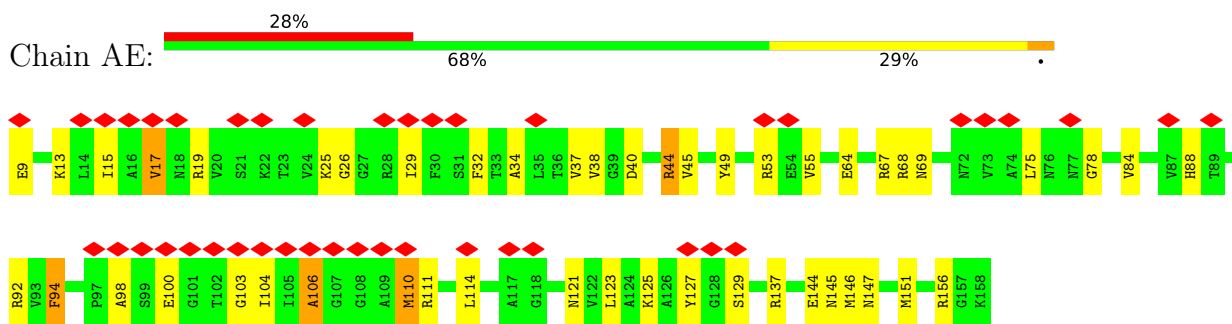
- Molecule 14: 30S ribosomal protein S3



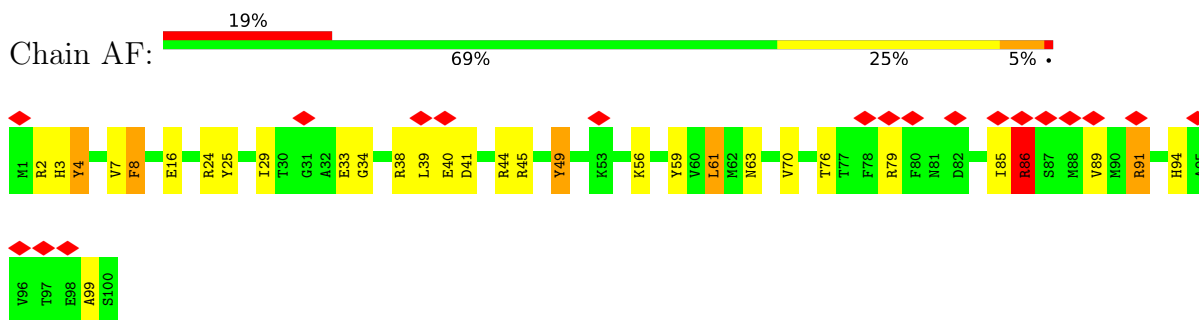
- Molecule 15: 30S ribosomal protein S4



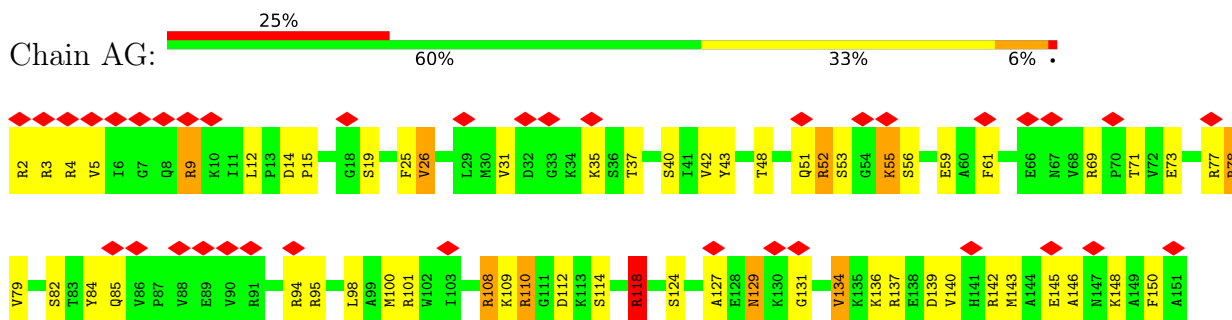
- Molecule 16: 30S ribosomal protein S5



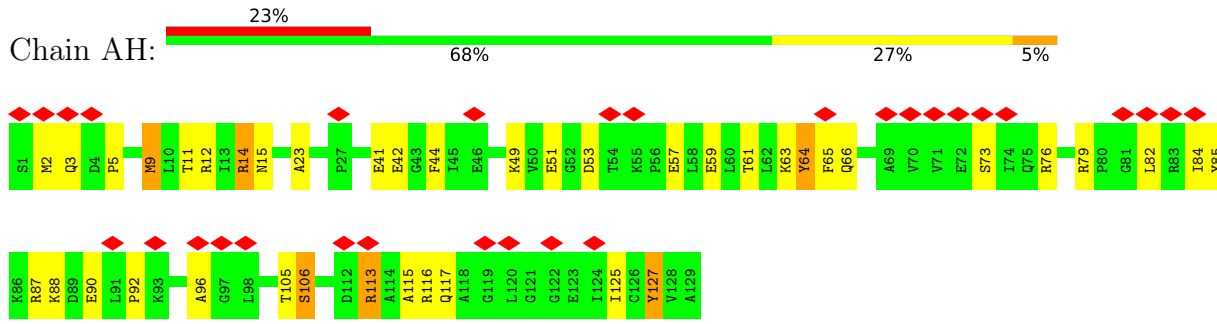
- Molecule 17: 30S ribosomal protein S6



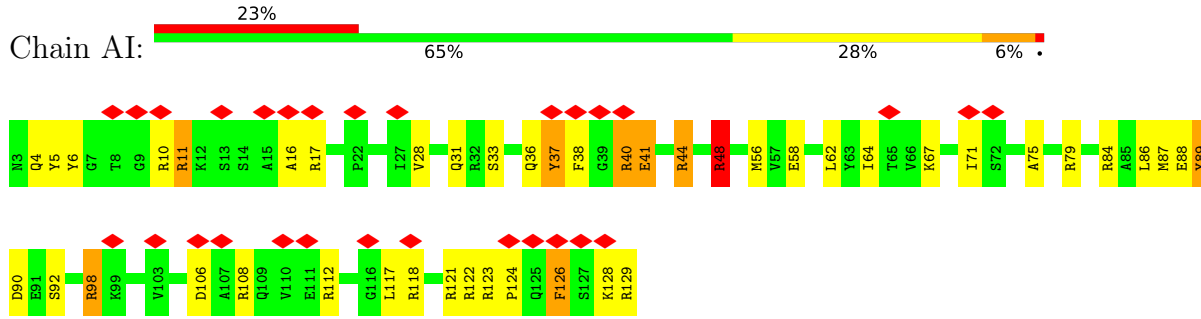
- Molecule 18: 30S ribosomal protein S7



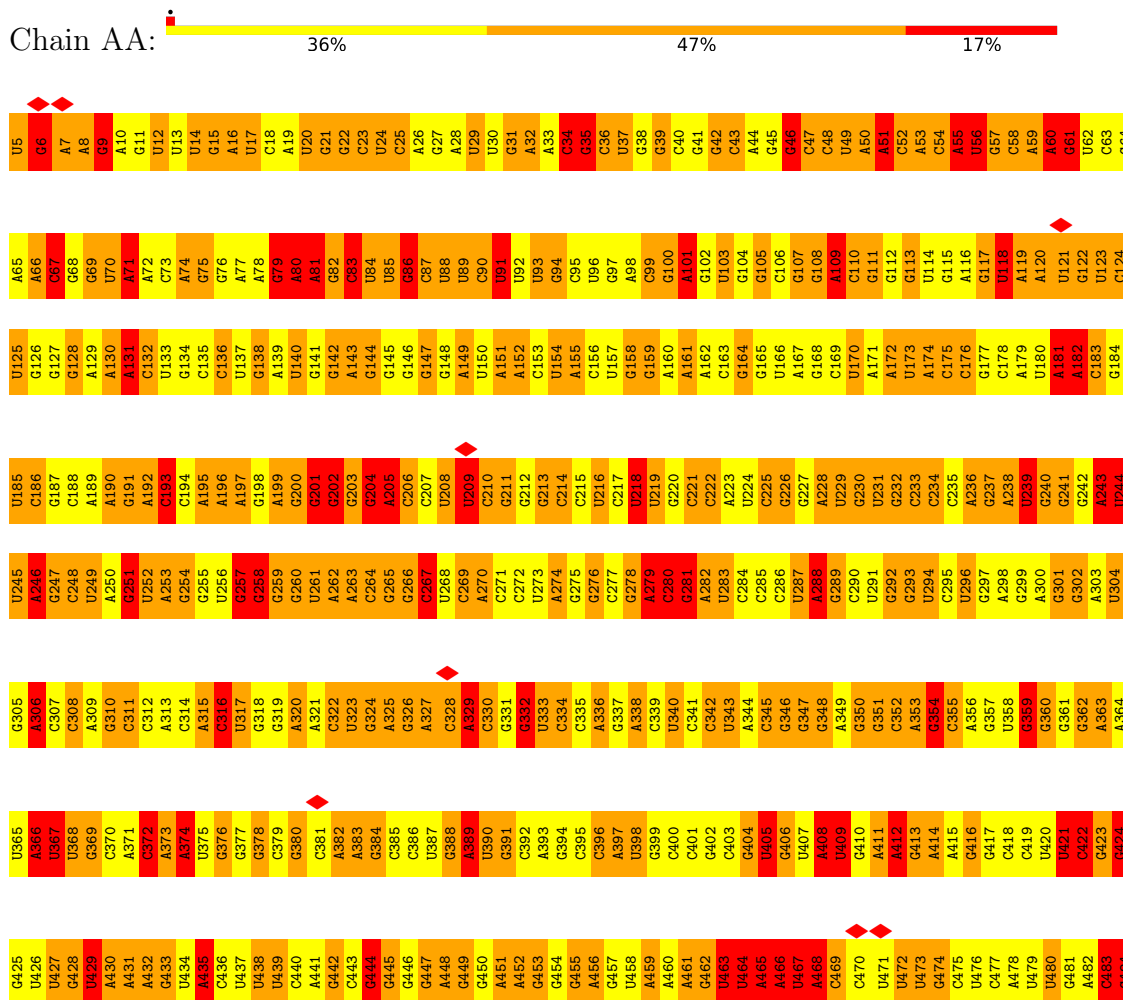
- Molecule 19: 30S ribosomal protein S8



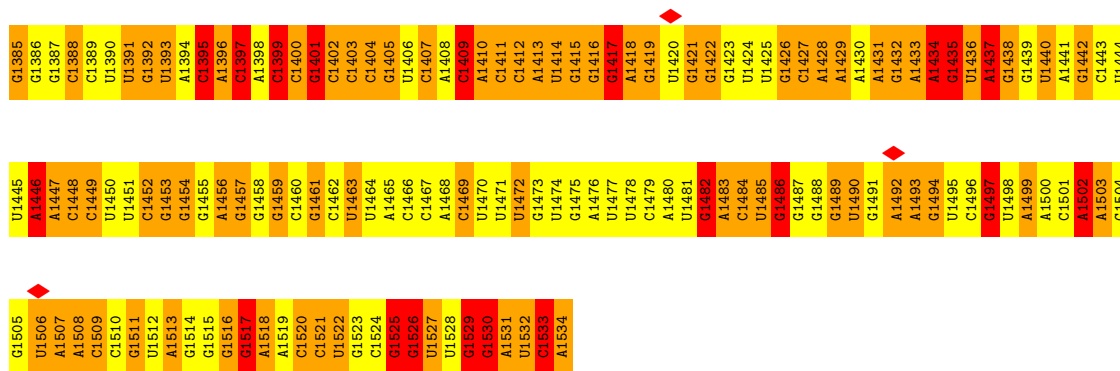
• Molecule 20: 30S ribosomal protein S9



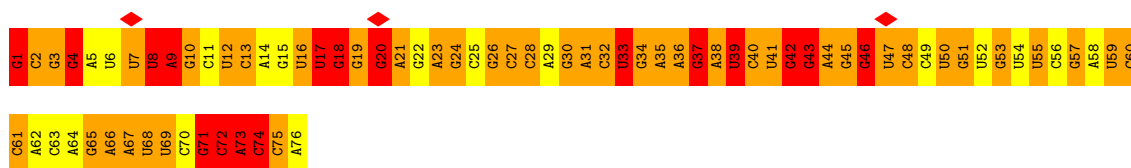
• Molecule 21: 16S rRNA



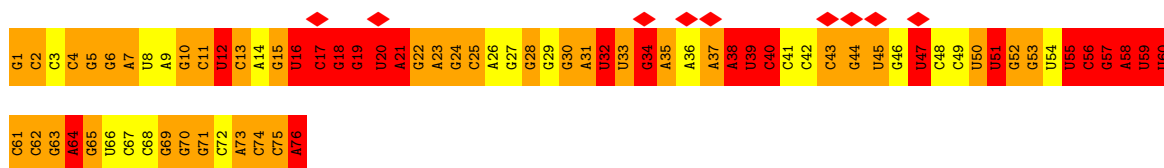
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C545	C546	C547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604
G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664
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G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784
G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844
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U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024
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• Molecule 22: A/T-site tRNA Phe



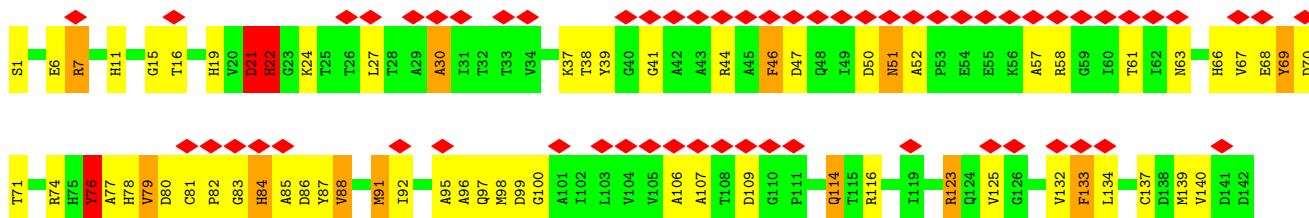
• Molecule 23: P-site tRNA fMet (Unmodified bases except for Thymine 54)

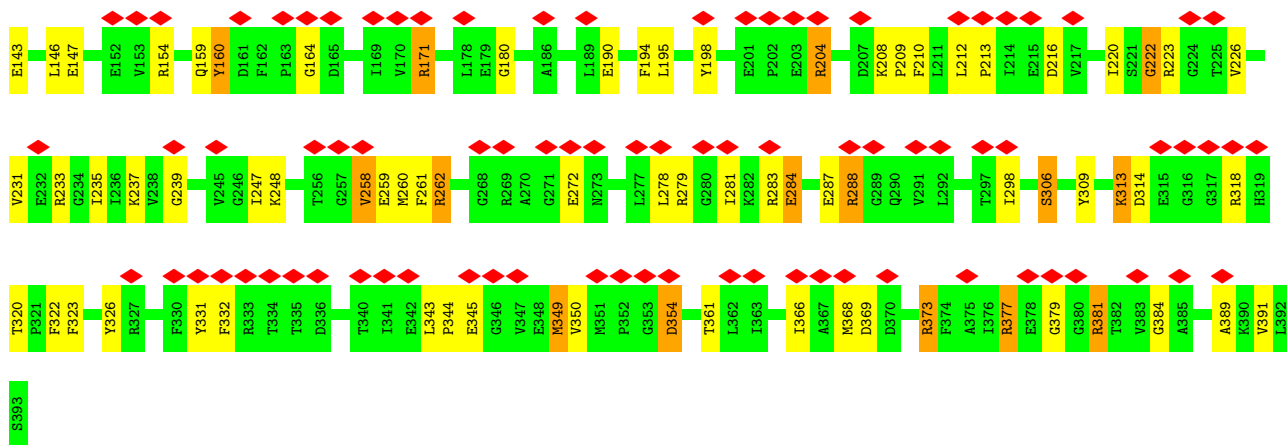


• Molecule 24: mRNA

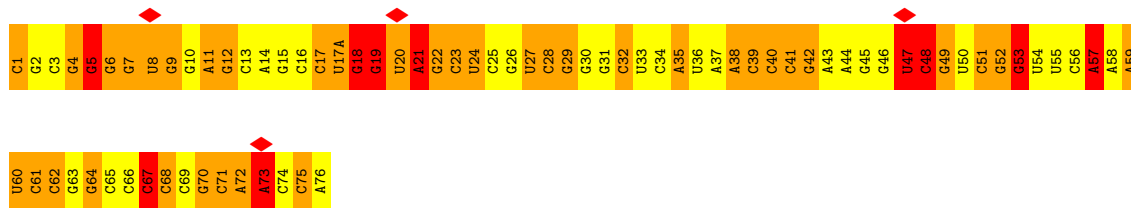


• Molecule 25: Elongation factor Tu

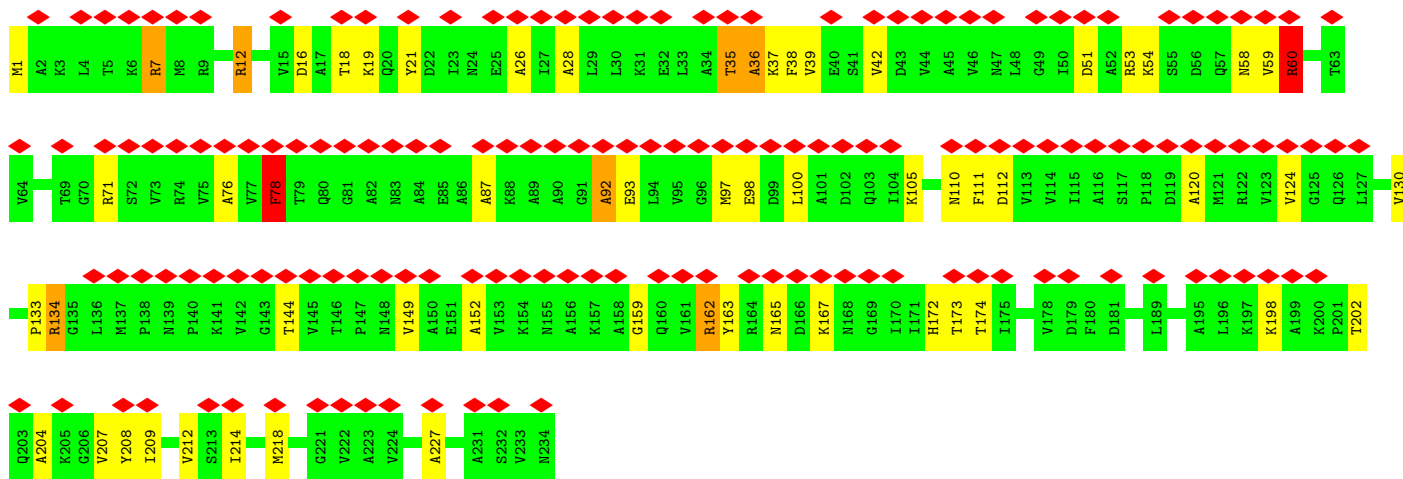
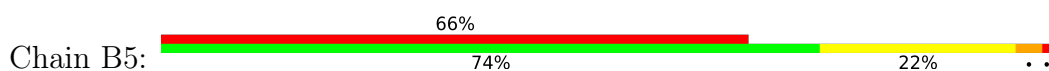




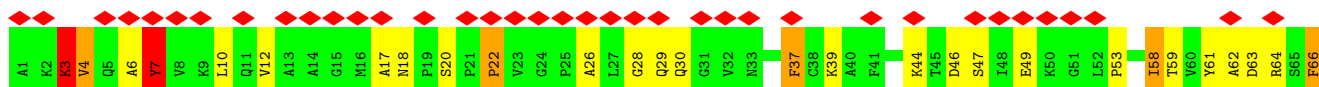
• Molecule 26: E-site tRNA Phe



• Molecule 27: 50S ribosomal protein L1

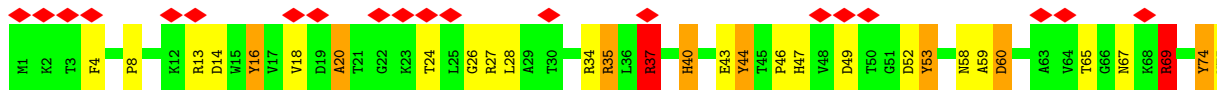


• Molecule 28: 50S ribosomal protein L11

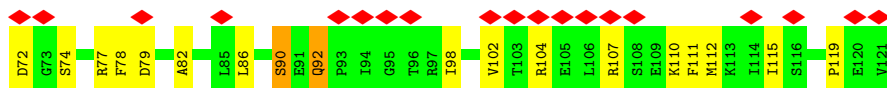
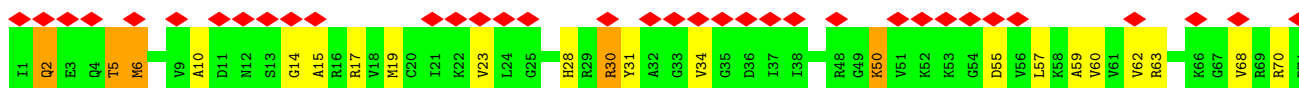




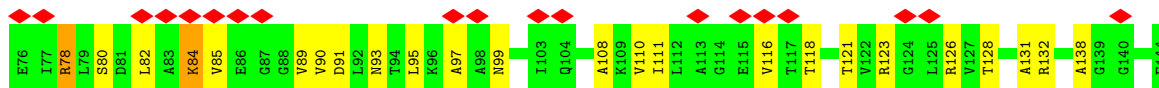
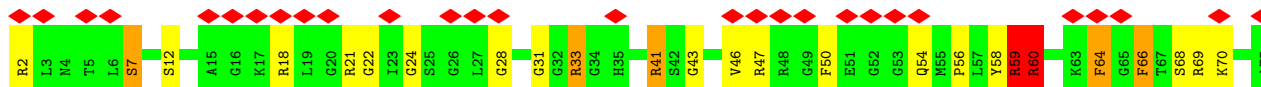
• Molecule 29: 50S ribosomal protein L13



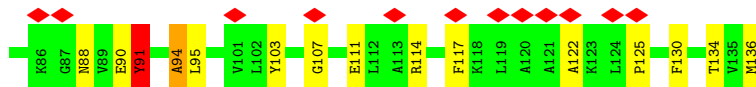
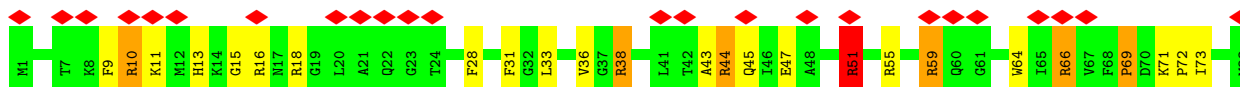
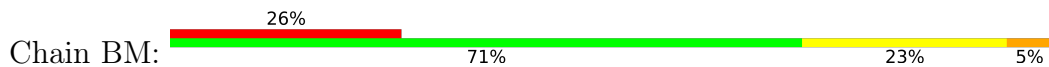
• Molecule 30: 50S ribosomal protein L14



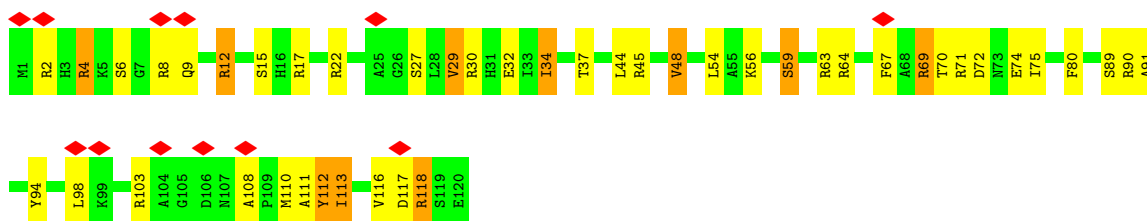
• Molecule 31: 50S ribosomal protein L15



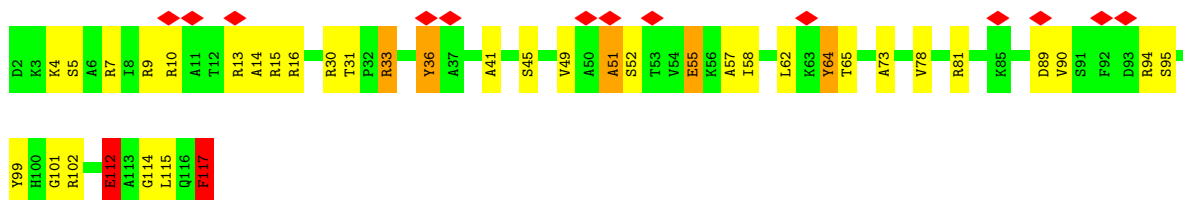
• Molecule 32: 50S ribosomal protein L16



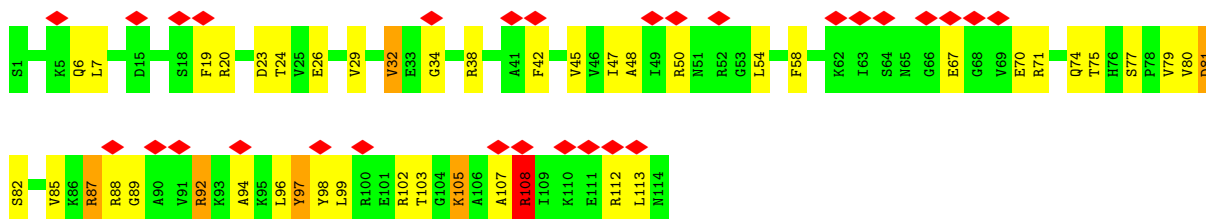
• Molecule 33: 50S ribosomal protein L17



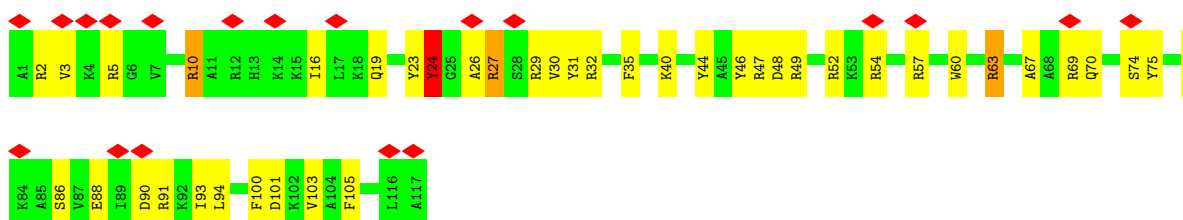
• Molecule 34: 50S ribosomal protein L18



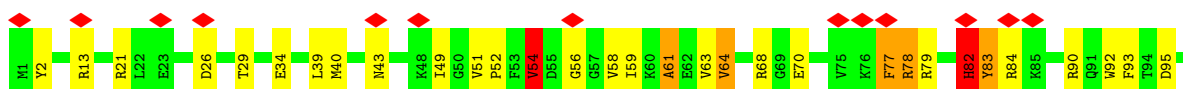
• Molecule 35: 50S ribosomal protein L19

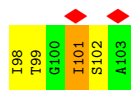


• Molecule 36: 50S ribosomal protein L20

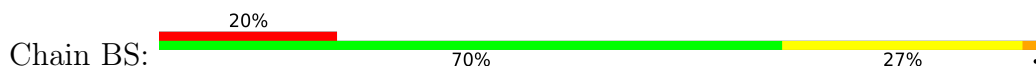


• Molecule 37: 50S ribosomal protein L21

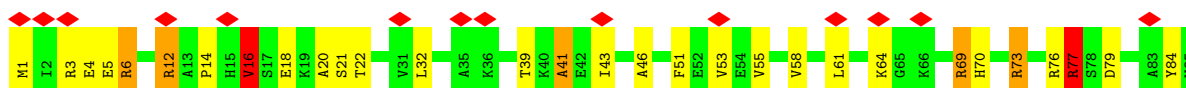




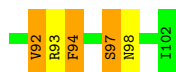
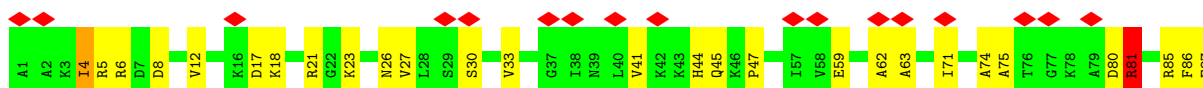
- Molecule 38: 50S ribosomal protein L22



- Molecule 39: 50S ribosomal protein L23



- Molecule 40: 50S ribosomal protein L24

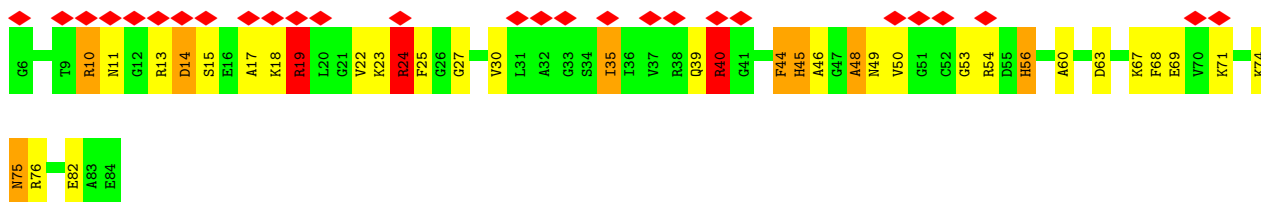


- Molecule 41: 50S ribosomal protein L25



- Molecule 42: 50S ribosomal protein L27





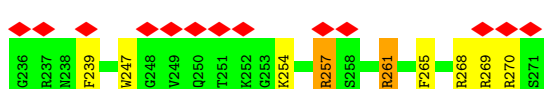
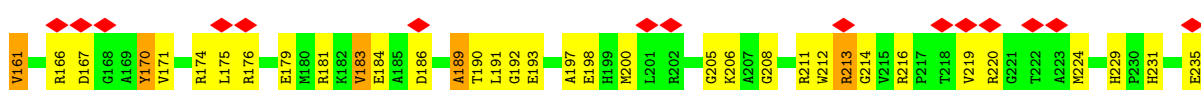
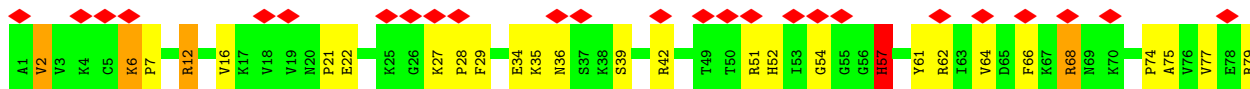
• Molecule 43: 50S ribosomal protein L28



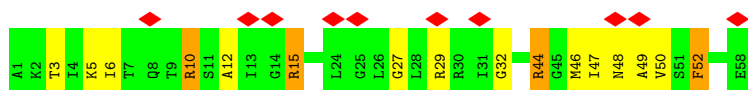
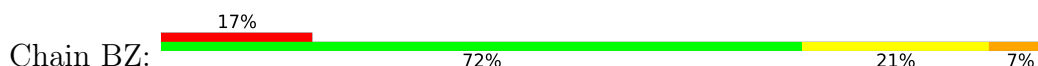
• Molecule 44: 50S ribosomal protein L29



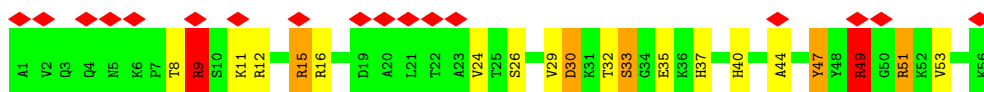
• Molecule 45: 50S ribosomal protein L2



• Molecule 46: 50S ribosomal protein L30



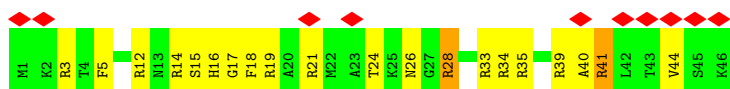
• Molecule 47: 50S ribosomal protein L32



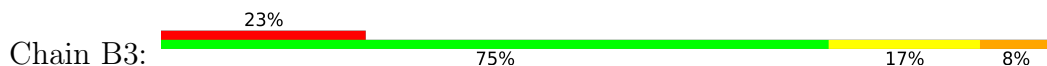
• Molecule 48: 50S ribosomal protein L33



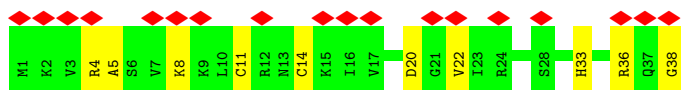
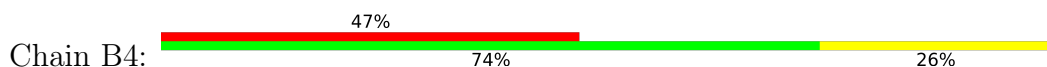
• Molecule 49: 50S ribosomal protein L34



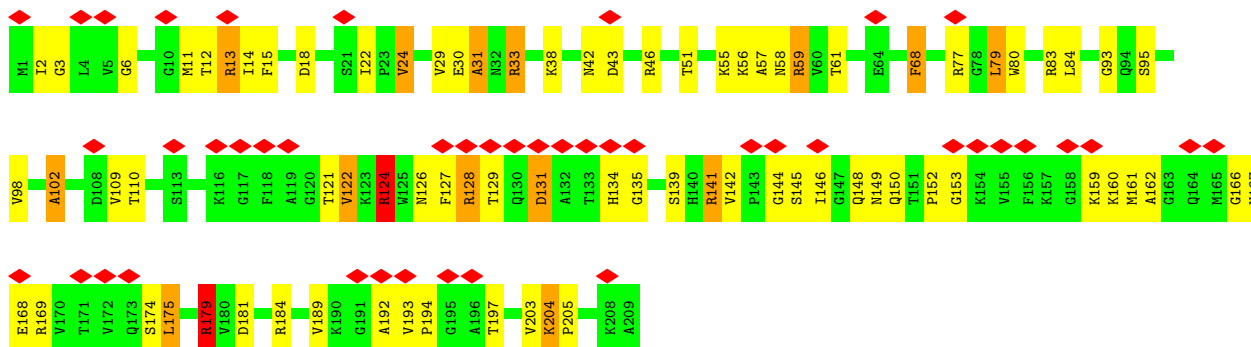
• Molecule 50: 50S ribosomal protein L35



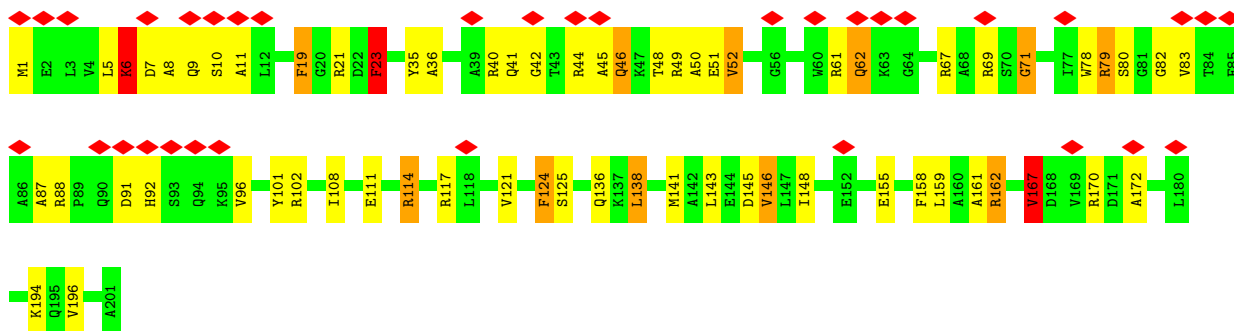
• Molecule 51: 50S ribosomal protein L36



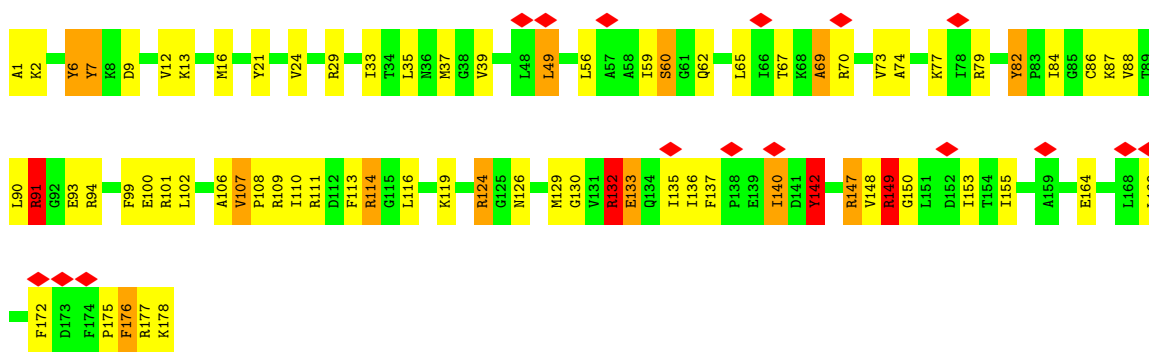
• Molecule 52: 50S ribosomal protein L3



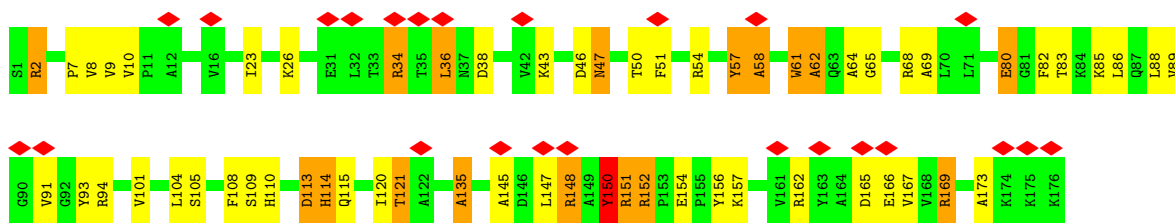
• Molecule 53: 50S ribosomal protein L4



• Molecule 54: 50S ribosomal protein L5

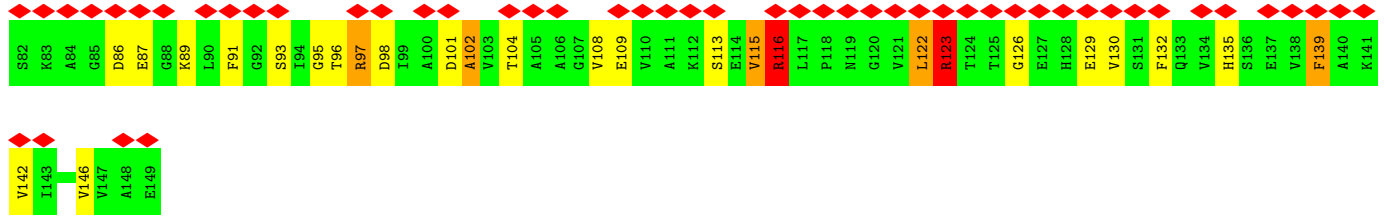


• Molecule 55: 50S ribosomal protein L6



• Molecule 56: 50S ribosomal protein L9





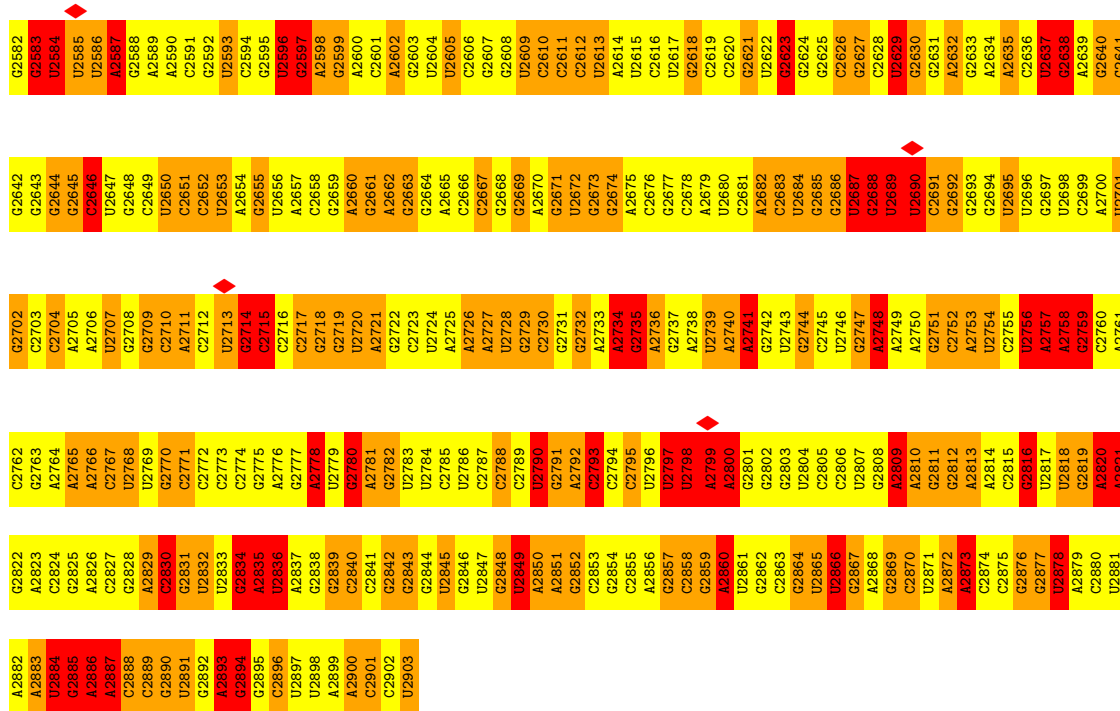
• Molecule 57: 23S ribosomal RNA



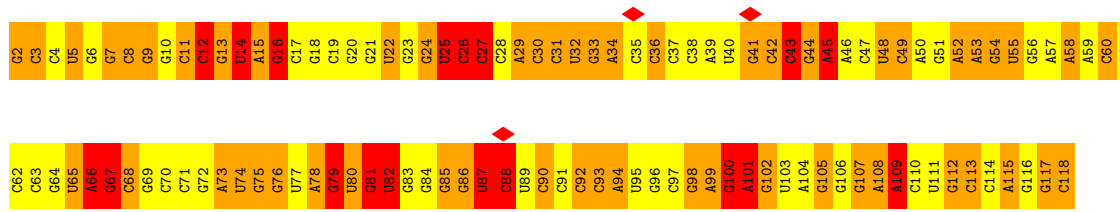
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C2575	C2515	U2395	A2335	C2275	C2215	A2095	G2035	C1974	U1915	U1855	C1795
U2576	A2516	G2396	G2336	G2276	U2216	C2096	C2036	G1975	A1916	U1856	U1796
G2577	C2517	U2397	G2337	A2277	C2217	A2097	A2037	U1976	U1917	G1857	G1797
U2578	U2518	G2398	C2338	G2278	G2218	U2098	G2038	A1977	A1918	A1858	U1798
C2579	U2519	C2399	U2339	A2279	U2219	U2099	U2039	A1978	A1919	A1859	U1799
U2580	C2520	G2400	A2340	G2280	U2220	G2100	G2040	U1979	C1920	U1860	C1800
G2581	U2401	U2401	G2341	A2281	G2221	C2160	U2401	A1980	G1921	G1861	A1801



● Molecule 58: 5S ribosomal RNA



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 i

5.1 Standard geometry i

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

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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 [i](#)

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 Torsions 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.

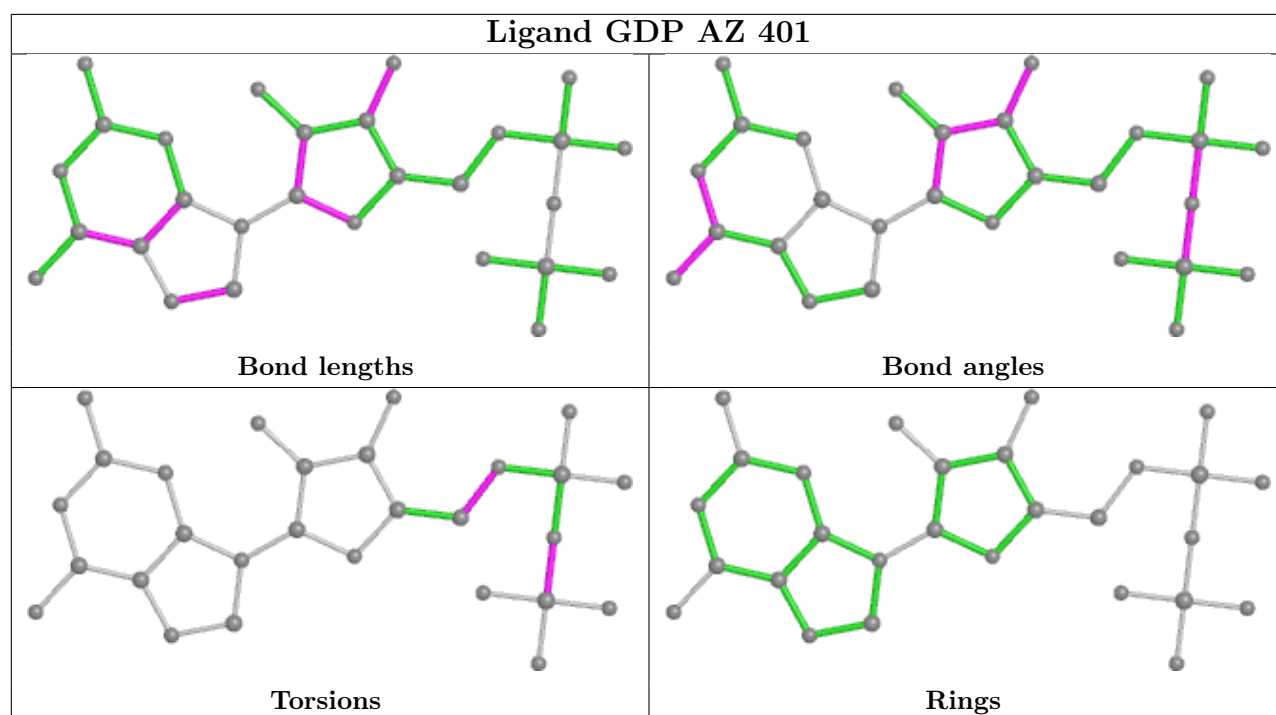
All (2) torsion outliers are listed below:

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.

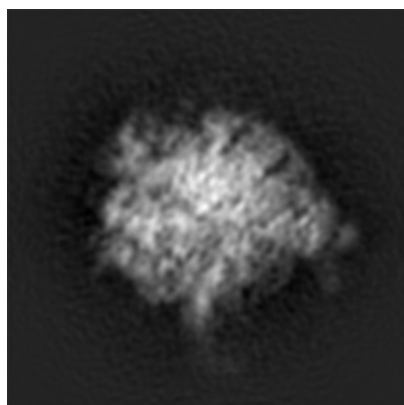
6 Map visualisation [i](#)

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.

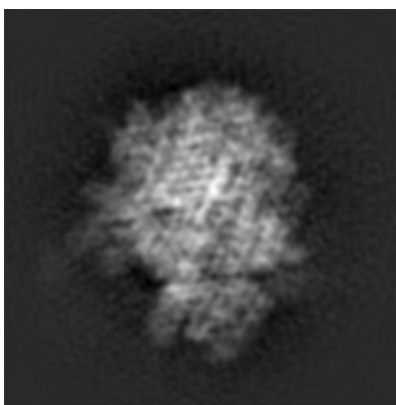
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

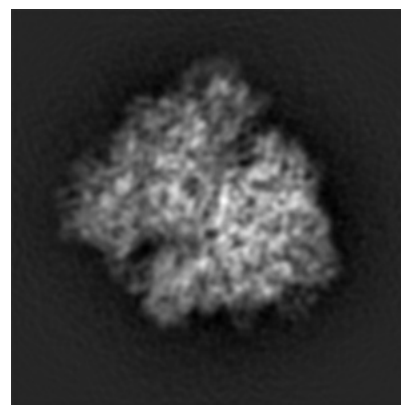
6.1.1 Primary map



X



Y

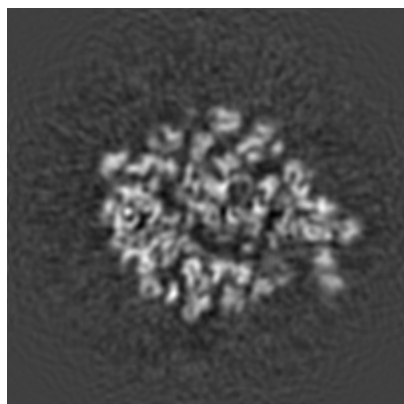


Z

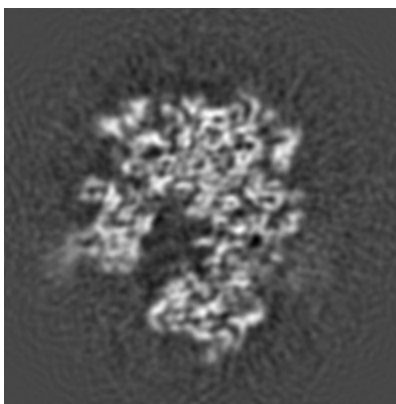
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

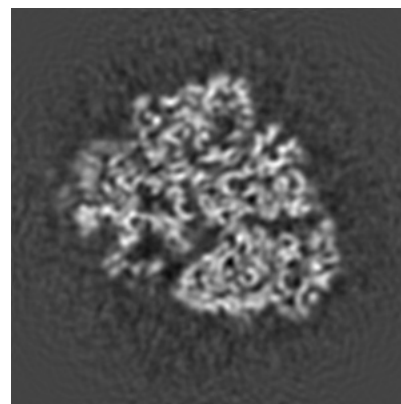
6.2.1 Primary map



X Index: 154



Y Index: 154

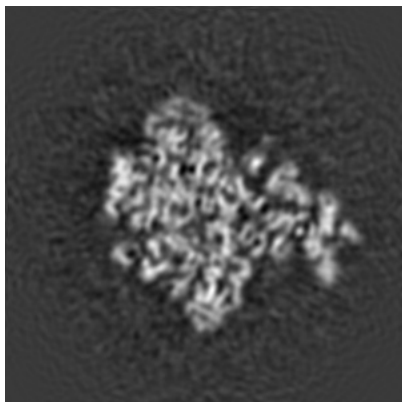


Z Index: 154

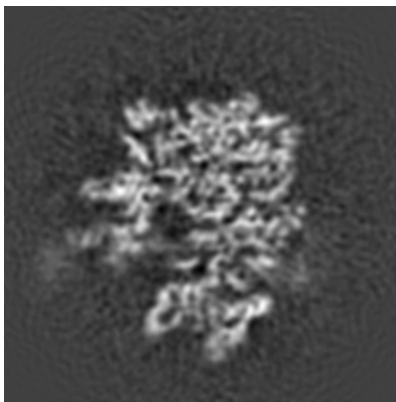
The images above show central slices of the map in three orthogonal directions.

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

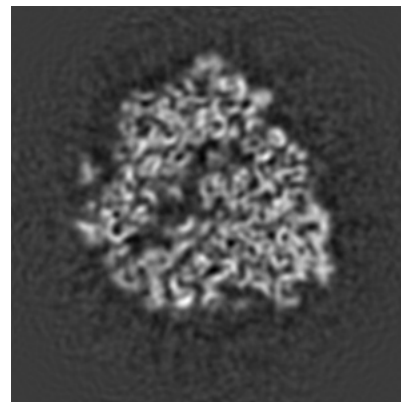
6.3.1 Primary map



X Index: 164



Y Index: 160

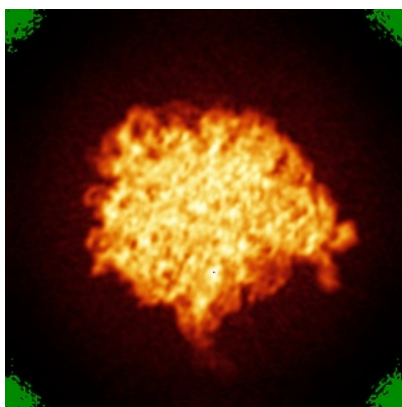


Z Index: 142

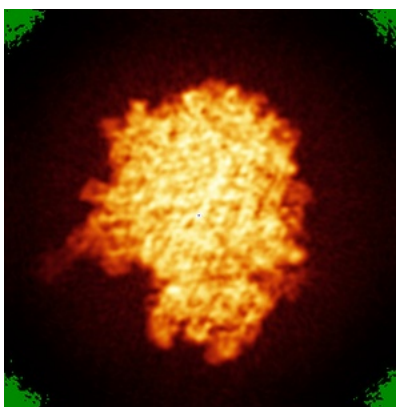
The images above show the largest variance slices of the map in three orthogonal directions.

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

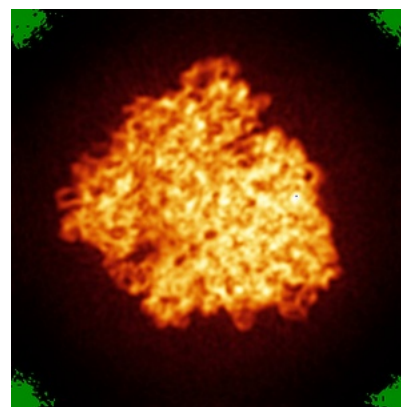
6.4.1 Primary map



X



Y

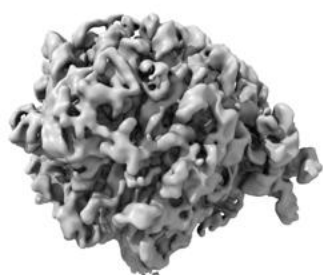


Z

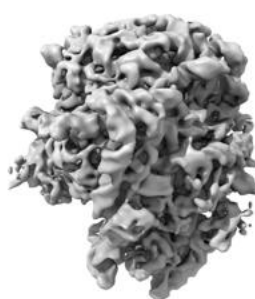
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

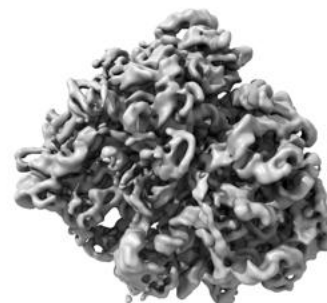
6.5.1 Primary map



X



Y



Z

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

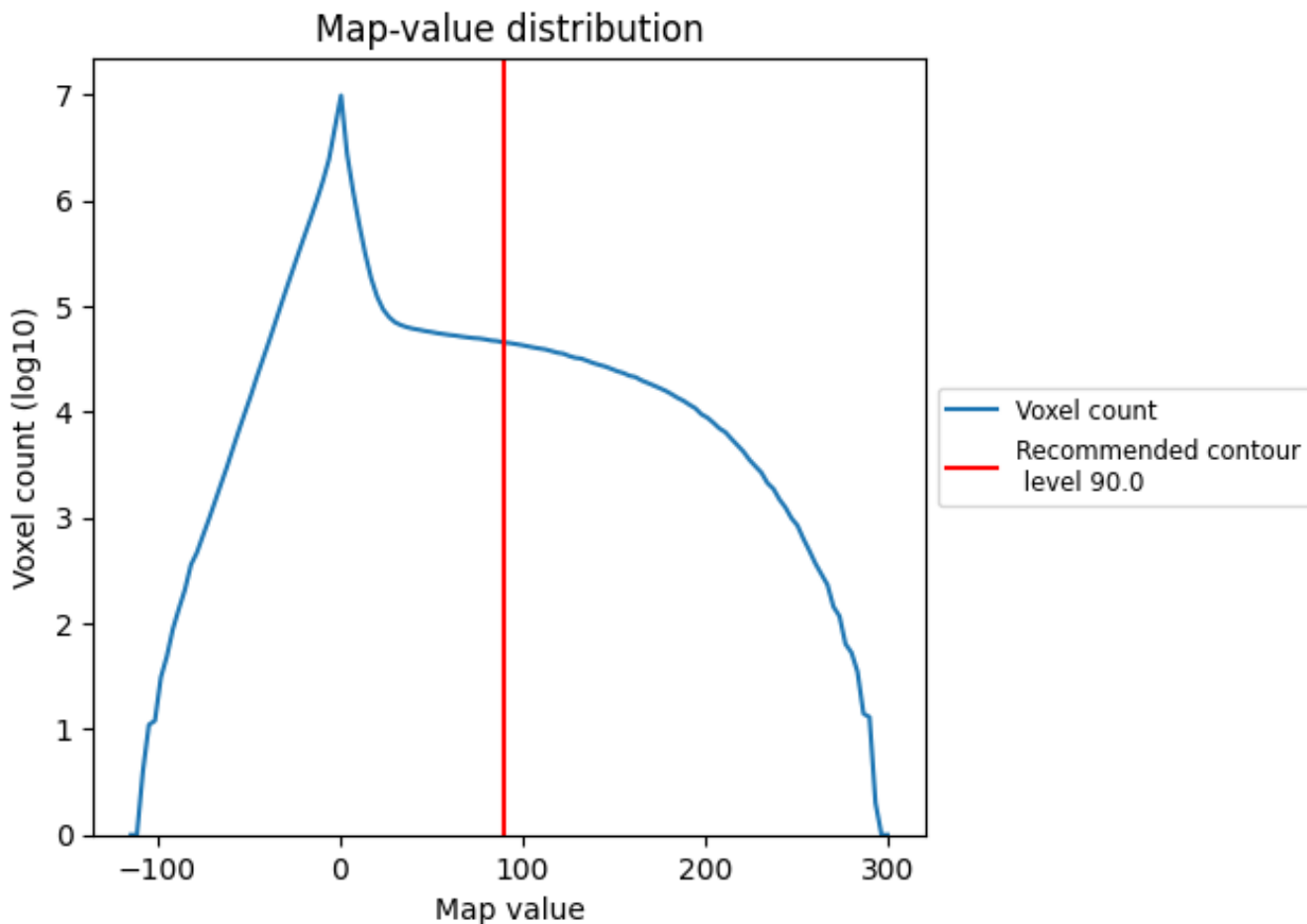
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

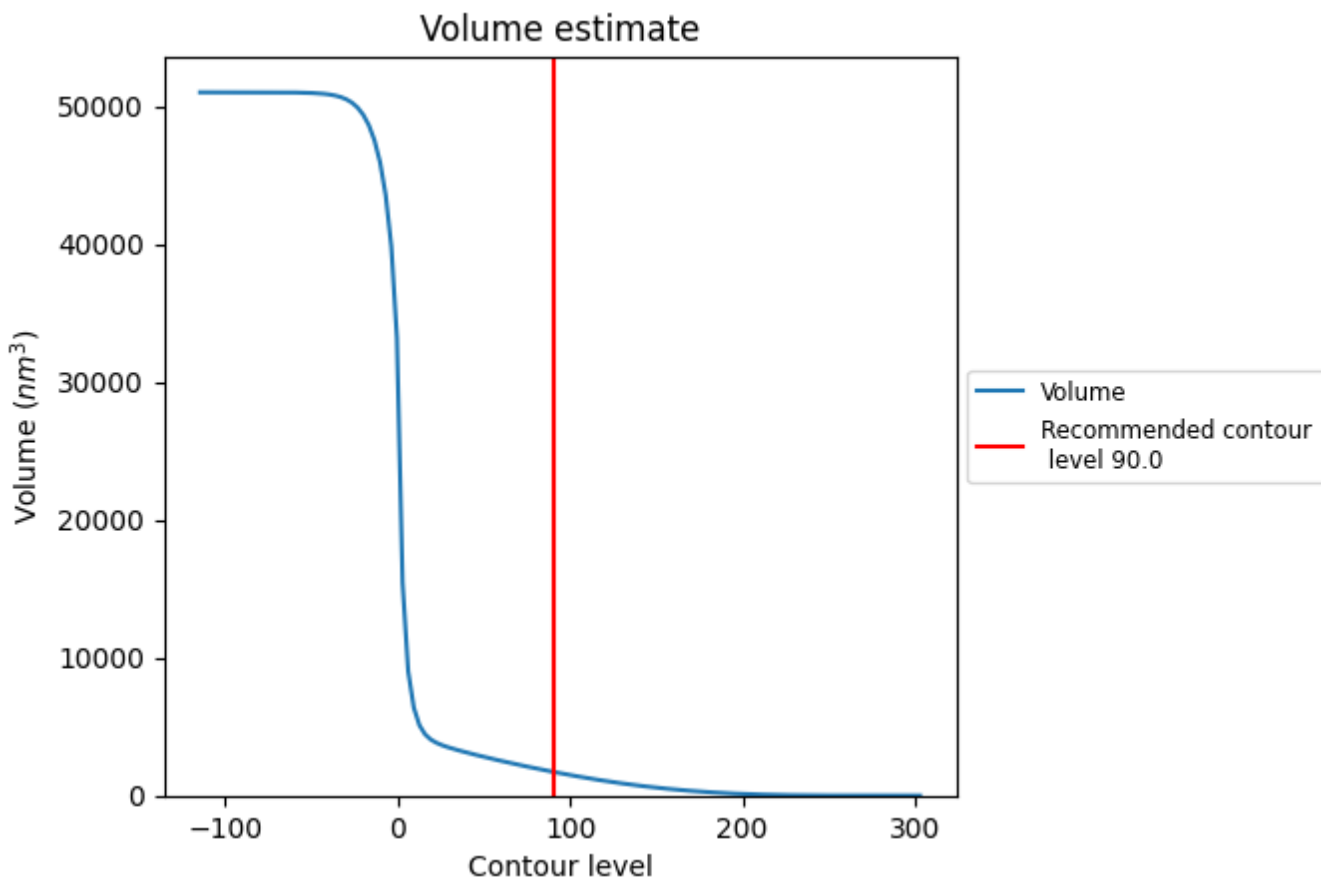
This section contains the results of statistical analysis of the map.

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.

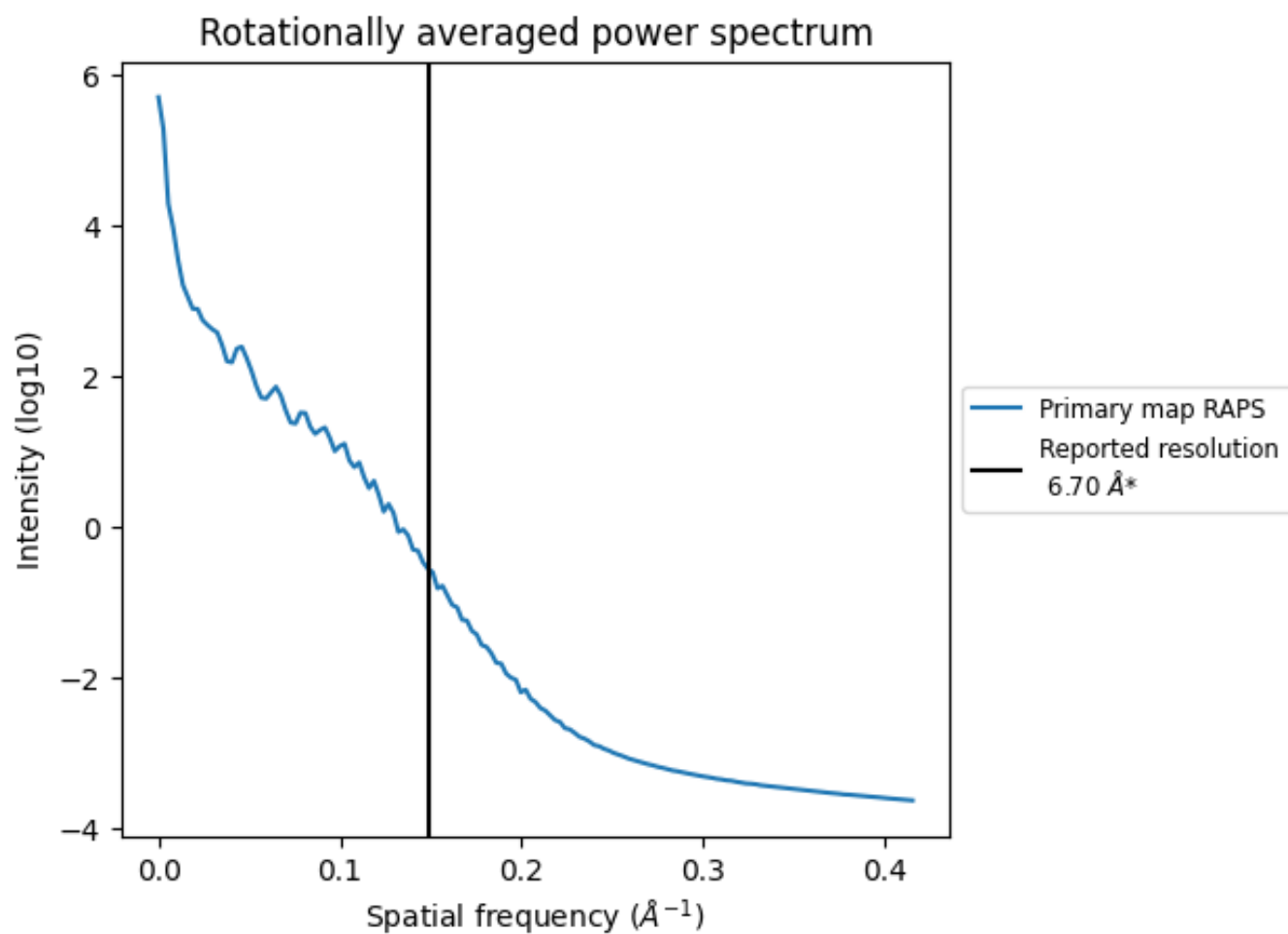
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.149\AA^{-1}

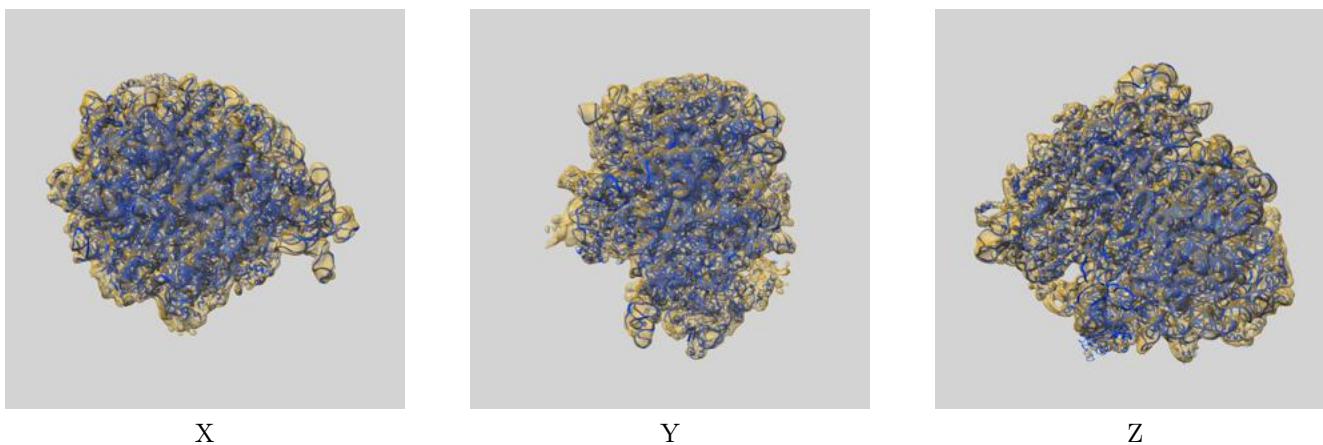
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

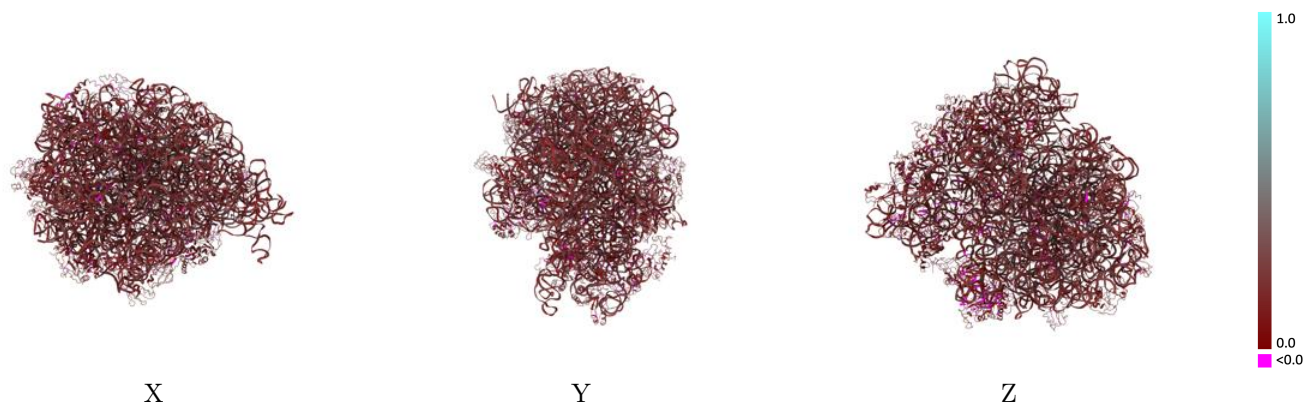
This section contains information regarding the fit between EMDB map EMD-5036 and PDB model 4V69. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



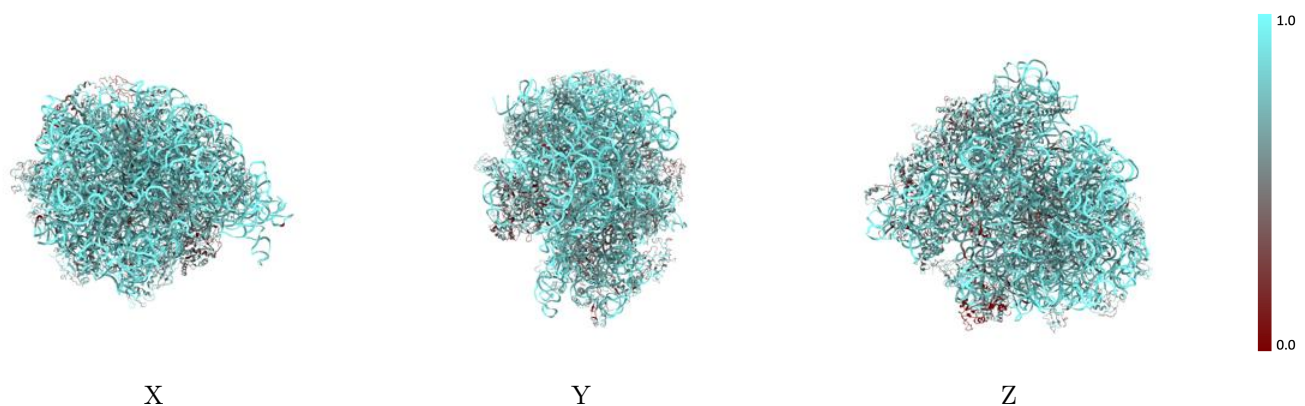
The images above show the 3D surface view of the map at the recommended contour level 90.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



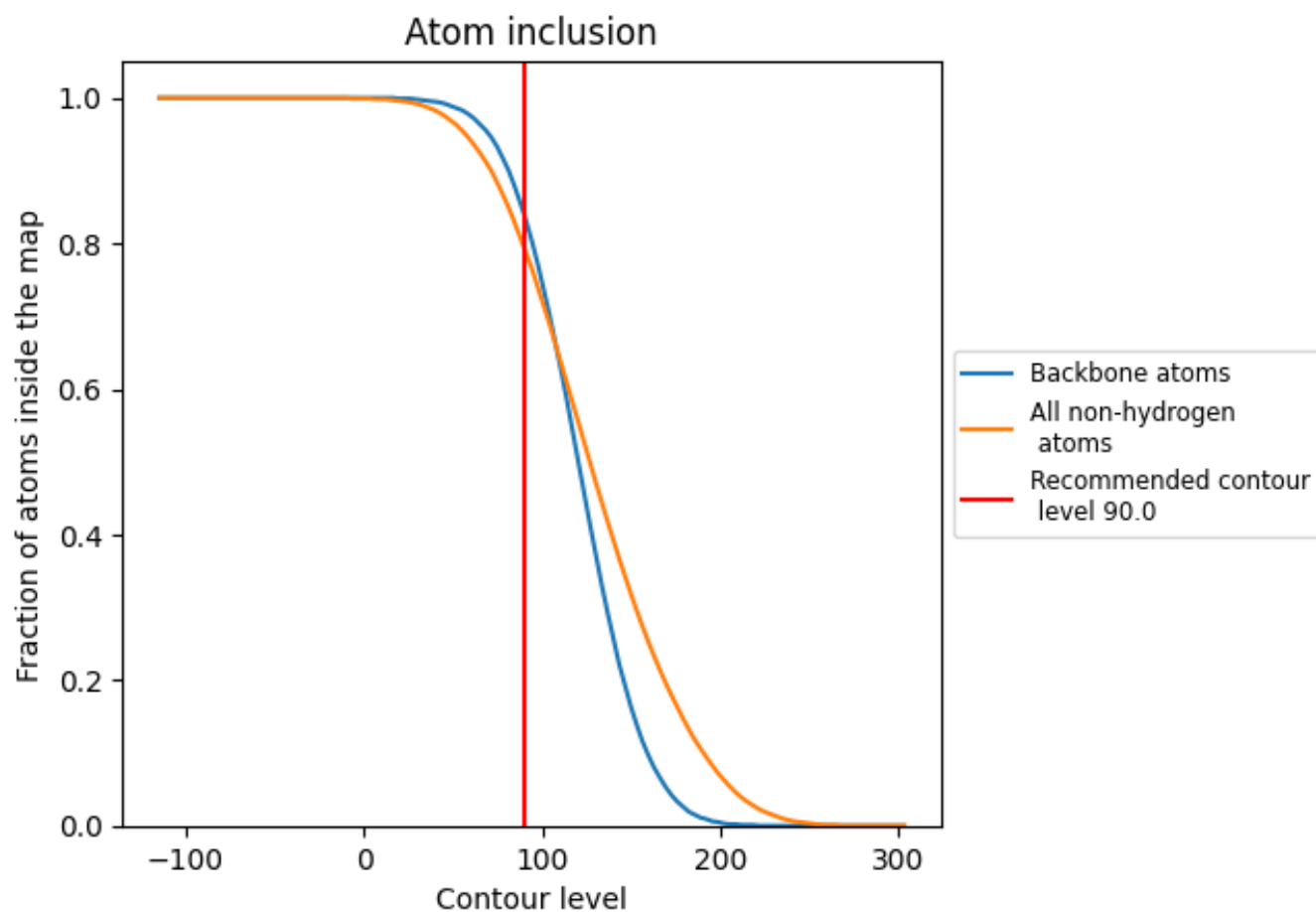
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.7930	 0.1860
AA	 0.8950	 0.2030
AB	 0.5980	 0.1550
AC	 0.6000	 0.1680
AD	 0.4980	 0.1540
AE	 0.5930	 0.1600
AF	 0.6510	 0.1650
AG	 0.6070	 0.1460
AH	 0.5600	 0.1590
AI	 0.6100	 0.1320
AJ	 0.4580	 0.1330
AK	 0.5100	 0.1580
AL	 0.4790	 0.1550
AM	 0.6190	 0.1590
AN	 0.6060	 0.1390
AO	 0.6230	 0.1520
AP	 0.6140	 0.1330
AQ	 0.6820	 0.1460
AR	 0.5490	 0.1480
AS	 0.6740	 0.1430
AT	 0.6030	 0.1520
AU	 0.7470	 0.2000
AV	 0.7940	 0.1990
AW	 0.7090	 0.1720
AX	 0.7540	 0.2270
AY	 0.7890	 0.1930
AZ	 0.4790	 0.1640
B0	 0.6400	 0.1350
B1	 0.6170	 0.1530
B2	 0.5970	 0.1010
B3	 0.5890	 0.1460
B4	 0.4970	 0.1260
B5	 0.3000	 0.0990
BA	 0.9240	 0.2090
BB	 0.9050	 0.2040



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Chain	Atom inclusion	Q-score
BC	 0.5800	 0.1420
BD	 0.5850	 0.1460
BE	 0.6170	 0.1630
BF	 0.7330	 0.1620
BG	 0.6840	 0.1710
BH	 0.4090	 0.1420
BI	 0.4640	 0.1380
BJ	 0.6030	 0.1590
BK	 0.4080	 0.1560
BL	 0.5300	 0.1450
BM	 0.5420	 0.1470
BN	 0.6650	 0.1340
BO	 0.7220	 0.1530
BP	 0.5630	 0.1700
BQ	 0.6130	 0.1150
BR	 0.6270	 0.1580
BS	 0.5920	 0.1460
BT	 0.6280	 0.1380
BU	 0.6730	 0.1560
BV	 0.7250	 0.1700
BW	 0.5380	 0.0990
BX	 0.5810	 0.1520
BY	 0.7060	 0.1360
BZ	 0.6590	 0.1660