wwPDB EM Validation Summary Report ⓘ

Jan 30, 2023 – 03:17 PM EST

PDB ID	:	4V6O
EMDB ID	:	EMD-5359
Title	:	Structural characterization of mRNA-tRNA translocation intermediates (class 4a of the six classes)
Authors	:	Agirrezabala, X.; Liao, H.; Schreiner, E.; Fu, J.; Ortiz-Meoz, R.F.; Schulten, K.; Green, R.; Frank, J.
Deposited on	:	2011-12-07
Resolution	:	14.70 Å(reported)
Based on initial model	:	2I2U

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

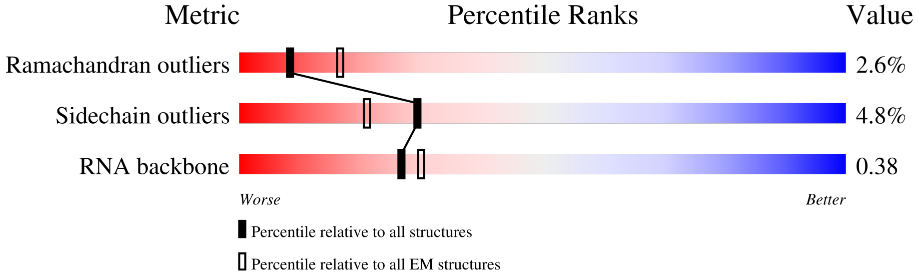
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance ⓘ

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

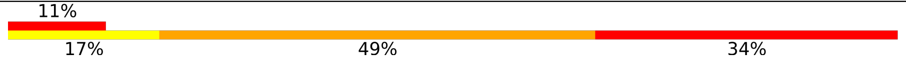
The reported resolution of this entry is 14.70 Å.

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)
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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1542	
2	AB	76	
3	AC	47	
4	AD	77	
5	AE	240	
6	AF	232	
7	AG	205	
8	AH	166	

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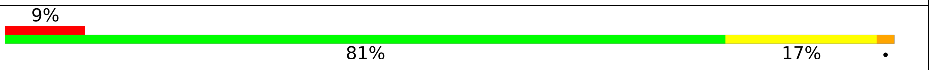
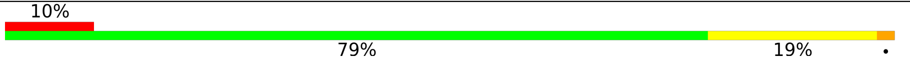
Mol	Chain	Length	Quality of chain
9	AI	135	
10	AJ	178	
11	AK	129	
12	AL	129	
13	AM	103	
14	AN	128	
15	AO	123	
16	AP	117	
17	AQ	100	
18	AR	88	
19	AS	82	
20	AT	83	
21	AU	74	
22	AV	91	
23	AW	86	
24	AX	70	
25	BA	120	
26	BB	2904	
27	BC	234	
28	BD	272	
29	BE	209	
30	BF	201	
31	BG	178	
32	BH	176	
33	BI	149	

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Mol	Chain	Length	Quality of chain
34	BJ	164	
35	BK	141	
36	BL	142	
37	BM	123	
38	BN	144	
39	BO	136	
40	BP	127	
41	BQ	117	
42	BR	114	
43	BS	117	
44	BT	103	
45	BU	110	
46	BV	100	
47	BW	103	
48	BX	94	
49	BY	84	
50	BZ	77	
51	B0	63	
52	B1	58	
53	B2	70	
54	B3	56	
55	B4	54	
56	B5	46	
57	B6	64	
58	B7	38	

2 Entry composition ⓘ

There are 60 unique types of molecules in this entry. The entry contains 152351 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1542	33089	14767	6064	10717	1541	0	0

- Molecule 2 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
2	AB	76	1627	731	287	532	75	2	0	0

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	AC	47	993	445	167	335	46	0	0

- Molecule 4 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
4	AD	77	1641	734	297	533	76	1	0	0

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	240	1872	1180	332	352	8	0	0

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AF	232	1822	1149	346	323	4	0	0

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AH	166	1225	761	232	226	6	0	0

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AI	135	1101	677	198	219	7	0	0

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AJ	178	1400	874	269	253	4	0	0

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AL	129	1036	642	208	183	3	0	0

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AM	103	825	514	158	151	2	0	0

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 17 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	AU	74	626	395	123	107	1	0	0

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	AV	91	727	464	139	122	2	0	0

- Molecule 23 is a protein called 30S ribosomal protein S20.

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

- Molecule 24 is a protein called 30S ribosomal protein S21.

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

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	BA	120	2566	1144	468	835	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	BB	2904	62351	27824	11469	20155	2903	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	BJ	164	1233	776	220	231	6	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	BN	144	1053	654	207	190	2	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	BP	127	1008	621	204	178	5	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B0	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

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

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

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B2	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	B4	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 56 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	B5	46	377	228	90	57	2	0	0

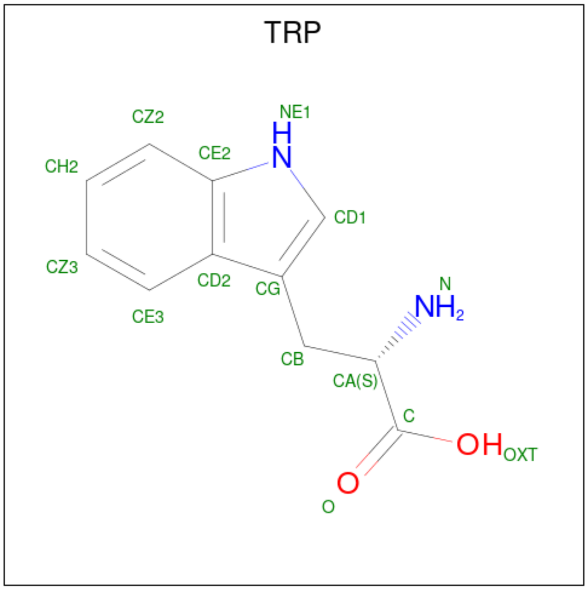
- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	B6	64	504	323	105	74	2	0	0

- Molecule 58 is a protein called 50S ribosomal protein L36.

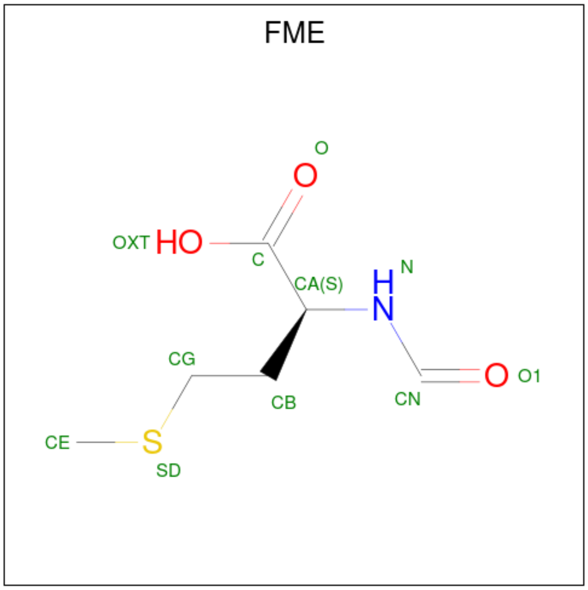
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	B7	38	302	185	65	48	4	0	0

- Molecule 59 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
59	AB	1	14	11	2	1	0

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).

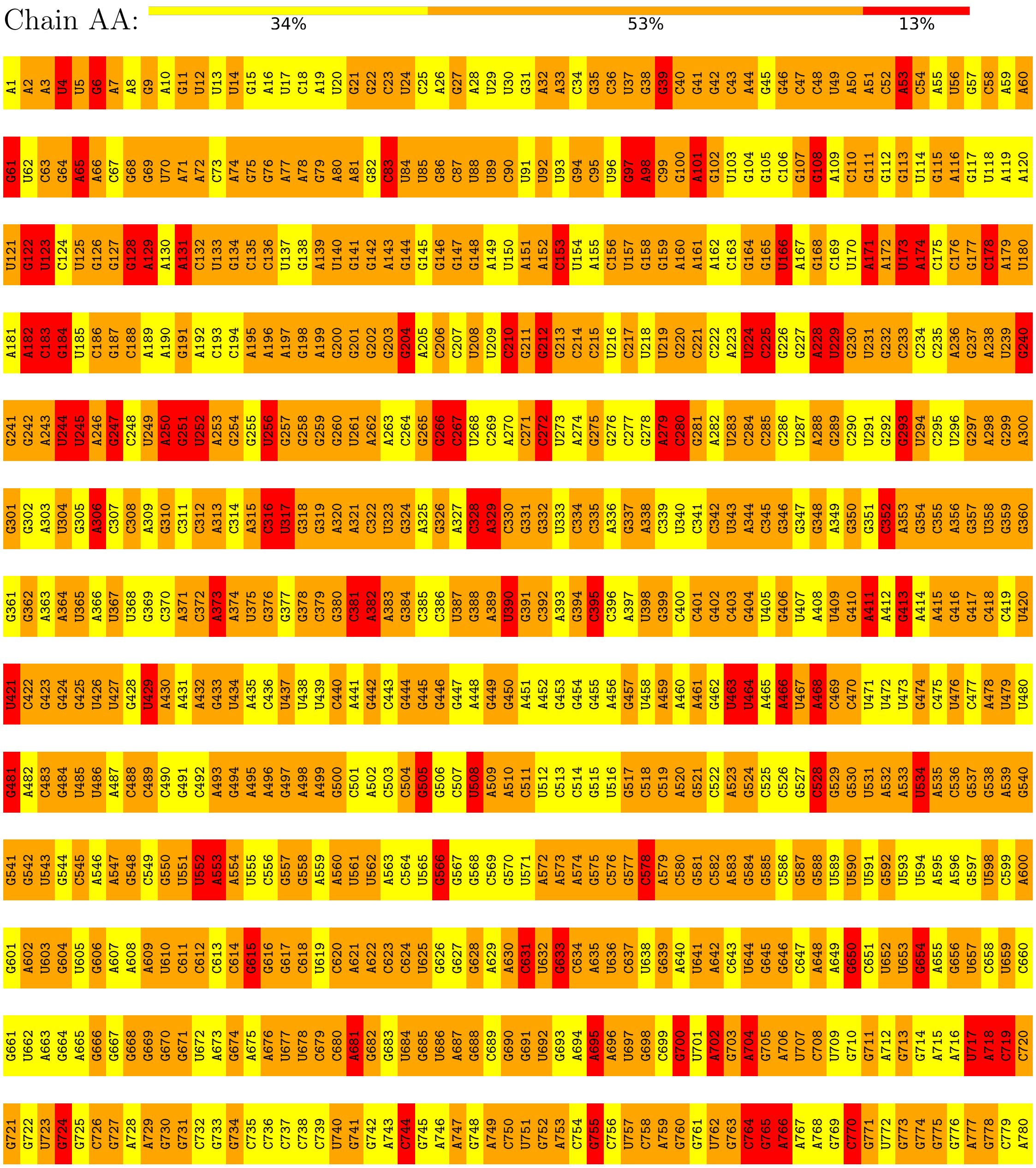


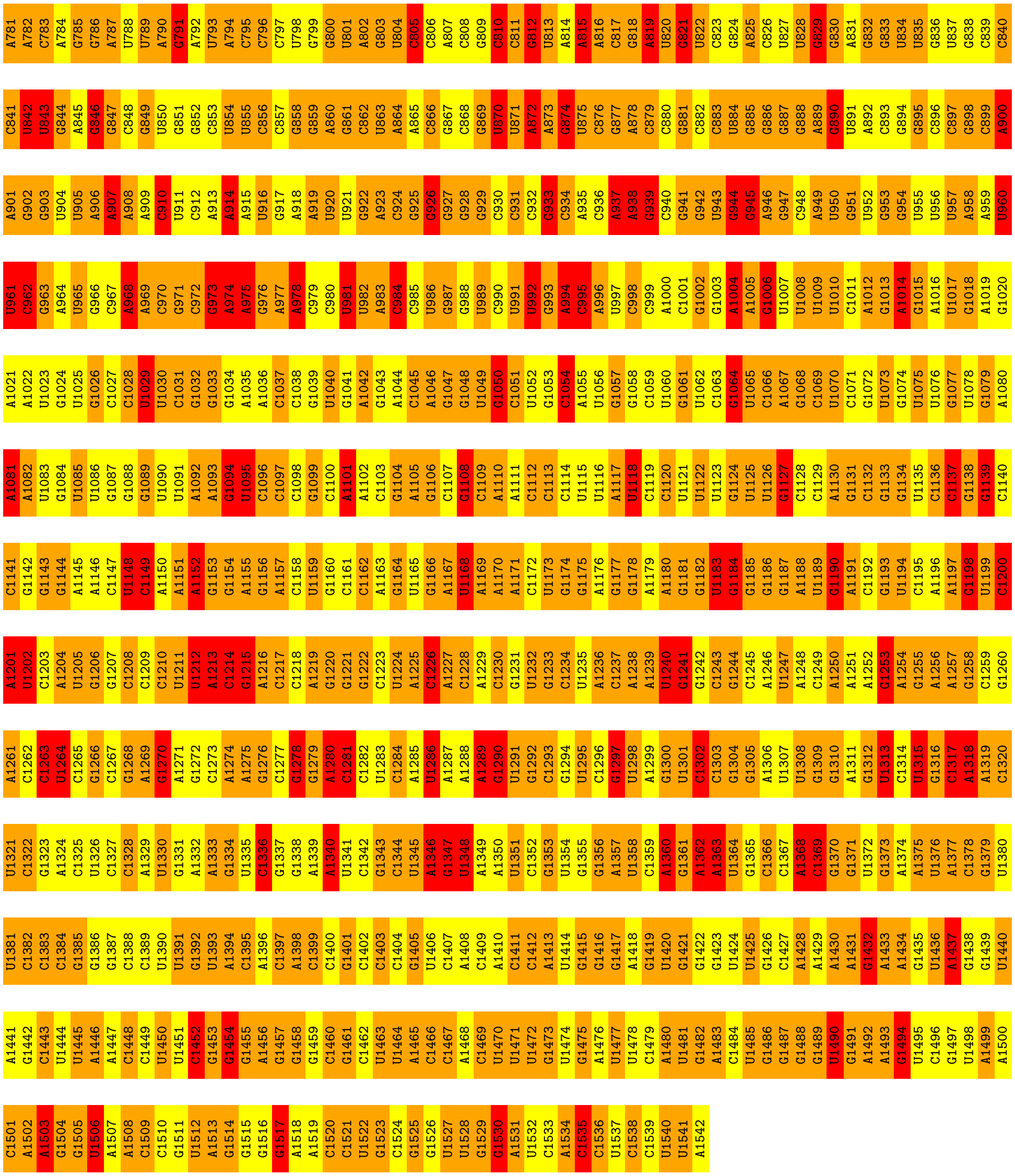
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	BB	1	10	6	1	2	1	0

3 Residue-property plots ⓘ

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

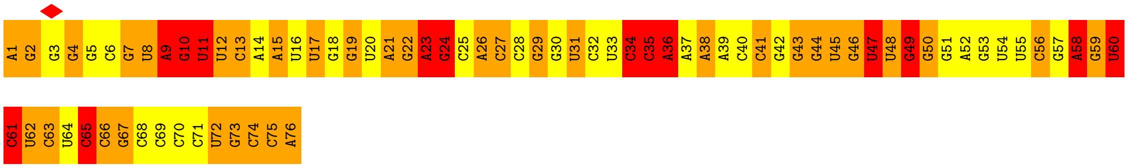
- Molecule 1: 16S ribosomal RNA





- Molecule 2: A site tRNA

Chain AB:

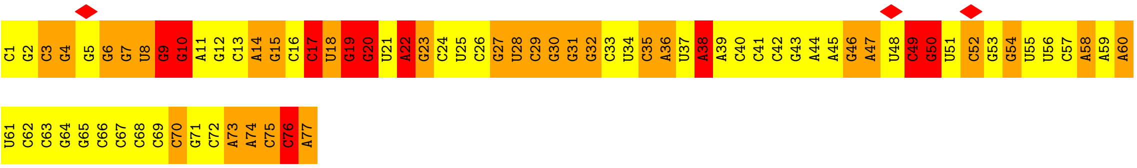


- Molecule 3: mRNA

Chain AC:

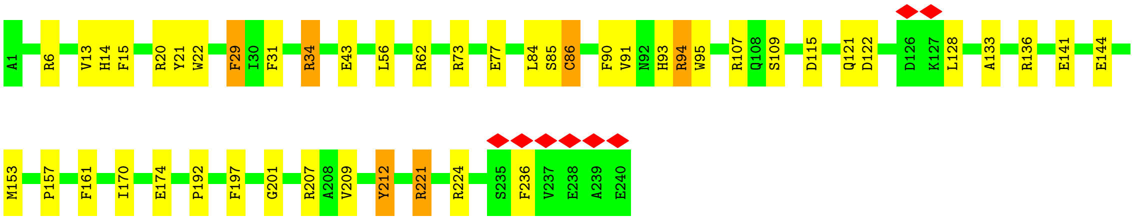
- Molecule 4: P site tRNA

Chain AD:



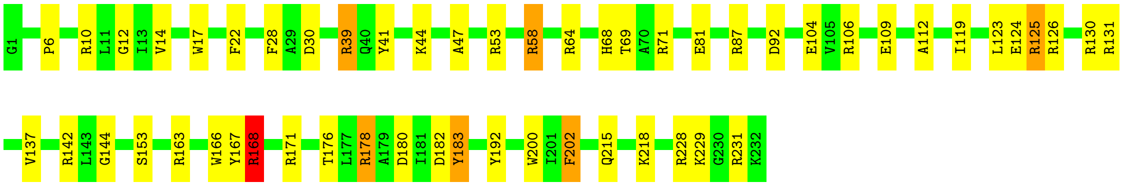
- Molecule 5: 30S ribosomal protein S2

Chain AE:



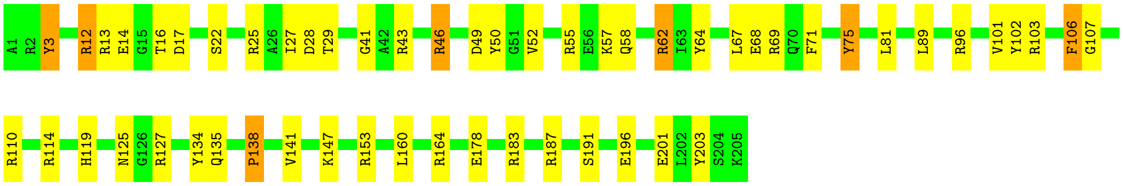
- Molecule 6: 30S ribosomal protein S3

Chain AF:



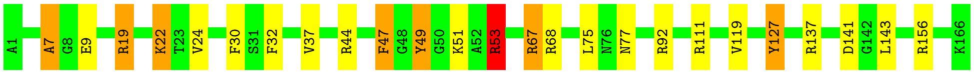
- Molecule 7: 30S ribosomal protein S4

Chain AG:



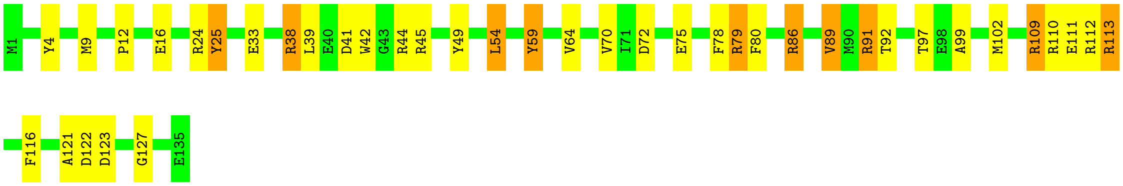
- Molecule 8: 30S ribosomal protein S5

Chain AH:



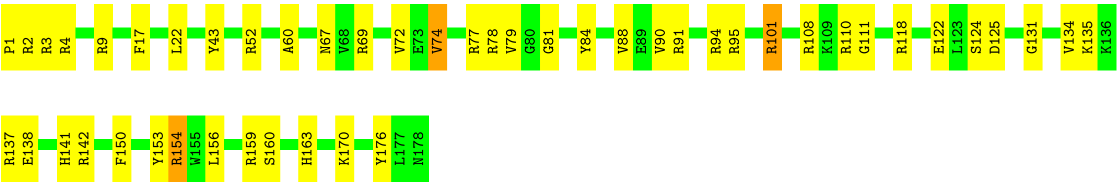
- Molecule 9: 30S ribosomal protein S6

Chain AI:



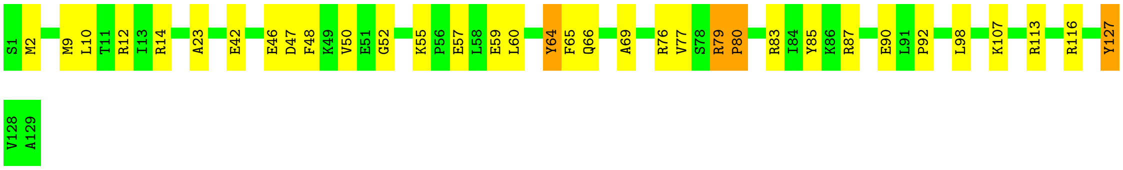
- Molecule 10: 30S ribosomal protein S7

Chain AJ:



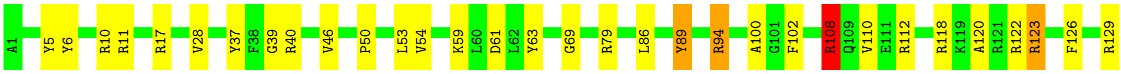
- Molecule 11: 30S ribosomal protein S8

Chain AK:



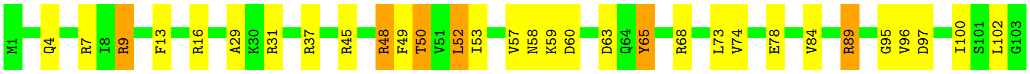
- Molecule 12: 30S ribosomal protein S9

Chain AL:

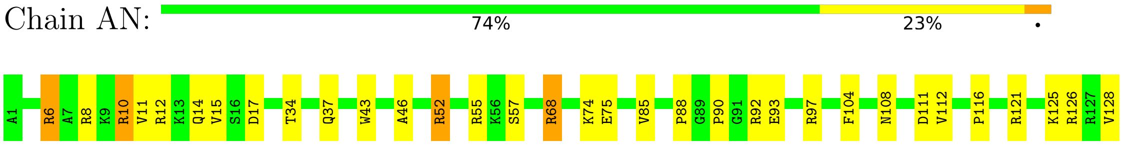


- Molecule 13: 30S ribosomal protein S10

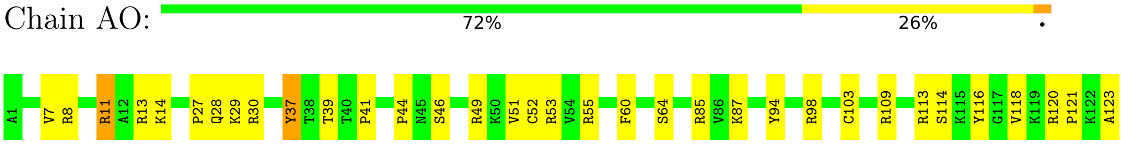
Chain AM:



- Molecule 14: 30S ribosomal protein S11



- Molecule 15: 30S ribosomal protein S12



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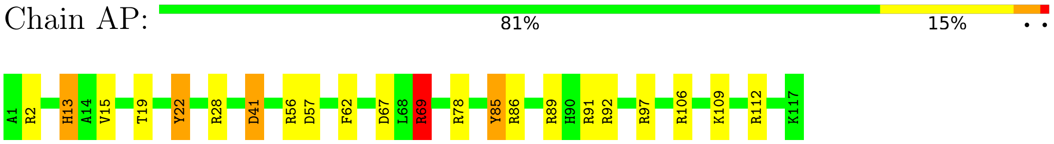

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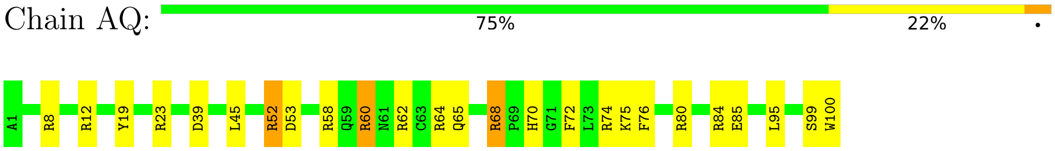
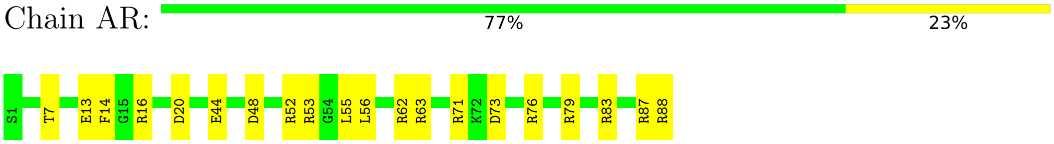


- Molecule 18: 30S ribosomal protein S15



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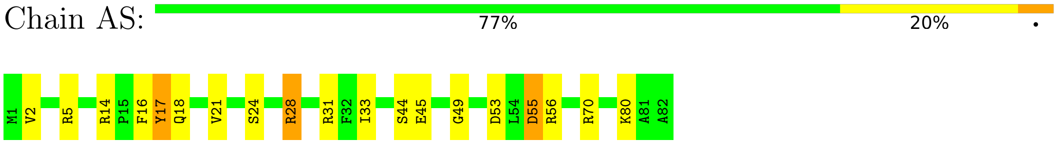

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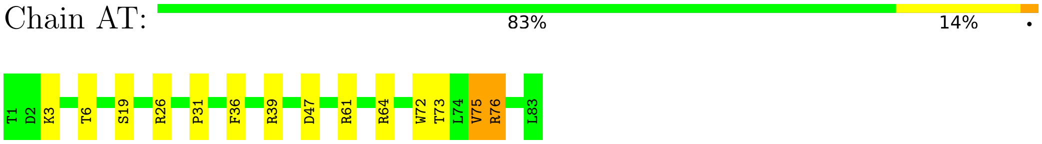

- Molecule 21: 30S ribosomal protein S18

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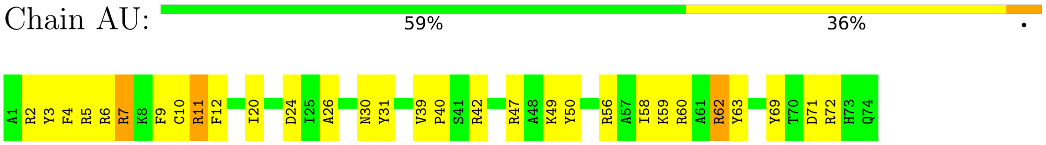

- Molecule 22: 30S ribosomal protein S19

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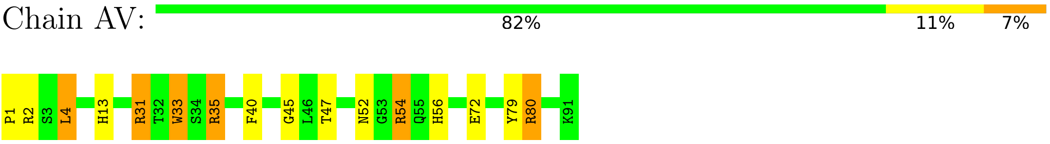

- Molecule 23: 30S ribosomal protein S20

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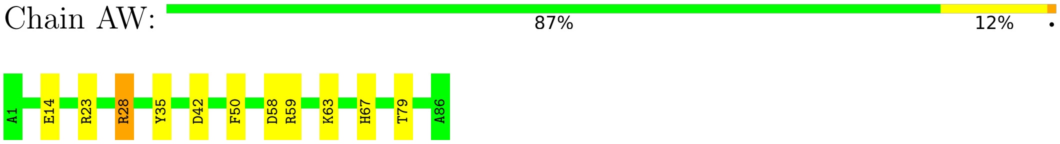

- Molecule 24: 30S ribosomal protein S21

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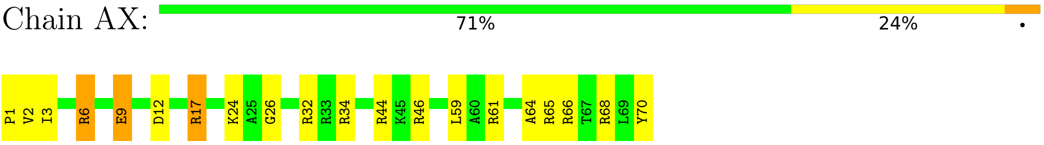

- Molecule 25: 5S ribosomal RNA

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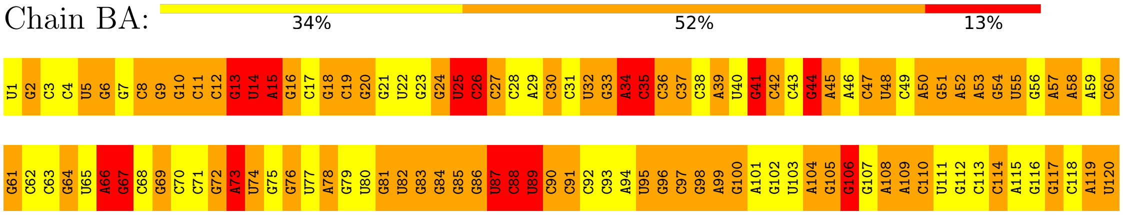

- Molecule 26: 23S ribosomal RNA

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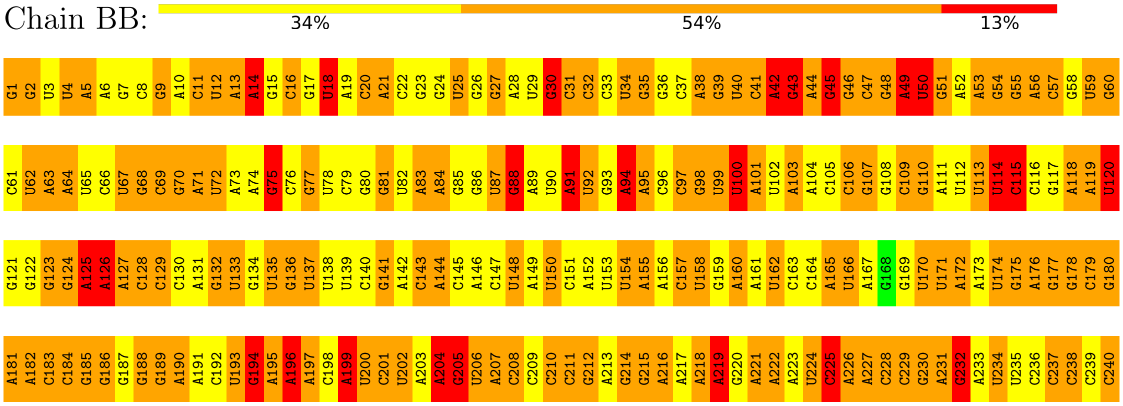

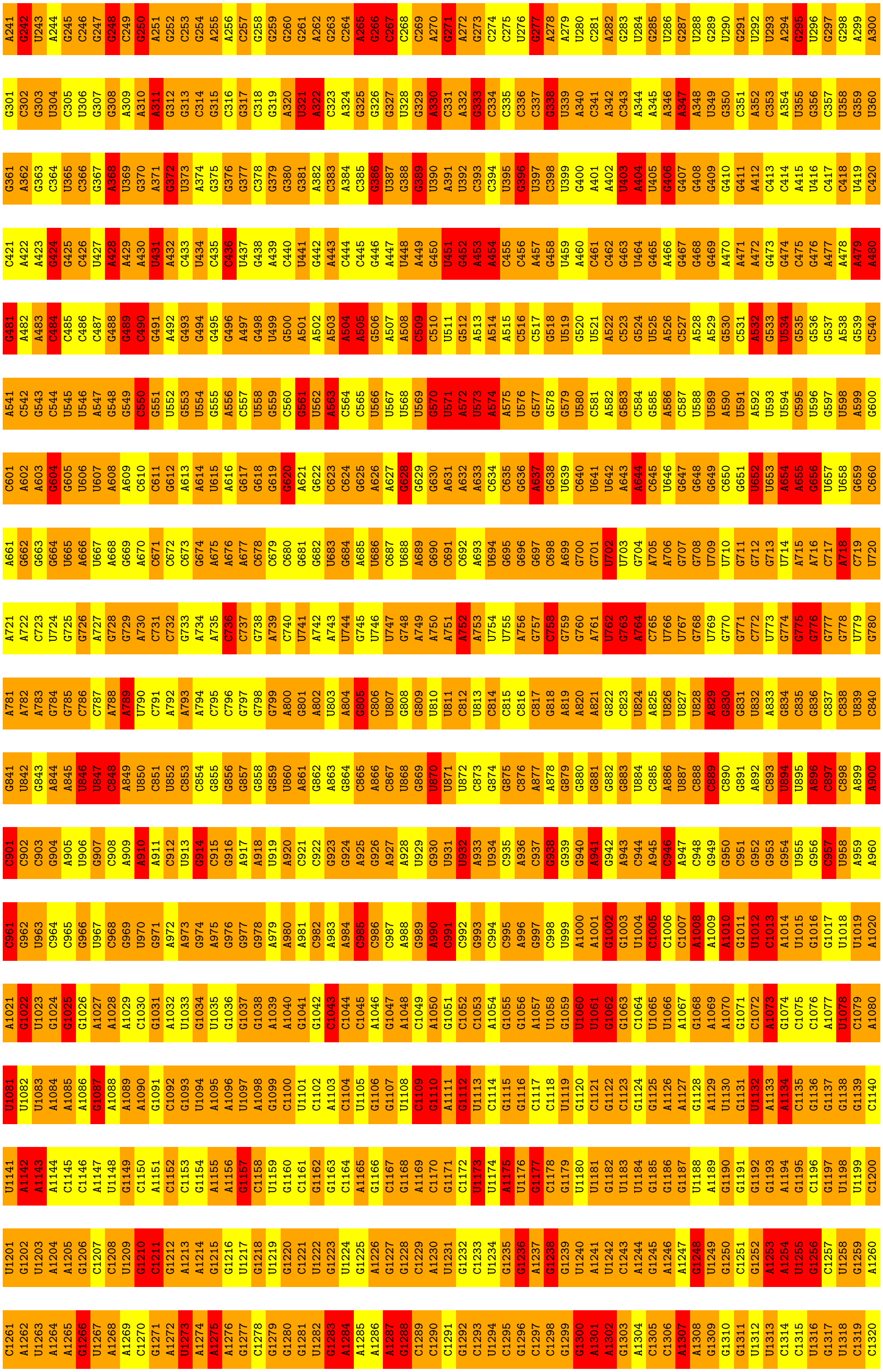

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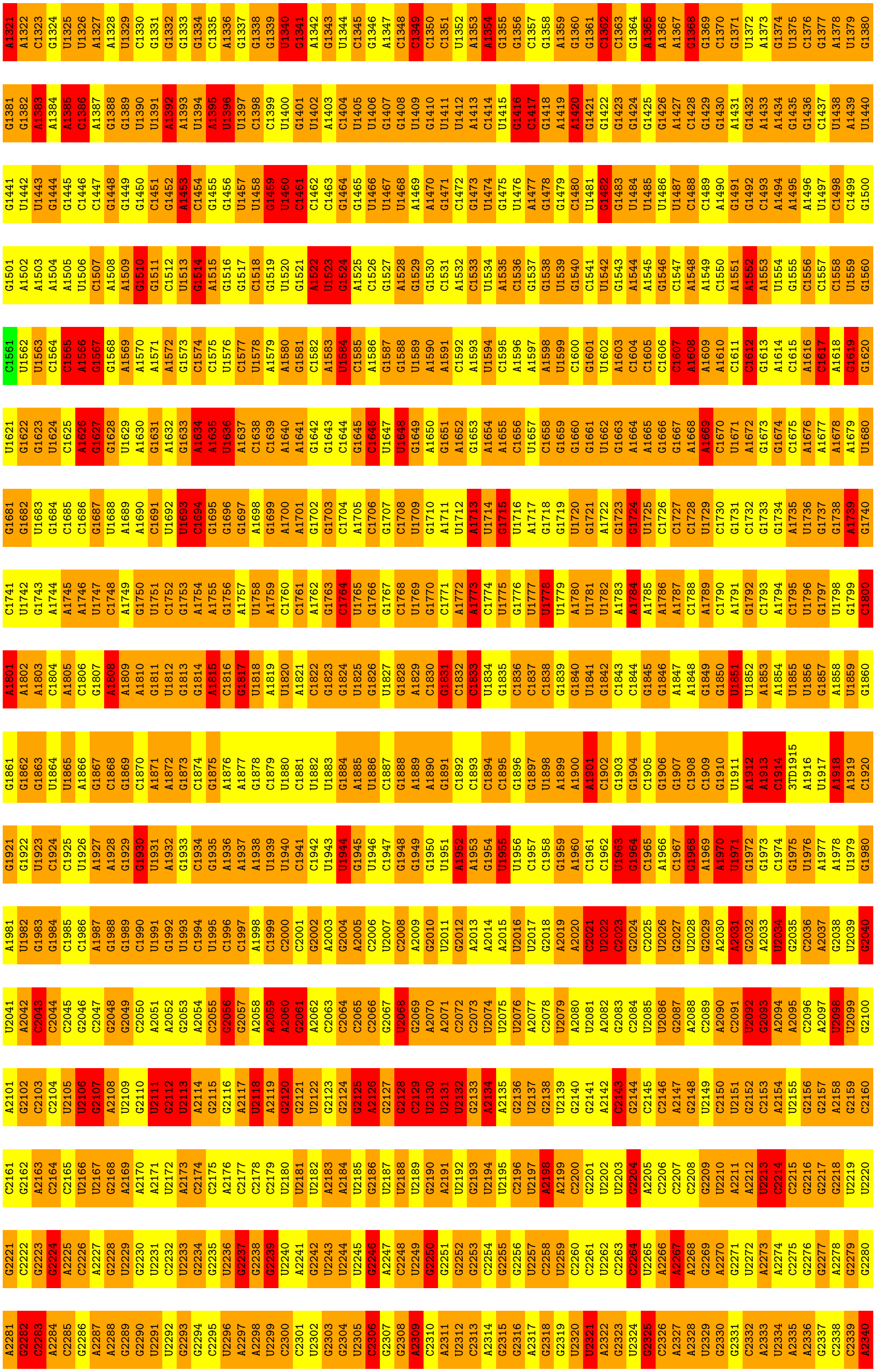

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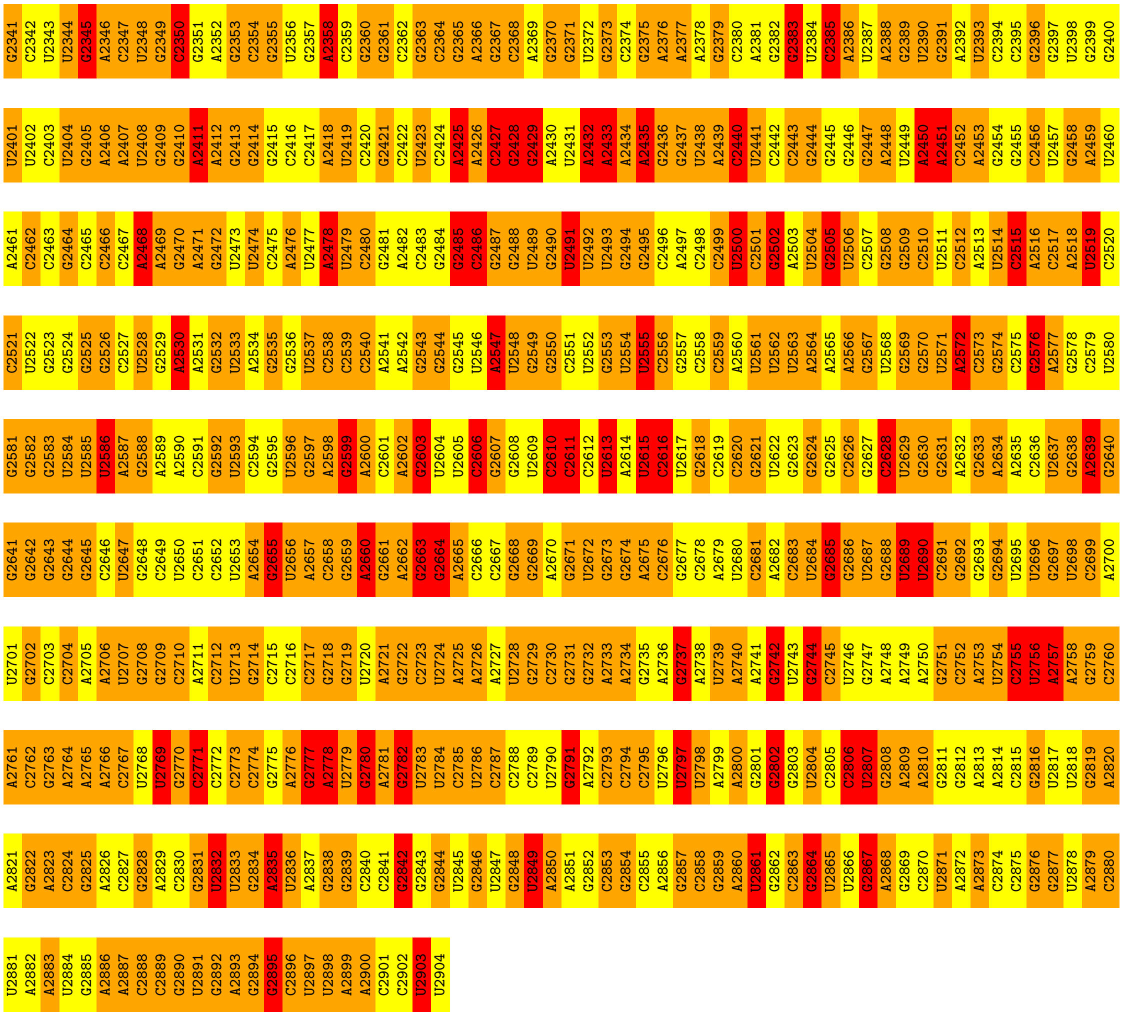
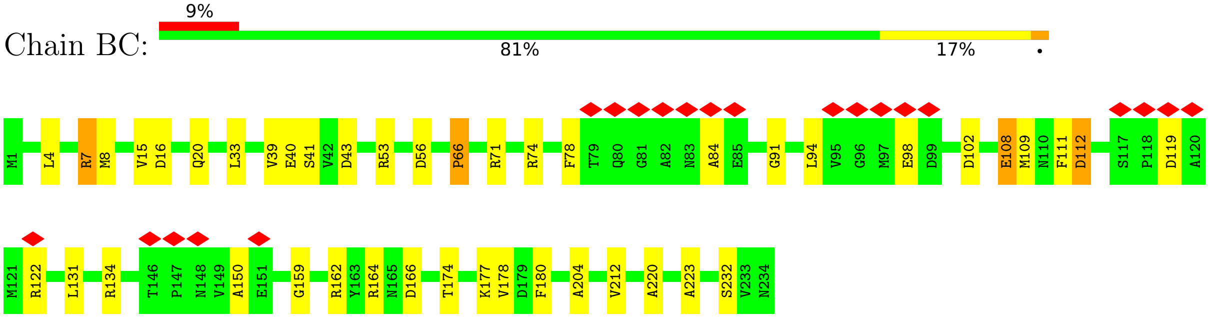


- Molecule 27: 50S ribosomal protein L1



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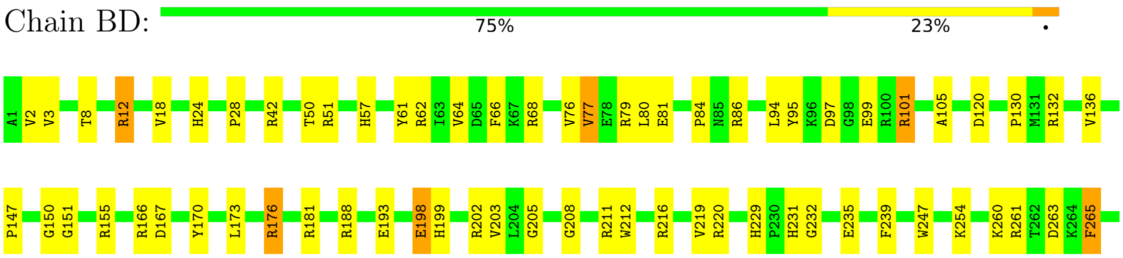

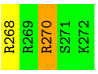

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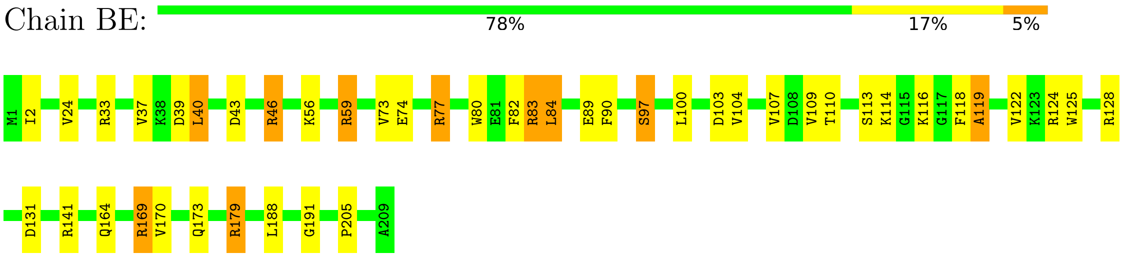

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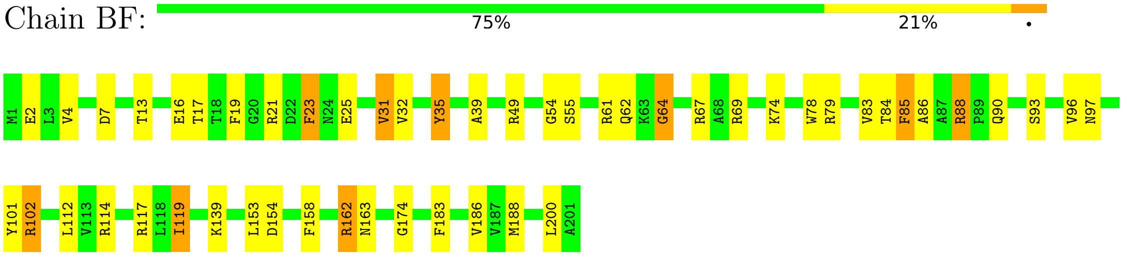
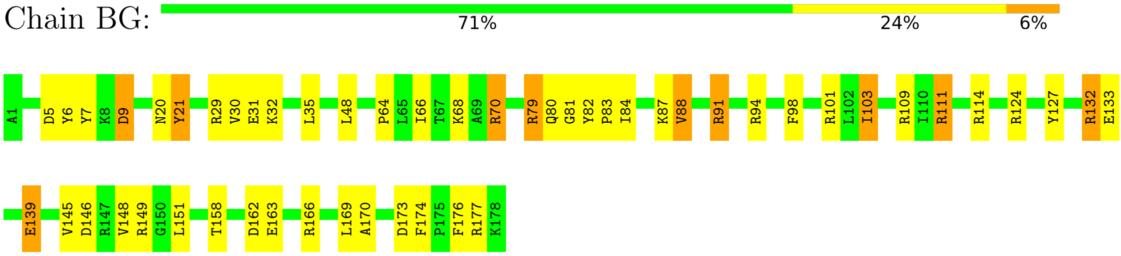
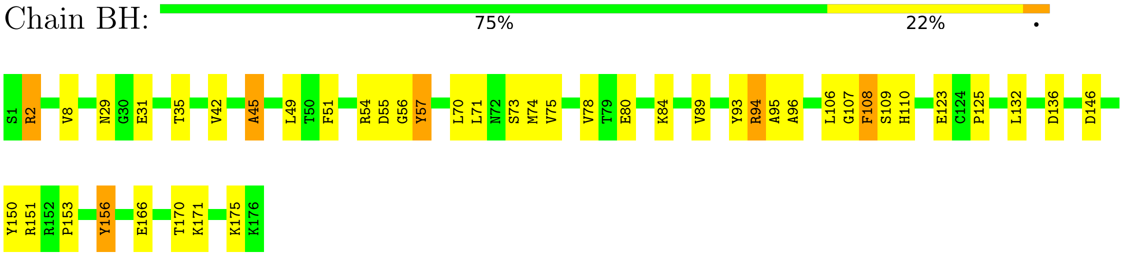


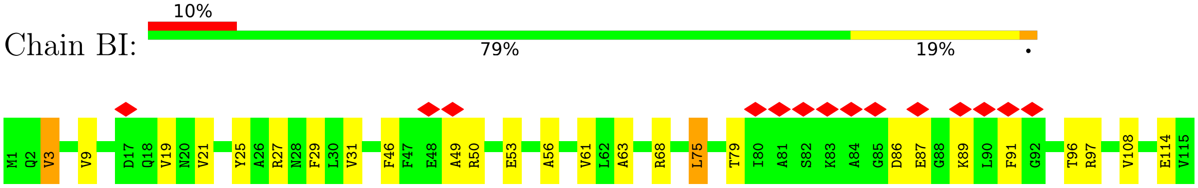
- Molecule 31: 50S ribosomal protein L5

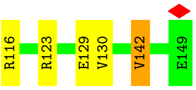


- Molecule 32: 50S ribosomal protein L6

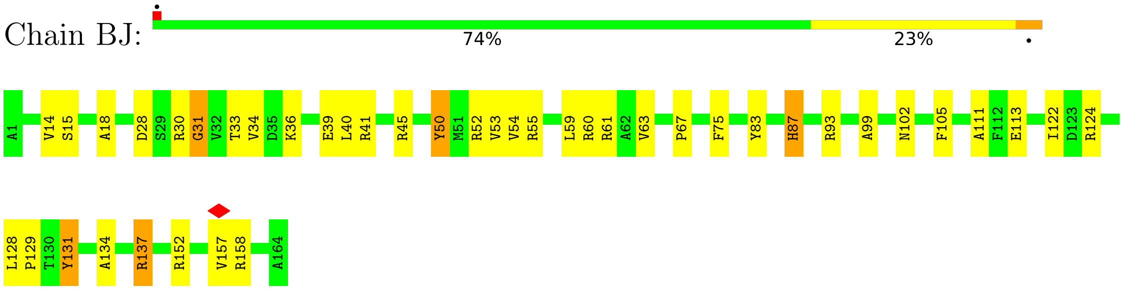


- Molecule 33: 50S ribosomal protein L9

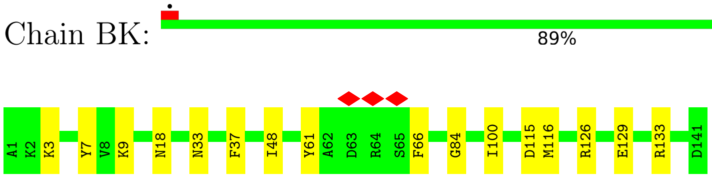




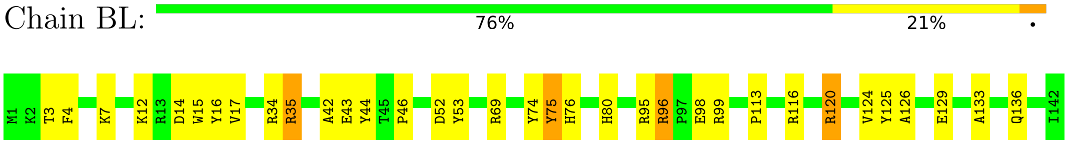
- Molecule 34: 50S ribosomal protein L10



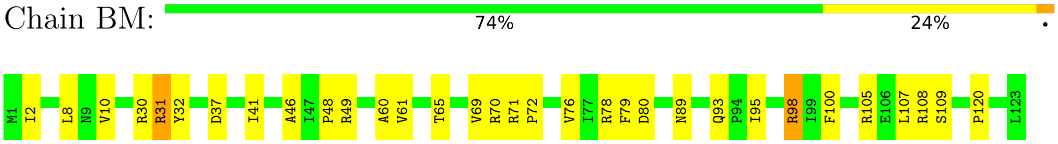
- Molecule 35: 50S ribosomal protein L11



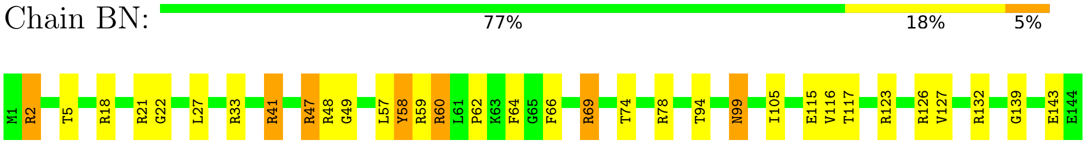
- Molecule 36: 50S ribosomal protein L13



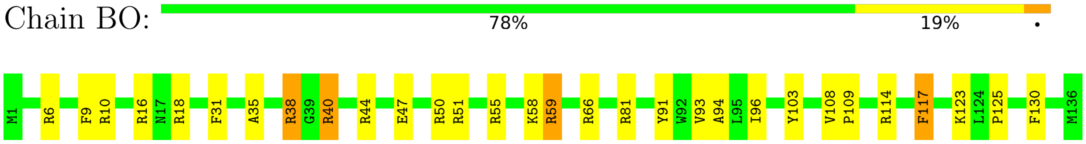
- Molecule 37: 50S ribosomal protein L14



- Molecule 38: 50S ribosomal protein L15

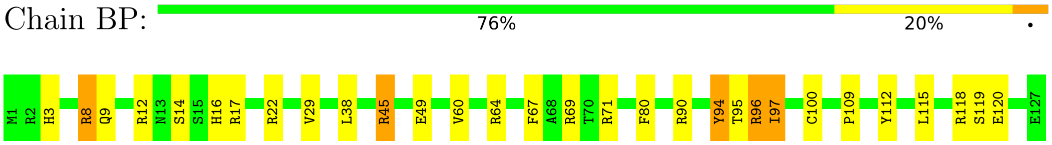


- Molecule 39: 50S ribosomal protein L16



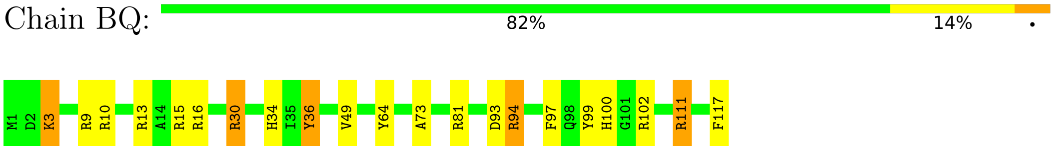
- Molecule 40: 50S ribosomal protein L17

Chain BP:



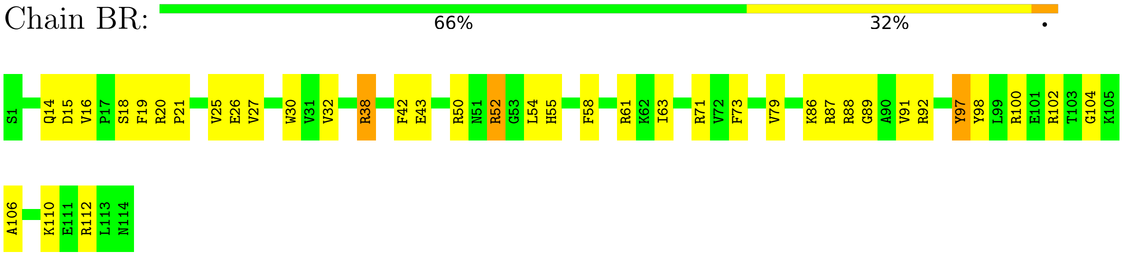
- Molecule 41: 50S ribosomal protein L18

Chain BQ:



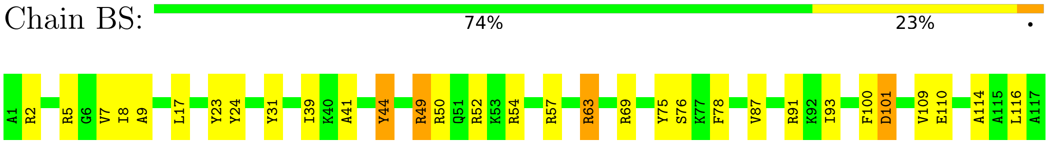
- Molecule 42: 50S ribosomal protein L19

Chain BR:



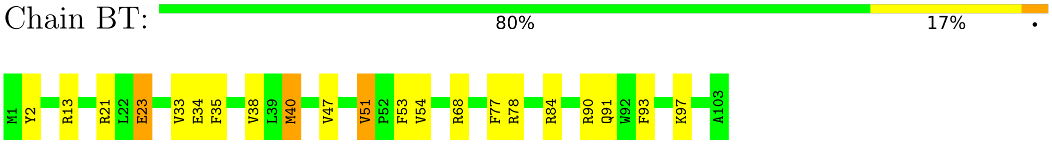
- Molecule 43: 50S ribosomal protein L20

Chain BS:



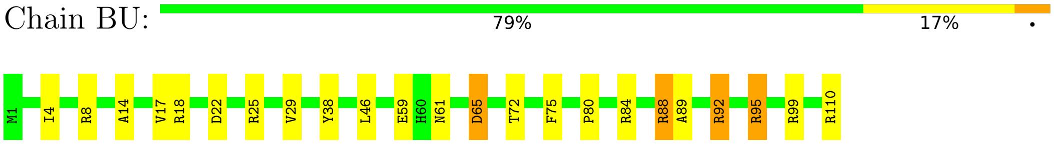
- Molecule 44: 50S ribosomal protein L21

Chain BT:



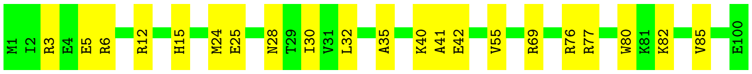
- Molecule 45: 50S ribosomal protein L22

Chain BU:



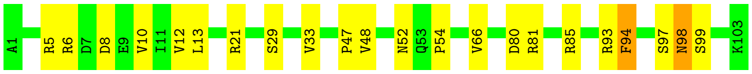
- Molecule 46: 50S ribosomal protein L23

Chain BV:



- Molecule 47: 50S ribosomal protein L24

Chain BW:

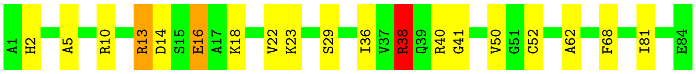



- Molecule 48: 50S ribosomal protein L25

Chain BX:

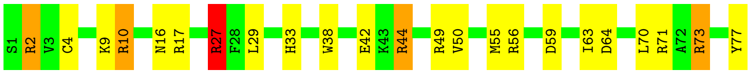

- Molecule 49: 50S ribosomal protein L27

Chain BY:

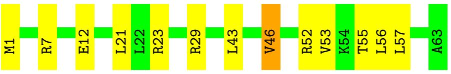
- Molecule 50: 50S ribosomal protein L28

Chain BZ:

- Molecule 51: 50S ribosomal protein L29

Chain B0:

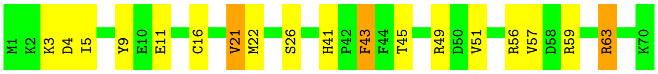



- Molecule 52: 50S ribosomal protein L30

Chain B1:

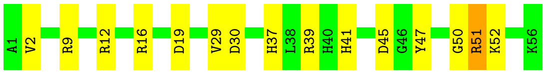

- Molecule 53: 50S ribosomal protein L31

Chain B2:

- Molecule 54: 50S ribosomal protein L32

Chain B3:



- Molecule 55: 50S ribosomal protein L33

Chain B4:

- Molecule 56: 50S ribosomal protein L34

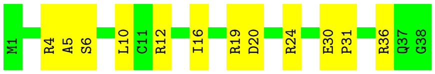
Chain B5:

- Molecule 57: 50S ribosomal protein L35

Chain B6:

- Molecule 58: 50S ribosomal protein L36

Chain B7:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Volumes were CTF-corrected in defocus groups	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	58269	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	1.422	Depositor
Minimum map value	-0.460	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.195	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	375.0, 375.0, 375.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5, 1.5, 1.5	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	3.08	3882/36769 (10.6%)	3.52	8356/57354 (14.6%)
2	AB	3.05	161/1600 (10.1%)	3.56	386/2492 (15.5%)
3	AC	3.23	133/1108 (12.0%)	3.55	250/1724 (14.5%)
4	AD	3.02	174/1721 (10.1%)	3.61	441/2683 (16.4%)
5	AE	1.50	9/1904 (0.5%)	1.89	37/2565 (1.4%)
6	AF	1.54	11/1852 (0.6%)	2.09	63/2490 (2.5%)
7	AG	1.51	9/1665 (0.5%)	1.95	48/2227 (2.2%)
8	AH	1.48	1/1239 (0.1%)	1.94	30/1664 (1.8%)
9	AI	1.57	5/1121 (0.4%)	2.07	36/1509 (2.4%)
10	AJ	1.54	9/1422 (0.6%)	2.04	43/1908 (2.3%)
11	AK	1.56	5/989 (0.5%)	1.94	28/1326 (2.1%)
12	AL	1.54	2/1048 (0.2%)	2.06	39/1394 (2.8%)
13	AM	1.43	1/835 (0.1%)	2.03	27/1127 (2.4%)
14	AN	1.53	5/982 (0.5%)	1.98	26/1323 (2.0%)
15	AO	1.52	2/969 (0.2%)	2.34	41/1300 (3.2%)
16	AP	1.47	2/919 (0.2%)	2.23	25/1226 (2.0%)
17	AQ	1.48	1/817 (0.1%)	2.06	30/1088 (2.8%)
18	AR	1.52	0/724	2.00	27/966 (2.8%)
19	AS	1.54	4/659 (0.6%)	2.11	21/884 (2.4%)
20	AT	1.56	2/681 (0.3%)	1.87	11/913 (1.2%)
21	AU	1.61	2/637 (0.3%)	2.24	27/851 (3.2%)
22	AV	1.45	4/744 (0.5%)	1.88	16/995 (1.6%)
23	AW	1.41	2/676 (0.3%)	1.66	7/895 (0.8%)
24	AX	1.56	2/598 (0.3%)	2.09	22/792 (2.8%)
25	BA	3.06	310/2869 (10.8%)	3.49	627/4474 (14.0%)
26	BB	3.07	7266/69257 (10.5%)	3.53	15668/108040 (14.5%)
27	BC	1.46	6/1748 (0.3%)	1.80	32/2355 (1.4%)
28	BD	1.54	14/2131 (0.7%)	1.94	53/2863 (1.9%)
29	BE	1.53	3/1586 (0.2%)	1.90	32/2134 (1.5%)
30	BF	1.46	7/1571 (0.4%)	2.00	43/2113 (2.0%)
31	BG	1.53	5/1444 (0.3%)	1.95	36/1937 (1.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	BH	1.45	3/1343 (0.2%)	1.88	31/1816 (1.7%)
33	BI	1.49	0/1122	1.97	30/1515 (2.0%)
34	BJ	1.53	6/1247 (0.5%)	1.94	35/1679 (2.1%)
35	BK	1.44	1/1046 (0.1%)	1.79	14/1410 (1.0%)
36	BL	1.54	6/1152 (0.5%)	1.93	29/1551 (1.9%)
37	BM	1.48	4/956 (0.4%)	1.93	27/1279 (2.1%)
38	BN	1.58	5/1062 (0.5%)	2.01	28/1413 (2.0%)
39	BO	1.54	4/1093 (0.4%)	2.04	35/1460 (2.4%)
40	BP	1.51	4/1021 (0.4%)	1.90	23/1364 (1.7%)
41	BQ	1.55	4/910 (0.4%)	2.05	22/1219 (1.8%)
42	BR	1.55	3/929 (0.3%)	2.15	32/1242 (2.6%)
43	BS	1.53	5/960 (0.5%)	2.10	34/1278 (2.7%)
44	BT	1.56	3/829 (0.4%)	1.93	17/1107 (1.5%)
45	BU	1.40	1/864 (0.1%)	1.89	21/1156 (1.8%)
46	BV	1.55	3/794 (0.4%)	2.06	19/1060 (1.8%)
47	BW	1.51	4/797 (0.5%)	1.86	18/1062 (1.7%)
48	BX	1.49	4/766 (0.5%)	1.82	17/1025 (1.7%)
49	BY	1.54	3/642 (0.5%)	1.90	17/848 (2.0%)
50	BZ	1.49	0/635	2.10	24/848 (2.8%)
51	B0	1.49	1/510 (0.2%)	1.95	10/677 (1.5%)
52	B1	1.46	3/453 (0.7%)	1.77	12/605 (2.0%)
53	B2	1.56	4/559 (0.7%)	1.96	10/745 (1.3%)
54	B3	1.53	2/450 (0.4%)	2.12	19/599 (3.2%)
55	B4	1.49	1/448 (0.2%)	1.90	7/594 (1.2%)
56	B5	1.52	1/380 (0.3%)	2.36	24/498 (4.8%)
57	B6	1.52	3/513 (0.6%)	1.68	6/676 (0.9%)
58	B7	1.41	2/303 (0.7%)	2.14	10/397 (2.5%)
All	All	2.69	12119/164069 (7.4%)	3.18	27099/244735 (11.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	888
2	AB	0	39
3	AC	0	23
4	AD	0	34
5	AE	0	6
6	AF	0	8
7	AG	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	AH	0	5
9	AI	0	11
10	AJ	0	6
11	AK	0	3
12	AL	0	5
13	AM	0	4
14	AN	0	5
15	AO	0	2
16	AP	0	3
17	AQ	0	1
19	AS	0	3
20	AT	0	1
21	AU	0	6
23	AW	0	2
24	AX	0	1
25	BA	0	71
26	BB	0	1680
27	BC	0	4
28	BD	0	11
29	BE	0	7
30	BF	0	6
31	BG	0	8
32	BH	0	3
34	BJ	0	6
36	BL	0	6
37	BM	0	3
38	BN	0	3
39	BO	0	2
40	BP	0	6
41	BQ	0	4
42	BR	0	4
43	BS	0	5
44	BT	0	1
45	BU	0	3
47	BW	0	2
48	BX	0	3
49	BY	0	5
50	BZ	0	4
51	B0	0	2
52	B1	0	2
53	B2	0	1
55	B4	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
56	B5	0	1
57	B6	0	3
58	B7	0	1
All	All	0	2927

The worst 5 of 12119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1076	U	C2-N3	18.65	1.50	1.37
26	BB	757	G	P-O5’	16.91	1.76	1.59
25	BA	50	A	N7-C5	16.16	1.49	1.39
26	BB	2569	G	P-O5’	16.09	1.75	1.59
26	BB	1039	A	N7-C5	-15.99	1.29	1.39

The worst 5 of 27099 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	AO	55	ARG	NE-CZ-NH2	-27.98	106.31	120.30
26	BB	2063	C	N3-C4-C5	-21.69	113.22	121.90
26	BB	2163	A	O4’-C1’-N9	21.36	125.29	108.20
26	BB	337	C	O4’-C1’-N1	21.12	125.10	108.20
1	AA	190	A	C8-N9-C4	-20.93	97.43	105.80

There are no chirality outliers.

5 of 2927 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	3	A	Sidechain
1	AA	4	U	Sidechain
1	AA	6	G	Sidechain
1	AA	7	A	Sidechain
1	AA	9	G	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	33089	0	16610	0	0
2	AB	1627	0	843	0	0
3	AC	993	0	497	0	0
4	AD	1641	0	841	0	0
5	AE	1872	0	1885	0	0
6	AF	1822	0	1913	0	0
7	AG	1643	0	1710	0	0
8	AH	1225	0	1273	0	0
9	AI	1101	0	1050	0	0
10	AJ	1400	0	1449	0	0
11	AK	979	0	1034	0	0
12	AL	1036	0	1084	0	0
13	AM	825	0	865	0	0
14	AN	965	0	997	0	0
15	AO	955	0	1019	0	0
16	AP	910	0	981	0	0
17	AQ	805	0	847	0	0
18	AR	716	0	742	0	0
19	AS	649	0	666	0	0
20	AT	672	0	716	0	0
21	AU	626	0	651	0	0
22	AV	727	0	769	0	0
23	AW	670	0	722	0	0
24	AX	590	0	631	0	0
25	BA	2566	0	1302	0	0
26	BB	62351	0	31246	0	0
27	BC	1733	0	1824	0	0
28	BD	2092	0	2170	0	0
29	BE	1565	0	1616	0	0
30	BF	1552	0	1619	0	0
31	BG	1420	0	1460	0	0
32	BH	1323	0	1374	0	0
33	BI	1111	0	1148	0	0
34	BJ	1233	0	1283	0	0
35	BK	1032	0	1088	0	0
36	BL	1129	0	1162	0	0
37	BM	947	0	1023	0	0
38	BN	1053	0	1129	0	0
39	BO	1074	0	1157	0	0
40	BP	1008	0	1045	0	0
41	BQ	900	0	935	0	0
42	BR	917	0	965	0	0
43	BS	947	0	1022	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BT	816	0	839	0	0
45	BU	857	0	922	0	0
46	BV	787	0	846	0	0
47	BW	789	0	847	0	0
48	BX	753	0	780	0	0
49	BY	634	0	656	0	0
50	BZ	625	0	655	0	0
51	B0	509	0	543	0	0
52	B1	449	0	491	0	0
53	B2	549	0	552	0	0
54	B3	444	0	461	0	0
55	B4	441	0	485	0	0
56	B5	377	0	418	0	0
57	B6	504	0	574	0	0
58	B7	302	0	343	0	0
59	AB	14	0	9	0	0
60	BB	10	0	10	0	0
All	All	152351	0	103794	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	238/240 (99%)	221 (93%)	13 (6%)	4 (2%)	9	42
6	AF	230/232 (99%)	200 (87%)	25 (11%)	5 (2%)	6	35
7	AG	203/205 (99%)	180 (89%)	18 (9%)	5 (2%)	5	32
8	AH	164/166 (99%)	141 (86%)	19 (12%)	4 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AI	133/135 (98%)	118 (89%)	11 (8%)	4 (3%)	4	28
10	AJ	176/178 (99%)	164 (93%)	11 (6%)	1 (1%)	25	66
11	AK	127/129 (98%)	114 (90%)	11 (9%)	2 (2%)	9	44
12	AL	127/129 (98%)	109 (86%)	17 (13%)	1 (1%)	19	60
13	AM	101/103 (98%)	90 (89%)	7 (7%)	4 (4%)	3	23
14	AN	126/128 (98%)	105 (83%)	18 (14%)	3 (2%)	6	33
15	AO	121/123 (98%)	102 (84%)	16 (13%)	3 (2%)	5	32
16	AP	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	17	57
17	AQ	98/100 (98%)	84 (86%)	10 (10%)	4 (4%)	3	23
18	AR	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
19	AS	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	5	32
20	AT	81/83 (98%)	71 (88%)	10 (12%)	0	100	100
21	AU	72/74 (97%)	63 (88%)	6 (8%)	3 (4%)	3	22
22	AV	89/91 (98%)	78 (88%)	10 (11%)	1 (1%)	14	52
23	AW	84/86 (98%)	79 (94%)	4 (5%)	1 (1%)	13	50
24	AX	68/70 (97%)	55 (81%)	9 (13%)	4 (6%)	1	17
27	BC	232/234 (99%)	208 (90%)	20 (9%)	4 (2%)	9	42
28	BD	270/272 (99%)	227 (84%)	37 (14%)	6 (2%)	6	35
29	BE	207/209 (99%)	171 (83%)	25 (12%)	11 (5%)	2	19
30	BF	199/201 (99%)	167 (84%)	26 (13%)	6 (3%)	4	28
31	BG	176/178 (99%)	144 (82%)	19 (11%)	13 (7%)	1	14
32	BH	174/176 (99%)	149 (86%)	16 (9%)	9 (5%)	2	19
33	BI	147/149 (99%)	132 (90%)	12 (8%)	3 (2%)	7	38
34	BJ	162/164 (99%)	140 (86%)	16 (10%)	6 (4%)	3	24
35	BK	139/141 (99%)	128 (92%)	9 (6%)	2 (1%)	11	46
36	BL	140/142 (99%)	118 (84%)	18 (13%)	4 (3%)	4	29
37	BM	121/123 (98%)	102 (84%)	14 (12%)	5 (4%)	3	23
38	BN	142/144 (99%)	113 (80%)	25 (18%)	4 (3%)	5	30
39	BO	134/136 (98%)	120 (90%)	13 (10%)	1 (1%)	22	63
40	BP	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
41	BQ	115/117 (98%)	103 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BR	112/114 (98%)	90 (80%)	16 (14%)	6 (5%)	2	19
43	BS	115/117 (98%)	105 (91%)	7 (6%)	3 (3%)	5	31
44	BT	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	15	55
45	BU	108/110 (98%)	100 (93%)	4 (4%)	4 (4%)	3	24
46	BV	98/100 (98%)	85 (87%)	12 (12%)	1 (1%)	15	55
47	BW	101/103 (98%)	84 (83%)	15 (15%)	2 (2%)	7	38
48	BX	92/94 (98%)	79 (86%)	11 (12%)	2 (2%)	6	35
49	BY	82/84 (98%)	64 (78%)	15 (18%)	3 (4%)	3	24
50	BZ	75/77 (97%)	63 (84%)	9 (12%)	3 (4%)	3	23
51	B0	61/63 (97%)	53 (87%)	6 (10%)	2 (3%)	4	26
52	B1	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
53	B2	68/70 (97%)	51 (75%)	12 (18%)	5 (7%)	1	14
54	B3	54/56 (96%)	38 (70%)	14 (26%)	2 (4%)	3	24
55	B4	52/54 (96%)	47 (90%)	4 (8%)	1 (2%)	8	38
56	B5	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	6	34
57	B6	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
58	B7	36/38 (95%)	28 (78%)	6 (17%)	2 (6%)	2	19
All	All	6319/6423 (98%)	5497 (87%)	658 (10%)	164 (3%)	8	31

5 of 164 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	84	LEU
5	AE	93	HIS
7	AG	3	TYR
8	AH	77	ASN
9	AI	99	ALA

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	
5	AE	198/198 (100%)	193 (98%)	5 (2%)	47	68
6	AF	189/189 (100%)	181 (96%)	8 (4%)	30	54
7	AG	172/172 (100%)	164 (95%)	8 (5%)	26	51
8	AH	125/125 (100%)	121 (97%)	4 (3%)	39	61
9	AI	116/116 (100%)	110 (95%)	6 (5%)	23	48
10	AJ	146/146 (100%)	140 (96%)	6 (4%)	30	55
11	AK	104/104 (100%)	98 (94%)	6 (6%)	20	45
12	AL	106/106 (100%)	103 (97%)	3 (3%)	43	65
13	AM	90/90 (100%)	84 (93%)	6 (7%)	16	41
14	AN	98/98 (100%)	94 (96%)	4 (4%)	30	55
15	AO	103/103 (100%)	100 (97%)	3 (3%)	42	64
16	AP	95/95 (100%)	90 (95%)	5 (5%)	22	47
17	AQ	83/83 (100%)	80 (96%)	3 (4%)	35	59
18	AR	76/76 (100%)	75 (99%)	1 (1%)	69	81
19	AS	65/65 (100%)	63 (97%)	2 (3%)	40	62
20	AT	77/77 (100%)	73 (95%)	4 (5%)	23	48
21	AU	64/64 (100%)	59 (92%)	5 (8%)	12	36
22	AV	78/78 (100%)	71 (91%)	7 (9%)	9	30
23	AW	65/65 (100%)	64 (98%)	1 (2%)	65	80
24	AX	60/60 (100%)	58 (97%)	2 (3%)	38	61
27	BC	181/181 (100%)	172 (95%)	9 (5%)	24	49
28	BD	217/217 (100%)	204 (94%)	13 (6%)	19	44
29	BE	164/164 (100%)	150 (92%)	14 (8%)	10	33
30	BF	165/165 (100%)	154 (93%)	11 (7%)	16	41
31	BG	149/149 (100%)	138 (93%)	11 (7%)	13	38
32	BH	137/137 (100%)	129 (94%)	8 (6%)	20	45
33	BI	114/114 (100%)	108 (95%)	6 (5%)	22	47
34	BJ	122/122 (100%)	116 (95%)	6 (5%)	25	50
35	BK	109/109 (100%)	105 (96%)	4 (4%)	34	58
36	BL	116/116 (100%)	113 (97%)	3 (3%)	46	66
37	BM	104/104 (100%)	101 (97%)	3 (3%)	42	64
38	BN	103/103 (100%)	96 (93%)	7 (7%)	16	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BO	109/109 (100%)	106 (97%)	3 (3%)	43	65
40	BP	103/103 (100%)	98 (95%)	5 (5%)	25	50
41	BQ	87/87 (100%)	84 (97%)	3 (3%)	37	60
42	BR	99/99 (100%)	93 (94%)	6 (6%)	18	44
43	BS	89/89 (100%)	87 (98%)	2 (2%)	52	71
44	BT	84/84 (100%)	79 (94%)	5 (6%)	19	44
45	BU	93/93 (100%)	90 (97%)	3 (3%)	39	61
46	BV	84/84 (100%)	77 (92%)	7 (8%)	11	34
47	BW	84/84 (100%)	80 (95%)	4 (5%)	25	51
48	BX	78/78 (100%)	73 (94%)	5 (6%)	17	42
49	BY	62/62 (100%)	60 (97%)	2 (3%)	39	61
50	BZ	67/67 (100%)	63 (94%)	4 (6%)	19	44
51	B0	55/55 (100%)	52 (94%)	3 (6%)	21	47
52	B1	48/48 (100%)	46 (96%)	2 (4%)	30	54
53	B2	62/62 (100%)	57 (92%)	5 (8%)	11	35
54	B3	47/47 (100%)	46 (98%)	1 (2%)	53	72
55	B4	48/48 (100%)	48 (100%)	0	100	100
56	B5	38/38 (100%)	37 (97%)	1 (3%)	46	66
57	B6	51/51 (100%)	48 (94%)	3 (6%)	19	45
58	B7	34/34 (100%)	33 (97%)	1 (3%)	42	64
All	All	5213/5213 (100%)	4964 (95%)	249 (5%)	29	51

5 of 249 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	BE	46	ARG
47	BW	98	ASN
31	BG	111	ARG
47	BW	81	ARG
52	B1	16	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1538/1542 (99%)	287 (18%)	93 (6%)
2	AB	74/76 (97%)	23 (31%)	7 (9%)
25	BA	119/120 (99%)	20 (16%)	13 (10%)
26	BB	2898/2904 (99%)	536 (18%)	180 (6%)
3	AC	47/47 (100%)	26 (55%)	14 (29%)
4	AD	76/77 (98%)	13 (17%)	4 (5%)
All	All	4752/4766 (99%)	905 (19%)	311 (6%)

5 of 905 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	6	G
1	AA	32	A
1	AA	36	C
1	AA	48	C

5 of 311 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BB	1697	G
26	BB	2500	U
26	BB	1786	A
26	BB	2129	C
26	BB	2756	U

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

49 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
1	5MC	AA	967	1	18,22,23	1.32	2 (11%)	26,32,35	1.20	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	OMG	BB	2251	26	18,26,27	1.53	4 (22%)	19,38,41	1.54	2 (10%)
2	OMC	AB	32	2	19,22,23	1.49	4 (21%)	26,31,34	1.62	5 (19%)
4	OMC	AD	33	4	19,22,23	1.46	3 (15%)	26,31,34	1.38	5 (19%)
2	MIA	AB	37	2	24,31,32	1.68	3 (12%)	26,44,47	3.01	9 (34%)
26	3TD	BB	1915	26	18,22,23	1.84	6 (33%)	22,32,35	1.17	0
26	PSU	BB	2457	26	18,21,22	1.12	2 (11%)	22,30,33	2.40	9 (40%)
26	CH	BB	2575	26	16,21,22	1.54	3 (18%)	20,30,33	2.28	7 (35%)
1	MA6	AA	1518	1	19,26,27	1.93	6 (31%)	18,38,41	1.83	4 (22%)
26	6MZ	BB	1618	26	18,25,26	1.85	4 (22%)	16,36,39	2.35	4 (25%)
4	PSU	AD	56	4	18,21,22	1.81	6 (33%)	22,30,33	1.33	3 (13%)
2	H2U	AB	17	2	18,21,22	1.35	3 (16%)	21,30,33	2.11	3 (14%)
1	2MG	AA	1516	1	18,26,27	2.19	8 (44%)	16,38,41	1.27	3 (18%)
1	5MC	AA	1407	1	18,22,23	1.44	2 (11%)	26,32,35	1.96	5 (19%)
2	H2U	AB	16	2	18,21,22	1.42	1 (5%)	21,30,33	1.89	7 (33%)
2	H2U	AB	20	2	18,21,22	1.49	3 (16%)	21,30,33	1.55	4 (19%)
26	PSU	BB	1917	26	18,21,22	1.45	3 (16%)	22,30,33	1.53	4 (18%)
26	5MC	BB	1962	26	18,22,23	1.70	6 (33%)	26,32,35	1.66	6 (23%)
26	6MZ	BB	2030	26	18,25,26	1.03	1 (5%)	16,36,39	1.54	3 (18%)
26	2MA	BB	2503	26	17,25,26	2.08	7 (41%)	17,37,40	1.27	1 (5%)
2	PSU	AB	55	2	18,21,22	1.49	3 (16%)	22,30,33	2.26	7 (31%)
1	4OC	AA	1402	-	20,23,24	1.32	3 (15%)	26,32,35	1.45	4 (15%)
1	PSU	AA	516	1	18,21,22	1.39	3 (16%)	22,30,33	2.88	7 (31%)
26	2MG	BB	1835	26	18,26,27	1.59	3 (16%)	16,38,41	1.97	5 (31%)
26	PSU	BB	2504	26	18,21,22	1.38	3 (16%)	22,30,33	1.87	7 (31%)
26	PSU	BB	1911	26	18,21,22	1.54	4 (22%)	22,30,33	2.16	3 (13%)
1	7MG	AA	527	1	22,26,27	4.13	6 (27%)	29,39,42	2.04	6 (20%)
1	UR3	AA	1498	1	19,22,23	1.12	1 (5%)	26,32,35	1.55	6 (23%)
26	PSU	BB	746	26	18,21,22	2.32	8 (44%)	22,30,33	2.14	8 (36%)
1	2MG	AA	966	1	18,26,27	1.34	3 (16%)	16,38,41	2.60	5 (31%)
4	H2U	AD	21	4	18,21,22	1.38	3 (16%)	21,30,33	2.19	5 (23%)
4	5MU	AD	55	4	19,22,23	1.33	4 (21%)	28,32,35	2.14	6 (21%)
26	2MG	BB	2445	26	18,26,27	2.20	6 (33%)	16,38,41	2.89	5 (31%)
4	4SU	AD	8	4	18,21,22	1.76	4 (22%)	26,30,33	2.03	7 (26%)
26	OMC	BB	2498	26	19,22,23	1.19	2 (10%)	26,31,34	1.34	3 (11%)
26	PSU	BB	2580	26	18,21,22	1.49	2 (11%)	22,30,33	1.75	9 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
26	5MU	BB	747	26	19,22,23	1.17	1 (5%)	28,32,35	1.62	7 (25%)
26	PSU	BB	2605	26	18,21,22	1.67	4 (22%)	22,30,33	1.75	3 (13%)
26	OMU	BB	2552	26	19,22,23	1.50	4 (21%)	26,31,34	2.10	8 (30%)
26	H2U	BB	2449	26	18,21,22	1.61	3 (16%)	21,30,33	1.77	4 (19%)
2	7MG	AB	46	2	22,26,27	4.77	5 (22%)	29,39,42	1.93	7 (24%)
2	4SU	AB	8	2	18,21,22	1.71	2 (11%)	26,30,33	1.95	5 (19%)
2	5MU	AB	54	2	19,22,23	0.95	1 (5%)	28,32,35	1.49	6 (21%)
26	1MG	BB	745	26	18,26,27	1.84	3 (16%)	19,39,42	1.81	6 (31%)
26	5MU	BB	1939	26	19,22,23	1.43	4 (21%)	28,32,35	2.03	11 (39%)
1	2MG	AA	1207	1	18,26,27	1.84	2 (11%)	16,38,41	1.37	1 (6%)
26	7MG	BB	2069	26	22,26,27	4.26	4 (18%)	29,39,42	1.87	7 (24%)
26	PSU	BB	955	26	18,21,22	1.70	3 (16%)	22,30,33	1.37	3 (13%)
1	MA6	AA	1519	1	19,26,27	1.59	4 (21%)	18,38,41	1.79	8 (44%)

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
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
26	OMG	BB	2251	26	-	0/5/27/28	0/3/3/3
2	OMC	AB	32	2	-	0/9/27/28	0/2/2/2
4	OMC	AD	33	4	-	0/9/27/28	0/2/2/2
2	MIA	AB	37	2	-	0/11/33/34	0/3/3/3
26	3TD	BB	1915	26	-	2/7/25/26	0/2/2/2
26	PSU	BB	2457	26	-	0/7/25/26	0/2/2/2
26	CH	BB	2575	26	-	0/5/25/26	0/2/2/2
1	MA6	AA	1518	1	-	2/7/29/30	0/3/3/3
26	6MZ	BB	1618	26	-	1/5/27/28	0/3/3/3
4	PSU	AD	56	4	-	0/7/25/26	0/2/2/2
2	H2U	AB	17	2	-	1/7/38/39	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
2	H2U	AB	16	2	-	0/7/38/39	0/2/2/2
2	H2U	AB	20	2	-	0/7/38/39	0/2/2/2
26	PSU	BB	1917	26	-	3/7/25/26	0/2/2/2
26	5MC	BB	1962	26	-	1/7/25/26	0/2/2/2
26	6MZ	BB	2030	26	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	2MA	BB	2503	26	-	0/3/25/26	0/3/3/3
2	PSU	AB	55	2	-	1/7/25/26	0/2/2/2
1	4OC	AA	1402	-	-	0/9/29/30	0/2/2/2
1	PSU	AA	516	1	-	0/7/25/26	0/2/2/2
26	2MG	BB	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	BB	2504	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	1911	26	-	1/7/25/26	0/2/2/2
1	7MG	AA	527	1	-	2/7/37/38	0/3/3/3
1	UR3	AA	1498	1	-	2/7/25/26	0/2/2/2
26	PSU	BB	746	26	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
4	H2U	AD	21	4	-	0/7/38/39	0/2/2/2
4	5MU	AD	55	4	-	0/7/25/26	0/2/2/2
26	2MG	BB	2445	26	-	0/5/27/28	0/3/3/3
4	4SU	AD	8	4	-	0/7/25/26	0/2/2/2
26	OMC	BB	2498	26	-	0/9/27/28	0/2/2/2
26	PSU	BB	2580	26	-	5/7/25/26	0/2/2/2
26	5MU	BB	747	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	2605	26	-	0/7/25/26	0/2/2/2
26	OMU	BB	2552	26	-	0/9/27/28	0/2/2/2
26	H2U	BB	2449	26	-	2/7/38/39	0/2/2/2
2	7MG	AB	46	2	-	3/7/37/38	0/3/3/3
2	4SU	AB	8	2	-	5/7/25/26	0/2/2/2
2	5MU	AB	54	2	-	1/7/25/26	0/2/2/2
26	1MG	BB	745	26	-	0/3/25/26	0/3/3/3
26	5MU	BB	1939	26	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	1/5/27/28	0/3/3/3
26	7MG	BB	2069	26	-	0/7/37/38	0/3/3/3
26	PSU	BB	955	26	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3

The worst 5 of 175 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	46	7MG	C8-N9	-20.90	1.34	1.46
26	BB	2069	7MG	C8-N9	-18.88	1.35	1.46
1	AA	527	7MG	C8-N9	-18.03	1.35	1.46
26	BB	955	PSU	C2-N1	6.15	1.45	1.36
26	BB	745	1MG	C8-N7	-6.03	1.24	1.35

The worst 5 of 254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AB	37	MIA	C11-S10-C2	12.41	111.53	102.27
26	BB	2445	2MG	O6-C6-N1	-8.97	110.06	120.65
2	AB	17	H2U	O4'-C1'-N1	8.59	121.00	109.30
1	AA	516	PSU	C6-C5-C4	8.47	124.12	118.20
26	BB	1911	PSU	C6-C5-C4	8.33	124.02	118.20

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1207	2MG	N3-C2-N2-CM2
2	AB	8	4SU	C2'-C1'-N1-C2
2	AB	8	4SU	C2'-C1'-N1-C6
2	AB	46	7MG	C4'-C5'-O5'-P
26	BB	1915	3TD	C2'-C1'-C5-C4

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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	TRP	AB	101	60,2	14,15,16	1.53	2 (14%)	13,20,22	2.28	7 (53%)
60	FME	BB	3001	59	8,9,10	1.63	1 (12%)	7,9,11	2.00	3 (42%)

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	TRP	AB	101	60,2	-	2/5/6/8	0/2/2/2
60	FME	BB	3001	59	-	2/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AB	101	TRP	OXT-C	-3.96	1.25	1.42
60	BB	3001	FME	CA-N	-3.74	1.41	1.46
59	AB	101	TRP	C-CA	2.56	1.56	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	AB	101	TRP	CB-CG-CD1	-3.98	123.06	127.97
60	BB	3001	FME	CG-CB-CA	3.44	122.50	112.95
59	AB	101	TRP	CZ3-CE3-CD2	3.18	125.30	120.89
59	AB	101	TRP	CZ2-CE2-NE1	2.88	138.77	130.80
59	AB	101	TRP	CH2-CZ2-CE2	2.70	123.97	120.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	BB	3001	FME	O1-CN-N-CA
60	BB	3001	FME	CB-CG-SD-CE
59	AB	101	TRP	N-CA-CB-CG
59	AB	101	TRP	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	BB	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BB	1614:A	O3'	1615:C	P	1.76

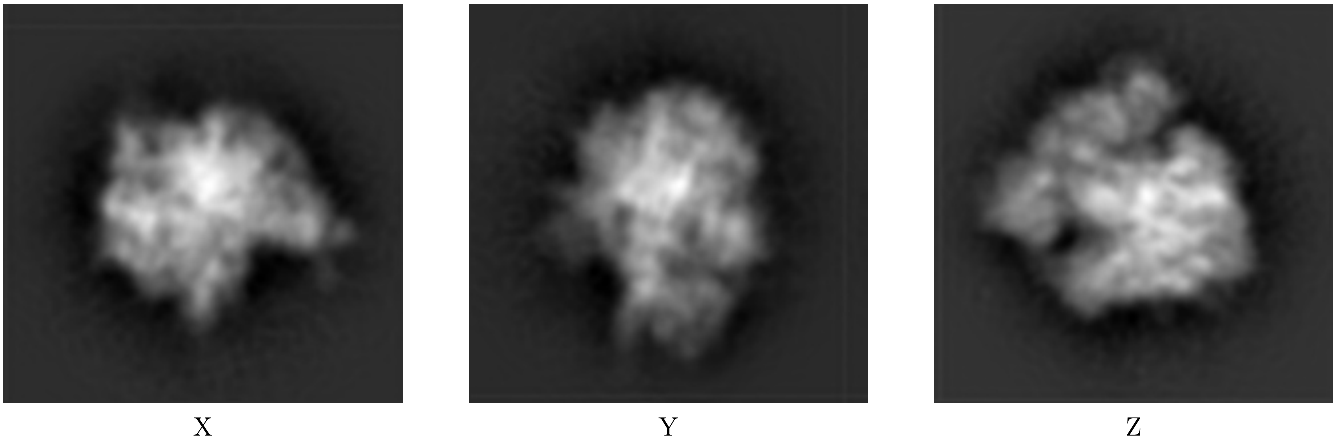
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-5359. 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 ⓘ

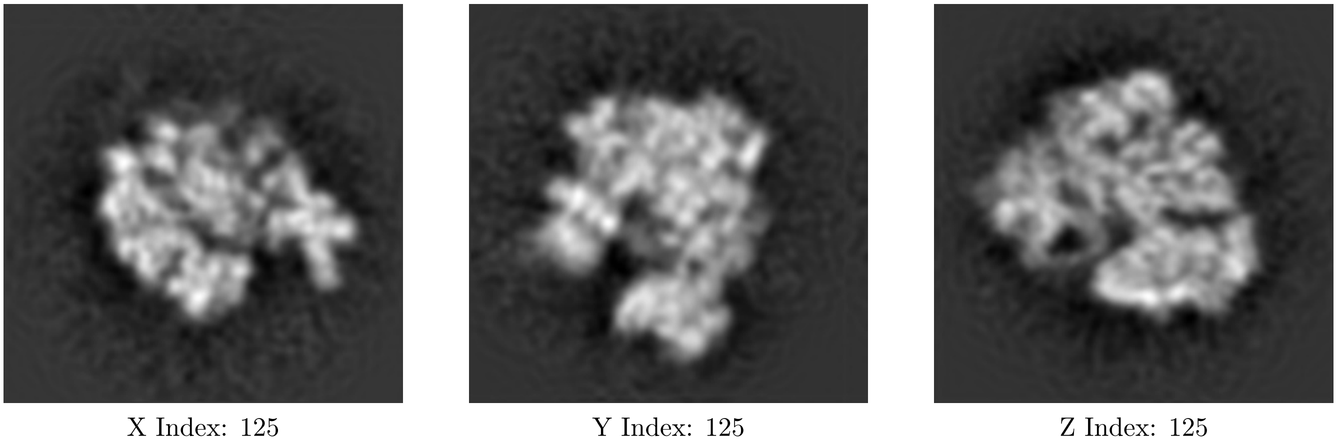
6.1.1 Primary map


X Y Z

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

6.2 Central slices ⓘ

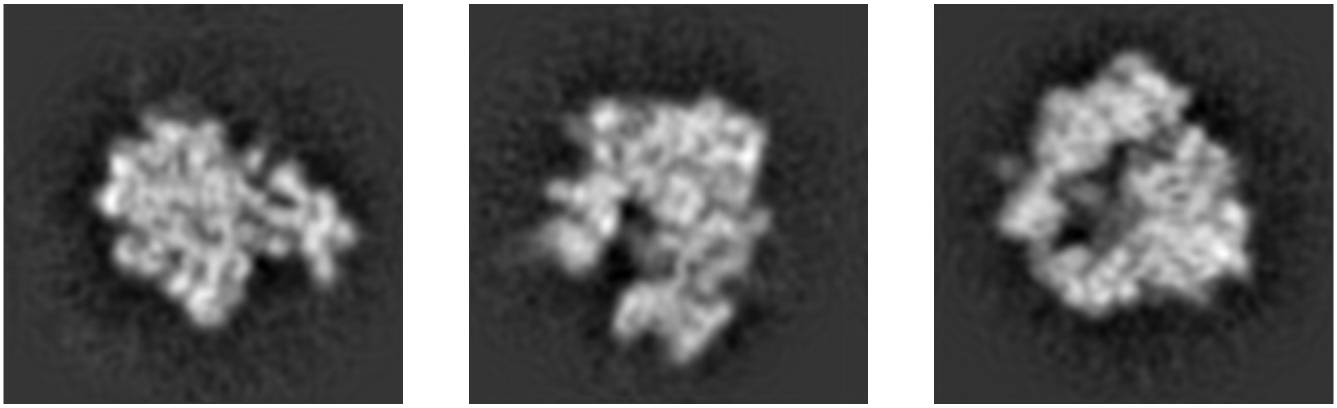
6.2.1 Primary map


X Index: 125 Y Index: 125 Z Index: 125

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

6.3 Largest variance slices (i)

6.3.1 Primary map

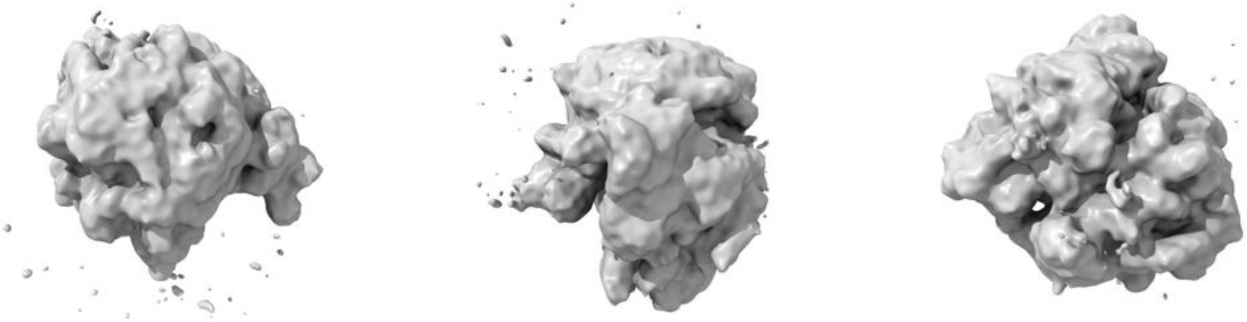


X Index: 131 Y Index: 129 Z Index: 114

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

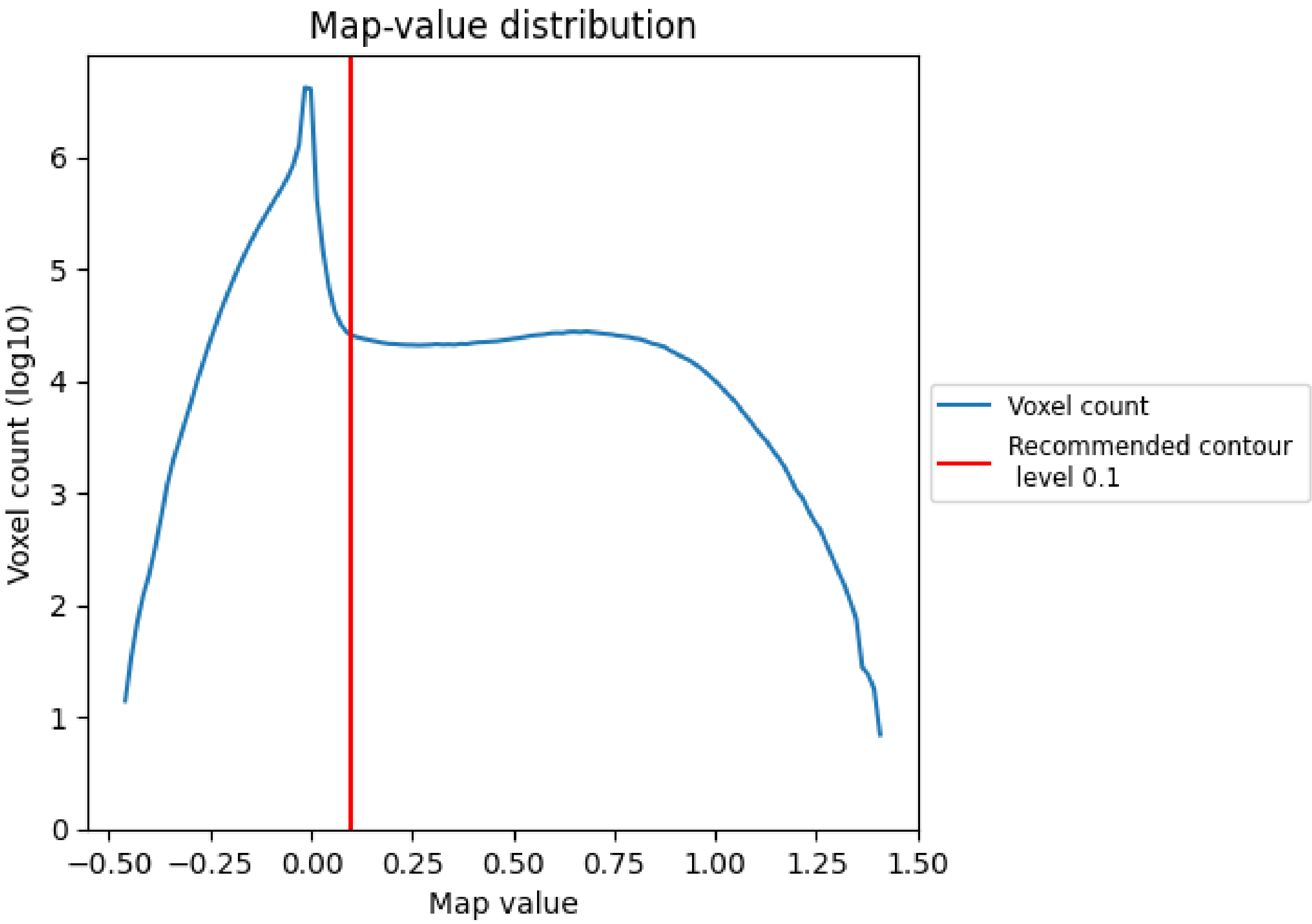
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

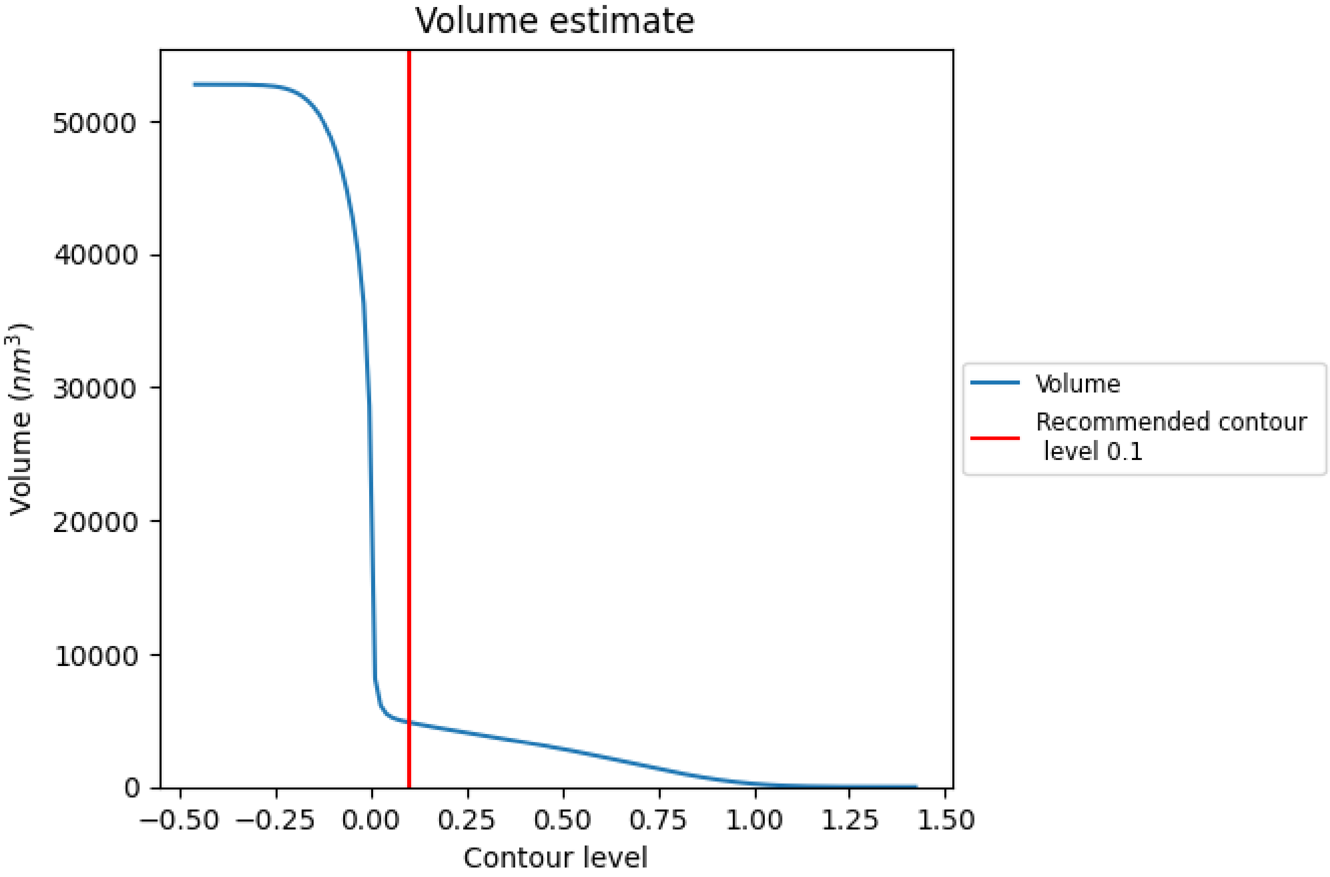
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

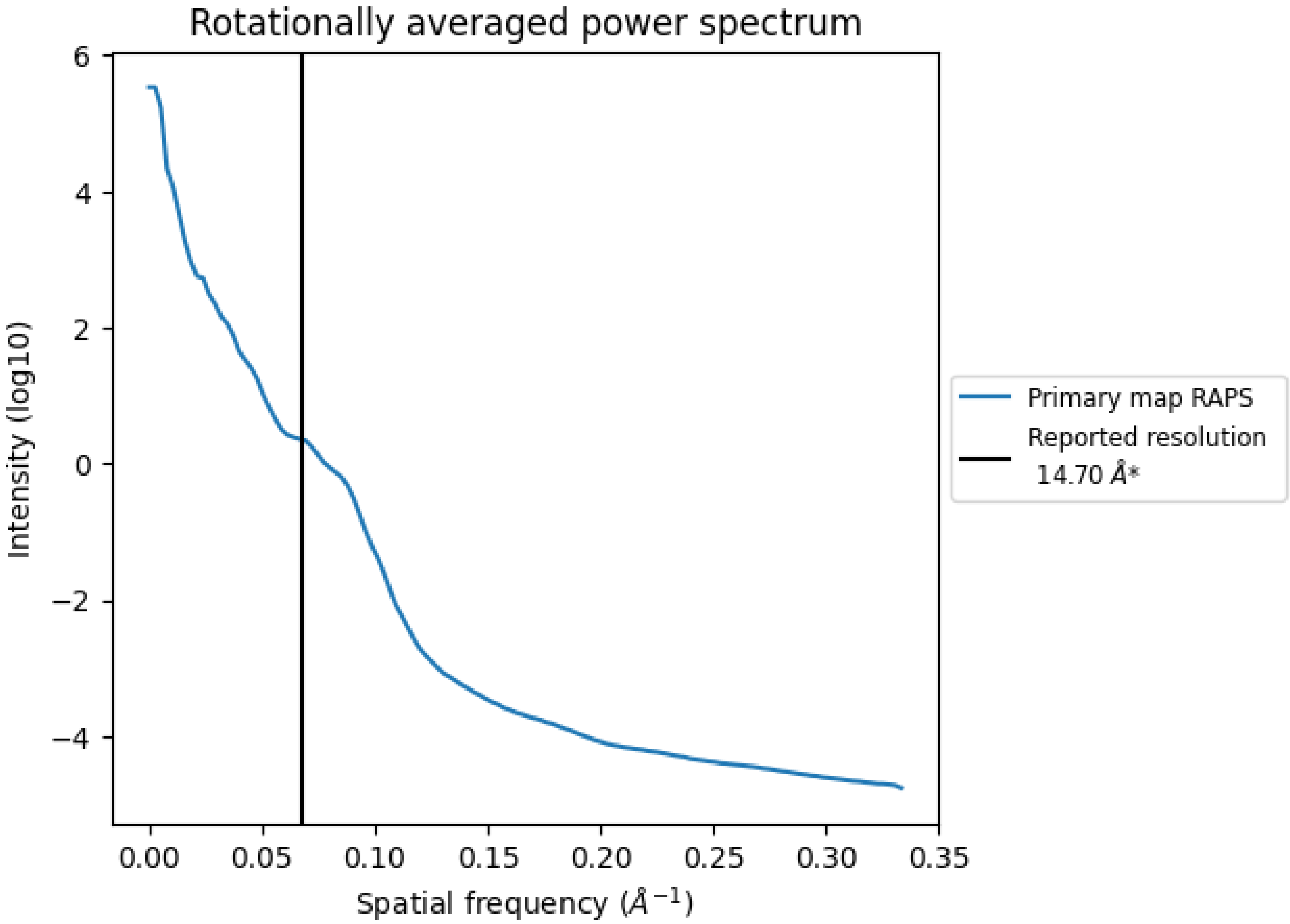
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 4871 nm^3; this corresponds to an approximate mass of 4400 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 0.068 Å^{-1}

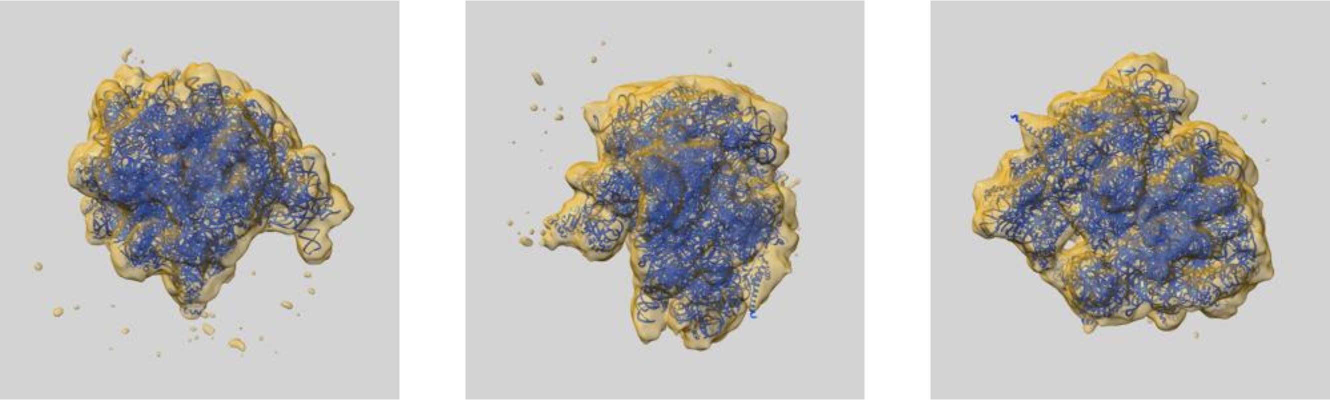
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-5359 and PDB model 4V6O. Per-residue inclusion information can be found in section 3 on page 15.

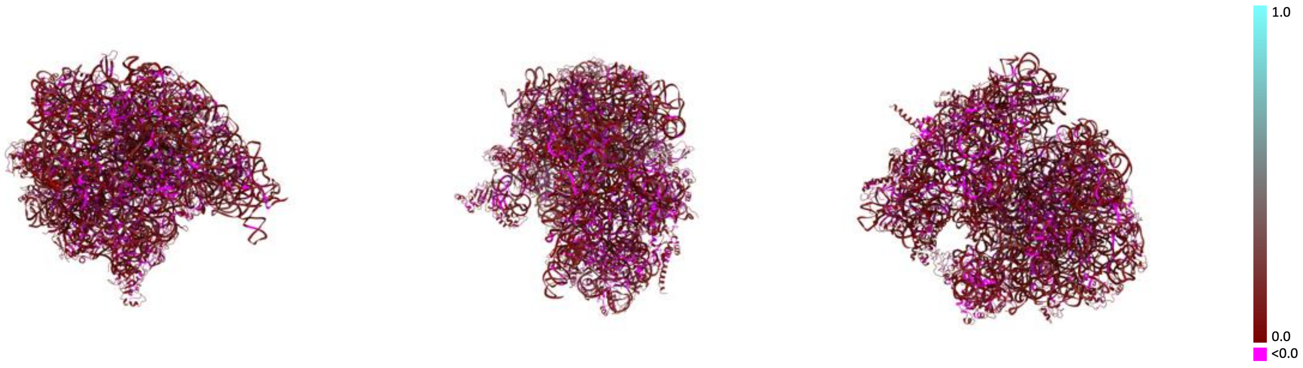
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

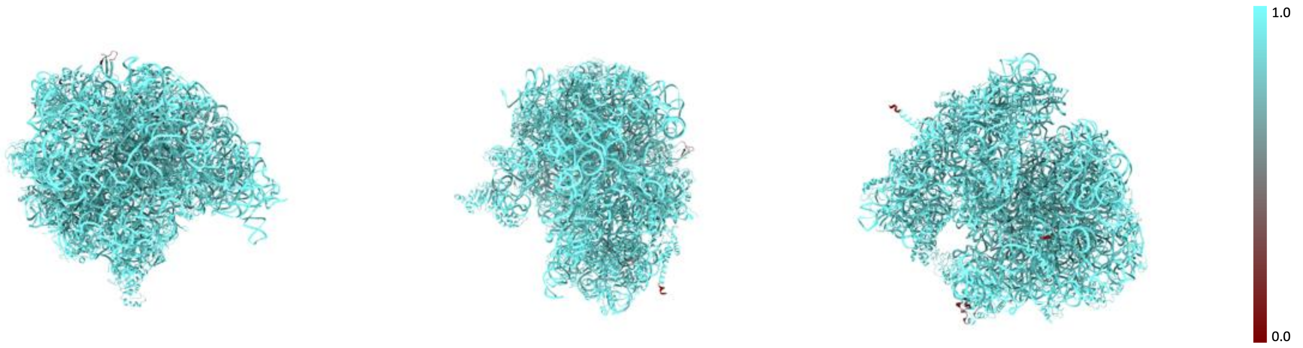
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

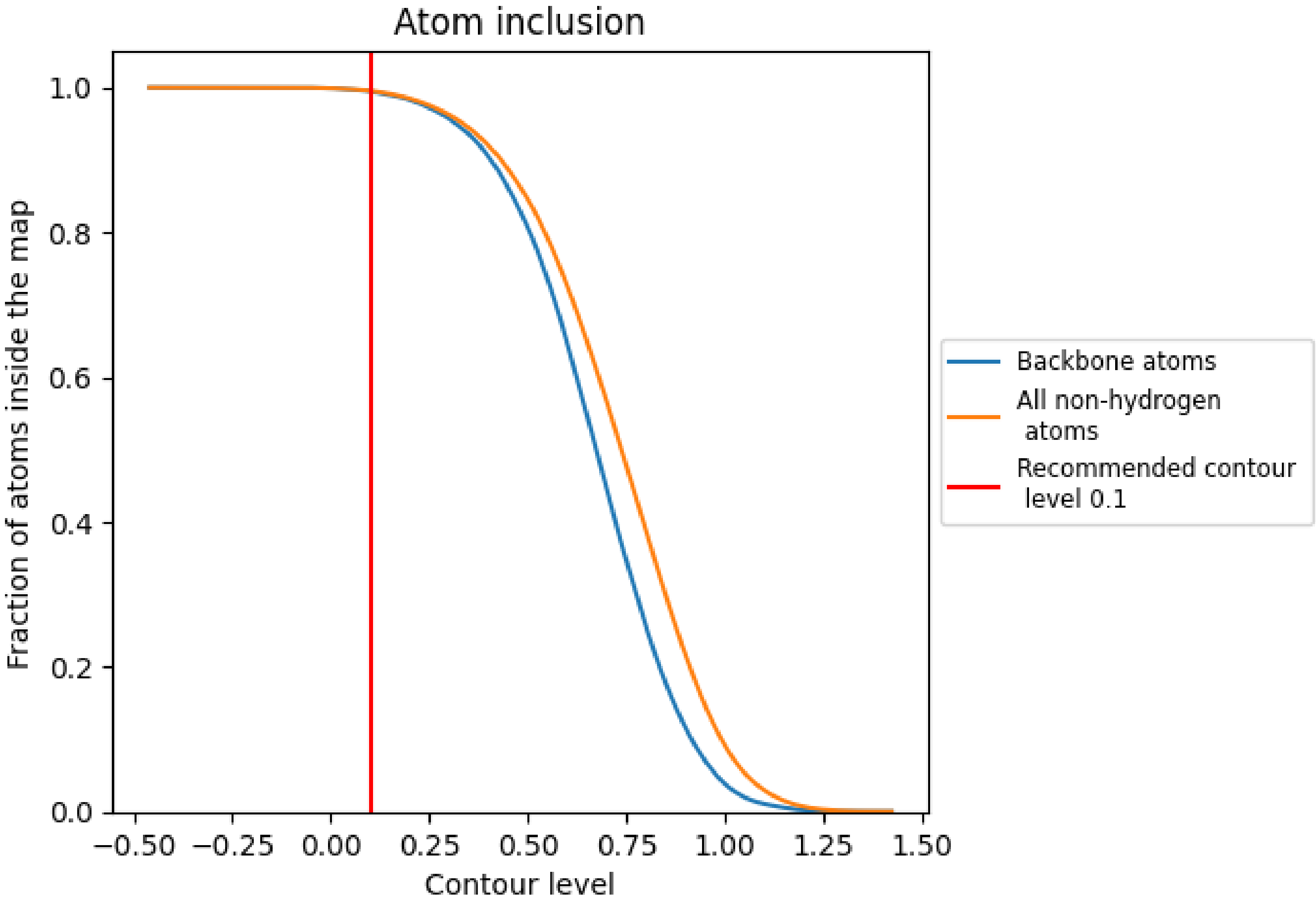
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9954	0.0650
AA	0.9999	0.0830
AB	0.9689	0.0430
AC	0.8943	-0.0220
AD	0.9519	0.0710
AE	0.9669	0.0380
AF	0.9972	0.0560
AG	1.0000	0.0330
AH	0.9975	0.0240
AI	0.9972	0.0450
AJ	1.0000	0.0640
AK	1.0000	0.0190
AL	0.9889	0.0450
AM	1.0000	0.0320
AN	0.9957	0.0540
AO	0.9891	0.0180
AP	0.9977	0.0630
AQ	1.0000	0.0310
AR	1.0000	0.0320
AS	1.0000	0.0250
AT	1.0000	0.0470
AU	1.0000	0.0490
AV	1.0000	0.0290
AW	1.0000	0.0250
AX	0.9982	0.0020
B0	1.0000	0.0290
B1	0.9954	0.0370
B2	0.9963	0.0110
B3	1.0000	0.0300
B4	1.0000	0.0400
B5	1.0000	0.0280
B6	1.0000	0.0010
B7	1.0000	0.0530
BA	1.0000	0.0950
BB	0.9999	0.0830

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Chain	Atom inclusion	Q-score
BC	🟦 0.9104	🟥 0.0280
BD	🟦 1.0000	🟥 0.0180
BE	🟦 0.9993	🟥 0.0270
BF	🟦 1.0000	🟥 0.0500
BG	🟦 1.0000	🟥 0.0610
BH	🟦 0.9992	🟥 0.0300
BI	🟦 0.8796	🟥 0.0350
BJ	🟦 0.9884	🟥 0.0510
BK	🟦 0.9755	🟥 0.0350
BL	🟦 1.0000	🟥 0.0130
BM	🟦 0.9902	🟥 0.0300
BN	🟦 1.0000	🟥 0.0050
BO	🟦 1.0000	🟥 0.0130
BP	🟦 1.0000	🟥 0.0190
BQ	🟦 0.9954	🟥 0.0460
BR	🟦 0.9921	🟥 0.0300
BS	🟦 1.0000	🟥 0.0050
BT	🟦 0.9987	🟥 0.0530
BU	🟦 0.9988	🟥 0.0180
BV	🟦 1.0000	🟥 0.0110
BW	🟦 1.0000	🟥 0.0510
BX	🟦 1.0000	🟥 0.0520
BY	🟦 1.0000	🟪 -0.0050
BZ	🟦 1.0000	🟥 0.0250