Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 03:58 PM EST

PDB ID	:	6VZ2
EMDB ID	:	EMD-21482
Title	:	Escherichia coli transcription-translation complex D1 (TTC-D1) containing mRNA with a 27 nt long spacer, NusG, and fMet-tRNAs at E-site and P-site
Authors	:	Molodtsov, V.; Wang, C.; Su, M.; Ebright, R.H.
Deposited on	:	2020-02-27
Resolution	:	10.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

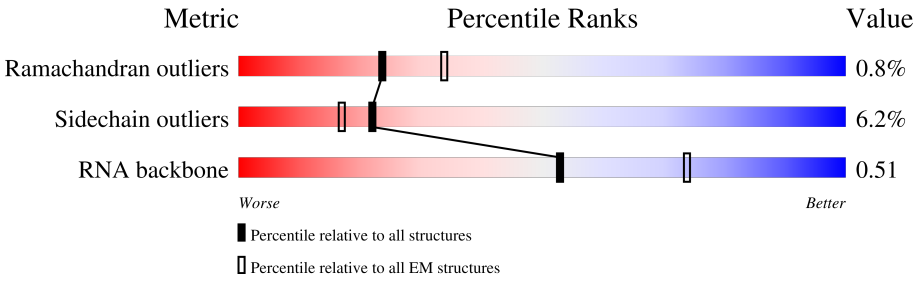
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 10.00 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	0	103	93% 7%
2	1	110	92% 8%
3	2	100	6% 89% 5% 6%
4	3	104	11% 91% 8%
5	4	94	96%
6	5	36	47% 17% 36%
7	6	36	64% 11% 25%
8	7	44	5% 16% 16% 5% 64%

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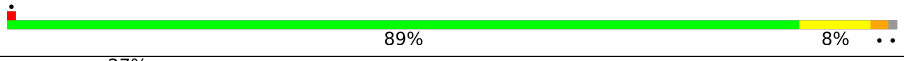
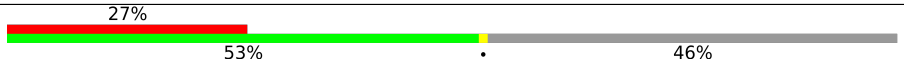
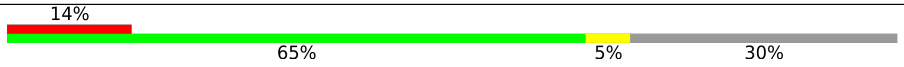
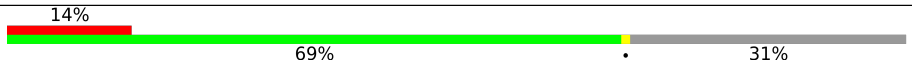
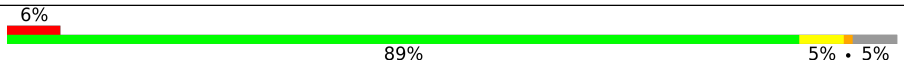
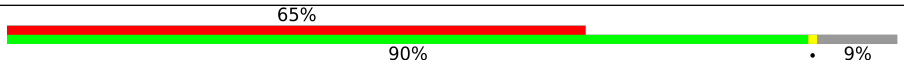
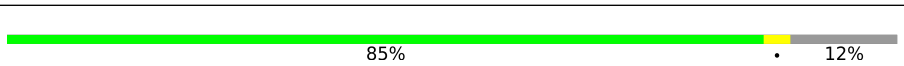
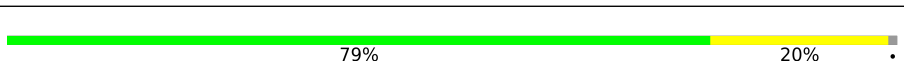
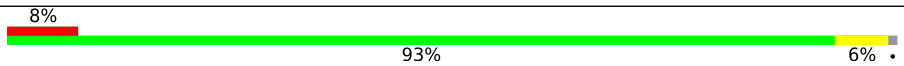
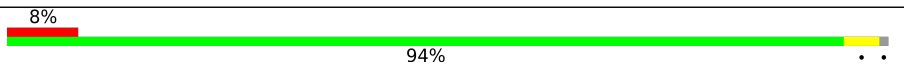
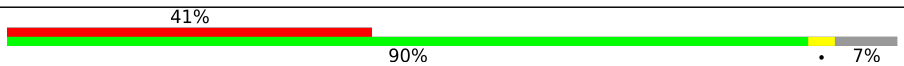
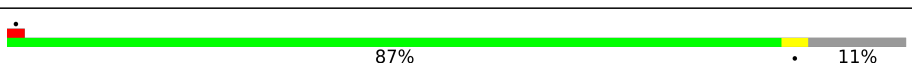
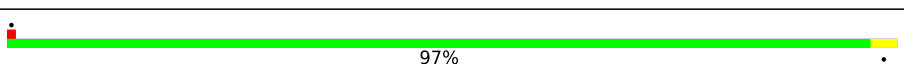
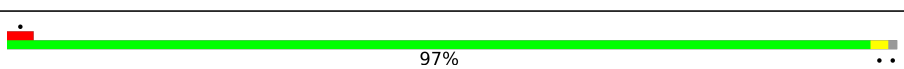
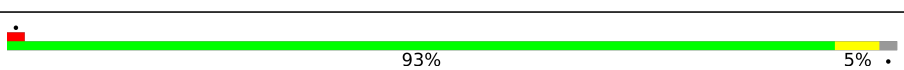
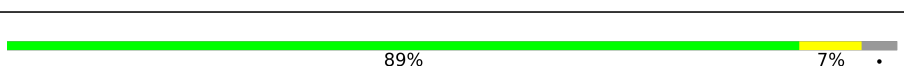
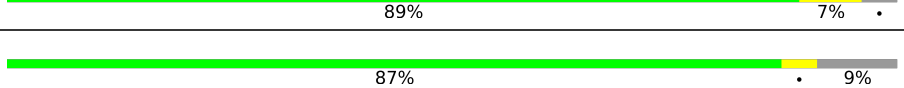
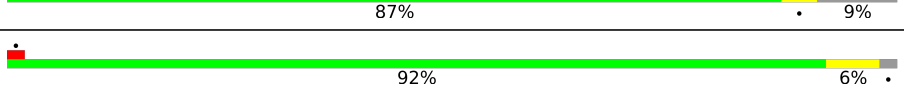
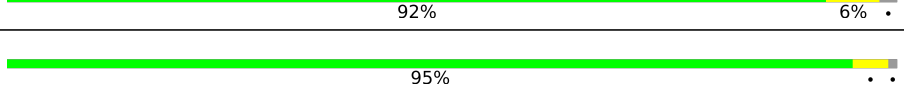
Mol	Chain	Length	Quality of chain
9	A	76	
9	B	76	
10	AA	1342	
11	AB	181	
12	AC	329	
12	AD	329	
13	AE	1407	
14	AF	91	
15	C	75	
16	D	1542	
17	E	87	
18	F	71	
19	G	241	
20	H	557	
21	I	233	
22	J	206	
23	K	167	
24	L	135	
25	M	179	
26	N	130	
27	O	130	
28	P	103	
29	Q	129	
30	R	124	
31	S	101	

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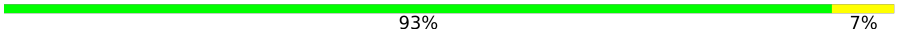
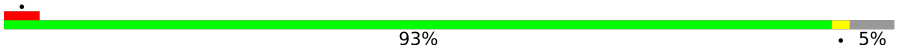
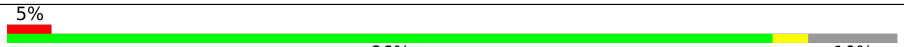
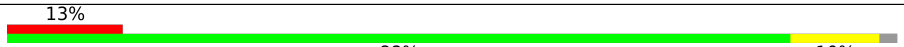
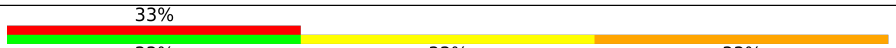
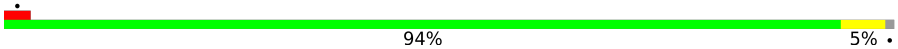
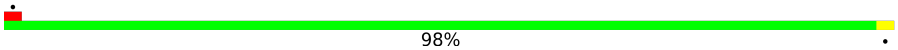
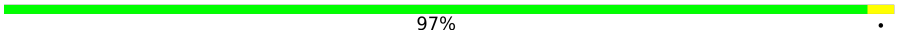
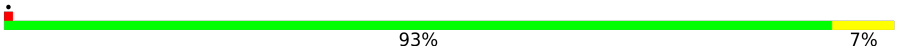
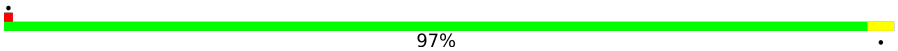
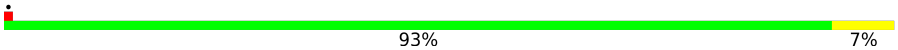
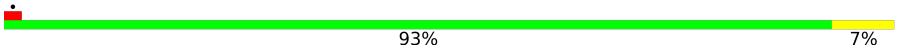
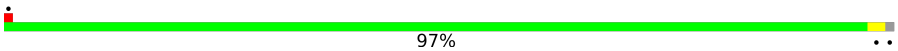
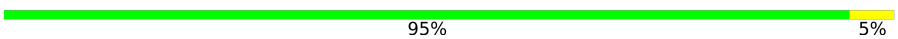
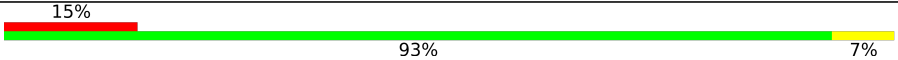
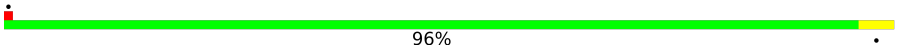
Mol	Chain	Length	Quality of chain
32	T	89	
33	U	82	
34	V	84	
35	W	92	
36	X	118	
37	Y	3	
38	a	2904	
39	b	85	
40	c	78	
41	d	120	
42	e	62	
43	f	58	
44	g	70	
45	h	271	
46	i	56	
47	j	209	
48	k	55	
49	l	201	
50	m	46	
51	n	177	
52	o	64	
53	p	177	
54	q	38	
55	r	149	
56	s	142	

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Mol	Chain	Length	Quality of chain
57	t	123	95% 5%
58	u	144	96%
59	v	136	96%
60	w	127	87% 6% 6%
61	x	117	94% 5%
62	y	115	95%
63	z	118	97%

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 299429 atoms, of which 125494 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 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	94	Total	C	H	N	O	S	0	0
			1557	470	811	140	134	2		

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	103	Total	C	H	N	O	0	0
			1632	498	844	148	142		

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	23	Total	C	H	N	O	P	0	0
			731	225	259	87	137	23		

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	27	Total	C	H	N	O	P	0	0
			847	259	305	89	167	27		

- Molecule 8 is a RNA chain called mRNA with 27 nt long spacer.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	16	Total	C	H	N	O	P	0	0
			516	154	169	62	115	16		

- Molecule 9 is a RNA chain called E-site and P-site tRNA (fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
9	A	76	Total	C	H	N	O	P	0	0
			2445	723	825	295	527	75		
9	B	76	Total	C	H	N	O	P	0	0
			2432	723	812	295	527	75		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AA	1322	Total	C	H	N	O	S	0	0
			20856	6539	10431	1817	2026	43		

- Molecule 11 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AB	98	Total	C	H	N	O	S	0	0
			1573	505	783	139	140	6		

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AC	230	Total	C	H	N	O	S	0	0
			3599	1112	1813	317	351	6		
12	AD	228	Total	C	H	N	O	S	0	0
			3556	1100	1789	312	349	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AE	1335	Total	C	H	N	O	S	0	0
			21000	6526	10612	1854	1958	50		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	1384	VAL	MET	conflict	UNP A0A4S1NBU2

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AF	83	Total	C	H	N	O	S	0	0
			1318	399	663	123	132	1		

- Molecule 15 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	C	66	Total	C	H	N	O	S	0	0
			1103	344	559	102	97	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	D	1523	Total	C	H	N	O	P	0	0
			49110	14575	16431	5998	10583	1523		

- Molecule 17 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	E	86	Total	C	H	N	O	S	0	0
			1388	414	719	138	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	F	70	Total	C	H	N	O	S	0	0
			1218	366	629	125	97	1		

- Molecule 19 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 20 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 21 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 22 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 23 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 24 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 25 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	M	151	Total	C	H	N	O	S	0	0
			2416	735	1235	227	215	4		

- Molecule 26 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	N	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 27 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	O	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

- Molecule 28 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	P	99	Total	C	H	N	O	S	0	0
			1621	495	831	151	143	1		

- Molecule 29 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Q	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	R	121	Total	C	H	N	O	S	0	0
			1940	580	1001	194	161	4		

- Molecule 31 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	S	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 32 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 33 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 34 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 35 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 36 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 37 is a RNA chain called mRNA in the ribosomal RNA entrance pore.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	Y	3	Total	C	H	N	O	P	0	0
			87	27	27	6	24	3		

- Molecule 38 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	a	2880	Total	C	H	N	O	P	0	0
			92918	27587	31077	11398	19976	2880		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 39 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	b	76	Total	C	H	N	O	S	0	0
			1181	360	599	117	104	1		

- Molecule 40 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	c	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 41 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	d	120	Total	C	H	N	O	P	0	0
			3869	1144	1300	468	837	120		

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	e	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 43 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	f	58	Total	C	H	N	O	S	0	0
			936	281	488	87	78	2		

- Molecule 44 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	g	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
45	h	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 46 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

- Molecule 47 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	j	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	k	52	Total	C	H	N	O	0	0
			890	275	464	78	73		

- Molecule 49 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	l	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	m	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 53 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 55 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 56 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	s	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 57 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 58 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	u	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 59 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 60 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 61 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	x	116	Total	C	H	N	O	0	0
			1815	552	923	178	162		

- Molecule 62 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	y	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 63 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	z	117	Total	C	H	N	O	0	0
			1967	604	1020	192	151		

- Molecule 64 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
64	AE	1	Total	Mg	0
			1	1	

- Molecule 65 is ZINC ION (three-letter code: ZN) (formula: Zn).

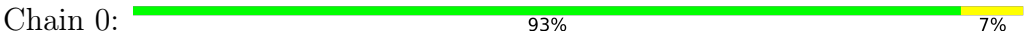
Mol	Chain	Residues	Atoms		AltConf
65	AE	2	Total	Zn	0
			2	2	

3 Residue-property plots (i)

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

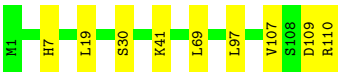
• Molecule 1: 50S ribosomal protein L21

Chain 0:



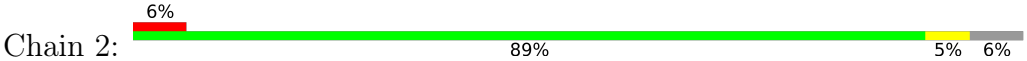
• Molecule 2: 50S ribosomal protein L22

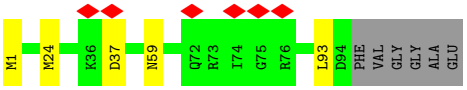
Chain 1:



• Molecule 3: 50S ribosomal protein L23

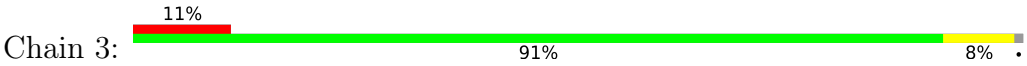
Chain 2:

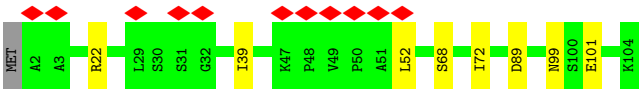




• Molecule 4: 50S ribosomal protein L24

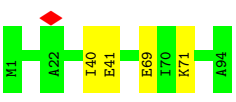
Chain 3:





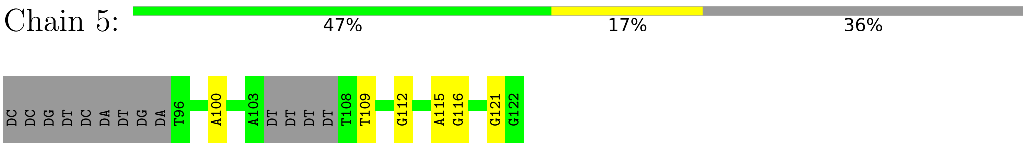
• Molecule 5: 50S ribosomal protein L25

Chain 4:



• Molecule 6: NT DNA

Chain 5:

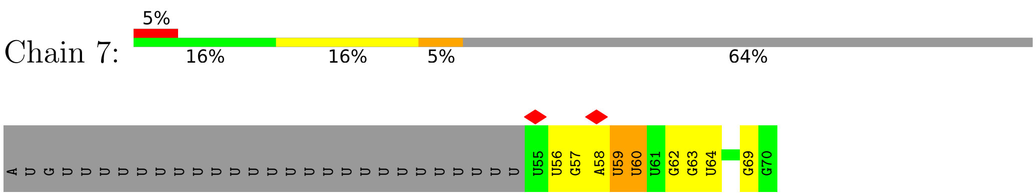


• Molecule 7: T DNA

Chain 6:

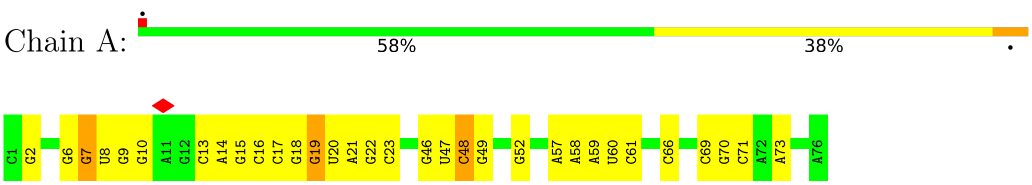
• Molecule 8: mRNA with 27 nt long spacer

Chain 7:



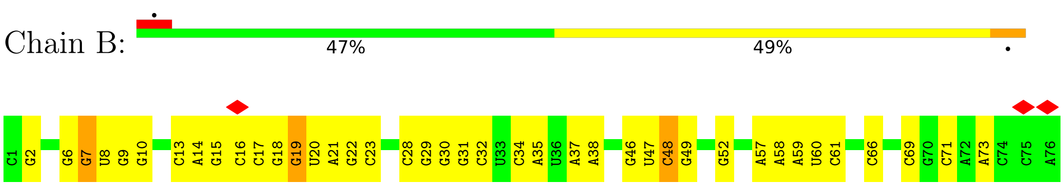
• Molecule 9: E-site and P-site tRNA (fMet)

Chain A:



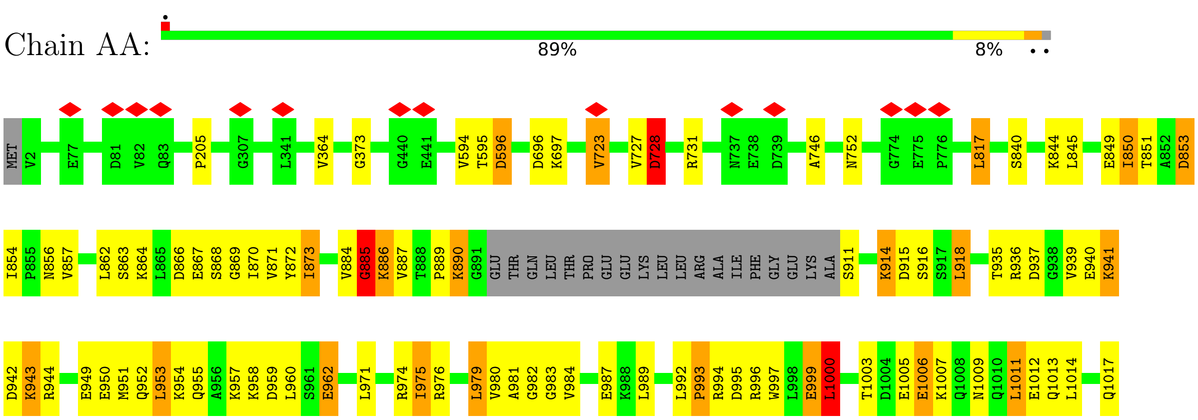
• Molecule 9: E-site and P-site tRNA (fMet)

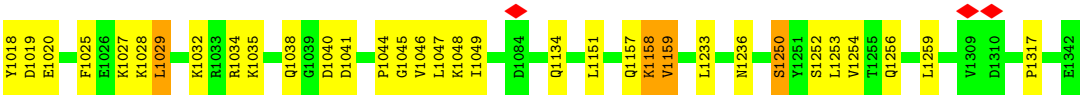
Chain B:



• Molecule 10: DNA-directed RNA polymerase subunit beta

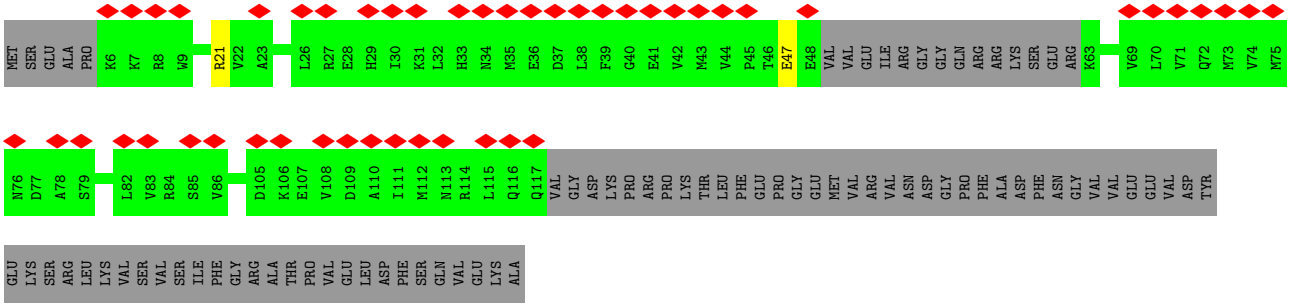
Chain AA:





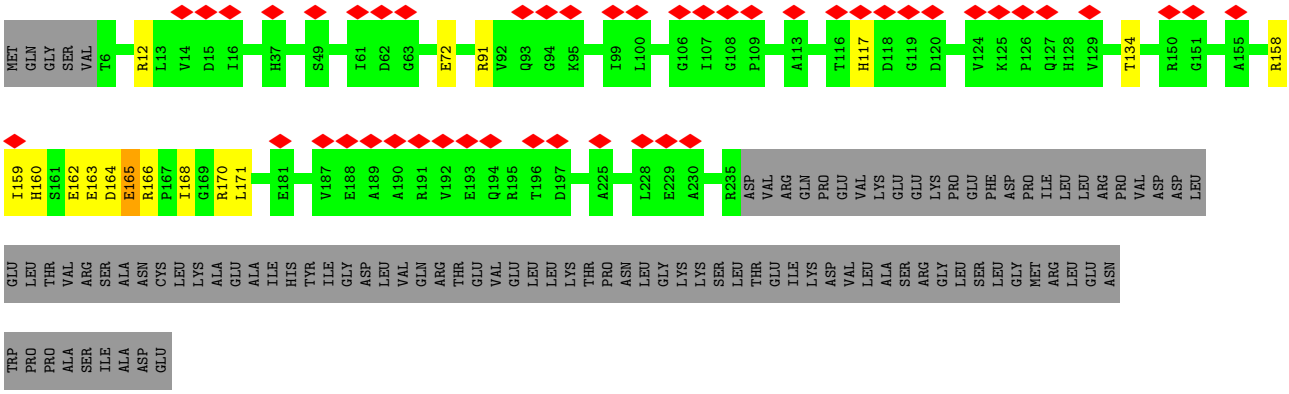
• Molecule 11: Transcription termination/antitermination protein NusG

Chain AB:



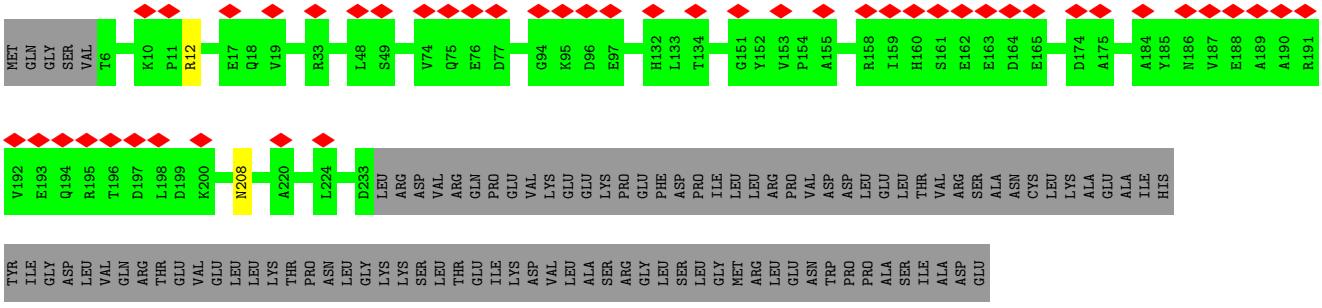
• Molecule 12: DNA-directed RNA polymerase subunit alpha

Chain AC:



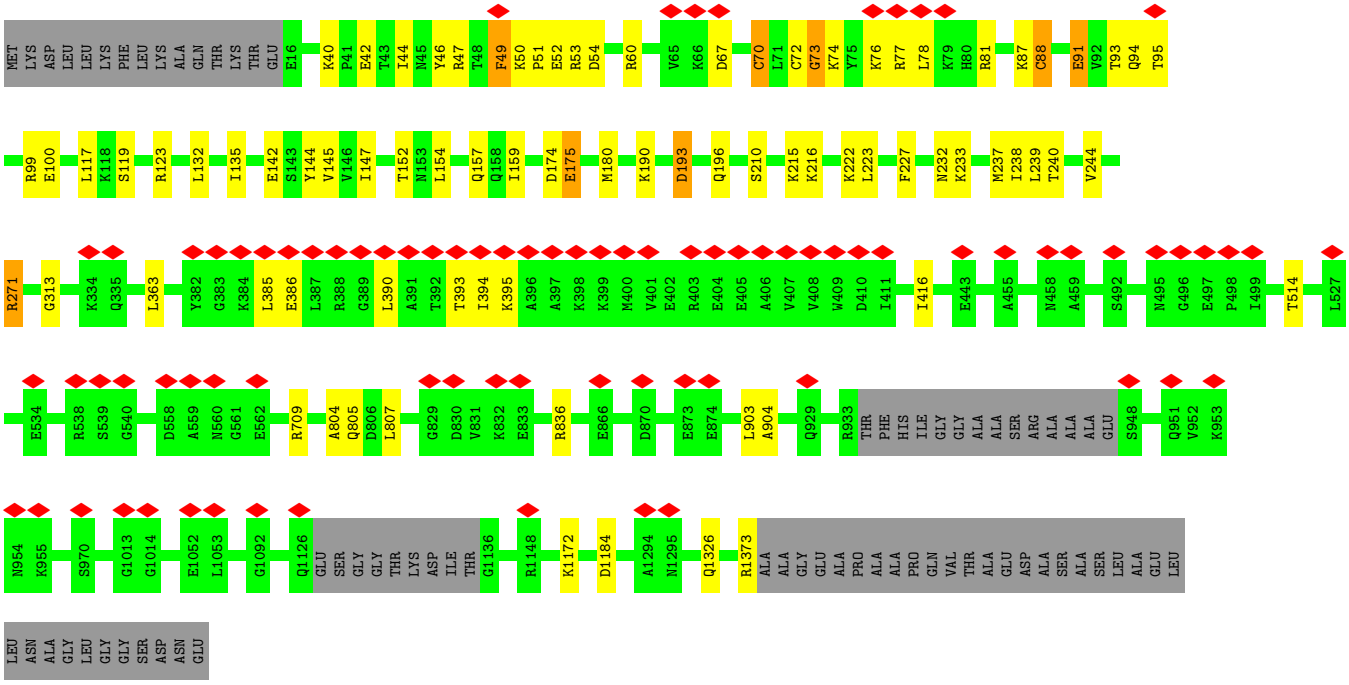
• Molecule 12: DNA-directed RNA polymerase subunit alpha

Chain AD:



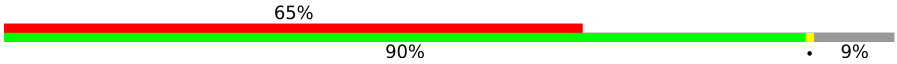
• Molecule 13: DNA-directed RNA polymerase subunit beta'

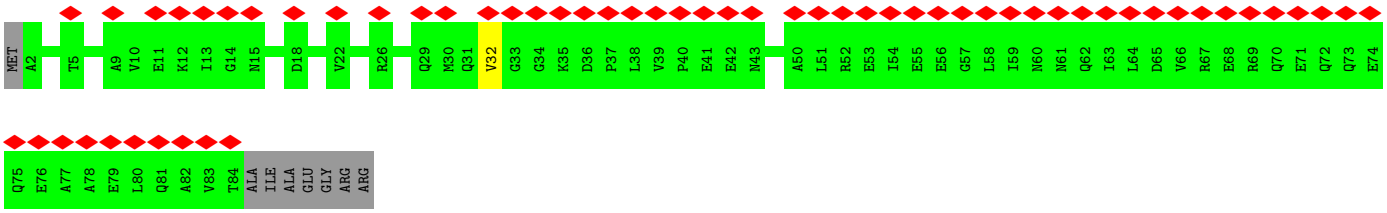
Chain AE:



• Molecule 14: DNA-directed RNA polymerase subunit omega

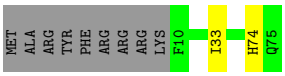
Chain AF:





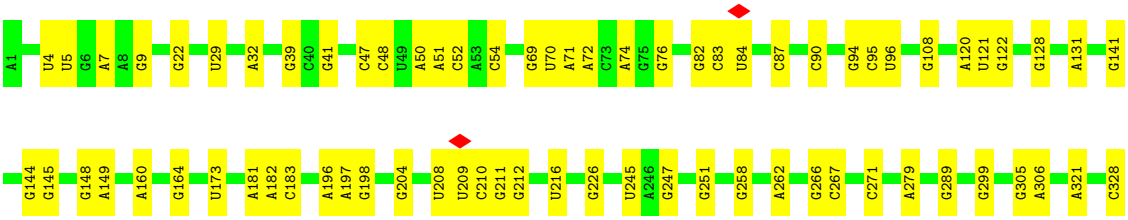
• Molecule 15: 30S ribosomal protein S18

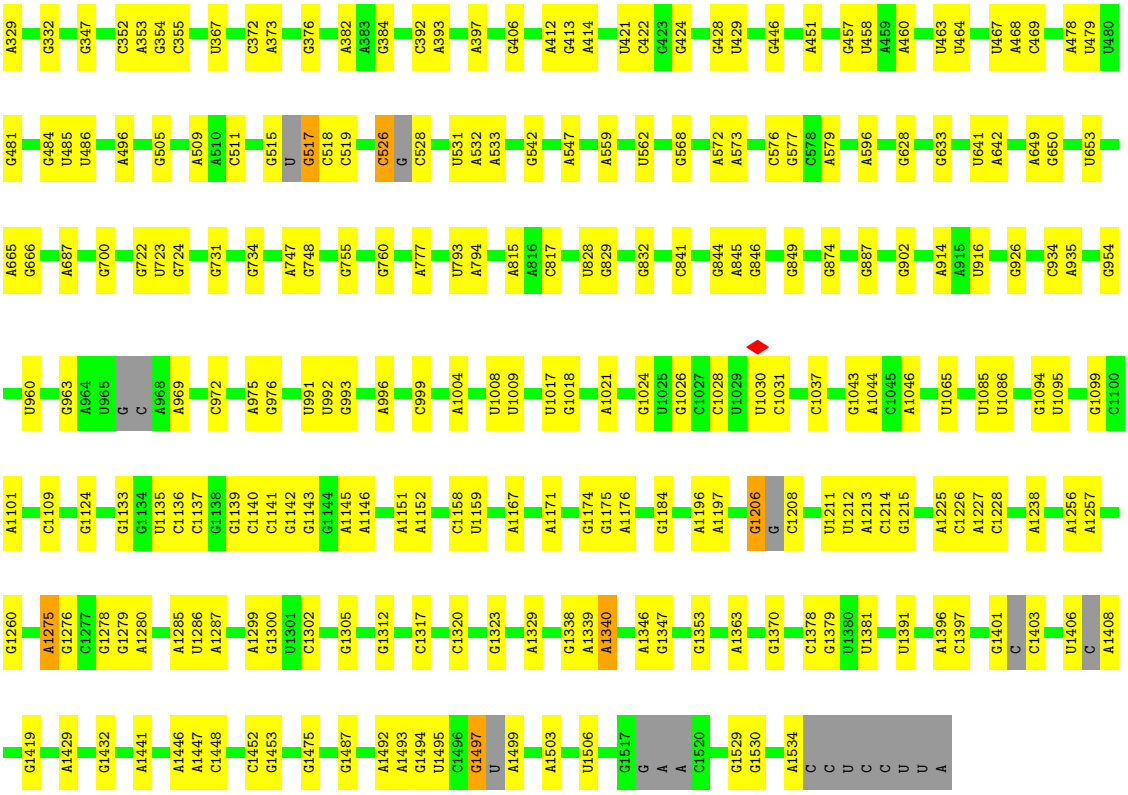
Chain C:



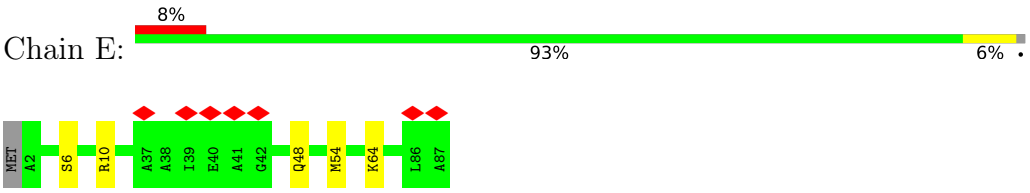
• Molecule 16: 16S rRNA

Chain D:

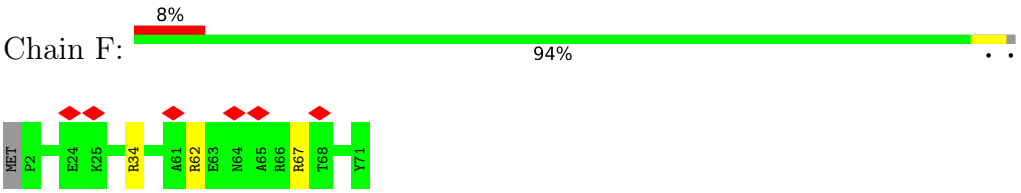




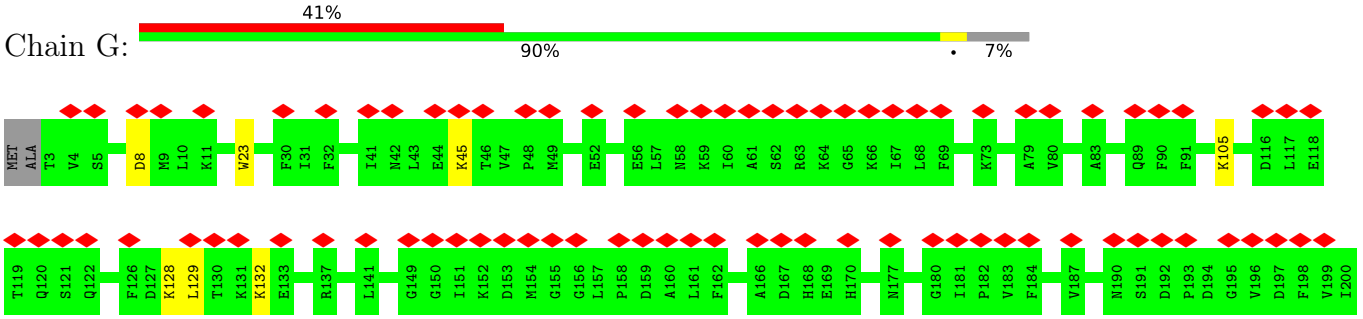
• Molecule 17: 30S ribosomal protein S20

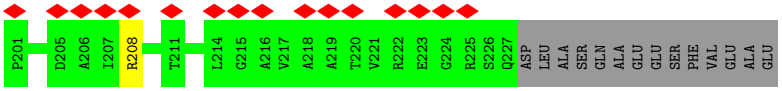


• Molecule 18: 30S ribosomal protein S21



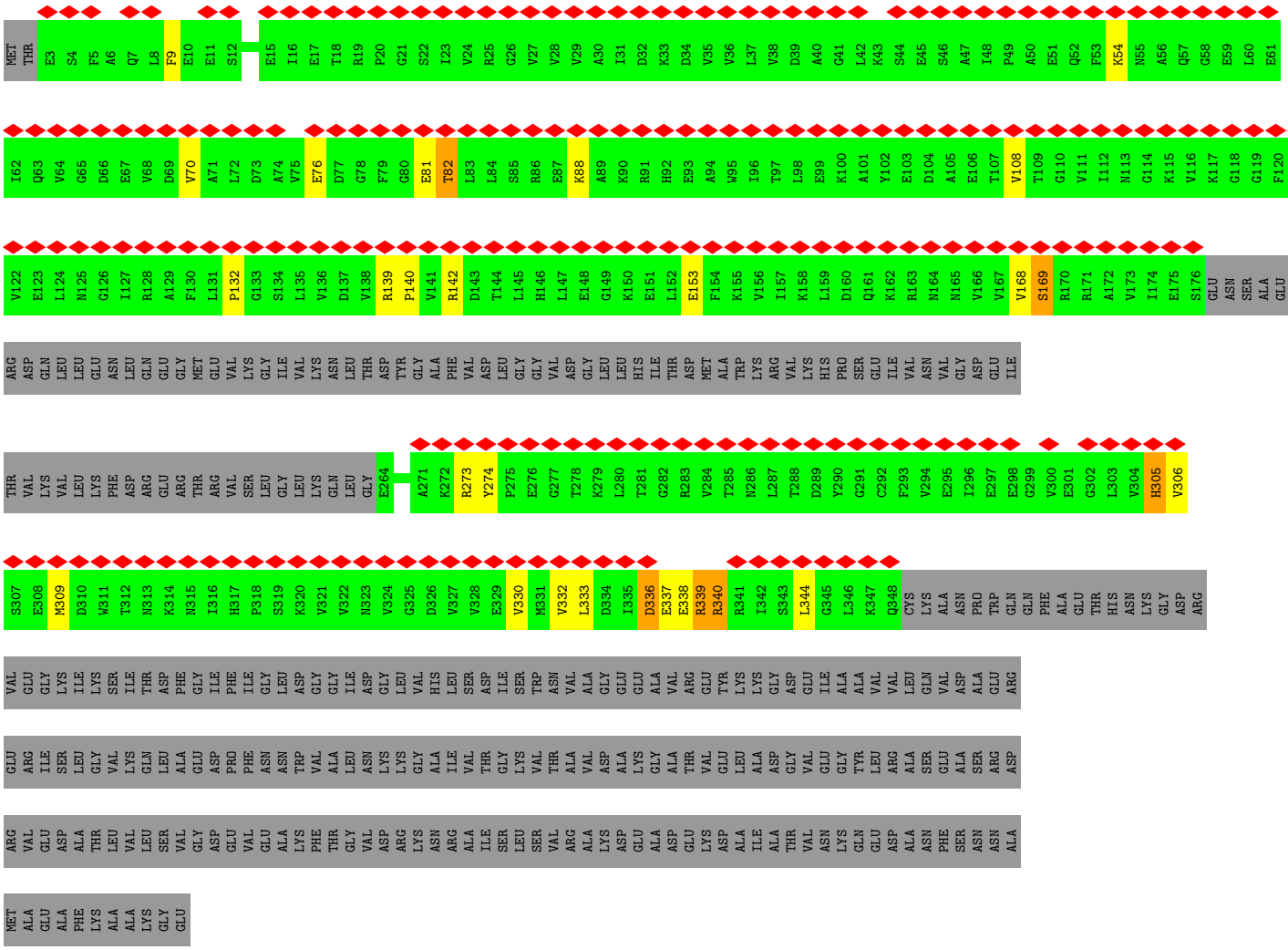
• Molecule 19: 30S ribosomal protein S2





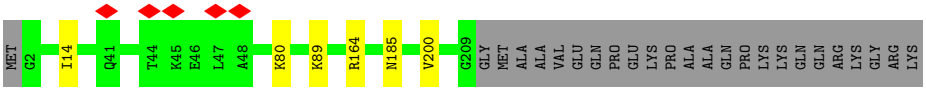
• Molecule 20: 30S ribosomal protein S1

Chain H:



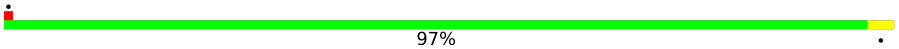
• Molecule 21: 30S ribosomal protein S3

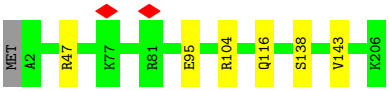
Chain I:



• Molecule 22: 30S ribosomal protein S4

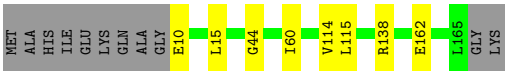
Chain J:





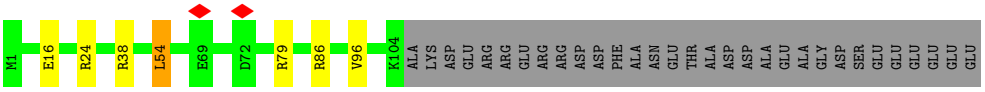
• Molecule 23: 30S ribosomal protein S5

Chain K:



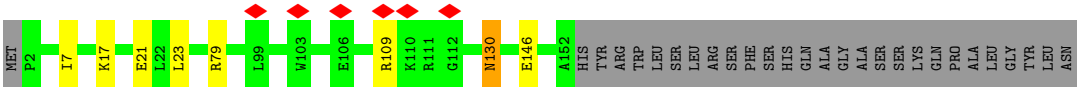
• Molecule 24: 30S ribosomal protein S6

Chain L:



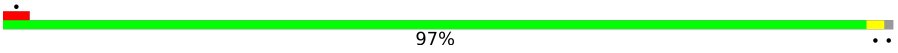
• Molecule 25: 30S ribosomal protein S7

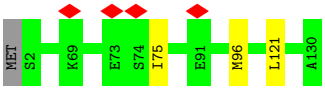
Chain M:



• Molecule 26: 30S ribosomal protein S8

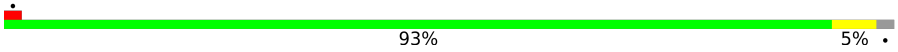
Chain N:

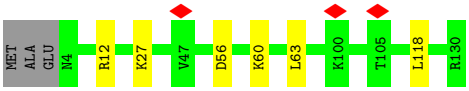




• Molecule 27: 30S ribosomal protein S9

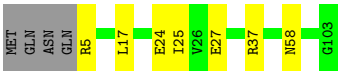
Chain O:





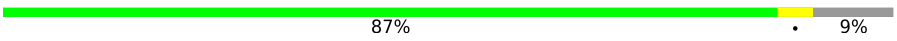
• Molecule 28: 30S ribosomal protein S10

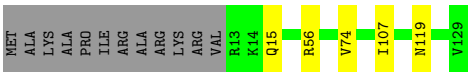
Chain P:



• Molecule 29: 30S ribosomal protein S11

Chain Q:



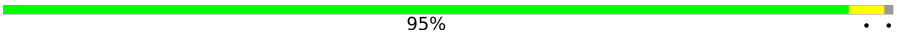


• Molecule 30: 30S ribosomal protein S12

Chain R:

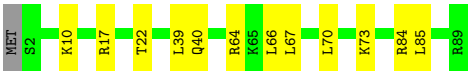
• Molecule 31: 30S ribosomal protein S14

Chain S:



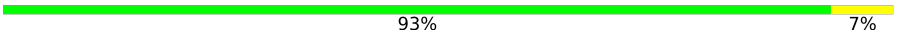
• Molecule 32: 30S ribosomal protein S15

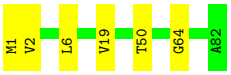
Chain T:



• Molecule 33: 30S ribosomal protein S16

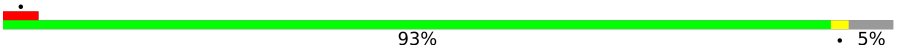
Chain U:

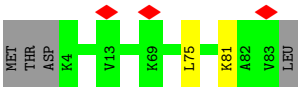




• Molecule 34: 30S ribosomal protein S17

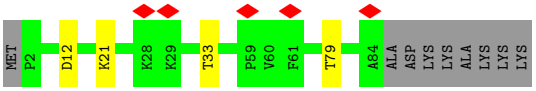
Chain V:





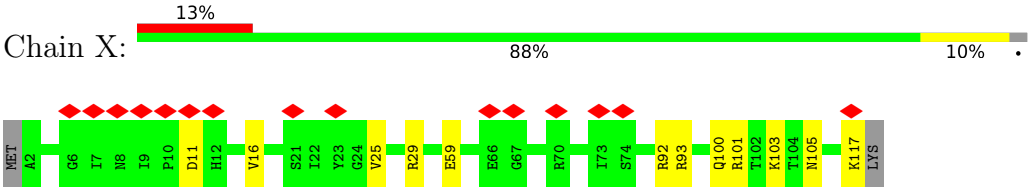
• Molecule 35: 30S ribosomal protein S19

Chain W:



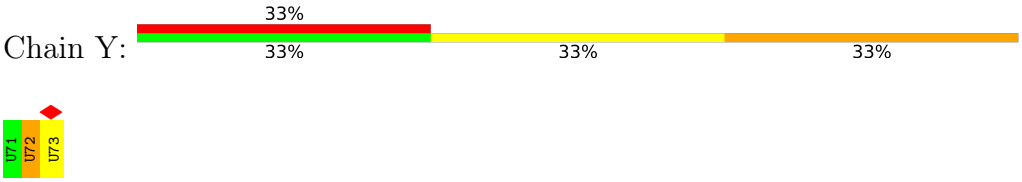
• Molecule 36: 30S ribosomal protein S13

Chain X:



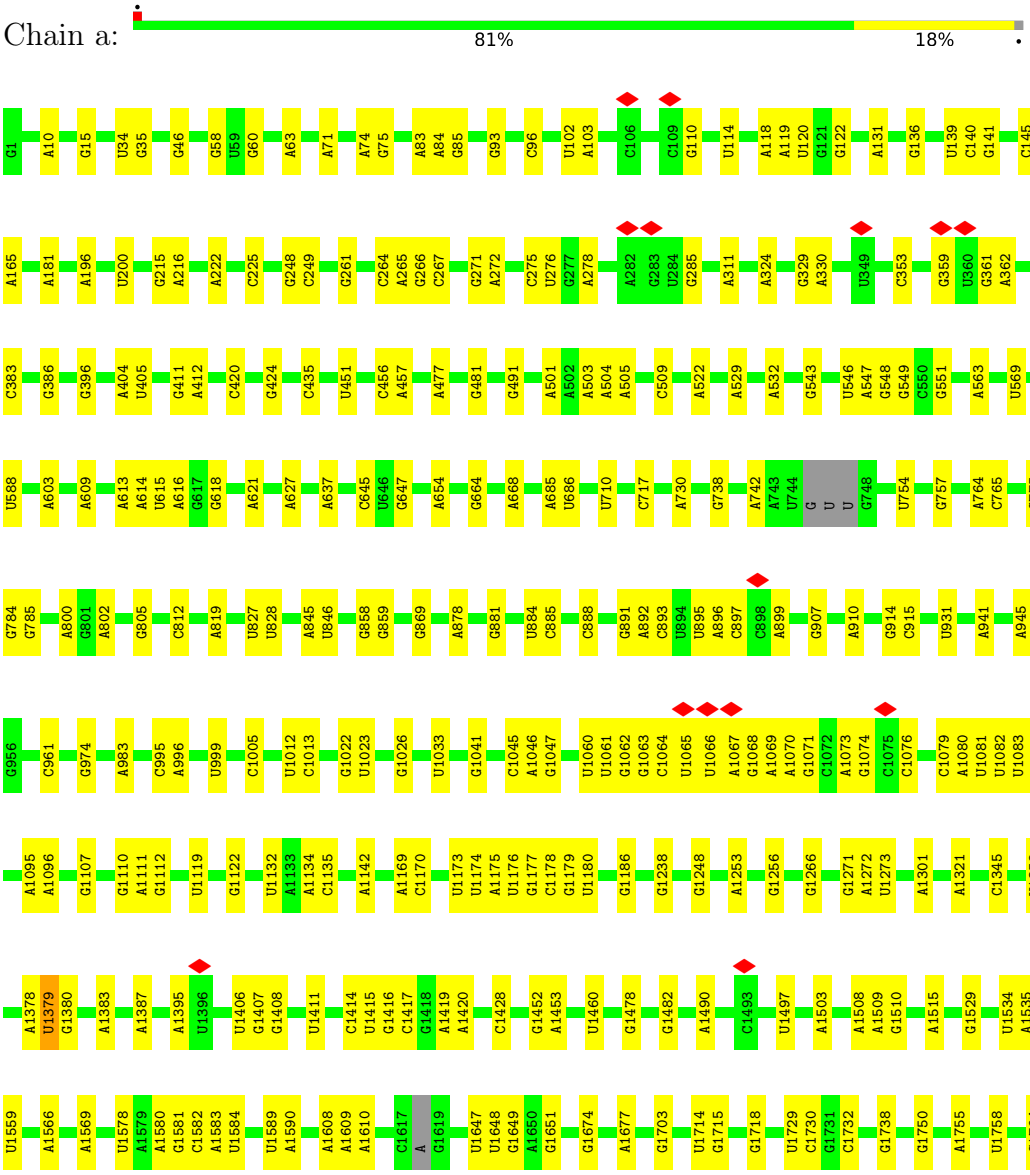
• Molecule 37: mRNA in the ribosomal RNA entrance pore

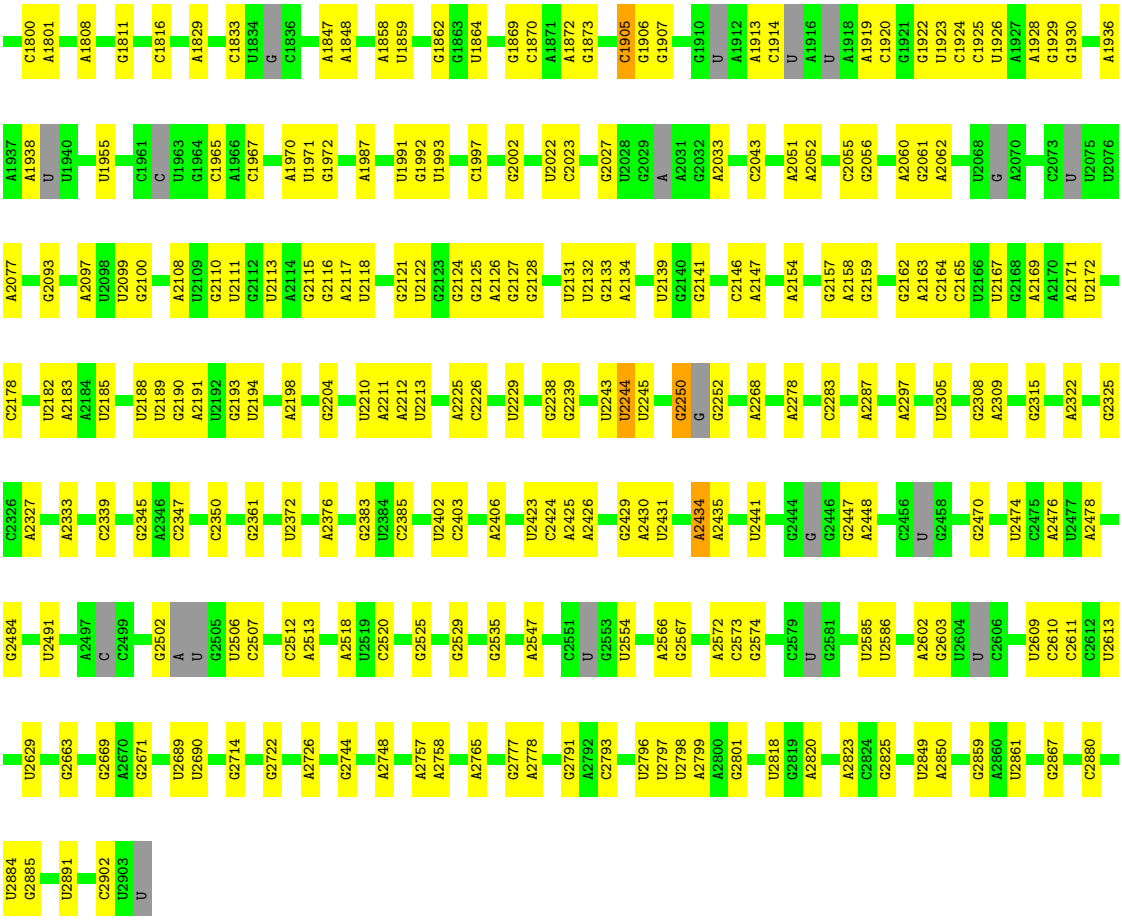
Chain Y:



• Molecule 38: 23S rRNA

Chain a:



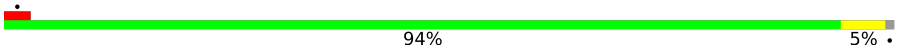


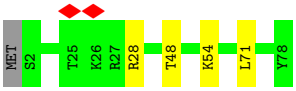
• Molecule 39: 50S ribosomal protein L27

Chain b:

• Molecule 40: 50S ribosomal protein L28

Chain c:



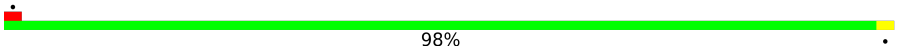


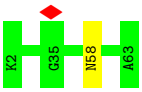
• Molecule 41: 5S rRNA

Chain d:

• Molecule 42: 50S ribosomal protein L29

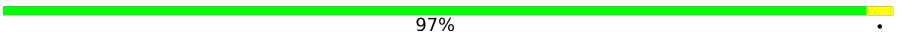
Chain e:

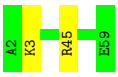




• Molecule 43: 50S ribosomal protein L30

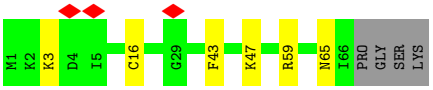
Chain f:





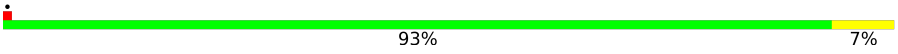
• Molecule 44: 50S ribosomal protein L31

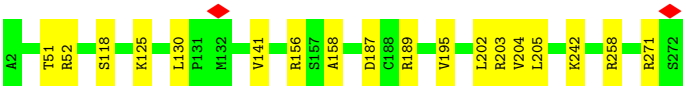
Chain g:



• Molecule 45: 50S ribosomal protein L2

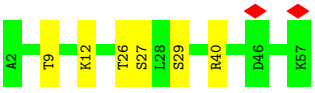
Chain h:





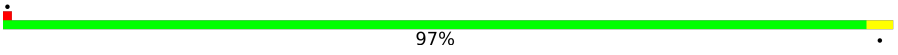
• Molecule 46: 50S ribosomal protein L32

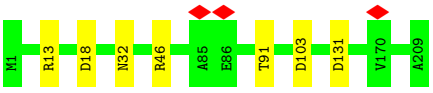
Chain i:



• Molecule 47: 50S ribosomal protein L3

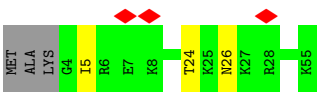
Chain j:





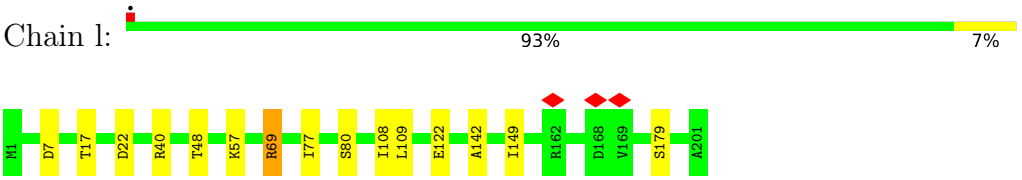
• Molecule 48: 50S ribosomal protein L33

Chain k:



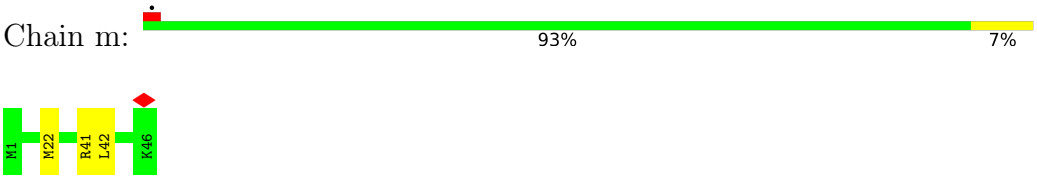
• Molecule 49: 50S ribosomal protein L4

Chain l:



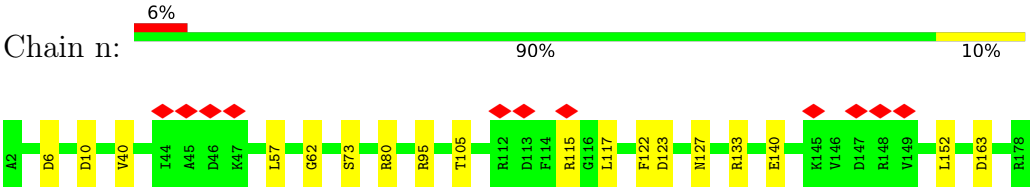
• Molecule 50: 50S ribosomal protein L34

Chain m:



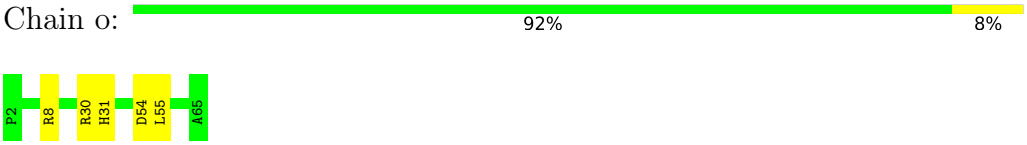
• Molecule 51: 50S ribosomal protein L5

Chain n:



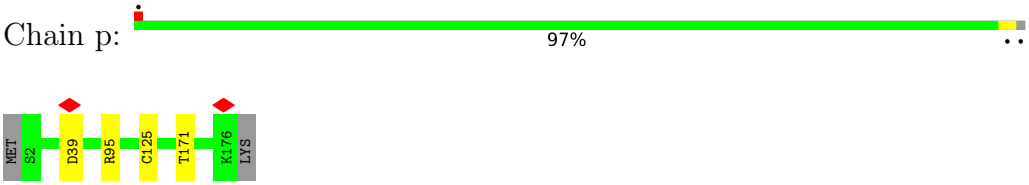
• Molecule 52: 50S ribosomal protein L35

Chain o:



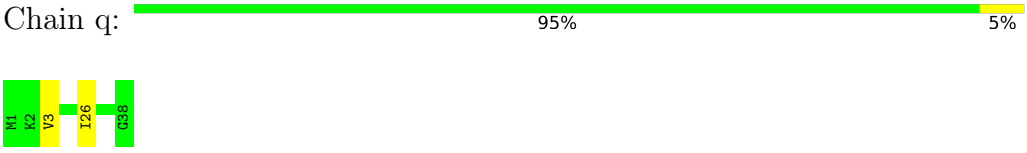
• Molecule 53: 50S ribosomal protein L6

Chain p:



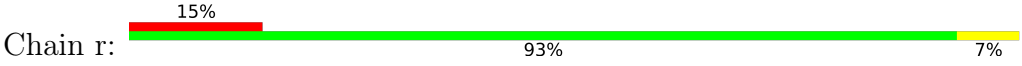
• Molecule 54: 50S ribosomal protein L36

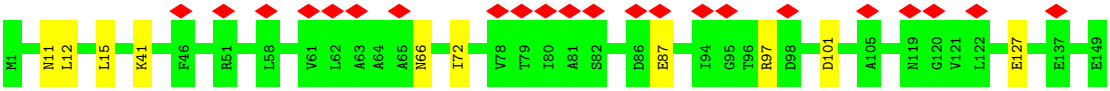
Chain q:



• Molecule 55: 50S ribosomal protein L9

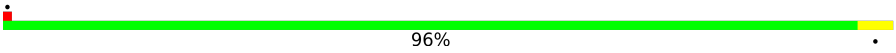
Chain r:





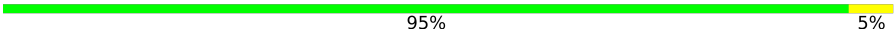
• Molecule 56: 50S ribosomal protein L13

Chain s:



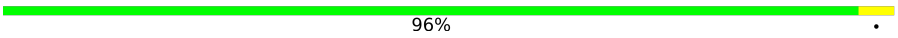
• Molecule 57: 50S ribosomal protein L14

Chain t:



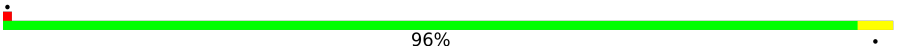
• Molecule 58: 50S ribosomal protein L15

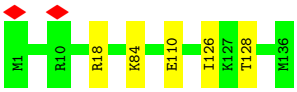
Chain u:



• Molecule 59: 50S ribosomal protein L16

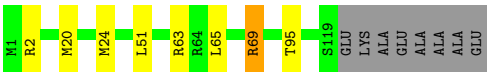
Chain v:





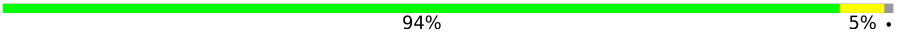
• Molecule 60: 50S ribosomal protein L17

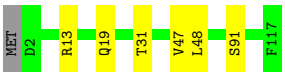
Chain w:



• Molecule 61: 50S ribosomal protein L18

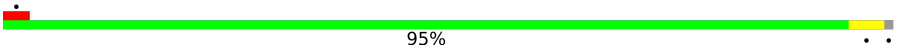
Chain x:

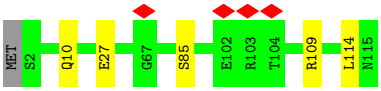




• Molecule 62: 50S ribosomal protein L19

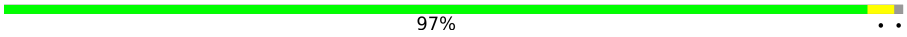
Chain y:

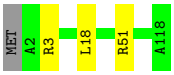




• Molecule 63: 50S ribosomal protein L20

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4207	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.325	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0342	Depositor
Map size (Å)	564.4608, 564.4608, 564.4608	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.9399002, 2.9399002, 2.9399002	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0	0.37	0/829	0.67	0/1107
2	1	0.48	0/864	0.82	0/1156
3	2	0.41	0/752	0.71	0/1005
4	3	0.35	0/796	0.67	2/1062 (0.2%)
5	4	0.40	0/766	0.68	0/1025
6	5	1.13	6/528 (1.1%)	0.97	1/810 (0.1%)
7	6	1.11	4/603 (0.7%)	0.97	0/926
8	7	0.95	4/388 (1.0%)	1.04	0/604
9	A	0.38	0/1810	0.75	1/2821 (0.0%)
9	B	0.43	0/1810	0.84	7/2821 (0.2%)
10	AA	0.59	4/10591 (0.0%)	0.77	24/14289 (0.2%)
11	AB	0.43	0/808	0.59	0/1088
12	AC	0.47	0/1808	0.61	1/2450 (0.0%)
12	AD	0.39	0/1789	0.56	0/2425
13	AE	0.51	3/10545 (0.0%)	0.66	5/14236 (0.0%)
14	AF	0.47	0/657	0.67	0/886
15	C	0.48	0/553	0.82	0/743
16	D	0.31	4/36582 (0.0%)	0.72	20/57043 (0.0%)
17	E	0.57	0/675	0.85	0/895
18	F	0.56	0/597	0.87	0/792
19	G	0.48	0/1791	0.71	0/2413
20	H	0.54	1/1746 (0.1%)	1.03	12/2382 (0.5%)
21	I	0.43	0/1663	0.70	0/2241
22	J	0.46	0/1665	0.74	0/2227
23	K	0.45	0/1165	0.75	0/1568
24	L	0.43	0/867	0.75	1/1171 (0.1%)
25	M	0.50	0/1195	0.81	0/1602
26	N	0.41	0/989	0.69	0/1326
27	O	0.43	0/1034	0.75	0/1375
28	P	0.39	0/800	0.75	0/1082
29	Q	0.40	0/893	0.69	0/1205
30	R	0.35	0/952	0.74	0/1274

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	S	0.49	0/817	0.78	0/1088
32	T	0.53	0/722	0.86	0/964
33	U	0.44	0/659	0.78	0/884
34	V	0.33	0/657	0.62	0/881
35	W	0.38	0/680	0.62	0/915
36	X	0.48	0/909	0.87	0/1215
37	Y	0.37	0/65	0.86	1/98 (1.0%)
38	a	0.37	3/69247 (0.0%)	0.72	17/107985 (0.0%)
39	b	0.39	0/589	0.71	0/779
40	c	0.48	0/635	0.81	1/848 (0.1%)
41	d	0.28	0/2872	0.69	0/4478
42	e	0.53	0/502	0.83	0/667
43	f	0.44	0/452	0.78	0/605
44	g	0.43	0/531	0.69	0/709
45	h	0.39	0/2121	0.78	0/2852
46	i	0.40	0/450	0.79	0/599
47	j	0.43	0/1586	0.70	0/2134
48	k	0.35	0/433	0.65	0/576
49	l	0.46	0/1571	0.77	2/2113 (0.1%)
50	m	0.53	0/380	0.99	0/498
51	n	0.49	0/1434	0.88	3/1926 (0.2%)
52	o	0.45	0/513	0.83	0/676
53	p	0.39	0/1333	0.67	0/1805
54	q	0.37	0/303	0.77	0/397
55	r	0.43	0/1122	0.69	0/1515
56	s	0.49	0/1152	0.75	0/1551
57	t	0.41	0/955	0.78	0/1279
58	u	0.40	0/1062	0.76	0/1413
59	v	0.47	0/1093	0.81	0/1460
60	w	0.52	0/964	0.87	1/1289 (0.1%)
61	x	0.46	0/902	0.81	0/1209
62	y	0.41	0/929	0.72	1/1242 (0.1%)
63	z	0.60	0/960	0.91	0/1278
All	All	0.42	29/187111 (0.0%)	0.73	100/275978 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	B	0	2
10	AA	0	13
13	AE	0	5
14	AF	0	1
20	H	0	3
36	X	0	1
All	All	0	27

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	AA	885	GLY	C-O	-13.35	1.02	1.23
16	D	1339	A	O3'-P	10.46	1.73	1.61
13	AE	88	CYS	CB-SG	-10.21	1.64	1.82
6	5	109	DT	O3'-P	8.69	1.71	1.61
10	AA	850	ILE	N-CA	-8.24	1.29	1.46
7	6	10	DG	C1'-N9	-8.24	1.35	1.47
16	D	196	A	O3'-P	8.21	1.71	1.61
16	D	145	G	O3'-P	8.02	1.70	1.61
16	D	1275	A	O3'-P	7.64	1.70	1.61
38	a	2434	A	O3'-P	7.61	1.70	1.61
20	H	169	SER	N-CA	7.51	1.61	1.46
6	5	121	DG	C1'-N9	-7.29	1.37	1.47
8	7	69	G	C1'-N9	-6.70	1.37	1.46
6	5	112	DG	C1'-N9	-6.68	1.37	1.47
38	a	2167	U	O3'-P	6.67	1.69	1.61
38	a	1905	C	O3'-P	6.65	1.69	1.61
6	5	100	DA	C1'-N9	-6.46	1.38	1.47
7	6	21	DA	C1'-N9	-6.42	1.38	1.47
13	AE	93	THR	CA-C	6.23	1.69	1.52
8	7	59	U	C1'-N1	6.07	1.57	1.48
6	5	116	DG	C1'-N9	-6.03	1.38	1.47
6	5	115	DA	C1'-N9	-6.00	1.38	1.47
13	AE	70	CYS	CA-CB	-5.82	1.41	1.53
8	7	60	U	C1'-N1	5.81	1.57	1.48
7	6	28	DA	C1'-N9	-5.69	1.39	1.47
8	7	64	U	C1'-N1	5.37	1.56	1.48
10	AA	953	LEU	N-CA	5.33	1.57	1.46
7	6	24	DT	C1'-N1	5.29	1.56	1.49
10	AA	1000	LEU	N-CA	5.14	1.56	1.46

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	AA	914	LYS	CA-CB-CG	12.10	140.02	113.40
10	AA	1250	SER	C-N-CA	11.17	149.63	121.70
38	a	2252	G	N9-C1'-C2'	-10.99	99.72	114.00
16	D	1401	G	N9-C1'-C2'	-10.73	100.05	114.00
51	n	73	SER	N-CA-CB	-10.57	94.65	110.50
16	D	1499	A	N9-C1'-C2'	-10.30	100.61	114.00
16	D	528	C	N1-C1'-C2'	-10.22	100.71	114.00
10	AA	914	LYS	CB-CG-CD	10.17	138.03	111.60
20	H	169	SER	N-CA-C	9.98	137.94	111.00
16	D	1339	A	P-O3'-C3'	9.95	131.63	119.70
9	B	29	G	N9-C1'-C2'	-9.69	101.34	112.00
9	B	28	C	P-O3'-C3'	9.52	131.12	119.70
13	AE	271	ARG	NE-CZ-NH2	-9.38	115.61	120.30
16	D	196	A	P-O3'-C3'	9.36	130.94	119.70
10	AA	863	SER	O-C-N	-8.98	108.34	122.70
16	D	526	C	N1-C1'-C2'	-8.82	102.30	112.00
20	H	88	LYS	C-N-CA	8.75	143.58	121.70
16	D	1208	C	N1-C1'-C2'	-8.55	102.59	112.00
10	AA	849	GLU	O-C-N	8.54	136.37	122.70
38	a	2167	U	P-O3'-C3'	8.53	129.93	119.70
16	D	1206	G	N9-C1'-C2'	-8.43	102.73	112.00
38	a	2434	A	P-O3'-C3'	8.22	129.56	119.70
16	D	1406	U	N1-C1'-C2'	-7.86	103.36	112.00
16	D	1275	A	P-O3'-C3'	7.84	129.11	119.70
38	a	1905	C	P-O3'-C3'	7.59	128.81	119.70
10	AA	979	LEU	CB-CA-C	7.58	124.61	110.20
20	H	305	HIS	N-CA-C	7.44	131.09	111.00
9	B	29	G	C3'-C2'-O2'	7.38	134.72	113.30
16	D	145	G	P-O3'-C3'	7.30	128.46	119.70
10	AA	999	GLU	O-C-N	-7.29	111.03	122.70
10	AA	979	LEU	N-CA-CB	-7.26	95.88	110.40
10	AA	975	ILE	CB-CA-C	7.24	126.08	111.60
16	D	1206	G	C4'-C3'-O3'	7.17	127.33	113.00
38	a	2245	U	N1-C1'-C2'	-7.12	104.17	112.00
10	AA	884	VAL	CA-C-N	7.08	130.36	116.20
10	AA	1029	LEU	CB-CG-CD1	-6.92	99.25	111.00
10	AA	962	GLU	C-N-CA	6.73	138.53	121.70
51	n	73	SER	CB-CA-C	6.72	122.87	110.10
10	AA	863	SER	CA-C-N	6.72	131.98	117.20
38	a	2250	G	C4'-C3'-O3'	-6.67	95.40	109.40
16	D	1401	G	C4'-C3'-O3'	6.63	126.27	113.00
38	a	1379	U	C2'-C3'-O3'	6.57	124.21	113.70
16	D	1403	C	N1-C1'-C2'	-6.57	104.78	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	a	2243	U	N1-C1'-C2'	-6.55	104.80	112.00
20	H	339	ARG	C-N-CA	6.47	137.87	121.70
16	D	515	G	N9-C1'-C2'	-6.41	104.94	112.00
16	D	1408	A	N9-C1'-C2'	-6.40	104.96	112.00
6	5	109	DT	P-O3'-C3'	6.39	127.37	119.70
10	AA	869	GLY	CA-C-O	-6.37	109.14	120.60
10	AA	885	GLY	CA-C-O	-6.34	109.18	120.60
16	D	1497	G	N9-C1'-C2'	-6.33	105.03	112.00
9	B	34	C	P-O3'-C3'	6.32	127.28	119.70
12	AC	117	HIS	CB-CA-C	-6.24	97.91	110.40
9	B	35	A	P-O3'-C3'	6.22	127.17	119.70
10	AA	884	VAL	CA-C-O	-6.12	107.25	120.10
10	AA	364	VAL	CA-CB-CG2	6.01	119.91	110.90
20	H	140	PRO	N-CA-CB	5.99	110.49	103.30
9	B	29	G	P-O3'-C3'	5.93	126.82	119.70
10	AA	727	VAL	N-CA-C	-5.90	95.07	111.00
20	H	330	VAL	N-CA-C	5.88	126.87	111.00
20	H	336	ASP	CB-CA-C	-5.86	98.68	110.40
20	H	132	PRO	N-CA-CB	5.85	110.32	103.30
38	a	754	U	N1-C1'-C2'	5.84	121.59	114.00
20	H	168	VAL	C-N-CA	5.82	136.24	121.70
13	AE	903	LEU	C-N-CA	5.76	136.09	121.70
16	D	517	G	C5'-C4'-C3'	5.71	125.14	116.00
10	AA	1029	LEU	CB-CG-CD2	-5.70	101.30	111.00
20	H	344	LEU	CA-CB-CG	5.70	128.42	115.30
51	n	127	ASN	CB-CA-C	5.65	121.71	110.40
38	a	2244	U	C1'-C2'-O2'	-5.62	93.75	110.60
13	AE	363	LEU	CA-CB-CG	5.58	128.14	115.30
24	L	54	LEU	CA-CB-CG	5.55	128.07	115.30
4	3	22	ARG	NE-CZ-NH1	5.55	123.07	120.30
10	AA	1233	LEU	CA-CB-CG	5.48	127.91	115.30
38	a	783	A	C4'-C3'-O3'	5.46	123.92	113.00
40	c	28	ARG	NE-CZ-NH2	-5.40	117.60	120.30
37	Y	72	U	P-O3'-C3'	5.40	126.18	119.70
10	AA	849	GLU	CA-C-N	-5.37	105.38	117.20
16	D	1340	A	C5'-C4'-C3'	5.30	124.47	116.00
4	3	22	ARG	NE-CZ-NH2	-5.29	117.65	120.30
10	AA	728	ASP	N-CA-C	5.27	125.22	111.00
62	y	109	ARG	NE-CZ-NH2	5.21	122.91	120.30
16	D	1340	A	C5'-C4'-O4'	5.21	115.35	109.10
38	a	742	A	C8-N9-C1'	-5.20	118.33	127.70
20	H	169	SER	N-CA-CB	-5.18	102.74	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	a	2244	U	C4'-C3'-O3'	5.17	123.34	113.00
10	AA	817	LEU	CB-CG-CD2	-5.16	102.22	111.00
38	a	404	A	C2'-C3'-O3'	5.14	121.92	113.70
38	a	2252	G	C4'-C3'-O3'	5.12	123.24	113.00
9	A	48	C	N1-C1'-C2'	5.08	120.61	114.00
9	B	48	C	N1-C1'-C2'	5.08	120.61	114.00
60	w	69	ARG	NE-CZ-NH2	5.05	122.83	120.30
49	l	69	ARG	NE-CZ-NH1	5.05	122.82	120.30
38	a	742	A	C4-N9-C1'	5.05	135.38	126.30
20	H	332	VAL	N-CA-C	5.04	124.61	111.00
13	AE	73	GLY	N-CA-C	5.04	125.70	113.10
13	AE	807	LEU	CB-CG-CD2	-5.04	102.44	111.00
10	AA	999	GLU	CA-C-N	5.03	128.26	117.20
38	a	2243	U	C4'-C3'-O3'	5.02	123.05	113.00
49	l	69	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	A	19	G	Sidechain
9	A	7	G	Sidechain
10	AA	1134	GLN	Peptide
10	AA	1157	GLN	Peptide
10	AA	1158	LYS	Peptide
10	AA	205	PRO	Peptide
10	AA	373	GLY	Mainchain
10	AA	594	VAL	Peptide
10	AA	595	THR	Peptide
10	AA	596	ASP	Mainchain
10	AA	696	ASP	Peptide
10	AA	746	ALA	Peptide
10	AA	885	GLY	Mainchain
10	AA	889	PRO	Mainchain
10	AA	981	ALA	Peptide
13	AE	1184	ASP	Peptide
13	AE	1326	GLN	Peptide
13	AE	313	GLY	Peptide
13	AE	416	ILE	Peptide
13	AE	804	ALA	Peptide
14	AF	32	VAL	Peptide
9	B	19	G	Sidechain

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Mol	Chain	Res	Type	Group
9	B	7	G	Sidechain
20	H	274	TYR	Peptide
20	H	81	GLU	Peptide
20	H	82	THR	Peptide
36	X	100	GLN	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	15 55
2	1	108/110 (98%)	104 (96%)	4 (4%)	0	100 100
3	2	92/100 (92%)	90 (98%)	2 (2%)	0	100 100
4	3	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	15 55
5	4	92/94 (98%)	90 (98%)	2 (2%)	0	100 100
10	AA	1318/1342 (98%)	1151 (87%)	135 (10%)	32 (2%)	6 33
11	AB	94/181 (52%)	88 (94%)	6 (6%)	0	100 100
12	AC	228/329 (69%)	214 (94%)	12 (5%)	2 (1%)	17 57
12	AD	226/329 (69%)	212 (94%)	14 (6%)	0	100 100
13	AE	1329/1407 (94%)	1199 (90%)	121 (9%)	9 (1%)	22 63
14	AF	81/91 (89%)	74 (91%)	7 (9%)	0	100 100
15	C	64/75 (85%)	63 (98%)	1 (2%)	0	100 100
17	E	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
18	F	68/71 (96%)	68 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	G	223/241 (92%)	210 (94%)	13 (6%)	0	100	100
20	H	255/557 (46%)	188 (74%)	55 (22%)	12 (5%)	2	21
21	I	206/233 (88%)	196 (95%)	9 (4%)	1 (0%)	29	69
22	J	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
23	K	154/167 (92%)	146 (95%)	7 (4%)	1 (1%)	25	66
24	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	15	55
25	M	149/179 (83%)	144 (97%)	4 (3%)	1 (1%)	22	63
26	N	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	19	60
27	O	125/130 (96%)	115 (92%)	9 (7%)	1 (1%)	19	60
28	P	97/103 (94%)	89 (92%)	7 (7%)	1 (1%)	15	55
29	Q	115/129 (89%)	104 (90%)	9 (8%)	2 (2%)	9	42
30	R	117/124 (94%)	116 (99%)	1 (1%)	0	100	100
31	S	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
32	T	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
33	U	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	12	48
34	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
35	W	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
36	X	114/118 (97%)	107 (94%)	5 (4%)	2 (2%)	8	40
39	b	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
40	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
42	e	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
43	f	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
44	g	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
45	h	269/271 (99%)	259 (96%)	9 (3%)	1 (0%)	34	72
46	i	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
47	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
48	k	50/55 (91%)	50 (100%)	0	0	100	100
49	l	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	29	69
50	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
51	n	175/177 (99%)	162 (93%)	11 (6%)	2 (1%)	14	52
52	o	62/64 (97%)	59 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	p	173/177 (98%)	161 (93%)	12 (7%)	0	100	100
54	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
55	r	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
56	s	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
57	t	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
58	u	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
59	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
60	w	117/127 (92%)	107 (92%)	10 (8%)	0	100	100
61	x	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
62	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
63	z	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	57
All	All	9136/10141 (90%)	8463 (93%)	599 (7%)	74 (1%)	24	60

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	AA	596	ASP
10	AA	890	LYS
10	AA	918	LEU
10	AA	937	ASP
10	AA	976	ARG
10	AA	984	VAL
10	AA	1000	LEU
10	AA	1003	THR
10	AA	1006	GLU
10	AA	1011	LEU
20	H	139	ARG
20	H	153	GLU
20	H	169	SER
20	H	306	VAL
20	H	340	ARG
27	O	56	ASP
36	X	103	LYS
10	AA	853	ASP
10	AA	856	ASN
10	AA	870	ILE
10	AA	873	ILE
10	AA	886	LYS

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Mol	Chain	Res	Type
10	AA	983	GLY
10	AA	1158	LYS
13	AE	175	GLU
20	H	108	VAL
20	H	309	MET
20	H	333	LEU
45	h	158	ALA
49	l	142	ALA
63	z	3	ARG
10	AA	723	VAL
10	AA	728	ASP
10	AA	862	LEU
10	AA	1045	GLY
12	AC	164	ASP
12	AC	165	GLU
13	AE	51	PRO
13	AE	805	GLN
20	H	76	GLU
20	H	142	ARG
25	M	130	ASN
28	P	58	ASN
29	Q	119	ASN
36	X	105	ASN
10	AA	940	GLU
10	AA	941	LYS
10	AA	943	LYS
10	AA	993	PRO
13	AE	174	ASP
13	AE	193	ASP
20	H	82	THR
21	I	80	LYS
51	n	40	VAL
10	AA	1044	PRO
13	AE	91	GLU
20	H	70	VAL
4	3	39	ILE
10	AA	982	GLY
13	AE	49	PHE
13	AE	904	ALA
10	AA	850	ILE
13	AE	73	GLY
24	L	96	VAL

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Mol	Chain	Res	Type
1	0	44	GLY
10	AA	697	LYS
10	AA	885	GLY
10	AA	1159	VAL
10	AA	1317	PRO
23	K	44	GLY
29	Q	74	VAL
33	U	64	GLY
26	N	75	ILE
51	n	62	GLY

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	0	84/84 (100%)	78 (93%)	6 (7%)	14 39
2	1	93/93 (100%)	84 (90%)	9 (10%)	8 27
3	2	81/84 (96%)	76 (94%)	5 (6%)	18 43
4	3	84/85 (99%)	78 (93%)	6 (7%)	14 39
5	4	78/78 (100%)	74 (95%)	4 (5%)	24 48
10	AA	1140/1157 (98%)	1044 (92%)	96 (8%)	11 33
11	AB	86/158 (54%)	84 (98%)	2 (2%)	50 70
12	AC	198/286 (69%)	184 (93%)	14 (7%)	14 39
12	AD	196/286 (68%)	194 (99%)	2 (1%)	76 86
13	AE	1120/1168 (96%)	1051 (94%)	69 (6%)	18 43
14	AF	70/75 (93%)	70 (100%)	0	100 100
15	C	57/65 (88%)	55 (96%)	2 (4%)	36 59
17	E	65/66 (98%)	60 (92%)	5 (8%)	13 37
18	F	60/61 (98%)	57 (95%)	3 (5%)	24 49
19	G	187/199 (94%)	179 (96%)	8 (4%)	29 53
20	H	137/461 (30%)	128 (93%)	9 (7%)	16 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	I	171/190 (90%)	166 (97%)	5 (3%)	42	64
22	J	172/173 (99%)	166 (96%)	6 (4%)	36	59
23	K	119/126 (94%)	112 (94%)	7 (6%)	19	45
24	L	91/116 (78%)	85 (93%)	6 (7%)	16	41
25	M	124/147 (84%)	116 (94%)	8 (6%)	17	42
26	N	104/105 (99%)	102 (98%)	2 (2%)	57	75
27	O	105/107 (98%)	100 (95%)	5 (5%)	25	51
28	P	86/90 (96%)	80 (93%)	6 (7%)	15	40
29	Q	90/99 (91%)	87 (97%)	3 (3%)	38	61
30	R	101/104 (97%)	94 (93%)	7 (7%)	15	40
31	S	83/84 (99%)	79 (95%)	4 (5%)	25	51
32	T	76/77 (99%)	64 (84%)	12 (16%)	2	13
33	U	65/65 (100%)	60 (92%)	5 (8%)	13	37
34	V	74/78 (95%)	72 (97%)	2 (3%)	44	65
35	W	72/79 (91%)	68 (94%)	4 (6%)	21	46
36	X	94/96 (98%)	85 (90%)	9 (10%)	8	27
39	b	58/63 (92%)	57 (98%)	1 (2%)	60	78
40	c	67/68 (98%)	64 (96%)	3 (4%)	27	52
42	e	54/54 (100%)	53 (98%)	1 (2%)	57	75
43	f	48/48 (100%)	46 (96%)	2 (4%)	30	54
44	g	59/62 (95%)	53 (90%)	6 (10%)	7	25
45	h	216/216 (100%)	199 (92%)	17 (8%)	12	35
46	i	47/47 (100%)	41 (87%)	6 (13%)	4	18
47	j	164/164 (100%)	157 (96%)	7 (4%)	29	53
48	k	47/49 (96%)	44 (94%)	3 (6%)	17	42
49	l	165/165 (100%)	151 (92%)	14 (8%)	10	33
50	m	38/38 (100%)	35 (92%)	3 (8%)	12	35
51	n	148/148 (100%)	134 (90%)	14 (10%)	8	27
52	o	51/51 (100%)	46 (90%)	5 (10%)	8	26
53	p	136/138 (99%)	132 (97%)	4 (3%)	42	64
54	q	34/34 (100%)	32 (94%)	2 (6%)	19	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	r	114/114 (100%)	104 (91%)	10 (9%)	10 31
56	s	116/116 (100%)	110 (95%)	6 (5%)	23 48
57	t	104/104 (100%)	98 (94%)	6 (6%)	20 45
58	u	103/103 (100%)	97 (94%)	6 (6%)	20 45
59	v	109/109 (100%)	104 (95%)	5 (5%)	27 52
60	w	99/103 (96%)	91 (92%)	8 (8%)	11 35
61	x	86/87 (99%)	80 (93%)	6 (7%)	15 40
62	y	99/100 (99%)	95 (96%)	4 (4%)	31 55
63	z	89/90 (99%)	87 (98%)	2 (2%)	52 71
All	All	7614/8413 (90%)	7142 (94%)	472 (6%)	22 43

All (472) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	LYS
1	0	13	ARG
1	0	48	LYS
1	0	51	VAL
1	0	68	ARG
1	0	86	GLN
2	1	7	HIS
2	1	19	LEU
2	1	30	SER
2	1	41	LYS
2	1	69	LEU
2	1	97	LEU
2	1	107	VAL
2	1	109	ASP
2	1	110	ARG
3	2	1	MET
3	2	24	MET
3	2	37	ASP
3	2	59	ASN
3	2	93	LEU
4	3	52	LEU
4	3	68	SER
4	3	72	ILE
4	3	89	ASP
4	3	99	ASN

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Mol	Chain	Res	Type
4	3	101	GLU
5	4	40	ILE
5	4	41	GLU
5	4	69	GLU
5	4	71	LYS
10	AA	723	VAL
10	AA	728	ASP
10	AA	731	ARG
10	AA	752	ASN
10	AA	817	LEU
10	AA	840	SER
10	AA	844	LYS
10	AA	845	LEU
10	AA	851	THR
10	AA	853	ASP
10	AA	854	ILE
10	AA	857	VAL
10	AA	864	LYS
10	AA	866	ASP
10	AA	867	GLU
10	AA	868	SER
10	AA	871	VAL
10	AA	872	TYR
10	AA	873	ILE
10	AA	886	LYS
10	AA	887	VAL
10	AA	890	LYS
10	AA	911	SER
10	AA	914	LYS
10	AA	915	ASP
10	AA	916	SER
10	AA	918	LEU
10	AA	935	THR
10	AA	936	ARG
10	AA	939	VAL
10	AA	941	LYS
10	AA	942	ASP
10	AA	943	LYS
10	AA	944	ARG
10	AA	949	GLU
10	AA	950	GLU
10	AA	951	MET

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Mol	Chain	Res	Type
10	AA	952	GLN
10	AA	953	LEU
10	AA	954	LYS
10	AA	955	GLN
10	AA	957	LYS
10	AA	958	LYS
10	AA	959	ASP
10	AA	960	LEU
10	AA	962	GLU
10	AA	971	LEU
10	AA	974	ARG
10	AA	975	ILE
10	AA	979	LEU
10	AA	980	VAL
10	AA	987	GLU
10	AA	989	LEU
10	AA	992	LEU
10	AA	993	PRO
10	AA	994	ARG
10	AA	995	ASP
10	AA	996	ARG
10	AA	997	TRP
10	AA	999	GLU
10	AA	1000	LEU
10	AA	1005	GLU
10	AA	1006	GLU
10	AA	1007	LYS
10	AA	1009	ASN
10	AA	1011	LEU
10	AA	1012	GLU
10	AA	1013	GLN
10	AA	1014	LEU
10	AA	1017	GLN
10	AA	1018	TYR
10	AA	1019	ASP
10	AA	1020	GLU
10	AA	1025	PHE
10	AA	1027	LYS
10	AA	1028	LYS
10	AA	1029	LEU
10	AA	1032	LYS
10	AA	1034	ARG

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Mol	Chain	Res	Type
10	AA	1035	LYS
10	AA	1038	GLN
10	AA	1040	ASP
10	AA	1041	ASP
10	AA	1046	VAL
10	AA	1047	LEU
10	AA	1048	LYS
10	AA	1049	ILE
10	AA	1151	LEU
10	AA	1159	VAL
10	AA	1236	ASN
10	AA	1250	SER
10	AA	1252	SER
10	AA	1253	LEU
10	AA	1254	VAL
10	AA	1256	GLN
10	AA	1259	LEU
11	AB	21	ARG
11	AB	47	GLU
12	AC	12	ARG
12	AC	72	GLU
12	AC	91	ARG
12	AC	134	THR
12	AC	158	ARG
12	AC	159	ILE
12	AC	160	HIS
12	AC	162	GLU
12	AC	163	GLU
12	AC	165	GLU
12	AC	166	ARG
12	AC	168	ILE
12	AC	170	ARG
12	AC	171	LEU
12	AD	12	ARG
12	AD	208	ASN
13	AE	40	LYS
13	AE	42	GLU
13	AE	44	ILE
13	AE	46	TYR
13	AE	47	ARG
13	AE	49	PHE
13	AE	50	LYS

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Mol	Chain	Res	Type
13	AE	52	GLU
13	AE	53	ARG
13	AE	54	ASP
13	AE	60	ARG
13	AE	67	ASP
13	AE	70	CYS
13	AE	72	CYS
13	AE	74	LYS
13	AE	76	LYS
13	AE	77	ARG
13	AE	78	LEU
13	AE	81	ARG
13	AE	87	LYS
13	AE	88	CYS
13	AE	91	GLU
13	AE	94	GLN
13	AE	95	THR
13	AE	99	ARG
13	AE	100	GLU
13	AE	117	LEU
13	AE	119	SER
13	AE	123	ARG
13	AE	132	LEU
13	AE	135	ILE
13	AE	142	GLU
13	AE	144	TYR
13	AE	145	VAL
13	AE	147	ILE
13	AE	152	THR
13	AE	154	LEU
13	AE	157	GLN
13	AE	159	ILE
13	AE	175	GLU
13	AE	180	MET
13	AE	190	LYS
13	AE	193	ASP
13	AE	196	GLN
13	AE	210	SER
13	AE	215	LYS
13	AE	216	LYS
13	AE	222	LYS
13	AE	223	LEU

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Mol	Chain	Res	Type
13	AE	227	PHE
13	AE	232	ASN
13	AE	233	LYS
13	AE	237	MET
13	AE	238	ILE
13	AE	239	LEU
13	AE	240	THR
13	AE	244	VAL
13	AE	271	ARG
13	AE	385	LEU
13	AE	386	GLU
13	AE	390	LEU
13	AE	393	THR
13	AE	394	ILE
13	AE	395	LYS
13	AE	514	THR
13	AE	709	ARG
13	AE	836	ARG
13	AE	1172	LYS
13	AE	1373	ARG
15	C	33	ILE
15	C	74	HIS
17	E	6	SER
17	E	10	ARG
17	E	48	GLN
17	E	54	MET
17	E	64	LYS
18	F	34	ARG
18	F	62	ARG
18	F	67	ARG
19	G	8	ASP
19	G	23	TRP
19	G	45	LYS
19	G	105	LYS
19	G	128	LYS
19	G	129	LEU
19	G	132	LYS
19	G	208	ARG
20	H	9	PHE
20	H	54	LYS
20	H	273	ARG
20	H	305	HIS

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Mol	Chain	Res	Type
20	H	336	ASP
20	H	337	GLU
20	H	338	GLU
20	H	339	ARG
20	H	340	ARG
21	I	14	ILE
21	I	89	LYS
21	I	164	ARG
21	I	185	ASN
21	I	200	VAL
22	J	47	ARG
22	J	95	GLU
22	J	104	ARG
22	J	116	GLN
22	J	138	SER
22	J	143	VAL
23	K	10	GLU
23	K	15	LEU
23	K	60	ILE
23	K	114	VAL
23	K	115	LEU
23	K	138	ARG
23	K	162	GLU
24	L	16	GLU
24	L	24	ARG
24	L	38	ARG
24	L	54	LEU
24	L	79	ARG
24	L	86	ARG
25	M	7	ILE
25	M	17	LYS
25	M	21	GLU
25	M	23	LEU
25	M	79	ARG
25	M	109	ARG
25	M	130	ASN
25	M	146	GLU
26	N	96	MET
26	N	121	LEU
27	O	12	ARG
27	O	27	LYS
27	O	60	LYS

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Mol	Chain	Res	Type
27	O	63	LEU
27	O	118	LEU
28	P	5	ARG
28	P	17	LEU
28	P	24	GLU
28	P	25	ILE
28	P	27	GLU
28	P	37	ARG
29	Q	15	GLN
29	Q	56	ARG
29	Q	107	ILE
30	R	5	ASN
30	R	12	ARG
30	R	24	LEU
30	R	56	ARG
30	R	62	GLU
30	R	74	LEU
30	R	102	LEU
31	S	45	VAL
31	S	46	LEU
31	S	89	MET
31	S	92	GLU
32	T	10	LYS
32	T	17	ARG
32	T	22	THR
32	T	39	LEU
32	T	40	GLN
32	T	64	ARG
32	T	66	LEU
32	T	67	LEU
32	T	70	LEU
32	T	73	LYS
32	T	84	ARG
32	T	85	LEU
33	U	1	MET
33	U	2	VAL
33	U	6	LEU
33	U	19	VAL
33	U	50	THR
34	V	75	LEU
34	V	81	LYS
35	W	12	ASP

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Mol	Chain	Res	Type
35	W	21	LYS
35	W	33	THR
35	W	79	THR
36	X	11	ASP
36	X	16	VAL
36	X	25	VAL
36	X	29	ARG
36	X	59	GLU
36	X	92	ARG
36	X	93	ARG
36	X	101	ARG
36	X	117	LYS
39	b	70	GLU
40	c	48	THR
40	c	54	LYS
40	c	71	LEU
42	e	58	ASN
43	f	3	LYS
43	f	45	ARG
44	g	3	LYS
44	g	16	CYS
44	g	43	PHE
44	g	47	LYS
44	g	59	ARG
44	g	65	ASN
45	h	51	THR
45	h	52	ARG
45	h	118	SER
45	h	125	LYS
45	h	130	LEU
45	h	141	VAL
45	h	156	ARG
45	h	187	ASP
45	h	189	ARG
45	h	195	VAL
45	h	202	LEU
45	h	203	ARG
45	h	204	VAL
45	h	205	LEU
45	h	242	LYS
45	h	258	ARG
45	h	271	ARG

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Mol	Chain	Res	Type
46	i	9	THR
46	i	12	LYS
46	i	26	THR
46	i	27	SER
46	i	29	SER
46	i	40	ARG
47	j	13	ARG
47	j	18	ASP
47	j	32	ASN
47	j	46	ARG
47	j	91	THR
47	j	103	ASP
47	j	131	ASP
48	k	5	ILE
48	k	24	THR
48	k	26	ASN
49	l	7	ASP
49	l	17	THR
49	l	22	ASP
49	l	40	ARG
49	l	48	THR
49	l	57	LYS
49	l	69	ARG
49	l	77	ILE
49	l	80	SER
49	l	108	ILE
49	l	109	LEU
49	l	122	GLU
49	l	149	ILE
49	l	179	SER
50	m	22	MET
50	m	41	ARG
50	m	42	LEU
51	n	6	ASP
51	n	10	ASP
51	n	57	LEU
51	n	80	ARG
51	n	95	ARG
51	n	105	THR
51	n	115	ARG
51	n	117	LEU
51	n	122	PHE

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Mol	Chain	Res	Type
51	n	123	ASP
51	n	133	ARG
51	n	140	GLU
51	n	152	LEU
51	n	163	ASP
52	o	8	ARG
52	o	30	ARG
52	o	31	HIS
52	o	54	ASP
52	o	55	LEU
53	p	39	ASP
53	p	95	ARG
53	p	125	CYS
53	p	171	THR
54	q	3	VAL
54	q	26	ILE
55	r	11	ASN
55	r	12	LEU
55	r	15	LEU
55	r	41	LYS
55	r	66	ASN
55	r	72	ILE
55	r	87	GLU
55	r	97	ARG
55	r	101	ASP
55	r	127	GLU
56	s	1	MET
56	s	14	ASP
56	s	30	THR
56	s	40	HIS
56	s	57	LEU
56	s	142	ILE
57	t	32	TYR
57	t	49	ARG
57	t	53	LYS
57	t	80	ASP
57	t	88	ASN
57	t	104	THR
58	u	5	THR
58	u	27	LEU
58	u	48	ARG
58	u	59	ARG

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Mol	Chain	Res	Type
58	u	76	GLU
58	u	78	ARG
59	v	18	ARG
59	v	84	LYS
59	v	110	GLU
59	v	126	ILE
59	v	128	THR
60	w	2	ARG
60	w	20	MET
60	w	24	MET
60	w	51	LEU
60	w	63	ARG
60	w	65	LEU
60	w	69	ARG
60	w	95	THR
61	x	13	ARG
61	x	19	GLN
61	x	31	THR
61	x	47	VAL
61	x	48	LEU
61	x	91	SER
62	y	10	GLN
62	y	27	GLU
62	y	85	SER
62	y	114	LEU
63	z	18	LEU
63	z	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
10	AA	1008	GLN
11	AB	81	HIS
19	G	18	HIS
23	K	61	GLN
32	T	40	GLN
36	X	105	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	D	1513/1542 (98%)	285 (18%)	33 (2%)
37	Y	2/3 (66%)	2 (100%)	0
38	a	2859/2904 (98%)	532 (18%)	0
41	d	119/120 (99%)	17 (14%)	0
8	7	15/44 (34%)	7 (46%)	0
9	A	75/76 (98%)	29 (38%)	6 (8%)
9	B	75/76 (98%)	34 (45%)	5 (6%)
All	All	4658/4765 (97%)	906 (19%)	44 (0%)

All (906) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	56	U
8	7	57	G
8	7	58	A
8	7	59	U
8	7	60	U
8	7	62	G
8	7	63	G
9	A	2	G
9	A	6	G
9	A	7	G
9	A	8	U
9	A	10	G
9	A	13	C
9	A	14	A
9	A	15	G
9	A	16	C
9	A	17	C
9	A	18	G
9	A	19	G
9	A	20	U
9	A	21	A
9	A	22	G
9	A	23	C
9	A	46	G
9	A	47	U
9	A	48	C
9	A	49	G
9	A	52	G
9	A	57	A
9	A	58	A
9	A	59	A

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Mol	Chain	Res	Type
9	A	61	C
9	A	66	C
9	A	69	C
9	A	71	C
9	A	73	A
9	B	2	G
9	B	6	G
9	B	7	G
9	B	8	U
9	B	10	G
9	B	13	C
9	B	14	A
9	B	15	G
9	B	16	C
9	B	17	C
9	B	18	G
9	B	19	G
9	B	20	U
9	B	21	A
9	B	22	G
9	B	23	C
9	B	30	G
9	B	31	G
9	B	32	C
9	B	37	A
9	B	38	A
9	B	46	G
9	B	47	U
9	B	48	C
9	B	49	G
9	B	52	G
9	B	57	A
9	B	58	A
9	B	59	A
9	B	61	C
9	B	66	C
9	B	69	C
9	B	71	C
9	B	73	A
16	D	4	U
16	D	5	U
16	D	9	G

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Mol	Chain	Res	Type
16	D	22	G
16	D	29	U
16	D	32	A
16	D	39	G
16	D	41	G
16	D	47	C
16	D	48	C
16	D	50	A
16	D	51	A
16	D	52	C
16	D	54	C
16	D	69	G
16	D	70	U
16	D	71	A
16	D	72	A
16	D	74	A
16	D	76	G
16	D	82	G
16	D	83	C
16	D	84	U
16	D	87	C
16	D	90	C
16	D	94	G
16	D	95	C
16	D	96	U
16	D	108	G
16	D	120	A
16	D	122	G
16	D	128	G
16	D	131	A
16	D	141	G
16	D	144	G
16	D	148	G
16	D	149	A
16	D	160	A
16	D	164	G
16	D	173	U
16	D	181	A
16	D	182	A
16	D	197	A
16	D	198	G
16	D	204	G

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Mol	Chain	Res	Type
16	D	208	U
16	D	209	U
16	D	210	C
16	D	211	G
16	D	212	G
16	D	216	U
16	D	226	G
16	D	245	U
16	D	247	G
16	D	251	G
16	D	258	G
16	D	262	A
16	D	266	G
16	D	267	C
16	D	271	C
16	D	279	A
16	D	289	G
16	D	299	G
16	D	306	A
16	D	321	A
16	D	328	C
16	D	329	A
16	D	332	G
16	D	347	G
16	D	352	C
16	D	353	A
16	D	354	G
16	D	355	C
16	D	367	U
16	D	372	C
16	D	373	A
16	D	376	G
16	D	382	A
16	D	384	G
16	D	392	C
16	D	393	A
16	D	397	A
16	D	406	G
16	D	412	A
16	D	413	G
16	D	414	A
16	D	421	U

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Mol	Chain	Res	Type
16	D	422	C
16	D	424	G
16	D	429	U
16	D	446	G
16	D	451	A
16	D	457	G
16	D	458	U
16	D	460	A
16	D	463	U
16	D	464	U
16	D	467	U
16	D	468	A
16	D	469	C
16	D	478	A
16	D	479	U
16	D	481	G
16	D	484	G
16	D	485	U
16	D	486	U
16	D	505	G
16	D	509	A
16	D	511	C
16	D	518	C
16	D	519	C
16	D	526	C
16	D	531	U
16	D	532	A
16	D	533	A
16	D	542	G
16	D	547	A
16	D	559	A
16	D	562	U
16	D	568	G
16	D	572	A
16	D	573	A
16	D	576	C
16	D	577	G
16	D	579	A
16	D	596	A
16	D	628	G
16	D	633	G
16	D	642	A

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Mol	Chain	Res	Type
16	D	649	A
16	D	650	G
16	D	653	U
16	D	665	A
16	D	666	G
16	D	687	A
16	D	700	G
16	D	723	U
16	D	724	G
16	D	731	G
16	D	734	G
16	D	747	A
16	D	748	G
16	D	755	G
16	D	760	G
16	D	777	A
16	D	793	U
16	D	794	A
16	D	815	A
16	D	817	C
16	D	828	U
16	D	829	G
16	D	832	G
16	D	841	C
16	D	844	G
16	D	845	A
16	D	846	G
16	D	849	G
16	D	874	G
16	D	887	G
16	D	902	G
16	D	914	A
16	D	916	U
16	D	926	G
16	D	934	C
16	D	935	A
16	D	954	G
16	D	960	U
16	D	963	G
16	D	969	A
16	D	972	C
16	D	975	A

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Mol	Chain	Res	Type
16	D	976	G
16	D	991	U
16	D	992	U
16	D	993	G
16	D	996	A
16	D	999	C
16	D	1004	A
16	D	1008	U
16	D	1009	U
16	D	1017	U
16	D	1018	G
16	D	1021	A
16	D	1024	G
16	D	1026	G
16	D	1028	C
16	D	1030	U
16	D	1031	C
16	D	1037	C
16	D	1043	G
16	D	1044	A
16	D	1046	A
16	D	1065	U
16	D	1085	U
16	D	1086	U
16	D	1094	G
16	D	1095	U
16	D	1099	G
16	D	1101	A
16	D	1124	G
16	D	1133	G
16	D	1135	U
16	D	1136	C
16	D	1137	C
16	D	1139	G
16	D	1140	C
16	D	1141	C
16	D	1142	G
16	D	1143	G
16	D	1145	A
16	D	1146	A
16	D	1151	A
16	D	1152	A

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Mol	Chain	Res	Type
16	D	1158	C
16	D	1159	U
16	D	1167	A
16	D	1171	A
16	D	1174	G
16	D	1175	G
16	D	1176	A
16	D	1184	G
16	D	1196	A
16	D	1197	A
16	D	1206	G
16	D	1211	U
16	D	1212	U
16	D	1213	A
16	D	1214	C
16	D	1215	G
16	D	1226	C
16	D	1227	A
16	D	1228	C
16	D	1238	A
16	D	1256	A
16	D	1257	A
16	D	1260	G
16	D	1275	A
16	D	1276	G
16	D	1278	G
16	D	1279	G
16	D	1280	A
16	D	1285	A
16	D	1286	U
16	D	1287	A
16	D	1299	A
16	D	1300	G
16	D	1302	C
16	D	1305	G
16	D	1312	G
16	D	1317	C
16	D	1320	C
16	D	1323	G
16	D	1329	A
16	D	1338	G
16	D	1340	A

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Mol	Chain	Res	Type
16	D	1346	A
16	D	1347	G
16	D	1353	G
16	D	1363	A
16	D	1370	G
16	D	1378	C
16	D	1379	G
16	D	1381	U
16	D	1391	U
16	D	1396	A
16	D	1397	C
16	D	1419	G
16	D	1429	A
16	D	1441	A
16	D	1446	A
16	D	1447	A
16	D	1448	C
16	D	1452	C
16	D	1453	G
16	D	1475	G
16	D	1487	G
16	D	1492	A
16	D	1494	G
16	D	1495	U
16	D	1497	G
16	D	1503	A
16	D	1506	U
16	D	1529	G
16	D	1530	G
16	D	1534	A
37	Y	72	U
37	Y	73	U
38	a	10	A
38	a	15	G
38	a	34	U
38	a	35	G
38	a	46	G
38	a	58	G
38	a	60	G
38	a	63	A
38	a	71	A
38	a	74	A

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Mol	Chain	Res	Type
38	a	75	G
38	a	83	A
38	a	84	A
38	a	85	G
38	a	93	G
38	a	96	C
38	a	102	U
38	a	103	A
38	a	110	G
38	a	114	U
38	a	118	A
38	a	119	A
38	a	120	U
38	a	122	G
38	a	131	A
38	a	136	G
38	a	139	U
38	a	140	C
38	a	141	G
38	a	145	C
38	a	163	C
38	a	165	A
38	a	181	A
38	a	196	A
38	a	200	U
38	a	215	G
38	a	216	A
38	a	222	A
38	a	225	C
38	a	248	G
38	a	249	C
38	a	261	G
38	a	264	C
38	a	265	A
38	a	266	G
38	a	267	C
38	a	271	G
38	a	272	A
38	a	275	C
38	a	276	U
38	a	278	A
38	a	285	G

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Mol	Chain	Res	Type
38	a	311	A
38	a	324	A
38	a	329	G
38	a	330	A
38	a	353	C
38	a	359	G
38	a	361	G
38	a	362	A
38	a	371	A
38	a	372	G
38	a	373	U
38	a	375	G
38	a	383	C
38	a	386	G
38	a	396	G
38	a	405	U
38	a	411	G
38	a	412	A
38	a	420	C
38	a	424	G
38	a	435	C
38	a	451	U
38	a	456	C
38	a	457	A
38	a	477	A
38	a	481	G
38	a	491	G
38	a	501	A
38	a	503	A
38	a	504	A
38	a	505	A
38	a	509	C
38	a	522	A
38	a	529	A
38	a	532	A
38	a	543	G
38	a	546	U
38	a	547	A
38	a	548	G
38	a	549	G
38	a	551	G
38	a	563	A

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Mol	Chain	Res	Type
38	a	569	U
38	a	573	U
38	a	575	A
38	a	588	U
38	a	603	A
38	a	609	A
38	a	613	A
38	a	614	A
38	a	615	U
38	a	616	A
38	a	618	G
38	a	621	A
38	a	627	A
38	a	637	A
38	a	645	C
38	a	647	G
38	a	654	A
38	a	664	G
38	a	668	A
38	a	685	A
38	a	686	U
38	a	710	U
38	a	717	C
38	a	730	A
38	a	738	G
38	a	757	G
38	a	764	A
38	a	765	C
38	a	775	G
38	a	776	G
38	a	782	A
38	a	784	G
38	a	785	G
38	a	800	A
38	a	802	A
38	a	805	G
38	a	812	C
38	a	819	A
38	a	827	U
38	a	828	U
38	a	845	A
38	a	846	U

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Mol	Chain	Res	Type
38	a	858	G
38	a	859	G
38	a	869	G
38	a	878	A
38	a	881	G
38	a	884	U
38	a	885	C
38	a	888	C
38	a	891	G
38	a	892	A
38	a	893	C
38	a	895	U
38	a	896	A
38	a	897	C
38	a	899	A
38	a	907	G
38	a	910	A
38	a	914	G
38	a	915	C
38	a	931	U
38	a	941	A
38	a	945	A
38	a	946	C
38	a	953	G
38	a	961	C
38	a	974	G
38	a	983	A
38	a	995	C
38	a	996	A
38	a	999	U
38	a	1005	C
38	a	1012	U
38	a	1013	C
38	a	1022	G
38	a	1023	U
38	a	1026	G
38	a	1033	U
38	a	1041	G
38	a	1045	C
38	a	1046	A
38	a	1047	G
38	a	1060	U

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Mol	Chain	Res	Type
38	a	1061	U
38	a	1062	G
38	a	1063	G
38	a	1064	C
38	a	1065	U
38	a	1066	U
38	a	1067	A
38	a	1068	G
38	a	1069	A
38	a	1070	A
38	a	1071	G
38	a	1073	A
38	a	1074	G
38	a	1076	C
38	a	1079	C
38	a	1080	A
38	a	1081	U
38	a	1082	U
38	a	1083	U
38	a	1084	A
38	a	1087	G
38	a	1088	A
38	a	1090	A
38	a	1095	A
38	a	1096	A
38	a	1107	G
38	a	1110	G
38	a	1111	A
38	a	1112	G
38	a	1119	U
38	a	1122	G
38	a	1132	U
38	a	1134	A
38	a	1135	C
38	a	1142	A
38	a	1169	A
38	a	1170	C
38	a	1173	U
38	a	1174	U
38	a	1175	A
38	a	1176	U
38	a	1177	G

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Mol	Chain	Res	Type
38	a	1178	C
38	a	1179	G
38	a	1180	U
38	a	1186	G
38	a	1238	G
38	a	1248	G
38	a	1253	A
38	a	1256	G
38	a	1266	G
38	a	1271	G
38	a	1272	A
38	a	1273	U
38	a	1301	A
38	a	1321	A
38	a	1345	C
38	a	1352	U
38	a	1365	A
38	a	1368	G
38	a	1378	A
38	a	1379	U
38	a	1380	G
38	a	1383	A
38	a	1387	A
38	a	1395	A
38	a	1406	U
38	a	1407	G
38	a	1408	G
38	a	1411	U
38	a	1414	C
38	a	1415	U
38	a	1416	G
38	a	1417	C
38	a	1419	A
38	a	1420	A
38	a	1428	C
38	a	1452	G
38	a	1453	A
38	a	1460	U
38	a	1478	G
38	a	1482	G
38	a	1490	A
38	a	1497	U

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Mol	Chain	Res	Type
38	a	1503	A
38	a	1508	A
38	a	1509	A
38	a	1510	G
38	a	1515	A
38	a	1529	G
38	a	1534	U
38	a	1535	A
38	a	1536	C
38	a	1537	G
38	a	1554	U
38	a	1559	U
38	a	1566	A
38	a	1569	A
38	a	1578	U
38	a	1580	A
38	a	1581	G
38	a	1582	C
38	a	1583	A
38	a	1584	U
38	a	1589	U
38	a	1590	A
38	a	1608	A
38	a	1609	A
38	a	1610	A
38	a	1647	U
38	a	1648	U
38	a	1649	G
38	a	1651	G
38	a	1674	G
38	a	1677	A
38	a	1703	G
38	a	1714	U
38	a	1715	G
38	a	1718	G
38	a	1729	U
38	a	1730	C
38	a	1732	C
38	a	1738	G
38	a	1750	G
38	a	1755	A
38	a	1758	U

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Mol	Chain	Res	Type
38	a	1764	C
38	a	1773	A
38	a	1791	A
38	a	1800	C
38	a	1801	A
38	a	1808	A
38	a	1811	G
38	a	1816	C
38	a	1829	A
38	a	1833	C
38	a	1847	A
38	a	1848	A
38	a	1858	A
38	a	1859	U
38	a	1862	G
38	a	1864	U
38	a	1869	G
38	a	1870	C
38	a	1872	A
38	a	1873	G
38	a	1905	C
38	a	1906	G
38	a	1907	G
38	a	1913	A
38	a	1914	C
38	a	1919	A
38	a	1920	C
38	a	1922	G
38	a	1923	U
38	a	1924	C
38	a	1925	C
38	a	1926	U
38	a	1928	A
38	a	1929	G
38	a	1930	G
38	a	1936	A
38	a	1938	A
38	a	1955	U
38	a	1965	C
38	a	1967	C
38	a	1970	A
38	a	1971	U

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Mol	Chain	Res	Type
38	a	1972	G
38	a	1987	A
38	a	1991	U
38	a	1992	G
38	a	1993	U
38	a	1997	C
38	a	2002	G
38	a	2022	U
38	a	2023	C
38	a	2027	G
38	a	2033	A
38	a	2043	C
38	a	2051	A
38	a	2052	A
38	a	2055	C
38	a	2056	G
38	a	2060	A
38	a	2061	G
38	a	2062	A
38	a	2077	A
38	a	2093	G
38	a	2097	A
38	a	2099	U
38	a	2100	G
38	a	2108	A
38	a	2110	G
38	a	2111	U
38	a	2113	U
38	a	2115	G
38	a	2116	G
38	a	2117	A
38	a	2118	U
38	a	2121	G
38	a	2122	U
38	a	2124	G
38	a	2125	G
38	a	2126	A
38	a	2127	G
38	a	2128	G
38	a	2131	U
38	a	2132	U
38	a	2133	G

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Mol	Chain	Res	Type
38	a	2134	A
38	a	2139	U
38	a	2141	G
38	a	2146	C
38	a	2147	A
38	a	2154	A
38	a	2157	G
38	a	2158	A
38	a	2159	G
38	a	2162	G
38	a	2163	A
38	a	2164	C
38	a	2165	C
38	a	2169	A
38	a	2171	A
38	a	2172	U
38	a	2178	C
38	a	2182	U
38	a	2183	A
38	a	2185	U
38	a	2188	U
38	a	2189	U
38	a	2190	G
38	a	2191	A
38	a	2193	G
38	a	2194	U
38	a	2198	A
38	a	2204	G
38	a	2210	U
38	a	2211	A
38	a	2212	A
38	a	2213	U
38	a	2225	A
38	a	2226	C
38	a	2229	U
38	a	2238	G
38	a	2239	G
38	a	2244	U
38	a	2250	G
38	a	2268	A
38	a	2278	A
38	a	2283	C

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Mol	Chain	Res	Type
38	a	2287	A
38	a	2297	A
38	a	2305	U
38	a	2308	G
38	a	2309	A
38	a	2315	G
38	a	2322	A
38	a	2325	G
38	a	2327	A
38	a	2333	A
38	a	2339	C
38	a	2345	G
38	a	2347	C
38	a	2350	C
38	a	2361	G
38	a	2372	U
38	a	2376	A
38	a	2383	G
38	a	2385	C
38	a	2402	U
38	a	2403	C
38	a	2406	A
38	a	2423	U
38	a	2424	C
38	a	2425	A
38	a	2426	A
38	a	2429	G
38	a	2430	A
38	a	2431	U
38	a	2434	A
38	a	2435	A
38	a	2441	U
38	a	2447	G
38	a	2448	A
38	a	2470	G
38	a	2474	U
38	a	2476	A
38	a	2478	A
38	a	2484	G
38	a	2491	U
38	a	2502	G
38	a	2506	U

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Mol	Chain	Res	Type
38	a	2507	C
38	a	2512	C
38	a	2513	A
38	a	2518	A
38	a	2520	C
38	a	2525	G
38	a	2529	G
38	a	2535	G
38	a	2547	A
38	a	2554	U
38	a	2566	A
38	a	2567	G
38	a	2572	A
38	a	2573	C
38	a	2574	G
38	a	2585	U
38	a	2586	U
38	a	2602	A
38	a	2603	G
38	a	2609	U
38	a	2610	C
38	a	2611	C
38	a	2613	U
38	a	2629	U
38	a	2663	G
38	a	2669	G
38	a	2671	G
38	a	2689	U
38	a	2690	U
38	a	2714	G
38	a	2722	G
38	a	2726	A
38	a	2744	G
38	a	2748	A
38	a	2757	A
38	a	2758	A
38	a	2765	A
38	a	2777	G
38	a	2778	A
38	a	2791	G
38	a	2793	C
38	a	2796	U

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Mol	Chain	Res	Type
38	a	2797	U
38	a	2798	U
38	a	2799	A
38	a	2801	G
38	a	2818	U
38	a	2820	A
38	a	2823	A
38	a	2825	G
38	a	2849	U
38	a	2850	A
38	a	2859	G
38	a	2861	U
38	a	2867	G
38	a	2880	C
38	a	2884	U
38	a	2885	G
38	a	2891	U
38	a	2902	C
41	d	2	G
41	d	9	G
41	d	13	G
41	d	16	G
41	d	17	C
41	d	35	C
41	d	36	C
41	d	45	A
41	d	51	G
41	d	56	G
41	d	64	G
41	d	66	A
41	d	88	C
41	d	89	U
41	d	90	C
41	d	99	A
41	d	109	A

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	6	G
9	A	7	G
9	A	9	G

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Mol	Chain	Res	Type
9	A	22	G
9	A	60	U
9	A	70	G
9	B	6	G
9	B	7	G
9	B	9	G
9	B	22	G
9	B	60	U
16	D	7	A
16	D	70	U
16	D	121	U
16	D	181	A
16	D	183	C
16	D	197	A
16	D	209	U
16	D	305	G
16	D	328	C
16	D	428	G
16	D	496	A
16	D	517	G
16	D	531	U
16	D	532	A
16	D	562	U
16	D	641	U
16	D	722	G
16	D	793	U
16	D	991	U
16	D	992	U
16	D	1109	C
16	D	1145	A
16	D	1196	A
16	D	1211	U
16	D	1212	U
16	D	1213	A
16	D	1214	C
16	D	1225	A
16	D	1299	A
16	D	1396	A
16	D	1432	G
16	D	1447	A
16	D	1493	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1515:G	O3'	1517:G	P	6.72

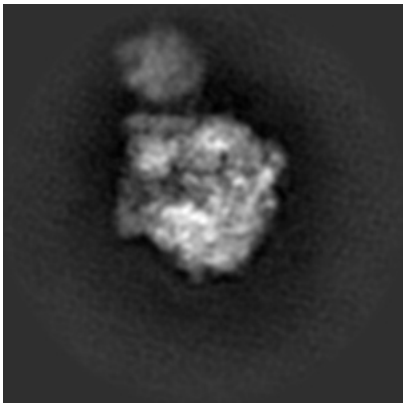
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21482. These allow visual inspection of the internal detail of the map and identification of artifacts.

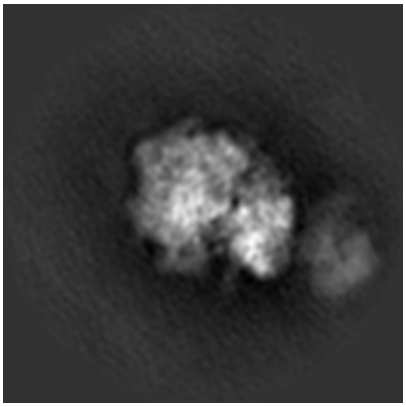
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

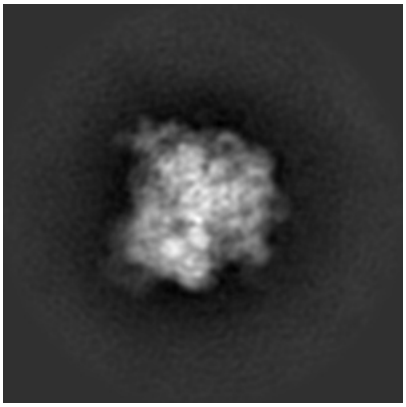
6.1.1 Primary map



X



Y

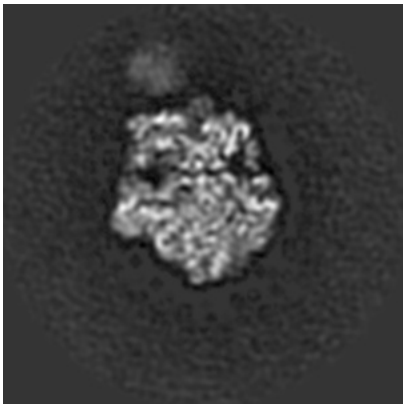


Z

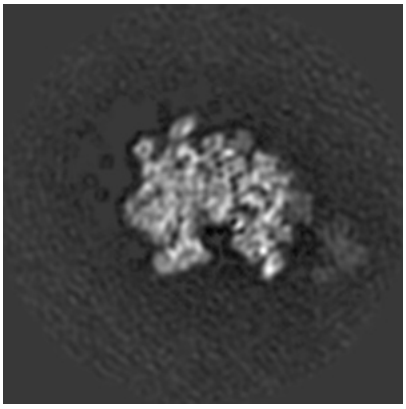
The images above show the map projected in three orthogonal directions.

6.2 Central slices

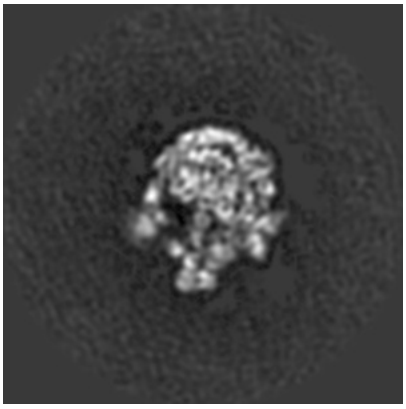
6.2.1 Primary map



X Index: 96



Y Index: 96

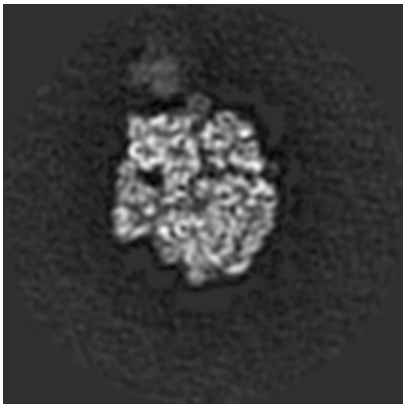


Z Index: 96

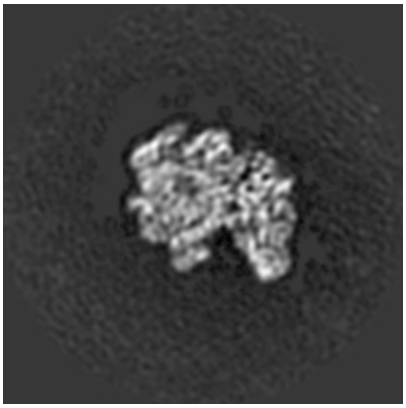
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

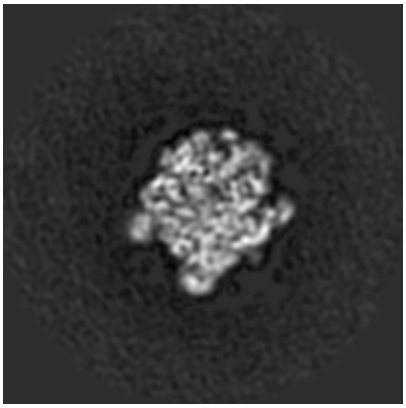
6.3.1 Primary map



X Index: 92



Y Index: 102



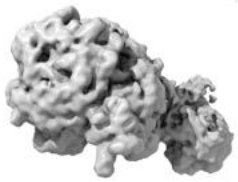
Z Index: 91

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

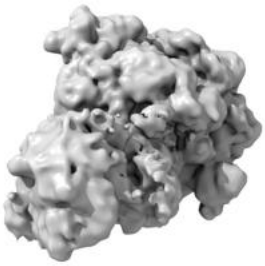
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0342. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

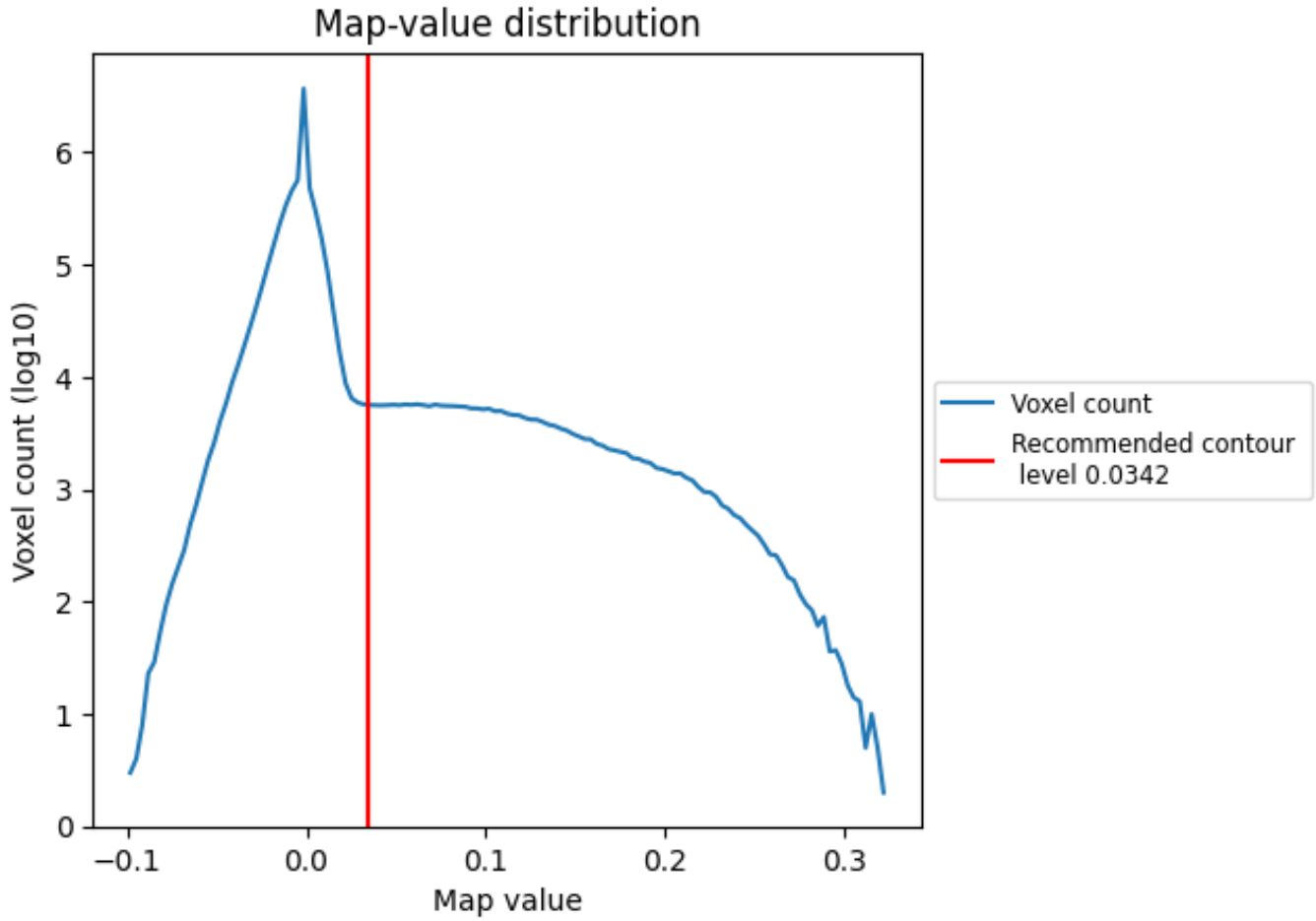
6.5 Mask visualisation (i)

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

7 Map analysis

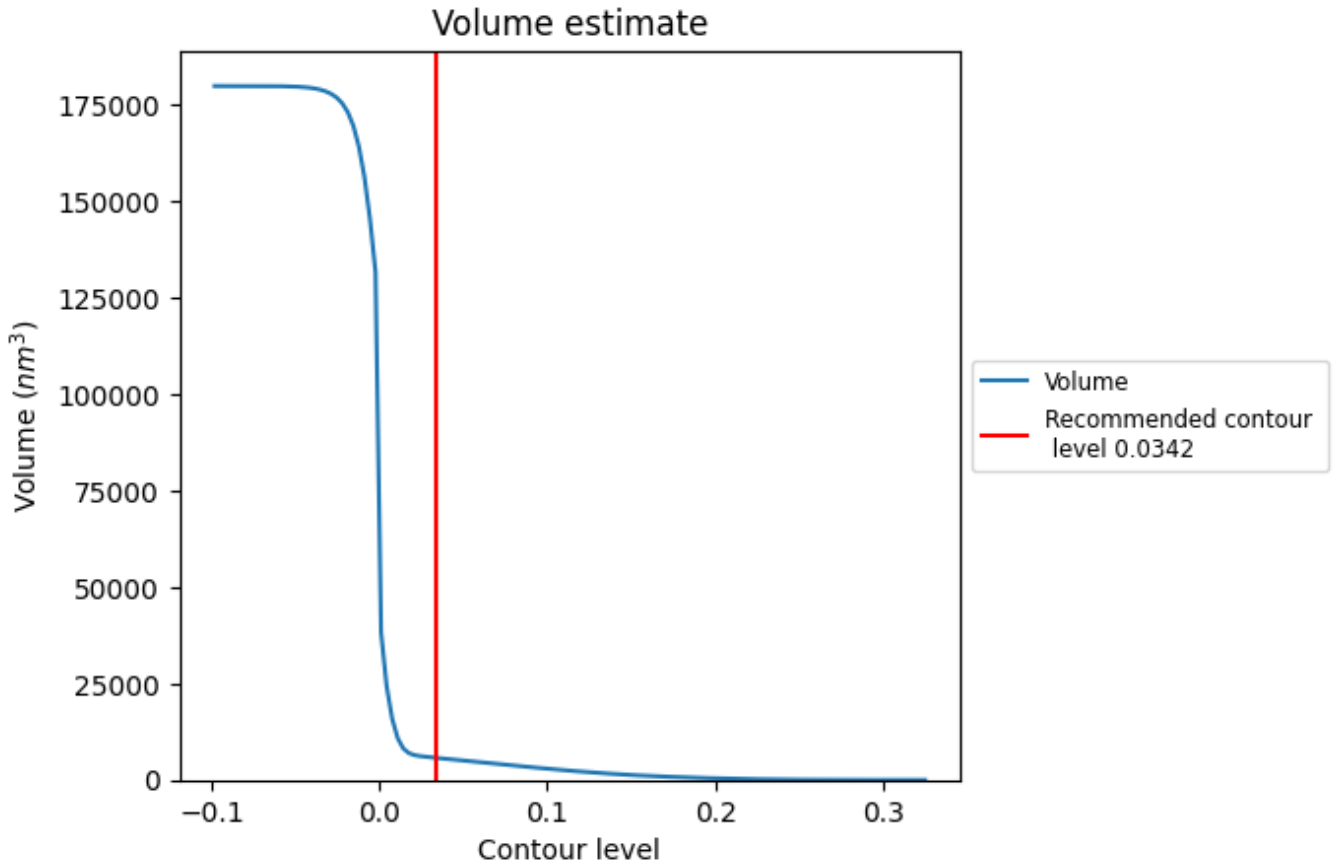
This section contains the results of statistical analysis of the map.

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.

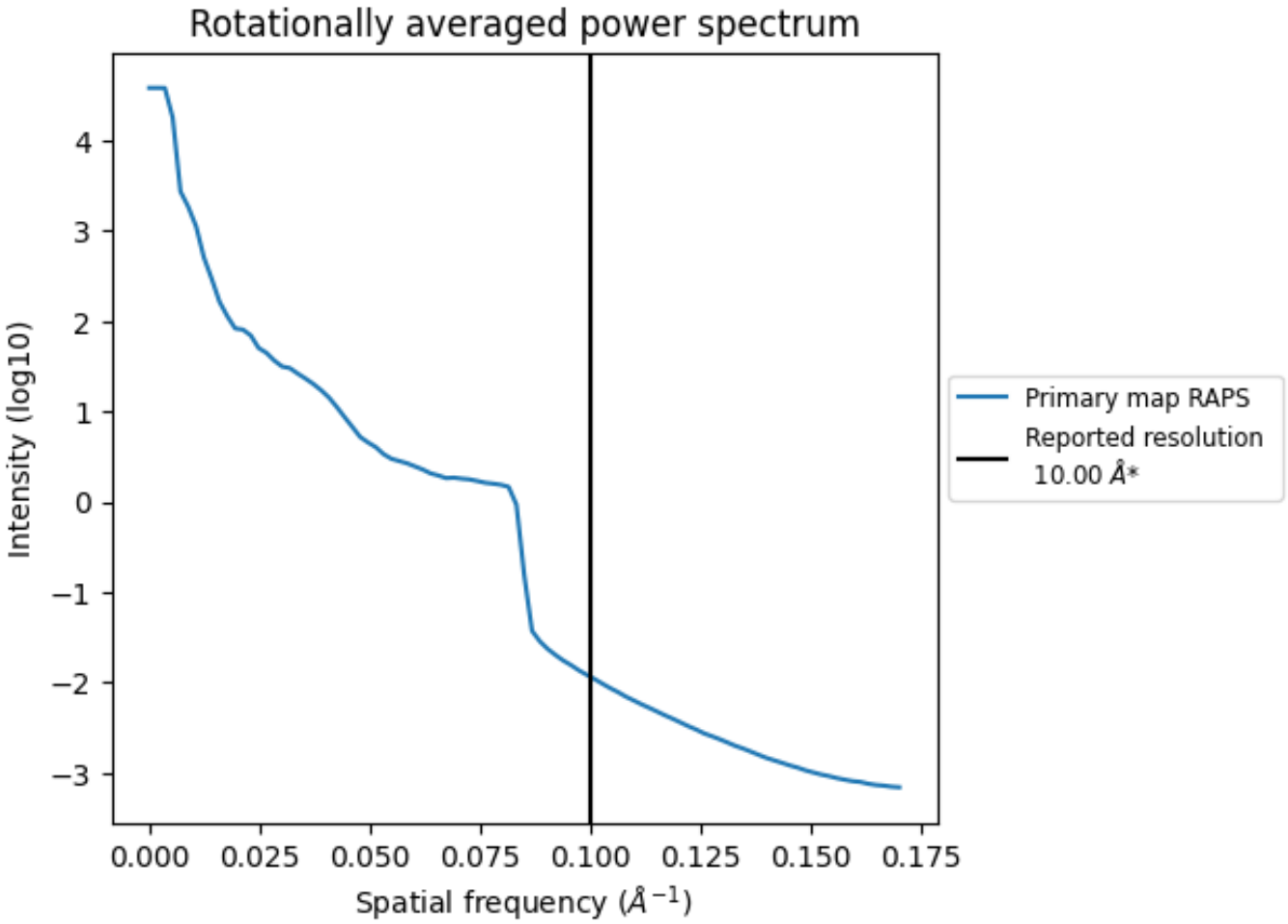
7.2 Volume estimate



The volume at the recommended contour level is 5708 nm^3; this corresponds to an approximate mass of 5157 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 0.100 $Å^{-1}$

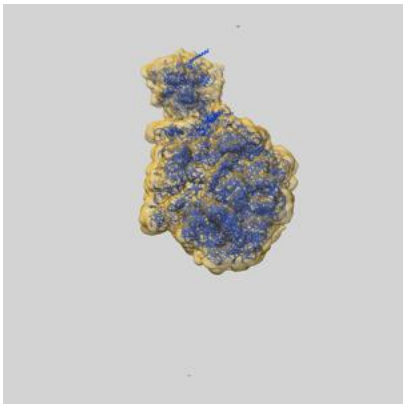
8 Fourier-Shell correlation (i)

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

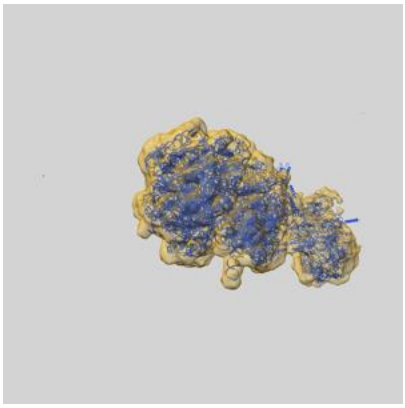
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21482 and PDB model 6VZ2. Per-residue inclusion information can be found in section 3 on page 16.

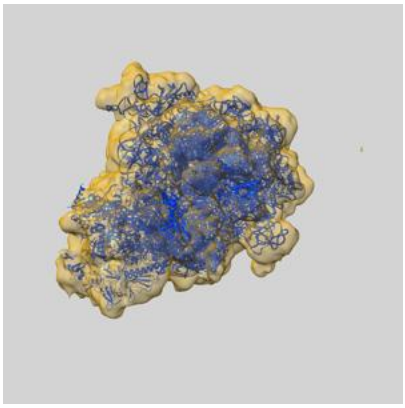
9.1 Map-model overlay



X



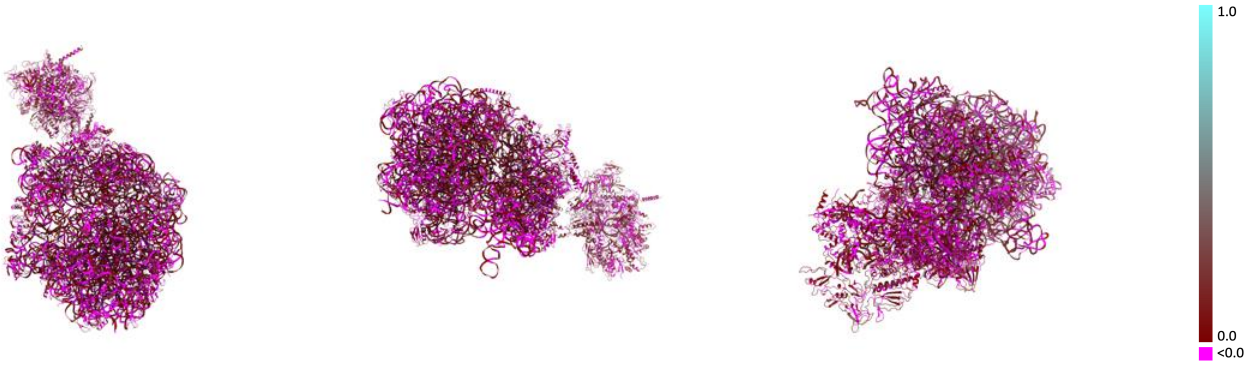
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0342 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.

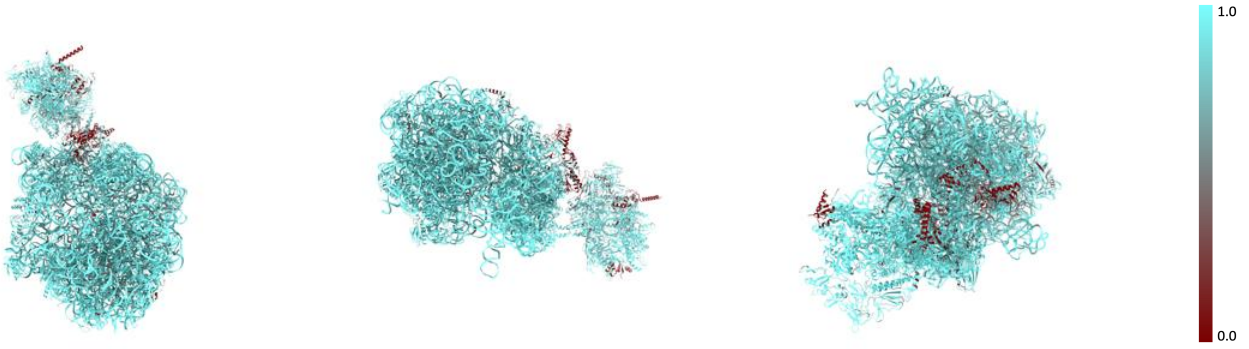
9.2 Q-score mapped to coordinate model (i)



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.

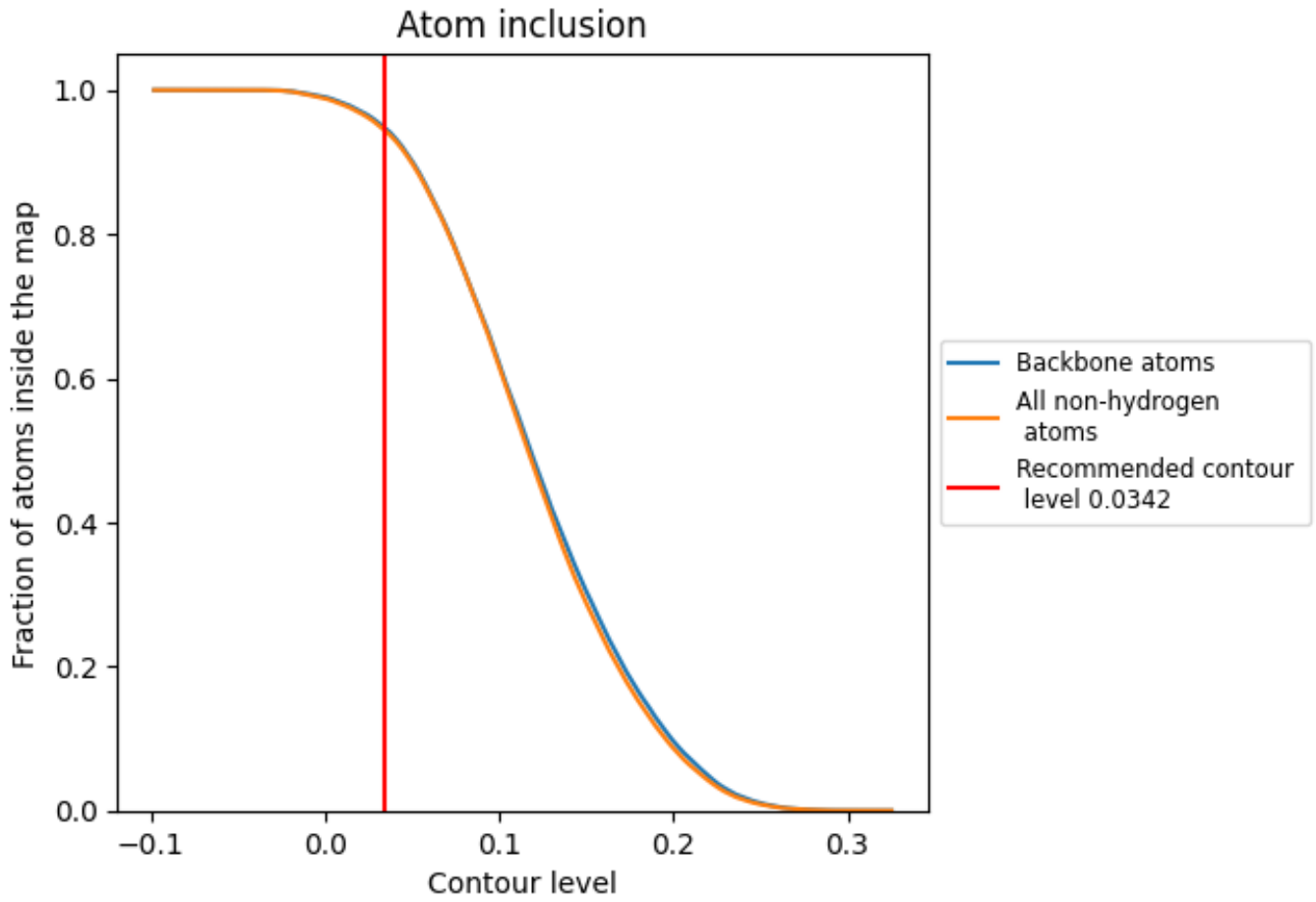
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0342).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.0342) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9439	0.0370
0	0.9987	0.0150
1	0.9976	0.0110
2	0.9274	-0.0210
3	0.8982	-0.0120
4	0.9837	0.0100
5	0.9979	0.1090
6	0.9945	0.0840
7	0.8732	0.0430
A	0.9111	0.0810
AA	0.9701	0.0510
AB	0.4508	-0.0110
AC	0.7500	0.0400
AD	0.7533	0.0410
AE	0.9219	0.0350
AF	0.2833	0.0220
B	0.8994	0.0500
C	1.0000	0.0040
D	0.9832	0.0510
E	0.9281	0.0060
F	0.8676	0.0340
G	0.5350	0.0060
H	0.0929	-0.0270
I	0.9591	-0.0040
J	0.9849	-0.0140
K	0.9920	0.0340
L	0.9541	0.0250
M	0.9476	0.0090
N	0.9521	-0.0060
O	0.9520	-0.0210
P	0.9987	0.0210
Q	0.9836	0.0400
R	0.9459	0.0500
S	1.0000	-0.0090
T	0.9826	0.0310

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Chain	Atom inclusion	Q-score
U	0.9984	0.0070
V	0.9351	0.0480
W	0.9181	0.0010
X	0.8698	-0.0040
Y	0.7667	-0.0420
a	0.9758	0.0490
b	1.0000	-0.0260
c	0.9617	0.0270
d	0.9763	0.0320
e	0.9571	-0.0280
f	1.0000	0.0130
g	0.9511	0.0270
h	0.9782	0.0270
i	0.9509	-0.0290
j	0.9785	-0.0130
k	0.9282	0.0100
l	0.9684	0.0100
m	0.9662	0.0030
n	0.9119	0.0290
o	0.9980	-0.0030
p	0.9798	0.0250
q	1.0000	-0.0170
r	0.7883	-0.0060
s	0.9855	-0.0070
t	0.9924	0.0180
u	1.0000	-0.0080
v	0.9750	0.0380
w	1.0000	-0.0090
x	0.9988	-0.0020
y	0.9482	-0.0210
z	1.0000	-0.0180