wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 02:17 pm BST

PDB ID	:	8CCS
EMDB ID	:	EMD-16563
Title	:	80S S. cerevisiae ribosome with ligands in hybrid-1 pre-translocation (PRE-H1) complex
Authors	:	Milicevic, N.; Jenner, L.; Myasnikov, A.; Yusupov, M.; Yusupova, G.
Deposited on	:	2023-01-27
Resolution	:	1.97 Å(reported)

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

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

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

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

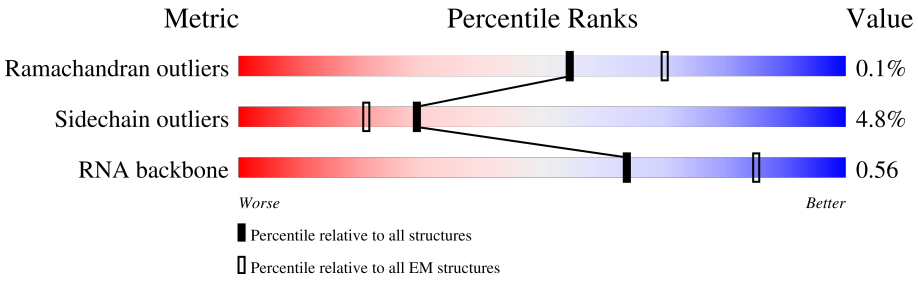
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.97 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%

Mol	Chain	Length	Quality of chain
1	0	135	91% 8% ·
2	1	108	62% · 35%
3	2	119	76% 5% 18%
4	3	82	98% ··
5	4	67	85% 9% 6%
6	5	56	80% 14% 5%
7	6	63	76% 8% 16%
8	7	319	87% 12%
9	8	152	22% · 76%

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Mol	Chain	Length	Quality of chain
10	A	199	98%
11	AA	3396	79% 15% 6%
12	B	184	83% 16%
13	BB	121	92% 8%
14	Bb	76	61% 39%
15	C	186	99%
16	CC	158	87% 13%
17	Cc	77	74% 25%
18	D	189	88% 5% 7%
19	DD	312	59% 37%
20	Dd	39	26% 8% 67%
21	E	172	97%
22	EE	254	98%
23	Ee	165	92%
24	F	160	95%
25	FF	387	97%
26	G	121	78% 20%
27	GG	362	97%
28	H	137	89% 5% 6%
29	HH	297	98%
30	I	155	40% 59%
31	II	176	86% 12%
32	J	142	83% 15%
33	JJ	244	89% 9%
34	K	127	95%

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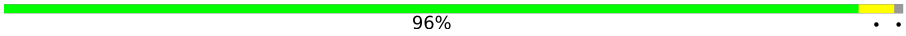
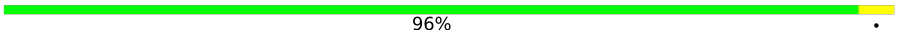
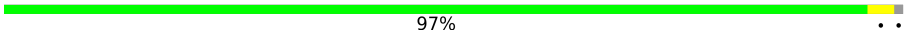
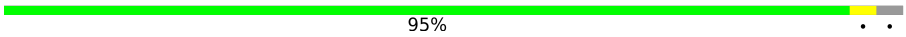
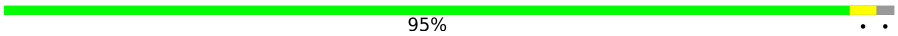
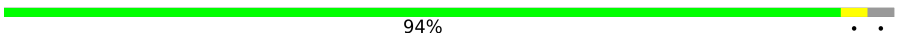
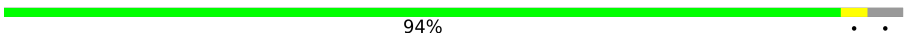
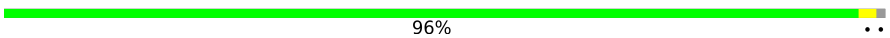
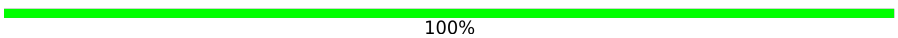
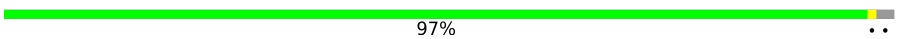
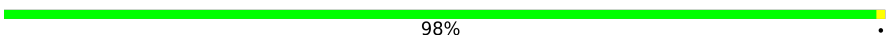
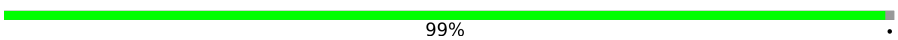
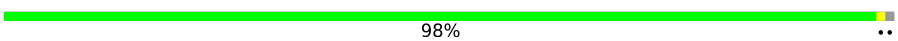
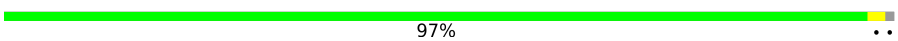
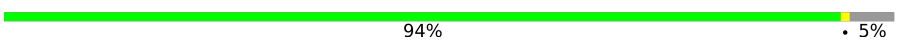
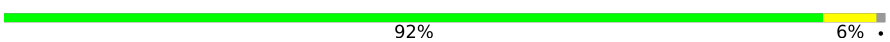
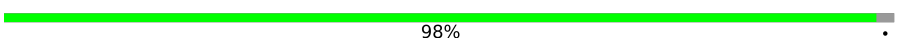
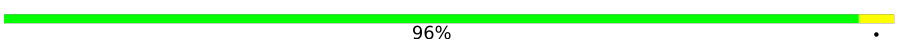
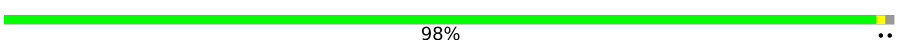
Mol	Chain	Length	Quality of chain
35	KK	256	
36	L	136	
37	LL	191	
38	M	149	
39	MM	221	
40	N	59	
41	NN	174	
42	O	105	
43	OO	199	
44	P	113	
45	PP	138	
46	Pp	2	
47	Q	130	
48	QQ	204	
49	R	107	
50	S	121	
51	T	120	
52	U	100	
53	V	88	
54	W	78	
55	X	51	
56	Y	128	
57	Z	25	
58	a	106	
59	b	92	

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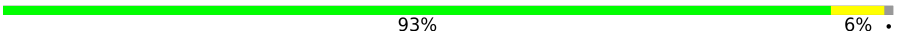
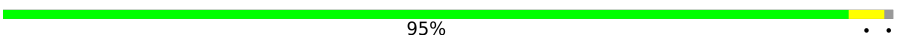
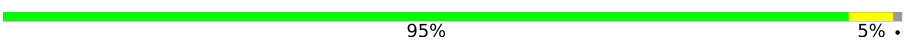
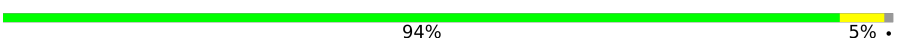
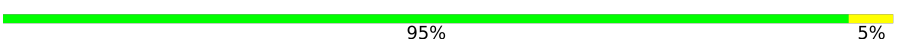
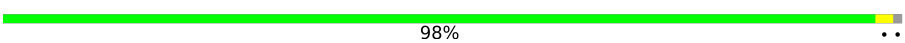
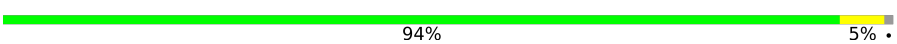
Mol	Chain	Length	Quality of chain
60	c	1800	
61	d	252	
62	e	255	
63	f	254	
64	g	240	
65	h	261	
66	i	225	
67	j	236	
68	k	190	
69	l	200	
70	m	197	
71	n	105	
72	o	156	
73	p	151	
74	q	137	
75	r	142	
76	s	143	
77	t	136	
78	u	146	
79	v	144	
80	w	121	
81	x	87	
82	y	130	
83	z	145	

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 201697 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	134	1073	676	208	189	0	0

- Molecule 2 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	70	563	360	104	99	0	0

- Molecule 3 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	97	769	475	160	129	5	0	0

- Molecule 4 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	81	610	382	110	113	5	0	0

- Molecule 5 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	63	497	306	99	91	1	0	0

- Molecule 6 is a protein called HLJ1_G0030400.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	53	442	274	92	72	4	0	0

- Molecule 7 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	53	Total	C	N	O	S	0	0
			427	269	88	69	1		

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	318	Total	C	N	O	S	0	0
			2436	1541	418	469	8		

- Molecule 9 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	36	Total	C	N	O	S	0	0
			276	173	54	45	4		

- Molecule 10 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 11 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	3190	Total	C	N	O	P	0	0
			68285	30524	12313	22258	3190		

- Molecule 12 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	B	154	Total	C	N	O	0	0
			1222	761	237	224		

- Molecule 13 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BB	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 14 is a RNA chain called Transfer RNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Bb	76	Total	C	N	O	P	0	0
			1638	736	294	533	75		

- Molecule 15 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 16 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CC	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 17 is a RNA chain called Transfer RNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Cc	77	Total	C	N	O	P	0	0
			1644	732	298	537	77		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cc	18	C	U	conflict	GB 170517292

- Molecule 18 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	D	176	Total	C	N	O	0	0
			1423	875	308	240		

- Molecule 19 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	DD	197	Total	C	N	O	S	0	0
			1531	980	266	281	4		

- Molecule 20 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Dd	13	Total	C	N	O	P	0	0
			278	125	50	90	13		

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	E	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 22 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	EE	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 23 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ee	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 24 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 25 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	FF	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 26 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	G	97	Total	C	N	O	0	0
			770	499	126	145		

- Molecule 27 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	GG	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 28 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	129	Total	C	N	O	S	0	0
			963	607	180	169	7		

- Molecule 29 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	HH	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 30 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	I	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 31 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	II	155	Total	C	N	O	S	0	0
			1230	795	221	213	1		

- Molecule 32 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 33 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	JJ	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 34 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	K	126	Total 993	C 625	N 192	O 176	0	0

- Molecule 35 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	KK	233	Total 1804	C 1151	N 323	O 327	S 3	0	0

- Molecule 36 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	L	135	Total 1092	C 710	N 202	O 180	0	0

- Molecule 37 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LL	191	Total 1518	C 963	N 274	O 277	S 4	0	0

- Molecule 38 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	M	148	Total 1173	C 749	N 231	O 190	S 3	0	0

- Molecule 39 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	MM	215	Total 1743	C 1102	N 331	O 303	S 7	0	0

- Molecule 40 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	N	58	Total 462	C 289	N 100	O 73	0	0

- Molecule 41 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	NN	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 42 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	O	97	Total	C	N	O	S	0	0
			742	479	124	138	1		

- Molecule 43 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	OO	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 44 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	P	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 45 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	PP	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 46 is a protein called di-peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Pp	2	Total	C	N	O	S	0	0
			19	14	2	2	1		

- Molecule 47 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Q	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 48 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	QQ	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 49 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	R	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 50 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	S	109	Total	C	N	O	S	0	0
			861	533	175	149	4		

- Molecule 51 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	T	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 52 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	U	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 53 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	V	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 54 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	W	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 55 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	X	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 56 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Y	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 57 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Z	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 58 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	a	102	Total	C	N	O	S	0	0
			819	514	166	134	5		

- Molecule 59 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	b	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 60 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	c	1604	Total	C	N	O	P	0	0
			34236	15322	6079	11231	1604		

- Molecule 61 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	d	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 62 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	e	212	Total	C	N	O	S	0	0
			1689	1073	303	309	4		

- Molecule 63 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	f	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 64 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	g	206	Total	C	N	O	S	0	0
			1601	1014	294	287	6		

- Molecule 65 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	h	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 66 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	i	199	Total	C	N	O	S	0	0
			1572	987	290	292	3		

- Molecule 67 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	j	219	Total	C	N	O	S	0	0
			1766	1108	341	314	3		

- Molecule 68 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	k	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 69 is a protein called 40S ribosomal protein S8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	l	184	Total	C	N	O	S	0	0
			1457	906	291	258	2		

- Molecule 70 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	m	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 71 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	n	91	Total	C	N	O	S	0	0
			772	503	123	144	2		

- Molecule 72 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	o	142	Total	C	N	O	S	0	0
			1146	735	217	191	3		

- Molecule 73 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	p	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 74 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	q	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 75 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	r	104	Total	C	N	O	S	0	0
			837	533	155	143	6		

- Molecule 76 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
76	s	137	Total	C	N	O	0	0
			1080	692	199	189		

- Molecule 77 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	t	121	Total	C	N	O	S	0	0
			961	599	182	178	2		

- Molecule 78 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	u	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 79 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	v	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 80 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	w	100	Total	C	N	O	S	0	0
			800	509	144	146	1		

- Molecule 81 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	x	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 82 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	y	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 83 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	z	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	2	1	Total	Zn	0
			1	1	
84	5	1	Total	Zn	0
			1	1	
84	8	1	Total	Zn	0
			1	1	
84	S	1	Total	Zn	0
			1	1	
84	V	1	Total	Zn	0
			1	1	
84	Y	1	Total	Zn	0
			1	1	
84	a	1	Total	Zn	0
			1	1	
84	b	1	Total	Zn	0
			1	1	

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	AA	205	Total	Mg	0
			205	205	
85	B	1	Total	Mg	0
			1	1	
85	BB	5	Total	Mg	0
			5	5	
85	Bb	1	Total	Mg	0
			1	1	
85	CC	3	Total	Mg	0
			3	3	
85	Cc	1	Total	Mg	0
			1	1	
85	Dd	1	Total	Mg	0
			1	1	
85	FF	1	Total	Mg	0
			1	1	
85	H	1	Total	Mg	0
			1	1	

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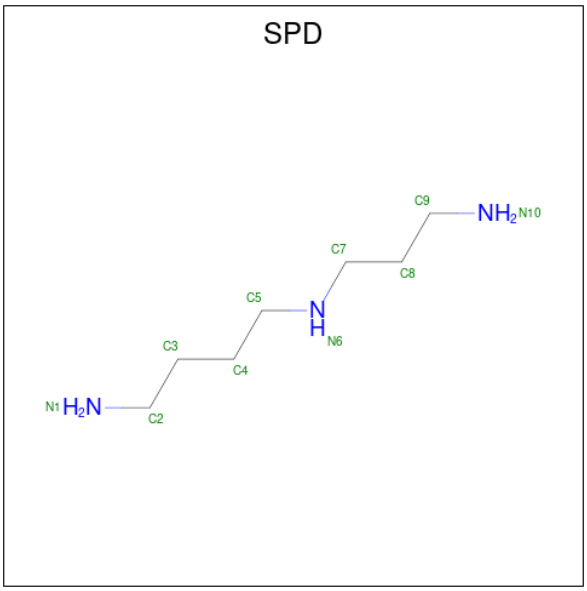
Mol	Chain	Residues	Atoms	AltConf
85	QQ	1	Total Mg 1 1	0
85	V	1	Total Mg 1 1	0
85	c	60	Total Mg 60 60	0

- Molecule 86 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
86	AA	12	Total K 12 12	0
86	EE	1	Total K 1 1	0
86	MM	1	Total K 1 1	0
86	Q	1	Total K 1 1	0
86	S	1	Total K 1 1	0
86	a	1	Total K 1 1	0
86	c	4	Total K 4 4	0
86	q	1	Total K 1 1	0

- Molecule 87 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
87	AA	1	Total C N 10 7 3	0
87	AA	1	Total C N 10 7 3	0
87	AA	1	Total C N 10 7 3	0
87	c	1	Total C N 10 7 3	0

- Molecule 88 is water.

Mol	Chain	Residues	Atoms	AltConf
88	2	1	Total O 1 1	0
88	A	2	Total O 2 2	0
88	AA	877	Total O 877 877	0
88	B	3	Total O 3 3	0
88	BB	12	Total O 12 12	0
88	Bb	5	Total O 5 5	0
88	CC	18	Total O 18 18	0
88	Cc	6	Total O 6 6	0

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Mol	Chain	Residues	Atoms	AltConf
88	D	4	Total O 4 4	0
88	Dd	4	Total O 4 4	0
88	EE	9	Total O 9 9	0
88	F	4	Total O 4 4	0
88	FF	4	Total O 4 4	0
88	GG	3	Total O 3 3	0
88	H	3	Total O 3 3	0
88	HH	1	Total O 1 1	0
88	J	1	Total O 1 1	0
88	JJ	2	Total O 2 2	0
88	LL	1	Total O 1 1	0
88	M	3	Total O 3 3	0
88	MM	2	Total O 2 2	0
88	N	1	Total O 1 1	0
88	Q	4	Total O 4 4	0
88	QQ	9	Total O 9 9	0
88	S	2	Total O 2 2	0
88	V	3	Total O 3 3	0
88	a	2	Total O 2 2	0
88	c	226	Total O 226 226	0
88	h	2	Total O 2 2	0

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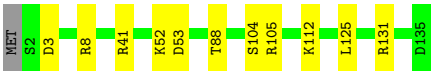
Mol	Chain	Residues	Atoms	AltConf
88	o	2	Total O 2 2	0
88	p	2	Total O 2 2	0
88	q	2	Total O 2 2	0
88	v	3	Total O 3 3	0
88	z	1	Total O 1 1	0

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. 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. 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.

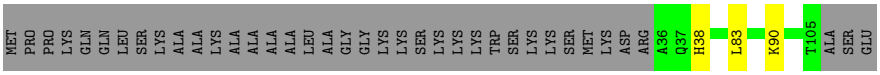
• Molecule 1: 40S ribosomal protein S24-A

Chain 0:



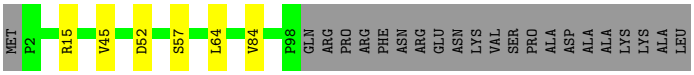
• Molecule 2: 40S ribosomal protein S25-A

Chain 1:



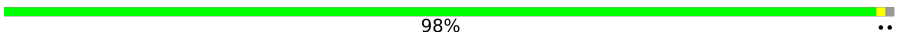
• Molecule 3: 40S ribosomal protein S26

Chain 2:



• Molecule 4: 40S ribosomal protein S27-A

Chain 3:



• Molecule 5: 40S ribosomal protein S28-A

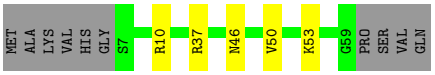
Chain 4:

• Molecule 6: HLJ1_G0030400.mRNA.1.CDS.1

Chain 5:

• Molecule 7: 40S ribosomal protein S30-A

Chain 6:

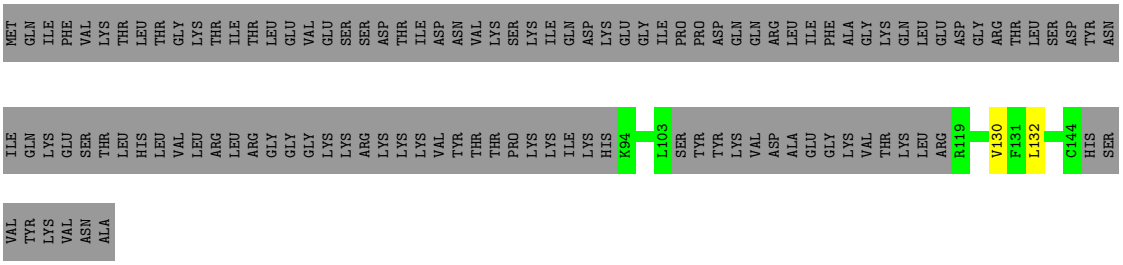


• Molecule 8: Guanine nucleotide-binding protein subunit beta-like protein

Chain 7:

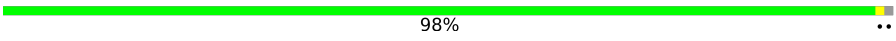
• Molecule 9: Ubiquitin-40S ribosomal protein S31

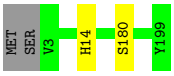
Chain 8:



• Molecule 10: 60S ribosomal protein L16-A

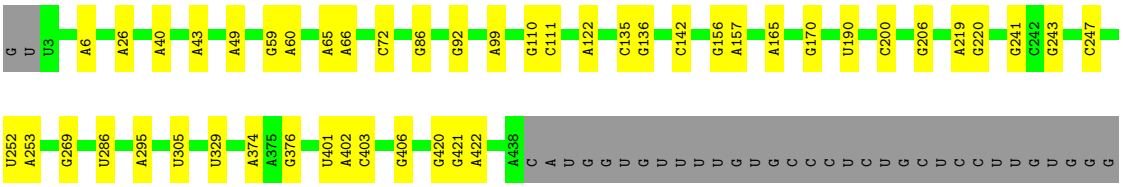
Chain A:

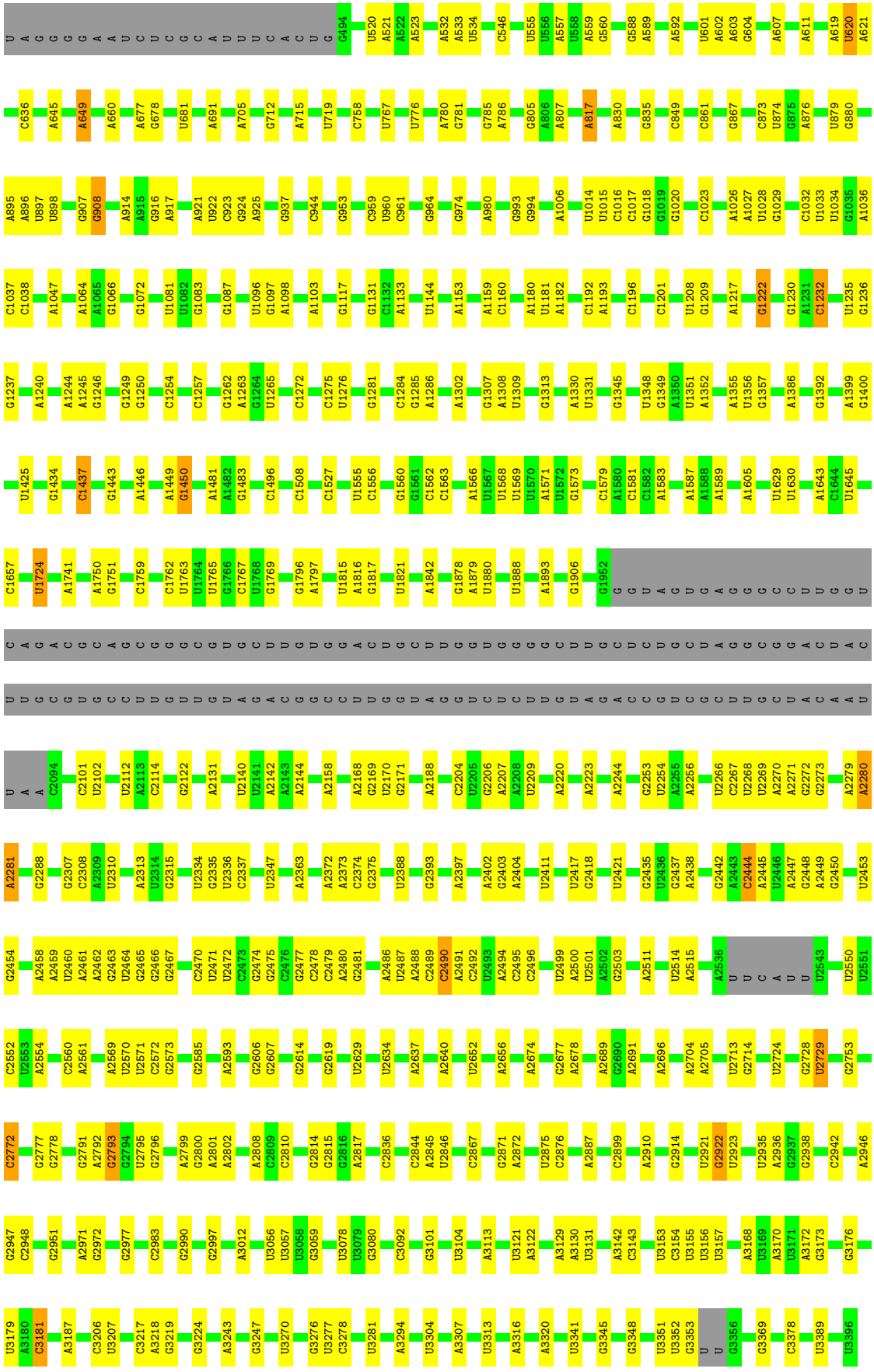




• Molecule 11: 25S ribosomal RNA

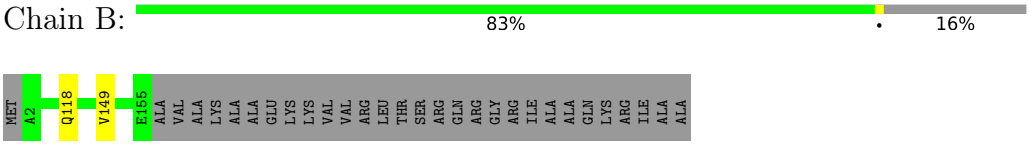
Chain AA:





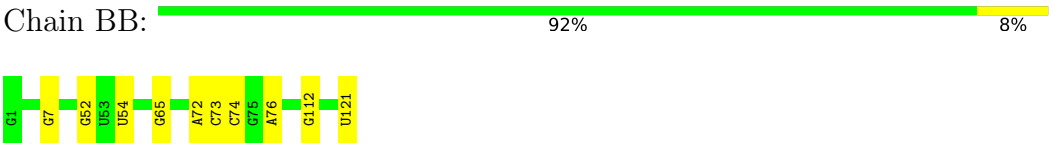
• Molecule 12: 60S ribosomal protein L17-A

Chain B:



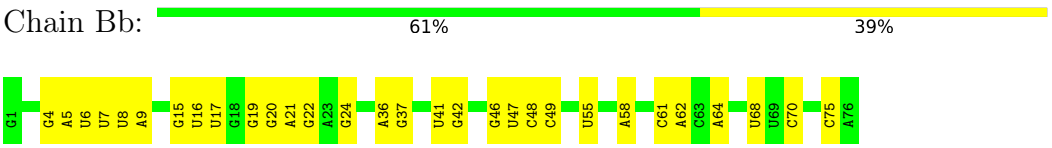
• Molecule 13: 5S ribosomal RNA

Chain BB:



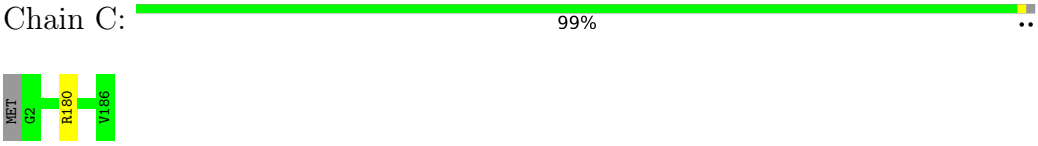
• Molecule 14: Transfer RNA Phe

Chain Bb:



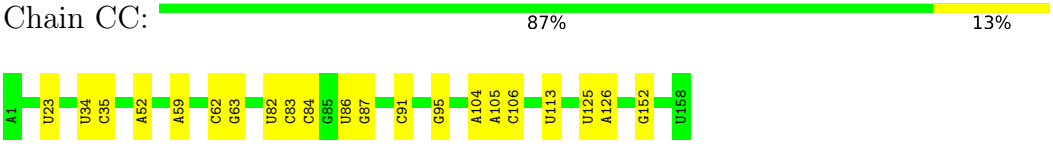
• Molecule 15: 60S ribosomal protein L18-A

Chain C:



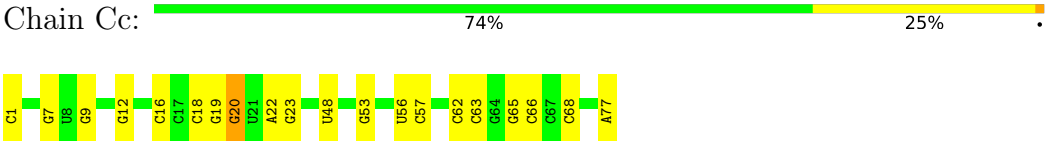
• Molecule 16: 5.8S ribosomal RNA

Chain CC:



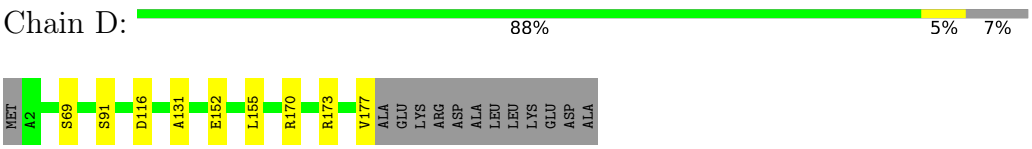
• Molecule 17: Transfer RNA fMet

Chain Cc:



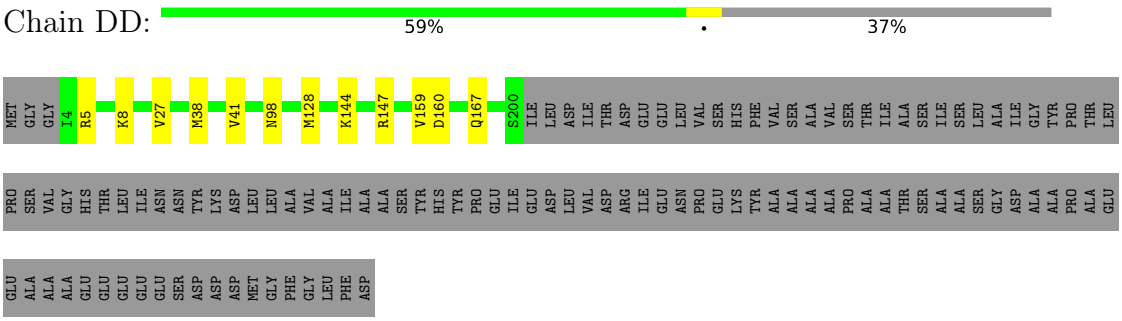
• Molecule 18: 60S ribosomal protein L19-A

Chain D:



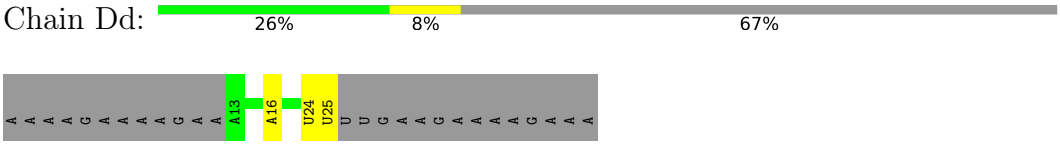
• Molecule 19: 60S acidic ribosomal protein P0

Chain DD:



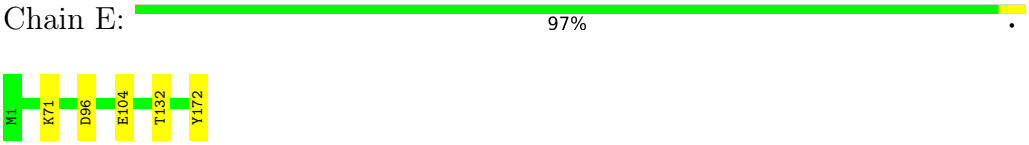
• Molecule 20: Messenger RNA

Chain Dd:



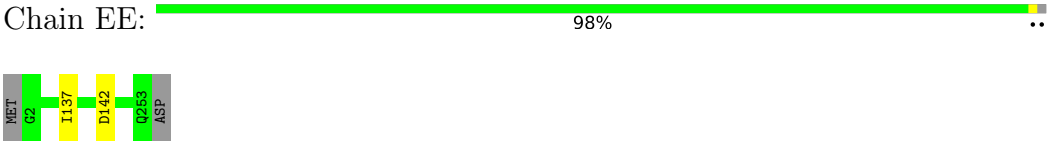
• Molecule 21: 60S ribosomal protein L20-A

Chain E:



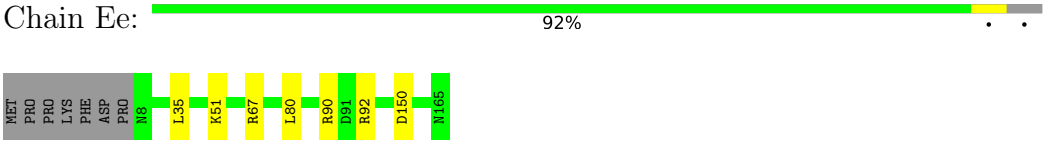
• Molecule 22: 60S ribosomal protein L2-A

Chain EE:



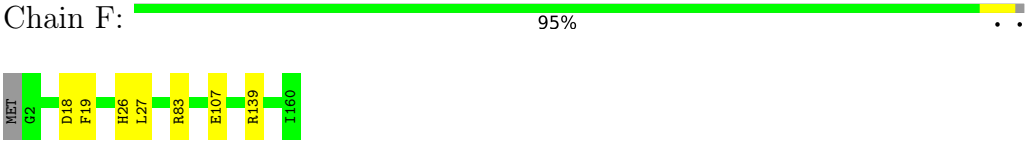
• Molecule 23: 60S ribosomal protein L12-A

Chain Ee:



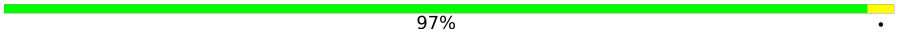
• Molecule 24: 60S ribosomal protein L21-A

Chain F:



• Molecule 25: 60S ribosomal protein L3

Chain FF:

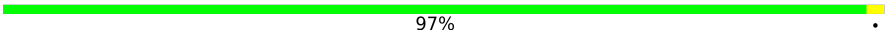


• Molecule 26: 60S ribosomal protein L22-A

Chain G:

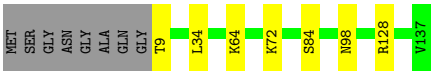
• Molecule 27: 60S ribosomal protein L4-A

Chain GG:



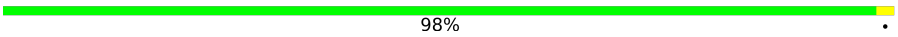
• Molecule 28: 60S ribosomal protein L23-A

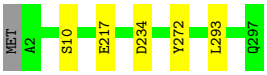
Chain H:



• Molecule 29: 60S ribosomal protein L5

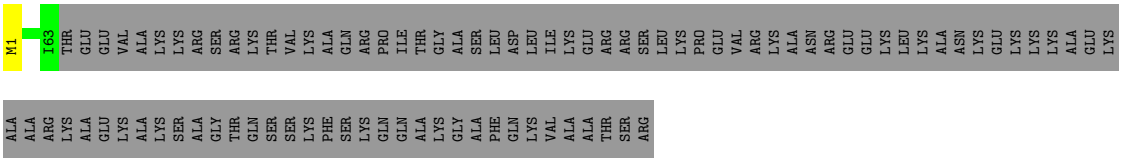
Chain HH:





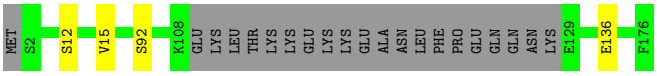
• Molecule 30: 60S ribosomal protein L24-A

Chain I:



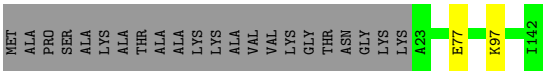
• Molecule 31: 60S ribosomal protein L6-A

Chain II:



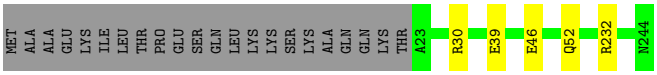
• Molecule 32: 60S ribosomal protein L25

Chain J:



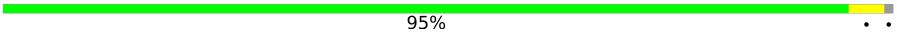
• Molecule 33: 60S ribosomal protein L7-A

Chain JJ:



• Molecule 34: 60S ribosomal protein L26-A

Chain K:

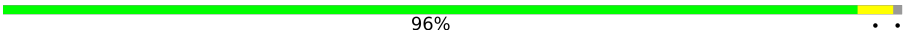


• Molecule 35: 60S ribosomal protein L8-A

Chain KK:

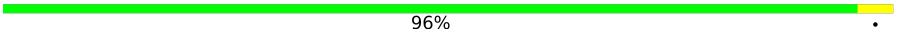
• Molecule 36: 60S ribosomal protein L27-A

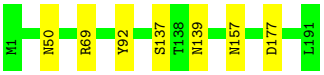
Chain L:



• Molecule 37: 60S ribosomal protein L9-A

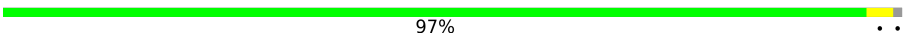
Chain LL:





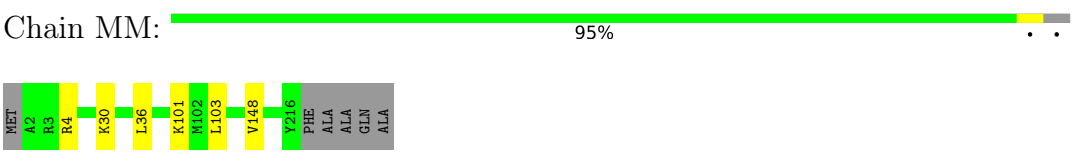
• Molecule 38: 60S ribosomal protein L28

Chain M:



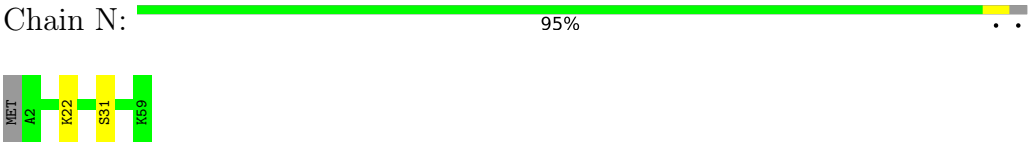
• Molecule 39: 60S ribosomal protein L10

Chain MM:



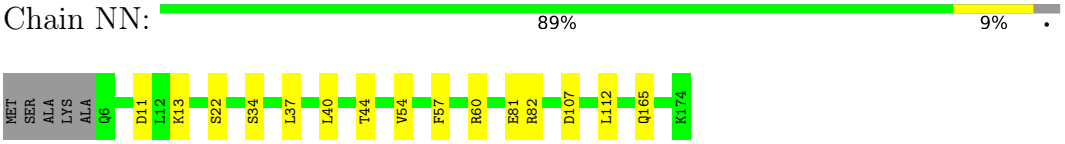
• Molecule 40: 60S ribosomal protein L29

Chain N:



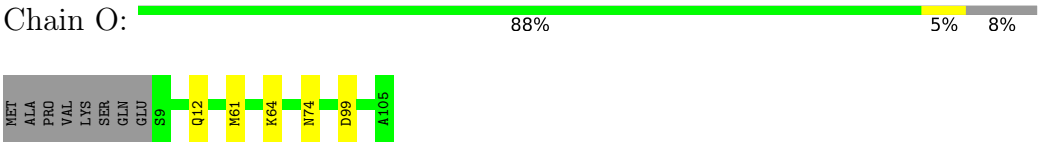
• Molecule 41: 60S ribosomal protein L11-A

Chain NN:



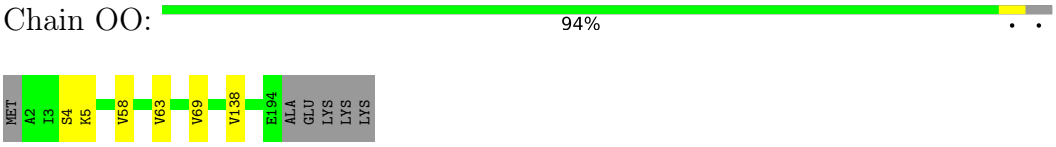
• Molecule 42: 60S ribosomal protein L30

Chain O:



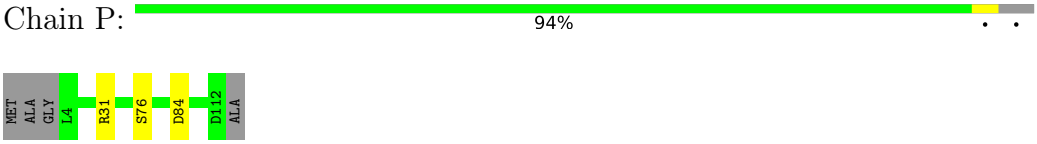
• Molecule 43: 60S ribosomal protein L13-A

Chain OO:



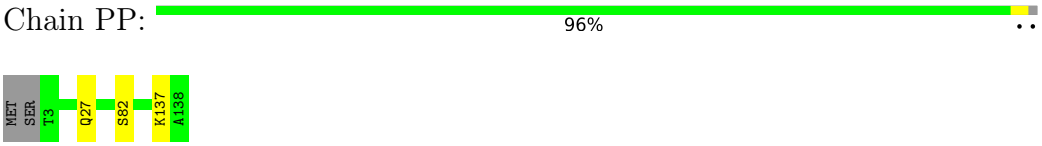
• Molecule 44: 60S ribosomal protein L31-A

Chain P:



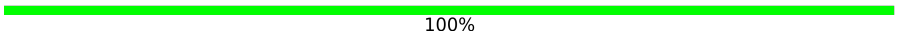
• Molecule 45: 60S ribosomal protein L14-A

Chain PP:



• Molecule 46: di-peptide

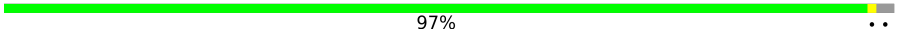
Chain Pp:

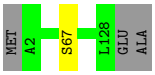


There are no outlier residues recorded for this chain.

• Molecule 47: 60S ribosomal protein L32

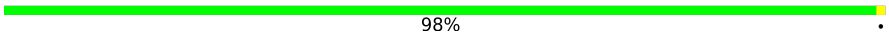
Chain Q:





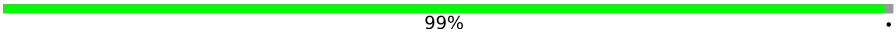
• Molecule 48: 60S ribosomal protein L15-A

Chain QQ:



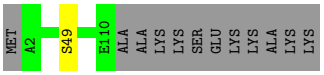
• Molecule 49: 60S ribosomal protein L33-A

Chain R:



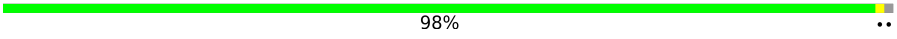
• Molecule 50: 60S ribosomal protein L34-A

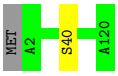
Chain S:



• Molecule 51: 60S ribosomal protein L35-A

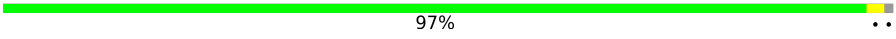
Chain T:





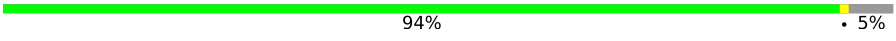
• Molecule 52: 60S ribosomal protein L36-A

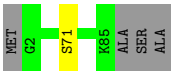
Chain U:



• Molecule 53: 60S ribosomal protein L37-A

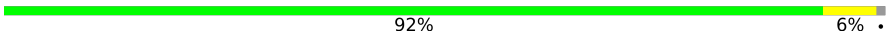
Chain V:





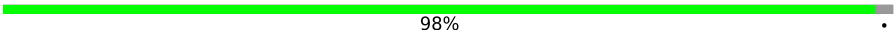
• Molecule 54: 60S ribosomal protein L38

Chain W:



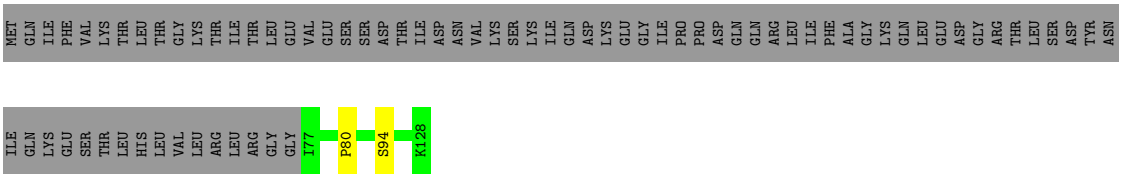
• Molecule 55: 60S ribosomal protein L39

Chain X:



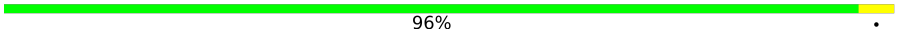
• Molecule 56: Ubiquitin-60S ribosomal protein L40

Chain Y:



• Molecule 57: 60S ribosomal protein L41-A

Chain Z:

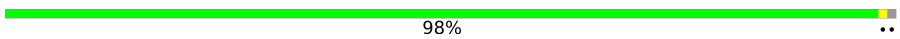


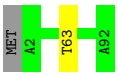
• Molecule 58: 60S ribosomal protein L42-A

Chain a:

• Molecule 59: 60S ribosomal protein L43-A

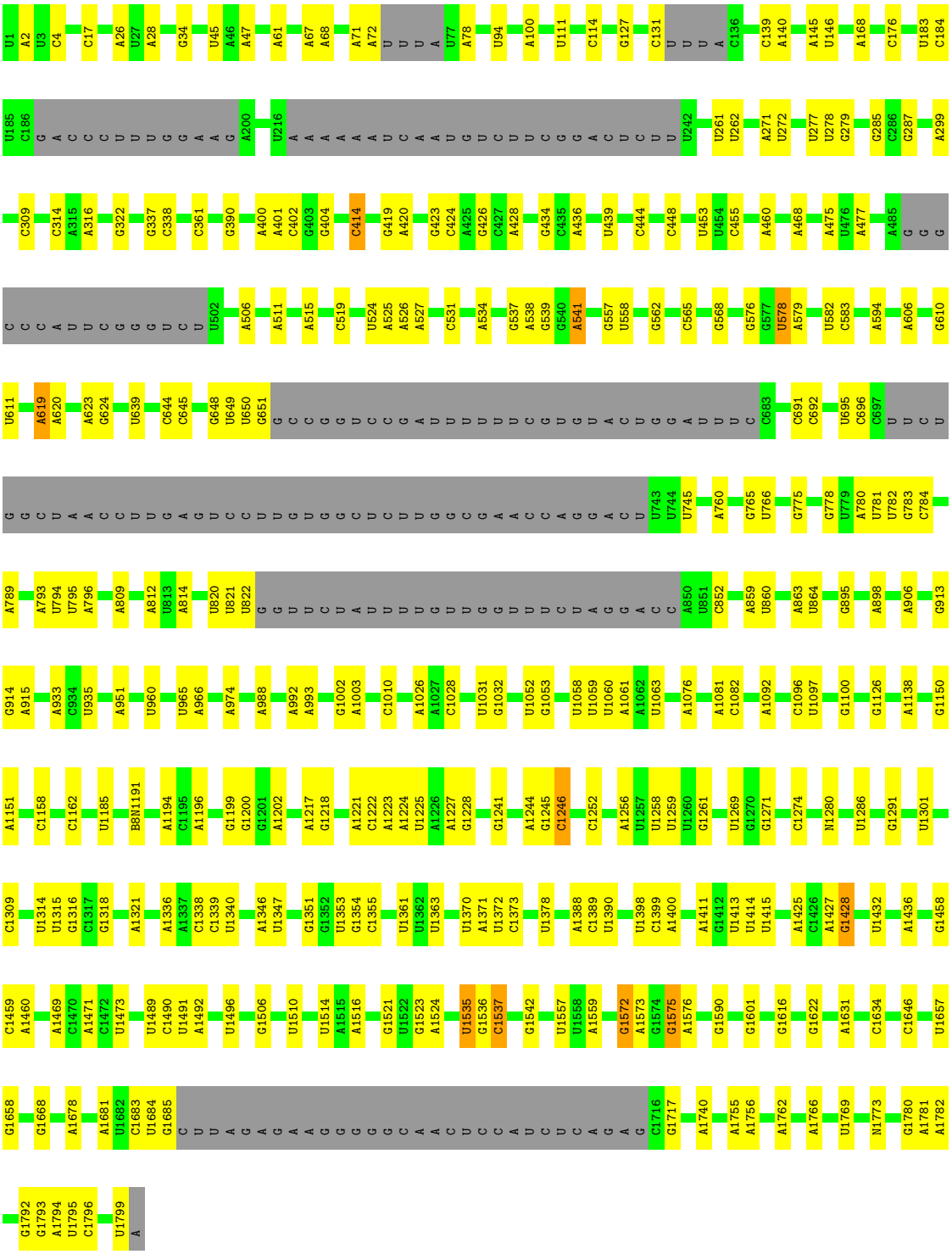
Chain b:





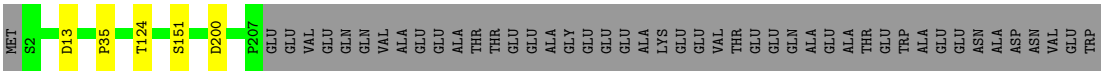
• Molecule 60: 18S ribosomal RNA

Chain c:



• Molecule 61: 40S ribosomal protein S0-A

Chain d:



• Molecule 62: 40S ribosomal protein S1-A

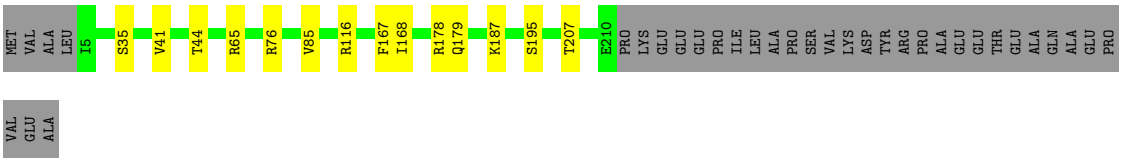
Chain e:

• Molecule 63: 40S ribosomal protein S2

Chain f:

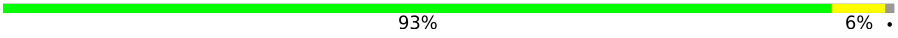
• Molecule 64: RPS3 isoform 1

Chain g:



• Molecule 65: 40S ribosomal protein S4-A

Chain h:

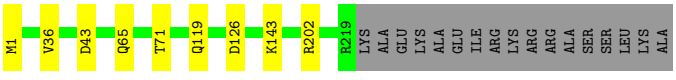


• Molecule 66: 40S ribosomal protein S5

Chain i:

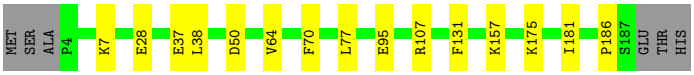
• Molecule 67: 40S ribosomal protein S6-A

Chain j:



• Molecule 68: 40S ribosomal protein S7-A

Chain k:

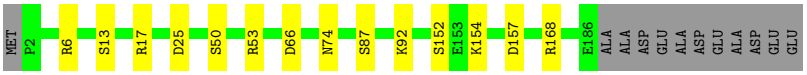


• Molecule 69: 40S ribosomal protein S8-B

Chain l:

• Molecule 70: 40S ribosomal protein S9-A

Chain m:



• Molecule 71: 40S ribosomal protein S10-A

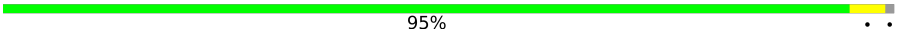
Chain n:

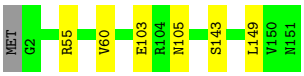
• Molecule 72: 40S ribosomal protein S11-A

Chain o:

• Molecule 73: 40S ribosomal protein S13

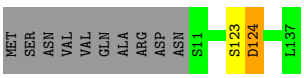
Chain p:





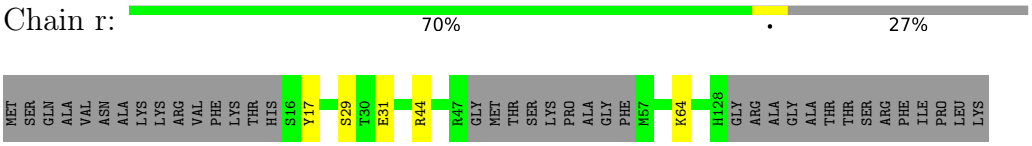
• Molecule 74: 40S ribosomal protein S14-A

Chain q:



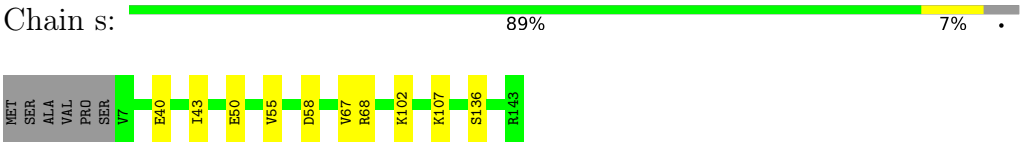
• Molecule 75: 40S ribosomal protein S15

Chain r:



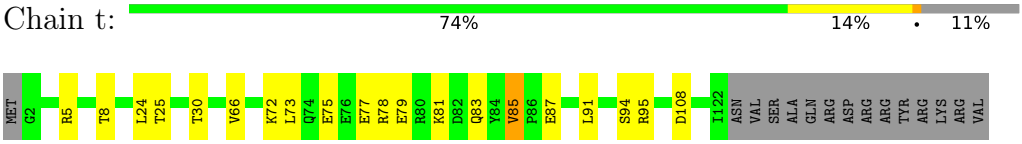
• Molecule 76: 40S ribosomal protein S16-A

Chain s:



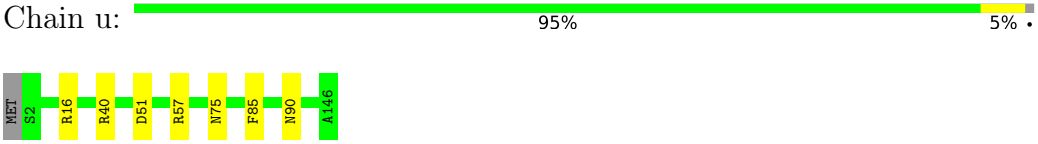
• Molecule 77: 40S ribosomal protein S17-A

Chain t:



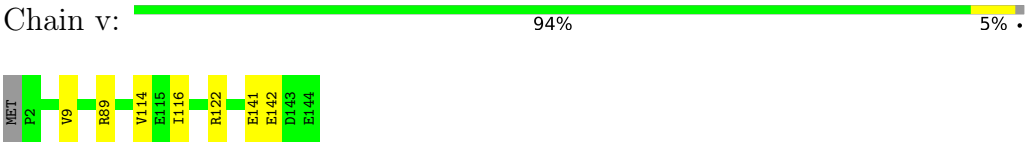
• Molecule 78: 40S ribosomal protein S18-A

Chain u:



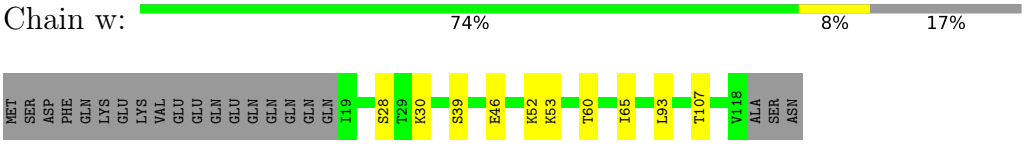
• Molecule 79: 40S ribosomal protein S19-A

Chain v:



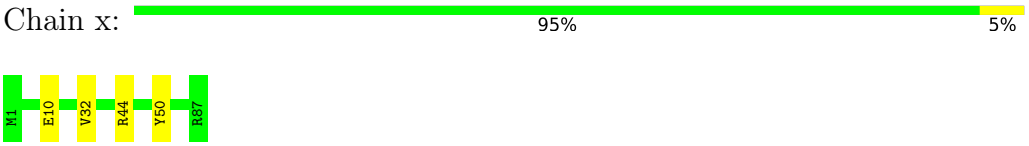
• Molecule 80: 40S ribosomal protein S20

Chain w:



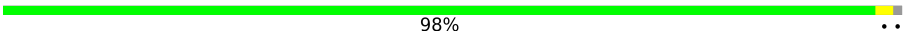
• Molecule 81: 40S ribosomal protein S21-A

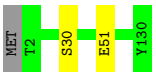
Chain x:



• Molecule 82: 40S ribosomal protein S22-A

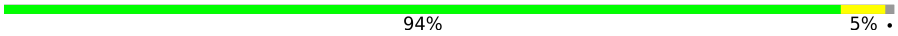
Chain y:





• Molecule 83: 40S ribosomal protein S23-A

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55455	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	270000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, ZN, 4AC, A2M, SPD, K, UR3, MG, 5MC, OMG, YYG, OMU, B8N, MA6, OMC, G7M

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	0.28	0/1087	0.55	0/1449
2	1	0.29	0/571	0.68	1/768 (0.1%)
3	2	0.29	0/782	0.62	0/1047
4	3	0.28	0/620	0.54	0/838
5	4	0.29	0/499	0.65	0/670
6	5	0.29	0/452	0.58	0/600
7	6	0.28	0/433	0.59	0/575
8	7	0.27	0/2489	0.58	0/3389
9	8	0.24	0/279	0.51	0/369
10	A	0.33	0/1585	0.54	0/2128
11	AA	0.53	0/75384	0.81	38/117530 (0.0%)
12	B	0.32	0/1245	0.54	0/1676
13	BB	0.48	0/2883	0.76	0/4491
14	Bb	0.30	0/1788	0.84	0/2786
15	C	0.30	0/1465	0.56	0/1965
16	CC	0.53	0/3746	0.78	0/5832
17	Cc	0.41	1/1836 (0.1%)	0.77	1/2859 (0.0%)
18	D	0.28	0/1440	0.58	0/1921
19	DD	0.27	0/1558	0.54	0/2107
20	Dd	0.41	0/311	0.72	0/482
21	E	0.32	0/1481	0.55	0/1990
22	EE	0.32	0/1948	0.58	0/2617
23	Ee	0.25	0/1210	0.52	0/1627
24	F	0.32	0/1300	0.53	0/1743
25	FF	0.32	0/3146	0.56	0/4228
26	G	0.31	0/786	0.49	0/1065
27	GG	0.30	0/2800	0.53	0/3790
28	H	0.32	0/978	0.56	0/1316
29	HH	0.30	0/2425	0.52	0/3271
30	I	0.30	0/533	0.53	0/707
31	II	0.32	0/1251	0.53	0/1682
32	J	0.32	0/974	0.54	0/1314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	JJ	0.32	0/1821	0.50	0/2451
34	K	0.30	0/1004	0.58	1/1341 (0.1%)
35	KK	0.30	0/1836	0.49	0/2481
36	L	0.32	0/1118	0.50	0/1497
37	LL	0.31	0/1539	0.53	0/2073
38	M	0.31	0/1204	0.55	0/1612
39	MM	0.31	0/1779	0.55	0/2386
40	N	0.28	0/473	0.52	0/629
41	NN	0.30	0/1374	0.57	0/1842
42	O	0.31	0/750	0.46	0/1008
43	OO	0.31	0/1568	0.59	0/2106
44	P	0.30	0/897	0.57	0/1205
45	PP	0.29	0/1068	0.51	0/1438
46	Pp	0.40	0/19	1.24	0/23
47	Q	0.30	0/1041	0.52	0/1394
48	QQ	0.33	0/1757	0.59	0/2354
49	R	0.35	0/868	0.57	0/1168
50	S	0.30	0/871	0.56	0/1164
51	T	0.29	0/978	0.53	0/1301
52	U	0.27	0/778	0.58	0/1034
53	V	0.33	0/680	0.60	0/901
54	W	0.31	0/618	0.59	0/826
55	X	0.30	0/443	0.65	0/588
56	Y	0.28	0/423	0.54	0/562
57	Z	0.27	0/234	0.70	0/300
58	a	0.31	0/831	0.59	0/1097
59	b	0.31	0/701	0.58	0/934
60	c	0.45	0/37665	0.81	29/58663 (0.0%)
61	d	0.30	0/1623	0.55	0/2222
62	e	0.29	0/1714	0.54	0/2308
63	f	0.30	0/1665	0.54	0/2263
64	g	0.30	0/1622	0.58	1/2180 (0.0%)
65	h	0.28	0/2097	0.54	0/2823
66	i	0.27	0/1591	0.56	0/2151
67	j	0.27	0/1790	0.57	0/2393
68	k	0.28	0/1506	0.56	1/2028 (0.0%)
69	l	0.28	0/1482	0.58	0/1980
70	m	0.27	0/1519	0.54	0/2035
71	n	0.31	0/792	0.57	0/1071
72	o	0.30	0/1172	0.54	0/1580
73	p	0.29	0/1215	0.53	0/1638
74	q	0.29	0/901	0.64	0/1217
75	r	0.30	0/853	0.54	0/1145

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	s	0.29	0/1099	0.55	0/1473
77	t	0.32	0/971	0.63	0/1303
78	u	0.27	0/1211	0.58	0/1628
79	v	0.29	0/1130	0.55	0/1517
80	w	0.29	0/810	0.54	0/1095
81	x	0.30	0/693	0.59	0/935
82	y	0.32	0/1038	0.57	0/1395
83	z	0.29	0/1139	0.55	0/1518
All	All	0.43	1/213256 (0.0%)	0.72	72/313108 (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
33	JJ	0	1
36	L	0	1
58	a	0	1
62	e	0	2
66	i	0	2
68	k	0	1
73	p	0	1
74	q	0	2
76	s	0	1
78	u	0	1
83	z	0	1
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Cc	1	C	OP3-P	-10.65	1.48	1.61

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	c	94	U	C2-N3-C4	13.64	135.18	127.00
11	AA	406	G	O4'-C1'-N9	9.27	115.61	108.20
11	AA	2269	U	N3-C2-O2	-7.76	116.77	122.20
60	c	1096	C	N1-C2-O2	7.71	123.52	118.90
60	c	1537	C	C2-N1-C1'	7.52	127.07	118.80

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	JJ	232	ARG	Peptide
36	L	102	GLU	Peptide
58	a	7	THR	Peptide
62	e	35	PRO	Peptide
62	e	38	PHE	Peptide

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	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
2	1	68/108 (63%)	62 (91%)	6 (9%)	0	100	100
3	2	95/119 (80%)	87 (92%)	8 (8%)	0	100	100
4	3	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
5	4	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
6	5	51/56 (91%)	51 (100%)	0	0	100	100
7	6	51/63 (81%)	47 (92%)	4 (8%)	0	100	100
8	7	316/319 (99%)	297 (94%)	19 (6%)	0	100	100
9	8	32/152 (21%)	22 (69%)	10 (31%)	0	100	100
10	A	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
12	B	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
15	C	183/186 (98%)	181 (99%)	2 (1%)	0	100	100
18	D	174/189 (92%)	170 (98%)	3 (2%)	1 (1%)	25	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	DD	195/312 (62%)	187 (96%)	8 (4%)	0	100	100
21	E	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
22	EE	250/254 (98%)	244 (98%)	6 (2%)	0	100	100
23	Ee	156/165 (94%)	153 (98%)	3 (2%)	0	100	100
24	F	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
25	FF	384/387 (99%)	374 (97%)	10 (3%)	0	100	100
26	G	95/121 (78%)	93 (98%)	2 (2%)	0	100	100
27	GG	359/362 (99%)	342 (95%)	17 (5%)	0	100	100
28	H	127/137 (93%)	126 (99%)	1 (1%)	0	100	100
29	HH	294/297 (99%)	284 (97%)	10 (3%)	0	100	100
30	I	61/155 (39%)	61 (100%)	0	0	100	100
31	II	151/176 (86%)	147 (97%)	4 (3%)	0	100	100
32	J	118/142 (83%)	114 (97%)	4 (3%)	0	100	100
33	JJ	220/244 (90%)	217 (99%)	3 (1%)	0	100	100
34	K	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
35	KK	231/256 (90%)	227 (98%)	4 (2%)	0	100	100
36	L	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
37	LL	189/191 (99%)	182 (96%)	7 (4%)	0	100	100
38	M	146/149 (98%)	138 (94%)	7 (5%)	1 (1%)	22	11
39	MM	213/221 (96%)	207 (97%)	6 (3%)	0	100	100
40	N	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
41	NN	167/174 (96%)	159 (95%)	8 (5%)	0	100	100
42	O	95/105 (90%)	95 (100%)	0	0	100	100
43	OO	191/199 (96%)	177 (93%)	13 (7%)	1 (0%)	29	16
44	P	107/113 (95%)	101 (94%)	6 (6%)	0	100	100
45	PP	134/138 (97%)	129 (96%)	5 (4%)	0	100	100
47	Q	125/130 (96%)	125 (100%)	0	0	100	100
48	QQ	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
49	R	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
50	S	107/121 (88%)	107 (100%)	0	0	100	100
51	T	117/120 (98%)	112 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	U	97/100 (97%)	89 (92%)	8 (8%)	0	100	100
53	V	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
54	W	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
55	X	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
56	Y	50/128 (39%)	50 (100%)	0	0	100	100
57	Z	23/25 (92%)	23 (100%)	0	0	100	100
58	a	100/106 (94%)	96 (96%)	4 (4%)	0	100	100
59	b	89/92 (97%)	89 (100%)	0	0	100	100
61	d	204/252 (81%)	190 (93%)	14 (7%)	0	100	100
62	e	210/255 (82%)	194 (92%)	16 (8%)	0	100	100
63	f	215/254 (85%)	202 (94%)	13 (6%)	0	100	100
64	g	204/240 (85%)	195 (96%)	9 (4%)	0	100	100
65	h	256/261 (98%)	249 (97%)	7 (3%)	0	100	100
66	i	195/225 (87%)	186 (95%)	9 (5%)	0	100	100
67	j	217/236 (92%)	208 (96%)	9 (4%)	0	100	100
68	k	182/190 (96%)	172 (94%)	10 (6%)	0	100	100
69	l	180/200 (90%)	168 (93%)	12 (7%)	0	100	100
70	m	183/197 (93%)	177 (97%)	6 (3%)	0	100	100
71	n	89/105 (85%)	80 (90%)	7 (8%)	2 (2%)	6	1
72	o	140/156 (90%)	132 (94%)	8 (6%)	0	100	100
73	p	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
74	q	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
75	r	100/142 (70%)	96 (96%)	4 (4%)	0	100	100
76	s	135/143 (94%)	127 (94%)	8 (6%)	0	100	100
77	t	119/136 (88%)	101 (85%)	14 (12%)	4 (3%)	3	0
78	u	143/146 (98%)	133 (93%)	10 (7%)	0	100	100
79	v	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
80	w	98/121 (81%)	97 (99%)	1 (1%)	0	100	100
81	x	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
82	y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
83	z	142/145 (98%)	129 (91%)	13 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	10968/12214 (90%)	10515 (96%)	444 (4%)	9 (0%)	54 42

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
77	t	94	SER
38	M	78	LEU
43	OO	63	VAL
71	n	48	SER
71	n	49	LEU

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	112/113 (99%)	101 (90%)	11 (10%)	8 1
2	1	61/89 (68%)	59 (97%)	2 (3%)	38 26
3	2	83/101 (82%)	77 (93%)	6 (7%)	14 5
4	3	70/71 (99%)	69 (99%)	1 (1%)	67 62
5	4	56/60 (93%)	50 (89%)	6 (11%)	6 1
6	5	47/49 (96%)	39 (83%)	8 (17%)	2 0
7	6	46/54 (85%)	41 (89%)	5 (11%)	6 1
8	7	259/262 (99%)	220 (85%)	39 (15%)	3 0
9	8	30/135 (22%)	28 (93%)	2 (7%)	16 6
10	A	160/162 (99%)	158 (99%)	2 (1%)	69 64
12	B	125/146 (86%)	123 (98%)	2 (2%)	62 56
15	C	150/151 (99%)	149 (99%)	1 (1%)	84 83
18	D	143/154 (93%)	135 (94%)	8 (6%)	21 9
19	DD	167/254 (66%)	155 (93%)	12 (7%)	14 5
21	E	156/156 (100%)	151 (97%)	5 (3%)	39 28
22	EE	193/196 (98%)	191 (99%)	2 (1%)	76 73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	Ee	129/136 (95%)	122 (95%)	7 (5%)	22 10
24	F	136/137 (99%)	129 (95%)	7 (5%)	24 12
25	FF	318/323 (98%)	306 (96%)	12 (4%)	33 21
26	G	84/107 (78%)	81 (96%)	3 (4%)	35 23
27	GG	288/289 (100%)	279 (97%)	9 (3%)	40 28
28	H	101/105 (96%)	94 (93%)	7 (7%)	15 6
29	HH	244/245 (100%)	239 (98%)	5 (2%)	55 48
30	I	55/129 (43%)	54 (98%)	1 (2%)	59 51
31	II	133/153 (87%)	129 (97%)	4 (3%)	41 29
32	J	104/118 (88%)	102 (98%)	2 (2%)	57 50
33	JJ	186/205 (91%)	182 (98%)	4 (2%)	52 46
34	K	109/110 (99%)	105 (96%)	4 (4%)	34 22
35	KK	187/208 (90%)	180 (96%)	7 (4%)	34 22
36	L	115/116 (99%)	111 (96%)	4 (4%)	36 24
37	LL	171/171 (100%)	164 (96%)	7 (4%)	30 18
38	M	118/119 (99%)	115 (98%)	3 (2%)	47 39
39	MM	184/187 (98%)	178 (97%)	6 (3%)	38 26
40	N	46/47 (98%)	44 (96%)	2 (4%)	29 17
41	NN	147/150 (98%)	132 (90%)	15 (10%)	7 1
42	O	81/88 (92%)	76 (94%)	5 (6%)	18 8
43	OO	154/159 (97%)	149 (97%)	5 (3%)	39 28
44	P	94/97 (97%)	91 (97%)	3 (3%)	39 28
45	PP	107/109 (98%)	104 (97%)	3 (3%)	43 32
46	Pp	2/2 (100%)	2 (100%)	0	100 100
47	Q	109/111 (98%)	108 (99%)	1 (1%)	78 77
48	QQ	175/176 (99%)	172 (98%)	3 (2%)	60 53
49	R	90/91 (99%)	90 (100%)	0	100 100
50	S	94/103 (91%)	93 (99%)	1 (1%)	73 70
51	T	104/105 (99%)	103 (99%)	1 (1%)	76 73
52	U	81/82 (99%)	79 (98%)	2 (2%)	47 39
53	V	69/71 (97%)	68 (99%)	1 (1%)	67 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
54	W	68/69 (99%)	63 (93%)	5 (7%)	13 5
55	X	45/46 (98%)	45 (100%)	0	100 100
56	Y	47/116 (40%)	45 (96%)	2 (4%)	29 17
57	Z	23/23 (100%)	22 (96%)	1 (4%)	29 17
58	a	87/91 (96%)	83 (95%)	4 (5%)	27 14
59	b	71/72 (99%)	70 (99%)	1 (1%)	67 62
61	d	165/210 (79%)	160 (97%)	5 (3%)	41 29
62	e	189/224 (84%)	177 (94%)	12 (6%)	18 7
63	f	176/205 (86%)	167 (95%)	9 (5%)	24 12
64	g	167/195 (86%)	154 (92%)	13 (8%)	12 4
65	h	220/222 (99%)	205 (93%)	15 (7%)	16 6
66	i	172/191 (90%)	160 (93%)	12 (7%)	15 6
67	j	188/201 (94%)	179 (95%)	9 (5%)	25 13
68	k	165/170 (97%)	152 (92%)	13 (8%)	12 3
69	l	146/161 (91%)	139 (95%)	7 (5%)	25 13
70	m	158/166 (95%)	144 (91%)	14 (9%)	9 2
71	n	84/98 (86%)	82 (98%)	2 (2%)	49 41
72	o	127/137 (93%)	121 (95%)	6 (5%)	26 13
73	p	127/128 (99%)	122 (96%)	5 (4%)	32 19
74	q	81/105 (77%)	80 (99%)	1 (1%)	71 67
75	r	89/118 (75%)	84 (94%)	5 (6%)	21 9
76	s	114/119 (96%)	105 (92%)	9 (8%)	12 3
77	t	105/124 (85%)	88 (84%)	17 (16%)	2 0
78	u	128/129 (99%)	122 (95%)	6 (5%)	26 13
79	v	115/116 (99%)	108 (94%)	7 (6%)	18 8
80	w	94/114 (82%)	84 (89%)	10 (11%)	6 1
81	x	74/74 (100%)	70 (95%)	4 (5%)	22 10
82	y	110/111 (99%)	108 (98%)	2 (2%)	59 51
83	z	119/120 (99%)	113 (95%)	6 (5%)	24 12
All	All	9327/10257 (91%)	8879 (95%)	448 (5%)	29 13

5 of 448 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	P	31	ARG
83	z	41	SER
64	g	44	THR
81	x	44	ARG
77	t	25	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
63	f	147	ASN
67	j	65	GLN
74	q	99	GLN
68	k	108	GLN
55	X	33	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	3185/3396 (93%)	472 (14%)	21 (0%)
13	BB	120/121 (99%)	9 (7%)	1 (0%)
14	Bb	75/76 (98%)	29 (38%)	0
16	CC	157/158 (99%)	21 (13%)	0
17	Cc	76/77 (98%)	19 (25%)	0
20	Dd	12/39 (30%)	3 (25%)	0
60	c	1589/1800 (88%)	283 (17%)	0
All	All	5214/5667 (92%)	836 (16%)	22 (0%)

5 of 836 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	AA	6	A
11	AA	26	A
11	AA	40	A
11	AA	43	A
11	AA	49	A

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	AA	2490	C
11	AA	2922	OMG

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Mol	Chain	Res	Type
11	AA	2792	A
11	AA	2971	A
11	AA	993	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	OMG	AA	2815	11	18,26,27	1.19	2 (11%)	19,38,41	0.91	1 (5%)
11	A2M	AA	2640	11	18,25,26	3.62	8 (44%)	18,36,39	3.26	4 (22%)
60	A2M	c	28	60	18,25,26	3.61	8 (44%)	18,36,39	3.32	3 (16%)
11	OMG	AA	2922	14,11	18,26,27	1.32	2 (11%)	19,38,41	0.94	1 (5%)
60	MA6	c	1781	60	18,26,27	1.08	2 (11%)	19,38,41	3.43	2 (10%)
11	OMG	AA	2793	11	18,26,27	1.26	3 (16%)	19,38,41	0.86	1 (5%)
60	OMU	c	1269	60	19,22,23	2.97	8 (42%)	26,31,34	1.70	5 (19%)
11	OMC	AA	663	11	19,22,23	0.63	0	26,31,34	0.73	0
11	OMC	AA	2197	86,11	19,22,23	0.61	0	26,31,34	0.67	0
11	A2M	AA	2256	11	18,25,26	3.58	7 (38%)	18,36,39	3.50	4 (22%)
11	OMC	AA	2959	11,85	19,22,23	0.64	0	26,31,34	0.64	0
11	A2M	AA	876	11	18,25,26	3.59	7 (38%)	18,36,39	3.38	4 (22%)
11	OMU	AA	2421	11	19,22,23	2.95	8 (42%)	26,31,34	1.75	5 (19%)
60	OMG	c	1126	60	18,26,27	1.19	2 (11%)	19,38,41	0.85	1 (5%)
11	OMG	AA	908	11	18,26,27	1.25	2 (11%)	19,38,41	0.84	1 (5%)
11	A2M	AA	1449	11,85	18,25,26	3.58	7 (38%)	18,36,39	3.36	4 (22%)
14	YYG	Bb	37	14,85	31,42,43	2.23	8 (25%)	33,62,65	1.79	10 (30%)
11	OMU	AA	2729	11	19,22,23	2.94	8 (42%)	26,31,34	1.66	5 (19%)
11	OMU	AA	2921	11,85	19,22,23	2.95	8 (42%)	26,31,34	1.71	5 (19%)
60	MA6	c	1782	60	18,26,27	1.06	2 (11%)	19,38,41	3.54	2 (10%)
11	OMG	AA	2791	11	18,26,27	1.22	2 (11%)	19,38,41	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	A2M	AA	2220	11	18,25,26	3.60	8 (44%)	18,36,39	3.38	3 (16%)
11	1MA	AA	645	11,85	16,25,26	1.00	2 (12%)	18,37,40	1.11	2 (11%)
60	A2M	c	974	60	18,25,26	3.62	9 (50%)	18,36,39	3.34	3 (16%)
60	OMG	c	562	60	18,26,27	1.16	2 (11%)	19,38,41	0.87	1 (5%)
11	UR3	AA	2634	11	19,22,23	2.79	7 (36%)	26,32,35	1.31	1 (3%)
60	OMG	c	1572	60	18,26,27	1.20	2 (11%)	19,38,41	0.87	1 (5%)
11	OMU	AA	1888	11	19,22,23	3.00	8 (42%)	26,31,34	1.81	6 (23%)
11	A2M	AA	2280	11	18,25,26	3.62	8 (44%)	18,36,39	3.30	3 (16%)
11	A2M	AA	817	11,85	18,25,26	3.59	7 (38%)	18,36,39	3.50	3 (16%)
60	B8N	c	1191	60	24,29,30	3.03	7 (29%)	29,42,45	1.69	5 (17%)
60	OMC	c	1007	60	19,22,23	0.59	0	26,31,34	0.63	0
60	OMC	c	1639	85,60	19,22,23	0.64	0	26,31,34	0.54	0
11	OMG	AA	1450	11	18,26,27	1.20	2 (11%)	19,38,41	0.77	1 (5%)
11	OMG	AA	2619	11	18,26,27	1.21	2 (11%)	19,38,41	0.83	1 (5%)
60	A2M	c	436	60	18,25,26	3.62	8 (44%)	18,36,39	3.39	3 (16%)
11	5MC	AA	2870	86,11	18,22,23	0.80	0	26,32,35	0.66	0
60	A2M	c	619	85,60	18,25,26	3.65	8 (44%)	18,36,39	3.50	3 (16%)
11	OMG	AA	2288	11	18,26,27	1.21	2 (11%)	19,38,41	0.81	1 (5%)
11	OMC	AA	2948	11	19,22,23	0.62	0	26,31,34	0.75	1 (3%)
60	OMU	c	578	60	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
60	OMG	c	1271	60	18,26,27	1.18	2 (11%)	19,38,41	0.87	1 (5%)
11	1MA	AA	2142	11,85	16,25,26	1.02	2 (12%)	18,37,40	1.10	2 (11%)
11	A2M	AA	649	11	18,25,26	3.65	7 (38%)	18,36,39	3.26	3 (16%)
60	OMC	c	414	60	19,22,23	0.63	0	26,31,34	0.78	1 (3%)
60	A2M	c	420	60	18,25,26	3.60	8 (44%)	18,36,39	3.30	3 (16%)
60	A2M	c	796	60	18,25,26	3.62	8 (44%)	18,36,39	3.38	3 (16%)
11	OMG	AA	867	86,11	18,26,27	1.27	2 (11%)	19,38,41	0.88	1 (5%)
11	A2M	AA	2946	11,85	18,25,26	3.61	7 (38%)	18,36,39	3.40	3 (16%)
11	A2M	AA	2281	11	18,25,26	3.72	8 (44%)	18,36,39	3.32	4 (22%)
11	OMC	AA	2337	11	19,22,23	0.62	0	26,31,34	0.77	1 (3%)
60	A2M	c	100	85,60	18,25,26	3.63	9 (50%)	18,36,39	3.33	4 (22%)
11	OMU	AA	2347	11	19,22,23	3.00	8 (42%)	26,31,34	1.71	5 (19%)
11	OMU	AA	2417	11	19,22,23	2.92	8 (42%)	26,31,34	1.75	5 (19%)
11	5MC	AA	2278	11,85	18,22,23	0.63	0	26,32,35	0.60	0
60	4AC	c	1773	60	21,24,25	3.36	10 (47%)	29,34,37	1.55	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
60	4AC	c	1280	60	21,24,25	3.40	10 (47%)	29,34,37	1.58	5 (17%)
11	OMU	AA	2724	11	19,22,23	2.95	8 (42%)	26,31,34	1.70	5 (19%)
11	OMG	AA	805	11	18,26,27	1.23	3 (16%)	19,38,41	0.86	1 (5%)
60	OMG	c	1428	85,60	18,26,27	1.20	2 (11%)	19,38,41	0.86	1 (5%)
11	OMU	AA	898	11	19,22,23	2.93	8 (42%)	26,31,34	1.69	5 (19%)
60	A2M	c	541	60	18,25,26	3.58	8 (44%)	18,36,39	3.44	5 (27%)
60	G7M	c	1575	60,17	20,26,27	2.34	7 (35%)	17,39,42	1.33	2 (11%)
11	A2M	AA	807	11	18,25,26	3.60	8 (44%)	18,36,39	3.36	3 (16%)
11	OMC	AA	1437	11,85	19,22,23	0.64	0	26,31,34	0.85	1 (3%)
11	A2M	AA	1133	11,85	18,25,26	3.62	8 (44%)	18,36,39	3.46	3 (16%)
11	OMC	AA	650	11,85	19,22,23	0.62	0	26,31,34	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMG	AA	2815	11	-	0/5/27/28	0/3/3/3
11	A2M	AA	2640	11	-	1/5/27/28	0/3/3/3
60	A2M	c	28	60	-	1/5/27/28	0/3/3/3
11	OMG	AA	2922	14,11	-	2/5/27/28	0/3/3/3
60	MA6	c	1781	60	-	0/7/29/30	0/3/3/3
11	OMG	AA	2793	11	-	0/5/27/28	0/3/3/3
60	OMU	c	1269	60	-	0/9/27/28	0/2/2/2
11	OMC	AA	663	11	-	1/9/27/28	0/2/2/2
11	OMC	AA	2197	86,11	-	4/9/27/28	0/2/2/2
11	A2M	AA	2256	11	-	3/5/27/28	0/3/3/3
11	OMC	AA	2959	11,85	-	0/9/27/28	0/2/2/2
11	A2M	AA	876	11	-	2/5/27/28	0/3/3/3
11	OMU	AA	2421	11	-	0/9/27/28	0/2/2/2
60	OMG	c	1126	60	-	1/5/27/28	0/3/3/3
11	OMG	AA	908	11	-	1/5/27/28	0/3/3/3
11	A2M	AA	1449	11,85	-	0/5/27/28	0/3/3/3
14	YYG	Bb	37	14,85	-	9/20/42/43	0/3/4/4
11	OMU	AA	2729	11	-	0/9/27/28	0/2/2/2
11	OMU	AA	2921	11,85	-	0/9/27/28	0/2/2/2
60	MA6	c	1782	60	-	3/7/29/30	0/3/3/3
11	OMG	AA	2791	11	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	A2M	AA	2220	11	-	0/5/27/28	0/3/3/3
11	1MA	AA	645	11,85	-	0/3/25/26	0/3/3/3
60	A2M	c	974	60	-	0/5/27/28	0/3/3/3
60	OMG	c	562	60	-	0/5/27/28	0/3/3/3
11	UR3	AA	2634	11	-	0/7/25/26	0/2/2/2
60	OMG	c	1572	60	-	2/5/27/28	0/3/3/3
11	OMU	AA	1888	11	-	0/9/27/28	0/2/2/2
11	A2M	AA	2280	11	-	2/5/27/28	0/3/3/3
11	A2M	AA	817	11,85	-	3/5/27/28	0/3/3/3
60	B8N	c	1191	60	-	1/16/34/35	0/2/2/2
60	OMC	c	1007	60	-	0/9/27/28	0/2/2/2
60	OMC	c	1639	85,60	-	0/9/27/28	0/2/2/2
11	OMG	AA	1450	11	-	2/5/27/28	0/3/3/3
11	OMG	AA	2619	11	-	1/5/27/28	0/3/3/3
60	A2M	c	436	60	-	0/5/27/28	0/3/3/3
11	5MC	AA	2870	86,11	-	4/7/25/26	0/2/2/2
60	A2M	c	619	85,60	-	3/5/27/28	0/3/3/3
11	OMG	AA	2288	11	-	0/5/27/28	0/3/3/3
11	OMC	AA	2948	11	-	0/9/27/28	0/2/2/2
60	OMU	c	578	60	-	4/9/27/28	0/2/2/2
60	OMG	c	1271	60	-	1/5/27/28	0/3/3/3
11	1MA	AA	2142	11,85	-	0/3/25/26	0/3/3/3
11	A2M	AA	649	11	-	1/5/27/28	0/3/3/3
60	OMC	c	414	60	-	3/9/27/28	0/2/2/2
60	A2M	c	420	60	-	1/5/27/28	0/3/3/3
60	A2M	c	796	60	-	0/5/27/28	0/3/3/3
11	OMG	AA	867	86,11	-	2/5/27/28	0/3/3/3
11	A2M	AA	2946	11,85	-	0/5/27/28	0/3/3/3
11	A2M	AA	2281	11	-	1/5/27/28	0/3/3/3
11	OMC	AA	2337	11	-	0/9/27/28	0/2/2/2
60	A2M	c	100	85,60	-	2/5/27/28	0/3/3/3
11	OMU	AA	2347	11	-	0/9/27/28	0/2/2/2
11	OMU	AA	2417	11	-	1/9/27/28	0/2/2/2
11	5MC	AA	2278	11,85	-	0/7/25/26	0/2/2/2
60	4AC	c	1773	60	-	2/11/29/30	0/2/2/2
60	4AC	c	1280	60	-	4/11/29/30	0/2/2/2
11	OMU	AA	2724	11	-	1/9/27/28	0/2/2/2
11	OMG	AA	805	11	-	0/5/27/28	0/3/3/3
60	OMG	c	1428	85,60	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMU	AA	898	11	-	0/9/27/28	0/2/2/2
60	A2M	c	541	60	-	3/5/27/28	0/3/3/3
60	G7M	c	1575	60,17	-	2/3/25/26	0/3/3/3
11	A2M	AA	807	11	-	3/5/27/28	0/3/3/3
11	OMC	AA	1437	11,85	-	2/9/27/28	0/2/2/2
11	A2M	AA	1133	11,85	-	0/5/27/28	0/3/3/3
11	OMC	AA	650	11,85	-	0/9/27/28	0/2/2/2

The worst 5 of 325 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	c	796	A2M	C3'-C4'	-8.98	1.30	1.53
60	c	100	A2M	C3'-C4'	-8.92	1.30	1.53
11	AA	1133	A2M	C3'-C4'	-8.88	1.30	1.53
60	c	619	A2M	C3'-C4'	-8.88	1.30	1.53
60	c	28	A2M	C3'-C4'	-8.88	1.30	1.53

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	c	1782	MA6	N1-C6-N6	-14.10	102.21	117.06
60	c	1781	MA6	N1-C6-N6	-13.64	102.70	117.06
11	AA	817	A2M	C5-C6-N6	11.00	137.06	120.35
11	AA	1133	A2M	C5-C6-N6	10.94	136.97	120.35
60	c	619	A2M	C5-C6-N6	10.88	136.88	120.35

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AA	663	OMC	C1'-C2'-O2'-CM2
11	AA	1437	OMC	C1'-C2'-O2'-CM2
11	AA	1450	OMG	O4'-C4'-C5'-O5'
11	AA	2197	OMC	C2'-C1'-N1-C2
11	AA	2197	OMC	C2'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 315 ligands modelled in this entry, 311 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	SPD	AA	3620	-	9,9,9	0.28	0	8,8,8	0.76	0
87	SPD	AA	3619	-	9,9,9	0.32	0	8,8,8	0.88	0
87	SPD	c	1965	-	9,9,9	0.29	0	8,8,8	0.81	0
87	SPD	AA	3618	-	9,9,9	0.31	0	8,8,8	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	AA	3620	-	-	4/7/7/7	-
87	SPD	AA	3619	-	-	0/7/7/7	-
87	SPD	c	1965	-	-	1/7/7/7	-
87	SPD	AA	3618	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	AA	3620	SPD	C3-C4-C5-N6
87	AA	3620	SPD	C2-C3-C4-C5
87	AA	3620	SPD	C4-C5-N6-C7

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Mol	Chain	Res	Type	Atoms
87	AA	3618	SPD	N1-C2-C3-C4
87	c	1965	SPD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16563. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.