



## wwPDB EM Validation Summary Report ⓘ

Jan 24, 2024 – 03:11 pm GMT

PDB ID : 8Q5I  
EMDB ID : EMD-18156  
Title : Structure of Candida albicans 80S ribosome in complex with cephaeline  
Authors : Kolosova, O.; Zgadzay, Y.; Stetsenko, A.; Atamas, A.; Guskov, A.; Yusupov, M.  
Deposited on : 2023-08-09  
Resolution : 2.45 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](mailto: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>.

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

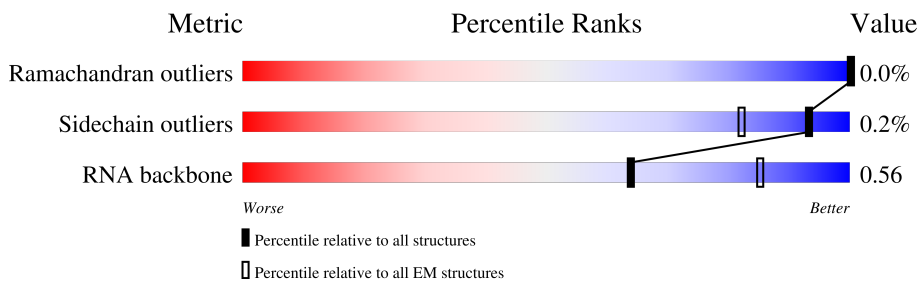
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.45 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	3359	
2	3	121	
3	4	158	
4	10	14	
5	j	254	
6	k	389	
7	l	363	
8	m	298	

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Mol	Chain	Length	Quality of chain
9	n	176	18% 88% 12%
10	o	241	1% 94% 6%
11	p	262	11% 89% 11%
12	q	191	7% 98% 5%
13	r	220	6% 95% 5%
14	s	174	34% 98% 2% 2%
15	t	202	8% 95% 5%
16	u	131	7% 98% 2% 2%
17	v	204	99%
18	w	200	1% 100%
19	x	185	8% 92% 2% 7%
20	y	186	99%
21	z	190	17% 94% 6%
22	0	172	1% 99% 1%
23	2	160	10% 99% 2% 2%
24	5	124	36% 80% 2% 19%
25	6	137	1% 96% 1%
26	7	155	1% 41% 59%
27	8	142	6% 85% 2% 15%
28	9	127	1% 98% 2% 2%
29	AA	136	11% 99% 1%
30	AB	149	1% 99% 1%
31	AC	63	16% 90% 10%
32	AD	106	8% 91% 9%
33	AE	112	7% 92% 8%

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Mol	Chain	Length	Quality of chain
34	AF	131	5% 95% 5%
35	AG	107	99% .
36	AH	122	9% 92% 8%
37	AI	120	6% 99% .
38	AJ	99	11% 97% ..
39	AK	90	. 96% .
40	AL	78	27% 99% .
41	AM	51	6% 98% .
42	AN	52	. 100%
43	AO	25	32% 100%
44	AP	106	8% 97% .
45	AQ	92	5% 99% .
46	A	1787	11% 67% 20% 13%
47	B	261	16% 80% 20%
48	C	256	47% 83% 16%
49	D	249	5% 87% 13%
50	E	251	56% 82% 18%
51	F	262	9% 99% .
52	G	225	79% 92% 8%
53	H	236	58% 96% .
54	I	186	53% 98% .
55	J	206	32% 90% 10%
56	K	189	10% 94% 6%
57	L	118	69% 77% 21%
58	M	155	14% 86% 13%

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Mol	Chain	Length	Quality of chain
59	O	151	15% 99%
60	P	132	30% 95%
61	Q	142	62% 82% 17%
62	R	142	76% 99%
63	S	137	69% 91% 9%
64	T	145	78% 98%
65	U	145	84% 97%
66	V	119	62% 82% 16%
67	W	87	13% 100%
68	X	130	99%
69	Y	145	99%
70	Z	135	22% 98%
71	b	119	19% 84% 16%
72	c	82	30% 99%
73	d	67	72% 93% 7%
74	e	56	14% 98%
75	f	63	32% 89% 11%
76	g	5	100% 80% 20%

## 2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 189590 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	3073	65690	29348	11807	21462	3073	0	0

- Molecule 2 is a RNA chain called 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	3	121	2579	1153	463	842	121	0	0

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	158	3353	1500	585	1110	158	0	0

- Molecule 4 is a RNA chain called Mixture of endogenous E-tRNAs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	10	9	187	84	31	63	9	0	0

- Molecule 5 is a protein called 60S ribosomal protein L2-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	j	249	1894	1185	377	330	2	1	0

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	k	386	3084	1955	584	538	7	1	0

- Molecule 7 is a protein called 60S ribosomal protein L4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	l	361	2751	1729	529	490	3	0	0

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	m	292	2394	1526	416	450	2	0	0

- Molecule 9 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	n	155	1237	794	226	217	1	0

- Molecule 10 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	o	226	1824	1170	336	317	1	0	

- Molecule 11 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	p	232	1800	1153	320	324	3	0	0

- Molecule 12 is a protein called 60S ribosomal protein L9-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	q	188	1501	948	274	275	4	0	0

- Molecule 13 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	r	208	1689	1069	322	291	7	0	0

- Molecule 14 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	s	172	Total	C	N	O	S	1	0
			1385	864	262	255	4		

- Molecule 15 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	t	191	Total	C	N	O	S	0	0
			1545	970	307	268			

- Molecule 16 is a protein called 60S ribosomal protein L14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	u	130	Total	C	N	O	S	0	0
			1029	660	193	175	1		

- Molecule 17 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	v	203	Total	C	N	O	S	0	0
			1713	1075	356	280	2		

- Molecule 18 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	w	199	Total	C	N	O	S	0	0
			1590	1025	294	269	2		

- Molecule 19 is a protein called Ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	x	172	Total	C	N	O	S	0	0
			1375	850	279	246			

- Molecule 20 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	y	185	Total	C	N	O	S	3	0
			1478	930	302	246			

- Molecule 21 is a protein called 60S ribosomal protein L19-A.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	z	179	Total	C	N	O	S	1	0
			1462	904	311	244	3		

- Molecule 22 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	171	Total	C	N	O	S	2	0
			1442	933	262	244	3		

- Molecule 23 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	159	Total	C	N	O	S	2	0
			1276	807	244	223	2		

- Molecule 24 is a protein called 60S ribosomal protein L22-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	5	101	Total	C	N	O	2	0
			833	544	136	153		

- Molecule 25 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	131	Total	C	N	O	S	1	0
			986	621	186	171	8		

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	7	63	Total	C	N	O	S	0	0
			524	334	103	86	1		

- Molecule 27 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	8	121	Total	C	N	O	S	0	0
			974	622	175	176	1		

- Molecule 28 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	9	125	Total	C	N	O	0	0
			980	613	189	178		

- Molecule 29 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AA	135	Total	C	N	O	S	0	0
			1087	705	197	183	2		

- Molecule 30 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AB	148	Total	C	N	O	S	0	0
			1170	741	231	197	1		

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AC	57	Total	C	N	O	S	1	0
			464	291	99	73	1		

- Molecule 32 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AD	96	Total	C	N	O	S	0	0
			729	469	121	137	2		

- Molecule 33 is a protein called 60S ribosomal protein L31-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AE	103	Total	C	N	O	S	0	0
			839	536	161	140	2		

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AF	125	Total	C	N	O	S	1	0
			1015	649	197	168	1		

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	AG	106	867	558	166	142	1	3	0

- Molecule 36 is a protein called 60S ribosomal protein L34-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	AH	112	913	567	188	154	4	4	0

- Molecule 37 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	AI	119	990	629	195	166	1	0

- Molecule 38 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	AJ	97	764	476	157	130	1	1	0

- Molecule 39 is a protein called 60S ribosomal protein L37-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	AK	86	677	413	148	110	6	0	0

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	AL	77	623	398	116	109	1	0

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	AM	50	446	280	100	66	1	0

- Molecule 42 is a protein called 60S ribosomal protein L40-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AN	52	Total	C	N	O	S	1	0
			427	265	89	67	6		

- Molecule 43 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AO	25	Total	C	N	O	S	0	0
			236	144	63	28	1		

- Molecule 44 is a protein called 60S ribosomal protein L42-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AP	103	Total	C	N	O	S	2	0
			843	533	168	137	5		

- Molecule 45 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AQ	91	Total	C	N	O	S	0	0
			698	430	140	124	4		

- Molecule 46 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	A	1558	Total	C	N	O	P	0	0
			33257	14866	5947	10886	1558		

- Molecule 47 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	B	208	Total	C	N	O	S	0	0
			1627	1041	284	297	5		

- Molecule 48 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	C	214	Total	C	N	O	S	0	0
			1724	1094	313	313	4		

- Molecule 49 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	D	216	Total	C	N	O	S	0	0
			1620	1033	287	295	5		

- Molecule 50 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	E	206	Total	C	N	O	S	0	0
			1582	1010	292	276	4		

- Molecule 51 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	F	260	Total	C	N	O	S	0	0
			2055	1306	386	358	5		

- Molecule 52 is a protein called Ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	G	206	Total	C	N	O	S	0	0
			1614	1008	301	301	4		

- Molecule 53 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	H	226	Total	C	N	O	S	0	0
			1820	1133	351	330	6		

- Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	I	182	Total	C	N	O	0	0
			1466	939	264	263		

- Molecule 55 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	J	185	Total	C	N	O	S	0	0
			1461	902	297	261	1		

- Molecule 56 is a protein called Ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	K	178	1453	918	286	248	1	0	0

- Molecule 57 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	L	93	783	511	129	142	1	0	0

- Molecule 58 is a protein called 40S ribosomal protein S11A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	M	135	1084	694	202	185	3	0	0

- Molecule 59 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	O	150	1187	757	219	210	1	0	0

- Molecule 60 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	P	127	942	579	186	174	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	119	IAS	ASP	conflict	UNP A0A8H6F0V4

- Molecule 61 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	Q	118	935	598	169	162	6	0	0

- Molecule 62 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	R	140	Total	C	N	O	S	0	0
			1091	700	198	192	1		

- Molecule 63 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	S	125	Total	C	N	O	S	0	0
			1002	631	184	186	1		

- Molecule 64 is a protein called 40S ribosomal protein S18-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	T	142	Total	C	N	O	S	0	0
			1169	733	228	205	3		

- Molecule 65 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	U	141	Total	C	N	O	S	0	0
			1100	689	210	200	1		

- Molecule 66 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	V	100	Total	C	N	O	S	0	0
			790	499	146	143	2		

- Molecule 67 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	W	87	Total	C	N	O	S	0	0
			676	415	126	133	2		

- Molecule 68 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	X	129	Total	C	N	O	S	0	0
			1032	655	191	183	3		

- Molecule 69 is a protein called Ribosomal protein S23 (S12).

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Y	143	Total	C	N	O	S	0	0
			1110	701	219	188	2		

- Molecule 70 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Z	132	Total	C	N	O	S	0	0
			1072	670	216	186			

- Molecule 71 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	b	100	Total	C	N	O	S	0	0
			799	494	169	130	6		

- Molecule 72 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	c	81	Total	C	N	O	S	0	0
			614	383	110	114	7		

- Molecule 73 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	d	62	Total	C	N	O	S	0	0
			487	299	98	88	2		

- Molecule 74 is a protein called 40S ribosomal protein S29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	e	55	Total	C	N	O	S	0	0
			454	281	94	75	4		

- Molecule 75 is a protein called 40S ribosomal protein S30.

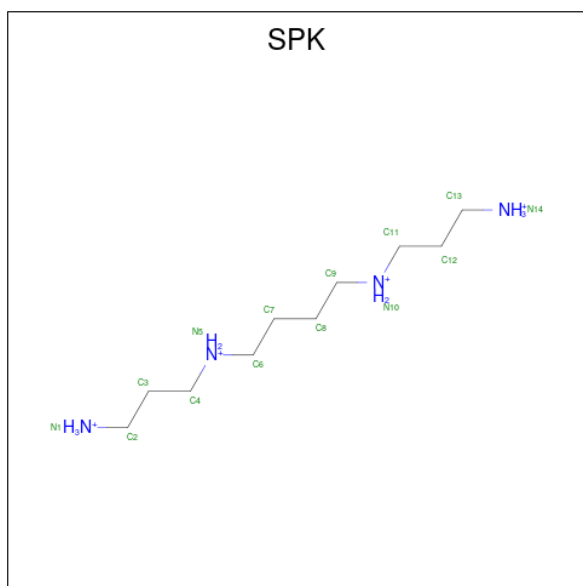
Mol	Chain	Residues	Atoms					AltConf	Trace
75	f	56	Total	C	N	O	S	0	0
			444	278	89	75	2		

- Molecule 76 is a RNA chain called DNA (5'-R(P\*GP\*GP\*CP\*AP\*G)-3').



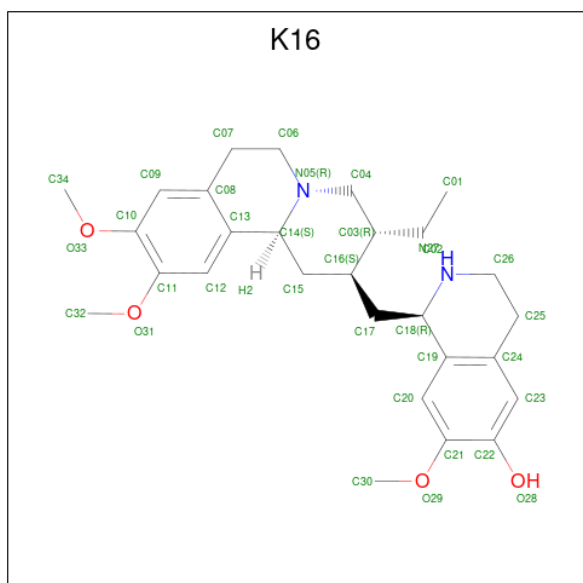
Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
76	g	5	111	49	23	34	5	0	0

- Molecule 77 is SPERMINE (FULLY PROTONATED FORM) (three-letter code: SPK) (formula:  $C_{10}H_{30}N_4$ ).



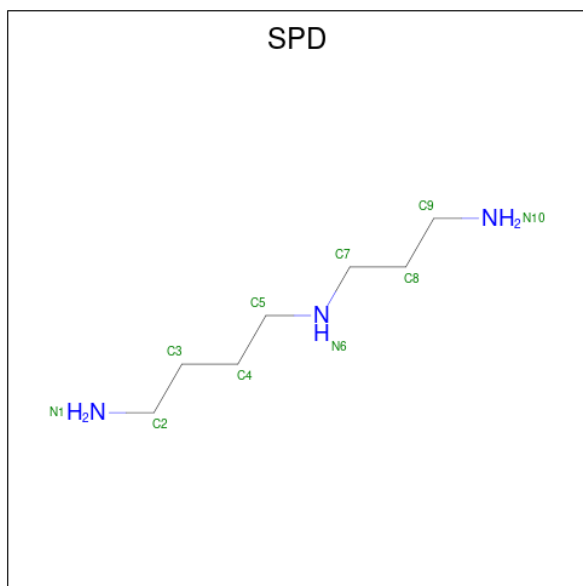
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
77	1	1	14	10	4	0

- Molecule 78 is Cephaeline (three-letter code: K16) (formula:  $C_{28}H_{38}N_2O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
78	1	1	Total 34	C 28	N 2	O 4	0
78	1	1	Total 34	C 28	N 2	O 4	0
78	A	1	Total 34	C 28	N 2	O 4	0

- Molecule 79 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
79	1	1	Total 10	C 7	N 3	0

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
80	1	255	Total 255	Mg 255	0
80	3	1	Total 1	Mg 1	0
80	4	2	Total 2	Mg 2	0
80	j	1	Total 1	Mg 1	0
80	k	1	Total 1	Mg 1	0
80	o	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms	AltConf
80	r	1	Total Mg 1 1	0
80	v	1	Total Mg 1 1	0
80	x	1	Total Mg 1 1	0
80	6	1	Total Mg 1 1	0
80	AH	1	Total Mg 1 1	0
80	AP	1	Total Mg 1 1	0
80	A	97	Total Mg 97 97	0
80	C	1	Total Mg 1 1	0
80	X	1	Total Mg 1 1	0
80	Y	1	Total Mg 1 1	0

- Molecule 81 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
81	AK	1	Total Zn 1 1	0
81	AN	1	Total Zn 1 1	0
81	AP	1	Total Zn 1 1	0
81	AQ	1	Total Zn 1 1	0
81	b	1	Total Zn 1 1	0
81	c	1	Total Zn 1 1	0
81	e	1	Total Zn 1 1	0

- Molecule 82 is water.

Mol	Chain	Residues	Atoms		AltConf
82	1	632	Total 632	O 632	0
82	3	2	Total 2	O 2	0
82	4	14	Total 14	O 14	0
82	10	1	Total 1	O 1	0
82	j	17	Total 17	O 17	0
82	k	16	Total 16	O 16	0
82	l	11	Total 11	O 11	0
82	m	2	Total 2	O 2	0
82	o	5	Total 5	O 5	0
82	q	2	Total 2	O 2	0
82	r	5	Total 5	O 5	0
82	t	1	Total 1	O 1	0
82	v	7	Total 7	O 7	0
82	w	3	Total 3	O 3	0
82	x	8	Total 8	O 8	0
82	y	1	Total 1	O 1	0
82	z	1	Total 1	O 1	0
82	2	1	Total 1	O 1	0
82	6	6	Total 6	O 6	0
82	8	2	Total 2	O 2	0
82	AA	1	Total 1	O 1	0
82	AB	1	Total 1	O 1	0

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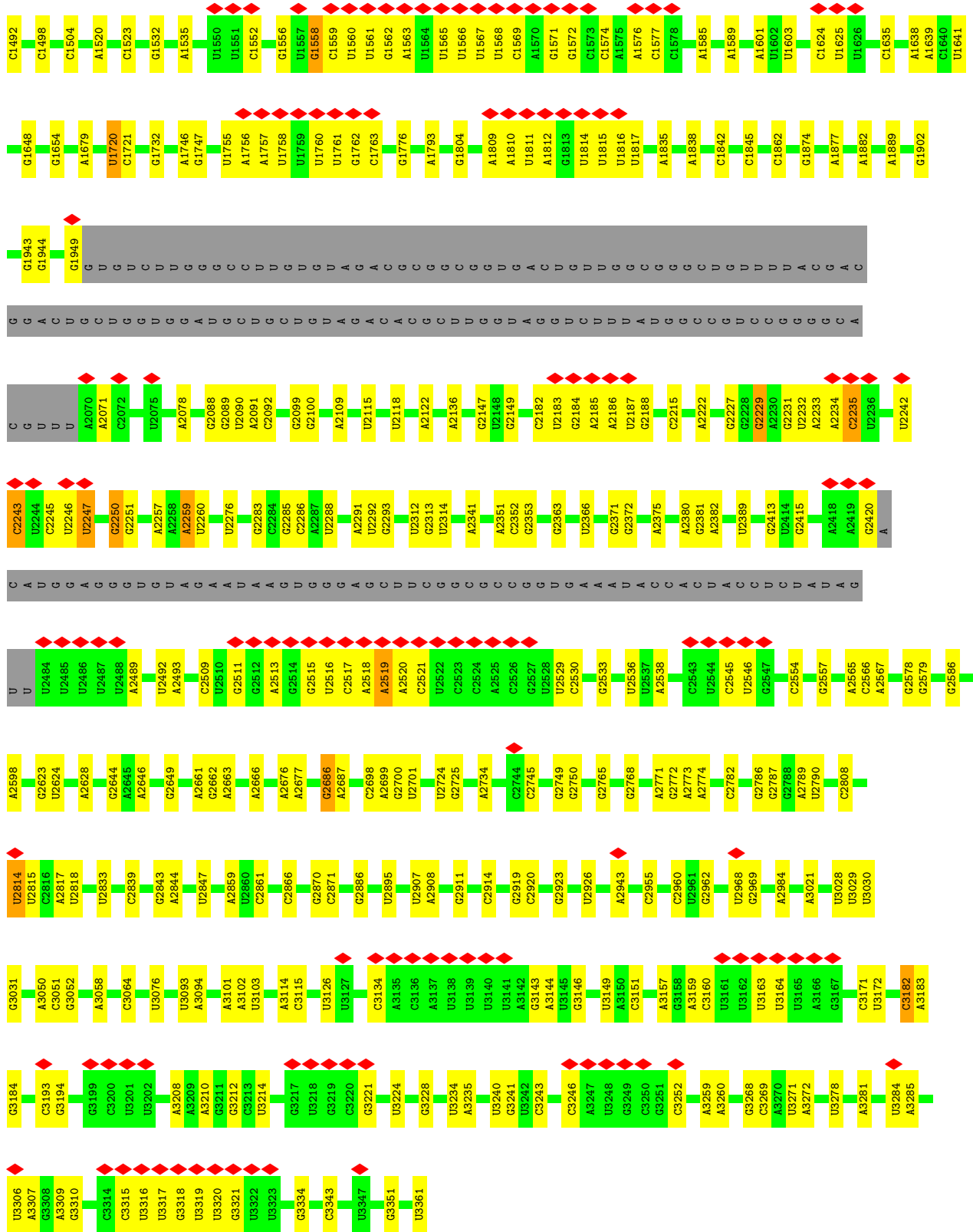
Mol	Chain	Residues	Atoms		AltConf
82	AC	3	Total 3	O 3	0
82	AF	5	Total 5	O 5	0
82	AG	3	Total 3	O 3	0
82	AH	4	Total 4	O 4	0
82	AI	2	Total 2	O 2	0
82	AK	7	Total 7	O 7	0
82	AP	3	Total 3	O 3	0
82	AQ	2	Total 2	O 2	0
82	A	321	Total 321	O 321	0
82	C	1	Total 1	O 1	0
82	D	5	Total 5	O 5	0
82	F	3	Total 3	O 3	0
82	H	3	Total 3	O 3	0
82	I	6	Total 6	O 6	0
82	J	5	Total 5	O 5	0
82	K	1	Total 1	O 1	0
82	M	5	Total 5	O 5	0
82	O	7	Total 7	O 7	0
82	P	1	Total 1	O 1	0
82	W	1	Total 1	O 1	0
82	X	15	Total 15	O 15	0

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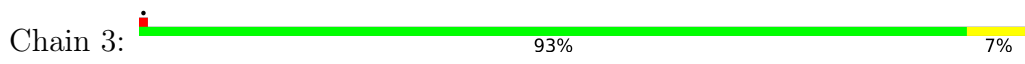
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
82	Y	11	Total 11	O 11	0
82	b	9	Total 9	O 9	0
82	c	3	Total 3	O 3	0
82	e	1	Total 1	O 1	0

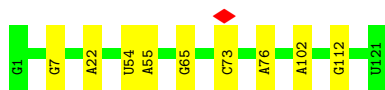




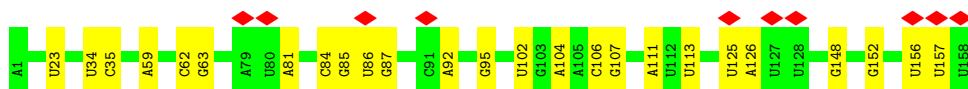
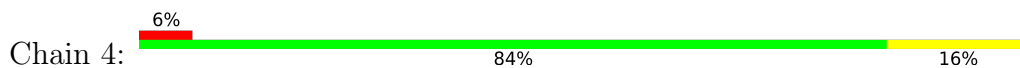
• Molecule 2: 5S







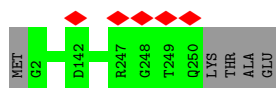
- Molecule 3: 5.8S rRNA



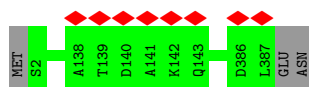
- Molecule 4: Mixture of endogenous E-tRNAs



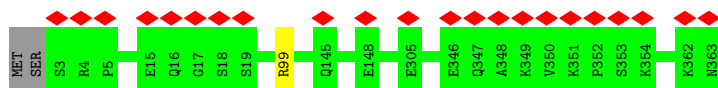
- Molecule 5: 60S ribosomal protein L2-B



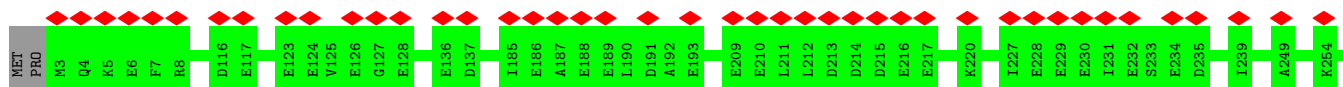
- Molecule 6: 60S ribosomal protein L3

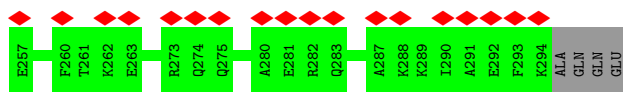


- Molecule 7: 60S ribosomal protein L4-B

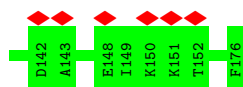
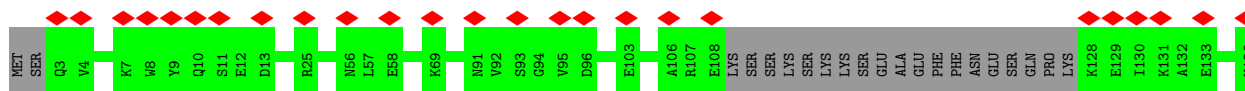
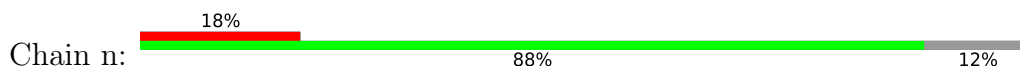


- Molecule 8: 60S ribosomal protein L5

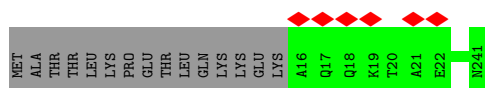




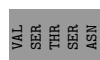
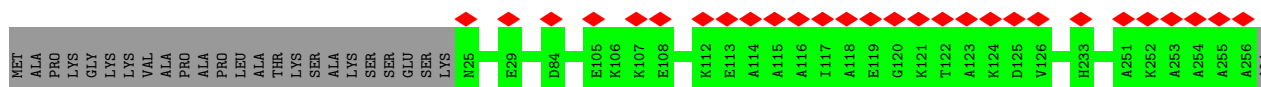
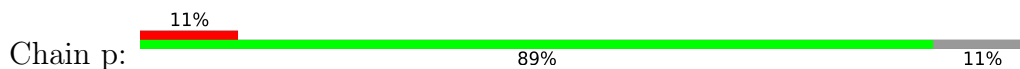
- Molecule 9: 60S ribosomal protein L6



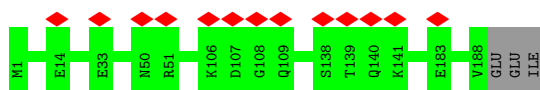
- Molecule 10: 60S ribosomal protein L7-A



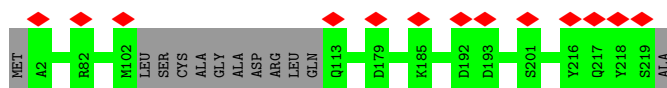
- Molecule 11: 60S ribosomal protein L8



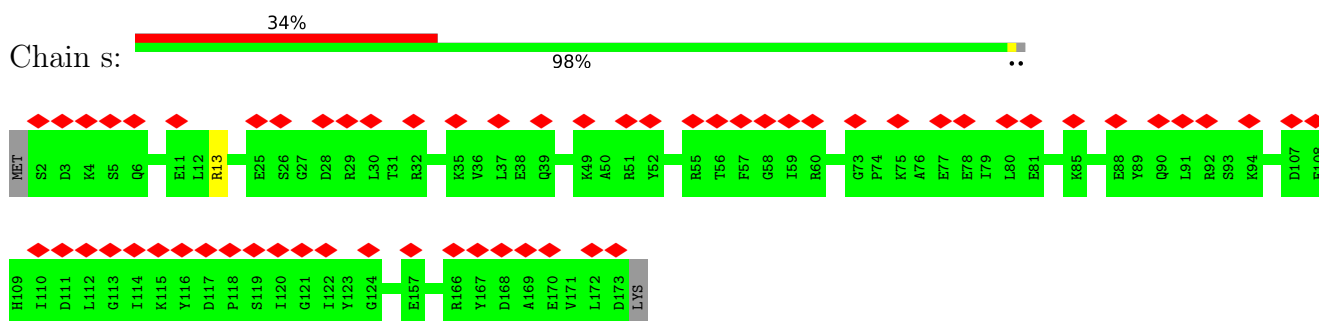
- Molecule 12: 60S ribosomal protein L9-B



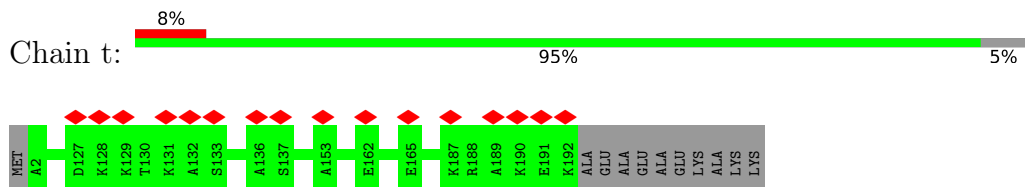
- Molecule 13: 60S ribosomal protein L10



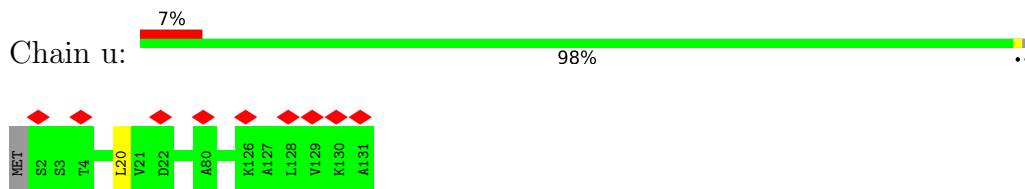
- Molecule 14: 60S ribosomal protein L11-B



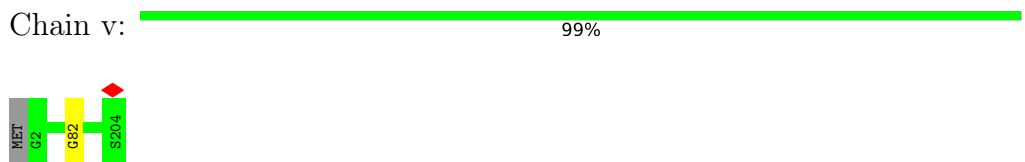
- Molecule 15: 60S ribosomal protein L13



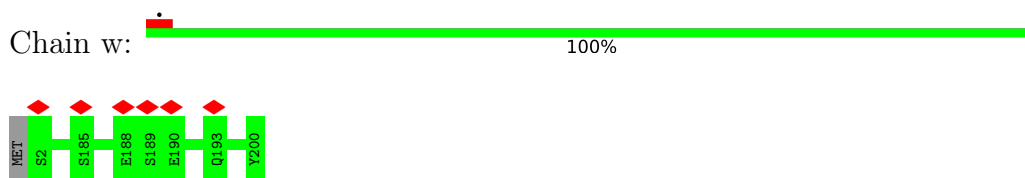
- Molecule 16: 60S ribosomal protein L14-B



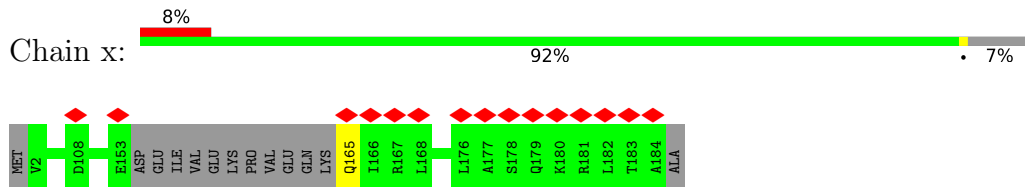
- Molecule 17: 60S ribosomal protein L15-A



- Molecule 18: Ribosomal protein L13



- Molecule 19: Ribosomal protein L22

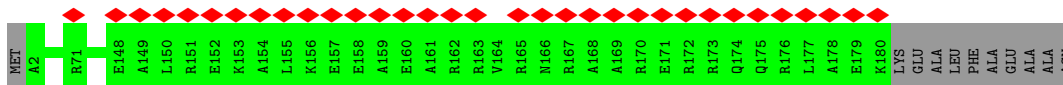
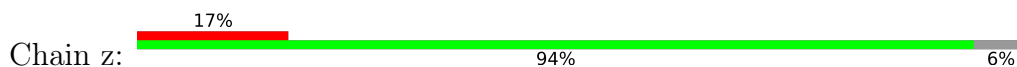


- Molecule 20: 60S ribosomal protein L18-A

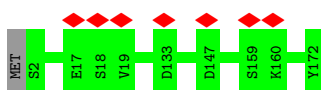




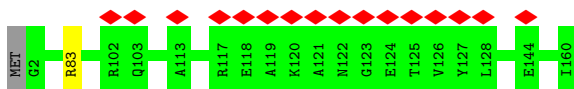
- Molecule 21: 60S ribosomal protein L19-A



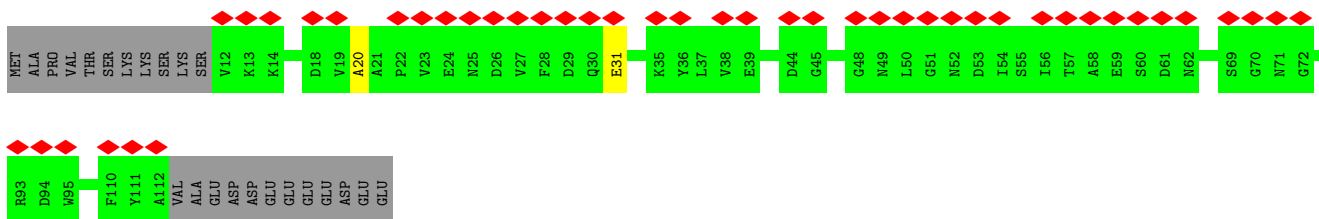
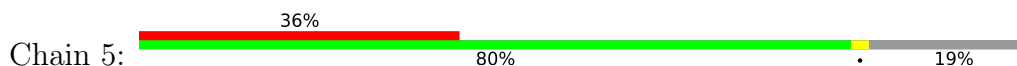
- Molecule 22: 60S ribosomal protein L20



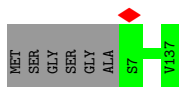
- Molecule 23: 60S ribosomal protein L21-A



- Molecule 24: 60S ribosomal protein L22-B

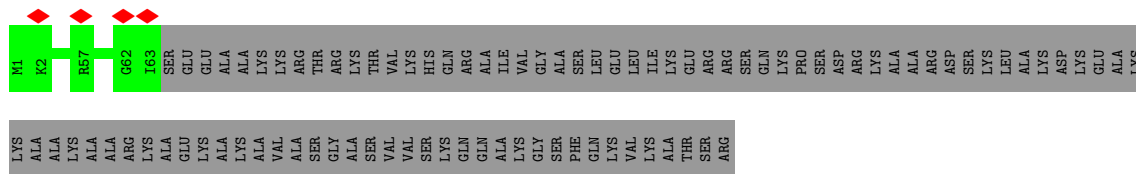


- Molecule 25: 60S ribosomal protein L23-A

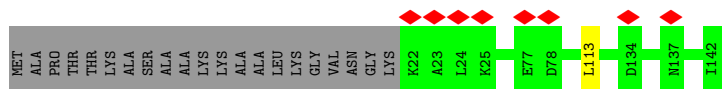
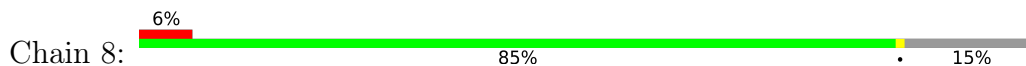


- Molecule 26: 60S ribosomal protein L24-A

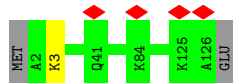




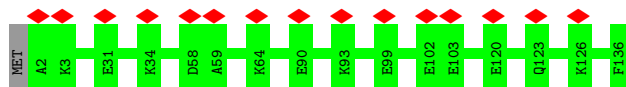
• Molecule 27: 60S ribosomal protein L25



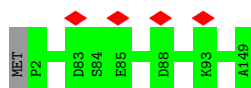
• Molecule 28: Ribosomal protein L24



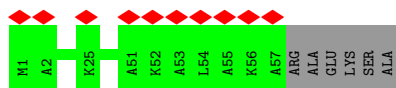
• Molecule 29: 60S ribosomal protein L27



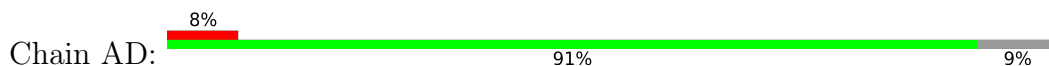
• Molecule 30: 60S ribosomal protein L28

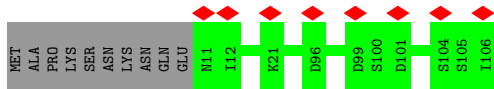


• Molecule 31: 60S ribosomal protein L29

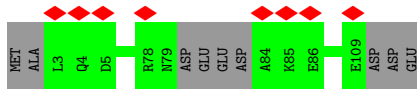


• Molecule 32: 60S ribosomal protein L30

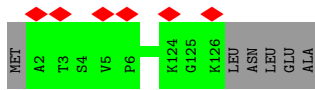




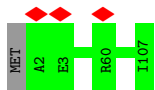
- Molecule 33: 60S ribosomal protein L31-B



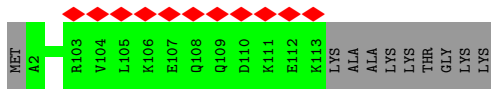
- Molecule 34: 60S ribosomal protein L32



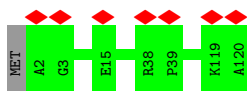
- Molecule 35: 60S ribosomal protein L33-A



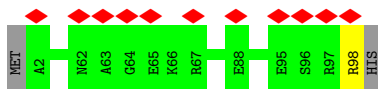
- Molecule 36: 60S ribosomal protein L34-B



- Molecule 37: Ribosomal protein L29

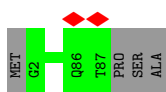


- Molecule 38: 60S ribosomal protein L36



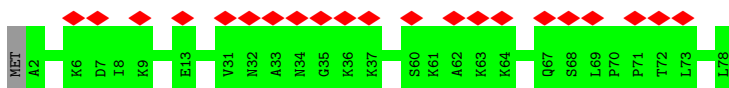
- Molecule 39: 60S ribosomal protein L37-B

Chain AK:  96%



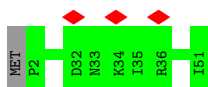
- Molecule 40: 60S ribosomal protein L38

Chain AL:  27% 99%



- Molecule 41: 60S ribosomal protein L39

Chain AM:  6% 98%



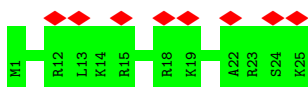
- Molecule 42: 60S ribosomal protein L40-B

Chain AN:  100%



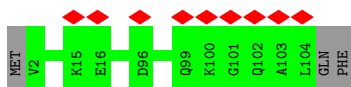
- Molecule 43: 60S ribosomal protein L41

Chain AO:  32% 100%



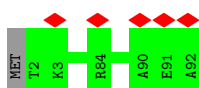
- Molecule 44: 60S ribosomal protein L42-B

Chain AP:  8% 97%

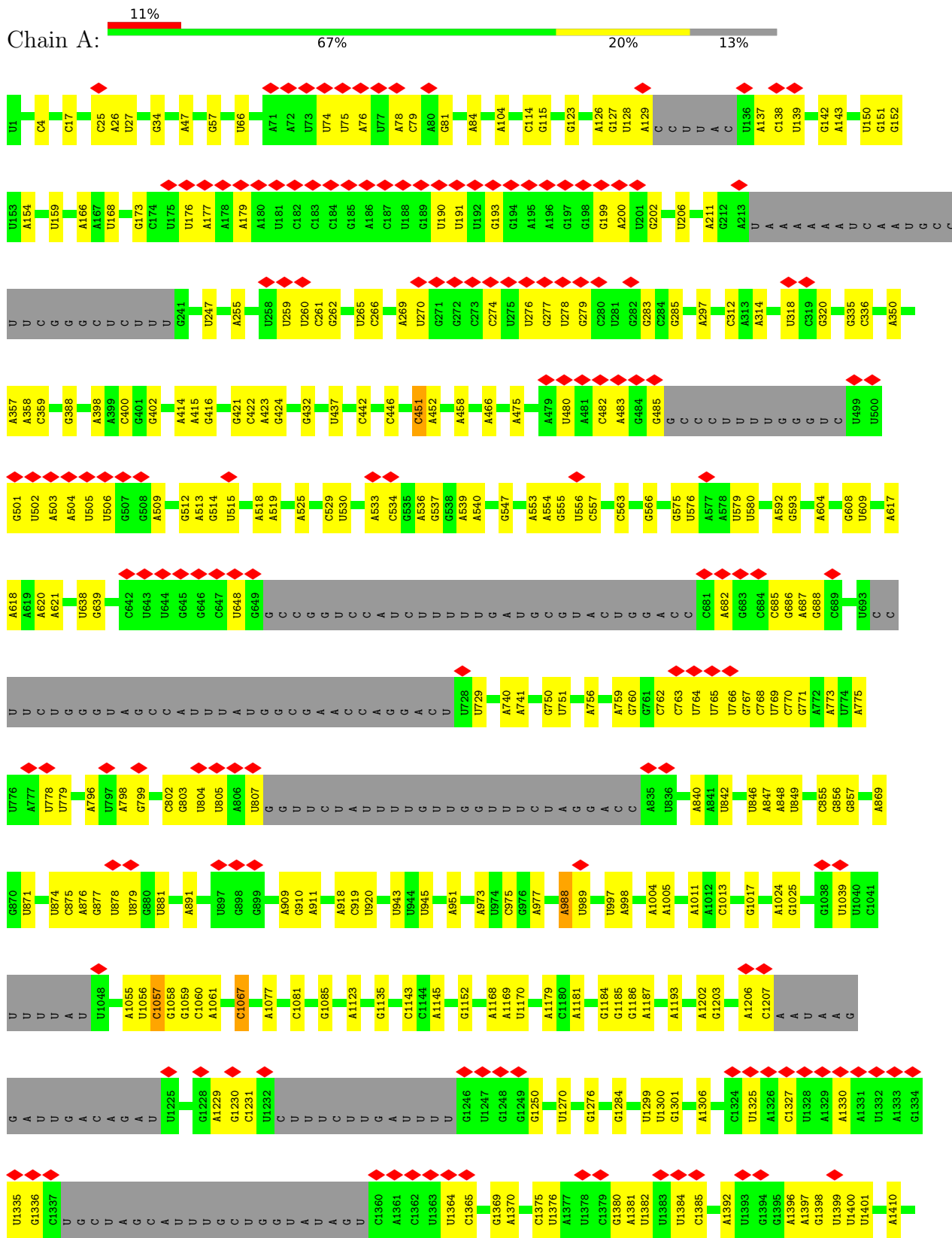


- Molecule 45: 60S ribosomal protein L43-A

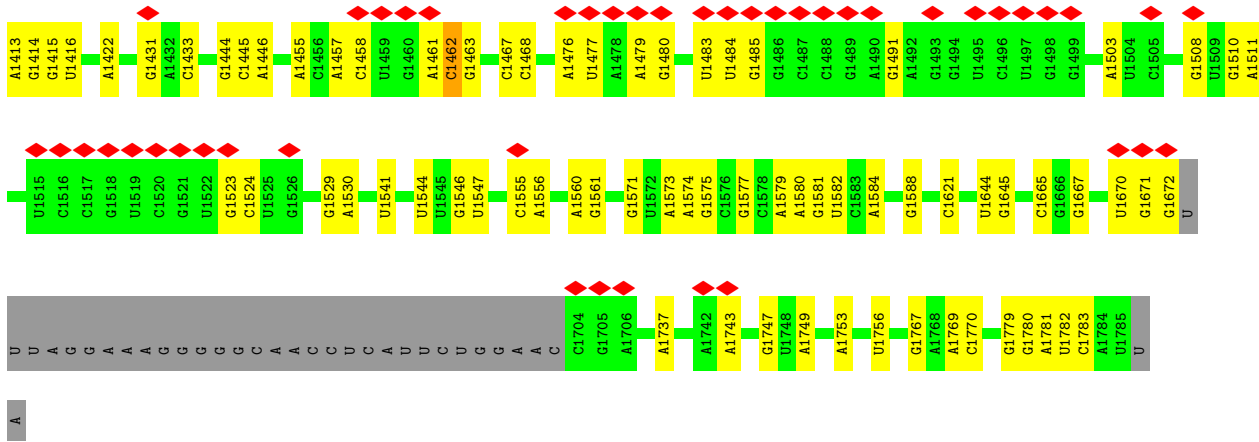
Chain AQ:  5% 99%



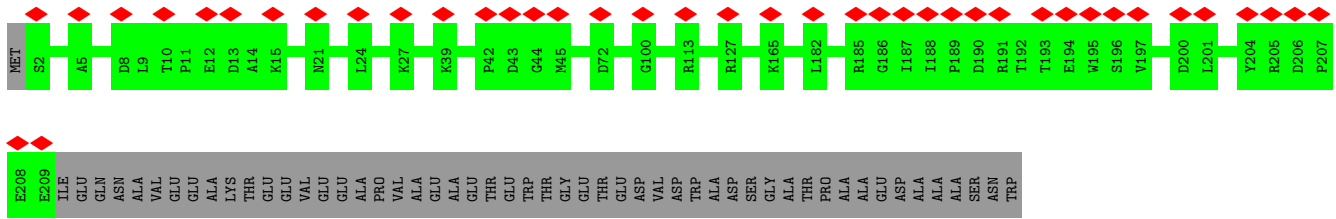
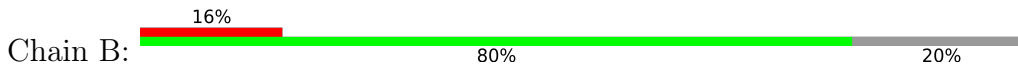
• Molecule 46: 18S ribosomal RNA



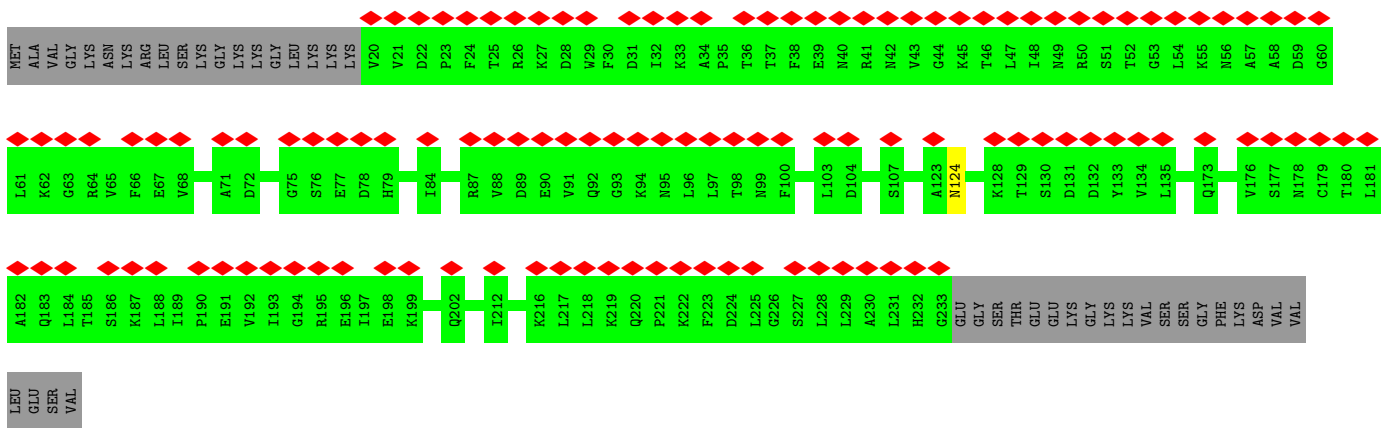
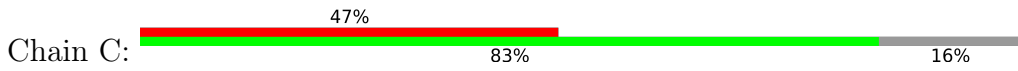




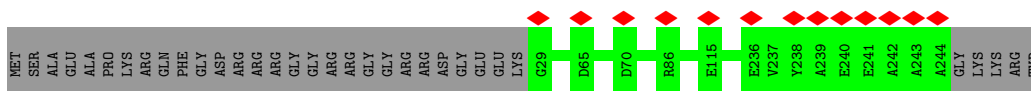
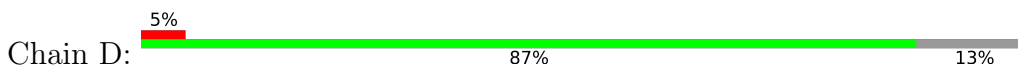
• Molecule 47: 40S ribosomal protein S0



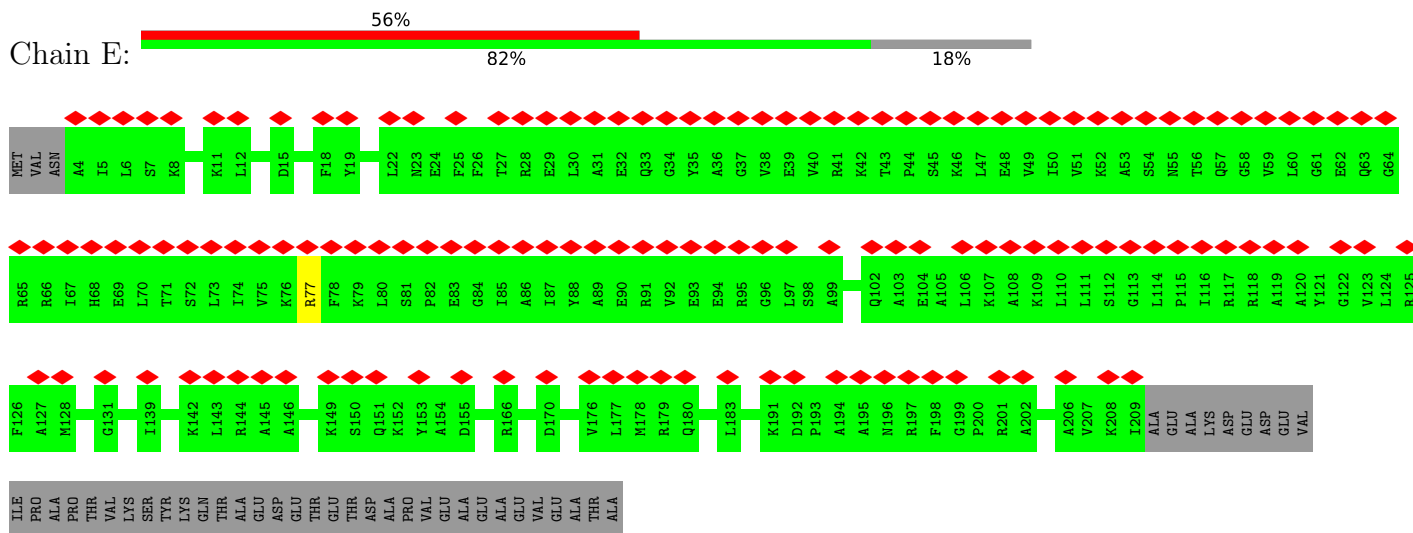
• Molecule 48: 40S ribosomal protein S1



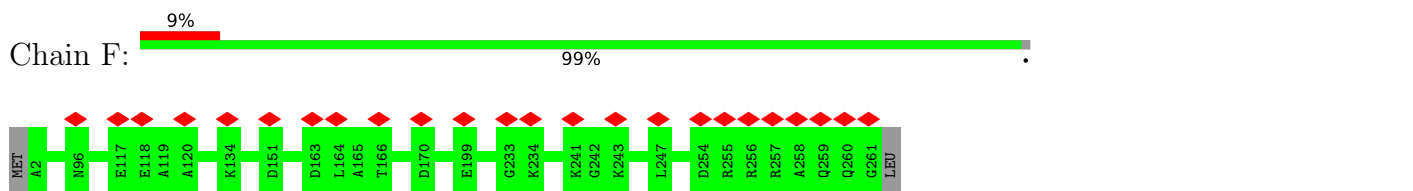
• Molecule 49: Ribosomal protein S5



• Molecule 50: Ribosomal protein S3



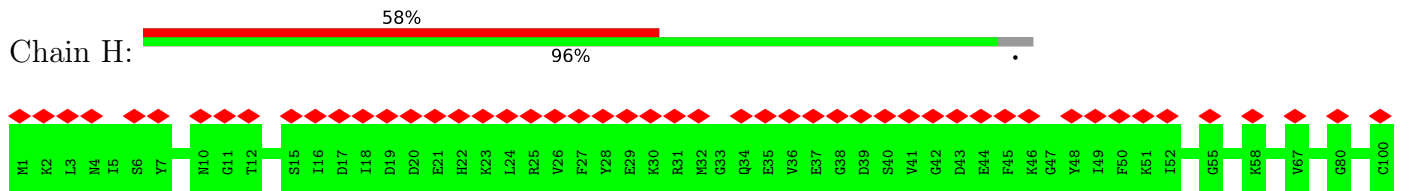
- Molecule 51: 40S ribosomal protein S4

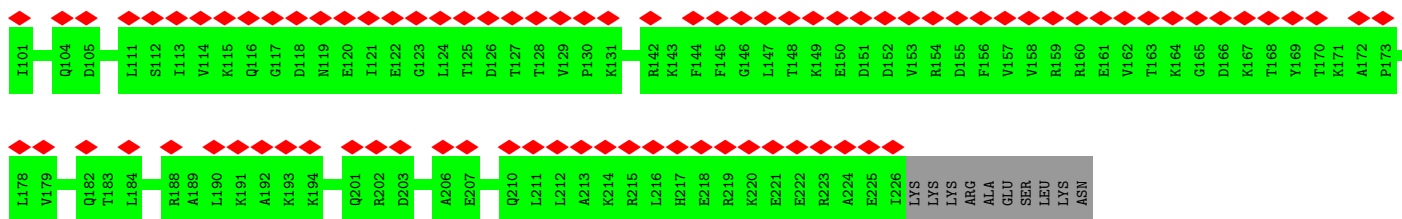


- Molecule 52: Ribosomal protein S7



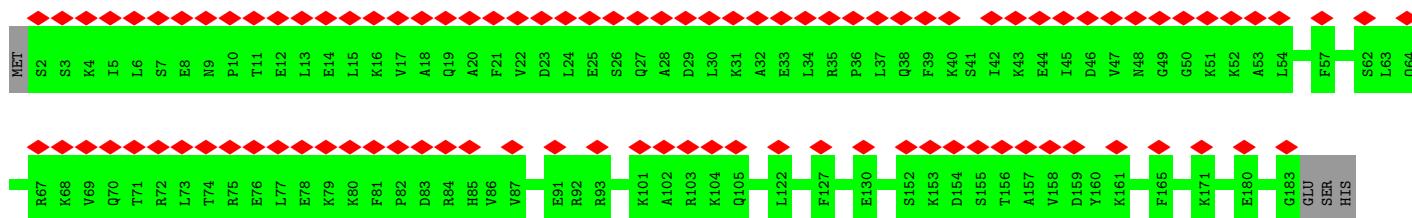
- Molecule 53: 40S ribosomal protein S6





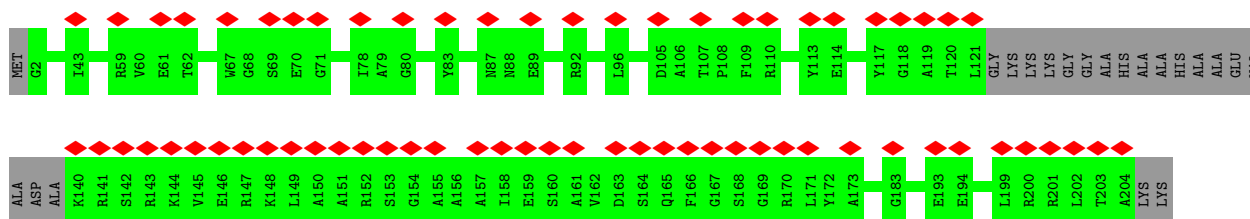
- Molecule 54: 40S ribosomal protein S7

Chain I: 53% 98%



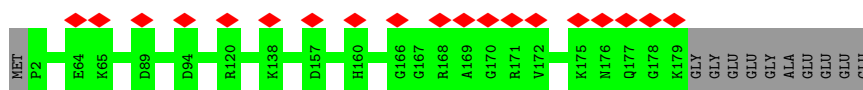
- Molecule 55: 40S ribosomal protein S8

Chain J: 32% 90% 10%



- Molecule 56: Ribosomal protein S4

Chain K: 10% 94% 6%

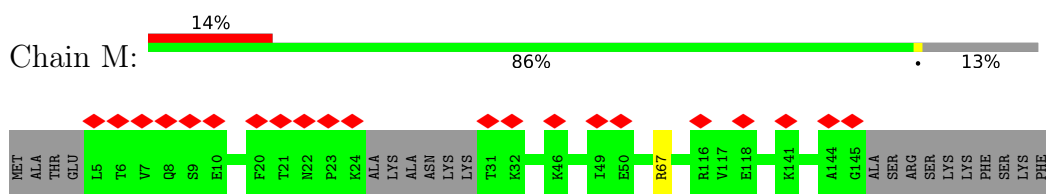


- Molecule 57: 40S ribosomal protein S10-A

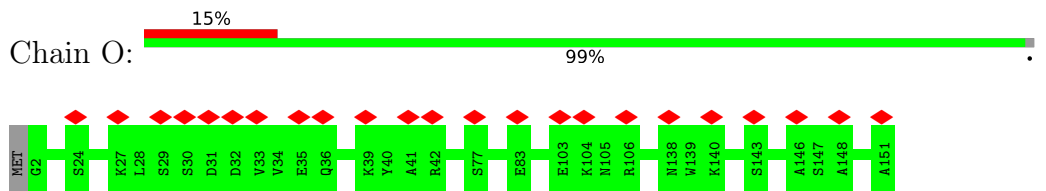
Chain L: 69% 77% 21%



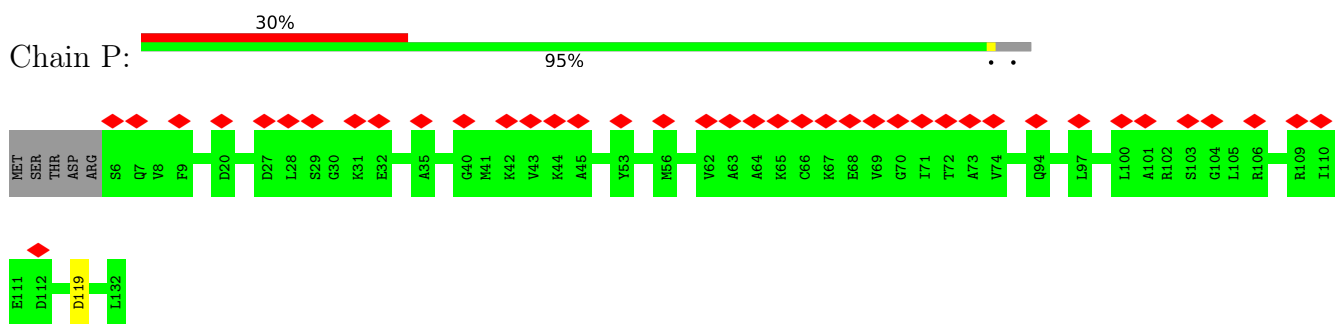
- Molecule 58: 40S ribosomal protein S11A



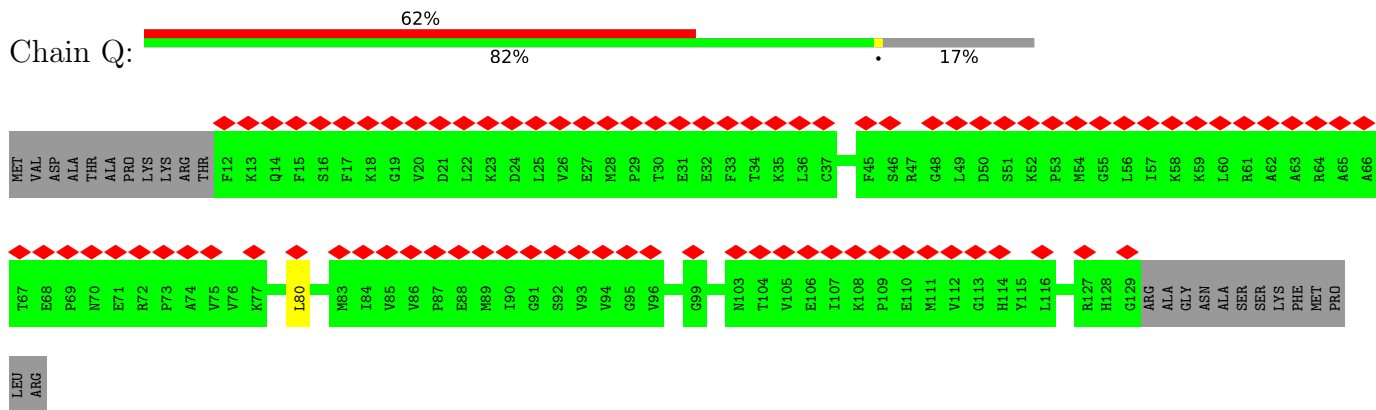
- Molecule 59: 40S ribosomal protein S13



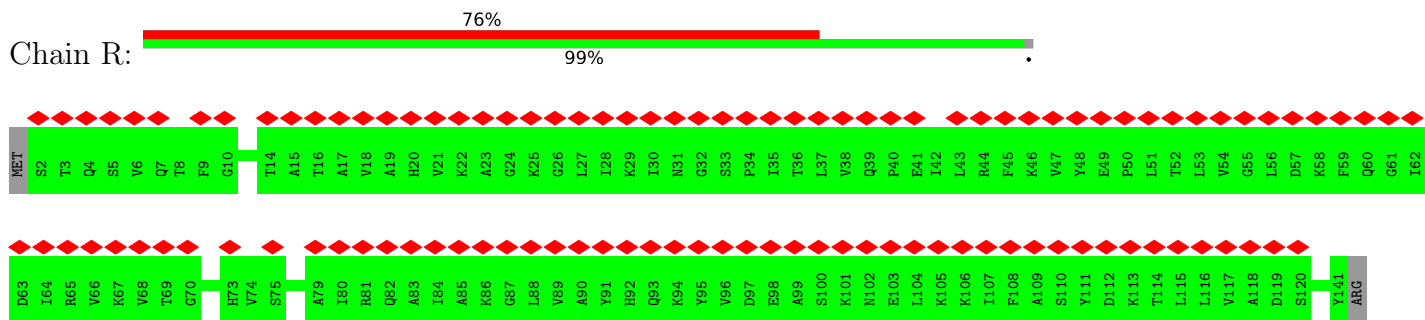
- Molecule 60: 40S ribosomal protein S14-A



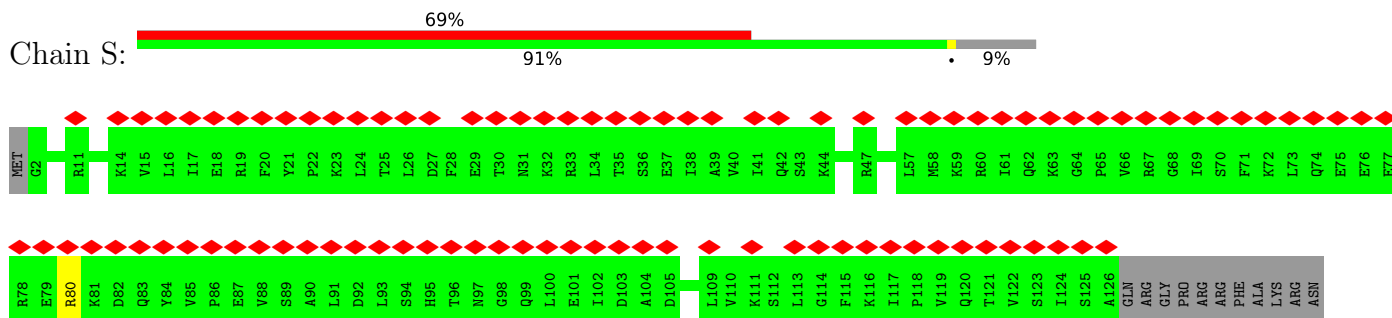
- Molecule 61: 40S ribosomal protein S15



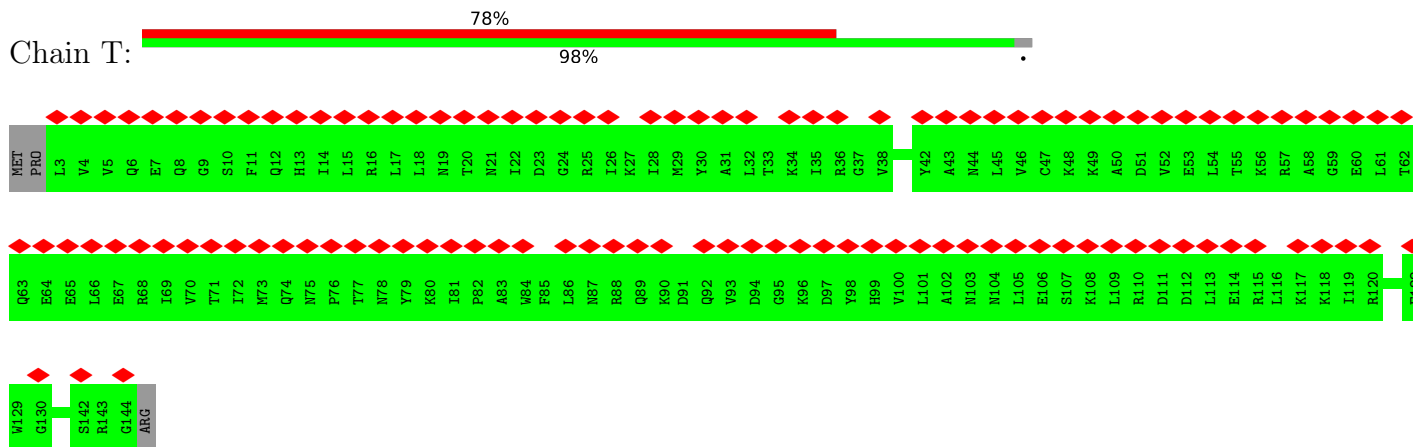
- Molecule 62: 40S ribosomal protein S16



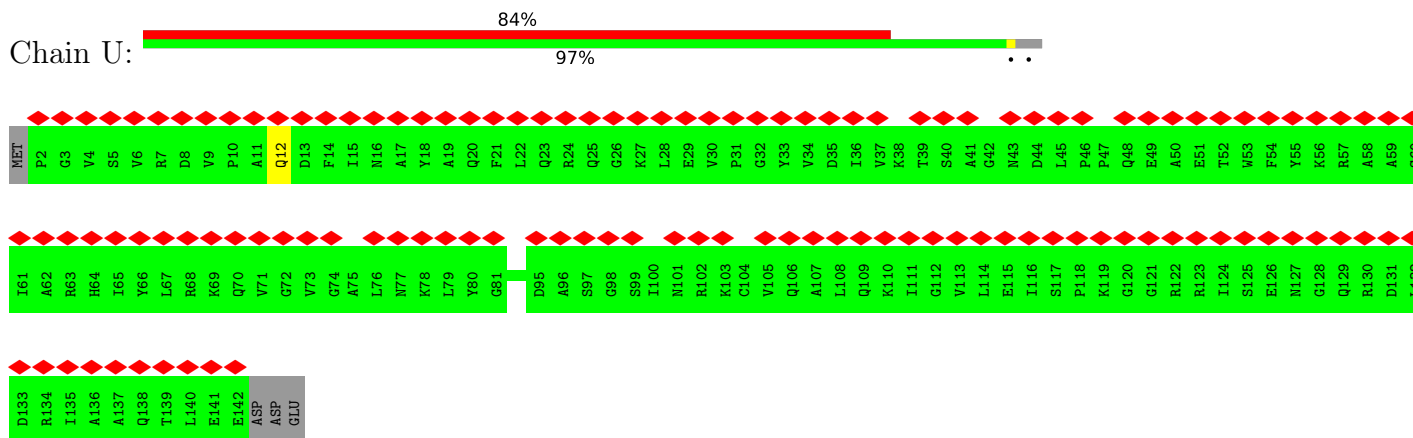
- Molecule 63: 40S ribosomal protein S17-B



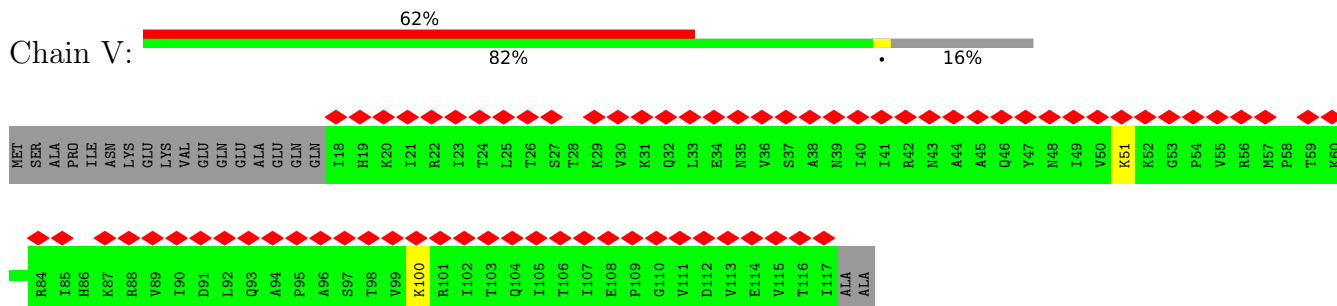
• Molecule 64: 40S ribosomal protein S18-B



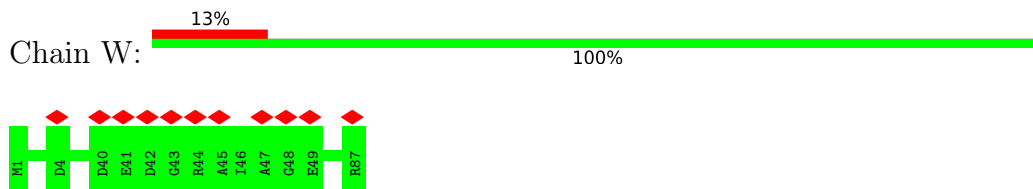
• Molecule 65: 40S ribosomal protein S19-A



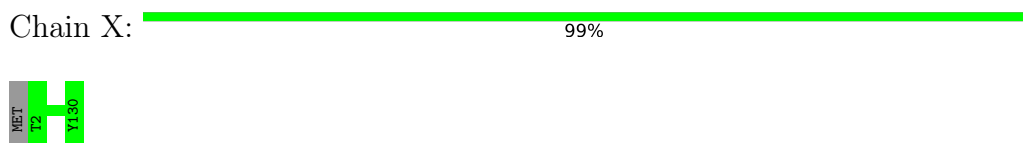
• Molecule 66: Ribosomal protein S10



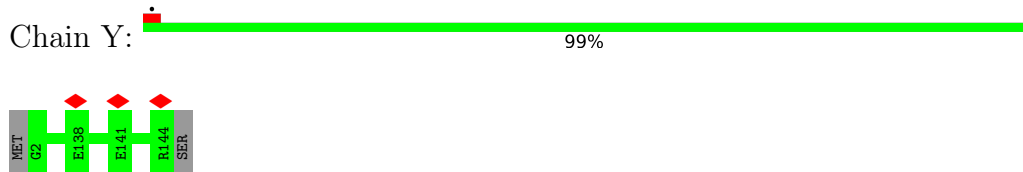
- Molecule 67: 40S ribosomal protein S21



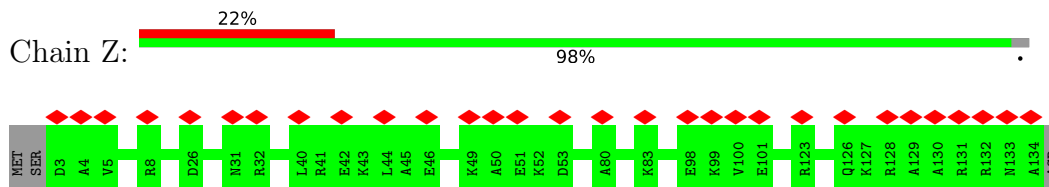
- Molecule 68: 40S ribosomal protein S22-A



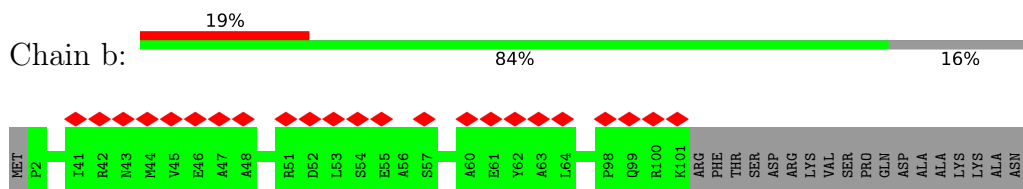
- Molecule 69: Ribosomal protein S23 (S12)



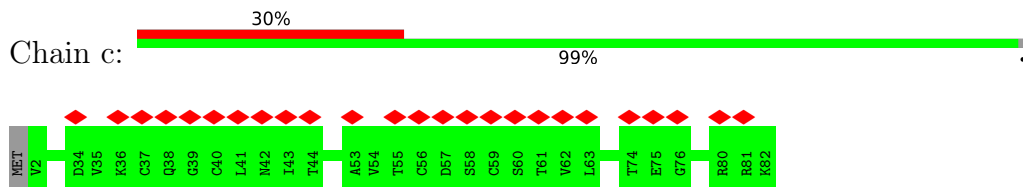
- Molecule 70: 40S ribosomal protein S24



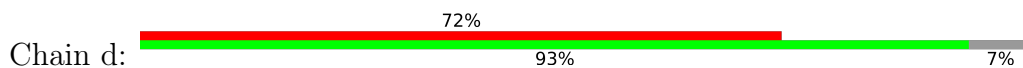
- Molecule 71: 40S ribosomal protein S26

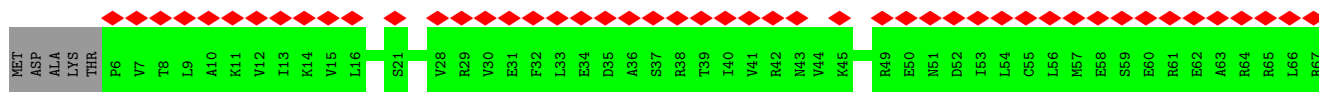


- Molecule 72: 40S ribosomal protein S27

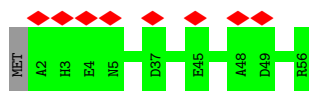


- Molecule 73: 40S ribosomal protein S28-B

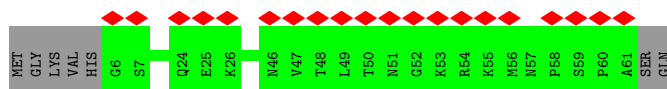
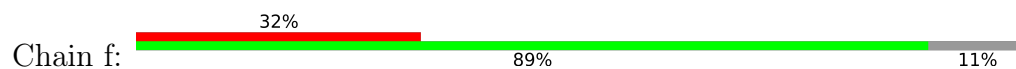




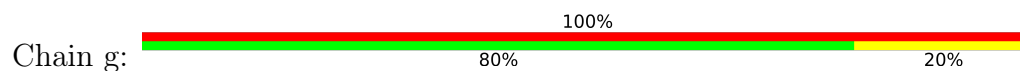
- Molecule 74: 40S ribosomal protein S29A



- Molecule 75: 40S ribosomal protein S30



- Molecule 76: DNA (5'-R(P\*GP\*GP\*CP\*AP\*G)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	254047	Depositor
Resolution determination method	FSC 3 SIGMA CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.815	Depositor
Minimum map value	-0.331	Depositor
Average map value	0.023	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.274	Depositor
Map size (Å)	426.36002, 426.36002, 426.36002	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.836, 0.836, 0.836	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: SPK, SPD, MG, K16, MLZ, OMG, IAS, ZN, OMC

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	1	0.76	0/73469	0.87	64/114528 (0.1%)
2	3	0.65	0/2884	0.77	0/4492
3	4	0.73	0/3746	0.80	0/5832
4	10	0.34	0/207	0.84	0/319
5	j	0.43	0/1931	0.60	0/2592
6	k	0.40	0/3156	0.58	0/4246
7	l	0.37	0/2799	0.56	0/3777
8	m	0.35	0/2447	0.53	0/3294
9	n	0.34	0/1258	0.54	0/1696
10	o	0.40	0/1860	0.56	0/2499
11	p	0.35	0/1830	0.51	0/2465
12	q	0.35	0/1519	0.57	0/2043
13	r	0.38	0/1724	0.57	0/2314
14	s	0.31	0/1404	0.58	0/1880
15	t	0.36	0/1572	0.59	0/2109
16	u	0.33	0/1044	0.57	1/1407 (0.1%)
17	v	0.46	1/1753 (0.1%)	0.63	0/2347
18	w	0.40	0/1620	0.55	0/2167
19	x	0.40	0/1398	0.60	0/1879
20	y	0.36	0/1511	0.62	0/2022
21	z	0.36	0/1483	0.61	0/1972
22	0	0.40	0/1483	0.58	0/1997
23	2	0.41	0/1305	0.56	0/1749
24	5	0.35	0/856	0.50	0/1156
25	6	0.39	0/994	0.61	0/1339
26	7	0.41	0/536	0.59	0/712
27	8	0.39	0/990	0.59	1/1337 (0.1%)
28	9	0.35	0/990	0.58	0/1322
29	AA	0.36	0/1112	0.52	0/1488
30	AB	0.40	0/1199	0.55	0/1607
31	AC	0.36	0/477	0.54	0/633
32	AD	0.37	0/738	0.53	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	AE	0.37	0/851	0.60	0/1141
34	AF	0.40	0/1039	0.57	0/1390
35	AG	0.42	0/895	0.56	0/1201
36	AH	0.39	0/934	0.61	0/1242
37	AI	0.36	0/1004	0.62	0/1337
38	AJ	0.35	0/772	0.62	0/1023
39	AK	0.42	0/690	0.68	0/916
40	AL	0.37	0/632	0.59	0/842
41	AM	0.32	0/458	0.63	0/609
42	AN	0.36	0/436	0.61	0/577
43	AO	0.32	0/237	0.79	0/304
44	AP	0.39	0/840	0.57	0/1108
45	AQ	0.40	0/705	0.64	0/940
46	A	0.68	0/37205	0.88	32/57962 (0.1%)
47	B	0.35	0/1666	0.55	0/2273
48	C	0.29	0/1750	0.58	0/2354
49	D	0.39	0/1648	0.55	0/2237
50	E	0.31	0/1604	0.59	0/2150
51	F	0.35	0/2096	0.57	0/2822
52	G	0.27	0/1631	0.56	0/2199
53	H	0.29	0/1845	0.59	0/2464
54	I	0.31	0/1490	0.57	0/2004
55	J	0.32	0/1485	0.63	0/1987
56	K	0.36	0/1478	0.60	0/1978
57	L	0.31	0/801	0.62	0/1081
58	M	0.40	0/1108	0.58	0/1492
59	O	0.34	0/1210	0.56	0/1631
60	P	0.32	0/944	0.63	0/1265
61	Q	0.33	0/954	0.60	1/1282 (0.1%)
62	R	0.29	0/1109	0.57	0/1486
63	S	0.29	0/1014	0.59	0/1361
64	T	0.27	0/1186	0.58	0/1590
65	U	0.28	0/1120	0.57	0/1508
66	V	0.31	0/800	0.59	0/1082
67	W	0.37	0/683	0.60	0/918
68	X	0.44	0/1049	0.60	0/1412
69	Y	0.40	0/1128	0.63	0/1505
70	Z	0.33	0/1086	0.59	0/1447
71	b	0.37	0/811	0.63	0/1085
72	c	0.32	0/624	0.56	0/843
73	d	0.29	0/489	0.69	0/654
74	e	0.36	0/466	0.58	0/620
75	f	0.31	0/451	0.59	0/601

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	g	0.22	0/124	0.81	0/192
All	All	0.61	1/201843 (0.0%)	0.77	99/296329 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	v	82	GLY	C-N	-5.18	1.22	1.34

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	A	451	C	N1-C2-O2	8.84	124.20	118.90
1	1	406	G	O4'-C1'-N9	8.59	115.07	108.20
46	A	451	C	N3-C2-O2	-8.11	116.23	121.90
46	A	451	C	C2-N1-C1'	8.05	127.66	118.80
1	1	2243	C	O5'-P-OP1	-8.02	98.48	105.70

There are no chirality outliers.

There are no planarity outliers.

## 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	
5	j	248/254 (98%)	241 (97%)	7 (3%)	0	100	100
6	k	385/389 (99%)	374 (97%)	11 (3%)	0	100	100
7	l	359/363 (99%)	350 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	m	290/298 (97%)	280 (97%)	10 (3%)	0	100	100
9	n	152/176 (86%)	150 (99%)	2 (1%)	0	100	100
10	o	225/241 (93%)	217 (96%)	8 (4%)	0	100	100
11	p	230/262 (88%)	225 (98%)	5 (2%)	0	100	100
12	q	186/191 (97%)	182 (98%)	4 (2%)	0	100	100
13	r	204/220 (93%)	201 (98%)	3 (2%)	0	100	100
14	s	171/174 (98%)	166 (97%)	5 (3%)	0	100	100
15	t	189/202 (94%)	187 (99%)	2 (1%)	0	100	100
16	u	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
17	v	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
18	w	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
19	x	168/185 (91%)	165 (98%)	3 (2%)	0	100	100
20	y	186/186 (100%)	182 (98%)	4 (2%)	0	100	100
21	z	178/190 (94%)	175 (98%)	3 (2%)	0	100	100
22	0	171/172 (99%)	170 (99%)	1 (1%)	0	100	100
23	2	159/160 (99%)	157 (99%)	2 (1%)	0	100	100
24	5	101/124 (82%)	96 (95%)	4 (4%)	1 (1%)	15	16
25	6	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
26	7	61/155 (39%)	61 (100%)	0	0	100	100
27	8	119/142 (84%)	118 (99%)	1 (1%)	0	100	100
28	9	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
29	AA	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
30	AB	146/149 (98%)	138 (94%)	8 (6%)	0	100	100
31	AC	56/63 (89%)	55 (98%)	1 (2%)	0	100	100
32	AD	94/106 (89%)	93 (99%)	1 (1%)	0	100	100
33	AE	99/112 (88%)	98 (99%)	1 (1%)	0	100	100
34	AF	124/131 (95%)	123 (99%)	1 (1%)	0	100	100
35	AG	107/107 (100%)	104 (97%)	3 (3%)	0	100	100
36	AH	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
37	AI	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
38	AJ	96/99 (97%)	95 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	AK	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
40	AL	76/78 (97%)	73 (96%)	3 (4%)	0	100	100
41	AM	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
42	AN	51/52 (98%)	51 (100%)	0	0	100	100
43	AO	23/25 (92%)	23 (100%)	0	0	100	100
44	AP	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
45	AQ	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
47	B	206/261 (79%)	200 (97%)	6 (3%)	0	100	100
48	C	212/256 (83%)	207 (98%)	5 (2%)	0	100	100
49	D	214/249 (86%)	210 (98%)	4 (2%)	0	100	100
50	E	204/251 (81%)	202 (99%)	2 (1%)	0	100	100
51	F	258/262 (98%)	255 (99%)	3 (1%)	0	100	100
52	G	204/225 (91%)	197 (97%)	7 (3%)	0	100	100
53	H	224/236 (95%)	222 (99%)	2 (1%)	0	100	100
54	I	180/186 (97%)	174 (97%)	6 (3%)	0	100	100
55	J	181/206 (88%)	180 (99%)	1 (1%)	0	100	100
56	K	176/189 (93%)	175 (99%)	1 (1%)	0	100	100
57	L	91/118 (77%)	84 (92%)	5 (6%)	2 (2%)	6	4
58	M	131/155 (84%)	130 (99%)	1 (1%)	0	100	100
59	O	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
60	P	123/132 (93%)	119 (97%)	4 (3%)	0	100	100
61	Q	116/142 (82%)	107 (92%)	9 (8%)	0	100	100
62	R	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
63	S	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
64	T	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
65	U	139/145 (96%)	137 (99%)	2 (1%)	0	100	100
66	V	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
67	W	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
68	X	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
69	Y	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
70	Z	130/135 (96%)	130 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	b	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
72	c	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
73	d	60/67 (90%)	55 (92%)	5 (8%)	0	100	100
74	e	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
75	f	54/63 (86%)	52 (96%)	2 (4%)	0	100	100
All	All	10253/11113 (92%)	10025 (98%)	225 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	L	88	PRO
24	5	20	ALA
57	L	17	GLN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	j	191/194 (98%)	191 (100%)	0	100	100
6	k	326/328 (99%)	326 (100%)	0	100	100
7	l	290/292 (99%)	289 (100%)	1 (0%)	92	95
8	m	247/252 (98%)	247 (100%)	0	100	100
9	n	135/154 (88%)	135 (100%)	0	100	100
10	o	191/204 (94%)	191 (100%)	0	100	100
11	p	193/216 (89%)	193 (100%)	0	100	100
12	q	167/170 (98%)	167 (100%)	0	100	100
13	r	178/186 (96%)	178 (100%)	0	100	100
14	s	148/149 (99%)	147 (99%)	1 (1%)	84	90
15	t	161/168 (96%)	161 (100%)	0	100	100
16	u	108/109 (99%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	v	177/178 (99%)	177 (100%)	0	100	100
18	w	166/167 (99%)	166 (100%)	0	100	100
19	x	142/154 (92%)	141 (99%)	1 (1%)	84	90
20	y	156/154 (101%)	156 (100%)	0	100	100
21	z	147/153 (96%)	147 (100%)	0	100	100
22	0	158/157 (101%)	158 (100%)	0	100	100
23	2	135/134 (101%)	134 (99%)	1 (1%)	84	90
24	5	93/112 (83%)	91 (98%)	2 (2%)	52	64
25	6	101/103 (98%)	101 (100%)	0	100	100
26	7	57/127 (45%)	57 (100%)	0	100	100
27	8	108/121 (89%)	108 (100%)	0	100	100
28	9	110/112 (98%)	109 (99%)	1 (1%)	78	86
29	AA	117/118 (99%)	117 (100%)	0	100	100
30	AB	120/121 (99%)	120 (100%)	0	100	100
31	AC	46/49 (94%)	46 (100%)	0	100	100
32	AD	81/90 (90%)	81 (100%)	0	100	100
33	AE	92/100 (92%)	92 (100%)	0	100	100
34	AF	111/115 (96%)	111 (100%)	0	100	100
35	AG	94/92 (102%)	94 (100%)	0	100	100
36	AH	99/102 (97%)	99 (100%)	0	100	100
37	AI	106/106 (100%)	106 (100%)	0	100	100
38	AJ	78/79 (99%)	77 (99%)	1 (1%)	69	79
39	AK	70/73 (96%)	70 (100%)	0	100	100
40	AL	69/69 (100%)	69 (100%)	0	100	100
41	AM	47/47 (100%)	47 (100%)	0	100	100
42	AN	48/47 (102%)	48 (100%)	0	100	100
43	AO	24/24 (100%)	24 (100%)	0	100	100
44	AP	88/89 (99%)	88 (100%)	0	100	100
45	AQ	72/73 (99%)	72 (100%)	0	100	100
47	B	176/215 (82%)	176 (100%)	0	100	100
48	C	194/229 (85%)	193 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	D	174/198 (88%)	174 (100%)	0	100	100
50	E	160/196 (82%)	159 (99%)	1 (1%)	86	91
51	F	218/220 (99%)	218 (100%)	0	100	100
52	G	178/197 (90%)	178 (100%)	0	100	100
53	H	195/204 (96%)	195 (100%)	0	100	100
54	I	163/167 (98%)	163 (100%)	0	100	100
55	J	149/160 (93%)	149 (100%)	0	100	100
56	K	153/160 (96%)	153 (100%)	0	100	100
57	L	87/104 (84%)	87 (100%)	0	100	100
58	M	118/134 (88%)	117 (99%)	1 (1%)	81	88
59	O	129/130 (99%)	129 (100%)	0	100	100
60	P	96/101 (95%)	96 (100%)	0	100	100
61	Q	102/121 (84%)	102 (100%)	0	100	100
62	R	114/116 (98%)	114 (100%)	0	100	100
63	S	112/122 (92%)	111 (99%)	1 (1%)	78	86
64	T	126/129 (98%)	126 (100%)	0	100	100
65	U	113/117 (97%)	112 (99%)	1 (1%)	78	86
66	V	90/105 (86%)	88 (98%)	2 (2%)	52	64
67	W	71/71 (100%)	71 (100%)	0	100	100
68	X	112/113 (99%)	112 (100%)	0	100	100
69	Y	116/118 (98%)	116 (100%)	0	100	100
70	Z	109/112 (97%)	109 (100%)	0	100	100
71	b	86/102 (84%)	86 (100%)	0	100	100
72	c	72/73 (99%)	72 (100%)	0	100	100
73	d	54/58 (93%)	54 (100%)	0	100	100
74	e	47/48 (98%)	47 (100%)	0	100	100
75	f	48/54 (89%)	48 (100%)	0	100	100
All	All	8809/9362 (94%)	8794 (100%)	15 (0%)	93	96

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	AJ	98	ARG

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Mol	Chain	Res	Type
66	V	51	LYS
48	C	124	ASN
66	V	100	LYS
63	S	80	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
47	B	30	GLN
51	F	130	GLN
73	d	27	GLN
64	T	89	GLN
24	5	30	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3067/3359 (91%)	512 (16%)	35 (1%)
2	3	120/121 (99%)	9 (7%)	0
3	4	157/158 (99%)	24 (15%)	3 (1%)
4	10	8/14 (57%)	1 (12%)	0
46	A	1546/1787 (86%)	327 (21%)	41 (2%)
76	g	4/5 (80%)	1 (25%)	0
All	All	4902/5444 (90%)	874 (17%)	79 (1%)

5 of 874 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	24	U
1	1	25	A
1	1	29	G
1	1	39	A
1	1	42	A

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	A	638	U
46	A	1467	C
46	A	740	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
46	A	1168	A
46	A	1555	C

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

6 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
1	OMG	1	2765	1	18,26,27	2.38	8 (44%)	19,38,41	1.57	5 (26%)
44	MLZ	AP	40	44	8,9,10	0.67	0	4,9,11	1.05	0
1	OMC	1	2808	1	19,22,23	2.88	8 (42%)	26,31,34	1.15	3 (11%)
60	IAS	P	119	60	6,7,8	1.04	0	6,8,10	1.47	2 (33%)
25	MLZ	6	110	25	8,9,10	0.72	0	4,9,11	0.97	0
44	MLZ	AP	55	44	8,9,10	0.65	0	4,9,11	0.73	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
1	OMG	1	2765	1	-	0/5/27/28	0/3/3/3
44	MLZ	AP	40	44	-	0/7/8/10	-
1	OMC	1	2808	1	-	3/9/27/28	0/2/2/2
60	IAS	P	119	60	-	0/7/7/8	-
25	MLZ	6	110	25	-	3/7/8/10	-
44	MLZ	AP	55	44	-	3/7/8/10	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2808	OMC	C6-C5	5.86	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2808	OMC	C2-N3	5.78	1.48	1.36
1	1	2765	OMG	C2-N3	5.16	1.45	1.33
1	1	2808	OMC	C2-N1	4.73	1.50	1.40
1	1	2808	OMC	C4-N4	4.56	1.44	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2765	OMG	C5-C6-N1	3.69	120.47	113.95
1	1	2808	OMC	O2-C2-N3	-3.49	116.66	122.33
1	1	2765	OMG	C2-N1-C6	-2.83	119.88	125.10
1	1	2765	OMG	C8-N7-C5	2.64	108.02	102.99
1	1	2765	OMG	O6-C6-C5	-2.36	119.76	124.37

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	2808	OMC	O4'-C1'-N1-C2
1	1	2808	OMC	O4'-C1'-N1-C6
1	1	2808	OMC	C1'-C2'-O2'-CM2
25	6	110	MLZ	N-CA-CB-CG
44	AP	55	MLZ	CG-CD-CE-NZ

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 379 ligands modelled in this entry, 374 are monoatomic - leaving 5 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$
79	SPD	1	3404	-	9,9,9	0.33	0	8,8,8	1.05	0
78	K16	A	1801	-	38,38,38	2.96	19 (50%)	50,55,55	2.03	19 (38%)
78	K16	1	3402	-	38,38,38	3.07	21 (55%)	50,55,55	1.93	16 (32%)
78	K16	1	3403	-	38,38,38	3.00	21 (55%)	50,55,55	1.91	15 (30%)
77	SPK	1	3401	-	13,13,13	0.36	0	12,12,12	0.70	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
79	SPD	1	3404	-	-	1/7/7/7	-
78	K16	A	1801	-	-	8/12/47/47	0/5/5/5
78	K16	1	3402	-	-	6/12/47/47	0/5/5/5
78	K16	1	3403	-	-	2/12/47/47	1/5/5/5
77	SPK	1	3401	-	-	7/11/11/11	-

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	1	3402	K16	C15-C14	8.69	1.63	1.53
78	1	3403	K16	C15-C14	7.33	1.61	1.53
78	A	1801	K16	C15-C14	6.02	1.60	1.53
78	A	1801	K16	C17-C18	5.68	1.59	1.53
78	1	3402	K16	C17-C16	5.47	1.64	1.53

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	1	3402	K16	C25-C26-N27	4.70	115.55	109.04
78	A	1801	K16	C25-C26-N27	4.55	115.34	109.04
78	1	3403	K16	C04-N05-C14	4.34	116.45	110.12
78	A	1801	K16	C15-C16-C03	4.30	117.72	110.55
78	1	3403	K16	C06-N05-C14	4.10	119.44	111.27

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

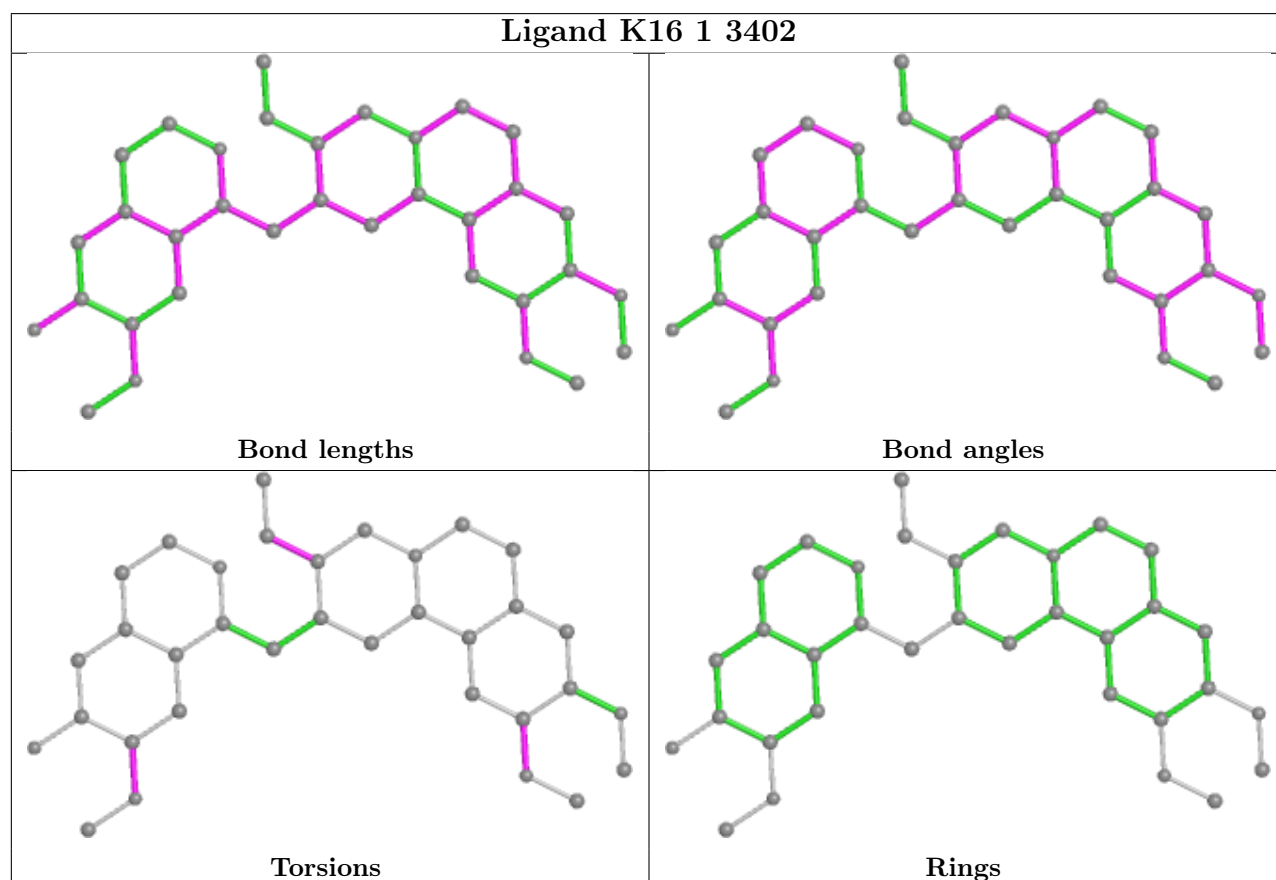
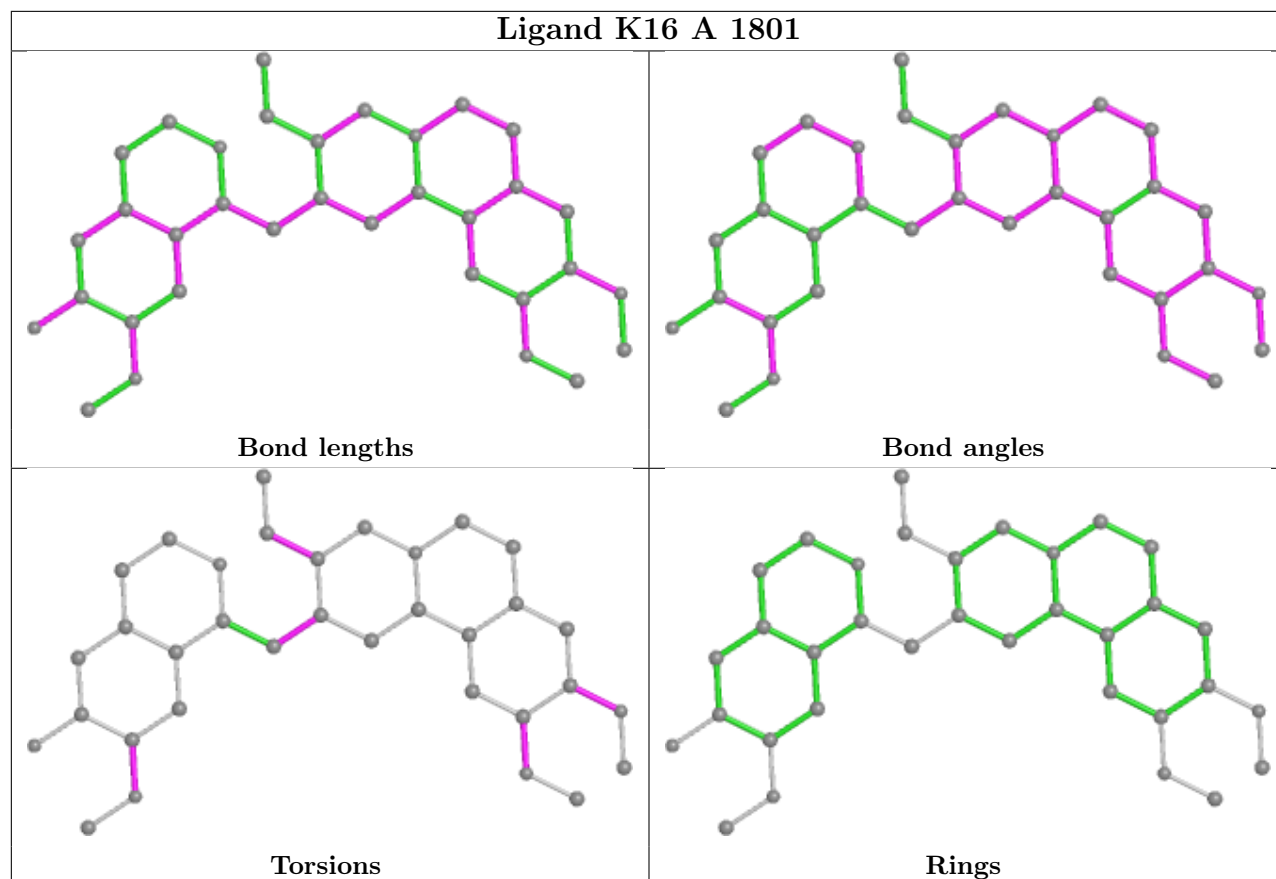
Mol	Chain	Res	Type	Atoms
78	1	3402	K16	C01-C02-C03-C04
78	A	1801	K16	C01-C02-C03-C16
78	A	1801	K16	C01-C02-C03-C04
78	A	1801	K16	C10-C11-O31-C32
77	1	3401	SPK	C7-C8-C9-N10

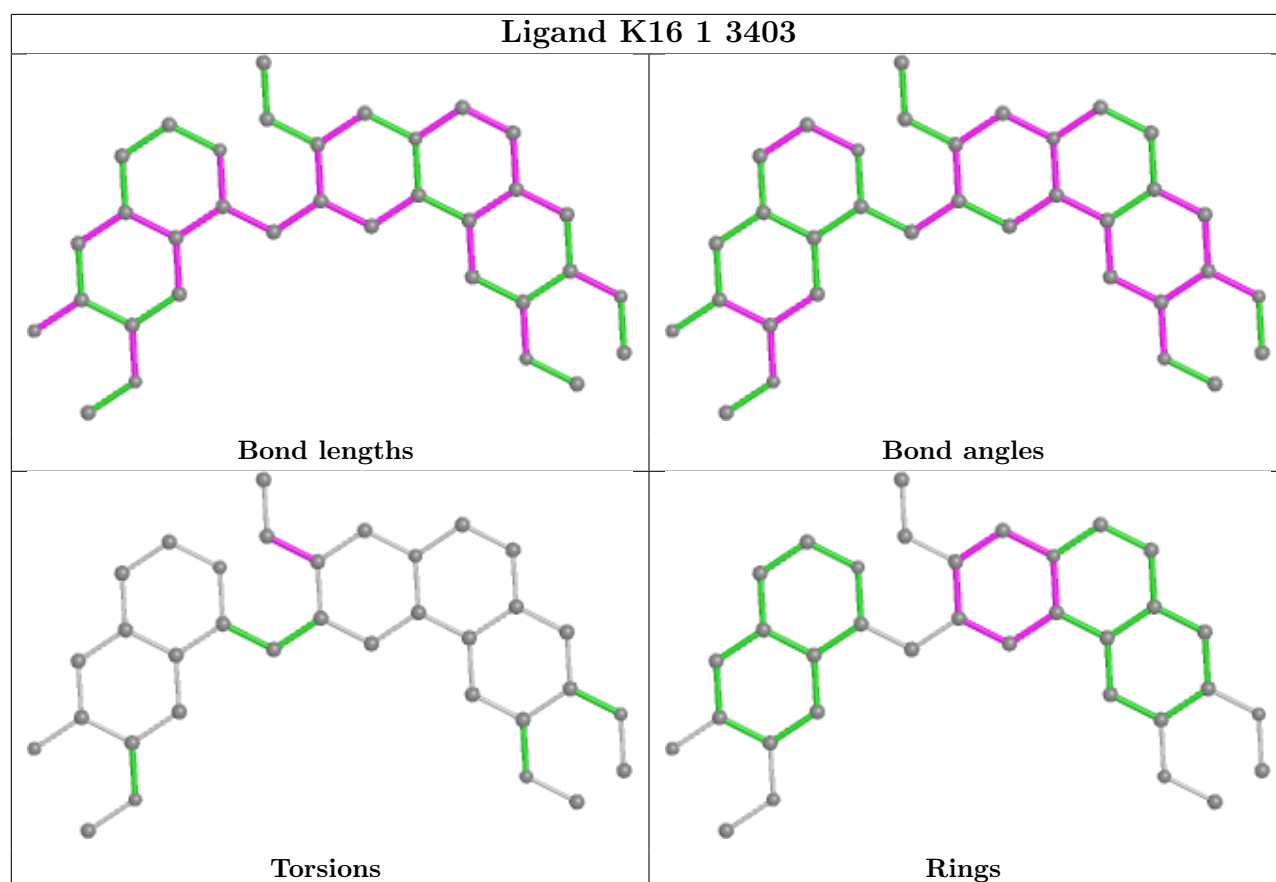
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
78	1	3403	K16	C03-C04-C14-C15-C16-N05

No monomer is involved in short contacts.

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

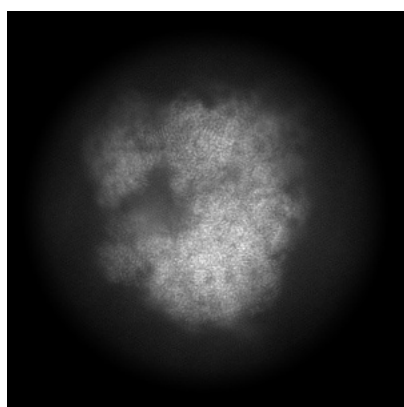
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18156. These allow visual inspection of the internal detail of the map and identification of artifacts.

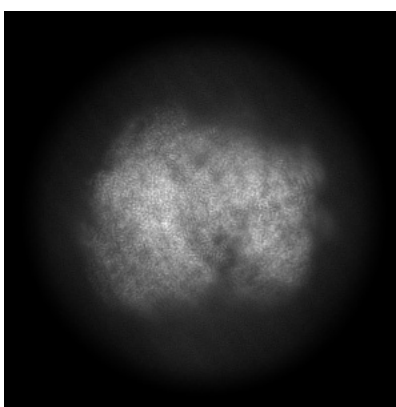
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

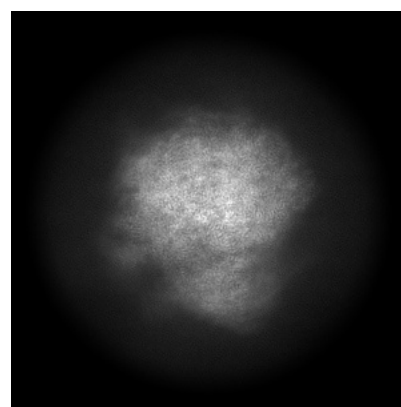
#### 6.1.1 Primary map



X



Y

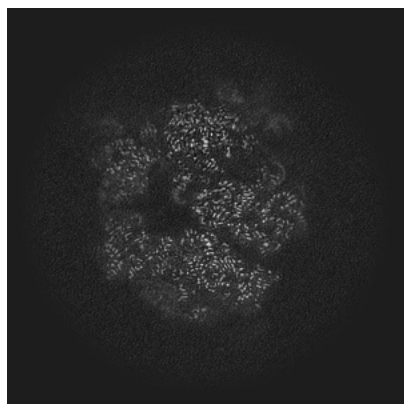


Z

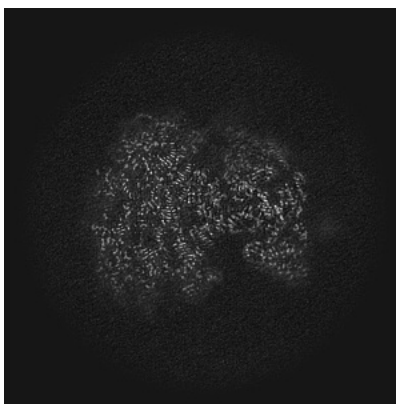
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

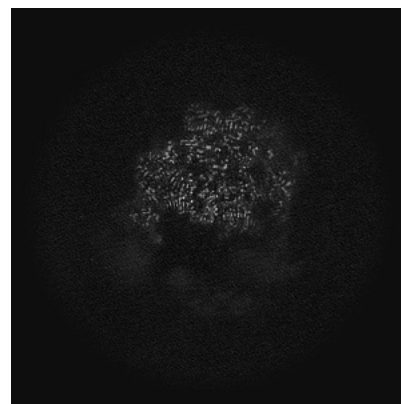
#### 6.2.1 Primary map



X Index: 255



Y Index: 255



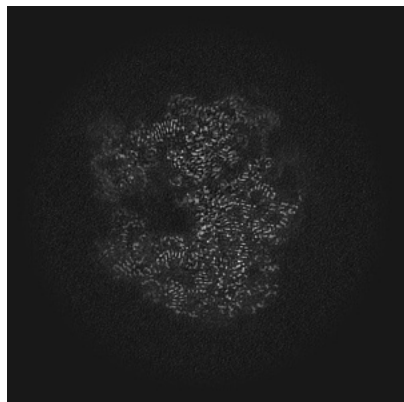
Z Index: 255



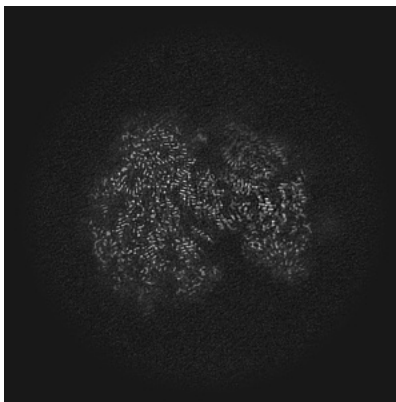
The images above show central slices of the map in three orthogonal directions.

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

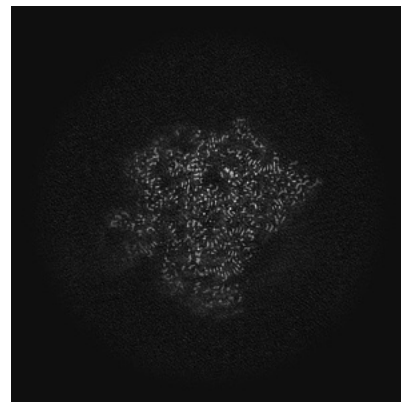
### 6.3.1 Primary map



X Index: 274



Y Index: 252

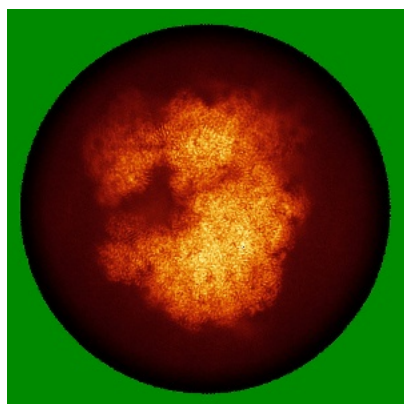


Z Index: 206

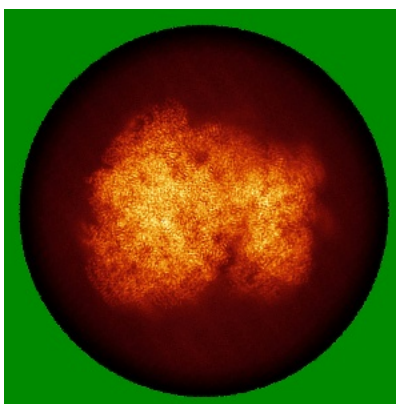
The images above show the largest variance slices of the map in three orthogonal directions.

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

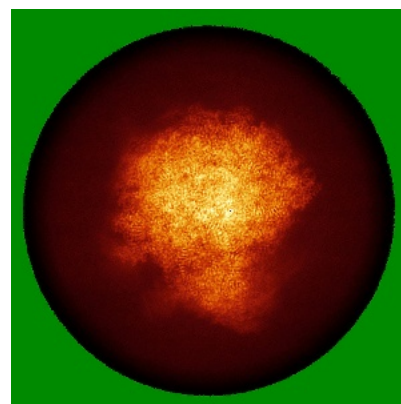
### 6.4.1 Primary map



X



Y

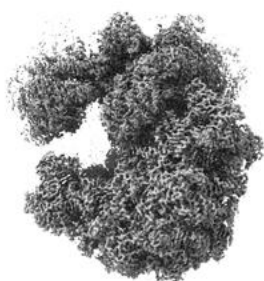


Z

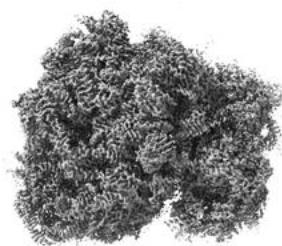
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.274. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

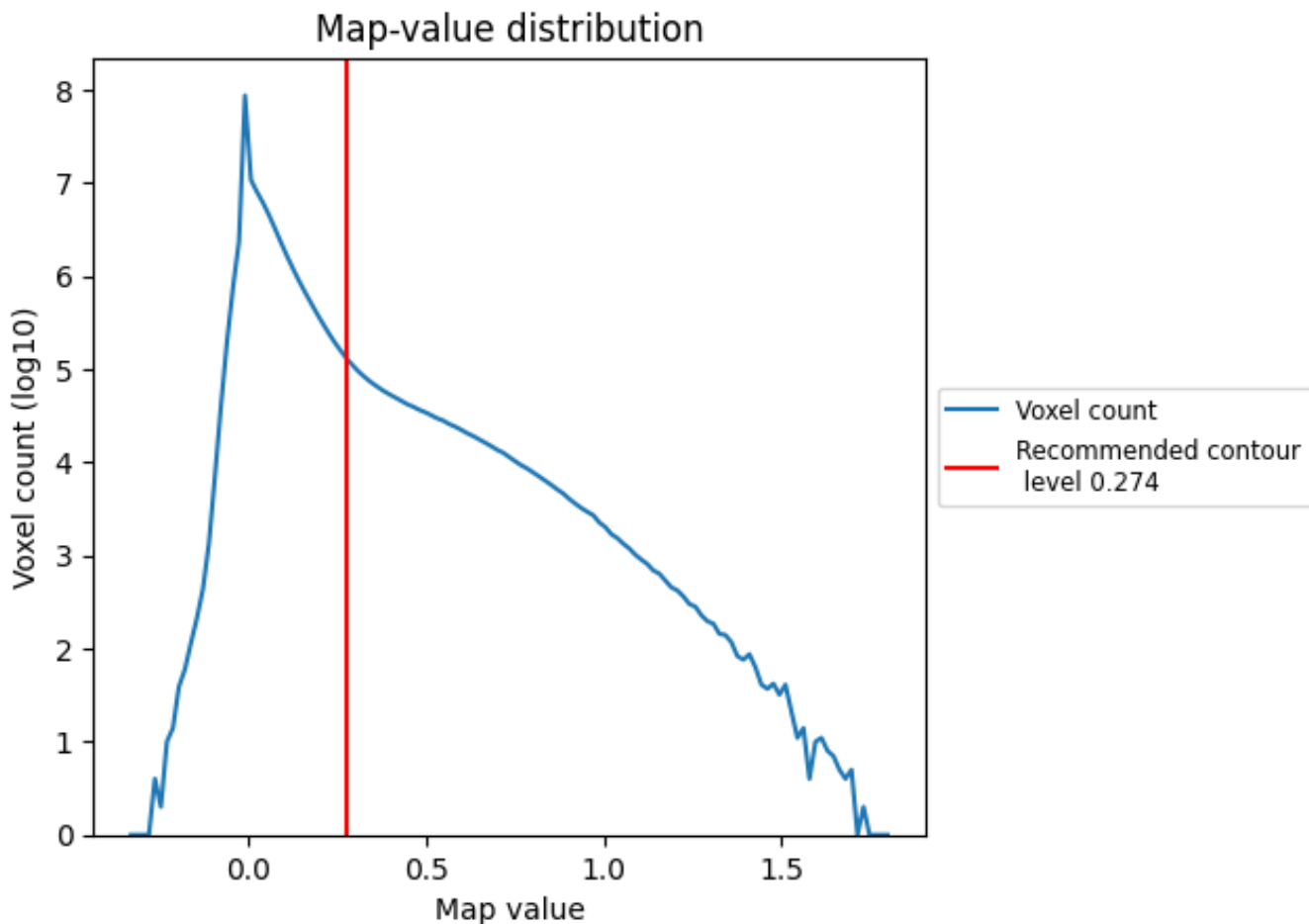
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

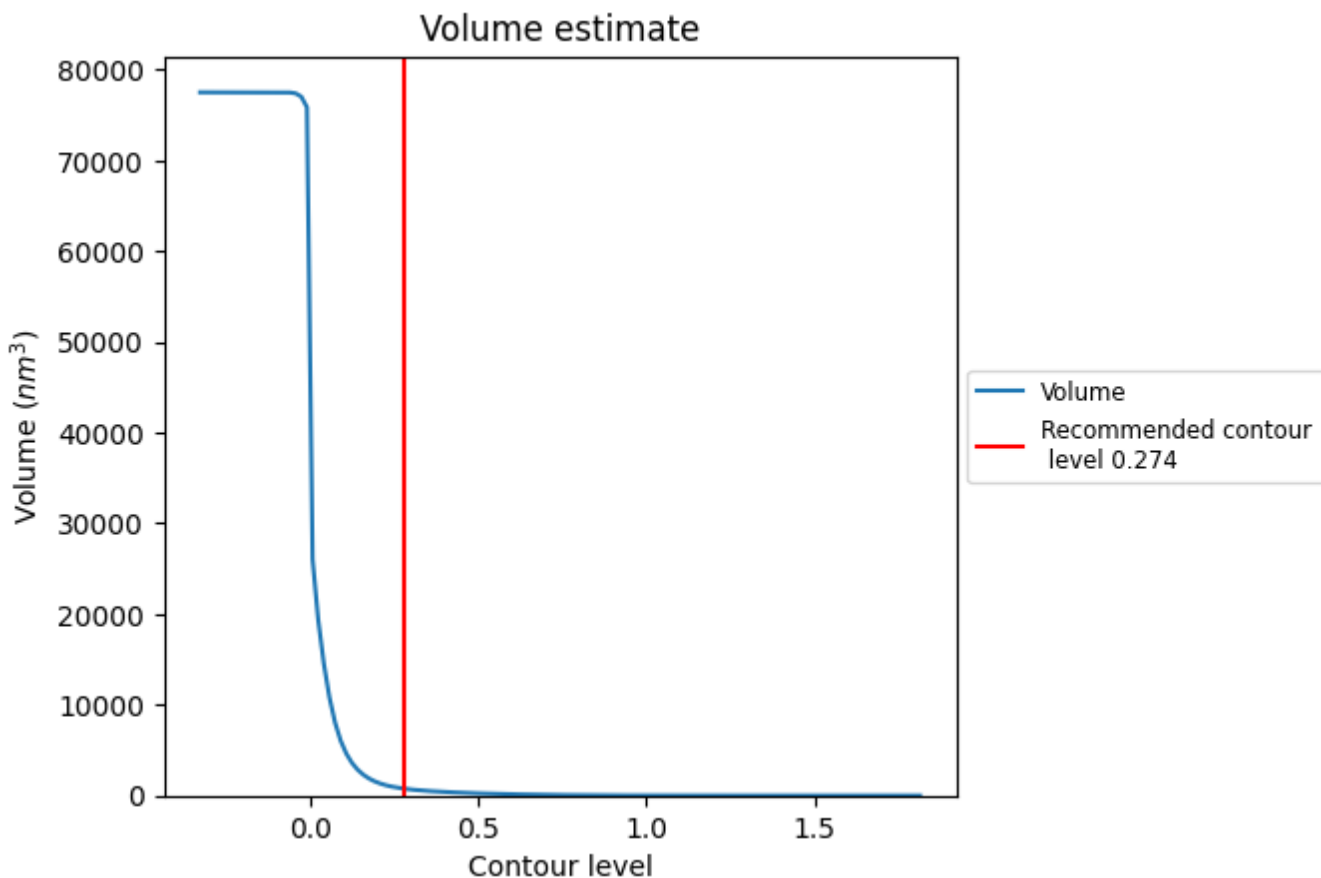
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

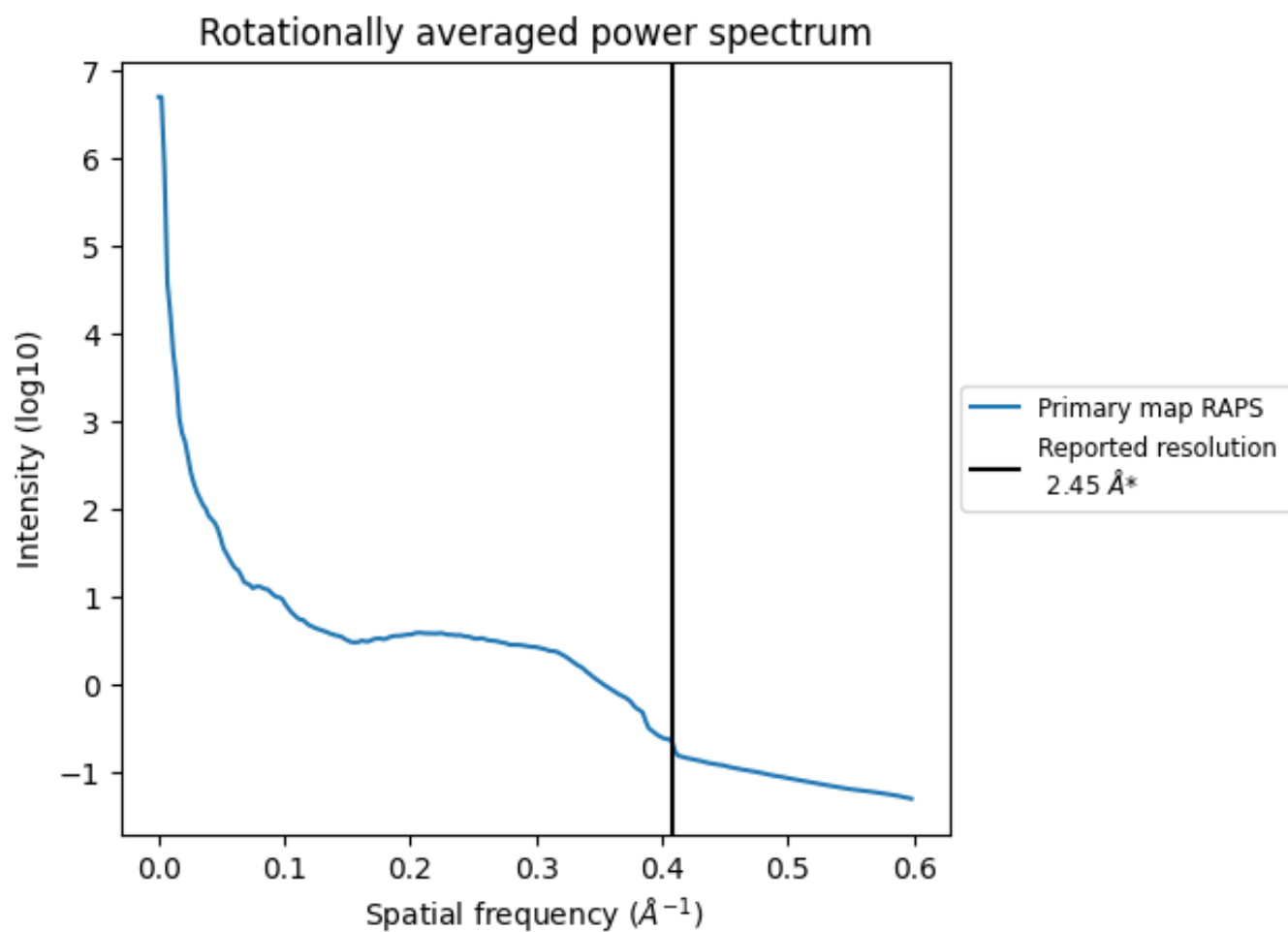
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 775 nm<sup>3</sup>; this corresponds to an approximate mass of 700 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 0.408 Å<sup>-1</sup>

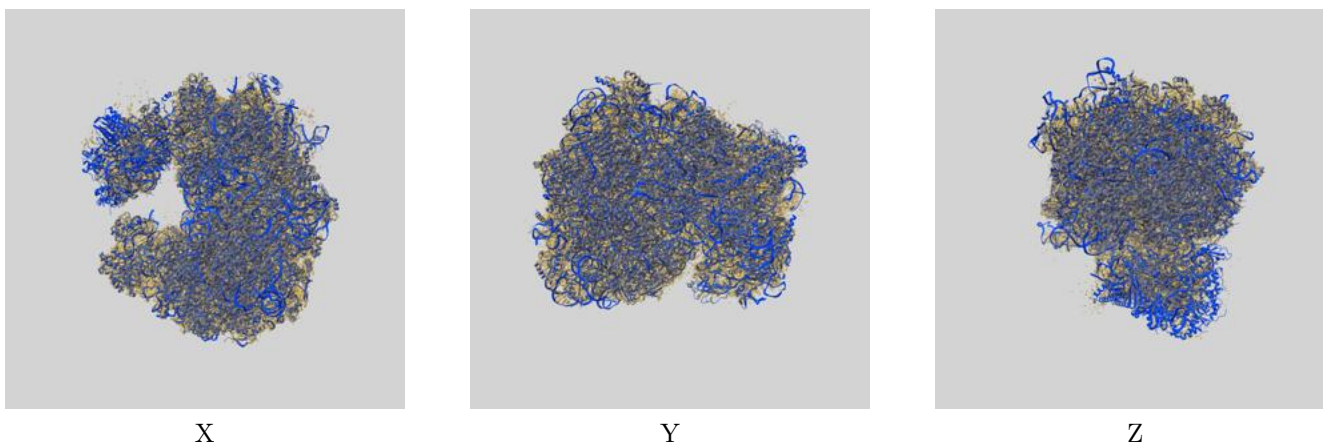
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

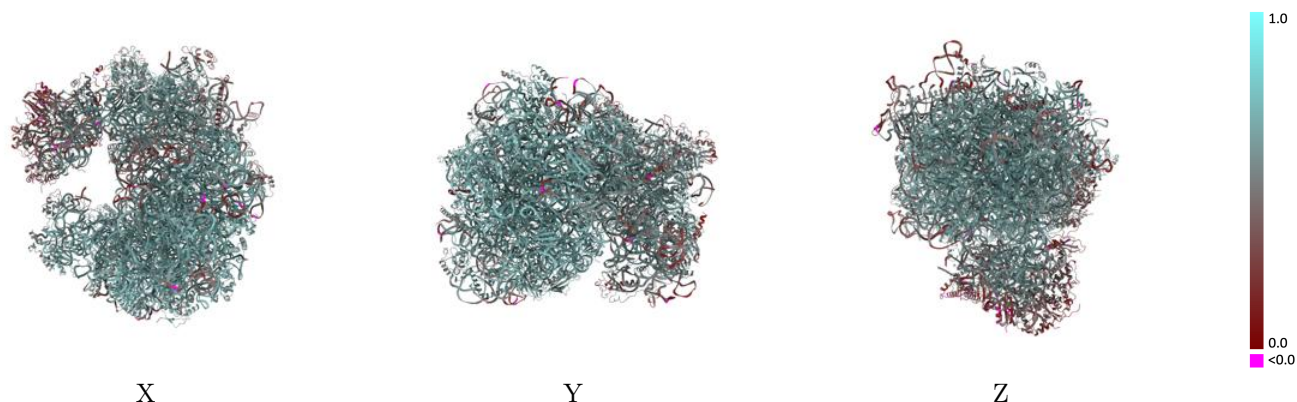
This section contains information regarding the fit between EMDB map EMD-18156 and PDB model 8Q5I. Per-residue inclusion information can be found in section 3 on page 23.

### 9.1 Map-model overlay [i](#)



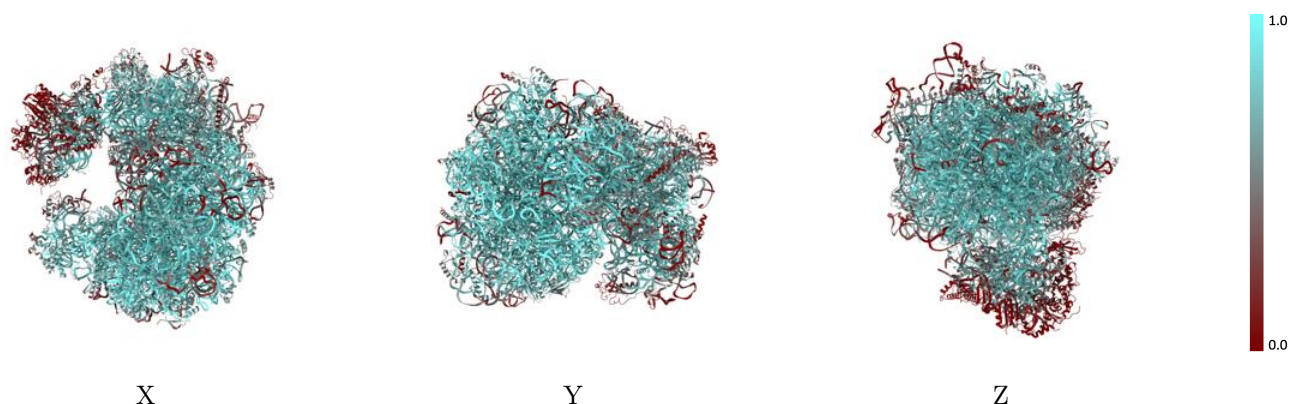
The images above show the 3D surface view of the map at the recommended contour level 0.274 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

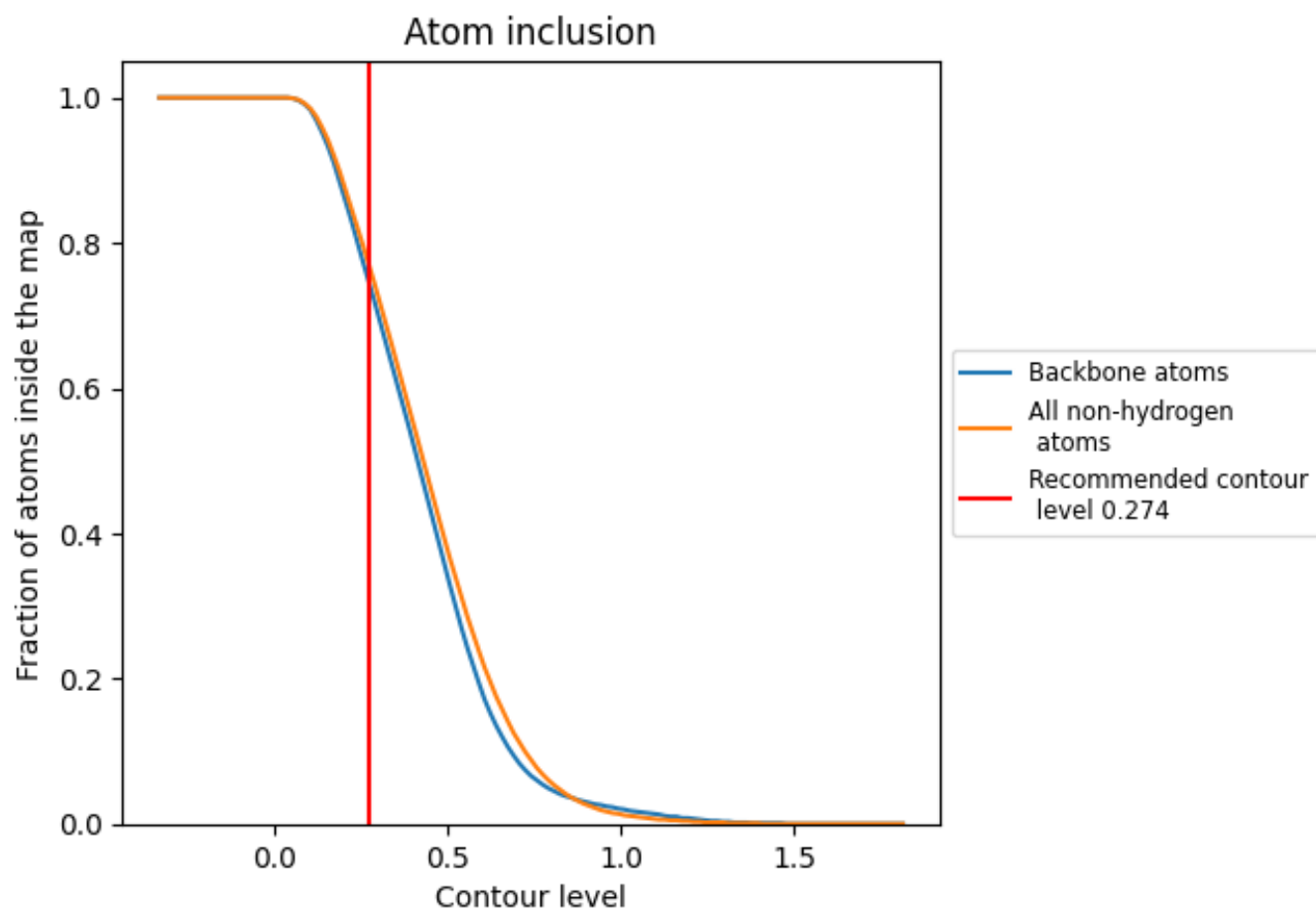
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.274).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 77% 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 (0.274) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.5940
0	 0.8470	 0.6540
1	 0.8760	 0.6310
10	 0.1870	 0.3830
2	 0.7950	 0.6290
3	 0.9040	 0.6390
4	 0.9000	 0.6400
5	 0.4390	 0.5030
6	 0.8840	 0.6550
7	 0.8440	 0.6420
8	 0.8180	 0.6480
9	 0.7950	 0.6360
A	 0.7820	 0.5630
AA	 0.7160	 0.6080
AB	 0.8960	 0.6730
AC	 0.7280	 0.5900
AD	 0.7600	 0.6140
AE	 0.8420	 0.6530
AF	 0.8490	 0.6550
AG	 0.8800	 0.6760
AH	 0.8110	 0.6370
AI	 0.7750	 0.6240
AJ	 0.7110	 0.5910
AK	 0.9100	 0.6810
AL	 0.6170	 0.5640
AM	 0.8510	 0.6470
AN	 0.7760	 0.6320
AO	 0.5670	 0.5460
AP	 0.7810	 0.6460
AQ	 0.8340	 0.6450
B	 0.6420	 0.5530
C	 0.3840	 0.4380
D	 0.8190	 0.6180
E	 0.2930	 0.4040
F	 0.7160	 0.5760



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Chain	Atom inclusion	Q-score
G	0.1550	0.3440
H	0.3420	0.4270
I	0.3980	0.4720
J	0.5330	0.5140
K	0.7310	0.5890
L	0.1510	0.3320
M	0.7130	0.6030
O	0.6850	0.5600
P	0.5190	0.5020
Q	0.2620	0.4200
R	0.2260	0.3720
S	0.2510	0.3940
T	0.2190	0.3810
U	0.1580	0.3710
V	0.2350	0.3360
W	0.7250	0.5950
X	0.9310	0.6540
Y	0.8660	0.6220
Z	0.5500	0.5230
b	0.6980	0.5680
c	0.5850	0.5270
d	0.1540	0.3400
e	0.6990	0.5750
f	0.5120	0.4770
g	0.0000	0.3270
j	0.9240	0.6850
k	0.8750	0.6600
l	0.8270	0.6420
m	0.6610	0.5820
n	0.6220	0.5850
o	0.8600	0.6650
p	0.7130	0.6110
q	0.7350	0.6120
r	0.7810	0.6260
s	0.5190	0.5330
t	0.7920	0.6290
u	0.7660	0.6150
v	0.9320	0.6850
w	0.8630	0.6590
x	0.8280	0.6480
y	0.8940	0.6650
z	0.7470	0.5950