



## wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 04:27 PM UTC

PDB ID : 8CDL / pdb\_00008cdl  
EMDB ID : EMD-16591  
Title : 80S *S. cerevisiae* ribosome with ligands in hybrid-2 pre-translocation (PRE-H2) complex  
Authors : Milicevic, N.; Jenner, L.; Myasnikov, A.; Yusupov, M.; Yusupova, G.  
Deposited on : 2023-01-31  
Resolution : 2.72 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:

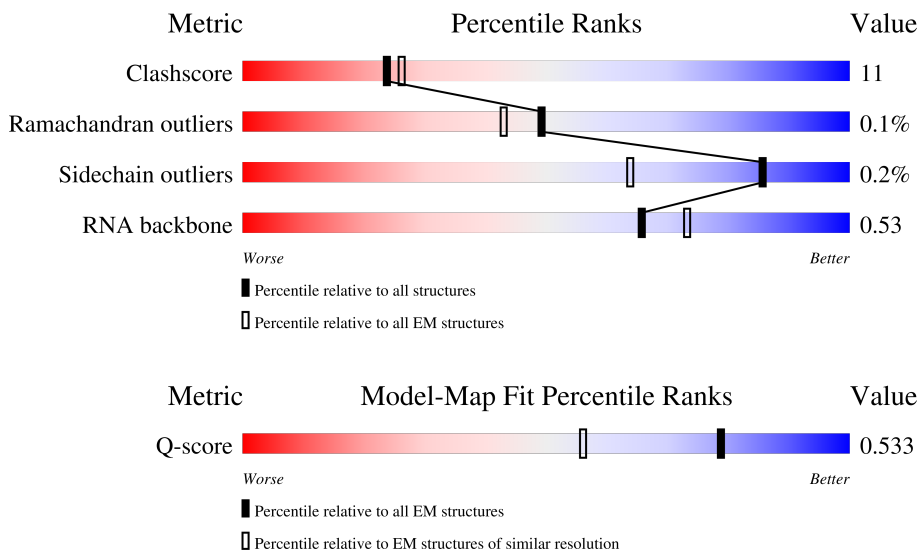
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 2.72 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.



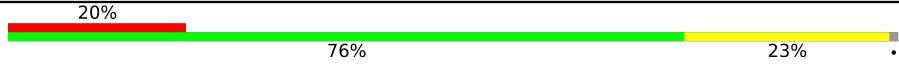
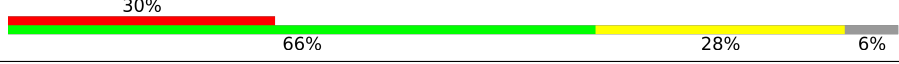
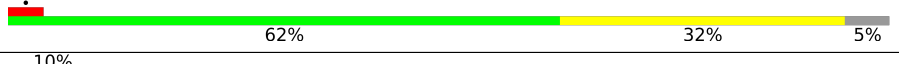

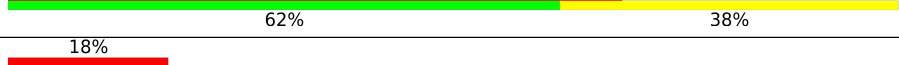
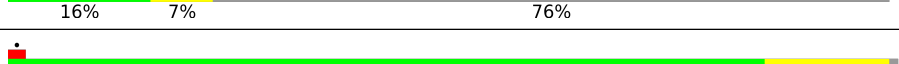

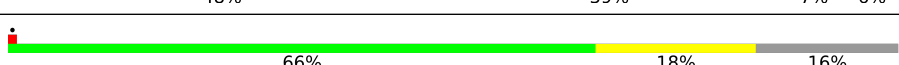
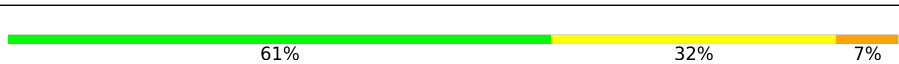
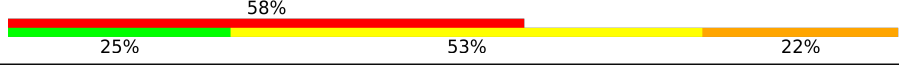

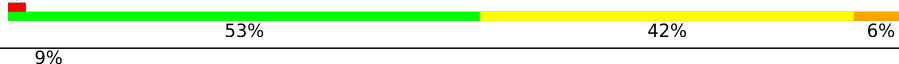
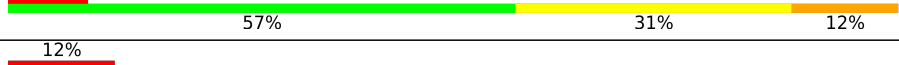

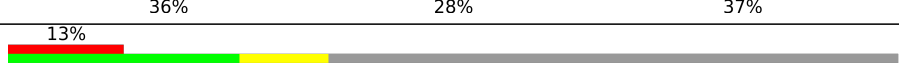


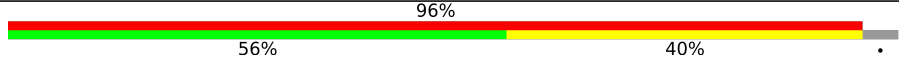







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10355 ( 2.22 - 3.22 )

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	0	135	41% (Poor fit) 61% (0 outliers) 39% (1 outlier) . (2 outliers)
2	1	108	33% (Poor fit) 38% (0 outliers) 27% (1 outlier) 35% (2 outliers)
3	2	119	5% (Poor fit) 58% (0 outliers) 24% (1 outlier) 18% (2 outliers)

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Mol	Chain	Length	Quality of chain
4	3	82	
5	4	67	
6	5	56	
7	6	63	
8	7	319	
9	8	152	
10	A	199	
11	AA	3396	
12	B	184	
13	BB	121	
14	Bb	76	
15	C	186	
16	CC	158	
17	Cc	77	
18	D	189	
19	DD	312	
20	Dd	39	
21	E	172	
22	EE	254	
23	Ee	165	
24	F	160	
25	FF	387	
26	G	121	
27	GG	362	
28	H	129	

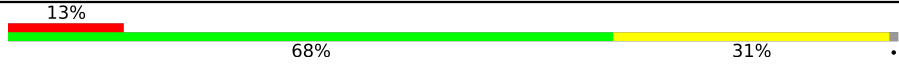
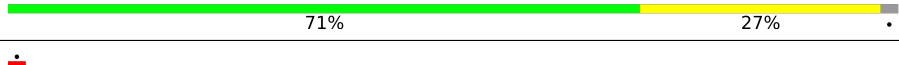


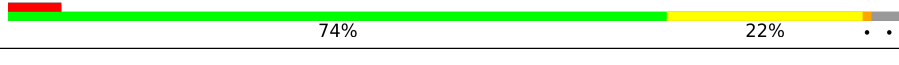
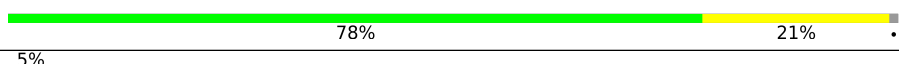
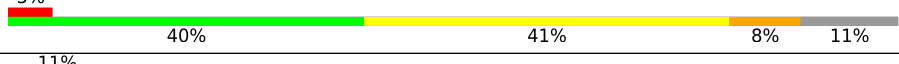
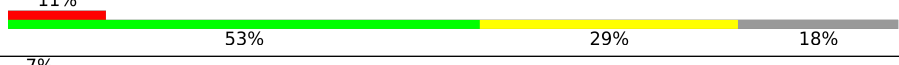
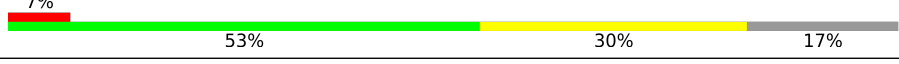



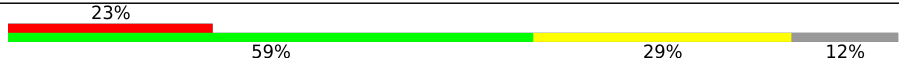
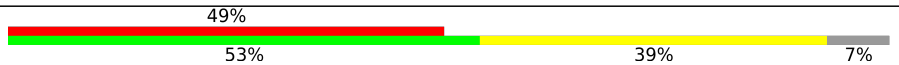
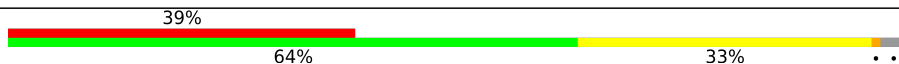
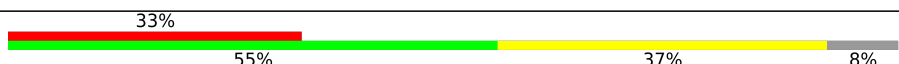
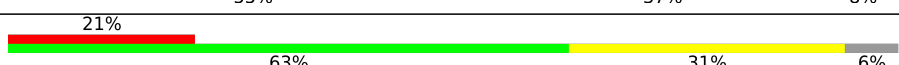
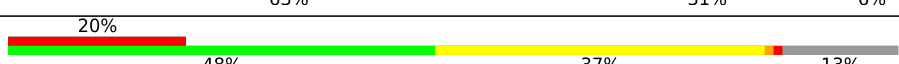


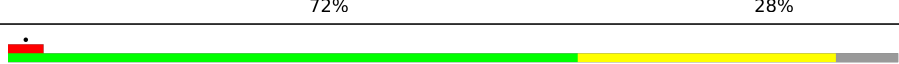



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Mol	Chain	Length	Quality of chain
29	HH	297	
30	I	155	
31	II	176	
32	J	142	
33	JJ	244	
34	K	127	
35	KK	256	
36	L	136	
37	LL	191	
38	M	149	
39	MM	221	
40	N	59	
41	NN	174	
42	O	105	
43	OO	199	
44	P	113	
45	PP	138	
46	Pp	2	
47	Q	130	
48	QQ	204	
49	R	107	
50	S	121	
51	T	120	
52	U	100	
53	V	88	

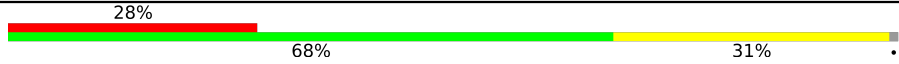

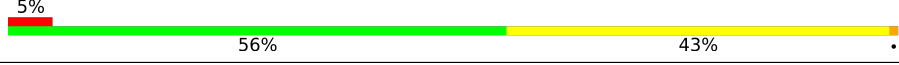


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Mol	Chain	Length	Quality of chain
54	W	78	
55	X	51	
56	Y	128	
57	Z	25	
58	a	106	
59	b	92	
60	c	1800	
61	d	252	
62	e	255	
63	f	254	
64	g	240	
65	h	261	
66	i	225	
67	j	236	
68	k	190	
69	l	200	
70	m	197	
71	n	105	
72	o	156	
73	p	151	
74	q	137	
75	r	142	
76	s	143	
77	t	136	
78	u	146	

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Mol	Chain	Length	Quality of chain
79	v	144	
80	w	121	
81	x	87	
82	y	130	
83	z	145	

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 201553 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
			Total	C	N	O	S		
7	6	53	427	269	88	69	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O		
18	D	176	1423	875	308	240	0	0

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

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

- Molecule 20 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Dd	14	Total	C	N	O	P	0	0
			298	134	52	98	14		

- 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	C	N	O	0	0
			993	625	192	176		

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

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

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

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

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

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

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

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

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

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

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

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

- 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 dipeptide.

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
			Total	C	N	O	S		
48	QQ	203	1720	1077	361	281	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
69	l	184	1457	906	291	258	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	AA	191	Total 191	Mg 191	0
85	B	1	Total 1	Mg 1	0
85	BB	4	Total 4	Mg 4	0
85	Bb	1	Total 1	Mg 1	0
85	CC	4	Total 4	Mg 4	0
85	Cc	1	Total 1	Mg 1	0
85	Dd	1	Total 1	Mg 1	0
85	FF	1	Total 1	Mg 1	0
85	H	1	Total 1	Mg 1	0

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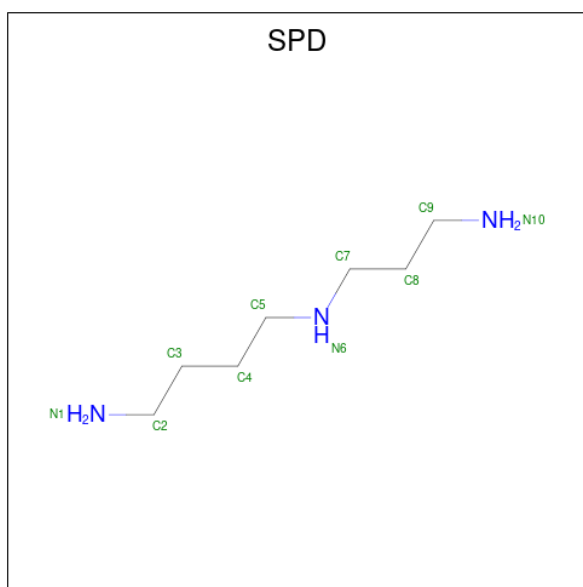
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Mol	Chain	Residues	Atoms		AltConf
85	JJ	1	Total 1	Mg 1	0
85	MM	1	Total 1	Mg 1	0
85	QQ	2	Total 2	Mg 2	0
85	V	1	Total 1	Mg 1	0
85	a	1	Total 1	Mg 1	0
85	c	46	Total 46	Mg 46	0
85	q	1	Total 1	Mg 1	0

- Molecule 86 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
86	AA	11	Total 11	K 11	0
86	EE	1	Total 1	K 1	0
86	MM	1	Total 1	K 1	0
86	Q	1	Total 1	K 1	0
86	S	1	Total 1	K 1	0
86	a	1	Total 1	K 1	0
86	c	4	Total 4	K 4	0
86	q	1	Total 1	K 1	0

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



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	2	Total O 2 2	0
88	A	3	Total O 3 3	0
88	AA	804	Total O 804 804	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	5	Total O 5 5	0
88	D	4	Total O 4 4	0

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Mol	Chain	Residues	Atoms		AltConf
88	Dd	4	Total 4	O 4	0
88	EE	6	Total 6	O 6	0
88	F	4	Total 4	O 4	0
88	FF	5	Total 5	O 5	0
88	GG	3	Total 3	O 3	0
88	H	3	Total 3	O 3	0
88	J	2	Total 2	O 2	0
88	LL	2	Total 2	O 2	0
88	M	3	Total 3	O 3	0
88	MM	2	Total 2	O 2	0
88	N	1	Total 1	O 1	0
88	OO	1	Total 1	O 1	0
88	P	1	Total 1	O 1	0
88	Q	3	Total 3	O 3	0
88	QQ	6	Total 6	O 6	0
88	S	2	Total 2	O 2	0
88	V	3	Total 3	O 3	0
88	a	4	Total 4	O 4	0
88	c	170	Total 170	O 170	0
88	f	1	Total 1	O 1	0
88	o	1	Total 1	O 1	0

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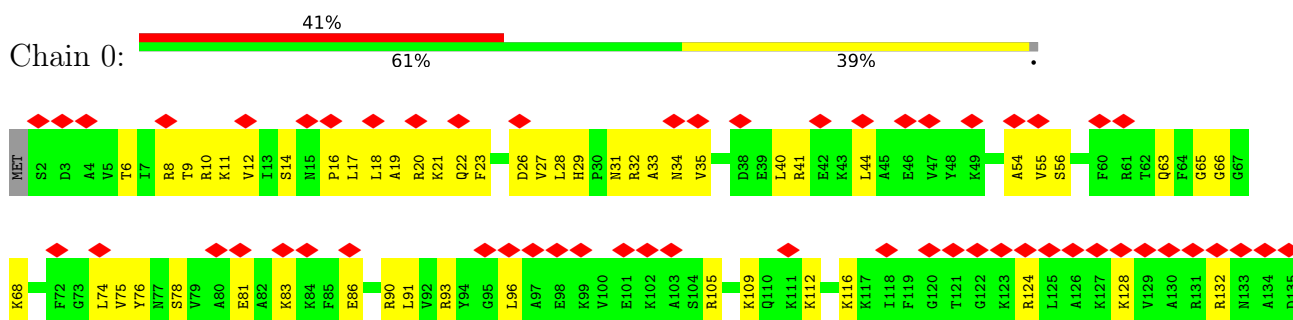
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
88	p	1	Total 1	O 1	0
88	q	2	Total 2	O 2	0
88	z	1	Total 1	O 1	0

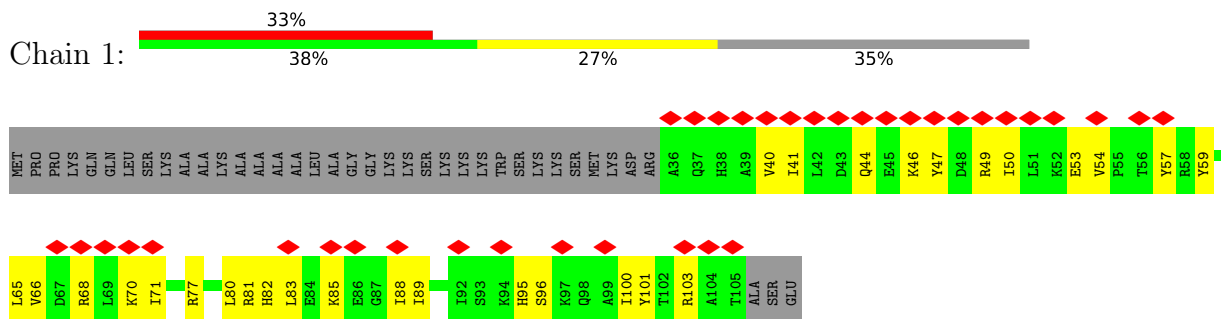
### 3 Residue-property plots [i](#)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

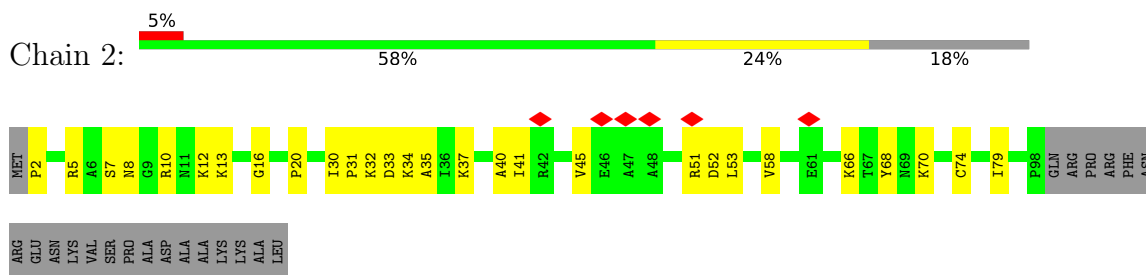
- Molecule 1: 40S ribosomal protein S24-A



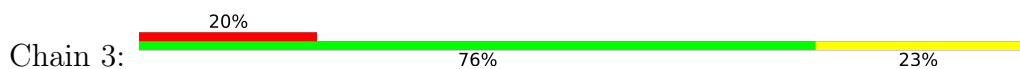
- Molecule 2: 40S ribosomal protein S25-A

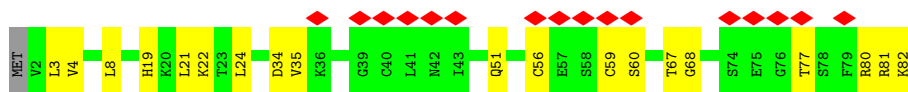


- Molecule 3: 40S ribosomal protein S26

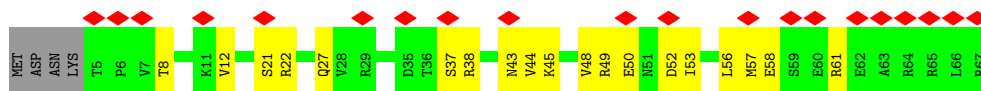


- Molecule 4: 40S ribosomal protein S27-A

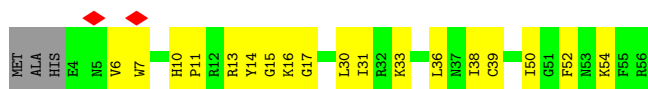




• Molecule 5: 40S ribosomal protein S28-A



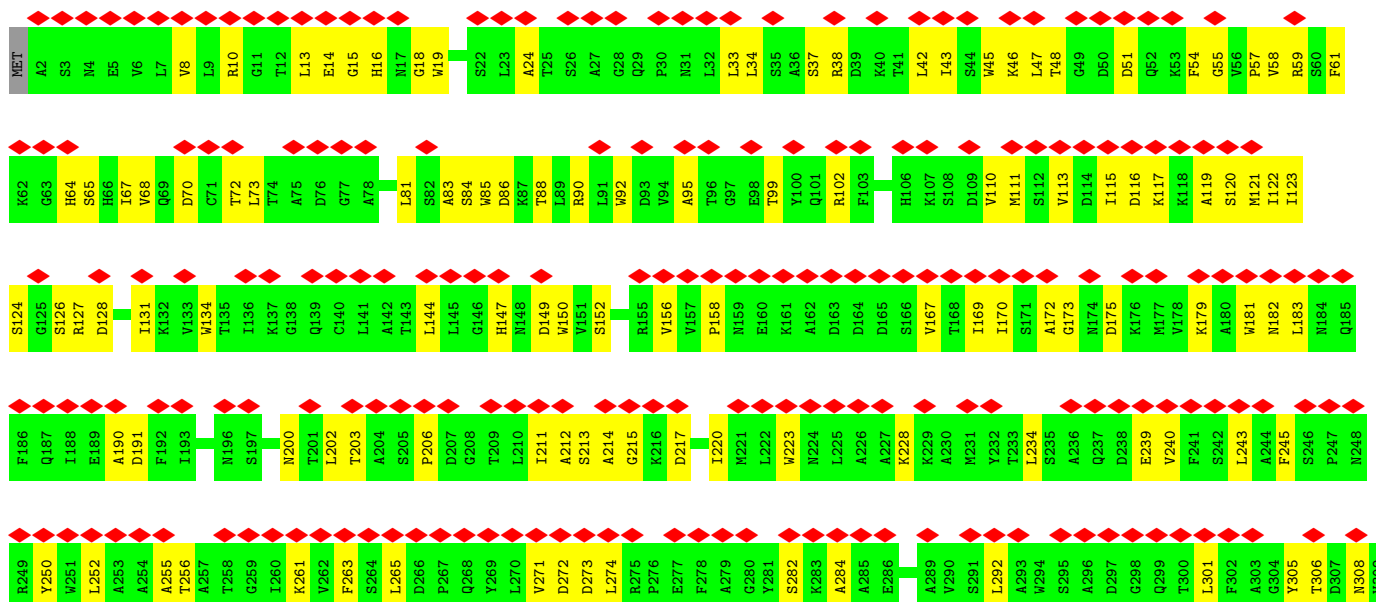
• Molecule 6: HLJ1\_G0030400.mRNA.1.CDS.1



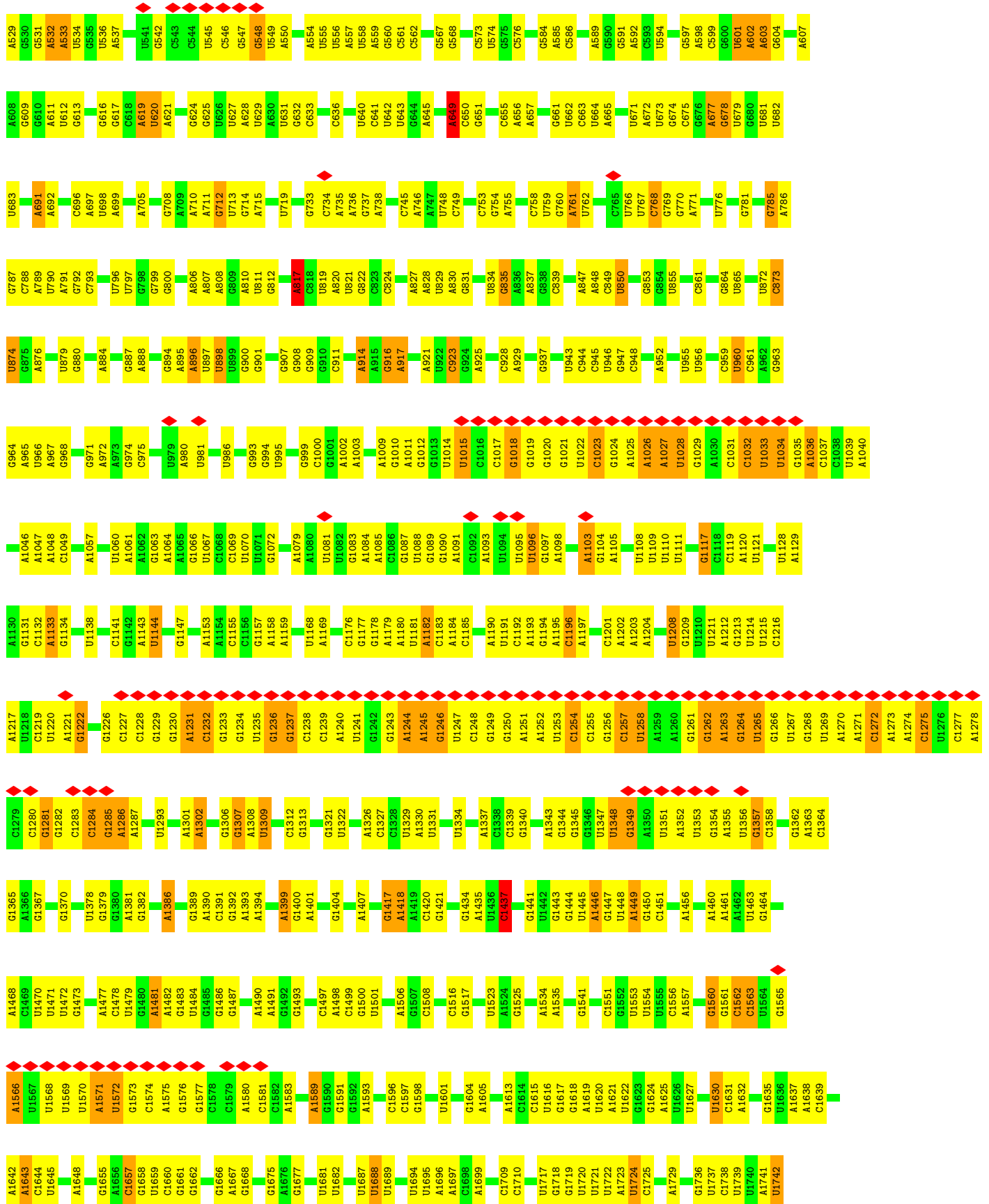
• Molecule 7: 40S ribosomal protein S30-A



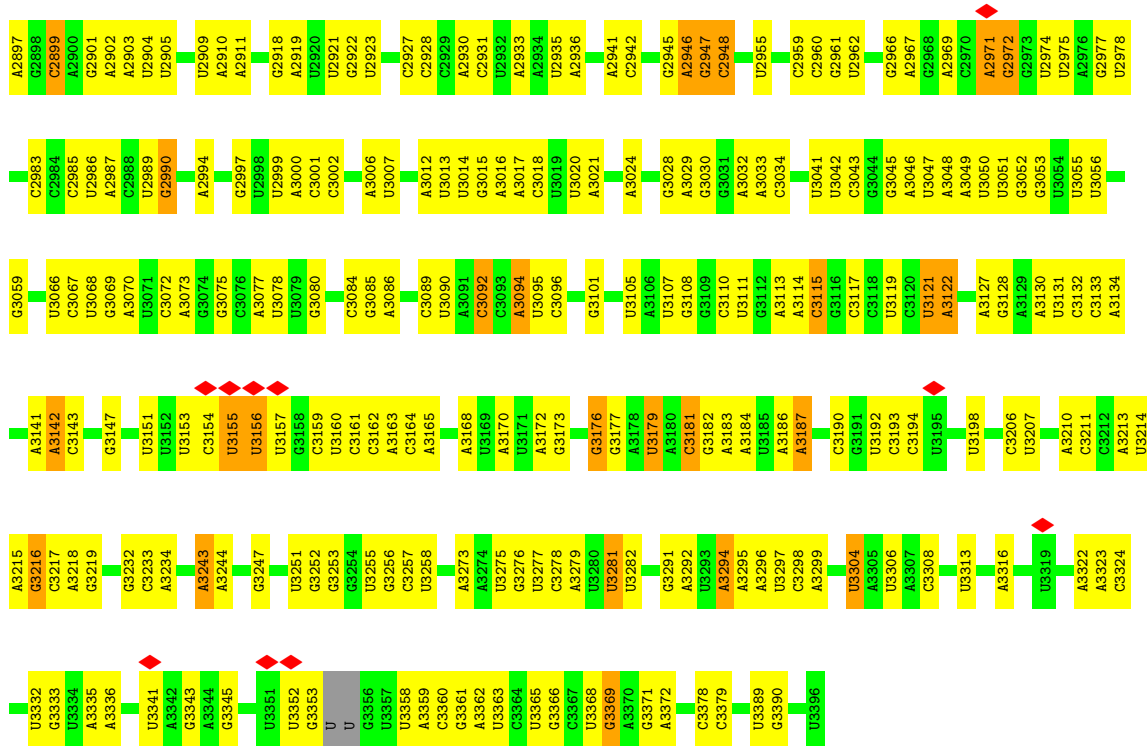
• Molecule 8: Guanine nucleotide-binding protein subunit beta-like protein

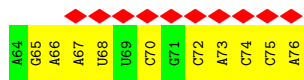




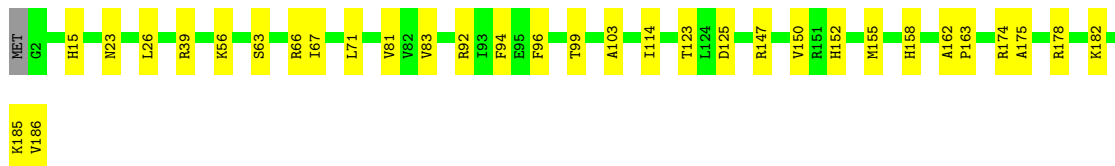
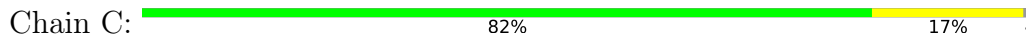




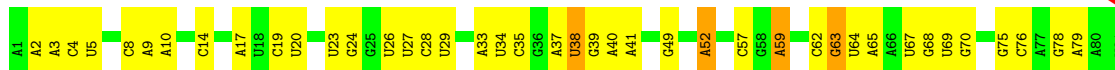




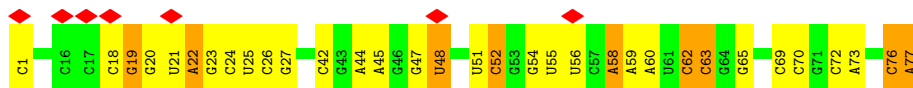
• Molecule 15: 60S ribosomal protein L18-A



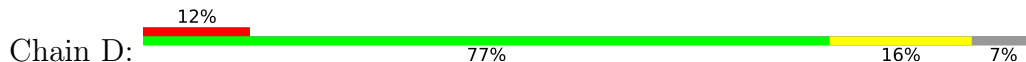
• Molecule 16: 5.8S ribosomal RNA



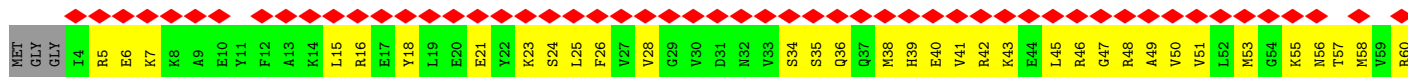
• Molecule 17: Transfer RNA fMet



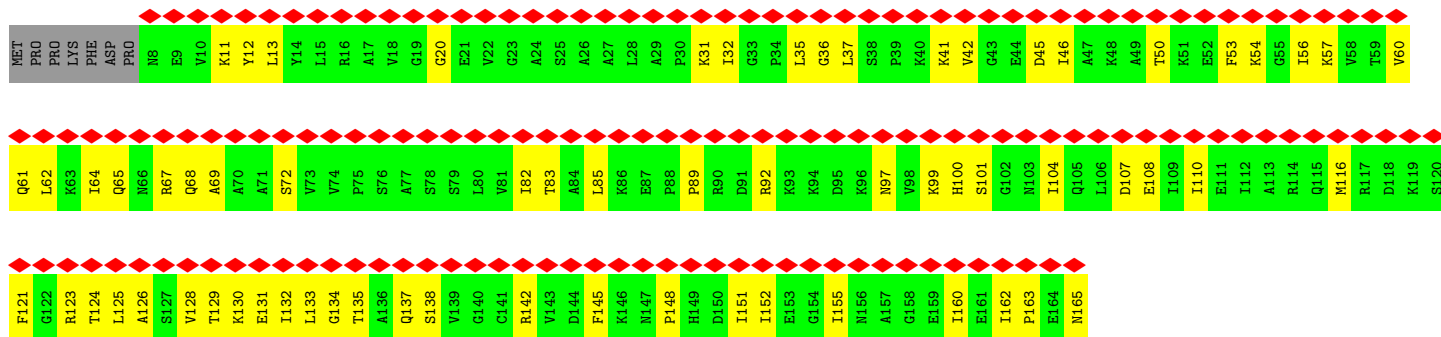
• Molecule 18: 60S ribosomal protein L19-A



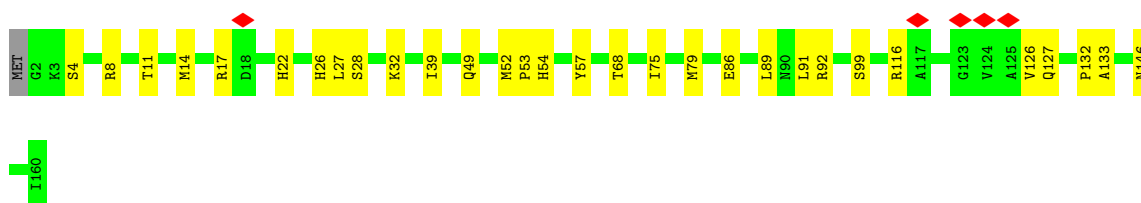
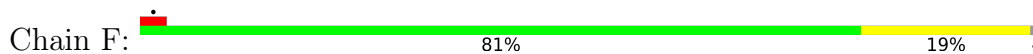
• Molecule 19: 60S acidic ribosomal protein P0



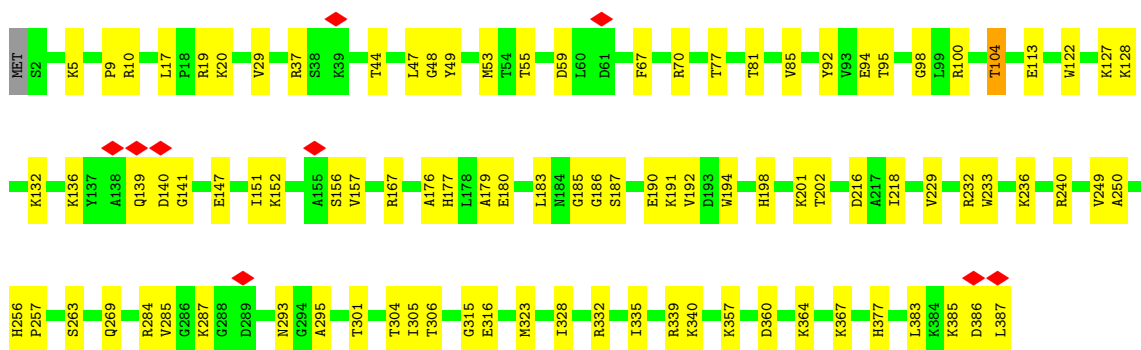
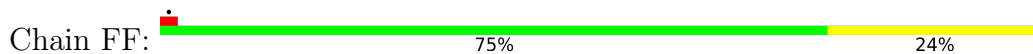




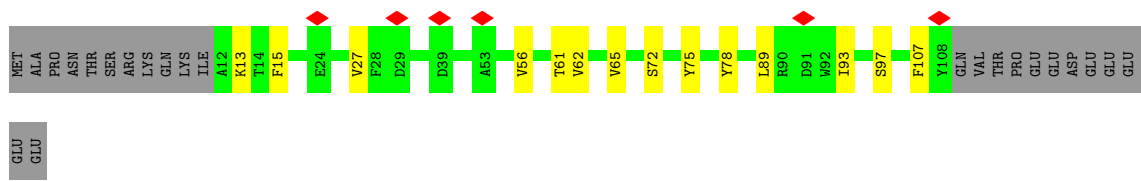
• Molecule 24: 60S ribosomal protein L21-A



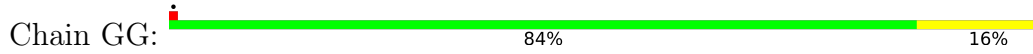
• Molecule 25: 60S ribosomal protein L3

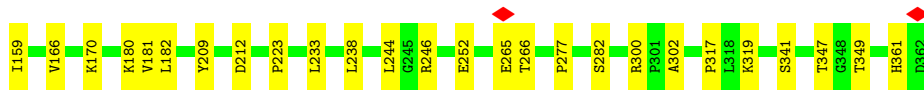
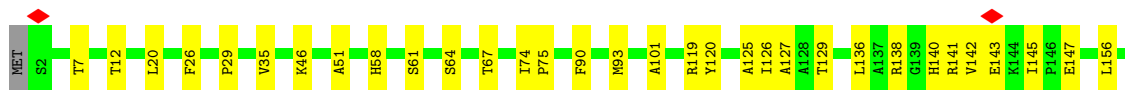


• Molecule 26: 60S ribosomal protein L22-A

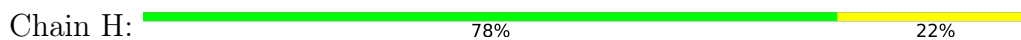


• Molecule 27: 60S ribosomal protein L4-A

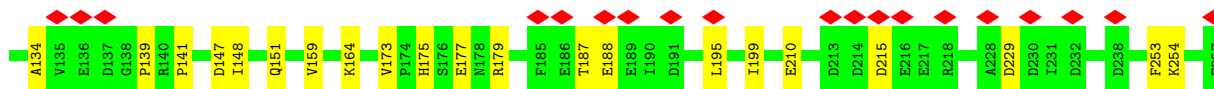
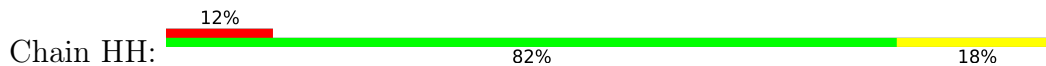




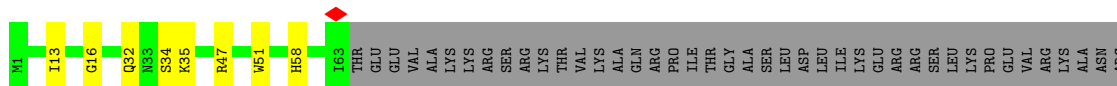
• Molecule 28: 60S ribosomal protein L23-A



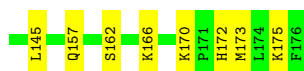
• Molecule 29: 60S ribosomal protein L5



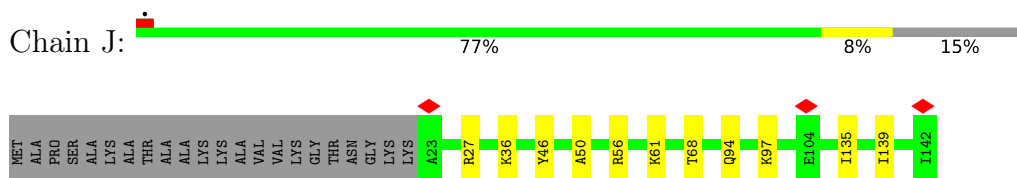
• Molecule 30: 60S ribosomal protein L24-A



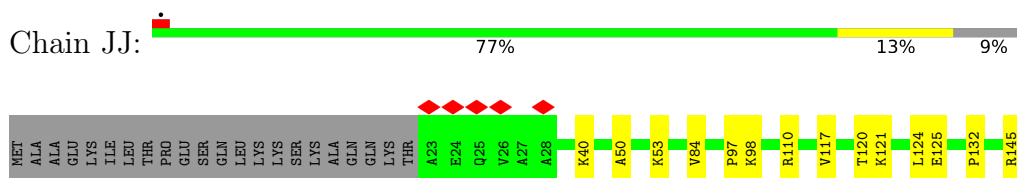
• Molecule 31: 60S ribosomal protein L6-A



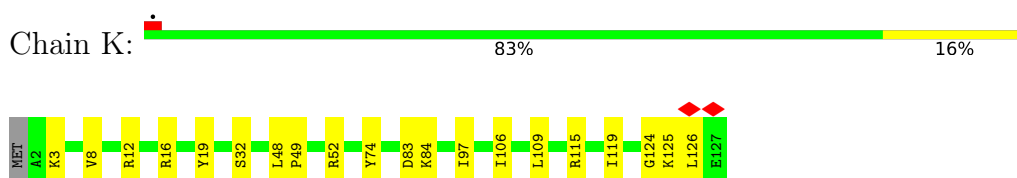
• Molecule 32: 60S ribosomal protein L25



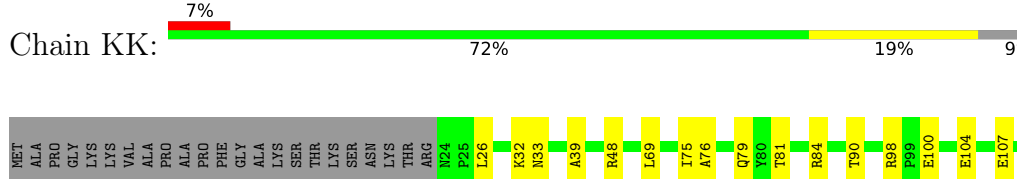
• Molecule 33: 60S ribosomal protein L7-A



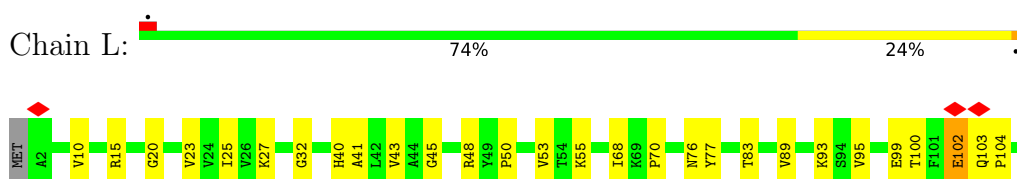
• Molecule 34: 60S ribosomal protein L26-A



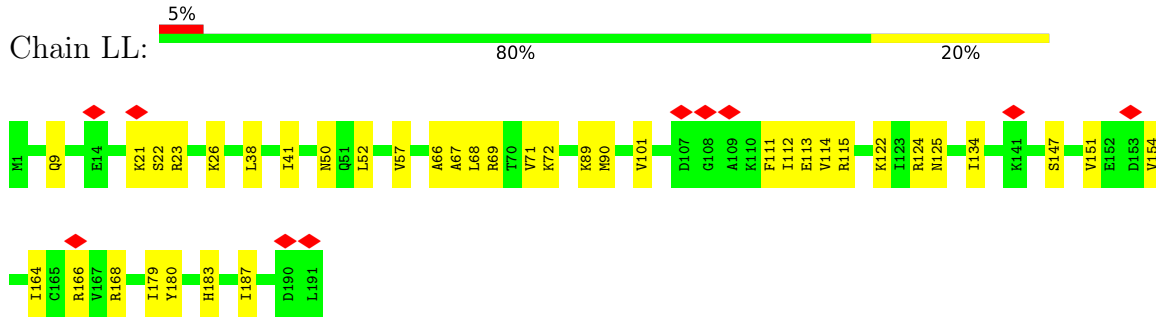
• Molecule 35: 60S ribosomal protein L8-A



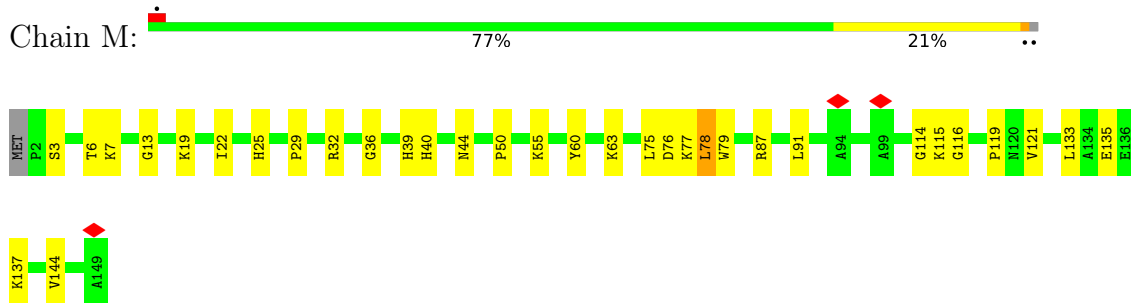
• Molecule 36: 60S ribosomal protein L27-A



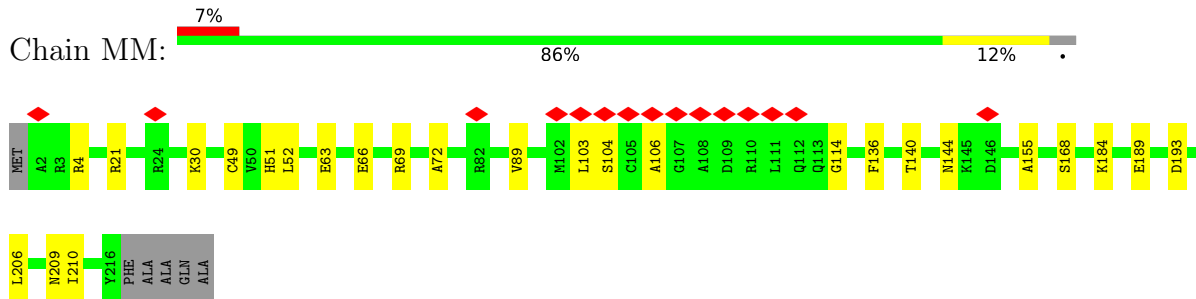
• Molecule 37: 60S ribosomal protein L9-A



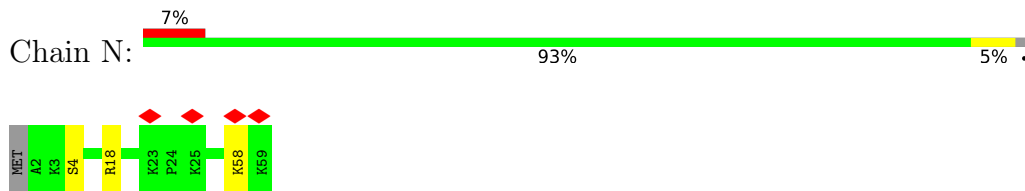
• Molecule 38: 60S ribosomal protein L28



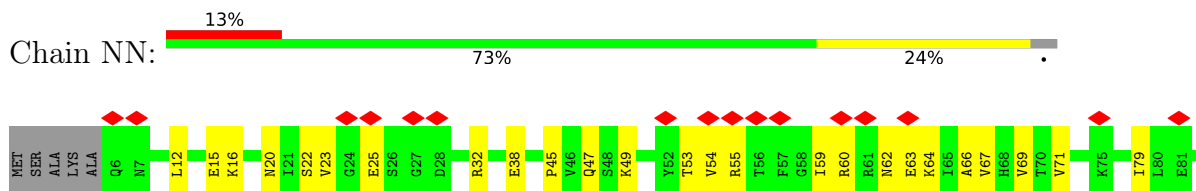
• Molecule 39: 60S ribosomal protein L10

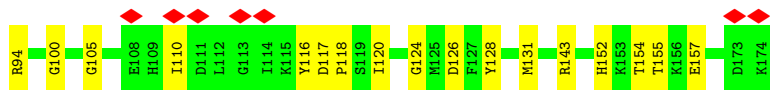


• Molecule 40: 60S ribosomal protein L29

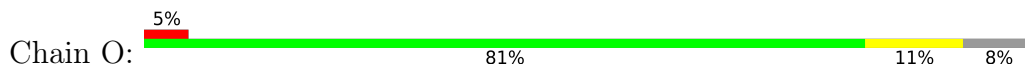


• Molecule 41: 60S ribosomal protein L11-A

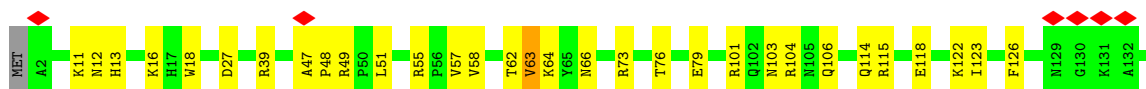
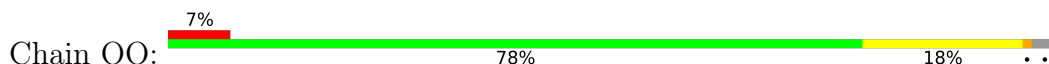




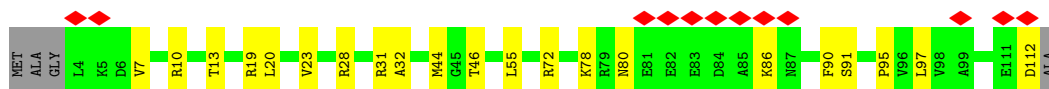
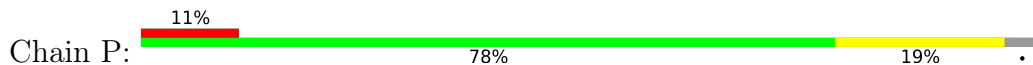
• Molecule 42: 60S ribosomal protein L30



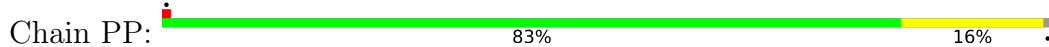
• Molecule 43: 60S ribosomal protein L13-A



• Molecule 44: 60S ribosomal protein L31-A



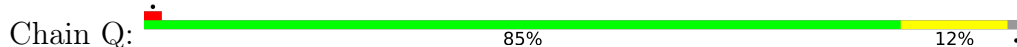
• Molecule 45: 60S ribosomal protein L14-A

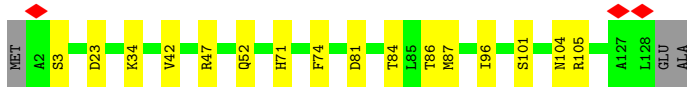


• Molecule 46: dipeptide



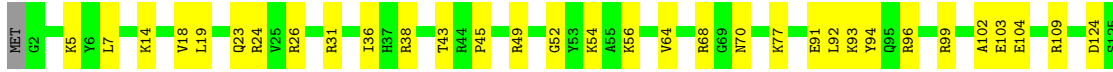
• Molecule 47: 60S ribosomal protein L32





- Molecule 48: 60S ribosomal protein L15-A

Chain QQ: 75% 25%



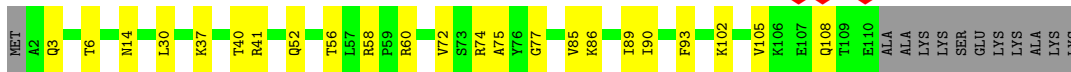
- Molecule 49: 60S ribosomal protein L33-A

Chain R: 82% 17%



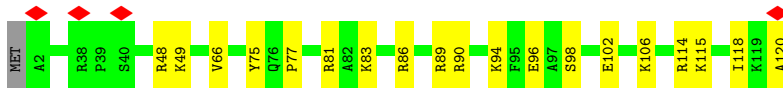
- Molecule 50: 60S ribosomal protein L34-A

Chain S: 71% 19% 10%



- Molecule 51: 60S ribosomal protein L35-A

Chain T: 83% 16%



- Molecule 52: 60S ribosomal protein L36-A

Chain U: 7% 76% 23%

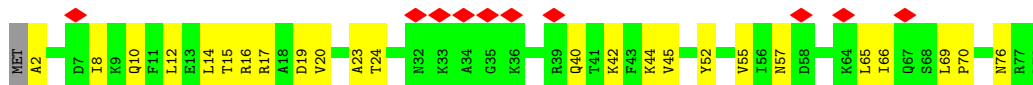


- Molecule 53: 60S ribosomal protein L37-A

Chain V: 68% 27% 5%



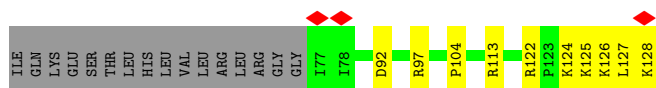
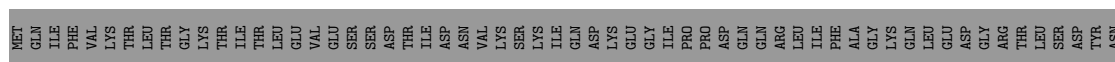
• Molecule 54: 60S ribosomal protein L38



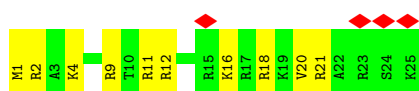
• Molecule 55: 60S ribosomal protein L39



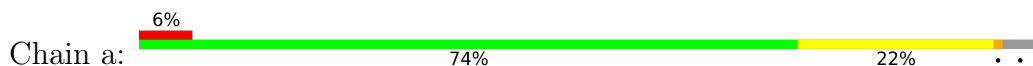
• Molecule 56: Ubiquitin-60S ribosomal protein L40



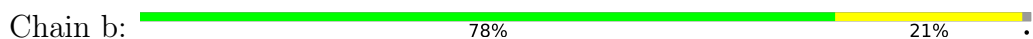
• Molecule 57: 60S ribosomal protein L41-A



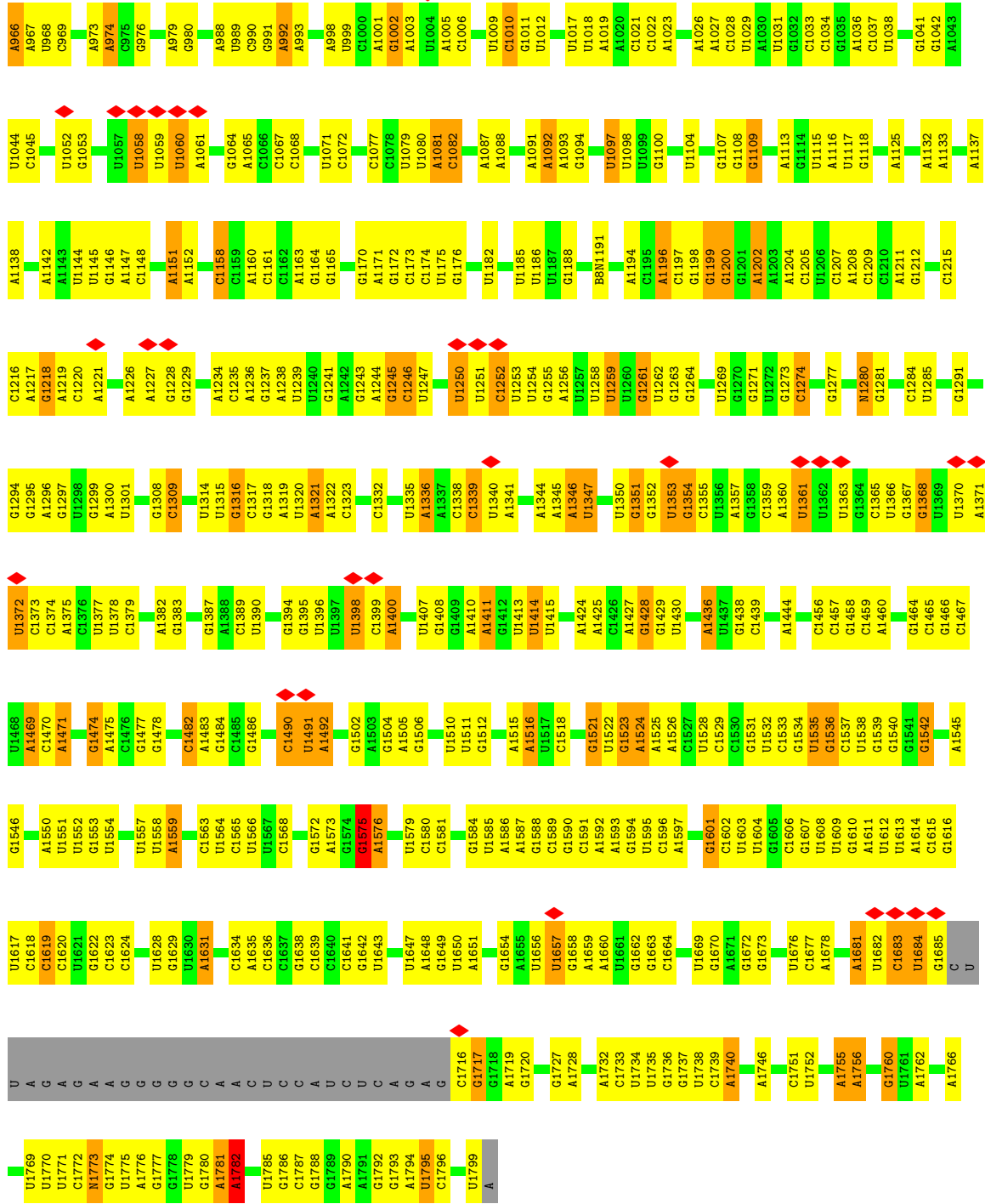
• Molecule 58: 60S ribosomal protein L42-A



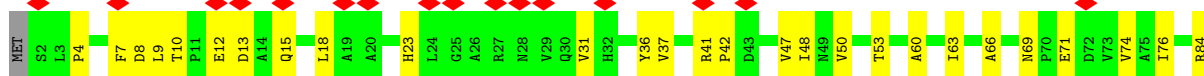
• Molecule 59: 60S ribosomal protein L43-A

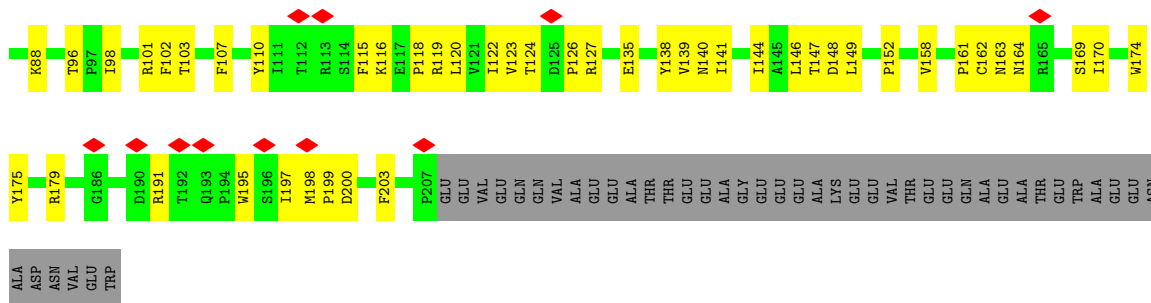




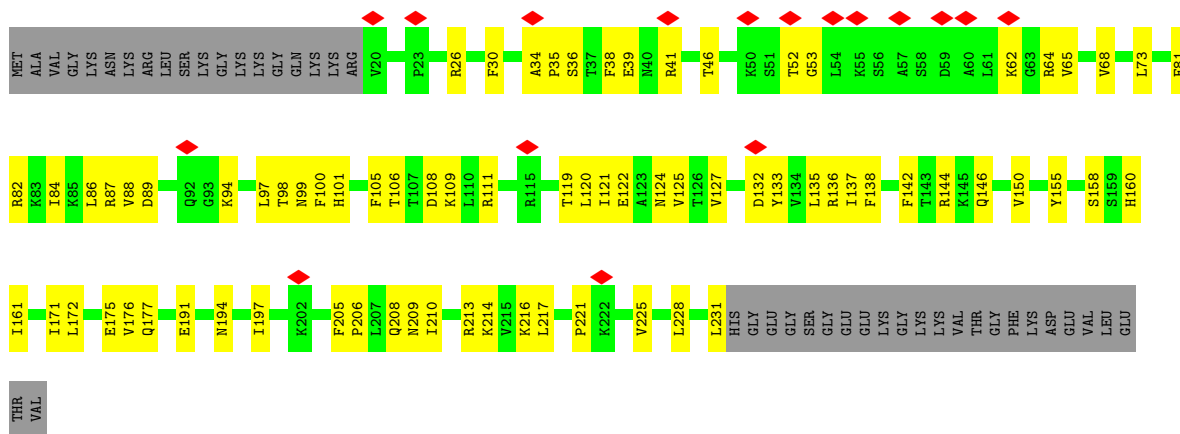


• Molecule 61: 40S ribosomal protein S0-A

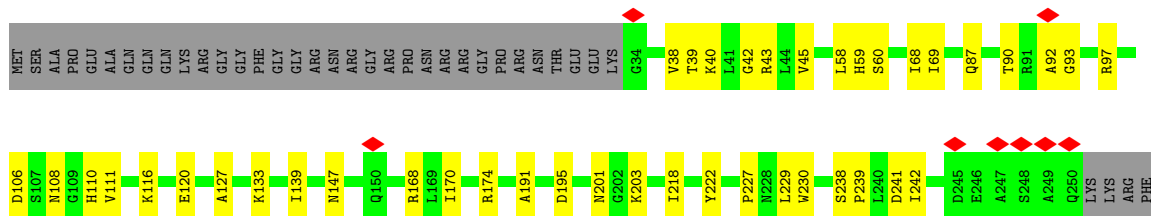




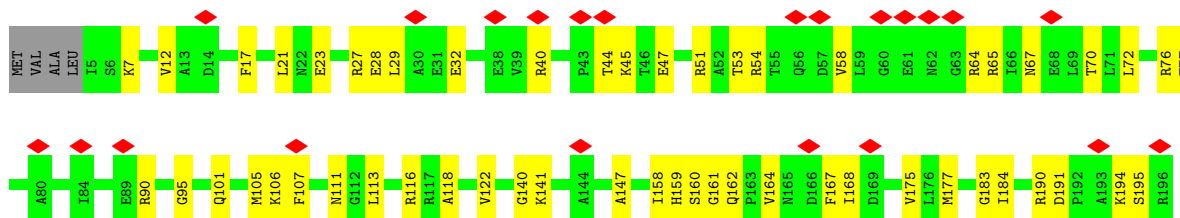
- Molecule 62: 40S ribosomal protein S1-A

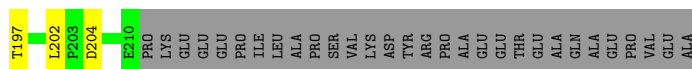


- Molecule 63: 40S ribosomal protein S2

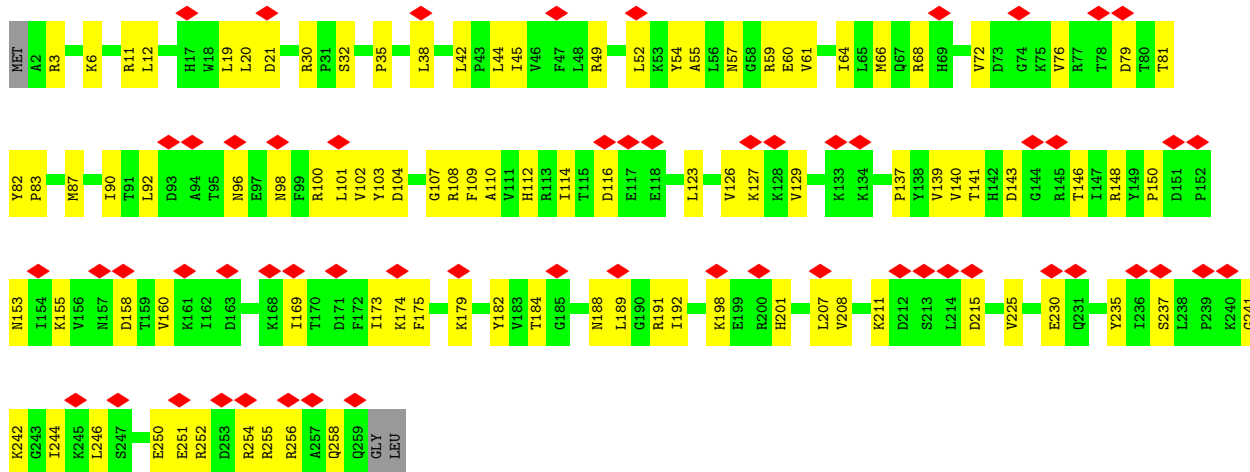


- Molecule 64: RPS3 isoform 1

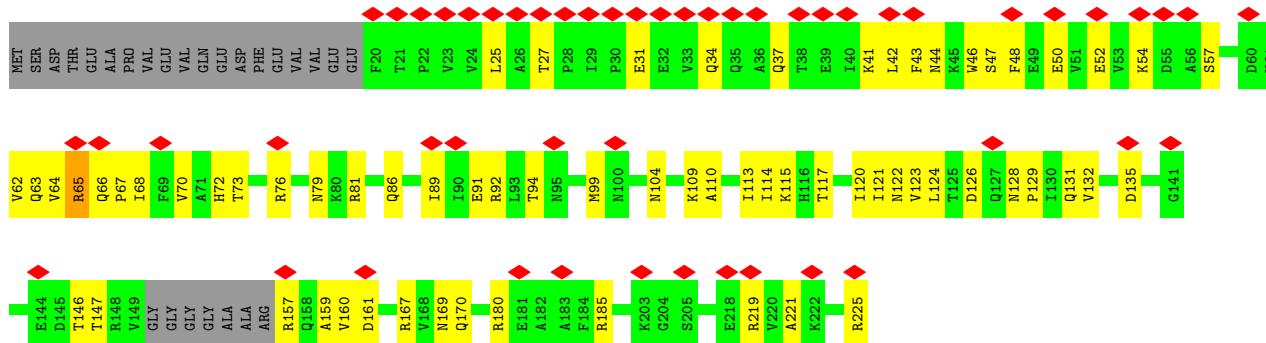




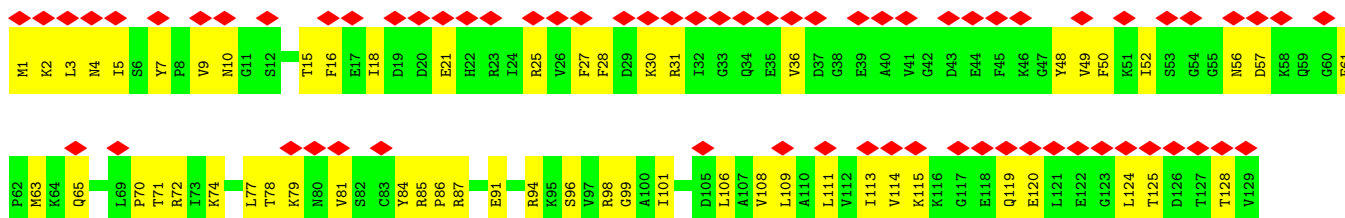
- Molecule 65: 40S ribosomal protein S4-A

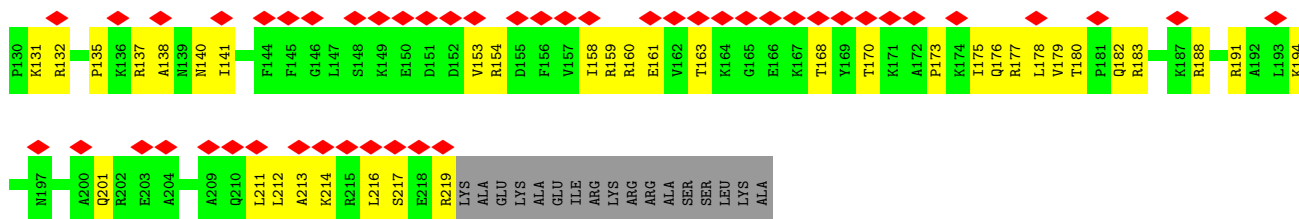


- Molecule 66: 40S ribosomal protein S5

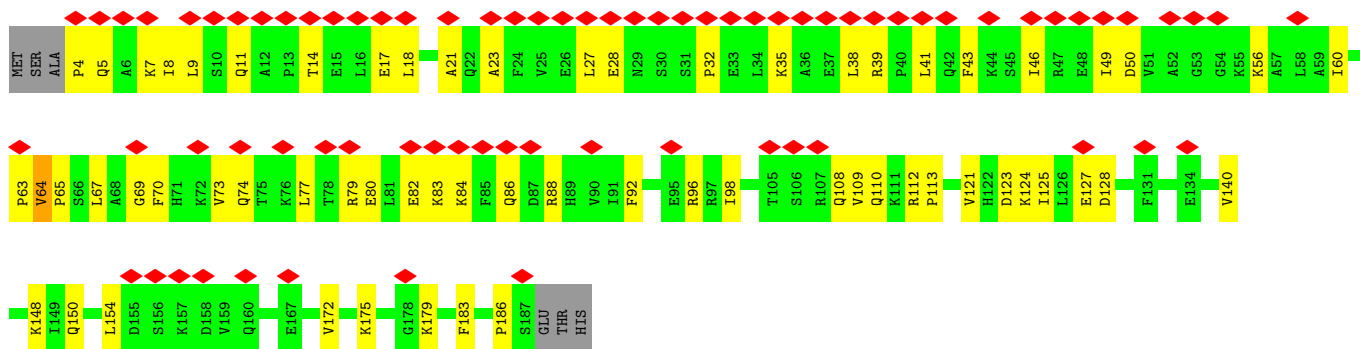
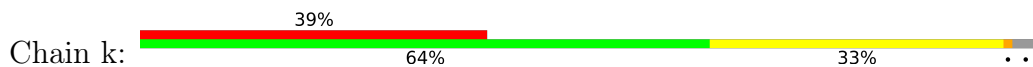


- Molecule 67: 40S ribosomal protein S6-A

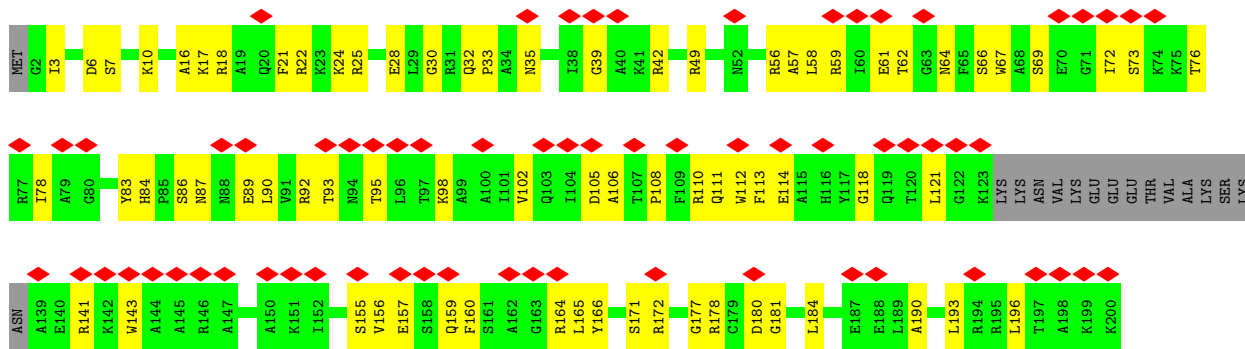




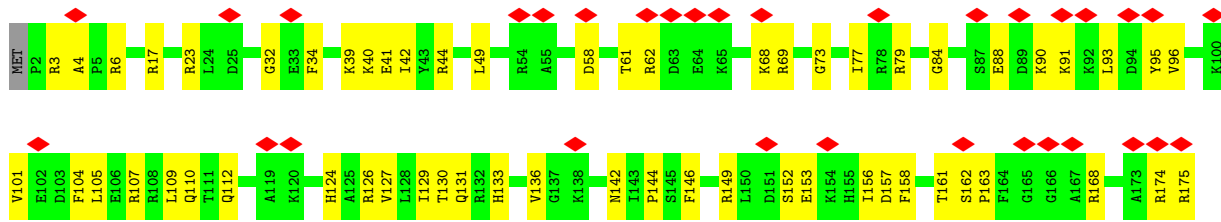
• Molecule 68: 40S ribosomal protein S7-A

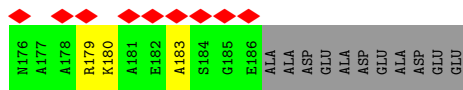


• Molecule 69: 40S ribosomal protein S8-B

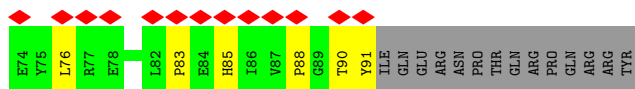
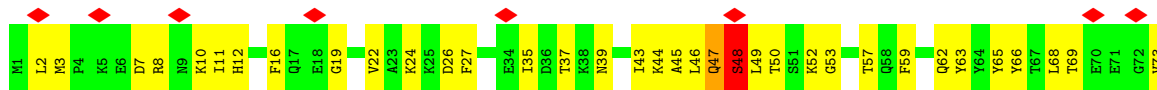


• Molecule 70: 40S ribosomal protein S9-A

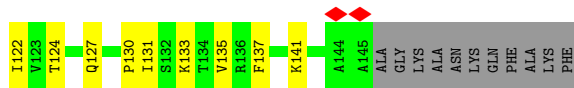
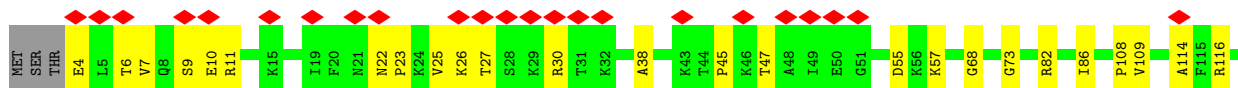




• Molecule 71: 40S ribosomal protein S10-A



• Molecule 72: 40S ribosomal protein S11-A



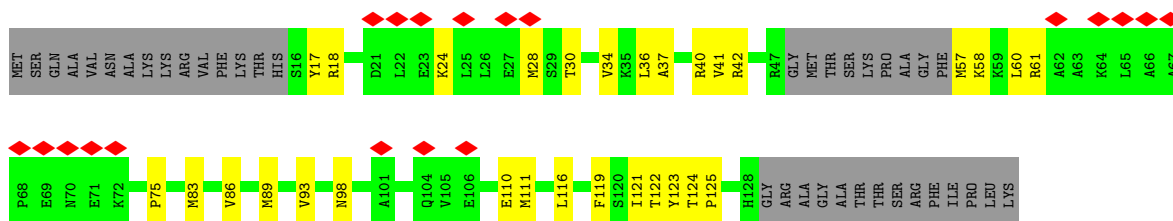
• Molecule 73: 40S ribosomal protein S13



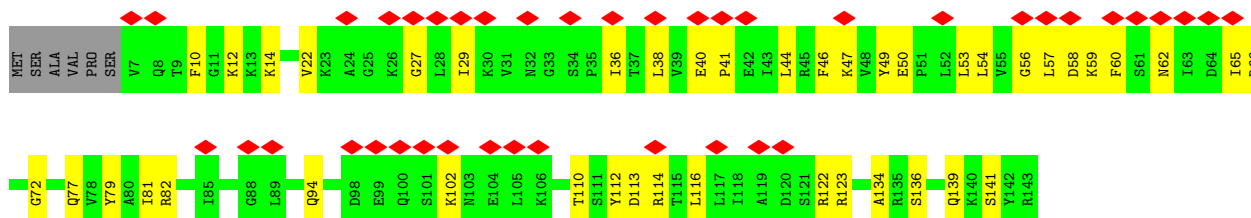
• Molecule 74: 40S ribosomal protein S14-A



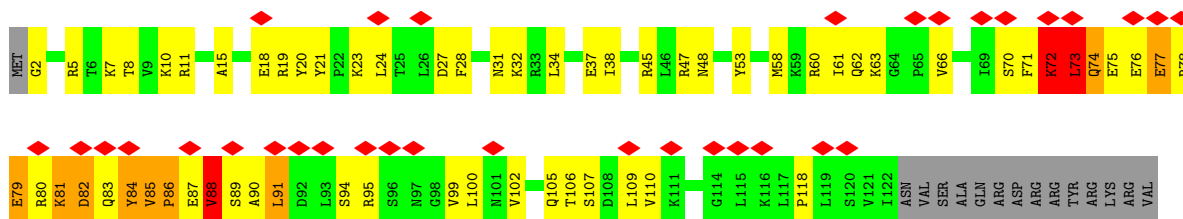
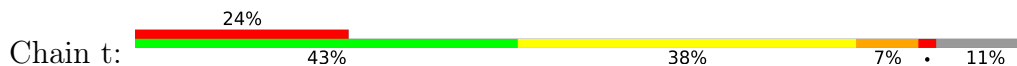
• Molecule 75: 40S ribosomal protein S15



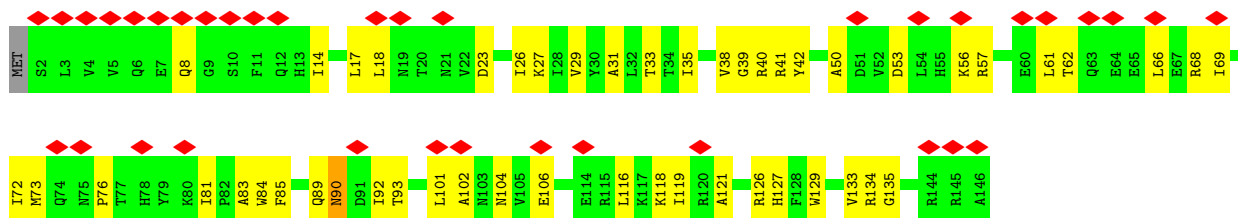
• Molecule 76: 40S ribosomal protein S16-A



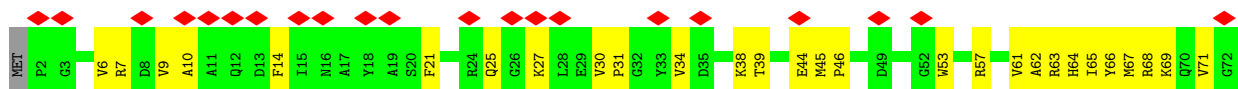
• Molecule 77: 40S ribosomal protein S17-A

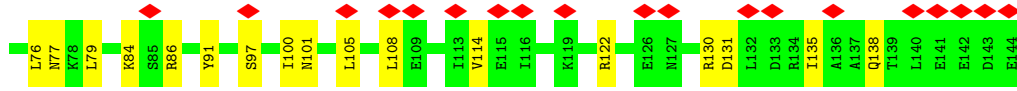


• Molecule 78: 40S ribosomal protein S18-A

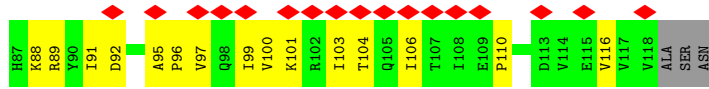
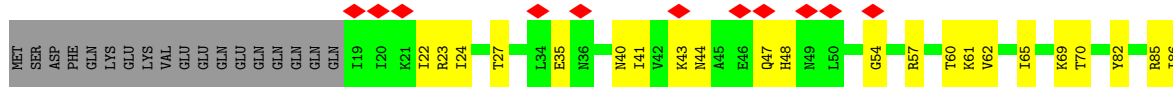


• Molecule 79: 40S ribosomal protein S19-A

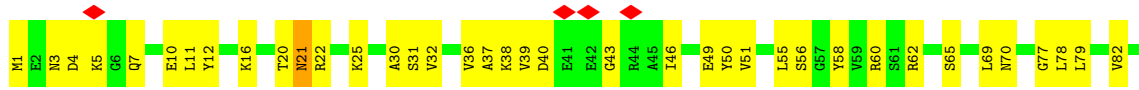




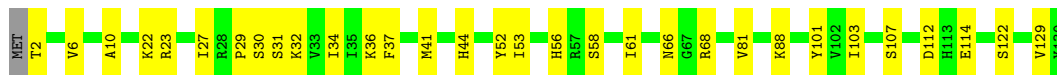
• Molecule 80: 40S ribosomal protein S20



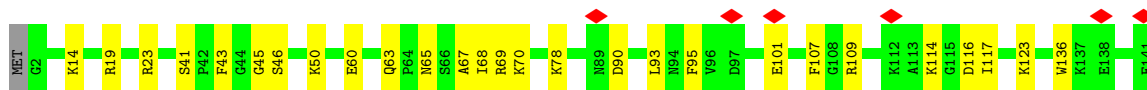
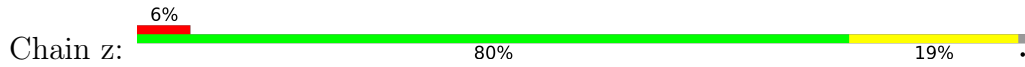
• Molecule 81: 40S ribosomal protein S21-A



• Molecule 82: 40S ribosomal protein S22-A



• Molecule 83: 40S ribosomal protein S23-A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68945	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.864	Depositor
Minimum map value	-0.437	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.141	Depositor
Map size (Å)	418.176, 418.176, 418.176	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.726, 0.726, 0.726	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: 5MC, UR3, K, OMG, G7M, YYG, 4AC, OMC, ZN, MA6, 1MA, SPD, MG, OMU, A2M, B8N

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	0.12	0/1087	0.36	0/1449
2	1	0.15	0/571	0.48	0/768
3	2	0.13	0/782	0.35	0/1047
4	3	0.13	0/620	0.37	0/838
5	4	0.14	0/499	0.36	0/670
6	5	0.14	0/452	0.35	0/600
7	6	0.13	0/433	0.47	0/575
8	7	0.14	0/2489	0.44	0/3389
9	8	0.12	0/279	0.42	0/369
10	A	0.18	0/1585	0.33	0/2128
11	AA	0.18	0/75384	0.27	0/117530
12	B	0.16	0/1245	0.31	0/1676
13	BB	0.14	0/2883	0.22	0/4491
14	Bb	0.14	0/1788	0.42	3/2786 (0.1%)
15	C	0.16	0/1465	0.31	0/1965
16	CC	0.16	0/3746	0.28	0/5832
17	Cc	0.11	0/1836	0.23	0/2859
18	D	0.15	0/1440	0.31	0/1921
19	DD	0.13	0/1558	0.38	0/2107
20	Dd	0.13	0/333	0.18	0/516
21	E	0.16	0/1481	0.37	0/1990
22	EE	0.15	0/1948	0.29	0/2617
23	Ee	0.12	0/1210	0.37	0/1627
24	F	0.14	0/1300	0.30	0/1743
25	FF	0.16	0/3146	0.33	0/4228
26	G	0.14	0/786	0.38	0/1065
27	GG	0.15	0/2800	0.30	0/3790
28	H	0.17	0/978	0.37	0/1316
29	HH	0.12	0/2425	0.29	0/3271
30	I	0.16	0/533	0.33	0/707
31	II	0.14	0/1251	0.29	0/1682
32	J	0.15	0/974	0.33	0/1314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	JJ	0.15	0/1821	0.29	0/2451
34	K	0.15	0/1004	0.34	0/1341
35	KK	0.14	0/1836	0.30	0/2481
36	L	0.16	0/1118	0.42	0/1497
37	LL	0.17	0/1539	0.37	0/2073
38	M	0.17	0/1204	0.35	0/1612
39	MM	0.14	0/1779	0.30	0/2386
40	N	0.15	0/473	0.31	0/629
41	NN	0.15	0/1374	0.39	0/1842
42	O	0.12	0/750	0.26	0/1008
43	OO	0.15	0/1568	0.37	0/2106
44	P	0.16	0/897	0.33	0/1205
45	PP	0.13	0/1068	0.26	0/1438
46	Pp	0.05	0/19	0.18	0/23
47	Q	0.15	0/1041	0.26	0/1394
48	QQ	0.14	0/1757	0.32	0/2354
49	R	0.18	0/868	0.32	0/1168
50	S	0.16	0/871	0.31	0/1164
51	T	0.14	0/978	0.28	0/1301
52	U	0.16	0/778	0.37	0/1034
53	V	0.18	0/680	0.36	0/901
54	W	0.17	0/618	0.37	0/826
55	X	0.16	0/443	0.43	0/588
56	Y	0.14	0/423	0.31	0/562
57	Z	0.13	0/234	0.27	0/300
58	a	0.15	0/831	0.35	0/1097
59	b	0.15	0/701	0.34	0/934
60	c	0.16	1/37665 (0.0%)	0.27	0/58663
61	d	0.15	0/1623	0.37	0/2222
62	e	0.16	0/1714	0.42	0/2308
63	f	0.16	0/1665	0.41	0/2263
64	g	0.16	0/1622	0.38	0/2180
65	h	0.13	0/2097	0.34	0/2823
66	i	0.16	0/1591	0.42	2/2151 (0.1%)
67	j	0.14	0/1790	0.39	0/2393
68	k	0.16	0/1506	0.42	0/2028
69	l	0.14	0/1482	0.43	0/1980
70	m	0.16	0/1519	0.37	0/2035
71	n	0.20	0/792	0.54	2/1071 (0.2%)
72	o	0.13	0/1172	0.37	0/1580
73	p	0.14	0/1215	0.35	0/1638
74	q	0.18	0/901	0.44	0/1217
75	r	0.15	0/853	0.38	0/1145

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	s	0.14	0/1099	0.41	0/1473
77	t	0.31	0/971	0.60	1/1303 (0.1%)
78	u	0.15	0/1211	0.38	0/1628
79	v	0.13	0/1130	0.35	0/1517
80	w	0.16	0/810	0.41	0/1095
81	x	0.17	0/693	0.42	0/935
82	y	0.16	0/1038	0.37	0/1395
83	z	0.15	0/1139	0.36	0/1518
All	All	0.16	1/213278 (0.0%)	0.31	8/313142 (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
66	i	0	1
68	k	0	1
71	n	0	1
76	s	0	1
78	u	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	c	1575	G7M	O3'-P	5.07	1.61	1.56

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Bb	37	YYG	O3'-P-O5'	-12.44	85.33	104.00
14	Bb	37	YYG	OP2-P-O3'	8.02	132.06	108.00
77	t	73	LEU	N-CA-C	-6.39	105.38	113.43
14	Bb	37	YYG	P-O3'-C3'	-5.45	112.03	120.20
71	n	47	GLN	CA-C-N	5.15	131.38	121.54

There are no chirality outliers.

5 of 8 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
66	i	65	ARG	Peptide
68	k	64	VAL	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1073	0	1132	52	0
2	1	563	0	603	28	0
3	2	769	0	814	26	0
4	3	610	0	633	15	0
5	4	497	0	535	18	0
6	5	442	0	428	18	0
7	6	427	0	476	14	0
8	7	2436	0	2386	104	0
9	8	276	0	288	12	0
10	A	1555	0	1659	20	0
11	AA	68285	0	34370	1186	0
12	B	1222	0	1231	26	0
13	BB	2579	0	1304	41	0
14	Bb	1638	0	835	44	0
15	C	1441	0	1543	25	0
16	CC	3353	0	1695	60	0
17	Cc	1644	0	837	24	0
18	D	1423	0	1510	25	0
19	DD	1531	0	1571	67	0
20	Dd	298	0	149	2	0
21	E	1445	0	1487	38	0
22	EE	1914	0	1981	37	0
23	Ee	1196	0	1257	51	0
24	F	1276	0	1323	24	0
25	FF	3075	0	3142	66	0
26	G	770	0	780	11	0
27	GG	2748	0	2859	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	H	963	0	1015	16	0
29	HH	2375	0	2325	44	0
30	I	521	0	551	6	0
31	II	1230	0	1320	21	0
32	J	959	0	1023	11	0
33	JJ	1784	0	1862	23	0
34	K	993	0	1081	16	0
35	KK	1804	0	1877	35	0
36	L	1092	0	1155	25	0
37	LL	1518	0	1587	28	0
38	M	1173	0	1215	32	0
39	MM	1743	0	1785	20	0
40	N	462	0	491	3	0
41	NN	1353	0	1383	32	0
42	O	742	0	797	8	0
43	OO	1543	0	1608	35	0
44	P	883	0	918	13	0
45	PP	1053	0	1149	16	0
46	Pp	19	0	20	1	0
47	Q	1020	0	1090	11	0
48	QQ	1720	0	1779	43	0
49	R	850	0	880	15	0
50	S	861	0	918	20	0
51	T	969	0	1078	17	0
52	U	771	0	849	20	0
53	V	665	0	668	24	0
54	W	612	0	682	17	0
55	X	436	0	475	17	0
56	Y	417	0	455	9	0
57	Z	233	0	282	9	0
58	a	819	0	886	25	0
59	b	694	0	734	13	0
60	c	34236	0	17249	751	0
61	d	1583	0	1578	60	0
62	e	1689	0	1763	55	0
63	f	1635	0	1723	34	0
64	g	1601	0	1682	45	0
65	h	2056	0	2140	71	0
66	i	1572	0	1639	63	0
67	j	1766	0	1859	85	0
68	k	1481	0	1572	53	0
69	l	1457	0	1488	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	m	1494	0	1573	52	0
71	n	772	0	760	35	0
72	o	1146	0	1213	22	0
73	p	1192	0	1255	31	0
74	q	891	0	883	38	0
75	r	837	0	868	26	0
76	s	1080	0	1140	44	0
77	t	961	0	999	63	0
78	u	1192	0	1222	50	0
79	v	1112	0	1124	36	0
80	w	800	0	869	32	0
81	x	684	0	672	30	0
82	y	1021	0	1060	24	0
83	z	1121	0	1196	23	0
84	2	1	0	0	0	0
84	5	1	0	0	0	0
84	8	1	0	0	0	0
84	S	1	0	0	0	0
84	V	1	0	0	0	0
84	Y	1	0	0	0	0
84	a	1	0	0	0	0
84	b	1	0	0	0	0
85	AA	191	0	0	0	0
85	B	1	0	0	0	0
85	BB	4	0	0	0	0
85	Bb	1	0	0	0	0
85	CC	4	0	0	0	0
85	Cc	1	0	0	0	0
85	Dd	1	0	0	0	0
85	FF	1	0	0	0	0
85	H	1	0	0	0	0
85	JJ	1	0	0	0	0
85	MM	1	0	0	0	0
85	QQ	2	0	0	0	0
85	V	1	0	0	0	0
85	a	1	0	0	0	0
85	c	46	0	0	0	0
85	q	1	0	0	0	0
86	AA	11	0	0	0	0
86	EE	1	0	0	0	0
86	MM	1	0	0	0	0
86	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	S	1	0	0	0	0
86	a	1	0	0	0	0
86	c	4	0	0	0	0
86	q	1	0	0	0	0
87	AA	30	0	57	4	0
87	c	10	0	19	2	0
88	2	2	0	0	0	0
88	A	3	0	0	1	0
88	AA	804	0	0	38	0
88	BB	12	0	0	0	0
88	Bb	5	0	0	0	0
88	CC	18	0	0	0	0
88	Cc	5	0	0	0	0
88	D	4	0	0	0	0
88	Dd	4	0	0	0	0
88	EE	6	0	0	0	0
88	F	4	0	0	0	0
88	FF	5	0	0	1	0
88	GG	3	0	0	0	0
88	H	3	0	0	0	0
88	J	2	0	0	0	0
88	LL	2	0	0	0	0
88	M	3	0	0	0	0
88	MM	2	0	0	0	0
88	N	1	0	0	0	0
88	OO	1	0	0	0	0
88	P	1	0	0	0	0
88	Q	3	0	0	0	0
88	QQ	6	0	0	0	0
88	S	2	0	0	0	0
88	V	3	0	0	0	0
88	a	4	0	0	0	0
88	c	170	0	0	9	0
88	f	1	0	0	0	0
88	o	1	0	0	0	0
88	p	1	0	0	0	0
88	q	2	0	0	0	0
88	z	1	0	0	0	0
All	All	201553	0	148369	3794	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 3794 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AA:1018:G:OP1	11:AA:1035:G:N2	1.74	1.19
11:AA:403:C:O3'	88:AA:3703:HOH:O	1.56	1.18
11:AA:1451:C:OP1	88:AA:3702:HOH:O	1.56	1.18
11:AA:2250:G:H1	11:AA:2266:U:H3	1.14	0.95
11:AA:1257:C:H42	11:AA:1261:G:H22	1.13	0.94

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
2	1	68/108 (63%)	60 (88%)	8 (12%)	0	100	100
3	2	95/119 (80%)	87 (92%)	8 (8%)	0	100	100
4	3	79/82 (96%)	75 (95%)	4 (5%)	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%)	49 (96%)	2 (4%)	0	100	100
8	7	316/319 (99%)	293 (93%)	23 (7%)	0	100	100
9	8	32/152 (21%)	26 (81%)	6 (19%)	0	100	100
10	A	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
12	B	152/184 (83%)	150 (99%)	2 (1%)	0	100	100
15	C	183/186 (98%)	181 (99%)	2 (1%)	0	100	100
18	D	174/189 (92%)	170 (98%)	4 (2%)	0	100	100
19	DD	195/312 (62%)	190 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	E	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
22	EE	250/254 (98%)	248 (99%)	2 (1%)	0	100	100
23	Ee	156/165 (94%)	148 (95%)	8 (5%)	0	100	100
24	F	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
25	FF	384/387 (99%)	373 (97%)	11 (3%)	0	100	100
26	G	95/121 (78%)	95 (100%)	0	0	100	100
27	GG	359/362 (99%)	348 (97%)	11 (3%)	0	100	100
28	H	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
29	HH	294/297 (99%)	289 (98%)	5 (2%)	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%)	115 (98%)	3 (2%)	0	100	100
33	JJ	220/244 (90%)	217 (99%)	3 (1%)	0	100	100
34	K	124/127 (98%)	124 (100%)	0	0	100	100
35	KK	231/256 (90%)	228 (99%)	3 (1%)	0	100	100
36	L	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
37	LL	189/191 (99%)	183 (97%)	6 (3%)	0	100	100
38	M	146/149 (98%)	140 (96%)	5 (3%)	1 (1%)	18	39
39	MM	213/221 (96%)	208 (98%)	5 (2%)	0	100	100
40	N	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
41	NN	167/174 (96%)	160 (96%)	7 (4%)	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%)	24	46
44	P	107/113 (95%)	102 (95%)	5 (5%)	0	100	100
45	PP	134/138 (97%)	132 (98%)	2 (2%)	0	100	100
47	Q	125/130 (96%)	125 (100%)	0	0	100	100
48	QQ	201/204 (98%)	194 (96%)	7 (4%)	0	100	100
49	R	104/107 (97%)	104 (100%)	0	0	100	100
50	S	107/121 (88%)	107 (100%)	0	0	100	100
51	T	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
52	U	97/100 (97%)	90 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	V	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
54	W	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
55	X	48/51 (94%)	44 (92%)	4 (8%)	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%)	97 (97%)	3 (3%)	0	100	100
59	b	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
61	d	204/252 (81%)	190 (93%)	14 (7%)	0	100	100
62	e	210/255 (82%)	199 (95%)	11 (5%)	0	100	100
63	f	215/254 (85%)	206 (96%)	9 (4%)	0	100	100
64	g	204/240 (85%)	196 (96%)	8 (4%)	0	100	100
65	h	256/261 (98%)	248 (97%)	8 (3%)	0	100	100
66	i	195/225 (87%)	187 (96%)	8 (4%)	0	100	100
67	j	217/236 (92%)	208 (96%)	9 (4%)	0	100	100
68	k	182/190 (96%)	173 (95%)	9 (5%)	0	100	100
69	l	180/200 (90%)	171 (95%)	9 (5%)	0	100	100
70	m	183/197 (93%)	178 (97%)	5 (3%)	0	100	100
71	n	89/105 (85%)	83 (93%)	4 (4%)	2 (2%)	5	13
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%)	98 (98%)	2 (2%)	0	100	100
76	s	135/143 (94%)	126 (93%)	9 (7%)	0	100	100
77	t	119/136 (88%)	102 (86%)	14 (12%)	3 (2%)	4	10
78	u	143/146 (98%)	132 (92%)	11 (8%)	0	100	100
79	v	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
80	w	98/121 (81%)	97 (99%)	1 (1%)	0	100	100
81	x	85/87 (98%)	80 (94%)	5 (6%)	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
All	All	10968/12206 (90%)	10575 (96%)	386 (4%)	7 (0%)	49	72

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
77	t	88	VAL
43	OO	63	VAL
71	n	48	SER
71	n	49	LEU
77	t	72	LYS

### 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%)	112 (100%)	0	100	100
2	1	61/89 (68%)	61 (100%)	0	100	100
3	2	83/101 (82%)	83 (100%)	0	100	100
4	3	70/71 (99%)	70 (100%)	0	100	100
5	4	56/60 (93%)	56 (100%)	0	100	100
6	5	47/49 (96%)	47 (100%)	0	100	100
7	6	46/54 (85%)	46 (100%)	0	100	100
8	7	259/262 (99%)	259 (100%)	0	100	100
9	8	30/135 (22%)	30 (100%)	0	100	100
10	A	160/162 (99%)	160 (100%)	0	100	100
12	B	125/146 (86%)	125 (100%)	0	100	100
15	C	150/151 (99%)	150 (100%)	0	100	100
18	D	143/154 (93%)	143 (100%)	0	100	100
19	DD	167/254 (66%)	167 (100%)	0	100	100
21	E	156/156 (100%)	156 (100%)	0	100	100
22	EE	193/196 (98%)	193 (100%)	0	100	100
23	Ee	129/136 (95%)	129 (100%)	0	100	100
24	F	136/137 (99%)	136 (100%)	0	100	100
25	FF	320/323 (99%)	319 (100%)	1 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	G	84/107 (78%)	84 (100%)	0	100	100
27	GG	288/289 (100%)	287 (100%)	1 (0%)	86	93
28	H	101/101 (100%)	101 (100%)	0	100	100
29	HH	244/245 (100%)	244 (100%)	0	100	100
30	I	55/129 (43%)	55 (100%)	0	100	100
31	II	133/153 (87%)	133 (100%)	0	100	100
32	J	104/118 (88%)	104 (100%)	0	100	100
33	JJ	186/205 (91%)	186 (100%)	0	100	100
34	K	109/110 (99%)	109 (100%)	0	100	100
35	KK	187/208 (90%)	187 (100%)	0	100	100
36	L	115/116 (99%)	115 (100%)	0	100	100
37	LL	171/171 (100%)	170 (99%)	1 (1%)	78	90
38	M	118/119 (99%)	118 (100%)	0	100	100
39	MM	184/187 (98%)	184 (100%)	0	100	100
40	N	46/47 (98%)	46 (100%)	0	100	100
41	NN	147/150 (98%)	147 (100%)	0	100	100
42	O	81/88 (92%)	81 (100%)	0	100	100
43	OO	154/159 (97%)	154 (100%)	0	100	100
44	P	94/97 (97%)	94 (100%)	0	100	100
45	PP	107/109 (98%)	107 (100%)	0	100	100
46	Pp	2/2 (100%)	2 (100%)	0	100	100
47	Q	109/111 (98%)	109 (100%)	0	100	100
48	QQ	175/176 (99%)	175 (100%)	0	100	100
49	R	90/91 (99%)	90 (100%)	0	100	100
50	S	94/103 (91%)	94 (100%)	0	100	100
51	T	104/105 (99%)	104 (100%)	0	100	100
52	U	81/82 (99%)	81 (100%)	0	100	100
53	V	69/71 (97%)	69 (100%)	0	100	100
54	W	68/69 (99%)	68 (100%)	0	100	100
55	X	45/46 (98%)	45 (100%)	0	100	100
56	Y	47/116 (40%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	Z	23/23 (100%)	23 (100%)	0	100	100
58	a	87/91 (96%)	87 (100%)	0	100	100
59	b	71/72 (99%)	71 (100%)	0	100	100
61	d	165/210 (79%)	165 (100%)	0	100	100
62	e	189/224 (84%)	189 (100%)	0	100	100
63	f	176/205 (86%)	176 (100%)	0	100	100
64	g	167/195 (86%)	167 (100%)	0	100	100
65	h	220/222 (99%)	220 (100%)	0	100	100
66	i	172/191 (90%)	172 (100%)	0	100	100
67	j	188/201 (94%)	188 (100%)	0	100	100
68	k	165/170 (97%)	165 (100%)	0	100	100
69	l	146/161 (91%)	146 (100%)	0	100	100
70	m	158/166 (95%)	158 (100%)	0	100	100
71	n	84/98 (86%)	84 (100%)	0	100	100
72	o	127/137 (93%)	127 (100%)	0	100	100
73	p	127/128 (99%)	127 (100%)	0	100	100
74	q	81/105 (77%)	81 (100%)	0	100	100
75	r	89/118 (75%)	89 (100%)	0	100	100
76	s	114/119 (96%)	114 (100%)	0	100	100
77	t	105/124 (85%)	93 (89%)	12 (11%)	5	13
78	u	128/129 (99%)	128 (100%)	0	100	100
79	v	115/116 (99%)	115 (100%)	0	100	100
80	w	94/114 (82%)	94 (100%)	0	100	100
81	x	74/74 (100%)	73 (99%)	1 (1%)	59	80
82	y	110/111 (99%)	110 (100%)	0	100	100
83	z	119/120 (99%)	119 (100%)	0	100	100
All	All	9329/10253 (91%)	9313 (100%)	16 (0%)	85	95

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
77	t	91	LEU
77	t	88	VAL

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Mol	Chain	Res	Type
77	t	79	GLU
77	t	85	VAL
77	t	78	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
51	T	113	GLN
66	i	95	ASN
58	a	38	GLN
64	g	111	ASN
69	l	52	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AA	3185/3396 (93%)	474 (14%)	16 (0%)
13	BB	120/121 (99%)	10 (8%)	1 (0%)
14	Bb	75/76 (98%)	29 (38%)	0
16	CC	157/158 (99%)	22 (14%)	0
17	Cc	76/77 (98%)	14 (18%)	0
20	Dd	13/39 (33%)	1 (7%)	0
60	c	1594/1800 (88%)	279 (17%)	0
All	All	5220/5667 (92%)	829 (15%)	17 (0%)

5 of 829 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 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	AA	3121	U
13	BB	72	A
11	AA	2101	C

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Mol	Chain	Res	Type
11	AA	2253	G
11	AA	2487	U

## 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	A2M	AA	2946	85,11	22,25,26	3.23	10 (45%)	30,36,39	2.97	11 (36%)
60	OMC	c	1639	85,60	19,22,23	0.53	0	25,31,34	0.61	0
11	A2M	AA	2220	11	22,25,26	3.20	10 (45%)	30,36,39	2.89	10 (33%)
11	OMG	AA	867	86,11	23,26,27	0.48	0	32,38,41	0.51	0
11	UR3	AA	2634	11	19,22,23	2.89	7 (36%)	26,32,35	1.66	4 (15%)
11	OMC	AA	650	85,11	19,22,23	0.55	0	25,31,34	0.68	0
11	A2M	AA	1449	85,11	22,25,26	3.21	10 (45%)	30,36,39	2.92	10 (33%)
11	OMG	AA	2619	11	23,26,27	0.47	0	32,38,41	0.48	0
11	5MC	AA	2870	86,11	19,22,23	0.65	0	26,32,35	0.59	0
60	A2M	c	619	85,60	22,25,26	3.24	10 (45%)	30,36,39	2.97	11 (36%)
11	OMU	AA	2421	11	19,22,23	3.05	8 (42%)	25,31,34	1.83	5 (20%)
60	MA6	c	1781	60	23,26,27	1.41	4 (17%)	33,38,41	3.21	12 (36%)
11	5MC	AA	2278	85,11	19,22,23	0.54	0	26,32,35	0.66	0
60	A2M	c	541	60	22,25,26	3.21	9 (40%)	30,36,39	2.94	10 (33%)
11	OMU	AA	2729	11	19,22,23	3.03	8 (42%)	25,31,34	1.78	5 (20%)
60	OMG	c	1126	60	23,26,27	0.49	0	32,38,41	0.54	0
60	OMC	c	414	60	19,22,23	0.53	0	25,31,34	0.69	0
11	OMG	AA	2922	11	23,26,27	0.49	0	32,38,41	0.47	0
11	OMU	AA	2921	11	19,22,23	3.04	8 (42%)	25,31,34	1.79	5 (20%)
11	1MA	AA	2142	85,11	21,25,26	0.48	0	30,37,40	0.79	1 (3%)
60	OMG	c	1428	85,60	23,26,27	0.47	0	32,38,41	0.46	0
11	A2M	AA	2256	11	22,25,26	3.20	10 (45%)	30,36,39	3.04	12 (40%)
11	OMC	AA	2959	11	19,22,23	0.55	0	25,31,34	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	OMG	c	1572	60	23,26,27	0.51	0	32,38,41	0.52	0
60	OMC	c	1007	60	19,22,23	0.51	0	25,31,34	0.66	0
11	OMC	AA	663	11	19,22,23	0.55	0	25,31,34	0.73	0
60	B8N	c	1191	60	25,29,30	3.37	8 (32%)	28,42,45	2.07	9 (32%)
11	A2M	AA	1133	85,11	22,25,26	3.23	10 (45%)	30,36,39	2.98	11 (36%)
11	A2M	AA	2281	11	22,25,26	3.21	10 (45%)	30,36,39	3.09	14 (46%)
11	OMU	AA	2417	11	19,22,23	3.05	8 (42%)	25,31,34	1.80	5 (20%)
11	A2M	AA	876	11	22,25,26	3.21	10 (45%)	30,36,39	2.89	10 (33%)
14	YYG	Bb	37	14	38,42,43	2.29	11 (28%)	45,62,65	2.18	12 (26%)
60	OMU	c	1269	60	19,22,23	3.08	8 (42%)	25,31,34	1.84	5 (20%)
11	A2M	AA	2640	11	22,25,26	3.23	9 (40%)	30,36,39	2.91	10 (33%)
11	OMG	AA	805	11	23,26,27	0.47	0	32,38,41	0.53	0
11	A2M	AA	2280	11	22,25,26	3.21	9 (40%)	30,36,39	2.97	10 (33%)
11	A2M	AA	649	11	22,25,26	3.21	10 (45%)	30,36,39	2.91	10 (33%)
11	A2M	AA	807	11	22,25,26	3.23	10 (45%)	30,36,39	2.95	11 (36%)
11	OMG	AA	2793	11	23,26,27	0.49	0	32,38,41	0.56	0
11	OMC	AA	2948	11	19,22,23	0.55	0	25,31,34	0.92	2 (8%)
60	MA6	c	1782	60	23,26,27	1.40	4 (17%)	33,38,41	3.27	12 (36%)
11	OMG	AA	1450	11	23,26,27	0.48	0	32,38,41	0.47	0
11	OMG	AA	2791	11	23,26,27	0.48	0	32,38,41	0.47	0
60	OMG	c	1271	60	23,26,27	0.46	0	32,38,41	0.46	0
60	4AC	c	1280	60	21,24,25	3.52	10 (47%)	28,34,37	1.79	6 (21%)
60	OMU	c	578	60	19,22,23	3.10	8 (42%)	25,31,34	1.79	5 (20%)
60	A2M	c	436	60	22,25,26	3.23	9 (40%)	30,36,39	2.92	11 (36%)
11	OMC	AA	1437	85,11	19,22,23	0.57	0	25,31,34	1.10	2 (8%)
60	A2M	c	100	85,60	22,25,26	3.23	9 (40%)	30,36,39	2.96	11 (36%)
11	OMG	AA	908	11	23,26,27	0.51	0	32,38,41	0.48	0
11	OMG	AA	2288	11	23,26,27	0.48	0	32,38,41	0.45	0
60	OMG	c	562	60	23,26,27	0.45	0	32,38,41	0.47	0
11	1MA	AA	645	85,11	21,25,26	0.49	0	30,37,40	0.75	1 (3%)
60	4AC	c	1773	60	21,24,25	3.44	10 (47%)	28,34,37	1.69	5 (17%)
11	OMU	AA	898	11	19,22,23	3.04	8 (42%)	25,31,34	1.76	5 (20%)
11	OMC	AA	2197	86,11	19,22,23	0.54	0	25,31,34	0.63	0
60	G7M	c	1575	60	23,26,27	2.65	8 (34%)	34,39,42	2.37	10 (29%)
11	OMU	AA	2724	11	19,22,23	3.05	8 (42%)	25,31,34	1.80	5 (20%)
11	OMC	AA	2337	11	19,22,23	0.54	0	25,31,34	0.70	0
60	A2M	c	420	60	22,25,26	3.21	9 (40%)	30,36,39	2.95	12 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	A2M	AA	817	85,11	22,25,26	3.22	10 (45%)	30,36,39	2.92	11 (36%)
60	A2M	c	28	60	22,25,26	3.22	10 (45%)	30,36,39	2.93	10 (33%)
60	A2M	c	974	60	22,25,26	3.23	10 (45%)	30,36,39	2.90	10 (33%)
11	OMU	AA	1888	11	19,22,23	3.05	8 (42%)	25,31,34	1.86	5 (20%)
60	A2M	c	796	60	22,25,26	3.26	10 (45%)	30,36,39	2.98	11 (36%)
11	OMU	AA	2347	11	19,22,23	3.07	8 (42%)	25,31,34	1.80	5 (20%)
11	OMG	AA	2815	11	23,26,27	0.47	0	32,38,41	0.47	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	A2M	AA	2946	85,11	-	0/9/27/28	0/3/3/3
60	OMC	c	1639	85,60	-	0/9/27/28	0/2/2/2
11	A2M	AA	2220	11	-	1/9/27/28	0/3/3/3
11	OMG	AA	867	86,11	-	2/9/27/28	0/3/3/3
11	UR3	AA	2634	11	-	0/7/25/26	0/2/2/2
11	OMC	AA	650	85,11	-	0/9/27/28	0/2/2/2
11	A2M	AA	1449	85,11	-	0/9/27/28	0/3/3/3
11	OMG	AA	2619	11	-	1/9/27/28	0/3/3/3
11	5MC	AA	2870	86,11	-	4/7/25/26	0/2/2/2
60	A2M	c	619	85,60	-	2/9/27/28	0/3/3/3
11	OMU	AA	2421	11	-	0/9/27/28	0/2/2/2
60	MA6	c	1781	60	-	0/11/29/30	0/3/3/3
11	5MC	AA	2278	85,11	-	0/7/25/26	0/2/2/2
60	A2M	c	541	60	-	4/9/27/28	0/3/3/3
11	OMU	AA	2729	11	-	1/9/27/28	0/2/2/2
60	OMG	c	1126	60	-	0/9/27/28	0/3/3/3
60	OMC	c	414	60	-	2/9/27/28	0/2/2/2
11	OMG	AA	2922	11	-	2/9/27/28	0/3/3/3
11	OMU	AA	2921	11	-	0/9/27/28	0/2/2/2
11	1MA	AA	2142	85,11	-	0/7/25/26	0/3/3/3
60	OMG	c	1428	85,60	-	2/9/27/28	0/3/3/3
11	A2M	AA	2256	11	-	3/9/27/28	0/3/3/3
11	OMC	AA	2959	11	-	0/9/27/28	0/2/2/2
60	OMG	c	1572	60	-	3/9/27/28	0/3/3/3
60	OMC	c	1007	60	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMC	AA	663	11	-	1/9/27/28	0/2/2/2
60	B8N	c	1191	60	-	5/16/34/35	0/2/2/2
11	A2M	AA	1133	85,11	-	0/9/27/28	0/3/3/3
11	A2M	AA	2281	11	-	4/9/27/28	0/3/3/3
11	OMU	AA	2417	11	-	1/9/27/28	0/2/2/2
11	A2M	AA	876	11	-	0/9/27/28	0/3/3/3
14	YYG	Bb	37	14	-	12/24/42/43	0/4/4/4
60	OMU	c	1269	60	-	0/9/27/28	0/2/2/2
11	A2M	AA	2640	11	-	1/9/27/28	0/3/3/3
11	OMG	AA	805	11	-	0/9/27/28	0/3/3/3
11	A2M	AA	2280	11	-	2/9/27/28	0/3/3/3
11	A2M	AA	649	11	-	1/9/27/28	0/3/3/3
11	A2M	AA	807	11	-	3/9/27/28	0/3/3/3
11	OMG	AA	2793	11	-	0/9/27/28	0/3/3/3
11	OMC	AA	2948	11	-	1/9/27/28	0/2/2/2
60	MA6	c	1782	60	-	2/11/29/30	0/3/3/3
11	OMG	AA	1450	11	-	2/9/27/28	0/3/3/3
11	OMG	AA	2791	11	-	0/9/27/28	0/3/3/3
60	OMG	c	1271	60	-	1/9/27/28	0/3/3/3
60	4AC	c	1280	60	-	5/11/29/30	0/2/2/2
60	OMU	c	578	60	-	7/9/27/28	0/2/2/2
60	A2M	c	436	60	-	0/9/27/28	0/3/3/3
11	OMC	AA	1437	85,11	-	3/9/27/28	0/2/2/2
60	A2M	c	100	85,60	-	2/9/27/28	0/3/3/3
11	OMG	AA	908	11	-	1/9/27/28	0/3/3/3
11	OMG	AA	2288	11	-	0/9/27/28	0/3/3/3
60	OMG	c	562	60	-	0/9/27/28	0/3/3/3
11	1MA	AA	645	85,11	-	2/7/25/26	0/3/3/3
60	4AC	c	1773	60	-	2/11/29/30	0/2/2/2
11	OMU	AA	898	11	-	1/9/27/28	0/2/2/2
11	OMC	AA	2197	86,11	-	4/9/27/28	0/2/2/2
60	G7M	c	1575	60	-	2/7/25/26	0/3/3/3
11	OMU	AA	2724	11	-	1/9/27/28	0/2/2/2
11	OMC	AA	2337	11	-	0/9/27/28	0/2/2/2
60	A2M	c	420	60	-	1/9/27/28	0/3/3/3
11	A2M	AA	817	85,11	-	1/9/27/28	0/3/3/3
60	A2M	c	28	60	-	1/9/27/28	0/3/3/3
60	A2M	c	974	60	-	0/9/27/28	0/3/3/3
11	OMU	AA	1888	11	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	A2M	c	796	60	-	0/9/27/28	0/3/3/3
11	OMU	AA	2347	11	-	0/9/27/28	0/2/2/2
11	OMG	AA	2815	11	-	0/9/27/28	0/3/3/3

The worst 5 of 336 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AA	807	A2M	C3'-C4'	-9.06	1.30	1.53
11	AA	2946	A2M	C3'-C4'	-8.97	1.30	1.53
60	c	619	A2M	C3'-C4'	-8.96	1.30	1.53
11	AA	1133	A2M	C3'-C4'	-8.95	1.30	1.53
60	c	796	A2M	C3'-C4'	-8.95	1.30	1.53

The worst 5 of 342 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	c	1782	MA6	N1-C6-N6	-11.99	102.25	116.86
60	c	1781	MA6	N1-C6-N6	-11.65	102.66	116.86
60	c	1782	MA6	C5-C6-N6	8.06	138.08	125.33
60	c	1781	MA6	C5-C6-N6	7.79	137.67	125.33
14	Bb	37	YYG	C5-C4-N3	-7.78	117.68	123.99

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AA	649	A2M	C1'-C2'-O2'-CM'
11	AA	663	OMC	C1'-C2'-O2'-CM2
11	AA	898	OMU	C1'-C2'-O2'-CM2
11	AA	1437	OMC	C1'-C2'-O2'-CM2
11	AA	1450	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

40 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AA	2946	A2M	2	0
60	c	1639	OMC	1	0
11	AA	2220	A2M	3	0
11	AA	650	OMC	2	0
11	AA	1449	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AA	2619	OMG	1	0
11	AA	2870	5MC	1	0
60	c	1781	MA6	2	0
60	c	541	A2M	1	0
11	AA	2729	OMU	1	0
60	c	414	OMC	1	0
60	c	1428	OMG	1	0
11	AA	2256	A2M	1	0
11	AA	2959	OMC	1	0
11	AA	663	OMC	1	0
11	AA	1133	A2M	1	0
11	AA	2417	OMU	1	0
14	Bb	37	YYG	10	0
11	AA	2640	A2M	1	0
11	AA	649	A2M	3	0
11	AA	2793	OMG	3	0
11	AA	2948	OMC	2	0
60	c	1782	MA6	1	0
60	c	1271	OMG	1	0
60	c	1280	4AC	4	0
60	c	578	OMU	1	0
60	c	436	A2M	1	0
11	AA	1437	OMC	2	0
60	c	562	OMG	1	0
60	c	1773	4AC	3	0
11	AA	898	OMU	2	0
60	c	1575	G7M	3	0
11	AA	2724	OMU	3	0
60	c	420	A2M	1	0
11	AA	817	A2M	1	0
60	c	28	A2M	2	0
60	c	974	A2M	1	0
60	c	796	A2M	1	0
11	AA	2347	OMU	1	0
11	AA	2815	OMG	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 291 ligands modelled in this entry, 287 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	c	1951	-	9,9,9	0.34	0	8,8,8	0.86	0
87	SPD	AA	3604	-	9,9,9	0.32	0	8,8,8	0.78	0
87	SPD	AA	3605	-	9,9,9	0.32	0	8,8,8	0.88	0
87	SPD	AA	3603	-	9,9,9	0.33	0	8,8,8	0.84	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	c	1951	-	-	3/7/7/7	-
87	SPD	AA	3604	-	-	4/7/7/7	-
87	SPD	AA	3605	-	-	2/7/7/7	-
87	SPD	AA	3603	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	AA	3605	SPD	C8-C7-N6-C5
87	c	1951	SPD	N6-C7-C8-C9
87	AA	3604	SPD	C3-C4-C5-N6
87	AA	3604	SPD	C2-C3-C4-C5
87	AA	3604	SPD	C7-C8-C9-N10

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	c	1951	SPD	2	0
87	AA	3604	SPD	3	0
87	AA	3603	SPD	1	0

## 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.

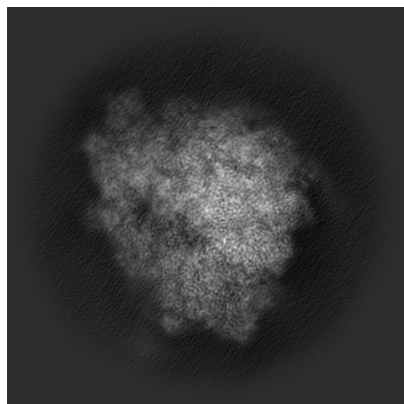
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16591. These allow visual inspection of the internal detail of the map and identification of artifacts.

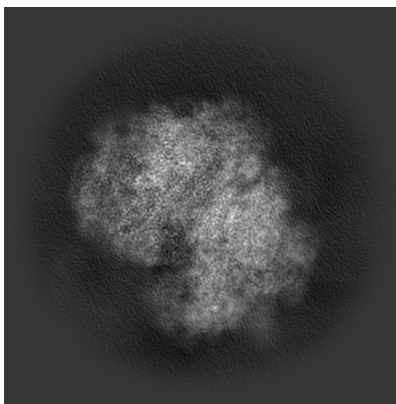
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

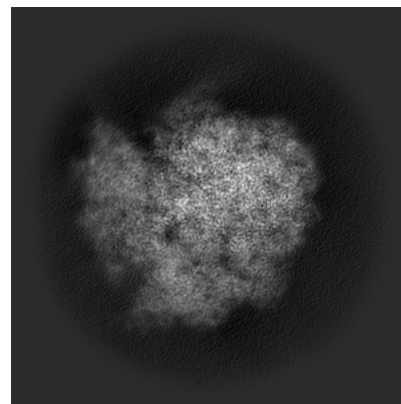
#### 6.1.1 Primary map



X

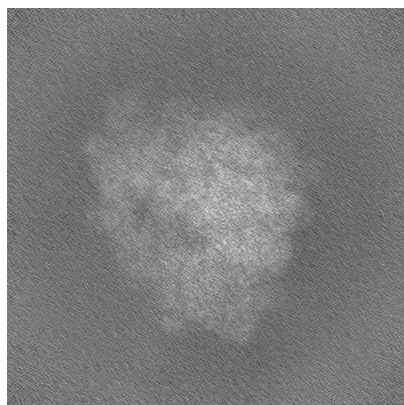


Y

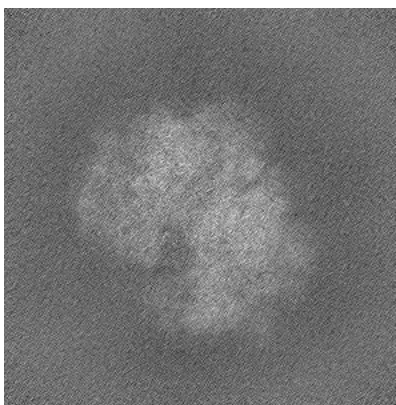


Z

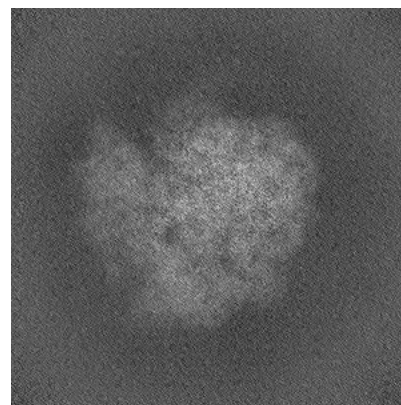
#### 6.1.2 Raw map



X



Y

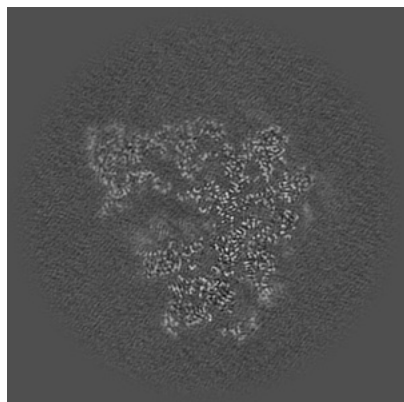


Z

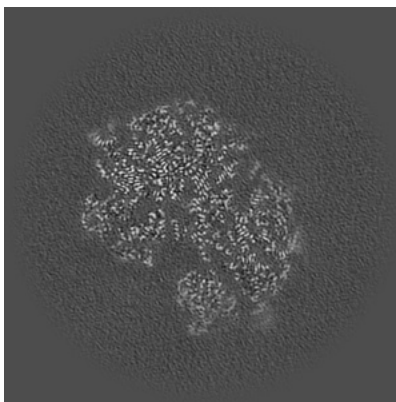
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

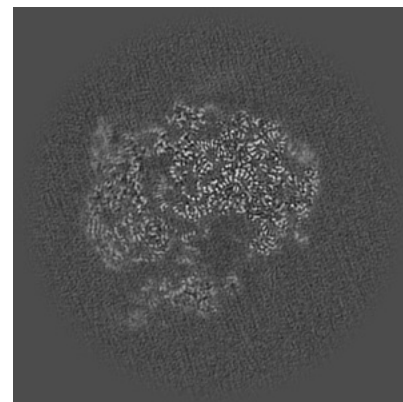
### 6.2.1 Primary map



X Index: 288

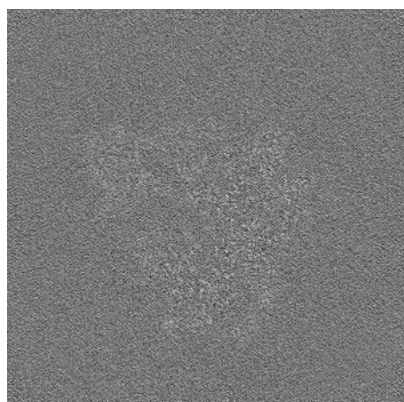


Y Index: 288

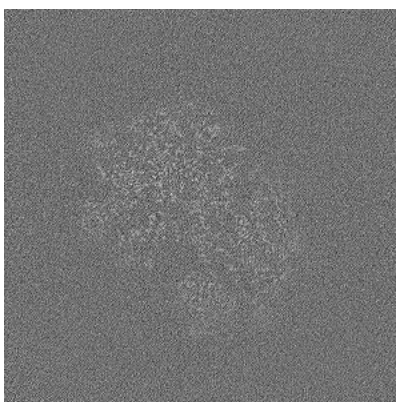


Z Index: 288

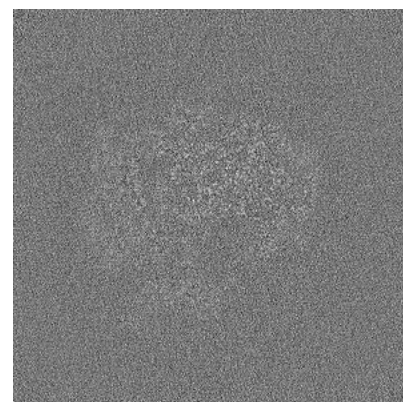
### 6.2.2 Raw map



X Index: 288



Y Index: 288

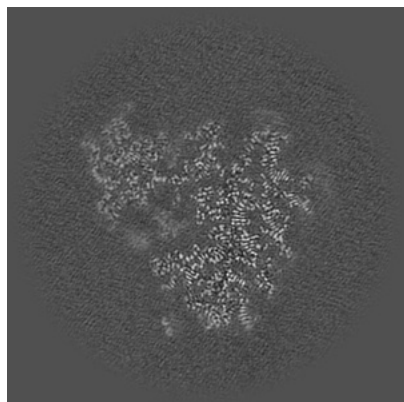


Z Index: 288

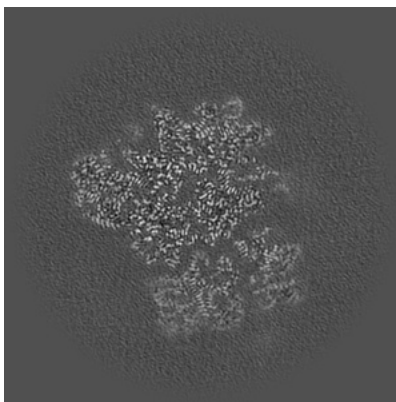
The images above show central slices of the map in three orthogonal directions.

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

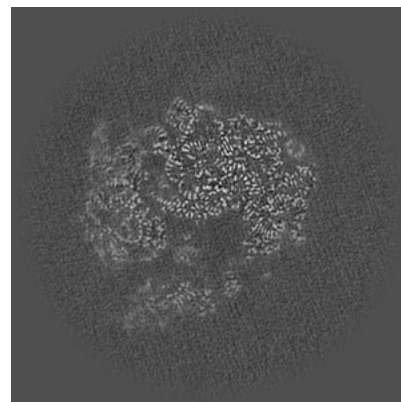
### 6.3.1 Primary map



X Index: 273

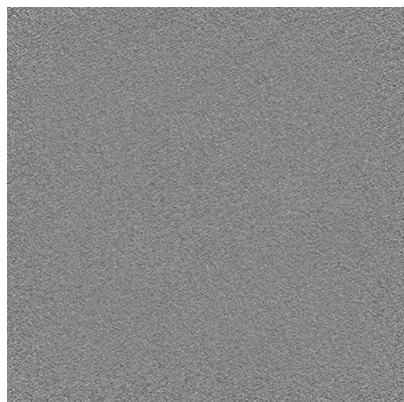


Y Index: 321

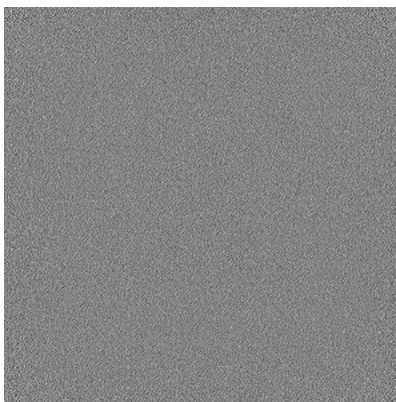


Z Index: 284

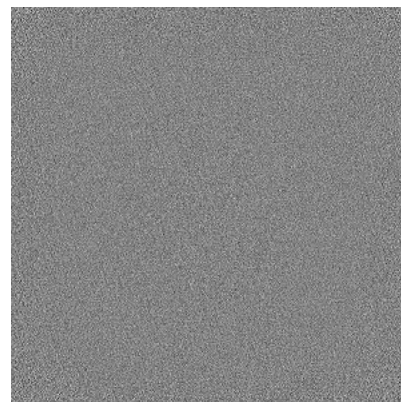
### 6.3.2 Raw map



X Index: 0



Y Index: 0

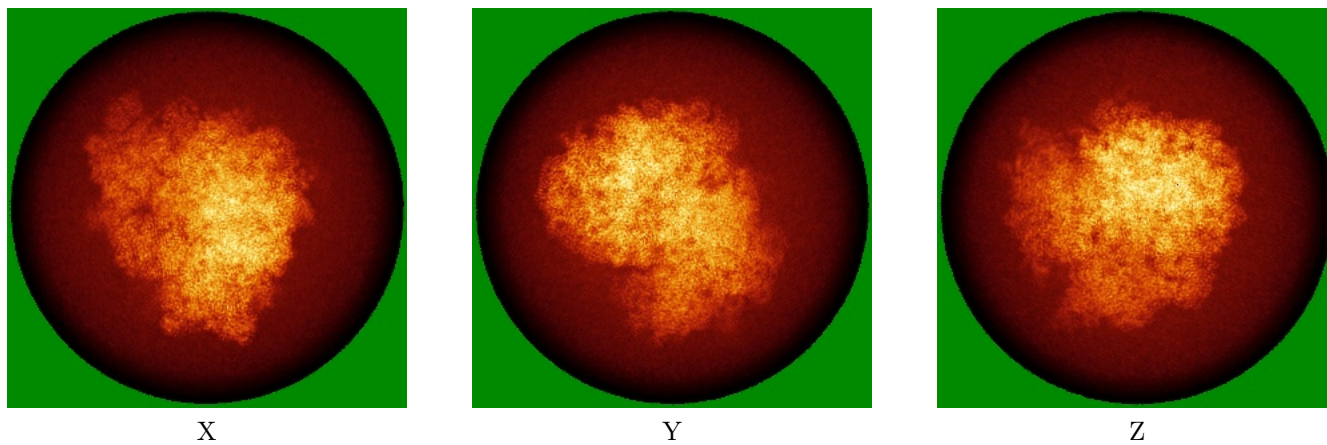


Z Index: 0

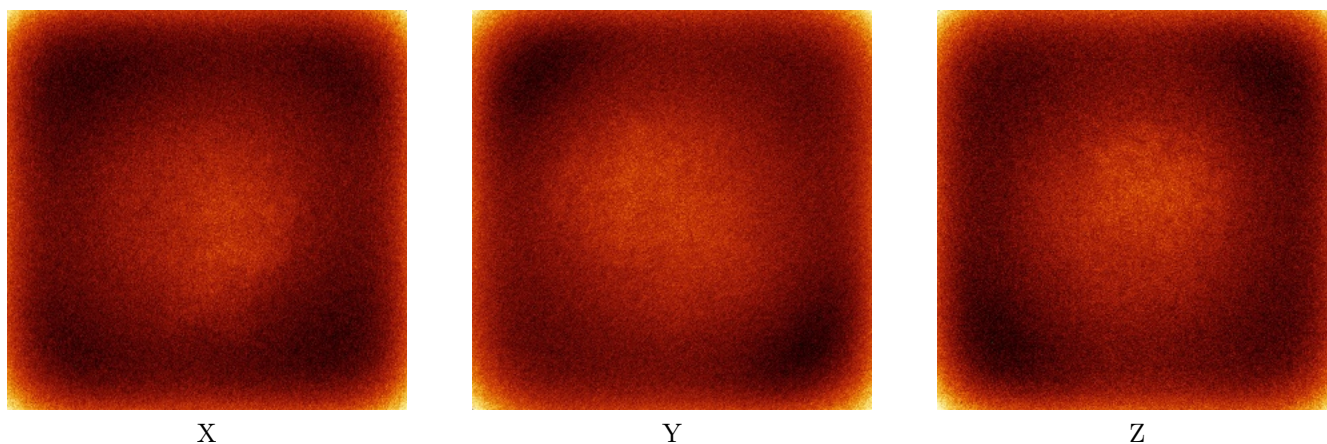
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

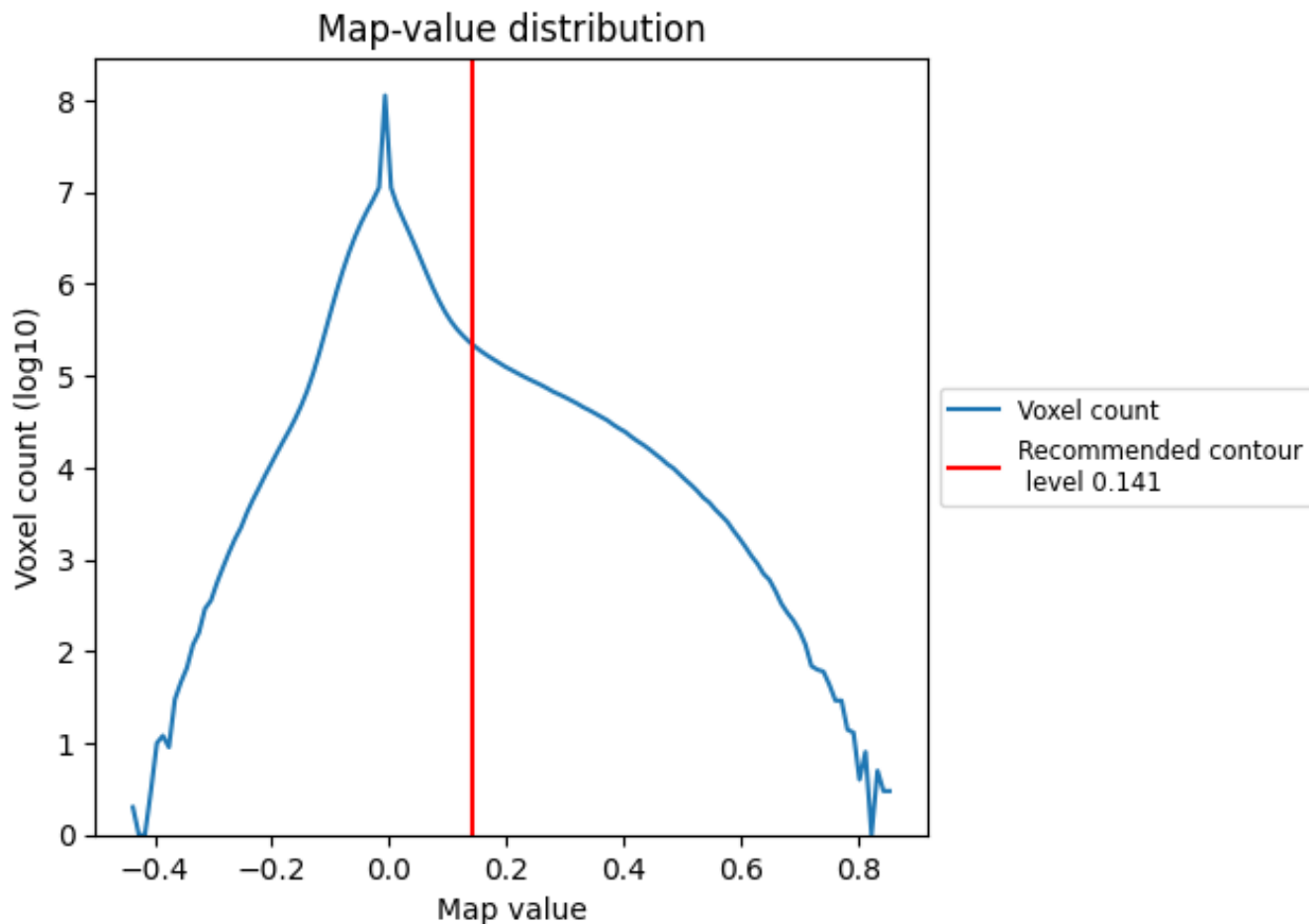
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

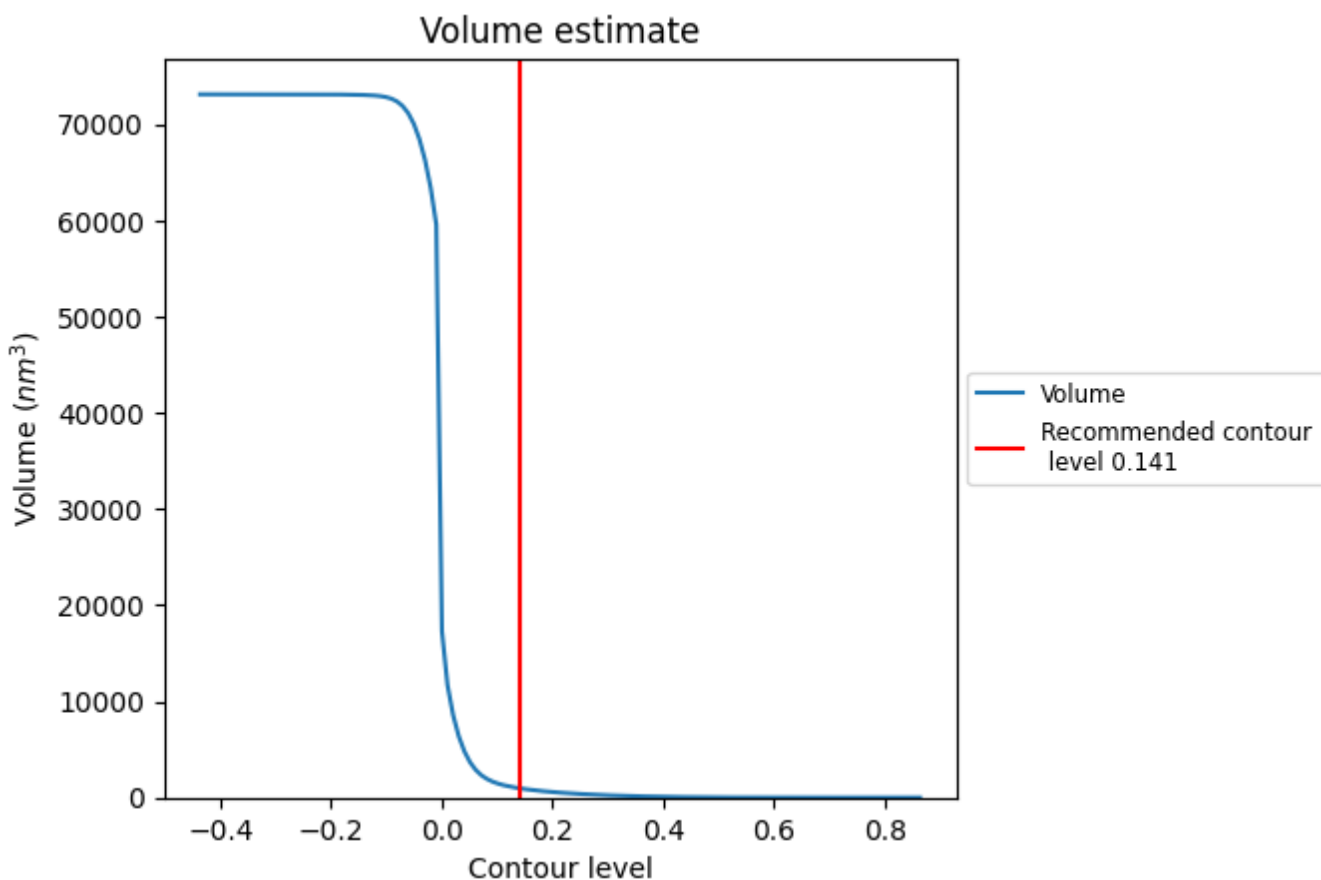
This section contains the results of statistical analysis of the map.

### 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.

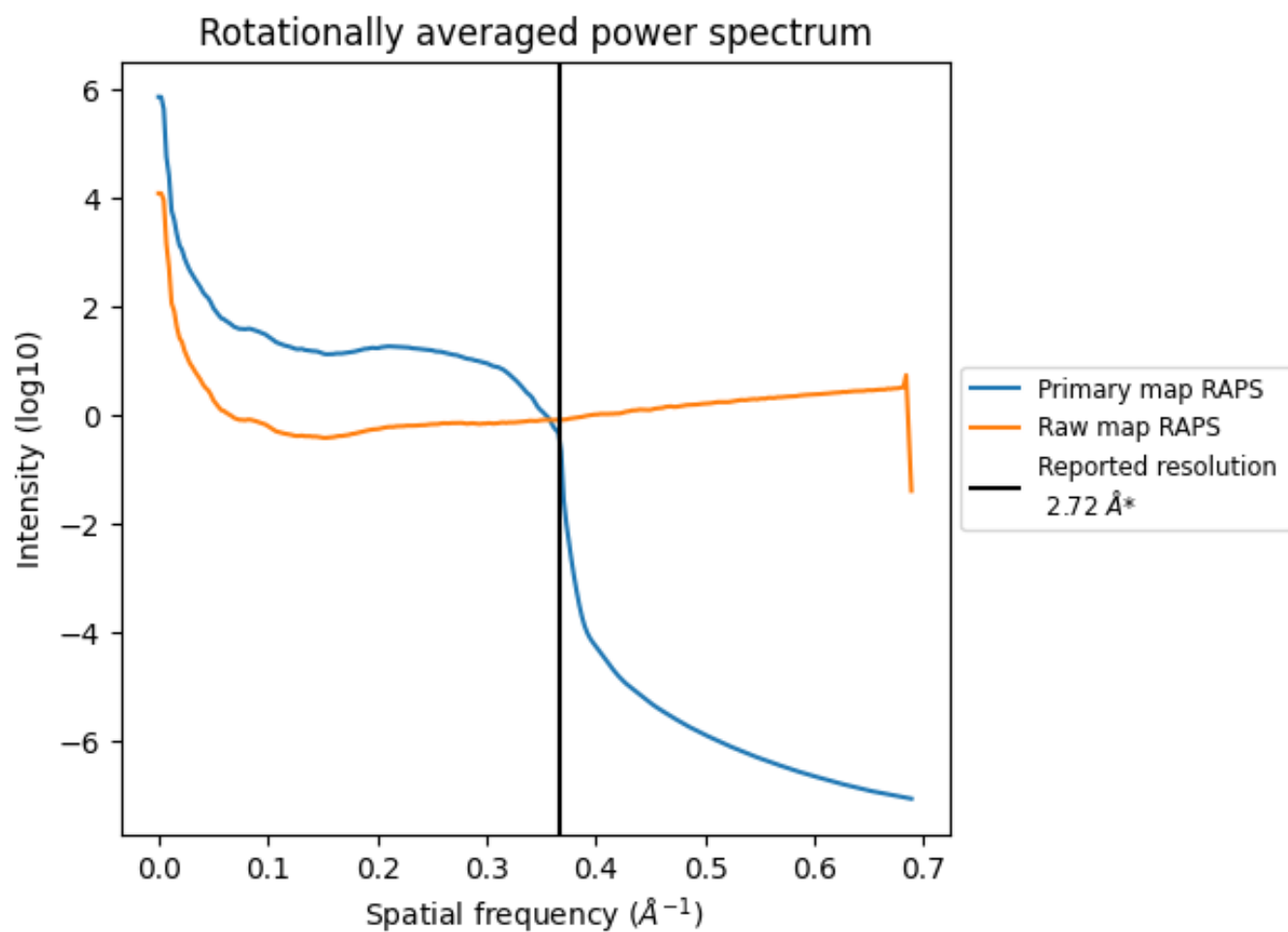
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 959 nm<sup>3</sup>; this corresponds to an approximate mass of 866 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](#)

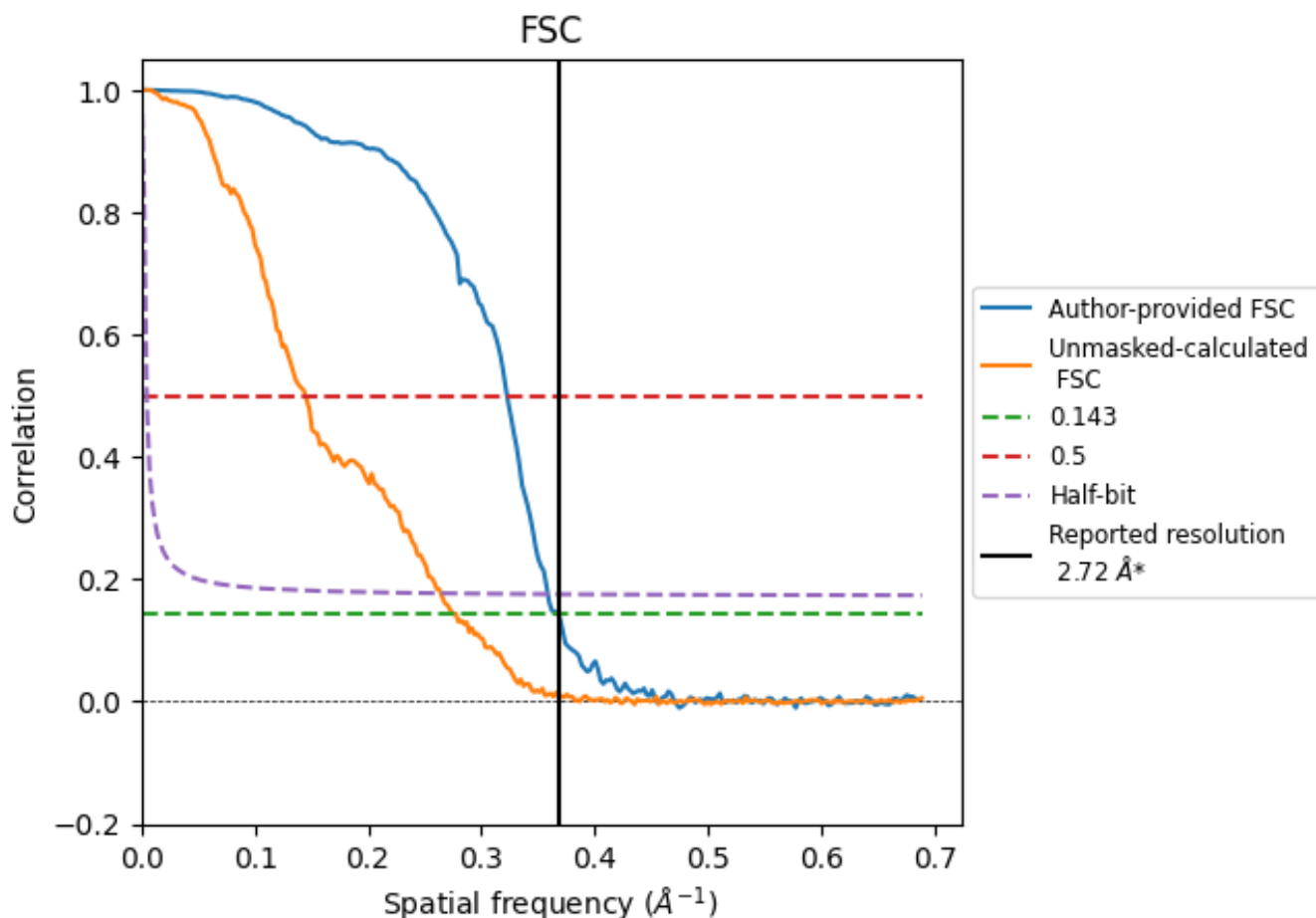


\*Reported resolution corresponds to spatial frequency of 0.368 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.368 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

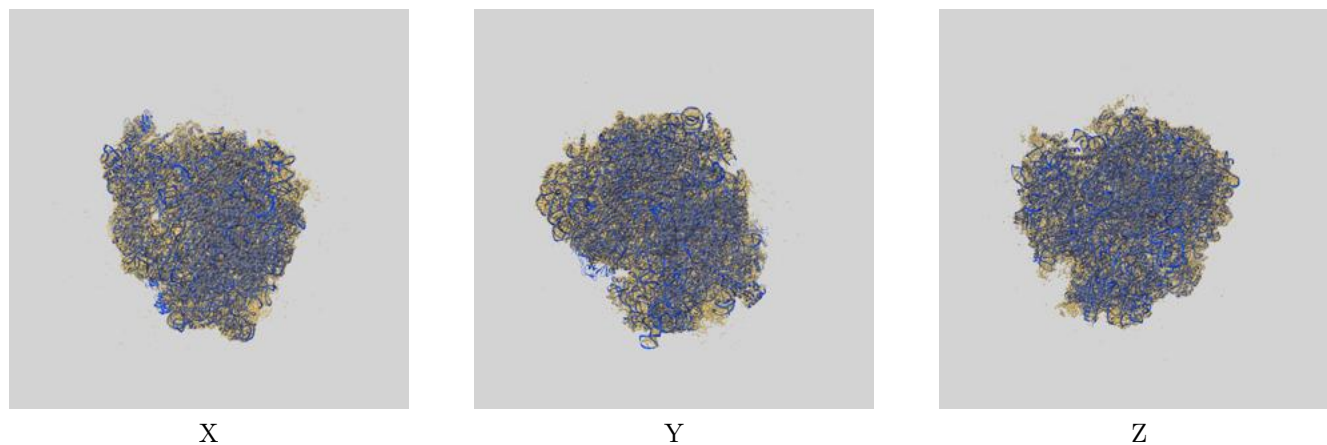
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.72	3.10	2.79
Unmasked-calculated*	3.64	6.91	3.78

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.64 differs from the reported value 2.72 by more than 10 %

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

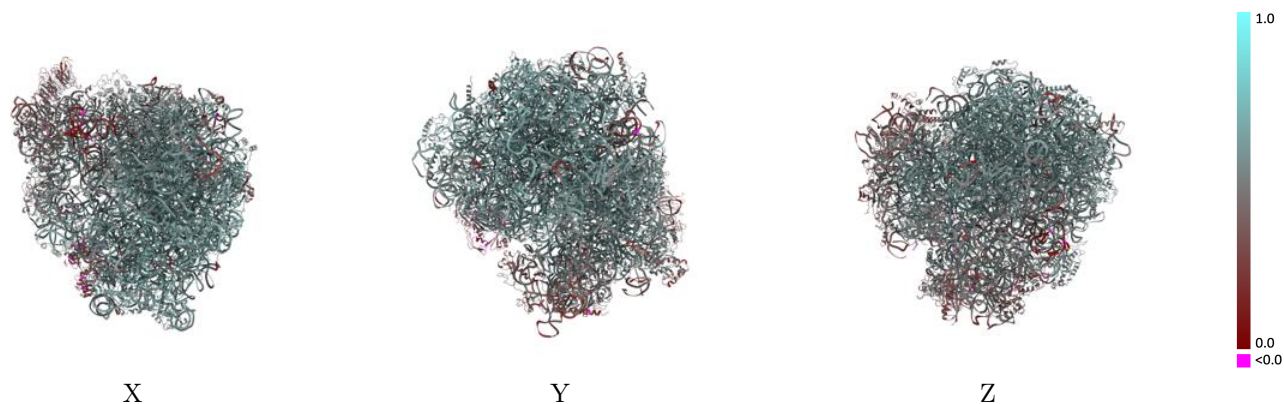
This section contains information regarding the fit between EMDB map EMD-16591 and PDB model 8CDL. Per-residue inclusion information can be found in section 3 on page 24.

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



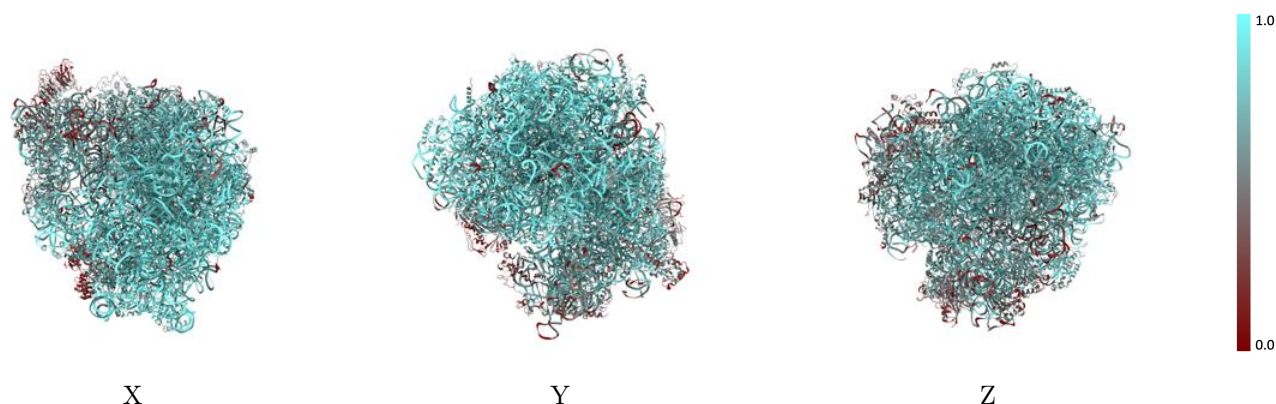
The images above show the 3D surface view of the map at the recommended contour level 0.141 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



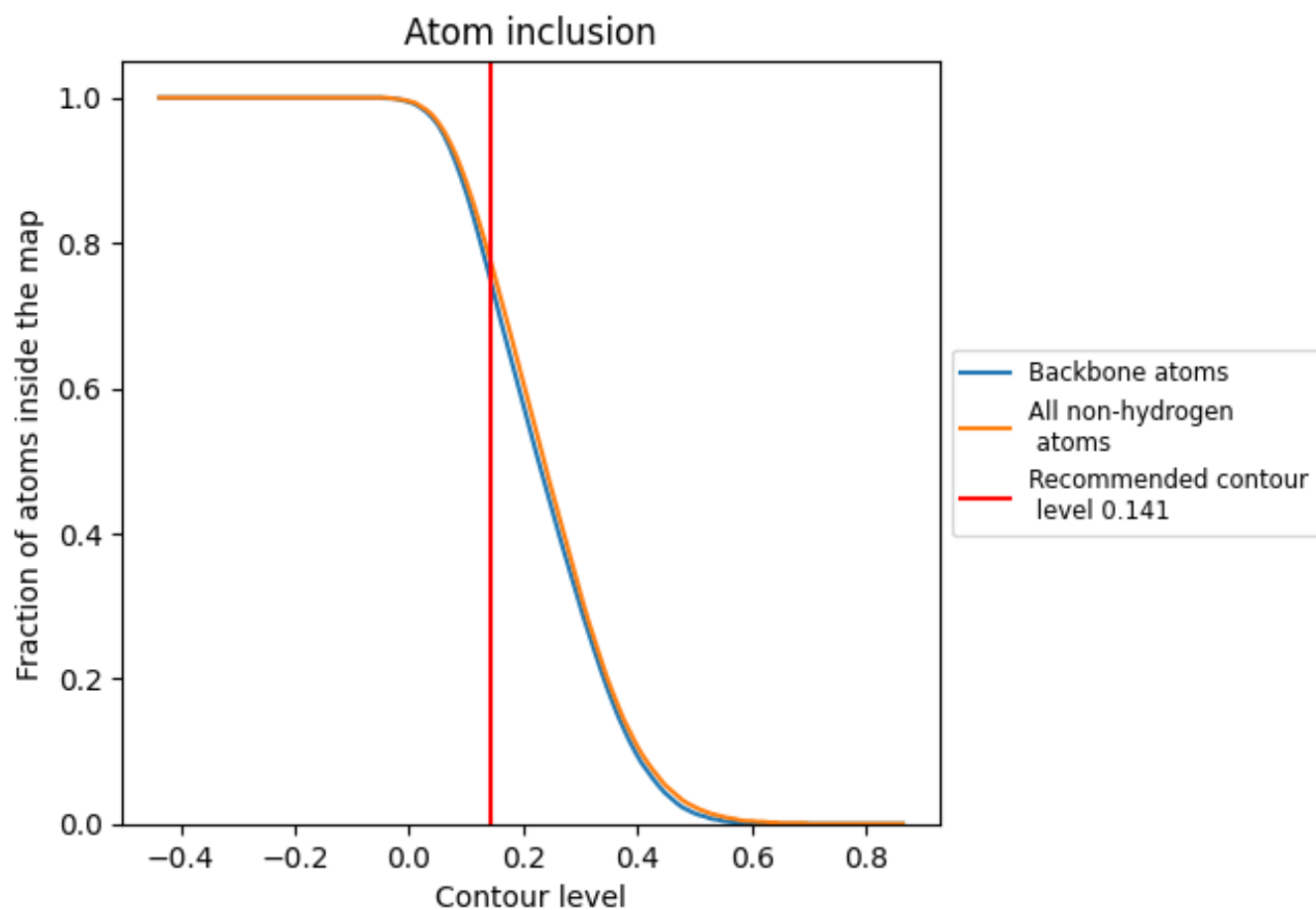
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.141).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 78% 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 (0.141) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7790	 0.5330
0	 0.4740	 0.4080
1	 0.3450	 0.3370
2	 0.7580	 0.5510
3	 0.6570	 0.5040
4	 0.5160	 0.4590
5	 0.7970	 0.5360
6	 0.6470	 0.4660
7	 0.3140	 0.3450
8	 0.2430	 0.2800
A	 0.8490	 0.5920
AA	 0.8770	 0.5630
B	 0.8820	 0.6050
BB	 0.9330	 0.5750
Bb	 0.3970	 0.3900
C	 0.8620	 0.5930
CC	 0.9340	 0.5960
Cc	 0.6470	 0.4380
D	 0.7570	 0.5500
DD	 0.0320	 0.1580
Dd	 0.6320	 0.5240
E	 0.8480	 0.5950
EE	 0.8430	 0.6050
Ee	 0.0110	 0.1480
F	 0.8290	 0.5830
FF	 0.8520	 0.5800
G	 0.7200	 0.5250
GG	 0.8550	 0.5980
H	 0.8180	 0.5920
HH	 0.7140	 0.5170
I	 0.8260	 0.5800
II	 0.8290	 0.5640
J	 0.8240	 0.5860
JJ	 0.8720	 0.5970
K	 0.8360	 0.5920

















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Chain	Atom inclusion	Q-score
KK	0.7310	0.5330
L	0.7900	0.5560
LL	0.7600	0.5550
M	0.8380	0.5770
MM	0.7960	0.5760
N	0.7590	0.5600
NN	0.6590	0.4890
O	0.7360	0.5670
OO	0.7930	0.5550
P	0.7910	0.5500
PP	0.8230	0.5760
Pp	0.1580	0.3770
Q	0.8870	0.6160
QQ	0.8880	0.6060
R	0.9000	0.6170
S	0.8330	0.5910
T	0.8190	0.5760
U	0.7170	0.5100
V	0.9140	0.6170
W	0.6610	0.5120
X	0.8480	0.5850
Y	0.7550	0.5850
Z	0.7220	0.5710
a	0.7660	0.5720
b	0.7970	0.5930
c	0.8120	0.5170
d	0.6610	0.4880
e	0.6860	0.5250
f	0.7510	0.5490
g	0.6510	0.5000
h	0.5670	0.4580
i	0.5360	0.4450
j	0.3910	0.3840
k	0.4850	0.4420
l	0.5170	0.4440
m	0.5900	0.4490
n	0.5710	0.4600
o	0.6420	0.5050
p	0.7590	0.5490
q	0.7230	0.5270
r	0.6330	0.4850
s	0.5660	0.4550

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Chain	Atom inclusion	Q-score
t	 0.5520	 0.4400
u	 0.5730	 0.4380
v	 0.5480	 0.4320
w	 0.5410	 0.4410
x	 0.7330	 0.5260
y	 0.8230	 0.5800
z	 0.7610	 0.5690