



## wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 06:32 PM JST

PDB ID : 8JDL / pdb\_00008jdl  
EMDB ID : EMD-36180  
Title : Structure of the Human cytoplasmic Ribosome with human tRNA  
Tyr(GalQ34) and mRNA(UAU) (non-rotated state)  
Authors : Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.  
Deposited on : 2023-05-14  
Resolution : 2.42 Å(reported)  
Based on initial model : 6Y0G

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 : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

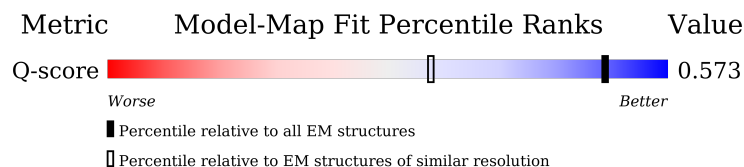
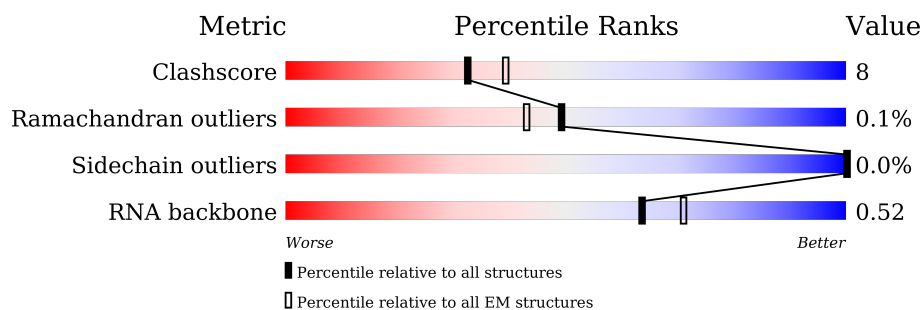
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.42 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.









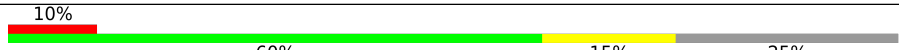
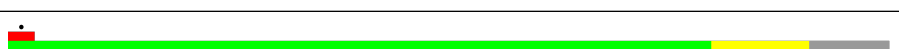

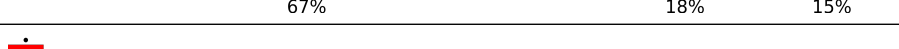
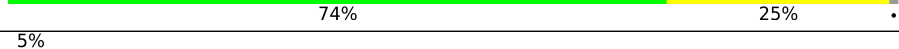














Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5729 ( 1.92 - 2.92 )

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	A	14	<div> <div>36%</div> <div>43%</div> <div>36%</div> <div>21%</div> </div>
2	B	76	<div> <div>74%</div> <div>42%</div> <div>38%</div> <div>16%</div> <div>.</div> </div>
3	D	5070	<div> <div>8%</div> <div>43%</div> <div>21%</div> <div>5%</div> <div>31%</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	120	
5	F	156	
6	G	257	
7	H	403	
8	I	427	
9	J	297	
10	K	288	
11	L	248	
12	M	266	
13	N	192	
14	O	214	
15	P	178	
16	Q	211	
17	R	215	
18	S	204	
19	T	203	
20	U	184	
21	V	188	
22	W	196	
23	X	176	
24	Y	160	
25	Z	128	
26	a	140	
27	b	157	
28	c	156	

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Mol	Chain	Length	Quality of chain
29	d	145	
30	e	136	
31	f	148	
32	g	159	
33	h	115	
34	i	125	
35	j	135	
36	k	110	
37	l	117	
38	m	123	
39	n	105	
40	o	97	
41	p	70	
42	q	51	
43	r	128	
44	s	25	
45	t	106	
46	u	92	
47	v	137	
48	w	1869	
49	x	295	
50	y	264	
51	z	293	
52	0	243	
53	1	263	

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Mol	Chain	Length	Quality of chain
54	2	204	
55	3	249	
56	4	194	
57	5	208	
58	6	194	
59	7	165	
60	8	158	
61	9	151	
62	AA	151	
63	AB	145	
64	AC	146	
65	AD	135	
66	AE	152	
67	AF	145	
68	AG	119	
69	AH	83	
70	AI	130	
71	AJ	143	
72	AK	133	
73	AL	125	
74	AM	115	
75	AN	84	
76	AO	69	
77	AP	56	
78	AQ	59	

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Mol	Chain	Length	Quality of chain
79	AR	317	<div><div></div><div>98%</div><div>53%</div><div>46%</div><div></div></div>

## 2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 207902 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	11	Total	C	N	O	P	0	0
			226	102	31	82	11		

- Molecule 2 is a RNA chain called tRNA (Tyr).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	76	Total	C	N	O	P	0	0
			1647	746	288	538	75		

- Molecule 3 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	3512	Total	C	N	O	P	0	0
			75336	33585	13757	24482	3512		

- Molecule 4 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 5 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 6 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	247	Total	C	N	O	S	0	0
			1891	1185	388	312	6		

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	398	Total	C	N	O	S	0	0
			3211	2045	604	548	14		

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	363	Total	C	N	O	S	0	0
			2884	1815	577	478	14		

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	293	Total	C	N	O	S	0	0
			2379	1506	434	425	14		

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	217	Total	C	N	O	S	0	0
			1751	1128	332	287	4		

- Molecule 11 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 12 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	227	Total	C	N	O	S	0	0
			1832	1168	352	308	4		

- Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 14 is a protein called 60S ribosomal protein L10-like.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	206	Total	C	N	O	S	0	0
			1660	1053	319	275	13		

- Molecule 15 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 16 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	208	Total	C	N	O	S	0	0
			1682	1052	348	278	4		

- Molecule 17 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 18 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 19 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	200	Total	C	N	O	S	0	0
			1641	1058	320	258	5		

- Molecule 20 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	157	Total	C	N	O	S	0	0
			1273	797	246	221	9		

- Molecule 21 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 22 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 23 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 25 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	101	Total	C	N	O	S	0	0
			821	526	143	150	2		

- Molecule 26 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 27 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 28 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	120	Total	C	N	O	S	0	0
			981	628	185	167	1		

- Molecule 29 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 30 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 31 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	104	Total	C	N	O	S	0	0
			832	515	182	132	3		

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	97	Total	C	N	O	S	0	0
			755	479	133	137	6		

- Molecule 34 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 36 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 37 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	112	Total	C	N	O	S	0	0
			888	555	183	144	6		

- Molecule 38 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	121	Total	C	N	O	S	0	0
			1010	638	204	167	1		

- Molecule 39 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 40 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 41 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 42 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 43 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 44 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 45 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 46 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 47 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 48 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	1634	Total	C	N	O	P	0	0
			34933	15622	6267	11411	1633		

- Molecule 49 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	215	Total	C	N	O	S	0	0
			1695	1077	297	313	8		

- Molecule 50 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	212	Total	C	N	O	S	0	0
			1725	1096	308	307	14		

- Molecule 51 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	212	Total	C	N	O	S	0	0
			1633	1059	279	285	10		

- Molecule 52 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	212	Total	C	N	O	S	0	0
			1646	1050	299	290	7		

- Molecule 53 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	262	Total	C	N	O	S	0	0
			2070	1321	383	358	8		

- Molecule 54 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	187	Total	C	N	O	S	0	0
			1464	916	276	265	7		

- Molecule 55 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	237	Total	C	N	O	S	0	0
			1917	1197	384	329	7		

- Molecule 56 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	187	Total	C	N	O	S	0	0
			1510	963	278	268	1		

- Molecule 57 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	206	Total	C	N	O	S	0	0
			1674	1049	329	291	5		

- Molecule 58 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	6	182	Total	C	N	O	S	0	0
			1506	959	300	245	2		

- Molecule 59 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	7	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 60 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	8	142	Total	C	N	O	S	0	0
			1150	732	215	197	6		

- Molecule 61 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	9	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 62 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AA	134	Total	C	N	O	S	0	0
			1002	612	197	187	6		

- Molecule 63 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AB	134	Total	C	N	O	S	0	0
			1103	703	208	185	7		

- Molecule 64 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AC	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 65 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AD	131	Total	C	N	O	S	0	0
			1057	665	197	191	4		

- Molecule 66 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AE	144	Total	C	N	O	S	0	0
			1169	731	236	201	1		

- Molecule 67 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AF	143	Total	C	N	O	S	0	0
			1111	696	213	198	4		

- Molecule 68 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AG	102	Total	C	N	O	S	0	0
			799	501	153	141	4		

- Molecule 69 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AH	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 70 is a protein called 40S ribosomal protein S15a.



Mol	Chain	Residues	Atoms					AltConf	Trace
70	AI	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 71 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AJ	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 72 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AK	123	Total	C	N	O	S	0	0
			1002	634	196	167	5		

- Molecule 73 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AL	86	Total	C	N	O	S	0	0
			680	436	127	116	1		

- Molecule 74 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AM	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 75 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AN	83	Total	C	N	O	S	0	0
			643	402	119	115	7		

- Molecule 76 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AO	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 77 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AP	45	Total	C	N	O	S	0	0
			370	228	77	60	5		

- Molecule 78 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AQ	57	Total	C	N	O	S	0	0
			452	279	99	73	1		

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AR	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

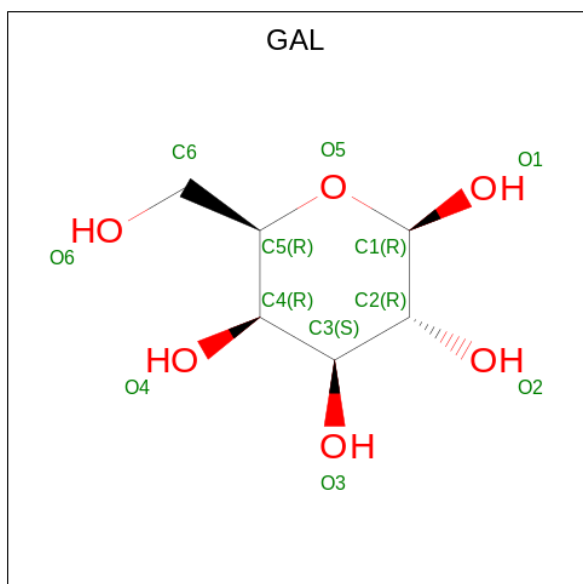
Mol	Chain	Residues	Atoms		AltConf
80	A	1	Total	Mg	0
			1	1	
80	D	401	Total	Mg	0
			401	401	
80	E	10	Total	Mg	0
			10	10	
80	F	5	Total	Mg	0
			5	5	
80	G	2	Total	Mg	0
			2	2	
80	H	1	Total	Mg	0
			1	1	
80	I	1	Total	Mg	0
			1	1	
80	N	1	Total	Mg	0
			1	1	
80	O	1	Total	Mg	0
			1	1	
80	S	1	Total	Mg	0
			1	1	
80	U	2	Total	Mg	0
			2	2	
80	V	2	Total	Mg	0
			2	2	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
80	X	1	Total 1	Mg 1	0
80	a	1	Total 1	Mg 1	0
80	g	1	Total 1	Mg 1	0
80	j	1	Total 1	Mg 1	0
80	k	1	Total 1	Mg 1	0
80	l	1	Total 1	Mg 1	0
80	w	100	Total 100	Mg 100	0
80	8	1	Total 1	Mg 1	0
80	AA	1	Total 1	Mg 1	0
80	AF	1	Total 1	Mg 1	0
80	AJ	1	Total 1	Mg 1	0
80	AM	1	Total 1	Mg 1	0

- Molecule 81 is beta-D-galactopyranose (CCD ID: GAL) (formula:  $C_6H_{12}O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
81	B	1	Total	C	O	0
			11	6	5	

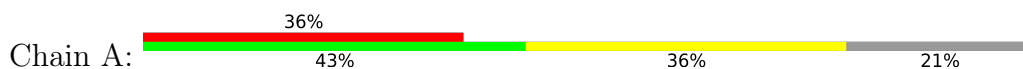
- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	o	1	Total	Zn	0
			1	1	
82	r	1	Total	Zn	0
			1	1	
82	t	1	Total	Zn	0
			1	1	
82	u	1	Total	Zn	0
			1	1	
82	AM	1	Total	Zn	0
			1	1	
82	AP	1	Total	Zn	0
			1	1	

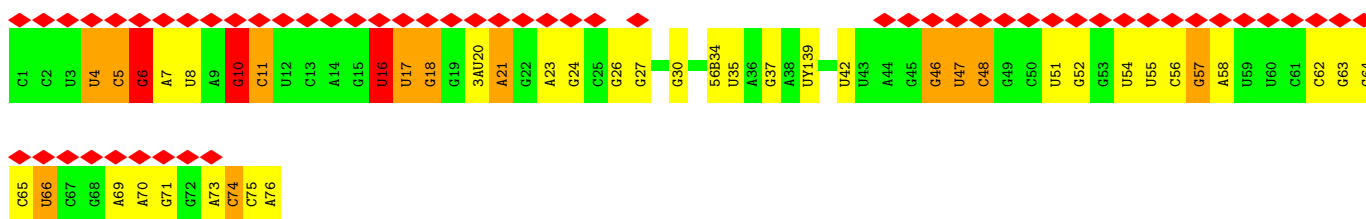
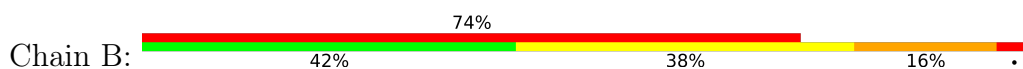
### 3 Residue-property plots

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

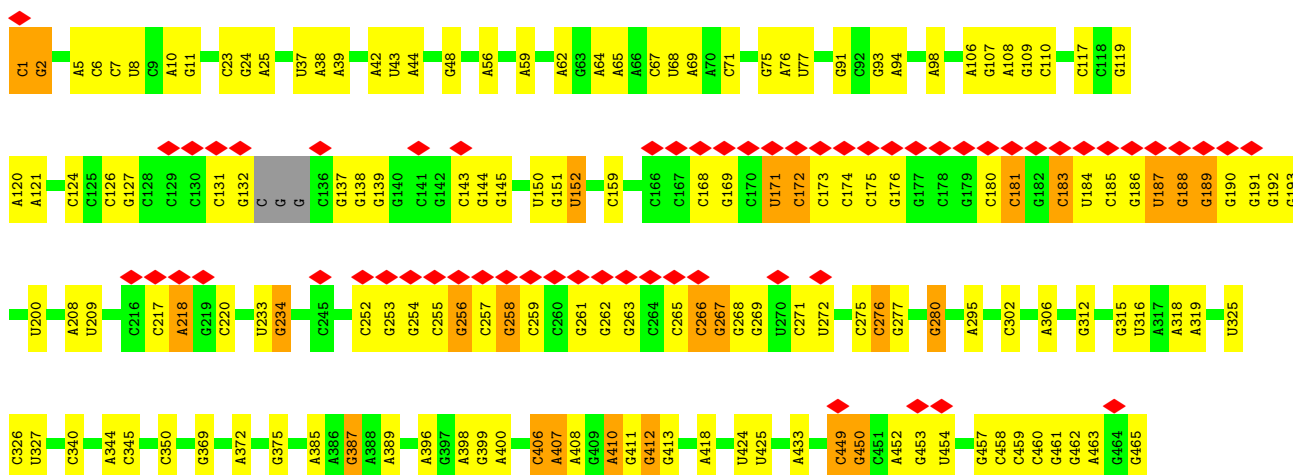
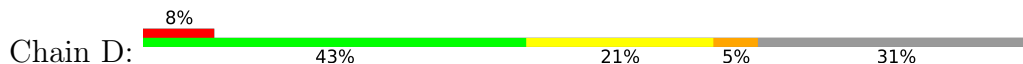
#### • Molecule 1: mRNA

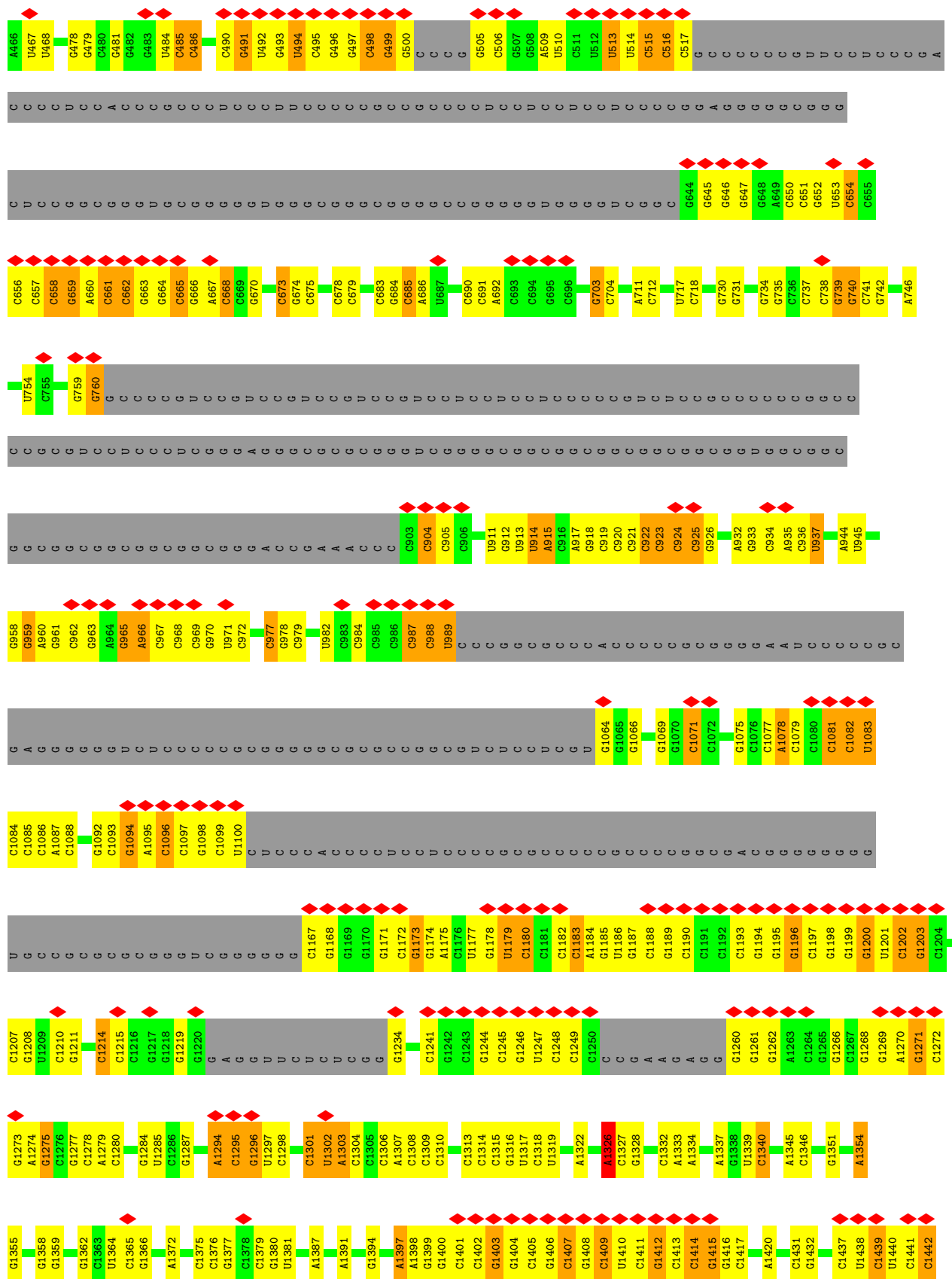


#### • Molecule 2: tRNA (Tyr)



#### • Molecule 3: 28S ribosomal RNA

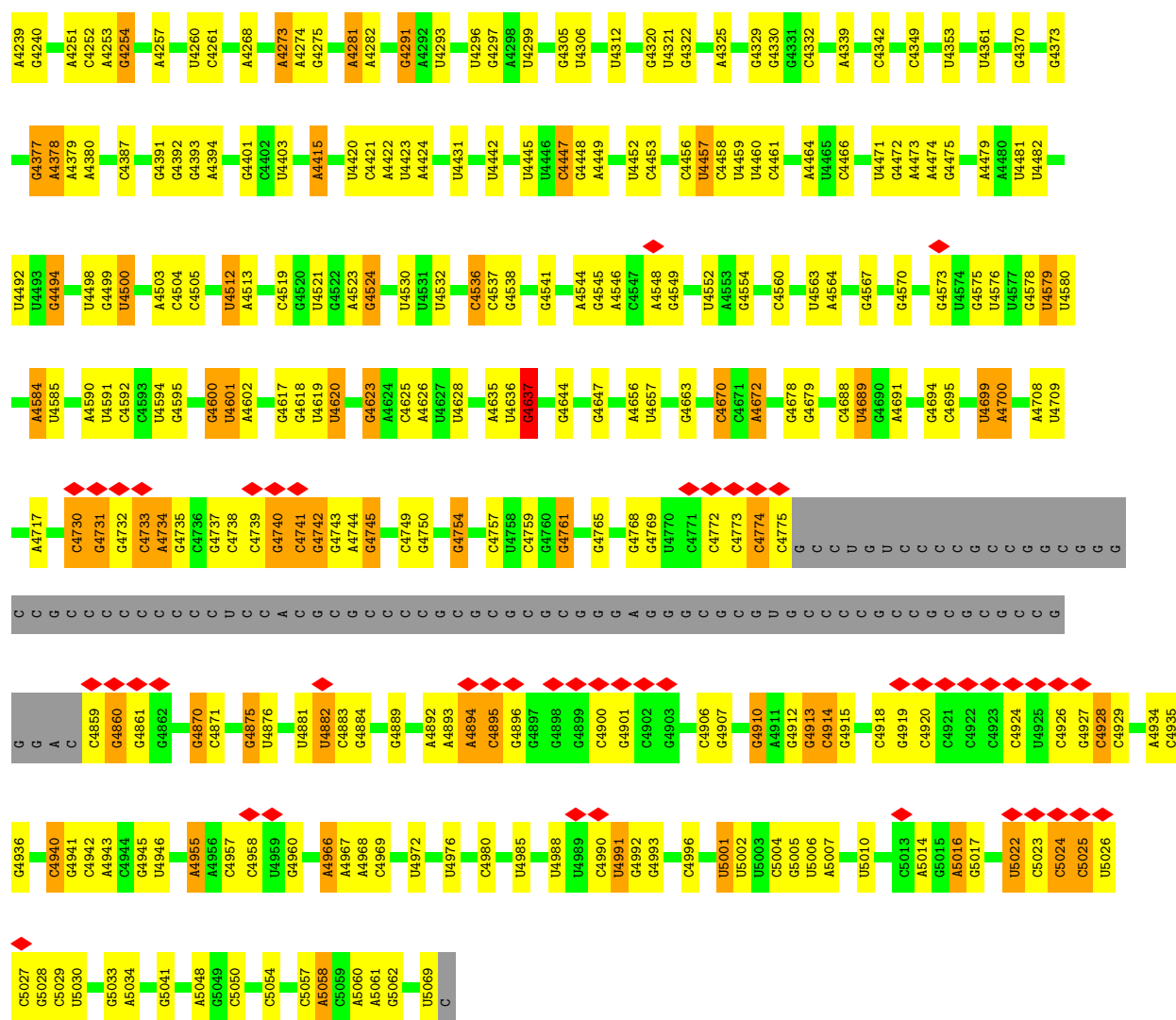




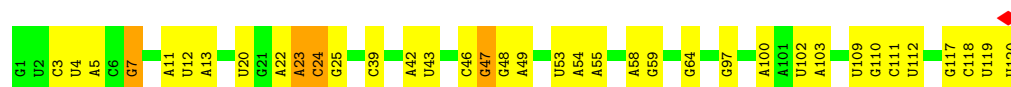




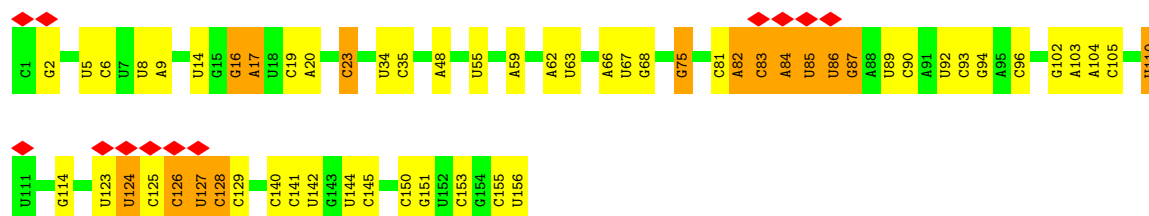





● Molecule 4: 5S ribosomal RNA

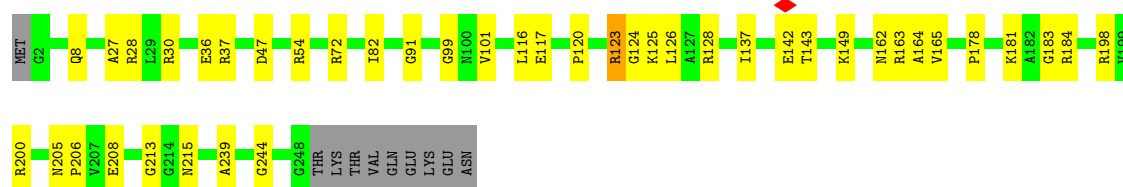


● Molecule 5: 5.8S ribosomal RNA




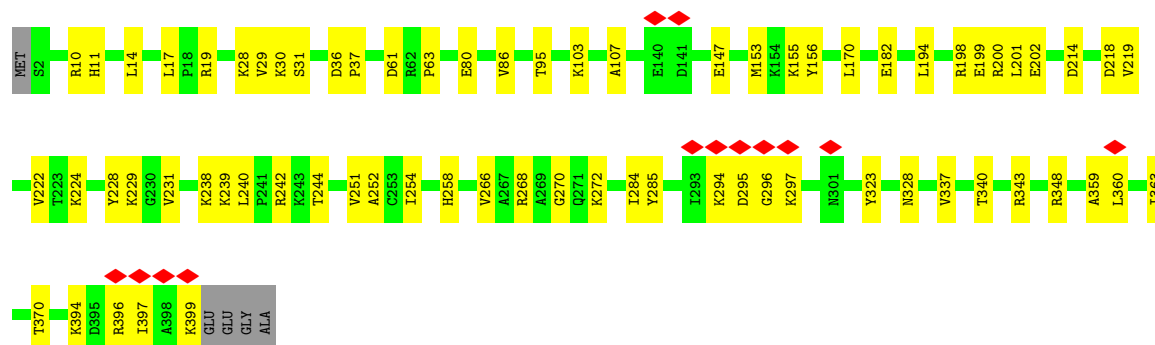
- Molecule 6: 60S ribosomal protein L8

Chain G: 



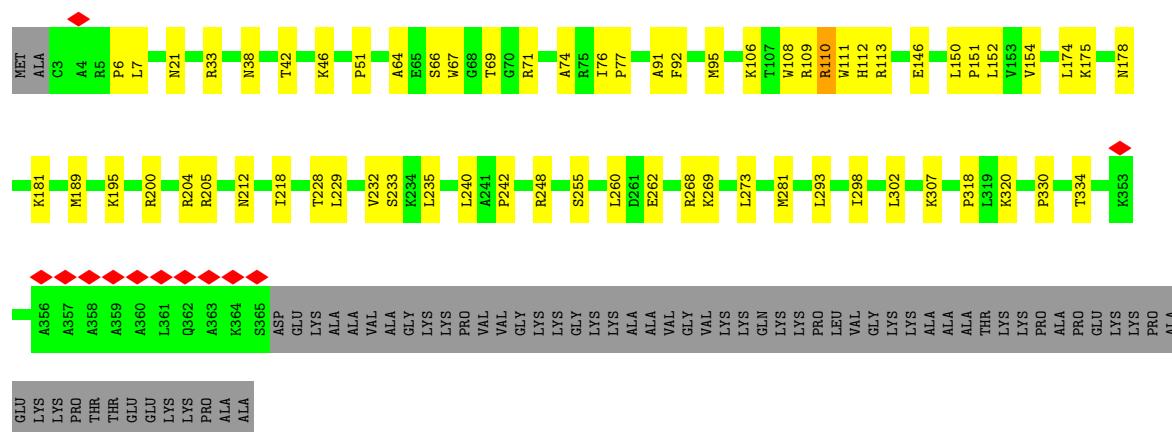
- Molecule 7: 60S ribosomal protein L3

Chain H: 




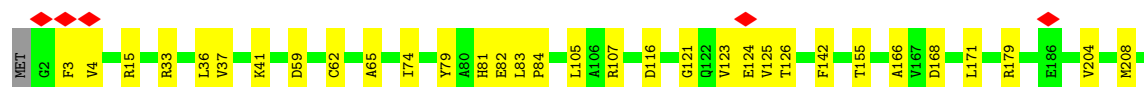
- Molecule 8: 60S ribosomal protein L4

Chain I: 

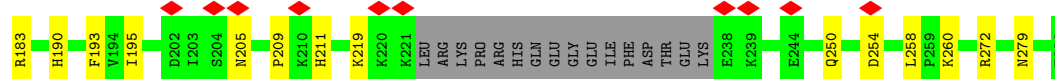
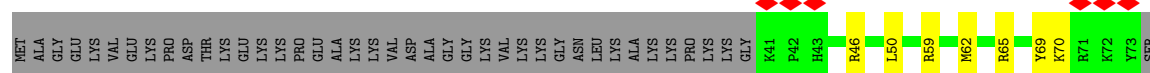


- Molecule 9: 60S ribosomal protein L5

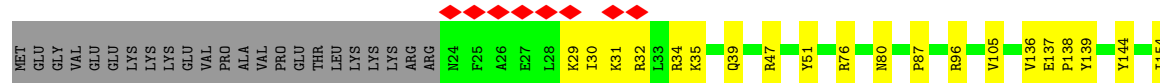
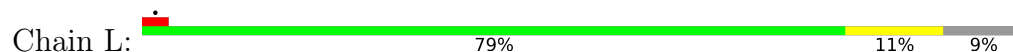
Chain J: 



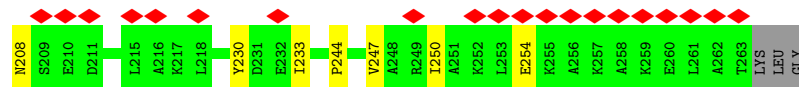
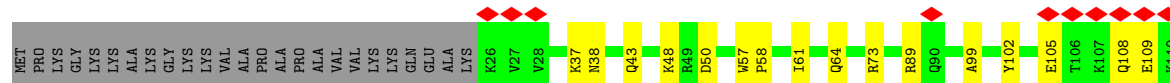
- Molecule 10: 60S ribosomal protein L6



- Molecule 11: 60S ribosomal protein L7

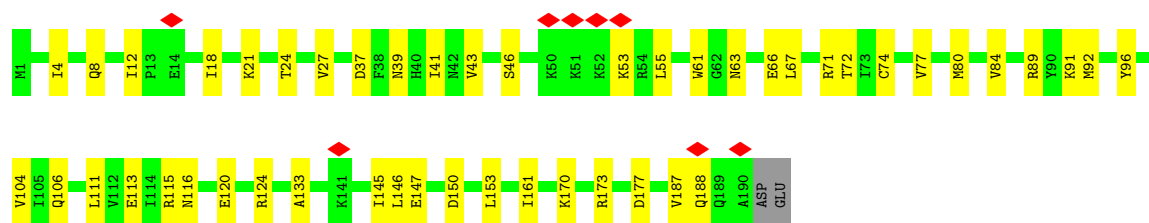


- Molecule 12: 60S ribosomal protein L7a

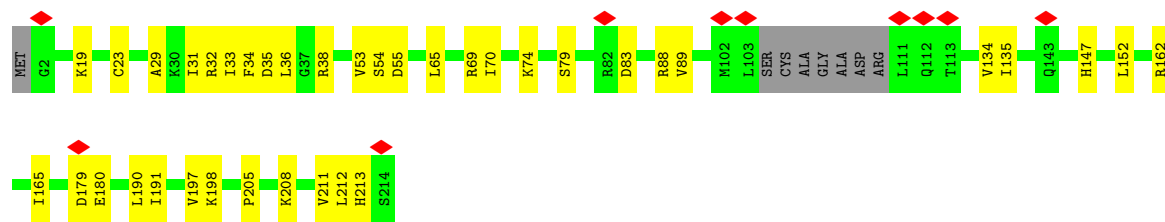
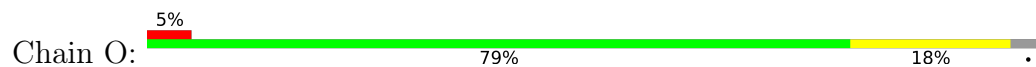


- Molecule 13: 60S ribosomal protein L9

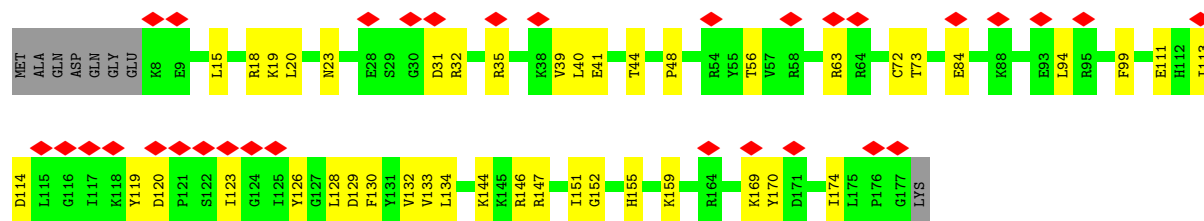




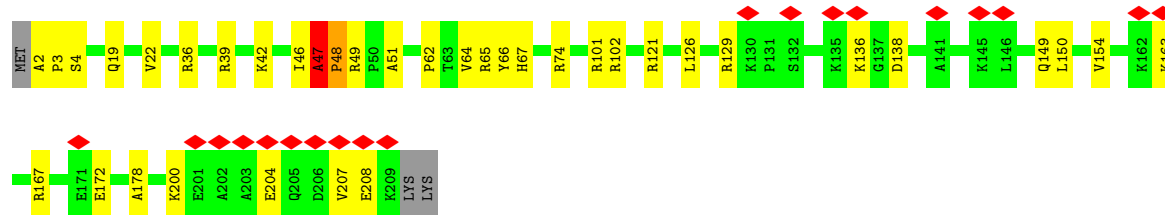
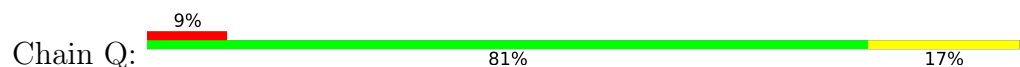
• Molecule 14: 60S ribosomal protein L10-like



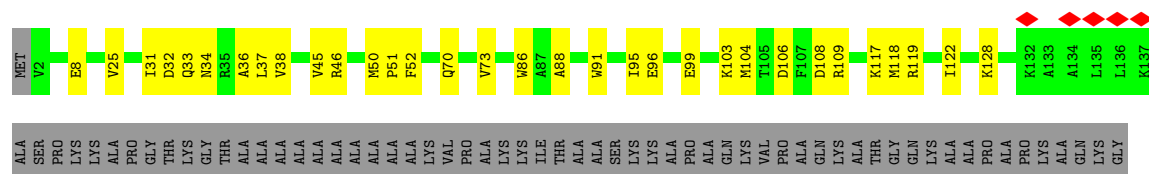
• Molecule 15: 60S ribosomal protein L11



• Molecule 16: 60S ribosomal protein L13




• Molecule 17: 60S ribosomal protein L14




GLN  
LYS  
ALA  
ALA  
PRO  
GLN  
LYS  
LYS  
ALA  
PRO  
PRO  
LYS  
ALA  
SER  
GLY  
LYS  
LYS  
ALA

- Molecule 18: 60S ribosomal protein L15

Chain S:  86% 14%

MET G2 A3 Y4 I7 K14 P45 R49 R67 R68 V75 T30 V85 W120 E123 D124 S125 F138 R143 R144 R145 P146 D147 R159 L164 H178 T183 I184 R188 R194 R202 Y203 R204


- Molecule 19: 60S ribosomal protein L13a

Chain T:  84% 14%

MET ALA GLU V4 Q5 D10 R37 P47 Y48 R49 Y54 R61 P70 F73 R74 F80 W81 R82 T83 V104 G107 I108 R140 E144 V145 G146 A151 T155 Y168 R176 A181 V185 E186 K187 I189 T193 K197 T198 H199

Y203

- Molecule 20: 60S ribosomal protein L17

Chain U:  73% 11% 15%

MET Y2 R3 Y4 F9 N10 K13 K16 S17 R18 G19 S20 N21 L22 T32 A35 Q54 V58 R69 W83 F90 M94 S111 P123 R131 H145 I149 E154 Q155 I156 V157 P158 LYS PRO GLU GLU VAL ALA GLN LYS LYS


ILE  
SER  
GLN  
LYS  
LEU  
LYS  
LYS  
GLN  
LEU  
MET  
ALA  
ARG  
GLU

- Molecule 21: 60S ribosomal protein L18

Chain V:  87% 12%

MET G2 R14 R15 K16 R33 F43 V47 L63 M66 D83 E94 V95 L98 T106 S107 R108 A109 P131 V148 Y149 R150 H151 F152 G157 T158 P159 H160 S161 R181 N188

- Molecule 22: 60S ribosomal protein L19

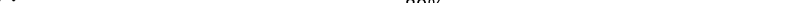
Chain W:  14% 82% 10% 8%

MET S2 R16 R38 Q39 R88 R89 P90 V93 M96 M99 L102 R103 R104 L105 R108 K136 R136 I137 L138 M139 E140 A150 Y151 L155 A156 D157 Q158 A159 E160 A161 R162 R163 S164 K165 T166 K167 E168 A169 R170 K171 R172 R173 E174 E175 R176 L177 Q178 A179

K180 K181 GLU GLU ILE ILE LYS THR LEU SER LYS GLU GLU THR LYS

- Molecule 23: 60S ribosomal protein L18a

Category	Count
MET	1
K2	1
L7	1
R15	1
C16	1
P20	11
K21	11
C22	11
H23	11
T24	11
L27	1
R43	1
W81	1
D85	1
A103	1
S123	1
M127	1
K128	1
V129	1
E130	1
F145	1
K151	1
P155	1
H156	1
K164	1
P165	1
T169	1
F176	1

- Chain Y:  6% 89% 10%

- Chain Z: 

Amino Acid	Count
MET	1
ALA	2
PRO	2
VAL	2
LYS	2
LEU	2
VAL	2
VAL	2
GLY	2
GLY	2
LYS	2
LYS	2
LYS	2
Q17	1
V18	1
I19	1
D24	1
C25	1
P28	1
V29	1
E30	1
D31	1
G32	1
T33	1
M34	1
D35	1
N38	1
F39	1
E40	1
D41	1
F42	1
I43	1
Q44	1
E45	1
R46	1
G54	1
N55	1
L56	1
O57	1
O58	1
O59	1
T62	1
I63	1
E64	1
R65	1
S66	1
K67	1
S68	1
K69	1
T73	1
S74	1

- Chain a:  81% 12% 6%

A horizontal bar chart showing the distribution of amino acid types across 1000 random sequences. The y-axis lists amino acid types: MET, SER, LYS, ARG, GLY, ARG, GLY, GLY, SER, S10, K13, G19, V22, K43, G44, I45, P53, V65, R73, S87, D92, G93, V94, Y97, N107, N108, K109, G110, E111, L128, R131, and A140. The x-axis represents the count of each type, ranging from 0 to 1000. The bars are colored in a repeating pattern of green, yellow, and grey. A red diamond marker is placed above the S10 bar, and another red diamond marker is placed above the N108 bar.

- Chain b:  38% 60%

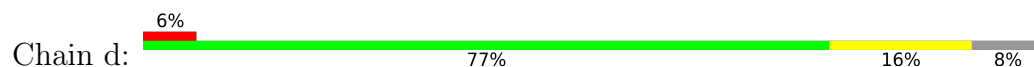
[illegible]

- Chain c:  67% 10% 23%

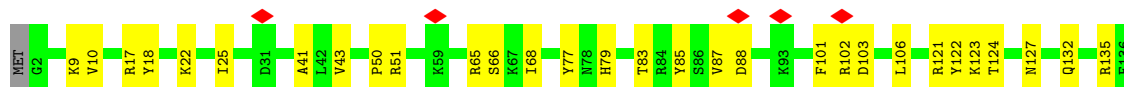
Category	Item	Value	Color	Label
A	MET	100	Grey	
	PRO	100	Grey	
	ALA	100	Grey	
	LYS	100	Grey	
	ALA	100	Grey	
	LYS	100	Grey	
	LYS	100	Grey	
	GLU	100	Grey	
	ALA	100	Grey	
	PRO	100	Grey	
	PRO	100	Grey	
	ALA	100	Grey	
	LYS	100	Grey	
	LYS	100	Grey	
	ALA	100	Grey	
	LEU	100	Grey	
	LYS	100	Grey	
	LYS	100	Grey	
B	ALA	100	Grey	
	VAL	100	Grey	
	LEU	100	Grey	
	LYS	100	Grey	
	GLY	100	Grey	
	VAL	100	Grey	
	HIS	100	Grey	
	SER	100	Grey	
	HIS	100	Grey	
	LYS	100	Grey	
	K37	100	Red	
	K38	100	Red	
C	K39	100	Red	
	I40	100	Yellow	
	R41	100	Yellow	
	I42	100	Yellow	
	R43	100	Yellow	
	R48	100	Yellow	
	S64	100	Yellow	
	D72	100	Yellow	
	H73	100	Yellow	
	I76	100	Yellow	
D	F79	100	Yellow	
	A112	100	Yellow	
	L116	100	Yellow	
	Y117	100	Yellow	
	D118	100	Red	



- Molecule 29: 60S ribosomal protein L26



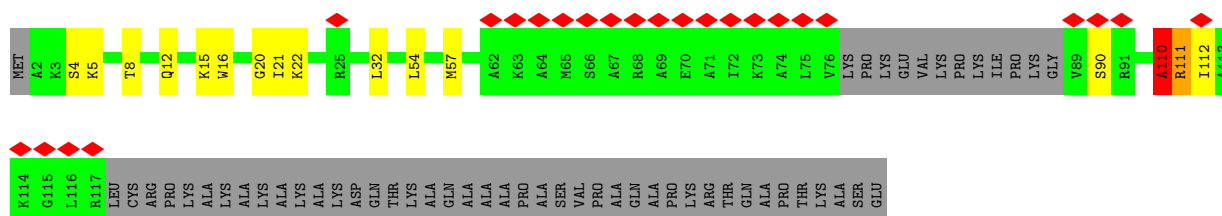
- Molecule 30: 60S ribosomal protein L27



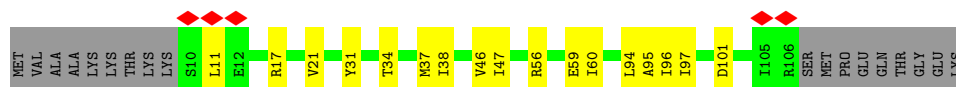
- Molecule 31: 60S ribosomal protein L27a



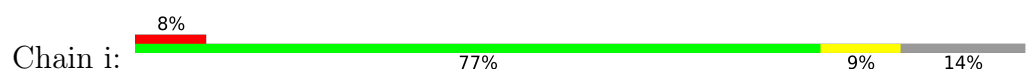
- Molecule 32: 60S ribosomal protein L29



- Molecule 33: 60S ribosomal protein L30

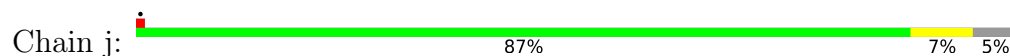


- Molecule 34: 60S ribosomal protein L31

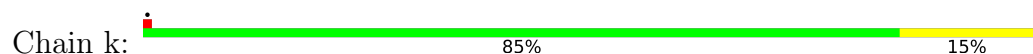




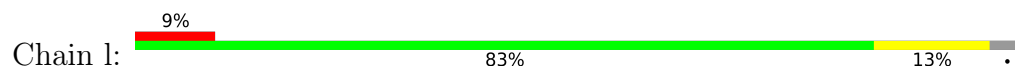
- Molecule 35: 60S ribosomal protein L32



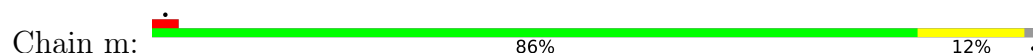
- Molecule 36: 60S ribosomal protein L35a



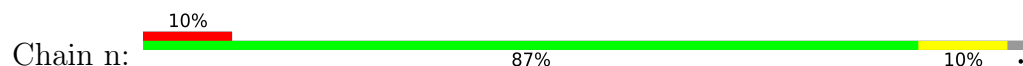
- Molecule 37: 60S ribosomal protein L34



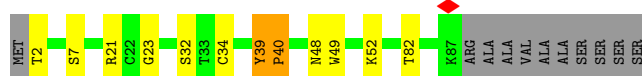
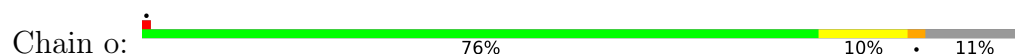
- Molecule 38: 60S ribosomal protein L35



- Molecule 39: 60S ribosomal protein L36

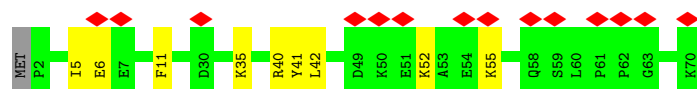
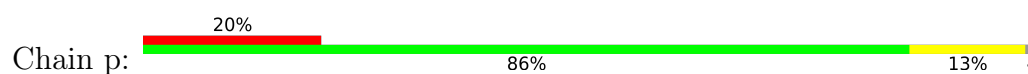


- Molecule 40: 60S ribosomal protein L37

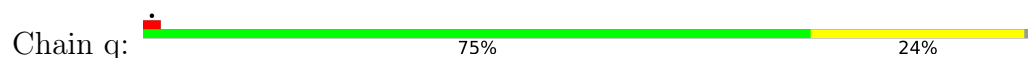


- Molecule 41: 60S ribosomal protein L38

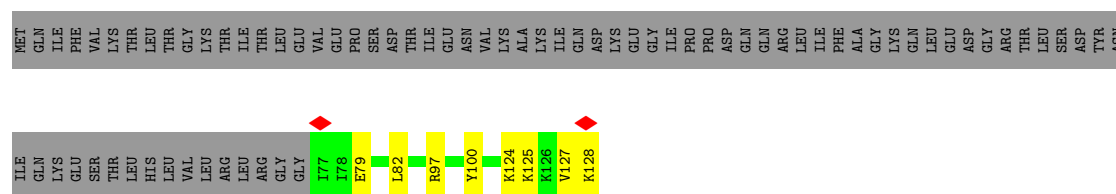
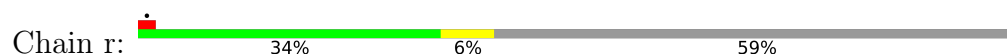




- Molecule 42: 60S ribosomal protein L39



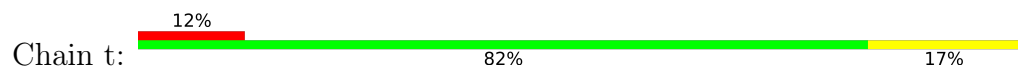
- Molecule 43: Ubiquitin-60S ribosomal protein L40



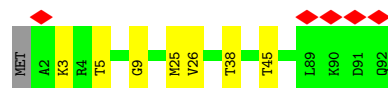
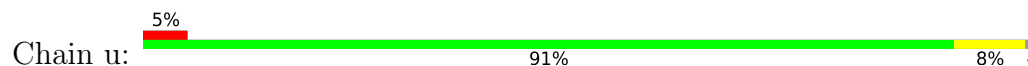
- Molecule 44: 60S ribosomal protein L41



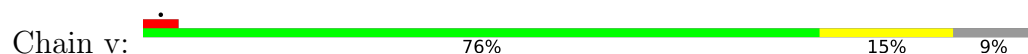
- Molecule 45: 60S ribosomal protein L36a



- Molecule 46: 60S ribosomal protein L37a



- Molecule 47: 60S ribosomal protein L28

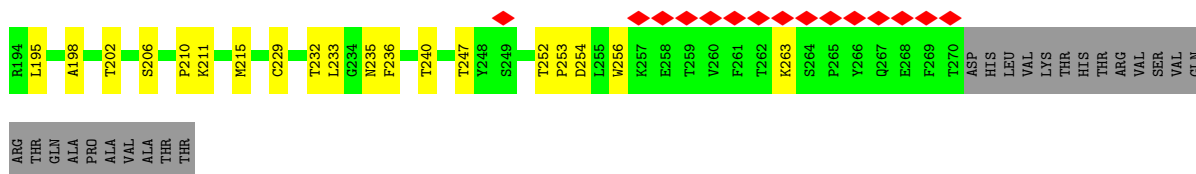


Chain w: 20% 37% 38% 12% 13%

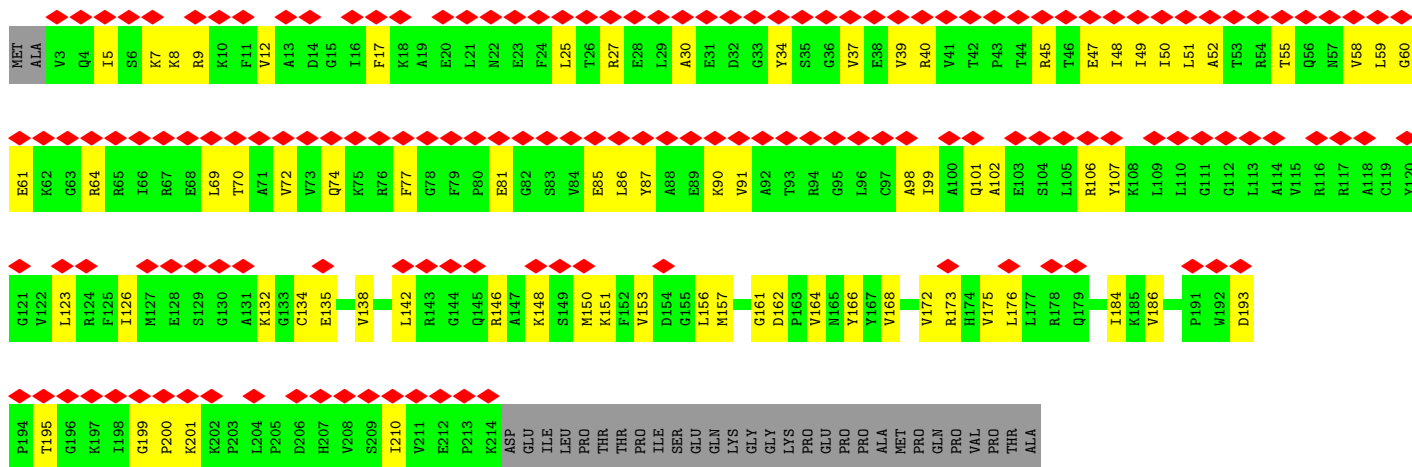


U	C	U1872	G1525	G1450	G1309	U1243	A1055	G956	U882	U814
C	U1601	U1673	G1526	G1451	U1310	U1244	A1056	G957	U883	U815
G	G1674	A1452	G1527	A1452	C1311	BSN1248	U1061	A963	U884	A816
G	G1603	C1453	G1528	A1453	G1312	A1251	A1062	A964	C884	G817
C	G1604	A1454			U1313	G1252	C1067	U965	U885	A818
C	G1605	U1457	G1532	U1457	U1314	C1253	G1068	U966	A886	G819
C	G1606	G1458	A1533	G1458	U1315	A1253	U1081	A972	U887	U820
A	A1607	G1459	C1534	U1397	G1316	C1254	U1082	C974	U888	G821
C	G1610	U1462	U1535	G1398	G1317	G1255	A1083	U980	U889	U822
G	G1611	U1463	U1536	U1398	G1318	G1256	A1084	A981	U890	U823
G	G1612	U1464	U1537	U1398	U1319	G1257	C1085	G982	C924	C924
C		U1465	G1540	A1401	U1320	A1258	U1088	U985	A827	A827
C	U1615	G1466	U1543	A1402	G1321	A1260	U1089	G986	G828	G828
C	U1616	U1467	C1544	C1403	G1322	C1261	G1098	G987	G829	A830
U	G1617	U1468	A1545	U1404	U1323	U1262	C1099	U989	G831	G831
G	C1618	C1471	G1546	A1405	U1324	U1263	G1101	A996	C832	C832
C	A1619	C1472	C1547	G1406	U1325	A1264	U1102	A997	C833	C833
C	A1620	G1473	G1548	U1407	G1326	A1265	U1103	A998	C834	C834
C	U1621	U1476	U1549	U1408	U1327	C1266	A1100	G999	C835	C835
C	U1622	U1477	C1550	A1409	U1328	U1267	G1099	G999	G836	G836
C	A1623	U1478	G1551	C1410	G1329	C1271	C1101	C1000	A837	A837
C	U1624	U1479	U1552	G1411	U1330	U1272	U1102	A1001	G838	G838
C	U1625	G1481	G1553	C1412	C1331	G1273	U1113	U1002	C839	C839
C	C1626	C1482	C1554	G1413	A1332	G1274	U1114	U1003	C840	C840
C	G1627	U1483	U1555	A1414	U1337	U1275	U1115	U1004	G841	G841
C	C1628	U1484	U1556	A1415	U1340	U1276	U1116	G1005	C842	C842
C	U1629	C1485	C1557	C1416	C1341	U1277	U1117	G1006	C843	C843
C	A1630	C1486	C1558	C1417	U1342	G1280	C1118	C1007	U844	U844
C	U1631	U1487	U1559	C1418	U1347	G1281	A1119	G1008	G845	G845
C	G1632	U1488	U1560	C1419	G1348	A1282	G1010	G1009	G846	G846
C	A1633	U1489	U1561	C1420	G1349	U1283	U1120	G1011	A847	A847
C	A1634	C1491	U1562	C1421	U1350	C1284	U1121	A1012	U848	U848
C	C1635	C1492	C1563	C1422	G1351	G1285	U1122	U1013	C912	C912
C	G1636	U1493	U1564	G1423	G1352	U1286	U1123	G1014	A913	A913
C	A1637	U1494	U1565	G1424	G1353	G1287	G1126	U1015	C851	C851
C	G1638	U1495	U1566	G1425	G1354	U1288	U1130	U1016	G852	G852
C	U1639	U1496	U1567	U1426	G1355	A1287	G1133	U1017	C856	C856
C	G1640	U1497	U1568	U1427	G1356	U1289	A1133	U1018		
C	U1641	U1498	U1569	G1428	G1357	U1290	G1134	A1023	A861	A861
C	A1643	G1501	U1570	G1429	U1367	G1291	G1135	U1024	U863	U863
C	C1644	U1502	U1571	C1430	U1371	A1291	G1136	U1025	U866	U866
C	C1645	U1503	G1572	C1431	U1372	G1292	U1137	U1026	G867	G867
C	G1646	U1504	G1573	U1432	U1373	A1293	C1138	U1027	G868	G868
C	A1647	U1505	C1574	C1433	G1374	G1294	G1139	A1030	A869	A869
C	U1648	U1506	U1575	C1434	C1375	A1295	G1140	A1031	U870	U870
C	U1649	U1507	U1576	C1435	G1376	U1296	G1141	U1045	A872	A872
C	U1653	U1508	U1577	C1436	U1377	U1297	G1142	G873	G873	G873
C	G1654	U1509	U1578	C1437	A1378	G1298	A1143	U945	G874	G874
C	A1663	U1510	A1580	U1438	G1379	U1299	A1144	U946	A875	A875
C	A1664	U1511	U1585	A1439	G1380	U1300	A1145	G952	C876	C876
C	A1665	G1514	U1586	C1440	G1381	A1301	U1148	C953	G877	G877
C	G1666	U1515	U1587	U1441	U1382	G1302		U946	C878	C878
C	A1667	U1516	U1588	U1442	A1383	U1303		G952	C879	C879
C	U1668	U1517	U1589	U1443	G1384	U1304		C953	G880	G880
C	G1669	U1518	U1590	U1444	G1385	C1305		U946	C881	C881
C	U1670	U1519	U1591	U1445		U1306				
C	C1671	U1520	U1592	U1446		U1307				
C		U1521	U1593	U1447		U1308				
C		U1522	U1594	U1448						
C		U1523	U1595	U1449						
C		U1524	U1596							
C		U1525	U1597							
C		U1526	U1598							
C		U1527	U1599							
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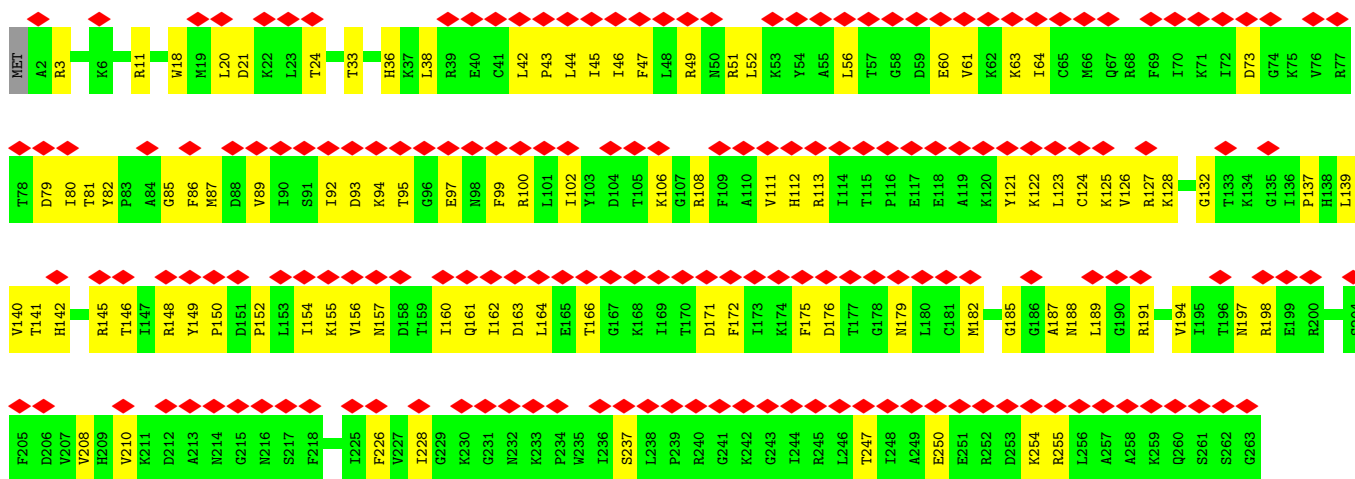


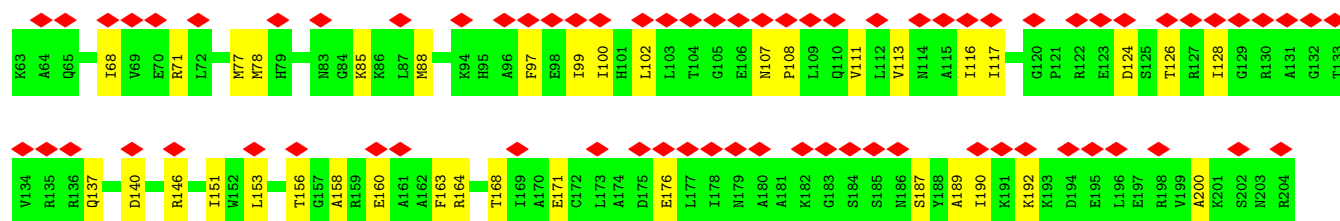


• Molecule 52: 40S ribosomal protein S3

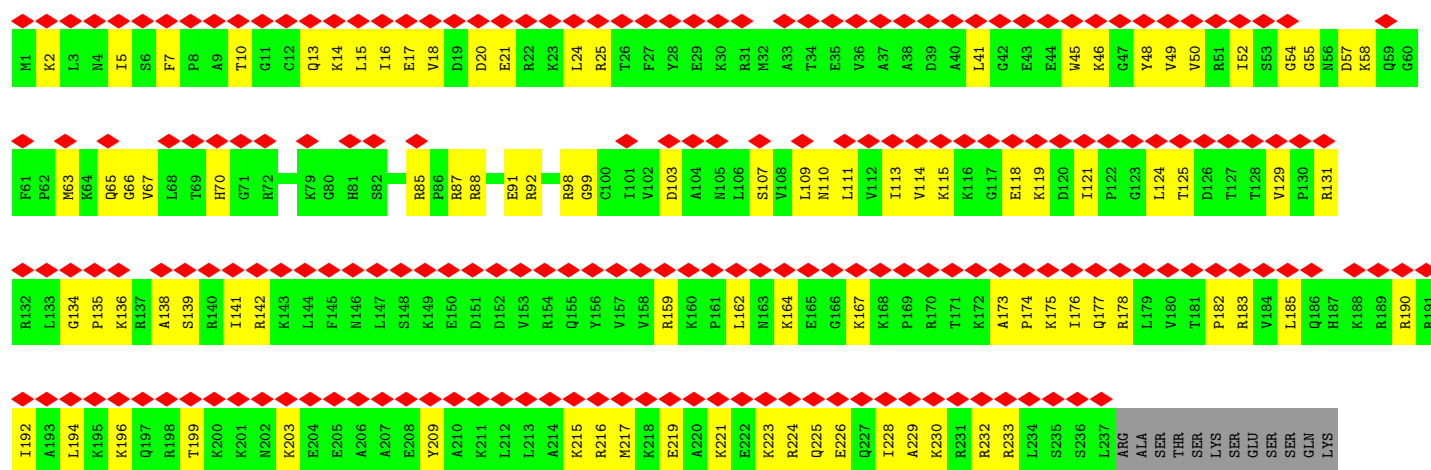
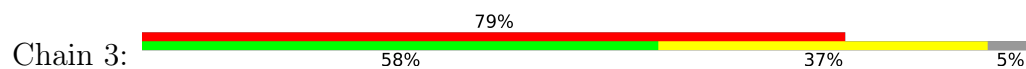


• Molecule 53: 40S ribosomal protein S4, X isoform

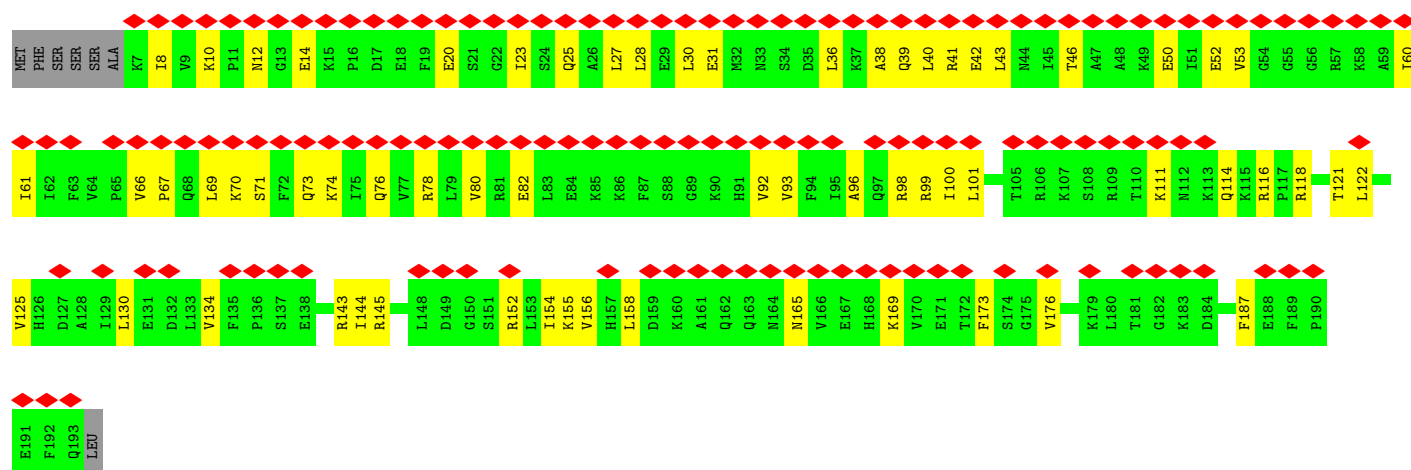
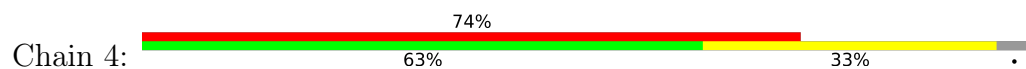




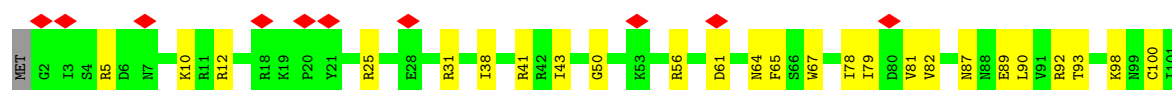
• Molecule 55: 40S ribosomal protein S6

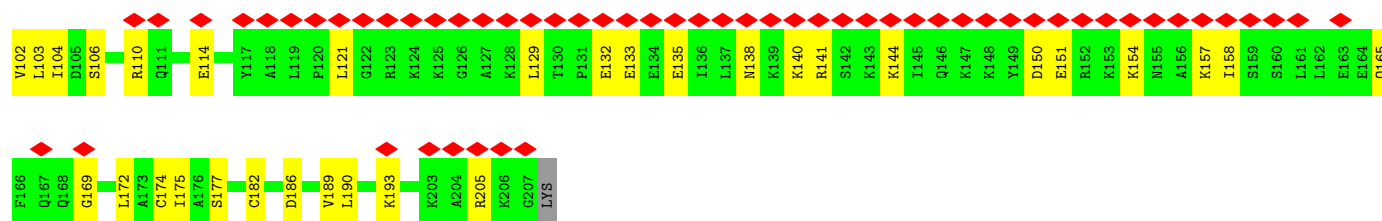


• Molecule 56: 40S ribosomal protein S7

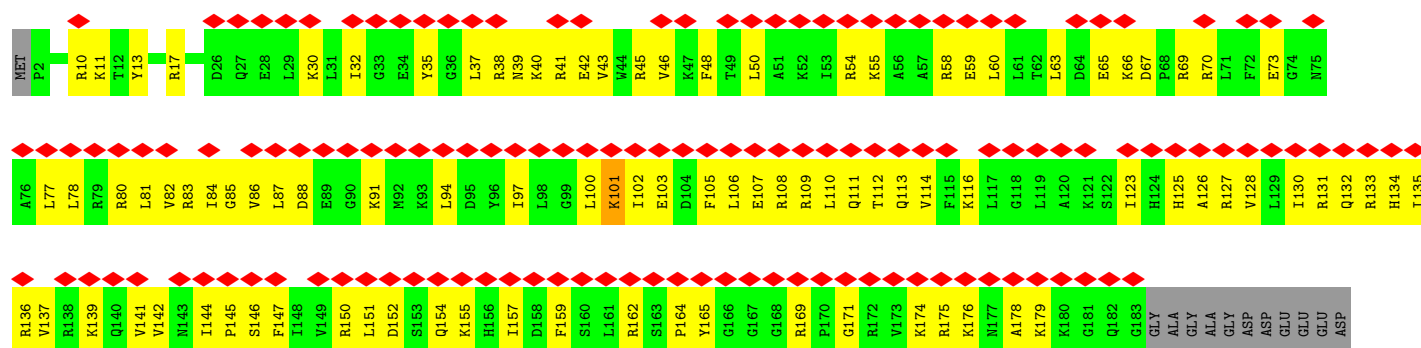


• Molecule 57: 40S ribosomal protein S8

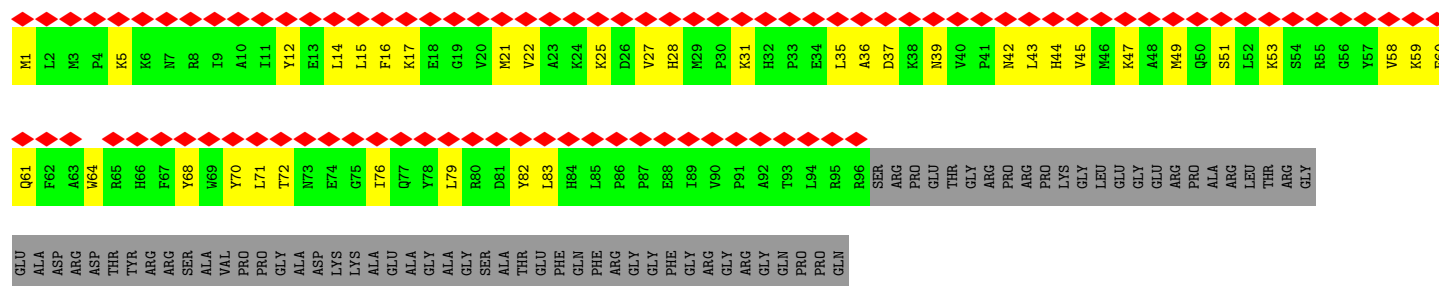




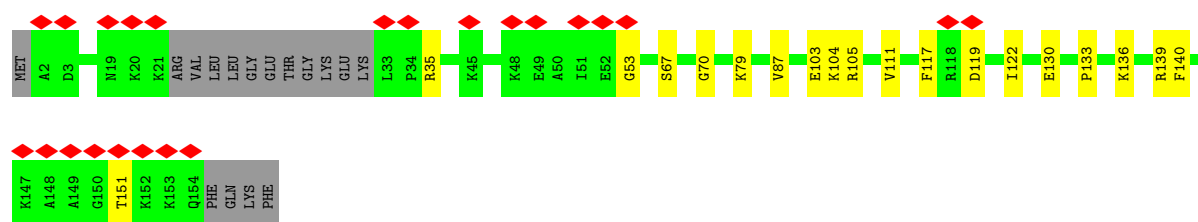
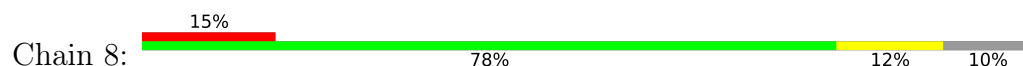
- Molecule 58: 40S ribosomal protein S9



- Molecule 59: 40S ribosomal protein S10

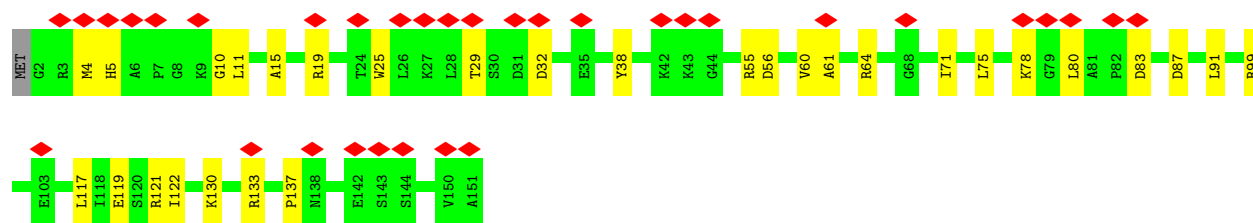


- Molecule 60: 40S ribosomal protein S11

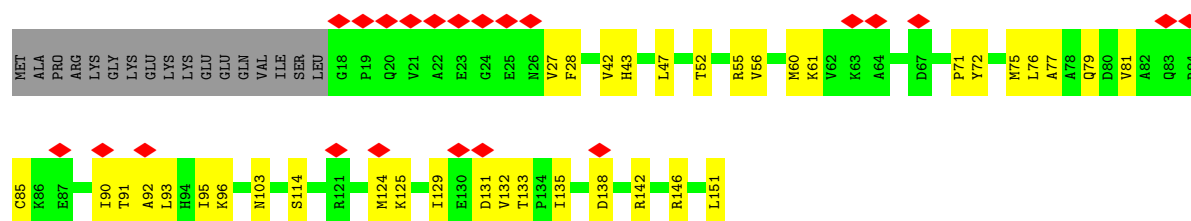


- Molecule 61: 40S ribosomal protein S13

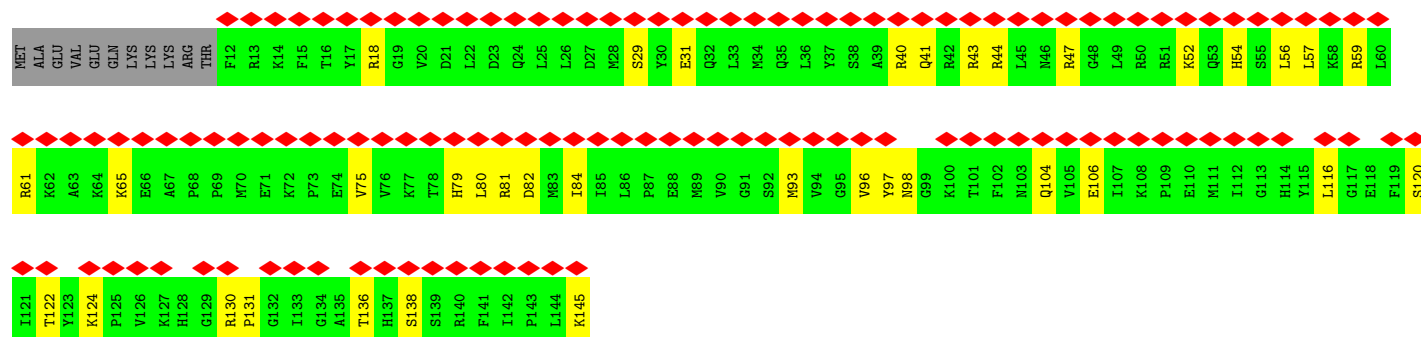
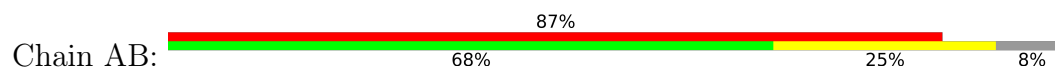




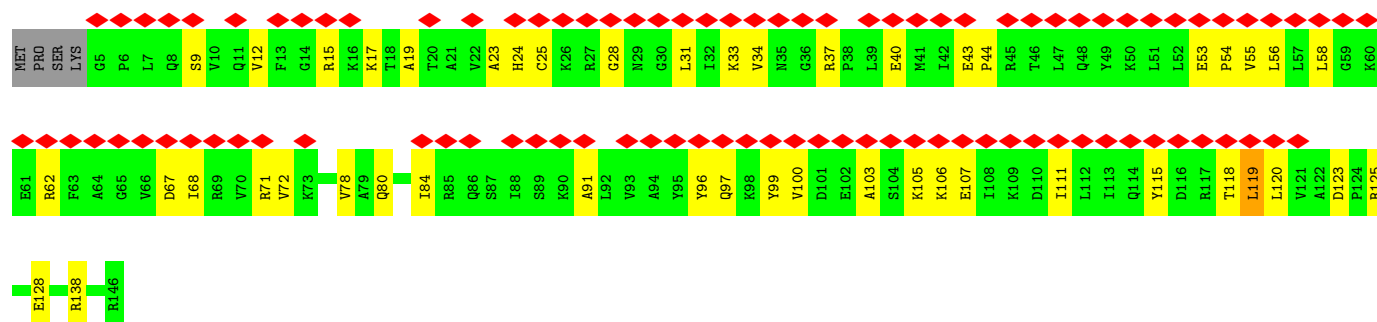
- Molecule 62: 40S ribosomal protein S14



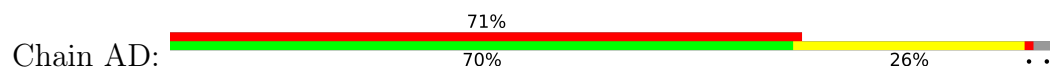
- Molecule 63: 40S ribosomal protein S15



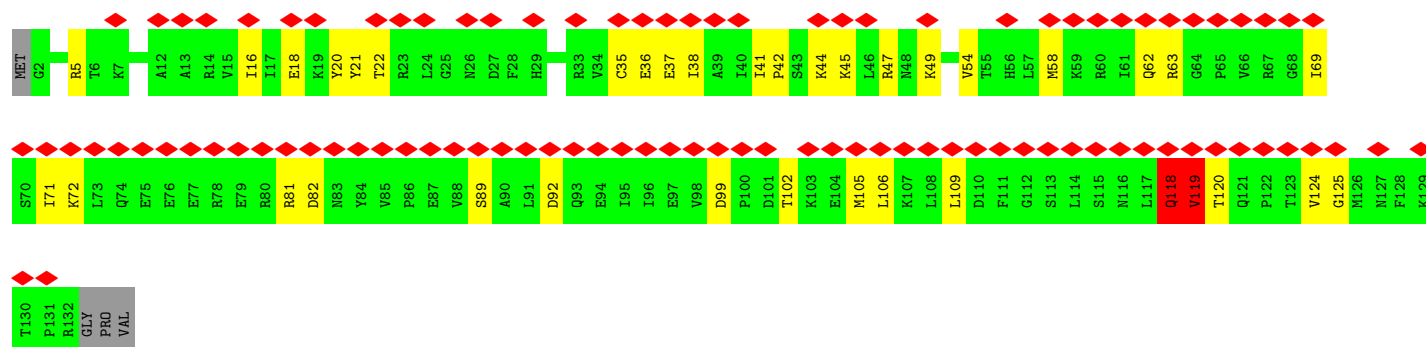
- Molecule 64: 40S ribosomal protein S16



- Molecule 65: 40S ribosomal protein S17

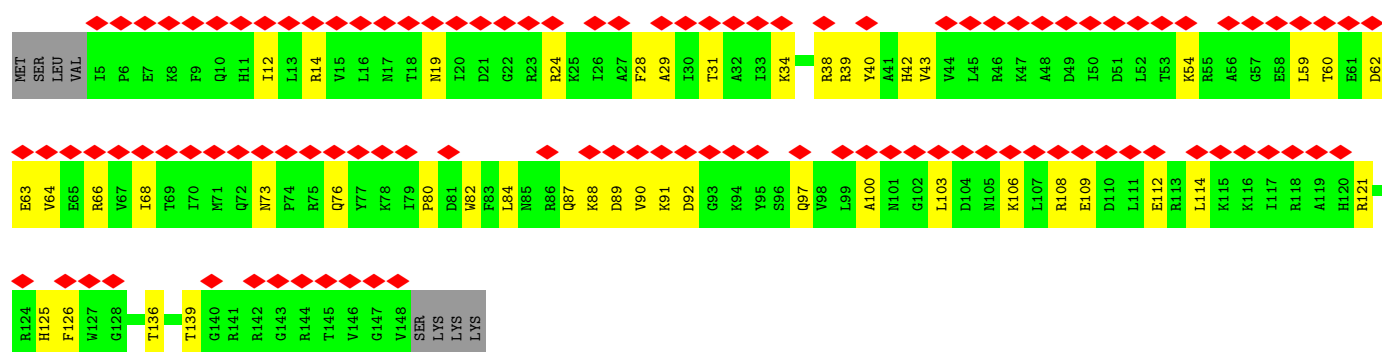






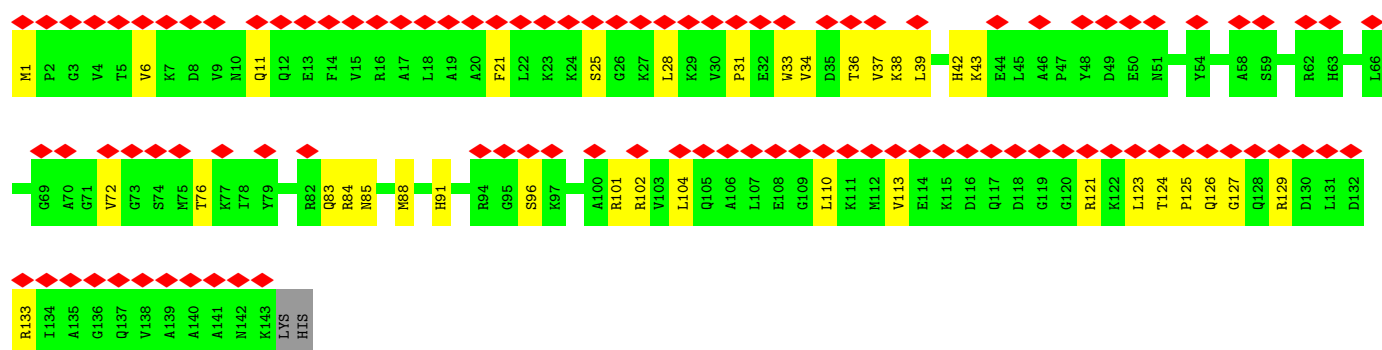
• Molecule 66: 40S ribosomal protein S18

Chain AE:



• Molecule 67: 40S ribosomal protein S19

Chain AF:



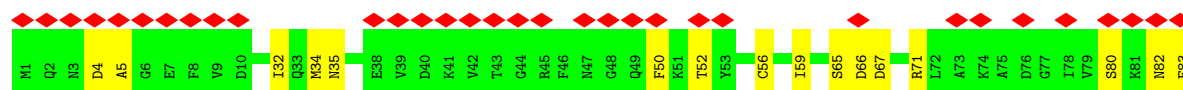
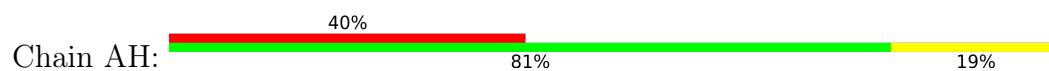
• Molecule 68: 40S ribosomal protein S20

Chain AG:

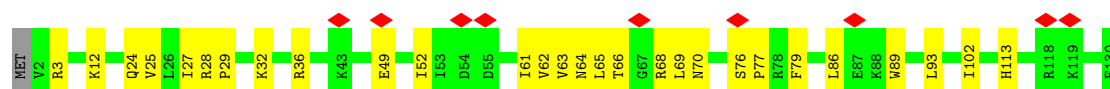
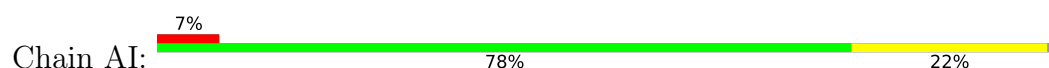




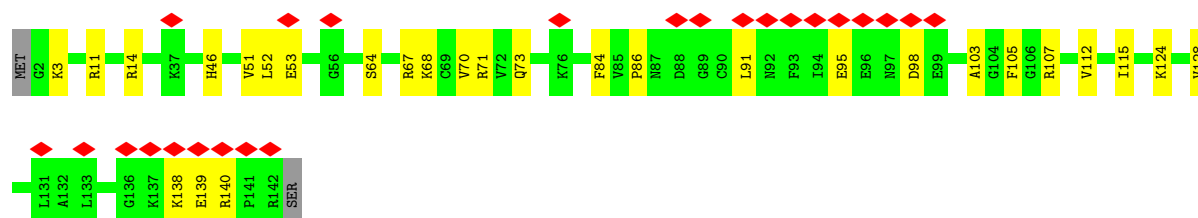
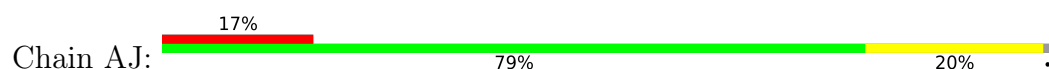
- Molecule 69: 40S ribosomal protein S21



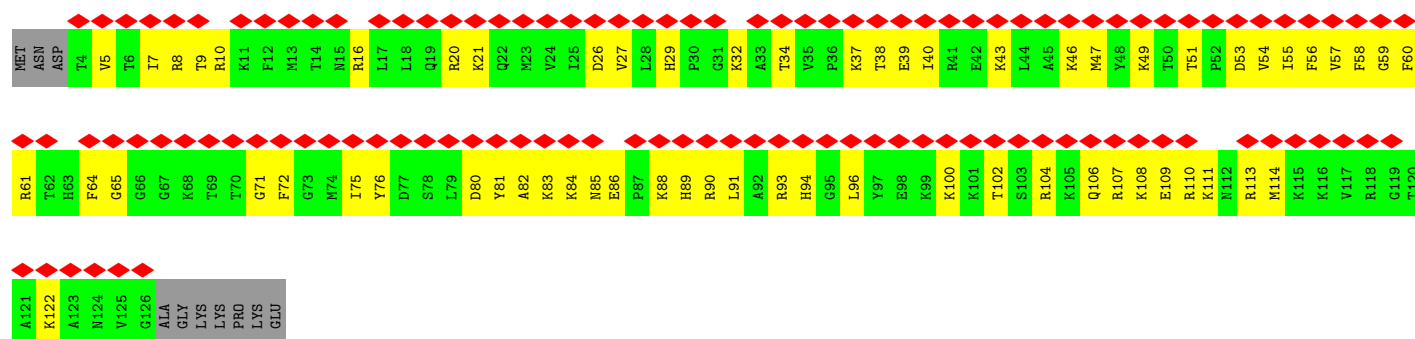
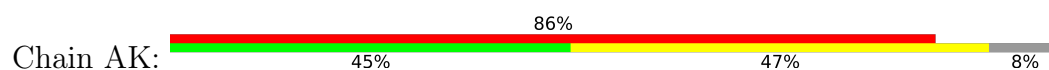
- Molecule 70: 40S ribosomal protein S15a



- Molecule 71: 40S ribosomal protein S23



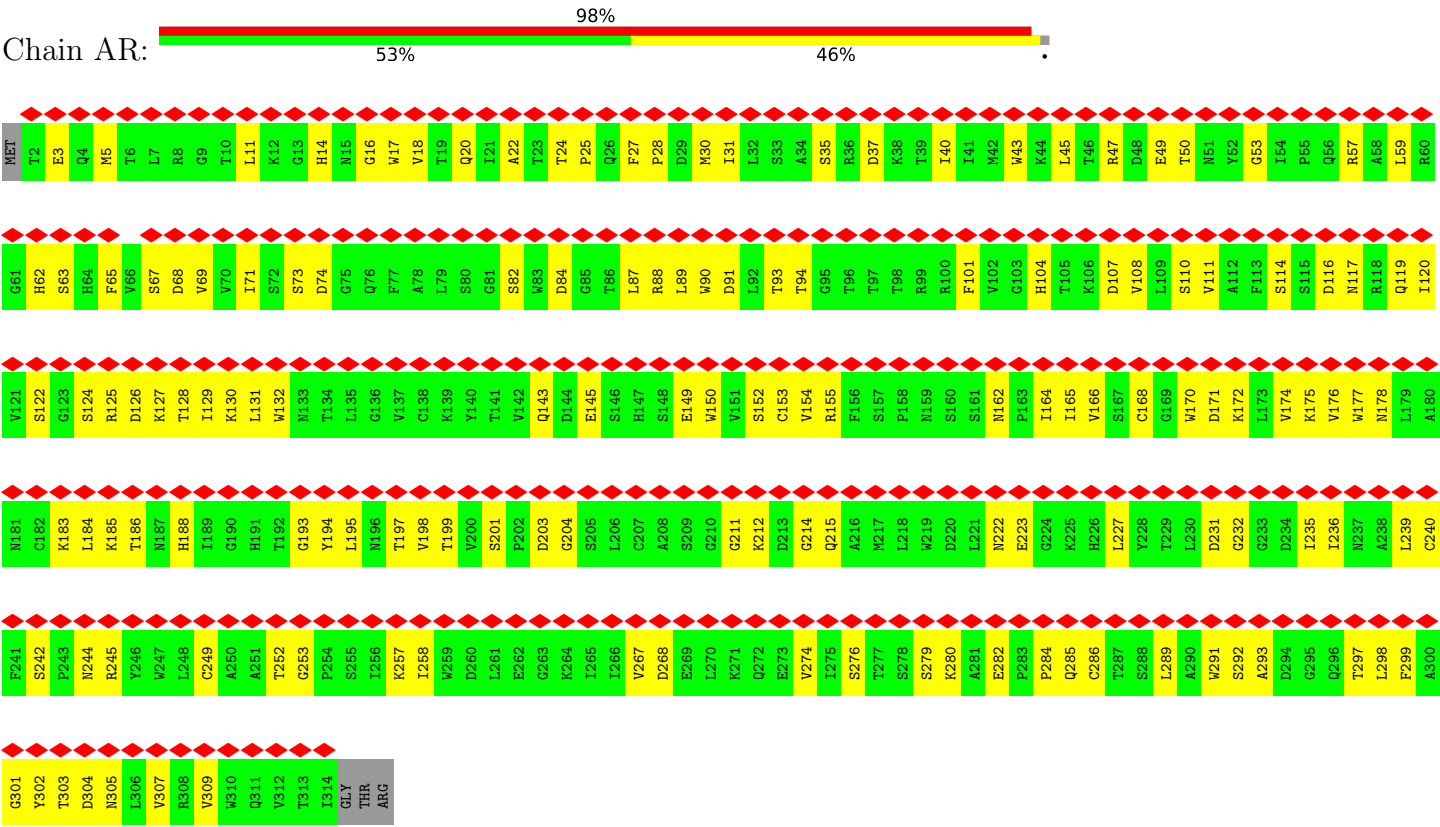
- Molecule 72: 40S ribosomal protein S24



- Molecule 73: 40S ribosomal protein S25







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	148464	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0191	Depositor
Map size ( $\text{\AA}$ )	439.9, 439.9, 439.9	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M2G, 2MG, 4AC, 1MG, ZN, OMG, OMC, 5MU, 6MZ, OMU, MG, UY1, 56B, GAL, B8N, MA6, 3AU, 1MA, H2U, PSU, G7M, A2M, 5MC, UR3

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	A	0.13	0/250	0.20	0/385
2	B	0.17	0/1402	0.27	0/2179
3	D	0.27	2/81567 (0.0%)	0.31	6/127232 (0.0%)
4	E	0.25	0/2858	0.27	0/4455
5	F	0.25	0/3675	0.29	0/5725
6	G	0.27	0/1929	0.48	0/2586
7	H	0.25	0/3279	0.44	0/4388
8	I	0.26	0/2938	0.44	0/3946
9	J	0.21	0/2425	0.42	0/3248
10	K	0.22	0/1785	0.46	0/2394
11	L	0.27	0/1905	0.47	0/2539
12	M	0.21	0/1863	0.45	1/2510 (0.0%)
13	N	0.23	0/1537	0.44	0/2066
14	O	0.22	0/1699	0.43	0/2270
15	P	0.19	0/1385	0.43	0/1852
16	Q	0.23	0/1713	0.43	0/2293
17	R	0.23	0/1142	0.44	0/1527
18	S	0.28	0/1746	0.44	0/2338
19	T	0.27	0/1673	0.44	0/2238
20	U	0.26	0/1300	0.45	0/1746
21	V	0.27	0/1537	0.45	0/2052
22	W	0.23	0/1524	0.42	0/2013
23	X	0.26	0/1493	0.41	0/2003
24	Y	0.24	0/1326	0.41	0/1770
25	Z	0.18	0/835	0.44	0/1122
26	a	0.24	0/993	0.41	0/1332
27	b	0.21	0/541	0.37	0/720
28	c	0.22	0/998	0.41	0/1340
29	d	0.23	0/1132	0.41	0/1504
30	e	0.22	0/1130	0.41	0/1507
31	f	0.26	0/1191	0.39	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	g	0.22	0/844	0.50	0/1115
33	h	0.22	0/765	0.37	0/1027
34	i	0.24	0/903	0.44	0/1216
35	j	0.25	0/1071	0.37	0/1429
36	k	0.28	0/895	0.53	0/1198
37	l	0.25	0/898	0.49	0/1197
38	m	0.20	0/1018	0.38	0/1344
39	n	0.18	0/843	0.36	0/1115
40	o	0.26	0/720	0.48	0/952
41	p	0.21	0/575	0.44	0/761
42	q	0.24	0/454	0.37	0/599
43	r	0.22	0/435	0.40	0/575
44	s	0.24	0/240	0.48	0/305
45	t	0.24	0/876	0.48	0/1156
46	u	0.24	0/718	0.39	0/953
47	v	0.26	0/1017	0.45	0/1364
48	w	0.21	0/37158	0.30	0/57908
49	x	0.16	0/1732	0.42	0/2355
50	y	0.15	0/1752	0.37	0/2345
51	z	0.17	0/1668	0.39	0/2254
52	0	0.16	0/1672	0.40	0/2250
53	1	0.17	0/2112	0.42	0/2842
54	2	0.15	0/1485	0.43	0/1998
55	3	0.18	0/1940	0.43	0/2583
56	4	0.15	0/1533	0.45	0/2053
57	5	0.17	0/1703	0.40	0/2275
58	6	0.21	0/1531	0.50	0/2045
59	7	0.15	0/834	0.40	0/1125
60	8	0.17	0/1170	0.38	0/1568
61	9	0.17	0/1232	0.37	0/1656
62	AA	0.20	0/1015	0.49	0/1361
63	AB	0.14	0/1126	0.40	0/1505
64	AC	0.16	0/1146	0.44	0/1534
65	AD	0.17	0/1071	0.52	3/1438 (0.2%)
66	AE	0.17	0/1187	0.49	0/1593
67	AF	0.15	0/1130	0.39	0/1515
68	AG	0.15	0/809	0.44	0/1087
69	AH	0.16	0/643	0.35	0/860
70	AI	0.18	0/1051	0.40	0/1406
71	AJ	0.16	0/1116	0.38	0/1490
72	AK	0.17	0/1019	0.48	0/1355
73	AL	0.15	0/688	0.40	0/921
74	AM	0.20	0/805	0.43	0/1079

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	AN	0.17	0/657	0.41	0/883
76	AO	0.17	0/481	0.48	0/643
77	AP	0.18	0/375	0.49	0/492
78	AQ	0.18	0/458	0.54	0/602
79	AR	0.14	0/2493	0.46	0/3394
All	All	0.23	2/217835 (0.0%)	0.36	10/319592 (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
6	G	0	2
7	H	0	1
8	I	0	2
10	K	0	1
11	L	0	1
16	Q	0	1
20	U	0	1
21	V	0	1
22	W	0	1
24	Y	0	1
29	d	0	1
32	g	0	1
40	o	0	1
58	6	0	1
65	AD	0	1
All	All	0	17

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2415	OMU	O3'-P	5.14	1.61	1.56
3	D	3785	A2M	O3'-P	5.09	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2101	C	OP1-P-OP2	-13.30	79.71	119.60
3	D	2100	A	OP2-P-O3'	-12.50	70.50	108.00
3	D	2101	C	O5'-P-OP1	-9.67	78.98	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2100	A	OP1-P-O3'	9.52	136.56	108.00
3	D	2101	C	O5'-P-OP2	7.16	129.49	108.00

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	G	123	ARG	Peptide
6	G	239	ALA	Peptide
7	H	258	HIS	Peptide
8	I	110	ARG	Peptide
8	I	91	ALA	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	A	226	0	114	3	0
2	B	1647	0	832	20	0
3	D	75336	0	38155	798	0
4	E	2558	0	1296	23	0
5	F	3315	0	1685	41	0
6	G	1891	0	1986	31	0
7	H	3211	0	3356	49	0
8	I	2884	0	3060	43	0
9	J	2379	0	2408	35	0
10	K	1751	0	1905	35	0
11	L	1870	0	1996	22	0
12	M	1832	0	1962	33	0
13	N	1518	0	1601	32	0
14	O	1660	0	1692	22	0
15	P	1362	0	1399	33	0
16	Q	1682	0	1792	34	0
17	R	1120	0	1187	24	0
18	S	1701	0	1749	21	0
19	T	1641	0	1788	22	0
20	U	1273	0	1304	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	V	1513	0	1628	16	0
22	W	1508	0	1664	14	0
23	X	1453	0	1490	15	0
24	Y	1298	0	1366	11	0
25	Z	821	0	839	13	0
26	a	979	0	1039	10	0
27	b	528	0	541	2	0
28	c	981	0	1062	13	0
29	d	1115	0	1205	19	0
30	e	1107	0	1182	23	0
31	f	1162	0	1213	23	0
32	g	832	0	883	13	0
33	h	755	0	791	9	0
34	i	888	0	930	8	0
35	j	1053	0	1147	7	0
36	k	876	0	912	12	0
37	l	888	0	981	14	0
38	m	1010	0	1143	11	0
39	n	832	0	917	12	0
40	o	705	0	737	8	0
41	p	569	0	637	5	0
42	q	444	0	483	8	0
43	r	429	0	466	7	0
44	s	239	0	289	0	0
45	t	862	0	930	13	0
46	u	708	0	756	5	0
47	v	1002	0	1068	16	0
48	w	34933	0	17694	668	0
49	x	1695	0	1690	35	0
50	y	1725	0	1800	32	0
51	z	1633	0	1716	29	0
52	0	1646	0	1734	54	0
53	1	2070	0	2166	78	0
54	2	1464	0	1505	42	0
55	3	1917	0	2078	77	0
56	4	1510	0	1606	52	0
57	5	1674	0	1739	46	0
58	6	1506	0	1618	104	0
59	7	810	0	836	27	0
60	8	1150	0	1199	15	0
61	9	1208	0	1294	25	0
62	AA	1002	0	1023	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	AB	1103	0	1156	30	0
64	AC	1128	0	1195	36	0
65	AD	1057	0	1110	33	0
66	AE	1169	0	1198	37	0
67	AF	1111	0	1144	27	0
68	AG	799	0	850	41	0
69	AH	636	0	637	11	0
70	AI	1034	0	1080	24	0
71	AJ	1098	0	1167	21	0
72	AK	1002	0	1067	67	0
73	AL	680	0	744	18	0
74	AM	792	0	842	13	0
75	AN	643	0	650	15	0
76	AO	479	0	507	6	0
77	AP	370	0	373	18	0
78	AQ	452	0	494	18	0
79	AR	2436	0	2393	107	0
80	8	1	0	0	0	0
80	A	1	0	0	0	0
80	AA	1	0	0	0	0
80	AF	1	0	0	0	0
80	AJ	1	0	0	0	0
80	AM	1	0	0	0	0
80	D	401	0	0	0	0
80	E	10	0	0	0	0
80	F	5	0	0	0	0
80	G	2	0	0	0	0
80	H	1	0	0	0	0
80	I	1	0	0	0	0
80	N	1	0	0	0	0
80	O	1	0	0	0	0
80	S	1	0	0	0	0
80	U	2	0	0	0	0
80	V	2	0	0	0	0
80	X	1	0	0	0	0
80	a	1	0	0	0	0
80	g	1	0	0	0	0
80	j	1	0	0	0	0
80	k	1	0	0	0	0
80	l	1	0	0	0	0
80	w	100	0	0	0	0
81	B	11	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	AM	1	0	0	0	0
82	AP	1	0	0	0	0
82	o	1	0	0	0	0
82	r	1	0	0	0	0
82	t	1	0	0	0	0
82	u	1	0	0	0	0
All	All	207902	0	153881	3001	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 8.

The worst 5 of 3001 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)
3:D:4745:G:H1	3:D:4955:A:N6	1.41	1.16
3:D:1:C:N4	5:F:156:U:H3	1.48	1.09
48:w:1471:C:N4	48:w:1476:A:H62	1.63	0.97
48:w:1471:C:H42	48:w:1476:A:H62	1.14	0.96
48:w:39:A:H62	48:w:515:G:H21	1.10	0.95

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	
6	G	245/257 (95%)	228 (93%)	17 (7%)	0	100	100
7	H	396/403 (98%)	375 (95%)	21 (5%)	0	100	100
8	I	361/427 (84%)	338 (94%)	23 (6%)	0	100	100
9	J	291/297 (98%)	271 (93%)	20 (7%)	0	100	100
10	K	211/288 (73%)	189 (90%)	22 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	L	223/248 (90%)	213 (96%)	10 (4%)	0	100	100
12	M	223/266 (84%)	208 (93%)	15 (7%)	0	100	100
13	N	188/192 (98%)	176 (94%)	12 (6%)	0	100	100
14	O	202/214 (94%)	187 (93%)	15 (7%)	0	100	100
15	P	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
16	Q	206/211 (98%)	189 (92%)	15 (7%)	2 (1%)	12	18
17	R	134/215 (62%)	122 (91%)	12 (9%)	0	100	100
18	S	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
19	T	198/203 (98%)	191 (96%)	7 (4%)	0	100	100
20	U	155/184 (84%)	143 (92%)	12 (8%)	0	100	100
21	V	185/188 (98%)	174 (94%)	11 (6%)	0	100	100
22	W	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
23	X	173/176 (98%)	160 (92%)	13 (8%)	0	100	100
24	Y	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
25	Z	99/128 (77%)	92 (93%)	6 (6%)	1 (1%)	12	18
26	a	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
27	b	61/157 (39%)	59 (97%)	2 (3%)	0	100	100
28	c	118/156 (76%)	110 (93%)	8 (7%)	0	100	100
29	d	132/145 (91%)	123 (93%)	9 (7%)	0	100	100
30	e	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
31	f	145/148 (98%)	132 (91%)	13 (9%)	0	100	100
32	g	100/159 (63%)	92 (92%)	6 (6%)	2 (2%)	6	7
33	h	95/115 (83%)	94 (99%)	1 (1%)	0	100	100
34	i	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
35	j	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
36	k	107/110 (97%)	101 (94%)	6 (6%)	0	100	100
37	l	110/117 (94%)	104 (94%)	6 (6%)	0	100	100
38	m	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
39	n	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
40	o	84/97 (87%)	79 (94%)	4 (5%)	1 (1%)	10	15
41	p	67/70 (96%)	60 (90%)	7 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	q	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	r	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
44	s	23/25 (92%)	23 (100%)	0	0	100	100
45	t	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
46	u	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
47	v	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
49	x	213/295 (72%)	205 (96%)	7 (3%)	1 (0%)	24	35
50	y	210/264 (80%)	196 (93%)	14 (7%)	0	100	100
51	z	210/293 (72%)	198 (94%)	11 (5%)	1 (0%)	24	35
52	0	210/243 (86%)	190 (90%)	20 (10%)	0	100	100
53	1	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
54	2	185/204 (91%)	169 (91%)	16 (9%)	0	100	100
55	3	235/249 (94%)	227 (97%)	8 (3%)	0	100	100
56	4	185/194 (95%)	168 (91%)	17 (9%)	0	100	100
57	5	204/208 (98%)	196 (96%)	8 (4%)	0	100	100
58	6	180/194 (93%)	166 (92%)	14 (8%)	0	100	100
59	7	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
60	8	138/158 (87%)	128 (93%)	10 (7%)	0	100	100
61	9	148/151 (98%)	140 (95%)	8 (5%)	0	100	100
62	AA	132/151 (87%)	120 (91%)	12 (9%)	0	100	100
63	AB	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
64	AC	140/146 (96%)	124 (89%)	15 (11%)	1 (1%)	18	27
65	AD	129/135 (96%)	108 (84%)	19 (15%)	2 (2%)	7	10
66	AE	142/152 (93%)	128 (90%)	14 (10%)	0	100	100
67	AF	141/145 (97%)	131 (93%)	10 (7%)	0	100	100
68	AG	100/119 (84%)	92 (92%)	8 (8%)	0	100	100
69	AH	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
70	AI	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
71	AJ	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
72	AK	121/133 (91%)	115 (95%)	6 (5%)	0	100	100
73	AL	84/125 (67%)	76 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	AM	97/115 (84%)	93 (96%)	4 (4%)	0	100	100
75	AN	81/84 (96%)	69 (85%)	11 (14%)	1 (1%)	10	15
76	AO	59/69 (86%)	53 (90%)	6 (10%)	0	100	100
77	AP	43/56 (77%)	43 (100%)	0	0	100	100
78	AQ	55/59 (93%)	48 (87%)	7 (13%)	0	100	100
79	AR	311/317 (98%)	268 (86%)	43 (14%)	0	100	100
All	All	10947/12400 (88%)	10216 (93%)	719 (7%)	12 (0%)	49	63

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	48	PRO
32	g	111	ARG
64	AC	119	LEU
65	AD	119	VAL
32	g	110	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	189/199 (95%)	189 (100%)	0	100	100
7	H	346/349 (99%)	346 (100%)	0	100	100
8	I	301/348 (86%)	301 (100%)	0	100	100
9	J	245/250 (98%)	245 (100%)	0	100	100
10	K	193/252 (77%)	193 (100%)	0	100	100
11	L	194/215 (90%)	194 (100%)	0	100	100
12	M	195/223 (87%)	195 (100%)	0	100	100
13	N	169/171 (99%)	169 (100%)	0	100	100
14	O	174/181 (96%)	174 (100%)	0	100	100
15	P	143/149 (96%)	143 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Q	174/177 (98%)	174 (100%)	0	100	100
17	R	116/161 (72%)	116 (100%)	0	100	100
18	S	171/172 (99%)	171 (100%)	0	100	100
19	T	172/174 (99%)	172 (100%)	0	100	100
20	U	138/163 (85%)	138 (100%)	0	100	100
21	V	164/165 (99%)	164 (100%)	0	100	100
22	W	159/175 (91%)	159 (100%)	0	100	100
23	X	156/157 (99%)	156 (100%)	0	100	100
24	Y	139/140 (99%)	139 (100%)	0	100	100
25	Z	90/115 (78%)	90 (100%)	0	100	100
26	a	101/107 (94%)	101 (100%)	0	100	100
27	b	55/126 (44%)	55 (100%)	0	100	100
28	c	107/133 (80%)	107 (100%)	0	100	100
29	d	124/135 (92%)	124 (100%)	0	100	100
30	e	117/118 (99%)	117 (100%)	0	100	100
31	f	120/121 (99%)	120 (100%)	0	100	100
32	g	81/126 (64%)	81 (100%)	0	100	100
33	h	82/97 (84%)	82 (100%)	0	100	100
34	i	98/110 (89%)	98 (100%)	0	100	100
35	j	114/121 (94%)	114 (100%)	0	100	100
36	k	88/89 (99%)	88 (100%)	0	100	100
37	l	96/100 (96%)	96 (100%)	0	100	100
38	m	109/110 (99%)	109 (100%)	0	100	100
39	n	86/89 (97%)	86 (100%)	0	100	100
40	o	73/80 (91%)	72 (99%)	1 (1%)	59	77
41	p	64/65 (98%)	64 (100%)	0	100	100
42	q	47/48 (98%)	47 (100%)	0	100	100
43	r	48/116 (41%)	48 (100%)	0	100	100
44	s	24/24 (100%)	24 (100%)	0	100	100
45	t	93/94 (99%)	93 (100%)	0	100	100
46	u	74/75 (99%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	v	109/121 (90%)	109 (100%)	0	100	100
49	x	178/243 (73%)	178 (100%)	0	100	100
50	y	194/231 (84%)	194 (100%)	0	100	100
51	z	176/225 (78%)	176 (100%)	0	100	100
52	0	175/202 (87%)	175 (100%)	0	100	100
53	1	223/225 (99%)	223 (100%)	0	100	100
54	2	154/170 (91%)	154 (100%)	0	100	100
55	3	206/218 (94%)	206 (100%)	0	100	100
56	4	168/174 (97%)	168 (100%)	0	100	100
57	5	175/180 (97%)	175 (100%)	0	100	100
58	6	160/168 (95%)	160 (100%)	0	100	100
59	7	87/136 (64%)	87 (100%)	0	100	100
60	8	125/142 (88%)	125 (100%)	0	100	100
61	9	130/131 (99%)	130 (100%)	0	100	100
62	AA	104/119 (87%)	104 (100%)	0	100	100
63	AB	120/130 (92%)	120 (100%)	0	100	100
64	AC	117/121 (97%)	117 (100%)	0	100	100
65	AD	117/122 (96%)	117 (100%)	0	100	100
66	AE	119/132 (90%)	118 (99%)	1 (1%)	73	85
67	AF	113/115 (98%)	113 (100%)	0	100	100
68	AG	89/107 (83%)	89 (100%)	0	100	100
69	AH	67/67 (100%)	67 (100%)	0	100	100
70	AI	112/113 (99%)	112 (100%)	0	100	100
71	AJ	113/115 (98%)	113 (100%)	0	100	100
72	AK	106/115 (92%)	106 (100%)	0	100	100
73	AL	73/103 (71%)	73 (100%)	0	100	100
74	AM	86/98 (88%)	86 (100%)	0	100	100
75	AN	73/76 (96%)	73 (100%)	0	100	100
76	AO	54/62 (87%)	54 (100%)	0	100	100
77	AP	39/49 (80%)	39 (100%)	0	100	100
78	AQ	46/48 (96%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
79	AR	272/275 (99%)	272 (100%)	0	100	100
All	All	9509/10553 (90%)	9507 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	o	48	ASN
66	AE	87	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
54	2	137	GLN
66	AE	101	ASN
55	3	70	HIS
60	8	18	GLN
69	AH	2	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	10/14 (71%)	1 (10%)	0
2	B	75/76 (98%)	18 (24%)	3 (4%)
3	D	3496/5070 (68%)	616 (17%)	24 (0%)
4	E	119/120 (99%)	14 (11%)	0
48	w	1624/1869 (86%)	418 (25%)	0
5	F	155/156 (99%)	28 (18%)	2 (1%)
All	All	5479/7305 (75%)	1095 (19%)	29 (0%)

5 of 1095 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	21	U
2	B	4	U
2	B	5	C
2	B	6	2MG
2	B	11	C

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	2101	C
5	F	16	G
3	D	2763	U
3	D	4699	U
3	D	2675	G

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

211 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$
48	PSU	w	109	48	18,21,22	1.08	1 (5%)	22,30,33	1.84	5 (22%)
48	OMU	w	121	48	19,22,23	2.87	6 (31%)	26,31,34	1.60	5 (19%)
3	OMG	D	3792	3	23,26,27	2.56	8 (34%)	33,38,41	1.89	9 (27%)
3	6MZ	D	4220	3	22,25,26	2.84	4 (18%)	30,36,39	2.20	10 (33%)
3	UR3	D	4530	80,3	19,22,23	2.66	7 (36%)	26,32,35	1.30	2 (7%)
48	A2M	w	468	48	22,25,26	1.55	2 (9%)	31,36,39	1.02	2 (6%)
3	PSU	D	4361	3	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
3	1MA	D	1322	3	21,25,26	0.71	1 (4%)	31,37,40	0.79	1 (3%)
3	PSU	D	4471	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
3	A2M	D	400	3	22,25,26	1.41	1 (4%)	31,36,39	0.98	2 (6%)
3	A2M	D	1524	3	22,25,26	1.48	2 (9%)	31,36,39	1.04	3 (9%)
3	A2M	D	3825	3	22,25,26	1.37	1 (4%)	31,36,39	1.02	2 (6%)
48	PSU	w	1056	48	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
48	PSU	w	1625	48	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
2	PSU	B	35	2,1	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
48	PSU	w	863	48	18,21,22	1.07	1 (5%)	22,30,33	1.80	4 (18%)
3	A2M	D	3724	3	22,25,26	1.40	1 (4%)	31,36,39	0.97	3 (9%)
48	PSU	w	814	48	18,21,22	1.02	1 (5%)	22,30,33	1.70	4 (18%)
48	A2M	w	1678	48	22,25,26	1.49	3 (13%)	31,36,39	1.04	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	A2M	w	1031	48	22,25,26	1.39	1 (4%)	31,36,39	1.00	1 (3%)
48	MA6	w	1851	48	23,26,27	1.28	4 (17%)	34,38,41	2.29	11 (32%)
48	PSU	w	686	48	18,21,22	1.06	1 (5%)	22,30,33	1.82	4 (18%)
48	OMG	w	436	48	23,26,27	2.61	8 (34%)	33,38,41	1.97	9 (27%)
5	OMG	F	75	5	23,26,27	2.59	8 (34%)	33,38,41	1.91	9 (27%)
3	PSU	D	3762	3	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
48	A2M	w	159	48	22,25,26	1.62	4 (18%)	31,36,39	1.02	3 (9%)
48	PSU	w	649	48	18,21,22	1.07	1 (5%)	22,30,33	1.81	5 (22%)
3	PSU	D	4299	3	18,21,22	1.02	1 (5%)	22,30,33	1.74	4 (18%)
3	OMU	D	4498	80,3	19,22,23	2.79	6 (31%)	26,31,34	1.73	5 (19%)
48	PSU	w	822	48	18,21,22	1.10	1 (5%)	22,30,33	1.74	4 (18%)
2	56B	B	34	2,81	29,35,36	2.84	10 (34%)	36,52,55	2.30	7 (19%)
3	PSU	D	4403	80,3	18,21,22	1.07	1 (5%)	22,30,33	1.80	5 (22%)
3	OMG	D	2424	3	23,26,27	2.59	9 (39%)	33,38,41	1.92	10 (30%)
3	OMU	D	4620	3	19,22,23	2.79	6 (31%)	26,31,34	1.73	5 (19%)
3	OMC	D	4456	3	19,22,23	2.86	8 (42%)	26,31,34	0.77	0
3	PSU	D	1782	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
48	OMG	w	683	48	23,26,27	2.60	8 (34%)	33,38,41	1.92	9 (27%)
48	OMU	w	1442	80,48	19,22,23	2.93	8 (42%)	26,31,34	1.68	4 (15%)
3	PSU	D	3734	3	18,21,22	1.06	1 (5%)	22,30,33	1.85	5 (22%)
48	OMG	w	1490	80,48	23,26,27	2.61	8 (34%)	33,38,41	1.90	9 (27%)
3	OMG	D	3899	3	23,26,27	2.55	9 (39%)	33,38,41	1.96	10 (30%)
3	A2M	D	2815	3	22,25,26	1.51	1 (4%)	31,36,39	1.01	3 (9%)
3	A2M	D	3830	3	22,25,26	1.38	1 (4%)	31,36,39	1.07	2 (6%)
3	OMC	D	2351	80,3	19,22,23	2.85	8 (42%)	26,31,34	0.92	2 (7%)
3	OMG	D	3944	3	23,26,27	2.61	8 (34%)	33,38,41	1.96	9 (27%)
3	OMG	D	4494	3	23,26,27	2.58	9 (39%)	33,38,41	1.93	9 (27%)
3	5MC	D	4447	80,3	18,22,23	3.66	7 (38%)	26,32,35	1.14	1 (3%)
3	A2M	D	1326	3	22,25,26	1.36	1 (4%)	31,36,39	1.01	2 (6%)
48	PSU	w	105	48	18,21,22	1.04	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	4353	3	18,21,22	1.05	1 (5%)	22,30,33	1.85	4 (18%)
48	G7M	w	1639	2,48	23,26,27	2.82	8 (34%)	35,39,42	1.75	8 (22%)
48	OMU	w	116	48	19,22,23	2.90	7 (36%)	26,31,34	1.67	4 (15%)
48	PSU	w	1004	48	18,21,22	1.03	1 (5%)	22,30,33	1.77	4 (18%)
2	UY1	B	39	2	19,22,23	1.24	2 (10%)	22,31,34	0.97	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	4AC	w	1842	48	21,24,25	0.57	0	29,34,37	1.19	4 (13%)
3	PSU	D	4457	3	18,21,22	1.02	1 (5%)	22,30,33	1.75	5 (22%)
3	OMC	D	4536	3	19,22,23	2.86	8 (42%)	26,31,34	0.75	0
3	PSU	D	5001	80,3	18,21,22	1.05	1 (5%)	22,30,33	1.77	4 (18%)
3	OMC	D	2365	80,3	19,22,23	2.85	8 (42%)	26,31,34	0.69	0
3	PSU	D	3637	80,3	18,21,22	1.01	1 (5%)	22,30,33	1.81	4 (18%)
3	OMC	D	3841	3	19,22,23	2.86	8 (42%)	26,31,34	0.70	0
3	PSU	D	4423	3	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
48	PSU	w	210	48	18,21,22	1.09	1 (5%)	22,30,33	1.76	4 (18%)
48	PSU	w	406	48	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	D	4228	3	23,26,27	2.55	9 (39%)	33,38,41	1.95	10 (30%)
48	PSU	w	801	48	18,21,22	1.09	1 (5%)	22,30,33	1.71	4 (18%)
48	OMU	w	1326	48	19,22,23	2.91	8 (42%)	26,31,34	1.70	4 (15%)
48	PSU	w	1445	48	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
48	A2M	w	512	48	22,25,26	1.50	1 (4%)	31,36,39	1.04	2 (6%)
48	OMG	w	601	48	23,26,27	2.60	8 (34%)	33,38,41	1.90	9 (27%)
3	OMG	D	4196	80,2,3	23,26,27	2.56	8 (34%)	33,38,41	1.90	9 (27%)
2	2MG	B	10	2	23,26,27	2.67	7 (30%)	32,38,41	2.18	10 (31%)
3	OMG	D	4499	3	23,26,27	2.58	9 (39%)	33,38,41	1.93	10 (30%)
2	H2U	B	16	2	18,21,22	1.00	2 (11%)	21,30,33	1.27	2 (9%)
3	PSU	D	3764	3	18,21,22	1.02	1 (5%)	22,30,33	1.73	4 (18%)
3	PSU	D	5010	3	18,21,22	1.03	1 (5%)	22,30,33	1.80	4 (18%)
48	PSU	w	651	48	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	1744	80,3	18,21,22	1.01	1 (5%)	22,30,33	1.85	4 (18%)
48	PSU	w	815	48	18,21,22	1.05	1 (5%)	22,30,33	1.84	5 (22%)
48	OMG	w	1328	48	23,26,27	2.61	8 (34%)	33,38,41	1.94	9 (27%)
48	OMU	w	627	48	19,22,23	2.96	8 (42%)	26,31,34	1.67	4 (15%)
2	1MA	B	58	2	21,25,26	0.96	2 (9%)	31,37,40	0.75	0
3	PSU	D	4576	3	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
3	OMG	D	4370	3	23,26,27	2.57	9 (39%)	33,38,41	1.95	10 (30%)
2	3AU	B	20	2	24,28,29	2.78	9 (37%)	33,40,43	1.40	5 (15%)
3	PSU	D	3639	3	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	3695	3	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
48	PSU	w	1046	48	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
48	PSU	w	93	48	18,21,22	1.04	1 (5%)	22,30,33	1.67	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	B8N	w	1248	48	24,29,30	0.91	1 (4%)	29,42,45	1.05	1 (3%)
2	5MC	B	48	2	18,22,23	3.82	8 (44%)	26,32,35	1.02	2 (7%)
3	OMG	D	4392	3	23,26,27	2.56	9 (39%)	33,38,41	1.94	10 (30%)
3	A2M	D	2401	80,3	22,25,26	1.38	1 (4%)	31,36,39	0.99	2 (6%)
2	2MG	B	6	2	23,26,27	2.66	7 (30%)	32,38,41	2.12	9 (28%)
48	A2M	w	166	48	22,25,26	1.57	3 (13%)	31,36,39	1.05	4 (12%)
3	OMG	D	4623	3	23,26,27	2.55	9 (39%)	33,38,41	1.96	10 (30%)
48	OMG	w	509	48	23,26,27	2.61	8 (34%)	33,38,41	1.96	10 (30%)
48	PSU	w	34	48	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
2	M2G	B	26	2	24,27,28	1.09	2 (8%)	35,40,43	0.85	1 (2%)
48	OMU	w	1288	48	19,22,23	2.97	8 (42%)	26,31,34	1.66	4 (15%)
3	PSU	D	4296	3	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
3	OMG	D	1760	3	23,26,27	2.65	8 (34%)	33,38,41	1.94	9 (27%)
3	UY1	D	3818	80,3	19,22,23	1.14	1 (5%)	22,31,34	0.94	1 (4%)
3	PSU	D	1792	3	18,21,22	1.01	1 (5%)	22,30,33	1.73	4 (18%)
48	OMC	w	174	48	19,22,23	3.03	8 (42%)	26,31,34	0.69	0
3	PSU	D	1781	3	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
48	PSU	w	1177	48	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	1862	3	18,21,22	1.02	1 (5%)	22,30,33	1.83	4 (18%)
3	A2M	D	398	3	22,25,26	1.41	1 (4%)	31,36,39	1.03	3 (9%)
48	A2M	w	27	48	22,25,26	1.43	1 (4%)	31,36,39	0.98	1 (3%)
48	PSU	w	1081	48	18,21,22	1.02	1 (5%)	22,30,33	1.82	5 (22%)
3	PSU	D	1677	80,3	18,21,22	1.04	1 (5%)	22,30,33	1.76	3 (13%)
48	PSU	w	1045	48	18,21,22	1.02	1 (5%)	22,30,33	1.77	4 (18%)
3	OMU	D	1773	3	19,22,23	2.95	8 (42%)	26,31,34	1.64	4 (15%)
2	M2G	B	27	2	24,27,28	1.14	2 (8%)	35,40,43	0.86	1 (2%)
2	1MG	B	37	2	22,26,27	2.67	7 (31%)	33,39,42	1.75	8 (24%)
3	OMU	D	4227	3	19,22,23	2.82	6 (31%)	26,31,34	1.79	4 (15%)
3	PSU	D	4628	3	18,21,22	1.01	1 (5%)	22,30,33	1.77	4 (18%)
3	A2M	D	3718	3	22,25,26	1.37	1 (4%)	31,36,39	0.98	3 (9%)
3	A2M	D	2787	3	22,25,26	1.35	1 (4%)	31,36,39	1.00	2 (6%)
3	PSU	D	4312	3	18,21,22	1.02	1 (5%)	22,30,33	1.82	4 (18%)
48	OMC	w	1391	48	19,22,23	2.99	8 (42%)	26,31,34	0.68	0
3	PSU	D	4972	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
2	PSU	B	55	2	18,21,22	1.11	1 (5%)	22,30,33	1.74	4 (18%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	D	3758	3	18,21,22	0.97	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4500	3	18,21,22	1.04	1 (5%)	22,30,33	1.89	5 (22%)
3	PSU	D	4689	3	18,21,22	1.07	1 (5%)	22,30,33	1.81	4 (18%)
48	OMU	w	428	48	19,22,23	2.89	7 (36%)	26,31,34	1.72	4 (15%)
48	OMC	w	462	48	19,22,23	3.02	8 (42%)	26,31,34	0.78	0
48	OMG	w	644	48	23,26,27	2.61	8 (34%)	33,38,41	1.93	10 (30%)
3	PSU	D	4579	3	18,21,22	1.02	1 (5%)	22,30,33	1.81	4 (18%)
48	OMU	w	799	48	19,22,23	2.93	8 (42%)	26,31,34	1.69	5 (19%)
48	A2M	w	576	48	22,25,26	1.44	2 (9%)	31,36,39	1.10	4 (12%)
3	A2M	D	1871	80,3	22,25,26	1.42	2 (9%)	31,36,39	1.10	2 (6%)
48	PSU	w	1232	48	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
3	PSU	D	4552	3	18,21,22	1.06	1 (5%)	22,30,33	1.83	4 (18%)
3	OMG	D	2364	3	23,26,27	2.54	9 (39%)	33,38,41	1.93	9 (27%)
3	OMG	D	3744	3	23,26,27	2.57	9 (39%)	33,38,41	1.93	10 (30%)
48	PSU	w	1692	48	18,21,22	1.02	1 (5%)	22,30,33	1.77	4 (18%)
3	OMC	D	2422	80,3	19,22,23	2.90	8 (42%)	26,31,34	0.72	0
3	A2M	D	3785	80,3	22,25,26	1.41	1 (4%)	31,36,39	1.26	3 (9%)
3	OMU	D	3925	3	19,22,23	2.80	6 (31%)	26,31,34	1.74	4 (15%)
48	PSU	w	609	48	18,21,22	1.03	1 (5%)	22,30,33	1.89	5 (22%)
48	A2M	w	1383	48	22,25,26	1.43	1 (4%)	31,36,39	1.12	4 (12%)
3	PSU	D	3851	3	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	1536	3	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
48	4AC	w	1337	48	21,24,25	0.63	0	29,34,37	1.17	5 (17%)
2	5MU	B	54	2	19,22,23	4.74	5 (26%)	28,32,35	3.60	9 (32%)
3	PSU	D	4532	3	18,21,22	1.01	1 (5%)	22,30,33	1.72	4 (18%)
3	PSU	D	1860	3	18,21,22	1.04	1 (5%)	22,30,33	1.83	5 (22%)
48	6MZ	w	1832	80,48	22,25,26	2.80	4 (18%)	30,36,39	2.21	10 (33%)
3	PSU	D	4293	3	18,21,22	0.99	1 (5%)	22,30,33	1.65	4 (18%)
3	PSU	D	3920	80,3	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
3	OMC	D	3887	3	19,22,23	2.87	8 (42%)	26,31,34	0.76	0
3	PSU	D	4420	3	18,21,22	1.05	1 (5%)	22,30,33	1.67	4 (18%)
48	PSU	w	572	48	18,21,22	1.12	1 (5%)	22,30,33	1.78	4 (18%)
48	PSU	w	1643	80,48	18,21,22	1.08	1 (5%)	22,30,33	1.76	4 (18%)
3	PSU	D	4431	3	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	D	3730	3	18,21,22	1.03	1 (5%)	22,30,33	1.77	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	A2M	D	1534	80,3	22,25,26	1.36	1 (4%)	31,36,39	1.29	6 (19%)
3	PSU	D	1683	80,3	18,21,22	1.08	1 (5%)	22,30,33	1.87	4 (18%)
3	OMU	D	4306	3	19,22,23	2.75	6 (31%)	26,31,34	1.72	5 (19%)
3	OMG	D	4618	3	23,26,27	2.57	9 (39%)	33,38,41	1.95	10 (30%)
3	PSU	D	3715	3	18,21,22	1.03	1 (5%)	22,30,33	1.73	4 (18%)
48	OMC	w	1703	80,48	19,22,23	2.94	8 (42%)	26,31,34	0.70	0
3	OMC	D	2824	3	19,22,23	2.89	8 (42%)	26,31,34	0.76	0
3	OMU	D	2415	3	19,22,23	2.83	6 (31%)	26,31,34	1.88	5 (19%)
48	PSU	w	1174	80,48	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
48	A2M	w	590	48	22,25,26	1.51	2 (9%)	31,36,39	1.01	1 (3%)
2	G7M	B	46	2	23,26,27	2.82	9 (39%)	35,39,42	1.68	8 (22%)
3	PSU	D	4442	3	18,21,22	1.04	2 (11%)	22,30,33	1.86	5 (22%)
3	OMG	D	3627	3	23,26,27	2.56	9 (39%)	33,38,41	1.98	10 (30%)
48	OMC	w	517	80,48	19,22,23	3.00	8 (42%)	26,31,34	0.76	0
3	OMU	D	2837	3	19,22,23	2.77	6 (31%)	26,31,34	1.83	5 (19%)
3	PSU	D	3768	3	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)
48	A2M	w	668	80,48	22,25,26	1.52	2 (9%)	31,36,39	0.98	1 (3%)
48	OMU	w	172	48	19,22,23	2.91	7 (36%)	26,31,34	1.72	5 (19%)
3	OMC	D	2861	3	19,22,23	2.89	8 (42%)	26,31,34	0.68	0
48	MA6	w	1850	48	23,26,27	1.36	4 (17%)	34,38,41	2.20	10 (29%)
3	OMG	D	1316	3	23,26,27	2.57	10 (43%)	33,38,41	1.95	9 (27%)
3	5MC	D	3782	80,3	18,22,23	3.64	8 (44%)	26,32,35	1.06	2 (7%)
2	H2U	B	47	2	18,21,22	1.03	2 (11%)	21,30,33	0.77	0
48	PSU	w	218	48	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
48	PSU	w	866	48	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
48	PSU	w	119	48	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
3	PSU	D	3770	3	18,21,22	1.07	1 (5%)	22,30,33	1.82	4 (18%)
48	PSU	w	1367	48	18,21,22	1.06	1 (5%)	22,30,33	1.80	5 (22%)
3	A2M	D	2363	80,3	22,25,26	1.37	2 (9%)	31,36,39	0.97	2 (6%)
2	H2U	B	17	2	18,21,22	1.01	2 (11%)	21,30,33	0.89	2 (9%)
3	OMG	D	1625	80,3	23,26,27	2.59	8 (34%)	33,38,41	1.91	9 (27%)
48	A2M	w	484	48	22,25,26	1.46	1 (4%)	31,36,39	1.00	2 (6%)
3	PSU	D	2508	3	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
48	PSU	w	966	48	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
48	PSU	w	1238	48	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	OMU	w	1804	48	19,22,23	2.89	8 (42%)	26,31,34	1.76	5 (19%)
48	PSU	w	36	48	18,21,22	1.06	1 (5%)	22,30,33	1.78	5 (22%)
3	PSU	D	4521	80,3	18,21,22	1.05	1 (5%)	22,30,33	1.86	4 (18%)
3	OMG	D	4637	3	23,26,27	2.56	9 (39%)	33,38,41	1.92	9 (27%)
48	PSU	w	1244	48	18,21,22	1.07	1 (5%)	22,30,33	1.79	5 (22%)
3	OMC	D	1340	3	19,22,23	2.84	8 (42%)	26,31,34	0.75	0
3	OMC	D	3808	3	19,22,23	2.86	8 (42%)	26,31,34	0.80	0
48	PSU	w	681	80,48	18,21,22	1.05	1 (5%)	22,30,33	1.79	4 (18%)
3	OMG	D	1522	3	23,26,27	2.57	9 (39%)	33,38,41	1.98	10 (30%)
3	OMC	D	3701	80,3	19,22,23	2.87	8 (42%)	26,31,34	0.73	0
48	PSU	w	1347	48	18,21,22	1.02	1 (5%)	22,30,33	1.78	4 (18%)
48	A2M	w	99	80,48	22,25,26	1.41	1 (4%)	31,36,39	1.03	2 (6%)
3	OMC	D	2804	3	19,22,23	2.86	8 (42%)	26,31,34	0.86	1 (3%)
3	PSU	D	2632	3	18,21,22	1.02	1 (5%)	22,30,33	1.71	4 (18%)
3	PSU	D	3853	80,3	18,21,22	0.99	1 (5%)	22,30,33	1.66	4 (18%)
3	A2M	D	3760	3	22,25,26	1.54	3 (13%)	31,36,39	1.09	3 (9%)
3	A2M	D	4523	80,3	22,25,26	1.42	1 (4%)	31,36,39	1.08	3 (9%)

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
48	PSU	w	109	48	-	0/7/25/26	0/2/2/2
48	OMU	w	121	48	-	0/9/27/28	0/2/2/2
3	OMG	D	3792	3	-	0/9/27/28	0/3/3/3
3	6MZ	D	4220	3	-	0/9/27/28	0/3/3/3
3	UR3	D	4530	80,3	-	0/7/25/26	0/2/2/2
48	A2M	w	468	48	-	3/9/27/28	0/3/3/3
3	PSU	D	4361	3	-	0/7/25/26	0/2/2/2
3	1MA	D	1322	3	-	2/7/25/26	0/3/3/3
3	PSU	D	4471	3	-	0/7/25/26	0/2/2/2
3	A2M	D	400	3	-	0/9/27/28	0/3/3/3
3	A2M	D	1524	3	-	3/9/27/28	0/3/3/3
3	A2M	D	3825	3	-	0/9/27/28	0/3/3/3
48	PSU	w	1056	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1625	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	B	35	2,1	-	0/7/25/26	0/2/2/2
48	PSU	w	863	48	-	0/7/25/26	0/2/2/2
3	A2M	D	3724	3	-	1/9/27/28	0/3/3/3
48	PSU	w	814	48	-	0/7/25/26	0/2/2/2
48	A2M	w	1678	48	-	1/9/27/28	0/3/3/3
48	A2M	w	1031	48	-	0/9/27/28	0/3/3/3
48	MA6	w	1851	48	-	3/11/29/30	0/3/3/3
48	PSU	w	686	48	-	0/7/25/26	0/2/2/2
48	OMG	w	436	48	-	0/9/27/28	0/3/3/3
5	OMG	F	75	5	-	0/9/27/28	0/3/3/3
3	PSU	D	3762	3	-	0/7/25/26	0/2/2/2
48	A2M	w	159	48	-	4/9/27/28	0/3/3/3
48	PSU	w	649	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4299	3	-	0/7/25/26	0/2/2/2
3	OMU	D	4498	80,3	-	0/9/27/28	0/2/2/2
48	PSU	w	822	48	-	0/7/25/26	0/2/2/2
2	56B	B	34	2,81	-	2/12/43/44	0/4/4/4
3	PSU	D	4403	80,3	-	0/7/25/26	0/2/2/2
3	OMG	D	2424	3	-	2/9/27/28	0/3/3/3
3	OMU	D	4620	3	-	0/9/27/28	0/2/2/2
3	OMC	D	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	D	1782	3	-	0/7/25/26	0/2/2/2
48	OMG	w	683	48	-	0/9/27/28	0/3/3/3
48	OMU	w	1442	80,48	-	1/9/27/28	0/2/2/2
3	PSU	D	3734	3	-	0/7/25/26	0/2/2/2
48	OMG	w	1490	80,48	-	3/9/27/28	0/3/3/3
3	OMG	D	3899	3	-	0/9/27/28	0/3/3/3
3	A2M	D	2815	3	-	3/9/27/28	0/3/3/3
3	A2M	D	3830	3	-	0/9/27/28	0/3/3/3
3	OMC	D	2351	80,3	-	4/9/27/28	0/2/2/2
3	OMG	D	3944	3	-	3/9/27/28	0/3/3/3
3	OMG	D	4494	3	-	1/9/27/28	0/3/3/3
3	5MC	D	4447	80,3	-	4/7/25/26	0/2/2/2
3	A2M	D	1326	3	-	1/9/27/28	0/3/3/3
48	PSU	w	105	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4353	3	-	0/7/25/26	0/2/2/2
48	G7M	w	1639	2,48	-	2/7/25/26	0/3/3/3
48	OMU	w	116	48	-	1/9/27/28	0/2/2/2
48	PSU	w	1004	48	-	0/7/25/26	0/2/2/2
2	UY1	B	39	2	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	4AC	w	1842	48	-	0/11/29/30	0/2/2/2
3	PSU	D	4457	3	-	0/7/25/26	0/2/2/2
3	OMC	D	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	D	5001	80,3	-	0/7/25/26	0/2/2/2
3	OMC	D	2365	80,3	-	0/9/27/28	0/2/2/2
3	PSU	D	3637	80,3	-	0/7/25/26	0/2/2/2
3	OMC	D	3841	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4423	3	-	0/7/25/26	0/2/2/2
48	PSU	w	210	48	-	0/7/25/26	0/2/2/2
48	PSU	w	406	48	-	0/7/25/26	0/2/2/2
3	OMG	D	4228	3	-	0/9/27/28	0/3/3/3
48	PSU	w	801	48	-	0/7/25/26	0/2/2/2
48	OMU	w	1326	48	-	4/9/27/28	0/2/2/2
48	PSU	w	1445	48	-	0/7/25/26	0/2/2/2
48	A2M	w	512	48	-	0/9/27/28	0/3/3/3
48	OMG	w	601	48	-	1/9/27/28	0/3/3/3
3	OMG	D	4196	80,2,3	-	1/9/27/28	0/3/3/3
2	2MG	B	10	2	-	0/9/27/28	0/3/3/3
3	OMG	D	4499	3	-	0/9/27/28	0/3/3/3
2	H2U	B	16	2	-	6/7/38/39	0/2/2/2
3	PSU	D	3764	3	-	0/7/25/26	0/2/2/2
3	PSU	D	5010	3	-	0/7/25/26	0/2/2/2
48	PSU	w	651	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1744	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	815	48	-	0/7/25/26	0/2/2/2
48	OMG	w	1328	48	-	1/9/27/28	0/3/3/3
48	OMU	w	627	48	-	0/9/27/28	0/2/2/2
2	1MA	B	58	2	-	0/7/25/26	0/3/3/3
3	PSU	D	4576	3	-	0/7/25/26	0/2/2/2
3	OMG	D	4370	3	-	2/9/27/28	0/3/3/3
2	3AU	B	20	2	-	8/16/34/35	0/2/2/2
3	PSU	D	3639	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3695	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1046	48	-	0/7/25/26	0/2/2/2
48	PSU	w	93	48	-	0/7/25/26	0/2/2/2
48	B8N	w	1248	48	-	2/16/34/35	0/2/2/2
2	5MC	B	48	2	-	0/7/25/26	0/2/2/2
3	OMG	D	4392	3	-	0/9/27/28	0/3/3/3
3	A2M	D	2401	80,3	-	1/9/27/28	0/3/3/3
2	2MG	B	6	2	-	2/9/27/28	0/3/3/3
48	A2M	w	166	48	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	D	4623	3	-	0/9/27/28	0/3/3/3
48	OMG	w	509	48	-	0/9/27/28	0/3/3/3
48	PSU	w	34	48	-	3/7/25/26	0/2/2/2
2	M2G	B	26	2	-	0/11/29/30	0/3/3/3
48	OMU	w	1288	48	-	1/9/27/28	0/2/2/2
3	PSU	D	4296	3	-	0/7/25/26	0/2/2/2
3	OMG	D	1760	3	-	2/9/27/28	0/3/3/3
3	UY1	D	3818	80,3	-	4/9/27/28	0/2/2/2
3	PSU	D	1792	3	-	0/7/25/26	0/2/2/2
48	OMC	w	174	48	-	0/9/27/28	0/2/2/2
3	PSU	D	1781	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1177	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1862	3	-	0/7/25/26	0/2/2/2
3	A2M	D	398	3	-	1/9/27/28	0/3/3/3
48	A2M	w	27	48	-	0/9/27/28	0/3/3/3
48	PSU	w	1081	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1677	80,3	-	4/7/25/26	0/2/2/2
48	PSU	w	1045	48	-	0/7/25/26	0/2/2/2
3	OMU	D	1773	3	-	0/9/27/28	0/2/2/2
2	M2G	B	27	2	-	0/11/29/30	0/3/3/3
2	1MG	B	37	2	-	0/7/25/26	0/3/3/3
3	OMU	D	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4628	3	-	0/7/25/26	0/2/2/2
3	A2M	D	3718	3	-	0/9/27/28	0/3/3/3
3	A2M	D	2787	3	-	3/9/27/28	0/3/3/3
3	PSU	D	4312	3	-	0/7/25/26	0/2/2/2
48	OMC	w	1391	48	-	0/9/27/28	0/2/2/2
3	PSU	D	4972	3	-	0/7/25/26	0/2/2/2
2	PSU	B	55	2	-	1/7/25/26	0/2/2/2
3	PSU	D	3758	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4500	3	-	4/7/25/26	0/2/2/2
3	PSU	D	4689	3	-	0/7/25/26	0/2/2/2
48	OMU	w	428	48	-	7/9/27/28	0/2/2/2
48	OMC	w	462	48	-	1/9/27/28	0/2/2/2
48	OMG	w	644	48	-	3/9/27/28	0/3/3/3
3	PSU	D	4579	3	-	0/7/25/26	0/2/2/2
48	OMU	w	799	48	-	3/9/27/28	0/2/2/2
48	A2M	w	576	48	-	2/9/27/28	0/3/3/3
3	A2M	D	1871	80,3	-	0/9/27/28	0/3/3/3
48	PSU	w	1232	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	D	4552	3	-	0/7/25/26	0/2/2/2
3	OMG	D	2364	3	-	2/9/27/28	0/3/3/3
3	OMG	D	3744	3	-	1/9/27/28	0/3/3/3
48	PSU	w	1692	48	-	0/7/25/26	0/2/2/2
3	OMC	D	2422	80,3	-	1/9/27/28	0/2/2/2
3	A2M	D	3785	80,3	-	3/9/27/28	0/3/3/3
3	OMU	D	3925	3	-	1/9/27/28	0/2/2/2
48	PSU	w	609	48	-	0/7/25/26	0/2/2/2
48	A2M	w	1383	48	-	1/9/27/28	0/3/3/3
3	PSU	D	3851	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1536	3	-	0/7/25/26	0/2/2/2
48	4AC	w	1337	48	-	0/11/29/30	0/2/2/2
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2
3	PSU	D	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1860	3	-	0/7/25/26	0/2/2/2
48	6MZ	w	1832	80,48	-	2/9/27/28	0/3/3/3
3	PSU	D	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3920	80,3	-	0/7/25/26	0/2/2/2
3	OMC	D	3887	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4420	3	-	0/7/25/26	0/2/2/2
48	PSU	w	572	48	-	2/7/25/26	0/2/2/2
48	PSU	w	1643	80,48	-	0/7/25/26	0/2/2/2
3	PSU	D	4431	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3730	3	-	0/7/25/26	0/2/2/2
3	A2M	D	1534	80,3	-	3/9/27/28	0/3/3/3
3	PSU	D	1683	80,3	-	0/7/25/26	0/2/2/2
3	OMU	D	4306	3	-	0/9/27/28	0/2/2/2
3	OMG	D	4618	3	-	0/9/27/28	0/3/3/3
3	PSU	D	3715	3	-	0/7/25/26	0/2/2/2
48	OMC	w	1703	80,48	-	2/9/27/28	0/2/2/2
3	OMC	D	2824	3	-	1/9/27/28	0/2/2/2
3	OMU	D	2415	3	-	1/9/27/28	0/2/2/2
48	PSU	w	1174	80,48	-	0/7/25/26	0/2/2/2
48	A2M	w	590	48	-	4/9/27/28	0/3/3/3
2	G7M	B	46	2	-	3/7/25/26	0/3/3/3
3	PSU	D	4442	3	-	0/7/25/26	0/2/2/2
3	OMG	D	3627	3	-	0/9/27/28	0/3/3/3
48	OMC	w	517	80,48	-	0/9/27/28	0/2/2/2
3	OMU	D	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	D	3768	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A2M	w	668	80,48	-	2/9/27/28	0/3/3/3
48	OMU	w	172	48	-	0/9/27/28	0/2/2/2
3	OMC	D	2861	3	-	0/9/27/28	0/2/2/2
48	MA6	w	1850	48	-	0/11/29/30	0/3/3/3
3	OMG	D	1316	3	-	0/9/27/28	0/3/3/3
3	5MC	D	3782	80,3	-	0/7/25/26	0/2/2/2
2	H2U	B	47	2	-	2/7/38/39	0/2/2/2
48	PSU	w	218	48	-	0/7/25/26	0/2/2/2
48	PSU	w	866	48	-	0/7/25/26	0/2/2/2
48	PSU	w	119	48	-	0/7/25/26	0/2/2/2
3	PSU	D	3770	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1367	48	-	0/7/25/26	0/2/2/2
3	A2M	D	2363	80,3	-	0/9/27/28	0/3/3/3
2	H2U	B	17	2	-	1/7/38/39	0/2/2/2
3	OMG	D	1625	80,3	-	0/9/27/28	0/3/3/3
48	A2M	w	484	48	-	0/9/27/28	0/3/3/3
3	PSU	D	2508	3	-	0/7/25/26	0/2/2/2
48	PSU	w	966	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1238	48	-	2/7/25/26	0/2/2/2
48	OMU	w	1804	48	-	1/9/27/28	0/2/2/2
48	PSU	w	36	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4521	80,3	-	0/7/25/26	0/2/2/2
3	OMG	D	4637	3	-	1/9/27/28	0/3/3/3
48	PSU	w	1244	48	-	0/7/25/26	0/2/2/2
3	OMC	D	1340	3	-	0/9/27/28	0/2/2/2
3	OMC	D	3808	3	-	0/9/27/28	0/2/2/2
48	PSU	w	681	80,48	-	0/7/25/26	0/2/2/2
3	OMG	D	1522	3	-	0/9/27/28	0/3/3/3
3	OMC	D	3701	80,3	-	4/9/27/28	0/2/2/2
48	PSU	w	1347	48	-	0/7/25/26	0/2/2/2
48	A2M	w	99	80,48	-	1/9/27/28	0/3/3/3
3	OMC	D	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	D	2632	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3853	80,3	-	0/7/25/26	0/2/2/2
3	A2M	D	3760	3	-	2/9/27/28	0/3/3/3
3	A2M	D	4523	80,3	-	0/9/27/28	0/3/3/3

The worst 5 of 770 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4220	6MZ	C6-N6	12.21	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	1832	6MZ	C6-N6	12.03	1.47	1.34
2	B	54	5MU	C2-N1	10.87	1.55	1.38
2	B	54	5MU	C6-N1	10.82	1.56	1.38
3	D	4447	5MC	C6-C5	9.48	1.50	1.34

The worst 5 of 925 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	5MU	C5-C4-N3	12.08	125.63	115.31
2	B	54	5MU	C5-C6-N1	-9.63	113.43	123.34
2	B	34	56B	C1'-N9-C4	-7.46	104.36	126.50
2	B	34	56B	C5-C4-N3	-6.44	119.98	127.52
2	B	10	2MG	C2-N3-C4	6.38	119.95	112.04

There are no chirality outliers.

5 of 158 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6	2MG	O4'-C4'-C5'-O5'
2	B	6	2MG	C3'-C4'-C5'-O5'
2	B	16	H2U	O4'-C1'-N1-C2
2	B	16	H2U	O4'-C1'-N1-C6
2	B	20	3AU	O4'-C1'-N1-C2

There are no ring outliers.

78 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	w	121	OMU	1	0
3	D	4220	6MZ	1	0
48	w	468	A2M	1	0
3	D	3825	A2M	1	0
3	D	3724	A2M	2	0
48	w	1678	A2M	2	0
48	w	1031	A2M	1	0
48	w	686	PSU	1	0
5	F	75	OMG	1	0
48	w	159	A2M	2	0
3	D	2424	OMG	1	0
3	D	4620	OMU	2	0
48	w	1442	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3734	PSU	1	0
48	w	1490	OMG	1	0
3	D	2815	A2M	1	0
3	D	2351	OMC	3	0
3	D	3944	OMG	2	0
3	D	4494	OMG	1	0
3	D	4447	5MC	1	0
3	D	1326	A2M	2	0
48	w	1639	G7M	2	0
48	w	116	OMU	3	0
48	w	1004	PSU	2	0
48	w	1842	4AC	1	0
3	D	4457	PSU	1	0
3	D	4536	OMC	1	0
3	D	5001	PSU	1	0
48	w	801	PSU	1	0
48	w	512	A2M	1	0
3	D	4196	OMG	1	0
2	B	10	2MG	1	0
2	B	16	H2U	1	0
48	w	815	PSU	1	0
48	w	1328	OMG	1	0
48	w	627	OMU	1	0
2	B	6	2MG	1	0
48	w	166	A2M	1	0
3	D	4623	OMG	1	0
48	w	509	OMG	2	0
48	w	34	PSU	1	0
48	w	1288	OMU	1	0
3	D	1760	OMG	1	0
3	D	3818	UY1	1	0
48	w	174	OMC	1	0
48	w	27	A2M	1	0
3	D	1677	PSU	1	0
3	D	1773	OMU	2	0
3	D	3718	A2M	3	0
48	w	1391	OMC	2	0
3	D	4689	PSU	1	0
48	w	428	OMU	1	0
48	w	462	OMC	1	0
48	w	644	OMG	2	0
3	D	4579	PSU	2	0

*Continued on next page...*



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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	w	799	OMU	1	0
48	w	576	A2M	3	0
3	D	1871	A2M	1	0
3	D	2364	OMG	1	0
3	D	3744	OMG	1	0
48	w	1692	PSU	1	0
3	D	2422	OMC	1	0
3	D	3925	OMU	1	0
48	w	572	PSU	2	0
48	w	1643	PSU	1	0
3	D	1534	A2M	1	0
48	w	1703	OMC	1	0
3	D	2824	OMC	1	0
3	D	2415	OMU	5	0
48	w	590	A2M	4	0
48	w	1850	MA6	1	0
3	D	2363	A2M	1	0
48	w	1804	OMU	2	0
48	w	36	PSU	1	0
3	D	4637	OMG	2	0
3	D	1340	OMC	1	0
3	D	2804	OMC	1	0
3	D	2632	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 546 ligands modelled in this entry, 545 are monoatomic - leaving 1 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
81	GAL	B	101	2	11,11,12	2.07	4 (36%)	15,15,17	1.69	4 (26%)

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
81	GAL	B	101	2	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	B	101	GAL	O5-C1	-3.53	1.38	1.43
81	B	101	GAL	C2-C3	3.31	1.57	1.52
81	B	101	GAL	C4-C5	2.61	1.58	1.53
81	B	101	GAL	C1-C2	2.14	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	B	101	GAL	O2-C2-C3	-3.29	103.56	110.14
81	B	101	GAL	O4-C4-C5	-2.55	102.97	109.30
81	B	101	GAL	C2-C3-C4	-2.40	106.75	110.89
81	B	101	GAL	C6-C5-C4	-2.14	108.00	113.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

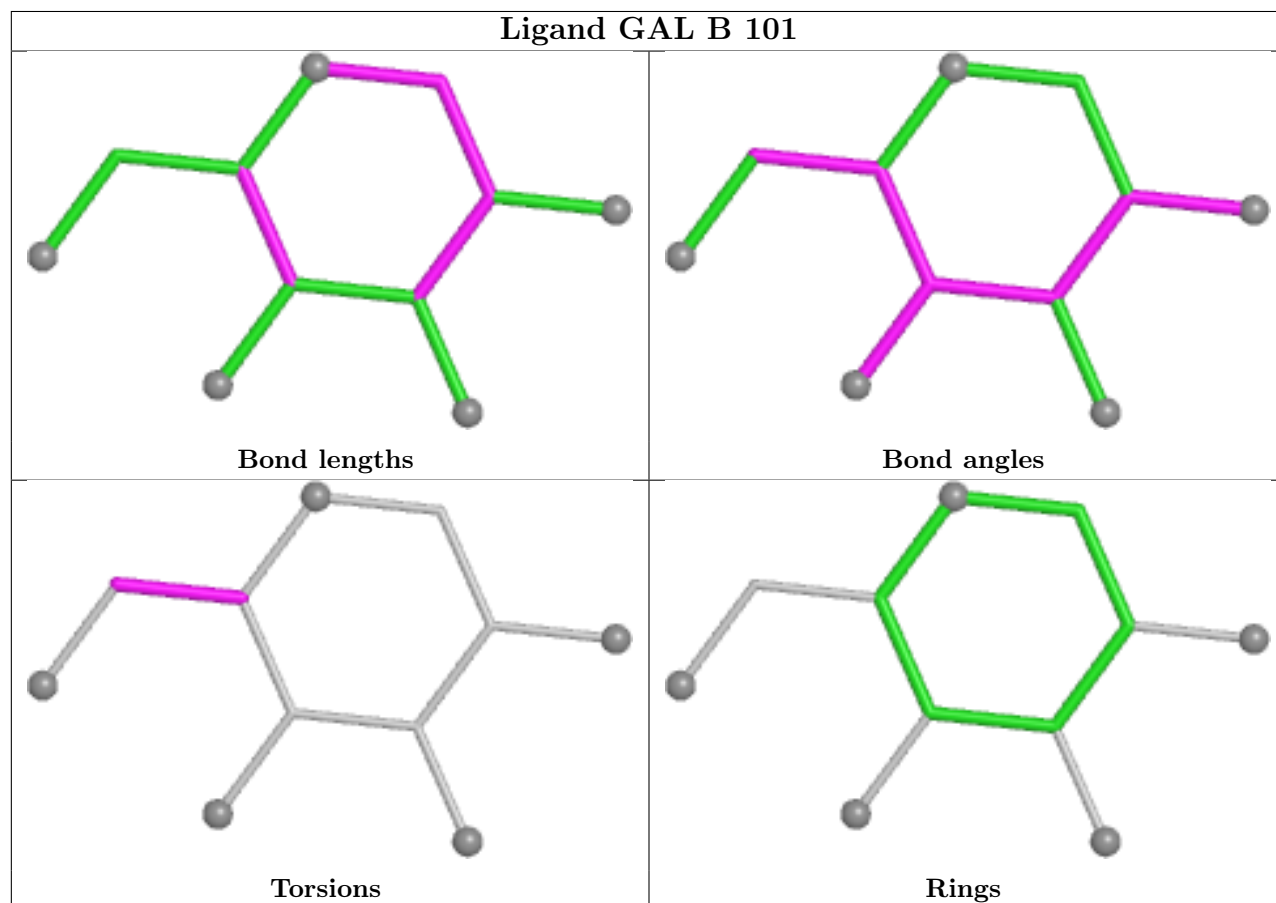
Mol	Chain	Res	Type	Atoms
81	B	101	GAL	O5-C5-C6-O6
81	B	101	GAL	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

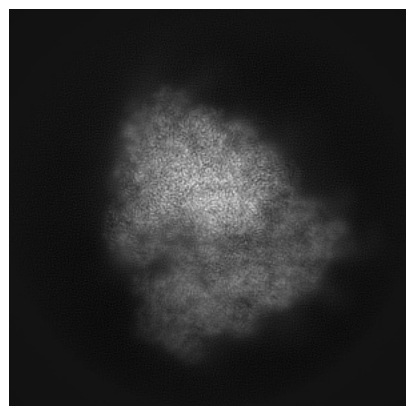
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36180. These allow visual inspection of the internal detail of the map and identification of artifacts.

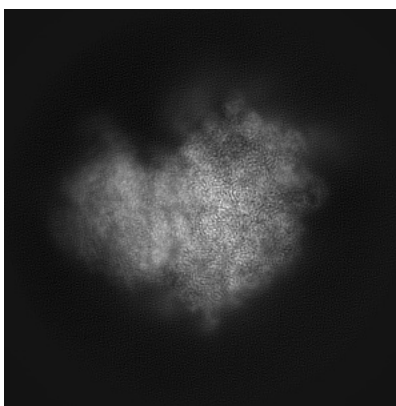
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

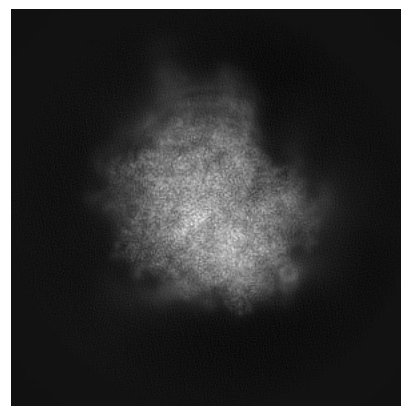
#### 6.1.1 Primary map



X

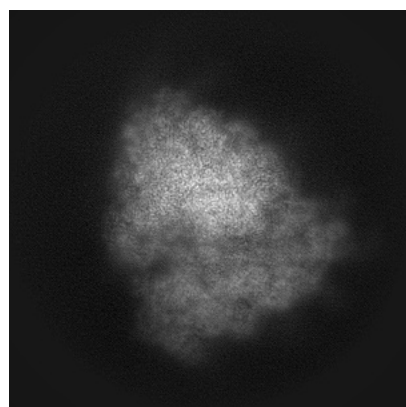


Y

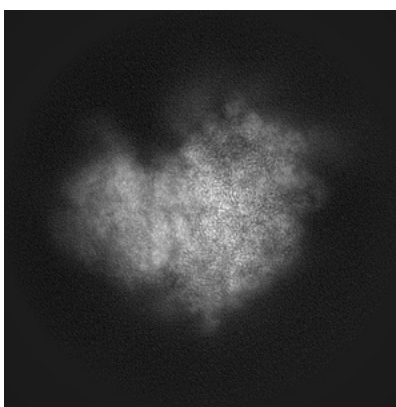


Z

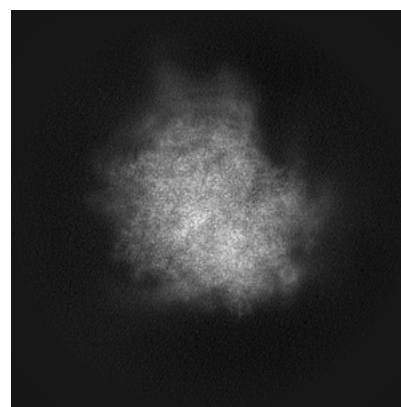
#### 6.1.2 Raw map



X



Y

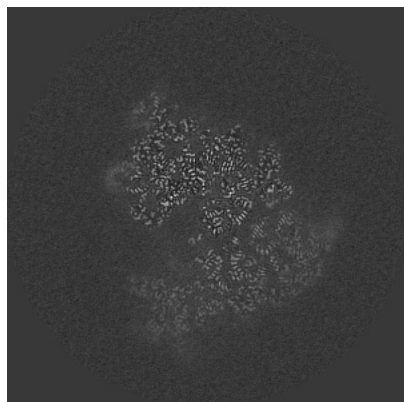


Z

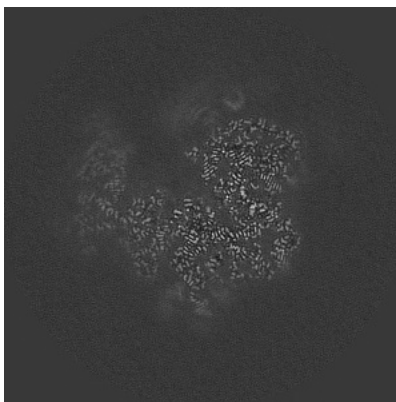
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

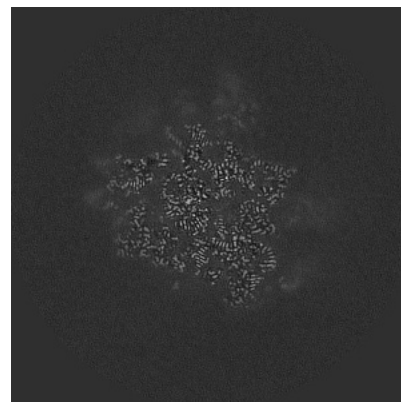
### 6.2.1 Primary map



X Index: 265

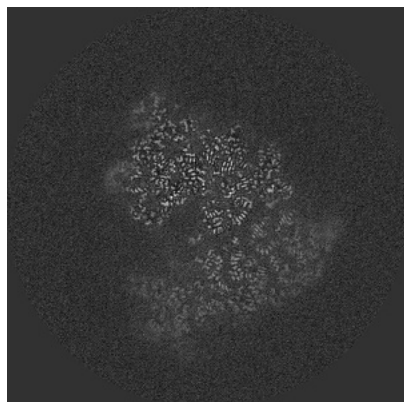


Y Index: 265

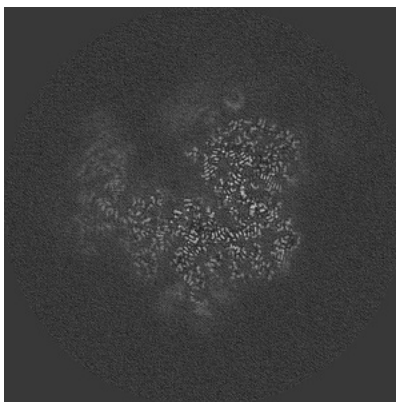


Z Index: 265

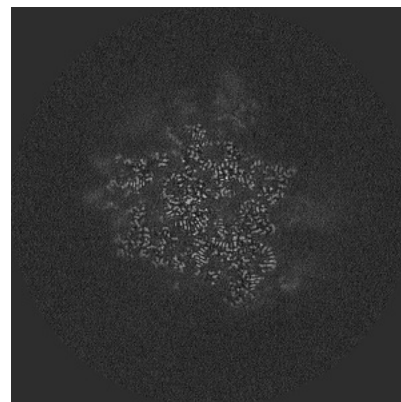
### 6.2.2 Raw map



X Index: 265



Y Index: 265



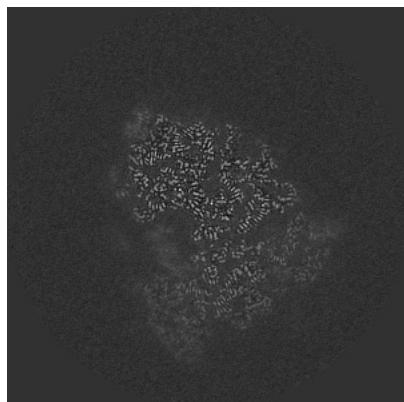
Z Index: 265

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

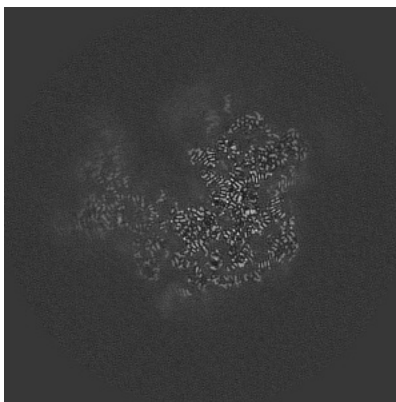


## 6.3 Largest variance slices [i](#)

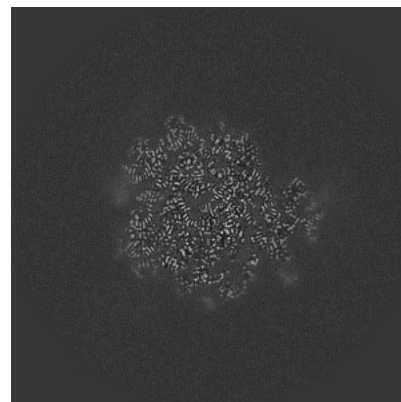
### 6.3.1 Primary map



X Index: 253

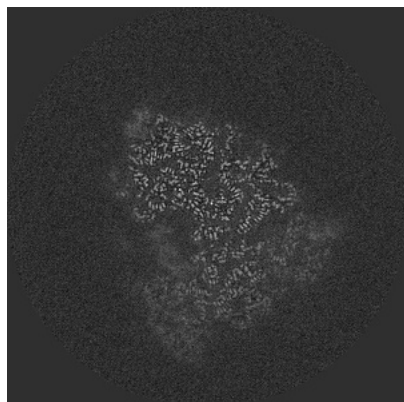


Y Index: 258

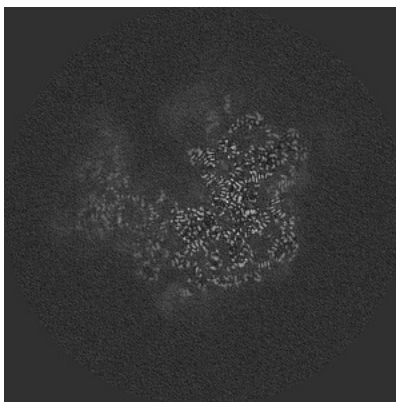


Z Index: 300

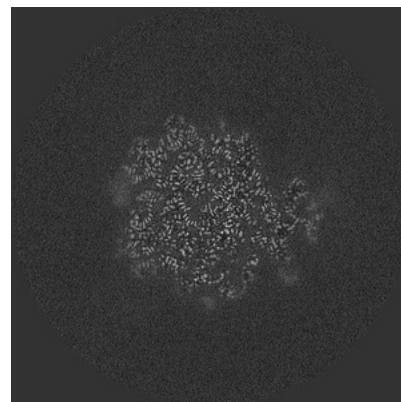
### 6.3.2 Raw map



X Index: 253



Y Index: 258

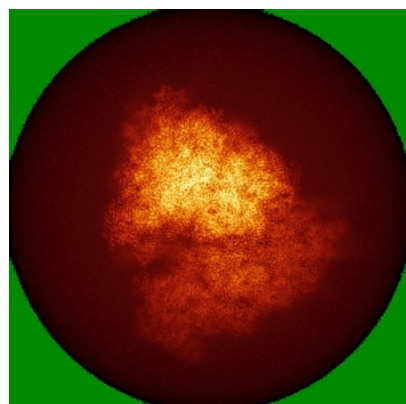


Z Index: 300

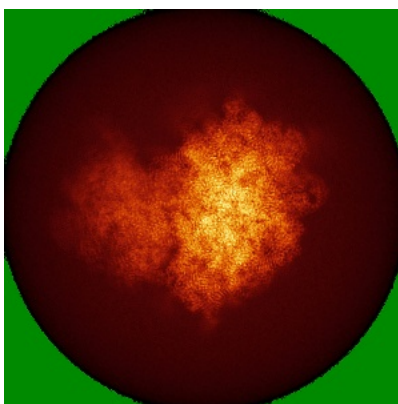
The images above show the largest variance slices of the map in three orthogonal directions.

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

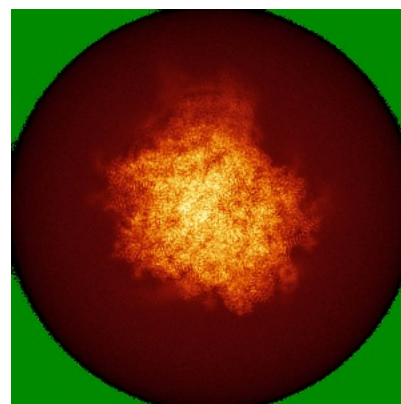
### 6.4.1 Primary map



X

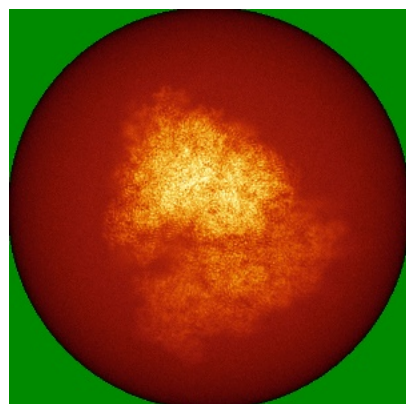


Y

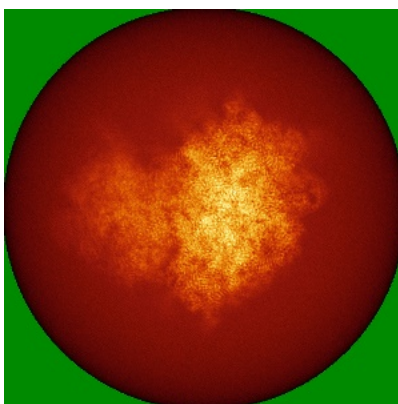


Z

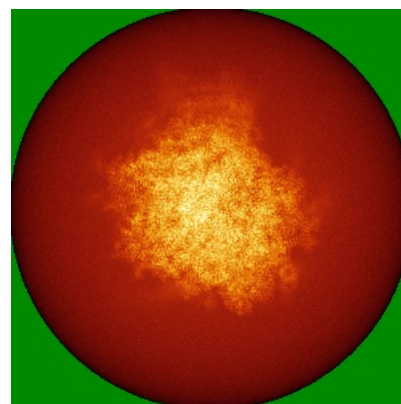
### 6.4.2 Raw map



X



Y

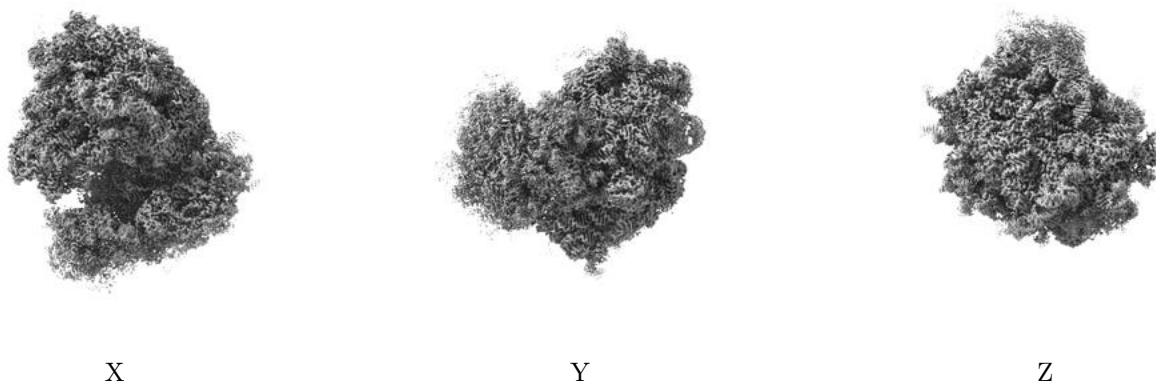


Z

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

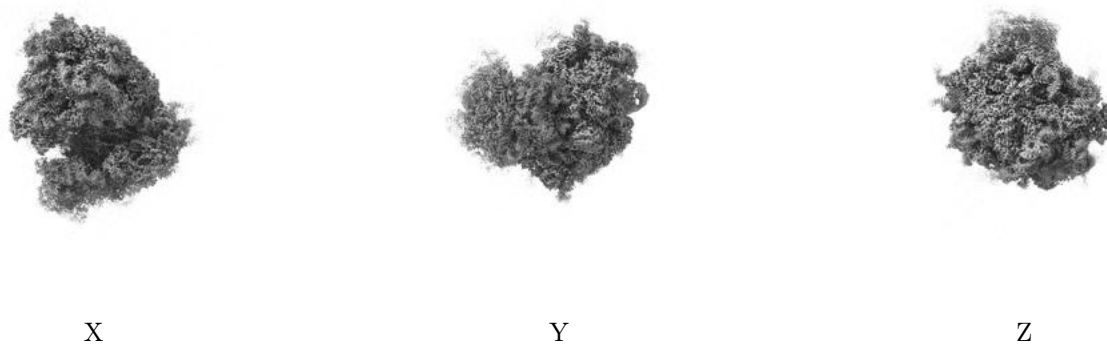
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0191. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

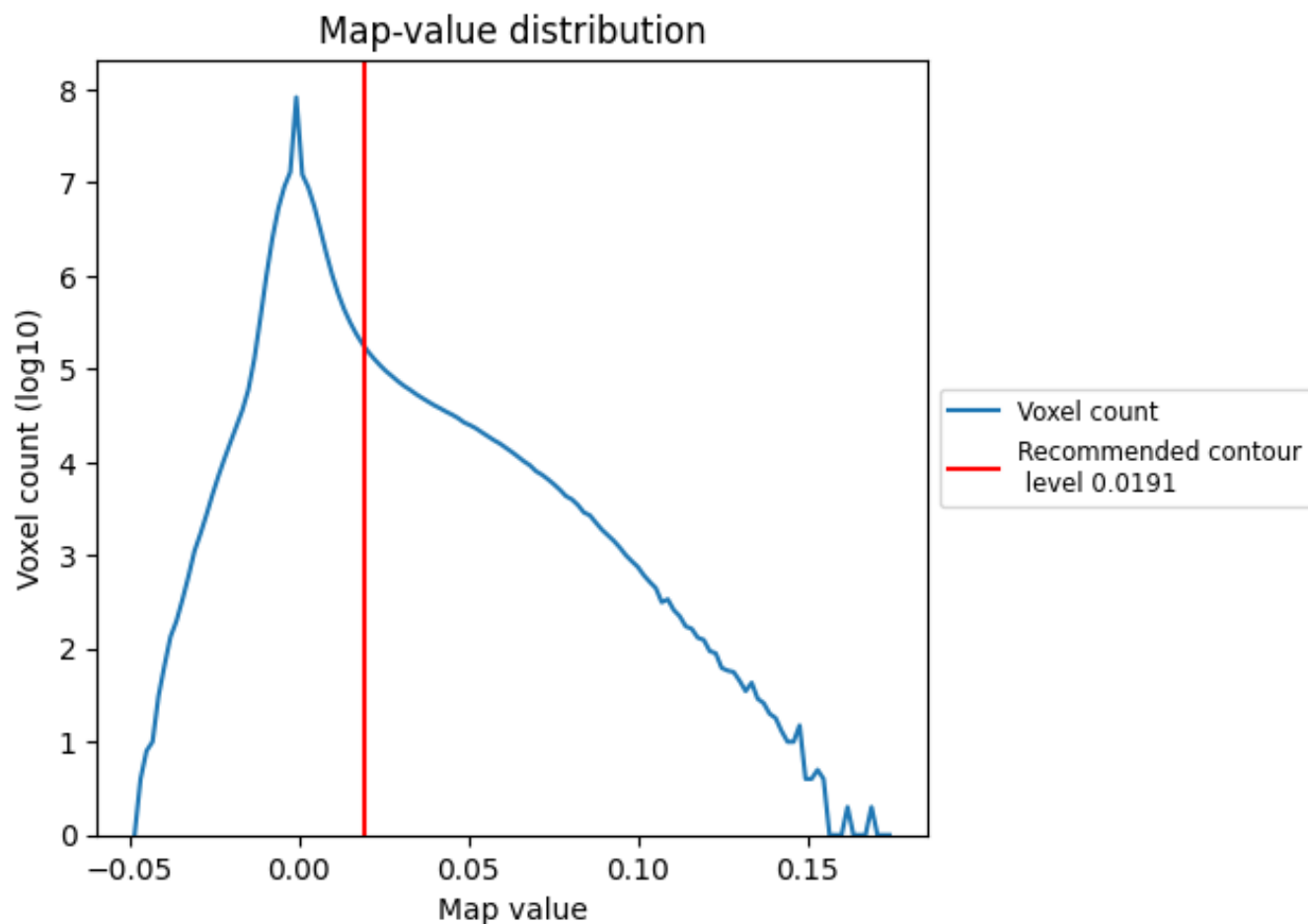
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

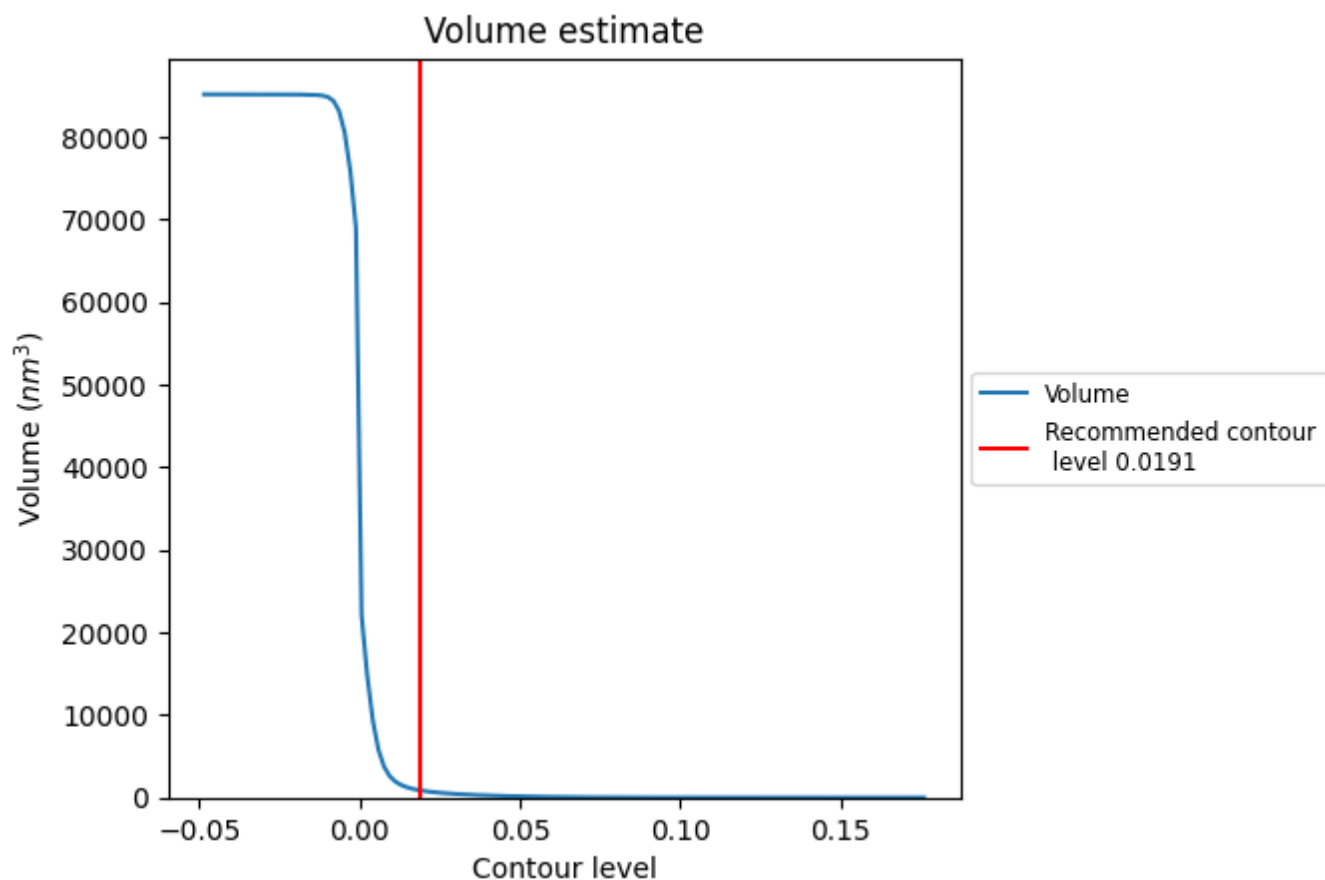
This section contains the results of statistical analysis of the map.

### 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.

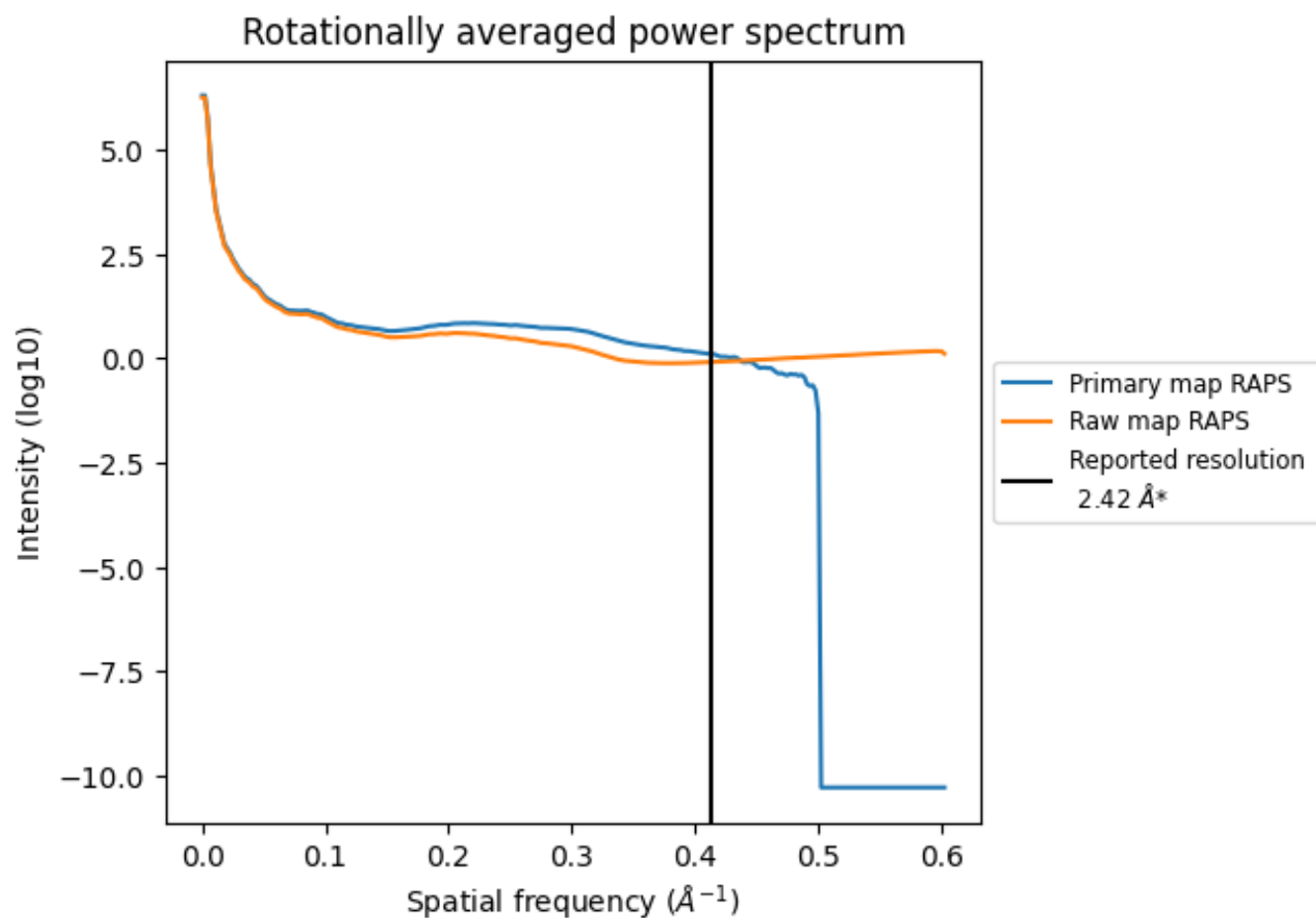
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 860  $\text{nm}^3$ ; this corresponds to an approximate mass of 777 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

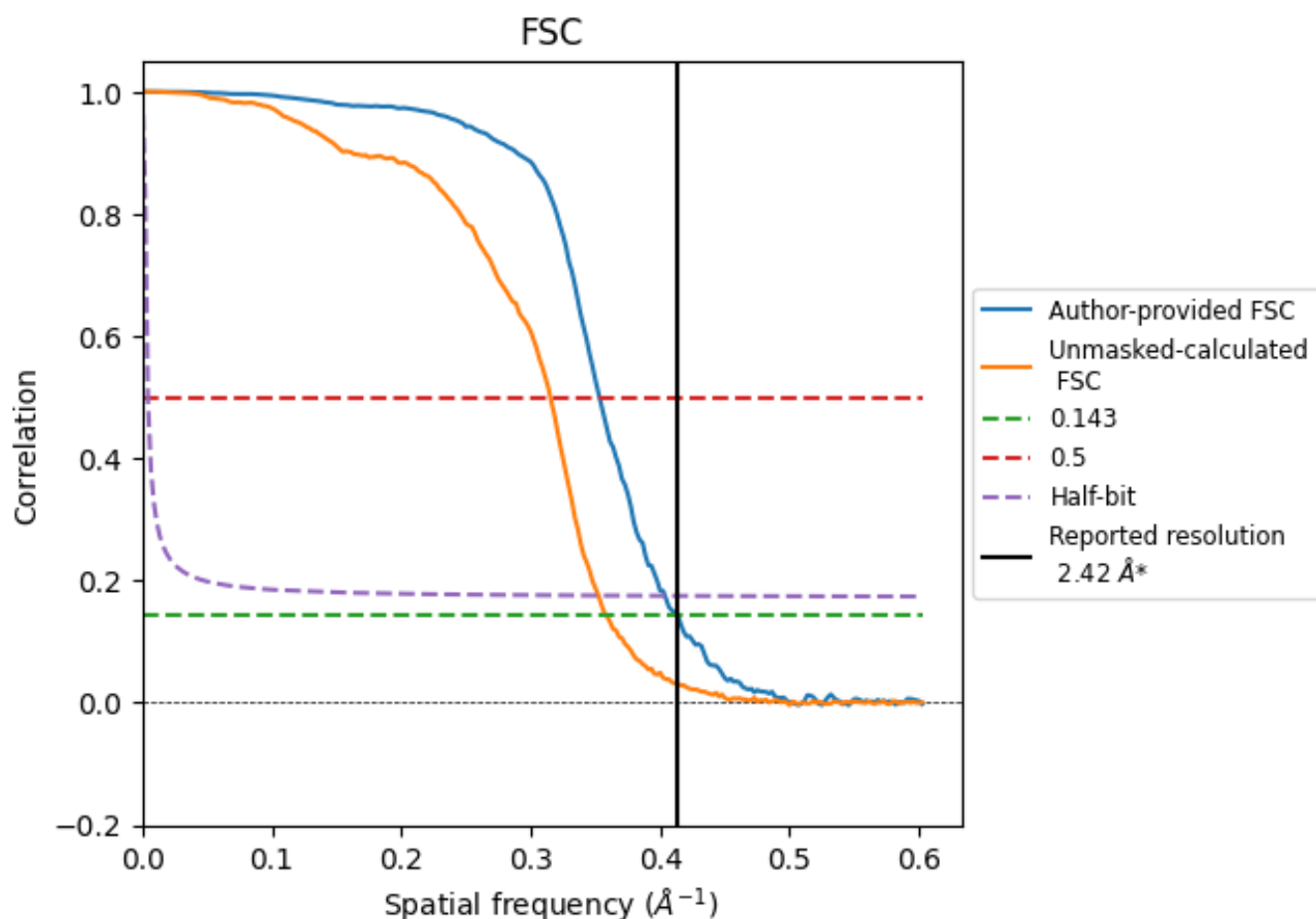


\*Reported resolution corresponds to spatial frequency of 0.413 Å<sup>-1</sup>

## 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 0.413  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

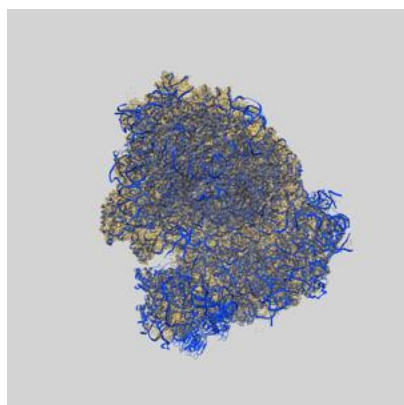
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.83	2.48
Unmasked-calculated*	2.79	3.17	2.84

\*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 2.79 differs from the reported value 2.42 by more than 10 %

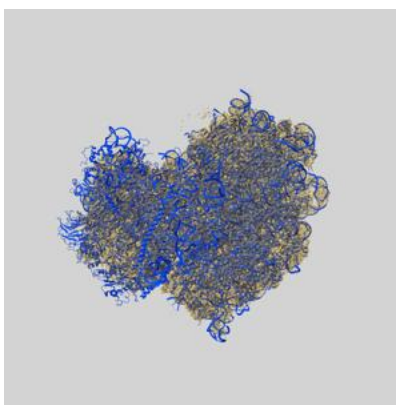
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36180 and PDB model 8JDL. Per-residue inclusion information can be found in section [3](#) on page [21](#).

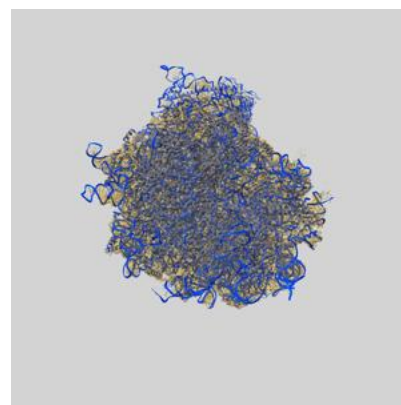
### 9.1 Map-model overlay [i](#)



X



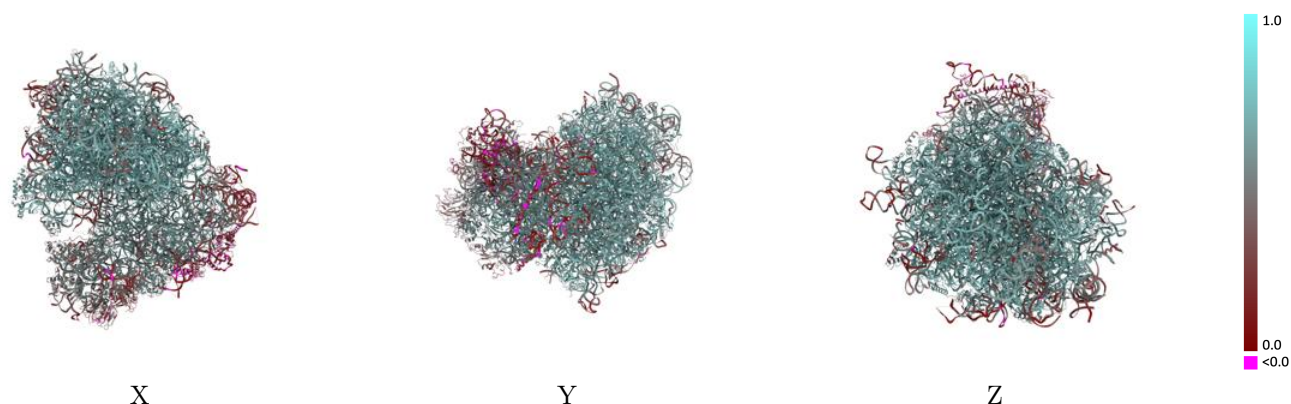
Y



Z

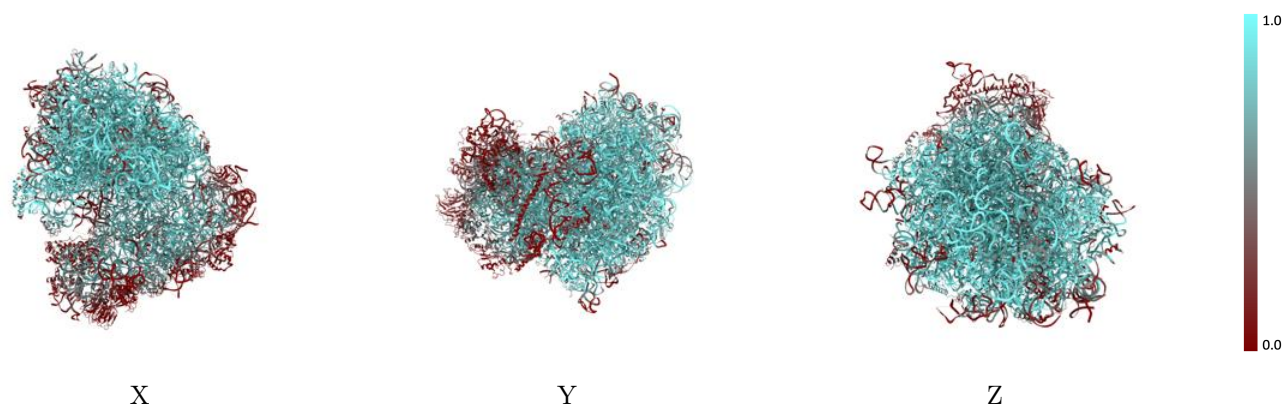
The images above show the 3D surface view of the map at the recommended contour level 0.0191 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



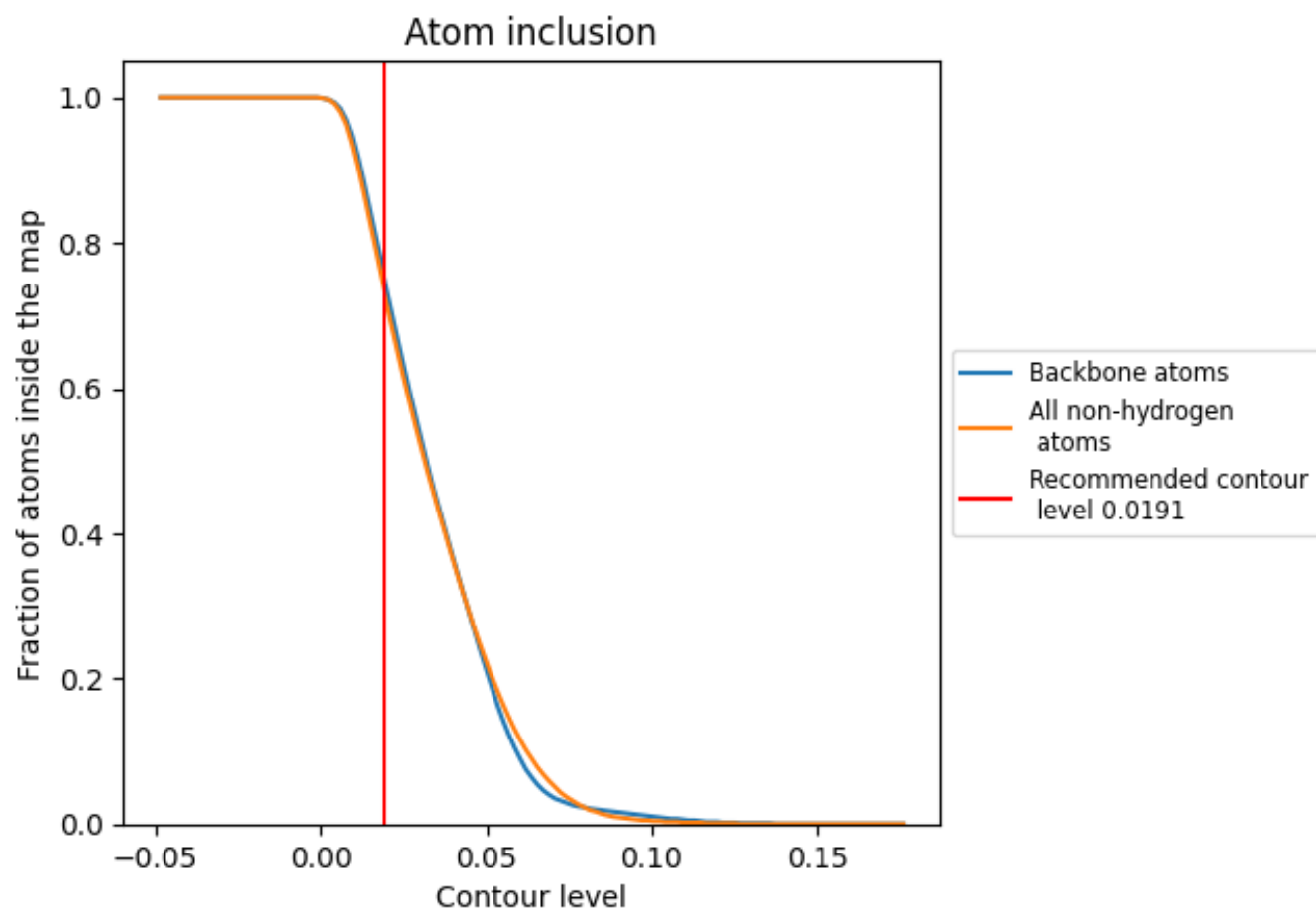
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0191).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.0191) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7350	 0.5730
0	 0.2460	 0.4230
1	 0.3220	 0.3450
2	 0.3830	 0.4840
3	 0.1560	 0.2800
4	 0.2200	 0.4010
5	 0.5270	 0.5120
6	 0.2500	 0.2290
7	 0.0520	 0.3010
8	 0.6910	 0.5920
9	 0.6360	 0.5790
A	 0.4890	 0.4710
AA	 0.6660	 0.5800
AB	 0.1410	 0.3950
AC	 0.3210	 0.4620
AD	 0.2250	 0.4190
AE	 0.2540	 0.4570
AF	 0.2730	 0.4540
AG	 0.2290	 0.3700
AH	 0.4820	 0.5530
AI	 0.7290	 0.6070
AJ	 0.6450	 0.5500
AK	 0.1130	 0.1930
AL	 0.1580	 0.3970
AM	 0.7120	 0.5870
AN	 0.4150	 0.4820
AO	 0.3510	 0.4680
AP	 0.5180	 0.5330
AQ	 0.1330	 0.2160
AR	 0.0240	 0.2980
B	 0.2670	 0.3860
D	 0.8520	 0.6160
E	 0.9700	 0.6660
F	 0.9050	 0.6340
G	 0.9540	 0.6890









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Chain	Atom inclusion	Q-score
H	 0.8850	 0.6660
I	 0.9040	 0.6550
J	 0.7840	 0.6120
K	 0.7610	 0.6050
L	 0.9050	 0.6690
M	 0.7080	 0.5780
N	 0.8240	 0.6330
O	 0.8550	 0.6460
P	 0.6500	 0.5430
Q	 0.8040	 0.6190
R	 0.8570	 0.6290
S	 0.9640	 0.6900
T	 0.9120	 0.6760
U	 0.8900	 0.6710
V	 0.9410	 0.6790
W	 0.7820	 0.6030
X	 0.9260	 0.6730
Y	 0.8550	 0.6440
Z	 0.5890	 0.5300
a	 0.9130	 0.6770
b	 0.8660	 0.6640
c	 0.8430	 0.6310
d	 0.8170	 0.6280
e	 0.8170	 0.6280
f	 0.9070	 0.6730
g	 0.7150	 0.5750
h	 0.8350	 0.6270
i	 0.8310	 0.6390
j	 0.9450	 0.6880
k	 0.9410	 0.6780
l	 0.8570	 0.6390
m	 0.8290	 0.6290
n	 0.7720	 0.6160
o	 0.9500	 0.6850
p	 0.6460	 0.5650
q	 0.9010	 0.6590
r	 0.8750	 0.6560
s	 0.8810	 0.6610
t	 0.8060	 0.6260
u	 0.8790	 0.6670
v	 0.9020	 0.6410
w	 0.6880	 0.5150

*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
x	 0.4640	 0.5430
y	 0.5690	 0.5650
z	 0.6350	 0.5760