



## wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 05:37 PM JST

PDB ID : 8JDM / pdb\_00008jdm  
EMDB ID : EMD-36181  
Title : Structure of the Human cytoplasmic Ribosome with human tRNA  
Tyr(GalQ34) and mRNA(UAU) (rotated state)  
Authors : Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.  
Deposited on : 2023-05-14  
Resolution : 2.67 Å (reported)  
Based on initial models : 6Y57, 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:

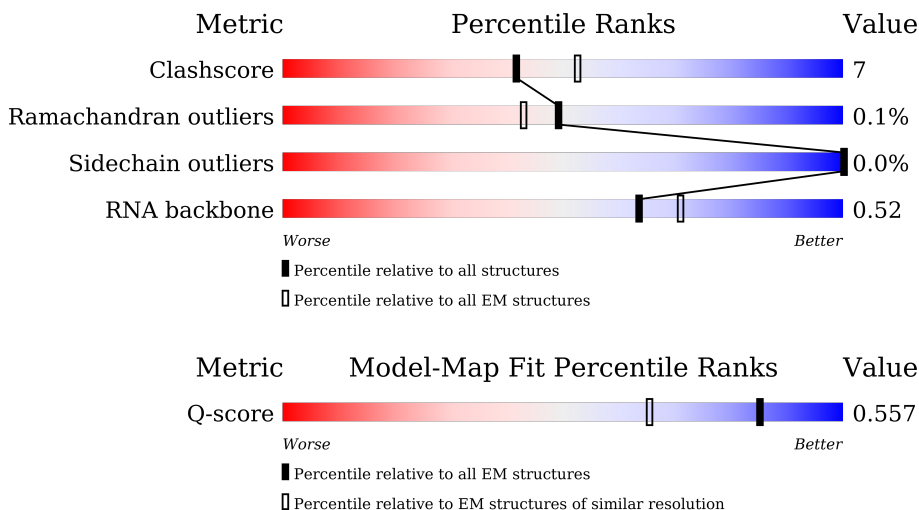
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 2.67 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.











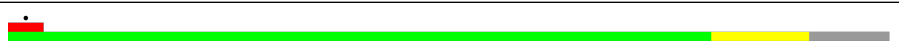

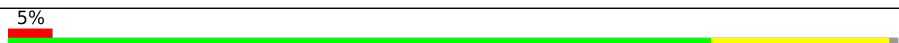


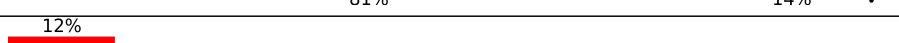
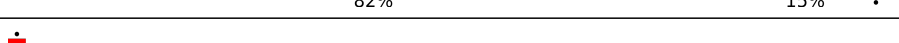
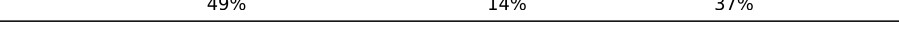
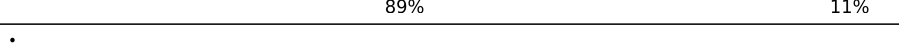
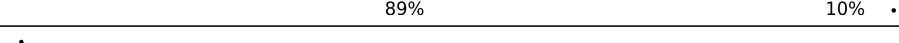
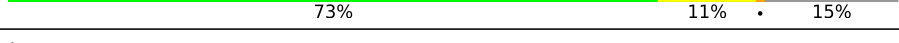



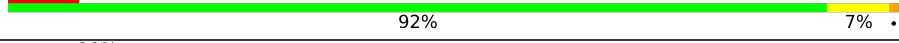


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9182 ( 2.17 - 3.17 )

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	
2	B	76	
2	C	76	

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Mol	Chain	Length	Quality of chain
3	D	5070	
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	

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Mol	Chain	Length	Quality of chain
28	c	156	63% 14% 23%
29	d	145	6% 78% 14% 8%
30	e	136	7% 83% 16%
31	f	148	78% 21%
32	g	159	15% 59% 5% 35%
33	h	115	10% 71% 13% 16%
34	i	125	6% 76% 9% 14%
35	j	135	90% 5% 5%
36	k	110	81% 18%
37	l	117	9% 85% 11%
38	m	123	91% 7%
39	n	105	13% 89% 9%
40	o	97	77% 9% 11%
41	p	70	21% 80% 19%
42	q	51	75% 24%
43	r	128	30% 11% 59%
44	s	25	100%
45	t	106	13% 76% 23%
46	u	92	87% 12%
47	v	137	75% 16% 9%
48	w	1869	18% 48% 31% 9% 13%
49	x	295	30% 53% 20% 27%
50	y	264	33% 61% 19% 20%
51	z	293	15% 61% 11% 28%
52	0	243	59% 68% 19% 13%

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Mol	Chain	Length	Quality of chain
53	1	263	73% 72% 27%
54	2	204	61% 70% 22% 8%
55	3	249	86% 64% 31% 5%
56	4	194	80% 61% 35%
57	5	208	67% 68% 31%
58	6	194	66% 64% 30% 6%
59	7	165	55% 41% 17% 42%
60	8	158	30% 76% 14% 10%
61	9	151	34% 79% 20%
62	AA	151	22% 66% 23% 11%
63	AB	145	59% 68% 25% 8%
64	AC	146	63% 73% 25%
65	AD	135	73% 71% 24%
66	AE	152	64% 59% 36% 5%
67	AF	145	62% 79% 19%
68	AG	119	64% 51% 34% 14%
69	AH	83	39% 76% 24%
70	AI	130	8% 75% 24%
71	AJ	143	21% 85% 13%
72	AK	133	86% 56% 36% 8%
73	AL	125	54% 43% 14% 42%
74	AM	115	21% 69% 17% 14%
75	AN	84	56% 63% 36%
76	AO	69	57% 59% 29% 12%
77	AP	56	18% 61% 20% 20%

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Mol	Chain	Length	Quality of chain
78	AQ	59	
79	AR	317	

## 2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 209349 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
			Total	C	N	O	P		
1	A	14	288	130	40	104	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	73	1580	715	281	512	72	0	0
2	C	73	1580	715	281	512	72	0	0

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
34	i	107	888	560	171	155	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	P		
48	w	1634	34933	15622	6267	11411	1633	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
62	AA	134	1002	612	197	187	6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	AL	72	574	368	104	101	1	0	0

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

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

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

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

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

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

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

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

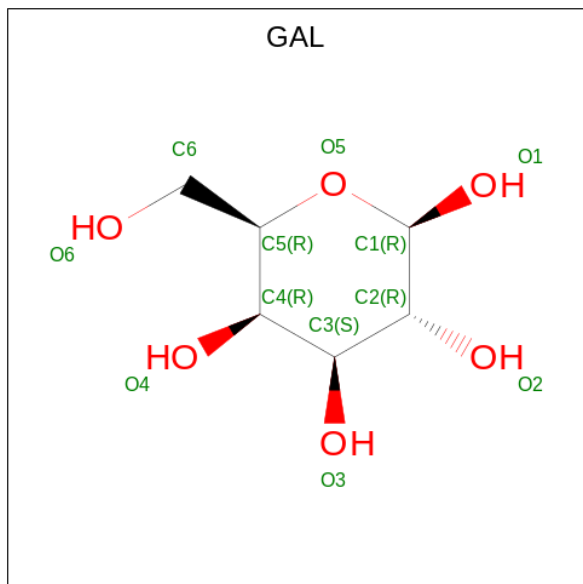
- Molecule 78 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	AQ	55	438	271	95	71	1	0	0

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

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

- Molecule 80 is beta-D-galactopyranose (CCD ID: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	D	391	Total	Mg	0
			391	391	
81	E	10	Total	Mg	0
			10	10	
81	F	5	Total	Mg	0
			5	5	
81	G	2	Total	Mg	0
			2	2	
81	H	1	Total	Mg	0
			1	1	
81	I	1	Total	Mg	0
			1	1	
81	N	1	Total	Mg	0
			1	1	
81	O	1	Total	Mg	0
			1	1	
81	S	1	Total	Mg	0
			1	1	
81	U	1	Total	Mg	0
			1	1	
81	V	2	Total	Mg	0
			2	2	
81	W	1	Total	Mg	0
			1	1	
81	X	1	Total	Mg	0
			1	1	
81	a	1	Total	Mg	0
			1	1	
81	g	1	Total	Mg	0
			1	1	
81	j	1	Total	Mg	0
			1	1	
81	k	1	Total	Mg	0
			1	1	
81	l	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
81	w	93	Total 93	Mg 93	0
81	2	1	Total 1	Mg 1	0
81	AA	1	Total 1	Mg 1	0
81	AG	1	Total 1	Mg 1	0
81	AM	1	Total 1	Mg 1	0

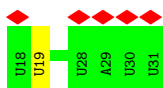
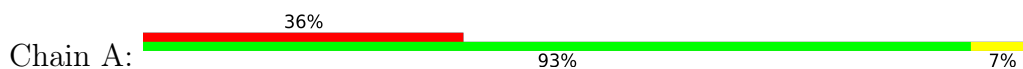
- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	o	1	Total 1	Zn 1	0
82	r	1	Total 1	Zn 1	0
82	t	1	Total 1	Zn 1	0
82	u	1	Total 1	Zn 1	0
82	w	1	Total 1	Zn 1	0
82	AA	1	Total 1	Zn 1	0

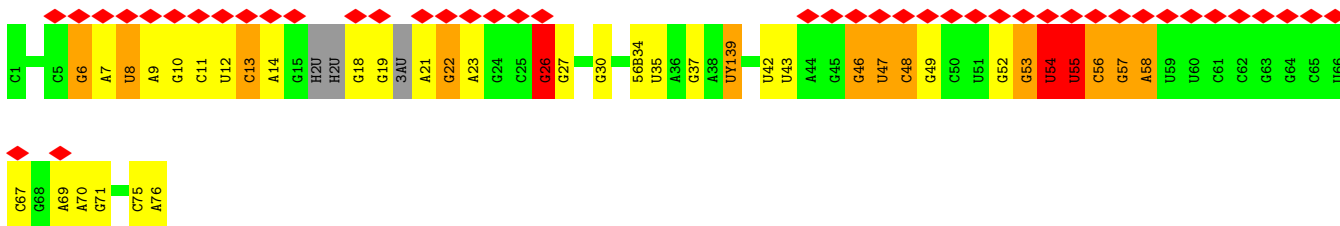
### 3 Residue-property plots [i](#)

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

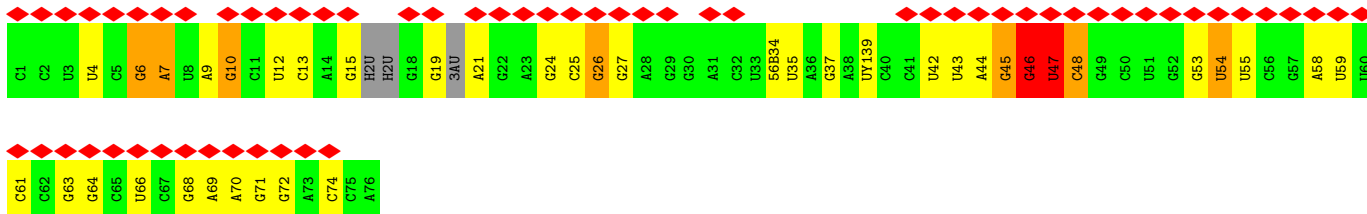
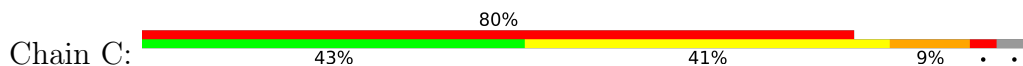
- Molecule 1: mRNA



- Molecule 2: tRNA (Tyr)

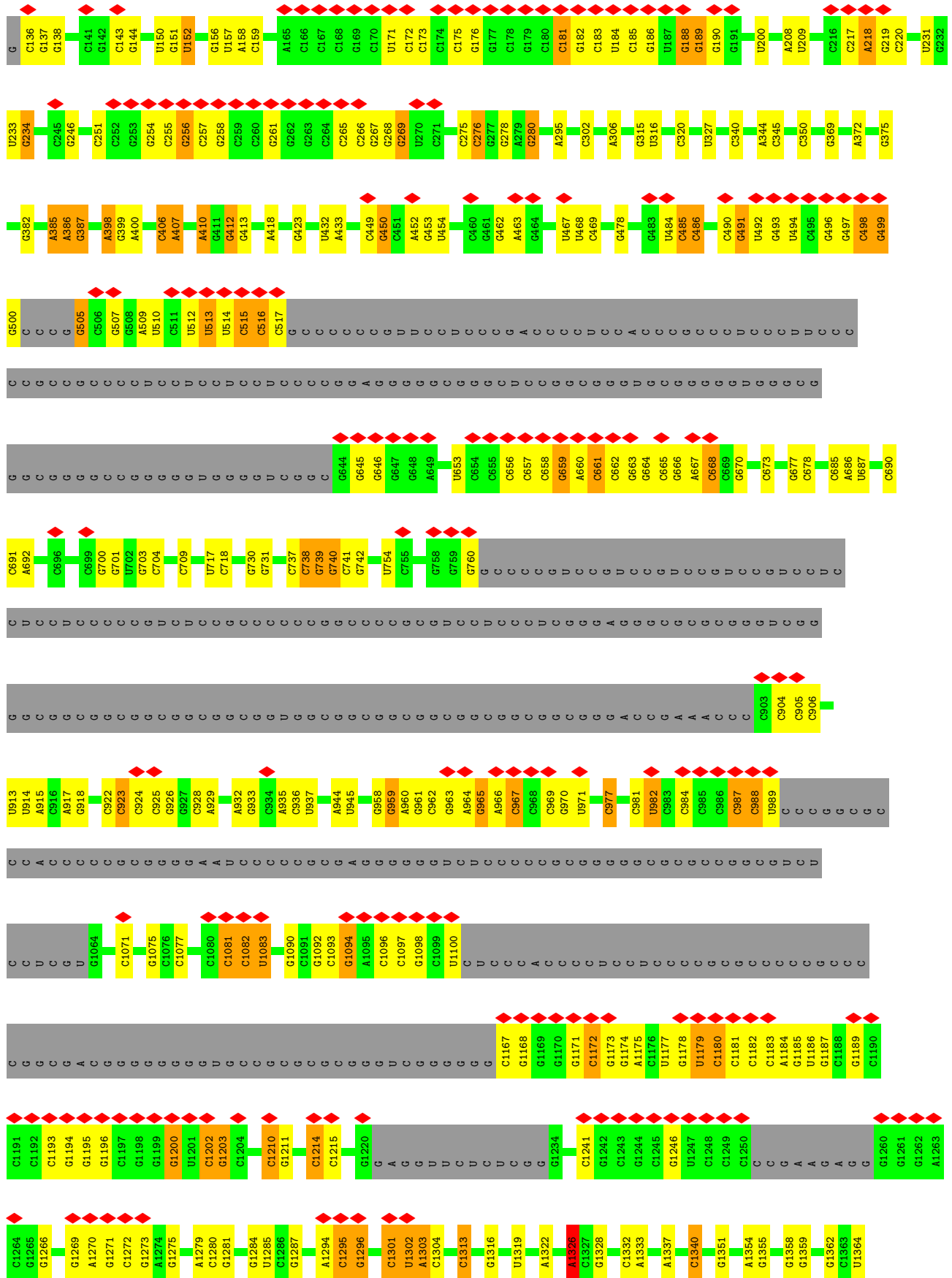


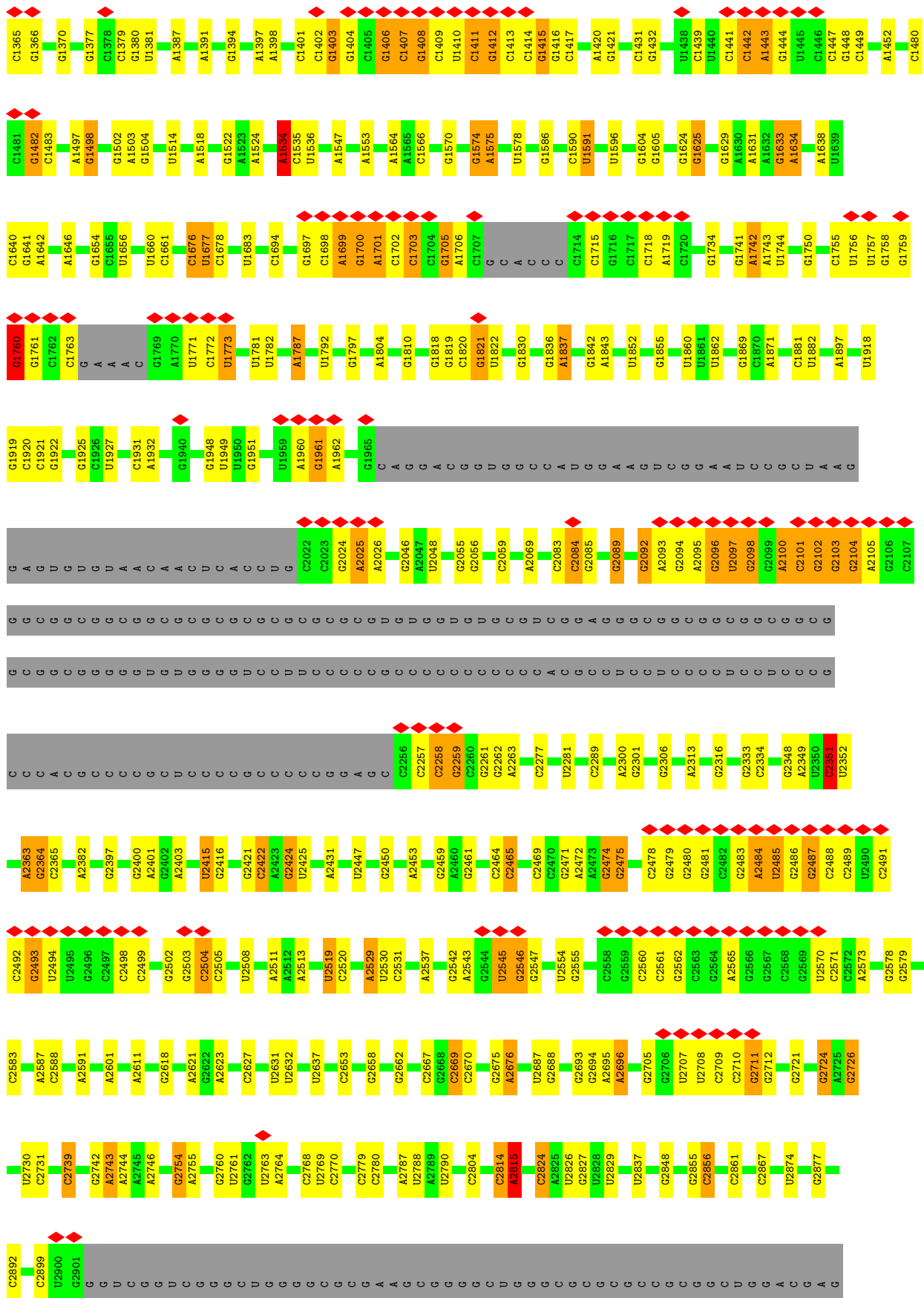
- Molecule 2: tRNA (Tyr)



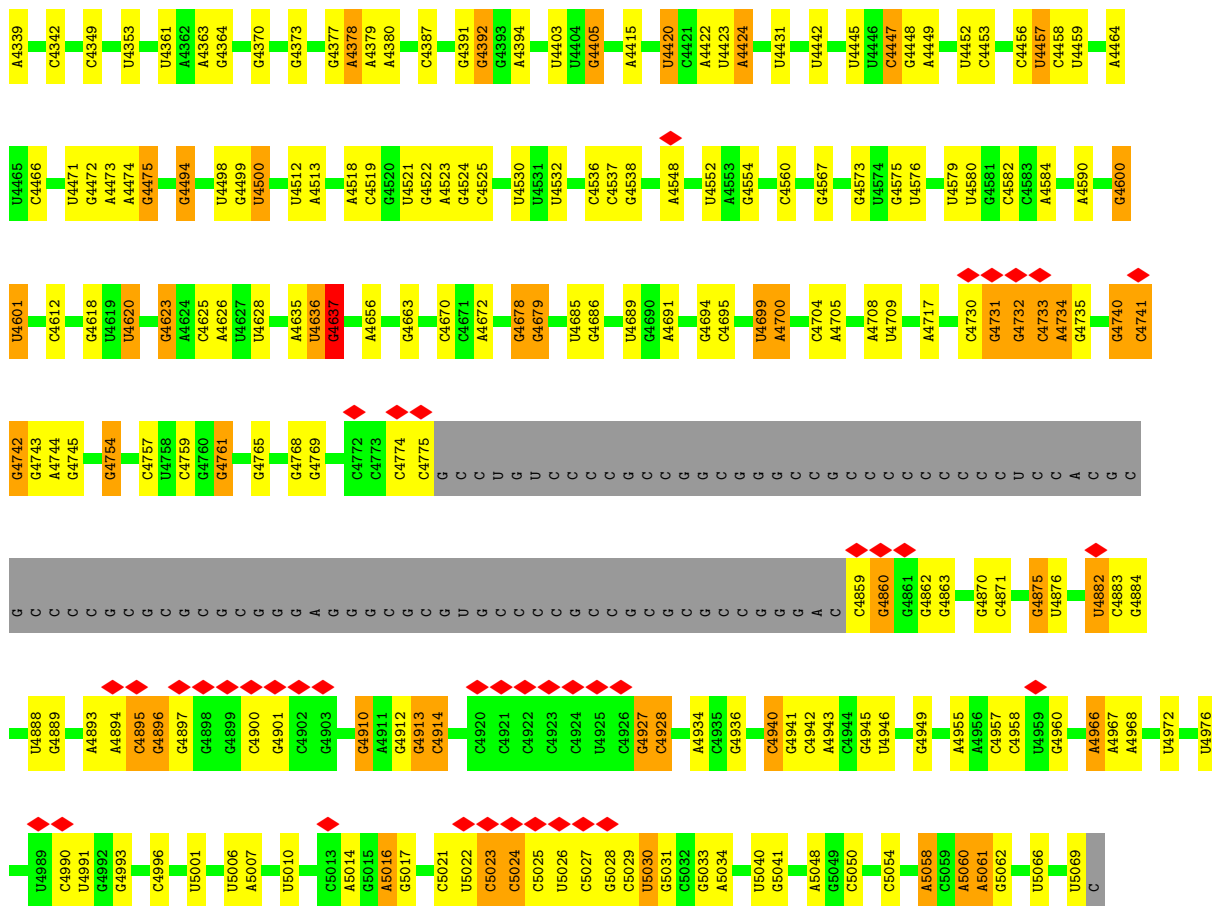
- Molecule 3: 28S ribosomal RNA



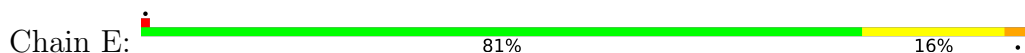




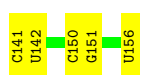
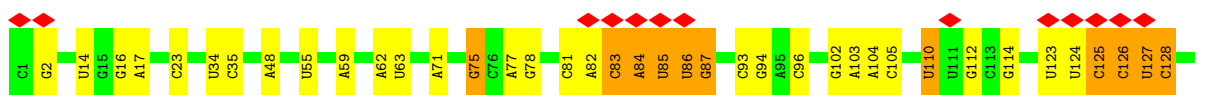




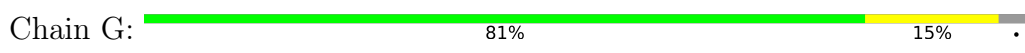
• Molecule 4: 5S ribosomal RNA

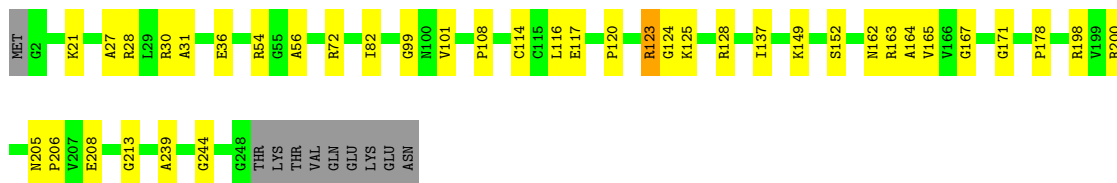


• Molecule 5: 5.8S ribosomal RNA

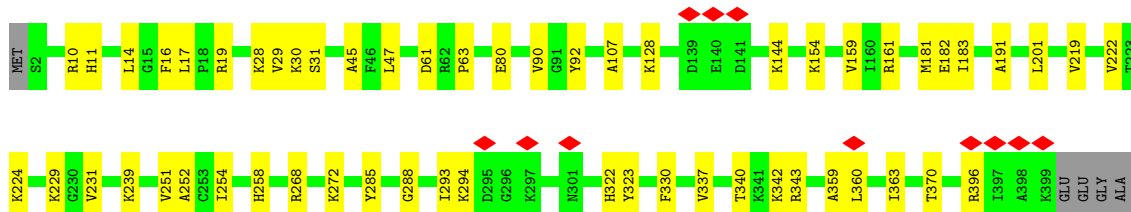
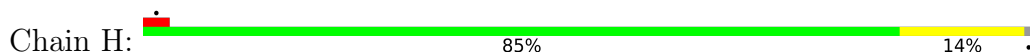


• Molecule 6: 60S ribosomal protein L8

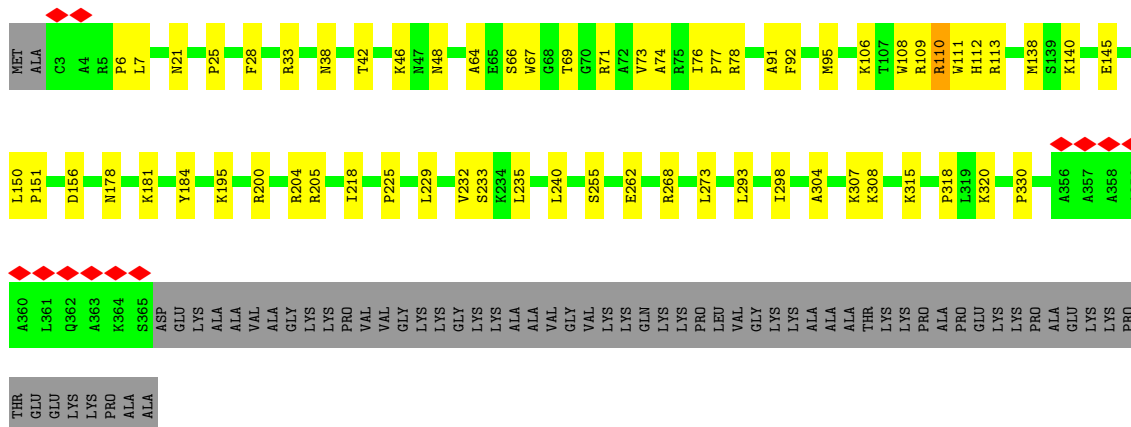




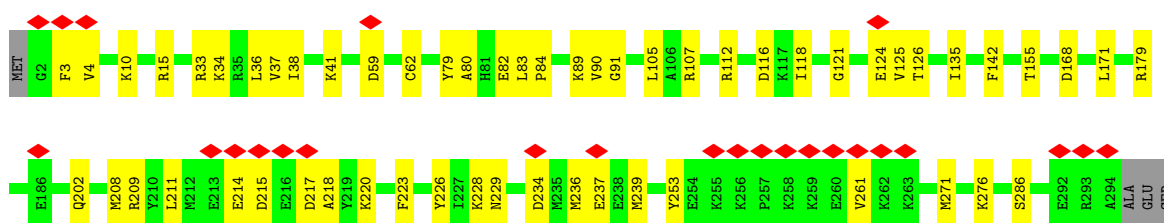
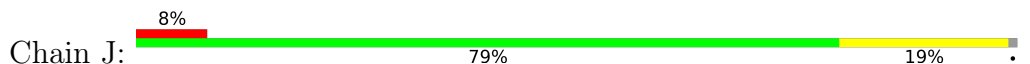
• Molecule 7: 60S ribosomal protein L3



• Molecule 8: 60S ribosomal protein L4

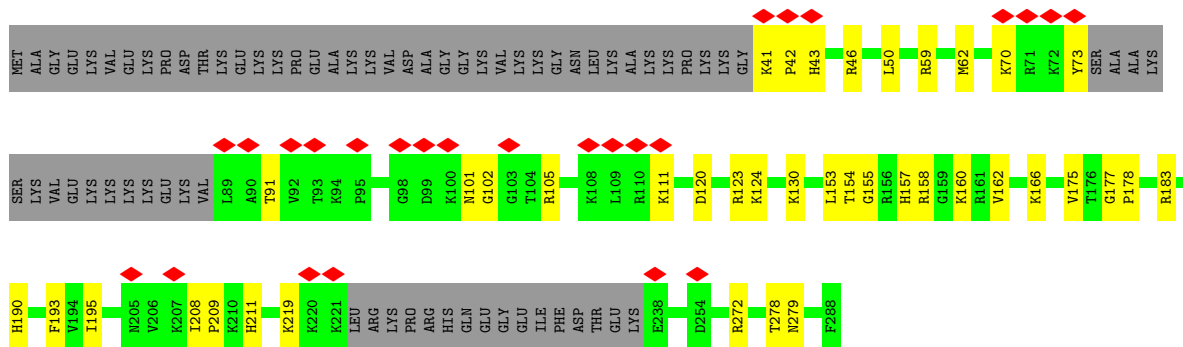


• Molecule 9: 60S ribosomal protein L5

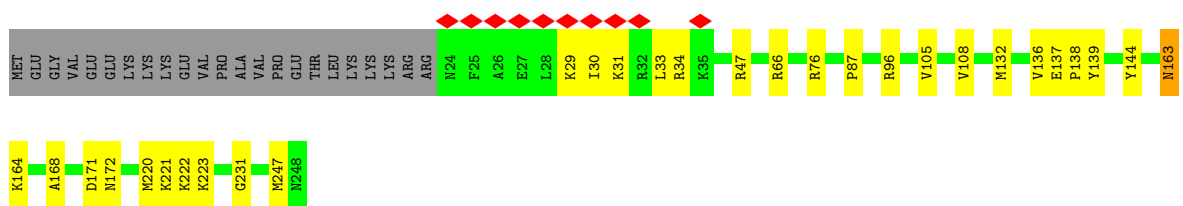
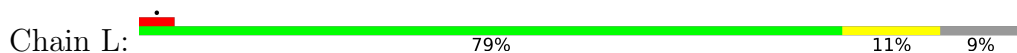


• Molecule 10: 60S ribosomal protein L6

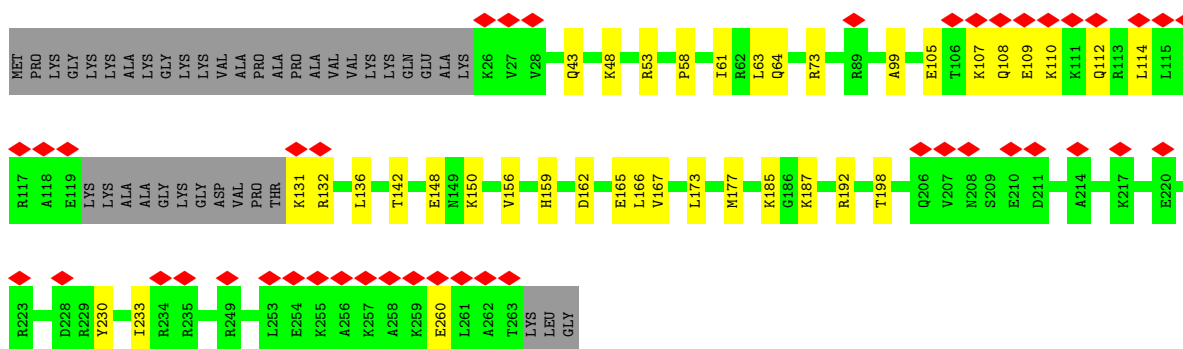




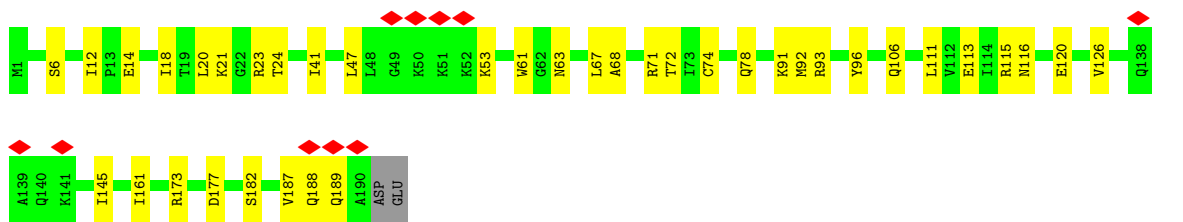
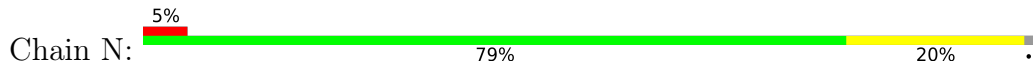
• Molecule 11: 60S ribosomal protein L7



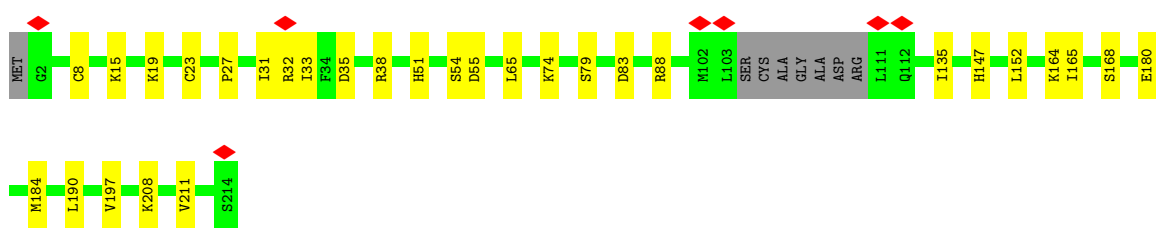
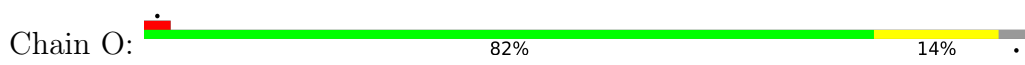
• Molecule 12: 60S ribosomal protein L7a



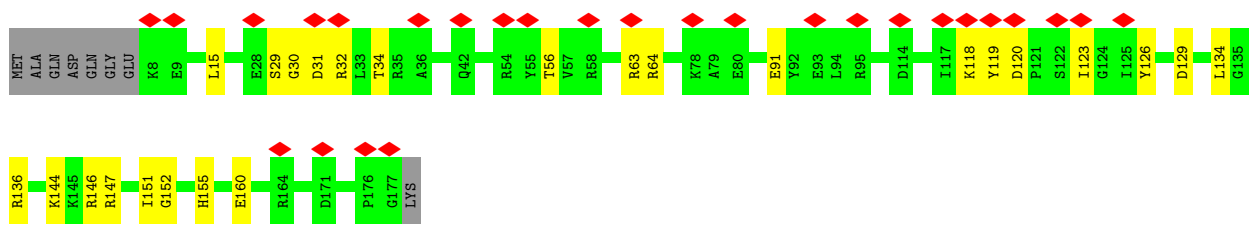
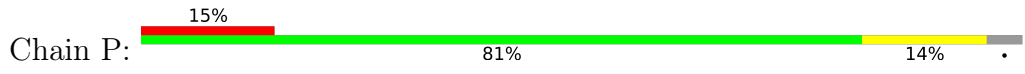
• Molecule 13: 60S ribosomal protein L9



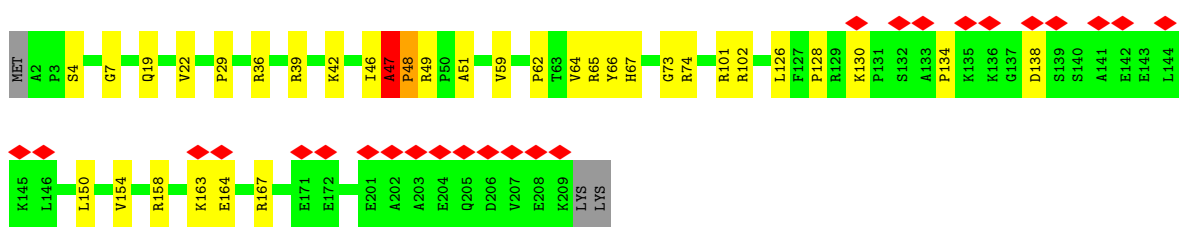
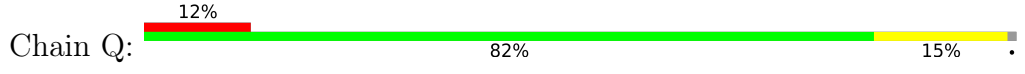
• Molecule 14: 60S ribosomal protein L10-like



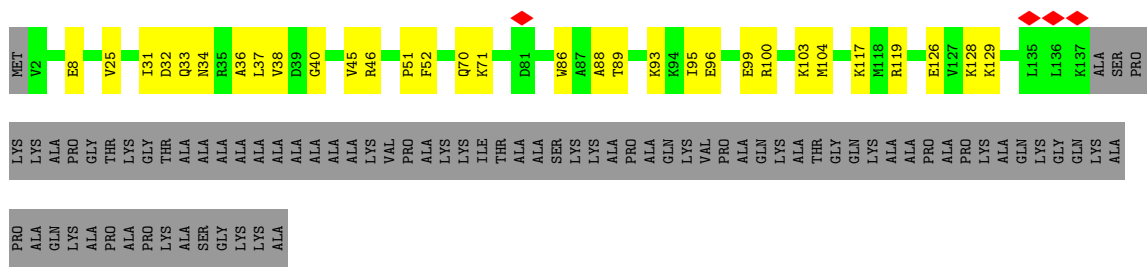
• Molecule 15: 60S ribosomal protein L11



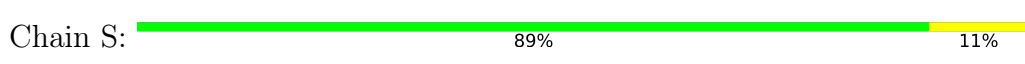
• Molecule 16: 60S ribosomal protein L13



• Molecule 17: 60S ribosomal protein L14

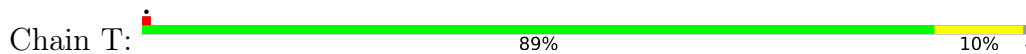


• Molecule 18: 60S ribosomal protein L15





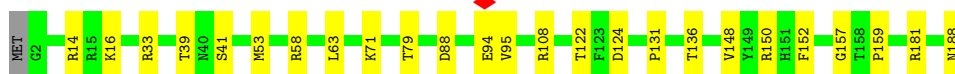
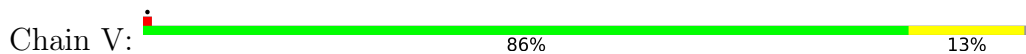
- Molecule 19: 60S ribosomal protein L13a



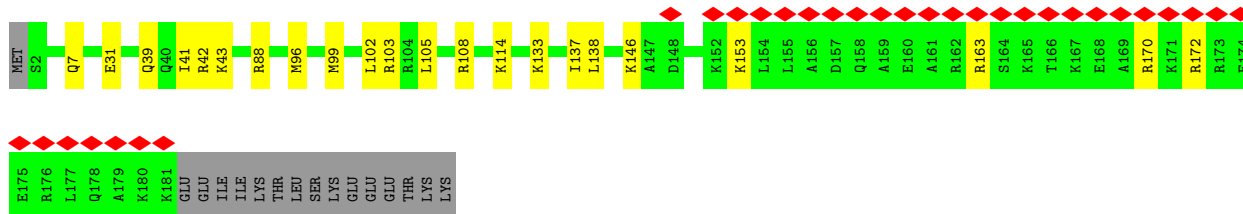
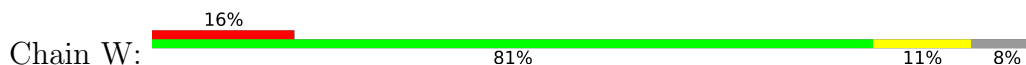
- Molecule 20: 60S ribosomal protein L17



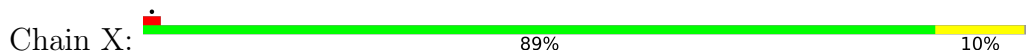
- Molecule 21: 60S ribosomal protein L18



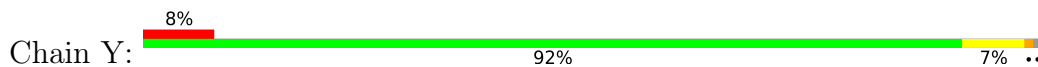
- Molecule 22: 60S ribosomal protein L19



- Molecule 23: 60S ribosomal protein L18a

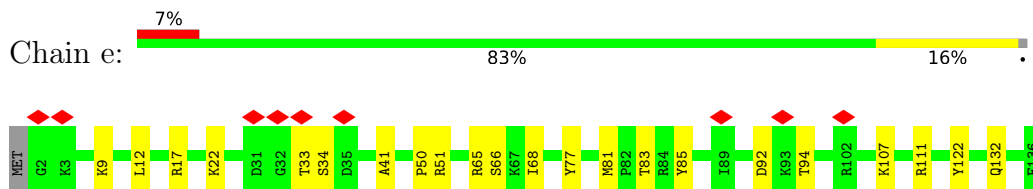


- Molecule 24: 60S ribosomal protein L21

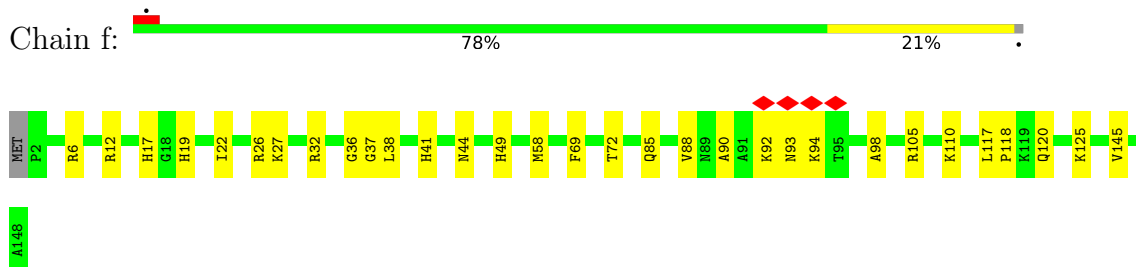




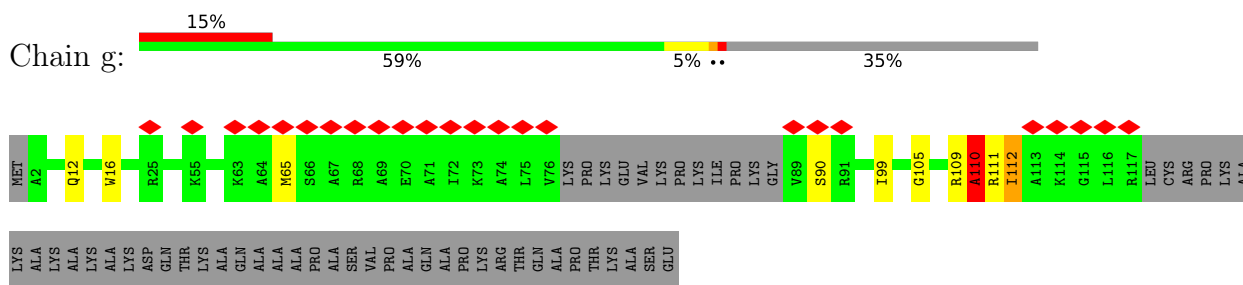
• Molecule 30: 60S ribosomal protein L27



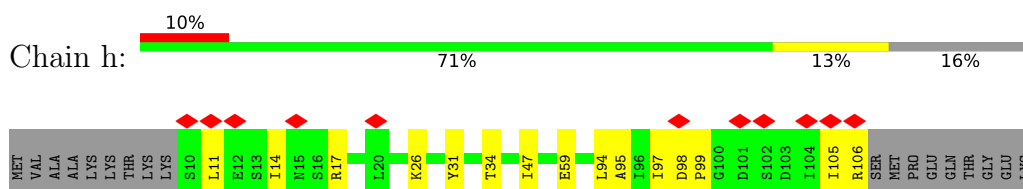
• Molecule 31: 60S ribosomal protein L27a



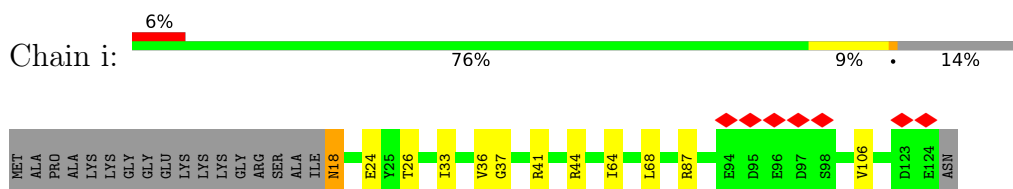
• Molecule 32: 60S ribosomal protein L29



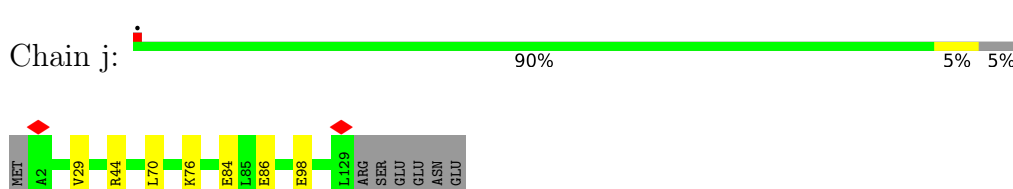
• Molecule 33: 60S ribosomal protein L30



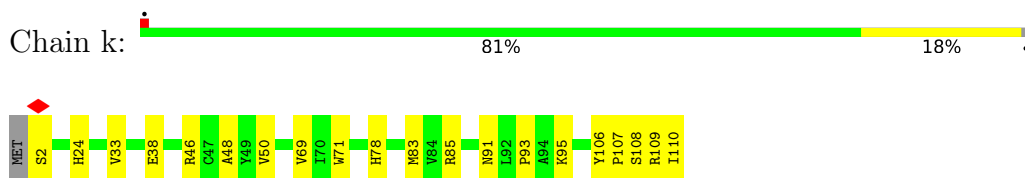
• Molecule 34: 60S ribosomal protein L31



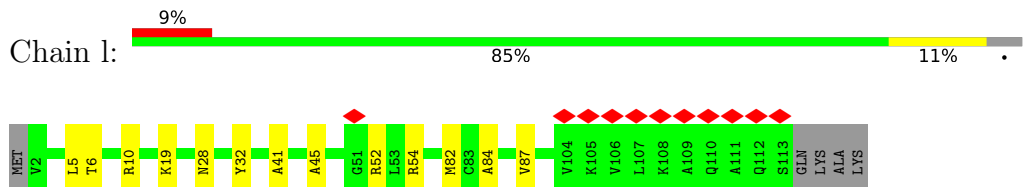
• Molecule 35: 60S ribosomal protein L32



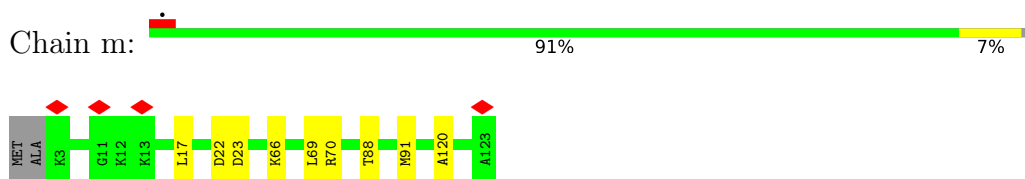
• Molecule 36: 60S ribosomal protein L35a



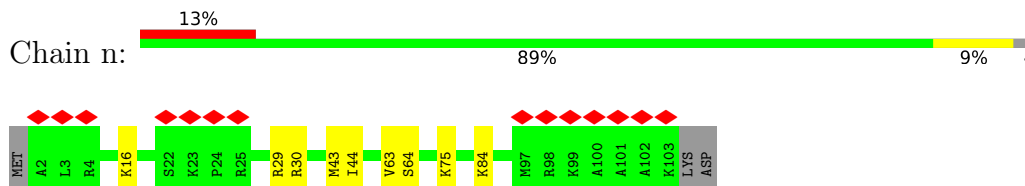
• Molecule 37: 60S ribosomal protein L34



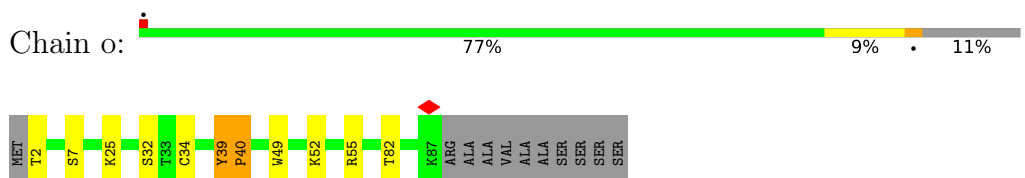
• Molecule 38: 60S ribosomal protein L35



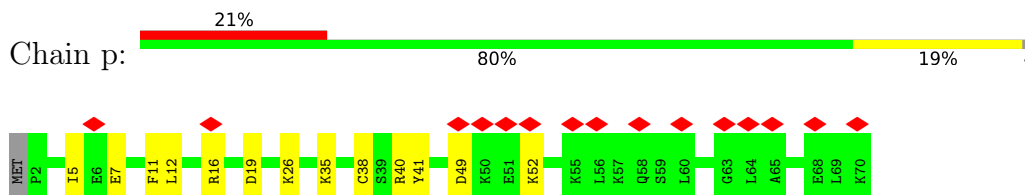
• Molecule 39: 60S ribosomal protein L36



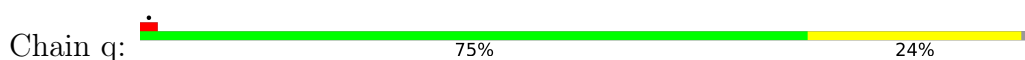
• Molecule 40: 60S ribosomal protein L37



• Molecule 41: 60S ribosomal protein L38

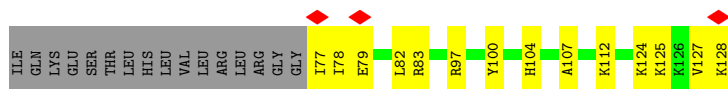
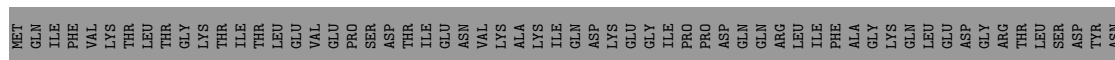


• Molecule 42: 60S ribosomal protein L39





• Molecule 43: Ubiquitin-60S ribosomal protein L40



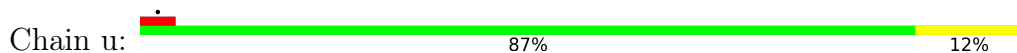
• Molecule 44: 60S ribosomal protein L41



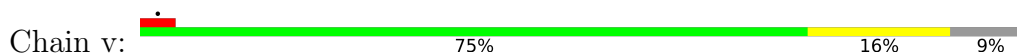
• Molecule 45: 60S ribosomal protein L36a



• Molecule 46: 60S ribosomal protein L37a

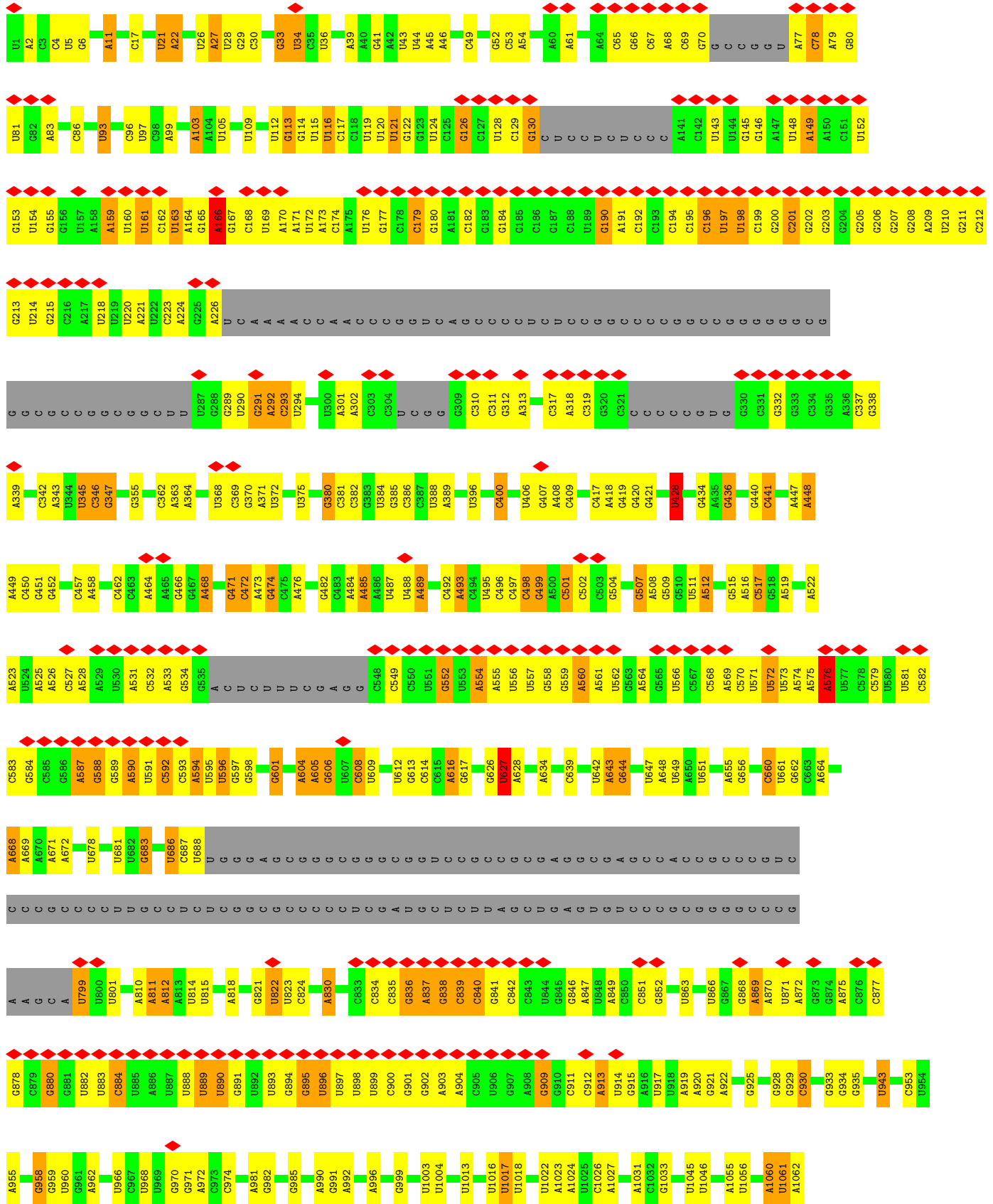


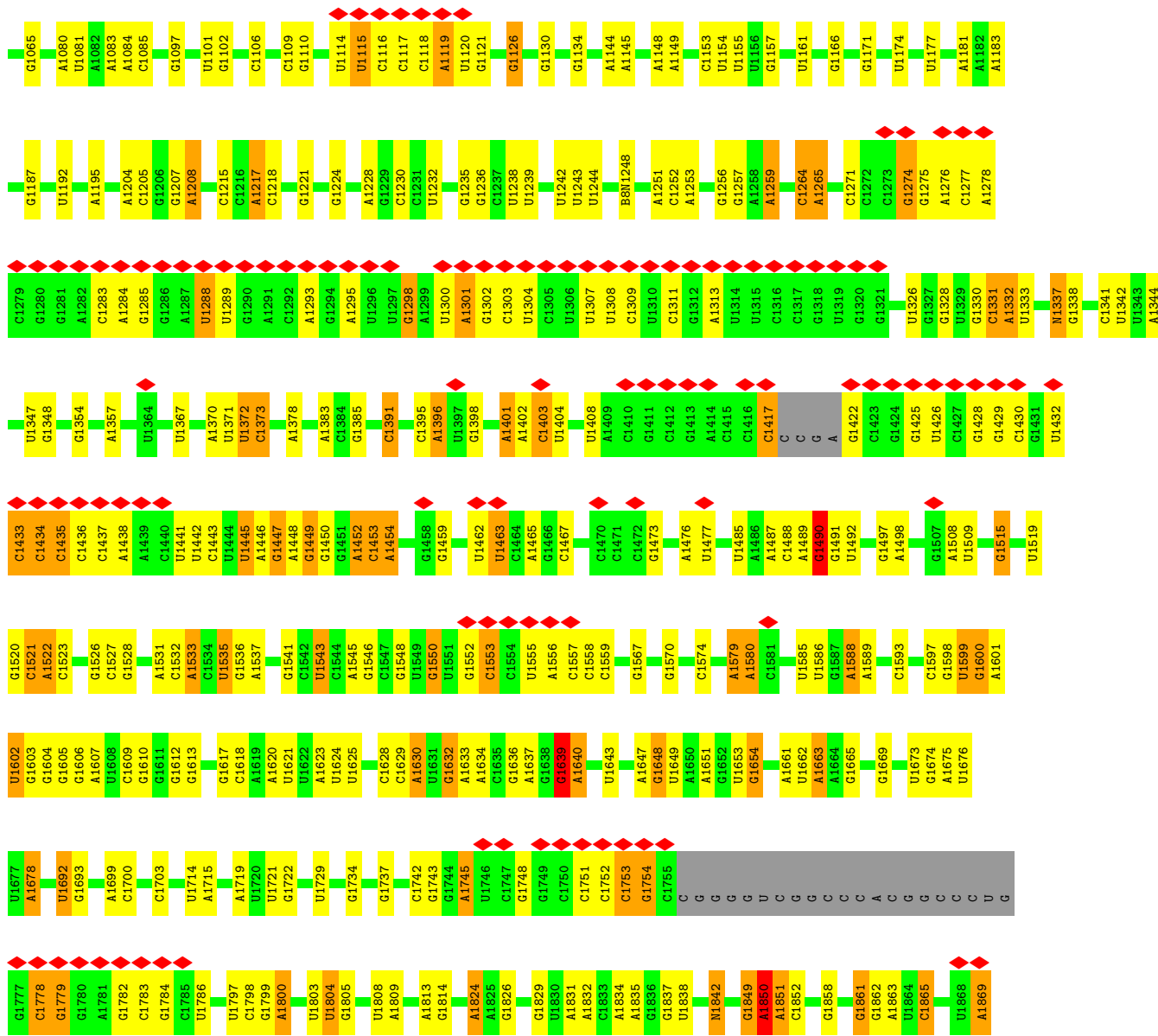
• Molecule 47: 60S ribosomal protein L28



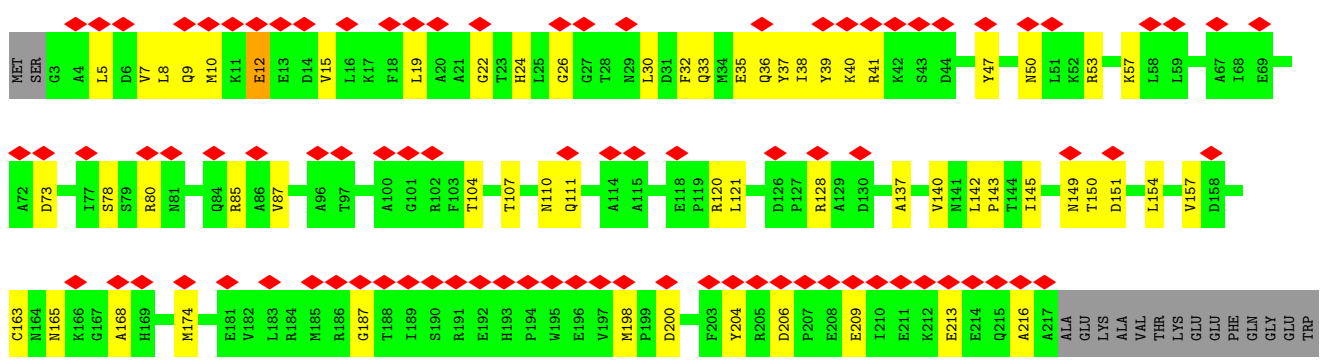
• Molecule 48: 18S ribosomal RNA



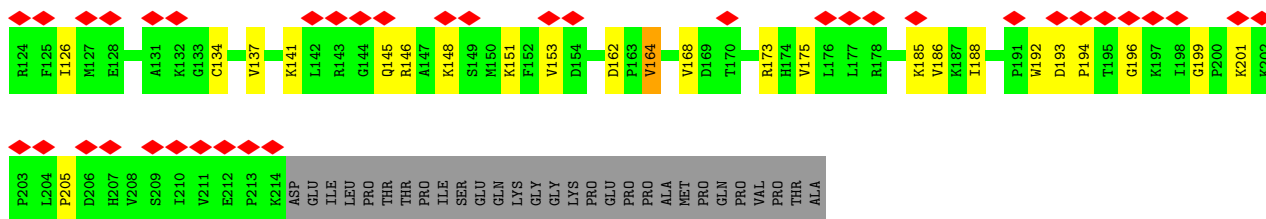




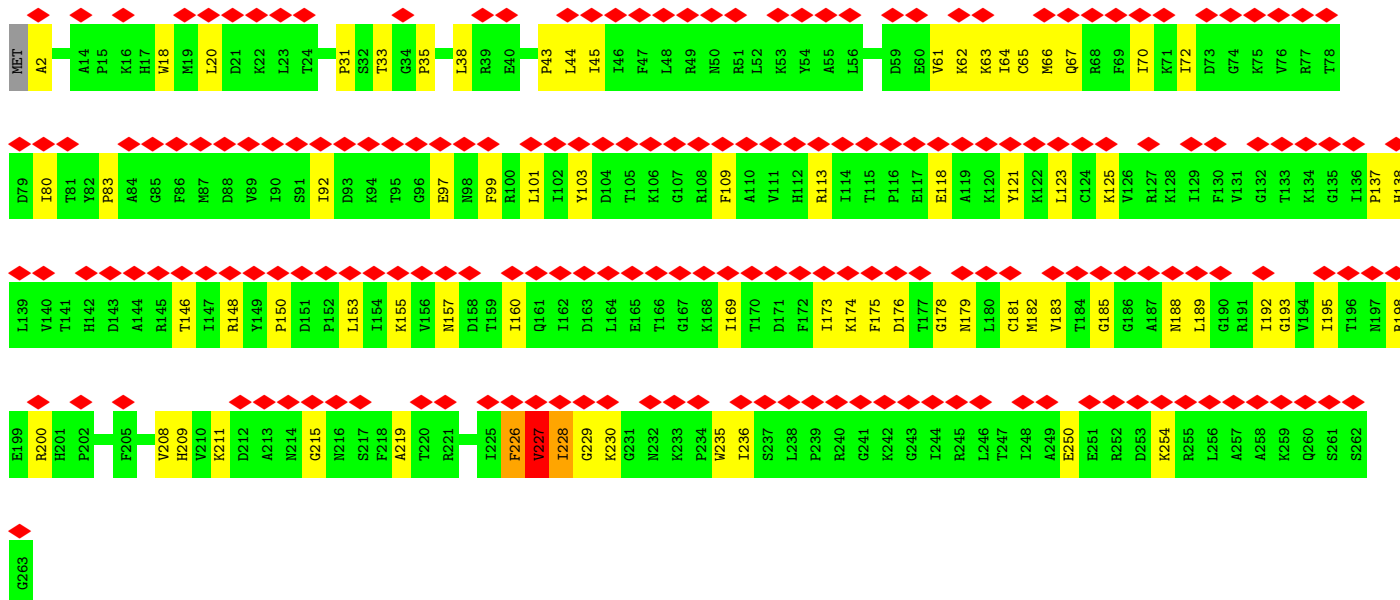
• Molecule 49: 40S ribosomal protein SA



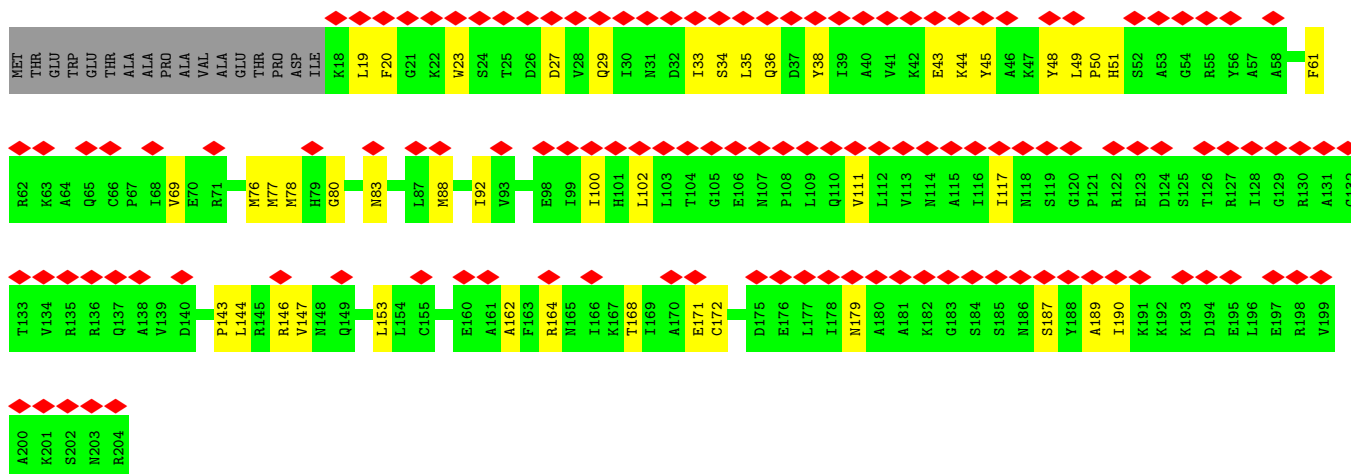




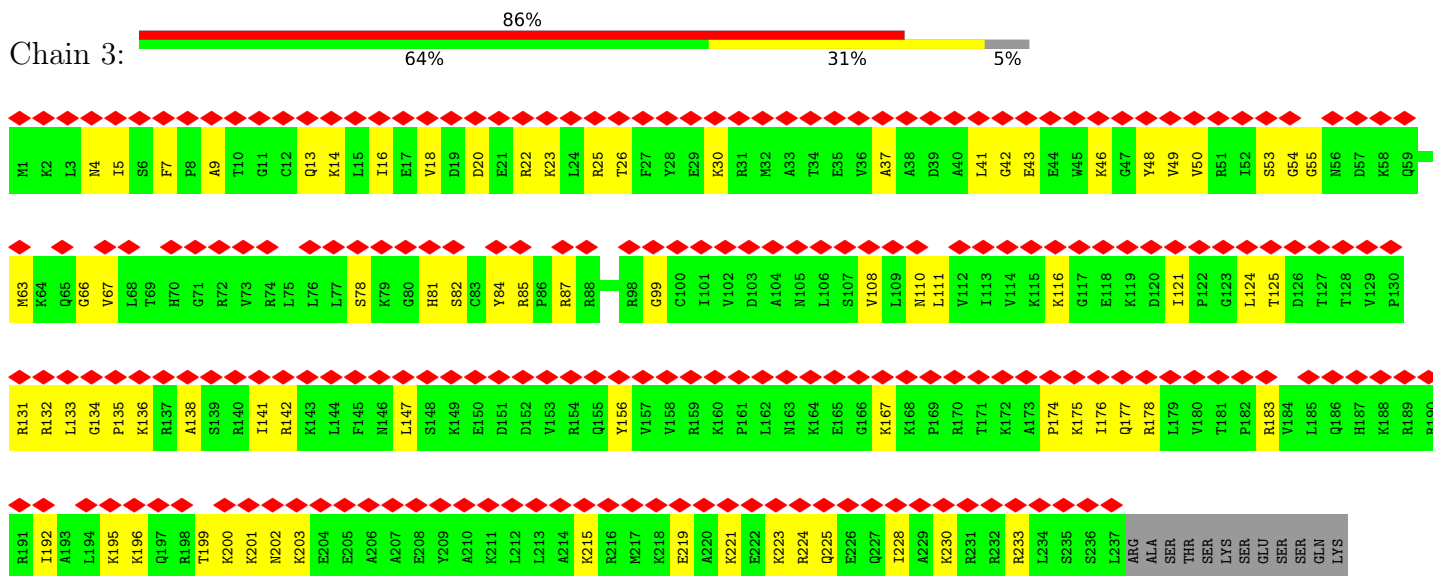
• Molecule 53: 40S ribosomal protein S4, X isoform



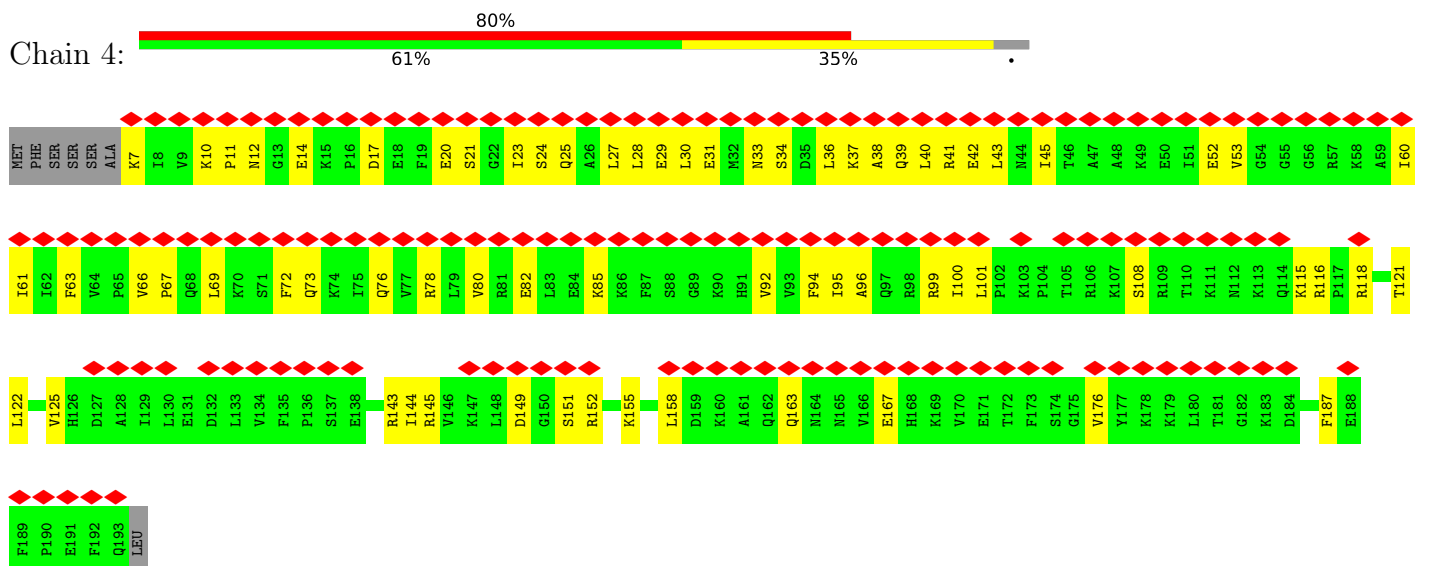
• Molecule 54: 40S ribosomal protein S5



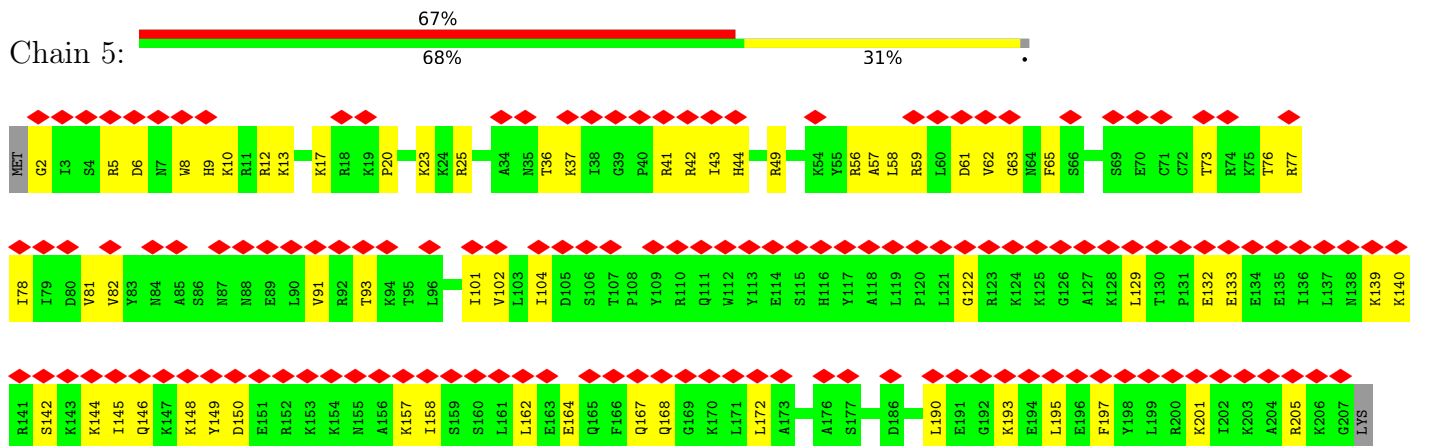
• Molecule 55: 40S ribosomal protein S6



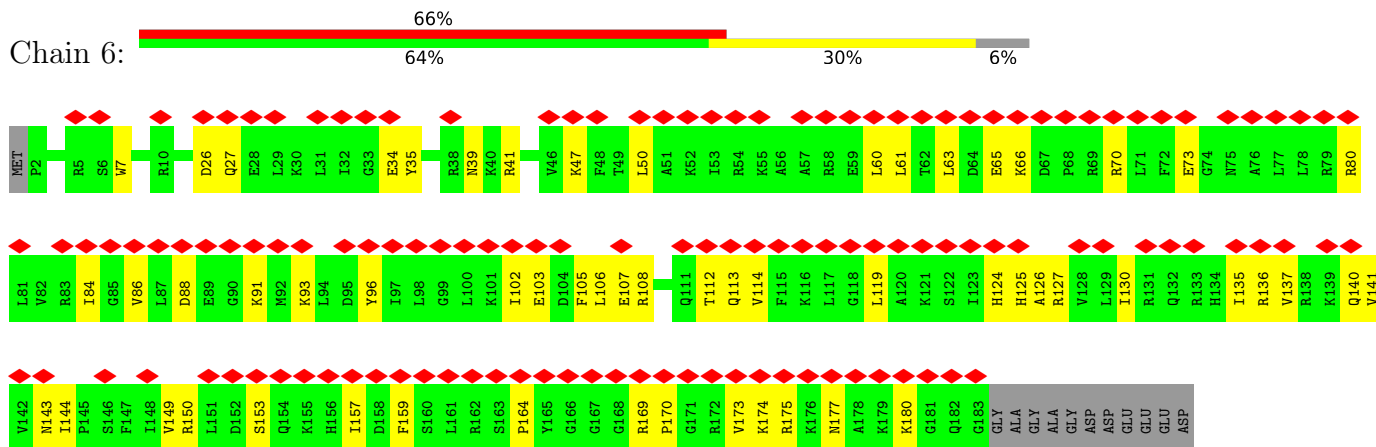
• Molecule 56: 40S ribosomal protein S7



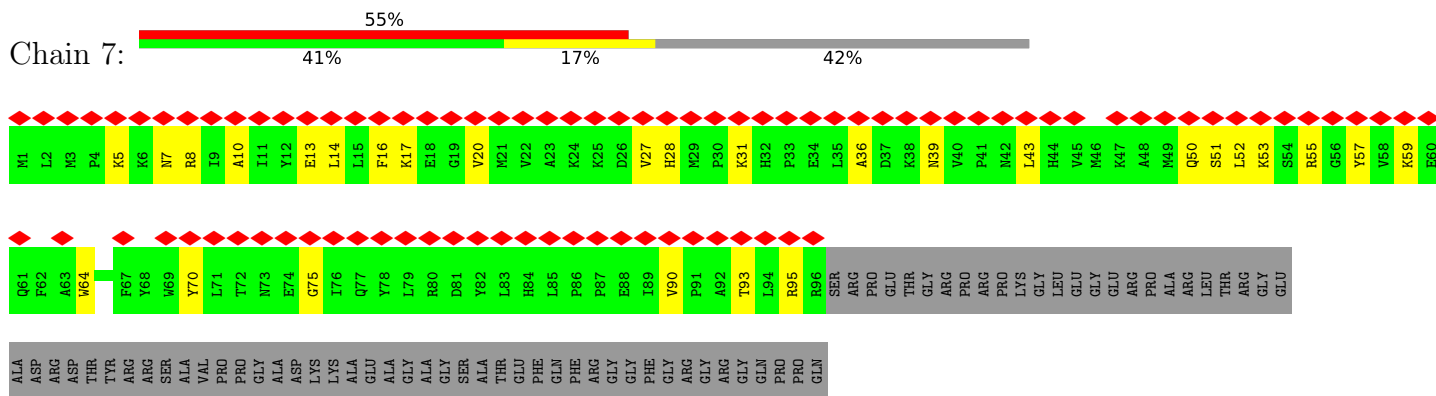
• Molecule 57: 40S ribosomal protein S8



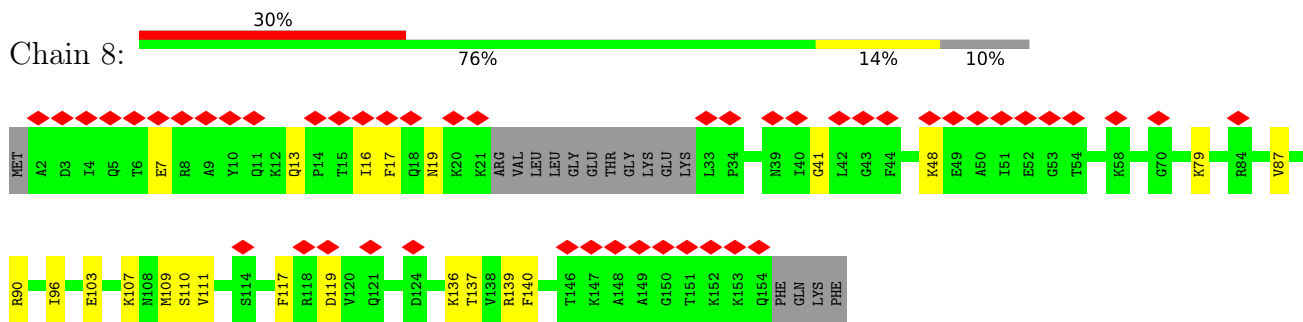
• Molecule 58: 40S ribosomal protein S9



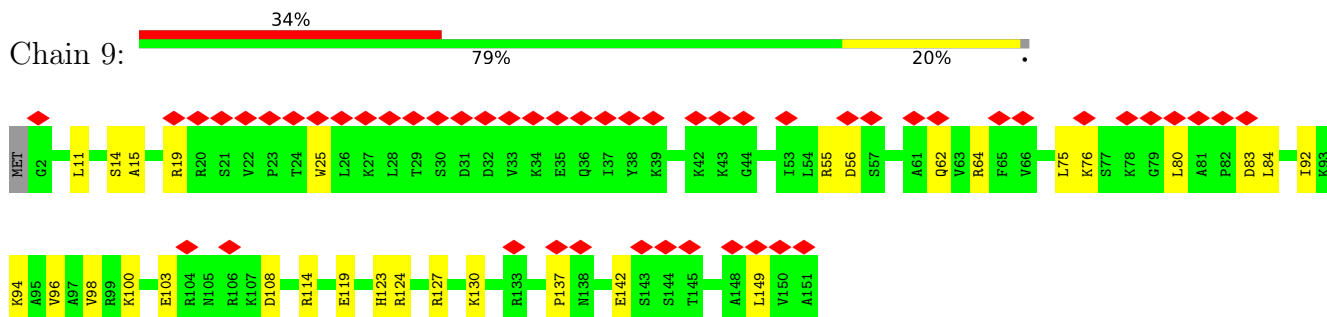
• Molecule 59: 40S ribosomal protein S10



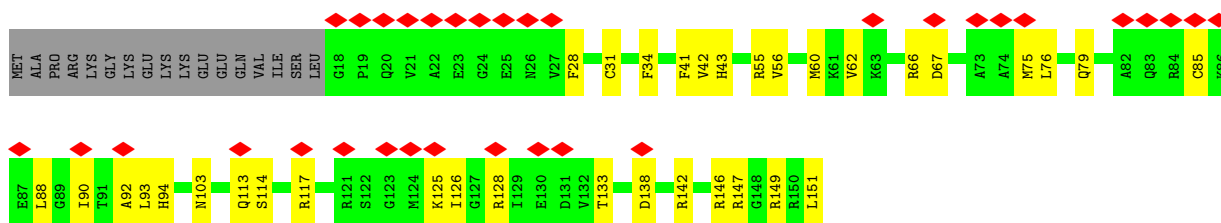
• Molecule 60: 40S ribosomal protein S11



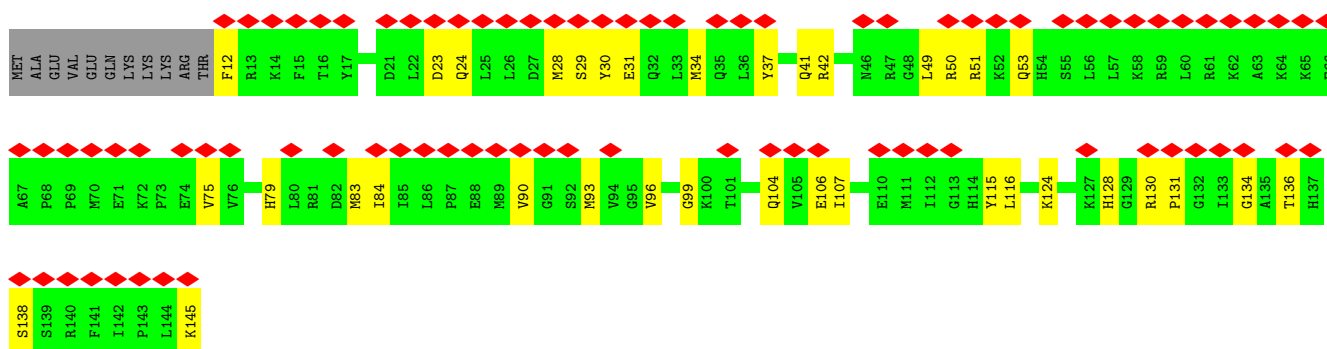
• Molecule 61: 40S ribosomal protein S13



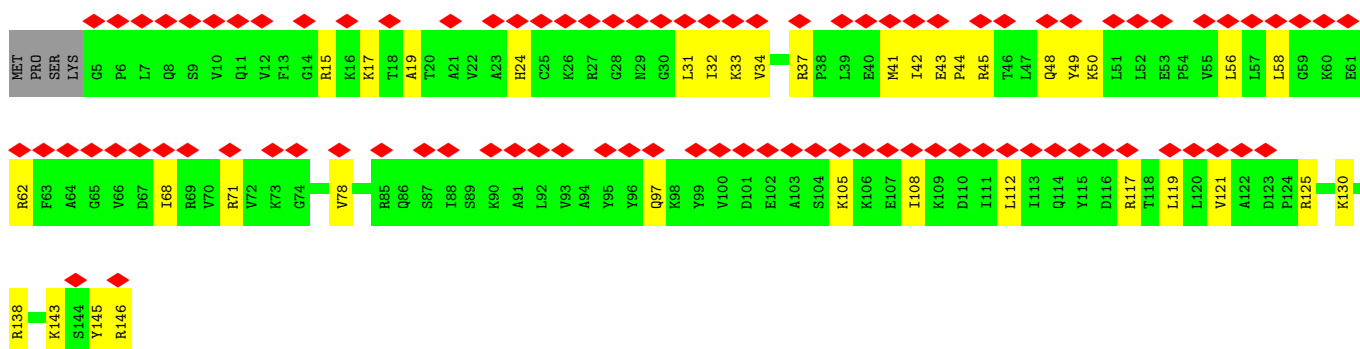
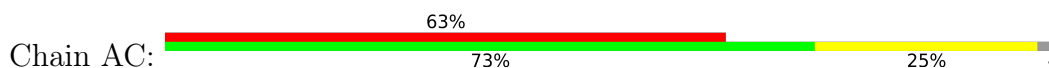
• Molecule 62: 40S ribosomal protein S14



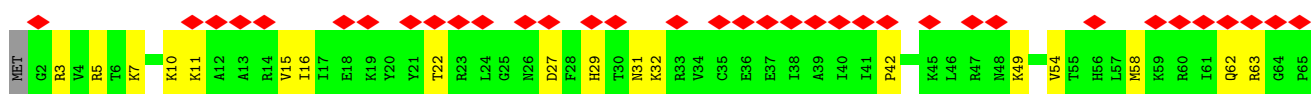
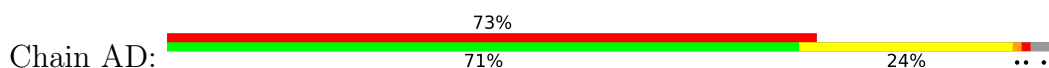
• Molecule 63: 40S ribosomal protein S15

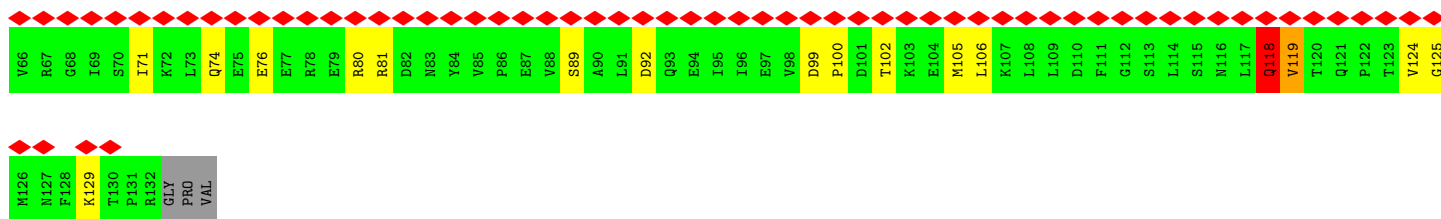


• Molecule 64: 40S ribosomal protein S16



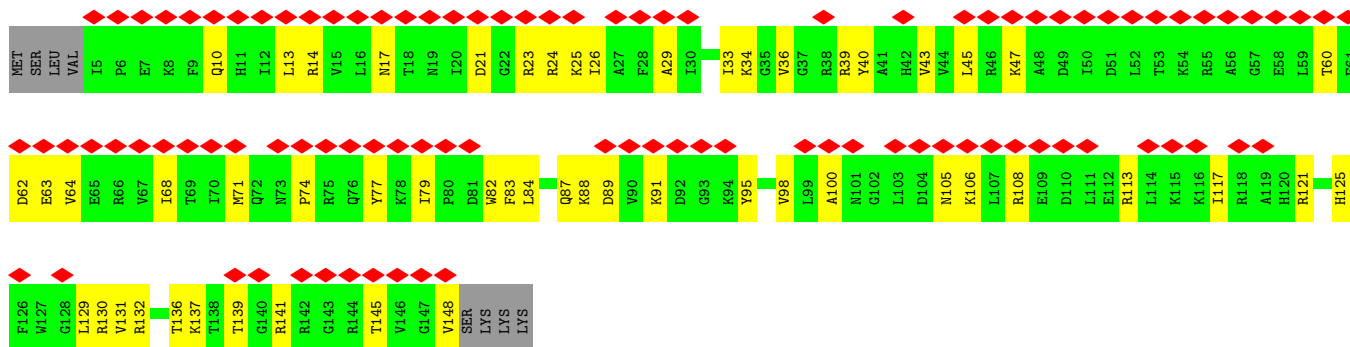
• Molecule 65: 40S ribosomal protein S17





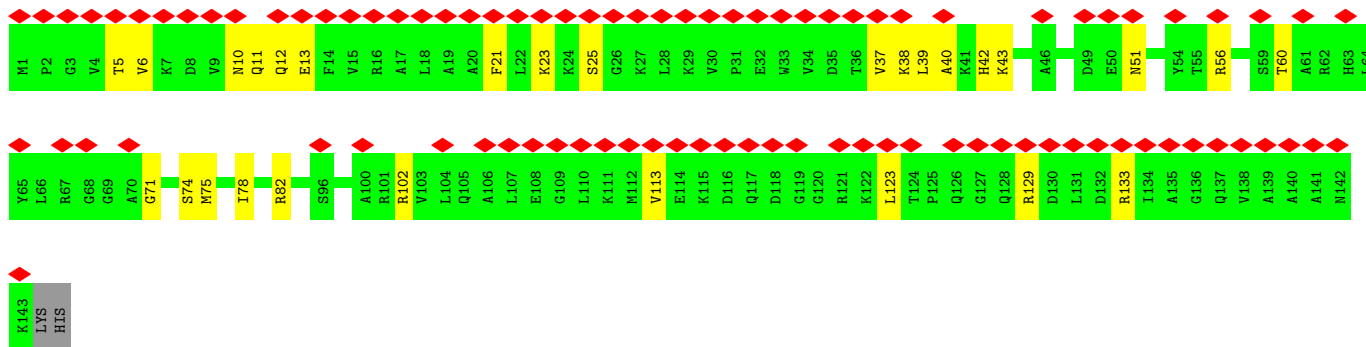
- Molecule 66: 40S ribosomal protein S18

Chain AE: 64%  
59% 36% 5%



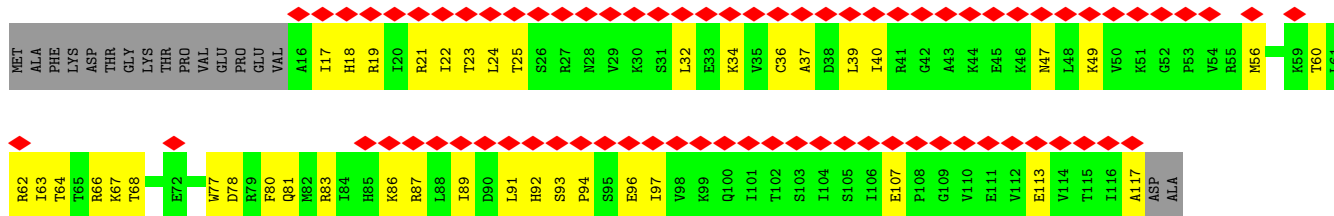
- Molecule 67: 40S ribosomal protein S19

Chain AF: 62%  
79% 19%

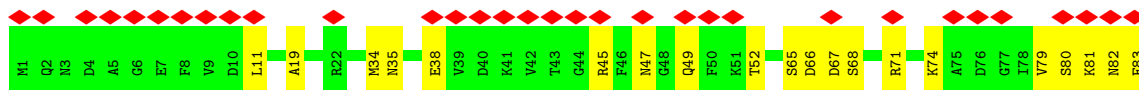
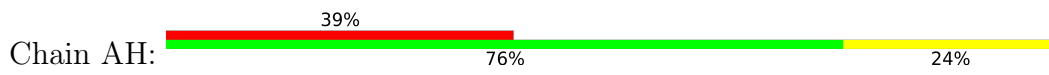


- Molecule 68: 40S ribosomal protein S20

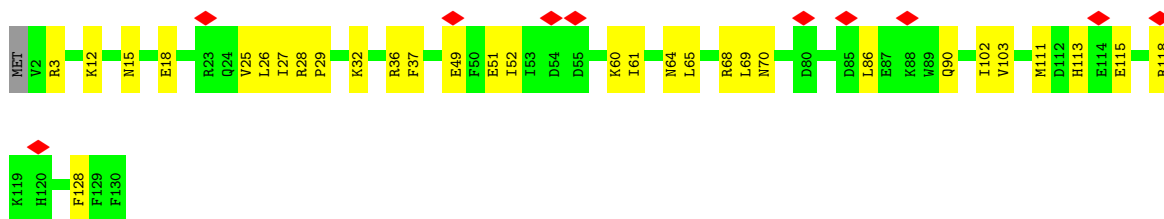
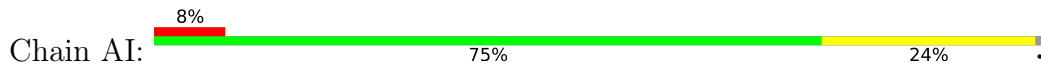
Chain AG: 64%  
51% 34% 14%



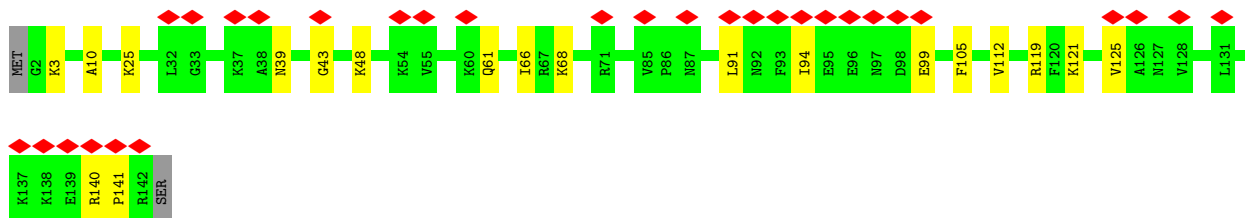
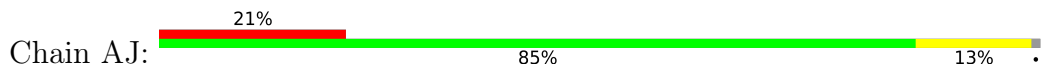
- Molecule 69: 40S ribosomal protein S21



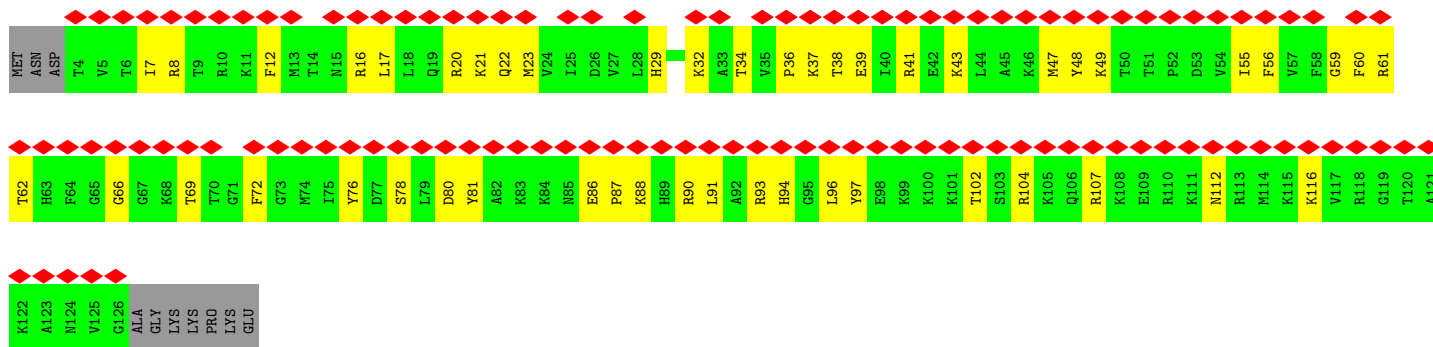
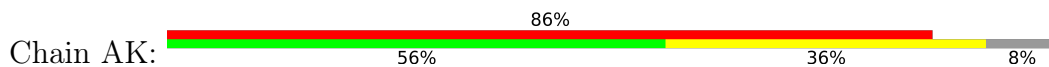
• Molecule 70: 40S ribosomal protein S15a



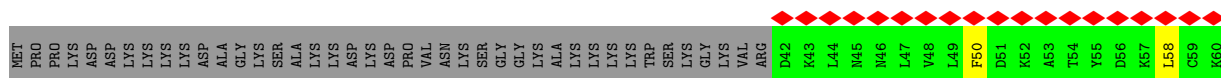
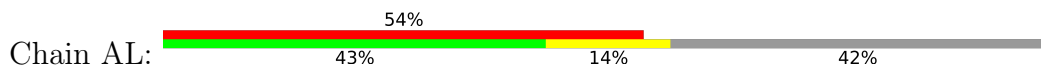
• Molecule 71: 40S ribosomal protein S23

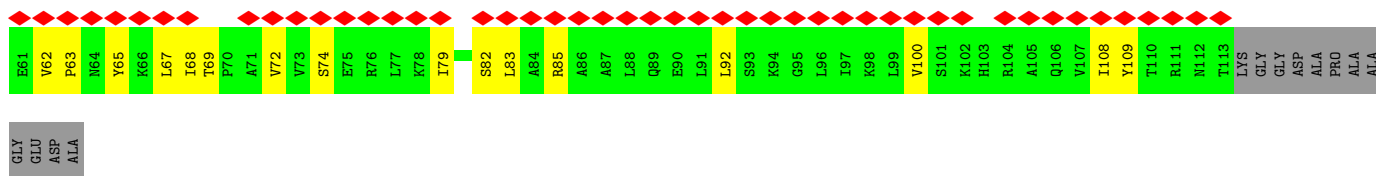


• Molecule 72: 40S ribosomal protein S24

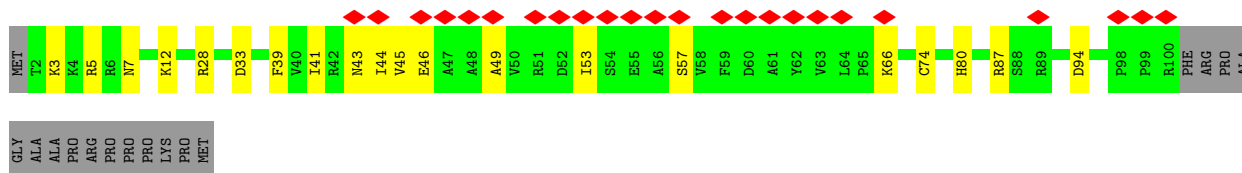


• Molecule 73: 40S ribosomal protein S25

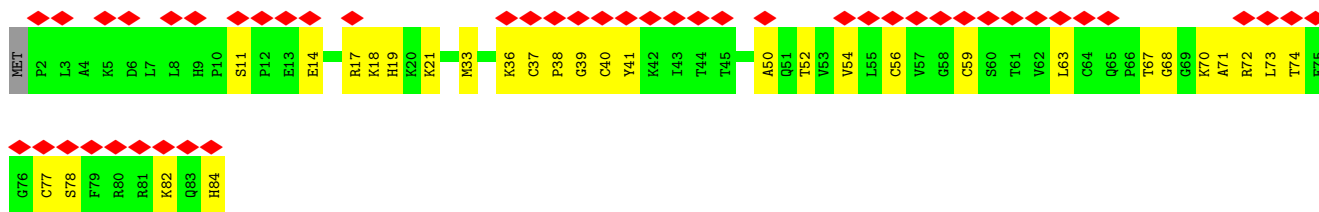




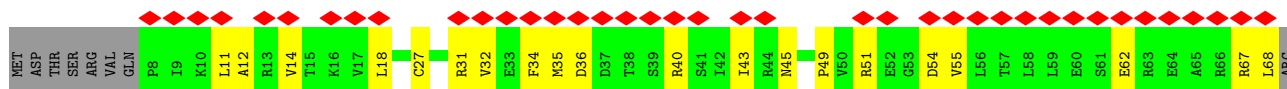
• Molecule 74: 40S ribosomal protein S26



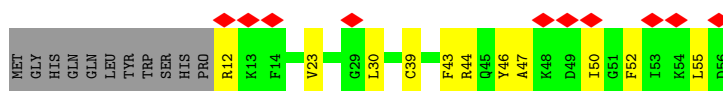
• Molecule 75: 40S ribosomal protein S27



• Molecule 76: 40S ribosomal protein S28



• Molecule 77: 40S ribosomal protein S29



• Molecule 78: 40S ribosomal protein S30





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75250	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	0.142	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0183	Depositor
Map size (Å)	439.9, 439.9, 439.9	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: UY1, 1MA, 56B, ZN, 2MG, M2G, B8N, 5MU, MA6, OMC, H2U, 4AC, A2M, PSU, 6MZ, G7M, OMG, 5MC, 1MG, GAL, MG, OMU, 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	0.14	0/319	0.15	0/492
2	B	0.19	0/1401	0.19	0/2175
2	C	0.16	0/1401	0.18	0/2175
3	D	0.31	1/81567 (0.0%)	0.26	6/127232 (0.0%)
4	E	0.30	0/2858	0.22	0/4455
5	F	0.30	0/3675	0.24	0/5725
6	G	0.31	0/1929	0.45	0/2586
7	H	0.29	0/3279	0.42	0/4388
8	I	0.30	0/2938	0.42	0/3946
9	J	0.25	0/2425	0.40	0/3248
10	K	0.24	0/1785	0.45	0/2394
11	L	0.31	0/1905	0.43	0/2539
12	M	0.24	0/1863	0.41	0/2510
13	N	0.26	0/1537	0.42	0/2066
14	O	0.26	0/1699	0.41	0/2270
15	P	0.20	0/1385	0.40	0/1852
16	Q	0.27	0/1713	0.46	1/2293 (0.0%)
17	R	0.26	0/1142	0.42	0/1527
18	S	0.32	0/1746	0.41	0/2338
19	T	0.31	0/1673	0.40	0/2238
20	U	0.29	0/1300	0.41	0/1746
21	V	0.31	0/1537	0.44	0/2052
22	W	0.25	0/1524	0.39	0/2013
23	X	0.30	0/1493	0.41	0/2003
24	Y	0.28	0/1326	0.38	0/1770
25	Z	0.20	0/835	0.39	0/1122
26	a	0.28	0/993	0.39	0/1332
27	b	0.26	0/541	0.41	0/720
28	c	0.24	0/998	0.36	0/1340
29	d	0.26	0/1132	0.40	0/1504
30	e	0.25	0/1130	0.37	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	f	0.30	0/1191	0.40	0/1591
32	g	0.24	0/844	0.52	1/1115 (0.1%)
33	h	0.25	0/765	0.33	0/1027
34	i	0.28	0/903	0.38	0/1216
35	j	0.30	0/1071	0.39	0/1429
36	k	0.32	0/895	0.50	0/1198
37	l	0.28	0/898	0.44	0/1197
38	m	0.24	0/1018	0.34	0/1344
39	n	0.21	0/843	0.37	0/1115
40	o	0.31	0/720	0.47	0/952
41	p	0.25	0/575	0.47	0/761
42	q	0.28	0/454	0.36	0/599
43	r	0.26	0/435	0.41	0/575
44	s	0.23	0/240	0.39	0/305
45	t	0.27	0/876	0.43	0/1156
46	u	0.28	0/718	0.37	0/953
47	v	0.30	0/1017	0.42	0/1364
48	w	0.21	0/37158	0.23	0/57908
49	x	0.18	0/1732	0.39	0/2355
50	y	0.17	0/1752	0.34	0/2345
51	z	0.18	0/1668	0.36	0/2254
52	0	0.15	0/1672	0.41	1/2250 (0.0%)
53	1	0.15	0/2112	0.37	0/2842
54	2	0.15	0/1485	0.38	0/1998
55	3	0.14	0/1940	0.36	0/2583
56	4	0.15	0/1533	0.39	0/2053
57	5	0.14	0/1703	0.40	0/2275
58	6	0.15	0/1531	0.40	0/2045
59	7	0.13	0/834	0.38	0/1125
60	8	0.18	0/1170	0.38	0/1568
61	9	0.17	0/1232	0.35	0/1656
62	AA	0.19	0/1015	0.44	0/1361
63	AB	0.16	0/1126	0.36	0/1505
64	AC	0.14	0/1146	0.38	0/1534
65	AD	0.18	0/1071	0.51	2/1438 (0.1%)
66	AE	0.17	0/1187	0.45	0/1593
67	AF	0.14	0/1130	0.36	0/1515
68	AG	0.15	0/809	0.40	0/1087
69	AH	0.18	0/643	0.40	0/860
70	AI	0.20	0/1051	0.38	0/1406
71	AJ	0.17	0/1116	0.35	0/1490
72	AK	0.14	0/1019	0.36	0/1355
73	AL	0.14	0/580	0.41	0/780

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
74	AM	0.20	0/805	0.42	0/1079
75	AN	0.19	0/657	0.42	0/883
76	AO	0.16	0/481	0.44	0/643
77	AP	0.18	0/375	0.40	0/492
78	AQ	0.13	0/443	0.41	0/582
79	AR	0.16	0/2493	0.45	0/3394
All	All	0.26	1/219181 (0.0%)	0.32	11/321709 (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	2
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
32	g	0	1
40	o	0	1
53	1	0	2
65	AD	0	1
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3785	A2M	O3'-P	5.11	1.61	1.56

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2101	C	OP1-P-OP2	-13.37	79.50	119.60
3	D	2100	A	OP2-P-O3'	-11.89	72.33	108.00
3	D	2101	C	O5'-P-OP1	-10.47	76.58	108.00
3	D	2100	A	OP1-P-O3'	9.64	136.93	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	0	164	VAL	N-CA-C	-7.71	106.39	113.71

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	G	123	ARG	Peptide
6	G	239	ALA	Peptide
7	H	16	PHE	Peptide
7	H	258	HIS	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	288	0	145	0	0
2	B	1580	0	794	16	0
2	C	1580	0	794	12	0
3	D	75336	0	38156	479	0
4	E	2558	0	1296	14	0
5	F	3315	0	1685	27	0
6	G	1891	0	1986	28	0
7	H	3211	0	3356	37	0
8	I	2884	0	3060	44	0
9	J	2379	0	2408	42	0
10	K	1751	0	1905	32	0
11	L	1870	0	1996	22	0
12	M	1832	0	1962	28	0
13	N	1518	0	1601	28	0
14	O	1660	0	1692	20	0
15	P	1362	0	1399	21	0
16	Q	1682	0	1792	31	0
17	R	1120	0	1187	24	0
18	S	1701	0	1749	21	0
19	T	1641	0	1788	15	0
20	U	1273	0	1304	18	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	19	0
23	X	1453	0	1490	13	0
24	Y	1298	0	1366	9	0
25	Z	821	0	839	15	0
26	a	979	0	1039	8	0
27	b	528	0	541	3	0
28	c	981	0	1062	18	0
29	d	1115	0	1205	17	0
30	e	1107	0	1182	15	0
31	f	1162	0	1213	24	0
32	g	832	0	883	7	0
33	h	755	0	791	8	0
34	i	888	0	930	10	0
35	j	1053	0	1147	7	0
36	k	876	0	912	13	0
37	l	888	0	981	12	0
38	m	1010	0	1143	8	0
39	n	832	0	917	8	0
40	o	705	0	737	8	0
41	p	569	0	637	9	0
42	q	444	0	483	9	0
43	r	429	0	466	12	0
44	s	239	0	289	0	0
45	t	862	0	930	17	0
46	u	708	0	756	9	0
47	v	1002	0	1068	16	0
48	w	34933	0	17693	406	0
49	x	1695	0	1690	45	0
50	y	1725	0	1800	40	0
51	z	1633	0	1716	21	0
52	0	1646	0	1734	33	0
53	1	2070	0	2166	54	0
54	2	1464	0	1505	39	0
55	3	1917	0	2078	63	0
56	4	1510	0	1606	49	0
57	5	1674	0	1739	52	0
58	6	1506	0	1618	47	0
59	7	810	0	836	22	0
60	8	1150	0	1199	16	0
61	9	1208	0	1294	22	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	29	0
64	AC	1128	0	1195	29	0
65	AD	1057	0	1110	30	0
66	AE	1169	0	1198	39	0
67	AF	1111	0	1144	22	0
68	AG	799	0	850	33	0
69	AH	636	0	637	14	0
70	AI	1034	0	1080	25	0
71	AJ	1098	0	1167	14	0
72	AK	1002	0	1067	37	0
73	AL	574	0	627	14	0
74	AM	792	0	845	16	0
75	AN	643	0	650	25	0
76	AO	479	0	507	16	0
77	AP	370	0	377	11	0
78	AQ	438	0	484	11	0
79	AR	2436	0	2393	116	0
80	B	11	0	10	0	0
80	C	11	0	10	0	0
81	2	1	0	0	0	0
81	AA	1	0	0	0	0
81	AG	1	0	0	0	0
81	AM	1	0	0	0	0
81	D	391	0	0	0	0
81	E	10	0	0	0	0
81	F	5	0	0	0	0
81	G	2	0	0	0	0
81	H	1	0	0	0	0
81	I	1	0	0	0	0
81	N	1	0	0	0	0
81	O	1	0	0	0	0
81	S	1	0	0	0	0
81	U	1	0	0	0	0
81	V	2	0	0	0	0
81	W	1	0	0	0	0
81	X	1	0	0	0	0
81	a	1	0	0	0	0
81	g	1	0	0	0	0
81	j	1	0	0	0	0
81	k	1	0	0	0	0
81	l	1	0	0	0	0
81	w	93	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	AA	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
82	w	1	0	0	0	0
All	All	209349	0	154558	2220	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 7.

The worst 5 of 2220 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:1:C:H42	5:F:156:U:H3	1.15	0.95
34:i:18:ASN:HD22	34:i:18:ASN:N	1.66	0.93
3:D:1303:A:N6	3:D:2316:G:N7	2.16	0.92
3:D:4092:G:H21	3:D:4093:G:H1	1.20	0.89
17:R:96:GLU:HA	17:R:99:GLU:HG3	1.56	0.88

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%)	227 (93%)	18 (7%)	0	100	100
7	H	396/403 (98%)	367 (93%)	29 (7%)	0	100	100
8	I	361/427 (84%)	338 (94%)	23 (6%)	0	100	100
9	J	291/297 (98%)	274 (94%)	17 (6%)	0	100	100
10	K	211/288 (73%)	191 (90%)	20 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	L	223/248 (90%)	212 (95%)	11 (5%)	0	100	100
12	M	223/266 (84%)	207 (93%)	16 (7%)	0	100	100
13	N	188/192 (98%)	174 (93%)	14 (7%)	0	100	100
14	O	202/214 (94%)	186 (92%)	16 (8%)	0	100	100
15	P	168/178 (94%)	155 (92%)	13 (8%)	0	100	100
16	Q	206/211 (98%)	190 (92%)	14 (7%)	2 (1%)	12	28
17	R	134/215 (62%)	123 (92%)	11 (8%)	0	100	100
18	S	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
19	T	198/203 (98%)	195 (98%)	3 (2%)	0	100	100
20	U	155/184 (84%)	143 (92%)	12 (8%)	0	100	100
21	V	185/188 (98%)	176 (95%)	9 (5%)	0	100	100
22	W	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
23	X	173/176 (98%)	162 (94%)	11 (6%)	0	100	100
24	Y	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
25	Z	99/128 (77%)	92 (93%)	7 (7%)	0	100	100
26	a	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
27	b	61/157 (39%)	60 (98%)	1 (2%)	0	100	100
28	c	118/156 (76%)	112 (95%)	6 (5%)	0	100	100
29	d	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
30	e	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
31	f	145/148 (98%)	130 (90%)	15 (10%)	0	100	100
32	g	100/159 (63%)	92 (92%)	6 (6%)	2 (2%)	6	14
33	h	95/115 (83%)	94 (99%)	1 (1%)	0	100	100
34	i	105/125 (84%)	101 (96%)	4 (4%)	0	100	100
35	j	126/135 (93%)	123 (98%)	3 (2%)	0	100	100
36	k	107/110 (97%)	97 (91%)	10 (9%)	0	100	100
37	l	110/117 (94%)	101 (92%)	9 (8%)	0	100	100
38	m	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
39	n	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
40	o	84/97 (87%)	79 (94%)	4 (5%)	1 (1%)	10	24
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%)	83 (93%)	6 (7%)	0	100	100
47	v	123/137 (90%)	115 (94%)	8 (6%)	0	100	100
49	x	213/295 (72%)	197 (92%)	15 (7%)	1 (0%)	24	45
50	y	210/264 (80%)	198 (94%)	12 (6%)	0	100	100
51	z	210/293 (72%)	200 (95%)	10 (5%)	0	100	100
52	0	210/243 (86%)	190 (90%)	20 (10%)	0	100	100
53	1	260/263 (99%)	243 (94%)	15 (6%)	2 (1%)	16	34
54	2	185/204 (91%)	171 (92%)	14 (8%)	0	100	100
55	3	235/249 (94%)	228 (97%)	7 (3%)	0	100	100
56	4	185/194 (95%)	166 (90%)	19 (10%)	0	100	100
57	5	204/208 (98%)	186 (91%)	18 (9%)	0	100	100
58	6	180/194 (93%)	171 (95%)	9 (5%)	0	100	100
59	7	94/165 (57%)	88 (94%)	6 (6%)	0	100	100
60	8	138/158 (87%)	127 (92%)	11 (8%)	0	100	100
61	9	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
62	AA	132/151 (87%)	122 (92%)	10 (8%)	0	100	100
63	AB	132/145 (91%)	126 (96%)	6 (4%)	0	100	100
64	AC	140/146 (96%)	129 (92%)	11 (8%)	0	100	100
65	AD	129/135 (96%)	109 (84%)	18 (14%)	2 (2%)	7	18
66	AE	142/152 (93%)	125 (88%)	17 (12%)	0	100	100
67	AF	141/145 (97%)	132 (94%)	9 (6%)	0	100	100
68	AG	100/119 (84%)	94 (94%)	6 (6%)	0	100	100
69	AH	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
70	AI	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
71	AJ	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
72	AK	121/133 (91%)	119 (98%)	2 (2%)	0	100	100
73	AL	70/125 (56%)	66 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	AM	97/115 (84%)	92 (95%)	5 (5%)	0	100	100
75	AN	81/84 (96%)	67 (83%)	13 (16%)	1 (1%)	10	24
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	53/59 (90%)	51 (96%)	2 (4%)	0	100	100
79	AR	311/317 (98%)	270 (87%)	41 (13%)	0	100	100
All	All	10931/12400 (88%)	10208 (93%)	712 (6%)	11 (0%)	49	71

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	48	PRO
32	g	111	ARG
53	l	227	VAL
32	g	110	ALA
65	AD	118	GLN

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	89 (99%)	1 (1%)	65	83
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%)	97 (99%)	1 (1%)	68	84
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%)	73 (100%)	0	100	100
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%)	119 (100%)	0	100	100
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	64/103 (62%)	64 (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	45/48 (94%)	45 (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	9499/10553 (90%)	9497 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
25	Z	95	ASN
34	i	18	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
54	2	36	GLN
59	7	77	GLN
54	2	149	GLN
56	4	76	GLN
63	AB	114	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	13/14 (92%)	1 (7%)	0
2	B	70/76 (92%)	24 (34%)	1 (1%)
2	C	70/76 (92%)	20 (28%)	0
3	D	3497/5070 (68%)	609 (17%)	26 (0%)
4	E	119/120 (99%)	13 (10%)	0
48	w	1624/1869 (86%)	392 (24%)	0
5	F	155/156 (99%)	25 (16%)	1 (0%)
All	All	5548/7381 (75%)	1084 (19%)	28 (0%)

5 of 1084 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	19	U
2	B	6	2MG
2	B	7	A
2	B	8	U
2	B	9	A

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	2102	G
5	F	86	U
3	D	3673	C
3	D	4699	U
3	D	3614	G

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

222 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
2	G7M	B	46	2	23,26,27	2.84	9 (39%)	35,39,42	1.77	7 (20%)
3	PSU	D	4500	3	18,21,22	1.04	1 (5%)	22,30,33	1.87	4 (18%)
48	OMC	w	462	48	19,22,23	2.98	8 (42%)	26,31,34	0.72	0
48	OMC	w	1391	48	19,22,23	2.96	8 (42%)	26,31,34	0.72	0
3	A2M	D	2363	3,81	22,25,26	1.38	2 (9%)	31,36,39	0.98	3 (9%)
48	OMU	w	627	48	19,22,23	2.91	8 (42%)	26,31,34	1.68	4 (15%)
2	5MU	B	54	2	19,22,23	4.75	5 (26%)	28,32,35	3.62	9 (32%)
3	A2M	D	1534	3,81	22,25,26	1.34	1 (4%)	31,36,39	1.31	6 (19%)
48	4AC	w	1842	48	21,24,25	0.57	0	29,34,37	1.17	4 (13%)
3	OMC	D	3701	3,81	19,22,23	2.85	8 (42%)	26,31,34	0.76	0
48	A2M	w	590	48	22,25,26	1.49	2 (9%)	31,36,39	1.06	2 (6%)
3	OMG	D	1760	3	23,26,27	2.64	8 (34%)	33,38,41	1.94	9 (27%)
48	PSU	w	1347	48	18,21,22	1.01	1 (5%)	22,30,33	1.79	4 (18%)
48	A2M	w	1383	48	22,25,26	1.47	1 (4%)	31,36,39	1.11	3 (9%)
48	OMG	w	601	48	23,26,27	2.59	9 (39%)	33,38,41	1.93	10 (30%)
48	OMU	w	799	48	19,22,23	2.95	8 (42%)	26,31,34	1.67	5 (19%)
3	PSU	D	3695	3	18,21,22	1.02	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	3762	3	18,21,22	1.05	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	UY1	D	3818	3,81	19,22,23	1.10	1 (5%)	22,31,34	0.93	1 (4%)
48	PSU	w	34	48	18,21,22	1.10	1 (5%)	22,30,33	1.79	4 (18%)
48	OMU	w	172	48	19,22,23	2.90	7 (36%)	26,31,34	1.73	5 (19%)
3	A2M	D	3830	3	22,25,26	1.38	1 (4%)	31,36,39	1.07	1 (3%)
3	PSU	D	4403	3,81	18,21,22	1.04	1 (5%)	22,30,33	1.84	4 (18%)
3	PSU	D	3758	3	18,21,22	0.96	1 (5%)	22,30,33	1.86	5 (22%)
48	A2M	w	576	48	22,25,26	1.41	2 (9%)	31,36,39	1.05	2 (6%)
3	OMG	D	4618	3	23,26,27	2.54	9 (39%)	33,38,41	1.90	10 (30%)
3	A2M	D	2787	3,81	22,25,26	1.38	1 (4%)	31,36,39	1.04	2 (6%)
2	PSU	B	35	2,1	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
2	2MG	B	6	2	23,26,27	2.60	8 (34%)	32,38,41	2.24	13 (40%)
3	OMC	D	2422	3,81	19,22,23	2.87	8 (42%)	26,31,34	0.72	0
3	OMU	D	4620	3	19,22,23	2.75	6 (31%)	26,31,34	1.79	5 (19%)
48	PSU	w	109	48	18,21,22	1.06	1 (5%)	22,30,33	1.85	5 (22%)
3	PSU	D	1781	3	18,21,22	1.02	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4312	3	18,21,22	1.02	1 (5%)	22,30,33	1.89	5 (22%)
3	OMC	D	2804	3	19,22,23	2.86	8 (42%)	26,31,34	0.68	0
3	PSU	D	5010	3	18,21,22	1.04	1 (5%)	22,30,33	1.85	4 (18%)
2	1MG	C	37	2	22,26,27	2.65	7 (31%)	33,39,42	1.73	8 (24%)
48	OMG	w	509	48	23,26,27	2.58	8 (34%)	33,38,41	1.97	10 (30%)
3	6MZ	D	4220	3	22,25,26	2.81	4 (18%)	30,36,39	2.25	10 (33%)
2	M2G	C	27	2	24,27,28	1.09	2 (8%)	35,40,43	0.87	1 (2%)
3	PSU	D	3715	3	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)
3	OMU	D	4227	3	19,22,23	2.79	6 (31%)	26,31,34	1.78	4 (15%)
48	PSU	w	1625	48	18,21,22	1.08	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	4628	3	18,21,22	1.05	1 (5%)	22,30,33	1.89	4 (18%)
48	PSU	w	815	48	18,21,22	1.08	1 (5%)	22,30,33	1.88	5 (22%)
3	1MA	D	1322	3	21,25,26	0.70	0	31,37,40	0.79	1 (3%)
48	PSU	w	1177	48	18,21,22	1.04	1 (5%)	22,30,33	1.82	4 (18%)
2	PSU	C	55	2	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
3	OMC	D	2365	3,81	19,22,23	2.83	8 (42%)	26,31,34	0.72	0
3	OMG	D	2364	3	23,26,27	2.53	9 (39%)	33,38,41	1.95	10 (30%)
3	A2M	D	4523	3,81	22,25,26	1.45	2 (9%)	31,36,39	1.07	2 (6%)
48	PSU	w	36	48	18,21,22	1.06	1 (5%)	22,30,33	1.81	5 (22%)
2	M2G	B	26	2	24,27,28	1.11	3 (12%)	35,40,43	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	PSU	w	1692	48	18,21,22	1.03	1 (5%)	22,30,33	1.81	4 (18%)
3	A2M	D	1871	3,81	22,25,26	1.44	1 (4%)	31,36,39	1.17	3 (9%)
3	OMC	D	2351	3,81	19,22,23	2.80	7 (36%)	26,31,34	0.83	1 (3%)
3	PSU	D	5001	3,81	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	2632	3	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	D	3792	3	23,26,27	2.56	9 (39%)	33,38,41	1.90	9 (27%)
3	OMG	D	4228	3	23,26,27	2.53	9 (39%)	33,38,41	1.97	10 (30%)
3	OMG	D	3627	3	23,26,27	2.56	9 (39%)	33,38,41	1.98	10 (30%)
3	PSU	D	3853	3,81	18,21,22	1.03	1 (5%)	22,30,33	1.77	4 (18%)
48	OMG	w	683	48	23,26,27	2.60	9 (39%)	33,38,41	1.95	9 (27%)
3	OMG	D	3944	3	23,26,27	2.61	8 (34%)	33,38,41	1.92	9 (27%)
48	PSU	w	966	48	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
48	PSU	w	1046	48	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
48	PSU	w	1643	81,48	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)
3	OMU	D	3925	3	19,22,23	2.77	6 (31%)	26,31,34	1.82	5 (19%)
2	UY1	B	39	2	19,22,23	1.19	1 (5%)	22,31,34	0.96	1 (4%)
3	A2M	D	3724	3	22,25,26	1.43	1 (4%)	31,36,39	1.04	1 (3%)
48	PSU	w	866	48	18,21,22	1.07	1 (5%)	22,30,33	1.84	5 (22%)
48	PSU	w	1174	81,48	18,21,22	1.04	1 (5%)	22,30,33	1.77	4 (18%)
48	OMU	w	1442	81,48	19,22,23	2.91	8 (42%)	26,31,34	1.71	5 (19%)
3	OMC	D	2861	3	19,22,23	2.86	8 (42%)	26,31,34	0.67	0
3	OMC	D	4536	3	19,22,23	2.84	8 (42%)	26,31,34	0.72	0
3	PSU	D	4420	3	18,21,22	1.05	1 (5%)	22,30,33	1.84	6 (27%)
3	OMU	D	1773	3	19,22,23	2.96	8 (42%)	26,31,34	1.61	5 (19%)
3	A2M	D	3760	3	22,25,26	1.47	1 (4%)	31,36,39	1.05	1 (3%)
48	OMC	w	1703	81,48	19,22,23	2.94	8 (42%)	26,31,34	0.72	0
48	A2M	w	1678	48	22,25,26	1.48	1 (4%)	31,36,39	0.99	2 (6%)
48	A2M	w	1031	48	22,25,26	1.40	1 (4%)	31,36,39	1.01	2 (6%)
48	PSU	w	1056	48	18,21,22	1.05	1 (5%)	22,30,33	1.82	5 (22%)
48	PSU	w	105	48	18,21,22	1.09	1 (5%)	22,30,33	1.92	5 (22%)
3	OMC	D	1340	3	19,22,23	2.82	8 (42%)	26,31,34	0.70	0
2	5MC	C	48	2	18,22,23	3.83	8 (44%)	26,32,35	1.04	2 (7%)
3	PSU	D	4521	3,81	18,21,22	1.07	2 (11%)	22,30,33	1.88	5 (22%)
3	PSU	D	3920	3,81	18,21,22	1.07	2 (11%)	22,30,33	1.87	4 (18%)
3	PSU	D	4299	3	18,21,22	1.02	1 (5%)	22,30,33	1.87	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	D	3734	3	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4361	3	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
48	OMU	w	1804	48	19,22,23	2.90	7 (36%)	26,31,34	1.74	4 (15%)
3	A2M	D	400	3	22,25,26	1.40	1 (4%)	31,36,39	1.03	2 (6%)
48	MA6	w	1850	48	23,26,27	1.36	4 (17%)	34,38,41	2.22	11 (32%)
3	OMC	D	3808	3	19,22,23	2.84	8 (42%)	26,31,34	0.74	0
2	1MA	C	58	2	21,25,26	0.91	1 (4%)	31,37,40	0.77	1 (3%)
48	G7M	w	1639	2,48	23,26,27	2.82	8 (34%)	35,39,42	1.80	8 (22%)
48	A2M	w	166	48	22,25,26	1.46	2 (9%)	31,36,39	1.04	2 (6%)
3	PSU	D	3768	3	18,21,22	1.04	1 (5%)	22,30,33	1.75	3 (13%)
3	PSU	D	1862	3	18,21,22	1.03	1 (5%)	22,30,33	1.95	5 (22%)
3	PSU	D	1860	3	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
3	OMC	D	3841	3	19,22,23	2.81	8 (42%)	26,31,34	0.70	0
2	UY1	C	39	2	19,22,23	1.28	2 (10%)	22,31,34	0.95	1 (4%)
3	A2M	D	1524	3	22,25,26	1.48	2 (9%)	31,36,39	1.09	3 (9%)
3	PSU	D	4423	3	18,21,22	1.06	1 (5%)	22,30,33	1.85	4 (18%)
48	OMC	w	517	48	19,22,23	3.01	8 (42%)	26,31,34	0.72	0
48	PSU	w	609	48	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)
48	OMU	w	1326	48	19,22,23	2.89	8 (42%)	26,31,34	1.72	4 (15%)
48	OMG	w	1328	48	23,26,27	2.60	8 (34%)	33,38,41	1.92	9 (27%)
48	PSU	w	119	48	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
48	PSU	w	863	48	18,21,22	1.07	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4431	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
48	PSU	w	686	48	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
3	OMU	D	4306	3	19,22,23	2.72	6 (31%)	26,31,34	1.74	5 (19%)
3	PSU	D	4353	3	18,21,22	1.04	2 (11%)	22,30,33	1.83	4 (18%)
3	PSU	D	4579	3	18,21,22	1.05	2 (11%)	22,30,33	1.84	4 (18%)
3	OMG	D	4637	3	23,26,27	2.55	10 (43%)	33,38,41	1.94	9 (27%)
48	PSU	w	93	48	18,21,22	1.09	1 (5%)	22,30,33	1.75	4 (18%)
48	PSU	w	1004	48	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
48	PSU	w	822	48	18,21,22	1.06	1 (5%)	22,30,33	1.84	4 (18%)
2	56B	C	34	2,80	29,35,36	2.81	10 (34%)	36,52,55	2.35	8 (22%)
48	A2M	w	27	48	22,25,26	1.44	1 (4%)	31,36,39	1.00	2 (6%)
3	PSU	D	3637	3,81	18,21,22	1.05	1 (5%)	22,30,33	1.85	2 (9%)
3	PSU	D	4689	3	18,21,22	1.03	1 (5%)	22,30,33	1.81	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	H2U	B	47	2	18,21,22	1.03	2 (11%)	21,30,33	0.78	0
3	OMC	D	4456	3	19,22,23	2.84	8 (42%)	26,31,34	0.69	0
48	PSU	w	210	48	18,21,22	1.09	1 (5%)	22,30,33	1.77	4 (18%)
2	5MC	B	48	2	18,22,23	3.82	8 (44%)	26,32,35	1.10	2 (7%)
3	PSU	D	1677	3,81	18,21,22	1.06	2 (11%)	22,30,33	1.80	4 (18%)
48	PSU	w	814	48	18,21,22	1.06	1 (5%)	22,30,33	1.85	5 (22%)
48	OMG	w	644	48	23,26,27	2.61	8 (34%)	33,38,41	1.94	10 (30%)
2	2MG	B	10	2	23,26,27	2.67	7 (30%)	32,38,41	2.12	9 (28%)
3	OMU	D	2837	3	19,22,23	2.78	6 (31%)	26,31,34	1.88	5 (19%)
3	PSU	D	4442	3	18,21,22	1.05	2 (11%)	22,30,33	1.89	6 (27%)
48	OMU	w	121	48	19,22,23	2.90	8 (42%)	26,31,34	1.67	5 (19%)
48	OMG	w	1490	81,48	23,26,27	2.59	8 (34%)	33,38,41	1.91	9 (27%)
3	A2M	D	3785	3,81	22,25,26	1.41	1 (4%)	31,36,39	1.32	3 (9%)
48	OMU	w	116	48	19,22,23	2.93	8 (42%)	26,31,34	1.69	4 (15%)
48	MA6	w	1851	48	23,26,27	1.29	4 (17%)	34,38,41	2.31	12 (35%)
3	PSU	D	3851	3	18,21,22	1.05	2 (11%)	22,30,33	1.84	4 (18%)
3	5MC	D	4447	3,81	18,22,23	3.63	7 (38%)	26,32,35	1.15	1 (3%)
48	A2M	w	512	48	22,25,26	1.45	1 (4%)	31,36,39	1.09	3 (9%)
48	OMU	w	1288	48	19,22,23	2.96	8 (42%)	26,31,34	1.70	4 (15%)
3	PSU	D	1536	3	18,21,22	1.06	2 (11%)	22,30,33	1.88	4 (18%)
3	5MC	D	3782	3,81	18,22,23	3.59	8 (44%)	26,32,35	1.08	2 (7%)
48	PSU	w	1445	48	18,21,22	1.05	1 (5%)	22,30,33	1.78	5 (22%)
3	OMG	D	2424	3	23,26,27	2.59	9 (39%)	33,38,41	1.92	10 (30%)
2	PSU	B	55	2	18,21,22	1.08	1 (5%)	22,30,33	1.74	6 (27%)
3	OMG	D	4499	2,3	23,26,27	2.58	9 (39%)	33,38,41	1.97	10 (30%)
2	2MG	C	10	2	23,26,27	2.68	7 (30%)	32,38,41	2.22	9 (28%)
3	OMG	D	4392	3	23,26,27	2.54	10 (43%)	33,38,41	1.93	9 (27%)
3	OMG	D	4370	3	23,26,27	2.56	9 (39%)	33,38,41	1.95	9 (27%)
3	PSU	D	1792	3	18,21,22	0.99	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	1744	3,81	18,21,22	1.02	1 (5%)	22,30,33	1.83	4 (18%)
2	PSU	C	35	2,1	18,21,22	1.01	1 (5%)	22,30,33	1.81	5 (22%)
3	A2M	D	398	3	22,25,26	1.41	1 (4%)	31,36,39	1.01	3 (9%)
3	A2M	D	2815	3	22,25,26	1.51	1 (4%)	31,36,39	1.02	3 (9%)
3	UR3	D	4530	3,81	19,22,23	2.64	7 (36%)	26,32,35	1.27	1 (3%)
48	PSU	w	801	48	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMG	D	1522	3	23,26,27	2.53	9 (39%)	33,38,41	1.99	10 (30%)
48	PSU	w	1244	48	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
2	G7M	C	46	2	23,26,27	2.83	9 (39%)	35,39,42	1.74	9 (25%)
48	OMU	w	428	48	19,22,23	2.92	8 (42%)	26,31,34	1.72	5 (19%)
3	OMC	D	3887	3	19,22,23	2.87	8 (42%)	26,31,34	0.78	0
48	PSU	w	1367	48	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
2	5MU	C	54	2	19,22,23	4.73	5 (26%)	28,32,35	3.60	9 (32%)
48	PSU	w	1232	48	18,21,22	1.04	1 (5%)	22,30,33	1.83	5 (22%)
48	PSU	w	218	48	18,21,22	1.08	1 (5%)	22,30,33	1.82	4 (18%)
2	1MA	B	58	2	21,25,26	0.92	1 (4%)	31,37,40	0.76	0
48	PSU	w	649	48	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
48	A2M	w	484	48	22,25,26	1.46	1 (4%)	31,36,39	1.00	3 (9%)
48	A2M	w	668	81,48	22,25,26	1.53	2 (9%)	31,36,39	1.04	3 (9%)
3	PSU	D	4471	3	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
2	2MG	C	6	2	23,26,27	2.67	7 (30%)	32,38,41	2.16	9 (28%)
48	PSU	w	1081	48	18,21,22	1.01	1 (5%)	22,30,33	1.76	5 (22%)
3	PSU	D	1782	3	18,21,22	1.01	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	4532	3	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	D	4296	3	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
3	OMU	D	4498	3,81	19,22,23	2.77	6 (31%)	26,31,34	1.72	4 (15%)
3	OMG	D	4196	3,81	23,26,27	2.56	9 (39%)	33,38,41	1.91	9 (27%)
3	PSU	D	1683	3,81	18,21,22	1.04	2 (11%)	22,30,33	1.92	5 (22%)
3	PSU	D	4552	3	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
3	PSU	D	3770	3	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
2	1MG	B	37	2	22,26,27	2.65	7 (31%)	33,39,42	1.71	7 (21%)
3	PSU	D	4972	3,81	18,21,22	1.02	1 (5%)	22,30,33	1.88	5 (22%)
48	A2M	w	159	48	22,25,26	1.53	2 (9%)	31,36,39	1.07	3 (9%)
48	A2M	w	468	48	22,25,26	1.58	2 (9%)	31,36,39	1.11	3 (9%)
3	OMU	D	2415	3	19,22,23	2.83	6 (31%)	26,31,34	1.97	6 (23%)
48	PSU	w	681	48	18,21,22	1.04	2 (11%)	22,30,33	1.84	4 (18%)
48	PSU	w	651	48	18,21,22	1.07	1 (5%)	22,30,33	1.83	5 (22%)
48	OMG	w	436	48	23,26,27	2.60	8 (34%)	33,38,41	1.97	9 (27%)
48	PSU	w	1238	48	18,21,22	1.08	1 (5%)	22,30,33	1.73	4 (18%)
3	PSU	D	4457	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	3730	3	18,21,22	1.01	1 (5%)	22,30,33	1.86	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	4AC	w	1337	48	21,24,25	0.66	0	29,34,37	1.19	4 (13%)
2	H2U	C	47	2	18,21,22	1.08	2 (11%)	21,30,33	1.38	2 (9%)
3	A2M	D	1326	3	22,25,26	1.34	1 (4%)	31,36,39	1.01	2 (6%)
2	M2G	B	27	2	24,27,28	1.14	2 (8%)	35,40,43	0.89	1 (2%)
3	PSU	D	3764	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
3	OMG	D	1625	3,81	23,26,27	2.59	8 (34%)	33,38,41	1.92	9 (27%)
2	M2G	C	26	2	24,27,28	1.12	2 (8%)	35,40,43	0.84	0
2	56B	B	34	2,80	29,35,36	2.79	10 (34%)	36,52,55	2.31	8 (22%)
48	A2M	w	99	81,48	22,25,26	1.41	1 (4%)	31,36,39	1.03	2 (6%)
48	PSU	w	1045	48	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
48	OMC	w	174	48	19,22,23	3.01	8 (42%)	26,31,34	0.71	0
3	OMG	D	3899	3	23,26,27	2.54	10 (43%)	33,38,41	1.97	10 (30%)
5	OMG	F	75	5	23,26,27	2.57	9 (39%)	33,38,41	1.95	10 (30%)
3	PSU	D	2508	3	18,21,22	1.02	1 (5%)	22,30,33	1.85	5 (22%)
3	PSU	D	4576	3	18,21,22	1.02	1 (5%)	22,30,33	1.85	5 (22%)
3	OMG	D	4623	3	23,26,27	2.53	9 (39%)	33,38,41	1.94	10 (30%)
48	PSU	w	406	48	18,21,22	1.04	1 (5%)	22,30,33	1.85	5 (22%)
48	PSU	w	572	48	18,21,22	1.11	1 (5%)	22,30,33	1.80	5 (22%)
3	A2M	D	3825	3	22,25,26	1.40	1 (4%)	31,36,39	1.05	2 (6%)
3	OMG	D	1316	3	23,26,27	2.55	10 (43%)	33,38,41	1.98	10 (30%)
3	OMG	D	4494	3	23,26,27	2.58	9 (39%)	33,38,41	1.93	9 (27%)
48	6MZ	w	1832	81,48	22,25,26	2.82	4 (18%)	30,36,39	2.20	9 (30%)
3	A2M	D	2401	3	22,25,26	1.40	1 (4%)	31,36,39	1.01	2 (6%)
3	OMG	D	3744	3	23,26,27	2.57	9 (39%)	33,38,41	1.96	10 (30%)
48	B8N	w	1248	48	24,29,30	0.82	0	29,42,45	0.94	2 (6%)
3	OMC	D	2824	3	19,22,23	2.88	8 (42%)	26,31,34	0.70	0
3	PSU	D	3639	3	18,21,22	1.03	2 (11%)	22,30,33	1.85	4 (18%)
3	A2M	D	3718	3	22,25,26	1.40	1 (4%)	31,36,39	1.01	2 (6%)
3	PSU	D	4293	3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)

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
2	G7M	B	46	2	-	2/7/25/26	0/3/3/3
3	PSU	D	4500	3	-	5/7/25/26	0/2/2/2
48	OMC	w	462	48	-	0/9/27/28	0/2/2/2
48	OMC	w	1391	48	-	0/9/27/28	0/2/2/2
3	A2M	D	2363	3,81	-	0/9/27/28	0/3/3/3
48	OMU	w	627	48	-	8/9/27/28	0/2/2/2
2	5MU	B	54	2	-	2/7/25/26	0/2/2/2
3	A2M	D	1534	3,81	-	3/9/27/28	0/3/3/3
48	4AC	w	1842	48	-	0/11/29/30	0/2/2/2
3	OMC	D	3701	3,81	-	4/9/27/28	0/2/2/2
48	A2M	w	590	48	-	2/9/27/28	0/3/3/3
3	OMG	D	1760	3	-	2/9/27/28	0/3/3/3
48	PSU	w	1347	48	-	0/7/25/26	0/2/2/2
48	A2M	w	1383	48	-	0/9/27/28	0/3/3/3
48	OMG	w	601	48	-	0/9/27/28	0/3/3/3
48	OMU	w	799	48	-	3/9/27/28	0/2/2/2
3	PSU	D	3695	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3762	3	-	2/7/25/26	0/2/2/2
3	UY1	D	3818	3,81	-	4/9/27/28	0/2/2/2
48	PSU	w	34	48	-	3/7/25/26	0/2/2/2
48	OMU	w	172	48	-	0/9/27/28	0/2/2/2
3	A2M	D	3830	3	-	0/9/27/28	0/3/3/3
3	PSU	D	4403	3,81	-	0/7/25/26	0/2/2/2
3	PSU	D	3758	3	-	2/7/25/26	0/2/2/2
48	A2M	w	576	48	-	2/9/27/28	0/3/3/3
3	OMG	D	4618	3	-	0/9/27/28	0/3/3/3
3	A2M	D	2787	3,81	-	3/9/27/28	0/3/3/3
2	PSU	B	35	2,1	-	0/7/25/26	0/2/2/2
2	2MG	B	6	2	-	0/9/27/28	0/3/3/3
3	OMC	D	2422	3,81	-	1/9/27/28	0/2/2/2
3	OMU	D	4620	3	-	0/9/27/28	0/2/2/2
48	PSU	w	109	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1781	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4312	3	-	0/7/25/26	0/2/2/2
3	OMC	D	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	D	5010	3	-	0/7/25/26	0/2/2/2
2	1MG	C	37	2	-	0/7/25/26	0/3/3/3
48	OMG	w	509	48	-	1/9/27/28	0/3/3/3
3	6MZ	D	4220	3	-	0/9/27/28	0/3/3/3
2	M2G	C	27	2	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	D	3715	3	-	2/7/25/26	0/2/2/2
3	OMU	D	4227	3	-	0/9/27/28	0/2/2/2
48	PSU	w	1625	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4628	3	-	0/7/25/26	0/2/2/2
48	PSU	w	815	48	-	0/7/25/26	0/2/2/2
3	1MA	D	1322	3	-	2/7/25/26	0/3/3/3
48	PSU	w	1177	48	-	0/7/25/26	0/2/2/2
2	PSU	C	55	2	-	2/7/25/26	0/2/2/2
3	OMC	D	2365	3,81	-	0/9/27/28	0/2/2/2
3	OMG	D	2364	3	-	2/9/27/28	0/3/3/3
3	A2M	D	4523	3,81	-	0/9/27/28	0/3/3/3
48	PSU	w	36	48	-	0/7/25/26	0/2/2/2
2	M2G	B	26	2	-	2/11/29/30	0/3/3/3
48	PSU	w	1692	48	-	0/7/25/26	0/2/2/2
3	A2M	D	1871	3,81	-	0/9/27/28	0/3/3/3
3	OMC	D	2351	3,81	-	2/9/27/28	0/2/2/2
3	PSU	D	5001	3,81	-	0/7/25/26	0/2/2/2
3	PSU	D	2632	3	-	0/7/25/26	0/2/2/2
3	OMG	D	3792	3	-	1/9/27/28	0/3/3/3
3	OMG	D	4228	3	-	0/9/27/28	0/3/3/3
3	OMG	D	3627	3	-	0/9/27/28	0/3/3/3
3	PSU	D	3853	3,81	-	0/7/25/26	0/2/2/2
48	OMG	w	683	48	-	0/9/27/28	0/3/3/3
3	OMG	D	3944	3	-	3/9/27/28	0/3/3/3
48	PSU	w	966	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1046	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1643	81,48	-	0/7/25/26	0/2/2/2
3	OMU	D	3925	3	-	1/9/27/28	0/2/2/2
2	UY1	B	39	2	-	2/9/27/28	0/2/2/2
3	A2M	D	3724	3	-	1/9/27/28	0/3/3/3
48	PSU	w	866	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1174	81,48	-	0/7/25/26	0/2/2/2
48	OMU	w	1442	81,48	-	1/9/27/28	0/2/2/2
3	OMC	D	2861	3	-	0/9/27/28	0/2/2/2
3	OMC	D	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4420	3	-	0/7/25/26	0/2/2/2
3	OMU	D	1773	3	-	1/9/27/28	0/2/2/2
3	A2M	D	3760	3	-	0/9/27/28	0/3/3/3
48	OMC	w	1703	81,48	-	2/9/27/28	0/2/2/2
48	A2M	w	1678	48	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A2M	w	1031	48	-	0/9/27/28	0/3/3/3
48	PSU	w	1056	48	-	0/7/25/26	0/2/2/2
48	PSU	w	105	48	-	0/7/25/26	0/2/2/2
3	OMC	D	1340	3	-	0/9/27/28	0/2/2/2
2	5MC	C	48	2	-	2/7/25/26	0/2/2/2
3	PSU	D	4521	3,81	-	2/7/25/26	0/2/2/2
3	PSU	D	3920	3,81	-	0/7/25/26	0/2/2/2
3	PSU	D	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3734	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4361	3	-	0/7/25/26	0/2/2/2
48	OMU	w	1804	48	-	2/9/27/28	0/2/2/2
3	A2M	D	400	3	-	0/9/27/28	0/3/3/3
48	MA6	w	1850	48	-	0/11/29/30	0/3/3/3
3	OMC	D	3808	3	-	0/9/27/28	0/2/2/2
2	1MA	C	58	2	-	0/7/25/26	0/3/3/3
48	G7M	w	1639	2,48	-	2/7/25/26	0/3/3/3
48	A2M	w	166	48	-	3/9/27/28	0/3/3/3
3	PSU	D	3768	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1860	3	-	0/7/25/26	0/2/2/2
3	OMC	D	3841	3	-	0/9/27/28	0/2/2/2
2	UY1	C	39	2	-	0/9/27/28	0/2/2/2
3	A2M	D	1524	3	-	1/9/27/28	0/3/3/3
3	PSU	D	4423	3	-	0/7/25/26	0/2/2/2
48	OMC	w	517	48	-	1/9/27/28	0/2/2/2
48	PSU	w	609	48	-	0/7/25/26	0/2/2/2
48	OMU	w	1326	48	-	3/9/27/28	0/2/2/2
48	OMG	w	1328	48	-	0/9/27/28	0/3/3/3
48	PSU	w	119	48	-	1/7/25/26	0/2/2/2
48	PSU	w	863	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4431	3	-	0/7/25/26	0/2/2/2
48	PSU	w	686	48	-	0/7/25/26	0/2/2/2
3	OMU	D	4306	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4579	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	93	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1004	48	-	0/7/25/26	0/2/2/2
48	PSU	w	822	48	-	2/7/25/26	0/2/2/2
2	56B	C	34	2,80	-	2/12/43/44	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A2M	w	27	48	-	0/9/27/28	0/3/3/3
3	PSU	D	3637	3,81	-	0/7/25/26	0/2/2/2
3	PSU	D	4689	3	-	0/7/25/26	0/2/2/2
2	H2U	B	47	2	-	3/7/38/39	0/2/2/2
3	OMC	D	4456	3	-	0/9/27/28	0/2/2/2
48	PSU	w	210	48	-	0/7/25/26	0/2/2/2
2	5MC	B	48	2	-	3/7/25/26	0/2/2/2
3	PSU	D	1677	3,81	-	3/7/25/26	0/2/2/2
48	PSU	w	814	48	-	0/7/25/26	0/2/2/2
48	OMG	w	644	48	-	3/9/27/28	0/3/3/3
2	2MG	B	10	2	-	0/9/27/28	0/3/3/3
3	OMU	D	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4442	3	-	0/7/25/26	0/2/2/2
48	OMU	w	121	48	-	0/9/27/28	0/2/2/2
48	OMG	w	1490	81,48	-	4/9/27/28	0/3/3/3
3	A2M	D	3785	3,81	-	3/9/27/28	0/3/3/3
48	OMU	w	116	48	-	0/9/27/28	0/2/2/2
48	MA6	w	1851	48	-	2/11/29/30	0/3/3/3
3	PSU	D	3851	3	-	0/7/25/26	0/2/2/2
3	5MC	D	4447	3,81	-	4/7/25/26	0/2/2/2
48	A2M	w	512	48	-	2/9/27/28	0/3/3/3
48	OMU	w	1288	48	-	1/9/27/28	0/2/2/2
3	PSU	D	1536	3	-	0/7/25/26	0/2/2/2
3	5MC	D	3782	3,81	-	0/7/25/26	0/2/2/2
48	PSU	w	1445	48	-	0/7/25/26	0/2/2/2
3	OMG	D	2424	3	-	2/9/27/28	0/3/3/3
2	PSU	B	55	2	-	2/7/25/26	0/2/2/2
3	OMG	D	4499	2,3	-	0/9/27/28	0/3/3/3
2	2MG	C	10	2	-	0/9/27/28	0/3/3/3
3	OMG	D	4392	3	-	0/9/27/28	0/3/3/3
3	OMG	D	4370	3	-	0/9/27/28	0/3/3/3
3	PSU	D	1792	3	-	0/7/25/26	0/2/2/2
3	PSU	D	1744	3,81	-	0/7/25/26	0/2/2/2
2	PSU	C	35	2,1	-	0/7/25/26	0/2/2/2
3	A2M	D	398	3	-	0/9/27/28	0/3/3/3
3	A2M	D	2815	3	-	2/9/27/28	0/3/3/3
3	UR3	D	4530	3,81	-	0/7/25/26	0/2/2/2
48	PSU	w	801	48	-	0/7/25/26	0/2/2/2
3	OMG	D	1522	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	w	1244	48	-	0/7/25/26	0/2/2/2
2	G7M	C	46	2	-	2/7/25/26	0/3/3/3
48	OMU	w	428	48	-	7/9/27/28	0/2/2/2
3	OMC	D	3887	3	-	1/9/27/28	0/2/2/2
48	PSU	w	1367	48	-	0/7/25/26	0/2/2/2
2	5MU	C	54	2	-	2/7/25/26	0/2/2/2
48	PSU	w	1232	48	-	0/7/25/26	0/2/2/2
48	PSU	w	218	48	-	0/7/25/26	0/2/2/2
2	1MA	B	58	2	-	2/7/25/26	0/3/3/3
48	PSU	w	649	48	-	0/7/25/26	0/2/2/2
48	A2M	w	484	48	-	0/9/27/28	0/3/3/3
48	A2M	w	668	81,48	-	3/9/27/28	0/3/3/3
3	PSU	D	4471	3	-	0/7/25/26	0/2/2/2
2	2MG	C	6	2	-	3/9/27/28	0/3/3/3
48	PSU	w	1081	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1782	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4296	3	-	0/7/25/26	0/2/2/2
3	OMU	D	4498	3,81	-	0/9/27/28	0/2/2/2
3	OMG	D	4196	3,81	-	0/9/27/28	0/3/3/3
3	PSU	D	1683	3,81	-	0/7/25/26	0/2/2/2
3	PSU	D	4552	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3770	3	-	0/7/25/26	0/2/2/2
2	1MG	B	37	2	-	1/7/25/26	0/3/3/3
3	PSU	D	4972	3,81	-	0/7/25/26	0/2/2/2
48	A2M	w	159	48	-	2/9/27/28	0/3/3/3
48	A2M	w	468	48	-	2/9/27/28	0/3/3/3
3	OMU	D	2415	3	-	1/9/27/28	0/2/2/2
48	PSU	w	681	48	-	0/7/25/26	0/2/2/2
48	PSU	w	651	48	-	0/7/25/26	0/2/2/2
48	OMG	w	436	48	-	0/9/27/28	0/3/3/3
48	PSU	w	1238	48	-	2/7/25/26	0/2/2/2
3	PSU	D	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3730	3	-	0/7/25/26	0/2/2/2
48	4AC	w	1337	48	-	0/11/29/30	0/2/2/2
2	H2U	C	47	2	-	3/7/38/39	0/2/2/2
3	A2M	D	1326	3	-	1/9/27/28	0/3/3/3
2	M2G	B	27	2	-	0/11/29/30	0/3/3/3
3	PSU	D	3764	3	-	0/7/25/26	0/2/2/2
3	OMG	D	1625	3,81	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M2G	C	26	2	-	0/11/29/30	0/3/3/3
2	56B	B	34	2,80	-	3/12/43/44	0/4/4/4
48	A2M	w	99	81,48	-	2/9/27/28	0/3/3/3
48	PSU	w	1045	48	-	0/7/25/26	0/2/2/2
48	OMC	w	174	48	-	0/9/27/28	0/2/2/2
3	OMG	D	3899	3	-	0/9/27/28	0/3/3/3
5	OMG	F	75	5	-	1/9/27/28	0/3/3/3
3	PSU	D	2508	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4576	3	-	0/7/25/26	0/2/2/2
3	OMG	D	4623	3	-	0/9/27/28	0/3/3/3
48	PSU	w	406	48	-	0/7/25/26	0/2/2/2
48	PSU	w	572	48	-	0/7/25/26	0/2/2/2
3	A2M	D	3825	3	-	0/9/27/28	0/3/3/3
3	OMG	D	1316	3	-	0/9/27/28	0/3/3/3
3	OMG	D	4494	3	-	0/9/27/28	0/3/3/3
48	6MZ	w	1832	81,48	-	2/9/27/28	0/3/3/3
3	A2M	D	2401	3	-	0/9/27/28	0/3/3/3
3	OMG	D	3744	3	-	0/9/27/28	0/3/3/3
48	B8N	w	1248	48	-	4/16/34/35	0/2/2/2
3	OMC	D	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	D	3639	3	-	0/7/25/26	0/2/2/2
3	A2M	D	3718	3	-	0/9/27/28	0/3/3/3
3	PSU	D	4293	3	-	0/7/25/26	0/2/2/2

The worst 5 of 832 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	1832	6MZ	C6-N6	12.19	1.47	1.34
3	D	4220	6MZ	C6-N6	12.03	1.47	1.34
2	B	54	5MU	C6-N1	11.03	1.56	1.38
2	C	54	5MU	C6-N1	10.87	1.56	1.38
2	B	54	5MU	C2-N1	10.70	1.55	1.38

The worst 5 of 1000 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	5MU	C5-C4-N3	12.25	125.76	115.31
2	C	54	5MU	C5-C4-N3	12.01	125.57	115.31
2	B	54	5MU	C5-C6-N1	-10.01	113.04	123.34
2	C	54	5MU	C5-C6-N1	-9.97	113.08	123.34
2	C	34	56B	C1'-N9-C4	-7.62	103.86	126.50

There are no chirality outliers.

5 of 174 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	26	M2G	C3'-C4'-C5'-O5'
2	B	34	56B	C11-C10-N10-C9
2	B	39	UY1	C3'-C4'-C5'-O5'
2	B	39	UY1	O4'-C4'-C5'-O5'
2	C	46	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

60 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	w	1391	OMC	1	0
3	D	2363	A2M	1	0
48	w	627	OMU	1	0
2	B	54	5MU	2	0
3	D	1534	A2M	1	0
48	w	1842	4AC	1	0
3	D	1760	OMG	1	0
48	w	601	OMG	1	0
48	w	799	OMU	2	0
3	D	3818	UY1	1	0
48	w	576	A2M	1	0
3	D	4620	OMU	2	0
3	D	4220	6MZ	1	0
3	D	2364	OMG	1	0
2	B	26	M2G	1	0
48	w	1692	PSU	1	0
3	D	2351	OMC	2	0
48	w	683	OMG	1	0
3	D	3925	OMU	1	0
3	D	3724	A2M	1	0
3	D	4420	PSU	1	0
3	D	1773	OMU	3	0
48	w	1678	A2M	1	0
3	D	1340	OMC	1	0
48	w	1850	MA6	1	0
48	w	1639	G7M	2	0
48	w	166	A2M	2	0
3	D	3768	PSU	1	0
48	w	517	OMC	2	0
48	w	686	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	4637	OMG	2	0
48	w	93	PSU	1	0
48	w	27	A2M	1	0
48	w	644	OMG	1	0
48	w	1490	OMG	3	0
3	D	3785	A2M	1	0
48	w	116	OMU	2	0
3	D	4447	5MC	1	0
48	w	512	A2M	1	0
48	w	1288	OMU	1	0
48	w	1445	PSU	1	0
2	B	55	PSU	3	0
3	D	4392	OMG	1	0
3	D	398	A2M	1	0
3	D	2815	A2M	1	0
2	C	46	G7M	2	0
48	w	428	OMU	2	0
3	D	2415	OMU	1	0
48	w	436	OMG	1	0
3	D	4457	PSU	1	0
48	w	1337	4AC	1	0
2	C	47	H2U	2	0
3	D	1326	A2M	1	0
2	C	26	M2G	2	0
5	F	75	OMG	1	0
3	D	4623	OMG	1	0
48	w	572	PSU	1	0
3	D	4494	OMG	1	0
3	D	2824	OMC	1	0
3	D	3718	A2M	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 528 ligands modelled in this entry, 526 are monoatomic - leaving 2 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
80	GAL	C	101	2	11,11,12	1.96	3 (27%)	15,15,17	1.82	6 (40%)
80	GAL	B	101	2	11,11,12	1.89	2 (18%)	15,15,17	1.99	6 (40%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
80	GAL	C	101	2	-	2/2/19/22	0/1/1/1
80	GAL	B	101	2	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	B	101	GAL	O5-C1	-3.65	1.37	1.43
80	C	101	GAL	O5-C1	-3.34	1.38	1.43
80	C	101	GAL	C2-C3	3.09	1.57	1.52
80	B	101	GAL	C2-C3	2.80	1.56	1.52
80	C	101	GAL	C4-C5	2.40	1.58	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	C	101	GAL	O2-C2-C3	-3.37	103.39	110.14
80	B	101	GAL	O4-C4-C5	-3.33	101.04	109.30
80	B	101	GAL	O2-C2-C3	-3.26	103.61	110.14
80	B	101	GAL	C6-C5-C4	-3.16	105.60	113.00
80	B	101	GAL	C2-C3-C4	-2.65	106.31	110.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	C	101	GAL	O5-C5-C6-O6
80	C	101	GAL	C4-C5-C6-O6

*Continued on next page...*

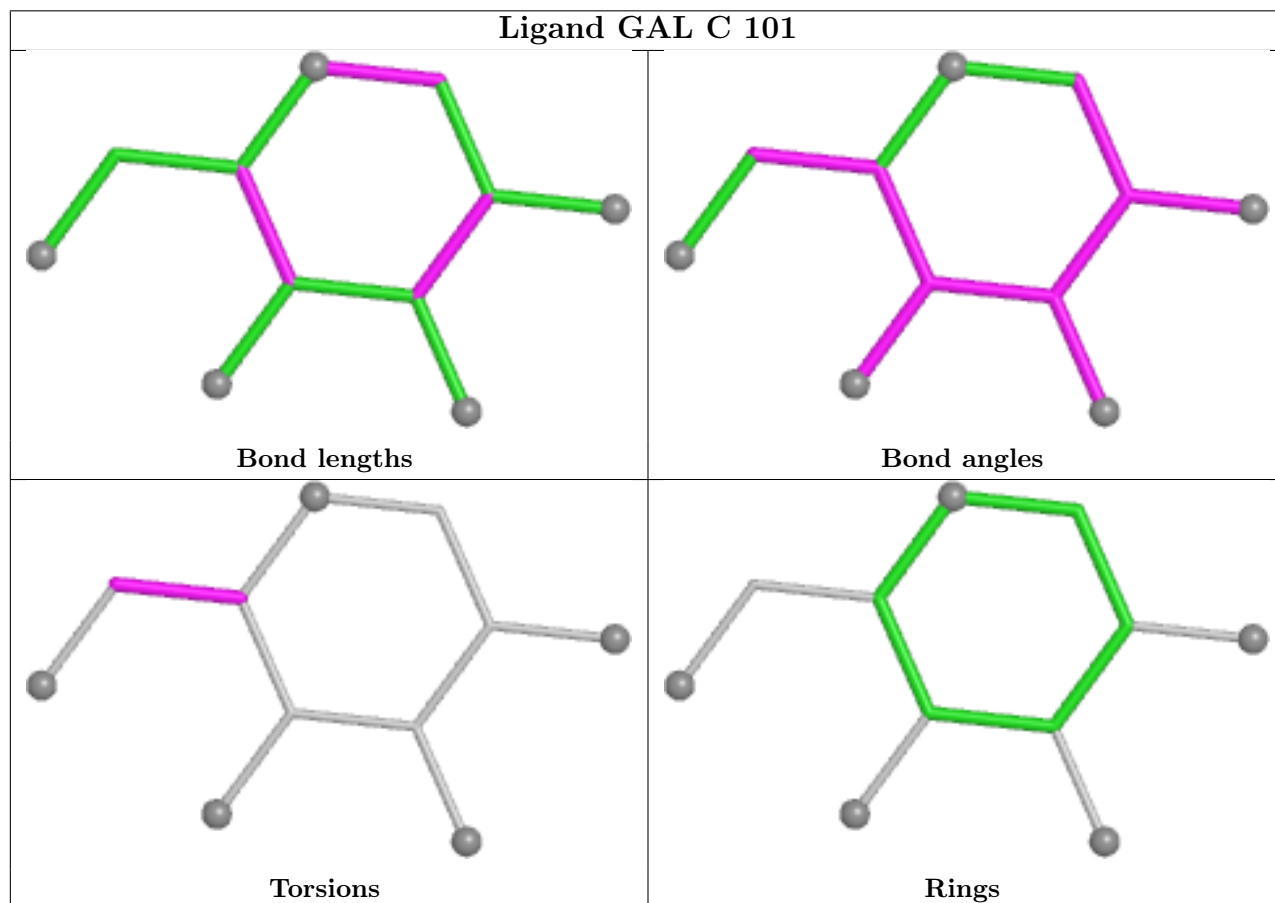
*Continued from previous page...*

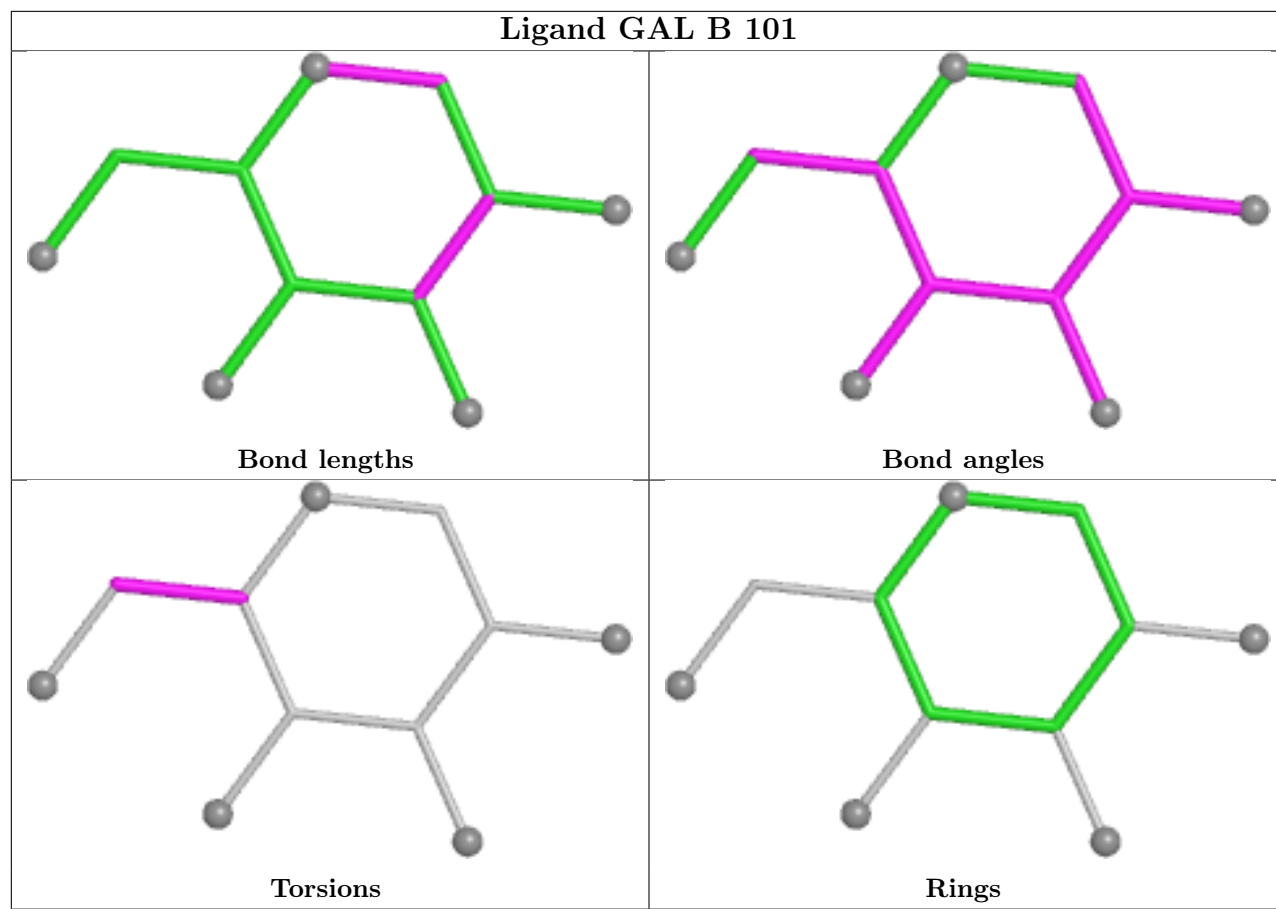
Mol	Chain	Res	Type	Atoms
80	B	101	GAL	O5-C5-C6-O6
80	B	101	GAL	C4-C5-C6-O6

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.

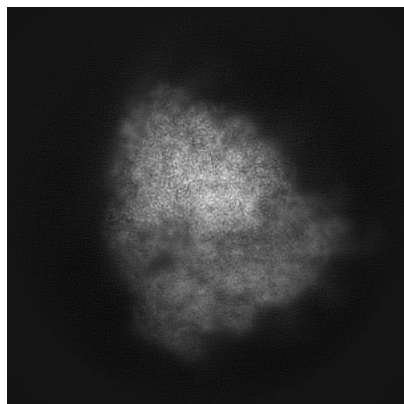
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36181. These allow visual inspection of the internal detail of the map and identification of artifacts.

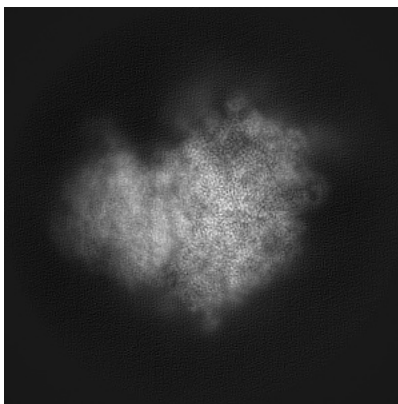
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

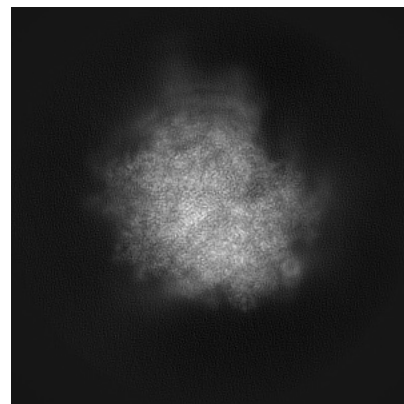
#### 6.1.1 Primary map



X

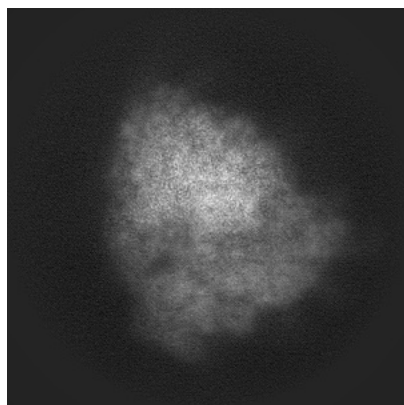


Y

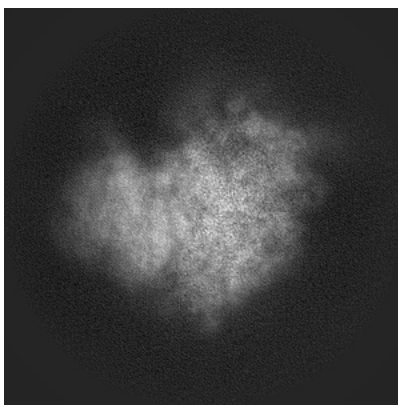


Z

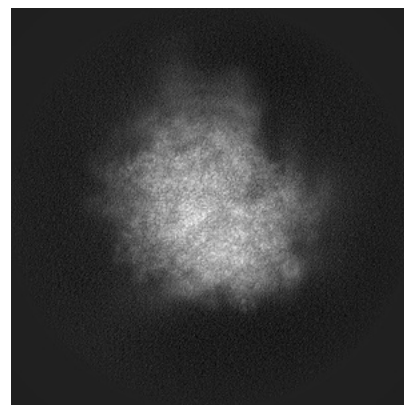
#### 6.1.2 Raw map



X



Y

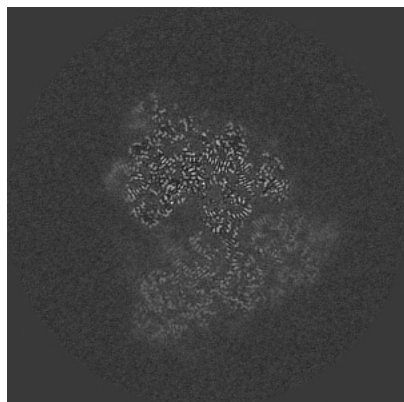


Z

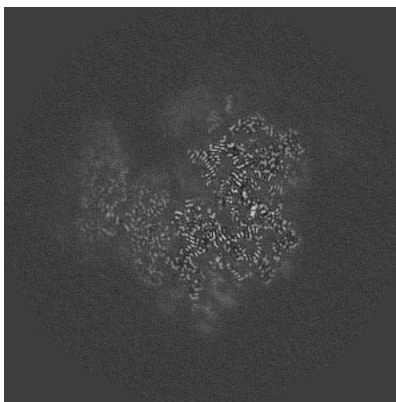
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

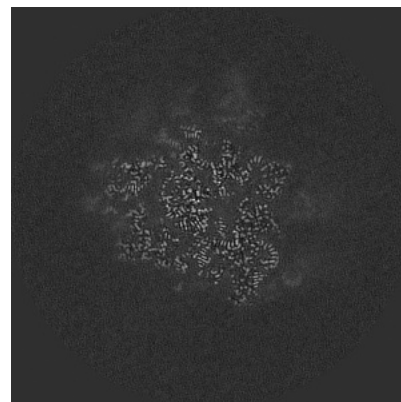
### 6.2.1 Primary map



X Index: 265

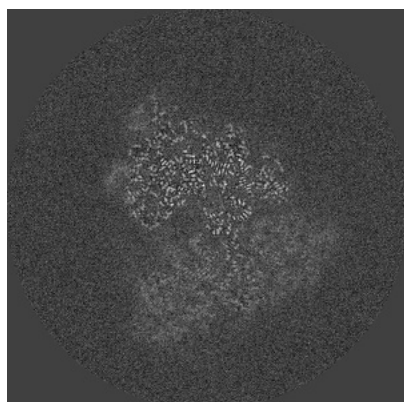


Y Index: 265

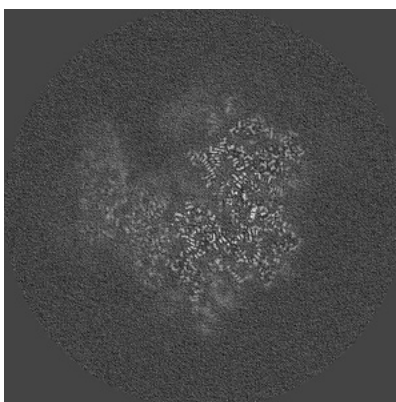


Z Index: 265

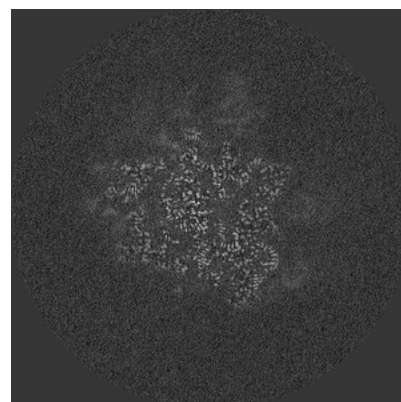
### 6.2.2 Raw map



X Index: 265



Y Index: 265

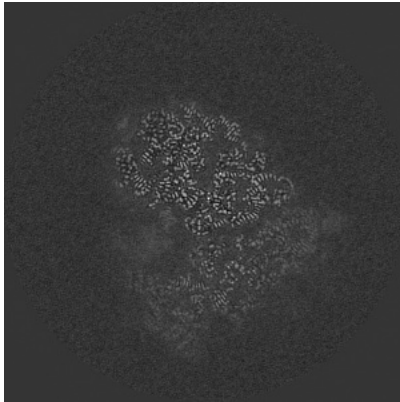


Z Index: 265

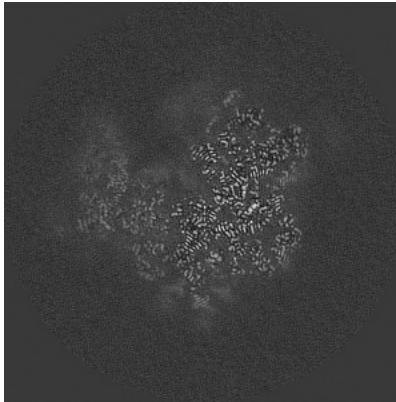
The images above show central slices of the map in three orthogonal directions.

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

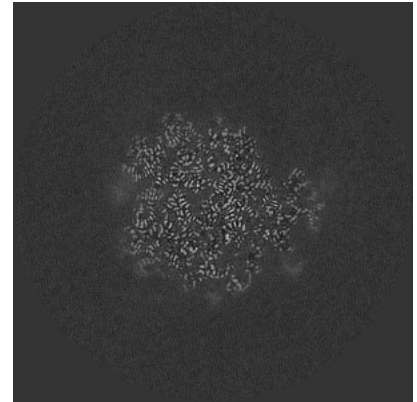
### 6.3.1 Primary map



X Index: 245

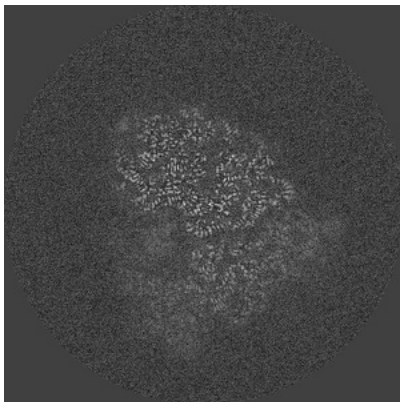


Y Index: 261

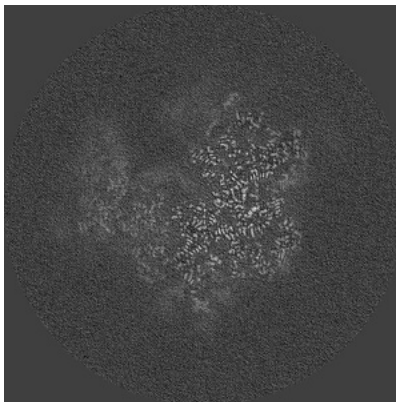


Z Index: 302

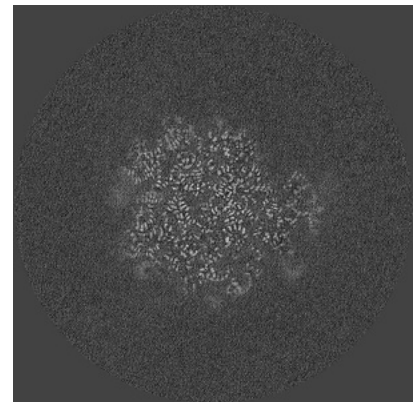
### 6.3.2 Raw map



X Index: 248



Y Index: 261

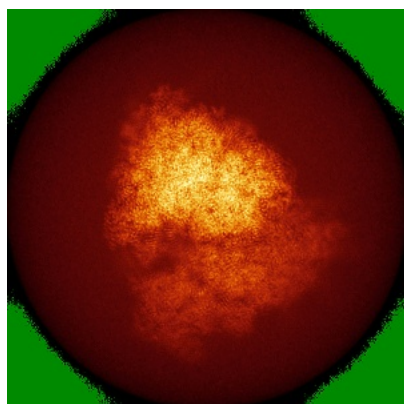


Z Index: 302

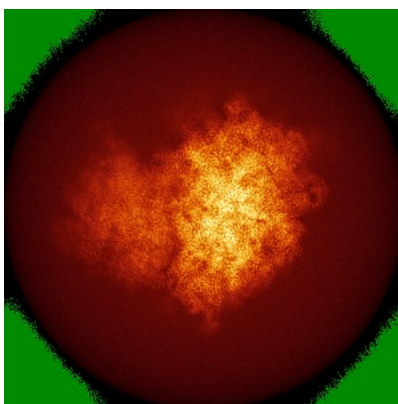
The images above show the largest variance slices of the map in three orthogonal directions.

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

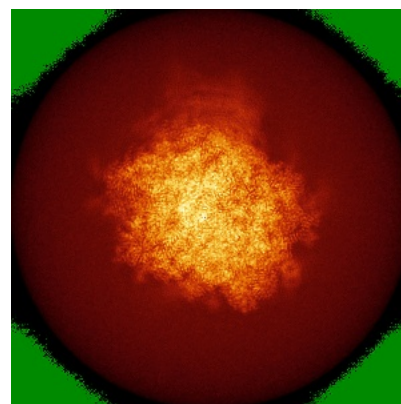
### 6.4.1 Primary map



X

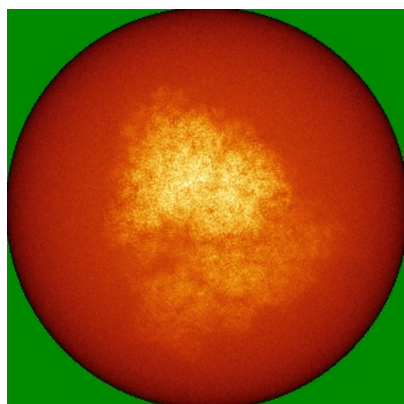


Y

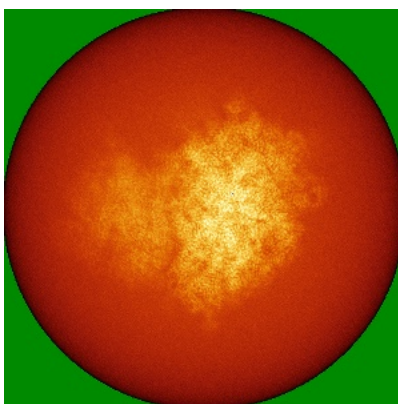


Z

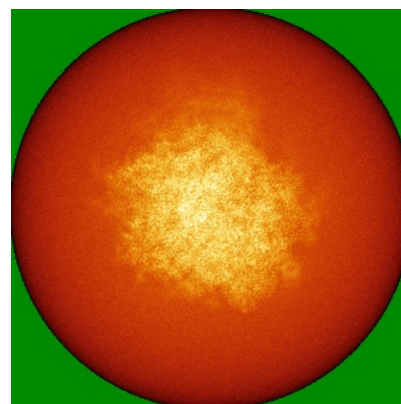
### 6.4.2 Raw map



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



X



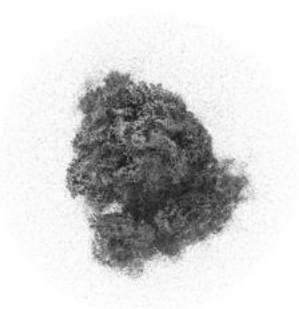
Y



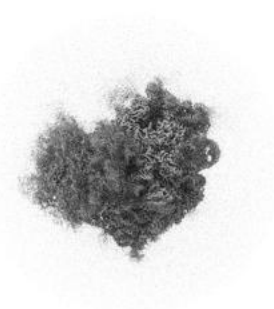
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0183. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

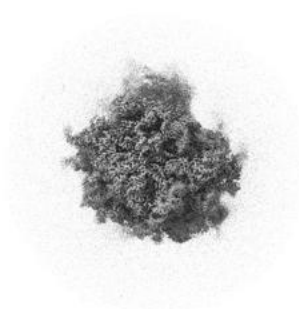
### 6.5.2 Raw map



X



Y



Z

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.

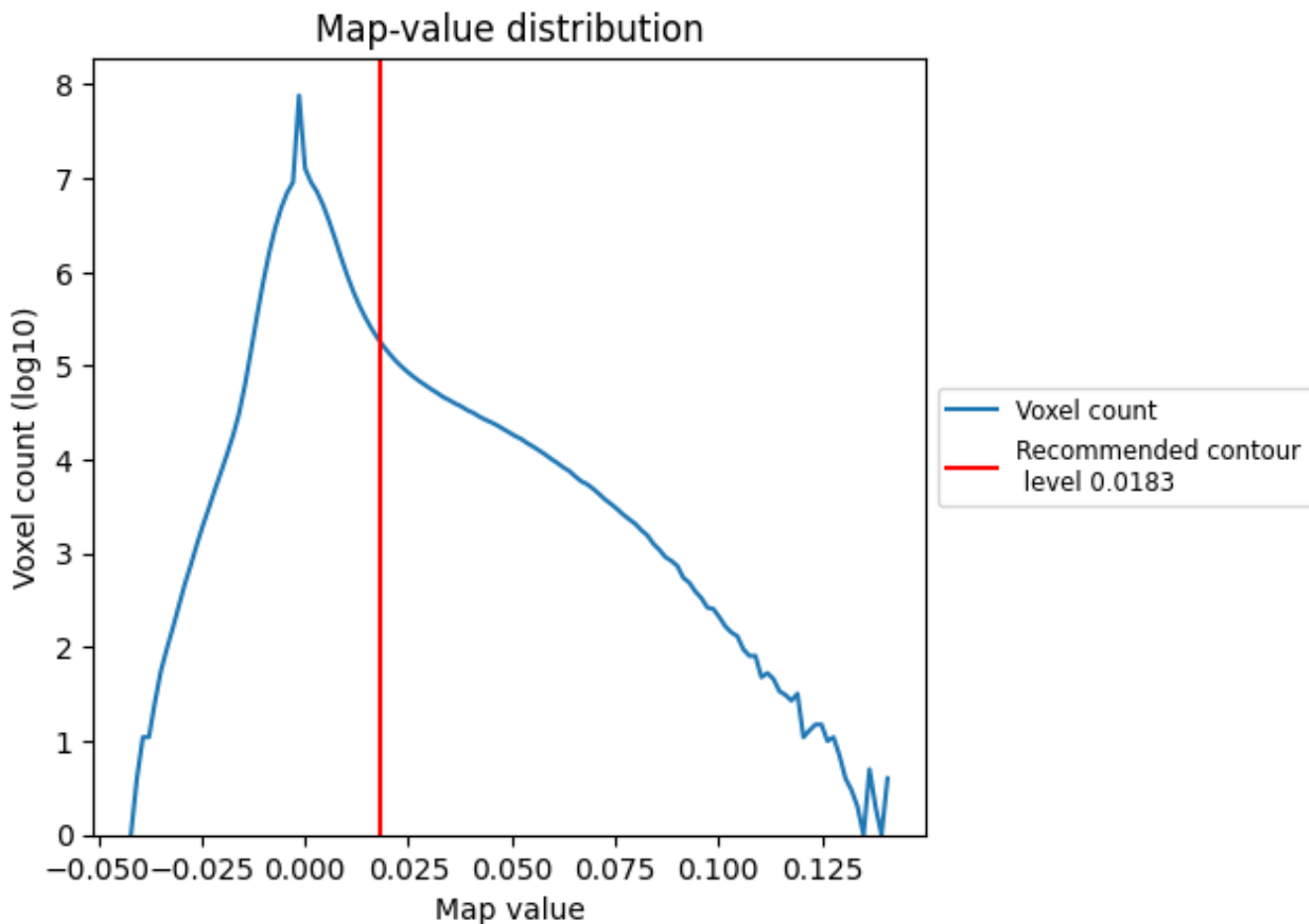
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

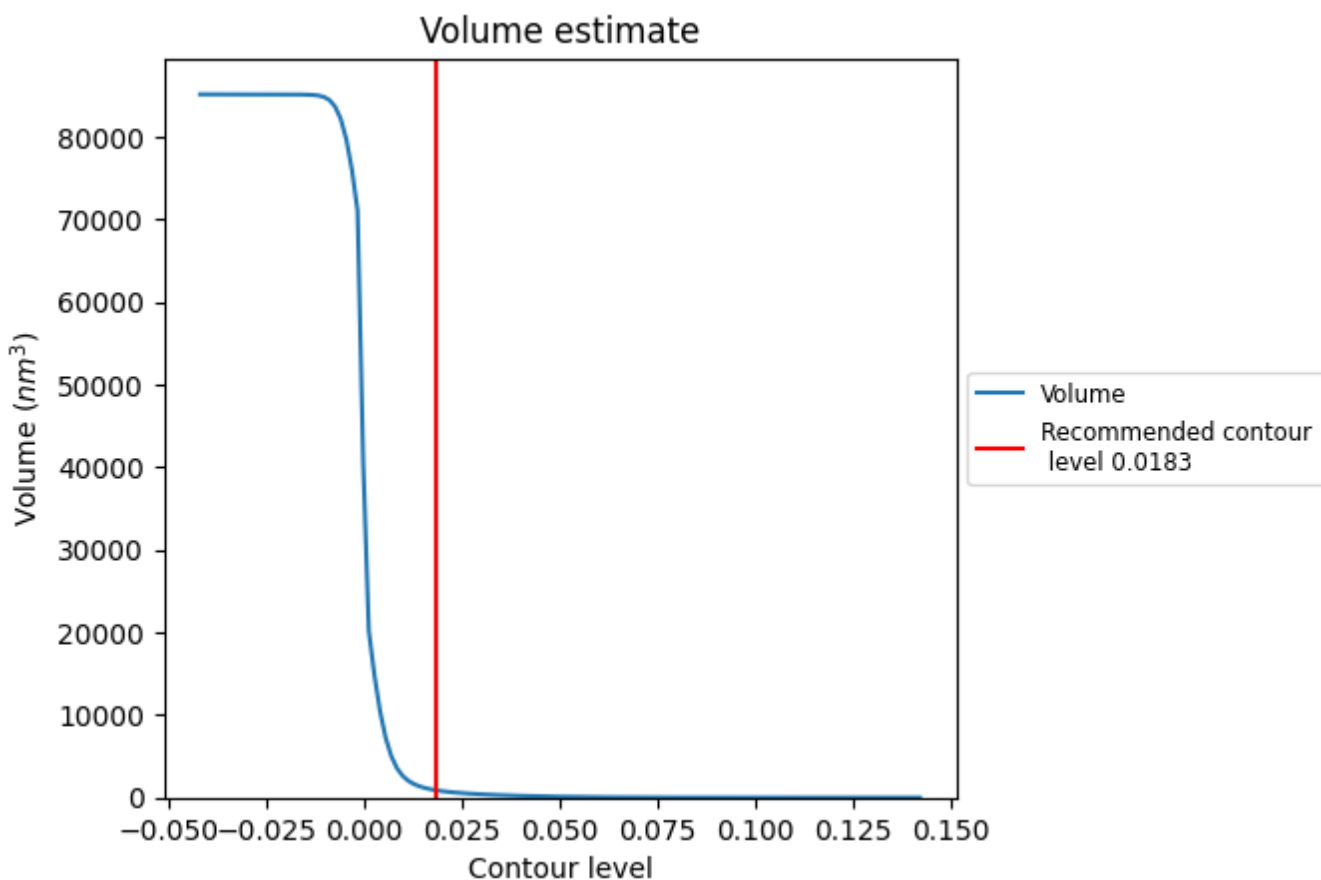
This section contains the results of statistical analysis of the map.

### 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.

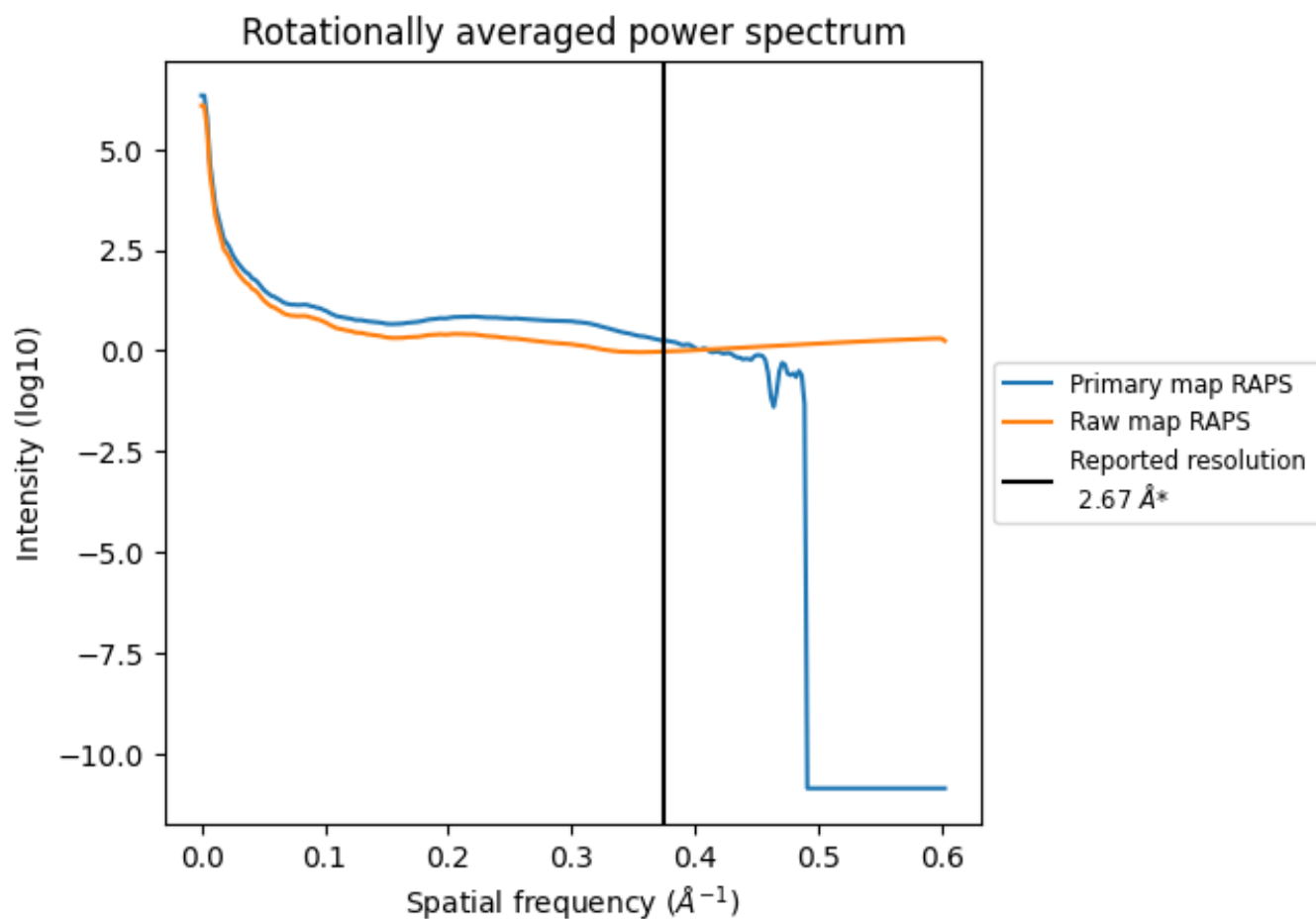
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 889 nm<sup>3</sup>; this corresponds to an approximate mass of 803 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

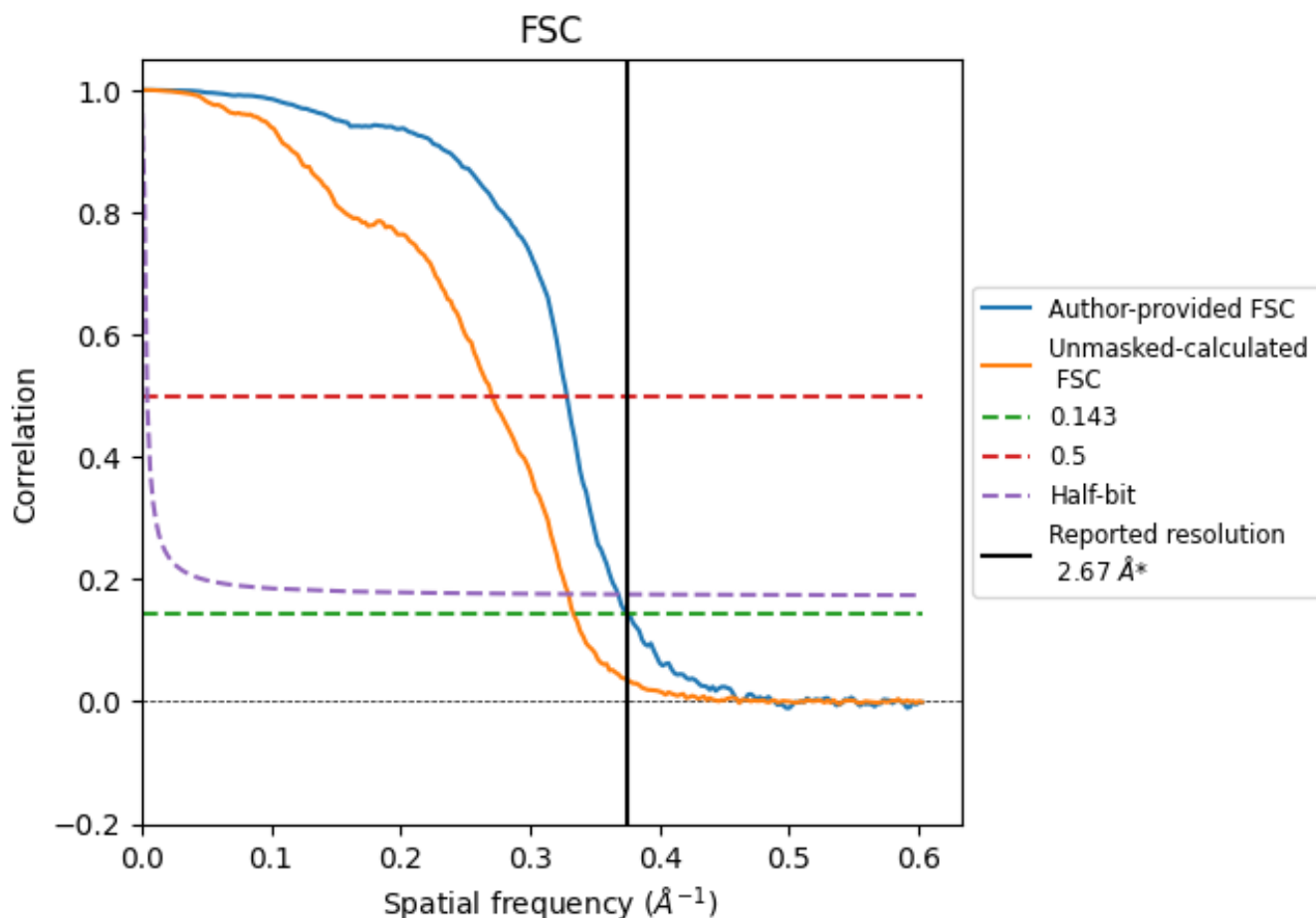


\*Reported resolution corresponds to spatial frequency of  $0.375 \text{ \AA}^{-1}$

## 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 0.375 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

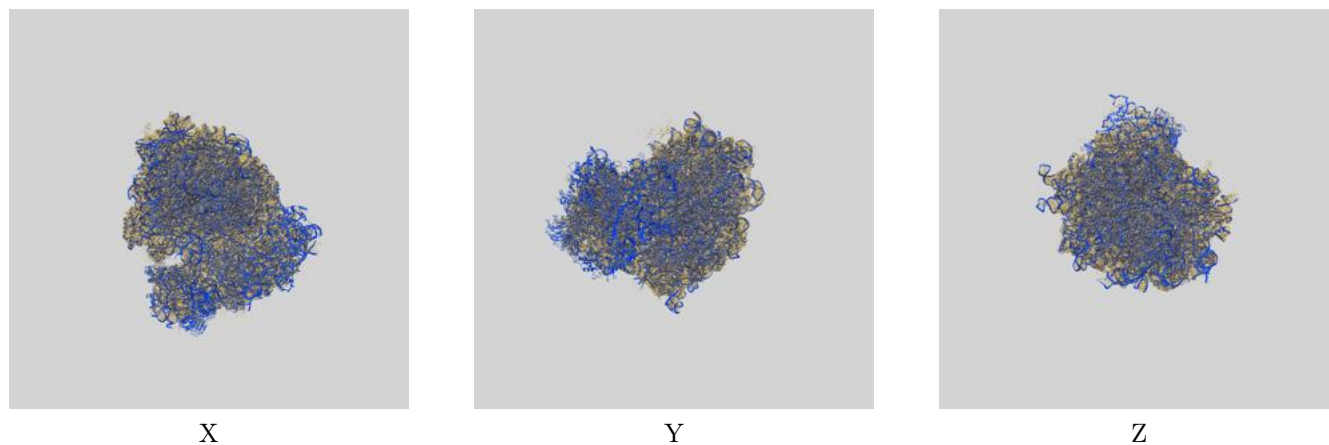
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.66	3.05	2.72
Unmasked-calculated*	3.00	3.70	3.03

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 2.67 by more than 10 %

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

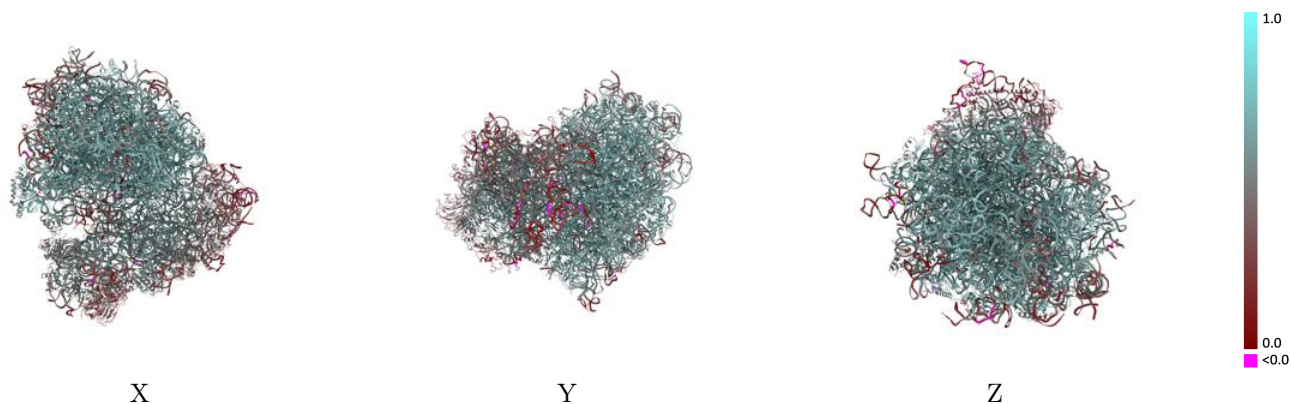
This section contains information regarding the fit between EMDB map EMD-36181 and PDB model 8JDM. Per-residue inclusion information can be found in section 3 on page 21.

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



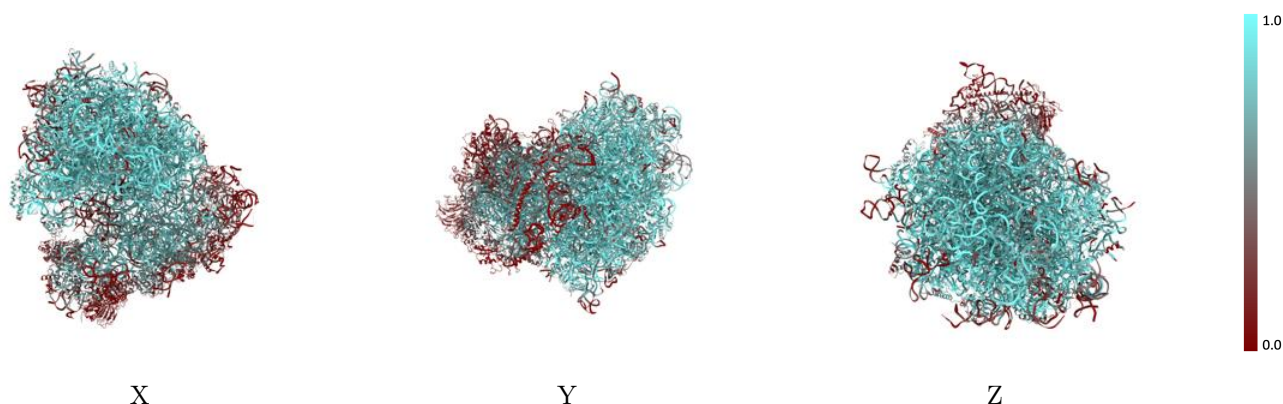
The images above show the 3D surface view of the map at the recommended contour level 0.0183 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



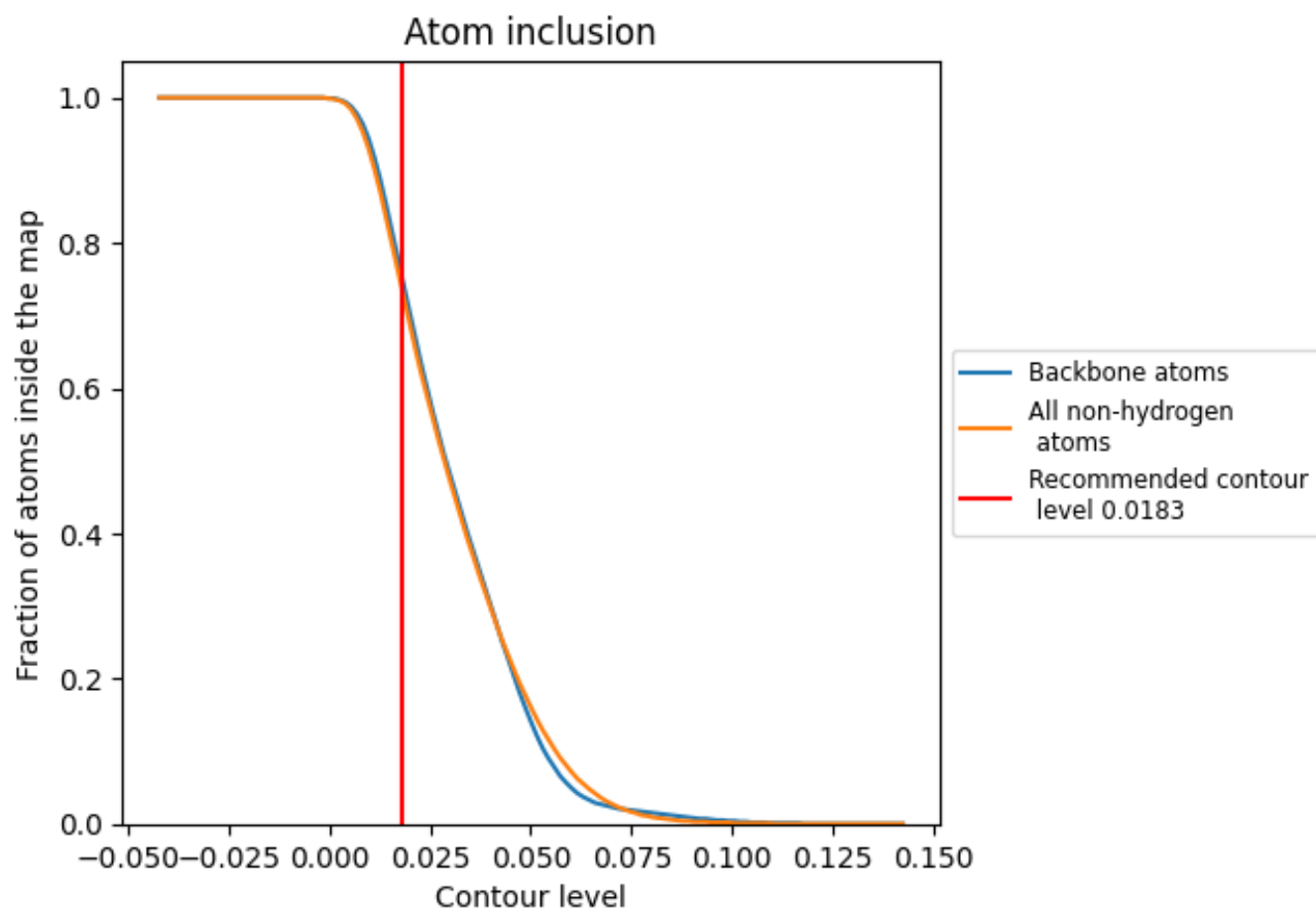
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0183).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 73% 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 (0.0183) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.5570
0	 0.2850	 0.4030
1	 0.2820	 0.4000
2	 0.3330	 0.4450
3	 0.1340	 0.2970
4	 0.1880	 0.3550
5	 0.2830	 0.3820
6	 0.3140	 0.4030
7	 0.1250	 0.3230
8	 0.5370	 0.5070
9	 0.5530	 0.5220
A	 0.6390	 0.4810
AA	 0.6000	 0.5160
AB	 0.3450	 0.4440
AC	 0.3380	 0.4510
AD	 0.2440	 0.3960
AE	 0.3440	 0.4500
AF	 0.3400	 0.4600
AG	 0.2430	 0.3470
AH	 0.4820	 0.5120
AI	 0.6960	 0.5720
AJ	 0.6390	 0.5460
AK	 0.1460	 0.3490
AL	 0.1360	 0.3880
AM	 0.6730	 0.5470
AN	 0.3770	 0.4270
AO	 0.2780	 0.4160
AP	 0.6050	 0.5410
AQ	 0.2670	 0.3780
AR	 0.0550	 0.2820
B	 0.4160	 0.3640
C	 0.2080	 0.3570
D	 0.8570	 0.5990
E	 0.9720	 0.6550
F	 0.9020	 0.6160











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Chain	Atom inclusion	Q-score
G	0.9470	0.6630
H	0.8740	0.6410
I	0.8890	0.6290
J	0.7820	0.5920
K	0.7550	0.5800
L	0.8980	0.6460
M	0.6930	0.5620
N	0.8040	0.6070
O	0.8480	0.6130
P	0.6540	0.5270
Q	0.7910	0.5920
R	0.8300	0.6060
S	0.9580	0.6670
T	0.9120	0.6530
U	0.8800	0.6420
V	0.9340	0.6560
W	0.7500	0.5740
X	0.9140	0.6490
Y	0.8550	0.6230
Z	0.5770	0.5140
a	0.8900	0.6460
b	0.8490	0.6200
c	0.8160	0.6050
d	0.8150	0.6020
e	0.7800	0.5940
f	0.9070	0.6490
g	0.7090	0.5380
h	0.7780	0.5940
i	0.8200	0.6110
j	0.9180	0.6600
k	0.9310	0.6540
l	0.8330	0.6120
m	0.8070	0.6050
n	0.7430	0.5910
o	0.9450	0.6600
p	0.6440	0.5400
q	0.9120	0.6390
r	0.8630	0.6290
s	0.8440	0.6250
t	0.7940	0.5960
u	0.8840	0.6480
v	0.8860	0.6240

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Chain	Atom inclusion	Q-score
w	 0.6900	 0.5140
x	 0.4430	 0.5020
y	 0.4980	 0.5220
z	 0.6020	 0.5380