wwPDB EM Validation Summary Report

Dec 17, 2023 – 03:47 AM JST

PDB ID	:	8JDJ
EMDB ID	:	EMD-36178
Title	:	Structure of the Human cytoplasmic Ribosome with human tRNA Asp(Q34) and mRNA(GAU)
Authors	:	Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.
Deposited on	:	2023-05-14
Resolution	:	2.50 Å(reported)
Based on initial model	:	6Y0G

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

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

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

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

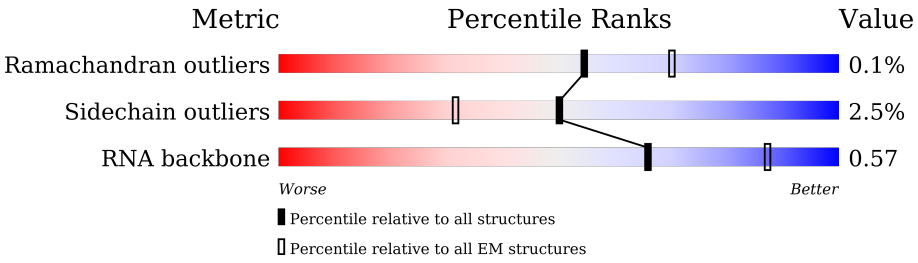
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



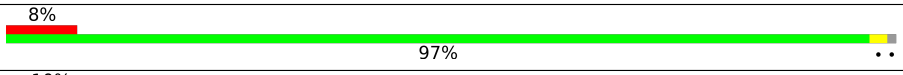
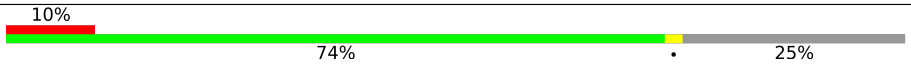
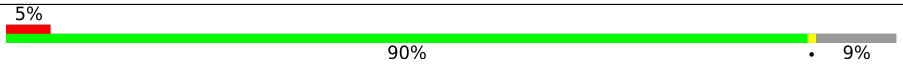
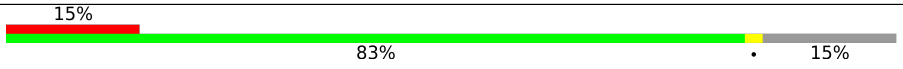
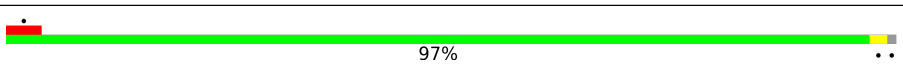
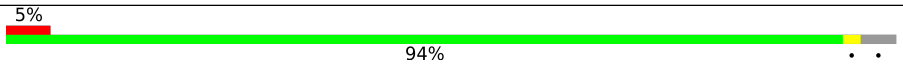
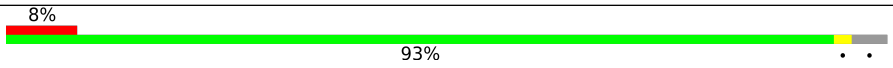
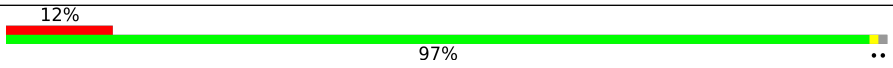
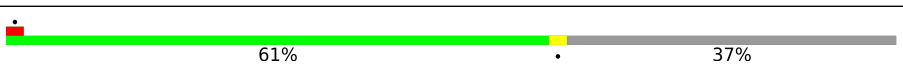
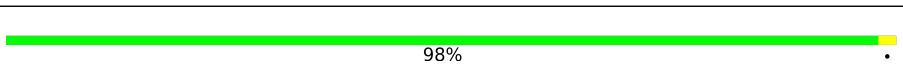
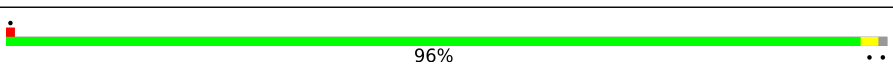
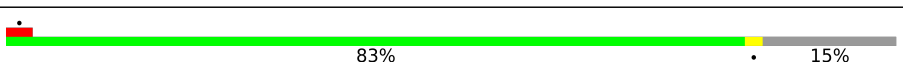
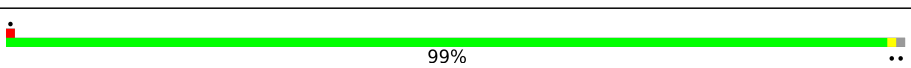
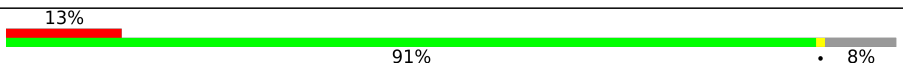
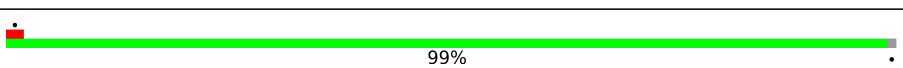
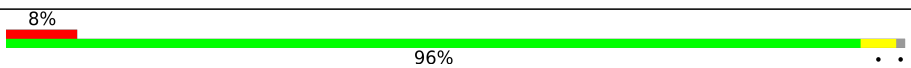
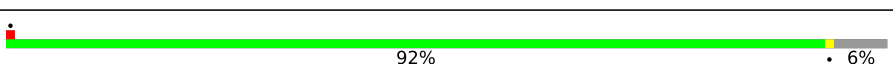
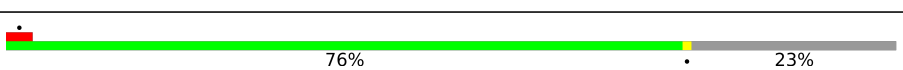
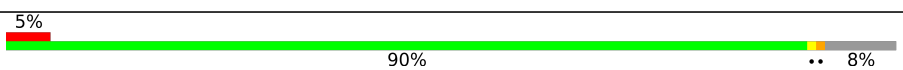
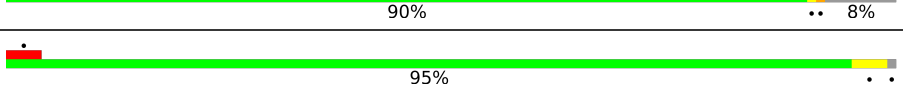
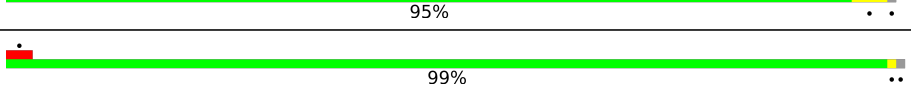
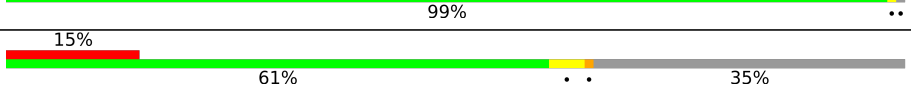
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	7% 93% 7%
2	B	75	11% 75% 19% 7%
2	C	75	21% 73% 20% 7%
3	D	5070	8% 55% 14% 31%
4	E	120	88% 12%
5	F	156	7% 80% 19%
6	G	257	95%
7	H	403	97%

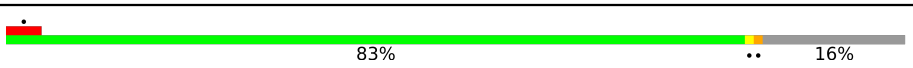
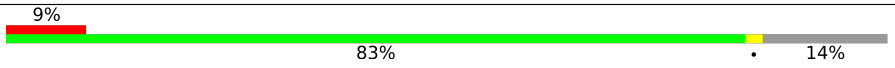
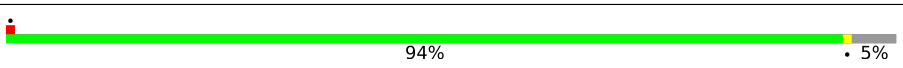
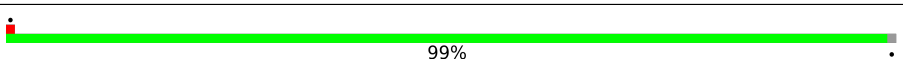
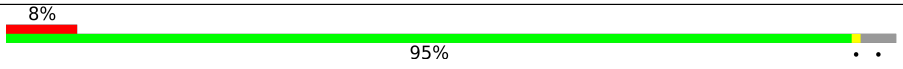
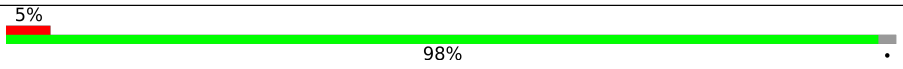
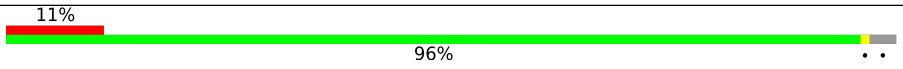
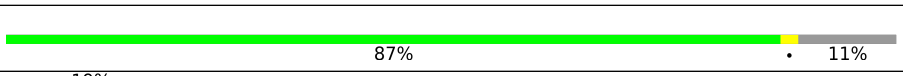
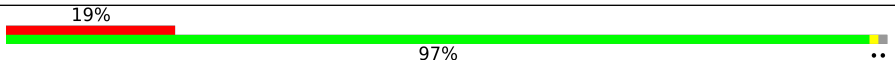
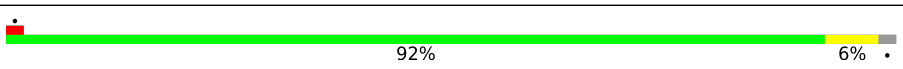
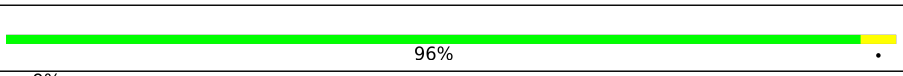
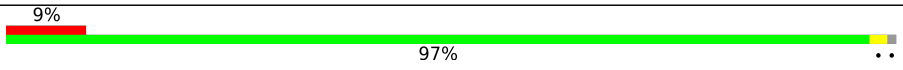
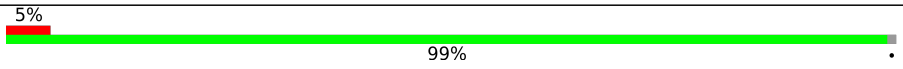
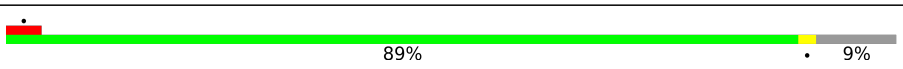
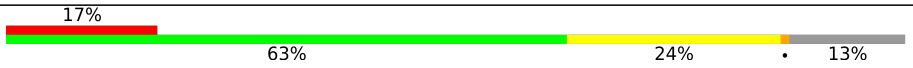
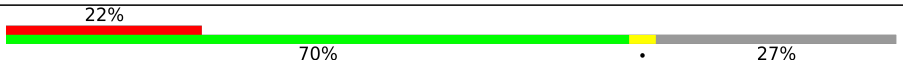
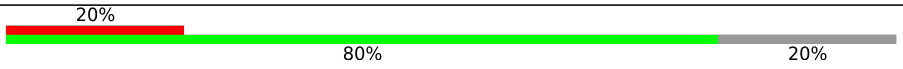
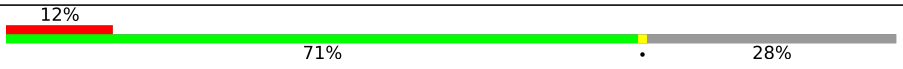
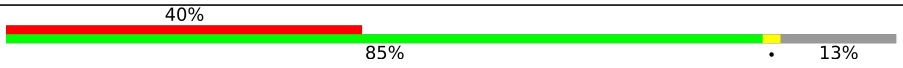
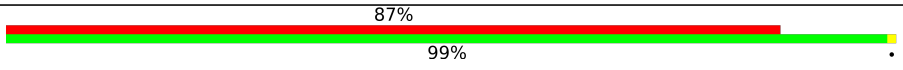
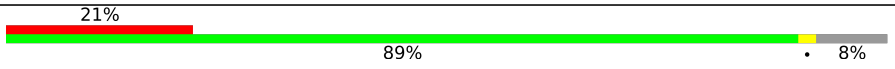
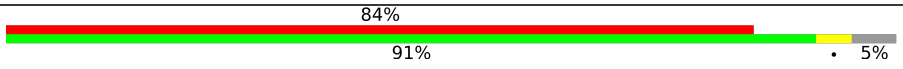
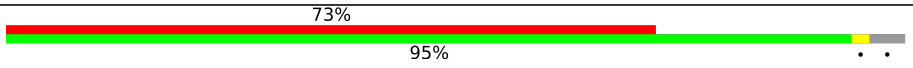
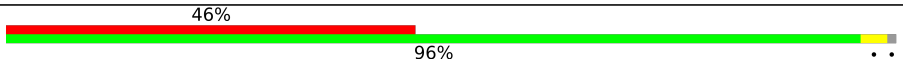
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	I	427	
9	J	297	
10	K	288	
11	L	248	
12	M	266	
13	N	192	
14	O	214	
15	P	178	
16	Q	211	
17	R	215	
18	S	204	
19	T	203	
20	U	184	
21	V	188	
22	W	196	
23	X	176	
24	Y	160	
25	Z	128	
26	a	140	
27	b	157	
28	c	156	
29	d	145	
30	e	136	
31	f	148	
32	g	159	

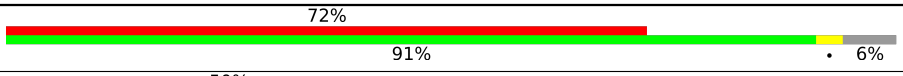
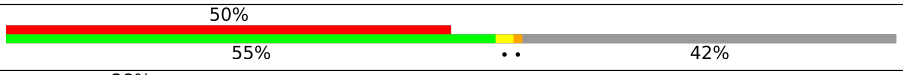
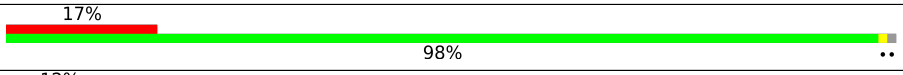
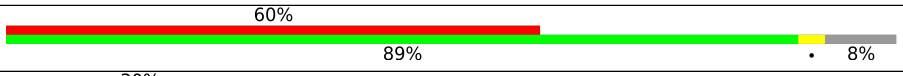
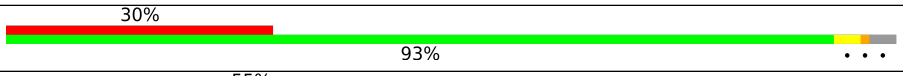
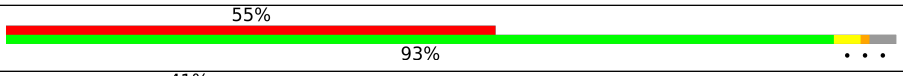
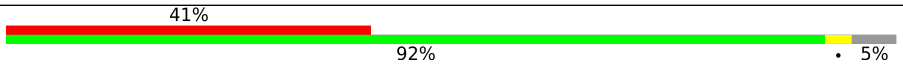
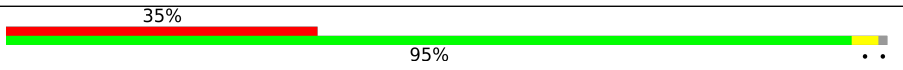
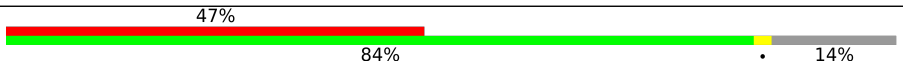
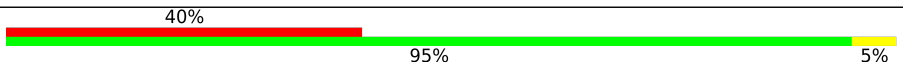
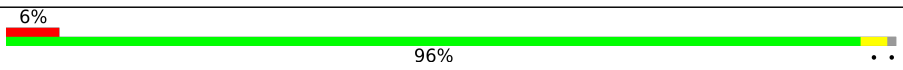
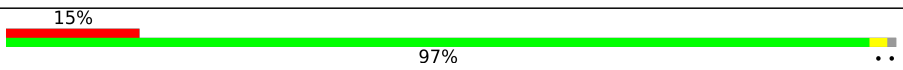
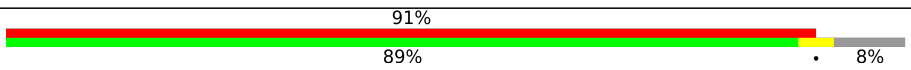
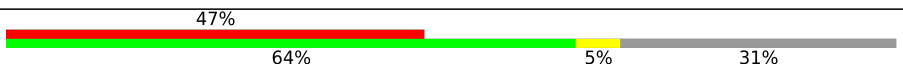
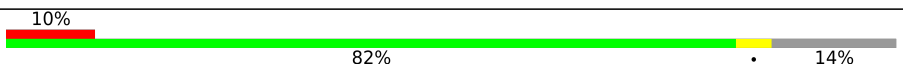
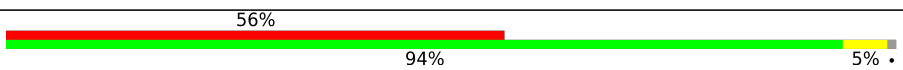
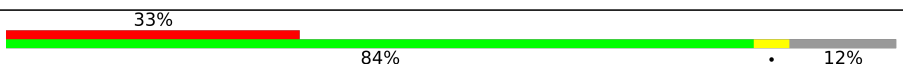
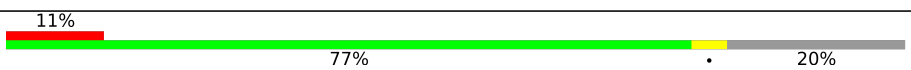
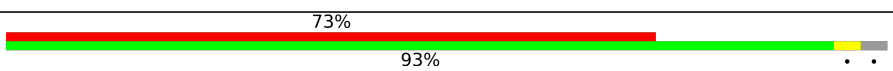
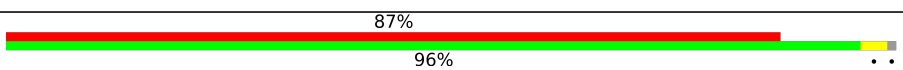
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	h	115	
34	i	125	
35	j	135	
36	k	110	
37	l	117	
38	m	123	
39	n	105	
40	o	97	
41	p	70	
42	q	51	
43	r	128	
44	s	25	
45	t	106	
46	u	92	
47	v	137	
48	w	1869	
49	x	295	
50	y	264	
51	z	293	
52	0	243	
53	1	263	
54	2	204	
55	3	249	
56	4	194	
57	5	208	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	6	194	
59	7	165	
60	8	158	
61	9	151	
62	AA	151	
63	AB	145	
64	AC	146	
65	AD	135	
66	AE	152	
67	AF	145	
68	AG	119	
69	AH	83	
70	AI	130	
71	AJ	143	
72	AK	133	
73	AL	125	
74	AM	115	
75	AN	84	
76	AO	69	
77	AP	56	
78	AQ	59	
79	AR	317	

2 Entry composition (i)

There are 81 unique types of molecules in this entry. The entry contains 209545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	14	Total	C	N	O	P	0	0
			303	135	55	99	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	75	Total	C	N	O	P	0	0
			1612	726	283	529	74		
2	C	75	Total	C	N	O	P	0	0
			1612	726	283	529	74		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	187	Total 1464	C 916	N 276	O 265	S 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
62	AA	134	Total	C	N	O	S	0	0
			1002	612	197	187	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		AltConf
80	A	1	Total	Mg	0
			1	1	
80	D	398	Total	Mg	0
			398	398	
80	E	10	Total	Mg	0
			10	10	
80	F	6	Total	Mg	0
			6	6	
80	G	2	Total	Mg	0
			2	2	
80	H	1	Total	Mg	0
			1	1	
80	I	1	Total	Mg	0
			1	1	
80	N	1	Total	Mg	0
			1	1	
80	O	2	Total	Mg	0
			2	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
80	S	1	Total Mg 1 1	0
80	U	2	Total Mg 2 2	0
80	V	2	Total Mg 2 2	0
80	X	1	Total Mg 1 1	0
80	a	1	Total Mg 1 1	0
80	g	1	Total Mg 1 1	0
80	j	1	Total Mg 1 1	0
80	k	1	Total Mg 1 1	0
80	l	1	Total Mg 1 1	0
80	u	1	Total Mg 1 1	0
80	w	103	Total Mg 103 103	0
80	AA	1	Total Mg 1 1	0
80	AF	1	Total Mg 1 1	0

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

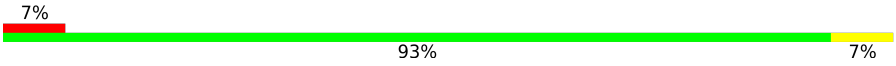
Mol	Chain	Residues	Atoms	AltConf
81	o	1	Total Zn 1 1	0
81	r	1	Total Zn 1 1	0
81	t	1	Total Zn 1 1	0
81	u	1	Total Zn 1 1	0
81	AM	1	Total Zn 1 1	0
81	AP	1	Total Zn 1 1	0

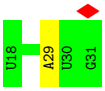
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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

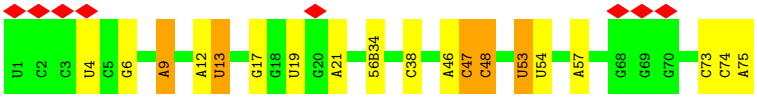
Chain A:





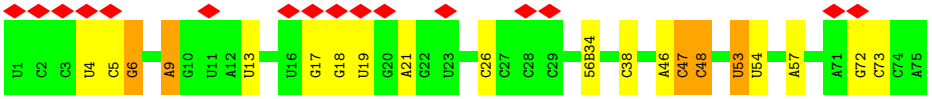
- Molecule 2: tRNA(Asp)

Chain B:



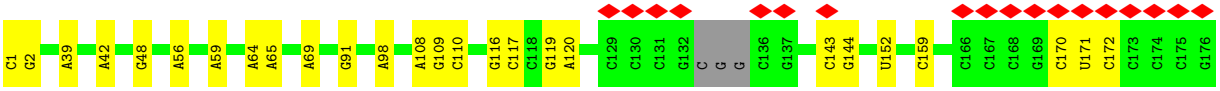
- Molecule 2: tRNA(Asp)

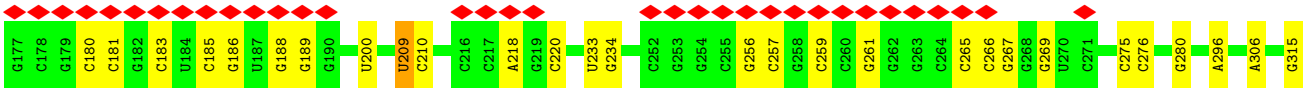
Chain C:

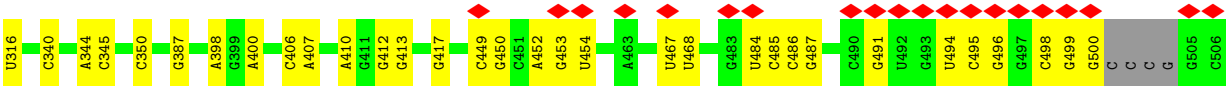


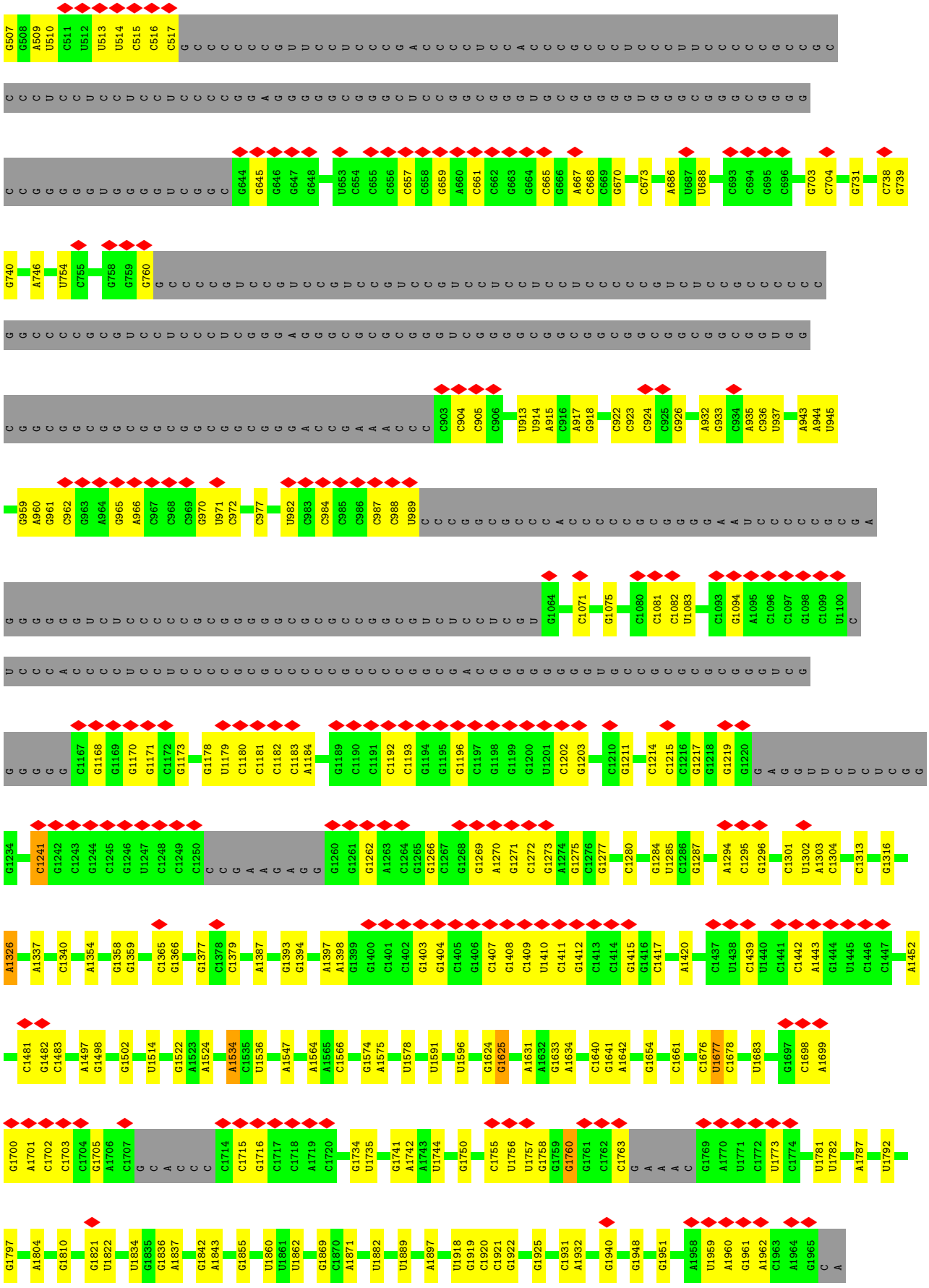
- Molecule 3: 28S ribosomal RNA

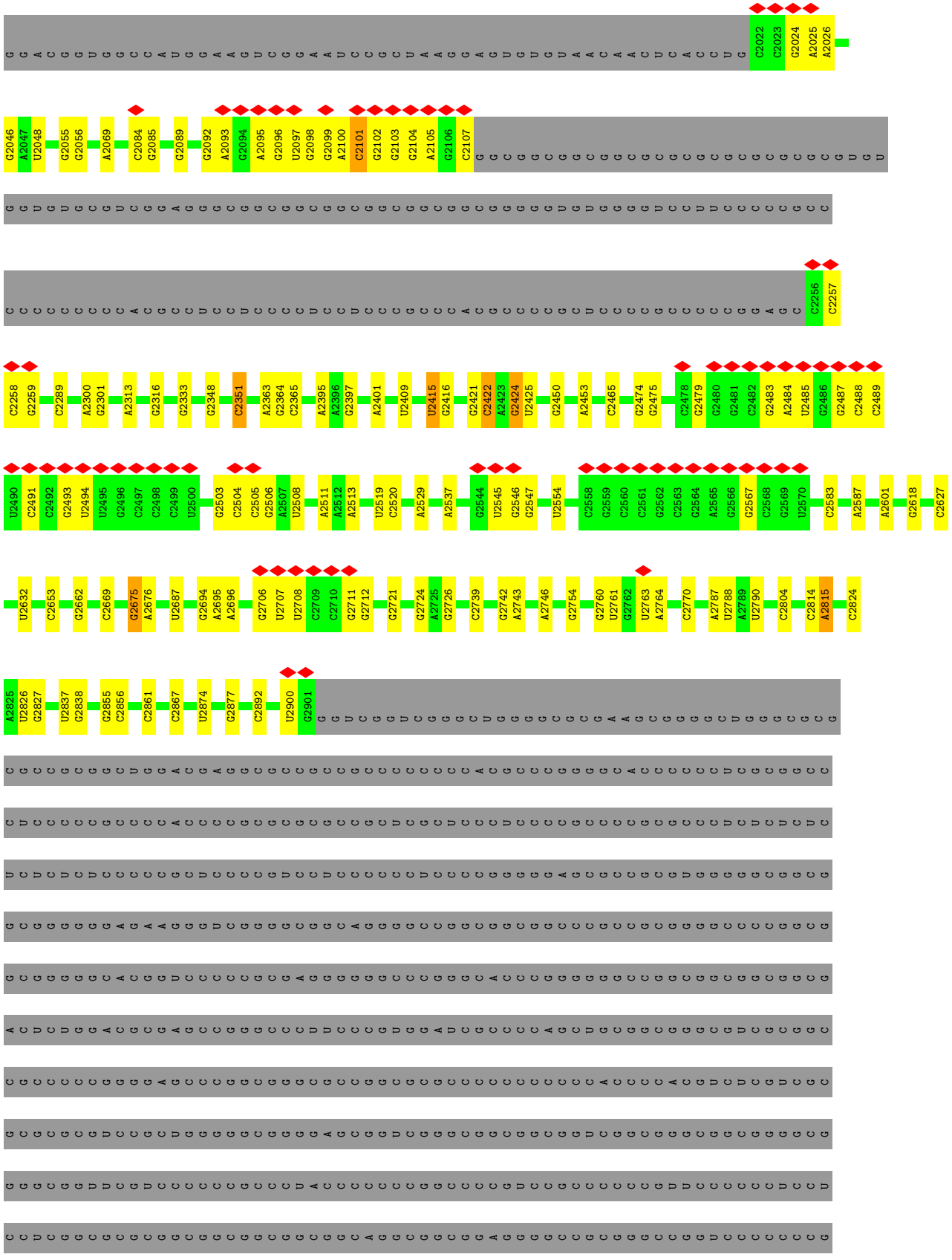
Chain D:

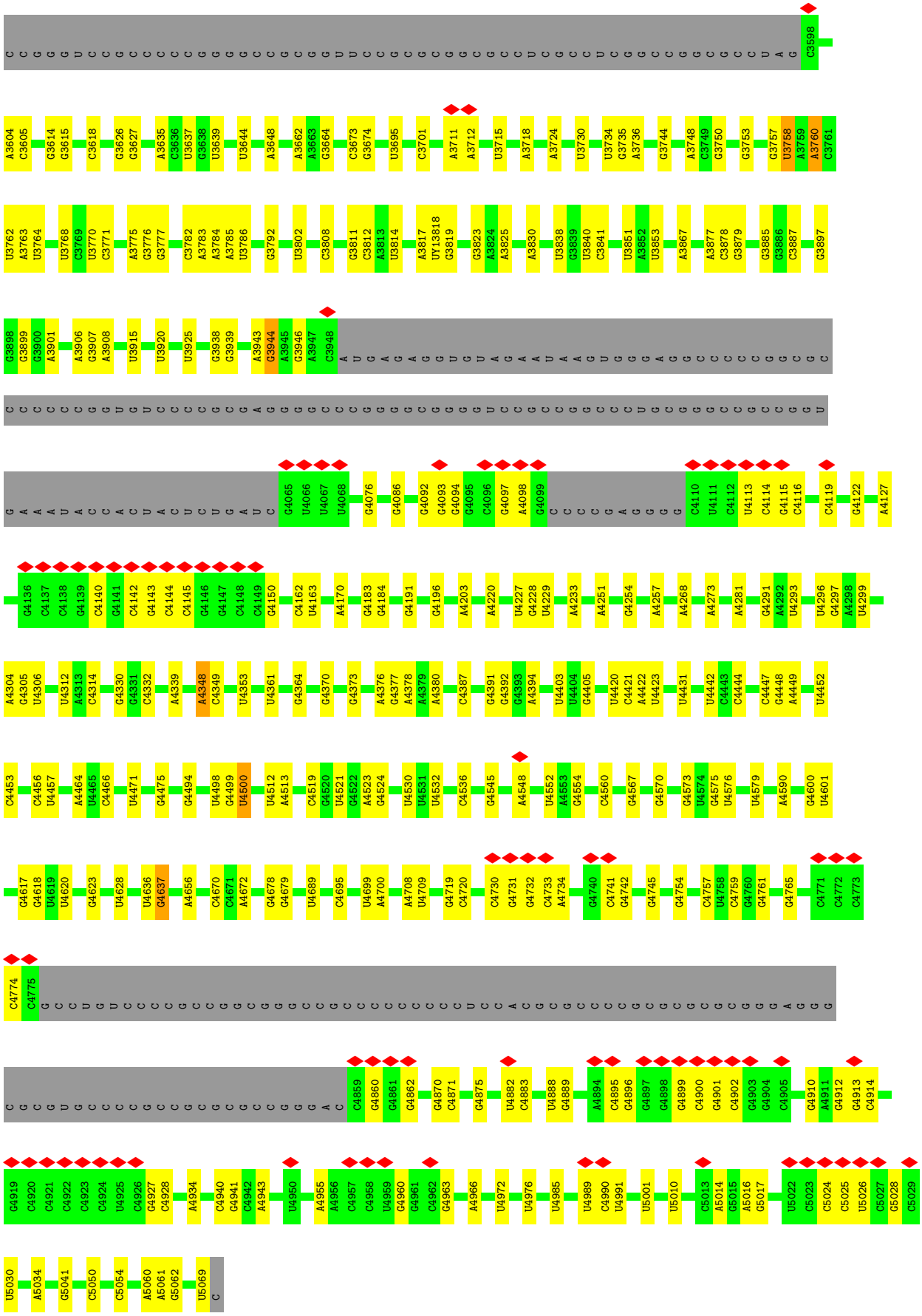






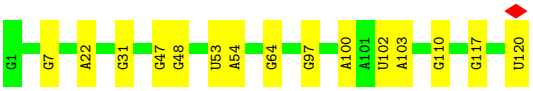






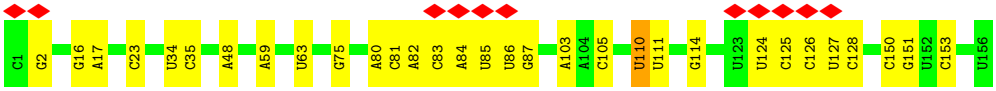
• Molecule 4: 5S ribosomal RNA

Chain E:



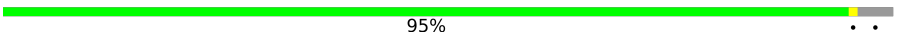
• Molecule 5: 5.8S ribosomal RNA

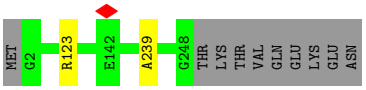
Chain F:



• Molecule 6: 60S ribosomal protein L8

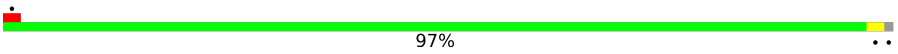
Chain G:

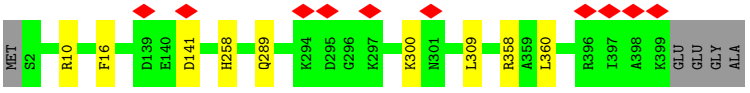




• Molecule 7: 60S ribosomal protein L3

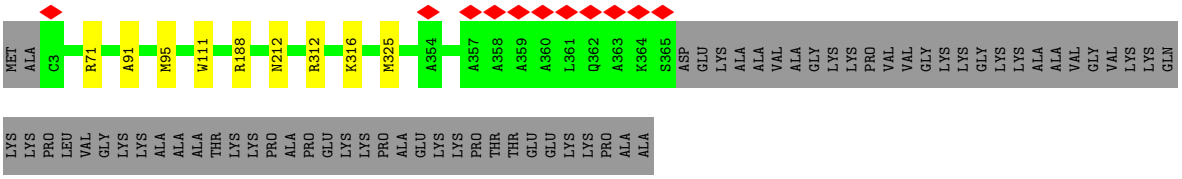
Chain H:





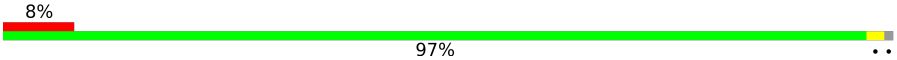
• Molecule 8: 60S ribosomal protein L4

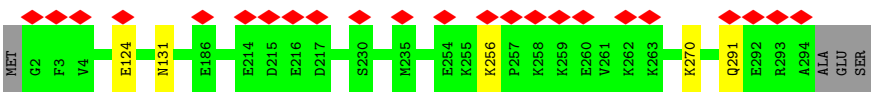
Chain I:



• Molecule 9: 60S ribosomal protein L5

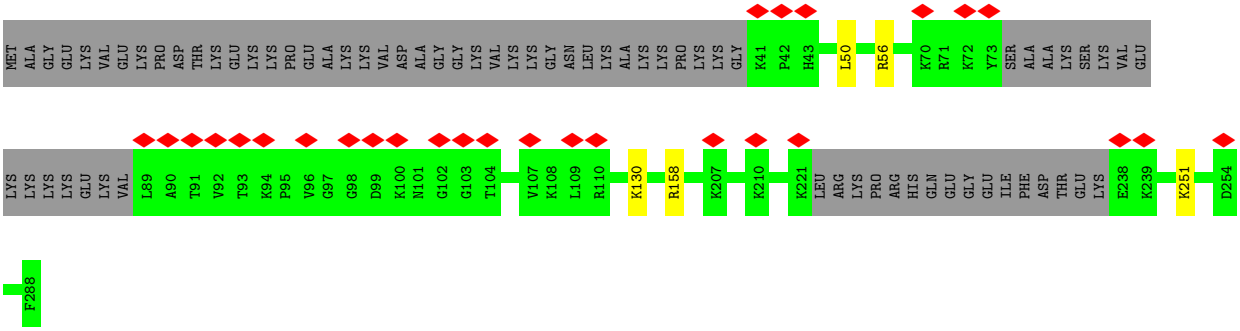
Chain J:



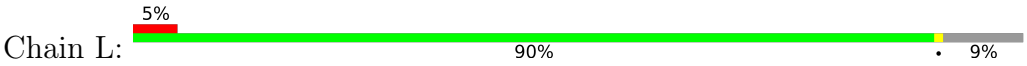


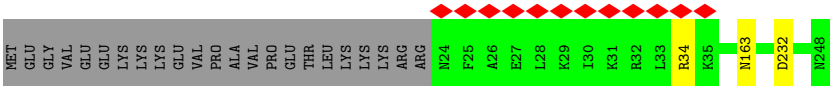
• Molecule 10: 60S ribosomal protein L6

Chain K:

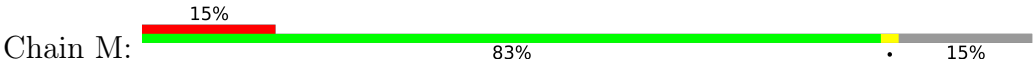


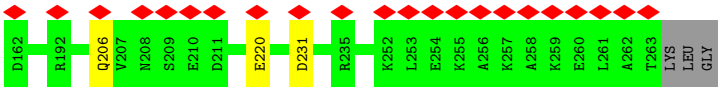
• Molecule 11: 60S ribosomal protein L7



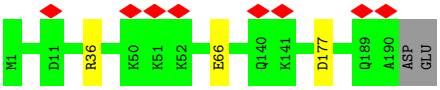


• Molecule 12: 60S ribosomal protein L7a

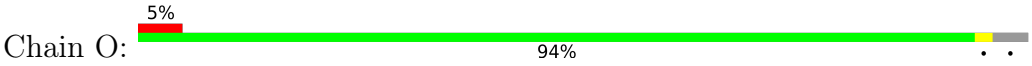


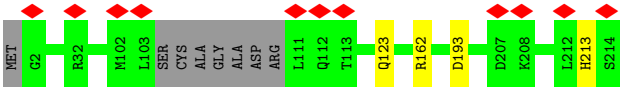


• Molecule 13: 60S ribosomal protein L9

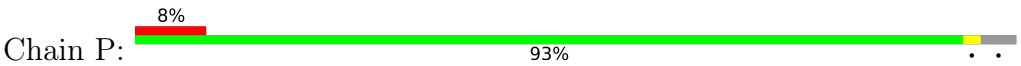


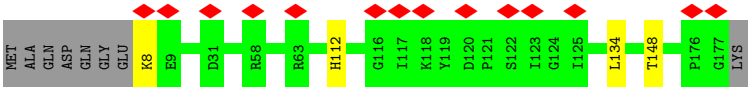
• Molecule 14: 60S ribosomal protein L10-like



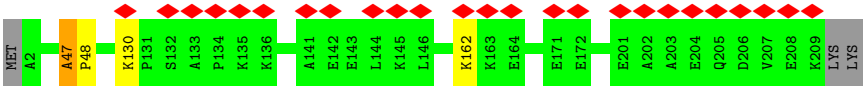


• Molecule 15: 60S ribosomal protein L11

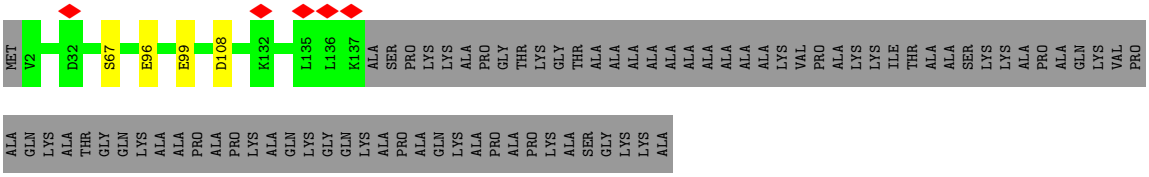




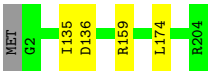
• Molecule 16: 60S ribosomal protein L13



• Molecule 17: 60S ribosomal protein L14

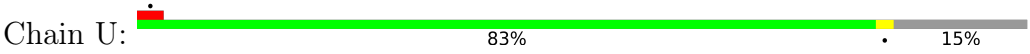


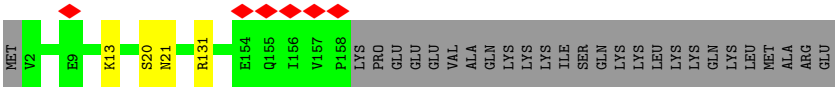
• Molecule 18: 60S ribosomal protein L15



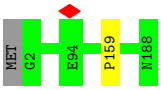
• Molecule 19: 60S ribosomal protein L13a

• Molecule 20: 60S ribosomal protein L17



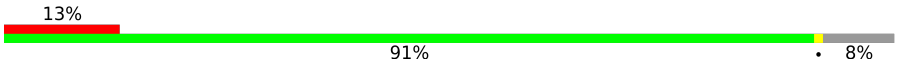


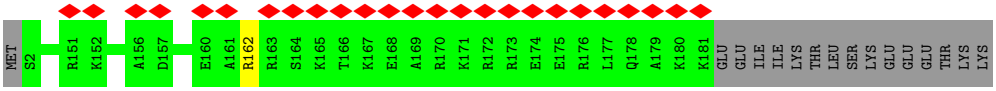
• Molecule 21: 60S ribosomal protein L18



• Molecule 22: 60S ribosomal protein L19

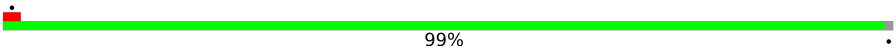
Chain W:

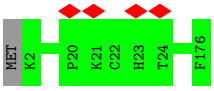




• Molecule 23: 60S ribosomal protein L18a

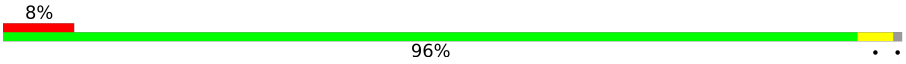
Chain X:

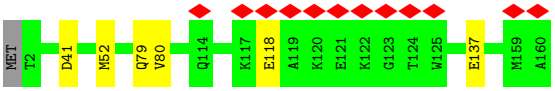




• Molecule 24: 60S ribosomal protein L21

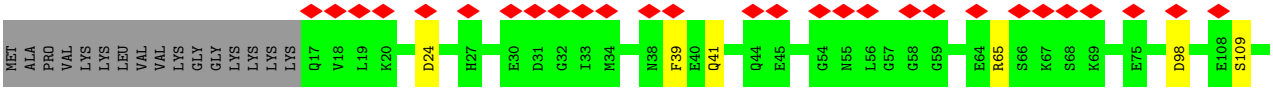
Chain Y:

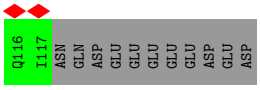




• Molecule 25: 60S ribosomal protein L22

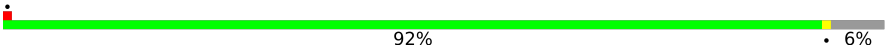
Chain Z:

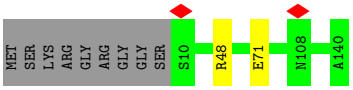




• Molecule 26: 60S ribosomal protein L23

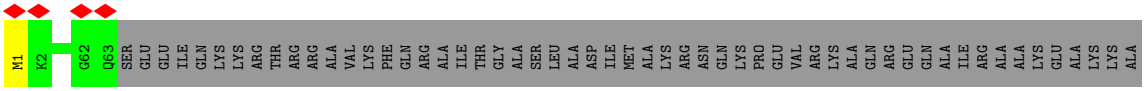
Chain a:





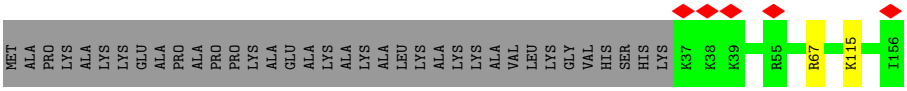
• Molecule 27: 60S ribosomal protein L24

Chain b:



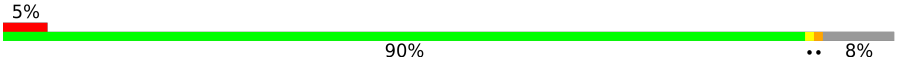
• Molecule 28: 60S ribosomal protein L23a

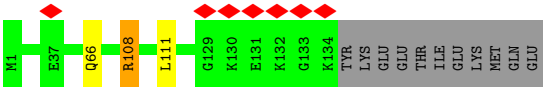
Chain c:



• Molecule 29: 60S ribosomal protein L26

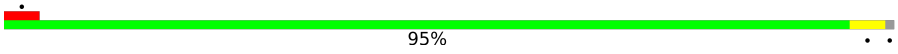
Chain d:

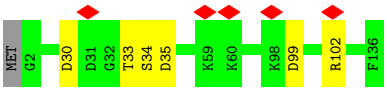




• Molecule 30: 60S ribosomal protein L27

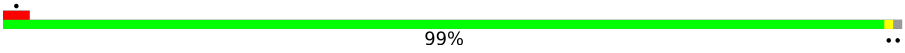
Chain e:

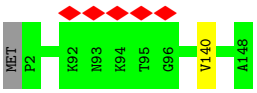




• Molecule 31: 60S ribosomal protein L27a

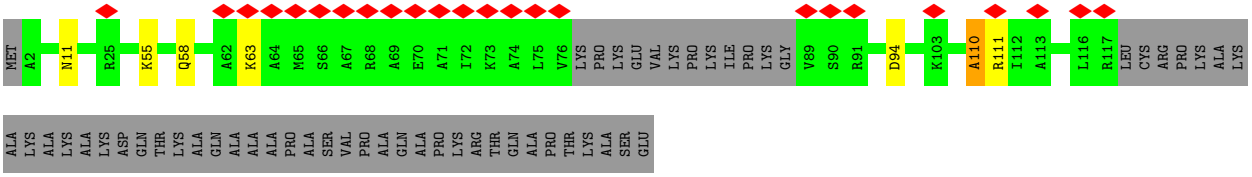
Chain f:





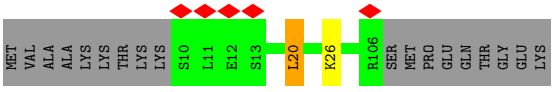
• Molecule 32: 60S ribosomal protein L29

Chain g:



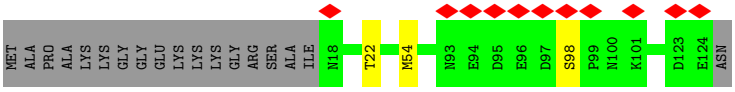
• Molecule 33: 60S ribosomal protein L30

Chain h:



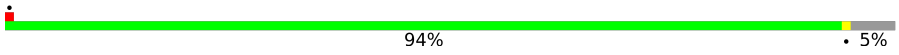
• Molecule 34: 60S ribosomal protein L31

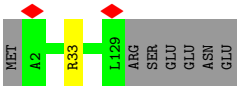
Chain i:



• Molecule 35: 60S ribosomal protein L32

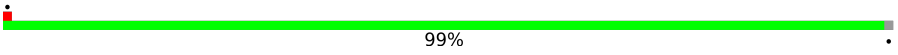
Chain j:





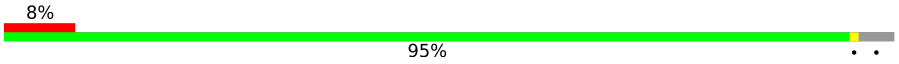
• Molecule 36: 60S ribosomal protein L35a

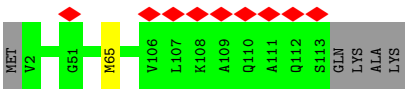
Chain k:



• Molecule 37: 60S ribosomal protein L34

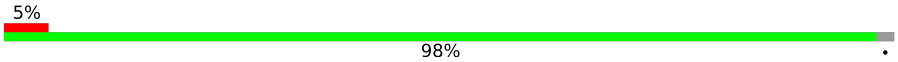
Chain l:

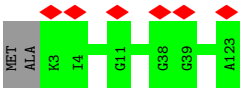




• Molecule 38: 60S ribosomal protein L35

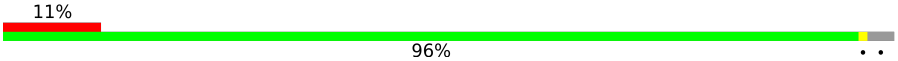
Chain m:

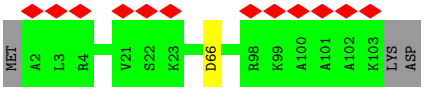




• Molecule 39: 60S ribosomal protein L36

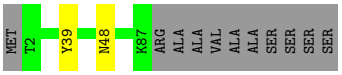
Chain n:





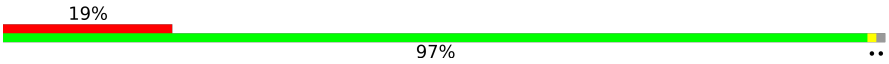
• Molecule 40: 60S ribosomal protein L37

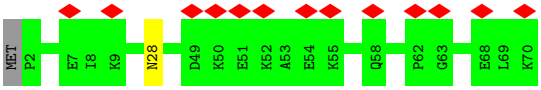
Chain o:



• Molecule 41: 60S ribosomal protein L38

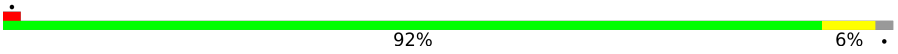
Chain p:

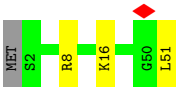




• Molecule 42: 60S ribosomal protein L39

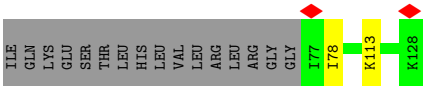
Chain q:





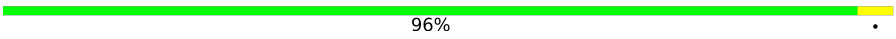
• Molecule 43: Ubiquitin-60S ribosomal protein L40

Chain r:



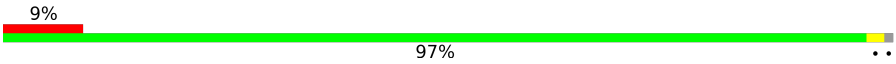
• Molecule 44: 60S ribosomal protein L41

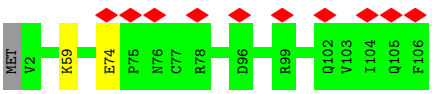
Chain s:



• Molecule 45: 60S ribosomal protein L36a

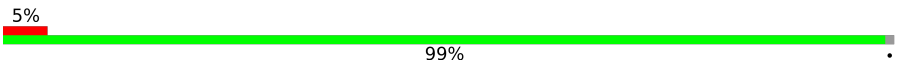
Chain t:

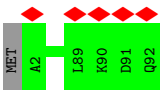




• Molecule 46: 60S ribosomal protein L37a

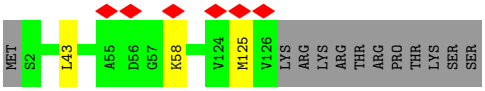
Chain u:





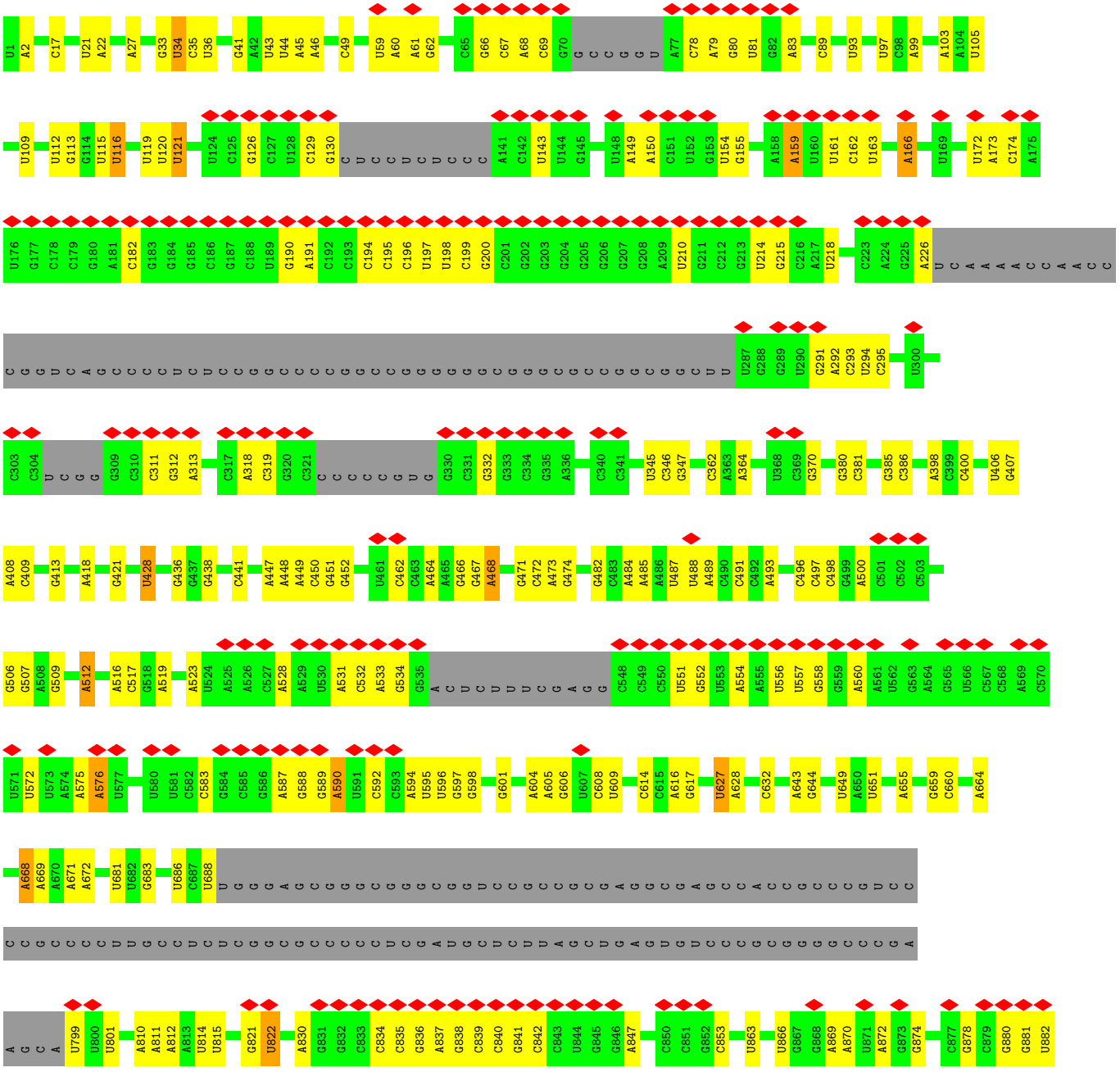
• Molecule 47: 60S ribosomal protein L28

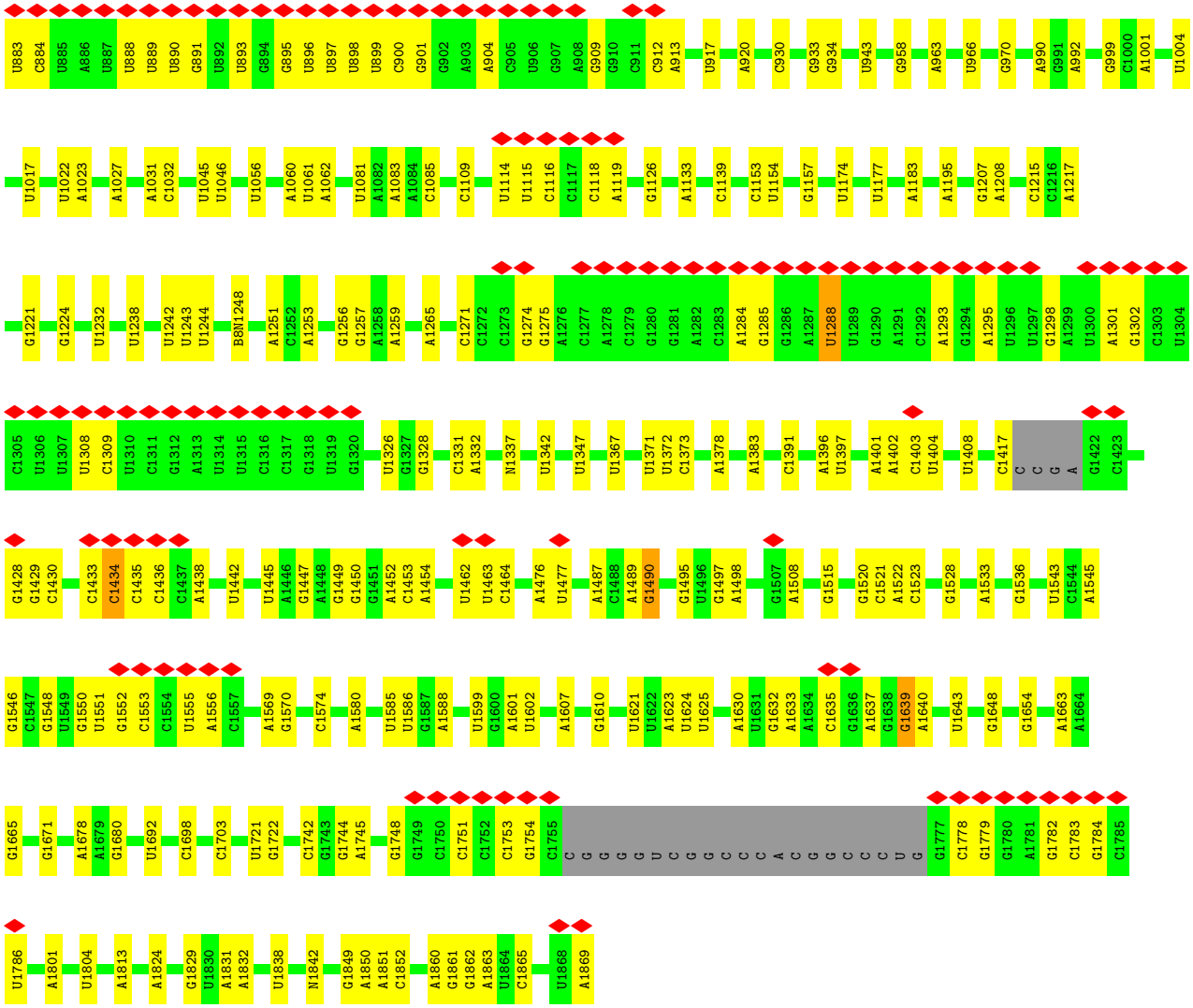
Chain v:



• Molecule 48: 18S ribosomal RNA

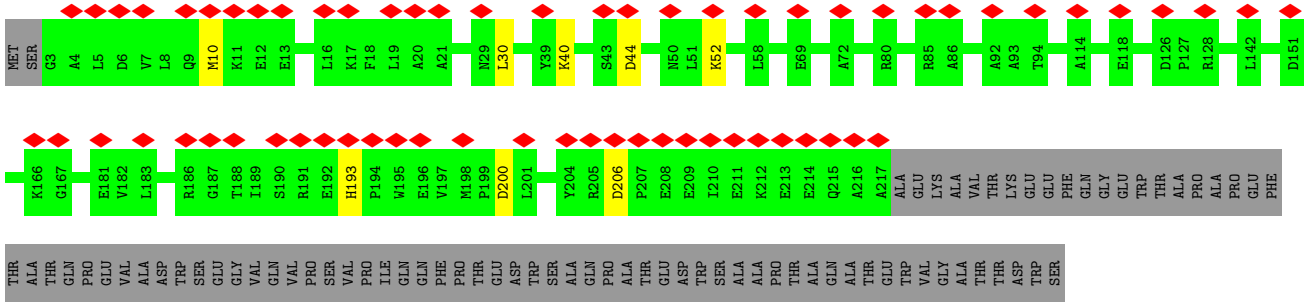
Chain w:





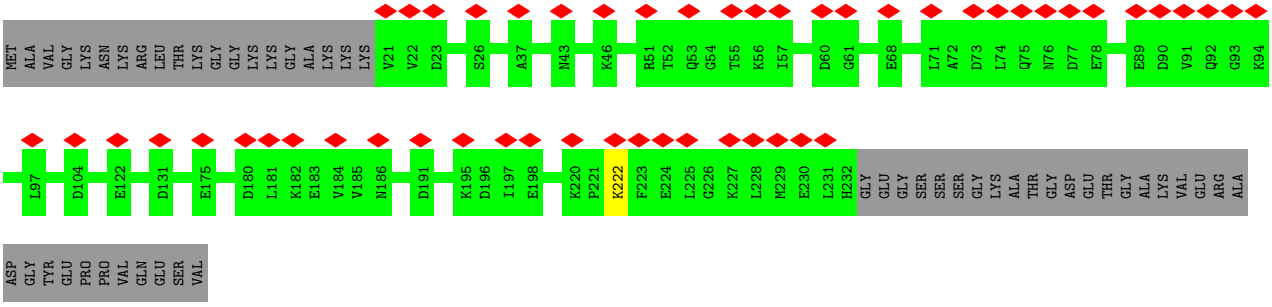
• Molecule 49: 40S ribosomal protein SA

Chain x:



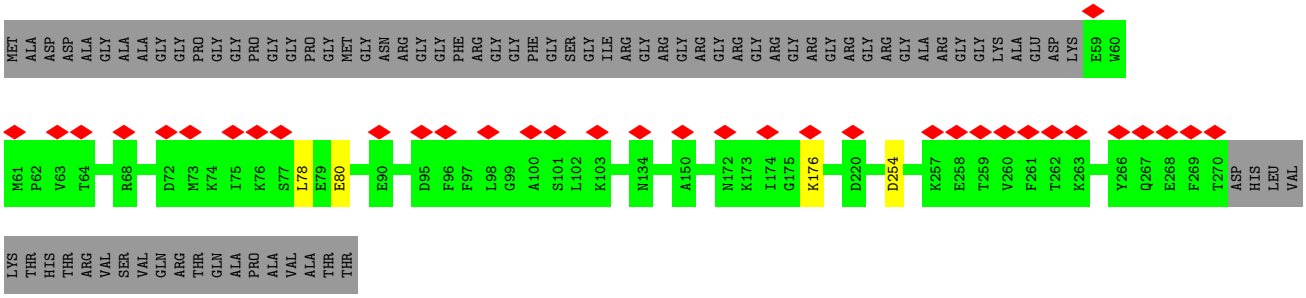
• Molecule 50: 40S ribosomal protein S3a

Chain y:



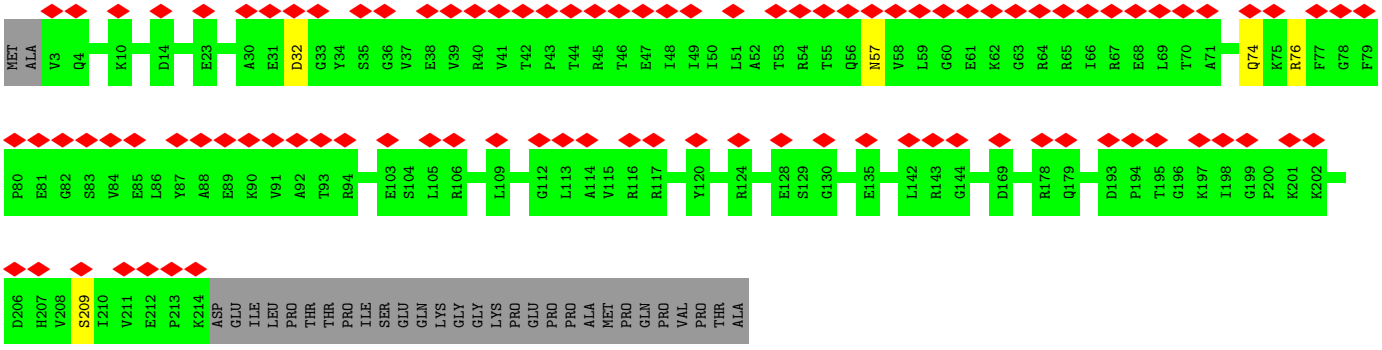
• Molecule 51: 40S ribosomal protein S2

Chain z:



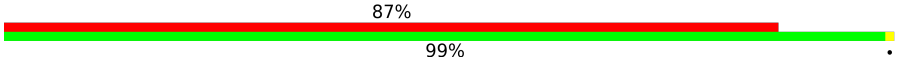
• Molecule 52: 40S ribosomal protein S3

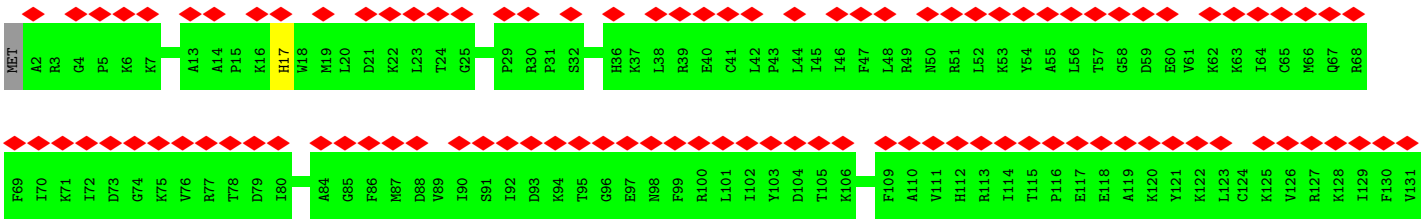
Chain 0:

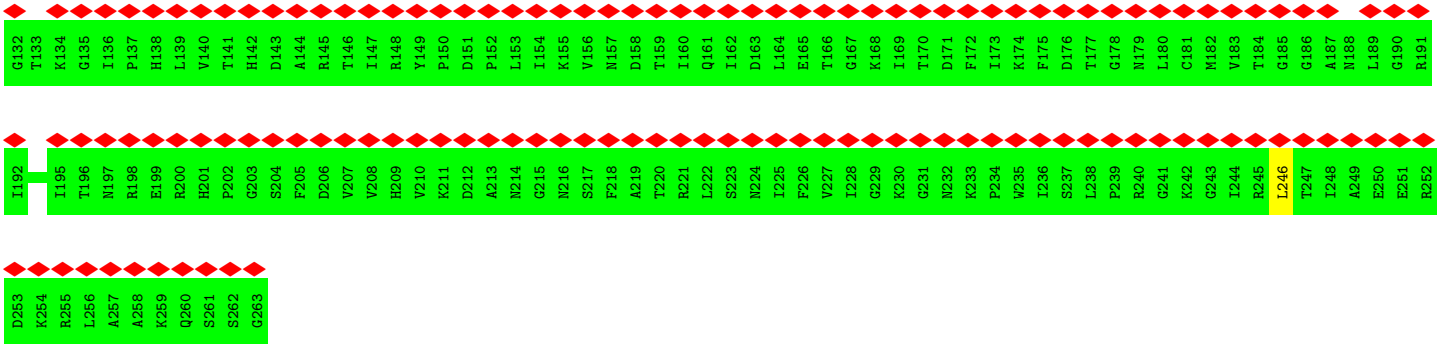


• Molecule 53: 40S ribosomal protein S4, X isoform

Chain 1:

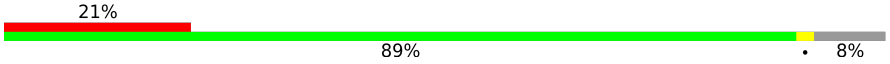


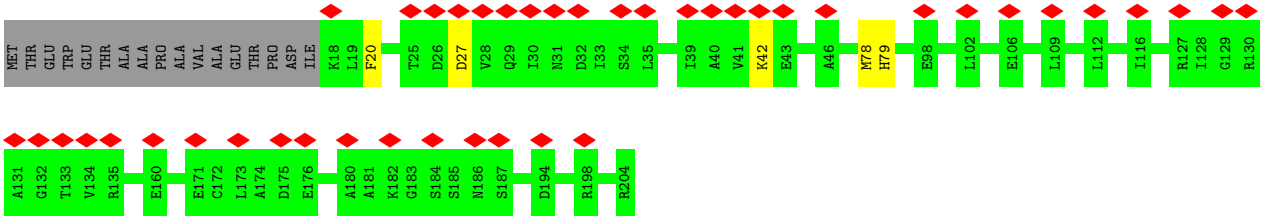




• Molecule 54: 40S ribosomal protein S5

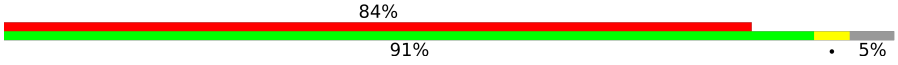
Chain 2:

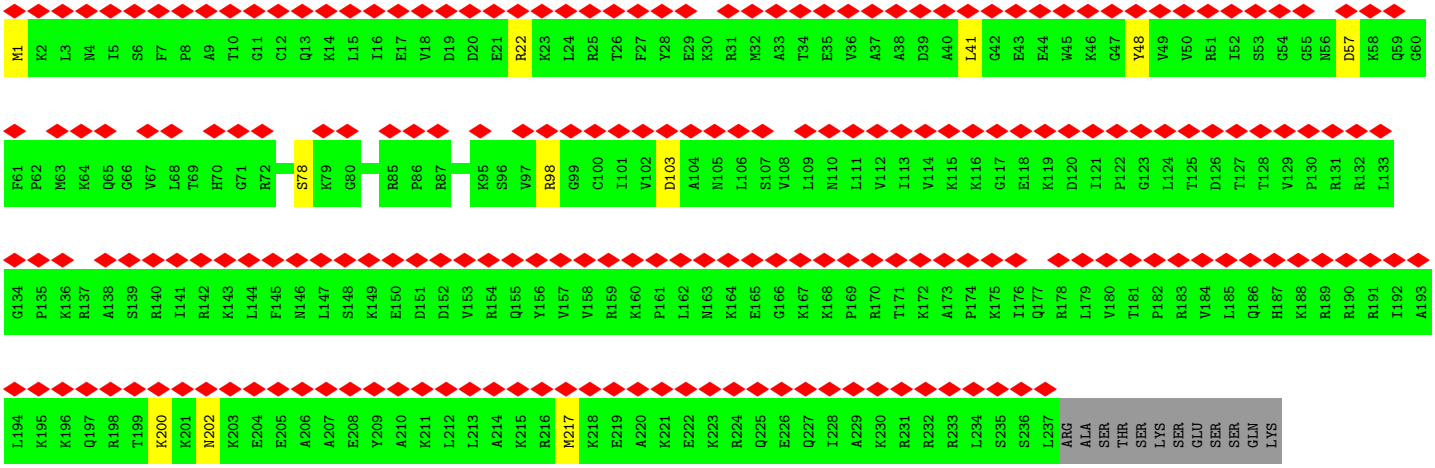




• Molecule 55: 40S ribosomal protein S6

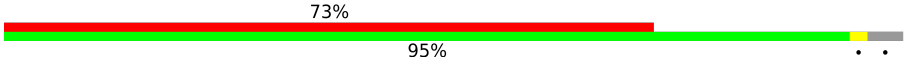
Chain 3:

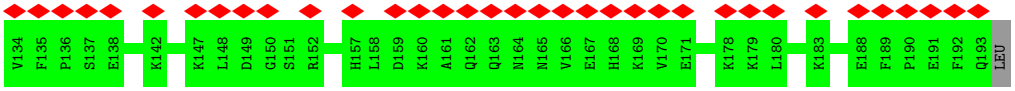




• Molecule 56: 40S ribosomal protein S7

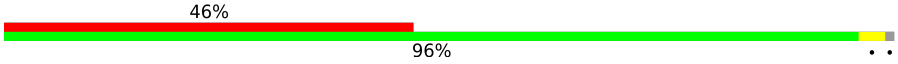
Chain 4:

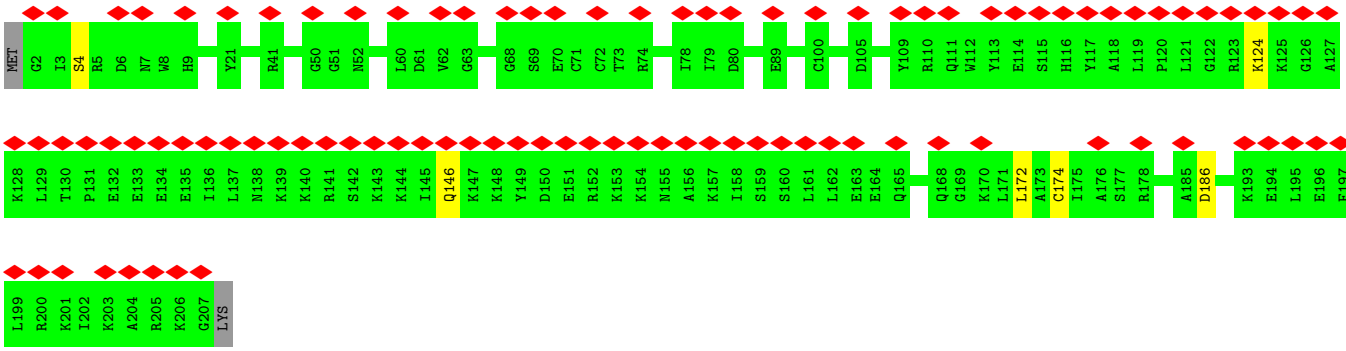




• Molecule 57: 40S ribosomal protein S8

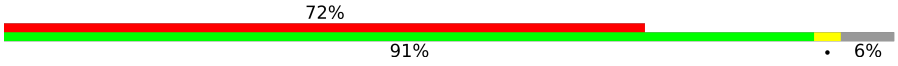
Chain 5:

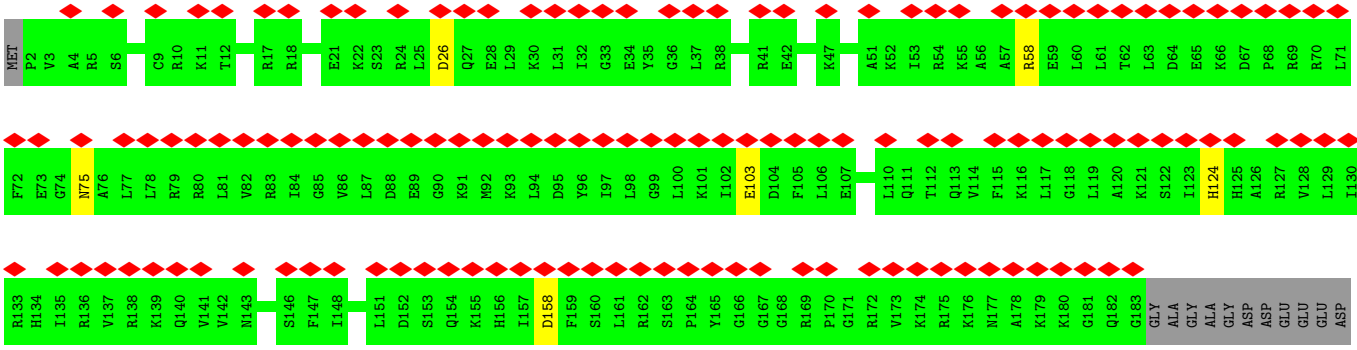




• Molecule 58: 40S ribosomal protein S9

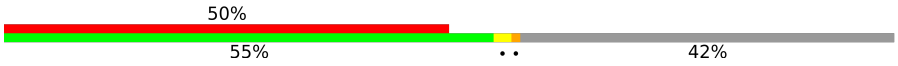
Chain 6:

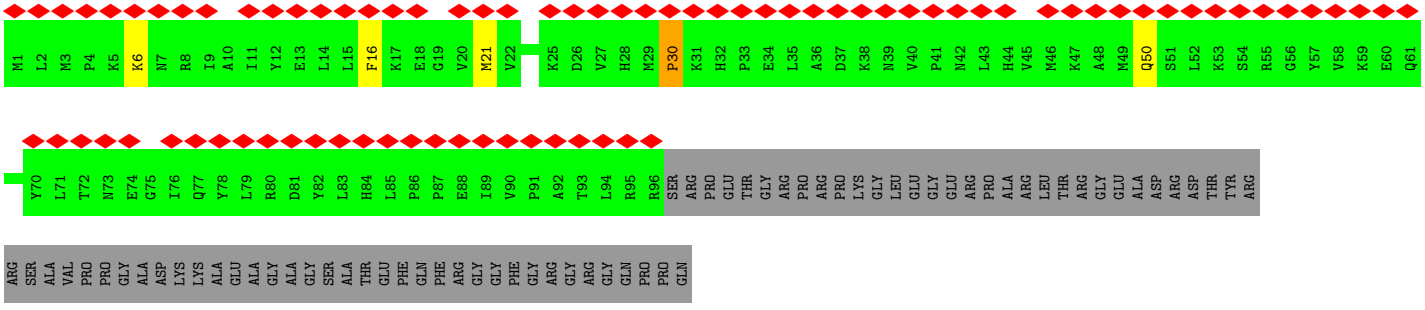




• Molecule 59: 40S ribosomal protein S10

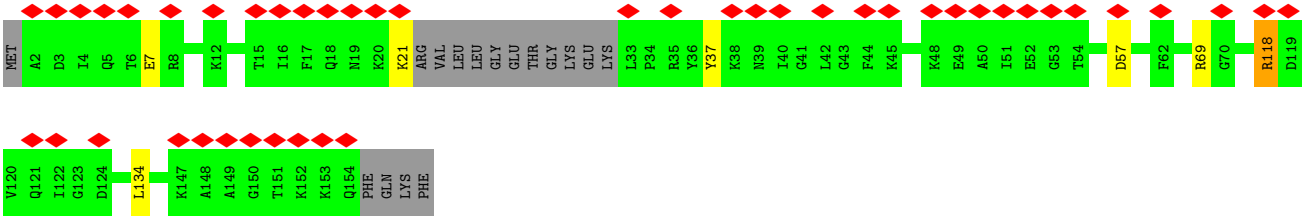
Chain 7:



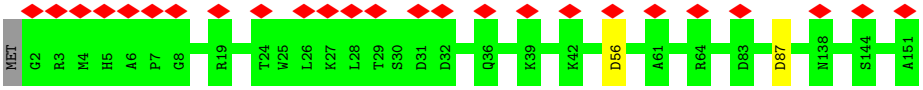


• Molecule 60: 40S ribosomal protein S11

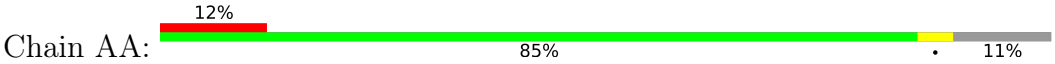
Chain 8:

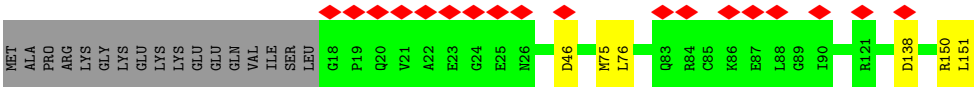


• Molecule 61: 40S ribosomal protein S13

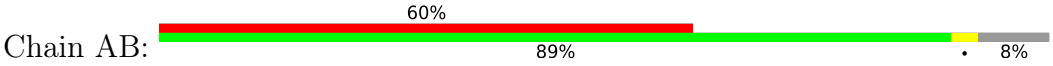


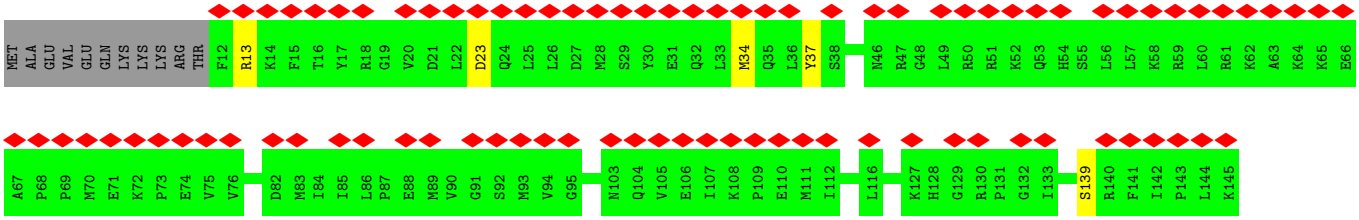
• Molecule 62: 40S ribosomal protein S14



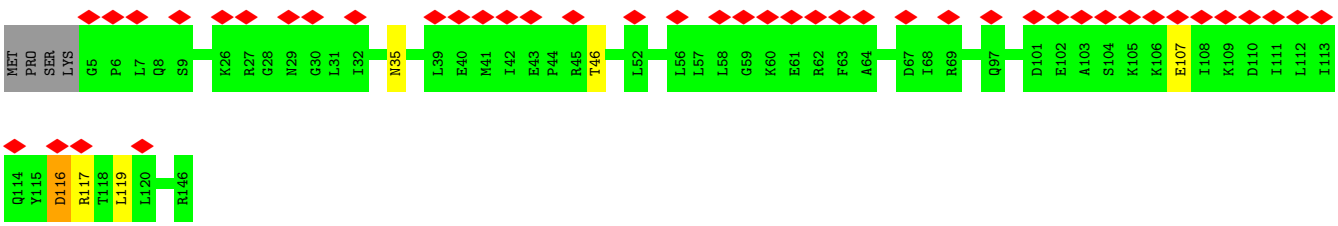


• Molecule 63: 40S ribosomal protein S15

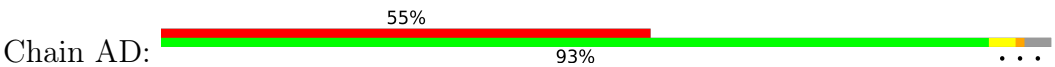


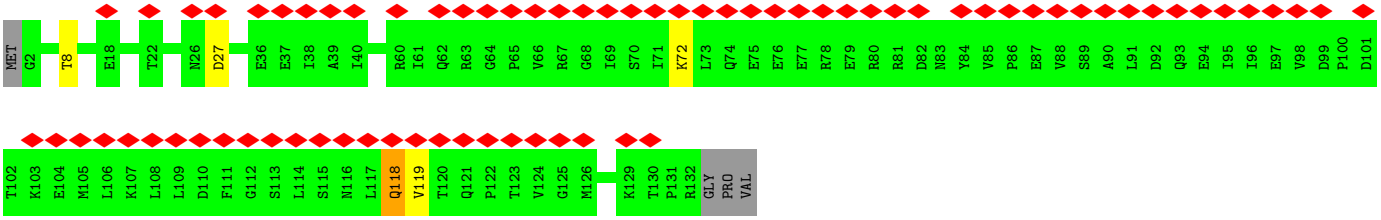


• Molecule 64: 40S ribosomal protein S16

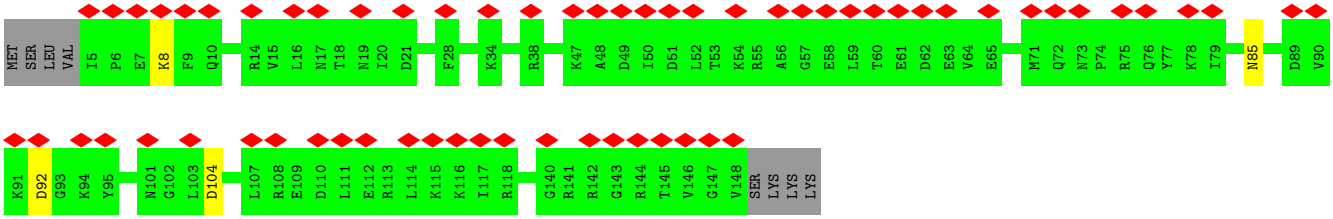


• Molecule 65: 40S ribosomal protein S17

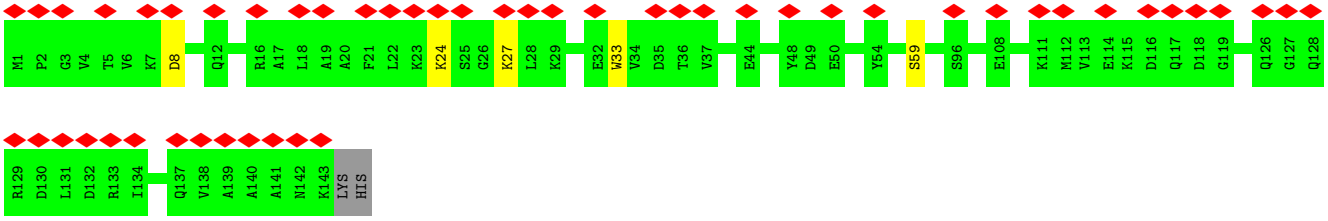




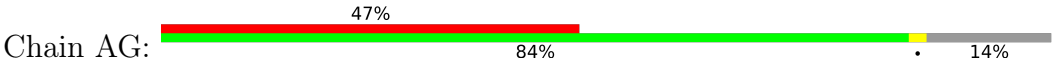
• Molecule 66: 40S ribosomal protein S18

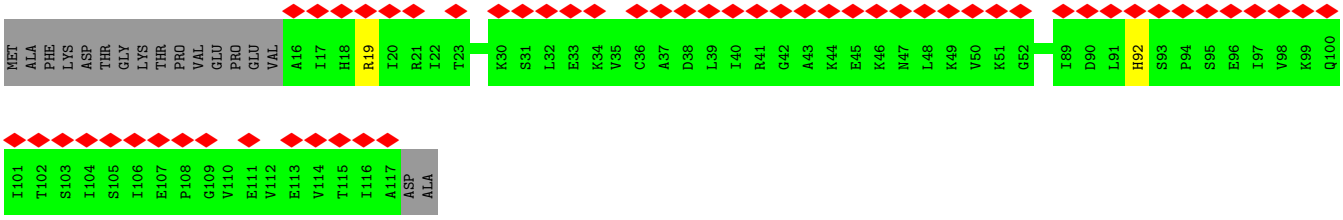


• Molecule 67: 40S ribosomal protein S19

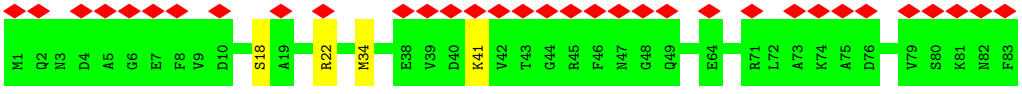


• Molecule 68: 40S ribosomal protein S20



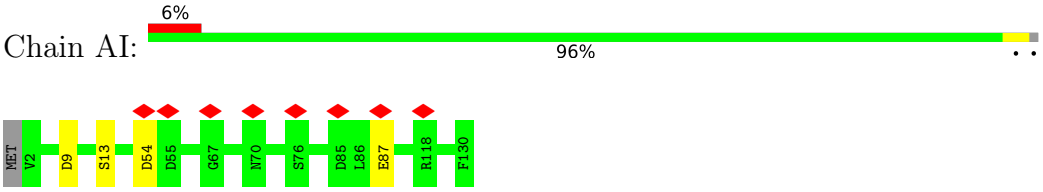


• Molecule 69: 40S ribosomal protein S21



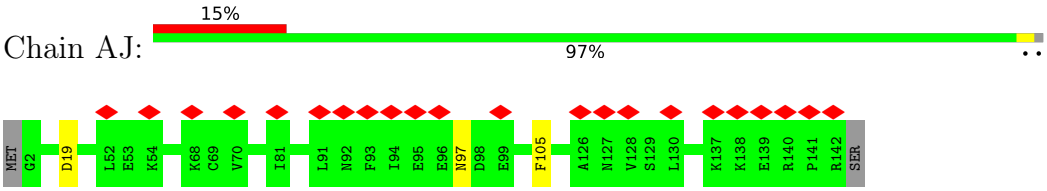
• Molecule 70: 40S ribosomal protein S15a

Chain AI:



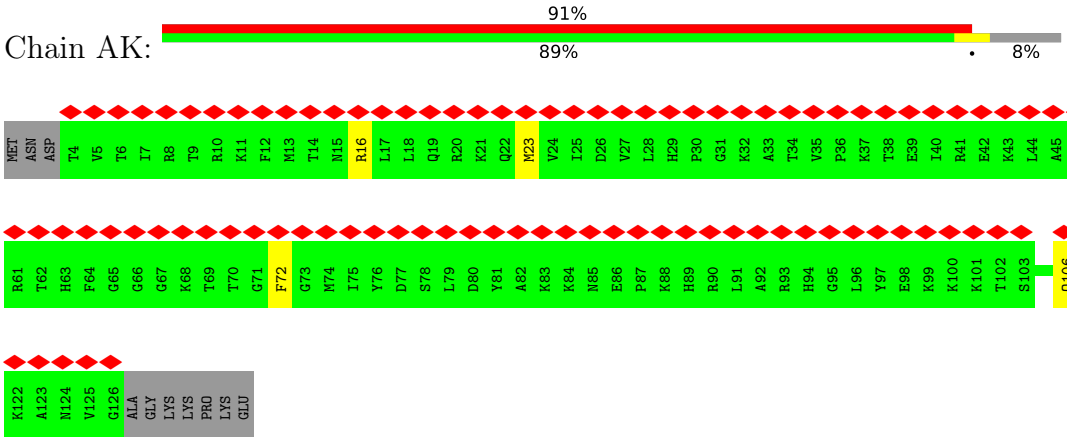
• Molecule 71: 40S ribosomal protein S23

Chain AJ:



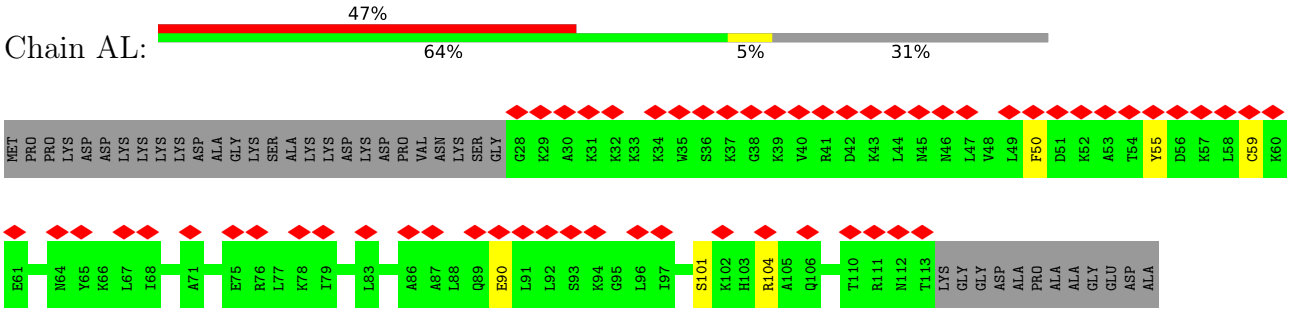
• Molecule 72: 40S ribosomal protein S24

Chain AK:



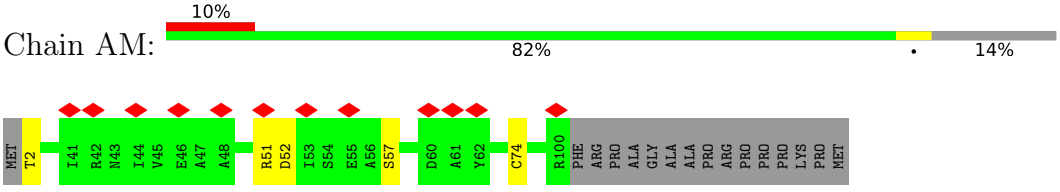
• Molecule 73: 40S ribosomal protein S25

Chain AL:



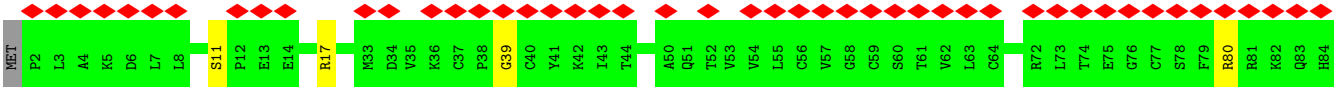
• Molecule 74: 40S ribosomal protein S26

Chain AM:

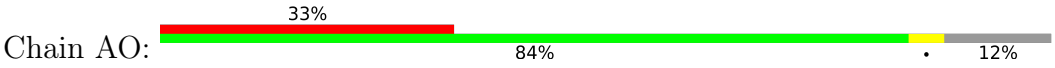


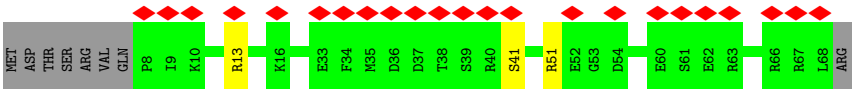
• Molecule 75: 40S ribosomal protein S27

Chain AN:

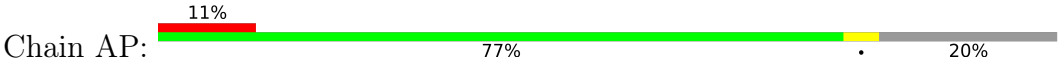


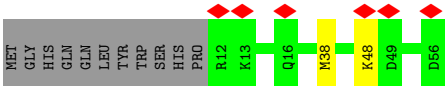
• Molecule 76: 40S ribosomal protein S28



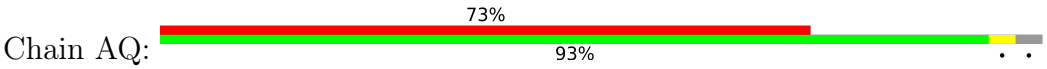


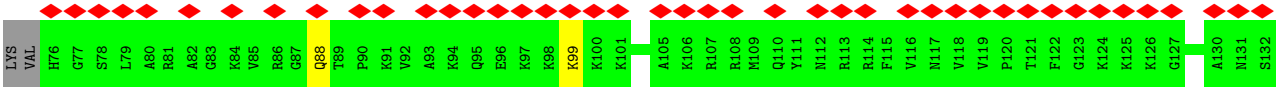
• Molecule 77: 40S ribosomal protein S29



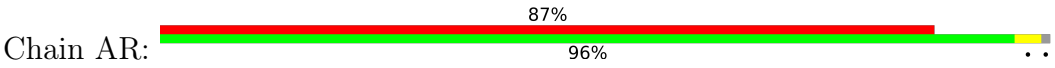


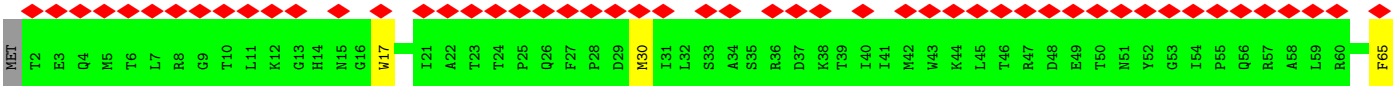
• Molecule 78: 40S ribosomal protein S30

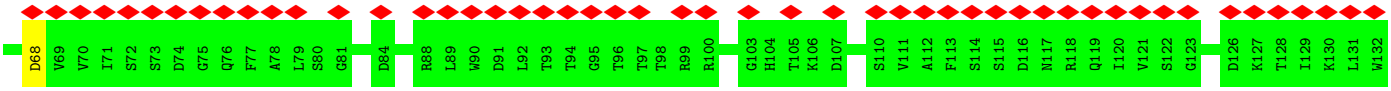


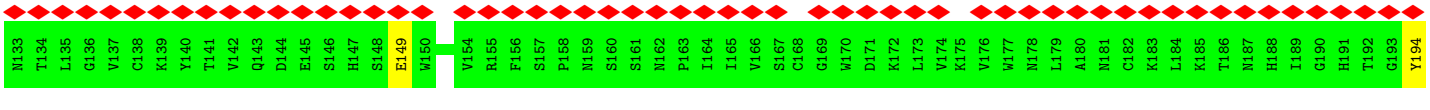


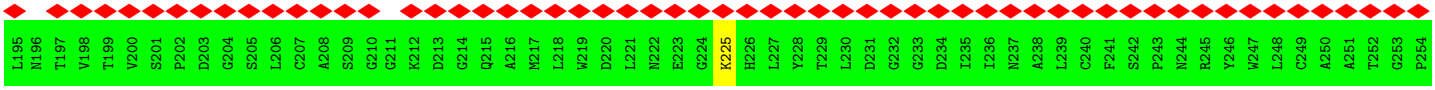
• Molecule 79: Receptor of activated protein C kinase 1

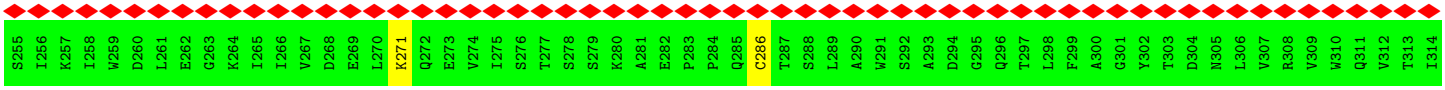












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	128240	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	0.163	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0204	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: UR3, G7M, OMC, 5MC, 5MU, 1MA, 56B, PSU, ZN, 4AC, MA6, A2M, OMG, 2MG, UY1, 6MZ, H2U, OMU, MG, B8N

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.43	0/339	0.68	0/527
2	B	0.40	0/1525	0.70	0/2375
2	C	0.30	0/1525	0.72	0/2375
3	D	0.65	0/81567	0.75	17/127232 (0.0%)
4	E	0.66	0/2858	0.71	0/4455
5	F	0.63	0/3675	0.75	4/5725 (0.1%)
6	G	0.38	0/1929	0.52	0/2586
7	H	0.37	0/3279	0.53	2/4388 (0.0%)
8	I	0.35	0/2938	0.50	1/3946 (0.0%)
9	J	0.36	0/2425	0.45	0/3248
10	K	0.32	0/1785	0.49	0/2394
11	L	0.37	0/1905	0.46	0/2539
12	M	0.33	0/1863	0.51	2/2510 (0.1%)
13	N	0.33	0/1537	0.49	0/2066
14	O	0.36	0/1699	0.50	1/2270 (0.0%)
15	P	0.31	0/1385	0.49	0/1852
16	Q	0.34	0/1713	0.47	0/2293
17	R	0.34	0/1142	0.47	0/1527
18	S	0.39	0/1746	0.48	1/2338 (0.0%)
19	T	0.38	0/1673	0.45	0/2238
20	U	0.38	0/1300	0.48	0/1746
21	V	0.38	0/1537	0.52	0/2052
22	W	0.32	0/1524	0.48	0/2013
23	X	0.38	0/1493	0.45	0/2003
24	Y	0.38	0/1326	0.49	0/1770
25	Z	0.31	0/835	0.50	0/1122
26	a	0.37	0/993	0.49	0/1332
27	b	0.36	0/541	0.42	0/720
28	c	0.33	0/998	0.50	0/1340
29	d	0.36	0/1132	0.48	0/1504
30	e	0.37	0/1130	0.48	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.37	0/1191	0.49	0/1591
32	g	0.30	0/844	0.46	0/1115
33	h	0.35	0/765	0.51	1/1027 (0.1%)
34	i	0.35	0/903	0.47	0/1216
35	j	0.38	0/1071	0.45	0/1429
36	k	0.40	0/895	0.55	0/1198
37	l	0.36	0/898	0.46	0/1197
38	m	0.32	0/1018	0.42	0/1344
39	n	0.30	0/843	0.43	0/1115
40	o	0.38	0/720	0.49	0/952
41	p	0.33	0/575	0.46	0/761
42	q	0.33	0/454	0.42	0/599
43	r	0.34	0/435	0.50	1/575 (0.2%)
44	s	0.31	0/240	0.36	0/305
45	t	0.37	0/876	0.50	0/1156
46	u	0.38	0/718	0.47	0/953
47	v	0.37	0/1017	0.50	0/1364
48	w	0.43	0/37158	0.75	13/57908 (0.0%)
49	x	0.28	0/1732	0.49	1/2355 (0.0%)
50	y	0.28	0/1752	0.48	0/2345
51	z	0.31	0/1668	0.49	0/2254
52	0	0.28	0/1672	0.47	0/2250
53	1	0.25	0/2112	0.46	0/2842
54	2	0.28	0/1485	0.47	0/1998
55	3	0.26	0/1940	0.50	0/2583
56	4	0.27	0/1533	0.52	0/2053
57	5	0.26	0/1703	0.48	1/2275 (0.0%)
58	6	0.25	0/1531	0.44	0/2045
59	7	0.32	0/834	0.64	2/1125 (0.2%)
60	8	0.30	0/1170	0.51	0/1568
61	9	0.27	0/1232	0.47	0/1656
62	AA	0.30	0/1015	0.53	1/1361 (0.1%)
63	AB	0.29	0/1126	0.50	0/1505
64	AC	0.31	0/1146	0.54	1/1534 (0.1%)
65	AD	0.27	0/1071	0.50	0/1438
66	AE	0.31	0/1187	0.58	0/1593
67	AF	0.29	0/1130	0.49	0/1515
68	AG	0.26	0/809	0.50	0/1087
69	AH	0.30	0/643	0.57	0/860
70	AI	0.29	0/1051	0.47	0/1406
71	AJ	0.27	0/1116	0.46	0/1490
72	AK	0.26	0/1019	0.54	0/1355
73	AL	0.26	0/688	0.50	0/921

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
74	AM	0.33	0/805	0.46	0/1079
75	AN	0.28	0/657	0.52	0/883
76	AO	0.28	0/481	0.61	0/643
77	AP	0.35	0/375	0.55	0/492
78	AQ	0.28	0/458	0.48	0/602
79	AR	0.26	0/2493	0.54	2/3394 (0.1%)
All	All	0.50	0/219572	0.66	51/322305 (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	1
9	J	0	1
10	K	0	1
11	L	0	1
16	Q	0	1
20	U	0	1
21	V	0	1
24	Y	0	1
29	d	0	1
32	g	0	1
40	o	0	1
54	2	0	1
65	AD	0	1
79	AR	0	1
All	All	0	18

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2101	C	O5'-P-OP1	-27.25	78.00	110.70
3	D	2101	C	OP1-P-OP2	-26.57	79.75	119.60
3	D	2101	C	O5'-P-OP2	16.09	130.01	110.70
3	D	2100	A	OP2-P-O3'	-15.46	71.19	105.20
3	D	2100	A	OP1-P-O3'	14.11	136.24	105.20

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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	245/257 (95%)	227 (93%)	18 (7%)	0	100	100
7	H	396/403 (98%)	375 (95%)	21 (5%)	0	100	100
8	I	361/427 (84%)	338 (94%)	23 (6%)	0	100	100
9	J	291/297 (98%)	271 (93%)	20 (7%)	0	100	100
10	K	211/288 (73%)	189 (90%)	22 (10%)	0	100	100
11	L	223/248 (90%)	212 (95%)	11 (5%)	0	100	100
12	M	223/266 (84%)	208 (93%)	14 (6%)	1 (0%)	34	54
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%)	158 (94%)	10 (6%)	0	100	100
16	Q	206/211 (98%)	192 (93%)	12 (6%)	2 (1%)	15	28
17	R	134/215 (62%)	120 (90%)	14 (10%)	0	100	100
18	S	201/204 (98%)	196 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	T	198/203 (98%)	195 (98%)	3 (2%)	0	100	100
20	U	155/184 (84%)	144 (93%)	11 (7%)	0	100	100
21	V	185/188 (98%)	173 (94%)	12 (6%)	0	100	100
22	W	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
23	X	173/176 (98%)	159 (92%)	14 (8%)	0	100	100
24	Y	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
25	Z	99/128 (77%)	93 (94%)	6 (6%)	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%)	111 (94%)	7 (6%)	0	100	100
29	d	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
30	e	133/136 (98%)	126 (95%)	6 (4%)	1 (1%)	19	35
31	f	145/148 (98%)	131 (90%)	14 (10%)	0	100	100
32	g	100/159 (63%)	90 (90%)	8 (8%)	2 (2%)	7	12
33	h	95/115 (83%)	91 (96%)	4 (4%)	0	100	100
34	i	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
35	j	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
36	k	107/110 (97%)	99 (92%)	8 (8%)	0	100	100
37	l	110/117 (94%)	106 (96%)	4 (4%)	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%)	5 (6%)	0	100	100
41	p	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
42	q	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	r	50/128 (39%)	49 (98%)	1 (2%)	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%)	84 (94%)	5 (6%)	0	100	100
47	v	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
49	x	213/295 (72%)	200 (94%)	13 (6%)	0	100	100
50	y	210/264 (80%)	193 (92%)	17 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	z	210/293 (72%)	200 (95%)	9 (4%)	1 (0%)	29 48
52	0	210/243 (86%)	188 (90%)	22 (10%)	0	100 100
53	1	260/263 (99%)	245 (94%)	15 (6%)	0	100 100
54	2	185/204 (91%)	166 (90%)	19 (10%)	0	100 100
55	3	235/249 (94%)	226 (96%)	9 (4%)	0	100 100
56	4	185/194 (95%)	168 (91%)	17 (9%)	0	100 100
57	5	204/208 (98%)	192 (94%)	12 (6%)	0	100 100
58	6	180/194 (93%)	171 (95%)	9 (5%)	0	100 100
59	7	94/165 (57%)	86 (92%)	7 (7%)	1 (1%)	14 26
60	8	138/158 (87%)	126 (91%)	11 (8%)	1 (1%)	22 39
61	9	148/151 (98%)	142 (96%)	6 (4%)	0	100 100
62	AA	132/151 (87%)	123 (93%)	9 (7%)	0	100 100
63	AB	132/145 (91%)	126 (96%)	6 (4%)	0	100 100
64	AC	140/146 (96%)	124 (89%)	15 (11%)	1 (1%)	22 39
65	AD	129/135 (96%)	107 (83%)	20 (16%)	2 (2%)	9 17
66	AE	142/152 (93%)	128 (90%)	14 (10%)	0	100 100
67	AF	141/145 (97%)	132 (94%)	9 (6%)	0	100 100
68	AG	100/119 (84%)	92 (92%)	8 (8%)	0	100 100
69	AH	81/83 (98%)	72 (89%)	9 (11%)	0	100 100
70	AI	127/130 (98%)	119 (94%)	8 (6%)	0	100 100
71	AJ	139/143 (97%)	135 (97%)	4 (3%)	0	100 100
72	AK	121/133 (91%)	118 (98%)	3 (2%)	0	100 100
73	AL	84/125 (67%)	74 (88%)	10 (12%)	0	100 100
74	AM	97/115 (84%)	91 (94%)	6 (6%)	0	100 100
75	AN	81/84 (96%)	71 (88%)	9 (11%)	1 (1%)	13 24
76	AO	59/69 (86%)	53 (90%)	6 (10%)	0	100 100
77	AP	43/56 (77%)	42 (98%)	1 (2%)	0	100 100
78	AQ	55/59 (93%)	50 (91%)	5 (9%)	0	100 100
79	AR	311/317 (98%)	261 (84%)	50 (16%)	0	100 100
All	All	10947/12400 (88%)	10208 (93%)	726 (7%)	13 (0%)	54 73

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	48	PRO
32	g	111	ARG
64	AC	119	LEU
51	z	78	LEU
65	AD	119	VAL

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%)	341 (99%)	5 (1%)	67	86
8	I	301/348 (86%)	294 (98%)	7 (2%)	50	76
9	J	245/250 (98%)	241 (98%)	4 (2%)	62	84
10	K	193/252 (77%)	189 (98%)	4 (2%)	53	78
11	L	194/215 (90%)	192 (99%)	2 (1%)	76	90
12	M	195/223 (87%)	192 (98%)	3 (2%)	65	85
13	N	169/171 (99%)	166 (98%)	3 (2%)	59	81
14	O	174/181 (96%)	171 (98%)	3 (2%)	60	82
15	P	143/149 (96%)	139 (97%)	4 (3%)	43	70
16	Q	174/177 (98%)	172 (99%)	2 (1%)	73	89
17	R	116/161 (72%)	112 (97%)	4 (3%)	37	63
18	S	171/172 (99%)	168 (98%)	3 (2%)	59	81
19	T	172/174 (99%)	167 (97%)	5 (3%)	42	69
20	U	138/163 (85%)	135 (98%)	3 (2%)	52	77
21	V	164/165 (99%)	164 (100%)	0	100	100
22	W	159/175 (91%)	158 (99%)	1 (1%)	86	95
23	X	156/157 (99%)	156 (100%)	0	100	100
24	Y	139/140 (99%)	134 (96%)	5 (4%)	35	61
25	Z	90/115 (78%)	84 (93%)	6 (7%)	16	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	a	101/107 (94%)	99 (98%)	2 (2%)	55 79
27	b	55/126 (44%)	54 (98%)	1 (2%)	59 81
28	c	107/133 (80%)	105 (98%)	2 (2%)	57 80
29	d	124/135 (92%)	121 (98%)	3 (2%)	49 74
30	e	117/118 (99%)	112 (96%)	5 (4%)	29 53
31	f	120/121 (99%)	119 (99%)	1 (1%)	81 93
32	g	81/126 (64%)	76 (94%)	5 (6%)	18 35
33	h	82/97 (84%)	80 (98%)	2 (2%)	49 74
34	i	98/110 (89%)	95 (97%)	3 (3%)	40 67
35	j	114/121 (94%)	113 (99%)	1 (1%)	78 92
36	k	88/89 (99%)	88 (100%)	0	100 100
37	l	96/100 (96%)	95 (99%)	1 (1%)	76 90
38	m	109/110 (99%)	109 (100%)	0	100 100
39	n	86/89 (97%)	85 (99%)	1 (1%)	71 88
40	o	73/80 (91%)	72 (99%)	1 (1%)	67 86
41	p	64/65 (98%)	63 (98%)	1 (2%)	62 84
42	q	47/48 (98%)	44 (94%)	3 (6%)	17 33
43	r	48/116 (41%)	47 (98%)	1 (2%)	53 78
44	s	24/24 (100%)	23 (96%)	1 (4%)	30 54
45	t	93/94 (99%)	91 (98%)	2 (2%)	52 77
46	u	74/75 (99%)	74 (100%)	0	100 100
47	v	109/121 (90%)	106 (97%)	3 (3%)	43 70
49	x	178/243 (73%)	171 (96%)	7 (4%)	32 57
50	y	194/231 (84%)	193 (100%)	1 (0%)	88 96
51	z	176/225 (78%)	173 (98%)	3 (2%)	60 82
52	0	175/202 (87%)	170 (97%)	5 (3%)	42 69
53	1	223/225 (99%)	221 (99%)	2 (1%)	78 92
54	2	154/170 (91%)	150 (97%)	4 (3%)	46 72
55	3	206/218 (94%)	195 (95%)	11 (5%)	22 43
56	4	168/174 (97%)	165 (98%)	3 (2%)	59 81
57	5	175/180 (97%)	170 (97%)	5 (3%)	42 69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
58	6	160/168 (95%)	154 (96%)	6 (4%)	33 58
59	7	87/136 (64%)	83 (95%)	4 (5%)	27 50
60	8	125/142 (88%)	118 (94%)	7 (6%)	21 40
61	9	130/131 (99%)	128 (98%)	2 (2%)	65 85
62	AA	104/119 (87%)	99 (95%)	5 (5%)	25 48
63	AB	120/130 (92%)	115 (96%)	5 (4%)	30 54
64	AC	117/121 (97%)	112 (96%)	5 (4%)	29 53
65	AD	117/122 (96%)	114 (97%)	3 (3%)	46 72
66	AE	119/132 (90%)	115 (97%)	4 (3%)	37 63
67	AF	113/115 (98%)	108 (96%)	5 (4%)	28 52
68	AG	89/107 (83%)	87 (98%)	2 (2%)	52 77
69	AH	67/67 (100%)	63 (94%)	4 (6%)	19 37
70	AI	112/113 (99%)	108 (96%)	4 (4%)	35 61
71	AJ	113/115 (98%)	110 (97%)	3 (3%)	44 71
72	AK	106/115 (92%)	101 (95%)	5 (5%)	26 49
73	AL	73/103 (71%)	67 (92%)	6 (8%)	11 22
74	AM	86/98 (88%)	81 (94%)	5 (6%)	20 38
75	AN	73/76 (96%)	70 (96%)	3 (4%)	30 55
76	AO	54/62 (87%)	51 (94%)	3 (6%)	21 40
77	AP	39/49 (80%)	37 (95%)	2 (5%)	24 45
78	AQ	46/48 (96%)	44 (96%)	2 (4%)	29 53
79	AR	272/275 (99%)	265 (97%)	7 (3%)	46 72
All	All	9509/10553 (90%)	9273 (98%)	236 (2%)	50 73

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	0	57	ASN
75	AN	80	ARG
57	5	186	ASP
75	AN	11	SER
70	AI	87	GLU

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

Mol	Chain	Res	Type
75	AN	83	GLN
78	AQ	88	GLN
79	AR	143	GLN
79	AR	117	ASN
55	3	110	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	13/14 (92%)	1 (7%)	0
2	B	73/75 (97%)	13 (17%)	0
2	C	73/75 (97%)	12 (16%)	2 (2%)
3	D	3494/5070 (68%)	621 (17%)	26 (0%)
4	E	119/120 (99%)	15 (12%)	0
48	w	1618/1869 (86%)	388 (23%)	0
5	F	155/156 (99%)	28 (18%)	3 (1%)
All	All	5545/7379 (75%)	1078 (19%)	31 (0%)

5 of 1078 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	29	A
2	B	4	U
2	B	9	1MA
2	B	12	A
2	B	13	PSU

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	2102	G
3	D	5016	A
3	D	3673	C
5	F	86	U
3	D	4678	G

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

216 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	5MC	B	47	2	18,22,23	3.75	8 (44%)	26,32,35	1.05	2 (7%)
48	A2M	w	668	48,80	18,25,26	1.58	2 (11%)	18,36,39	0.95	1 (5%)
48	PSU	w	1625	48	18,21,22	1.07	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	1677	3	18,21,22	1.06	2 (11%)	22,30,33	1.75	4 (18%)
2	5MU	B	53	2	19,22,23	4.66	5 (26%)	28,32,35	3.64	8 (28%)
3	PSU	D	3762	3	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
3	6MZ	D	4220	3	18,25,26	2.01	2 (11%)	16,36,39	2.08	3 (18%)
3	OMC	D	2351	80,3	19,22,23	2.80	7 (36%)	26,31,34	0.77	0
48	PSU	w	119	48	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
3	UY1	D	3818	80,3	19,22,23	1.10	2 (10%)	22,31,34	0.92	1 (4%)
2	2MG	C	6	2	18,26,27	2.20	5 (27%)	16,38,41	1.44	3 (18%)
3	PSU	D	4972	80,3	18,21,22	1.02	1 (5%)	22,30,33	1.85	4 (18%)
3	PSU	D	4500	2,3	18,21,22	1.10	1 (5%)	22,30,33	1.84	4 (18%)
48	PSU	w	966	48	18,21,22	1.03	1 (5%)	22,30,33	1.82	5 (22%)
48	OMU	w	116	48	19,22,23	2.92	8 (42%)	26,31,34	1.70	4 (15%)
48	4AC	w	1842	48	21,24,25	0.56	0	29,34,37	1.16	4 (13%)
48	A2M	w	27	48	18,25,26	1.50	1 (5%)	18,36,39	0.98	0
48	PSU	w	1347	48	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	D	4552	3	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
2	5MC	C	48	2	18,22,23	3.79	8 (44%)	26,32,35	1.02	2 (7%)
3	PSU	D	3770	3	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4420	3	18,21,22	1.04	1 (5%)	22,30,33	1.80	5 (22%)
3	OMG	D	4228	3	18,26,27	2.73	8 (44%)	19,38,41	1.57	4 (21%)
3	PSU	D	4521	80,3	18,21,22	1.04	1 (5%)	22,30,33	1.88	5 (22%)
48	PSU	w	686	48	18,21,22	1.05	1 (5%)	22,30,33	1.82	4 (18%)
48	PSU	w	406	48	18,21,22	1.03	1 (5%)	22,30,33	1.86	5 (22%)
3	OMG	D	3944	3	18,26,27	2.81	8 (44%)	19,38,41	1.50	4 (21%)
48	B8N	w	1248	48	24,29,30	0.80	0	29,42,45	0.97	2 (6%)
3	A2M	D	3825	3	18,25,26	1.49	1 (5%)	18,36,39	1.04	1 (5%)
3	A2M	D	1326	3	18,25,26	1.45	1 (5%)	18,36,39	1.03	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PSU	D	5001	80,3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	1860	3	18,21,22	1.05	1 (5%)	22,30,33	1.86	4 (18%)
48	A2M	w	99	48,80	18,25,26	1.47	1 (5%)	18,36,39	1.02	1 (5%)
48	OMG	w	1490	48,80	18,26,27	2.76	8 (44%)	19,38,41	1.47	4 (21%)
3	OMU	D	2837	3	19,22,23	2.75	6 (31%)	26,31,34	1.85	5 (19%)
48	MA6	w	1850	48	19,26,27	1.03	1 (5%)	18,38,41	1.60	3 (16%)
3	OMC	D	4456	3	19,22,23	2.82	8 (42%)	26,31,34	0.69	0
2	H2U	C	19	2	18,21,22	1.06	2 (11%)	21,30,33	0.80	0
48	PSU	w	1045	48	18,21,22	1.04	1 (5%)	22,30,33	1.87	5 (22%)
2	1MA	C	9	2	16,25,26	0.96	1 (6%)	18,37,40	0.82	0
48	PSU	w	93	48	18,21,22	1.05	1 (5%)	22,30,33	1.78	3 (13%)
3	PSU	D	3764	3	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	OMC	D	2824	3	19,22,23	2.86	8 (42%)	26,31,34	0.72	0
3	PSU	D	4442	3	18,21,22	1.05	1 (5%)	22,30,33	1.86	6 (27%)
3	PSU	D	3851	3	18,21,22	1.03	1 (5%)	22,30,33	1.87	5 (22%)
3	OMU	D	2415	3	19,22,23	2.83	6 (31%)	26,31,34	1.94	6 (23%)
3	PSU	D	2508	3	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	D	4293	3	18,21,22	1.06	2 (11%)	22,30,33	1.83	4 (18%)
3	OMG	D	4499	2,3	18,26,27	2.74	8 (44%)	19,38,41	1.50	4 (21%)
48	PSU	w	1004	48	18,21,22	1.06	1 (5%)	22,30,33	1.82	4 (18%)
48	4AC	w	1337	48	21,24,25	0.56	0	29,34,37	1.19	5 (17%)
3	PSU	D	3730	3	18,21,22	1.02	1 (5%)	22,30,33	1.82	5 (22%)
48	PSU	w	815	48	18,21,22	1.08	1 (5%)	22,30,33	1.86	5 (22%)
48	PSU	w	1643	48,80	18,21,22	1.04	1 (5%)	22,30,33	1.81	5 (22%)
2	5MC	C	47	2	18,22,23	3.79	8 (44%)	26,32,35	1.04	2 (7%)
3	1MA	D	1322	3	16,25,26	0.87	0	18,37,40	0.88	0
3	OMG	D	4637	3	18,26,27	2.73	8 (44%)	19,38,41	1.50	4 (21%)
48	OMU	w	1326	48	19,22,23	2.88	7 (36%)	26,31,34	1.78	6 (23%)
2	H2U	B	19	2	18,21,22	1.09	2 (11%)	21,30,33	0.82	0
3	OMU	D	1773	3	19,22,23	2.92	8 (42%)	26,31,34	1.68	4 (15%)
3	OMU	D	4498	80,3	19,22,23	2.79	6 (31%)	26,31,34	1.75	5 (19%)
2	5MU	C	53	2	19,22,23	4.66	6 (31%)	28,32,35	3.61	9 (32%)
3	OMG	D	1316	3	18,26,27	2.73	8 (44%)	19,38,41	1.55	4 (21%)
3	OMG	D	1522	3	18,26,27	2.68	8 (44%)	19,38,41	1.50	4 (21%)
3	PSU	D	3920	80,3	18,21,22	1.02	1 (5%)	22,30,33	1.85	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	OMG	w	644	48	18,26,27	2.83	8 (44%)	19,38,41	1.50	4 (21%)
48	OMC	w	1703	48,80	19,22,23	2.89	8 (42%)	26,31,34	0.73	0
3	OMU	D	3925	3	19,22,23	2.78	6 (31%)	26,31,34	1.84	5 (19%)
3	PSU	D	4576	3	18,21,22	1.02	1 (5%)	22,30,33	1.84	4 (18%)
48	PSU	w	1367	48	18,21,22	1.04	1 (5%)	22,30,33	1.87	5 (22%)
3	OMU	D	4227	3	19,22,23	2.81	6 (31%)	26,31,34	1.75	4 (15%)
2	5MC	B	48	2	18,22,23	3.79	8 (44%)	26,32,35	1.03	2 (7%)
2	1MA	C	57	2	16,25,26	0.94	1 (6%)	18,37,40	0.85	0
3	A2M	D	1524	3	18,25,26	1.59	2 (11%)	18,36,39	1.00	1 (5%)
3	OMG	D	4494	3	18,26,27	2.75	8 (44%)	19,38,41	1.51	4 (21%)
48	PSU	w	822	48	18,21,22	1.08	1 (5%)	22,30,33	1.75	5 (22%)
48	PSU	w	1056	48	18,21,22	1.02	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	1792	3	18,21,22	0.99	1 (5%)	22,30,33	1.76	3 (13%)
3	OMC	D	2422	80,3	19,22,23	2.87	8 (42%)	26,31,34	0.73	0
2	2MG	B	6	2	18,26,27	2.19	5 (27%)	16,38,41	1.47	3 (18%)
48	PSU	w	218	48	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
48	OMG	w	436	48	18,26,27	2.82	8 (44%)	19,38,41	1.55	4 (21%)
3	PSU	D	4423	3	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	3758	3	18,21,22	0.97	1 (5%)	22,30,33	1.81	4 (18%)
2	5MC	C	38	2	18,22,23	3.76	8 (44%)	26,32,35	1.02	2 (7%)
48	PSU	w	681	48,80	18,21,22	1.04	1 (5%)	22,30,33	1.90	5 (22%)
3	A2M	D	3785	80,3	18,25,26	1.55	2 (11%)	18,36,39	1.23	1 (5%)
3	OMG	D	4370	3	18,26,27	2.73	8 (44%)	19,38,41	1.50	4 (21%)
3	A2M	D	400	3	18,25,26	1.52	1 (5%)	18,36,39	1.03	1 (5%)
3	5MC	D	4447	80,3	18,22,23	3.60	7 (38%)	26,32,35	1.13	1 (3%)
2	56B	B	34	2	27,35,36	3.03	13 (48%)	28,52,55	4.60	4 (14%)
3	OMC	D	2861	3	19,22,23	2.85	8 (42%)	26,31,34	0.67	0
48	OMG	w	601	48	18,26,27	2.82	8 (44%)	19,38,41	1.50	4 (21%)
3	PSU	D	3715	3	18,21,22	1.05	1 (5%)	22,30,33	1.85	5 (22%)
48	PSU	w	651	48	18,21,22	1.03	1 (5%)	22,30,33	1.87	5 (22%)
3	PSU	D	3695	3	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
48	PSU	w	105	48	18,21,22	1.04	1 (5%)	22,30,33	1.81	5 (22%)
48	A2M	w	512	48	18,25,26	1.50	1 (5%)	18,36,39	1.08	1 (5%)
48	OMU	w	1288	48	19,22,23	2.96	8 (42%)	26,31,34	1.67	4 (15%)
48	OMU	w	1442	48,80	19,22,23	2.87	6 (31%)	26,31,34	1.70	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	PSU	w	1445	48	18,21,22	1.04	1 (5%)	22,30,33	1.81	5 (22%)
3	PSU	D	1536	3	18,21,22	1.05	2 (11%)	22,30,33	1.88	4 (18%)
3	PSU	D	4457	3	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
48	6MZ	w	1832	48,80	18,25,26	1.99	3 (16%)	16,36,39	1.87	2 (12%)
3	PSU	D	4471	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	4431	3	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
48	PSU	w	801	48	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	4579	3	18,21,22	1.04	1 (5%)	22,30,33	1.83	4 (18%)
3	OMU	D	4620	3	19,22,23	2.76	6 (31%)	26,31,34	1.78	5 (19%)
2	5MC	B	38	2	18,22,23	3.71	8 (44%)	26,32,35	1.06	2 (7%)
3	OMC	D	3701	80,3	19,22,23	2.85	8 (42%)	26,31,34	0.73	0
48	OMC	w	462	48	19,22,23	3.01	8 (42%)	26,31,34	0.74	0
3	A2M	D	3760	3	18,25,26	1.46	1 (5%)	18,36,39	1.25	2 (11%)
48	PSU	w	863	48	18,21,22	1.08	1 (5%)	22,30,33	1.82	5 (22%)
48	PSU	w	572	48	18,21,22	1.09	1 (5%)	22,30,33	1.79	3 (13%)
2	PSU	C	13	2	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
48	OMG	w	1328	48	18,26,27	2.82	8 (44%)	19,38,41	1.49	4 (21%)
48	A2M	w	468	48	18,25,26	1.59	1 (5%)	18,36,39	1.02	0
2	1MA	B	9	2	16,25,26	0.93	1 (6%)	18,37,40	0.86	0
5	OMG	F	75	5	18,26,27	2.77	8 (44%)	19,38,41	1.49	4 (21%)
48	OMU	w	428	48	19,22,23	2.93	8 (42%)	26,31,34	1.71	5 (19%)
3	PSU	D	3639	3	18,21,22	1.04	1 (5%)	22,30,33	1.76	4 (18%)
48	A2M	w	484	48	18,25,26	1.55	1 (5%)	18,36,39	1.03	1 (5%)
3	PSU	D	4299	3	18,21,22	1.03	1 (5%)	22,30,33	1.84	4 (18%)
3	A2M	D	398	3	18,25,26	1.46	1 (5%)	18,36,39	1.01	1 (5%)
2	56B	C	34	2	27,35,36	3.02	12 (44%)	28,52,55	4.67	4 (14%)
48	A2M	w	1678	48	18,25,26	1.50	1 (5%)	18,36,39	0.99	1 (5%)
48	OMU	w	1804	48	19,22,23	2.86	6 (31%)	26,31,34	1.76	4 (15%)
3	OMC	D	3808	3	19,22,23	2.84	8 (42%)	26,31,34	0.76	0
3	PSU	D	1862	3	18,21,22	1.03	1 (5%)	22,30,33	1.89	5 (22%)
48	OMU	w	121	48	19,22,23	2.94	8 (42%)	26,31,34	1.65	4 (15%)
48	A2M	w	159	48	18,25,26	1.57	1 (5%)	18,36,39	1.07	1 (5%)
2	PSU	B	13	2	18,21,22	1.03	1 (5%)	22,30,33	1.86	5 (22%)
3	PSU	D	4296	3	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	4353	3	18,21,22	1.03	1 (5%)	22,30,33	1.85	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
48	OMC	w	517	48,80	19,22,23	2.99	8 (42%)	26,31,34	0.76	0
3	PSU	D	1782	3	18,21,22	1.00	1 (5%)	22,30,33	1.84	4 (18%)
3	OMG	D	3744	3	18,26,27	2.76	8 (44%)	19,38,41	1.52	4 (21%)
3	PSU	D	1683	3	18,21,22	1.07	2 (11%)	22,30,33	1.95	5 (22%)
3	OMC	D	2365	80,3	19,22,23	2.84	8 (42%)	26,31,34	0.71	0
48	OMU	w	627	48	19,22,23	2.90	7 (36%)	26,31,34	1.72	5 (19%)
48	A2M	w	166	48	18,25,26	1.50	1 (5%)	18,36,39	1.09	1 (5%)
48	OMU	w	799	48	19,22,23	2.94	8 (42%)	26,31,34	1.68	4 (15%)
3	OMG	D	1760	3	18,26,27	2.83	8 (44%)	19,38,41	1.46	4 (21%)
48	PSU	w	1232	48	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
3	A2M	D	2815	3	18,25,26	1.55	1 (5%)	18,36,39	1.00	1 (5%)
2	PSU	C	54	2	18,21,22	1.08	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	D	3792	3	18,26,27	2.70	8 (44%)	19,38,41	1.47	4 (21%)
48	PSU	w	1046	48	18,21,22	1.04	1 (5%)	22,30,33	1.83	4 (18%)
48	G7M	w	1639	48,2	20,26,27	2.71	7 (35%)	17,39,42	1.23	2 (11%)
3	PSU	D	4403	80,3	18,21,22	1.06	1 (5%)	22,30,33	1.88	5 (22%)
48	PSU	w	1081	48	18,21,22	1.01	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	5010	3	18,21,22	1.03	1 (5%)	22,30,33	1.87	5 (22%)
3	PSU	D	2632	3	18,21,22	1.02	1 (5%)	22,30,33	1.80	4 (18%)
48	A2M	w	576	48	18,25,26	1.43	1 (5%)	18,36,39	1.04	1 (5%)
3	A2M	D	3718	3	18,25,26	1.48	1 (5%)	18,36,39	1.02	1 (5%)
48	PSU	w	34	48	18,21,22	1.06	1 (5%)	22,30,33	1.69	4 (18%)
3	PSU	D	3853	80,3	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
48	PSU	w	814	48	18,21,22	1.05	1 (5%)	22,30,33	1.80	4 (18%)
3	A2M	D	4523	80,3	18,25,26	1.59	2 (11%)	18,36,39	1.12	2 (11%)
3	OMC	D	4536	3	19,22,23	2.83	8 (42%)	26,31,34	0.74	0
3	PSU	D	4689	3	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
3	OMU	D	4306	3	19,22,23	2.76	6 (31%)	26,31,34	1.78	5 (19%)
3	OMG	D	4392	3	18,26,27	2.71	8 (44%)	19,38,41	1.52	4 (21%)
3	PSU	D	1744	80,3	18,21,22	1.02	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	D	4196	80,2,3	18,26,27	2.69	8 (44%)	19,38,41	1.45	4 (21%)
3	A2M	D	2363	80,3	18,25,26	1.47	2 (11%)	18,36,39	1.02	1 (5%)
3	PSU	D	3734	3	18,21,22	1.05	1 (5%)	22,30,33	1.86	5 (22%)
2	PSU	B	54	2	18,21,22	1.04	1 (5%)	22,30,33	1.76	4 (18%)
48	OMC	w	174	48	19,22,23	3.02	8 (42%)	26,31,34	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OMG	D	4618	3	18,26,27	2.75	8 (44%)	19,38,41	1.47	4 (21%)
48	PSU	w	210	48	18,21,22	1.09	1 (5%)	22,30,33	1.80	5 (22%)
48	PSU	w	866	48	18,21,22	1.05	1 (5%)	22,30,33	1.82	4 (18%)
3	A2M	D	2787	80,3	18,25,26	1.48	1 (5%)	18,36,39	1.08	1 (5%)
3	OMG	D	3899	3	18,26,27	2.71	8 (44%)	19,38,41	1.50	4 (21%)
3	PSU	D	4312	3	18,21,22	1.02	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	D	4628	3	18,21,22	1.05	1 (5%)	22,30,33	1.87	4 (18%)
3	A2M	D	1871	80,3	18,25,26	1.55	1 (5%)	18,36,39	1.15	1 (5%)
48	A2M	w	590	48	18,25,26	1.44	1 (5%)	18,36,39	1.05	1 (5%)
3	A2M	D	3830	3	18,25,26	1.48	1 (5%)	18,36,39	1.08	0
3	A2M	D	1534	80,3	18,25,26	1.42	1 (5%)	18,36,39	1.40	3 (16%)
2	1MA	B	57	2	16,25,26	0.97	1 (6%)	18,37,40	0.81	0
3	OMC	D	3841	3	19,22,23	2.81	8 (42%)	26,31,34	0.68	0
3	PSU	D	1781	3	18,21,22	1.05	1 (5%)	22,30,33	1.80	4 (18%)
3	A2M	D	2401	3	18,25,26	1.51	1 (5%)	18,36,39	1.02	1 (5%)
48	PSU	w	1177	48	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	D	1625	80,3	18,26,27	2.78	8 (44%)	19,38,41	1.51	4 (21%)
3	OMC	D	1340	3	19,22,23	2.82	8 (42%)	26,31,34	0.69	0
3	OMC	D	2804	3	19,22,23	2.85	8 (42%)	26,31,34	0.69	0
48	OMG	w	683	48	18,26,27	2.81	8 (44%)	19,38,41	1.54	4 (21%)
3	OMC	D	3887	3	19,22,23	2.86	8 (42%)	26,31,34	0.76	0
3	5MC	D	3782	80,3	18,22,23	3.61	7 (38%)	26,32,35	1.08	2 (7%)
48	PSU	w	1238	48	18,21,22	1.05	1 (5%)	22,30,33	1.82	5 (22%)
48	A2M	w	1383	48	18,25,26	1.48	1 (5%)	18,36,39	1.21	2 (11%)
3	PSU	D	3768	3	18,21,22	1.05	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4361	3	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4532	3	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
3	OMG	D	2364	3	18,26,27	2.68	8 (44%)	19,38,41	1.50	4 (21%)
3	OMG	D	2424	3	18,26,27	2.77	8 (44%)	19,38,41	1.51	4 (21%)
3	OMG	D	4623	3	18,26,27	2.72	8 (44%)	19,38,41	1.50	4 (21%)
48	PSU	w	109	48	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)
48	OMG	w	509	48	18,26,27	2.88	8 (44%)	19,38,41	1.49	4 (21%)
48	OMU	w	172	48	19,22,23	2.94	8 (42%)	26,31,34	1.71	5 (19%)
3	PSU	D	3637	80,3	18,21,22	1.04	1 (5%)	22,30,33	1.90	4 (18%)
48	PSU	w	609	48	18,21,22	1.06	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	OMG	D	3627	3	18,26,27	2.73	8 (44%)	19,38,41	1.55	4 (21%)
3	A2M	D	3724	3	18,25,26	1.47	1 (5%)	18,36,39	1.02	1 (5%)
3	UR3	D	4530	3	19,22,23	2.63	7 (36%)	26,32,35	1.30	2 (7%)
48	PSU	w	1244	48	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
48	PSU	w	36	48	18,21,22	1.08	1 (5%)	22,30,33	1.86	5 (22%)
48	A2M	w	1031	48	18,25,26	1.50	1 (5%)	18,36,39	1.00	0
48	PSU	w	649	48	18,21,22	1.04	1 (5%)	22,30,33	1.85	5 (22%)
48	PSU	w	1692	48	18,21,22	1.00	1 (5%)	22,30,33	1.82	4 (18%)
48	MA6	w	1851	48	19,26,27	1.00	1 (5%)	18,38,41	1.78	3 (16%)
48	OMC	w	1391	48	19,22,23	2.93	8 (42%)	26,31,34	0.74	0
48	PSU	w	1174	48,80	18,21,22	1.06	1 (5%)	22,30,33	1.77	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	5MC	B	47	2	-	3/7/25/26	0/2/2/2
48	A2M	w	668	48,80	-	3/5/27/28	0/3/3/3
48	PSU	w	1625	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1677	3	-	5/7/25/26	0/2/2/2
2	5MU	B	53	2	-	2/7/25/26	0/2/2/2
3	PSU	D	3762	3	-	0/7/25/26	0/2/2/2
3	6MZ	D	4220	3	-	0/5/27/28	0/3/3/3
3	OMC	D	2351	80,3	-	1/9/27/28	0/2/2/2
48	PSU	w	119	48	-	0/7/25/26	0/2/2/2
3	UY1	D	3818	80,3	-	4/9/27/28	0/2/2/2
2	2MG	C	6	2	-	0/5/27/28	0/3/3/3
3	PSU	D	4972	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	4500	2,3	-	3/7/25/26	0/2/2/2
48	PSU	w	966	48	-	0/7/25/26	0/2/2/2
48	OMU	w	116	48	-	2/9/27/28	0/2/2/2
48	4AC	w	1842	48	-	0/11/29/30	0/2/2/2
48	A2M	w	27	48	-	1/5/27/28	0/3/3/3
48	PSU	w	1347	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4552	3	-	0/7/25/26	0/2/2/2
2	5MC	C	48	2	-	2/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	D	3770	3	-	1/7/25/26	0/2/2/2
3	PSU	D	4420	3	-	0/7/25/26	0/2/2/2
3	OMG	D	4228	3	-	0/5/27/28	0/3/3/3
3	PSU	D	4521	80,3	-	2/7/25/26	0/2/2/2
48	PSU	w	686	48	-	0/7/25/26	0/2/2/2
48	PSU	w	406	48	-	0/7/25/26	0/2/2/2
3	OMG	D	3944	3	-	4/5/27/28	0/3/3/3
48	B8N	w	1248	48	-	4/16/34/35	0/2/2/2
3	A2M	D	3825	3	-	0/5/27/28	0/3/3/3
3	A2M	D	1326	3	-	0/5/27/28	0/3/3/3
3	PSU	D	5001	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	1860	3	-	0/7/25/26	0/2/2/2
48	A2M	w	99	48,80	-	2/5/27/28	0/3/3/3
48	OMG	w	1490	48,80	-	3/5/27/28	0/3/3/3
3	OMU	D	2837	3	-	0/9/27/28	0/2/2/2
48	MA6	w	1850	48	-	0/7/29/30	0/3/3/3
3	OMC	D	4456	3	-	0/9/27/28	0/2/2/2
2	H2U	C	19	2	-	0/7/38/39	0/2/2/2
48	PSU	w	1045	48	-	0/7/25/26	0/2/2/2
2	1MA	C	9	2	-	2/3/25/26	0/3/3/3
48	PSU	w	93	48	-	0/7/25/26	0/2/2/2
3	PSU	D	3764	3	-	0/7/25/26	0/2/2/2
3	OMC	D	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3851	3	-	1/7/25/26	0/2/2/2
3	OMU	D	2415	3	-	3/9/27/28	0/2/2/2
3	PSU	D	2508	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4293	3	-	0/7/25/26	0/2/2/2
3	OMG	D	4499	2,3	-	1/5/27/28	0/3/3/3
48	PSU	w	1004	48	-	0/7/25/26	0/2/2/2
48	4AC	w	1337	48	-	0/11/29/30	0/2/2/2
3	PSU	D	3730	3	-	0/7/25/26	0/2/2/2
48	PSU	w	815	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1643	48,80	-	0/7/25/26	0/2/2/2
2	5MC	C	47	2	-	3/7/25/26	0/2/2/2
3	1MA	D	1322	3	-	0/3/25/26	0/3/3/3
3	OMG	D	4637	3	-	1/5/27/28	0/3/3/3
48	OMU	w	1326	48	-	5/9/27/28	0/2/2/2
2	H2U	B	19	2	-	0/7/38/39	0/2/2/2
3	OMU	D	1773	3	-	1/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	D	4498	80,3	-	0/9/27/28	0/2/2/2
2	5MU	C	53	2	-	2/7/25/26	0/2/2/2
3	OMG	D	1316	3	-	0/5/27/28	0/3/3/3
3	OMG	D	1522	3	-	0/5/27/28	0/3/3/3
3	PSU	D	3920	80,3	-	0/7/25/26	0/2/2/2
48	OMG	w	644	48	-	3/5/27/28	0/3/3/3
48	OMC	w	1703	48,80	-	2/9/27/28	0/2/2/2
3	OMU	D	3925	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4576	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1367	48	-	0/7/25/26	0/2/2/2
3	OMU	D	4227	3	-	1/9/27/28	0/2/2/2
2	5MC	B	48	2	-	2/7/25/26	0/2/2/2
2	1MA	C	57	2	-	0/3/25/26	0/3/3/3
3	A2M	D	1524	3	-	1/5/27/28	0/3/3/3
3	OMG	D	4494	3	-	1/5/27/28	0/3/3/3
48	PSU	w	822	48	-	2/7/25/26	0/2/2/2
48	PSU	w	1056	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1792	3	-	0/7/25/26	0/2/2/2
3	OMC	D	2422	80,3	-	1/9/27/28	0/2/2/2
2	2MG	B	6	2	-	2/5/27/28	0/3/3/3
48	PSU	w	218	48	-	0/7/25/26	0/2/2/2
48	OMG	w	436	48	-	0/5/27/28	0/3/3/3
3	PSU	D	4423	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3758	3	-	0/7/25/26	0/2/2/2
2	5MC	C	38	2	-	0/7/25/26	0/2/2/2
48	PSU	w	681	48,80	-	0/7/25/26	0/2/2/2
3	A2M	D	3785	80,3	-	2/5/27/28	0/3/3/3
3	OMG	D	4370	3	-	1/5/27/28	0/3/3/3
3	A2M	D	400	3	-	0/5/27/28	0/3/3/3
3	5MC	D	4447	80,3	-	4/7/25/26	0/2/2/2
2	56B	B	34	2	-	3/6/43/44	0/4/4/4
3	OMC	D	2861	3	-	0/9/27/28	0/2/2/2
48	OMG	w	601	48	-	0/5/27/28	0/3/3/3
3	PSU	D	3715	3	-	0/7/25/26	0/2/2/2
48	PSU	w	651	48	-	0/7/25/26	0/2/2/2
3	PSU	D	3695	3	-	0/7/25/26	0/2/2/2
48	PSU	w	105	48	-	0/7/25/26	0/2/2/2
48	A2M	w	512	48	-	2/5/27/28	0/3/3/3
48	OMU	w	1288	48	-	3/9/27/28	0/2/2/2
48	OMU	w	1442	48,80	-	1/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	w	1445	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1536	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4457	3	-	0/7/25/26	0/2/2/2
48	6MZ	w	1832	48,80	-	2/5/27/28	0/3/3/3
3	PSU	D	4471	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4431	3	-	0/7/25/26	0/2/2/2
48	PSU	w	801	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4579	3	-	0/7/25/26	0/2/2/2
3	OMU	D	4620	3	-	0/9/27/28	0/2/2/2
2	5MC	B	38	2	-	0/7/25/26	0/2/2/2
3	OMC	D	3701	80,3	-	4/9/27/28	0/2/2/2
48	OMC	w	462	48	-	1/9/27/28	0/2/2/2
3	A2M	D	3760	3	-	2/5/27/28	0/3/3/3
48	PSU	w	863	48	-	0/7/25/26	0/2/2/2
48	PSU	w	572	48	-	0/7/25/26	0/2/2/2
2	PSU	C	13	2	-	0/7/25/26	0/2/2/2
48	OMG	w	1328	48	-	0/5/27/28	0/3/3/3
48	A2M	w	468	48	-	2/5/27/28	0/3/3/3
2	1MA	B	9	2	-	2/3/25/26	0/3/3/3
5	OMG	F	75	5	-	0/5/27/28	0/3/3/3
48	OMU	w	428	48	-	7/9/27/28	0/2/2/2
3	PSU	D	3639	3	-	0/7/25/26	0/2/2/2
48	A2M	w	484	48	-	0/5/27/28	0/3/3/3
3	PSU	D	4299	3	-	0/7/25/26	0/2/2/2
3	A2M	D	398	3	-	2/5/27/28	0/3/3/3
2	56B	C	34	2	-	3/6/43/44	0/4/4/4
48	A2M	w	1678	48	-	1/5/27/28	0/3/3/3
48	OMU	w	1804	48	-	2/9/27/28	0/2/2/2
3	OMC	D	3808	3	-	0/9/27/28	0/2/2/2
3	PSU	D	1862	3	-	0/7/25/26	0/2/2/2
48	OMU	w	121	48	-	0/9/27/28	0/2/2/2
48	A2M	w	159	48	-	2/5/27/28	0/3/3/3
2	PSU	B	13	2	-	2/7/25/26	0/2/2/2
3	PSU	D	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4353	3	-	0/7/25/26	0/2/2/2
48	OMC	w	517	48,80	-	0/9/27/28	0/2/2/2
3	PSU	D	1782	3	-	0/7/25/26	0/2/2/2
3	OMG	D	3744	3	-	0/5/27/28	0/3/3/3
3	PSU	D	1683	3	-	0/7/25/26	0/2/2/2
3	OMC	D	2365	80,3	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMU	w	627	48	-	5/9/27/28	0/2/2/2
48	A2M	w	166	48	-	2/5/27/28	0/3/3/3
48	OMU	w	799	48	-	3/9/27/28	0/2/2/2
3	OMG	D	1760	3	-	2/5/27/28	0/3/3/3
48	PSU	w	1232	48	-	0/7/25/26	0/2/2/2
3	A2M	D	2815	3	-	3/5/27/28	0/3/3/3
2	PSU	C	54	2	-	2/7/25/26	0/2/2/2
3	OMG	D	3792	3	-	0/5/27/28	0/3/3/3
48	PSU	w	1046	48	-	0/7/25/26	0/2/2/2
48	G7M	w	1639	48,2	-	2/3/25/26	0/3/3/3
3	PSU	D	4403	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	1081	48	-	0/7/25/26	0/2/2/2
3	PSU	D	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	D	2632	3	-	0/7/25/26	0/2/2/2
48	A2M	w	576	48	-	2/5/27/28	0/3/3/3
3	A2M	D	3718	3	-	0/5/27/28	0/3/3/3
48	PSU	w	34	48	-	3/7/25/26	0/2/2/2
3	PSU	D	3853	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	814	48	-	0/7/25/26	0/2/2/2
3	A2M	D	4523	80,3	-	0/5/27/28	0/3/3/3
3	OMC	D	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4689	3	-	0/7/25/26	0/2/2/2
3	OMU	D	4306	3	-	0/9/27/28	0/2/2/2
3	OMG	D	4392	3	-	0/5/27/28	0/3/3/3
3	PSU	D	1744	80,3	-	0/7/25/26	0/2/2/2
3	OMG	D	4196	80,2,3	-	1/5/27/28	0/3/3/3
3	A2M	D	2363	80,3	-	0/5/27/28	0/3/3/3
3	PSU	D	3734	3	-	0/7/25/26	0/2/2/2
2	PSU	B	54	2	-	0/7/25/26	0/2/2/2
48	OMC	w	174	48	-	1/9/27/28	0/2/2/2
3	OMG	D	4618	3	-	0/5/27/28	0/3/3/3
48	PSU	w	210	48	-	0/7/25/26	0/2/2/2
48	PSU	w	866	48	-	0/7/25/26	0/2/2/2
3	A2M	D	2787	80,3	-	0/5/27/28	0/3/3/3
3	OMG	D	3899	3	-	0/5/27/28	0/3/3/3
3	PSU	D	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4628	3	-	0/7/25/26	0/2/2/2
3	A2M	D	1871	80,3	-	0/5/27/28	0/3/3/3
48	A2M	w	590	48	-	2/5/27/28	0/3/3/3
3	A2M	D	3830	3	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	D	1534	80,3	-	3/5/27/28	0/3/3/3
2	1MA	B	57	2	-	0/3/25/26	0/3/3/3
3	OMC	D	3841	3	-	0/9/27/28	0/2/2/2
3	PSU	D	1781	3	-	0/7/25/26	0/2/2/2
3	A2M	D	2401	3	-	1/5/27/28	0/3/3/3
48	PSU	w	1177	48	-	0/7/25/26	0/2/2/2
3	OMG	D	1625	80,3	-	1/5/27/28	0/3/3/3
3	OMC	D	1340	3	-	0/9/27/28	0/2/2/2
3	OMC	D	2804	3	-	0/9/27/28	0/2/2/2
48	OMG	w	683	48	-	0/5/27/28	0/3/3/3
3	OMC	D	3887	3	-	1/9/27/28	0/2/2/2
3	5MC	D	3782	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	1238	48	-	2/7/25/26	0/2/2/2
48	A2M	w	1383	48	-	0/5/27/28	0/3/3/3
3	PSU	D	3768	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4361	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4532	3	-	0/7/25/26	0/2/2/2
3	OMG	D	2364	3	-	2/5/27/28	0/3/3/3
3	OMG	D	2424	3	-	2/5/27/28	0/3/3/3
3	OMG	D	4623	3	-	0/5/27/28	0/3/3/3
48	PSU	w	109	48	-	0/7/25/26	0/2/2/2
48	OMG	w	509	48	-	1/5/27/28	0/3/3/3
48	OMU	w	172	48	-	1/9/27/28	0/2/2/2
3	PSU	D	3637	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	609	48	-	0/7/25/26	0/2/2/2
3	OMG	D	3627	3	-	0/5/27/28	0/3/3/3
3	A2M	D	3724	3	-	0/5/27/28	0/3/3/3
3	UR3	D	4530	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1244	48	-	0/7/25/26	0/2/2/2
48	PSU	w	36	48	-	0/7/25/26	0/2/2/2
48	A2M	w	1031	48	-	0/5/27/28	0/3/3/3
48	PSU	w	649	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1692	48	-	0/7/25/26	0/2/2/2
48	MA6	w	1851	48	-	2/7/29/30	0/3/3/3
48	OMC	w	1391	48	-	0/9/27/28	0/2/2/2
48	PSU	w	1174	48,80	-	0/7/25/26	0/2/2/2

The worst 5 of 760 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	53	5MU	C2-N1	10.72	1.55	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	53	5MU	C6-N1	10.54	1.56	1.38
2	C	53	5MU	C2-N1	10.54	1.55	1.38
2	B	53	5MU	C6-N1	10.46	1.55	1.38
2	C	48	5MC	C6-C5	9.53	1.50	1.34

The worst 5 of 691 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	34	56B	C8-N9-C1'	23.29	146.11	125.48
2	B	34	56B	C8-N9-C1'	22.82	145.70	125.48
2	B	53	5MU	C5-C4-N3	12.26	125.77	115.31
2	C	53	5MU	C5-C4-N3	12.00	125.55	115.31
2	C	53	5MU	C5-C6-N1	-9.91	113.14	123.34

There are no chirality outliers.

5 of 168 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	34	56B	C14-C10-N10-C9
2	C	34	56B	C11-C10-N10-C9
2	C	34	56B	C14-C10-N10-C9
2	B	47	5MC	O4'-C4'-C5'-O5'
2	B	47	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 545 ligands modelled in this entry, 545 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

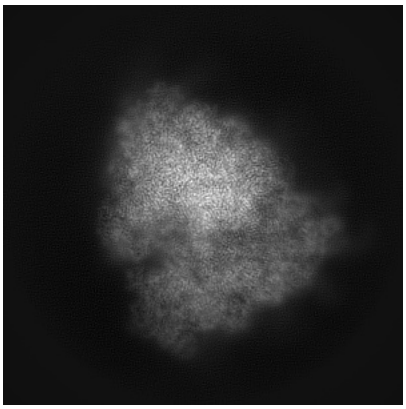
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36178. These allow visual inspection of the internal detail of the map and identification of artifacts.

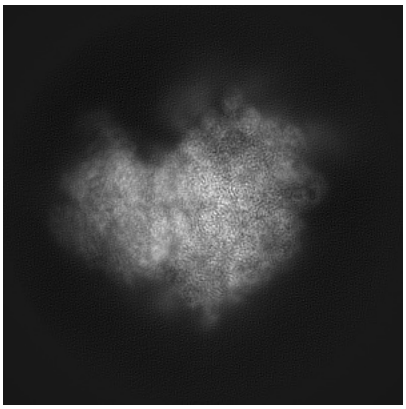
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

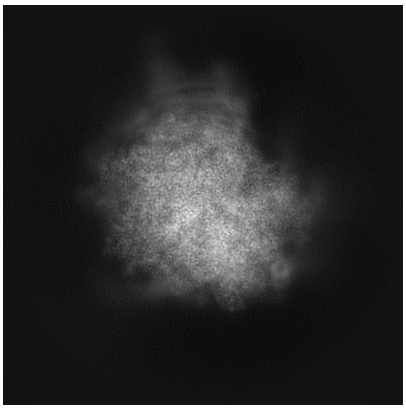
6.1.1 Primary map



X

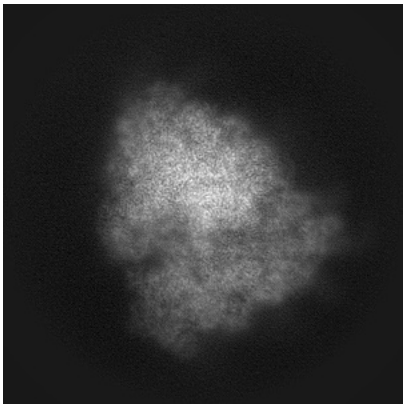


Y

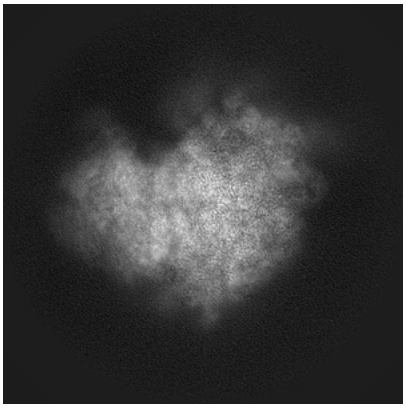


Z

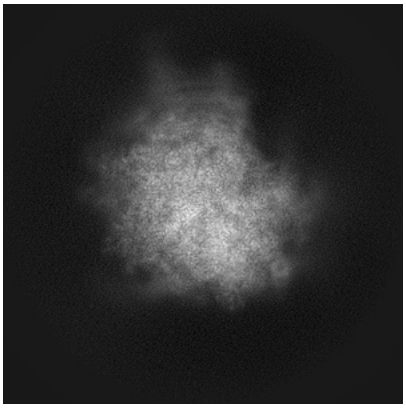
6.1.2 Raw map



X



Y

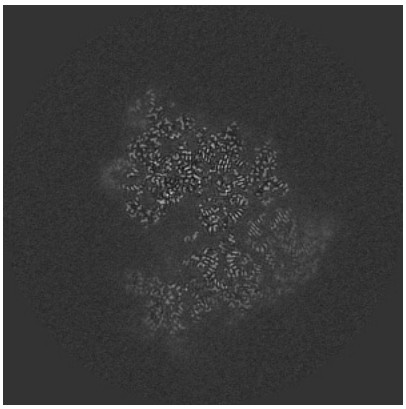


Z

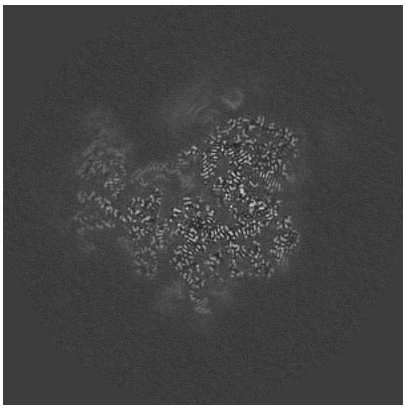
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

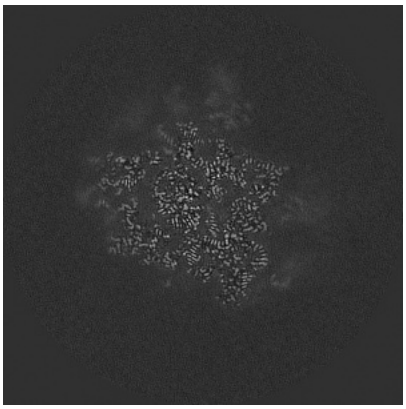
6.2.1 Primary map



X Index: 265

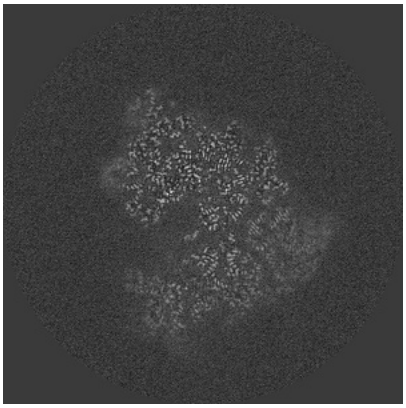


Y Index: 265

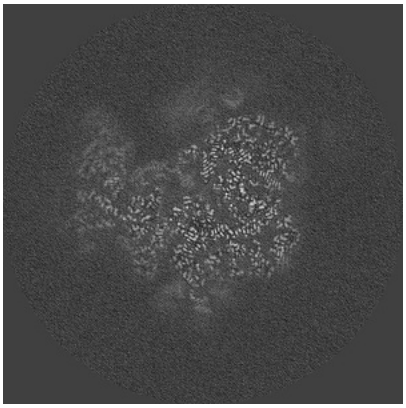


Z Index: 265

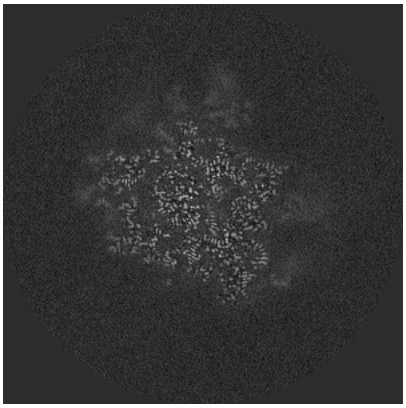
6.2.2 Raw map



X Index: 265



Y Index: 265

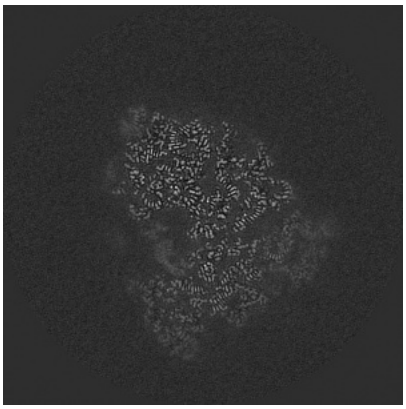


Z Index: 265

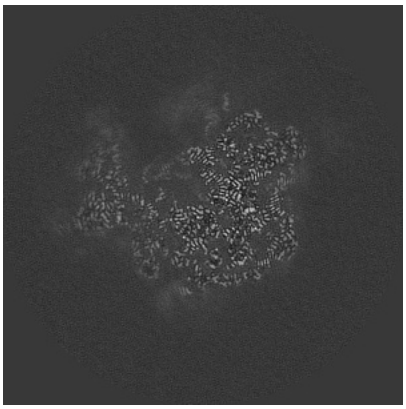
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

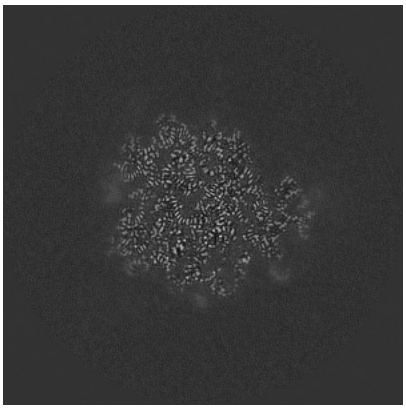
6.3.1 Primary map



X Index: 253

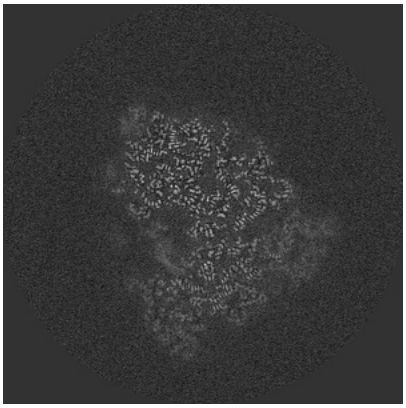


Y Index: 258

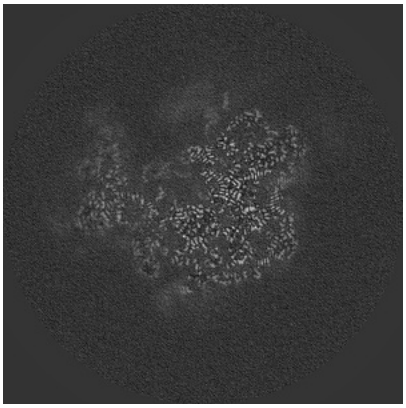


Z Index: 300

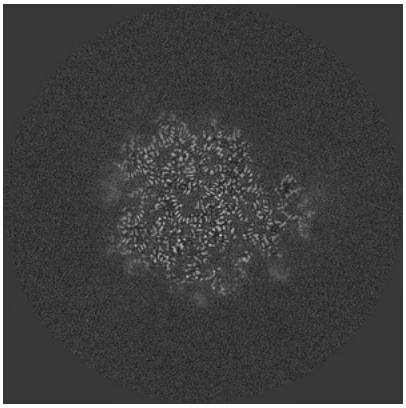
6.3.2 Raw map



X Index: 253



Y Index: 258

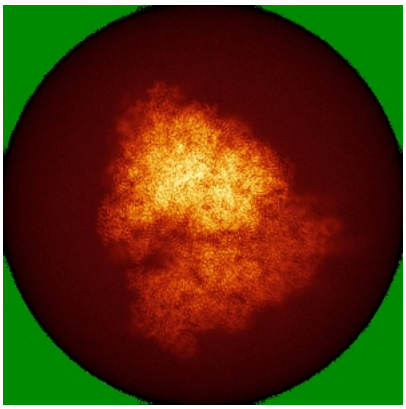


Z Index: 300

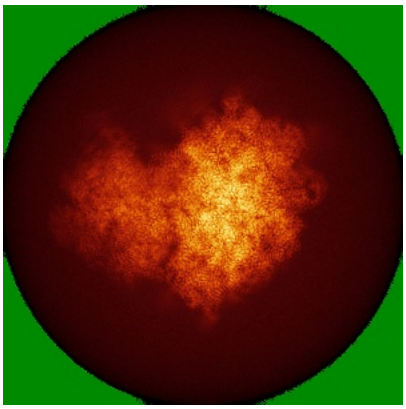
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

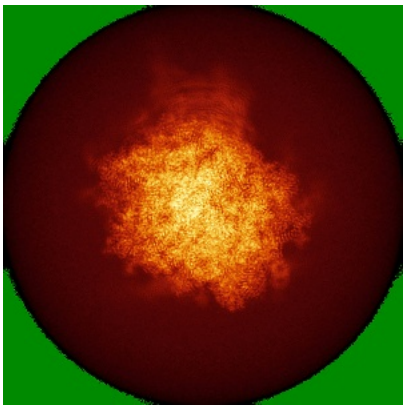
6.4.1 Primary map



X

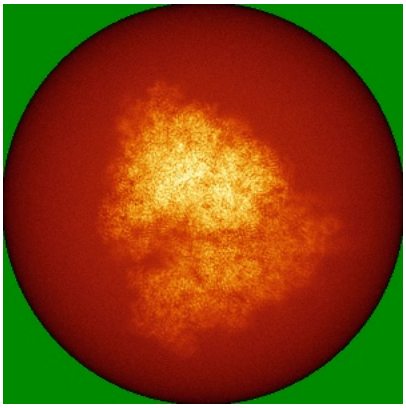


Y

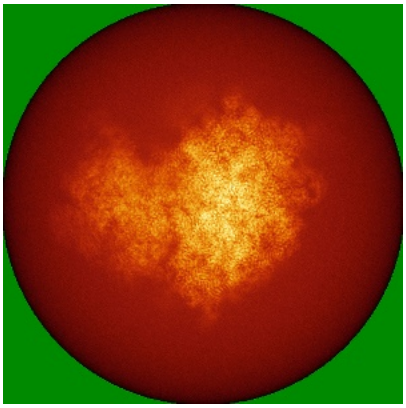


Z

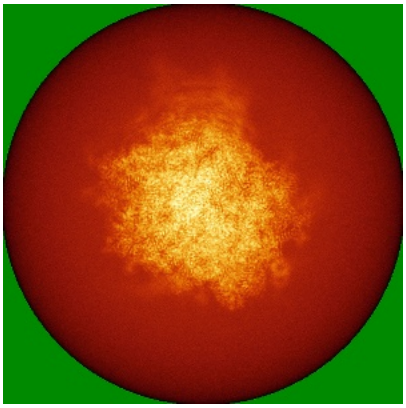
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0204. 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.

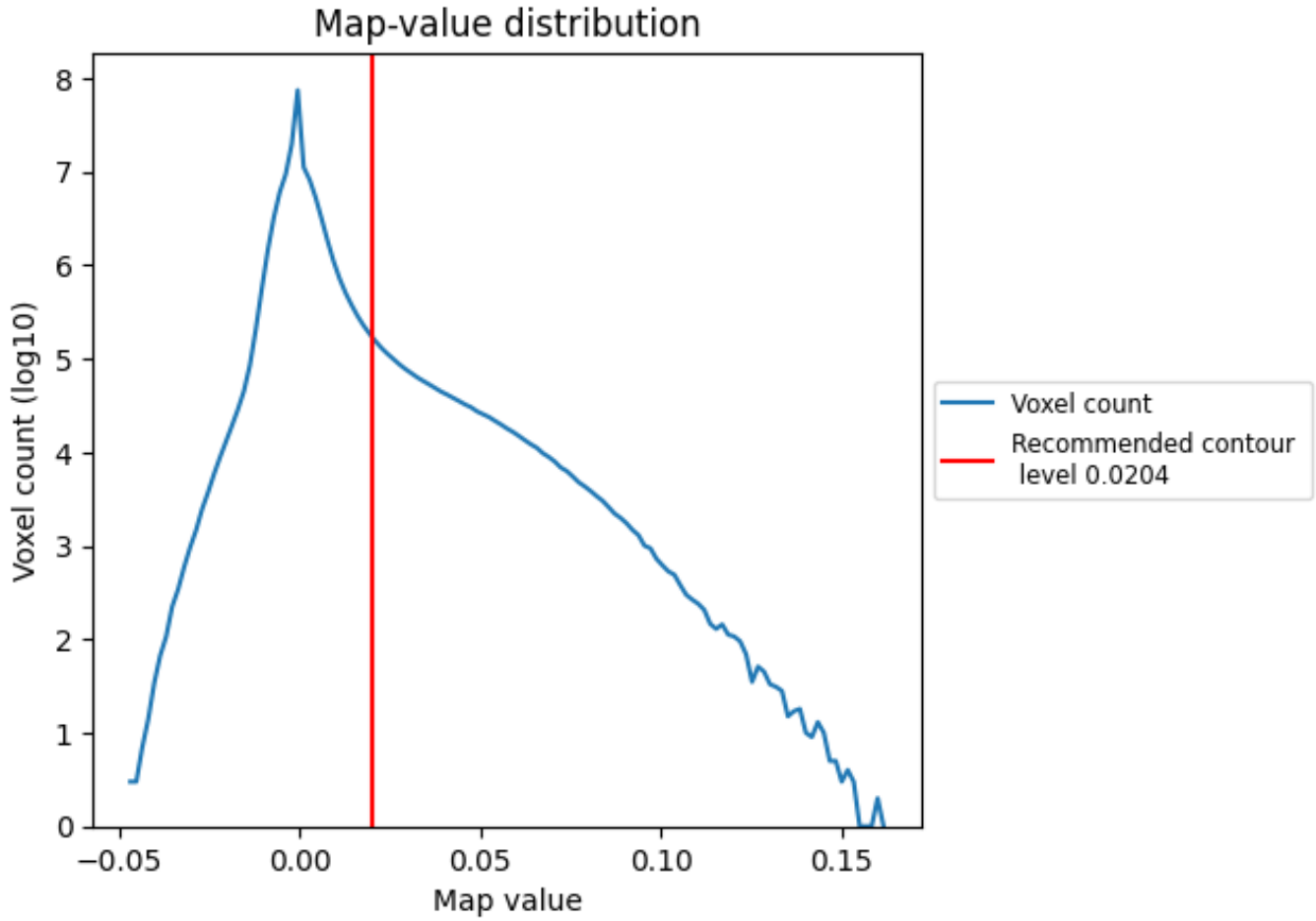
6.6 Mask visualisation (i)

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

7 Map analysis

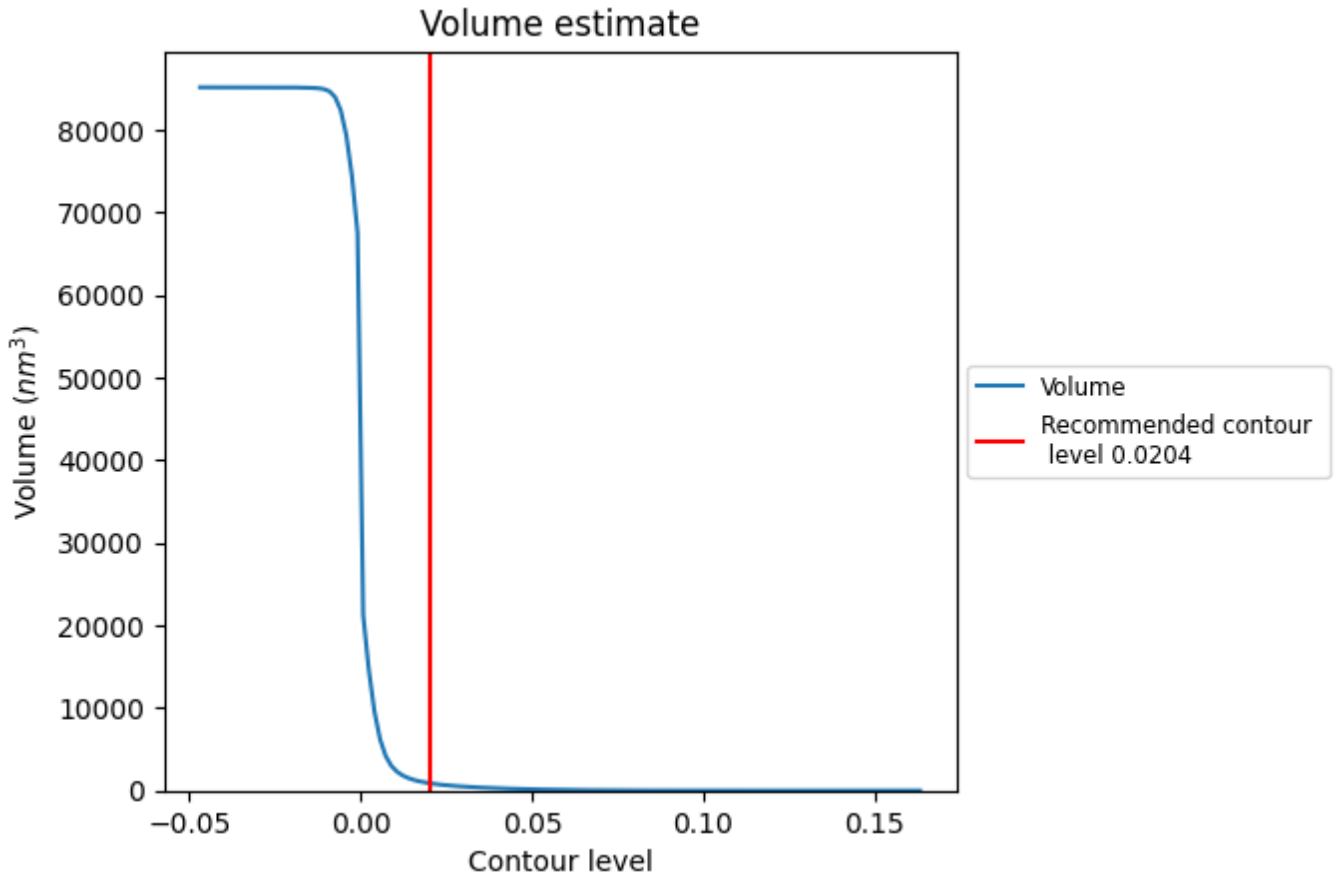
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

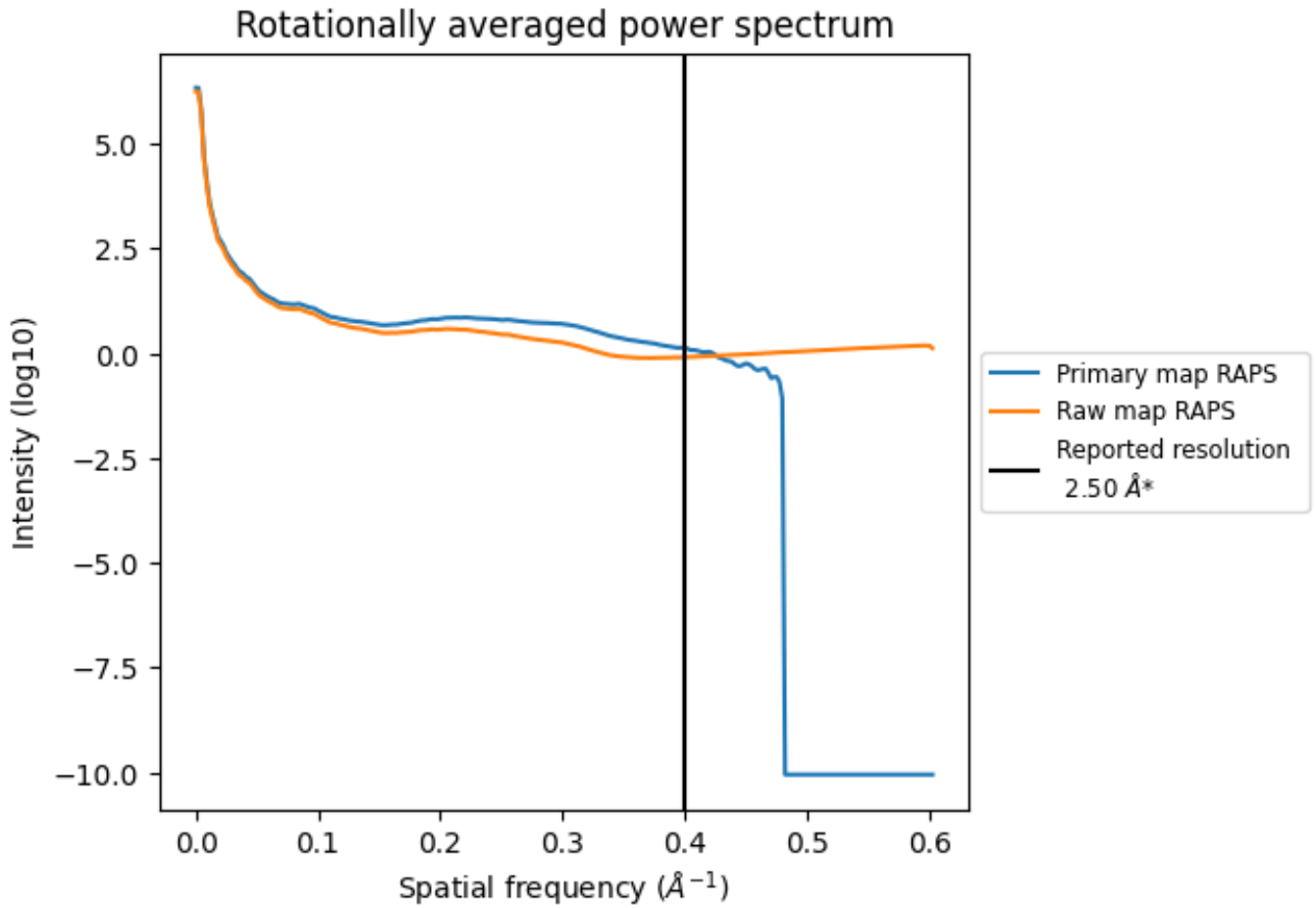
7.2 Volume estimate (i)



The volume at the recommended contour level is 872 nm^3; this corresponds to an approximate mass of 788 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)

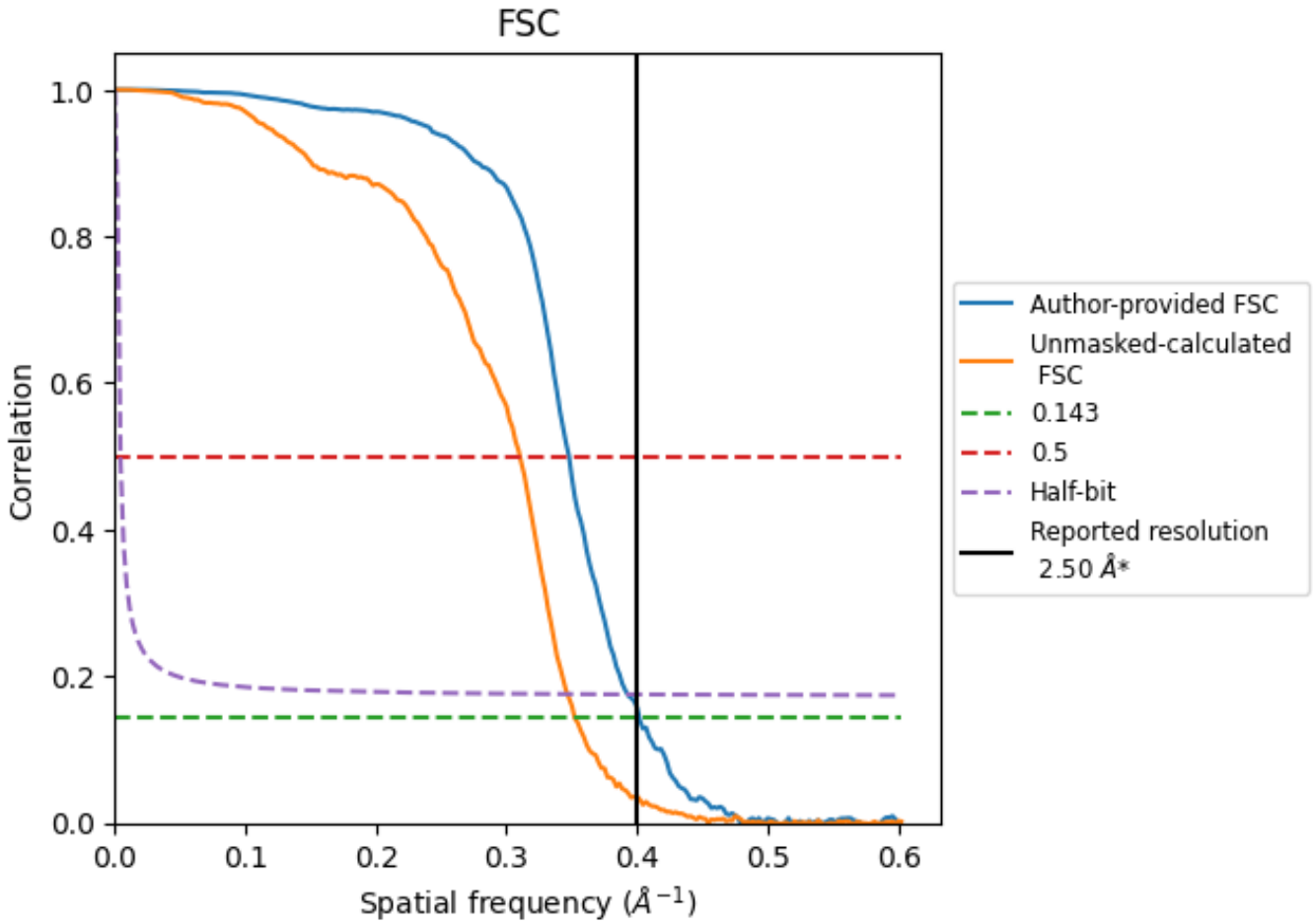


*Reported resolution corresponds to spatial frequency of 0.400 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

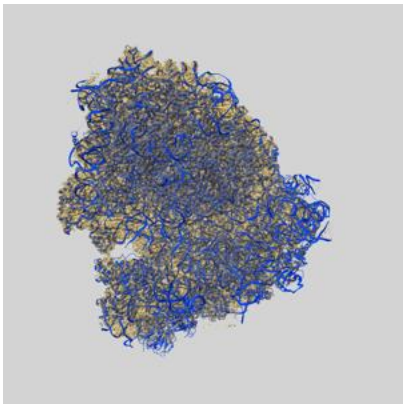
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.87	2.55
Unmasked-calculated*	2.84	3.22	2.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.84 differs from the reported value 2.5 by more than 10 %

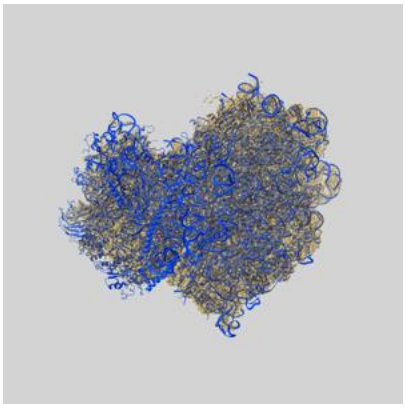
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36178 and PDB model 8JDJ. Per-residue inclusion information can be found in section 3 on page 19.

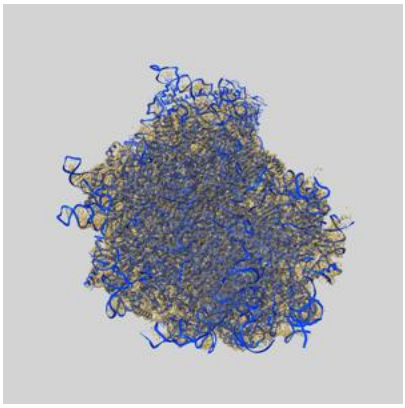
9.1 Map-model overlay



X



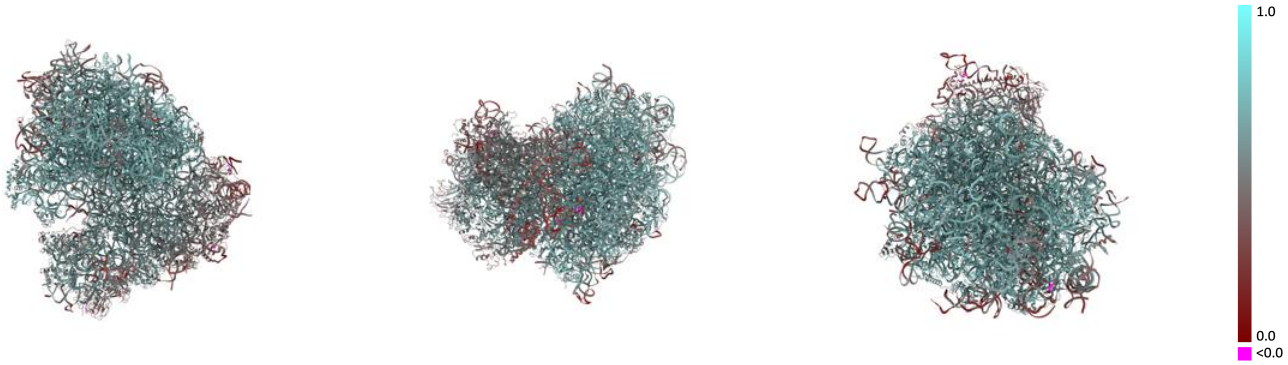
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0204 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.

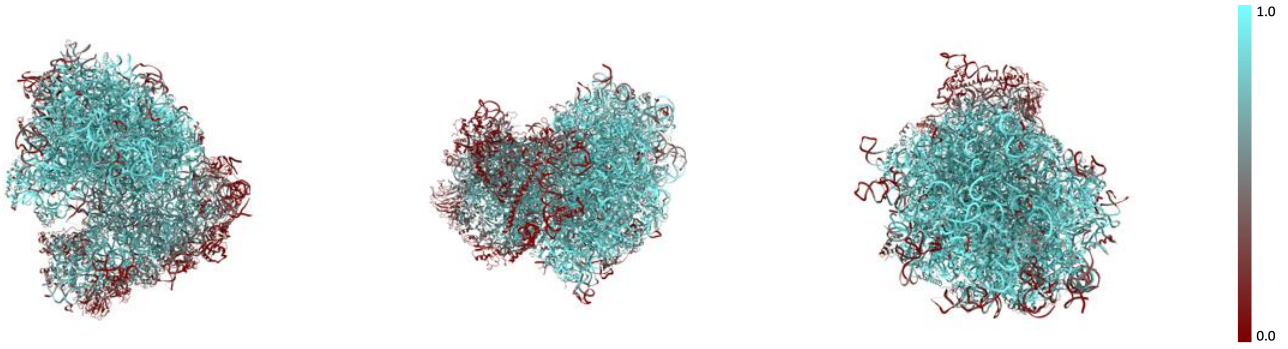
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

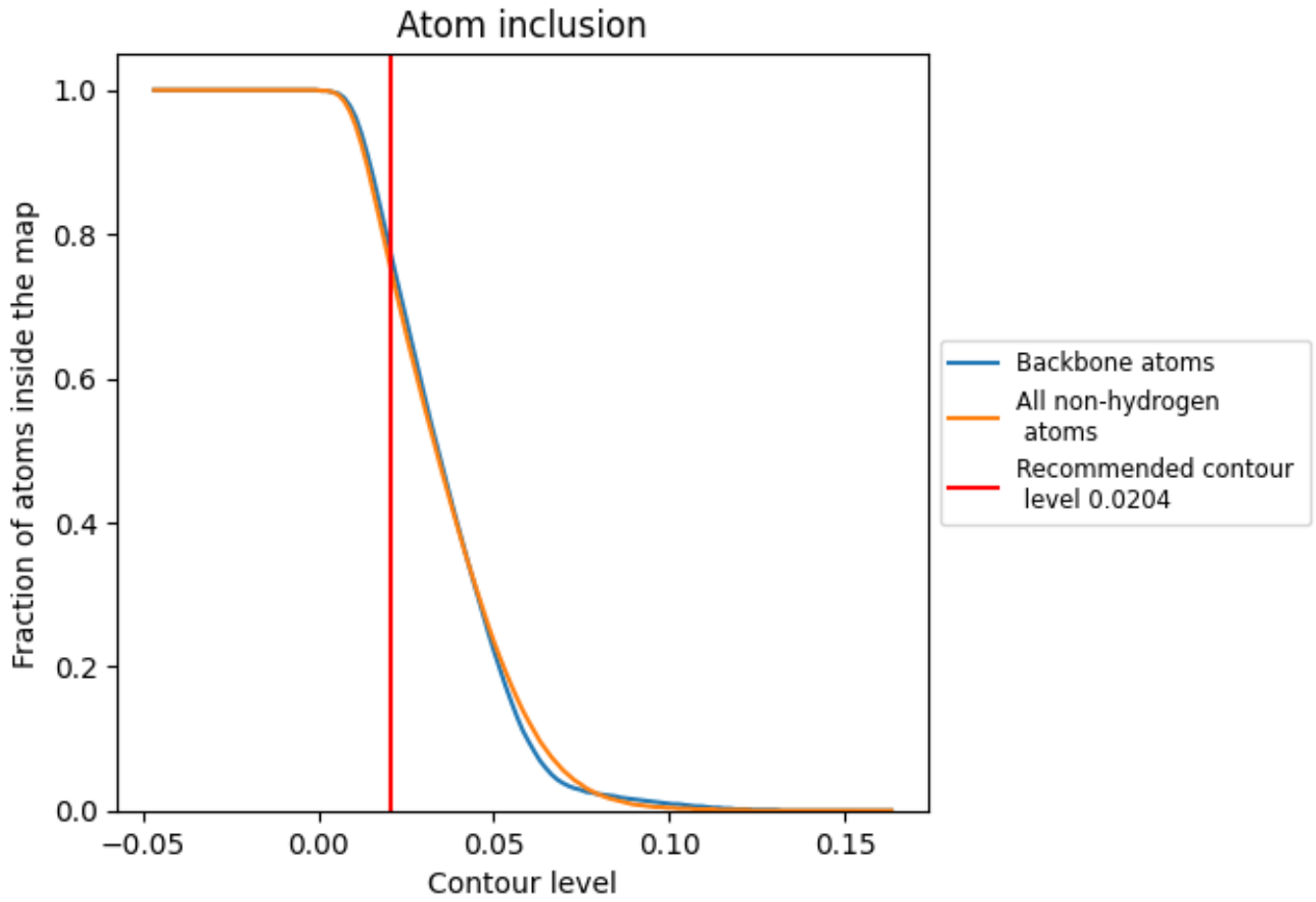
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0204).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 76% 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 (0.0204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7560	0.5940
0	0.4300	0.5030
1	0.1920	0.4160
2	0.5890	0.5570
3	0.1380	0.3760
4	0.2120	0.4330
5	0.4180	0.4690
6	0.2690	0.4200
7	0.1920	0.4090
8	0.5540	0.5380
9	0.6460	0.5830
A	0.7530	0.5730
AA	0.7120	0.5910
AB	0.3450	0.5030
AC	0.5690	0.5560
AD	0.3730	0.4790
AE	0.4660	0.5170
AF	0.5290	0.5460
AG	0.3960	0.4720
AH	0.5030	0.5610
AI	0.7210	0.6100
AJ	0.6570	0.5690
AK	0.0850	0.3780
AL	0.2980	0.4910
AM	0.7380	0.6020
AN	0.4170	0.5080
AO	0.4970	0.5270
AP	0.7720	0.6050
AQ	0.2430	0.4390
AR	0.1450	0.4090
B	0.7340	0.5560
C	0.5610	0.5650
D	0.8550	0.6220
E	0.9800	0.6730
F	0.9010	0.6360

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
G	0.9550	0.6850
H	0.8850	0.6650
I	0.8960	0.6530
J	0.7930	0.6250
K	0.7470	0.6060
L	0.8990	0.6680
M	0.7090	0.5960
N	0.8330	0.6410
O	0.8630	0.6450
P	0.7060	0.5940
Q	0.8040	0.6270
R	0.8490	0.6380
S	0.9710	0.6860
T	0.9130	0.6740
U	0.8890	0.6690
V	0.9320	0.6750
W	0.7920	0.6230
X	0.9190	0.6720
Y	0.8500	0.6450
Z	0.5790	0.5520
a	0.8970	0.6740
b	0.8780	0.6650
c	0.8270	0.6340
d	0.8200	0.6300
e	0.8170	0.6290
f	0.9170	0.6710
g	0.7080	0.5860
h	0.8250	0.6290
i	0.8220	0.6470
j	0.9330	0.6880
k	0.9370	0.6720
l	0.8510	0.6420
m	0.8160	0.6370
n	0.7680	0.6360
o	0.9550	0.6800
p	0.6550	0.5890
q	0.8960	0.6520
r	0.8750	0.6570
s	0.9130	0.6680
t	0.8330	0.6340
u	0.8800	0.6660
v	0.8920	0.6410

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
w	0.7260	0.5470
x	0.5390	0.5670
y	0.6030	0.5830
z	0.6630	0.5930