wwPDB EM Validation Summary Report (i)

Nov 8, 2022 – 04:09 AM EST

PDB ID	:	6MTC
EMDB ID	:	EMD-9239
Title	:	Rabbit 80S ribosome with Z-site tRNA and IFRD2 (unrotated state)
Authors	:	Brown, A.; Baird, M.R.; Yip, M.C.J.; Murray, J.; Shao, S.
Deposited on	:	2018-10-19
Resolution	:	3.40 Å(reported)
Based on initial model	:	5LZV

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:

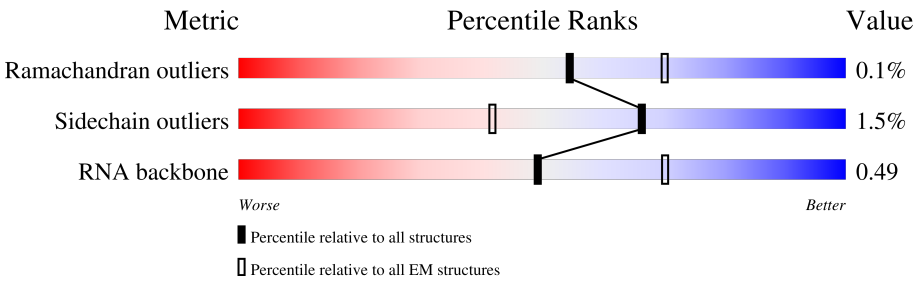
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.40 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	4	75	5% 45% 51% •
2	5	3597	• 67% 28% 5%
3	7	120	• 81% 18% •
4	8	151	• 74% 25% •
5	A	248	98% •
6	B	394	98% •
7	C	362	• 98% •
8	D	293	99% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	E	291	73% 26%
10	F	225	100%
11	G	319	71% 27%
12	H	190	97%
13	I	214	95%
14	J	170	99%
15	L	210	96%
16	M	138	99%
17	N	203	97%
18	O	199	98%
19	P	153	99%
20	Q	187	98%
21	R	180	99%
22	S	176	98%
23	T	159	98%
24	U	99	99%
25	V	131	98%
26	W	157	12% 66% 32%
27	X	118	100%
28	Y	134	97%
29	Z	135	99%
30	a	147	100%
31	b	245	5% 42% 58%
32	c	98	97%
33	d	107	98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	e	128	98%
35	f	109	99%
36	g	114	96%
37	h	122	99%
38	i	102	99%
39	j	86	99%
40	k	69	97%
41	l	50	94% 6%
42	m	52	98%
43	n	25	100%
44	o	103	98%
45	p	91	99%
46	r	124	98%
47	u	206	45% 97%
48	v	441	11% 78% 20%
49	9	1698	5% 70% 27%
50	AA	217	99%
51	BB	213	98%
52	CC	221	98%
53	DD	228	9% 97%
54	EE	262	98%
55	FF	204	88% 9%
56	GG	237	8% 97%
57	HH	194	6% 92% 5%
58	II	206	6% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	JJ	185	100%
60	KK	96	8%, 98%
61	LL	158	90%, 9%
62	MM	117	65%, 99%
63	NN	149	99%
64	OO	136	98%
65	PP	120	8%, 98%
66	QQ	142	96%
67	RR	132	99%
68	SS	144	6%, 100%
69	TT	141	98%
70	UU	100	9%, 100%
71	VV	83	99%
72	WW	129	98%
73	XX	141	98%
74	YY	124	99%
75	ZZ	75	5%, 100%
76	aa	101	100%
77	bb	83	99%
78	cc	62	5%, 98%
79	dd	55	98%
80	ee	55	18%, 98%
81	ff	68	59%, 99%
82	gg	313	9%, 99%

2 Entry composition (i)

There are 84 unique types of molecules in this entry. The entry contains 216975 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 Z-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	4	75	1593	712	281	526	74	0	0

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	3597	77254	34469	14127	25061	3597	0	0

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	7	120	2558	1141	456	842	119	0	0

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	8	151	3209	1433	564	1062	150	0	0

- Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	248	1898	1189	389	314	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	394	3172	2020	597	542	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	362	2884	1813	577	480	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	293	2391	1512	438	427	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	216	1729	1115	329	282	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	225	1875	1205	358	303	9	0	0

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	233	1879	1199	361	315	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	190	1516	954	284	272	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	205	1664	1056	321	274	13	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	L	210	1702	1065	354	279	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	M	138	1137	727	221	182	7	0	0

- Molecule 17 is a protein called 60S Ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	O	199	1630	1051	319	255	5	0	0

- Molecule 19 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	P	153	1242	777	241	215	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Q	187	1515	946	315	250	4	0	0

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

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

- Molecule 22 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	S	176	1462	930	285	236	11	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	U	99	809	519	141	147	2	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	W	106	860	538	174	144	4	0	0

- Molecule 27 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	X	118	967	618	181	167	1	0	0

- Molecule 28 is a protein called 60S ribosomal protein L26.

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

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

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

- Molecule 30 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	a	147	1162	734	239	185	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	b	104	848	527	189	129	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	c	98	761	481	134	140	6	0	0

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

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

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

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

- Molecule 35 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	f	109	876	555	174	143	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	g	114	906	566	187	147	6	0	0

- Molecule 37 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	h	122	1013	640	204	168	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	i	102	830	520	176	129	5	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	l	50	447	286	96	64	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	m	52	430	267	90	67	6	0	0

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

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

- Molecule 44 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	o	103	842	528	172	136	6	0	0

- Molecule 45 is a protein called 60S ribosomal protein L37a.

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

- Molecule 46 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	r	124	994	616	205	167	6	0	0

- Molecule 47 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	u	206	1654	1058	297	291	8	0	0

- Molecule 48 is a protein called Interferon-related developmental regulator 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	v	354	2737	1725	493	506	13	0	0

- Molecule 49 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	9	1698	36291	16217	6509	11868	1697	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	AA	217	1710	1086	300	316	8	0	0

- Molecule 51 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	BB	213	1729	1098	309	308	14	0	0

- Molecule 52 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	CC	221	1716	1111	295	301	9	0	0

- Molecule 53 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	DD	228	1768	1126	318	316	8	0	0

- Molecule 54 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	EE	262	2076	1324	386	358	8	0	0

- Molecule 55 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	FF	185	1471	921	277	266	7	0	0

- Molecule 56 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	GG	237	1923	1200	387	329	7	0	0

- Molecule 57 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	HH	185	1488	952	271	264	1	0	0

- Molecule 58 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	II	206	1686	1058	332	291	5	0	0

- Molecule 59 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	JJ	185	1525	969	306	248	2	0	0

- Molecule 60 is a protein called 40S ribosomal protein S10.

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

- Molecule 61 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	LL	143	1175	749	222	198	6	0	0

- Molecule 62 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	MM	117	908	570	161	169	8	0	0

- Molecule 63 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	NN	149	1202	770	228	203	1	0	0

- Molecule 64 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	OO	136	1016	621	199	190	6	0	0

- Molecule 65 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	PP	120	997	635	187	168	7	0	0

- Molecule 66 is a protein called 40S ribosomal protein S16.

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

- Molecule 67 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	RR	132	1068	670	199	195	4	0	0

- Molecule 68 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	SS	144	1190	746	241	202	1	0	0

- Molecule 69 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	TT	141	1097	688	211	195	3	0	0

- Molecule 70 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	UU	100	795	498	152	141	4	0	0

- Molecule 71 is a protein called 40S ribosomal protein S21.

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

- Molecule 72 is a protein called 40S ribosomal protein S15a.

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

- Molecule 73 is a protein called 40S ribosomal protein S23.

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

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	YY	124	1011	640	198	168	5	0	0

- Molecule 75 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	ZZ	75	598	382	111	104	1	0	0

- Molecule 76 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	aa	101	814	507	170	132	5	0	0

- Molecule 77 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	bb	83	651	408	121	115	7	0	0

- Molecule 78 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	cc	62	488	297	97	92	2	0	0

- Molecule 79 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	dd	55	459	286	94	74	5	0	0

- Molecule 80 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	ee	55	443	274	97	71	1	0	0

- Molecule 81 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	ff	68	555	351	103	94	7	0	0

- Molecule 82 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
83	5	202	202	202	0
83	7	7	7	7	0
83	8	6	6	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
83	A	1	1	1	0
83	P	1	1	1	0
83	V	1	1	1	0
83	9	77	77	77	0
83	LL	1	1	1	0
83	aa	1	1	1	0

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

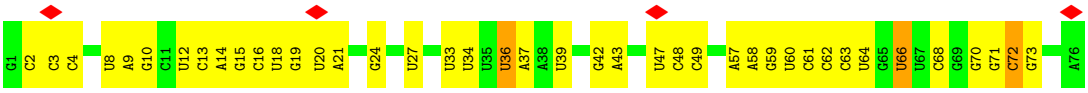
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
84	g	1	1	1	0
84	j	1	1	1	0
84	m	1	1	1	0
84	o	1	1	1	0
84	p	1	1	1	0
84	aa	1	1	1	0
84	dd	1	1	1	0
84	ff	1	1	1	0

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.

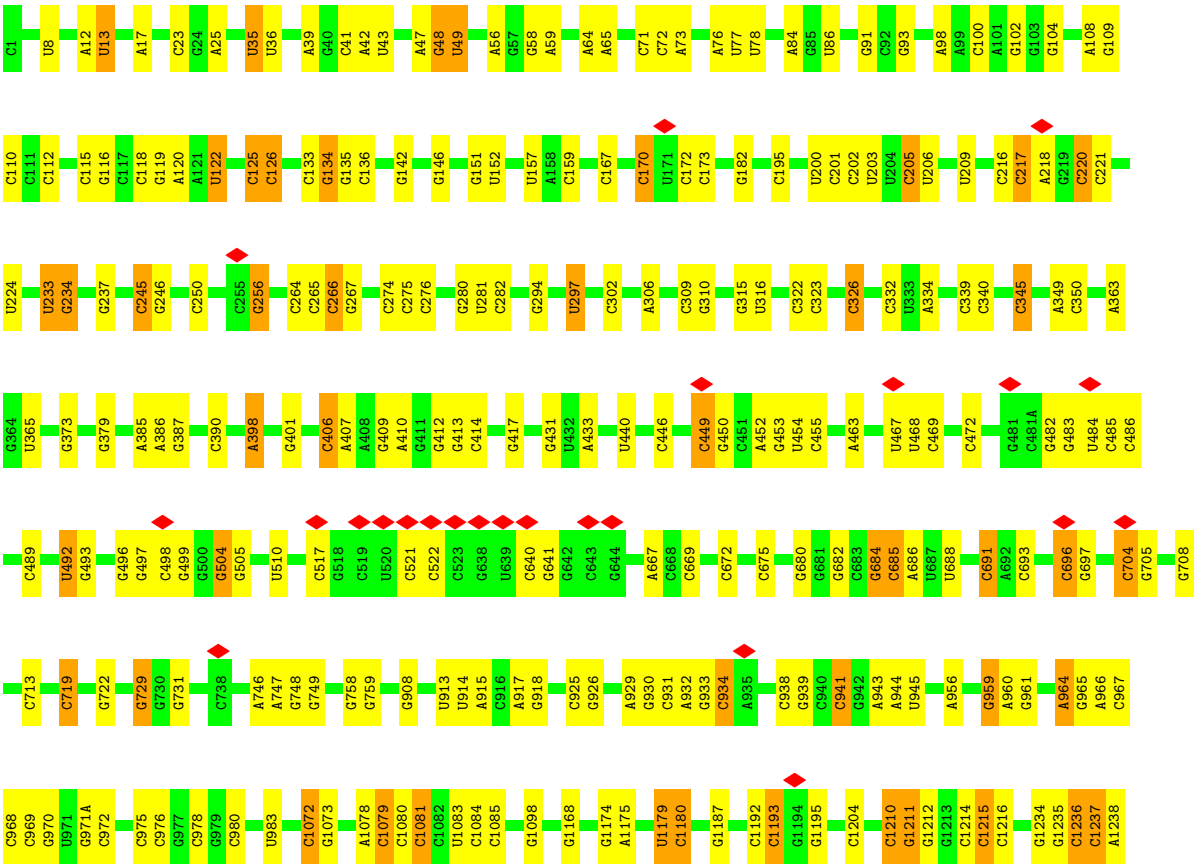
- Molecule 1: Z-site tRNA

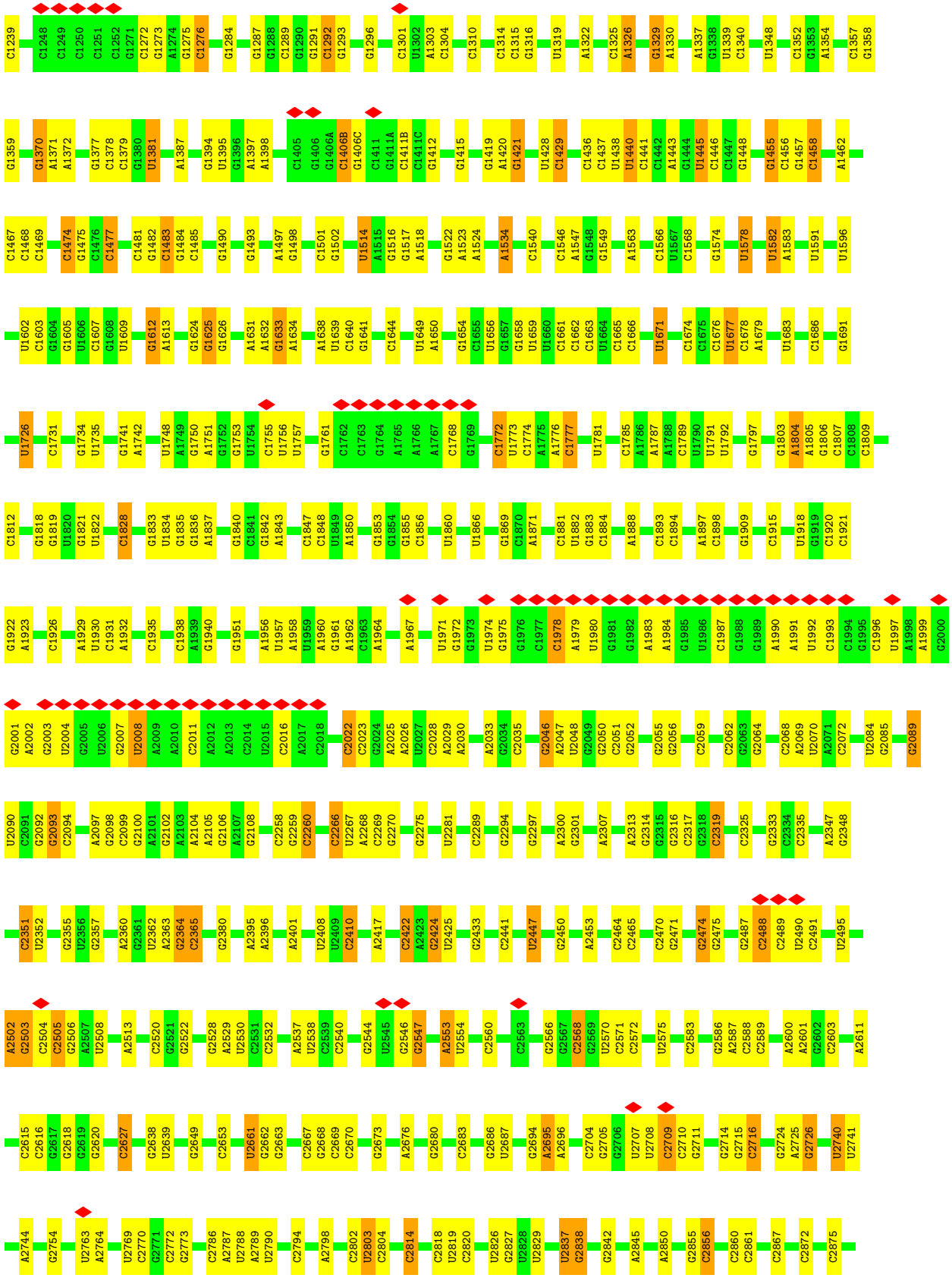
Chain 4:

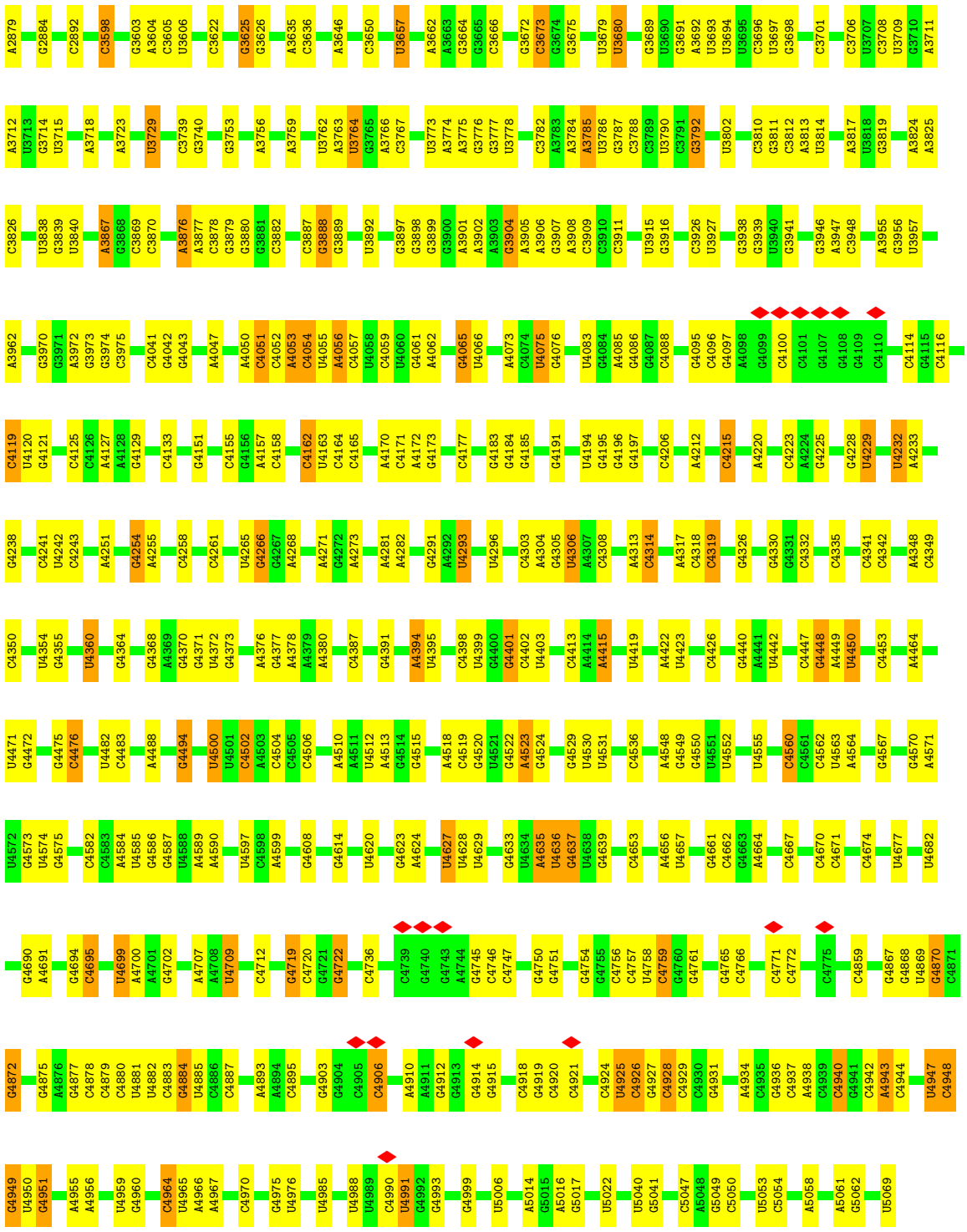


- Molecule 2: 28S rRNA

Chain 5:

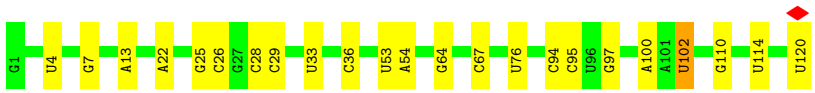



C1239 C1248 C1249 C1250 C1251 C1252 C1271 C1272 C1273 A1274 G1275 C1276 G1284 G1287 G1288 C1289 G1290 G1291 C1292 G1293 G1296 C1301 U1302 A1303 C1304 C1310 C1314 C1315 G1316 U1319 A1322 C1325 A1326 G1329 A1330 A1337 G1338 U1339 C1340 U1348 C1352 G1353 A1354 C1357 G1358
G1359 G1370 A1371 A1372 G1377 C1378 C1379 G1380 U1381 A1387 G1394 U1395 G1396 A1397 A1398 C1405 G1406 G1406A C1406B G1406C C1411 C1411A C1411B C1411C G1412 G1415 G1419 A1420 G1421 U1428 C1429 C1436 C1437 U1438 U1440 C1441 C1442 A1443 G1444 U1445 C1446 C1447 G1448 G1455 C1456 G1457 C1458 A1462
C1467 C1468 C1469 C1474 G1475 C1476 C1477 C1481 G1482 C1483 G1484 C1485 G1490 G1493 A1497 G1498 C1501 G1502 U1514 A1515 G1516 G1517 A1518 G1522 A1523 A1524 A1534 C1540 C1546 A1547 G1548 G1549 A1563 C1566 U1567 C1568 G1574 U1578 U1582 A1583 U1591 U1596
U1602 C1603 G1604 G1605 U1606 C1607 G1608 U1609 G1612 A1613 G1624 G1625 G1626 A1631 A1632 G1633 A1634 A1638 U1639 C1640 G1641 C1644 U1649 A1650 G1654 C1655 U1656 G1657 G1658 U1659 U1660 C1661 C1662 C1663 U1664 C1665 C1666 U1671 C1674 C1675 C1676 U1677 C1678 A1679 U1683 C1686 G1691
U1726 C1731 G1734 U1735 G1741 A1742 U1748 A1749 G1750 A1751 G1752 G1753 U1754 C1755 U1756 U1757 G1761 C1762 C1763 G1764 A1765 A1766 A1767 C1768 G1769 C1772 U1773 C1774 A1775 A1776 C1777 U1781 C1785 A1786 A1787 A1788 C1789 U1790 U1791 U1792 G1797 G1803 A1804 A1805 G1806 C1807 C1808 C1809
C1812 G1818 G1819 U1820 G1821 U1822 C1828 G1833 U1834 G1835 G1836 A1837 G1840 C1841 G1842 A1843 C1847 C1848 U1849 A1850 G1853 G1854 G1855 C1856 U1860 U1866 G1869 C1870 A1871 C1881 U1882 G1883 C1884 A1888 C1893 C1894 A1897 C1898 G1909 C1915 U1918 G1919 C1920 C1921
G1922 A1923 C1926 A1929 U1930 C1931 A1932 C1935 C1938 A1939 G1940 G1951 A1956 U1957 A1958 U1959 A1960 G1961 A1962 C1963 A1964 A1967 U1971 G1972 G1973 U1974 G1975 G1976 C1977 C1978 A1979 U1980 G1981 G1982 A1983 A1984 G1985 U1986 C1987 G1988 G1989 A1990 A1991 U1992 C1993 C1994 G1995 C1996 U1997 A1998 A1999 G2000
G2001 A2002 G2003 U2004 G2005 U2006 G2007 U2008 A2009 A2010 C2011 A2012 A2013 C2014 U2015 C2016 A2017 C2018 C2022 C2023 G2024 A2025 A2026 U2027 C2028 A2029 A2030 A2033 G2034 C2035 G2046 A2047 U2048 G2049 G2050 C2051 G2052 G2055 G2056 C2059 C2062 G2063 G2064 C2068 A2069 U2070 A2071 C2072 U2084 G2085 G2089
U2090 C2091 G2092 G2093 C2094 A2097 G2098 C2099 G2100 A2101 G2102 A2103 A2104 A2105 G2106 A2107 G2108 C2258 G2259 C2260 C2266 U2267 A2268 C2269 G2270 G2275 U2281 C2289 G2294 G2297 A2300 G2301 A2307 A2313 G2314 G2315 G2316 C2317 G2318 C2319 C2325 G2333 C2334 C2335 A2347 G2348
C2351 U2352 G2355 U2356 G2357 A2360 G2361 U2362 A2363 G2364 C2365 G2380 A2395 A2396 A2401 U2408 U2409 C2410 A2417 C2422 A2423 G2424 U2425 G2433 C2441 U2447 G2450 A2453 C2464 C2465 C2470 G2471 G2474 G2475 G2487 C2488 C2489 U2490 C2491 U2495
A2502 G2503 C2504 C2505 G2506 A2507 U2508 A2513 C2520 G2521 G2522 G2528 A2529 U2530 C2531 C2532 A2537 U2538 C2539 C2540 G2544 U2545 G2546 G2547 A2553 U2554 C2560 C2563 G2566 G2567 C2568 C2569 U2570 C2571 C2572 U2575 C2583 G2586 A2587 C2588 C2589 A2600 A2601 G2602 C2603 A2611
C2615 C2616 G2617 G2618 G2619 G2620 C2627 G2638 U2639 G2649 C2653 U2661 G2662 G2663 C2667 G2668 C2669 C2670 G2673 A2676 G2680 C2683 G2686 U2687 G2694 A2695 A2696 C2704 G2705 G2706 U2707 U2708 C2709 C2710 G2711 G2714 G2715 C2716 G2724 A2725 G2726 U2740 U2741
A2744 G2754 U2763 A2764 U2769 C2770 G2771 C2772 G2773 C2786 A2787 U2788 A2789 U2790 C2794 A2798 C2802 U2803 C2804 C2814 C2818 U2819 C2820 U2826 G2827 U2828 U2829 U2837 G2838 G2842 A2845 A2850 G2855 C2856 C2860 C2861 C2867 C2872 C2875



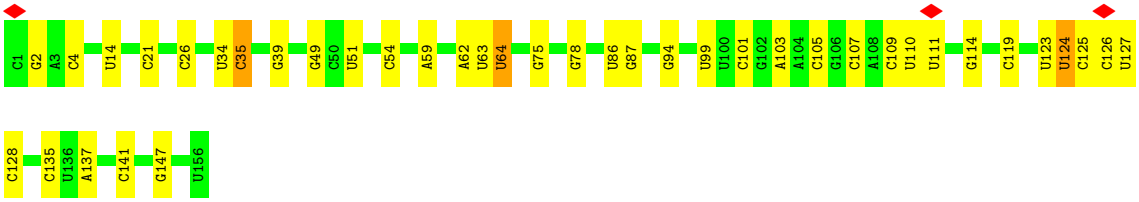
- Molecule 3: 5S rRNA

Chain 7:



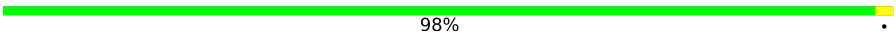
- Molecule 4: 5.8S rRNA

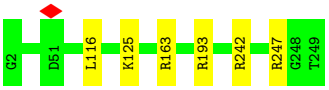
Chain 8:



- Molecule 5: 60S ribosomal protein L8

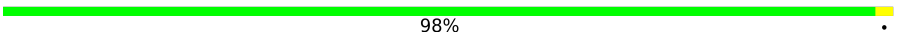
Chain A:

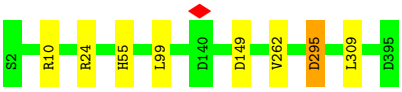




- Molecule 6: 60S ribosomal protein L3

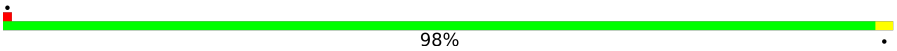
Chain B:

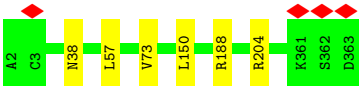




- Molecule 7: 60S ribosomal protein L4

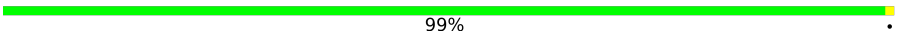
Chain C:





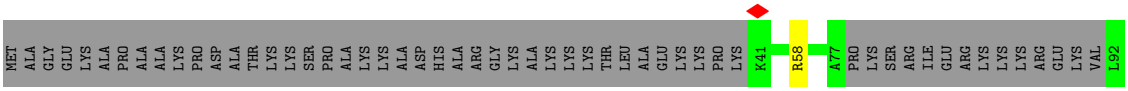
- Molecule 8: 60S ribosomal protein L5

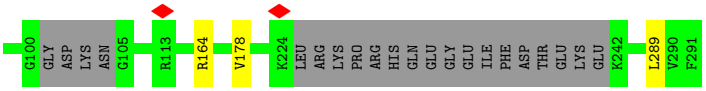
Chain D:



- Molecule 9: 60S ribosomal protein L6

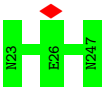
Chain E:





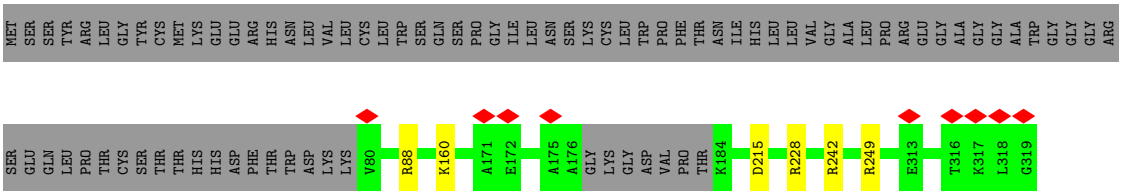
• Molecule 10: 60S ribosomal protein L7

Chain F: 100%



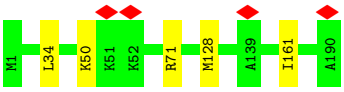
• Molecule 11: 60S ribosomal protein L7a

Chain G: 71% 27%



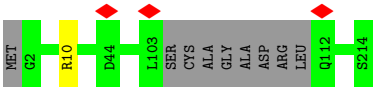
• Molecule 12: 60S ribosomal protein L9

Chain H: 97%



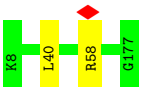
• Molecule 13: 60S ribosomal protein L10

Chain I: 95%



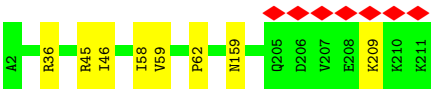
• Molecule 14: 60S ribosomal protein L11

Chain J: 99%

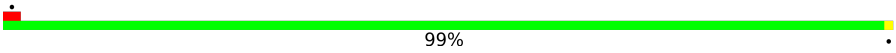


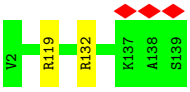
• Molecule 15: 60S ribosomal protein L13

Chain L: 96%

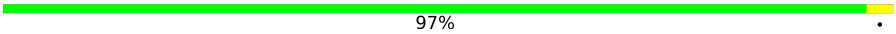


• Molecule 16: 60S ribosomal protein L14

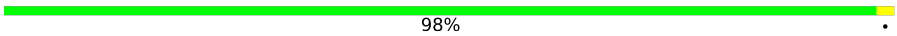
Chain M: 



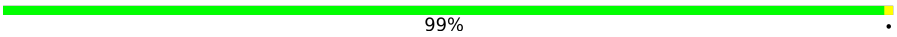
• Molecule 17: 60S Ribosomal protein L15

Chain N: 

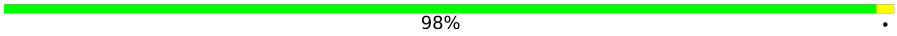
• Molecule 18: 60S ribosomal protein L13a

Chain O: 

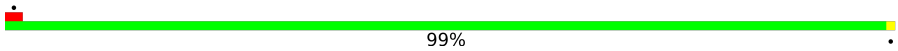
• Molecule 19: 60S ribosomal protein L17

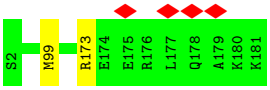
Chain P: 

• Molecule 20: 60S ribosomal protein L18

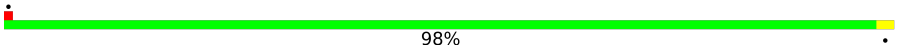
Chain Q: 

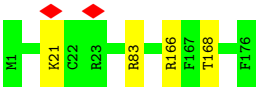
• Molecule 21: 60S ribosomal protein L19

Chain R: 



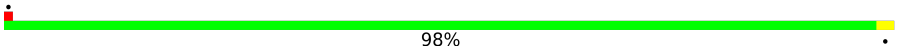
• Molecule 22: 60S ribosomal protein L18a

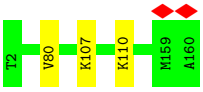
Chain S: 



• Molecule 23: 60S ribosomal protein L21

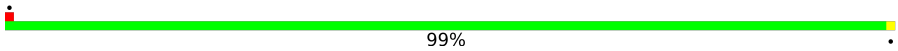
Chain T:

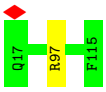




• Molecule 24: 60S ribosomal protein L22

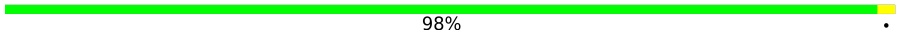
Chain U:

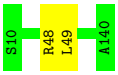




• Molecule 25: 60S ribosomal protein L23

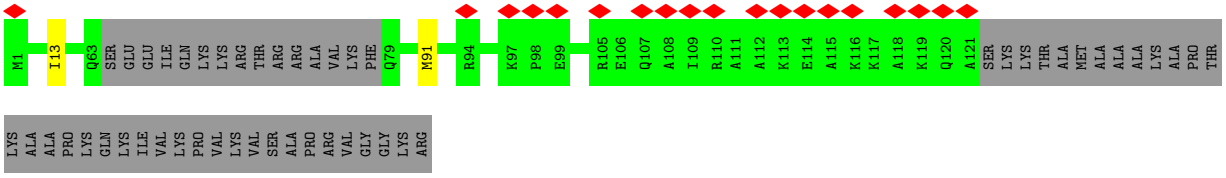
Chain V:





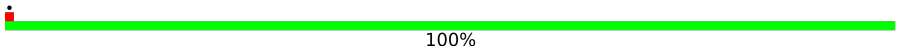
• Molecule 26: 60S ribosomal protein L24

Chain W:



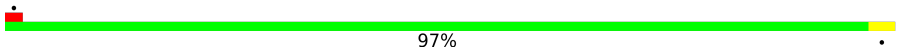
• Molecule 27: 60S ribosomal protein L23a

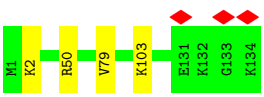
Chain X:



• Molecule 28: 60S ribosomal protein L26

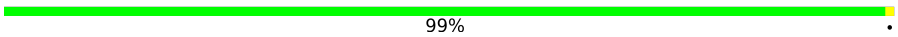
Chain Y:





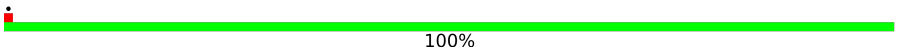
- Molecule 29: 60S ribosomal protein L27

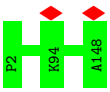
Chain Z:



- Molecule 30: 60S ribosomal protein L27a

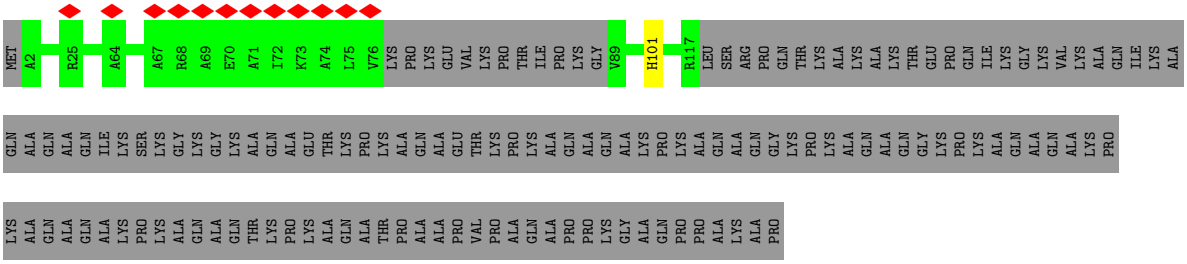
Chain a:





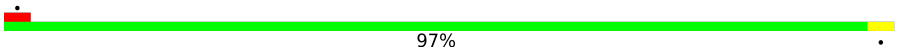
- Molecule 31: 60S ribosomal protein L29

Chain b:



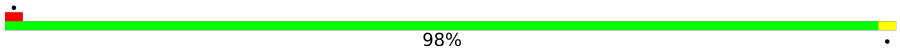
- Molecule 32: 60S ribosomal protein L30

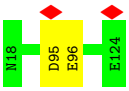
Chain c:



- Molecule 33: 60S ribosomal protein L31

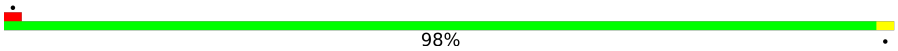
Chain d:

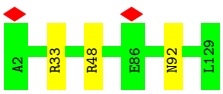




- Molecule 34: 60S ribosomal protein L32

Chain e:



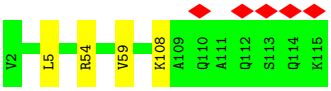


- Molecule 35: 60S ribosomal protein L35a

Chain f: 99%

• Molecule 36: 60S ribosomal protein L34

Chain g: 96%



• Molecule 37: 60S ribosomal protein L35

Chain h: 99%

• Molecule 38: 60S ribosomal protein L36

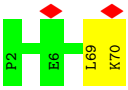
Chain i: 99%

• Molecule 39: 60S ribosomal protein L37

Chain j: 99%

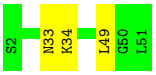
• Molecule 40: 60S ribosomal protein L38

Chain k: 97%



• Molecule 41: 60S ribosomal protein L39

Chain l: 94% 6%



• Molecule 42: 60S ribosomal protein L40

Chain m: 98%

I51 C73 K102

• Molecule 43: 60S ribosomal protein L41

Chain n: 100%

There are no outlier residues recorded for this chain.

• Molecule 44: 60S ribosomal protein L36a

Chain o: 98%

V2 M82 R99 I104

• Molecule 45: 60S ribosomal protein L37a

Chain p: 99%

A2 R84 Q92

• Molecule 46: 60S ribosomal protein L28

Chain r: 98%

S2 L106 R107 M125

• Molecule 47: 60S ribosomal protein L10a

Chain u: 45% 97%

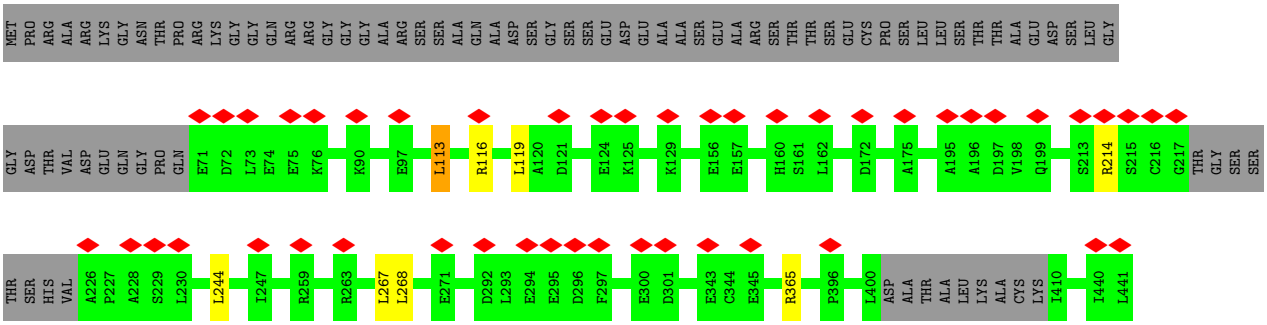
V5 S6 R7 D8 E12 R15 H19 G20 N21 Q22 R23 K24 R25 R26 E33 K39 K45 D46 K47 S50 V53 R54 L55 K56 R60 P61 V65 C66 V67 L68 G69 D70 Q71 Q72 D75 E76 A77 K78 A79 V80 D81 I82 D86 I87 E88 A89 L90 K91

K92 L93 N94 K95 N96 L99 L103 A104 K105 K106 Y107 D108 A112 S113 E114 S115 L116 I117 K118 Q119 I120 P121 R122 I123 P126 K130 A131 G132 S136 L137 L138 T139 H140 N141 E142 N143 M144 V145 A146 K147 V148 D149 E150 V151 T154 I155 K156 K173 M174 T175 D176 D177

E178 S192 L193 L194 K195 W198 Q199 I206 K207 S208 T209 M210

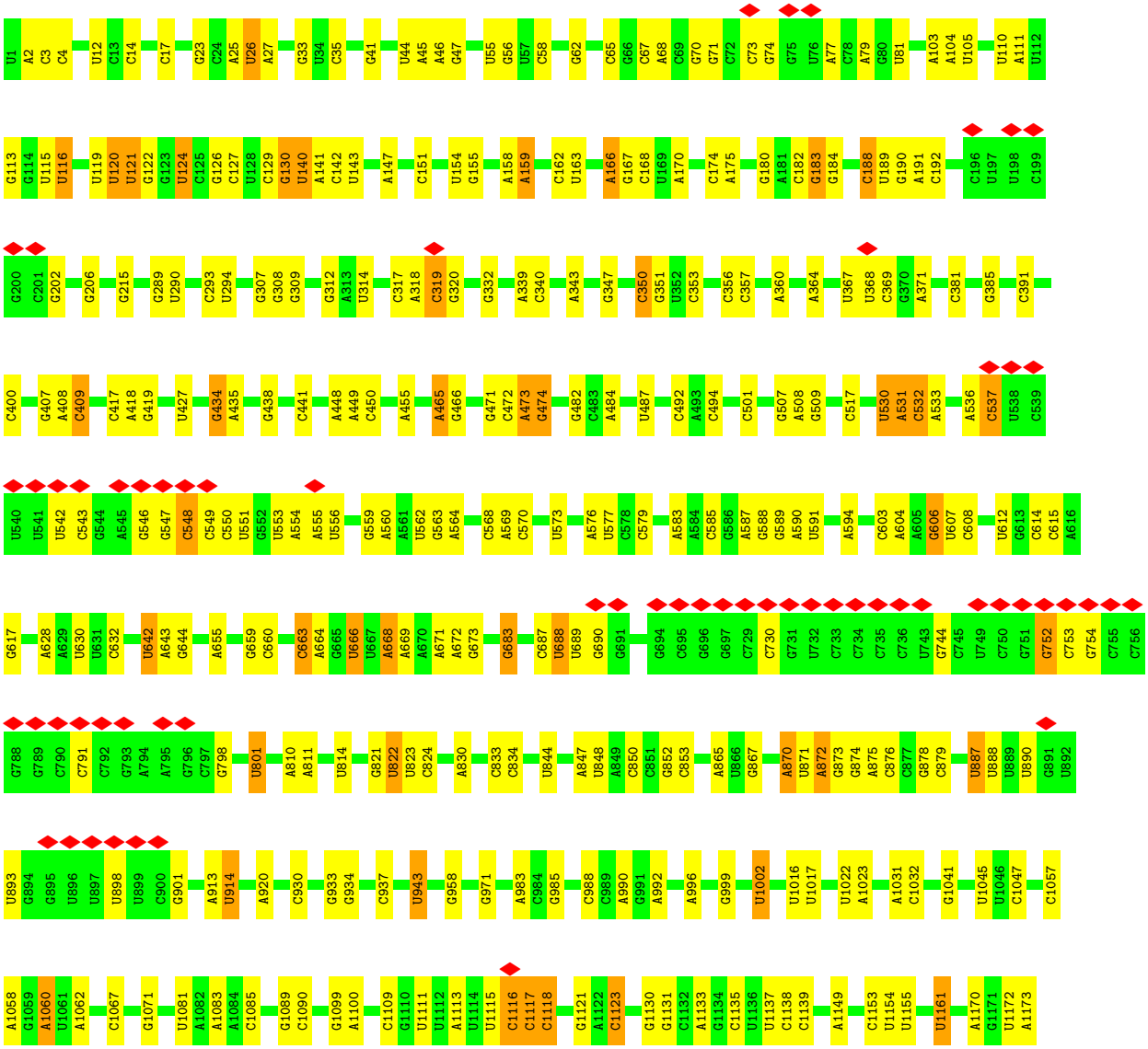
• Molecule 48: Interferon-related developmental regulator 2

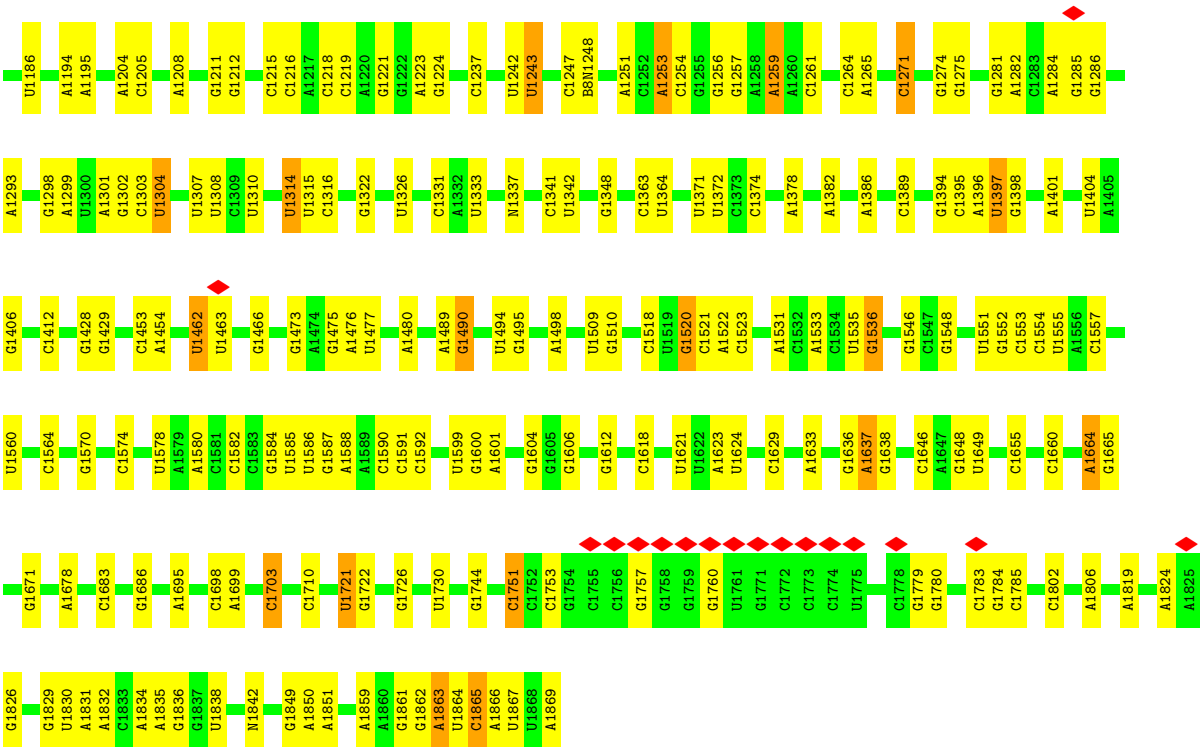
Chain v:



- Molecule 49: 18S rRNA

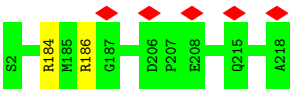
Chain 9:





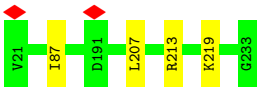
- Molecule 50: 40S ribosomal protein SA

Chain AA: 99%



- Molecule 51: 40S ribosomal protein S3a

Chain BB: 98%

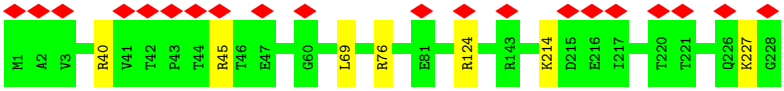


- Molecule 52: 40S ribosomal protein S2

Chain CC: 98%

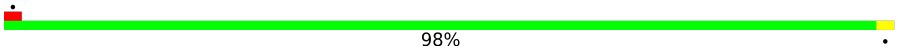
- Molecule 53: 40S ribosomal protein S3

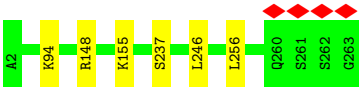
Chain DD: 9% 97%



• Molecule 54: 40S ribosomal protein S4, X isoform

Chain EE:



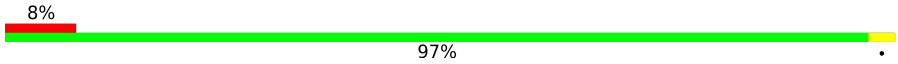


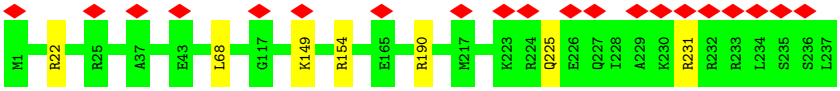
• Molecule 55: 40S ribosomal protein S5

Chain FF:

• Molecule 56: 40S ribosomal protein S6

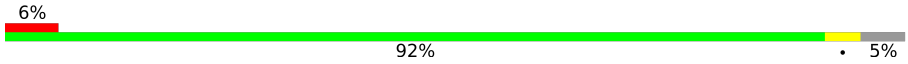
Chain GG:

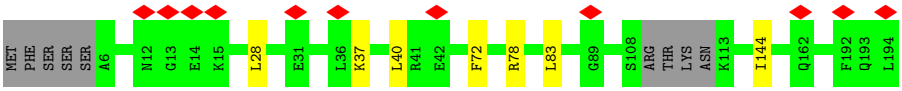




• Molecule 57: 40S ribosomal protein S7

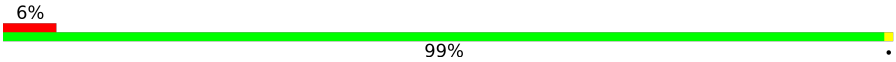
Chain HH:

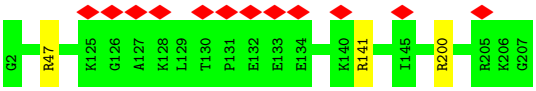




• Molecule 58: 40S ribosomal protein S8

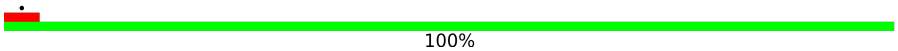
Chain II:

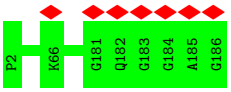




• Molecule 59: 40S ribosomal protein S9

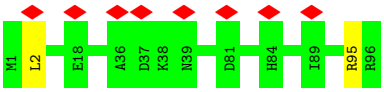
Chain JJ:





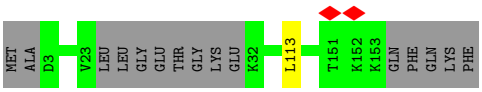
• Molecule 60: 40S ribosomal protein S10

Chain KK: 8% 98%



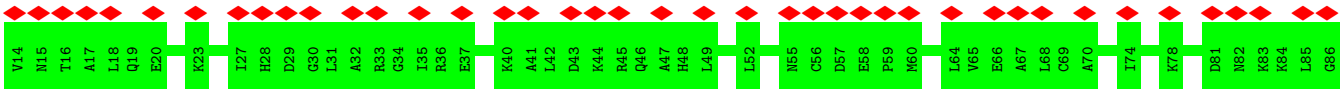
• Molecule 61: 40S ribosomal protein S11

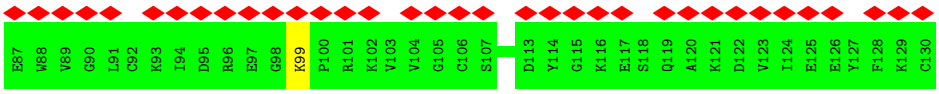
Chain LL: 90% 9%



• Molecule 62: 40S ribosomal protein S12

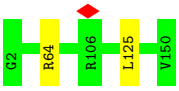
Chain MM: 65% 99%





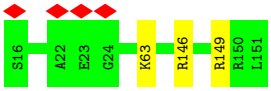
• Molecule 63: 40S ribosomal protein S13

Chain NN: 99%



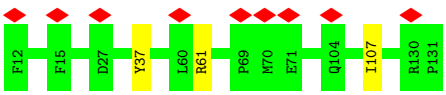
• Molecule 64: 40S ribosomal protein S14

Chain OO: 98%



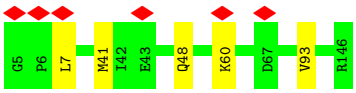
• Molecule 65: 40S ribosomal protein S15

Chain PP: 8% 98%

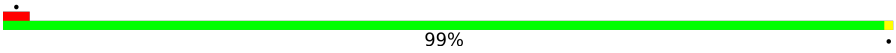


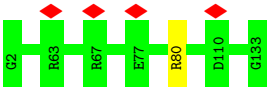
• Molecule 66: 40S ribosomal protein S16

Chain QQ: 96%

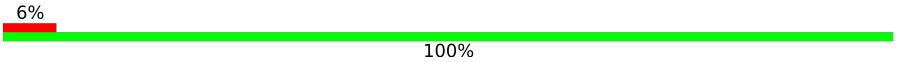


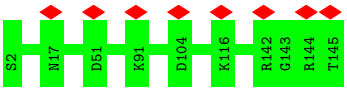
• Molecule 67: 40S ribosomal protein S17

Chain RR: 

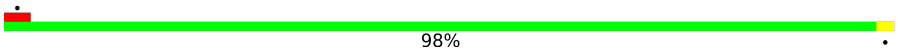


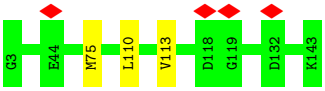
• Molecule 68: 40S ribosomal protein S18

Chain SS: 

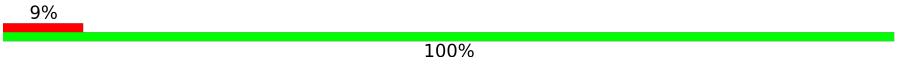


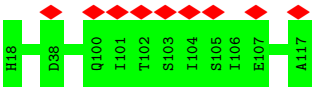
• Molecule 69: 40S ribosomal protein S19

Chain TT: 

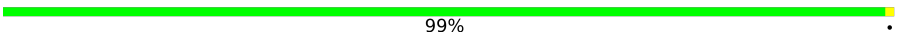


• Molecule 70: 40S ribosomal protein S20

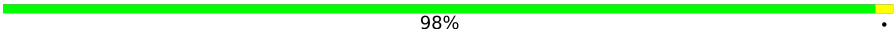
Chain UU: 

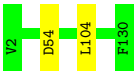


• Molecule 71: 40S ribosomal protein S21

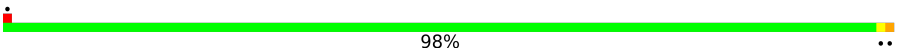
Chain VV: 

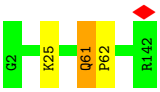
• Molecule 72: 40S ribosomal protein S15a

Chain WW: 

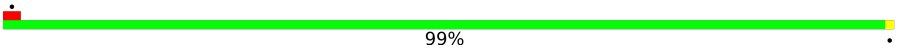


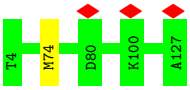
• Molecule 73: 40S ribosomal protein S23

Chain XX: 

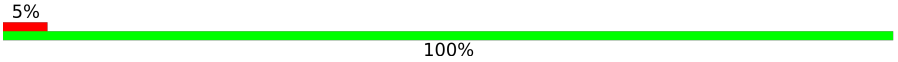


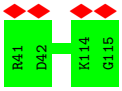
• Molecule 74: 40S ribosomal protein S24

Chain YY: 

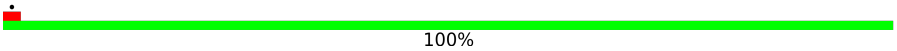


• Molecule 75: 40S ribosomal protein S25

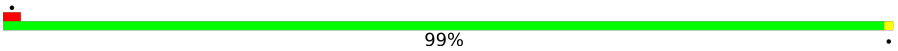
Chain ZZ: 

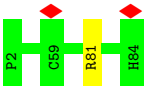


• Molecule 76: 40S ribosomal protein S26

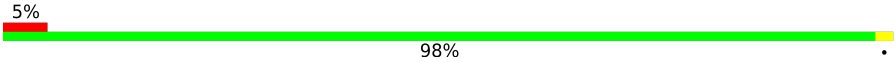
Chain aa: 

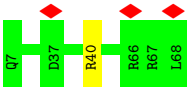
• Molecule 77: 40S ribosomal protein S27

Chain bb: 

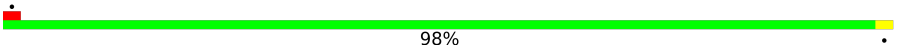


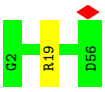
• Molecule 78: 40S ribosomal protein S28

Chain cc: 



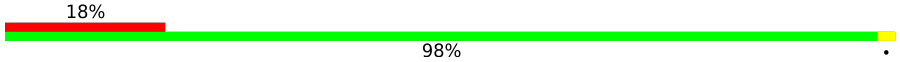
• Molecule 79: 40S ribosomal protein S29

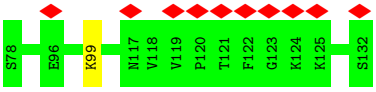
Chain dd: 



- Molecule 80: 40S ribosomal protein S30

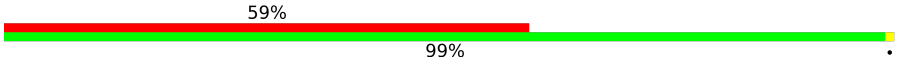
Chain ee:

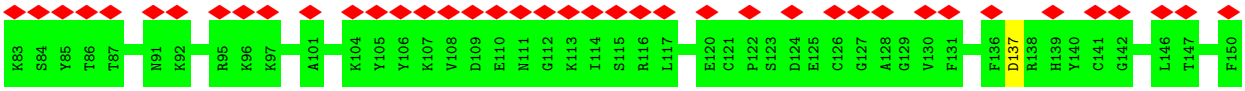




- Molecule 81: 40S ribosomal protein S27a

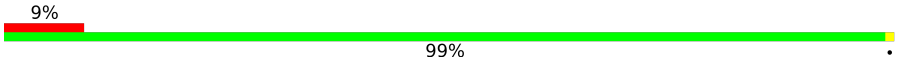
Chain ff:

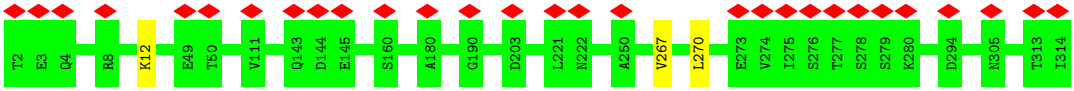




- Molecule 82: Receptor of activated protein C kinase 1

Chain gg:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74031	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.018	Depositor
Minimum map value	-0.622	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: E7G, I4U, B8H, B8Q, B8W, E6G, OMC, 5MC, OMG, P7G, B8N, MG, PSU, MA6, B9H, 4AC, UR3, BGH, OMU, M7A, 6MZ, 7MG, E3C, 2MG, A2M, MHG, MLZ, ZN, B9B, 1MA, P4U, 5MU, B8T, B8K

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	4	0.42	0/1779	1.19	17/2771 (0.6%)
2	5	0.90	0/83825	1.21	704/130614 (0.5%)
3	7	0.87	0/2858	1.14	15/4455 (0.3%)
4	8	0.90	0/3559	1.20	27/5543 (0.5%)
5	A	0.59	0/1936	0.72	1/2596 (0.0%)
6	B	0.55	0/3240	0.70	4/4339 (0.1%)
7	C	0.52	0/2927	0.64	0/3932
8	D	0.48	0/2437	0.58	0/3264
9	E	0.43	0/1762	0.64	1/2362 (0.0%)
10	F	0.54	0/1911	0.65	0/2549
11	G	0.47	0/1910	0.64	0/2569
12	H	0.48	0/1535	0.67	1/2063 (0.0%)
13	I	0.49	0/1702	0.60	0/2272
14	J	0.44	0/1385	0.68	1/1852 (0.1%)
15	L	0.46	0/1733	0.64	0/2316
16	M	0.51	0/1158	0.63	0/1547
17	N	0.60	0/1746	0.65	0/2338
18	O	0.54	0/1662	0.66	0/2222
19	P	0.56	0/1268	0.63	0/1700
20	Q	0.52	0/1539	0.67	0/2054
21	R	0.49	0/1524	0.70	2/2013 (0.1%)
22	S	0.56	0/1501	0.65	0/2012
23	T	0.54	0/1326	0.64	0/1770
24	U	0.41	0/823	0.67	0/1104
25	V	0.52	0/993	0.66	1/1332 (0.1%)
26	W	0.48	0/873	0.63	1/1158 (0.1%)
27	X	0.47	0/984	0.61	0/1323
28	Y	0.50	0/1132	0.65	0/1504
29	Z	0.52	0/1130	0.61	0/1507
30	a	0.56	0/1191	0.63	0/1590

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	b	0.40	0/861	0.61	0/1138
32	c	0.55	0/771	0.69	0/1034
33	d	0.50	0/903	0.65	0/1216
34	e	0.52	0/1071	0.58	0/1429
35	f	0.57	0/895	0.65	0/1198
36	g	0.51	0/916	0.66	0/1220
37	h	0.45	0/1021	0.62	0/1348
38	i	0.46	0/841	0.61	0/1112
39	j	0.55	0/720	0.68	0/952
40	k	0.43	0/575	0.61	0/761
41	l	0.51	0/459	0.67	1/608 (0.2%)
42	m	0.50	0/425	0.68	0/561
43	n	0.44	0/240	0.72	0/305
44	o	0.49	0/855	0.60	0/1128
45	p	0.57	0/718	0.62	0/953
46	r	0.55	0/1010	0.68	0/1354
47	u	0.33	0/1680	0.72	1/2255 (0.0%)
48	v	0.37	0/2779	0.71	5/3751 (0.1%)
49	9	0.76	0/39723	1.19	338/61870 (0.5%)
50	AA	0.48	0/1747	0.68	0/2374
51	BB	0.46	0/1756	0.67	0/2350
52	CC	0.49	0/1753	0.69	0/2369
53	DD	0.38	0/1796	0.67	1/2417 (0.0%)
54	EE	0.44	1/2118 (0.0%)	0.65	1/2849 (0.0%)
55	FF	0.42	0/1492	0.64	1/2005 (0.0%)
56	GG	0.38	0/1946	0.64	1/2590 (0.0%)
57	HH	0.40	0/1510	0.69	1/2022 (0.0%)
58	II	0.46	0/1715	0.63	0/2287
59	JJ	0.41	0/1550	0.61	0/2069
60	KK	0.37	0/834	0.65	1/1125 (0.1%)
61	LL	0.52	0/1195	0.63	1/1597 (0.1%)
62	MM	0.35	0/918	0.70	0/1233
63	NN	0.46	0/1226	0.68	1/1649 (0.1%)
64	OO	0.49	0/1029	0.65	0/1380
65	PP	0.39	0/1017	0.62	1/1358 (0.1%)
66	QQ	0.41	0/1146	0.65	1/1534 (0.1%)
67	RR	0.38	0/1082	0.65	0/1452
68	SS	0.36	0/1208	0.66	0/1618
69	TT	0.37	0/1115	0.60	1/1493 (0.1%)
70	UU	0.36	0/805	0.63	0/1081
71	VV	0.46	0/643	0.60	0/860
72	WW	0.50	0/1051	0.69	0/1406
73	XX	0.45	0/1116	0.67	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
74	YY	0.40	0/1028	0.56	0/1366
75	ZZ	0.35	0/604	0.62	0/810
76	aa	0.48	0/828	0.62	0/1109
77	bb	0.40	0/665	0.62	0/891
78	cc	0.40	0/490	0.61	0/656
79	dd	0.47	0/470	0.59	0/623
80	ee	0.38	0/447	0.59	0/587
81	ff	0.33	0/567	0.56	0/753
82	gg	0.35	0/2493	0.64	0/3394
All	All	0.72	1/229172 (0.0%)	1.02	1131/335661 (0.3%)

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	B	0	1
7	C	0	1
11	G	0	1
12	H	0	1
15	L	0	2
17	N	0	3
18	O	0	1
23	T	0	1
31	b	0	1
33	d	0	1
40	k	0	1
47	u	0	2
52	CC	0	1
54	EE	0	1
71	VV	0	1
72	WW	0	1
73	XX	0	1
81	ff	0	1
All	All	0	22

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	EE	237	SER	C-N	-5.43	1.21	1.34

The worst 5 of 1131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	9	501	C	C2-N1-C1'	12.91	133.00	118.80
2	5	1978	C	N1-C2-O2	12.32	126.29	118.90
49	9	501	C	N1-C2-O2	12.10	126.16	118.90
2	5	2505	C	N1-C2-O2	12.03	126.11	118.90
2	5	4056	A	OP1-P-O3'	-11.92	78.98	105.20

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B	55	HIS	Peptide
7	C	73	VAL	Peptide
11	G	215	ASP	Peptide
12	H	50	LYS	Peptide
15	L	46	ILE	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
5	A	246/248 (99%)	218 (89%)	28 (11%)	0	100 100
6	B	392/394 (100%)	364 (93%)	27 (7%)	1 (0%)	41 72
7	C	359/362 (99%)	343 (96%)	16 (4%)	0	100 100
8	D	291/293 (99%)	277 (95%)	14 (5%)	0	100 100
9	E	208/291 (72%)	193 (93%)	15 (7%)	0	100 100
10	F	223/225 (99%)	215 (96%)	8 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	G	229/319 (72%)	221 (96%)	8 (4%)	0	100	100
12	H	188/190 (99%)	179 (95%)	9 (5%)	0	100	100
13	I	201/214 (94%)	194 (96%)	7 (4%)	0	100	100
14	J	168/170 (99%)	166 (99%)	2 (1%)	0	100	100
15	L	208/210 (99%)	200 (96%)	7 (3%)	1 (0%)	29	61
16	M	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
17	N	201/203 (99%)	186 (92%)	15 (8%)	0	100	100
18	O	197/199 (99%)	193 (98%)	4 (2%)	0	100	100
19	P	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
20	Q	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
21	R	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
22	S	174/176 (99%)	164 (94%)	9 (5%)	1 (1%)	25	57
23	T	157/159 (99%)	148 (94%)	9 (6%)	0	100	100
24	U	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
25	V	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
26	W	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
27	X	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
28	Y	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
29	Z	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	19	51
30	a	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
31	b	100/245 (41%)	93 (93%)	7 (7%)	0	100	100
32	c	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
33	d	105/107 (98%)	95 (90%)	9 (9%)	1 (1%)	15	46
34	e	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
35	f	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
36	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
37	h	120/122 (98%)	120 (100%)	0	0	100	100
38	i	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
39	j	84/86 (98%)	75 (89%)	9 (11%)	0	100	100
40	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
41	l	48/50 (96%)	41 (85%)	7 (15%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	m	49/52 (94%)	43 (88%)	5 (10%)	1 (2%)	7	30
43	n	23/25 (92%)	23 (100%)	0	0	100	100
44	o	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
45	p	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
46	r	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
47	u	204/206 (99%)	173 (85%)	29 (14%)	2 (1%)	15	46
48	v	348/441 (79%)	320 (92%)	28 (8%)	0	100	100
50	AA	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
51	BB	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
52	CC	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
53	DD	226/228 (99%)	217 (96%)	9 (4%)	0	100	100
54	EE	260/262 (99%)	243 (94%)	17 (6%)	0	100	100
55	FF	181/204 (89%)	172 (95%)	9 (5%)	0	100	100
56	GG	235/237 (99%)	226 (96%)	9 (4%)	0	100	100
57	HH	181/194 (93%)	172 (95%)	9 (5%)	0	100	100
58	II	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
59	JJ	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
60	KK	94/96 (98%)	86 (92%)	8 (8%)	0	100	100
61	LL	139/158 (88%)	132 (95%)	7 (5%)	0	100	100
62	MM	115/117 (98%)	102 (89%)	13 (11%)	0	100	100
63	NN	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
64	OO	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
65	PP	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
66	QQ	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
67	RR	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
68	SS	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
69	TT	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
70	UU	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
71	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
72	WW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
73	XX	139/141 (99%)	130 (94%)	7 (5%)	2 (1%)	11	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	YY	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
75	ZZ	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
76	aa	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
77	bb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
78	cc	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
79	dd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
80	ee	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
81	ff	66/68 (97%)	58 (88%)	8 (12%)	0	100	100
82	gg	311/313 (99%)	279 (90%)	32 (10%)	0	100	100
All	All	11723/12395 (95%)	11060 (94%)	653 (6%)	10 (0%)	54	82

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	m	73	CYS
6	B	295	ASP
33	d	96	GLU
47	u	61	PRO
47	u	198	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	190/190 (100%)	185 (97%)	5 (3%)	46	72
6	B	342/342 (100%)	339 (99%)	3 (1%)	78	90
7	C	301/301 (100%)	296 (98%)	5 (2%)	60	80
8	D	247/247 (100%)	244 (99%)	3 (1%)	71	85
9	E	190/251 (76%)	187 (98%)	3 (2%)	62	81
10	F	196/196 (100%)	196 (100%)	0	100	100
11	G	200/272 (74%)	195 (98%)	5 (2%)	47	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	H	169/169 (100%)	166 (98%)	3 (2%)	59	79
13	I	175/181 (97%)	174 (99%)	1 (1%)	86	94
14	J	143/143 (100%)	142 (99%)	1 (1%)	84	92
15	L	175/175 (100%)	170 (97%)	5 (3%)	42	69
16	M	117/117 (100%)	115 (98%)	2 (2%)	60	80
17	N	171/171 (100%)	168 (98%)	3 (2%)	59	79
18	O	171/171 (100%)	169 (99%)	2 (1%)	71	85
19	P	134/134 (100%)	133 (99%)	1 (1%)	84	92
20	Q	164/164 (100%)	161 (98%)	3 (2%)	59	79
21	R	159/159 (100%)	158 (99%)	1 (1%)	86	94
22	S	157/157 (100%)	154 (98%)	3 (2%)	57	78
23	T	139/139 (100%)	137 (99%)	2 (1%)	67	83
24	U	89/89 (100%)	88 (99%)	1 (1%)	73	86
25	V	101/101 (100%)	100 (99%)	1 (1%)	76	88
26	W	86/126 (68%)	85 (99%)	1 (1%)	71	85
27	X	106/106 (100%)	106 (100%)	0	100	100
28	Y	124/124 (100%)	120 (97%)	4 (3%)	39	67
29	Z	117/117 (100%)	117 (100%)	0	100	100
30	a	119/119 (100%)	119 (100%)	0	100	100
31	b	84/184 (46%)	84 (100%)	0	100	100
32	c	84/84 (100%)	81 (96%)	3 (4%)	35	63
33	d	98/98 (100%)	98 (100%)	0	100	100
34	e	114/114 (100%)	111 (97%)	3 (3%)	46	72
35	f	88/88 (100%)	87 (99%)	1 (1%)	73	86
36	g	98/98 (100%)	94 (96%)	4 (4%)	30	59
37	h	109/109 (100%)	108 (99%)	1 (1%)	78	90
38	i	86/86 (100%)	85 (99%)	1 (1%)	71	85
39	j	73/73 (100%)	72 (99%)	1 (1%)	67	83
40	k	64/64 (100%)	63 (98%)	1 (2%)	62	81
41	l	47/47 (100%)	45 (96%)	2 (4%)	29	59
42	m	47/47 (100%)	47 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	n	24/24 (100%)	24 (100%)	0	100	100
44	o	91/91 (100%)	89 (98%)	2 (2%)	52	75
45	p	74/74 (100%)	73 (99%)	1 (1%)	67	83
46	r	108/108 (100%)	106 (98%)	2 (2%)	57	78
47	u	186/186 (100%)	183 (98%)	3 (2%)	62	81
48	v	289/355 (81%)	284 (98%)	5 (2%)	60	80
50	AA	180/181 (99%)	178 (99%)	2 (1%)	73	86
51	BB	194/194 (100%)	190 (98%)	4 (2%)	53	76
52	CC	187/187 (100%)	184 (98%)	3 (2%)	62	81
53	DD	190/190 (100%)	184 (97%)	6 (3%)	39	67
54	EE	224/224 (100%)	221 (99%)	3 (1%)	69	84
55	FF	158/170 (93%)	153 (97%)	5 (3%)	39	67
56	GG	207/207 (100%)	201 (97%)	6 (3%)	42	69
57	HH	165/174 (95%)	159 (96%)	6 (4%)	35	63
58	II	178/178 (100%)	175 (98%)	3 (2%)	60	80
59	JJ	161/161 (100%)	161 (100%)	0	100	100
60	KK	87/87 (100%)	86 (99%)	1 (1%)	73	86
61	LL	130/142 (92%)	130 (100%)	0	100	100
62	MM	99/99 (100%)	98 (99%)	1 (1%)	76	88
63	NN	130/130 (100%)	129 (99%)	1 (1%)	81	91
64	OO	106/106 (100%)	103 (97%)	3 (3%)	43	70
65	PP	109/109 (100%)	107 (98%)	2 (2%)	59	79
66	QQ	117/117 (100%)	113 (97%)	4 (3%)	37	65
67	RR	119/119 (100%)	118 (99%)	1 (1%)	81	91
68	SS	125/125 (100%)	125 (100%)	0	100	100
69	TT	111/111 (100%)	109 (98%)	2 (2%)	59	79
70	UU	92/92 (100%)	92 (100%)	0	100	100
71	VV	67/67 (100%)	67 (100%)	0	100	100
72	WW	112/112 (100%)	111 (99%)	1 (1%)	78	90
73	XX	113/113 (100%)	112 (99%)	1 (1%)	78	90
74	YY	107/107 (100%)	106 (99%)	1 (1%)	78	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	ZZ	66/66 (100%)	66 (100%)	0	100	100
76	aa	88/88 (100%)	88 (100%)	0	100	100
77	bb	75/75 (100%)	74 (99%)	1 (1%)	69	84
78	cc	55/55 (100%)	54 (98%)	1 (2%)	59	79
79	dd	48/48 (100%)	47 (98%)	1 (2%)	53	76
80	ee	46/46 (100%)	45 (98%)	1 (2%)	52	75
81	ff	61/61 (100%)	61 (100%)	0	100	100
82	gg	272/272 (100%)	269 (99%)	3 (1%)	73	86
All	All	10225/10604 (96%)	10074 (98%)	151 (2%)	66	82

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	GG	225	GLN
74	YY	74	MET
57	HH	72	PHE
64	OO	146	ARG
82	gg	270	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
19	P	64	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	4	74/75 (98%)	35 (47%)	1 (1%)
2	5	3526/3597 (98%)	884 (25%)	68 (1%)
3	7	119/120 (99%)	14 (11%)	0
4	8	149/151 (98%)	27 (18%)	1 (0%)
49	9	1671/1698 (98%)	388 (23%)	20 (1%)
All	All	5539/5641 (98%)	1348 (24%)	90 (1%)

5 of 1348 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	4	2	C
1	4	3	C
1	4	4	C
1	4	8	U
1	4	9	A

5 of 90 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	4075	U
49	9	140	U
2	5	4232	U
2	5	4884	G
49	9	553	U

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

137 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	A2M	5	1326	2	18,25,26	4.64	9 (50%)	18,36,39	2.76	4 (22%)
49	E3C	9	568	49	18,23,24	3.45	6 (33%)	21,33,36	2.47	5 (23%)
2	A2M	5	4523	83,2	18,25,26	4.78	8 (44%)	18,36,39	2.67	3 (16%)
49	PSU	9	823	49	18,21,22	1.03	1 (5%)	22,30,33	1.68	4 (18%)
2	B8K	5	4690	12,2	24,28,29	5.02	16 (66%)	30,42,45	2.66	13 (43%)
2	B8K	5	3897	2	24,28,29	4.79	17 (70%)	30,42,45	2.60	14 (46%)
2	I4U	5	1659	2	21,24,25	4.90	16 (76%)	27,34,37	1.38	2 (7%)
2	P4U	5	1348	83,2	21,24,25	3.37	8 (38%)	27,33,36	1.29	2 (7%)
2	2MG	5	729	2	18,26,27	2.45	7 (38%)	16,38,41	1.30	3 (18%)
2	2MG	5	1517	2	18,26,27	2.53	7 (38%)	16,38,41	1.59	3 (18%)
49	4AC	9	1337	49	21,24,25	3.16	10 (47%)	29,34,37	1.14	4 (13%)
2	OMG	5	1522	2	18,26,27	2.44	8 (44%)	19,38,41	1.62	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	B8T	5	4483	2	19,22,23	3.00	8 (42%)	26,31,34	1.12	2 (7%)
49	5MU	9	814	49	19,22,23	4.79	7 (36%)	28,32,35	3.53	11 (39%)
2	A2M	5	3718	2	18,25,26	4.78	10 (55%)	18,36,39	2.48	3 (16%)
2	PSU	5	4293	2	18,21,22	1.06	2 (11%)	22,30,33	1.76	4 (18%)
2	B9B	5	2754	83,2	21,28,29	6.28	9 (42%)	23,40,43	2.00	5 (21%)
49	PSU	9	1243	49	18,21,22	1.19	2 (11%)	22,30,33	1.32	4 (18%)
49	OMC	9	1703	49	19,22,23	2.93	7 (36%)	26,31,34	0.72	0
2	PSU	5	4500	2	18,21,22	1.02	3 (16%)	22,30,33	1.92	5 (22%)
49	UR3	9	1830	49	19,22,23	2.57	6 (31%)	26,32,35	1.65	4 (15%)
2	A2M	5	3825	2	18,25,26	4.67	8 (44%)	18,36,39	2.83	4 (22%)
4	OMU	8	14	4,2	19,22,23	2.78	7 (36%)	26,31,34	1.93	6 (23%)
2	OMC	5	3887	2	19,22,23	2.73	7 (36%)	26,31,34	0.86	1 (3%)
49	MA6	9	1851	49	19,26,27	1.06	1 (5%)	18,38,41	2.79	2 (11%)
2	6MZ	5	4220	2	18,25,26	2.18	4 (22%)	16,36,39	1.94	4 (25%)
2	5MC	5	4335	2	18,22,23	3.54	7 (38%)	26,32,35	1.25	3 (11%)
2	OMG	5	1625	83,2	18,26,27	2.36	8 (44%)	19,38,41	1.49	4 (21%)
2	7MG	5	4550	2	22,26,27	3.40	10 (45%)	29,39,42	2.03	10 (34%)
49	OMC	9	174	49	19,22,23	2.88	7 (36%)	26,31,34	0.71	0
2	5MU	5	4083	2	19,22,23	4.66	7 (36%)	28,32,35	3.73	11 (39%)
2	E7G	5	1797	2	24,27,28	3.60	11 (45%)	30,40,43	2.18	10 (33%)
49	A2M	9	27	83,49	18,25,26	4.75	9 (50%)	18,36,39	2.59	3 (16%)
2	E7G	5	2297	2	24,27,28	3.51	11 (45%)	30,40,43	2.14	9 (30%)
2	1MA	5	4415	2	16,25,26	3.92	4 (25%)	18,37,40	1.72	3 (16%)
2	PSU	5	4531	2	18,21,22	1.09	2 (11%)	22,30,33	1.86	5 (22%)
2	B9H	5	2786	2	20,25,26	2.91	3 (15%)	22,35,38	1.65	2 (9%)
49	6MZ	9	1832	83,49	18,25,26	2.25	3 (16%)	16,36,39	1.93	3 (18%)
49	OMG	9	509	83,49	18,26,27	2.40	8 (44%)	19,38,41	1.52	4 (21%)
49	OMU	9	121	49	19,22,23	2.85	7 (36%)	26,31,34	1.87	6 (23%)
2	OMC	5	2861	2	19,22,23	2.84	7 (36%)	26,31,34	1.04	2 (7%)
49	A2M	9	159	49	18,25,26	4.86	8 (44%)	18,36,39	2.65	4 (22%)
2	P7G	5	3880	2	24,28,29	3.89	10 (41%)	27,41,44	1.72	4 (14%)
2	B8W	5	4129	2	18,26,27	5.24	8 (44%)	21,38,41	5.97	10 (47%)
2	UR3	5	4530	2	19,22,23	2.65	7 (36%)	26,32,35	1.41	5 (19%)
2	OMG	5	4637	2	18,26,27	2.36	8 (44%)	19,38,41	1.56	4 (21%)
2	PSU	5	1677	2	18,21,22	1.19	3 (16%)	22,30,33	1.93	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	A2M	5	1524	2	18,25,26	4.66	11 (61%)	18,36,39	2.76	4 (22%)
2	PSU	5	4403	2	18,21,22	0.98	1 (5%)	22,30,33	1.85	5 (22%)
2	A2M	5	4571	2	18,25,26	4.77	9 (50%)	18,36,39	2.65	3 (16%)
2	OMC	5	2804	2	19,22,23	2.82	7 (36%)	26,31,34	0.88	1 (3%)
2	1MA	5	1322	83,2	16,25,26	3.67	4 (25%)	18,37,40	1.84	3 (16%)
2	OMG	5	4494	2	18,26,27	2.49	8 (44%)	19,38,41	1.68	6 (31%)
2	B8T	5	4671	2	19,22,23	3.02	8 (42%)	26,31,34	0.90	1 (3%)
2	B8H	5	4296	2	19,22,23	6.84	7 (36%)	22,32,35	2.46	5 (22%)
2	OMG	5	4370	2	18,26,27	2.46	8 (44%)	19,38,41	1.54	4 (21%)
2	A2M	5	398	2	18,25,26	4.78	9 (50%)	18,36,39	2.57	3 (16%)
49	4AC	9	1842	49	21,24,25	3.09	10 (47%)	29,34,37	1.29	4 (13%)
2	BGH	5	3899	83,2	25,29,30	4.13	16 (64%)	31,43,46	2.59	15 (48%)
2	B8Q	5	1456	2	17,22,23	2.76	5 (29%)	22,32,35	2.08	5 (22%)
2	A2M	5	3867	2	18,25,26	4.71	8 (44%)	18,36,39	2.55	3 (16%)
2	PSU	5	4442	2	18,21,22	1.06	2 (11%)	22,30,33	1.92	5 (22%)
49	A2M	9	1031	49	18,25,26	4.79	9 (50%)	18,36,39	2.54	3 (16%)
2	OMC	5	3869	2	19,22,23	2.77	7 (36%)	26,31,34	0.79	0
2	OMC	5	4536	2	19,22,23	2.75	7 (36%)	26,31,34	1.00	1 (3%)
2	A2M	5	2363	83,2	18,25,26	4.76	10 (55%)	18,36,39	2.69	4 (22%)
2	PSU	5	4636	2	18,21,22	1.11	2 (11%)	22,30,33	1.95	5 (22%)
2	OMG	5	1883	2	18,26,27	2.52	8 (44%)	19,38,41	1.69	5 (26%)
7	MLZ	C	333	7	8,9,10	0.88	0	4,9,11	0.81	0
2	5MC	5	3782	2	18,22,23	3.50	7 (38%)	26,32,35	1.15	2 (7%)
2	OMC	5	3909	2	19,22,23	2.81	7 (36%)	26,31,34	0.65	0
49	OMC	9	1710	49	19,22,23	2.91	7 (36%)	26,31,34	1.13	2 (7%)
2	PSU	5	4450	83,2	18,21,22	1.06	2 (11%)	22,30,33	2.08	4 (18%)
2	OMU	5	4306	2	19,22,23	2.66	7 (36%)	26,31,34	1.83	5 (19%)
49	OMU	9	116	49	19,22,23	2.78	7 (36%)	26,31,34	1.76	5 (19%)
49	OMG	9	683	49	18,26,27	2.50	8 (44%)	19,38,41	1.62	5 (26%)
49	A2M	9	668	83,49	18,25,26	4.65	9 (50%)	18,36,39	2.74	3 (16%)
2	OMG	5	373	2	18,26,27	2.47	8 (44%)	19,38,41	1.69	6 (31%)
2	A2M	5	3723	2	18,25,26	4.85	10 (55%)	18,36,39	2.61	3 (16%)
49	B8Q	9	1219	83,49	17,22,23	2.89	5 (29%)	22,32,35	2.62	7 (31%)
49	PSU	9	612	49	18,21,22	0.96	2 (11%)	22,30,33	1.66	5 (22%)
49	OMC	9	517	49	19,22,23	2.84	7 (36%)	26,31,34	0.98	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PSU	5	3715	2	18,21,22	1.00	1 (5%)	22,30,33	1.63	3 (13%)
2	B8W	5	4185	2	18,26,27	5.21	8 (44%)	21,38,41	5.94	10 (47%)
49	PSU	9	822	49	18,21,22	1.02	1 (5%)	22,30,33	1.79	5 (22%)
2	OMG	5	1316	2	18,26,27	2.50	8 (44%)	19,38,41	1.72	5 (26%)
49	5MC	9	1374	49	18,22,23	3.55	7 (38%)	26,32,35	1.05	1 (3%)
2	OMU	5	4620	2	19,22,23	2.68	7 (36%)	26,31,34	1.93	6 (23%)
2	7MG	5	1605	2	22,26,27	3.42	10 (45%)	29,39,42	2.04	9 (31%)
49	B8N	9	1248	49	24,29,30	2.78	6 (25%)	29,42,45	1.75	5 (17%)
2	PSU	5	4628	2	18,21,22	1.07	2 (11%)	22,30,33	2.08	4 (18%)
2	2MG	5	4872	16,2	18,26,27	2.66	7 (38%)	16,38,41	1.70	4 (25%)
2	B8W	5	2380	2	18,26,27	5.21	8 (44%)	21,38,41	6.19	8 (38%)
2	B8H	5	1860	2	19,22,23	6.79	6 (31%)	22,32,35	2.31	5 (22%)
49	M7A	9	1806	49	20,25,26	2.04	3 (15%)	28,37,40	3.67	8 (28%)
49	PSU	9	1081	49	18,21,22	1.08	3 (16%)	22,30,33	1.66	4 (18%)
2	OMC	5	2422	83,2	19,22,23	2.90	7 (36%)	26,31,34	0.79	0
2	PSU	5	3729	2	18,21,22	1.05	1 (5%)	22,30,33	1.70	4 (18%)
2	A2M	5	1871	83,2	18,25,26	4.67	8 (44%)	18,36,39	2.71	4 (22%)
2	PSU	5	3764	2	18,21,22	1.00	1 (5%)	22,30,33	1.58	4 (18%)
2	A2M	5	1534	83,2	18,25,26	4.66	10 (55%)	18,36,39	2.82	5 (27%)
2	5MC	5	4447	2	18,22,23	3.71	7 (38%)	26,32,35	1.11	1 (3%)
2	UR3	5	4597	2	19,22,23	2.58	6 (31%)	26,32,35	1.29	4 (15%)
49	A2M	9	1678	49	18,25,26	4.78	10 (55%)	18,36,39	2.69	3 (16%)
2	B8W	5	4529	83,2	18,26,27	5.21	8 (44%)	21,38,41	6.40	11 (52%)
2	OMG	5	2773	2	18,26,27	2.44	8 (44%)	19,38,41	1.49	4 (21%)
2	OMG	5	2050	2	18,26,27	2.42	8 (44%)	19,38,41	1.48	4 (21%)
2	E6G	5	4355	2	20,27,28	5.74	8 (40%)	22,39,42	2.42	7 (31%)
49	A2M	9	484	49	18,25,26	4.69	9 (50%)	18,36,39	2.78	4 (22%)
49	MA6	9	1850	49	19,26,27	1.05	1 (5%)	18,38,41	2.98	2 (11%)
2	OMC	5	3701	83,2	19,22,23	2.75	7 (36%)	26,31,34	0.84	0
2	OMG	5	4870	2	18,26,27	2.48	8 (44%)	19,38,41	1.48	4 (21%)
2	I4U	5	4194	2	21,24,25	4.90	16 (76%)	27,34,37	1.21	4 (14%)
2	OMC	5	2365	2	19,22,23	2.87	7 (36%)	26,31,34	0.93	0
2	OMG	5	2364	2	18,26,27	2.42	8 (44%)	19,38,41	1.61	4 (21%)
2	PSU	5	1582	2	18,21,22	1.16	1 (5%)	22,30,33	1.80	4 (18%)
2	A2M	5	2401	83,2	18,25,26	4.72	10 (55%)	18,36,39	2.61	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PSU	5	1683	2	18,21,22	1.20	2 (11%)	22,30,33	1.84	4 (18%)
2	B8W	5	4472	2	18,26,27	5.20	8 (44%)	21,38,41	5.87	9 (42%)
2	PSU	5	2508	2	18,21,22	0.99	1 (5%)	22,30,33	1.57	4 (18%)
2	OMG	5	3792	2	18,26,27	2.46	8 (44%)	19,38,41	1.58	4 (21%)
2	B9B	5	237	2	21,28,29	6.43	9 (42%)	23,40,43	2.39	7 (30%)
2	B8H	5	3762	2	19,22,23	6.80	6 (31%)	22,32,35	2.39	5 (22%)
2	OMG	5	4623	2	18,26,27	2.44	8 (44%)	19,38,41	1.56	4 (21%)
2	UR3	5	1866	2	19,22,23	2.43	6 (31%)	26,32,35	1.32	4 (15%)
2	A2M	5	3785	2	18,25,26	4.55	10 (55%)	18,36,39	2.61	3 (16%)
2	OMG	5	2424	2	18,26,27	2.53	8 (44%)	19,38,41	1.64	4 (21%)
49	A2M	9	166	49	18,25,26	4.86	8 (44%)	18,36,39	2.71	4 (22%)
49	OMG	9	644	49	18,26,27	2.43	8 (44%)	19,38,41	1.58	4 (21%)
2	OMG	5	4196	2	18,26,27	2.39	8 (44%)	19,38,41	1.54	4 (21%)
2	P7G	5	1909	2	24,28,29	4.09	10 (41%)	27,41,44	1.84	5 (18%)
42	MLZ	m	72	42	8,9,10	0.78	0	4,9,11	0.82	0
49	PSU	9	119	49	18,21,22	0.95	1 (5%)	22,30,33	1.61	4 (18%)
2	MHG	5	4371	2	29,32,33	3.99	11 (37%)	34,46,49	2.23	10 (29%)
2	7MG	5	2522	2	22,26,27	3.35	10 (45%)	29,39,42	2.05	8 (27%)
2	M7A	5	4564	2	20,25,26	2.00	3 (15%)	28,37,40	3.83	7 (25%)
2	B9B	5	1574	2	21,28,29	6.30	9 (42%)	23,40,43	2.13	7 (30%)

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	A2M	5	1326	2	-	0/5/27/28	0/3/3/3
49	E3C	9	568	49	-	6/9/44/45	0/2/2/2
2	A2M	5	4523	83,2	-	2/5/27/28	0/3/3/3
49	PSU	9	823	49	-	0/7/25/26	0/2/2/2
2	B8K	5	4690	12,2	-	0/11/41/42	0/3/3/3
2	B8K	5	3897	2	-	3/11/41/42	0/3/3/3
2	I4U	5	1659	2	-	2/9/29/30	0/2/2/2
2	P4U	5	1348	83,2	-	2/10/29/30	0/2/2/2
2	2MG	5	729	2	-	2/5/27/28	0/3/3/3
2	2MG	5	1517	2	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	4AC	9	1337	49	-	1/11/29/30	0/2/2/2
2	OMG	5	1522	2	-	0/5/27/28	0/3/3/3
2	B8T	5	4483	2	-	0/7/27/28	0/2/2/2
49	5MU	9	814	49	-	1/7/25/26	0/2/2/2
2	A2M	5	3718	2	-	0/5/27/28	0/3/3/3
2	PSU	5	4293	2	-	1/7/25/26	0/2/2/2
2	B9B	5	2754	83,2	-	3/7/29/30	0/3/3/3
49	PSU	9	1243	49	-	2/7/25/26	0/2/2/2
49	OMC	9	1703	49	-	2/9/27/28	0/2/2/2
2	PSU	5	4500	2	-	3/7/25/26	0/2/2/2
49	UR3	9	1830	49	-	2/7/25/26	0/2/2/2
2	A2M	5	3825	2	-	0/5/27/28	0/3/3/3
4	OMU	8	14	4,2	-	1/9/27/28	0/2/2/2
2	OMC	5	3887	2	-	1/9/27/28	0/2/2/2
49	MA6	9	1851	49	-	4/7/29/30	0/3/3/3
2	6MZ	5	4220	2	-	1/5/27/28	0/3/3/3
2	5MC	5	4335	2	-	0/7/25/26	0/2/2/2
2	OMG	5	1625	83,2	-	3/5/27/28	0/3/3/3
2	7MG	5	4550	2	-	0/7/37/38	0/3/3/3
49	OMC	9	174	49	-	0/9/27/28	0/2/2/2
2	5MU	5	4083	2	-	0/7/25/26	0/2/2/2
2	E7G	5	1797	2	-	3/9/39/40	0/3/3/3
49	A2M	9	27	83,49	-	0/5/27/28	0/3/3/3
2	E7G	5	2297	2	-	2/9/39/40	0/3/3/3
2	1MA	5	4415	2	-	2/3/25/26	0/3/3/3
2	PSU	5	4531	2	-	0/7/25/26	0/2/2/2
2	B9H	5	2786	2	-	2/12/47/48	0/2/2/2
49	6MZ	9	1832	83,49	-	1/5/27/28	0/3/3/3
49	OMG	9	509	83,49	-	2/5/27/28	0/3/3/3
49	OMU	9	121	49	-	2/9/27/28	0/2/2/2
2	OMC	5	2861	2	-	1/9/27/28	0/2/2/2
49	A2M	9	159	49	-	3/5/27/28	0/3/3/3
2	P7G	5	3880	2	-	3/10/40/41	0/3/3/3
2	B8W	5	4129	2	-	3/5/27/28	0/3/3/3
2	UR3	5	4530	2	-	1/7/25/26	0/2/2/2
2	OMG	5	4637	2	-	2/5/27/28	0/3/3/3
2	PSU	5	1677	2	-	0/7/25/26	0/2/2/2
2	A2M	5	1524	2	-	1/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	5	4403	2	-	2/7/25/26	0/2/2/2
2	A2M	5	4571	2	-	0/5/27/28	0/3/3/3
2	OMC	5	2804	2	-	0/9/27/28	0/2/2/2
2	1MA	5	1322	83,2	-	0/3/25/26	0/3/3/3
2	OMG	5	4494	2	-	4/5/27/28	0/3/3/3
2	B8T	5	4671	2	-	0/7/27/28	0/2/2/2
2	B8H	5	4296	2	-	0/7/25/26	0/2/2/2
2	OMG	5	4370	2	-	0/5/27/28	0/3/3/3
2	A2M	5	398	2	-	2/5/27/28	0/3/3/3
49	4AC	9	1842	49	-	0/11/29/30	0/2/2/2
2	BGH	5	3899	83,2	-	3/13/43/44	0/3/3/3
2	B8Q	5	1456	2	-	0/7/42/43	0/2/2/2
2	A2M	5	3867	2	-	2/5/27/28	0/3/3/3
2	PSU	5	4442	2	-	0/7/25/26	0/2/2/2
49	A2M	9	1031	49	-	0/5/27/28	0/3/3/3
2	OMC	5	3869	2	-	0/9/27/28	0/2/2/2
2	OMC	5	4536	2	-	0/9/27/28	0/2/2/2
2	A2M	5	2363	83,2	-	0/5/27/28	0/3/3/3
2	PSU	5	4636	2	-	3/7/25/26	0/2/2/2
2	OMG	5	1883	2	-	0/5/27/28	0/3/3/3
7	MLZ	C	333	7	-	2/7/8/10	-
2	5MC	5	3782	2	-	0/7/25/26	0/2/2/2
2	OMC	5	3909	2	-	0/9/27/28	0/2/2/2
49	OMC	9	1710	49	-	0/9/27/28	0/2/2/2
2	PSU	5	4450	83,2	-	4/7/25/26	0/2/2/2
2	OMU	5	4306	2	-	0/9/27/28	0/2/2/2
49	OMU	9	116	49	-	2/9/27/28	0/2/2/2
49	OMG	9	683	49	-	2/5/27/28	0/3/3/3
49	A2M	9	668	83,49	-	2/5/27/28	0/3/3/3
2	OMG	5	373	2	-	1/5/27/28	0/3/3/3
2	A2M	5	3723	2	-	0/5/27/28	0/3/3/3
49	B8Q	9	1219	83,49	-	1/7/42/43	0/2/2/2
49	PSU	9	612	49	-	0/7/25/26	0/2/2/2
49	OMC	9	517	49	-	2/9/27/28	0/2/2/2
2	PSU	5	3715	2	-	0/7/25/26	0/2/2/2
2	B8W	5	4185	2	-	4/5/27/28	0/3/3/3
49	PSU	9	822	49	-	2/7/25/26	0/2/2/2
2	OMG	5	1316	2	-	0/5/27/28	0/3/3/3
49	5MC	9	1374	49	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	5	4620	2	-	1/9/27/28	0/2/2/2
2	7MG	5	1605	2	-	0/7/37/38	0/3/3/3
49	B8N	9	1248	49	-	4/16/34/35	0/2/2/2
2	PSU	5	4628	2	-	0/7/25/26	0/2/2/2
2	2MG	5	4872	16,2	-	2/5/27/28	0/3/3/3
2	B8W	5	2380	2	-	4/5/27/28	0/3/3/3
2	B8H	5	1860	2	-	0/7/25/26	0/2/2/2
49	M7A	9	1806	49	-	0/7/37/38	0/3/3/3
49	PSU	9	1081	49	-	1/7/25/26	0/2/2/2
2	OMC	5	2422	83,2	-	1/9/27/28	0/2/2/2
2	PSU	5	3729	2	-	2/7/25/26	0/2/2/2
2	A2M	5	1871	83,2	-	0/5/27/28	0/3/3/3
2	PSU	5	3764	2	-	1/7/25/26	0/2/2/2
2	A2M	5	1534	83,2	-	2/5/27/28	0/3/3/3
2	5MC	5	4447	2	-	4/7/25/26	0/2/2/2
2	UR3	5	4597	2	-	0/7/25/26	0/2/2/2
49	A2M	9	1678	49	-	0/5/27/28	0/3/3/3
2	B8W	5	4529	83,2	-	3/5/27/28	0/3/3/3
2	OMG	5	2773	2	-	0/5/27/28	0/3/3/3
2	OMG	5	2050	2	-	0/5/27/28	0/3/3/3
2	E6G	5	4355	2	-	4/6/28/29	0/3/3/3
49	A2M	9	484	49	-	0/5/27/28	0/3/3/3
49	MA6	9	1850	49	-	0/7/29/30	0/3/3/3
2	OMC	5	3701	83,2	-	6/9/27/28	0/2/2/2
2	OMG	5	4870	2	-	3/5/27/28	0/3/3/3
2	I4U	5	4194	2	-	3/9/29/30	0/2/2/2
2	OMC	5	2365	2	-	2/9/27/28	0/2/2/2
2	OMG	5	2364	2	-	2/5/27/28	0/3/3/3
2	PSU	5	1582	2	-	2/7/25/26	0/2/2/2
2	A2M	5	2401	83,2	-	0/5/27/28	0/3/3/3
2	PSU	5	1683	2	-	0/7/25/26	0/2/2/2
2	B8W	5	4472	2	-	2/5/27/28	0/3/3/3
2	PSU	5	2508	2	-	0/7/25/26	0/2/2/2
2	OMG	5	3792	2	-	2/5/27/28	0/3/3/3
2	B9B	5	237	2	-	5/7/29/30	0/3/3/3
2	B8H	5	3762	2	-	2/7/25/26	0/2/2/2
2	OMG	5	4623	2	-	0/5/27/28	0/3/3/3
2	UR3	5	1866	2	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	5	3785	2	-	4/5/27/28	0/3/3/3
2	OMG	5	2424	2	-	2/5/27/28	0/3/3/3
49	A2M	9	166	49	-	2/5/27/28	0/3/3/3
49	OMG	9	644	49	-	1/5/27/28	0/3/3/3
2	OMG	5	4196	2	-	0/5/27/28	0/3/3/3
2	P7G	5	1909	2	-	1/10/40/41	0/3/3/3
42	MLZ	m	72	42	-	2/7/8/10	-
49	PSU	9	119	49	-	1/7/25/26	0/2/2/2
2	MHG	5	4371	2	-	8/16/46/47	0/3/3/3
2	7MG	5	2522	2	-	0/7/37/38	0/3/3/3
2	M7A	5	4564	2	-	0/7/37/38	0/3/3/3
2	B9B	5	1574	2	-	3/7/29/30	0/3/3/3

The worst 5 of 944 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	237	B9B	C2'-C1'	-18.12	1.26	1.53
2	5	1574	B9B	C2'-C1'	-18.07	1.26	1.53
2	5	2754	B9B	C2'-C1'	-17.90	1.26	1.53
2	5	237	B9B	O4'-C1'	17.12	1.65	1.41
2	5	2754	B9B	O4'-C1'	16.63	1.64	1.41

The worst 5 of 609 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	2380	B8W	N2-C2-N3	17.19	145.81	117.79
2	5	4529	B8W	N2-C2-N3	16.95	145.41	117.79
2	5	4185	B8W	N2-C2-N3	16.62	144.87	117.79
2	5	4472	B8W	N2-C2-N3	16.22	144.22	117.79
2	5	4129	B8W	N2-C2-N3	16.17	144.15	117.79

There are no chirality outliers.

5 of 191 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	333	MLZ	N-CA-CB-CG
7	C	333	MLZ	C-CA-CB-CG
2	5	237	B9B	C5-C6-O6-C61
2	5	237	B9B	N1-C6-O6-C61
2	5	237	B9B	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 305 ligands modelled in this entry, 305 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	5	43
49	9	18
4	8	1

The worst 5 of 62 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	40.50
1	5	1252:C	O3'	1271:G	P	34.93
1	5	1219:G	O3'	1233:G	P	21.40
1	5	1405:C	O3'	1406:G	P	20.69
1	5	1406(C):G	O3'	1411:C	P	20.19

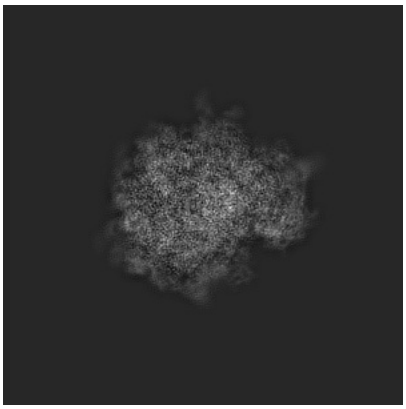
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9239. These allow visual inspection of the internal detail of the map and identification of artifacts.

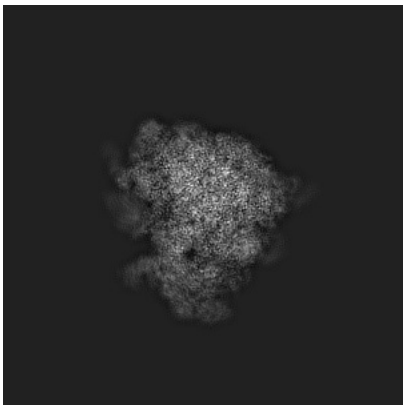
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

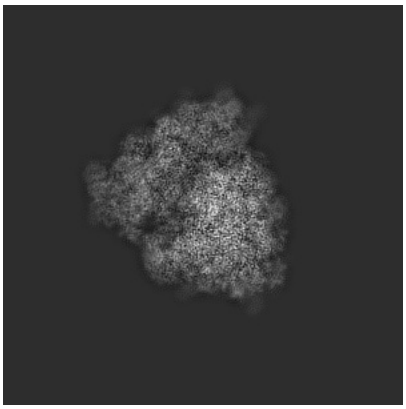
6.1.1 Primary map



X

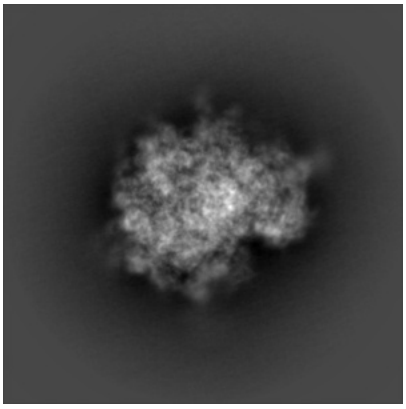


Y

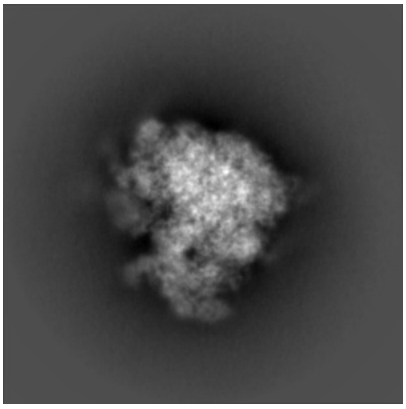


Z

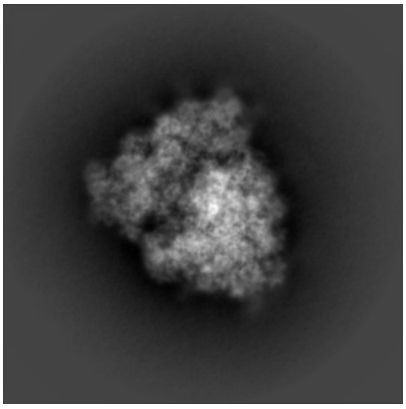
6.1.2 Raw map



X



Y

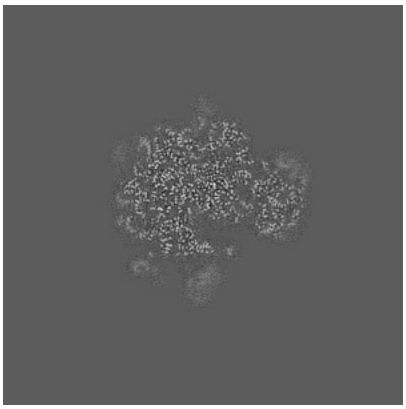


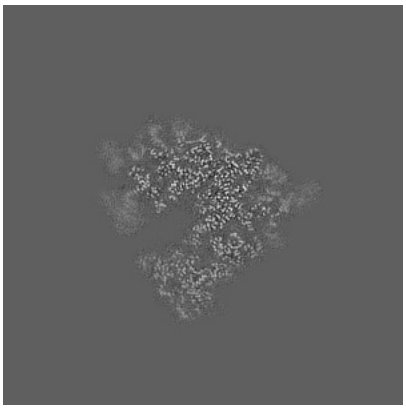
Z

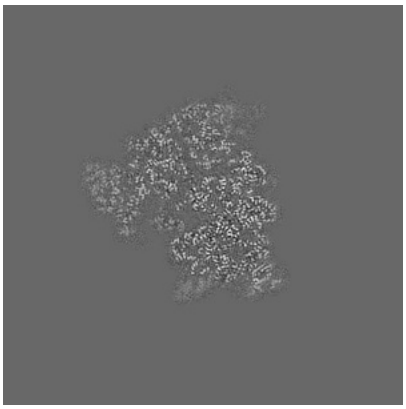
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

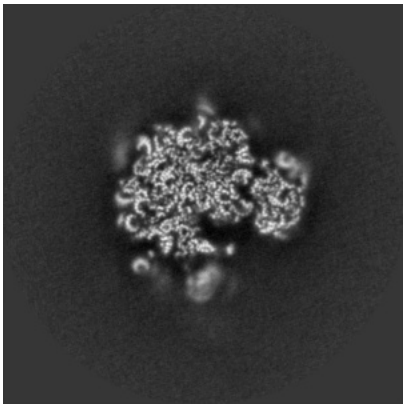
6.2.1 Primary map

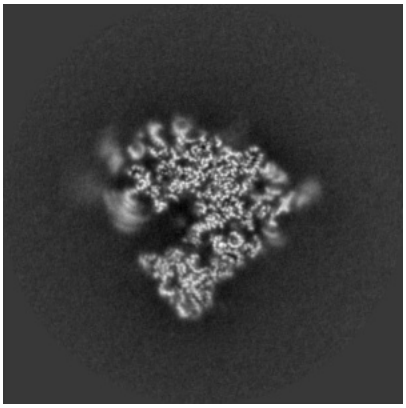

X Index: 200

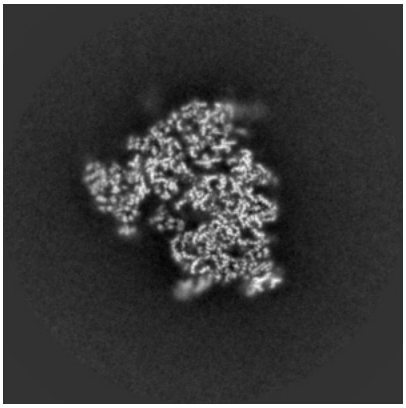

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

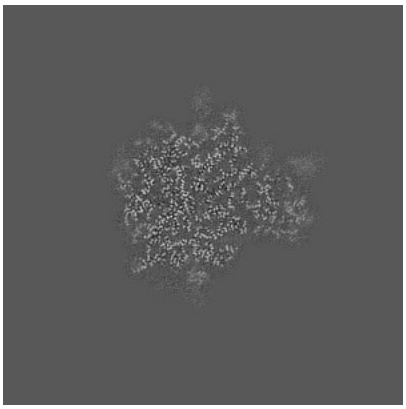

Y Index: 200


Z Index: 200

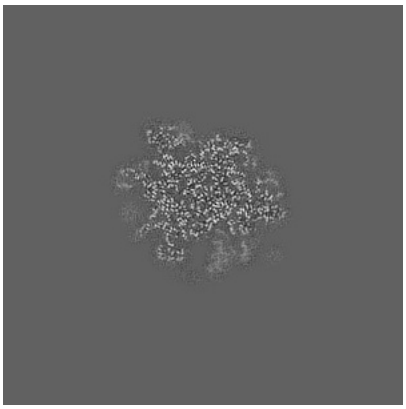
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

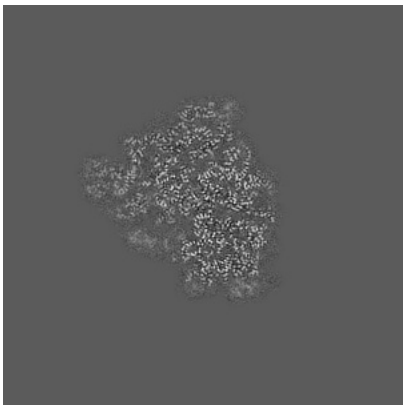
6.3.1 Primary map



X Index: 213

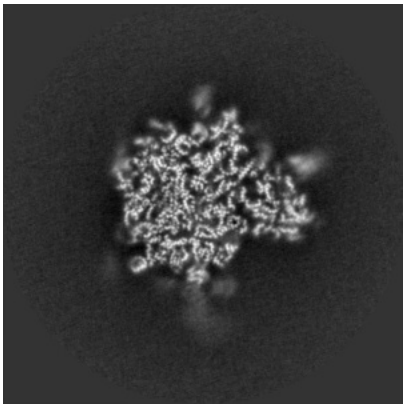


Y Index: 160

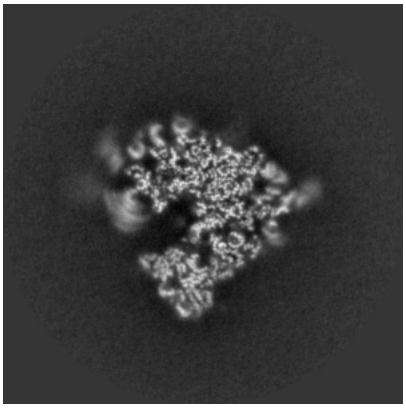


Z Index: 211

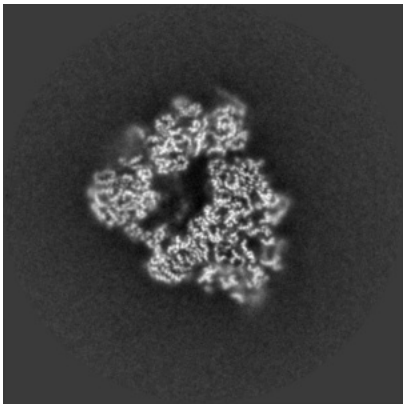
6.3.2 Raw map



X Index: 213



Y Index: 201

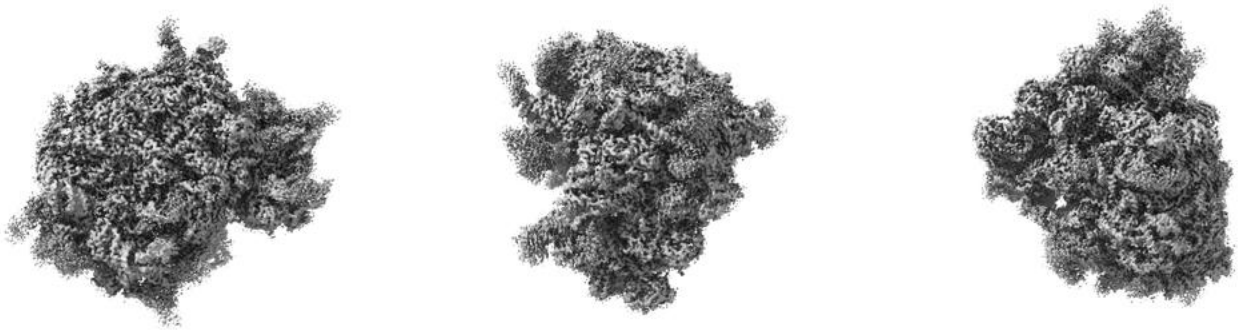


Z Index: 176

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

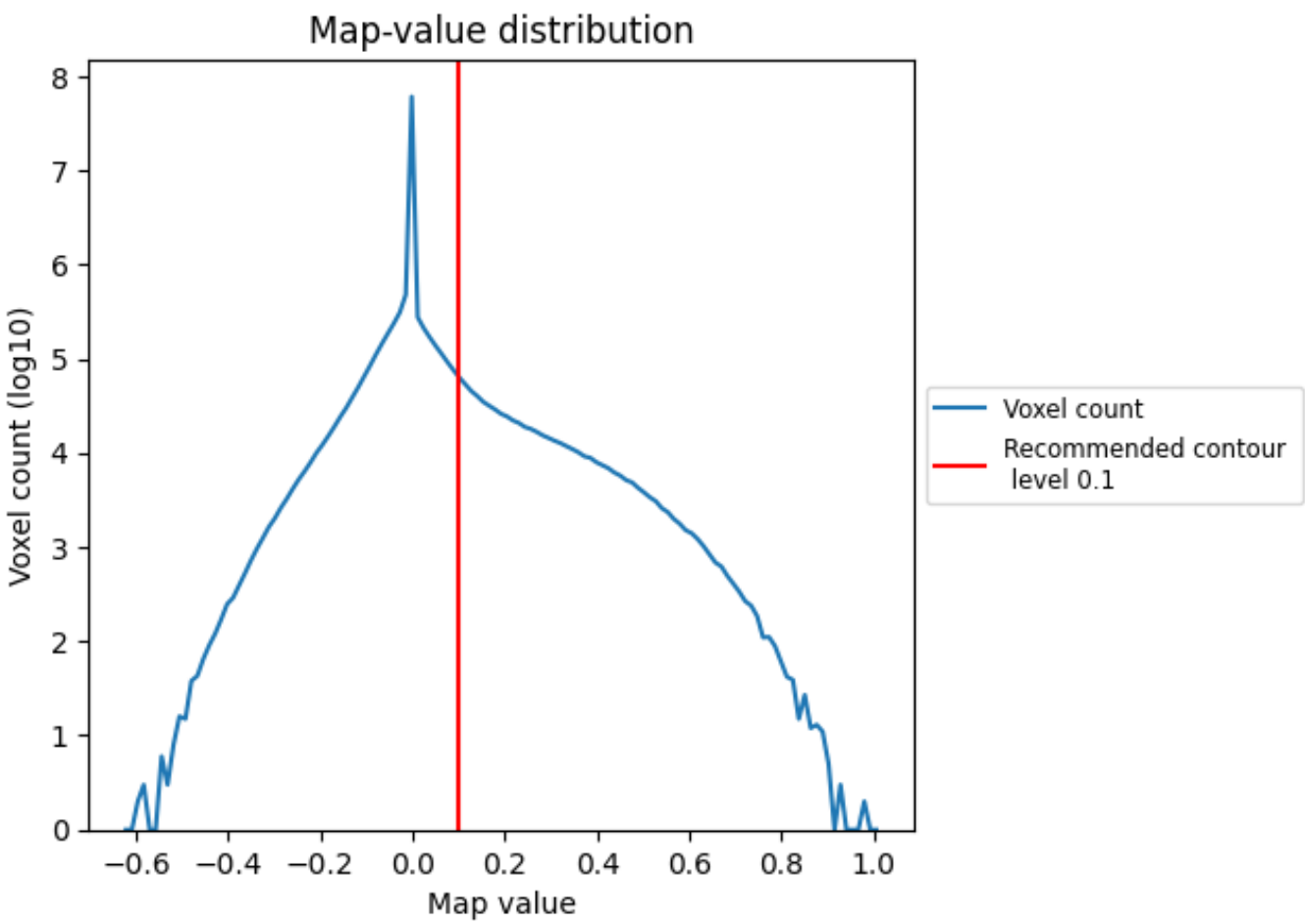
6.5 Mask visualisation (i)

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

7 Map analysis (i)

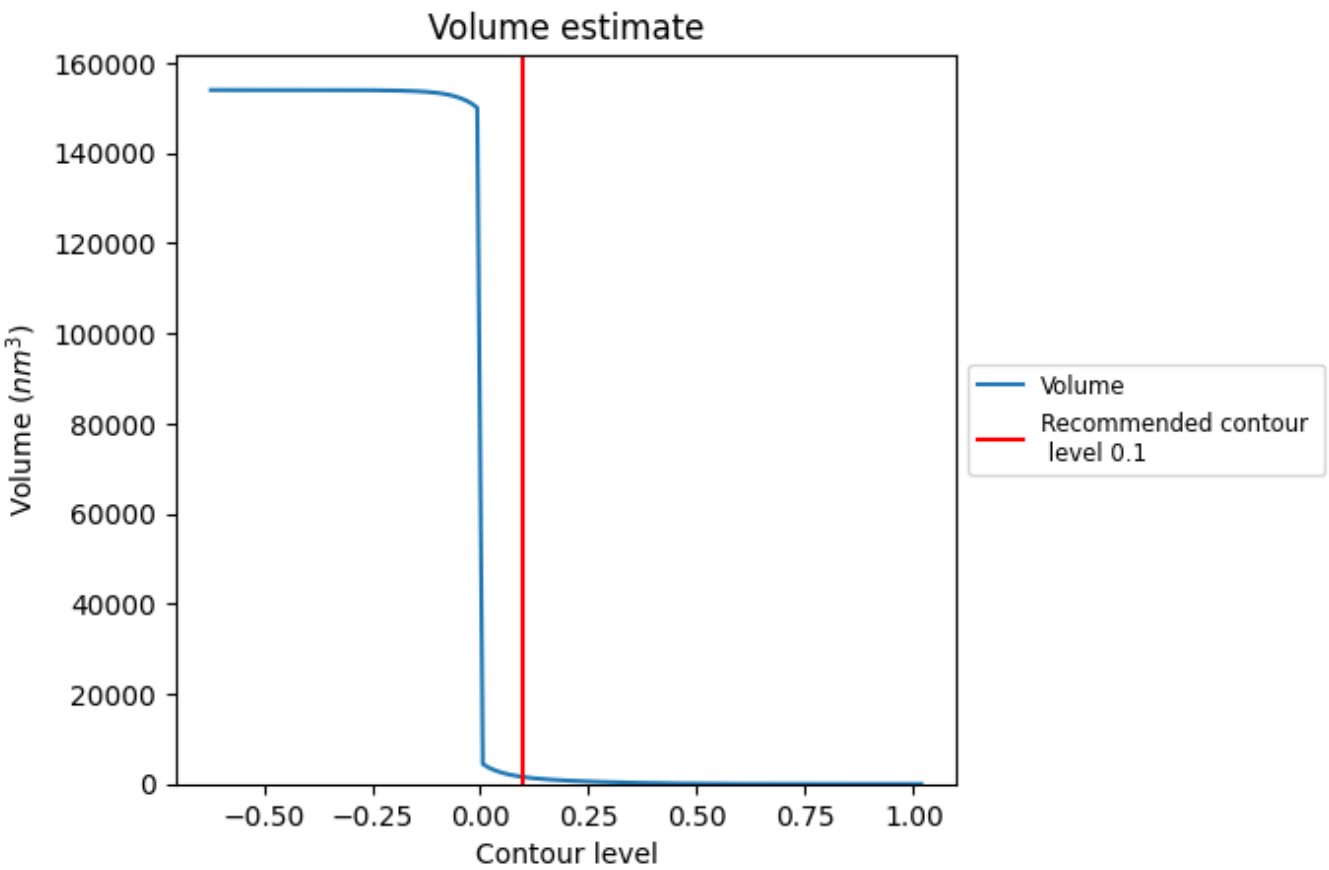
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

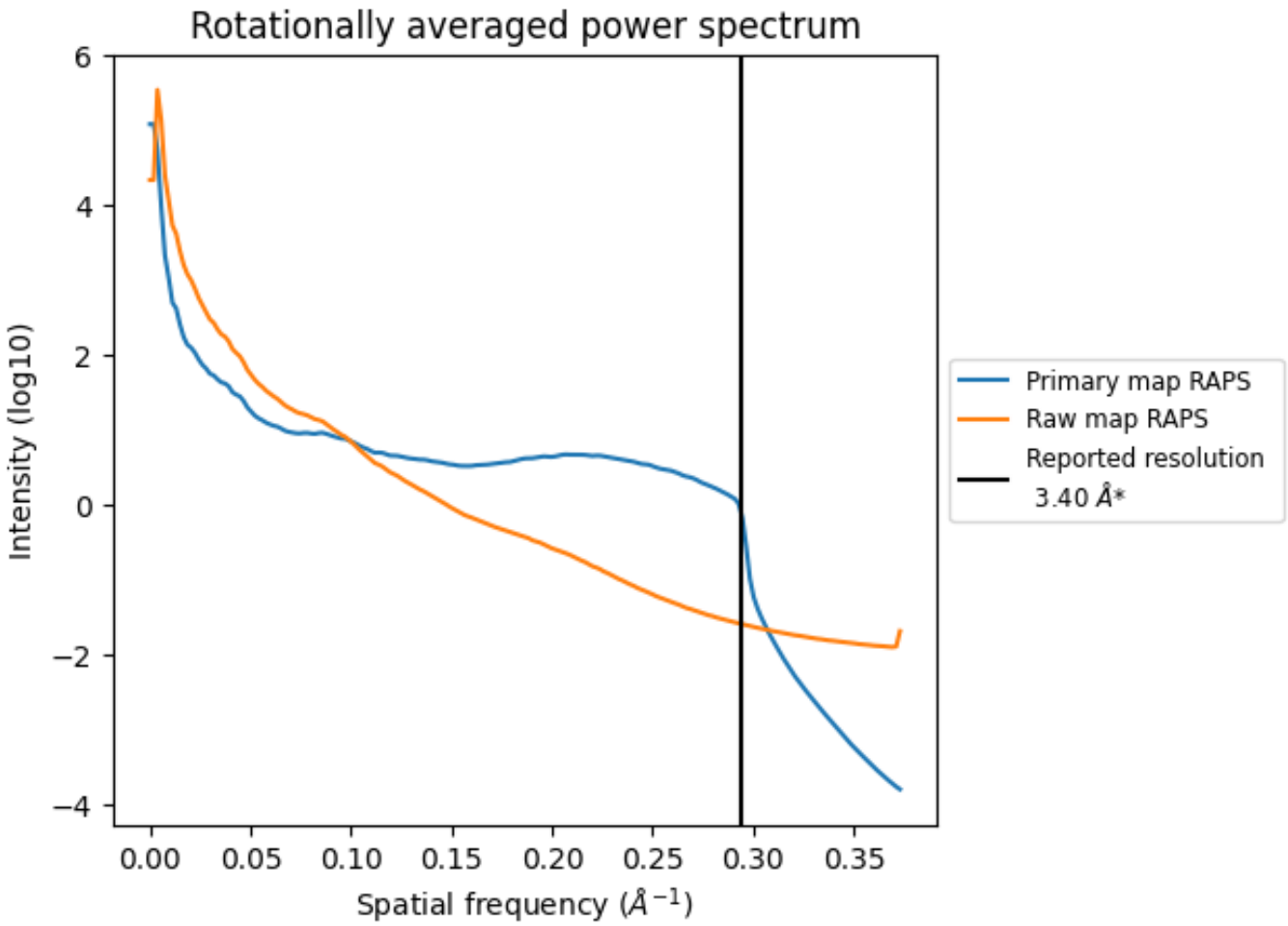
7.2 Volume estimate (i)



The volume at the recommended contour level is 1528 nm^3; this corresponds to an approximate mass of 1381 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)

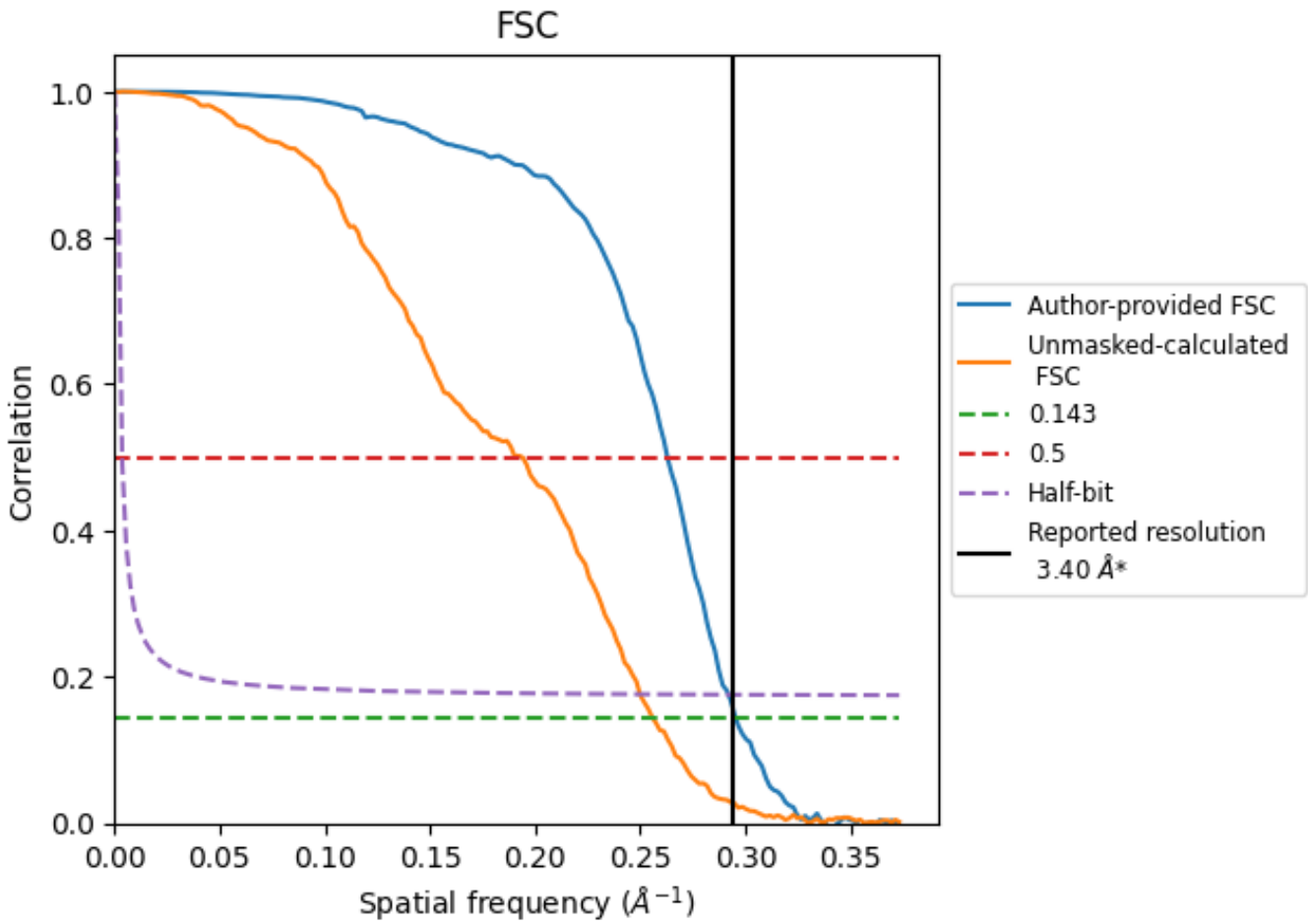


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

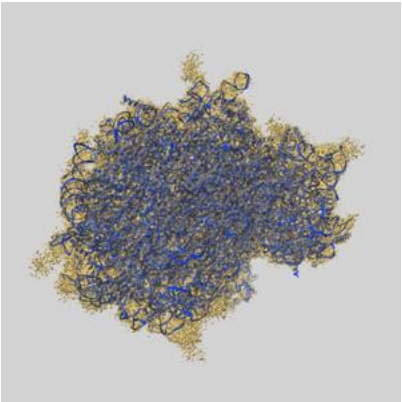
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.81	3.43
Unmasked-calculated*	3.91	5.16	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.4 by more than 10 %

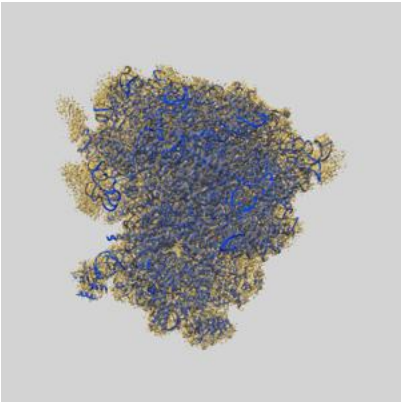
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9239 and PDB model 6MTC. Per-residue inclusion information can be found in section 3 on page 19.

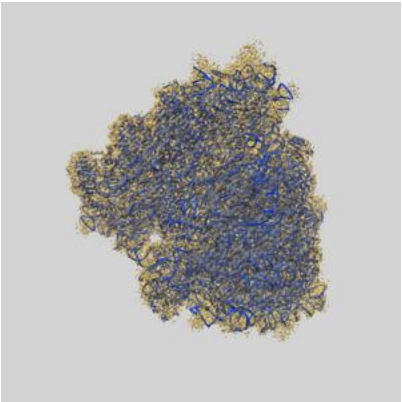
9.1 Map-model overlay (i)



X



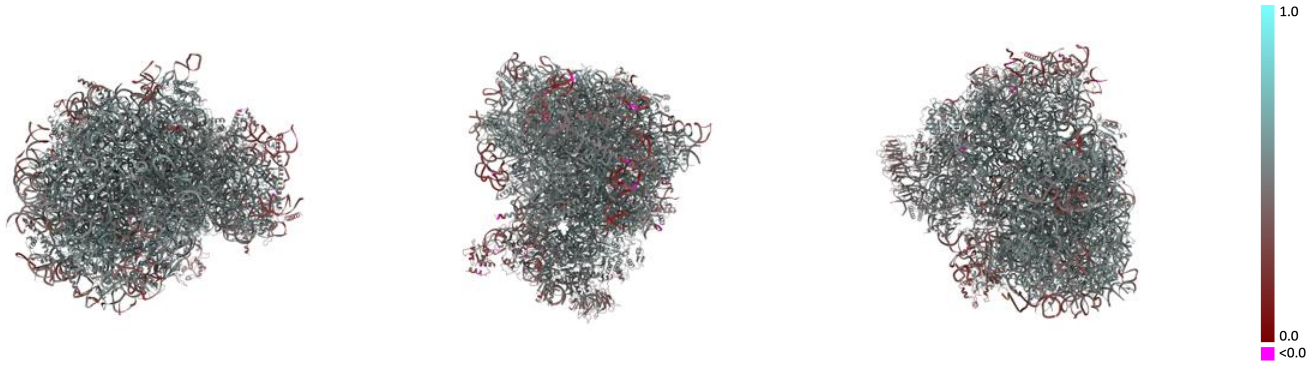
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

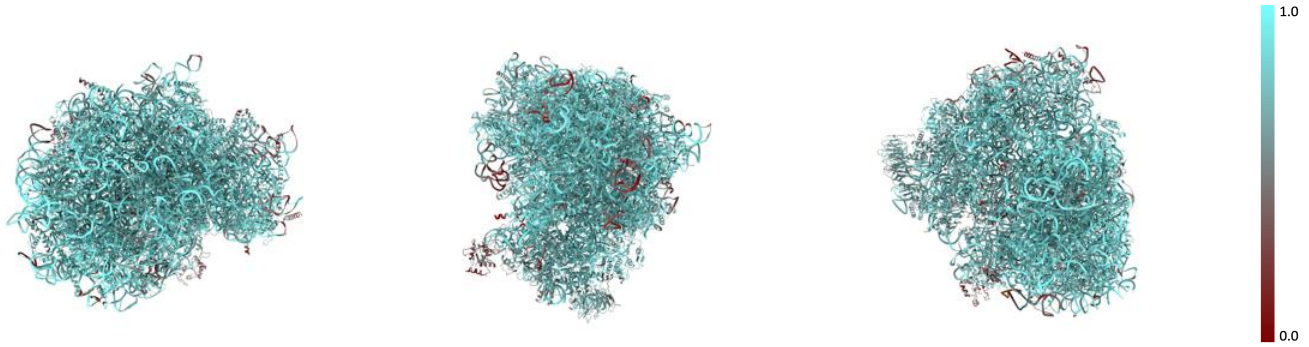
9.2 Q-score mapped to coordinate model (i)



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.

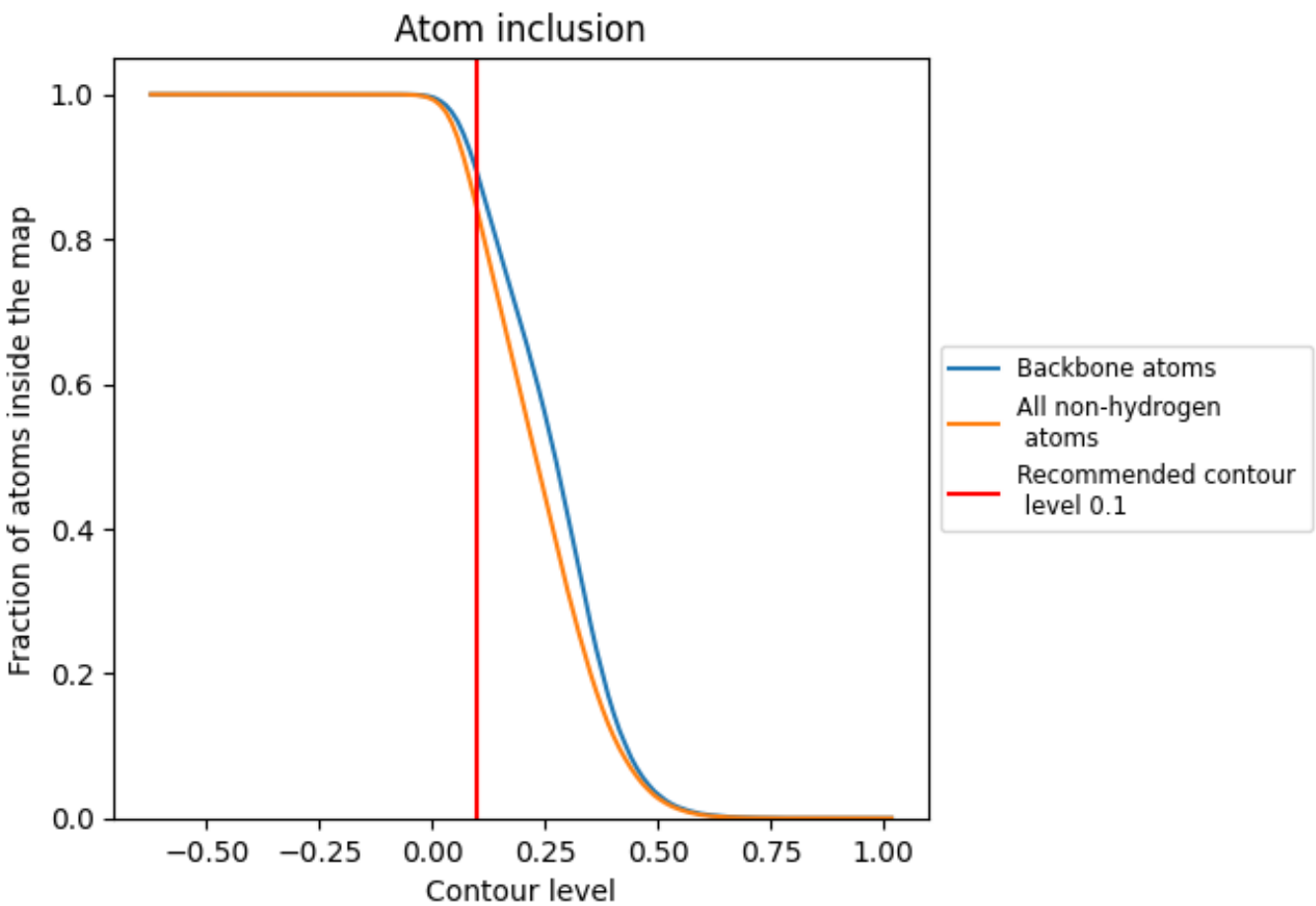
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8413	0.4970
4	0.7288	0.3350
5	0.8835	0.4920
7	0.9392	0.5210
8	0.9064	0.5060
9	0.8689	0.4760
A	0.8867	0.5620
AA	0.8131	0.5150
B	0.8750	0.5500
BB	0.8034	0.5210
C	0.8650	0.5490
CC	0.8266	0.5240
D	0.8504	0.5240
DD	0.6916	0.4640
E	0.8410	0.5280
EE	0.8099	0.5260
F	0.8567	0.5460
FF	0.7737	0.4930
G	0.7973	0.5110
GG	0.7181	0.4660
H	0.8200	0.5310
HH	0.7303	0.4720
I	0.8513	0.5440
II	0.7892	0.5150
J	0.7896	0.5020
JJ	0.8082	0.5050
KK	0.6709	0.4350
L	0.8268	0.5300
LL	0.8151	0.5350
M	0.8471	0.5280
MM	0.3098	0.2620
N	0.8926	0.5620
NN	0.8405	0.5300
O	0.8542	0.5430
OO	0.8075	0.5220

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
P	0.8641	0.5490
PP	0.6715	0.4330
Q	0.8690	0.5540
QQ	0.7399	0.4770
R	0.8119	0.5210
RR	0.7505	0.4860
S	0.8658	0.5520
SS	0.7223	0.4680
T	0.8456	0.5380
TT	0.7423	0.4730
U	0.7826	0.4850
UU	0.6809	0.4460
V	0.8580	0.5550
VV	0.8023	0.5250
W	0.6943	0.4530
WW	0.8545	0.5380
X	0.8298	0.5330
XX	0.8226	0.5300
Y	0.8525	0.5390
YY	0.7808	0.4960
Z	0.8611	0.5320
ZZ	0.7050	0.4620
a	0.8732	0.5560
aa	0.8327	0.5420
b	0.7485	0.4890
bb	0.7872	0.5180
c	0.8360	0.5290
cc	0.7383	0.5060
d	0.8308	0.5300
dd	0.8077	0.4980
e	0.8732	0.5590
ee	0.6948	0.4890
f	0.8907	0.5620
ff	0.3808	0.3280
g	0.8310	0.5430
gg	0.6386	0.4170
h	0.8264	0.5280
i	0.8354	0.5250
j	0.9019	0.5550
k	0.7684	0.5130
l	0.8431	0.5460
m	0.8537	0.5360

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
n	0.7936	0.5270
o	0.8531	0.5500
p	0.8389	0.5540
r	0.8840	0.5490
u	0.4539	0.3420
v	0.6271	0.4620