wwPDB EM Validation Summary Report (i)

Nov 27, 2022 – 09:47 AM EST

PDB ID	:	6OM0
EMDB ID	:	EMD-0596
Title	:	Human ribosome nascent chain complex (PCSK9-RNC) stalled by a drug-like molecule with AP and PE tRNAs
Authors	:	Li, W.; Cate, J.H.D.
Deposited on	:	2019-04-17
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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 (1)) were used in the production of this report:

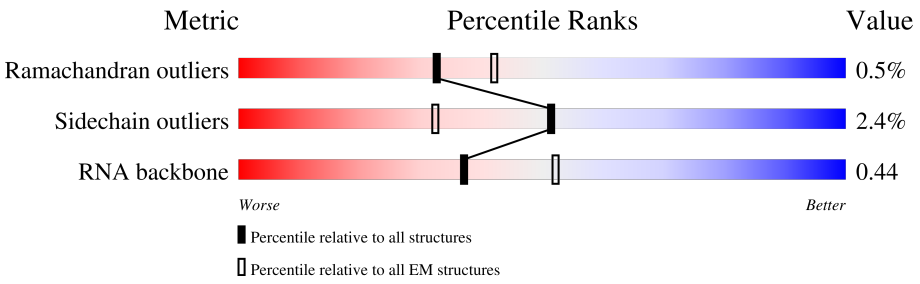
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.10 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	S2	1714	9% 64% 32% ·
2	SA	221	13% 95% 5%
3	SB	214	5% 99% ·
4	SD	226	18% 99% ·
5	SE	259	7% 98% ·
6	SF	189	17% 96% · ·
7	SH	189	31% 97% · ·
8	SI	204	15% 98% ·

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Mol	Chain	Length	Quality of chain
9	SK	98	21% 98%
10	SL	153	20% 97%
11	SP	127	11% 97%
12	SQ	146	12% 98%
13	SR	134	23% 97%
14	SS	145	8% 99%
15	ST	143	6% 97%
16	SU	104	30% 94% 5%
17	SV	82	6% 96%
18	SX	141	97%
19	Sa	102	10% 96%
20	Sc	64	30% 98%
21	Sd	55	7% 93% 7%
22	Sg	312	37% 97%
23	SC	220	11% 98%
24	SG	237	24% 95%
25	SJ	185	10% 94% 5%
26	SM	118	79% 96%
27	SN	150	99%
28	SO	137	9% 99%
29	SW	129	98%
30	SY	131	15% 98%
31	SZ	73	16% 97%
32	Sb	82	13% 100%
33	Se	57	19% 98%

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Mol	Chain	Length	Quality of chain
34	Sf	67	72% 94% 6%
35	A	252	96%
36	B	397	97%
37	C	363	5% 97%
38	D	157	8% 71% 27%
39	E	119	85% 15%
40	F	294	6% 96%
41	G	247	16% 91%
42	H	225	96%
43	I	234	11% 99%
44	J	191	97%
45	K	211	6% 96%
46	L	169	99%
47	M	205	10% 96%
48	N	139	99%
49	O	203	96%
50	P	195	96%
51	Q	153	98%
52	R	187	96%
53	S	181	9% 98%
54	T	175	98%
55	U	157	97%
56	V	99	9% 93% 7%
57	W	129	100%
58	X	61	98%

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Mol	Chain	Length	Quality of chain
59	Y	117	97%
60	Z	134	100%
61	a	134	98%
62	b	147	96%
63	c	121	13% 80% 17%
64	d	103	12% 96%
65	e	106	7% 98%
66	f	129	98%
67	g	109	94% 6%
68	h	114	7% 97%
69	i	122	6% 94% 6%
70	j	97	97%
71	k	84	98%
72	l	69	13% 99%
73	m	50	96%
74	n	50	98%
75	o	25	96%
76	p	105	8% 92% 7%
77	q	91	99%
78	r	122	94% 6%
79	t	3607	7% 72% 26%
80	u	76	20% 57% 39%
81	v	76	11% 59% 36% 5%
82	w	10	70% 20% 10%
83	y	26	88% 50% 50%

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 214893 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	S2	1714	36501	16306	6533	11949	1713	0	0

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SA	221	1741	1106	305	322	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SB	214	1738	1103	310	311	14	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SD	226	1757	1120	316	314	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SE	259	2059	1316	383	352	8	0	0

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SF	189	1495	934	284	270	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SH	186	1497	956	274	266	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SI	204	1673	1050	329	289	5	0	0

- Molecule 9 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SK	98	827	539	148	134	6	0	0

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SL	153	1247	793	234	214	6	0	0

- Molecule 11 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SP	127	1045	663	198	177	7	0	0

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SQ	146	1158	736	218	200	4	0	0

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SR	134	1082	680	201	197	4	0	0

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	SS	145	1198	751	242	203	2	0	0

- Molecule 15 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	ST	143	1112	697	214	198	3	0	0

- Molecule 16 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	SU	104	821	514	155	148	4	0	0

- Molecule 17 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	SV	82	625	384	116	120	5	0	0

- Molecule 18 is a protein called 40S ribosomal protein S23.

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

- Molecule 19 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Sa	102	821	512	171	133	5	0	0

- Molecule 20 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Sc	64	506	308	102	94	2	0	0

- Molecule 21 is a protein called 40S ribosomal protein S29.

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

- Molecule 22 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Sg	312	2429	1531	423	463	12	0	0

- Molecule 23 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	SC	220	1715	1109	296	300	10	1	0

- Molecule 24 is a protein called 40S ribosomal protein S6.

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

- Molecule 25 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	SJ	185	1533	974	309	248	2	1	0

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	SM	118	912	571	161	173	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	52	GLN	LEU	conflict	UNP P25398
SM	69	LEU	CYS	conflict	UNP P25398
SM	99	ASN	LYS	conflict	UNP P25398

- Molecule 27 is a protein called 40S ribosomal protein S13.

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

- Molecule 28 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	SO	137	1024	627	200	191	6	0	0

- Molecule 29 is a protein called 40S ribosomal protein S15a.

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

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	SY	131	1073	678	212	178	5	1	0

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	SZ	73	579	372	106	100	1	0	0

- Molecule 32 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Sb	82	640	402	118	113	7	0	0

- Molecule 33 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Se	57	452	281	99	71	1	0	0

- Molecule 34 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Sf	67	548	346	102	93	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	A	252	1930	1209	395	320	6	0	0

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	B	397	3202	2039	602	547	14	0	0

- Molecule 37 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	C	363	2888	1817	577	480	14	0	0

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	D	157	3337	1489	587	1104	157	0	0

- Molecule 39 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	E	119	2541	1132	454	836	119	0	0

- Molecule 40 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	F	294	2392	1510	436	432	14	0	0

- Molecule 41 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	G	236	1904	1222	361	317	4	0	0

- Molecule 42 is a protein called 60S ribosomal protein L7.

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

- Molecule 43 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	I	234	1880	1197	362	317	4	0	0

- Molecule 44 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	J	191	1526	960	285	275	6	0	0

- Molecule 45 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	K	208	1692	1074	327	278	13	0	0

- Molecule 46 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	L	169	1353	855	252	240	6	0	0

- Molecule 47 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	M	205	1657	1036	344	273	4	0	0

- Molecule 48 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	N	139	1138	730	218	183	7	0	0

- Molecule 49 is a protein called 60S ribosomal protein L15.

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

- Molecule 50 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	P	195	1606	1034	315	252	5	0	0

- Molecule 51 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Q	153	1242	776	241	216	9	0	0

- Molecule 52 is a protein called 60S ribosomal protein L18.

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

- Molecule 53 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	S	181	1517	938	329	241	9	0	0

- Molecule 54 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	T	175	1449	921	283	234	11	0	0

- Molecule 55 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	U	157	1284	815	250	214	5	0	0

- Molecule 56 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	V	99	808	518	141	147	2	0	0

- Molecule 57 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	W	129	969	613	182	169	5	0	0

- Molecule 58 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	X	61	511	327	100	82	2	0	0

- Molecule 59 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	Y	117	958	612	180	165	1	0	0

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

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

- Molecule 61 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	a	134	1103	712	207	181	3	0	0

- Molecule 62 is a protein called 60S ribosomal protein L27a.

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

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	c	100	814	506	179	125	4	0	0

- Molecule 64 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	d	103	801	508	141	145	7	0	0

- Molecule 65 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	e	106	879	555	170	152	2	0	0

- Molecule 66 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	f	129	1064	673	220	166	5	0	0

- Molecule 67 is a protein called 60S ribosomal protein L35a.

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

- Molecule 68 is a protein called 60S ribosomal protein L34.

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

- Molecule 69 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	i	122	1015	641	205	168	1	0	0

- Molecule 70 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	j	97	794	497	168	124	5	0	0

- Molecule 71 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	k	84	689	423	152	109	5	0	0

- Molecule 72 is a protein called 60S ribosomal protein L38.

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

- Molecule 73 is a protein called 60S ribosomal protein L39.

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

- Molecule 74 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	n	50	411	254	87	64	6	0	0

- Molecule 75 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	o	25	240	145	64	28	3	0	0

- Molecule 76 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	p	105	863	542	175	140	6	0	0

- Molecule 77 is a protein called 60S ribosomal protein L37a.

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

- Molecule 78 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	r	122	980	607	204	165	4	0	0

- Molecule 79 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
79	t	3607	77332	34436	14150	25139	3607	0	0

- Molecule 80 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
80	u	76	1613	720	283	535	75	0	0

- Molecule 81 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
81	v	76	1618	721	287	534	76	0	0

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
82	w	10	213	95	37	72	9	0	0

- Molecule 83 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
83	y	26	204	138	32	34	0	0

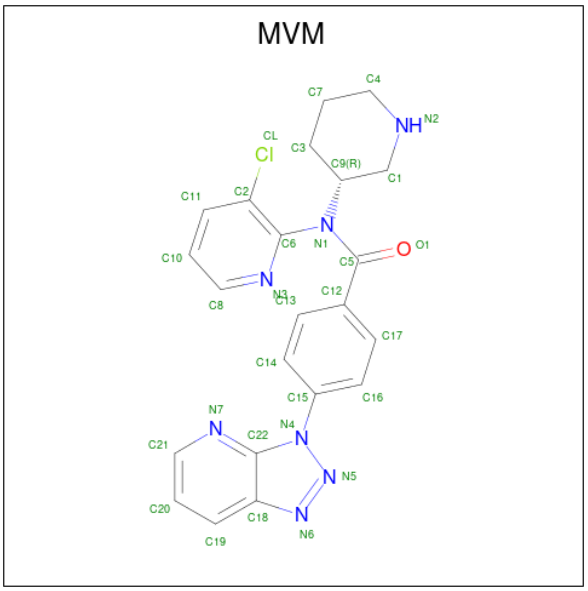
- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
84	S2	2	2	2	0
84	A	1	1	1	0
84	B	1	1	1	0
84	D	7	7	7	0
84	E	9	9	9	0
84	b	1	1	1	0
84	o	1	1	1	0
84	t	9	9	9	0

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
85	S2	1	1	1	0
85	Sa	1	1	1	0
85	Sf	1	1	1	0
85	k	1	1	1	0
85	p	1	1	1	0
85	q	1	1	1	0

- Molecule 86 is N-(3-chloropyridin-2-yl)-N-[(3R)-piperidin-3-yl]-4-(3H-[1,2,3]triazolo[4,5-b]pyridin-3-yl)benzamide (three-letter code: MVM) (formula: $C_{22}H_{20}ClN_7O$).



Mol	Chain	Residues	Atoms					AltConf
86	t	1	Total 31	C 22	Cl 1	N 7	O 1	0

- Molecule 87 is water.

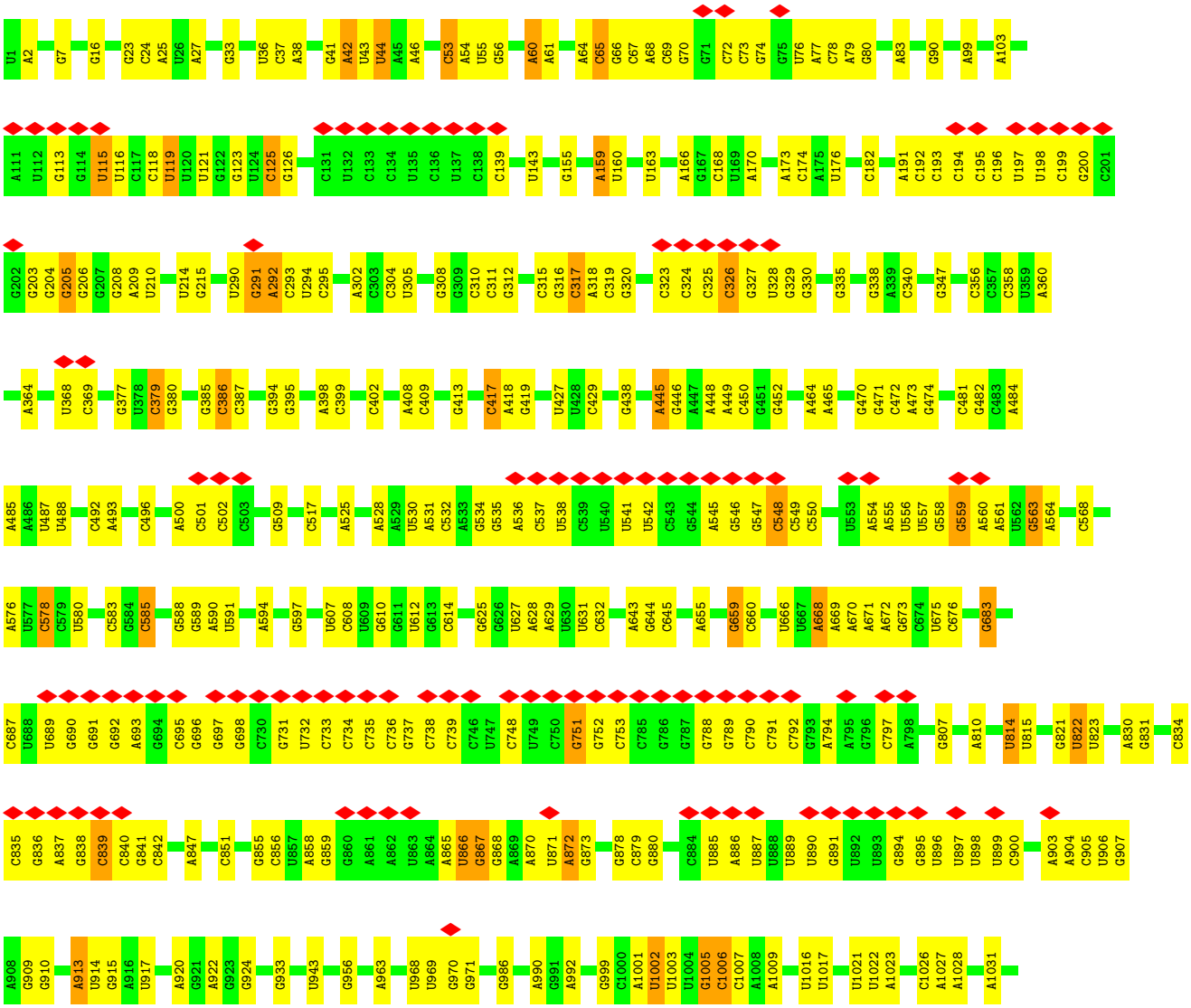
Mol	Chain	Residues	Atoms		AltConf
87	S2	6	Total 6	O 6	0
87	SA	1	Total 1	O 1	0
87	SP	1	Total 1	O 1	0
87	SQ	1	Total 1	O 1	0
87	SS	1	Total 1	O 1	0
87	SC	1	Total 1	O 1	0
87	SN	1	Total 1	O 1	0
87	Sf	1	Total 1	O 1	0
87	u	1	Total 1	O 1	0

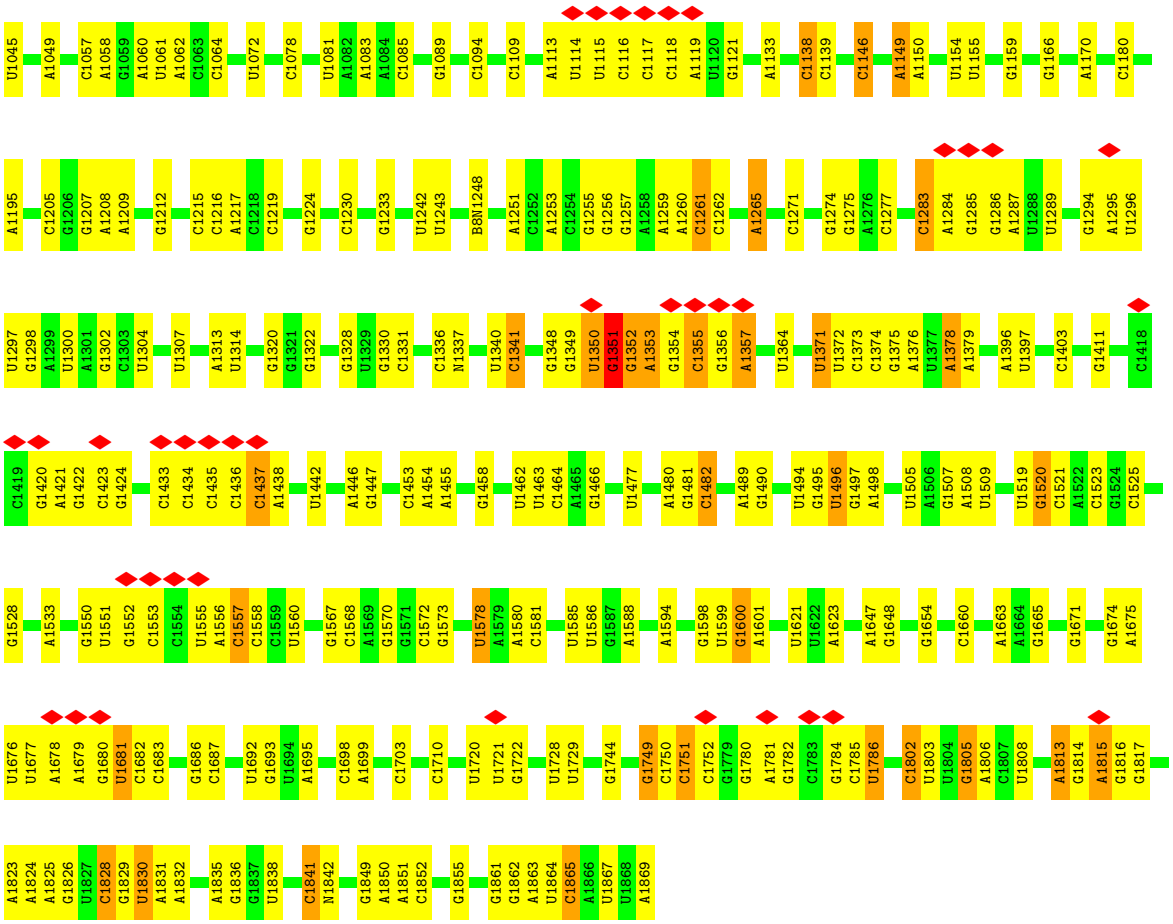
3 Residue-property plots (i)

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

- Molecule 1: 18S ribosomal RNA

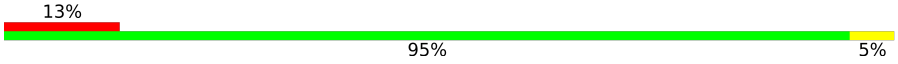
Chain S2:

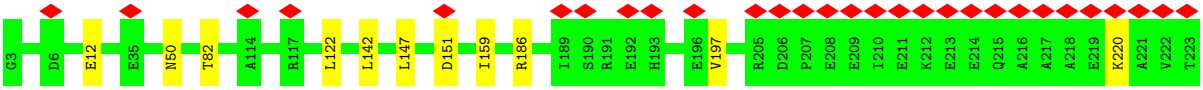




- Molecule 2: 40S ribosomal protein SA

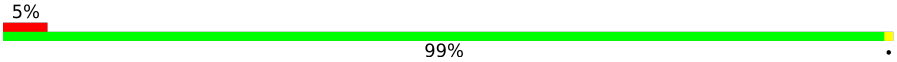
Chain SA:

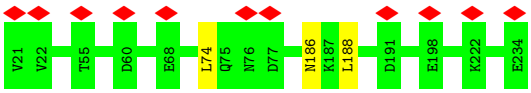




- Molecule 3: 40S ribosomal protein S3a

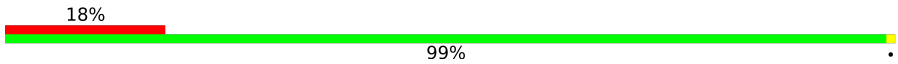
Chain SB:

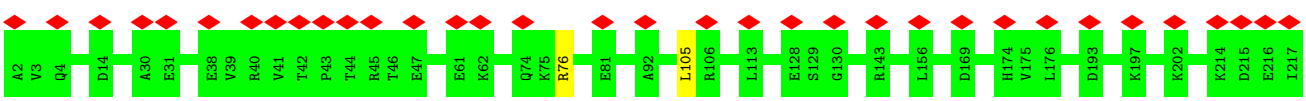


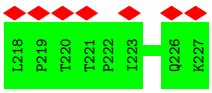


- Molecule 4: 40S ribosomal protein S3

Chain SD:

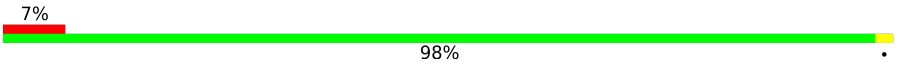


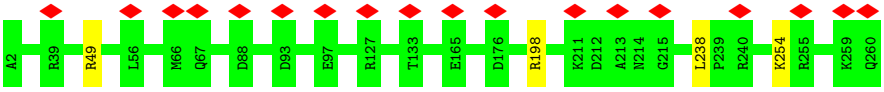




• Molecule 5: 40S ribosomal protein S4, X isoform

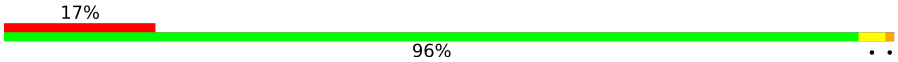
Chain SE:

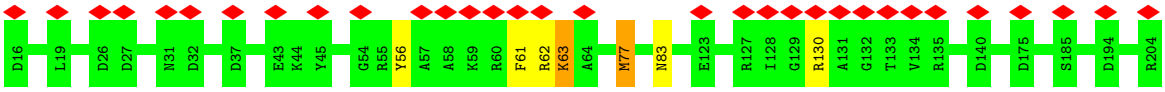




• Molecule 6: 40S ribosomal protein S5

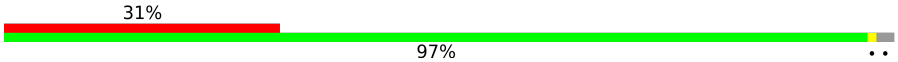
Chain SF:

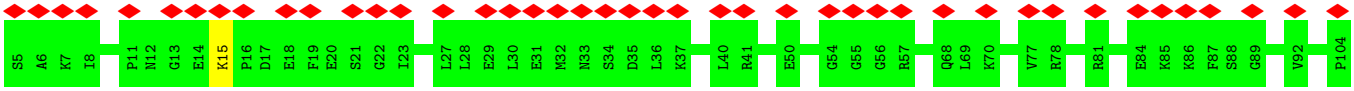


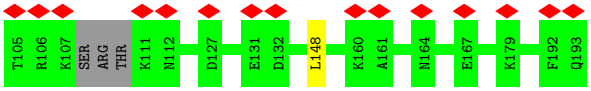


• Molecule 7: 40S ribosomal protein S7

Chain SH:

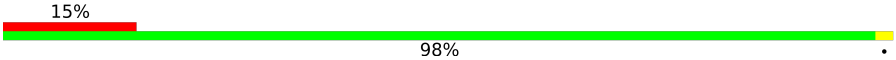


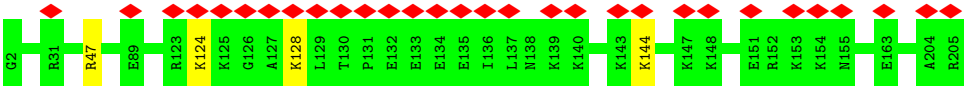




• Molecule 8: 40S ribosomal protein S8

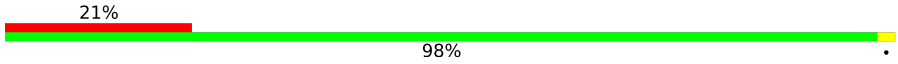
Chain SI:

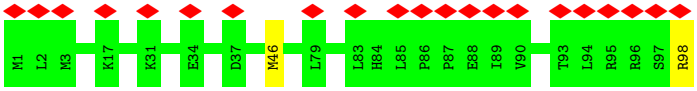




• Molecule 9: 40S ribosomal protein S10

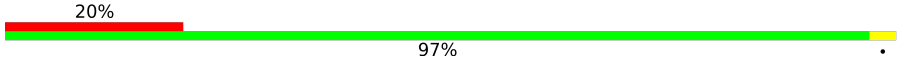
Chain SK:

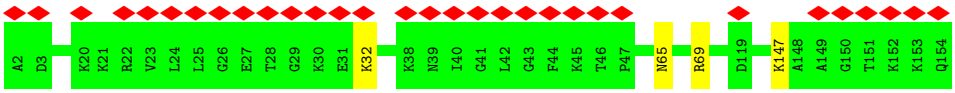




• Molecule 10: 40S ribosomal protein S11

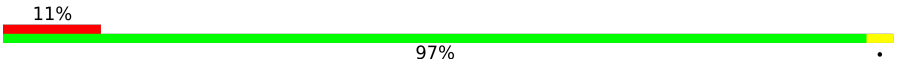
Chain SL:

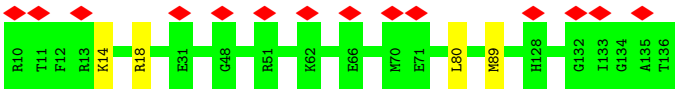




- Molecule 11: 40S ribosomal protein S15

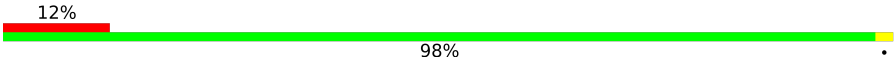
Chain SP:

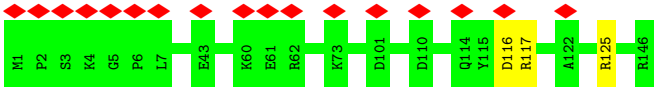




- Molecule 12: 40S ribosomal protein S16

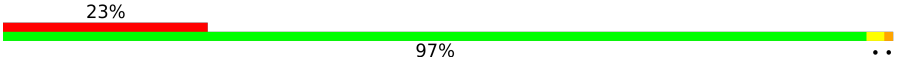
Chain SQ:

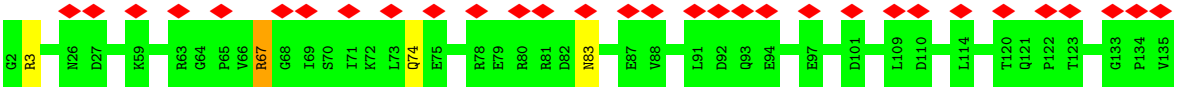




- Molecule 13: 40S ribosomal protein S17

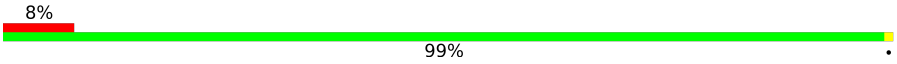
Chain SR:

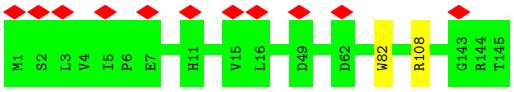




- Molecule 14: 40S ribosomal protein S18

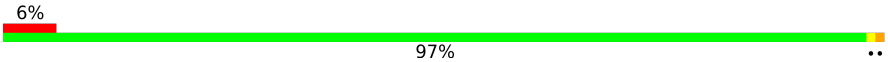
Chain SS:

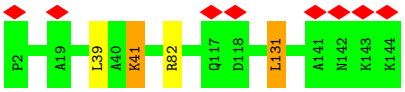




- Molecule 15: 40S ribosomal protein S19

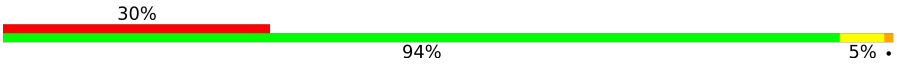
Chain ST:

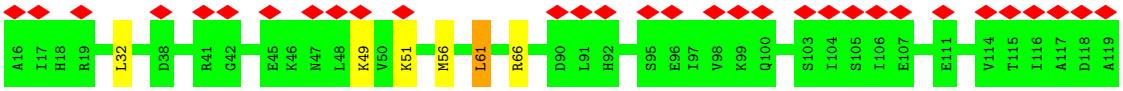




- Molecule 16: 40S ribosomal protein S20

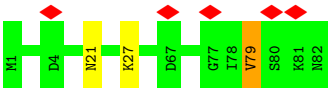
Chain SU:





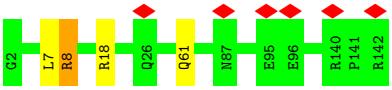
- Molecule 17: 40S ribosomal protein S21

Chain SV: 6% 96%



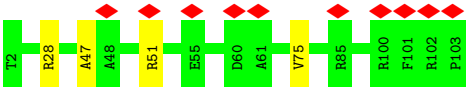
• Molecule 18: 40S ribosomal protein S23

Chain SX: 97%



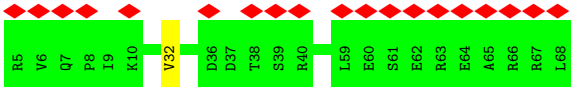
• Molecule 19: 40S ribosomal protein S26

Chain Sa: 10% 96%



• Molecule 20: 40S ribosomal protein S28

Chain Sc: 30% 98%

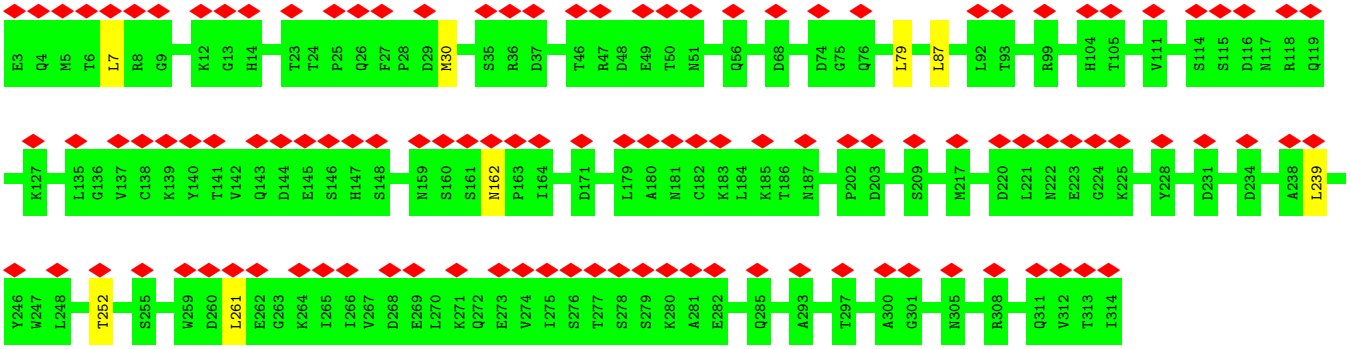


• Molecule 21: 40S ribosomal protein S29

Chain Sd: 7% 93% 7%

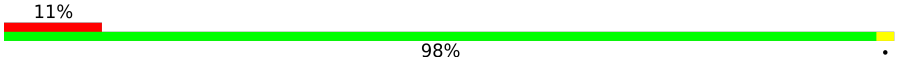
• Molecule 22: Receptor of activated protein C kinase 1

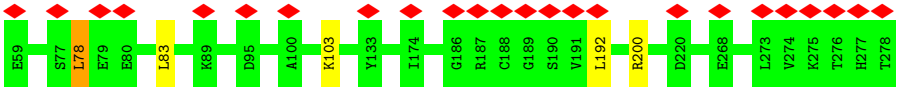
Chain Sg: 37% 97%



- Molecule 23: 40S ribosomal protein S2

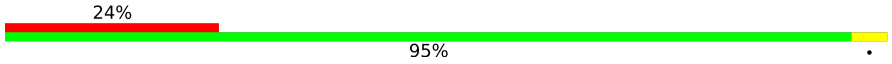
Chain SC:

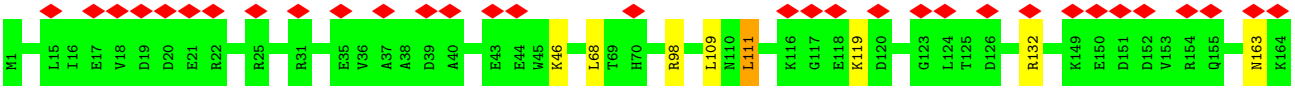


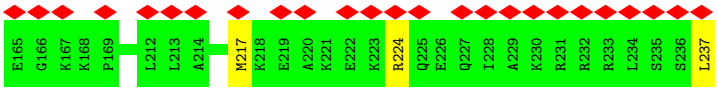


- Molecule 24: 40S ribosomal protein S6

Chain SG:

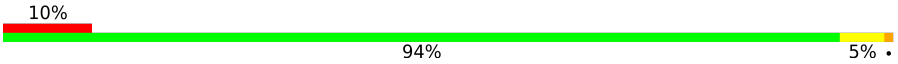


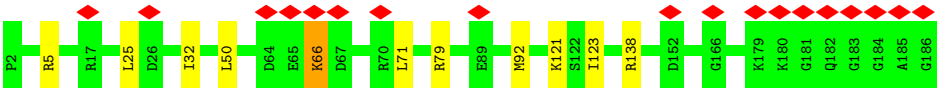




- Molecule 25: 40S ribosomal protein S9

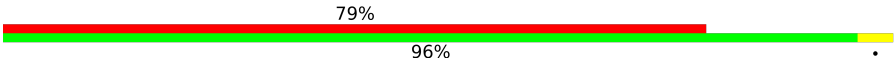
Chain SJ:

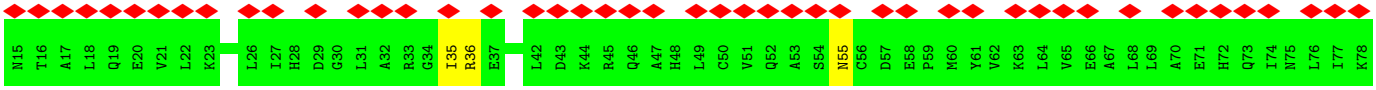


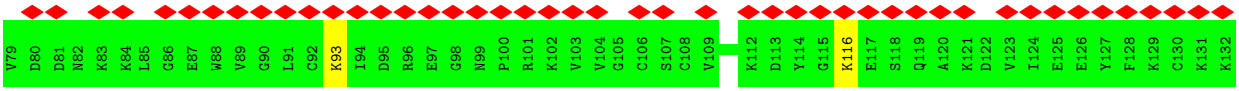


- Molecule 26: 40S ribosomal protein S12

Chain SM:

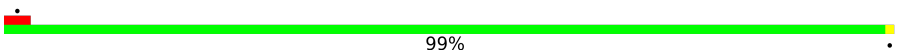


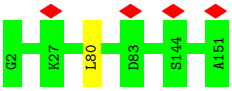




- Molecule 27: 40S ribosomal protein S13

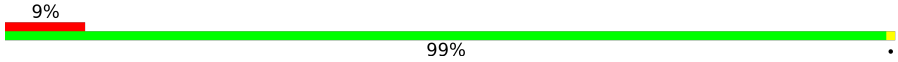
Chain SN:

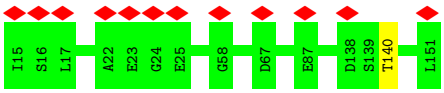




- Molecule 28: 40S ribosomal protein S14

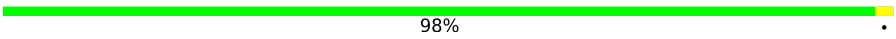
Chain SO:

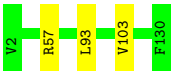




• Molecule 29: 40S ribosomal protein S15a

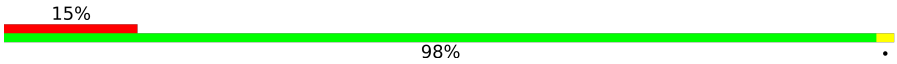
Chain SW:

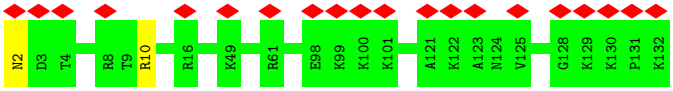




• Molecule 30: 40S ribosomal protein S24

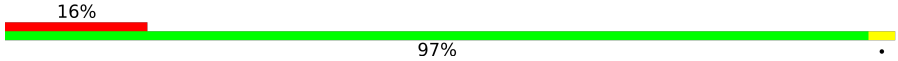
Chain SY:

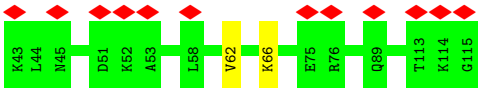




• Molecule 31: 40S ribosomal protein S25

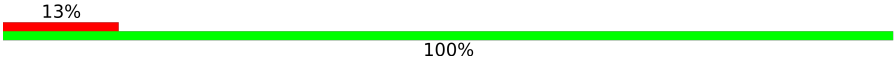
Chain SZ:

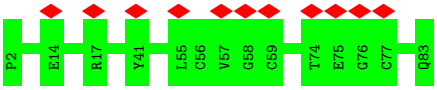




• Molecule 32: 40S ribosomal protein S27

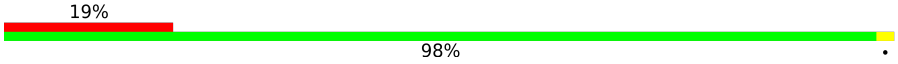
Chain Sb:

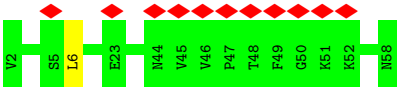




• Molecule 33: 40S ribosomal protein S30

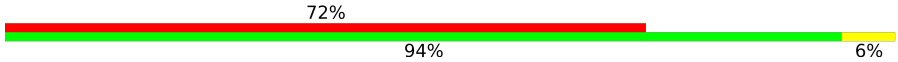
Chain Se:

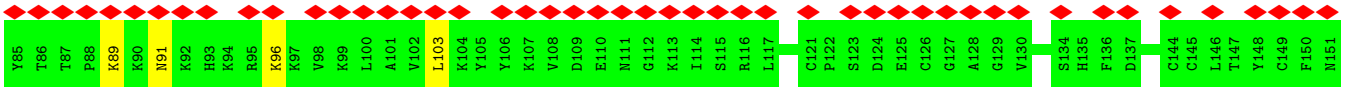




• Molecule 34: 40S ribosomal protein S27a

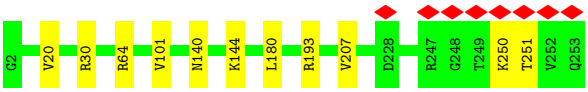
Chain Sf:





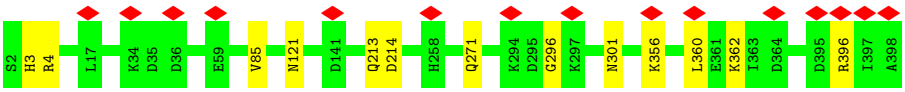
• Molecule 35: 60S ribosomal protein L8

Chain A: 96%



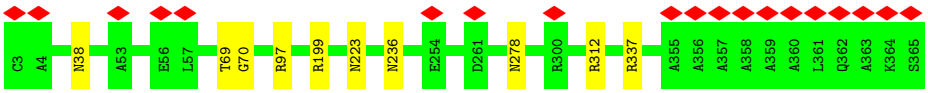
• Molecule 36: 60S ribosomal protein L3

Chain B: 97%



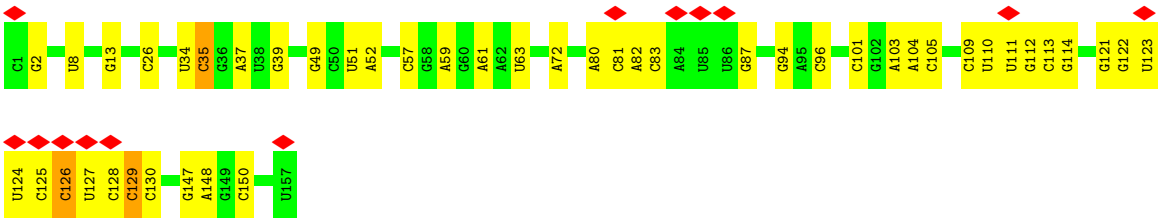
• Molecule 37: 60S ribosomal protein L4

Chain C: 5% 97%



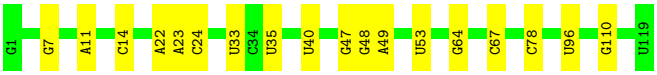
• Molecule 38: 5.8S ribosomal RNA

Chain D: 8% 71% 27%



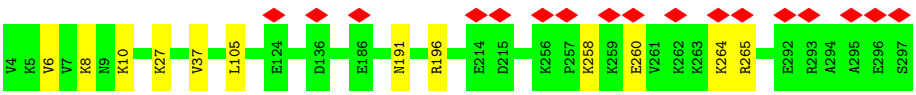
• Molecule 39: 5S ribosomal RNA

Chain E: 85% 15%



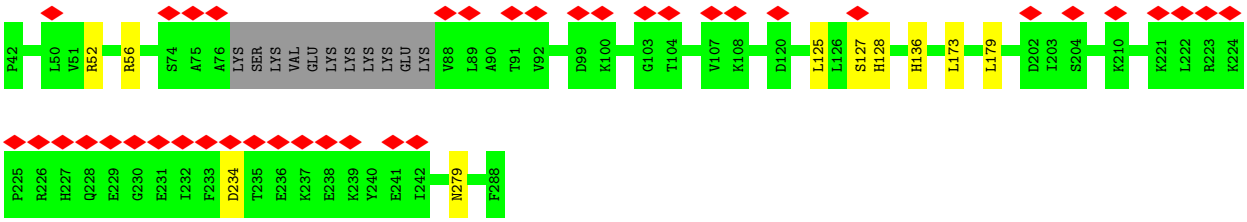
• Molecule 40: 60S ribosomal protein L5

Chain F: 6% 96%



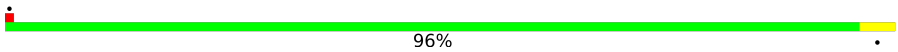
• Molecule 41: 60S ribosomal protein L6

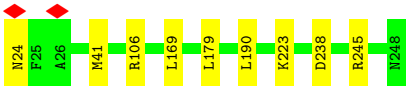
Chain G: 16% 91%



• Molecule 42: 60S ribosomal protein L7

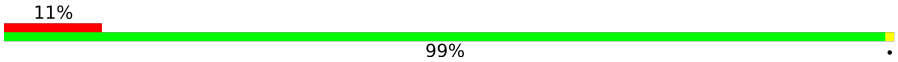
Chain H:

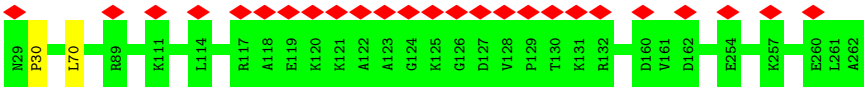




• Molecule 43: 60S ribosomal protein L7a

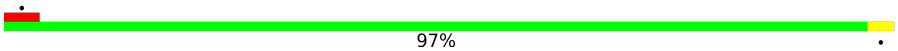
Chain I:

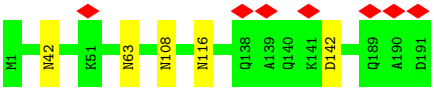




• Molecule 44: 60S ribosomal protein L9

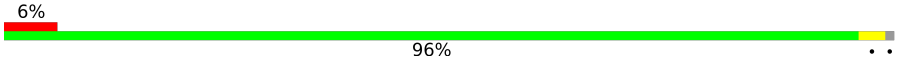
Chain J:

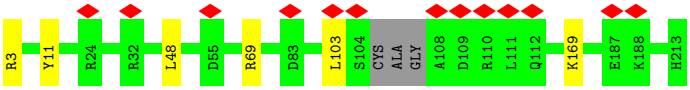




• Molecule 45: 60S ribosomal protein L10

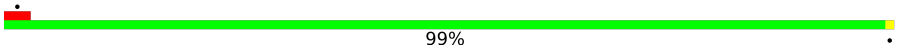
Chain K:

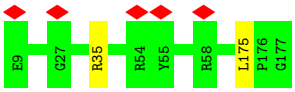




• Molecule 46: 60S ribosomal protein L11

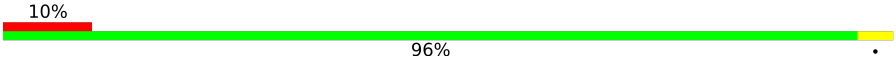
Chain L:

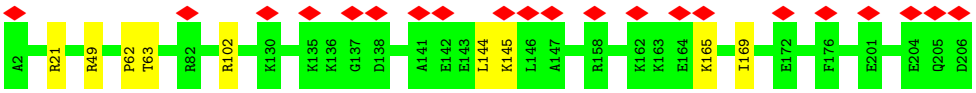




• Molecule 47: 60S ribosomal protein L13

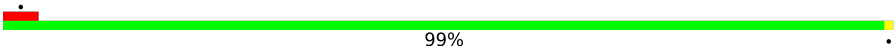
Chain M:

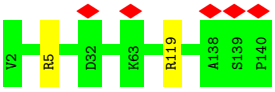




• Molecule 48: 60S ribosomal protein L14

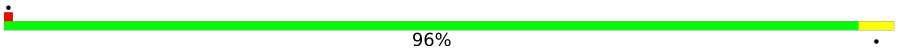
Chain N:

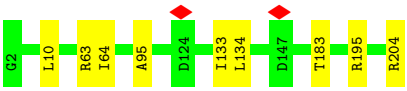




• Molecule 49: 60S ribosomal protein L15

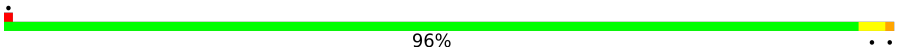
Chain O:

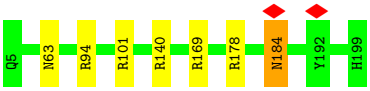




• Molecule 50: 60S ribosomal protein L13a

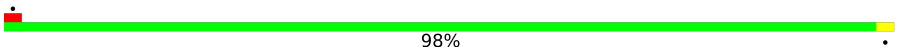
Chain P:

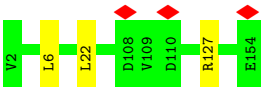




• Molecule 51: 60S ribosomal protein L17

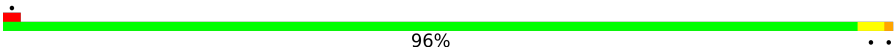
Chain Q:

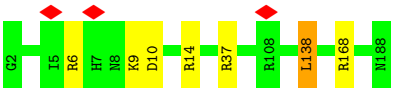




• Molecule 52: 60S ribosomal protein L18

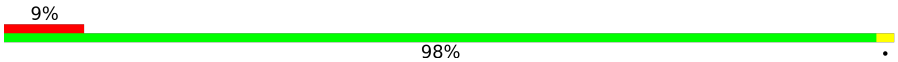
Chain R:

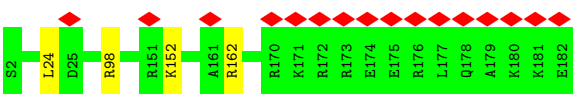




• Molecule 53: 60S ribosomal protein L19

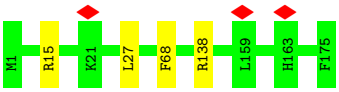
Chain S:





• Molecule 54: 60S ribosomal protein L18a

Chain T: 98%

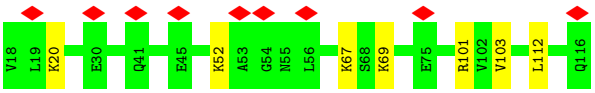


• Molecule 55: 60S ribosomal protein L21

Chain U: 97%

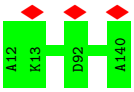
• Molecule 56: 60S ribosomal protein L22

Chain V: 9% 93% 7%



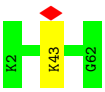
• Molecule 57: 60S ribosomal protein L23

Chain W: 100%



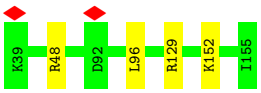
• Molecule 58: 60S ribosomal protein L24

Chain X: 98%



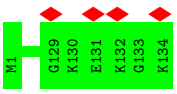
• Molecule 59: 60S ribosomal protein L23a

Chain Y: 97%



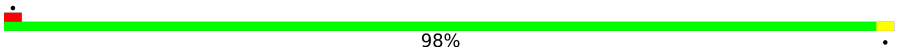
• Molecule 60: 60S ribosomal protein L26

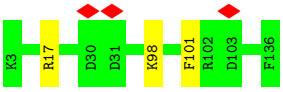
Chain Z: 100%



- Molecule 61: 60S ribosomal protein L27

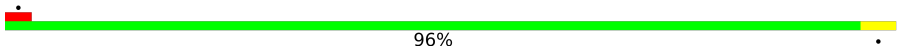
Chain a:

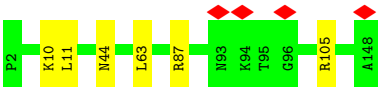




- Molecule 62: 60S ribosomal protein L27a

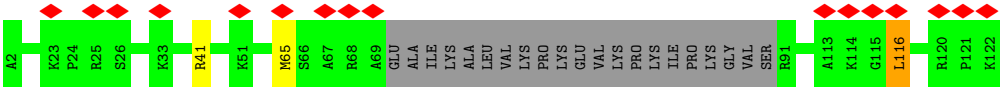
Chain b:





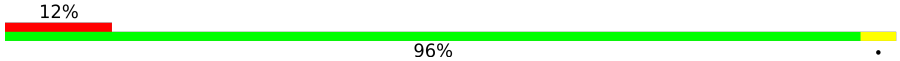
- Molecule 63: 60S ribosomal protein L29

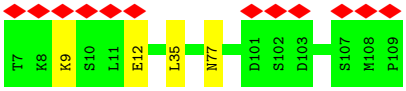
Chain c:



- Molecule 64: 60S ribosomal protein L30

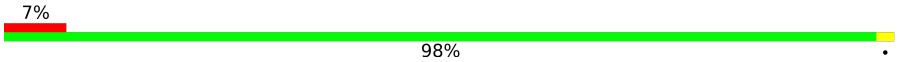
Chain d:

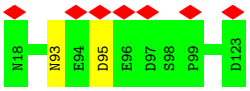




- Molecule 65: 60S ribosomal protein L31

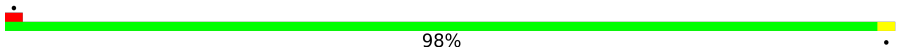
Chain e:





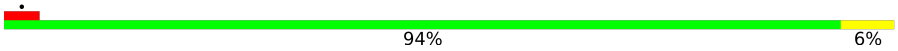
- Molecule 66: 60S ribosomal protein L32

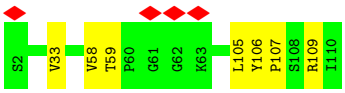
Chain f:



- Molecule 67: 60S ribosomal protein L35a

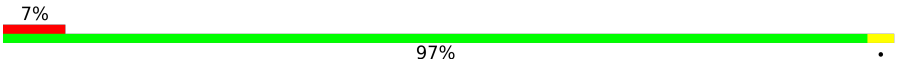
Chain g:

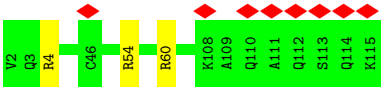




• Molecule 68: 60S ribosomal protein L34

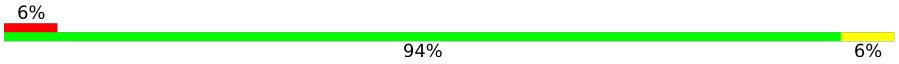
Chain h:

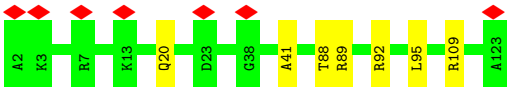




• Molecule 69: 60S ribosomal protein L35

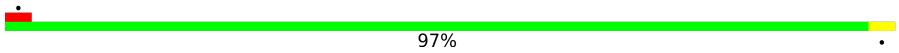
Chain i:

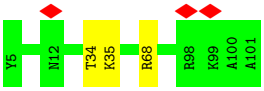




• Molecule 70: 60S ribosomal protein L36

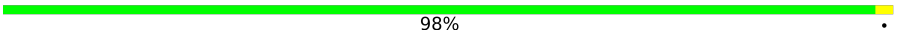
Chain j:





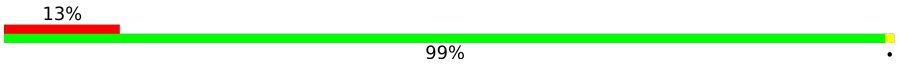
• Molecule 71: 60S ribosomal protein L37

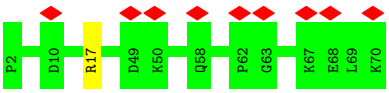
Chain k:



• Molecule 72: 60S ribosomal protein L38

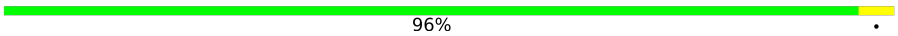
Chain l:

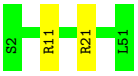




• Molecule 73: 60S ribosomal protein L39

Chain m:





• Molecule 74: 60S ribosomal protein L40

Chain n: 98%

I78 E79 K112 V127

• Molecule 75: 60S ribosomal protein L41

Chain o: 96%

M1 R9 K25

• Molecule 76: 60S ribosomal protein L36a

Chain p: 8% 92% 7%

V2 T10 K27 K30 R69 N76 C77 R78 R81 L93 G94 G95 R99 V103 I104 Q105 F106

• Molecule 77: 60S ribosomal protein L37a

Chain q: 99%

A2 R84 K90 D91 Q92

• Molecule 78: 60S ribosomal protein L28

Chain r: 94% 6%

S2 L5 N21 K22 Q23 N41 N83 K101 L106 P123

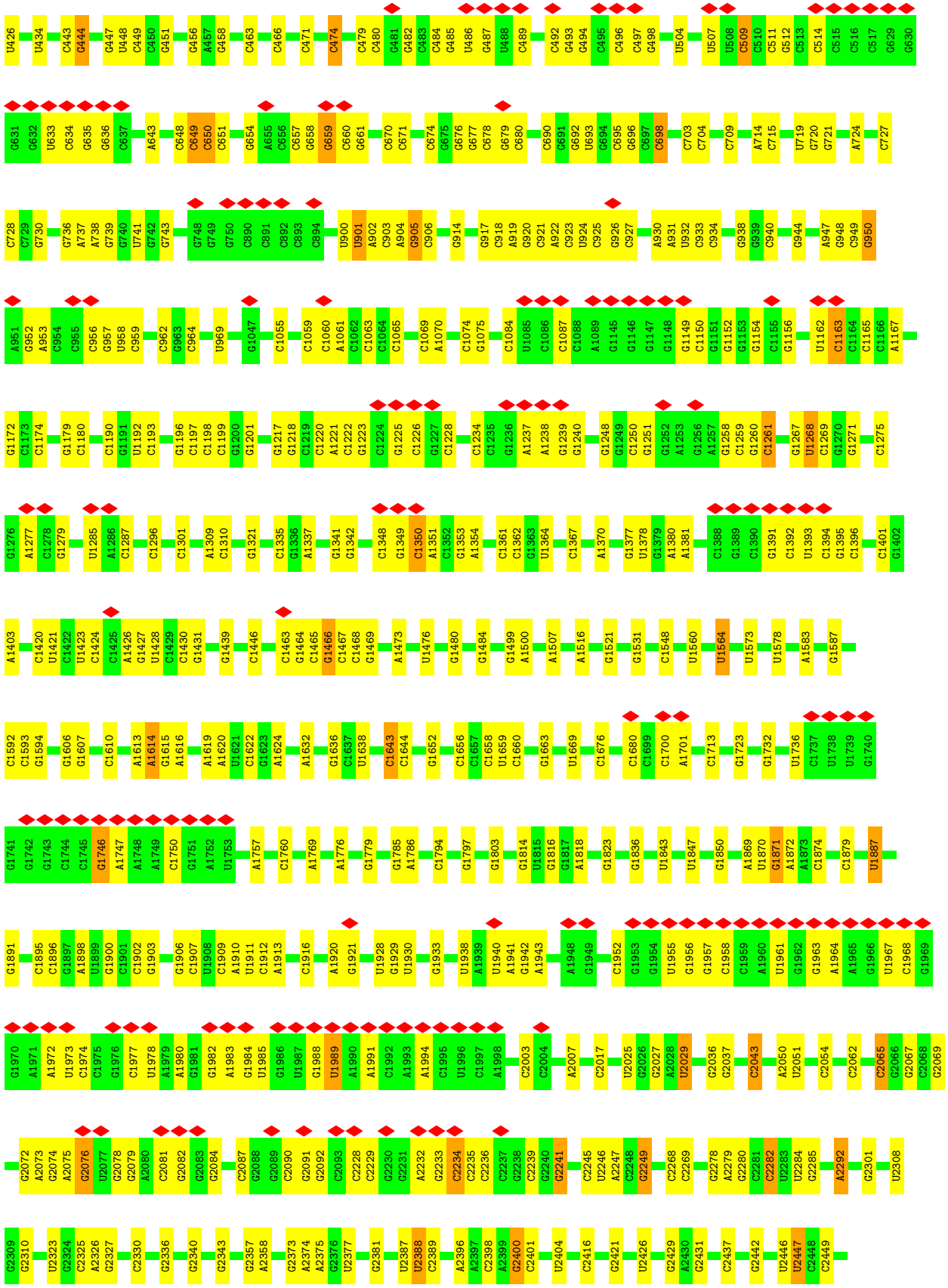
• Molecule 79: 28S ribosomal RNA

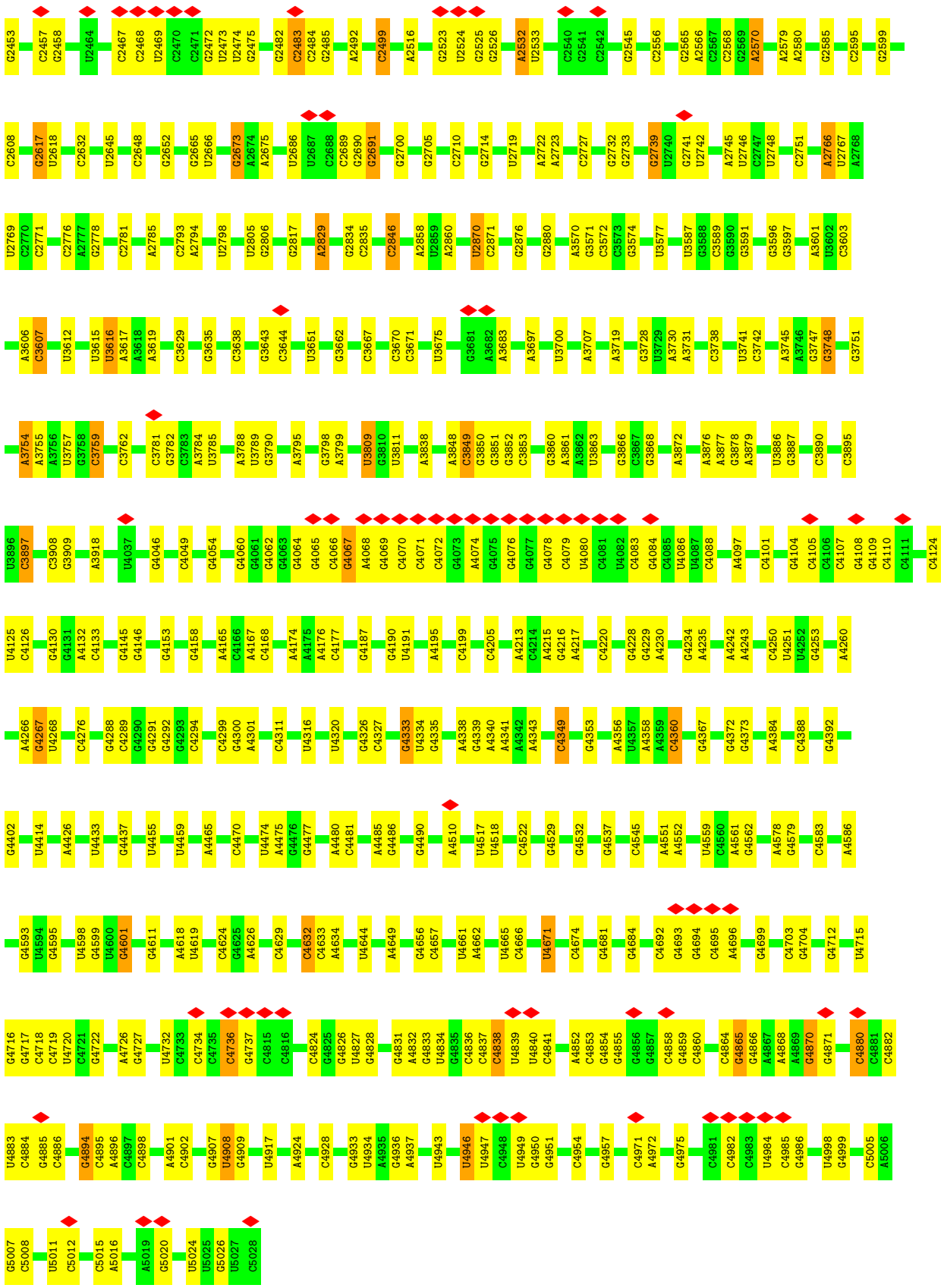
Chain t: 7% 72% 26%

C1 C6 C9 A10 G11 A17 C18 A25 C26 C27 C30 U31 G32 A39 G40 C41 A42 G48 U49 G58 A59 A64 A65 A66 C67 A70 C71 C72 A73 G74 G75 G91 C92 G93 A101 A108 G109 C110 C111 G116 C117 C118 G119 A120 C129

C130 C131 G132 C133 G134 G135 G136 G137 C138 G143 A144 G148 U149 G150 C156 G157 C169 G173 G174 C175 G176 U181 C182 G183 U184 G185 G190 C193 G196 U197 A205 U206 C207 C212 C213 C214 A215 G216 C217 C218 C219 C225 U228 G229 U230 G233

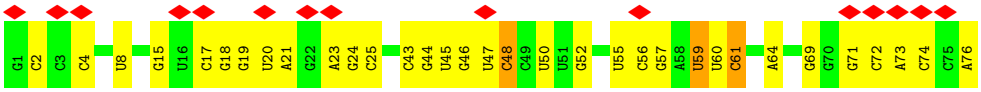
C236 G237 C242 C249 G250 G251 C252 G253 C256 G257 C258 C259 C260 G272 C276 G288 A289 A290 U291 A300 G309 U310 A311 A323 C334 C339 A343 C344 G367 A370 A379 A380 G381 A404 G405 G406 G407 C408 G409 U410 G411 G425


U426 U434 C443 G444 G447 U448 C449 C450 G451 G456 A457 G458 C463 C466 C471 C474 C479 C480 G481 G482 C483 C484 G485 U486 G487 U488 C489 C492 G493 G494 C495 C496 C497 G498 U504 U507 U508 C509 C510 C511 G512 C513 C514 C515 C516 C517 G629 G630
G631 G632 U633 C634 G635 G636 C637 A643 C648 G649 G650 C651 G654 A655 C656 C657 G658 G659 C660 C661 C670 C671 C674 G675 G676 G677 G678 G679 C680 C690 G691 G692 U693 G694 C695 G696 C697 G698 C703 C704 C709 A714 C715 U719 G720 G721 A724 C727
C728 G729 G730 G736 A737 A738 G739 G740 U741 G742 G743 G748 G749 G750 C890 C891 C892 C893 C894 U900 U901 A902 C903 A904 G905 C906 G914 G917 C918 A919 G920 C921 A922 C923 U924 C925 G926 C927 A930 A931 U932 C933 C934 G938 G939 C940 G944 A947 G948 C949 G950
A951 G952 A953 C954 C955 C956 G957 U958 C959 C962 G963 C964 U969 G1047 C1055 C1059 C1060 A1061 C1062 C1063 C1064 C1065 C1069 A1070 C1074 G1075 C1084 U1085 C1086 C1087 C1088 A1089 G1145 G1146 G1147 G1148 G1149 C1150 C1151 G1152 G1153 G1154 C1155 C1156 U1162 C1163 C1164 C1165 C1166 A1167
G1172 C1173 C1174 G1179 C1180 C1190 G1191 U1192 C1193 G1196 C1197 C1198 C1199 G1200 G1201 G1217 G1218 C1219 C1220 A1221 C1222 G1223 C1224 G1225 C1226 G1227 C1228 C1234 C1235 G1236 A1237 A1238 G1239 G1240 G1248 G1249 C1250 G1251 G1252 A1253 G1256 A1257 G1258 C1259 G1260 C1261 G1267 U1268 C1269 G1270 G1271 C1275
G1276 A1277 C1278 G1279 U1285 A1286 C1287 C1296 C1301 A1309 C1310 G1321 C1335 G1336 A1337 G1341 G1342 C1348 G1349 C1350 A1351 C1352 G1353 A1354 C1361 C1362 G1363 U1364 C1367 A1370 G1377 U1378 G1379 A1380 A1381 C1388 G1389 C1390 G1391 C1392 U1393 C1394 G1395 C1396 C1401 G1402
A1403 C1420 U1421 C1422 U1423 C1424 C1425 A1426 G1427 U1428 C1429 C1430 G1431 G1439 C1446 C1463 G1464 C1465 G1466 C1467 C1468 G1469 A1473 U1476 G1480 G1484 G1499 A1500 A1507 A1516 G1521 G1531 C1548 U1560 U1564 U1573 U1578 A1583 G1587
C1592 C1593 G1594 G1606 G1607 C1610 A1613 A1614 G1615 A1616 A1619 A1620 U1621 C1622 G1623 A1624 A1632 G1636 C1637 U1638 C1643 C1644 G1652 C1656 C1657 C1658 U1659 C1660 G1663 U1669 C1676 C1680 C1699 C1700 A1701 C1713 G1723 G1732 U1736 C1737 U1738 U1739 G1740
G1741 G1742 G1743 C1744 C1745 G1746 A1747 A1748 A1749 C1750 G1751 A1752 U1753 A1757 C1760 A1769 A1776 G1779 G1785 A1786 C1794 G1797 G1803 G1814 U1815 G1816 G1817 A1818 G1823 G1836 U1843 U1847 G1850 A1869 U1870 G1871 A1872 A1873 C1874 C1879 U1887
G1891 C1895 C1896 G1897 A1898 U1899 G1900 C1901 C1902 G1903 G1906 C1907 U1908 C1909 A1910 U1911 C1912 A1913 C1916 A1920 G1921 U1928 G1929 U1930 G1933 U1938 A1939 U1940 A1941 G1942 A1943 A1948 G1949 C1952 G1953 G1954 U1955 G1956 G1957 C1958 C1959 A1960 U1961 G1962 G1963 A1964 A1965 G1966 U1967 C1968 G1969
G1970 A1971 A1972 U1973 C1974 C1975 G1976 C1977 U1978 A1979 A1980 G1981 G1982 A1983 G1984 U1985 G1986 U1987 G1988 U1989 A1990 A1991 C1992 A1993 A1994 C1995 U1996 C1997 A1998 C2003 C2004 A2007 C2017 U2025 G2026 G2027 A2028 U2029 G2036 G2037 C2043 A2050 U2051 C2054 C2062 C2065 G2066 G2067 C2068 G2069
G2072 A2073 G2074 A2075 G2076 U2077 G2078 G2079 A2080 C2081 G2082 G2083 G2084 C2087 G2088 G2089 C2090 G2091 G2092 C2093 C2228 C2229 G2230 G2231 A2232 G2233 C2234 C2235 C2236 C2237 G2238 C2239 G2240 G2241 C2245 U2246 A2247 C2248 G2249 C2268 C2269 G2278 A2279 G2280 C2281 C2282 U2283 U2284 G2285 A2292 G2301 U2308
G2309 G2310 U2323 G2324 C2325 A2326 G2327 C2330 G2336 G2340 G2343 G2357 A2358 G2373 A2374 A2375 G2376 U2377 G2381 U2387 U2388 C2389 A2396 A2397 C2398 A2399 G2400 C2401 U2404 C2416 G2421 U2426 G2429 A2430 G2431 C2437 G2442 U2446 U2447 C2448 C2449



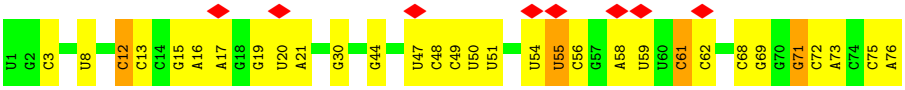
- Molecule 80: tRNA

Chain u:



- Molecule 81: tRNA

Chain v:

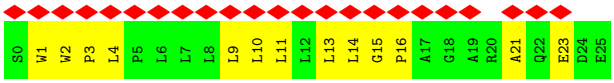


- Molecule 82: mRNA

Chain w:

- Molecule 83: Proprotein convertase subtilisin/kexin type 9

Chain y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.178	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	524.60004, 524.60004, 524.60004	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	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: B8Q, MG, E3C, OMG, 4AC, 5MC, 5MU, M7A, ZN, B8N, MA6, PSU, UR3, A2M, OMU, 6MZ, MVM, OMC

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	S2	0.66	20/39949 (0.1%)	1.14	273/62213 (0.4%)
2	SA	0.39	0/1778	0.71	5/2416 (0.2%)
3	SB	0.36	0/1765	0.65	2/2362 (0.1%)
4	SD	0.35	0/1785	0.67	0/2404
5	SE	0.35	0/2099	0.63	0/2822
6	SF	0.40	0/1514	0.78	4/2031 (0.2%)
7	SH	0.33	0/1518	0.66	1/2029 (0.0%)
8	SI	0.36	0/1702	0.64	0/2271
9	SK	0.38	0/851	0.67	0/1147
10	SL	0.39	0/1266	0.64	0/1690
11	SP	0.36	0/1065	0.65	1/1423 (0.1%)
12	SQ	0.38	0/1177	0.70	0/1575
13	SR	0.34	0/1097	0.68	0/1474
14	SS	0.35	0/1216	0.65	1/1628 (0.1%)
15	ST	0.34	0/1131	0.64	1/1515 (0.1%)
16	SU	0.33	0/831	0.71	2/1115 (0.2%)
17	SV	0.38	0/631	0.67	0/844
18	SX	0.41	0/1116	0.68	1/1490 (0.1%)
19	Sa	0.47	0/836	0.67	0/1121
20	Sc	0.34	0/508	0.71	0/680
21	Sd	0.47	0/470	0.75	1/623 (0.2%)
22	Sg	0.33	0/2486	0.70	5/3384 (0.1%)
23	SC	0.43	0/1753	0.74	3/2365 (0.1%)
24	SG	0.31	0/1946	0.66	4/2590 (0.2%)
25	SJ	0.51	1/1561 (0.1%)	0.88	5/2083 (0.2%)
26	SM	0.30	0/922	0.66	0/1238
27	SN	0.34	0/1232	0.63	1/1656 (0.1%)
28	SO	0.34	0/1037	0.67	0/1391
29	SW	0.38	0/1051	0.65	0/1406
30	SY	0.34	0/1094	0.63	0/1452
31	SZ	0.38	0/585	0.78	0/785

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Sb	0.34	0/653	0.58	0/876
33	Se	0.33	0/458	0.61	0/604
34	Sf	0.32	0/560	0.68	1/745 (0.1%)
35	A	0.45	0/1968	0.66	1/2639 (0.0%)
36	B	0.43	0/3270	0.71	2/4377 (0.0%)
37	C	0.42	0/2942	0.68	0/3951
38	D	0.72	1/3726 (0.0%)	1.09	21/5804 (0.4%)
39	E	0.70	0/2839	1.07	9/4425 (0.2%)
40	F	0.40	0/2437	0.65	1/3262 (0.0%)
41	G	0.38	0/1942	0.77	4/2606 (0.2%)
42	H	0.45	0/1905	0.70	2/2539 (0.1%)
43	I	0.38	0/1913	0.67	1/2576 (0.0%)
44	J	0.38	0/1545	0.67	1/2077 (0.0%)
45	K	0.41	0/1730	0.67	2/2311 (0.1%)
46	L	0.38	0/1376	0.67	1/1841 (0.1%)
47	M	0.41	0/1688	0.70	0/2260
48	N	0.40	0/1161	0.62	0/1554
49	O	0.48	0/1746	0.72	2/2338 (0.1%)
50	P	0.44	0/1638	0.64	0/2191
51	Q	0.44	0/1268	0.66	1/1701 (0.1%)
52	R	0.44	0/1537	0.72	1/2052 (0.0%)
53	S	0.42	0/1533	0.66	1/2025 (0.0%)
54	T	0.44	0/1488	0.68	1/1997 (0.1%)
55	U	0.45	0/1312	0.66	0/1753
56	V	0.36	0/822	0.63	1/1103 (0.1%)
57	W	0.41	0/983	0.62	0/1319
58	X	0.46	0/524	0.62	0/698
59	Y	0.38	0/975	0.66	0/1312
60	Z	0.44	0/1132	0.63	0/1504
61	a	0.41	0/1126	0.66	1/1502 (0.1%)
62	b	0.44	0/1191	0.75	1/1591 (0.1%)
63	c	0.33	0/826	0.65	1/1088 (0.1%)
64	d	0.44	0/812	0.70	0/1089
65	e	0.42	0/894	0.67	1/1204 (0.1%)
66	f	0.42	0/1082	0.68	2/1443 (0.1%)
67	g	0.45	0/895	0.69	1/1198 (0.1%)
68	h	0.44	0/916	0.75	1/1220 (0.1%)
69	i	0.36	0/1023	0.69	0/1351
70	j	0.35	0/805	0.64	0/1065
71	k	0.42	0/703	0.66	0/929
72	l	0.39	0/575	0.65	0/761
73	m	0.38	0/454	0.67	0/599
74	n	0.39	0/417	0.64	0/553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	o	0.36	0/241	0.66	0/305
76	p	0.47	0/877	0.73	1/1156 (0.1%)
77	q	0.43	0/718	0.65	0/953
78	r	0.46	0/995	0.76	2/1334 (0.1%)
79	t	0.73	3/86502 (0.0%)	1.10	428/134927 (0.3%)
80	u	0.46	0/1799	1.27	21/2800 (0.8%)
81	v	0.50	0/1802	1.23	18/2797 (0.6%)
82	w	0.64	0/235	1.31	3/365 (0.8%)
83	y	0.53	0/210	0.99	2/289 (0.7%)
All	All	0.60	25/230141 (0.0%)	0.98	846/338182 (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
1	S2	0	1
11	SP	0	1
13	SR	0	1
36	B	0	1
40	F	0	1
47	M	0	1
64	d	0	1
76	p	0	2
All	All	0	9

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1357	A	N7-C5	-14.86	1.30	1.39
1	S2	1351	G	N7-C5	-10.71	1.32	1.39
1	S2	1357	A	N9-C4	10.35	1.44	1.37
25	SJ	66	LYS	C-N	9.27	1.55	1.34
1	S2	1351	G	N9-C8	-9.17	1.31	1.37

The worst 5 of 846 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1350	U	C5-C6-N1	29.79	137.59	122.70
1	S2	1351	G	C8-N9-C4	-29.31	94.68	106.40
1	S2	1351	G	N7-C8-N9	26.21	126.21	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1350	U	C5-C4-O4	-24.49	111.21	125.90
1	S2	115	U	C2-N3-C4	21.74	140.04	127.00

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	B	296	GLY	Peptide
40	F	264	LYS	Peptide
1	S2	1351	G	Sidechain
11	SP	14	LYS	Peptide
13	SR	67	ARG	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
2	SA	219/221 (99%)	193 (88%)	25 (11%)	1 (0%)	29 64
3	SB	212/214 (99%)	189 (89%)	23 (11%)	0	100 100
4	SD	224/226 (99%)	194 (87%)	30 (13%)	0	100 100
5	SE	253/259 (98%)	232 (92%)	21 (8%)	0	100 100
6	SF	183/189 (97%)	163 (89%)	20 (11%)	0	100 100
7	SH	180/189 (95%)	158 (88%)	22 (12%)	0	100 100
8	SI	202/204 (99%)	183 (91%)	19 (9%)	0	100 100
9	SK	96/98 (98%)	84 (88%)	12 (12%)	0	100 100
10	SL	147/153 (96%)	130 (88%)	17 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	SP	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
12	SQ	144/146 (99%)	119 (83%)	23 (16%)	2 (1%)	11	40
13	SR	132/134 (98%)	115 (87%)	16 (12%)	1 (1%)	19	54
14	SS	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
15	ST	141/143 (99%)	133 (94%)	6 (4%)	2 (1%)	11	40
16	SU	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
17	SV	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	12	42
18	SX	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	22	57
19	Sa	100/102 (98%)	88 (88%)	11 (11%)	1 (1%)	15	49
20	Sc	62/64 (97%)	51 (82%)	10 (16%)	1 (2%)	9	37
21	Sd	53/55 (96%)	43 (81%)	9 (17%)	1 (2%)	8	33
22	Sg	310/312 (99%)	259 (84%)	51 (16%)	0	100	100
23	SC	215/220 (98%)	198 (92%)	16 (7%)	1 (0%)	29	64
24	SG	235/237 (99%)	215 (92%)	20 (8%)	0	100	100
25	SJ	184/185 (100%)	167 (91%)	16 (9%)	1 (0%)	29	64
26	SM	116/118 (98%)	100 (86%)	16 (14%)	0	100	100
27	SN	148/150 (99%)	141 (95%)	7 (5%)	0	100	100
28	SO	135/137 (98%)	121 (90%)	14 (10%)	0	100	100
29	SW	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
30	SY	130/131 (99%)	124 (95%)	6 (5%)	0	100	100
31	SZ	71/73 (97%)	61 (86%)	10 (14%)	0	100	100
32	Sb	80/82 (98%)	66 (82%)	14 (18%)	0	100	100
33	Se	55/57 (96%)	47 (86%)	8 (14%)	0	100	100
34	Sf	65/67 (97%)	50 (77%)	15 (23%)	0	100	100
35	A	250/252 (99%)	226 (90%)	22 (9%)	2 (1%)	19	54
36	B	395/397 (100%)	358 (91%)	34 (9%)	3 (1%)	19	54
37	C	361/363 (99%)	326 (90%)	33 (9%)	2 (1%)	25	59
40	F	292/294 (99%)	269 (92%)	22 (8%)	1 (0%)	41	73
41	G	232/247 (94%)	197 (85%)	32 (14%)	3 (1%)	12	42
42	H	223/225 (99%)	204 (92%)	17 (8%)	2 (1%)	17	52
43	I	232/234 (99%)	213 (92%)	18 (8%)	1 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	J	189/191 (99%)	172 (91%)	17 (9%)	0	100	100
45	K	204/211 (97%)	185 (91%)	18 (9%)	1 (0%)	29	64
46	L	167/169 (99%)	152 (91%)	15 (9%)	0	100	100
47	M	203/205 (99%)	172 (85%)	30 (15%)	1 (0%)	29	64
48	N	137/139 (99%)	126 (92%)	11 (8%)	0	100	100
49	O	201/203 (99%)	179 (89%)	21 (10%)	1 (0%)	29	64
50	P	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	29	64
51	Q	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
52	R	185/187 (99%)	169 (91%)	14 (8%)	2 (1%)	14	46
53	S	179/181 (99%)	168 (94%)	11 (6%)	0	100	100
54	T	173/175 (99%)	159 (92%)	14 (8%)	0	100	100
55	U	155/157 (99%)	137 (88%)	16 (10%)	2 (1%)	12	42
56	V	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
57	W	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
58	X	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
59	Y	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
60	Z	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
61	a	132/134 (98%)	119 (90%)	13 (10%)	0	100	100
62	b	145/147 (99%)	125 (86%)	20 (14%)	0	100	100
63	c	94/121 (78%)	80 (85%)	14 (15%)	0	100	100
64	d	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
65	e	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
66	f	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
67	g	107/109 (98%)	94 (88%)	12 (11%)	1 (1%)	17	52
68	h	112/114 (98%)	103 (92%)	9 (8%)	0	100	100
69	i	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	4	21
70	j	95/97 (98%)	89 (94%)	4 (4%)	2 (2%)	7	30
71	k	82/84 (98%)	72 (88%)	10 (12%)	0	100	100
72	l	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
73	m	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
74	n	48/50 (96%)	45 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
75	o	23/25 (92%)	23 (100%)	0	0	100 100
76	p	103/105 (98%)	95 (92%)	6 (6%)	2 (2%)	8 33
77	q	89/91 (98%)	82 (92%)	7 (8%)	0	100 100
78	r	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	5 27
83	y	24/26 (92%)	17 (71%)	3 (12%)	4 (17%)	0 0
All	All	11201/11416 (98%)	10107 (90%)	1043 (9%)	51 (0%)	32 64

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	SV	79	VAL
23	SC	78	LEU
52	R	10	ASP
67	g	107	PRO
69	i	89	ARG

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
2	SA	183/183 (100%)	178 (97%)	5 (3%)	44 74
3	SB	195/195 (100%)	194 (100%)	1 (0%)	88 94
4	SD	189/189 (100%)	187 (99%)	2 (1%)	73 89
5	SE	222/222 (100%)	218 (98%)	4 (2%)	59 82
6	SF	159/159 (100%)	153 (96%)	6 (4%)	33 66
7	SH	166/169 (98%)	165 (99%)	1 (1%)	86 94
8	SI	177/177 (100%)	173 (98%)	4 (2%)	50 77
9	SK	89/89 (100%)	87 (98%)	2 (2%)	52 78
10	SL	137/137 (100%)	133 (97%)	4 (3%)	42 72
11	SP	113/113 (100%)	111 (98%)	2 (2%)	59 82
12	SQ	121/121 (100%)	120 (99%)	1 (1%)	81 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	SR	121/121 (100%)	118 (98%)	3 (2%)	47	75
14	SS	126/126 (100%)	125 (99%)	1 (1%)	81	92
15	ST	113/113 (100%)	110 (97%)	3 (3%)	44	74
16	SU	94/94 (100%)	89 (95%)	5 (5%)	22	54
17	SV	66/66 (100%)	63 (96%)	3 (4%)	27	60
18	SX	113/113 (100%)	110 (97%)	3 (3%)	44	74
19	Sa	89/89 (100%)	86 (97%)	3 (3%)	37	69
20	Sc	57/57 (100%)	57 (100%)	0	100	100
21	Sd	48/48 (100%)	46 (96%)	2 (4%)	30	62
22	Sg	271/271 (100%)	268 (99%)	3 (1%)	73	89
23	SC	187/186 (100%)	184 (98%)	3 (2%)	62	84
24	SG	207/207 (100%)	199 (96%)	8 (4%)	32	65
25	SJ	162/161 (101%)	155 (96%)	7 (4%)	29	62
26	SM	98/100 (98%)	93 (95%)	5 (5%)	24	56
27	SN	130/130 (100%)	130 (100%)	0	100	100
28	SO	107/107 (100%)	106 (99%)	1 (1%)	78	91
29	SW	112/112 (100%)	109 (97%)	3 (3%)	44	74
30	SY	114/113 (101%)	112 (98%)	2 (2%)	59	82
31	SZ	64/64 (100%)	62 (97%)	2 (3%)	40	70
32	Sb	74/74 (100%)	74 (100%)	0	100	100
33	Se	46/46 (100%)	45 (98%)	1 (2%)	52	78
34	Sf	60/60 (100%)	57 (95%)	3 (5%)	24	57
35	A	194/194 (100%)	186 (96%)	8 (4%)	30	64
36	B	345/345 (100%)	338 (98%)	7 (2%)	55	80
37	C	302/302 (100%)	294 (97%)	8 (3%)	46	74
40	F	248/248 (100%)	239 (96%)	9 (4%)	35	67
41	G	209/220 (95%)	206 (99%)	3 (1%)	67	86
42	H	194/194 (100%)	189 (97%)	5 (3%)	46	74
43	I	199/199 (100%)	199 (100%)	0	100	100
44	J	170/170 (100%)	166 (98%)	4 (2%)	49	76
45	K	178/179 (99%)	175 (98%)	3 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	L	142/142 (100%)	141 (99%)	1 (1%)	84	93
47	M	171/171 (100%)	164 (96%)	7 (4%)	30	64
48	N	118/118 (100%)	116 (98%)	2 (2%)	60	83
49	O	171/171 (100%)	165 (96%)	6 (4%)	36	68
50	P	168/168 (100%)	161 (96%)	7 (4%)	30	62
51	Q	134/134 (100%)	132 (98%)	2 (2%)	65	85
52	R	164/164 (100%)	159 (97%)	5 (3%)	41	71
53	S	160/160 (100%)	157 (98%)	3 (2%)	57	81
54	T	156/156 (100%)	153 (98%)	3 (2%)	57	81
55	U	138/138 (100%)	135 (98%)	3 (2%)	52	78
56	V	89/89 (100%)	83 (93%)	6 (7%)	16	46
57	W	100/100 (100%)	100 (100%)	0	100	100
58	X	53/53 (100%)	52 (98%)	1 (2%)	57	81
59	Y	105/105 (100%)	101 (96%)	4 (4%)	33	66
60	Z	124/124 (100%)	124 (100%)	0	100	100
61	a	117/117 (100%)	115 (98%)	2 (2%)	60	83
62	b	120/120 (100%)	115 (96%)	5 (4%)	30	62
63	c	82/101 (81%)	79 (96%)	3 (4%)	34	66
64	d	88/88 (100%)	85 (97%)	3 (3%)	37	69
65	e	97/97 (100%)	96 (99%)	1 (1%)	76	90
66	f	115/115 (100%)	114 (99%)	1 (1%)	78	91
67	g	88/88 (100%)	83 (94%)	5 (6%)	20	52
68	h	98/98 (100%)	96 (98%)	2 (2%)	55	80
69	i	109/109 (100%)	106 (97%)	3 (3%)	43	73
70	j	83/83 (100%)	82 (99%)	1 (1%)	71	88
71	k	71/71 (100%)	69 (97%)	2 (3%)	43	73
72	l	64/64 (100%)	63 (98%)	1 (2%)	62	84
73	m	47/47 (100%)	45 (96%)	2 (4%)	29	62
74	n	46/46 (100%)	45 (98%)	1 (2%)	52	78
75	o	24/24 (100%)	23 (96%)	1 (4%)	30	62
76	p	93/93 (100%)	89 (96%)	4 (4%)	29	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
77	q	74/74 (100%)	73 (99%)	1 (1%)	67 86
78	r	106/106 (100%)	104 (98%)	2 (2%)	57 81
83	y	21/21 (100%)	13 (62%)	8 (38%)	0 0
All	All	9785/9818 (100%)	9547 (98%)	238 (2%)	51 76

5 of 238 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	C	337	ARG
74	n	112	LYS
47	M	63	THR
73	m	11	ARG
83	y	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
36	B	245	HIS
63	c	19	ASN
41	G	101	ASN
62	b	44	ASN
73	m	43	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1679/1714 (97%)	541 (32%)	34 (2%)
38	D	156/157 (99%)	39 (25%)	0
39	E	118/119 (99%)	13 (11%)	0
79	t	3590/3607 (99%)	879 (24%)	0
80	u	74/76 (97%)	28 (37%)	0
81	v	71/76 (93%)	28 (39%)	0
82	w	9/10 (90%)	2 (22%)	0
All	All	5697/5759 (98%)	1530 (26%)	34 (0%)

5 of 1530 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A

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Mol	Chain	Res	Type
1	S2	7	G
1	S2	16	G
1	S2	23	G
1	S2	24	C

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	1681	U
1	S2	1749	G
1	S2	1815	A
1	S2	445	A
1	S2	417	C

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

34 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	$\#\|Z\| > 2$
1	UR3	S2	1830	1	19,22,23	2.89	7 (36%)	26,32,35	2.99	7 (26%)
1	PSU	S2	1243	1	18,21,22	4.25	7 (38%)	22,30,33	1.88	5 (22%)
1	A2M	S2	1678	1	18,25,26	4.27	8 (44%)	18,36,39	3.51	9 (50%)
1	OMG	S2	644	1	18,26,27	2.51	8 (44%)	19,38,41	1.45	4 (21%)
1	M7A	S2	1806	1	20,25,26	1.97	3 (15%)	28,37,40	3.61	8 (28%)
1	PSU	S2	1081	1	18,21,22	4.11	8 (44%)	22,30,33	1.72	4 (18%)
1	OMG	S2	509	1	18,26,27	2.42	8 (44%)	19,38,41	1.42	4 (21%)
1	PSU	S2	823	1	18,21,22	4.27	8 (44%)	22,30,33	2.40	6 (27%)
1	OMC	S2	1703	1	19,22,23	3.47	7 (36%)	26,31,34	0.88	1 (3%)
1	OMC	S2	517	1	19,22,23	3.57	8 (42%)	26,31,34	0.82	1 (3%)
1	OMG	S2	683	1	18,26,27	2.47	8 (44%)	19,38,41	1.48	4 (21%)
1	MA6	S2	1851	1	19,26,27	1.05	1 (5%)	18,38,41	3.92	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	S2	1374	1	18,22,23	3.40	7 (38%)	26,32,35	1.07	2 (7%)
1	PSU	S2	822	1	18,21,22	4.34	7 (38%)	22,30,33	1.79	5 (22%)
1	A2M	S2	27	1	18,25,26	4.07	6 (33%)	18,36,39	3.58	4 (22%)
1	4AC	S2	1337	1	21,24,25	3.31	9 (42%)	29,34,37	0.98	2 (6%)
1	A2M	S2	484	1	18,25,26	4.10	7 (38%)	18,36,39	3.68	6 (33%)
1	OMU	S2	116	1	19,22,23	3.11	6 (31%)	26,31,34	1.74	5 (19%)
1	OMC	S2	1710	1	19,22,23	3.52	8 (42%)	26,31,34	0.73	0
1	5MU	S2	814	1	19,22,23	7.61	8 (42%)	28,32,35	3.44	12 (42%)
1	B8Q	S2	1219	1	17,22,23	4.59	6 (35%)	22,32,35	1.97	4 (18%)
1	E3C	S2	568	1	18,23,24	3.46	6 (33%)	21,33,36	2.48	5 (23%)
1	MA6	S2	1850	1	19,26,27	1.09	1 (5%)	18,38,41	4.05	3 (16%)
1	A2M	S2	1031	1	18,25,26	4.09	6 (33%)	18,36,39	3.53	5 (27%)
1	A2M	S2	668	1	18,25,26	4.05	6 (33%)	18,36,39	3.75	5 (27%)
1	A2M	S2	159	1	18,25,26	4.12	6 (33%)	18,36,39	3.44	6 (33%)
1	OMU	S2	121	1	19,22,23	3.06	6 (31%)	26,31,34	1.72	5 (19%)
1	PSU	S2	612	1	18,21,22	4.27	8 (44%)	22,30,33	2.04	5 (22%)
1	PSU	S2	119	1	18,21,22	4.41	7 (38%)	22,30,33	1.86	5 (22%)
1	A2M	S2	166	1	18,25,26	4.23	7 (38%)	18,36,39	3.36	5 (27%)
1	OMC	S2	174	1	19,22,23	3.56	8 (42%)	26,31,34	0.79	0
1	4AC	S2	1842	1	21,24,25	3.28	9 (42%)	29,34,37	1.28	4 (13%)
1	6MZ	S2	1832	1	18,25,26	2.08	4 (22%)	16,36,39	2.76	4 (25%)
1	B8N	S2	1248	1	24,29,30	2.84	5 (20%)	29,42,45	1.82	8 (27%)

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
1	UR3	S2	1830	1	-	4/7/25/26	0/2/2/2
1	PSU	S2	1243	1	-	1/7/25/26	0/2/2/2
1	A2M	S2	1678	1	-	2/5/27/28	0/3/3/3
1	OMG	S2	644	1	-	3/5/27/28	0/3/3/3
1	M7A	S2	1806	1	-	1/7/37/38	0/3/3/3
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
1	OMG	S2	509	1	-	0/5/27/28	0/3/3/3
1	PSU	S2	823	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	S2	1703	1	-	2/9/27/28	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	OMG	S2	683	1	-	2/5/27/28	0/3/3/3
1	MA6	S2	1851	1	-	4/7/29/30	0/3/3/3
1	5MC	S2	1374	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	27	1	-	1/5/27/28	0/3/3/3
1	4AC	S2	1337	1	-	2/11/29/30	0/2/2/2
1	A2M	S2	484	1	-	0/5/27/28	0/3/3/3
1	OMU	S2	116	1	-	2/9/27/28	0/2/2/2
1	OMC	S2	1710	1	-	0/9/27/28	0/2/2/2
1	5MU	S2	814	1	-	0/7/25/26	0/2/2/2
1	B8Q	S2	1219	1	-	0/7/42/43	0/2/2/2
1	E3C	S2	568	1	-	4/9/44/45	0/2/2/2
1	MA6	S2	1850	1	-	2/7/29/30	0/3/3/3
1	A2M	S2	1031	1	-	2/5/27/28	0/3/3/3
1	A2M	S2	668	1	-	2/5/27/28	0/3/3/3
1	A2M	S2	159	1	-	4/5/27/28	0/3/3/3
1	OMU	S2	121	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	612	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	2/7/25/26	0/2/2/2
1	A2M	S2	166	1	-	0/5/27/28	0/3/3/3
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	6MZ	S2	1832	1	-	1/5/27/28	0/3/3/3
1	B8N	S2	1248	1	-	2/16/34/35	0/2/2/2

The worst 5 of 224 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	814	5MU	C4-C5	22.37	1.81	1.44
1	S2	814	5MU	C6-N1	16.93	1.66	1.38
1	S2	814	5MU	C6-C5	-11.53	1.15	1.34
1	S2	1678	A2M	O4'-C1'	11.38	1.57	1.41
1	S2	119	PSU	C6-C5	11.23	1.48	1.35

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1850	MA6	N1-C6-N6	-15.15	101.11	117.06
1	S2	1851	MA6	N1-C6-N6	-14.94	101.33	117.06
1	S2	1806	M7A	C5-C6-N6	10.91	142.38	123.74
1	S2	668	A2M	C1'-N9-C4	-10.06	108.97	126.64
1	S2	1806	M7A	N6-C6-N1	-9.61	97.30	118.35

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	116	OMU	C3'-C4'-C5'-O5'
1	S2	116	OMU	O4'-C4'-C5'-O5'
1	S2	159	A2M	O4'-C4'-C5'-O5'
1	S2	159	A2M	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 38 ligands modelled in this entry, 37 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	MVM	t	5110	-	33,35,35	1.33	3 (9%)	36,49,49	1.32	5 (13%)

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
86	MVM	t	5110	-	-	4/20/28/28	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	t	5110	MVM	C1-N2	3.81	1.52	1.46
86	t	5110	MVM	N6-N5	-3.12	1.28	1.34
86	t	5110	MVM	C5-N1	2.95	1.41	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	t	5110	MVM	N6-N5-N4	3.25	109.99	106.37
86	t	5110	MVM	C1-C9-N1	-3.12	108.33	116.16
86	t	5110	MVM	C20-C19-C18	-3.06	115.68	120.08
86	t	5110	MVM	C21-N7-C22	-2.59	113.54	116.77
86	t	5110	MVM	O1-C5-N1	-2.40	118.43	121.48

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	t	5110	MVM	C16-C15-N4-C22
86	t	5110	MVM	C14-C15-N4-C22
86	t	5110	MVM	C16-C15-N4-N5
86	t	5110	MVM	C14-C15-N4-N5

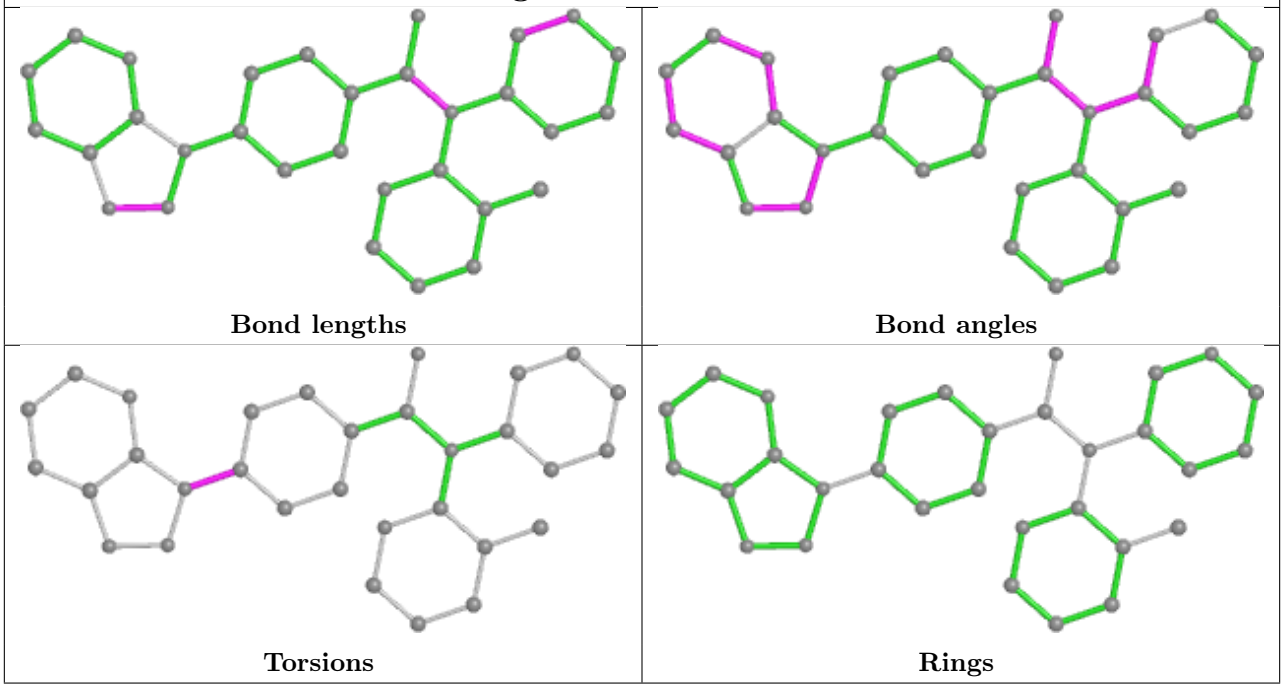
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MVM t 5110



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
1	S2	17
79	t	16
81	v	4
6	SF	2
23	SC	2
5	SE	2
10	SL	2
7	SH	1
63	c	1
80	u	1

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	1677:U	O3'	1678:A2M	P	60.95
1	S2	1353:A	O3'	1354:G	P	60.47
1	S2	1357:A	O3'	1358:U	P	59.69
1	SF	55:ARG	C	56:TYR	N	59.69
1	S2	503:C	O3'	504:G	P	59.61

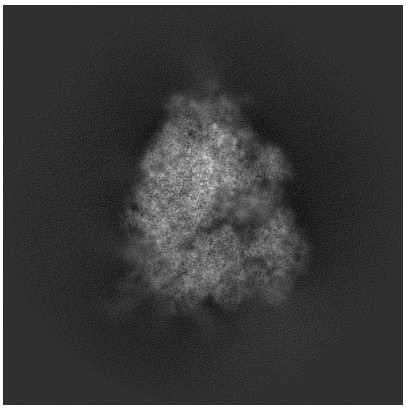
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0596. These allow visual inspection of the internal detail of the map and identification of artifacts.

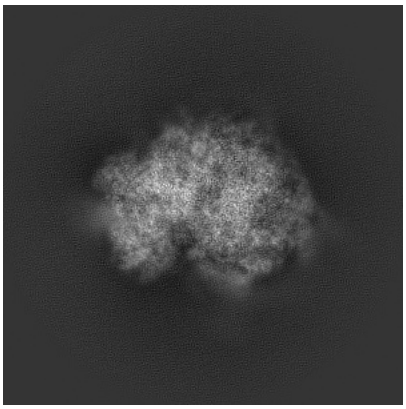
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

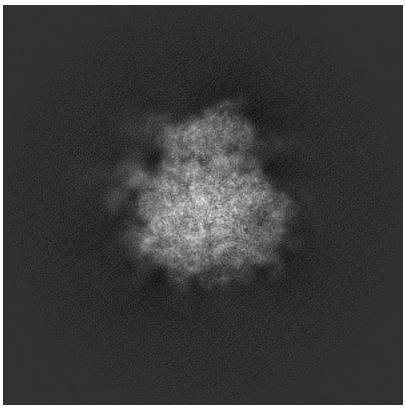
6.1.1 Primary map



X

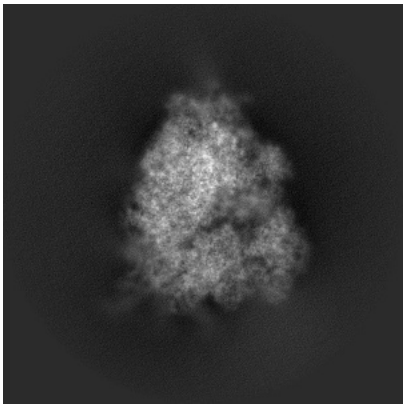


Y

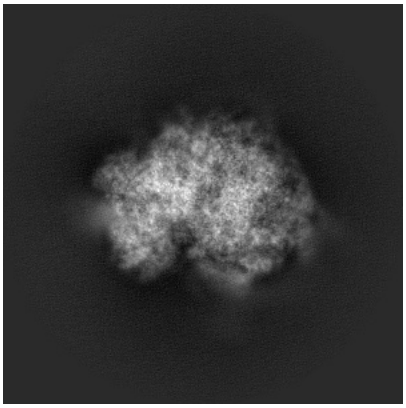


Z

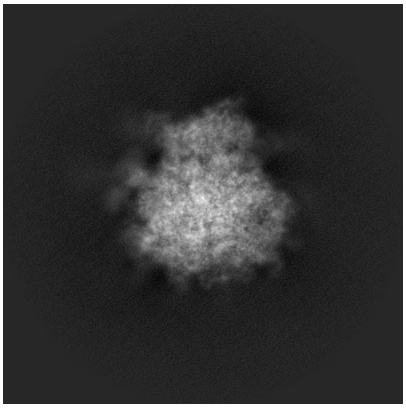
6.1.2 Raw map



X



Y

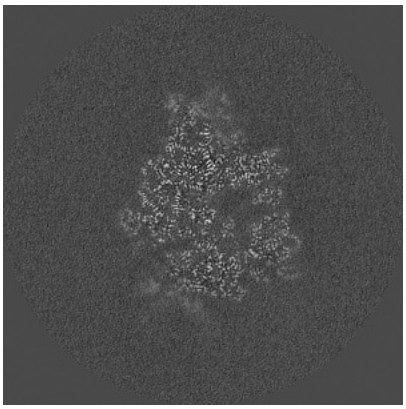


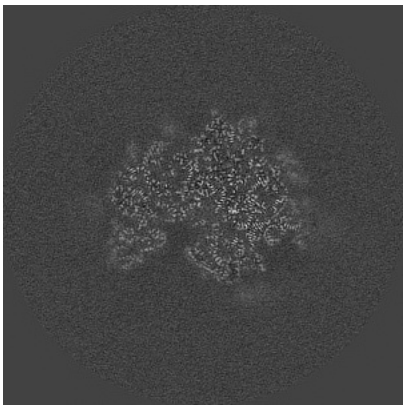
Z

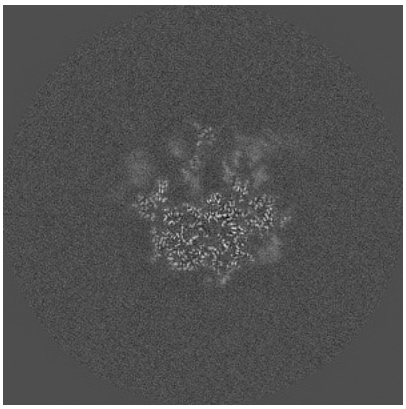
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

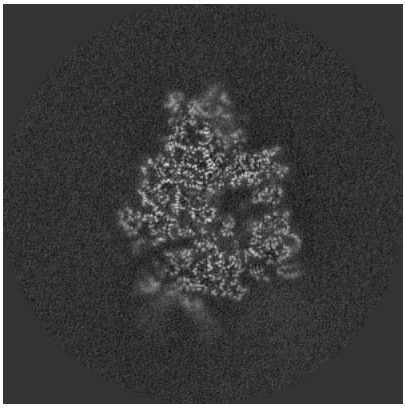
6.2.1 Primary map

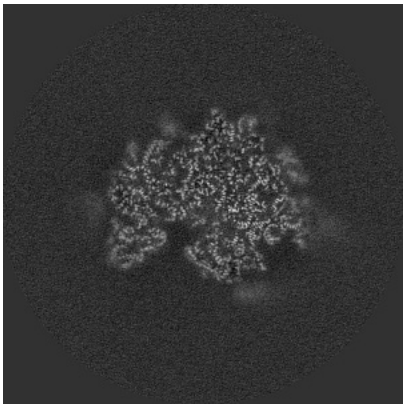

X Index: 215

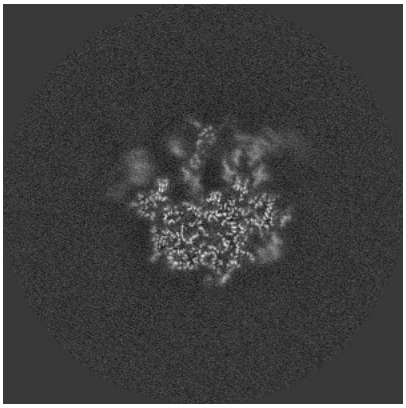

Y Index: 215


Z Index: 215

6.2.2 Raw map


X Index: 215

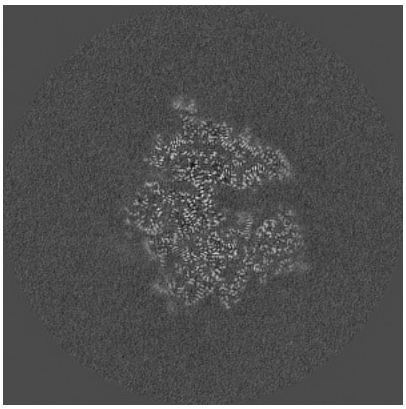

Y Index: 215

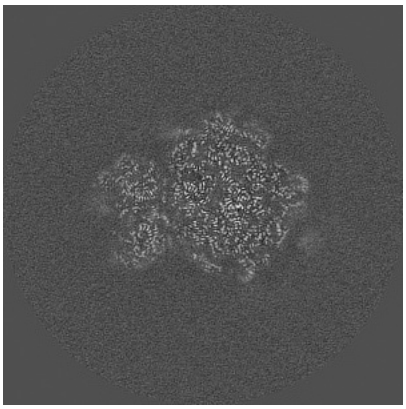

Z Index: 215

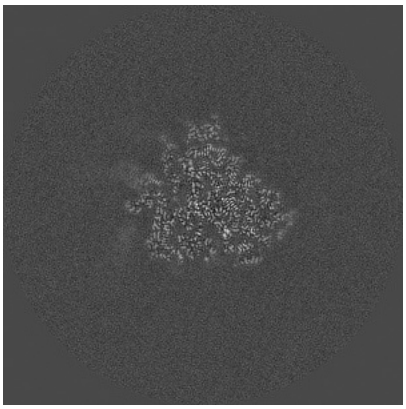
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

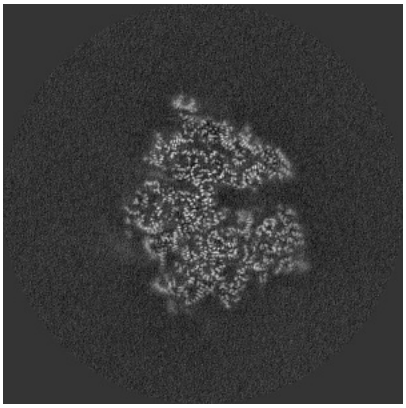
6.3.1 Primary map

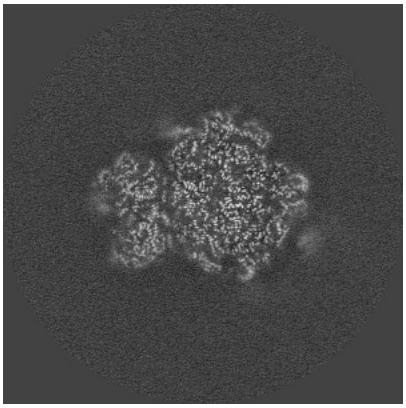

X Index: 231

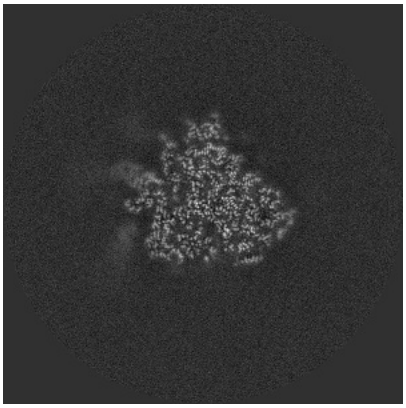

Y Index: 204


Z Index: 243

6.3.2 Raw map


X Index: 231


Y Index: 204


Z Index: 243

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 0.022. 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.

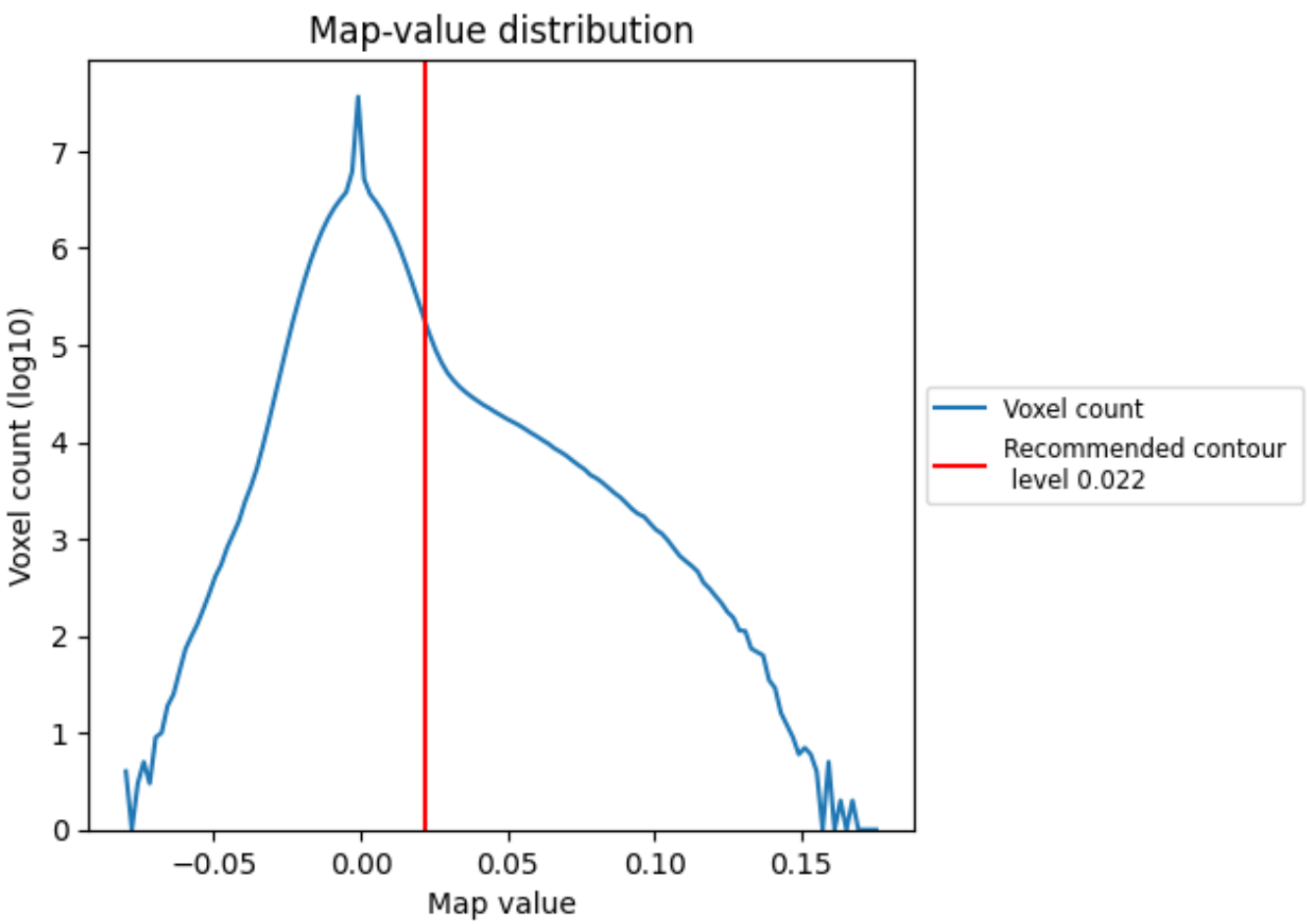
6.5 Mask visualisation (i)

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

7 Map analysis (i)

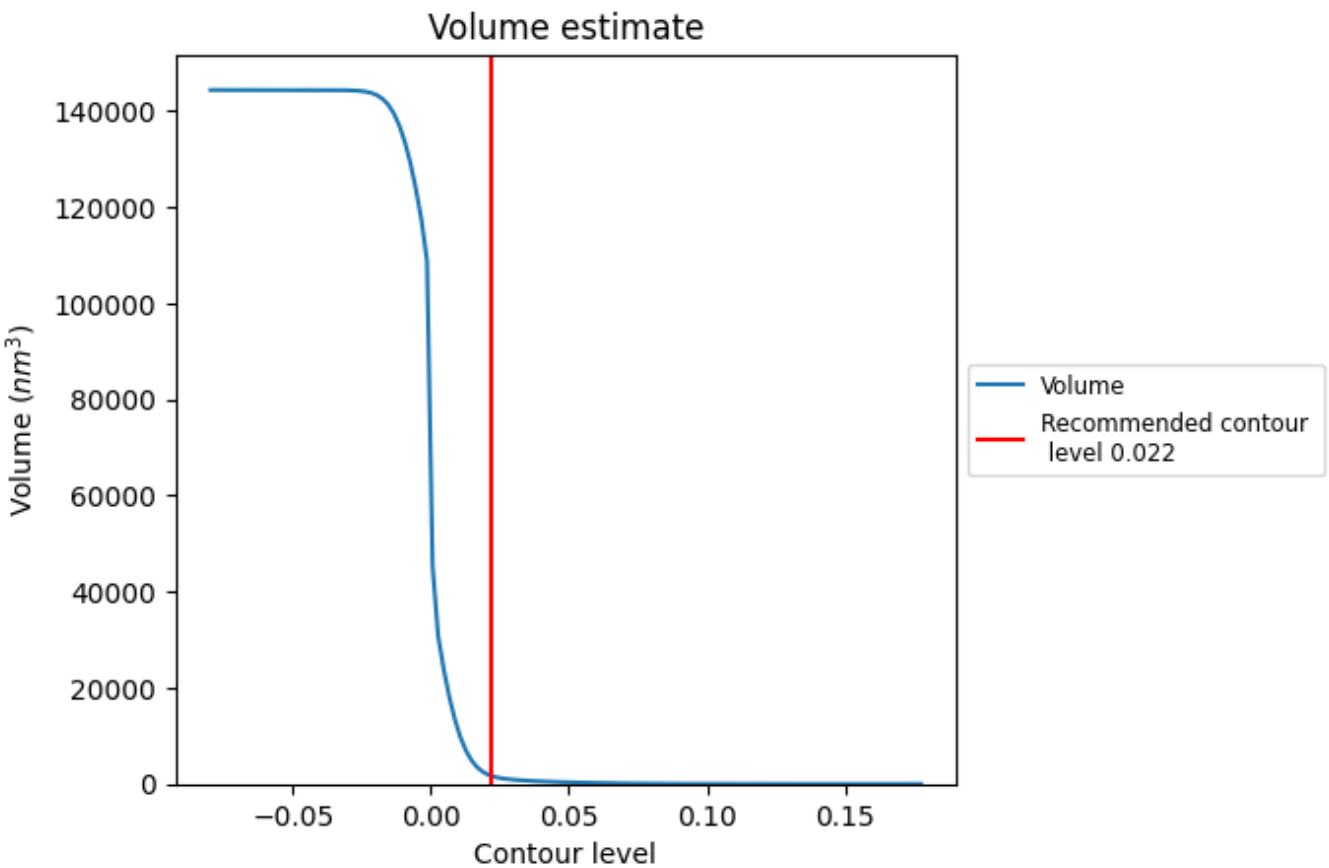
This section contains the results of statistical analysis of the map.

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.

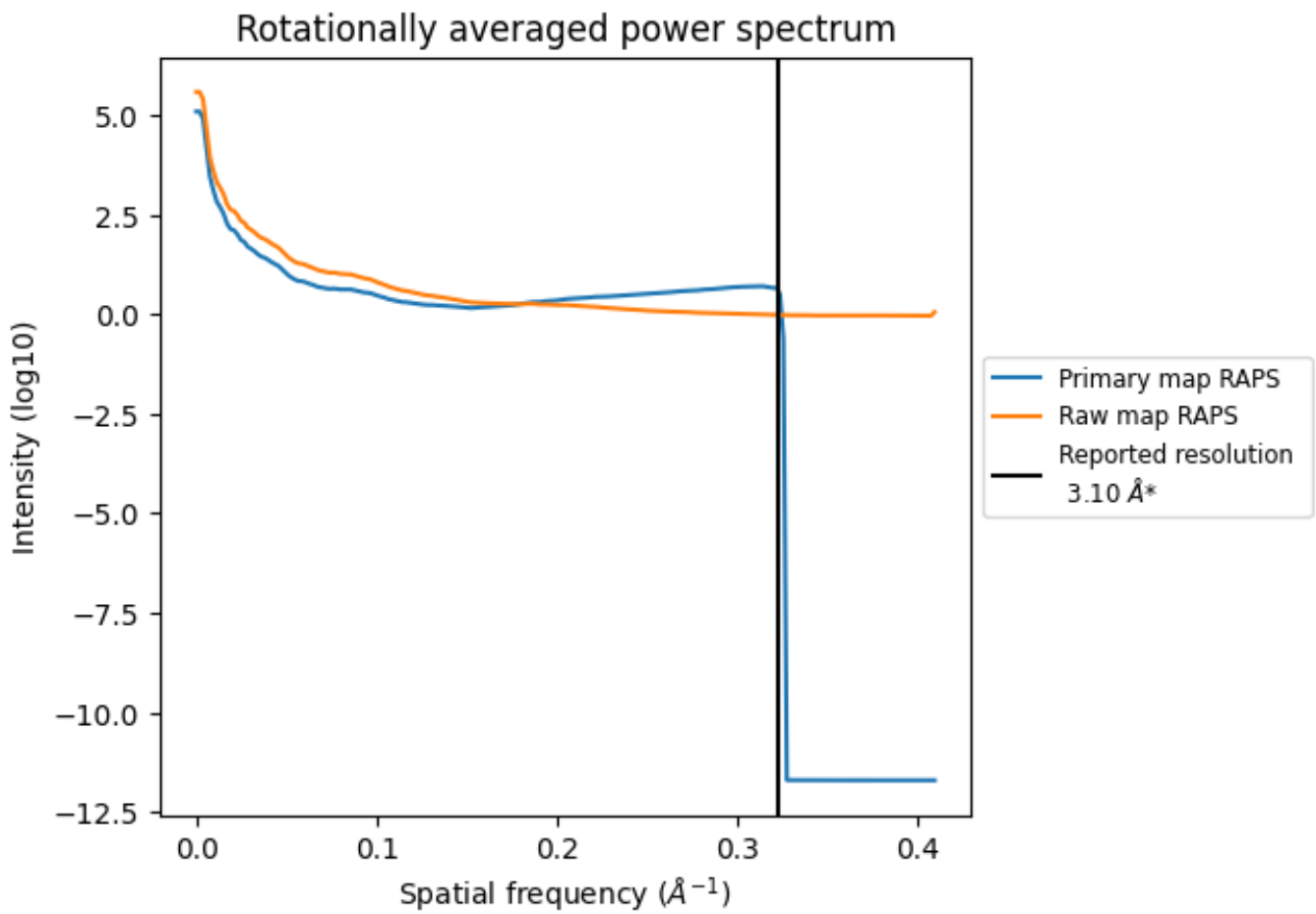
7.2 Volume estimate (i)



The volume at the recommended contour level is 1680 nm^3; this corresponds to an approximate mass of 1518 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)

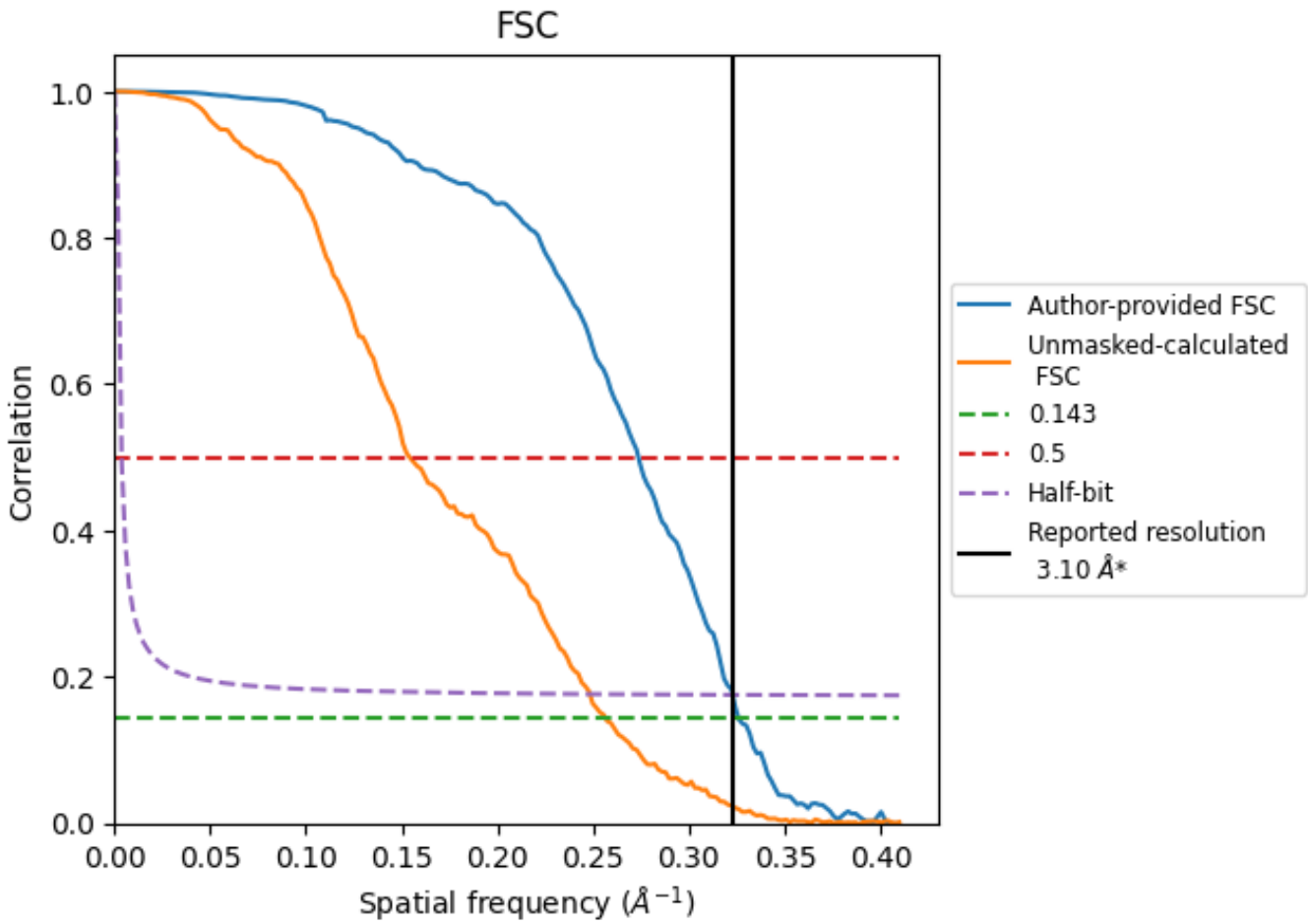


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

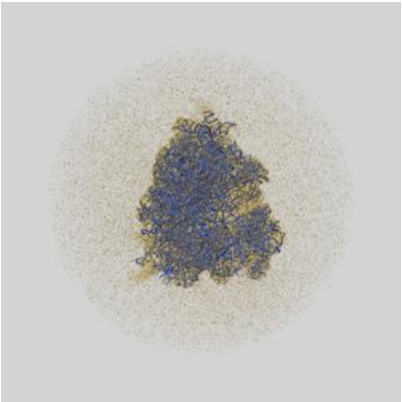
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.65	3.10
Unmasked-calculated*	3.90	6.49	4.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.90 differs from the reported value 3.1 by more than 10 %

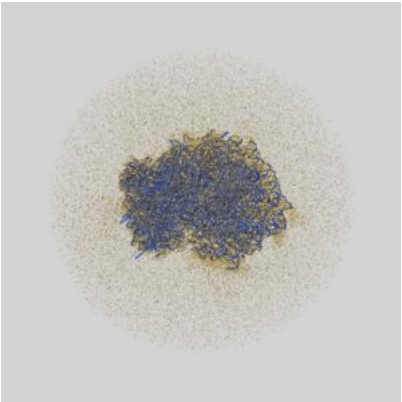
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0596 and PDB model 6OM0. Per-residue inclusion information can be found in section 3 on page 20.

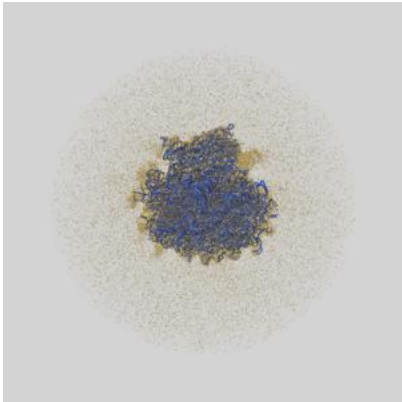
9.1 Map-model overlay (i)



X



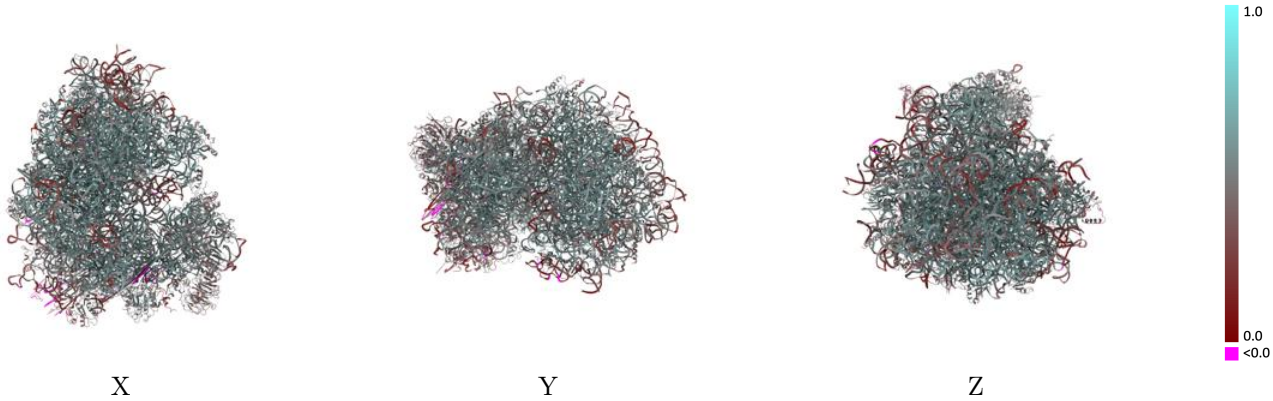
Y



Z

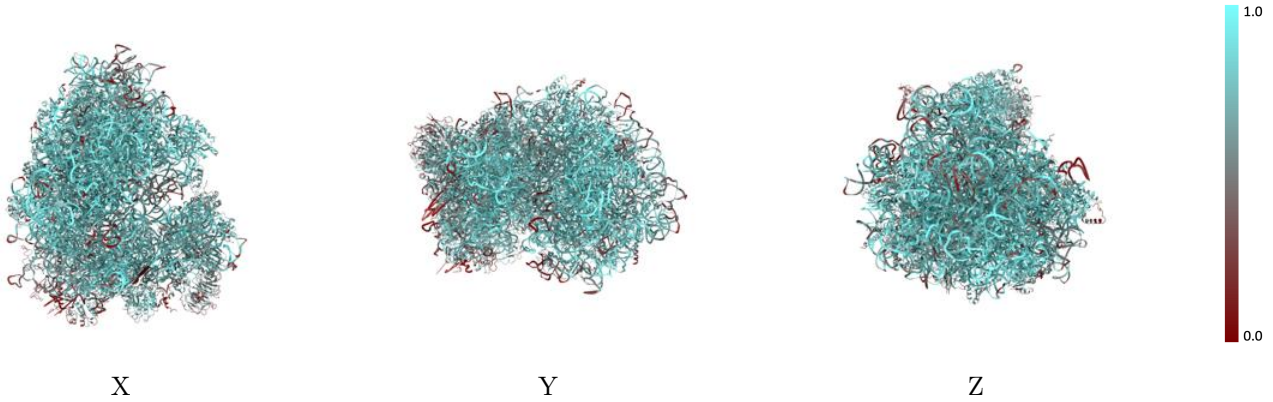
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



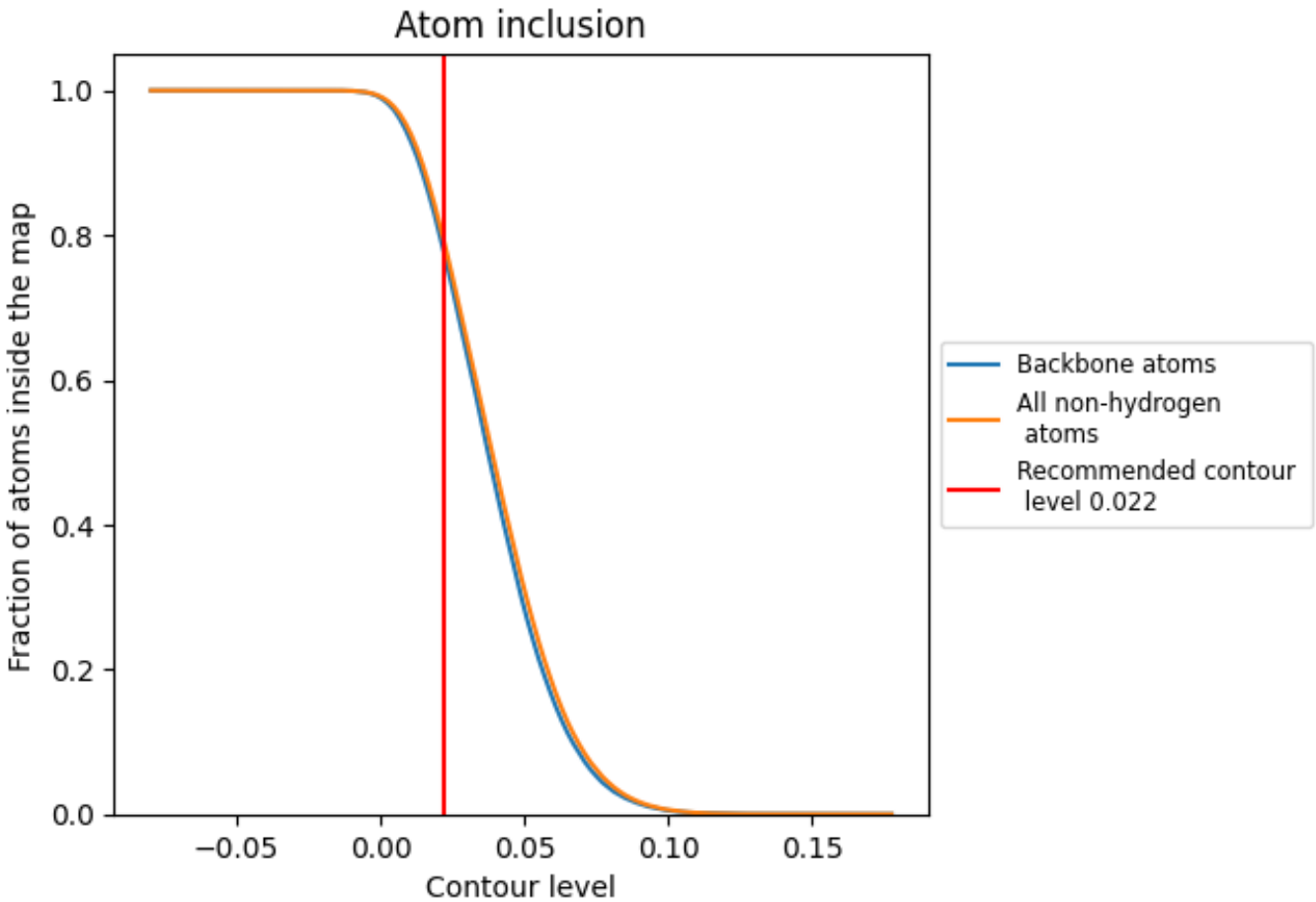
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 79% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7924	0.5110
A	0.8442	0.5700
B	0.7953	0.5320
C	0.8137	0.5430
D	0.8717	0.5480
E	0.9553	0.5870
F	0.7709	0.4980
G	0.6924	0.4610
H	0.8157	0.5450
I	0.7125	0.4920
J	0.7426	0.5130
K	0.7768	0.5310
L	0.7378	0.4980
M	0.7516	0.5070
N	0.7895	0.5220
O	0.8784	0.5710
P	0.8247	0.5430
Q	0.8325	0.5520
R	0.8232	0.5440
S	0.7138	0.4980
S2	0.8406	0.5160
SA	0.6694	0.4770
SB	0.7231	0.5040
SC	0.7104	0.5020
SD	0.6015	0.4500
SE	0.7062	0.4920
SF	0.6176	0.4400
SG	0.5736	0.4160
SH	0.5197	0.4010
SI	0.6617	0.4590
SJ	0.6962	0.4650
SK	0.5988	0.4320
SL	0.6502	0.4680
SM	0.2367	0.2420
SN	0.7423	0.5160

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Chain	Atom inclusion	Q-score
SO	0.7085	0.4980
SP	0.6795	0.4650
SQ	0.6631	0.4730
SR	0.5894	0.4430
SS	0.6956	0.4690
ST	0.7061	0.4800
SU	0.5587	0.4160
SV	0.7005	0.4850
SW	0.8030	0.5390
SX	0.7666	0.5220
SY	0.6357	0.4440
SZ	0.6113	0.4440
Sa	0.7389	0.5060
Sb	0.6815	0.4770
Sc	0.5185	0.4230
Sd	0.8005	0.5170
Se	0.6201	0.4420
Sf	0.2959	0.2930
Sg	0.4824	0.3750
T	0.8153	0.5370
U	0.7870	0.5230
V	0.6747	0.4470
W	0.7941	0.5560
X	0.8211	0.5500
Y	0.7830	0.5250
Z	0.7978	0.5320
a	0.7643	0.5040
b	0.8391	0.5580
c	0.7006	0.4870
d	0.7105	0.4850
e	0.7642	0.5250
f	0.8314	0.5620
g	0.8266	0.5470
h	0.7837	0.5410
i	0.7574	0.5070
j	0.7402	0.4920
k	0.8630	0.5660
l	0.6643	0.4710
m	0.8109	0.5510
n	0.7809	0.5340
o	0.7591	0.5130
p	0.7530	0.5150

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Chain	Atom inclusion	Q-score
q	0.7939	0.5560
r	0.8162	0.5320
t	0.8645	0.5290
u	0.5914	0.3780
v	0.6786	0.3970
w	0.8873	0.5610
y	0.1600	0.1540