



## wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 02:07 AM EDT

PDB ID : 6OLE / pdb\_00006ole  
EMDB ID : EMD-0600  
Title : Human ribosome nascent chain complex (CDH1-RNC) stalled by a drug-like molecule with AP and PE tRNAs  
Authors : Li, W.; Cate, J.H.D.  
Deposited on : 2019-04-16  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

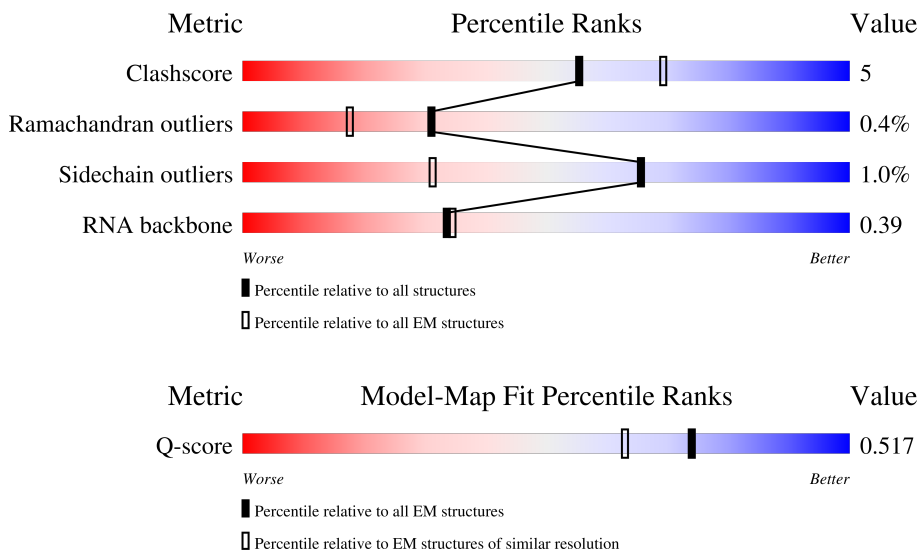
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 ( 2.50 - 3.50 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S2	1714	
2	SA	221	
3	SB	214	

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Mol	Chain	Length	Quality of chain
4	SD	226	23% 85% 14%
5	SE	259	11% 76% 23%
6	SF	189	14% 80% 19%
7	SH	189	33% 75% 23%
8	SI	204	19% 80% 20%
9	SK	98	24% 89% 11%
10	SL	153	19% 92% 7%
11	SP	127	17% 75% 23%
12	SQ	146	16% 82% 17%
13	SR	134	28% 77% 23%
14	SS	145	15% 85% 14%
15	ST	143	10% 81% 17%
16	SU	104	36% 79% 21%
17	SV	82	7% 83% 17%
18	SX	141	6% 87% 13%
19	Sa	102	11% 82% 17%
20	Sc	64	30% 72% 28%
21	Sd	55	11% 69% 27%
22	Sg	312	43% 78% 22%
23	SC	220	9% 82% 17%
24	SG	237	32% 83% 17%
25	SJ	185	15% 82% 17%
26	SM	118	83% 12%
27	SN	150	6% 84% 16%
28	SO	137	12% 82% 18%




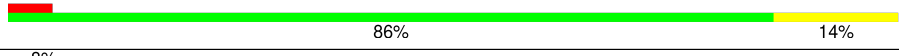
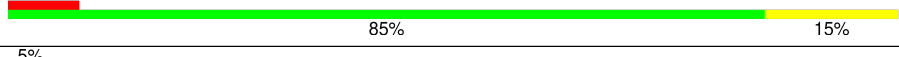



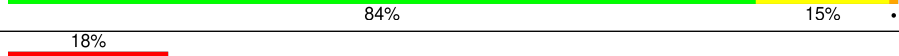
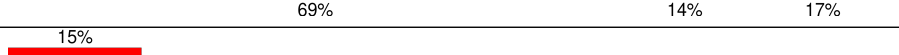
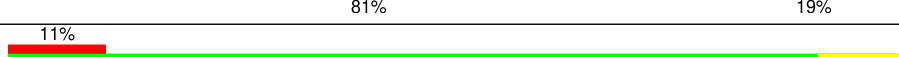
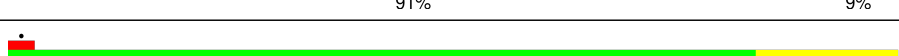

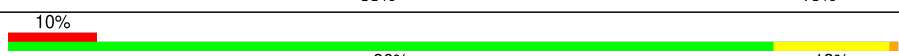
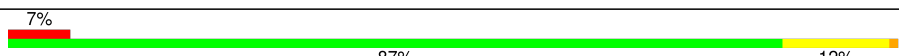
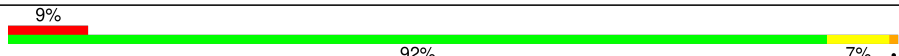





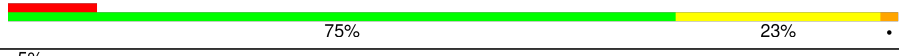



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Mol	Chain	Length	Quality of chain
29	SW	129	79% 21%
30	SY	131	86% 14% 18%
31	SZ	73	81% 19% 22%
32	Sb	82	87% 13% 20%
33	Se	57	93% 7% 25%
34	Sf	67	82% 16% 78%
35	A	252	84% 15%
36	B	397	81% 19% 5%
37	C	363	81% 18% 6%
38	D	157	66% 31% 9%
39	E	121	76% 20%
40	F	294	88% 11% 7%
41	G	247	73% 20% 15%
42	H	225	78% 20%
43	I	234	89% 11% 15%
44	J	191	84% 16% 6%
45	K	211	82% 16% 8%
46	L	169	89% 11% 8%
47	M	205	84% 16% 14%
48	N	139	82% 18% 6%
49	O	203	77% 22%
50	P	195	80% 20%
51	Q	153	82% 18%
52	R	187	83% 16%
53	S	181	76% 24% 13%

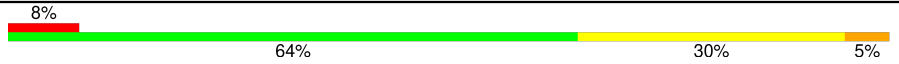


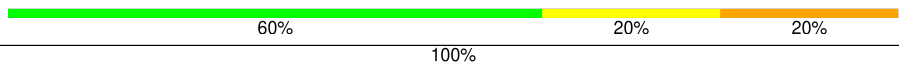

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Mol	Chain	Length	Quality of chain
54	T	175	 73% 26%
55	U	157	 84% 16%
56	V	99	 14% 88% 11%
57	W	129	 5% 86% 14%
58	X	61	 8% 85% 15%
59	Y	117	 5% 84% 15%
60	Z	134	 84% 16%
61	a	134	 78% 22%
62	b	147	 84% 15%
63	c	121	 18% 69% 14% 17%
64	d	103	 15% 81% 19%
65	e	106	 11% 91% 9%
66	f	129	 84% 16%
67	g	109	 83% 16%
68	h	114	 10% 86% 13%
69	i	122	 7% 87% 12%
70	j	97	 9% 92% 7%
71	k	84	 87% 13%
72	l	69	 25% 90% 10%
73	m	50	 6% 76% 24%
74	n	50	 8% 84% 16%
75	o	25	 76% 24%
76	p	105	 10% 75% 23%
77	q	91	 5% 87% 12%
78	r	122	 82% 18%

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Mol	Chain	Length	Quality of chain
79	t	3607	
80	u	76	
81	v	76	
82	w	10	
83	y	39	

## 2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 214951 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
14	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
34	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
76	p	105	Total	C	N	O	S	0	0
			863	542	175	140	6		

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

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

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

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

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

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

- Molecule 80 is a RNA chain called AP RNA.

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

- Molecule 81 is a RNA chain called PE RNA.

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

- Molecule 82 is a RNA chain called mRNA.

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

- Molecule 83 is a protein called Cadherin-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
83	y	39	262	180	40	42	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	6	ALA	-	insertion	UNP P12830

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	S2	3	Total 3	Mg 3	0
84	A	1	Total 1	Mg 1	0
84	B	1	Total 1	Mg 1	0
84	D	8	Total 8	Mg 8	0
84	E	9	Total 9	Mg 9	0
84	O	1	Total 1	Mg 1	0
84	Z	1	Total 1	Mg 1	0
84	b	1	Total 1	Mg 1	0
84	t	6	Total 6	Mg 6	0

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

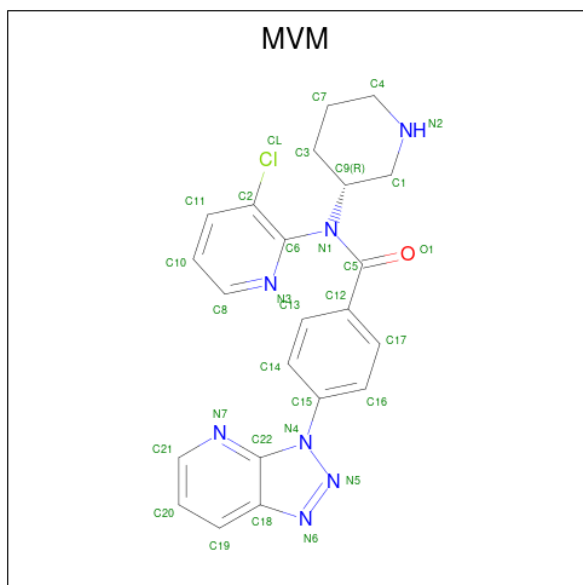
Mol	Chain	Residues	Atoms		AltConf
85	S2	1	Total 1	Zn 1	0
85	Sa	1	Total 1	Zn 1	0
85	Sf	1	Total 1	Zn 1	0
85	k	1	Total 1	Zn 1	0
85	p	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
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 (CCD ID: MVM) (formula: C<sub>22</sub>H<sub>20</sub>ClN<sub>7</sub>O).



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

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
87	S2	4	4	4	0
87	SP	1	1	1	0
87	SQ	1	1	1	0
87	SR	1	1	1	0
87	SS	2	2	2	0
87	SC	1	1	1	0
87	SN	1	1	1	0

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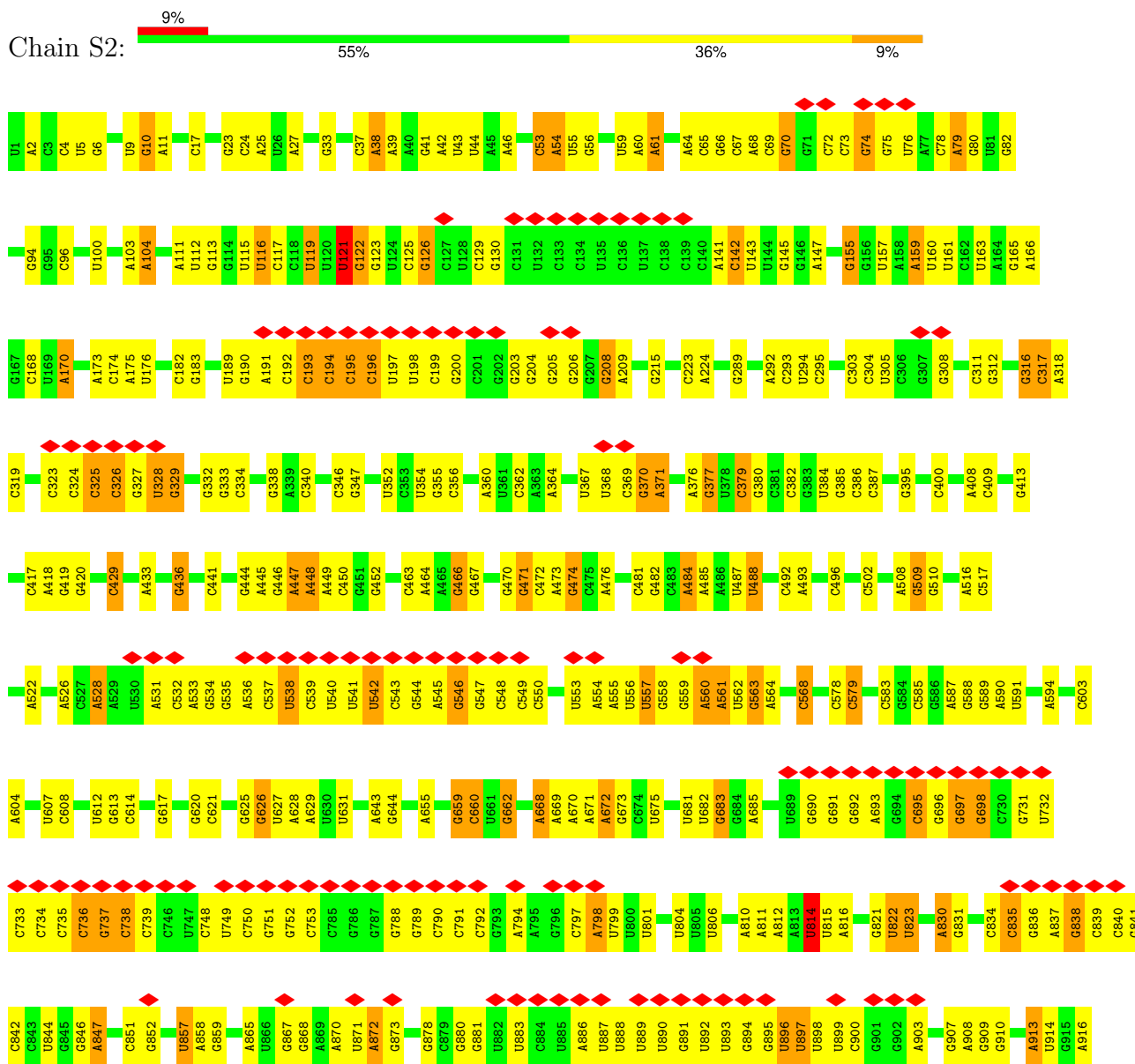
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
87	Sf	1	Total 1	O 1	0
87	u	1	Total 1	O 1	0
87	v	1	Total 1	O 1	0

### 3 Residue-property plots

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


- Molecule 1: 18S ribosomal RNA

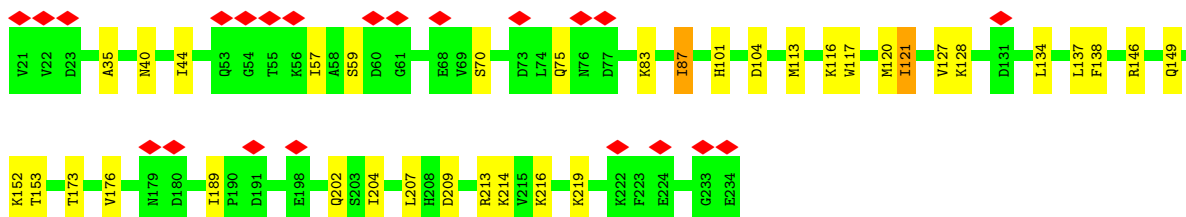





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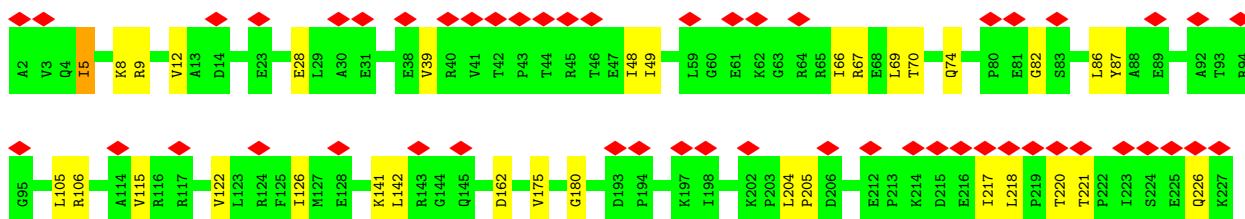
• Molecule 3: 40S ribosomal protein S3a

Chain SB:  10% 83% 16%




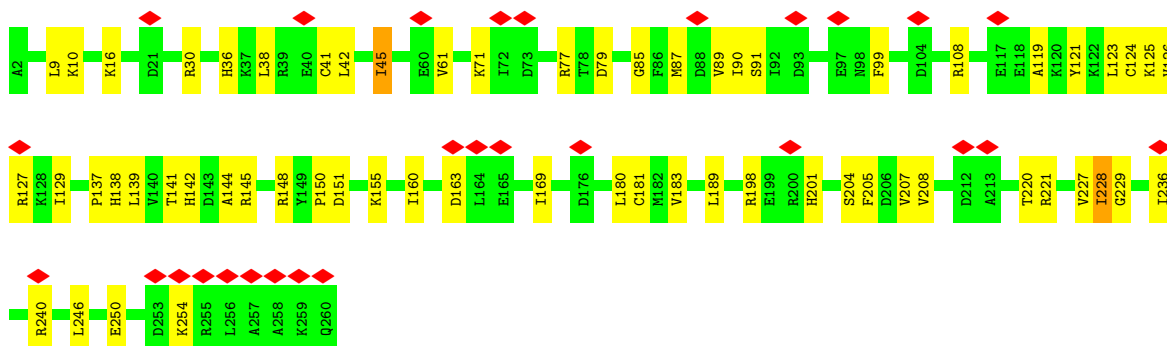
• Molecule 4: 40S ribosomal protein S3

Chain SD:  23% 85% 14%




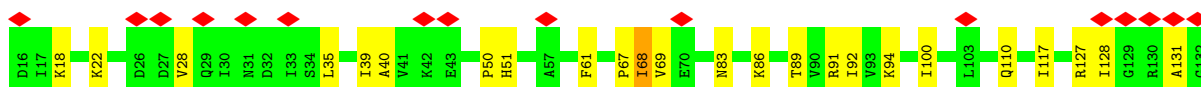
• Molecule 5: 40S ribosomal protein S4, X isoform

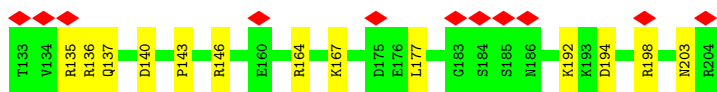
Chain SE:  11% 76% 23%



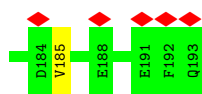
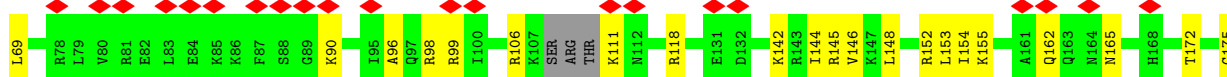
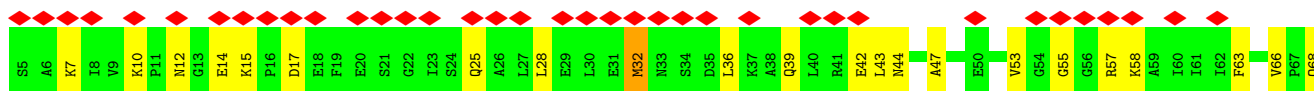
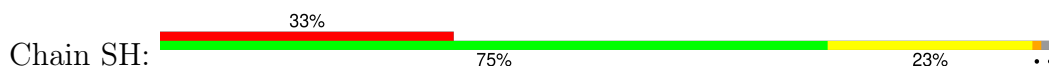
• Molecule 6: 40S ribosomal protein S5

Chain SF:  14% 80% 19%

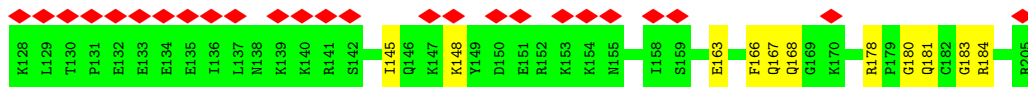
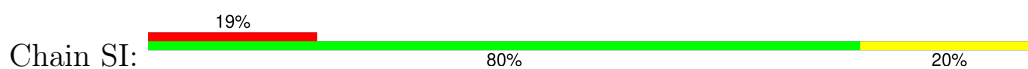




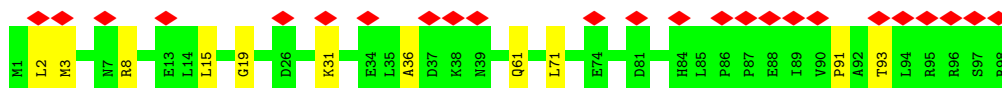
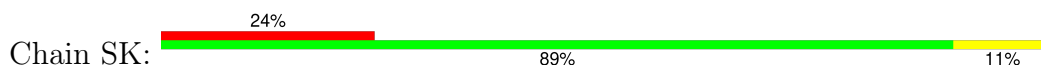
- Molecule 7: 40S ribosomal protein S7



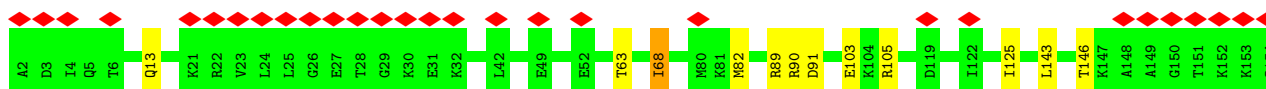
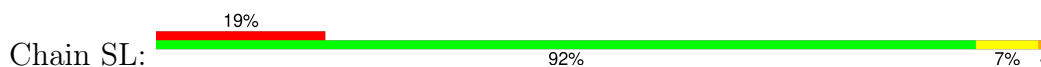
- Molecule 8: 40S ribosomal protein S8



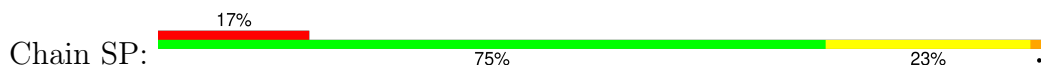
- Molecule 9: 40S ribosomal protein S10

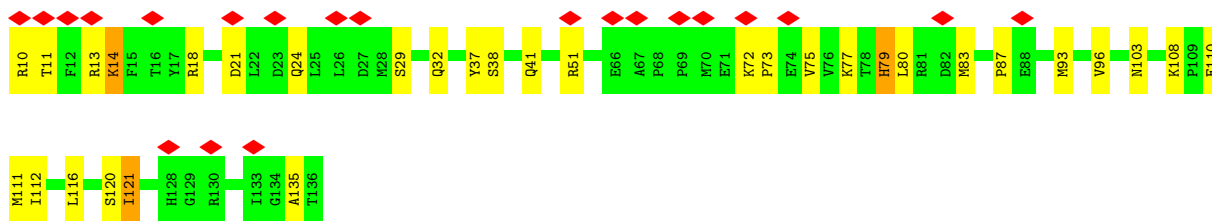


- Molecule 10: 40S ribosomal protein S11

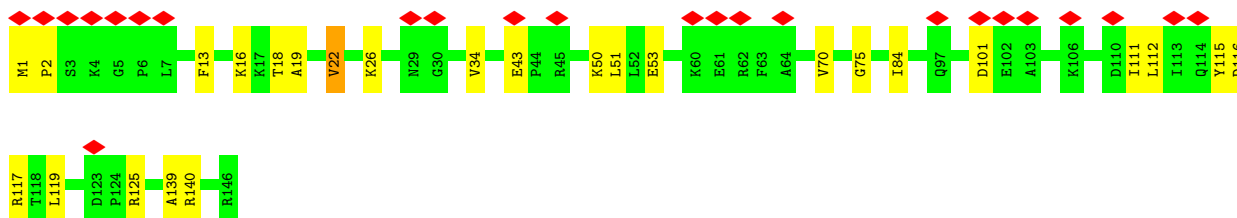
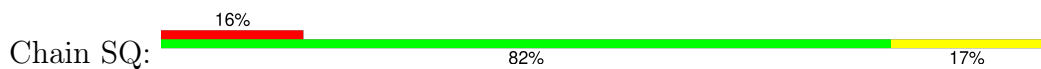


- Molecule 11: 40S ribosomal protein S15

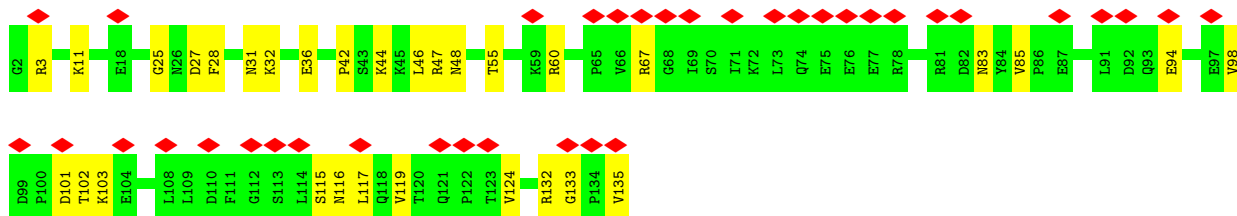
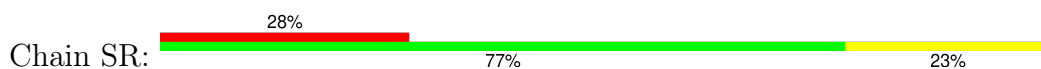




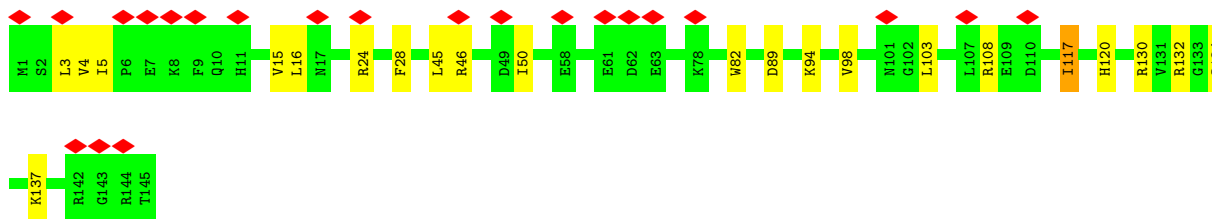
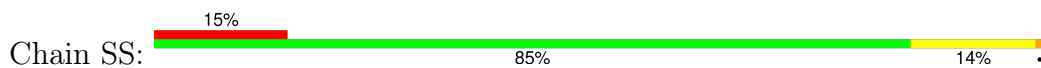
- Molecule 12: 40S ribosomal protein S16



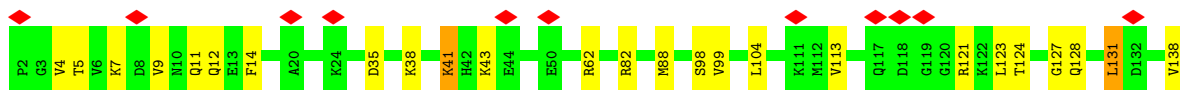
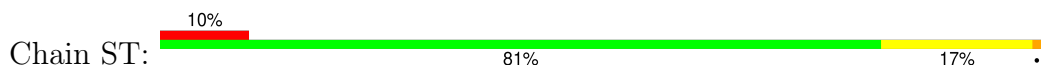
- Molecule 13: 40S ribosomal protein S17

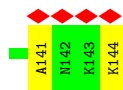


- Molecule 14: 40S ribosomal protein S18

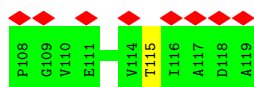
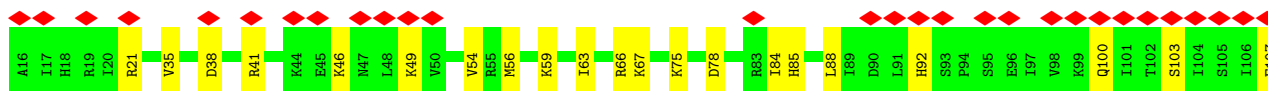
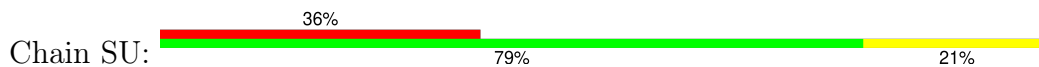


- Molecule 15: 40S ribosomal protein S19

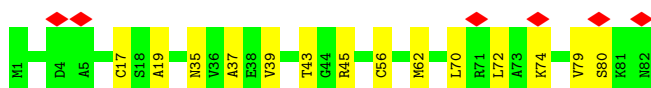
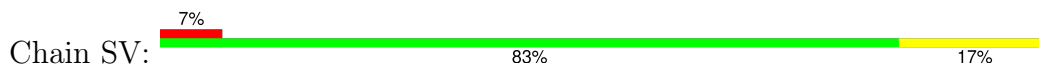




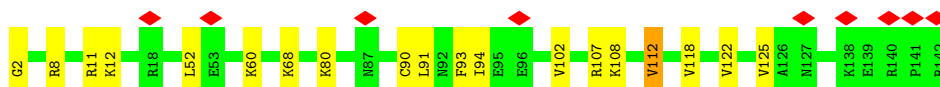
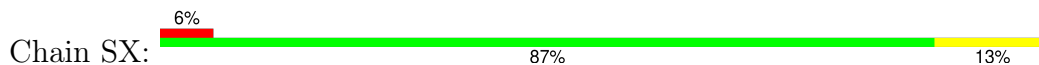
- Molecule 16: 40S ribosomal protein S20



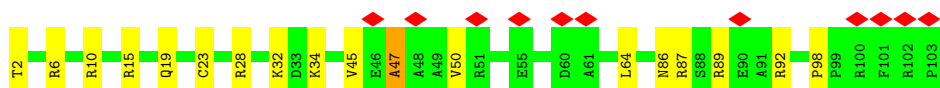
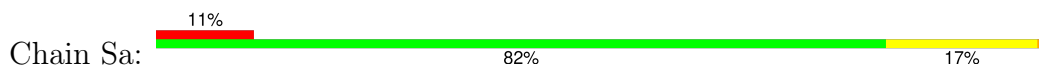
- Molecule 17: 40S ribosomal protein S21



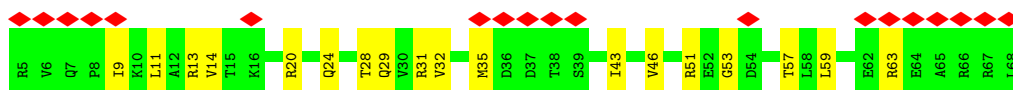
- Molecule 18: 40S ribosomal protein S23



- Molecule 19: 40S ribosomal protein S26

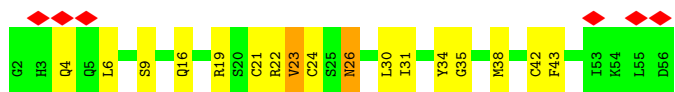


- Molecule 20: 40S ribosomal protein S28

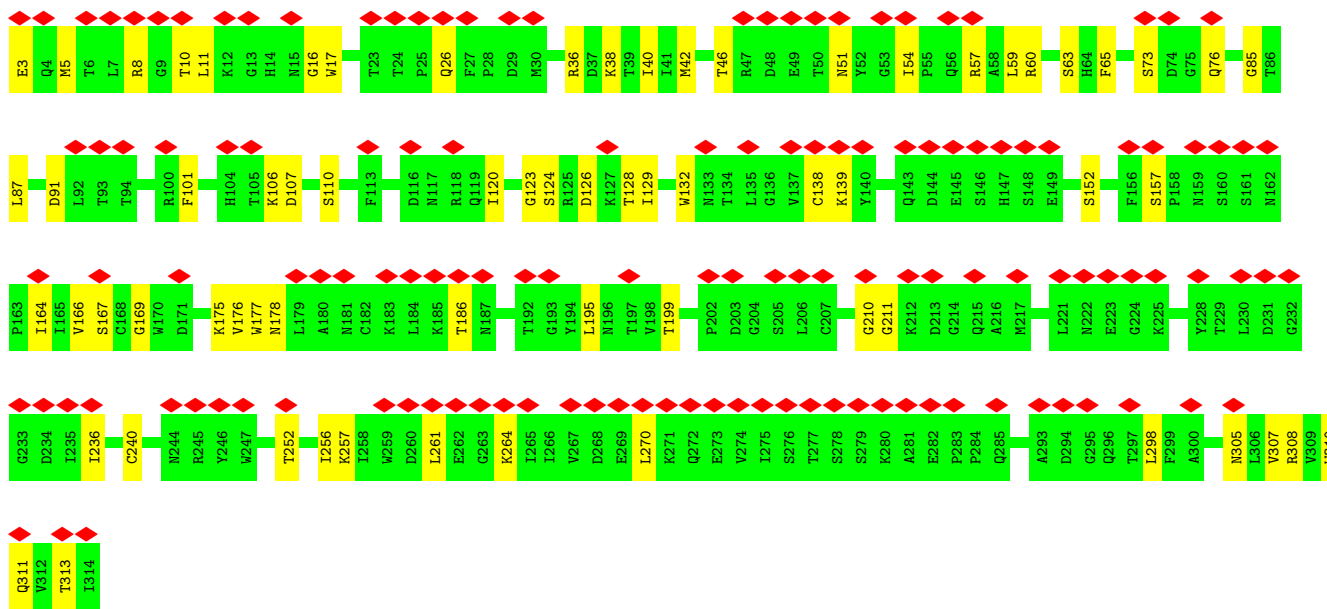
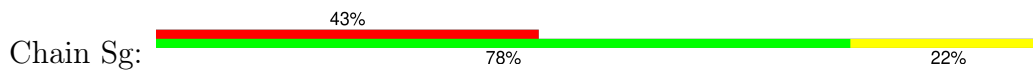


- Molecule 21: 40S ribosomal protein S29

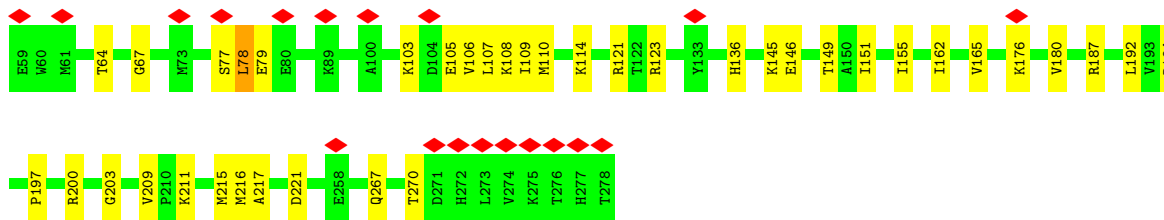
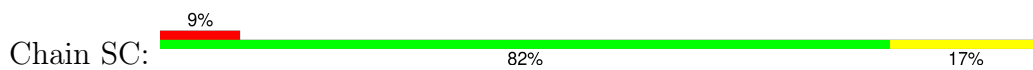




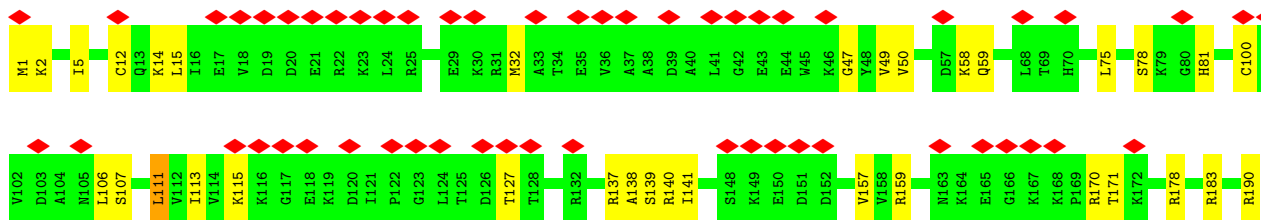
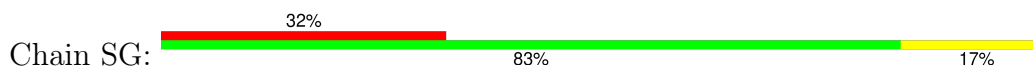
• Molecule 22: Receptor of activated protein C kinase 1

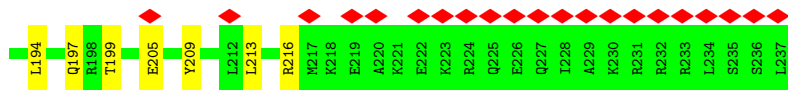


• Molecule 23: 40S ribosomal protein S2

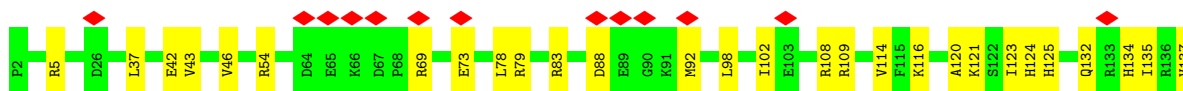
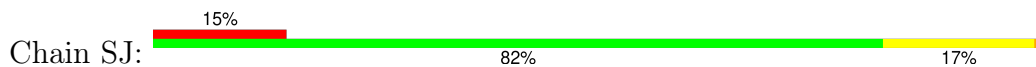


• Molecule 24: 40S ribosomal protein S6

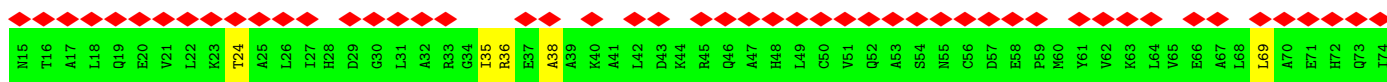
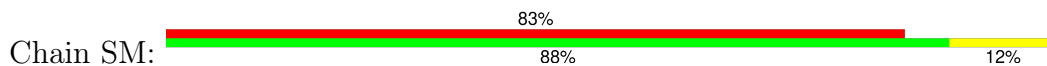




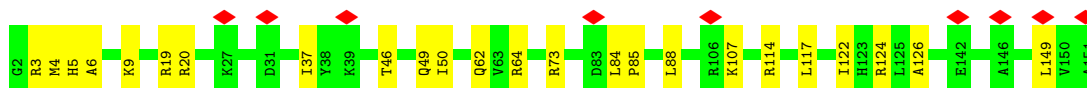
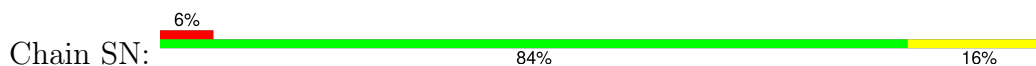
- Molecule 25: 40S ribosomal protein S9



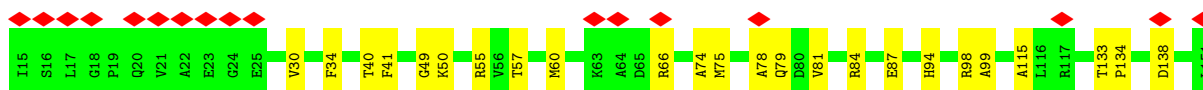
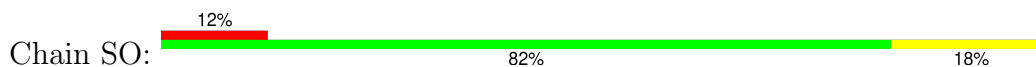
- Molecule 26: 40S ribosomal protein S12



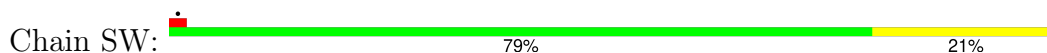
- Molecule 27: 40S ribosomal protein S13



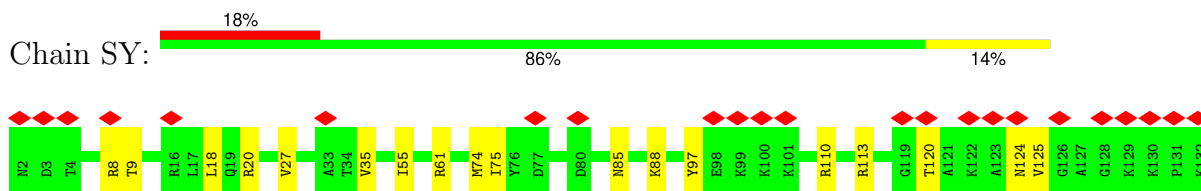
- Molecule 28: 40S ribosomal protein S14



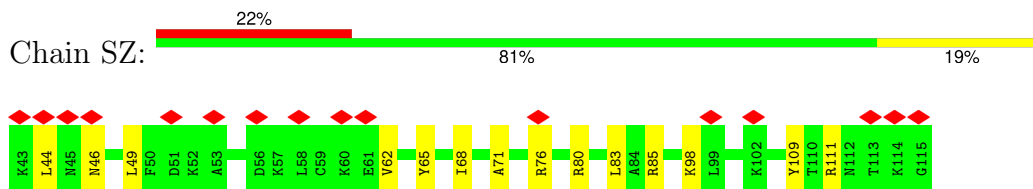
- Molecule 29: 40S ribosomal protein S15a



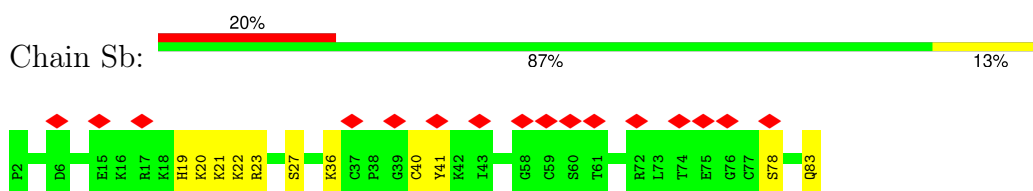
- Molecule 30: 40S ribosomal protein S24



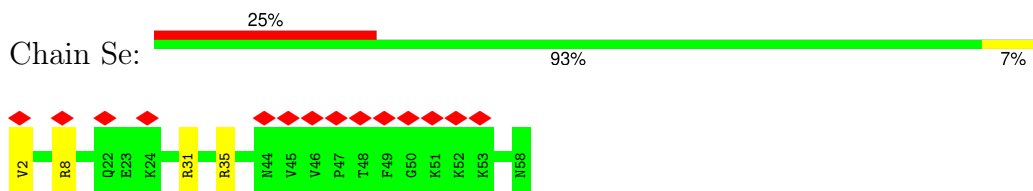
• Molecule 31: 40S ribosomal protein S25



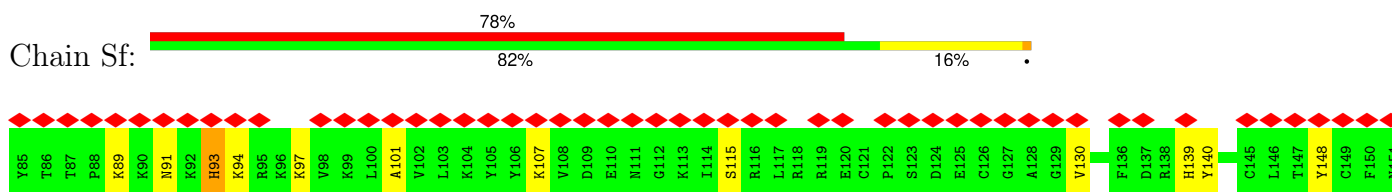
• Molecule 32: 40S ribosomal protein S27



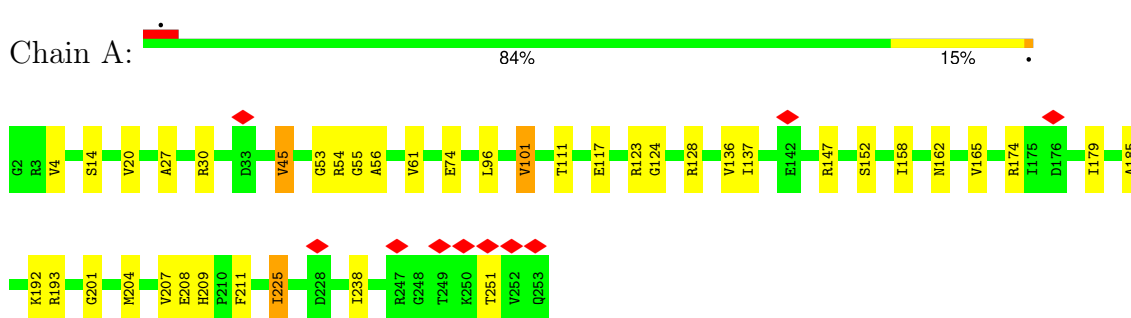
• Molecule 33: 40S ribosomal protein S30



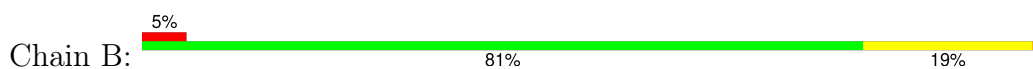
• Molecule 34: 40S ribosomal protein S27a

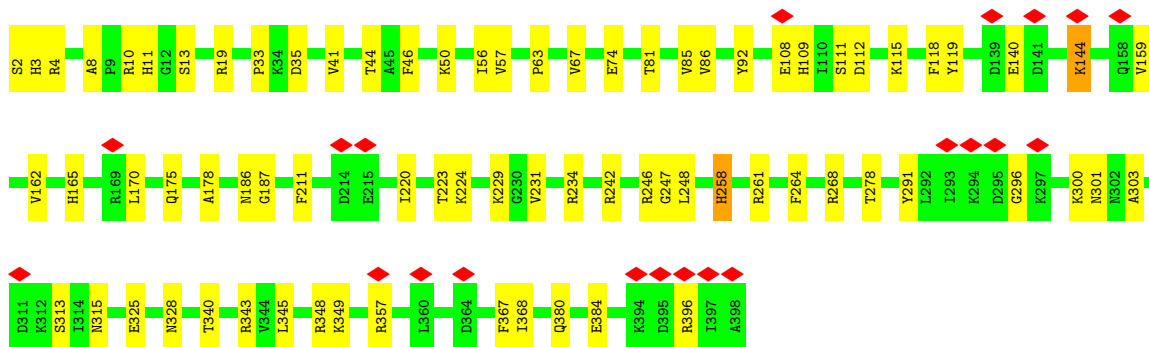


• Molecule 35: 60S ribosomal protein L8

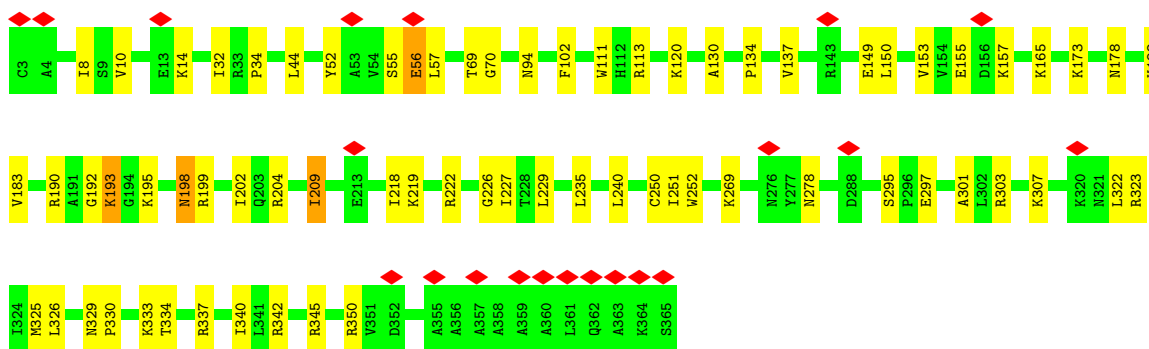
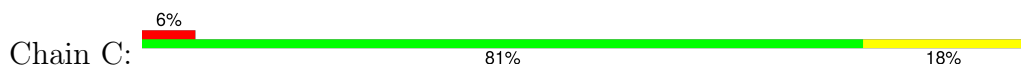


• Molecule 36: 60S ribosomal protein L3





• Molecule 37: 60S ribosomal protein L4



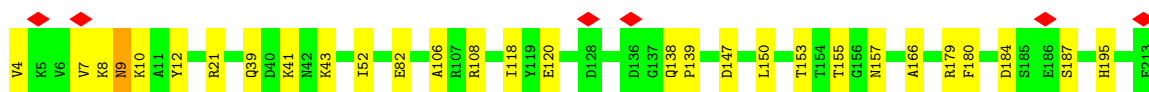
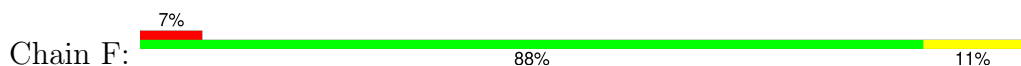
• Molecule 38: 5.8S ribosomal RNA

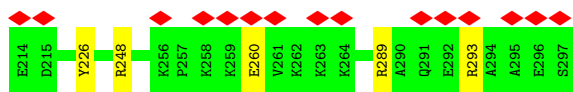


• Molecule 39: 5S ribosomal RNA

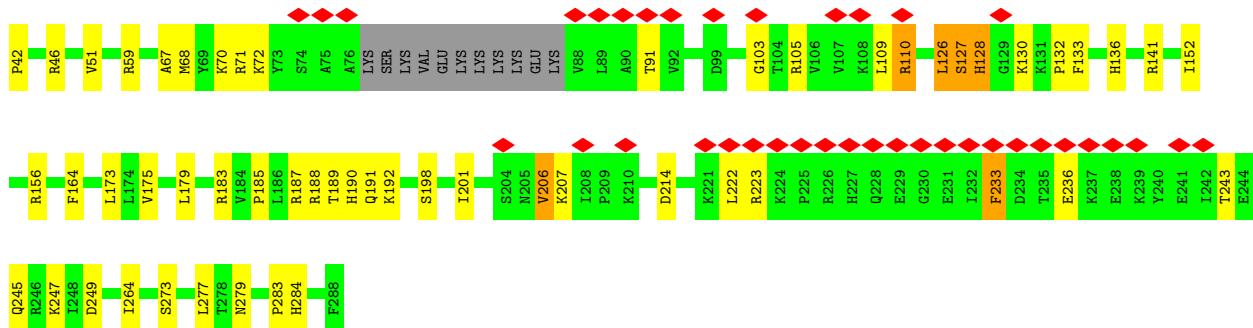
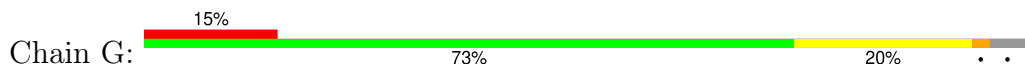


• Molecule 40: 60S ribosomal protein L5

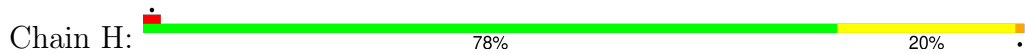




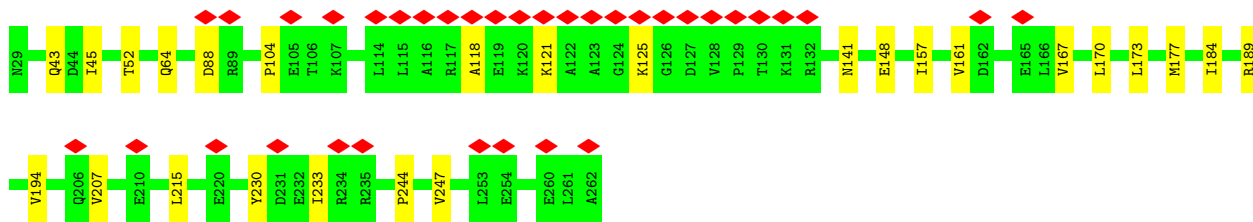
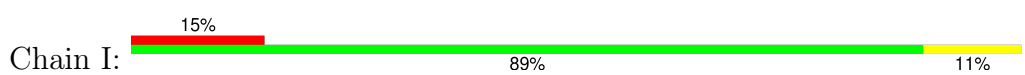
• Molecule 41: 60S ribosomal protein L6



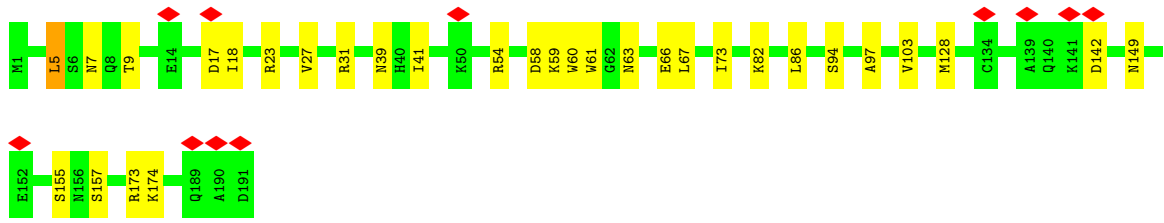
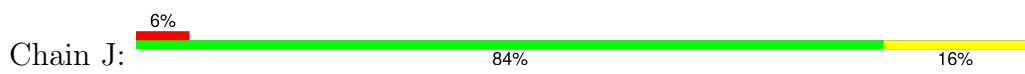
• Molecule 42: 60S ribosomal protein L7



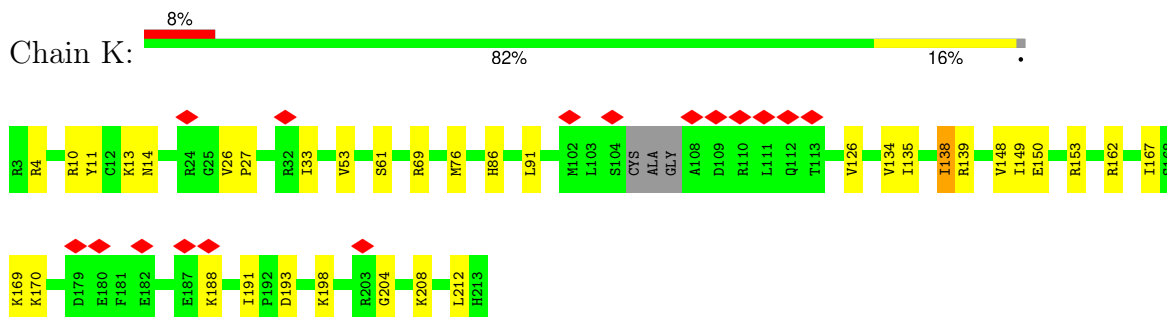
• Molecule 43: 60S ribosomal protein L7a



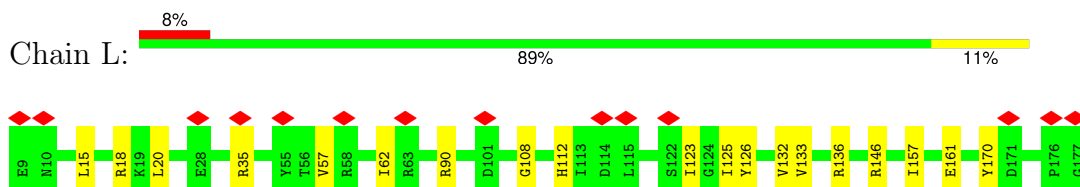
• Molecule 44: 60S ribosomal protein L9



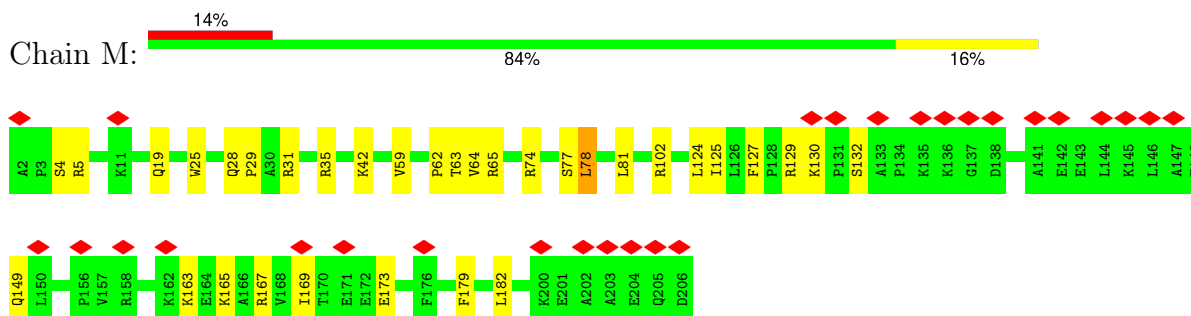
- Molecule 45: 60S ribosomal protein L10



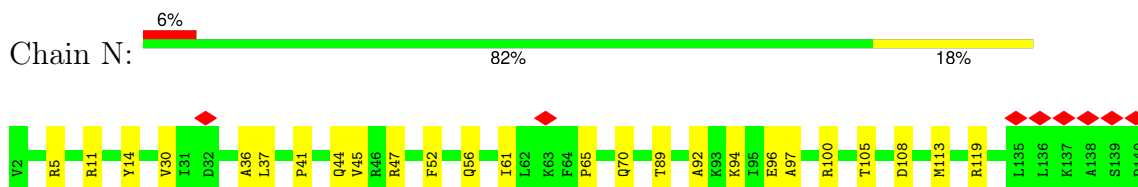
- Molecule 46: 60S ribosomal protein L11



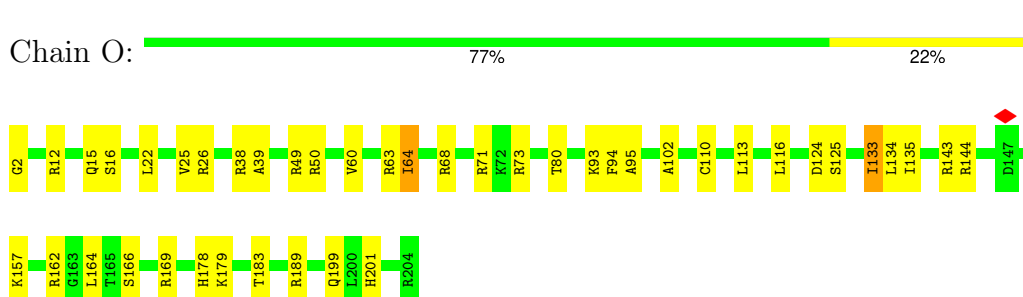
- Molecule 47: 60S ribosomal protein L13



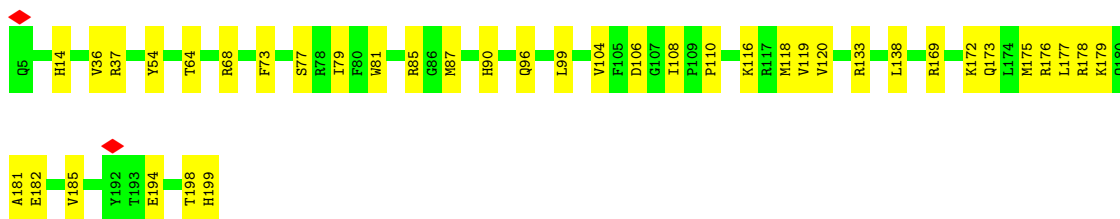
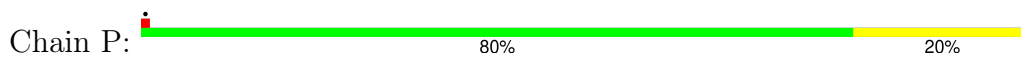
- Molecule 48: 60S ribosomal protein L14



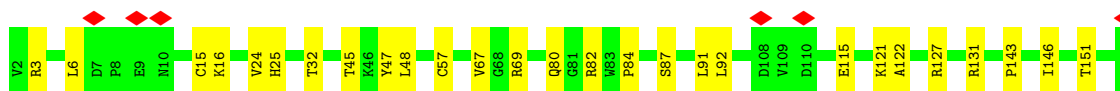
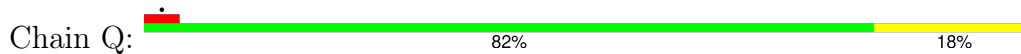
- Molecule 49: 60S ribosomal protein L15



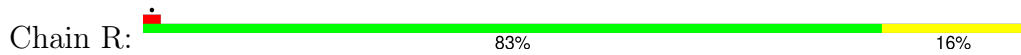
- Molecule 50: 60S ribosomal protein L13a



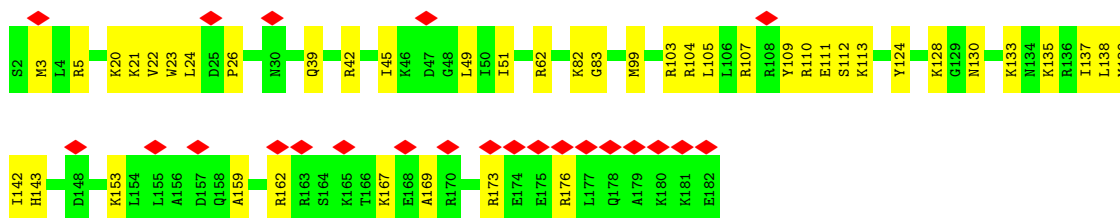
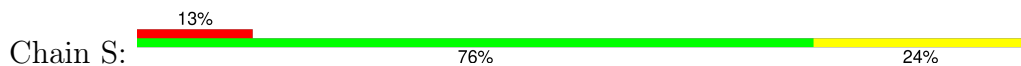
• Molecule 51: 60S ribosomal protein L17



• Molecule 52: 60S ribosomal protein L18



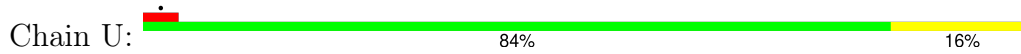
• Molecule 53: 60S ribosomal protein L19

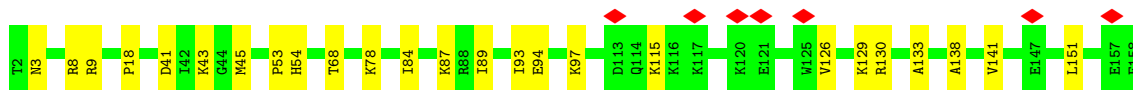


• Molecule 54: 60S ribosomal protein L18a

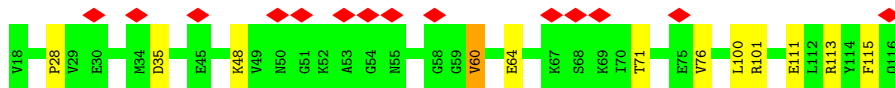
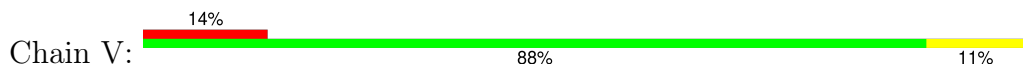


• Molecule 55: 60S ribosomal protein L21

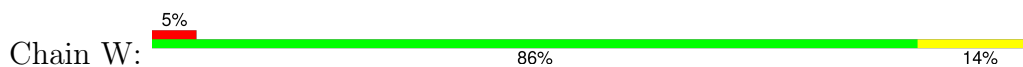




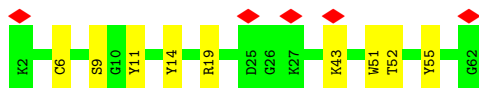
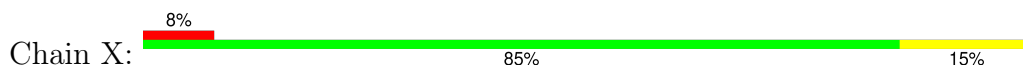
- Molecule 56: 60S ribosomal protein L22



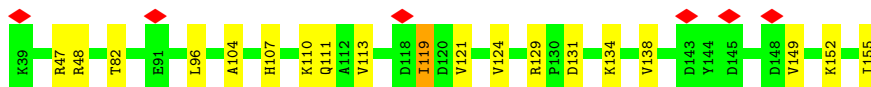
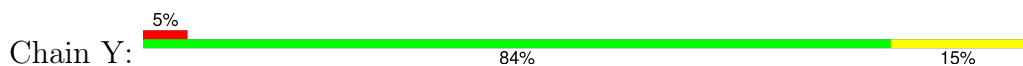
- Molecule 57: 60S ribosomal protein L23



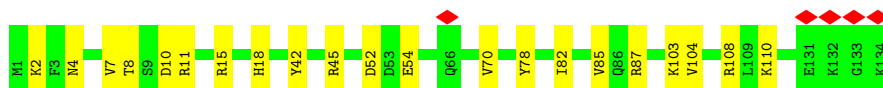
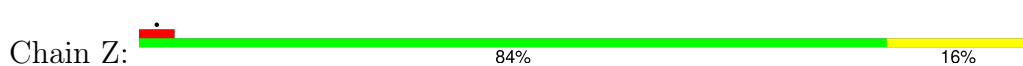
- Molecule 58: 60S ribosomal protein L24



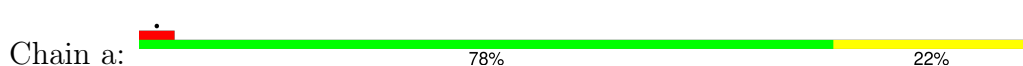
- Molecule 59: 60S ribosomal protein L23a



- Molecule 60: 60S ribosomal protein L26




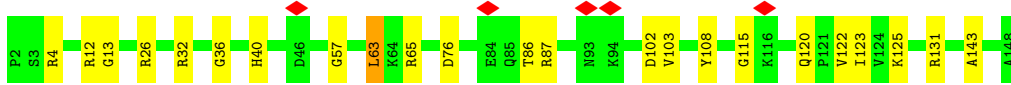
- Molecule 61: 60S ribosomal protein L27



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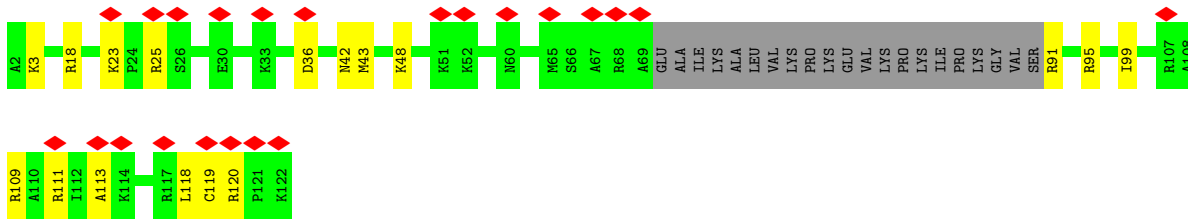
- Molecule 62: 60S ribosomal protein L27a

Chain b:  84% 15%




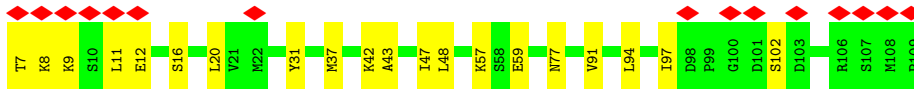
- Molecule 63: 60S ribosomal protein L29

Chain c:  18% 69% 14% 17%



- Molecule 64: 60S ribosomal protein L30

Chain d:  15% 81% 19%




- Molecule 65: 60S ribosomal protein L31

Chain e:  11% 91% 9%




- Molecule 66: 60S ribosomal protein L32

Chain f:  84% 16%

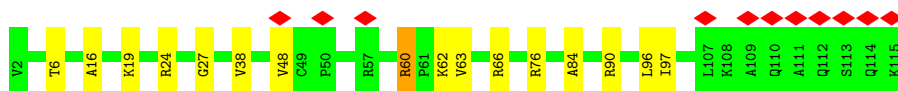
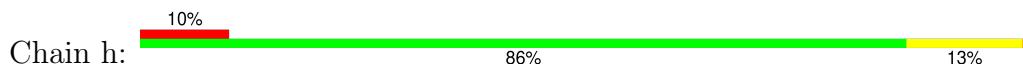


- Molecule 67: 60S ribosomal protein L35a

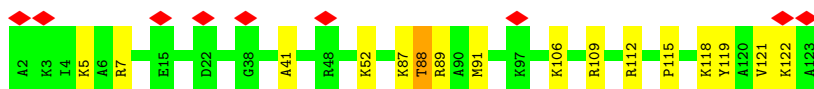
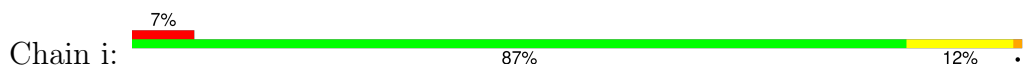
Chain g:  83% 16%



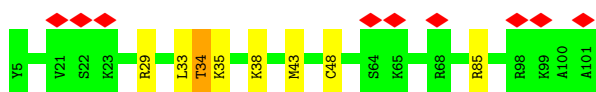
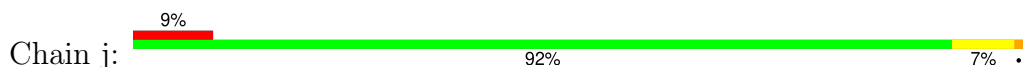
- Molecule 68: 60S ribosomal protein L34



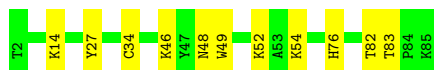
- Molecule 69: 60S ribosomal protein L35



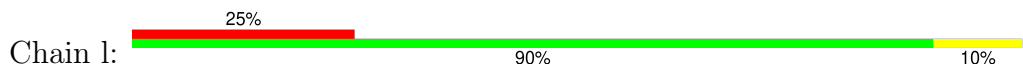
- Molecule 70: 60S ribosomal protein L36



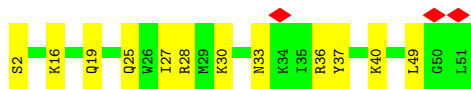
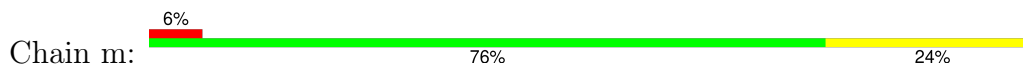
- Molecule 71: 60S ribosomal protein L37



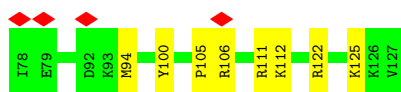
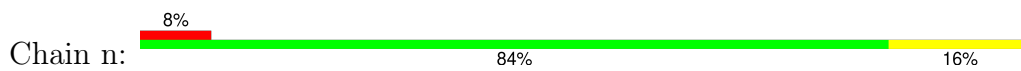
- Molecule 72: 60S ribosomal protein L38



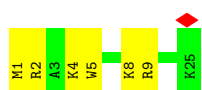
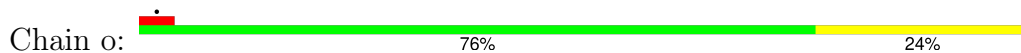
- Molecule 73: 60S ribosomal protein L39



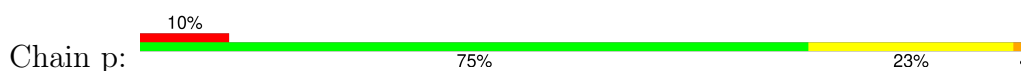
- Molecule 74: 60S ribosomal protein L40



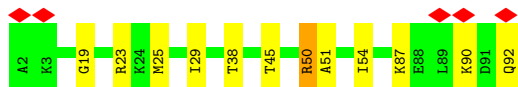
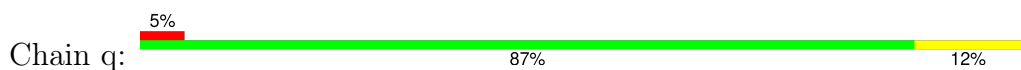
• Molecule 75: 60S ribosomal protein L41



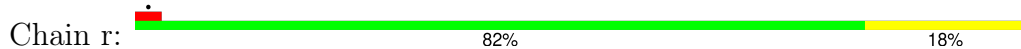
• Molecule 76: 60S ribosomal protein L36a



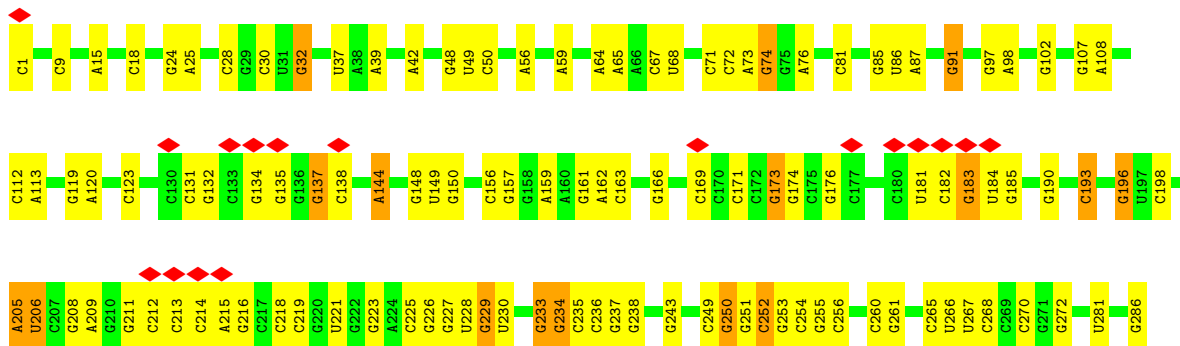
• Molecule 77: 60S ribosomal protein L37a



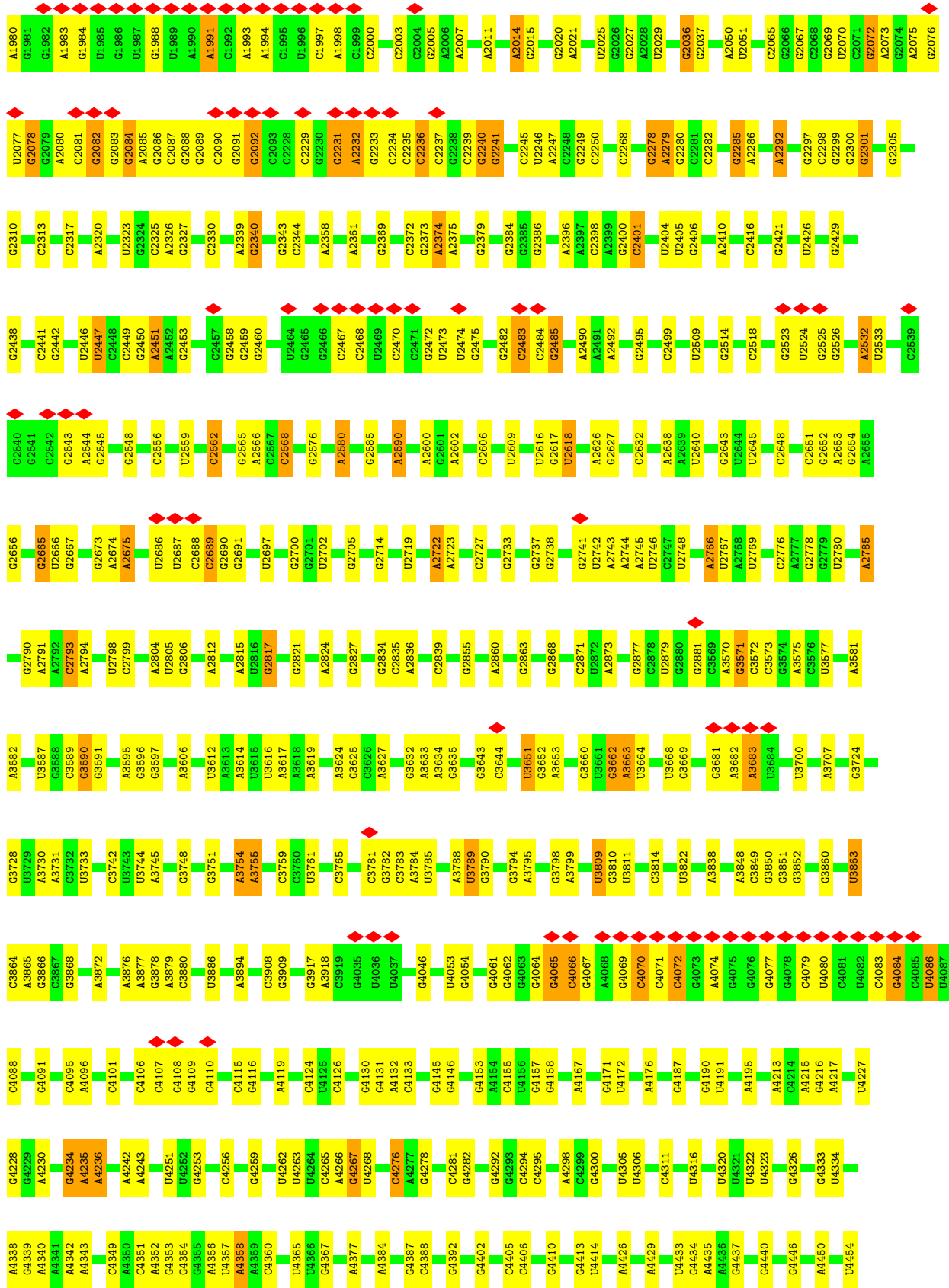
• Molecule 78: 60S ribosomal protein L28

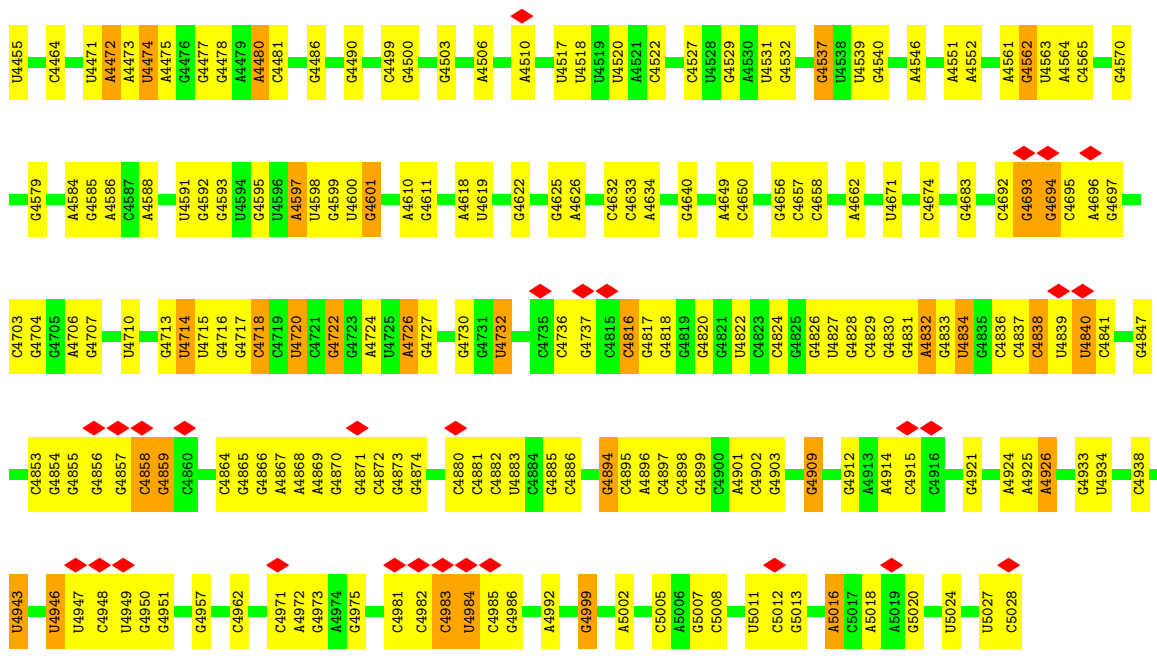


• Molecule 79: 28S ribosomal RNA

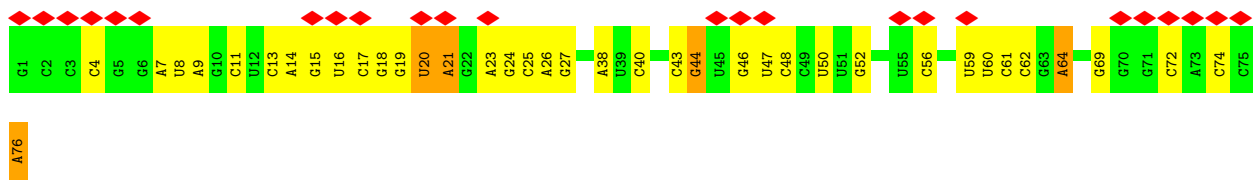




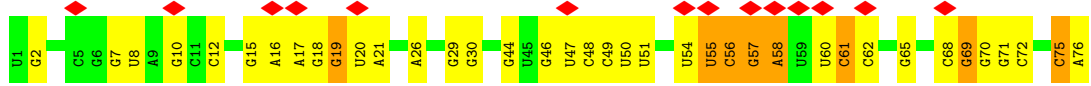




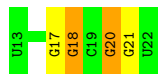
• Molecule 80: AP RNA



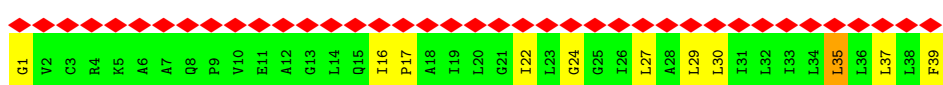
• Molecule 81: PE RNA



• Molecule 82: mRNA



• Molecule 83: Cadherin-1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73110	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 ( $e^-/\text{\AA}^2$ )	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	0.149	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	460.0, 460.0, 460.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.15, 1.15, 1.15	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: 5MC, PSU, OMC, MG, OMG, M7A, B8N, OMU, E3C, MA6, UR3, 6MZ, MVM, A2M, B8Q, ZN, 5MU, 4AC

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	0.31	0/39959	0.42	1/62253 (0.0%)
2	SA	0.32	0/1778	0.68	4/2416 (0.2%)
3	SB	0.30	0/1765	0.60	1/2362 (0.0%)
4	SD	0.30	0/1785	0.68	0/2404
5	SE	0.28	0/2101	0.64	0/2828
6	SF	0.33	0/1516	0.71	2/2037 (0.1%)
7	SH	0.28	0/1519	0.65	0/2033
8	SI	0.30	0/1702	0.63	0/2271
9	SK	0.29	0/851	0.68	0/1147
10	SL	0.31	0/1268	0.66	0/1696
11	SP	0.29	0/1065	0.66	0/1423
12	SQ	0.33	0/1177	0.80	2/1575 (0.1%)
13	SR	0.29	0/1097	0.72	0/1474
14	SS	0.27	0/1216	0.64	1/1628 (0.1%)
15	ST	0.32	0/1131	0.69	1/1515 (0.1%)
16	SU	0.30	0/831	0.70	2/1115 (0.2%)
17	SV	0.34	0/631	0.66	0/844
18	SX	0.33	0/1116	0.69	0/1490
19	Sa	0.39	0/836	0.69	0/1121
20	Sc	0.32	0/508	0.76	0/680
21	Sd	0.42	0/470	0.92	1/623 (0.2%)
22	Sg	0.26	0/2486	0.67	0/3384
23	SC	0.34	0/1755	0.71	1/2371 (0.0%)
24	SG	0.24	0/1946	0.64	0/2590
25	SJ	0.32	0/1561	0.78	1/2083 (0.0%)
26	SM	0.24	0/922	0.60	0/1238
27	SN	0.28	0/1232	0.53	0/1656
28	SO	0.31	0/1037	0.70	0/1391
29	SW	0.36	0/1051	0.66	0/1406
30	SY	0.26	0/1094	0.61	0/1452
31	SZ	0.31	0/585	0.81	0/785

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Sb	0.27	0/653	0.57	0/876
33	Se	0.25	0/458	0.61	0/604
34	Sf	0.28	0/560	0.89	2/745 (0.3%)
35	A	0.39	0/1968	0.68	0/2639
36	B	0.37	0/3270	0.73	1/4377 (0.0%)
37	C	0.40	0/2942	0.72	0/3951
38	D	0.33	0/3726	0.39	0/5804
39	E	0.33	0/2839	0.37	0/4425
40	F	0.34	0/2437	0.73	2/3262 (0.1%)
41	G	0.34	0/1942	0.89	12/2606 (0.5%)
42	H	0.41	0/1905	0.74	1/2539 (0.0%)
43	I	0.35	0/1913	0.66	0/2576
44	J	0.32	0/1545	0.66	1/2077 (0.0%)
45	K	0.33	0/1730	0.65	1/2311 (0.0%)
46	L	0.30	0/1376	0.67	2/1841 (0.1%)
47	M	0.37	0/1688	0.79	0/2260
48	N	0.33	0/1161	0.63	0/1554
49	O	0.41	0/1746	0.72	0/2338
50	P	0.37	0/1638	0.65	1/2191 (0.0%)
51	Q	0.37	0/1268	0.64	1/1701 (0.1%)
52	R	0.38	0/1537	0.82	5/2052 (0.2%)
53	S	0.36	0/1533	0.68	0/2025
54	T	0.39	0/1488	0.66	1/1997 (0.1%)
55	U	0.37	0/1312	0.70	0/1753
56	V	0.28	0/822	0.67	1/1103 (0.1%)
57	W	0.35	0/983	0.60	0/1319
58	X	0.35	0/524	0.62	0/698
59	Y	0.33	0/975	0.61	0/1312
60	Z	0.35	0/1132	0.66	2/1504 (0.1%)
61	a	0.34	0/1126	0.68	2/1502 (0.1%)
62	b	0.38	0/1191	0.81	0/1591
63	c	0.32	0/826	0.72	0/1088
64	d	0.35	0/812	0.67	0/1089
65	e	0.37	0/894	0.69	0/1204
66	f	0.39	0/1082	0.71	0/1443
67	g	0.46	1/895 (0.1%)	0.73	0/1198
68	h	0.37	0/916	0.77	3/1220 (0.2%)
69	i	0.32	0/1023	0.75	2/1351 (0.1%)
70	j	0.33	0/805	0.71	0/1065
71	k	0.38	0/703	0.62	0/929
72	l	0.30	0/575	0.59	0/761
73	m	0.40	0/454	0.67	0/599
74	n	0.32	0/417	0.67	0/553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	o	0.36	0/241	0.85	0/305
76	p	0.38	0/877	0.77	2/1156 (0.2%)
77	q	0.36	0/718	0.67	0/953
78	r	0.40	0/995	0.82	1/1334 (0.1%)
79	t	0.34	0/86502	0.41	4/134927 (0.0%)
80	u	0.24	0/1799	0.48	0/2800
81	v	0.24	0/1802	0.46	0/2797
82	w	0.31	0/235	0.65	1/365 (0.3%)
83	y	0.42	0/263	1.14	1/359 (0.3%)
All	All	0.33	1/230213 (0.0%)	0.54	66/338320 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	SA	0	1
7	SH	0	2
11	SP	0	1
13	SR	0	2
18	SX	0	1
21	Sd	0	2
31	SZ	0	1
36	B	0	1
37	C	0	1
40	F	0	1
44	J	0	1
67	g	0	1
76	p	0	1
All	All	0	16

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	g	59	THR	C-N	5.58	1.39	1.34

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	i	87	LYS	CA-C-N	8.28	137.35	121.54
69	i	87	LYS	C-N-CA	8.28	137.35	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	G	233	PHE	CA-C-N	7.53	135.91	121.54
41	G	233	PHE	C-N-CA	7.53	135.91	121.54
41	G	130	LYS	CA-C-N	7.09	130.79	120.51

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	SA	27	GLY	Peptide
7	SH	15	LYS	Peptide
7	SH	32	MET	Peptide
11	SP	14	LYS	Peptide
13	SR	67	ARG	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	36501	0	18404	262	0
2	SA	1741	0	1746	31	0
3	SB	1738	0	1809	27	0
4	SD	1757	0	1853	24	0
5	SE	2059	0	2164	43	0
6	SF	1495	0	1549	27	0
7	SH	1497	0	1590	30	0
8	SI	1673	0	1756	29	0
9	SK	827	0	854	8	0
10	SL	1247	0	1323	8	0
11	SP	1045	0	1095	22	0
12	SQ	1158	0	1232	16	0
13	SR	1082	0	1137	22	0
14	SS	1198	0	1261	15	0
15	ST	1112	0	1146	19	0
16	SU	821	0	883	14	0
17	SV	625	0	628	11	0
18	SX	1098	0	1167	14	0
19	Sa	821	0	870	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	Sc	506	0	536	13	0
21	Sd	459	0	449	11	0
22	Sg	2429	0	2386	41	0
23	SC	1715	0	1804	25	0
24	SG	1923	0	2089	30	0
25	SJ	1533	0	1653	22	0
26	SM	912	0	930	10	0
27	SN	1208	0	1294	16	0
28	SO	1024	0	1050	18	0
29	SW	1034	0	1080	19	0
30	SY	1073	0	1155	11	0
31	SZ	579	0	639	8	0
32	Sb	640	0	665	9	0
33	Se	452	0	498	3	0
34	Sf	548	0	552	11	0
35	A	1930	0	2030	24	0
36	B	3202	0	3343	48	0
37	C	2888	0	3064	46	0
38	D	3337	0	1692	20	0
39	E	2541	0	1285	7	0
40	F	2392	0	2425	23	0
41	G	1904	0	2055	40	0
42	H	1870	0	1996	34	0
43	I	1880	0	2018	16	0
44	J	1526	0	1605	18	0
45	K	1692	0	1744	19	0
46	L	1353	0	1386	12	0
47	M	1657	0	1764	24	0
48	N	1138	0	1204	18	0
49	O	1701	0	1749	36	0
50	P	1606	0	1745	33	0
51	Q	1242	0	1269	17	0
52	R	1513	0	1628	21	0
53	S	1517	0	1670	31	0
54	T	1449	0	1493	35	0
55	U	1284	0	1352	24	0
56	V	808	0	831	8	0
57	W	969	0	1031	11	0
58	X	511	0	521	6	0
59	Y	958	0	1029	10	0
60	Z	1115	0	1205	15	0
61	a	1103	0	1179	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	b	1162	0	1213	17	0
63	c	814	0	880	18	0
64	d	801	0	845	15	0
65	e	879	0	924	6	0
66	f	1064	0	1160	16	0
67	g	876	0	912	11	0
68	h	906	0	1002	10	0
69	i	1015	0	1148	13	0
70	j	794	0	870	6	0
71	k	689	0	717	8	0
72	l	569	0	637	6	0
73	m	444	0	483	9	0
74	n	411	0	443	7	0
75	o	240	0	289	4	0
76	p	863	0	931	16	0
77	q	708	0	756	8	0
78	r	980	0	1041	15	0
79	t	77332	0	39076	449	0
80	u	1613	0	822	10	0
81	v	1618	0	826	10	0
82	w	213	0	109	1	0
83	y	262	0	290	5	0
84	A	1	0	0	0	0
84	B	1	0	0	0	0
84	D	8	0	0	0	0
84	E	9	0	0	0	0
84	O	1	0	0	0	0
84	S2	3	0	0	0	0
84	Z	1	0	0	0	0
84	b	1	0	0	0	0
84	t	6	0	0	0	0
85	S2	1	0	0	0	0
85	Sa	1	0	0	0	0
85	Sf	1	0	0	0	0
85	k	1	0	0	0	0
85	p	1	0	0	0	0
85	q	1	0	0	0	0
86	y	31	0	0	0	0
87	S2	4	0	0	0	0
87	SC	1	0	0	0	0
87	SN	1	0	0	0	0
87	SP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	SQ	1	0	0	0	0
87	SR	1	0	0	0	0
87	SS	2	0	0	0	0
87	Sf	1	0	0	0	0
87	u	1	0	0	1	0
87	v	1	0	0	0	0
All	All	214951	0	158934	1670	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1670 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:814:5MU:C4	1:S2:814:5MU:C5	1.81	1.60
79:t:708:U:H3	79:t:938:G:H1	1.25	0.84
40:F:4:VAL:N	79:t:1760:C:HO2'	1.76	0.82
79:t:3663:A:H62	79:t:3794:G:H21	1.31	0.78
1:S2:1648:G:H5''	12:SQ:125:ARG:HB2	1.69	0.75

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SA	219/221 (99%)	194 (89%)	24 (11%)	1 (0%)	24	57
3	SB	212/214 (99%)	197 (93%)	15 (7%)	0	100	100
4	SD	224/226 (99%)	200 (89%)	24 (11%)	0	100	100
5	SE	257/259 (99%)	237 (92%)	20 (8%)	0	100	100
6	SF	187/189 (99%)	170 (91%)	17 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	SH	182/189 (96%)	160 (88%)	22 (12%)	0	100	100
8	SI	202/204 (99%)	180 (89%)	22 (11%)	0	100	100
9	SK	96/98 (98%)	85 (88%)	11 (12%)	0	100	100
10	SL	151/153 (99%)	134 (89%)	17 (11%)	0	100	100
11	SP	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
12	SQ	144/146 (99%)	121 (84%)	21 (15%)	2 (1%)	9	34
13	SR	132/134 (98%)	115 (87%)	17 (13%)	0	100	100
14	SS	143/145 (99%)	127 (89%)	16 (11%)	0	100	100
15	ST	141/143 (99%)	134 (95%)	6 (4%)	1 (1%)	18	49
16	SU	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
17	SV	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
18	SX	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
19	Sa	100/102 (98%)	88 (88%)	11 (11%)	1 (1%)	12	41
20	Sc	62/64 (97%)	50 (81%)	12 (19%)	0	100	100
21	Sd	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	6	27
22	Sg	310/312 (99%)	254 (82%)	56 (18%)	0	100	100
23	SC	219/220 (100%)	201 (92%)	17 (8%)	1 (0%)	24	57
24	SG	235/237 (99%)	210 (89%)	25 (11%)	0	100	100
25	SJ	184/185 (100%)	168 (91%)	15 (8%)	1 (0%)	24	57
26	SM	116/118 (98%)	98 (84%)	18 (16%)	0	100	100
27	SN	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
28	SO	135/137 (98%)	118 (87%)	17 (13%)	0	100	100
29	SW	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
30	SY	130/131 (99%)	119 (92%)	11 (8%)	0	100	100
31	SZ	71/73 (97%)	54 (76%)	17 (24%)	0	100	100
32	Sb	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
33	Se	55/57 (96%)	46 (84%)	9 (16%)	0	100	100
34	Sf	65/67 (97%)	49 (75%)	15 (23%)	1 (2%)	8	32
35	A	250/252 (99%)	226 (90%)	23 (9%)	1 (0%)	30	61
36	B	395/397 (100%)	359 (91%)	34 (9%)	2 (0%)	24	57
37	C	361/363 (99%)	329 (91%)	27 (8%)	5 (1%)	9	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	F	292/294 (99%)	263 (90%)	26 (9%)	3 (1%)	12	41
41	G	232/247 (94%)	193 (83%)	38 (16%)	1 (0%)	30	61
42	H	223/225 (99%)	206 (92%)	16 (7%)	1 (0%)	30	61
43	I	232/234 (99%)	213 (92%)	19 (8%)	0	100	100
44	J	189/191 (99%)	170 (90%)	17 (9%)	2 (1%)	11	39
45	K	204/211 (97%)	185 (91%)	18 (9%)	1 (0%)	24	57
46	L	167/169 (99%)	149 (89%)	18 (11%)	0	100	100
47	M	203/205 (99%)	173 (85%)	28 (14%)	2 (1%)	12	41
48	N	137/139 (99%)	127 (93%)	10 (7%)	0	100	100
49	O	201/203 (99%)	184 (92%)	16 (8%)	1 (0%)	24	57
50	P	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
51	Q	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
52	R	185/187 (99%)	170 (92%)	14 (8%)	1 (0%)	24	57
53	S	179/181 (99%)	168 (94%)	11 (6%)	0	100	100
54	T	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
55	U	155/157 (99%)	133 (86%)	20 (13%)	2 (1%)	9	35
56	V	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
57	W	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
58	X	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
59	Y	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
60	Z	132/134 (98%)	122 (92%)	10 (8%)	0	100	100
61	a	132/134 (98%)	118 (89%)	14 (11%)	0	100	100
62	b	145/147 (99%)	127 (88%)	18 (12%)	0	100	100
63	c	94/121 (78%)	79 (84%)	15 (16%)	0	100	100
64	d	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
65	e	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
66	f	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
67	g	107/109 (98%)	97 (91%)	10 (9%)	0	100	100
68	h	112/114 (98%)	103 (92%)	9 (8%)	0	100	100
69	i	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	7	30
70	j	95/97 (98%)	85 (90%)	8 (8%)	2 (2%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	k	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
72	l	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
73	m	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
74	n	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
75	o	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
76	p	103/105 (98%)	95 (92%)	7 (7%)	1 (1%)	12	41
77	q	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	11	39
78	r	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	7	30
83	y	37/39 (95%)	18 (49%)	18 (49%)	1 (3%)	4	20
All	All	11232/11429 (98%)	10097 (90%)	1095 (10%)	40 (0%)	31	61

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	ST	41	LYS
23	SC	78	LEU
34	Sf	93	HIS
41	G	127	SER
47	M	64	VAL

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SA	183/183 (100%)	181 (99%)	2 (1%)	65	78
3	SB	195/195 (100%)	192 (98%)	3 (2%)	57	75
4	SD	189/189 (100%)	187 (99%)	2 (1%)	65	78
5	SE	222/222 (100%)	220 (99%)	2 (1%)	70	80
6	SF	159/159 (100%)	157 (99%)	2 (1%)	61	77
7	SH	166/169 (98%)	165 (99%)	1 (1%)	78	83
8	SI	177/177 (100%)	176 (99%)	1 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	SK	89/89 (100%)	88 (99%)	1 (1%)	65	78
10	SL	137/137 (100%)	136 (99%)	1 (1%)	76	82
11	SP	113/113 (100%)	111 (98%)	2 (2%)	51	73
12	SQ	121/121 (100%)	119 (98%)	2 (2%)	53	74
13	SR	121/121 (100%)	118 (98%)	3 (2%)	42	69
14	SS	126/126 (100%)	125 (99%)	1 (1%)	73	81
15	ST	113/113 (100%)	111 (98%)	2 (2%)	51	73
16	SU	94/94 (100%)	94 (100%)	0	100	100
17	SV	66/66 (100%)	65 (98%)	1 (2%)	57	75
18	SX	113/113 (100%)	111 (98%)	2 (2%)	51	73
19	Sa	89/89 (100%)	89 (100%)	0	100	100
20	Sc	57/57 (100%)	57 (100%)	0	100	100
21	Sd	48/48 (100%)	47 (98%)	1 (2%)	47	71
22	Sg	271/271 (100%)	270 (100%)	1 (0%)	84	86
23	SC	187/186 (100%)	186 (100%)	1 (0%)	81	85
24	SG	207/207 (100%)	206 (100%)	1 (0%)	81	85
25	SJ	162/161 (101%)	160 (99%)	2 (1%)	63	78
26	SM	98/100 (98%)	98 (100%)	0	100	100
27	SN	130/130 (100%)	130 (100%)	0	100	100
28	SO	107/107 (100%)	107 (100%)	0	100	100
29	SW	112/112 (100%)	111 (99%)	1 (1%)	70	80
30	SY	114/113 (101%)	112 (98%)	2 (2%)	51	73
31	SZ	64/64 (100%)	63 (98%)	1 (2%)	55	75
32	Sb	74/74 (100%)	74 (100%)	0	100	100
33	Se	46/46 (100%)	46 (100%)	0	100	100
34	Sf	60/60 (100%)	60 (100%)	0	100	100
35	A	194/194 (100%)	189 (97%)	5 (3%)	40	68
36	B	345/345 (100%)	341 (99%)	4 (1%)	63	78
37	C	302/302 (100%)	297 (98%)	5 (2%)	53	74
40	F	248/248 (100%)	248 (100%)	0	100	100
41	G	209/220 (95%)	207 (99%)	2 (1%)	68	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	H	194/194 (100%)	191 (98%)	3 (2%)	57	75
43	I	199/199 (100%)	198 (100%)	1 (0%)	81	85
44	J	170/170 (100%)	169 (99%)	1 (1%)	78	83
45	K	178/179 (99%)	176 (99%)	2 (1%)	65	78
46	L	142/142 (100%)	142 (100%)	0	100	100
47	M	171/171 (100%)	169 (99%)	2 (1%)	63	78
48	N	118/118 (100%)	116 (98%)	2 (2%)	53	74
49	O	171/171 (100%)	168 (98%)	3 (2%)	51	73
50	P	168/168 (100%)	167 (99%)	1 (1%)	78	83
51	Q	134/134 (100%)	132 (98%)	2 (2%)	57	75
52	R	164/164 (100%)	162 (99%)	2 (1%)	63	78
53	S	160/160 (100%)	160 (100%)	0	100	100
54	T	156/156 (100%)	156 (100%)	0	100	100
55	U	138/138 (100%)	138 (100%)	0	100	100
56	V	89/89 (100%)	89 (100%)	0	100	100
57	W	100/100 (100%)	99 (99%)	1 (1%)	68	79
58	X	53/53 (100%)	52 (98%)	1 (2%)	50	73
59	Y	105/105 (100%)	103 (98%)	2 (2%)	50	73
60	Z	124/124 (100%)	122 (98%)	2 (2%)	55	75
61	a	117/117 (100%)	116 (99%)	1 (1%)	70	80
62	b	120/120 (100%)	118 (98%)	2 (2%)	53	74
63	c	82/101 (81%)	82 (100%)	0	100	100
64	d	88/88 (100%)	86 (98%)	2 (2%)	44	70
65	e	97/97 (100%)	96 (99%)	1 (1%)	68	79
66	f	115/115 (100%)	115 (100%)	0	100	100
67	g	88/88 (100%)	85 (97%)	3 (3%)	32	63
68	h	98/98 (100%)	96 (98%)	2 (2%)	48	72
69	i	109/109 (100%)	109 (100%)	0	100	100
70	j	83/83 (100%)	83 (100%)	0	100	100
71	k	71/71 (100%)	71 (100%)	0	100	100
72	l	64/64 (100%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	m	47/47 (100%)	47 (100%)	0	100	100
74	n	46/46 (100%)	46 (100%)	0	100	100
75	o	24/24 (100%)	24 (100%)	0	100	100
76	p	93/93 (100%)	89 (96%)	4 (4%)	26	57
77	q	74/74 (100%)	73 (99%)	1 (1%)	59	76
78	r	106/106 (100%)	106 (100%)	0	100	100
83	y	23/29 (79%)	20 (87%)	3 (13%)	4	18
All	All	9787/9826 (100%)	9689 (99%)	98 (1%)	65	79

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	I	45	ILE
52	R	138	LEU
45	K	26	VAL
49	O	64	ILE
59	Y	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 183 such sidechains are listed below:

Mol	Chain	Res	Type
42	H	131	ASN
51	Q	34	GLN
43	I	206	GLN
47	M	104	ASN
53	S	130	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1698/1714 (99%)	573 (33%)	31 (1%)
38	D	156/157 (99%)	37 (23%)	0
39	E	118/121 (97%)	21 (17%)	0
79	t	3593/3607 (99%)	892 (24%)	0
80	u	74/76 (97%)	30 (40%)	0
81	v	72/76 (94%)	31 (43%)	0
82	w	9/10 (90%)	4 (44%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	5720/5761 (99%)	1588 (27%)	31 (0%)

5 of 1588 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	4	C
1	S2	9	U
1	S2	10	G
1	S2	11	A

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	563	G
1	S2	1813	A
1	S2	872	A
1	S2	1815	A
1	S2	1661	A

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

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	A2M	S2	159	1	22,25,26	4.08	9 (40%)	30,36,39	3.09	16 (53%)
1	PSU	S2	823	1	18,21,22	4.45	8 (44%)	21,30,33	2.47	5 (23%)
1	5MU	S2	814	1	19,22,23	7.71	8 (42%)	27,32,35	3.49	12 (44%)
1	4AC	S2	1842	1	21,24,25	3.16	9 (42%)	28,34,37	1.20	5 (17%)
1	MA6	S2	1850	1	23,26,27	1.47	4 (17%)	33,38,41	3.58	14 (42%)
1	B8Q	S2	1219	1	18,22,23	4.78	7 (38%)	21,32,35	1.87	4 (19%)
1	OMC	S2	174	1	19,22,23	3.55	8 (42%)	25,31,34	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	S2	121	1	19,22,23	3.13	6 (31%)	25,31,34	1.82	6 (24%)
1	PSU	S2	1081	1	18,21,22	4.27	8 (44%)	21,30,33	1.75	3 (14%)
1	OMG	S2	509	1	23,26,27	2.43	7 (30%)	32,38,41	2.17	10 (31%)
1	5MC	S2	1374	1	19,22,23	3.58	8 (42%)	26,32,35	0.94	2 (7%)
1	A2M	S2	1678	1	22,25,26	4.21	9 (40%)	30,36,39	2.90	13 (43%)
1	PSU	S2	822	1	18,21,22	4.51	8 (44%)	21,30,33	1.91	4 (19%)
1	A2M	S2	484	1	22,25,26	4.07	9 (40%)	30,36,39	2.99	14 (46%)
1	OMC	S2	517	1	19,22,23	3.47	8 (42%)	25,31,34	0.72	0
1	M7A	S2	1806	1	19,25,26	1.64	2 (10%)	25,37,40	3.66	8 (32%)
1	A2M	S2	166	1	22,25,26	4.12	9 (40%)	30,36,39	2.87	14 (46%)
1	A2M	S2	1031	1	22,25,26	4.09	9 (40%)	30,36,39	2.99	11 (36%)
1	UR3	S2	1830	1	19,22,23	2.86	7 (36%)	26,32,35	2.98	8 (30%)
1	A2M	S2	27	1	22,25,26	4.08	9 (40%)	30,36,39	2.98	13 (43%)
1	MA6	S2	1851	1	23,26,27	1.47	5 (21%)	33,38,41	3.48	15 (45%)
1	PSU	S2	612	1	18,21,22	4.42	8 (44%)	21,30,33	2.34	6 (28%)
1	PSU	S2	119	1	18,21,22	4.41	7 (38%)	21,30,33	1.92	5 (23%)
1	OMG	S2	683	1	23,26,27	2.42	7 (30%)	32,38,41	2.06	10 (31%)
1	E3C	S2	568	1	19,23,24	3.51	7 (36%)	21,33,36	2.66	6 (28%)
1	PSU	S2	1243	1	18,21,22	4.38	7 (38%)	21,30,33	1.90	5 (23%)
1	OMG	S2	644	1	23,26,27	2.42	8 (34%)	32,38,41	2.20	10 (31%)
1	OMC	S2	1703	1	19,22,23	3.47	8 (42%)	25,31,34	0.75	1 (4%)
1	OMU	S2	116	1	19,22,23	3.13	6 (31%)	25,31,34	1.66	6 (24%)
1	4AC	S2	1337	1	21,24,25	3.33	9 (42%)	28,34,37	1.21	3 (10%)
1	A2M	S2	668	1	22,25,26	4.10	9 (40%)	30,36,39	3.11	14 (46%)
1	6MZ	S2	1832	1	22,25,26	2.58	6 (27%)	29,36,39	2.11	8 (27%)
1	B8N	S2	1248	1	25,29,30	3.13	7 (28%)	28,42,45	2.09	8 (28%)
1	OMC	S2	1710	1	19,22,23	3.54	8 (42%)	25,31,34	0.75	0

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	A2M	S2	159	1	-	3/9/27/28	0/3/3/3
1	PSU	S2	823	1	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	S2	814	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	MA6	S2	1850	1	-	2/11/29/30	0/3/3/3
1	B8Q	S2	1219	1	-	2/7/42/43	0/2/2/2
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	OMU	S2	121	1	-	3/9/27/28	0/2/2/2
1	PSU	S2	1081	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	509	1	-	1/9/27/28	0/3/3/3
1	5MC	S2	1374	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	822	1	-	2/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	0/9/27/28	0/3/3/3
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	M7A	S2	1806	1	-	3/7/37/38	0/3/3/3
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	1031	1	-	1/9/27/28	0/3/3/3
1	UR3	S2	1830	1	-	4/7/25/26	0/2/2/2
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
1	MA6	S2	1851	1	-	3/11/29/30	0/3/3/3
1	PSU	S2	612	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	119	1	-	2/7/25/26	0/2/2/2
1	OMG	S2	683	1	-	2/9/27/28	0/3/3/3
1	E3C	S2	568	1	-	4/9/44/45	0/2/2/2
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	OMG	S2	644	1	-	1/9/27/28	0/3/3/3
1	OMC	S2	1703	1	-	2/9/27/28	0/2/2/2
1	OMU	S2	116	1	-	3/9/27/28	0/2/2/2
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	A2M	S2	668	1	-	4/9/27/28	0/3/3/3
1	6MZ	S2	1832	1	-	2/9/27/28	0/3/3/3
1	B8N	S2	1248	1	-	0/16/34/35	0/2/2/2
1	OMC	S2	1710	1	-	0/9/27/28	0/2/2/2

The worst 5 of 254 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	814	5MU	C4-C5	22.66	1.81	1.44
1	S2	814	5MU	C6-N1	17.25	1.67	1.38
1	S2	823	PSU	C6-C5	11.94	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	814	5MU	C6-C5	-11.90	1.15	1.34
1	S2	822	PSU	C6-C5	11.70	1.48	1.35

The worst 5 of 259 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1851	MA6	N1-C6-N6	-12.22	101.97	116.86
1	S2	1850	MA6	N1-C6-N6	-11.97	102.27	116.86
1	S2	1806	M7A	C5-C6-N6	10.71	141.95	123.75
1	S2	814	5MU	C5-C4-N3	9.71	123.76	115.32
1	S2	1806	M7A	N6-C6-N1	-9.37	97.51	118.38

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	116	OMU	O4'-C4'-C5'-O5'
1	S2	121	OMU	O4'-C4'-C5'-O5'
1	S2	159	A2M	C1'-C2'-O2'-CM'
1	S2	509	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	814	5MU	1	0
1	S2	1850	MA6	1	0
1	S2	121	OMU	3	0
1	S2	509	OMG	4	0
1	S2	1678	A2M	1	0
1	S2	1337	4AC	1	0
1	S2	1832	6MZ	1	0

## 5.5 Carbohydrates

There are no oligosaccharides 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	y	101	-	35,35,35	1.82	4 (11%)	44,49,49	2.64	15 (34%)

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	y	101	-	-	1/20/28/28	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	y	101	MVM	N4-N5	-6.53	1.31	1.38
86	y	101	MVM	C5-N1	5.54	1.45	1.37
86	y	101	MVM	C6-N1	2.28	1.44	1.39
86	y	101	MVM	O1-C5	-2.10	1.18	1.22

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	y	101	MVM	N7-C22-N4	7.42	134.22	125.88
86	y	101	MVM	C15-N4-N5	6.58	125.17	119.25
86	y	101	MVM	C15-N4-C22	-6.51	124.76	130.55
86	y	101	MVM	C18-C22-N7	-4.47	121.05	127.18
86	y	101	MVM	C1-C9-N1	-4.39	105.14	116.16

There are no chirality outliers.

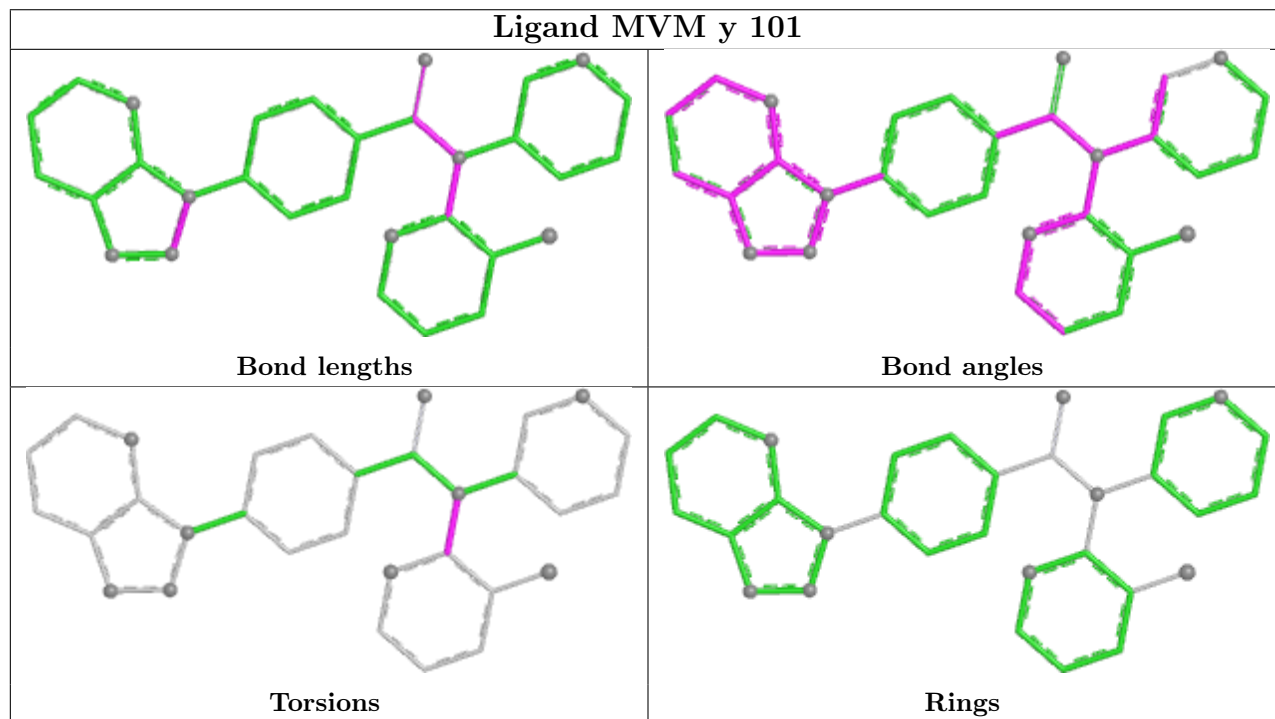
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	y	101	MVM	C2-C6-N1-C5

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
79	t	16
1	S2	5
81	v	4
63	c	1
80	u	1

The worst 5 of 27 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	26.07
1	t	750:G	O3'	890:C	P	19.83
1	t	3919:C	O3'	4035:G	P	18.64
1	t	517:C	O3'	629:G	P	17.24
1	t	1680:C	O3'	1699:C	P	16.67

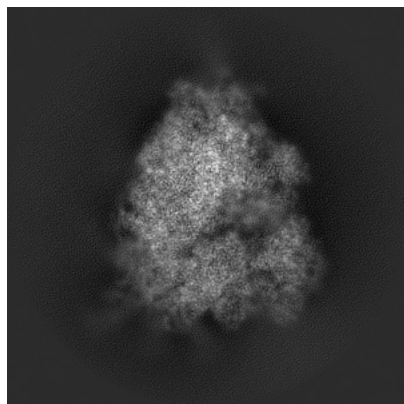
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0600. These allow visual inspection of the internal detail of the map and identification of artifacts.

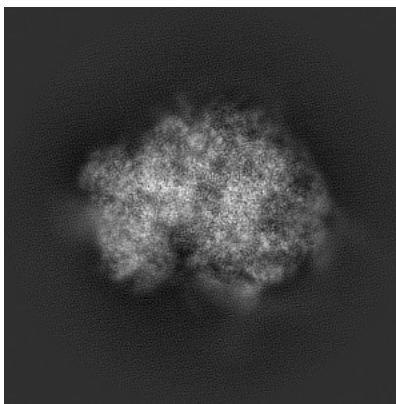
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

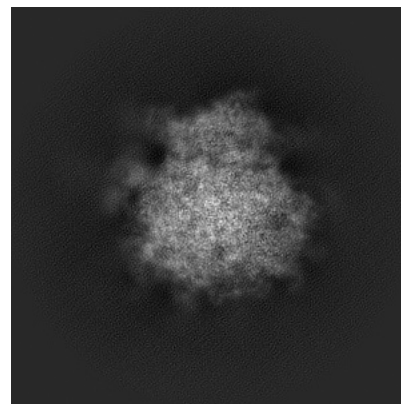
#### 6.1.1 Primary map



X

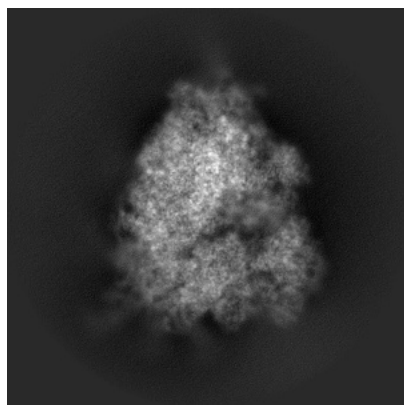


Y

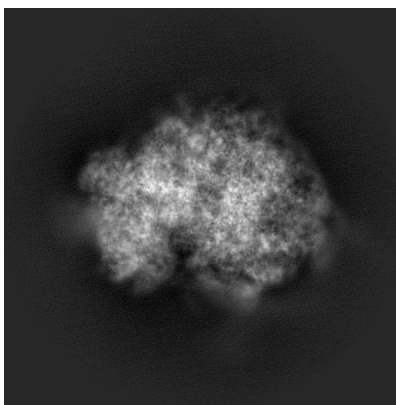


Z

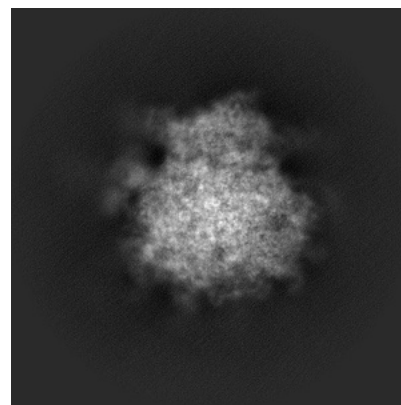
#### 6.1.2 Raw map



X



Y

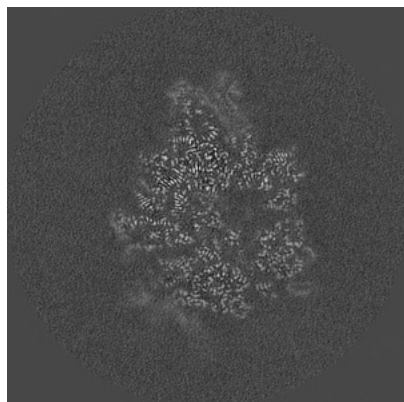


Z

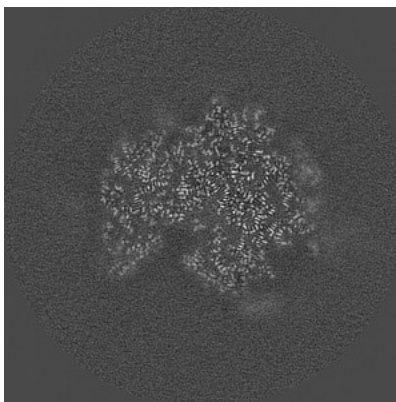
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

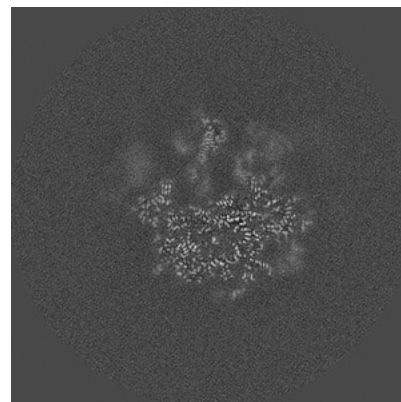
### 6.2.1 Primary map



X Index: 200

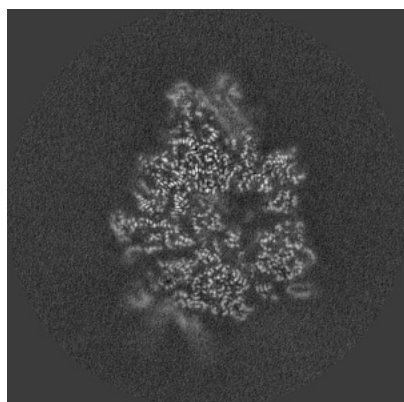


Y Index: 200

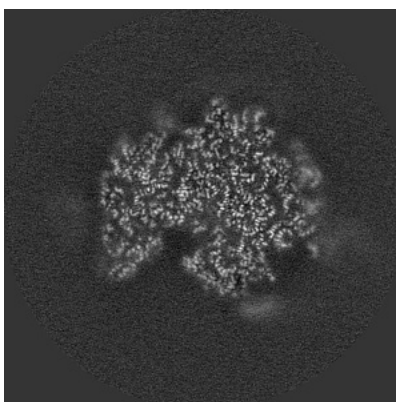


Z Index: 200

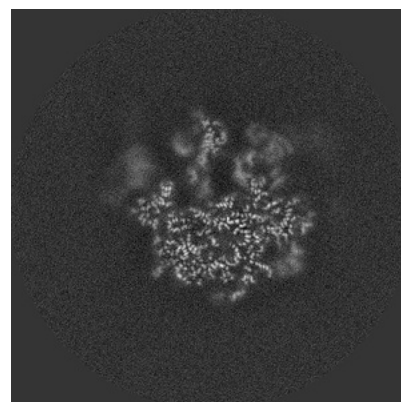
### 6.2.2 Raw map



X Index: 200



Y Index: 200

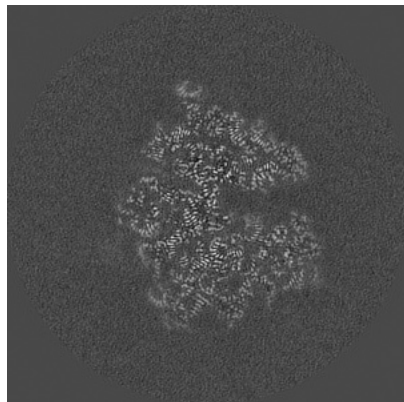


Z Index: 200

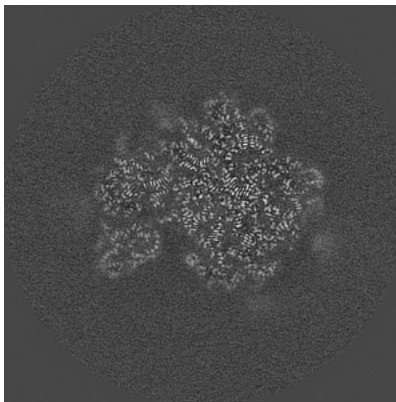
The images above show central slices of the map in three orthogonal directions.

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

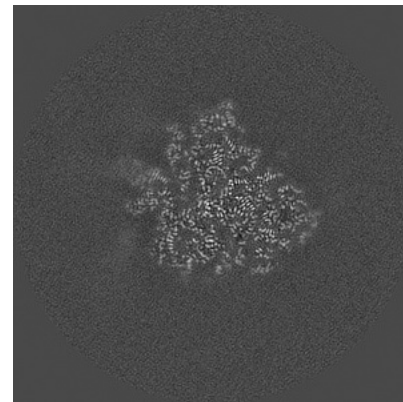
### 6.3.1 Primary map



X Index: 219

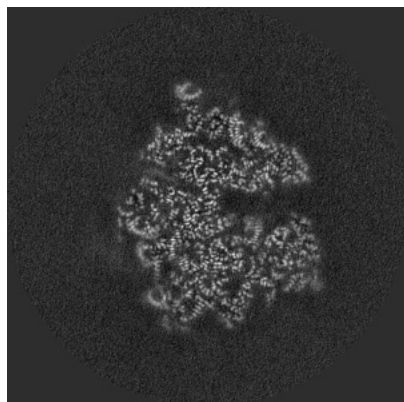


Y Index: 193

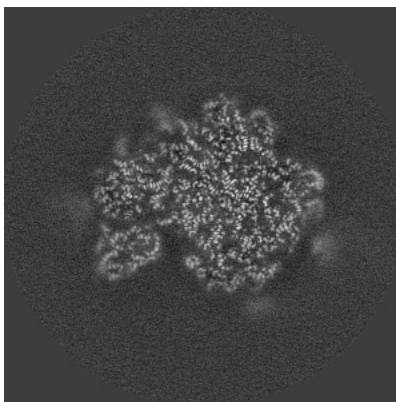


Z Index: 229

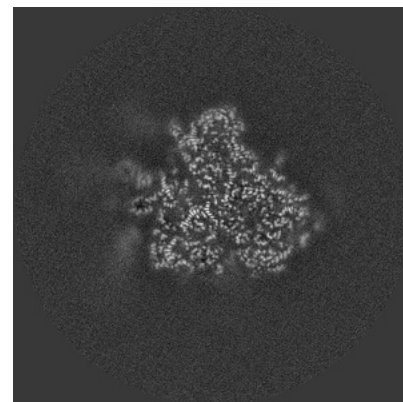
### 6.3.2 Raw map



X Index: 218



Y Index: 193

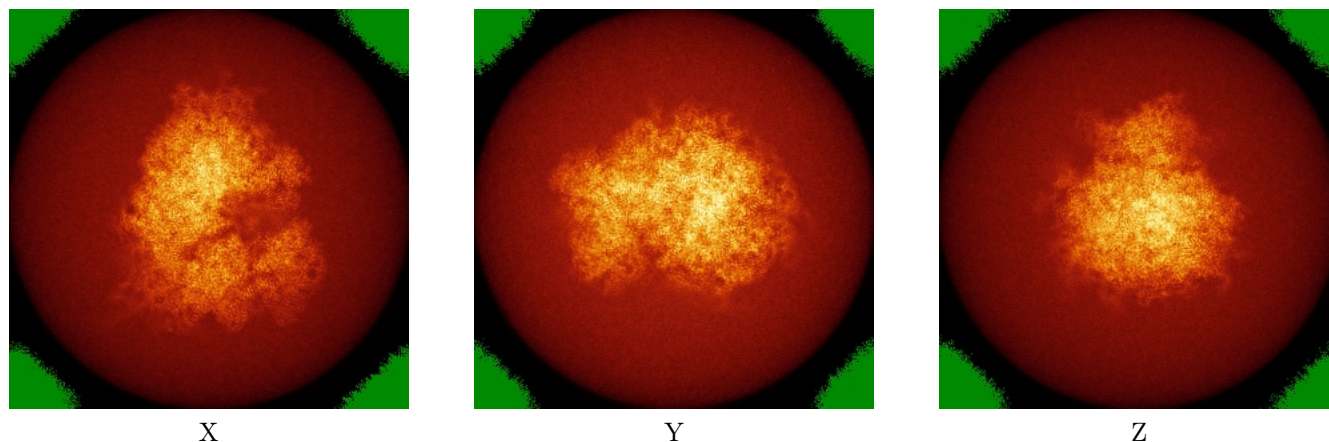


Z Index: 234

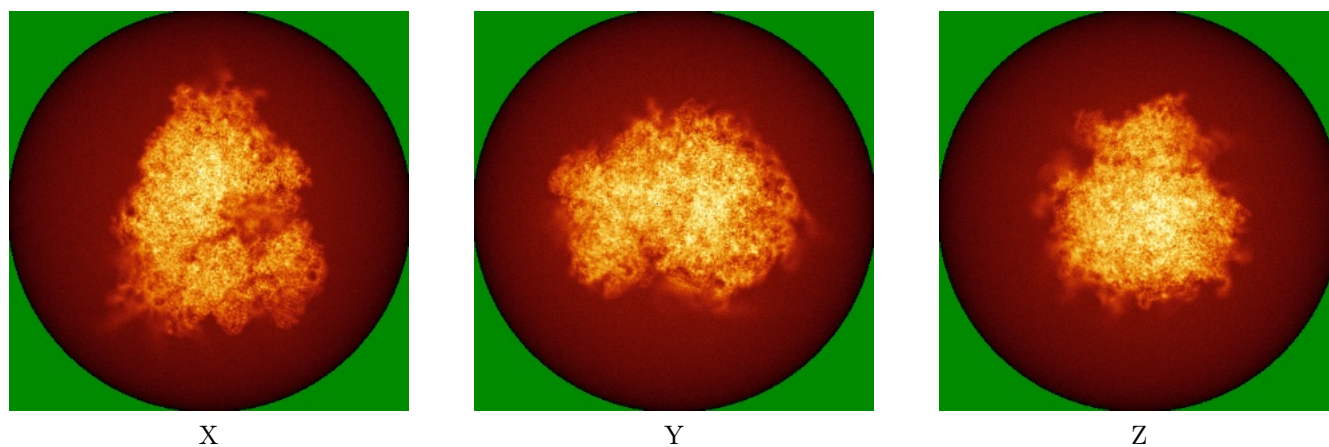
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



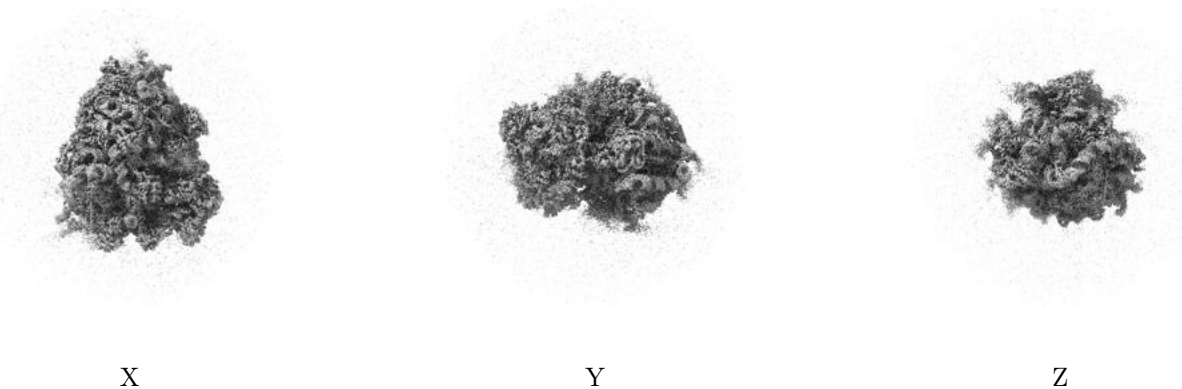
### 6.4.2 Raw map



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

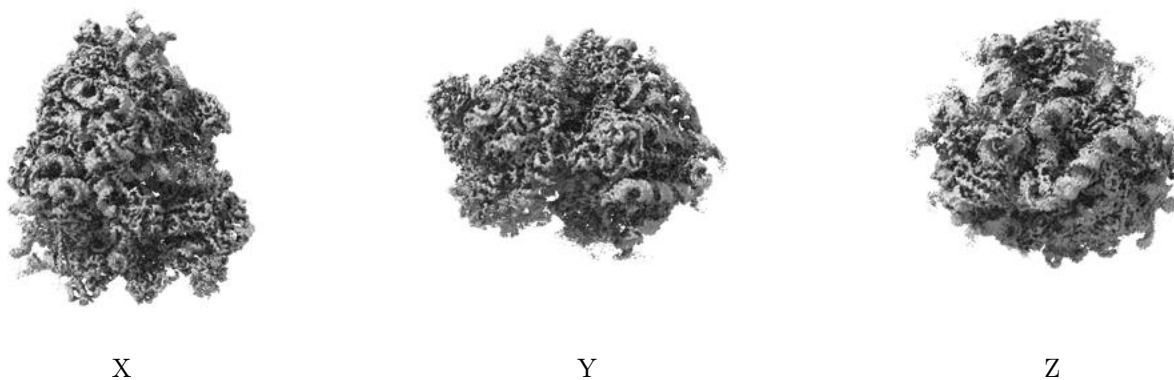
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

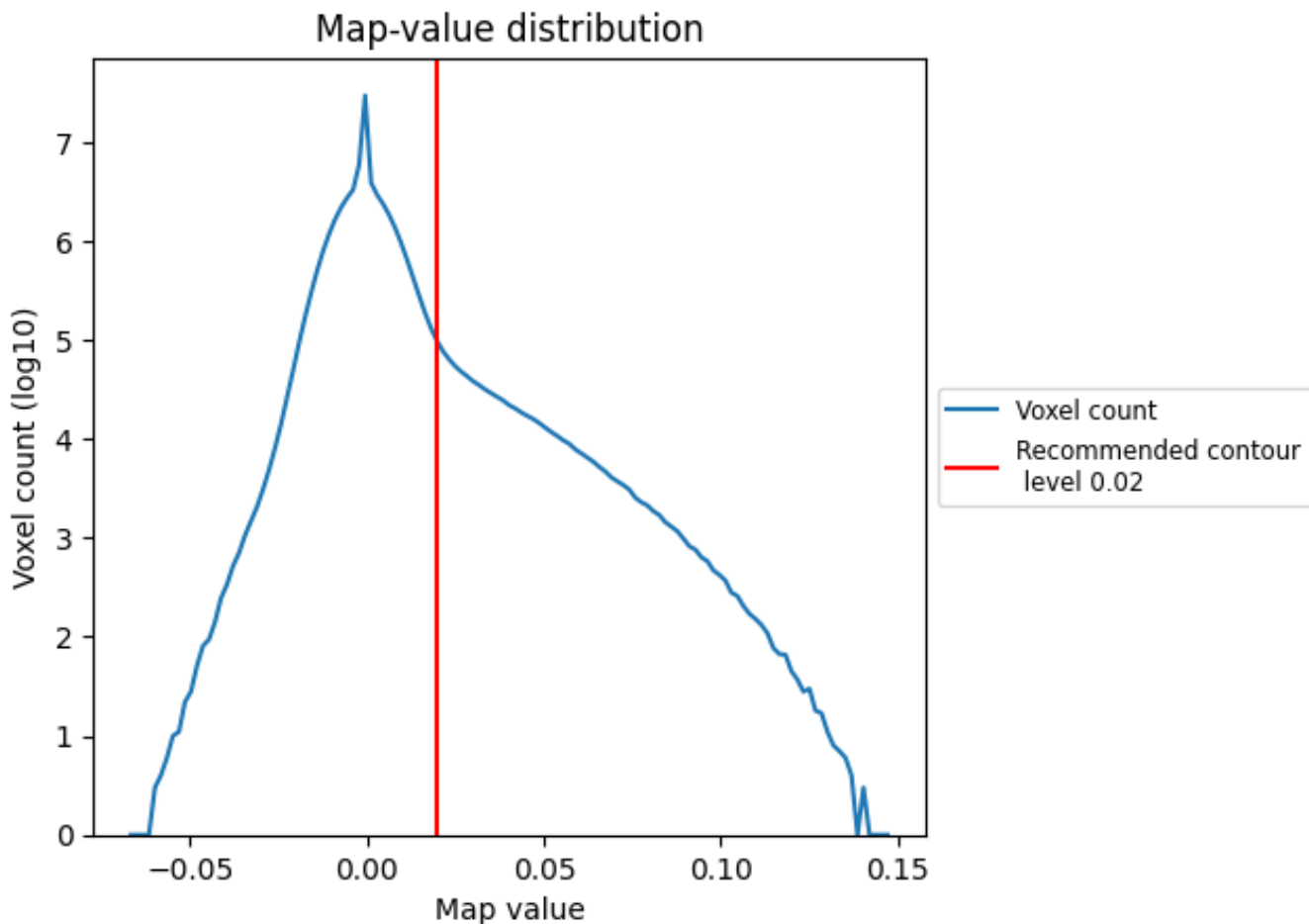
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

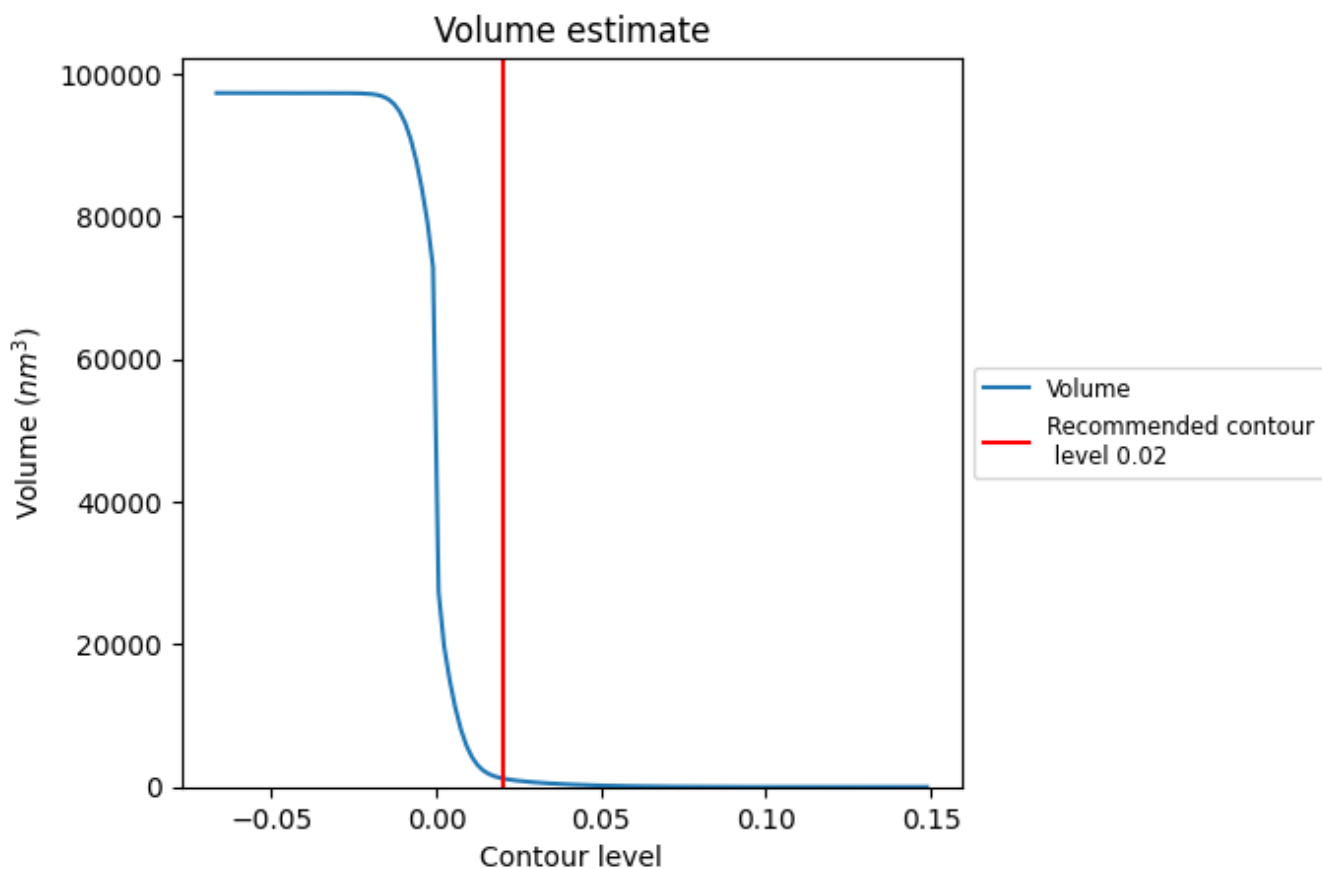
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

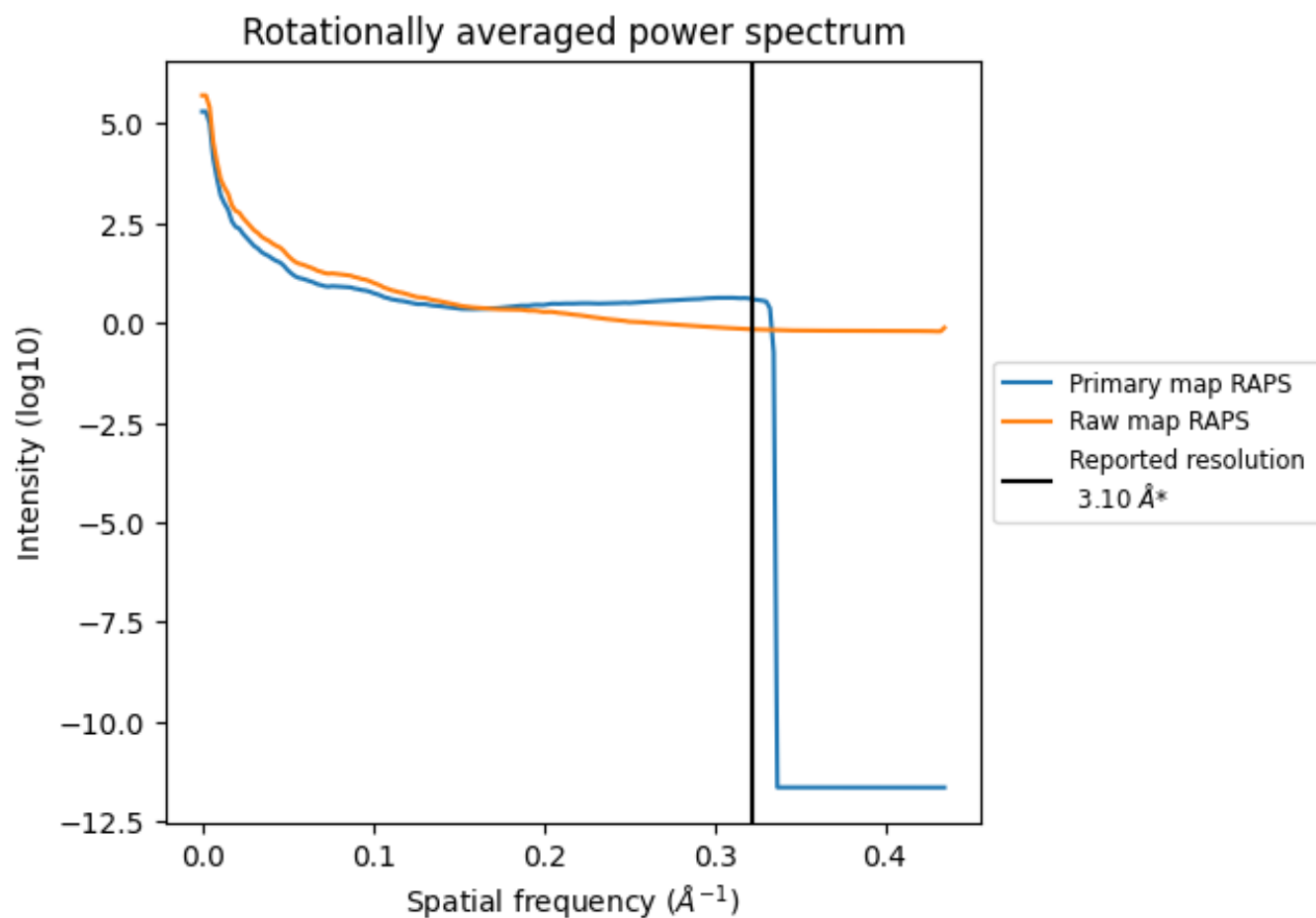
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1213  $\text{nm}^3$ ; this corresponds to an approximate mass of 1096 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](#)

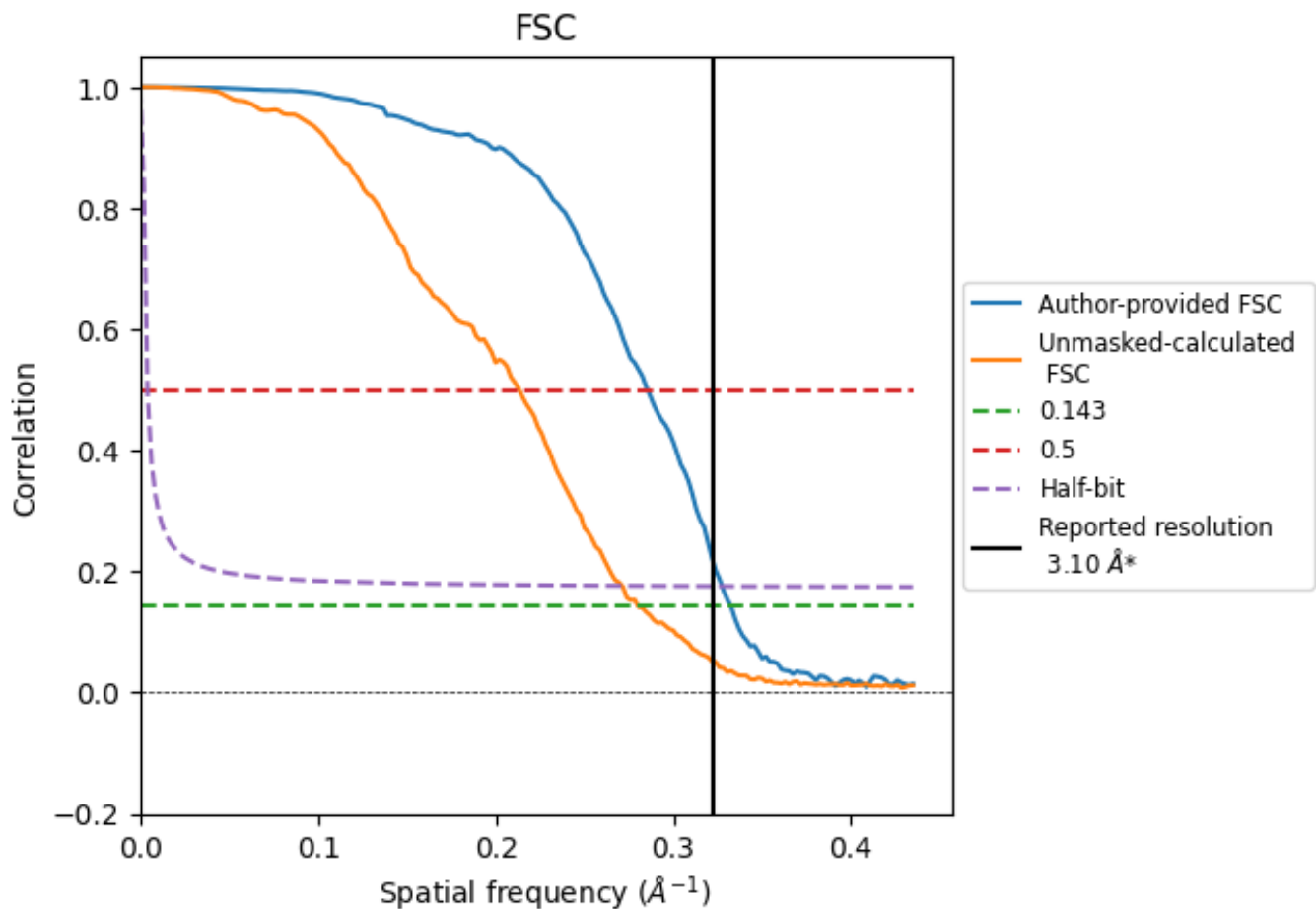


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

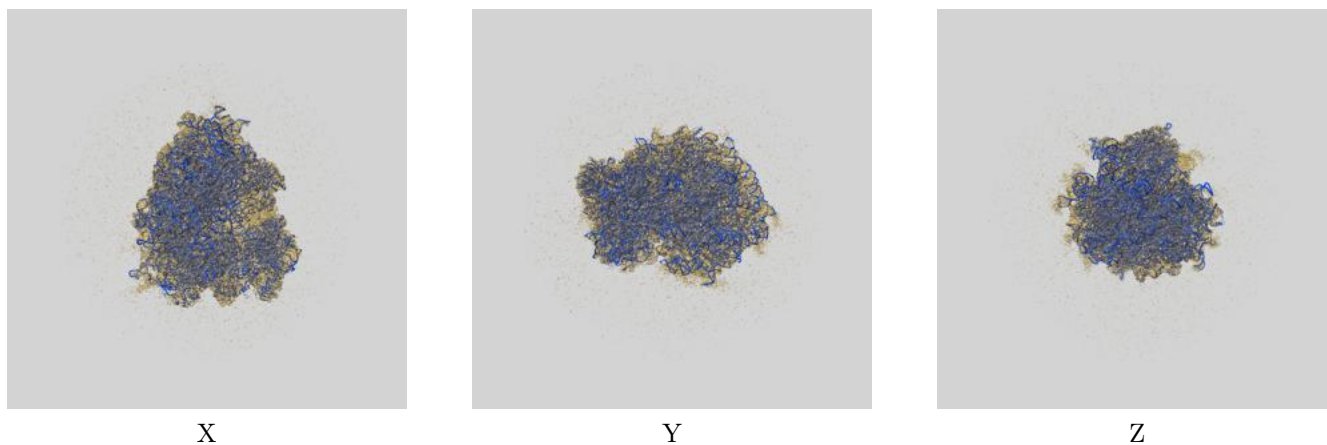
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.01	3.50	3.05
Unmasked-calculated*	3.57	4.69	3.69

\*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 3.57 differs from the reported value 3.1 by more than 10 %

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

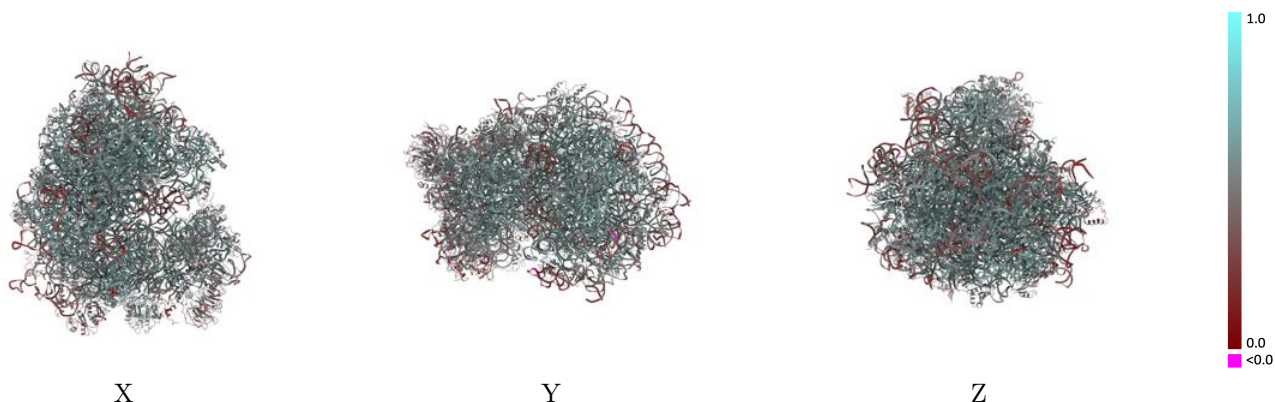
This section contains information regarding the fit between EMDB map EMD-0600 and PDB model 6OLE. Per-residue inclusion information can be found in section 3 on page 22.

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



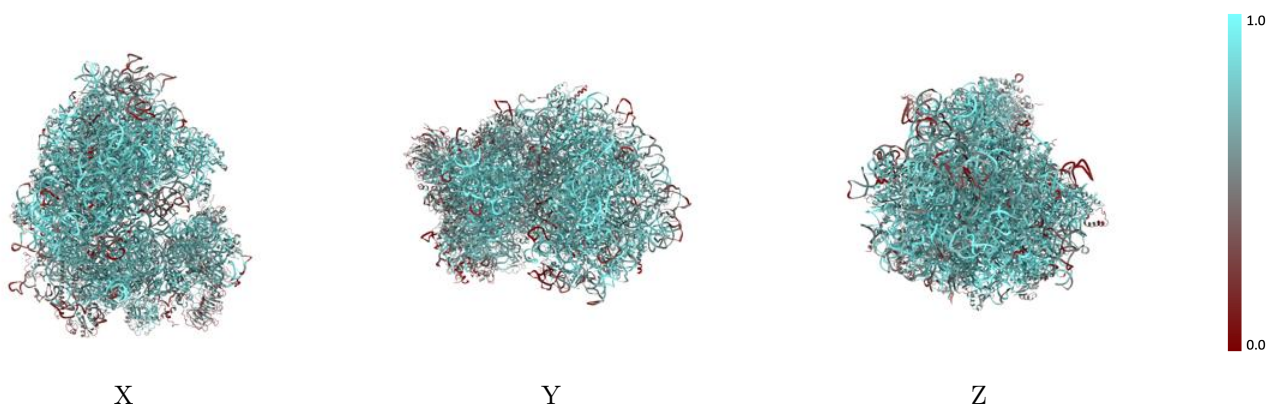
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



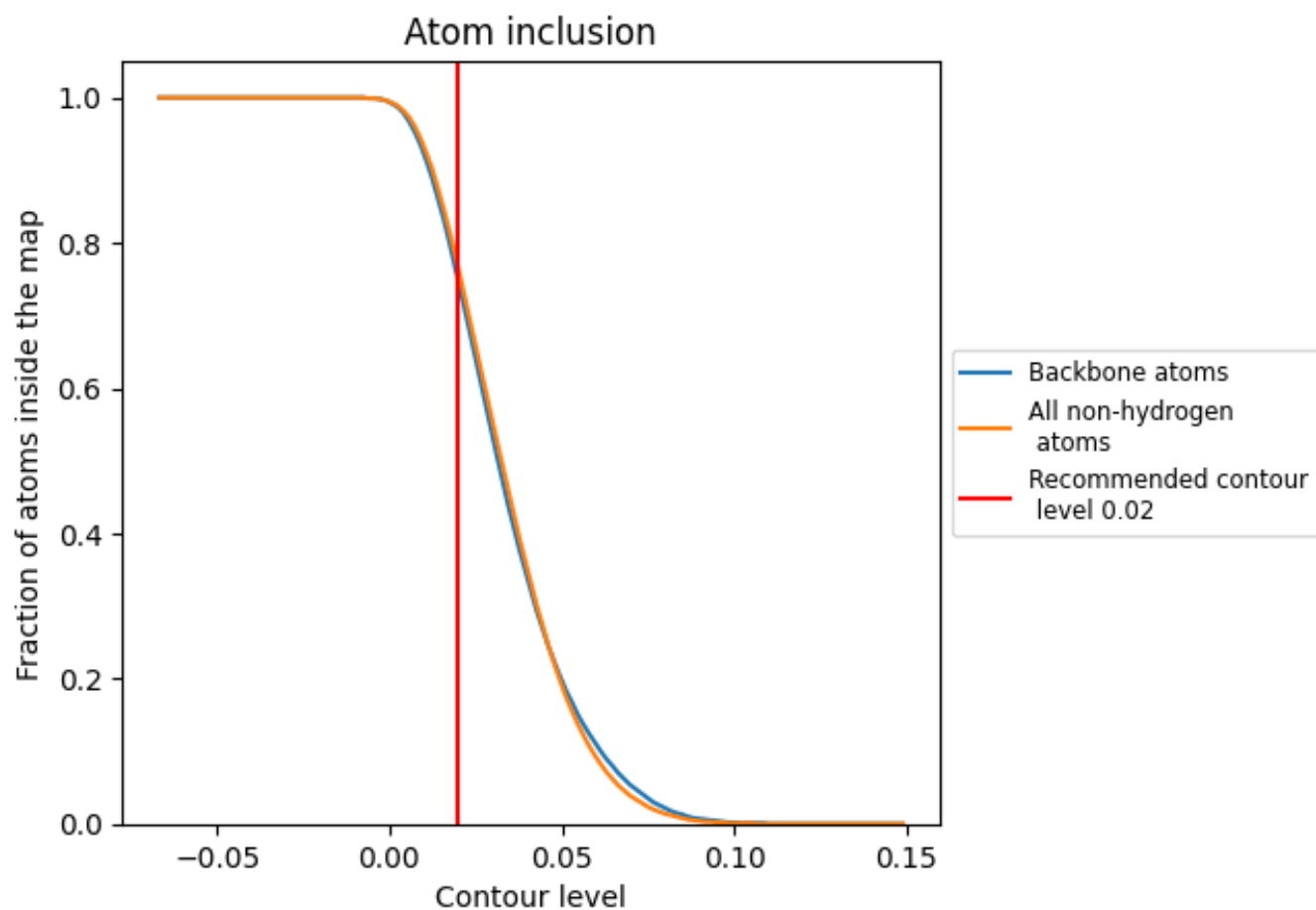
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7650	 0.5170
A	 0.8030	 0.5710
B	 0.7590	 0.5310
C	 0.7770	 0.5430
D	 0.8550	 0.5510
E	 0.9530	 0.5950
F	 0.7520	 0.5090
G	 0.6690	 0.4730
H	 0.7890	 0.5430
I	 0.6550	 0.4930
J	 0.6830	 0.5080
K	 0.7530	 0.5200
L	 0.7130	 0.5080
M	 0.7050	 0.4980
N	 0.7490	 0.5310
O	 0.8480	 0.5680
P	 0.7960	 0.5420
Q	 0.7780	 0.5510
R	 0.7910	 0.5480
S	 0.7110	 0.5020
S2	 0.8250	 0.5270
SA	 0.6690	 0.4920
SB	 0.6600	 0.5040
SC	 0.6890	 0.5100
SD	 0.5400	 0.4490
SE	 0.6470	 0.4970
SF	 0.6070	 0.4620
SG	 0.5020	 0.4070
SH	 0.4950	 0.4080
SI	 0.6050	 0.4500
SJ	 0.6350	 0.4690
SK	 0.5780	 0.4440
SL	 0.6350	 0.4970
SM	 0.1990	 0.2760
SN	 0.7010	 0.5180

















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Chain	Atom inclusion	Q-score
SO	 0.6720	 0.5010
SP	 0.6470	 0.4870
SQ	 0.6310	 0.4750
SR	 0.5550	 0.4360
SS	 0.6470	 0.4780
ST	 0.6820	 0.4940
SU	 0.5090	 0.4390
SV	 0.6740	 0.5050
SW	 0.7450	 0.5410
SX	 0.7140	 0.5250
SY	 0.5830	 0.4490
SZ	 0.5510	 0.4370
Sa	 0.7160	 0.5100
Sb	 0.6150	 0.4880
Sc	 0.5100	 0.4360
Sd	 0.7530	 0.5100
Se	 0.5630	 0.4540
Sf	 0.2420	 0.3010
Sg	 0.4400	 0.3760
T	 0.8050	 0.5430
U	 0.7610	 0.5260
V	 0.6350	 0.4560
W	 0.7630	 0.5510
X	 0.7700	 0.5350
Y	 0.7500	 0.5310
Z	 0.7550	 0.5230
a	 0.7290	 0.5190
b	 0.8050	 0.5580
c	 0.6690	 0.4850
d	 0.6610	 0.4840
e	 0.7220	 0.5230
f	 0.7960	 0.5550
g	 0.8400	 0.5610
h	 0.7200	 0.5240
i	 0.7190	 0.5120
j	 0.6780	 0.4860
k	 0.8480	 0.5720
l	 0.6120	 0.4730
m	 0.7750	 0.5440
n	 0.7930	 0.5320
o	 0.7170	 0.5130
p	 0.7060	 0.5150

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Chain	Atom inclusion	Q-score
q	 0.7550	 0.5420
r	 0.7710	 0.5300
t	 0.8450	 0.5350
u	 0.5430	 0.4010
v	 0.6080	 0.4040
w	 0.8830	 0.5620
y	 0.1840	 0.3040