



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 09:29 pm BST

PDB ID : 6GQV / pdb_00006gqv
EMDB ID : EMD-0049
Title : Cryo-EM reconstruction of yeast 80S ribosome in complex with mRNA, tRNA and eEF2 (GMPPCP)
Authors : Pellegrino, S.; Yusupov, M.; Yusupova, G.; Hashem, Y.
Deposited on : 2018-06-08
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

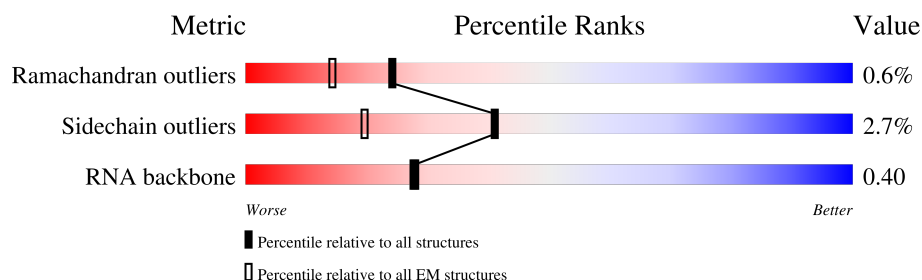
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



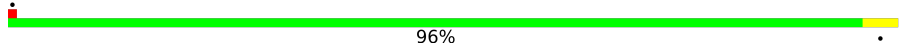

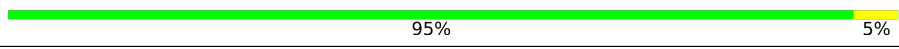
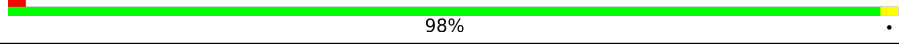
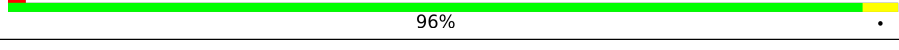
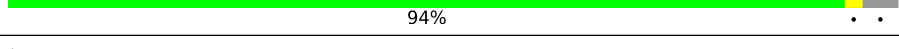
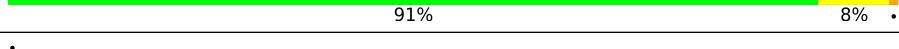
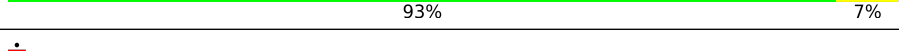
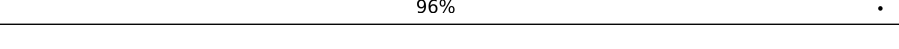
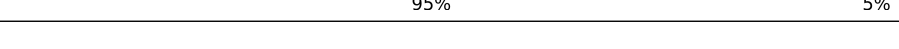
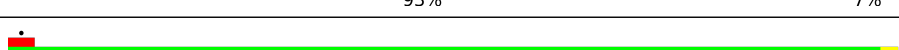
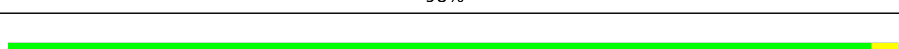
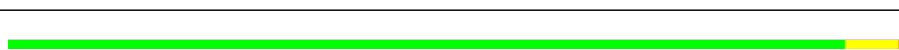
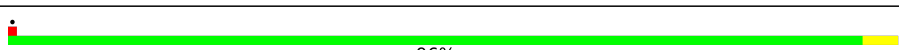
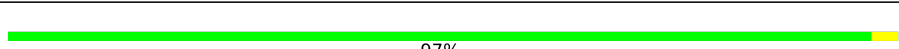
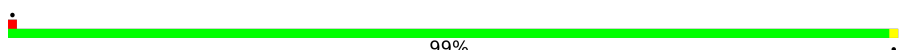

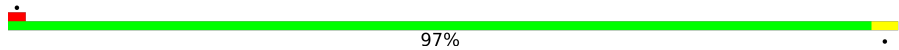
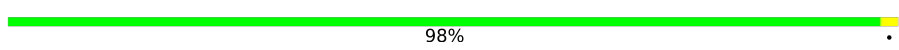
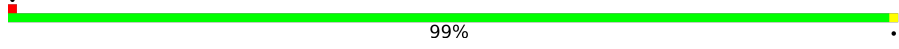
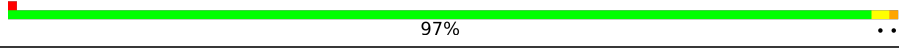
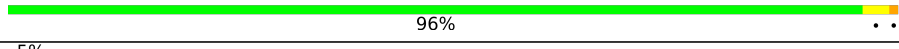
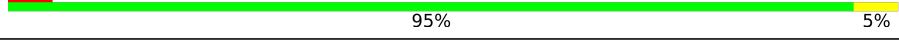
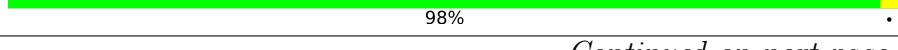

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1	3396	
2	3	121	
3	4	158	
4	P0	189	
5	P2	94	
6	A	252	
7	B	386	
8	C	361	

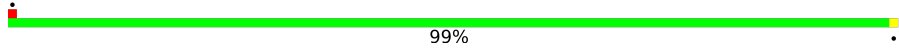
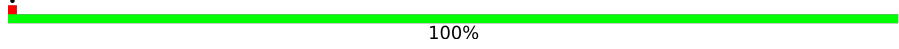
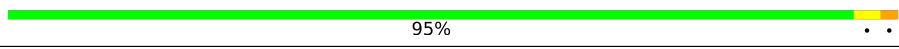
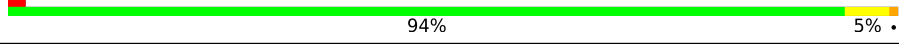
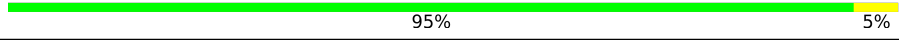
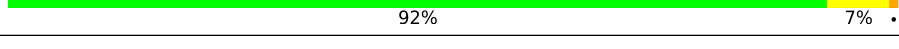
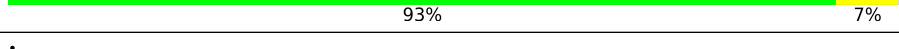
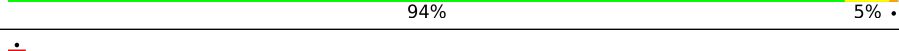
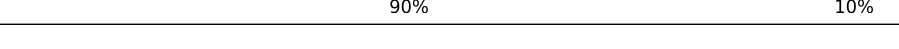
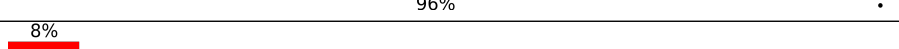
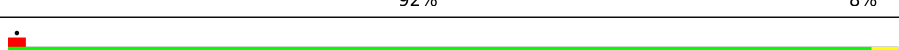
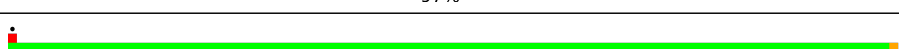

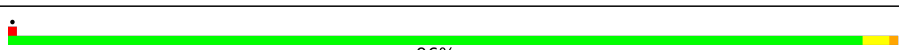
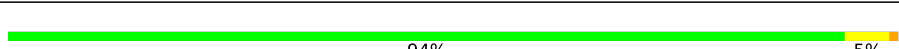

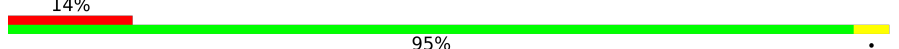
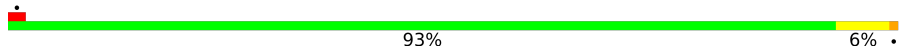
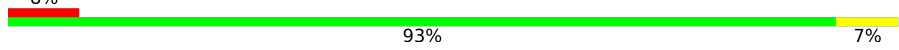

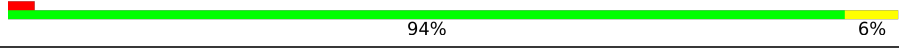
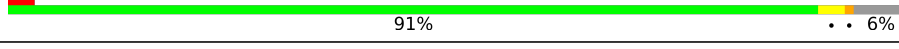
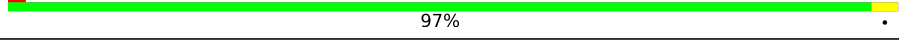


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Mol	Chain	Length	Quality of chain
9	D	296	
10	E	175	
11	F	222	
12	G	233	
13	H	191	
14	I	220	
15	J	169	
16	L	193	
17	M	136	
18	N	203	
19	O	197	
20	P	183	
21	Q	185	
22	R	188	
23	S	172	
24	T	159	
25	U	100	
26	V	136	
27	W	62	
28	X	121	
29	Y	126	
30	Z	135	
31	a	148	
32	b	58	
33	c	97	

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Mol	Chain	Length	Quality of chain
34	d	109	
35	e	127	
36	f	106	
37	g	112	
38	h	119	
39	i	99	
40	j	87	
41	k	77	
42	l	50	
43	m	52	
44	n	25	
45	o	105	
46	p	91	
47	2	1797	
48	q	206	
49	r	214	
50	s	217	
51	t	223	
52	u	260	
53	v	206	
54	w	223	
55	x	184	
56	y	199	
57	z	185	
58	AA	105	

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Mol	Chain	Length	Quality of chain
59	AB	153	
60	AC	124	
61	AD	150	
62	AE	127	
63	AF	124	
64	AG	141	
65	AH	125	
66	AI	145	
67	AJ	143	
68	AK	107	
69	AL	87	
70	AM	129	
71	AN	144	
72	AO	134	
73	AP	70	
74	AQ	97	
75	AR	81	
76	AS	63	
77	AT	53	
78	AU	60	
79	AV	318	
80	AW	37	
81	AX	837	
82	AY	76	
83	AZ	7	

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Mol	Chain	Length	Quality of chain
84	BA	204	<div><div></div><div>17%</div><div>94%</div><div>5%</div></div>

2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 212058 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3223	Total	C	N	O	P	0	0
			68931	30790	12416	22502	3223		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 4 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P0	189	Total	C	N	O	S	0	0
			1473	942	257	270	4		

- Molecule 5 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P2	94	Total	C	N	O	S	0	0
			723	448	138	135	2		

- Molecule 6 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 12 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	211	Total	C	N	O	S	0	0
			1705	1083	322	294	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	193	Total	C	N	O	S	0	0
			1543	962	315	266			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 19 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	183	Total	C	N	O	S	0	0
			1420	882	281	257			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	188	Total	C	N	O		0	0
			1521	935	326	260			

- Molecule 23 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	100	Total	C	N	O		0	0
			796	516	131	149			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	136	Total	C	N	O	S	0	0
			997	625	186	179	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	62	Total	C	N	O	S	0	0
			513	330	101	81	1		

- Molecule 28 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	126	Total	C	N	O		0	0
			993	625	192	176			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 31 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	58	Total	C	N	O		0	0
			462	289	100	73			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 36 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
41	k	77	Total	C	N	O	0	0
			612	391	115	106		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 45 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 46 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	1776	Total	C	N	O	P	0	0
			37845	16918	6702	12449	1776		

- Molecule 48 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	206	Total	C	N	O	S	0	0
			1577	1014	278	283	2		

- Molecule 49 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 50 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 51 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 52 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 54 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	223	Total	C	N	O	S	0	0
			1790	1123	346	318	3		

- Molecule 55 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	x	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 56 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	y	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 57 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	z	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 58 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AA	96	Total	C	N	O	S	0	0
			772	499	126	145	2		

- Molecule 59 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AB	153	Total	C	N	O	S	0	0
			1220	780	231	206	3		

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AC	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 61 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AD	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 62 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AF	124	Total	C	N	O	S	0	0
			977	622	182	166	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AG	141	Total	C	N	O		0	0
			1105	708	203	194			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AH	120	Total	C	N	O	S	0	0
			926	577	177	170	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AI	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AJ	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AK	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AL	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 70 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AM	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AN	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AO	134	Total	C	N	O		0	0
			1073	676	208	189			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AP	70	Total	C	N	O		0	0
			563	360	104	99			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AQ	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AR	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AS	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AT	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AU	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AV	318	Total	C	N	O	S	0	0
			2437	1541	418	470	8		

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AW	37	Total	C	N	O	S	0	0
			287	177	57	49	4		

- Molecule 81 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AX	837	Total	C	N	O	S	0	0
			6523	4143	1120	1231	29		

- Molecule 82 is a RNA chain called Transfer RNA - Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	AY	76	Total	C	N	O	P	0	0
			1626	725	293	532	76		

- Molecule 83 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	AZ	7	Total	C	N	O	P	0	0
			144	65	21	51	7		

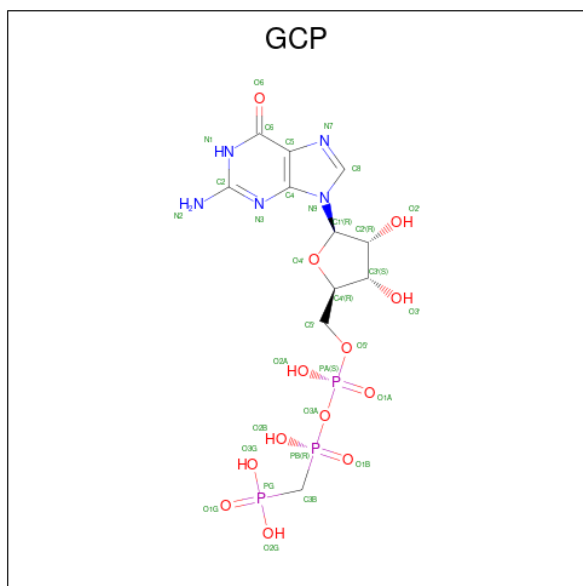
- Molecule 84 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	BA	204	Total	C	N	O	S	0	0
			1609	1031	279	290	9		

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

Mol	Chain	Residues	Atoms		AltConf
85	j	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	
85	AQ	1	Total	Zn	0
			1	1	
85	AR	1	Total	Zn	0
			1	1	
85	AT	1	Total	Zn	0
			1	1	
85	AW	1	Total	Zn	0
			1	1	

- Molecule 86 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

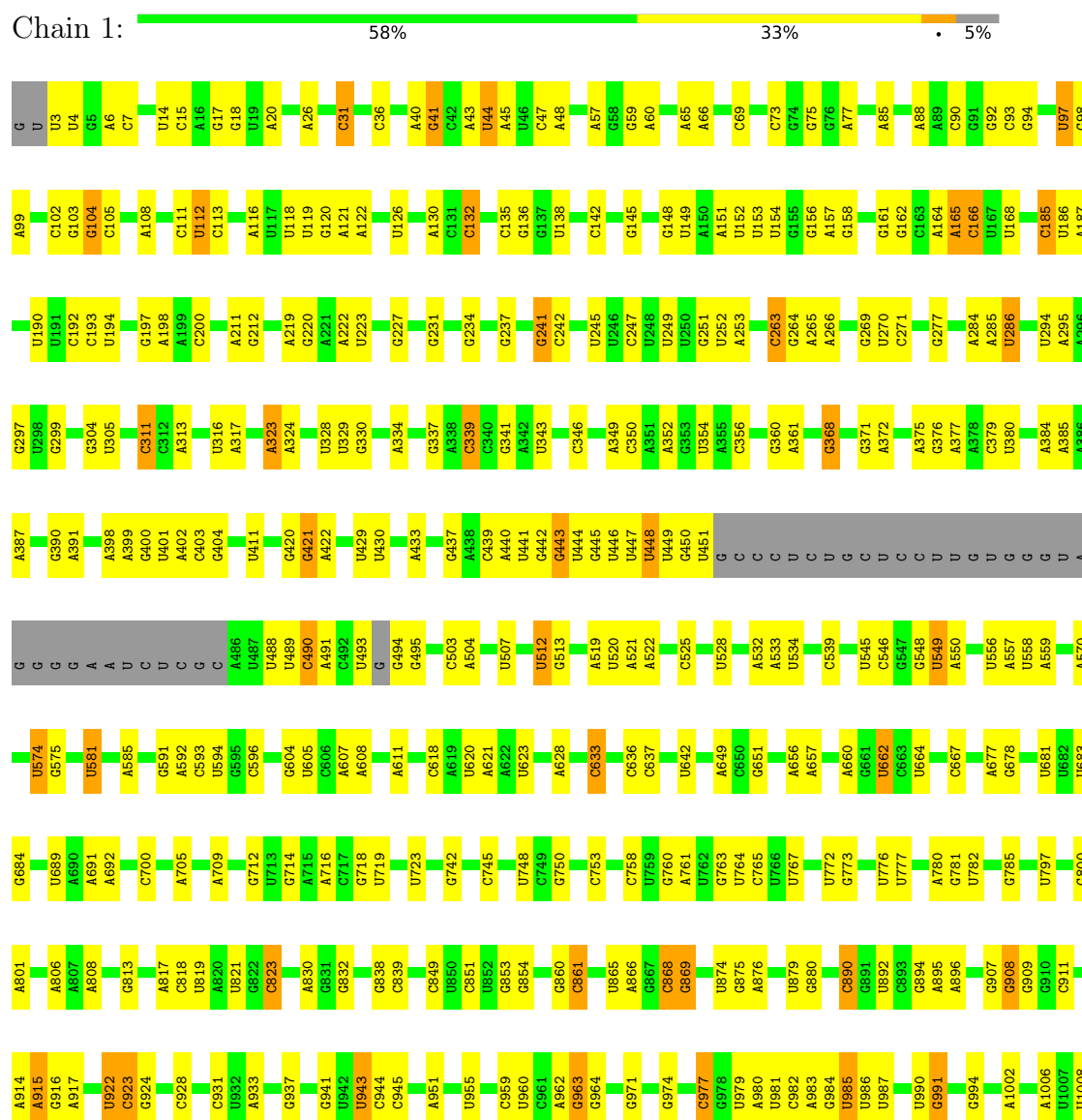


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
86	AX	1	32	11	5	13	3	0

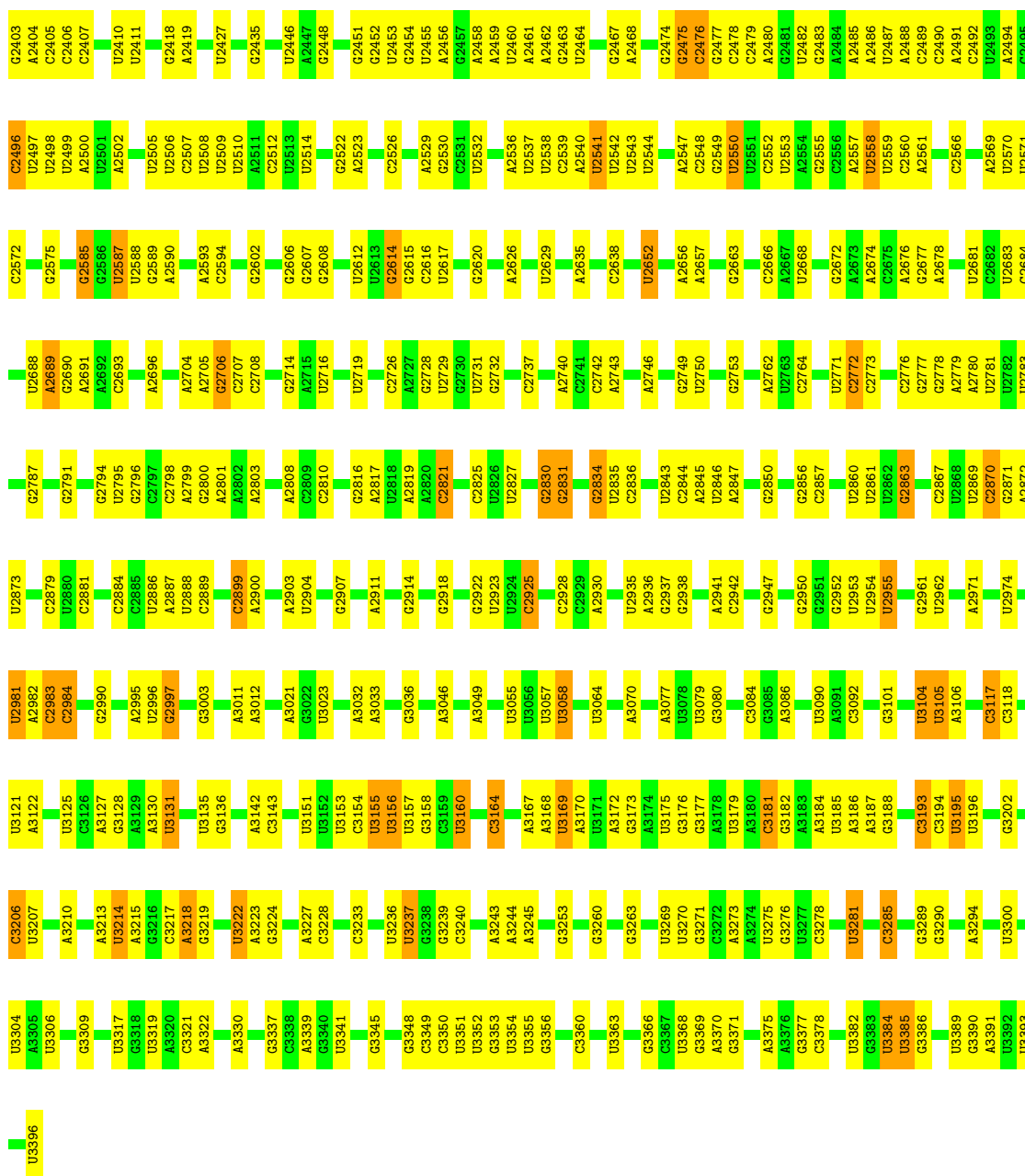
3 Residue-property plots

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: 25S ribosomal RNA



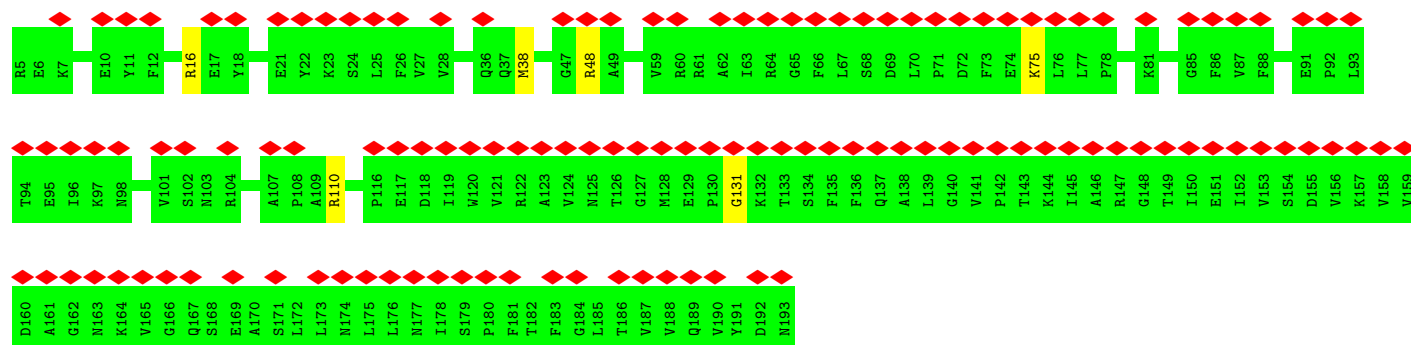
C2300	A2188	G1770	G1686	C1562	A1449	U1341	U1258	U1191	U1088	A1009
U2301	U2189	G1770	C1671	C1563	G1450	C1342	A1259	C1192	U1089	G1013
C2304	C2192	C1773	C1671	G1564	A1452	U1348	G1261	A1193	U1014	U1014
C2306	U2193	G1774	A1678	G1565	U1455	A1349	A1262	C1196	A1093	U1015
C2307	C2194	G1776	G1680	U1568	A1456	A1350	A1263	C1197	A1094	C1016
C2308	U2205	U1777	G1683	U1569	U1457	U1351	G1264	C1198	U1095	C1017
A2309	G2206	G1778	G1683	U1570	U1458	U1352	U1267	C1199	U1096	G1018
U2310	A2207	G1779	C1690	A1571	A1459	U1353	U1267	C1200	G1097	U1019
A2313	A2208	C1781	C1690	U1572	A1460	A1354	A1271	A1202	A1098	G1020
U2314	C2101	G1784	U1702	G1573	G1466	G1356	C1272	A1203	A1099	U1022
G2315	U2102	G1784	U1703	A1575	G1466	G1357	U1275	G1206	G1023	U1022
U2318	A2213	C1788	A1704	G1576	C1469	A1362	C1275	G1206	G1024	G1024
A2324	A2214	C1788	U1705	C1579	U1470	A1363	C1279	G1209	A1025	A1025
A2325	A2215	C1788	C1706	A1580	U1470	C1364	C1280	U1210	A1026	A1026
C2333	G2221	C1793	G1711	C1581	A1482	G1370	G1281	U1211	G1115	A1027
U2334	A2222	G1794	G1712	C1582	U1483	G1370	G1282	U1212	G1116	U1028
A2335	A2223	U1795	G1713	A1583	U1484	G1374	G1283	A1212	G1117	G1029
U2336	A2224	G1796	G1714	U1584	G1485	G1374	G1284	U1215	A1030	A1030
C2339	U2225	A1797	A1715	A1587	A1490	G1375	G1285	C1216	G1127	C1031
C2347	C2231	A1907	U1716	A1588	A1491	A1386	A1286	U1217	U1128	C1032
A2348	G2236	C1917	G1718	A1589	C1496	A1390	A1287	A1218	U1129	U1033
U2349	A2243	U1724	U1724	A1593	C1502	C1391	A1291	U1219	A1130	U1034
C2350	A2243	U1724	U1724	C1596	G1507	C1392	C1292	U1220	G1131	G1035
U2351	A2243	U1724	U1724	C1597	C1508	A1393	G1295	A1221	A1136	A1036
A2352	G2246	U1820	G1728	C1597	C1508	A1394	G1295	A1222	C1137	C1037
C2359	G2249	U1821	G1730	G1604	U1511	C1397	A1301	A1223	C1141	C1038
A2362	A2256	U1821	A1731	U1605	U1512	U1398	A1302	A1224	G1142	U1042
C2362	C2257	U1837	G1736	U1606	A1513	A1399	A1303	A1225	G1143	U1043
C2366	U2260	G1838	U1737	U1607	G1514	G1400	A1304	A1226	A1143	A1047
A2372	C2265	U1839	U1739	C1608	A1515	U1405	G1306	G1231	U1151	U1048
A2373	C2265	U1840	C1738	A1613	C1516	A1406	A1307	G1232	U1050	C1049
C2374	U2148	A1841	U1739	C1614	U1523	C1411	A1308	G1233	U1051	U1051
G2375	U2148	A1842	U1740	U1620	A1524	C1416	U1309	G1234	U1052	U1052
C2378	A2270	C1843	G1748	A1621	U1526	U1416	G1311	U1235	G1059	G1059
A2271	A2271	C1846	A1749	U1629	U1533	G1417	G1312	G1236	U1060	U1060
A2386	G2272	A1847	A1750	U1632	U1533	A1418	G1313	G1237	A1061	A1061
A2387	G2273	A1850	G1751	A1632	G1536	A1419	C1316	C1238	A1064	A1064
U2388	U2274	G1851	G1753	C1633	U1546	U1425	A1317	A1244	A1065	A1065
C2389	A2281	U1855	C1755	A1642	A1546	G1434	G1320	A1245	U1067	C1068
A2390	U2282	G1863	C1756	A1643	C1551	G1434	G1321	G1246	G1072	G1072
C2391	G2283	A1864	U1760	A1644	C1551	C1437	U1325	U1247	C1076	C1076
C2392	U2175	A1865	C1761	U1645	U1554	U1438	U1331	G1248	A1079	A1079
G2393	C2284	C1866	U1762	G1646	U1555	A1441	A1332	G1249	A1080	A1080
U2397	U2286	U1867	U1763	A1647	C1557	U1442	A1337	A1252	U1081	U1081
A2398	G2288	G1868	U1764	A1654	A1558	U1446	A1338	U1253	U1082	U1082
A2401	U2298	U1871	U1765	A1655	A1559	G1447	C1339	C1254	G1083	G1083
A2402	A2299	C1872	G1767	C1657	G1560	U1448	G1340	C1257	A1084	A1084
									A1085	A1085





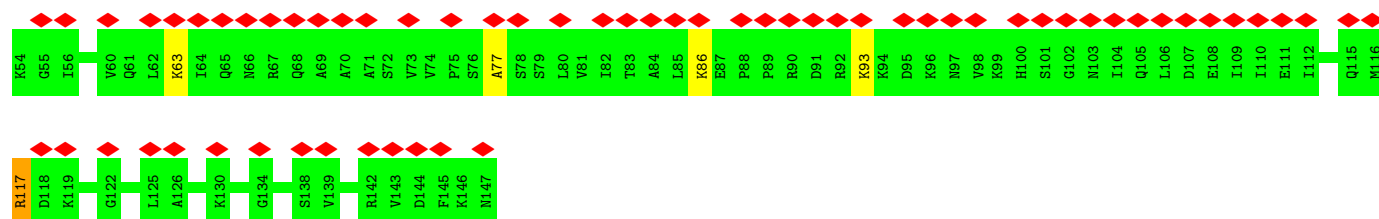
• Molecule 4: 60S acidic ribosomal protein P0

Chain P0: 67% 97%



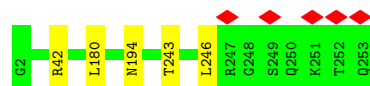
• Molecule 5: 60S ribosomal protein L12-A

Chain P2: 66% 95%



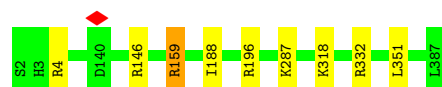
• Molecule 6: 60S ribosomal protein L2-A

Chain A: 98%



• Molecule 7: 60S ribosomal protein L3

Chain B: 98%



• Molecule 8: 60S ribosomal protein L4-A

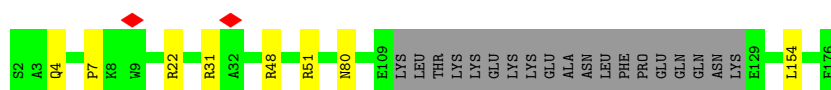
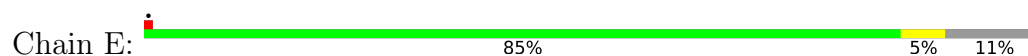
Chain C: 97%



- Molecule 9: 60S ribosomal protein L5



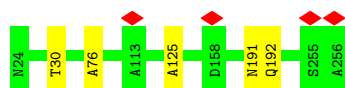
- Molecule 10: 60S ribosomal protein L6-A



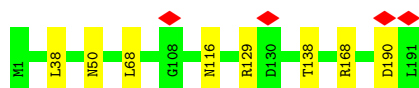
- Molecule 11: 60S ribosomal protein L7-A



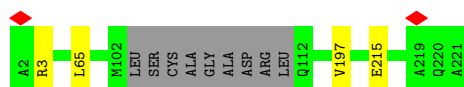
- Molecule 12: 60S ribosomal protein L8-A



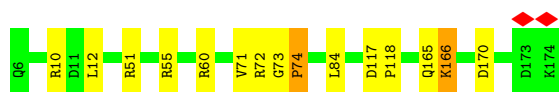
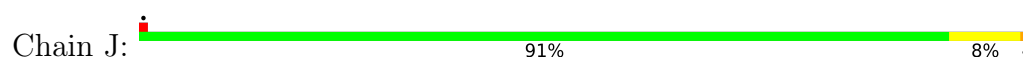
- Molecule 13: 60S ribosomal protein L9-A



- Molecule 14: 60S ribosomal protein L10



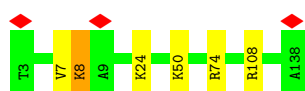
- Molecule 15: 60S ribosomal protein L11-B



- Molecule 16: 60S ribosomal protein L13-A



- Molecule 17: 60S ribosomal protein L14-A



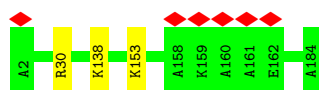
- Molecule 18: 60S ribosomal protein L15-A



- Molecule 19: 60S ribosomal protein L16-A



- Molecule 20: 60S ribosomal protein L17-A



- Molecule 21: 60S ribosomal protein L18-A



- Molecule 22: 60S ribosomal protein L19-A

Chain R:  94% 6%



- Molecule 23: 60S ribosomal protein L20-A

Chain S:  96%



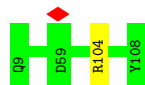
- Molecule 24: 60S ribosomal protein L21-A

Chain T:  97%



- Molecule 25: 60S ribosomal protein L22-A

Chain U:  99%



- Molecule 26: 60S ribosomal protein L23-A

Chain V:  97%



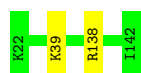
- Molecule 27: 60S ribosomal protein L24-A

Chain W:  97%



- Molecule 28: 60S ribosomal protein L25

Chain X:  98%



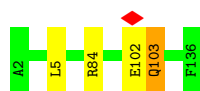
- Molecule 29: 60S ribosomal protein L26-A

Chain Y:  99%



- Molecule 30: 60S ribosomal protein L27-A

Chain Z:  97%



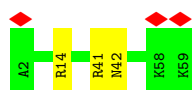
- Molecule 31: 60S ribosomal protein L28

Chain a:  96%



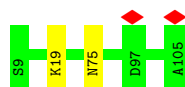
- Molecule 32: 60S ribosomal protein L29

Chain b:  5% 95% 5%



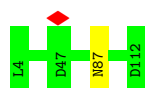
- Molecule 33: 60S ribosomal protein L30

Chain c:  98%



- Molecule 34: 60S ribosomal protein L31-A

Chain d:  99%



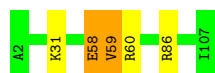
- Molecule 35: 60S ribosomal protein L32

Chain e:  100%



- Molecule 36: 60S ribosomal protein L33-A

Chain f:  95%



- Molecule 37: 60S ribosomal protein L34-A

Chain g:  94% 5%




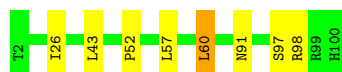
- Molecule 38: 60S ribosomal protein L35-A

Chain h:  95% 5%



- Molecule 39: 60S ribosomal protein L36-A

Chain i:  92% 7%



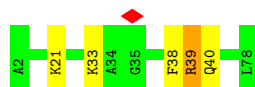
- Molecule 40: 60S ribosomal protein L37-A

Chain j:  93% 7%

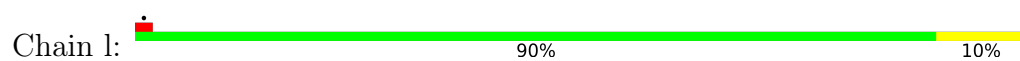


- Molecule 41: 60S ribosomal protein L38

Chain k:  94% 5%



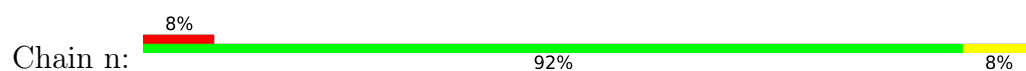
- Molecule 42: 60S ribosomal protein L39



- Molecule 43: Ubiquitin-60S ribosomal protein L40



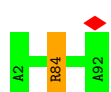
- Molecule 44: 60S ribosomal protein L41-B



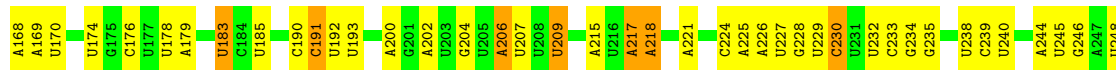
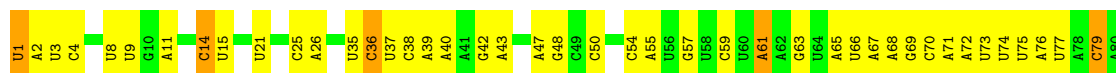
- Molecule 45: 60S ribosomal protein L42-A



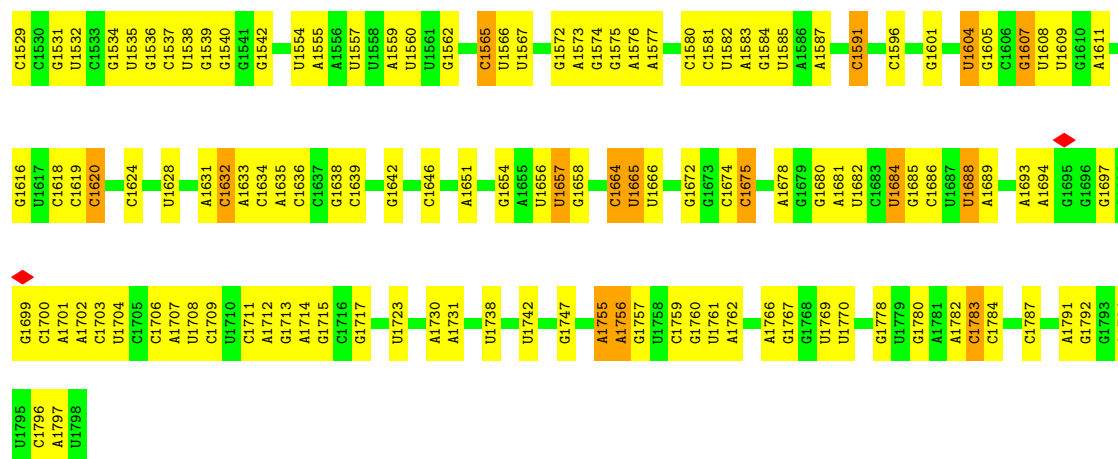
- Molecule 46: 60S ribosomal protein L43-A



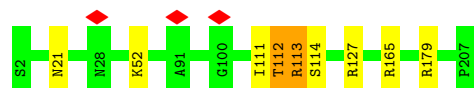
- Molecule 47: 18S ribosomal RNA



U1443	A1444	G1299	C1162	U	U960	U841	A760	G687	G597	G509	G430	A333	U249
A1445	G1445	A1300	A1163	U	U964	C842	A760	C691	U602	G510	C431	G334	C250
A1446	G1446	U1301	G1164	U	U965	U843	G765	C692	A606	A511	G432	G337	A256
C1447	G1447	U1306	G1165	U	A966	A844	U766	U695	G610	A515	C433	C338	C257
G1448	G1448	C1306	A1166	A	U966	G845	U767	U694	U611	G516	G434	C339	C258
U1449	A1382	U1381	U1167	A1062	G980	C849	C768	U695	U611	U517	A436	U345	U259
U1450	A1383	U1310	G1168	C1070	U981	A850	C775	C696	U611	A518	A437	U345	U260
C1451	G1384	U1311	G1169	U1071	G986	U851	G776	C697	A620	C519	A438	C351	U261
G1454	G1385	A1312	A1171	A1076	U986	C852	C777	U698	A619	U522	U439	U352	U262
G1455	A1313	U1314	C1173	A1076	C990	U853	U778	U699	A620	A525	U440	A352	A266
C1456	G1387	U1315	G1174	U1080	G991	A859	U779	C700	A623	A525	A441	A359	A266
C1457	A1388	U1315	C1174	A1081	A992	U860	A780	G702	A624	U532	C444	A360	C270
G1458	U1390	U1320	G1175	A1082	A993	A863	U781	U705	C627	U533	A445	A361	A271
A1460	U1391	A1321	G1176	C1082	U1000	U864	U782	A706	A630	A534	A446	G365	U272
C1461	U1392	A1326	G1177	G1083	A1001	U873	C784	C708	A635	A535	U447	A366	G274
G1462	G1394	C1327	U1181	A1091	G1002	U873	A789	C709	A635	C536	A452	A370	C275
C1463	G1395	G1328	U1182	A1092	A1003	A881	U790	C710	A636	G537	U453	A370	C276
G1466	C1332	C1332	A1183	C1096	A1004	U891	U790	U710	A636	A538	U454	G373	U277
C1467	U1397	U1397	A1184	U1097	A1005	G895	U791	U711	U638	G539	C455	G373	U278
U1468	C1398	U1398	U1185	U1098	C1006	U895	U792	G712	U639	G540	C455	G373	U279
G1469	C1399	C1399	U1186	U1099	C1007	A898	A793	A713	U640	A541	A460	C376	U280
A1471	A1400	U1335	U1186	G1100	C1010	U903	U794	G714	G641	A542	U463	C376	G281
C1482	G1407	A1336	G1113	G1113	G1011	U904	U795	U715	G642	C543	A464	U379	C282
G1486	G1408	C1337	U1115	U1115	G1011	G904	A799	C716	A545	A544	A465	U380	U283
A1487	G1409	A1344	U1116	U1117	C1021	U905	A800	C717	A546	A545	U466	A387	G287
G1488	U1412	A1345	G1118	G1118	C1022	A906	U801	U718	U547	U546	U467	G388	A288
U1413	G1413	U1346	U1119	G1119	G1015	U909	A806	U719	C653	G548	A468	G389	U289
U1414	U1414	A1347	G1201	G1201	C1016	U909	A806	U719	C653	G548	A468	G389	U289
U1415	U1415	G1348	G1202	G1202	C1016	U909	A806	U719	C653	G548	A468	G389	U289
A1492	G1416	G1349	G1203	G1203	C1016	U909	A806	U719	C653	G548	A468	G389	U289
A1493	G1416	G1350	G1204	G1204	C1016	U909	A806	U719	C653	G548	A468	G389	U289
G1506	G1419	G1352	G1205	G1205	A1020	U910	A810	U725	C654	G557	U476	A400	A299
G1507	G1420	U1353	U1206	U1206	C1021	U911	A811	U726	G655	U558	U477	A401	A299
U1508	A1421	G1354	C1207	C1207	A1027	U912	G815	U727	G656	C554	A478	A402	A300
C1509	G1425	C1355	U1208	U1208	U1029	U920	C818	G728	U657	C554	C479	A403	A301
U1510	C1426	U1356	G1273	G1273	U1030	U921	G819	G730	C658	C557	U482	A404	U302
U1511	A1427	A1357	C1274	C1274	U1031	G922	U820	C731	C658	C557	U482	A404	U302
G1526	G1428	U1360	U1276	U1276	G1032	A924	U821	G732	C	C572	G486	C411	C305
A1515	A1429	U1361	C1215	C1215	A1036	U928	G824	G733	G	C572	G487	C412	U306
A1516	U1362	G1284	C1216	C1216	C1037	U928	U825	U738	U	C572	G488	C413	U306
U1517	U1363	U1285	G1217	G1217	U1038	C931	U827	G739	U	C572	C489	C414	C309
C1518	G1364	U1286	A1218	A1218	A1039	U932	U831	A740	U	C572	C490	C415	A312
U1433	U1433	A1287	C1220	C1220	G1040	A933	U832	C741	U	C572	C491	C416	A313
U1434	U1434	G1288	A1221	A1221	A1043	U935	U833	U742	G676	C577	C491	A417	U313
G1435	G1367	U1289	C1156	C1156	A1043	U935	U834	U743	G677	C577	C491	A417	U313
A1436	U1290	U1290	G1157	G1157	G1051	A944	U835	U744	A678	C577	C491	A417	U313
U1524	U1370	U1293	C1158	C1158	U1052	U945	U836	U744	A678	C577	C491	A417	U313
A1525	A1371	U1293	C1159	C1159	G1053	A951	U839	C747	U679	A592	A506	C424	C321
C1527	C1440	U1226	A1160	A1160	U1053	A951	U839	U748	U680	A593	A507	A425	G322
U1528	U1227	U1227	C1161	C1161	U1056	A951	U840	U749	C686	A594	U507	G426	G322



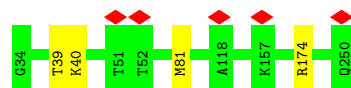
- Molecule 48: 40S ribosomal protein S0-A



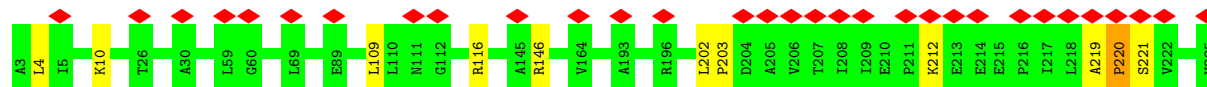
- Molecule 49: 40S ribosomal protein S1-A



- Molecule 50: 40S ribosomal protein S2



- Molecule 51: 40S ribosomal protein S3

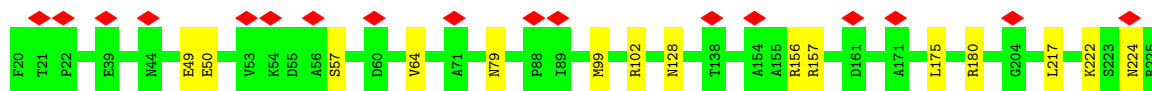
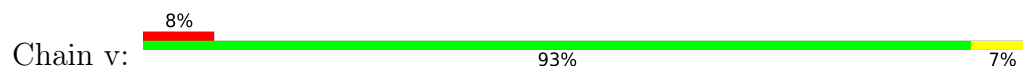


- Molecule 52: 40S ribosomal protein S4-A

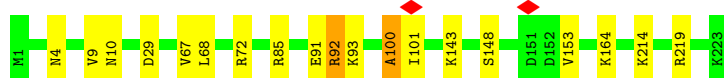




- Molecule 53: 40S ribosomal protein S5



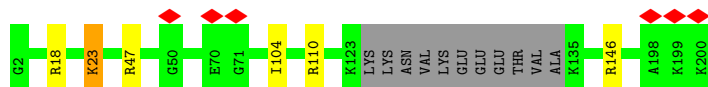
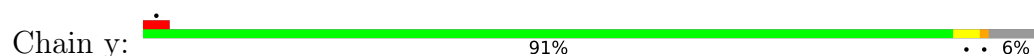
- Molecule 54: 40S ribosomal protein S6-A



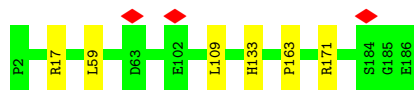
- Molecule 55: 40S ribosomal protein S7-A



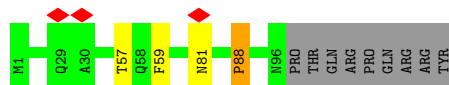
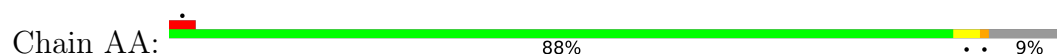
- Molecule 56: 40S ribosomal protein S8-A



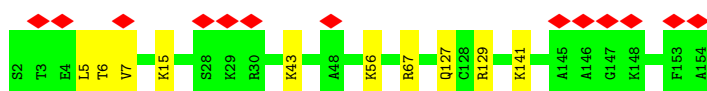
- Molecule 57: 40S ribosomal protein S9-A



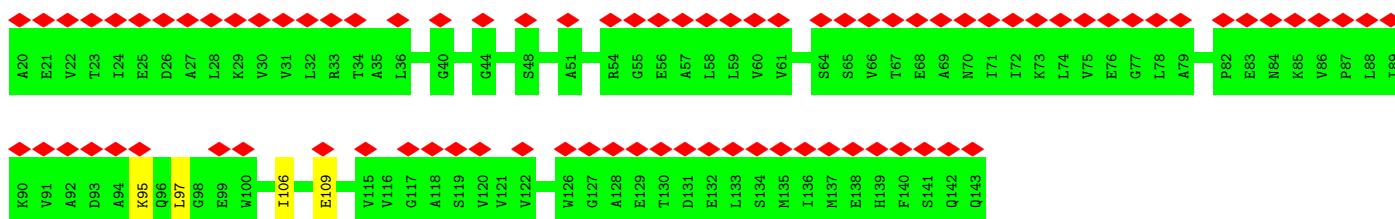
- Molecule 58: 40S ribosomal protein S10-A



- Molecule 59: 40S ribosomal protein S11-A



- Molecule 60: 40S ribosomal protein S12



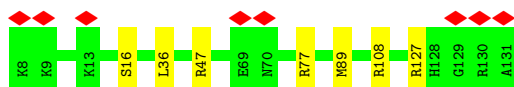
- Molecule 61: 40S ribosomal protein S13



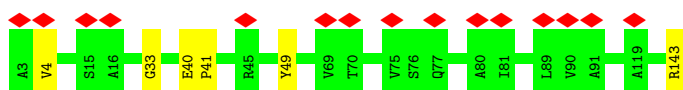
- Molecule 62: 40S ribosomal protein S14-B



- Molecule 63: 40S ribosomal protein S15

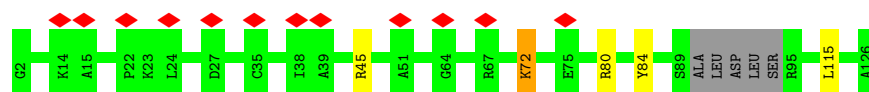


- Molecule 64: 40S ribosomal protein S16-A

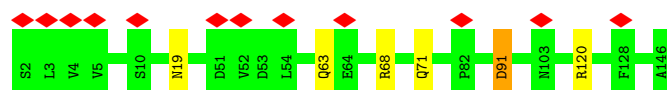


- Molecule 65: 40S ribosomal protein S17-B

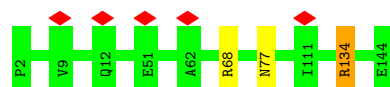




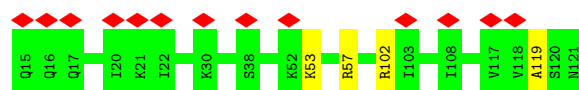
- Molecule 66: 40S ribosomal protein S18-A



- Molecule 67: 40S ribosomal protein S19-A



- Molecule 68: 40S ribosomal protein S20



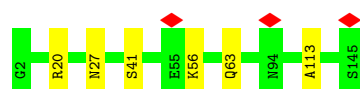
- Molecule 69: 40S ribosomal protein S21-A



- Molecule 70: 40S ribosomal protein S22-A



- Molecule 71: 40S ribosomal protein S23-A



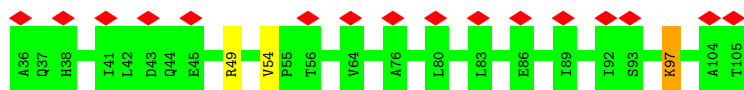
- Molecule 72: 40S ribosomal protein S24-A

Chain AO:  97%



- Molecule 73: 40S ribosomal protein S25-A

Chain AP:  23% 96%



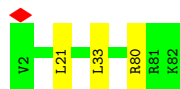
- Molecule 74: 40S ribosomal protein S26-B

Chain AQ:  94% 6%



- Molecule 75: 40S ribosomal protein S27-A

Chain AR:  96%



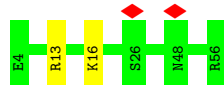
- Molecule 76: 40S ribosomal protein S28-A

Chain AS:  21% 97%



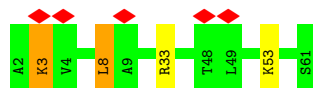
- Molecule 77: 40S ribosomal protein S29-A

Chain AT:  96%

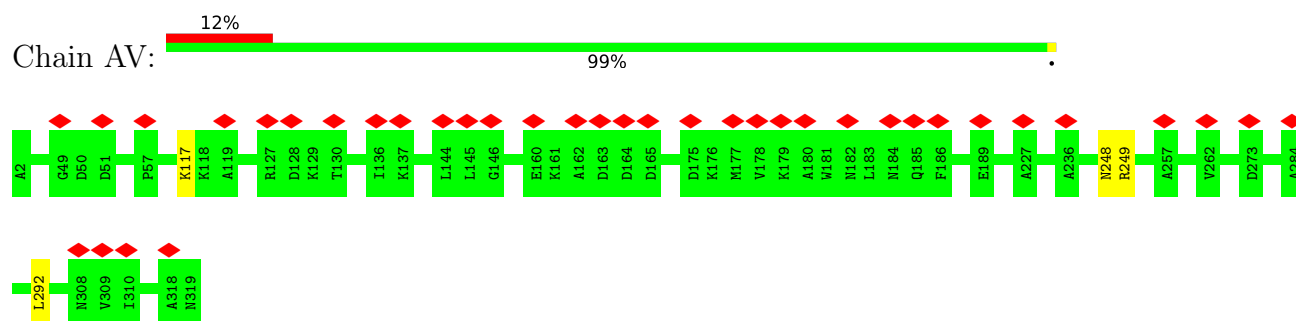


- Molecule 78: 40S ribosomal protein S30-A

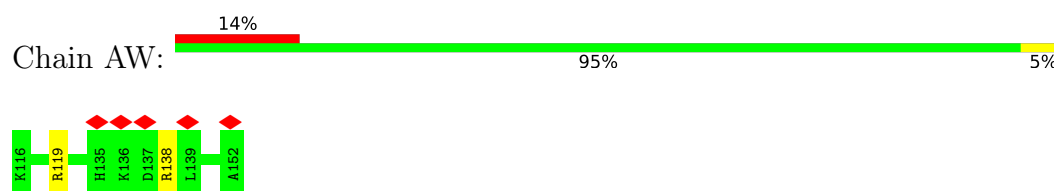
Chain AU:  8% 93%



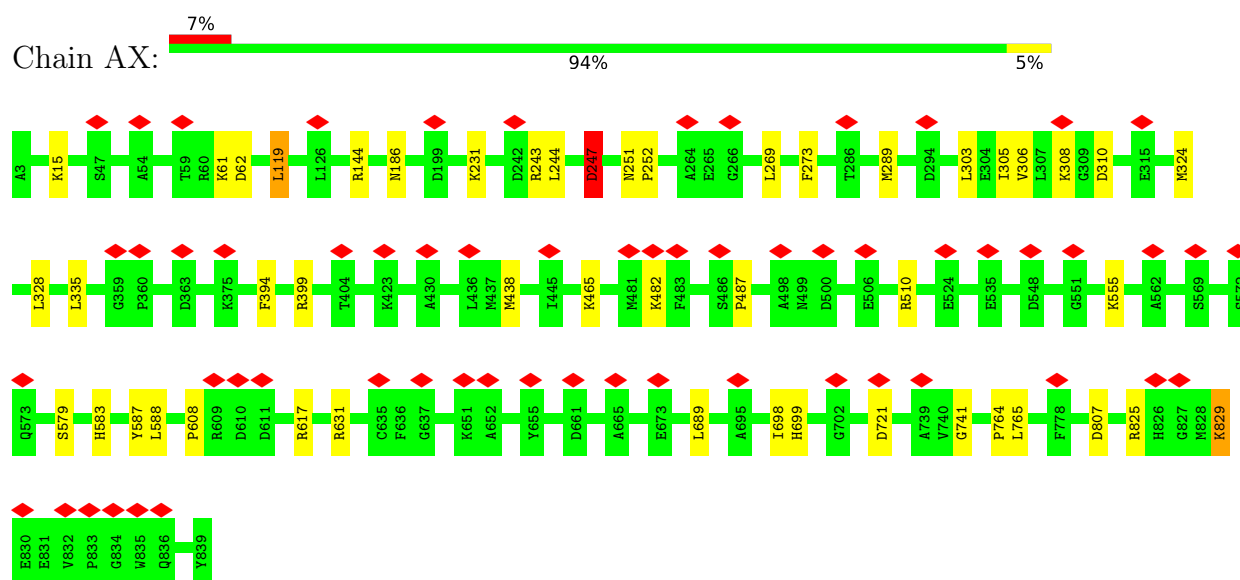
- Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein



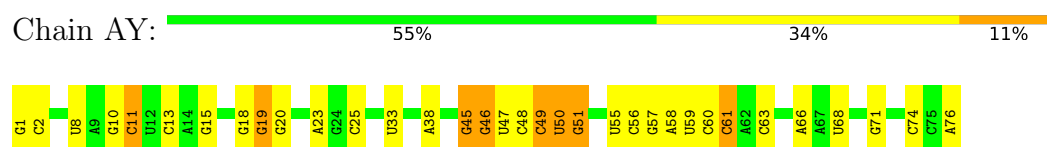
- Molecule 80: Ubiquitin-40S ribosomal protein S31



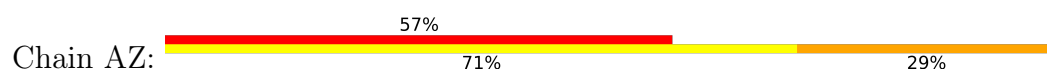
- Molecule 81: Elongation factor 2

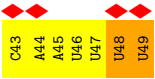


- Molecule 82: Transfer RNA - Phe

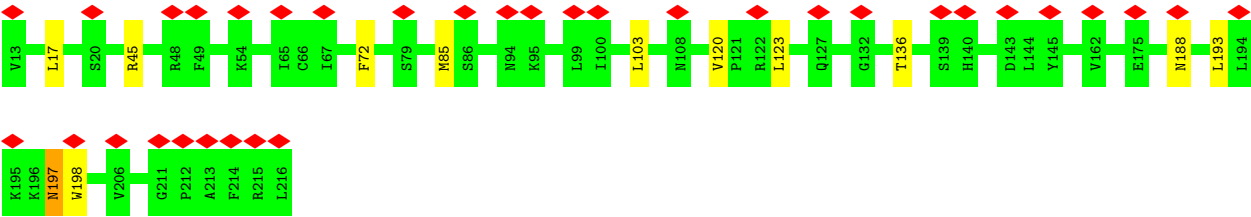


- Molecule 83: Messenger RNA





● Molecule 84: 60S ribosomal protein L1-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.306	Depositor
Minimum map value	-0.179	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.033	Depositor
Map size (\AA)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DDE, GCP, ZN

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	1	0.68	1/77157 (0.0%)	1.24	613/120295 (0.5%)
2	3	0.59	0/2883	1.18	20/4491 (0.4%)
3	4	0.67	0/3746	1.26	37/5832 (0.6%)
4	P0	0.32	0/1498	0.65	1/2025 (0.0%)
5	P2	0.34	0/728	0.78	2/975 (0.2%)
6	A	0.41	0/1948	0.71	2/2617 (0.1%)
7	B	0.37	0/3146	0.67	1/4228 (0.0%)
8	C	0.38	0/2800	0.68	1/3790 (0.0%)
9	D	0.35	0/2425	0.67	2/3271 (0.1%)
10	E	0.33	0/1260	0.66	0/1694
11	F	0.39	0/1821	0.68	0/2451
12	G	0.35	0/1836	0.64	1/2481 (0.0%)
13	H	0.37	0/1539	0.71	4/2073 (0.2%)
14	I	0.39	0/1741	0.64	0/2335
15	J	0.34	0/1374	0.74	1/1842 (0.1%)
16	L	0.36	0/1568	0.67	1/2106 (0.0%)
17	M	0.32	0/1068	0.62	0/1438
18	N	0.42	0/1757	0.67	1/2354 (0.0%)
19	O	0.40	0/1585	0.66	2/2128 (0.1%)
20	P	0.37	0/1443	0.62	0/1944
21	Q	0.37	0/1465	0.66	1/1965 (0.1%)
22	R	0.32	0/1538	0.67	3/2050 (0.1%)
23	S	0.39	0/1481	0.66	1/1990 (0.1%)
24	T	0.40	0/1300	0.62	0/1743
25	U	0.35	0/812	0.64	0/1099
26	V	0.41	0/1012	0.70	0/1362
27	W	0.36	0/525	0.65	1/696 (0.1%)
28	X	0.35	0/979	0.63	0/1321
29	Y	0.33	0/1004	0.65	1/1341 (0.1%)
30	Z	0.39	0/1118	0.66	1/1497 (0.1%)
31	a	0.37	0/1204	0.69	2/1612 (0.1%)
32	b	0.34	0/473	0.60	0/629

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.33	0/751	0.62	0/1008
34	d	0.40	0/897	0.68	0/1205
35	e	0.38	0/1041	0.64	0/1394
36	f	0.40	0/868	0.67	0/1168
37	g	0.38	0/890	0.72	1/1189 (0.1%)
38	h	0.32	0/978	0.70	1/1301 (0.1%)
39	i	0.36	0/778	0.73	2/1034 (0.2%)
40	j	0.38	0/696	0.72	0/923
41	k	0.32	0/618	0.79	1/826 (0.1%)
42	l	0.35	0/443	0.75	1/588 (0.2%)
43	m	0.36	0/423	0.63	0/562
44	n	0.34	0/234	0.67	0/300
45	o	0.37	0/860	0.71	0/1136
46	p	0.46	0/701	0.68	0/934
47	2	0.56	2/42328 (0.0%)	1.28	445/65955 (0.7%)
48	q	0.33	0/1617	0.69	0/2215
49	r	0.34	0/1735	0.81	5/2335 (0.2%)
50	s	0.32	0/1665	0.68	0/2263
51	t	0.32	0/1759	0.68	0/2368
52	u	0.33	0/2109	0.77	4/2839 (0.1%)
53	v	0.31	0/1629	0.74	3/2202 (0.1%)
54	w	0.34	0/1814	0.82	2/2425 (0.1%)
55	x	0.32	0/1506	0.74	1/2028 (0.0%)
56	y	0.33	0/1514	0.67	0/2021
57	z	0.33	0/1519	0.72	0/2035
58	AA	0.32	0/789	0.70	1/1067 (0.1%)
59	AB	0.37	0/1247	0.67	1/1681 (0.1%)
60	AC	0.28	0/898	0.69	1/1220 (0.1%)
61	AD	0.33	0/1215	0.72	1/1638 (0.1%)
62	AE	0.33	0/901	0.69	0/1217
63	AF	0.35	0/998	0.77	0/1341
64	AG	0.33	0/1125	0.71	0/1510
65	AH	0.32	0/935	0.71	0/1254
66	AI	0.31	0/1211	0.69	0/1628
67	AJ	0.30	0/1130	0.63	0/1517
68	AK	0.31	0/865	0.71	1/1169 (0.1%)
69	AL	0.36	0/693	0.82	1/935 (0.1%)
70	AM	0.34	0/1038	0.66	1/1395 (0.1%)
71	AN	0.38	0/1139	0.71	0/1518
72	AO	0.33	0/1087	0.63	0/1449
73	AP	0.34	0/571	0.75	0/768
74	AQ	0.34	0/782	0.77	0/1047
75	AR	0.30	0/620	0.79	2/838 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	AS	0.29	0/499	0.73	0/670
77	AT	0.36	0/452	0.65	0/600
78	AU	0.30	0/483	0.71	1/643 (0.2%)
79	AV	0.30	0/2490	0.69	0/3389
80	AW	0.29	0/292	0.65	0/390
81	AX	0.35	0/6626	0.78	12/8970 (0.1%)
82	AY	0.57	1/1818 (0.1%)	1.42	33/2831 (1.2%)
83	AZ	0.66	1/159 (0.6%)	1.65	5/244 (2.0%)
84	BA	0.33	0/1634	0.74	2/2195 (0.1%)
All	All	0.53	5/227304 (0.0%)	1.07	1227/333053 (0.4%)

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
4	P0	0	2
5	P2	0	1
7	B	0	1
8	C	0	1
9	D	0	4
10	E	0	2
11	F	0	2
12	G	0	3
14	I	0	3
15	J	0	6
16	L	0	2
17	M	0	2
18	N	0	1
19	O	0	3
22	R	0	1
23	S	0	2
30	Z	0	1
31	a	0	2
32	b	0	1
34	d	0	1
36	f	0	2
37	g	0	4
38	h	0	2
39	i	0	3
40	j	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	k	0	2
45	o	0	2
46	p	0	1
48	q	0	2
49	r	0	3
50	s	0	1
51	t	0	4
52	u	0	7
53	v	0	4
54	w	0	6
55	x	0	3
56	y	0	1
57	z	0	3
58	AA	0	2
59	AB	0	1
61	AD	0	2
62	AE	0	3
63	AF	0	2
64	AG	0	4
65	AH	0	1
66	AI	0	1
67	AJ	0	1
68	AK	0	2
69	AL	0	2
71	AN	0	2
73	AP	0	1
74	AQ	0	3
75	AR	0	1
76	AS	0	1
78	AU	0	1
80	AW	0	1
81	AX	0	15
84	BA	0	3
All	All	0	143

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	AY	1	G	OP3-P	-10.64	1.48	1.61
47	2	506	A	N9-C4	6.05	1.41	1.37
83	AZ	48	U	O3'-P	5.16	1.67	1.61
1	1	2149	A	N9-C4	-5.08	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	2	218	A	N9-C4	5.08	1.40	1.37

The worst 5 of 1227 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	94	U	C2-N3-C4	21.52	139.91	127.00
47	2	1706	C	N1-C2-O2	12.82	126.59	118.90
1	1	3155	U	N1-C2-O2	11.63	130.94	122.80
1	1	3155	U	C2-N1-C1'	11.51	131.52	117.70
47	2	94	U	N3-C4-C5	11.26	121.35	114.60

There are no chirality outliers.

5 of 143 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	B	159	ARG	Peptide
8	C	93	MET	Peptide
4	P0	16	ARG	Peptide
4	P0	38	MET	Peptide
5	P2	77	ALA	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P0	187/189 (99%)	145 (78%)	42 (22%)	0	100	100
5	P2	92/94 (98%)	64 (70%)	28 (30%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	250/252 (99%)	217 (87%)	33 (13%)	0	100	100
7	B	384/386 (100%)	335 (87%)	48 (12%)	1 (0%)	37	71
8	C	359/361 (99%)	305 (85%)	52 (14%)	2 (1%)	22	58
9	D	294/296 (99%)	248 (84%)	43 (15%)	3 (1%)	13	47
10	E	152/175 (87%)	137 (90%)	15 (10%)	0	100	100
11	F	220/222 (99%)	194 (88%)	25 (11%)	1 (0%)	25	61
12	G	231/233 (99%)	204 (88%)	27 (12%)	0	100	100
13	H	189/191 (99%)	168 (89%)	20 (11%)	1 (0%)	25	61
14	I	207/220 (94%)	178 (86%)	29 (14%)	0	100	100
15	J	167/169 (99%)	130 (78%)	34 (20%)	3 (2%)	7	36
16	L	191/193 (99%)	166 (87%)	23 (12%)	2 (1%)	13	47
17	M	134/136 (98%)	121 (90%)	12 (9%)	1 (1%)	19	55
18	N	201/203 (99%)	172 (86%)	29 (14%)	0	100	100
19	O	195/197 (99%)	171 (88%)	21 (11%)	3 (2%)	8	40
20	P	181/183 (99%)	161 (89%)	20 (11%)	0	100	100
21	Q	183/185 (99%)	165 (90%)	18 (10%)	0	100	100
22	R	186/188 (99%)	170 (91%)	16 (9%)	0	100	100
23	S	170/172 (99%)	151 (89%)	19 (11%)	0	100	100
24	T	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
25	U	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
26	V	134/136 (98%)	120 (90%)	14 (10%)	0	100	100
27	W	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
28	X	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
29	Y	124/126 (98%)	115 (93%)	9 (7%)	0	100	100
30	Z	133/135 (98%)	115 (86%)	17 (13%)	1 (1%)	16	53
31	a	146/148 (99%)	118 (81%)	25 (17%)	3 (2%)	5	33
32	b	56/58 (97%)	46 (82%)	10 (18%)	0	100	100
33	c	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
34	d	107/109 (98%)	95 (89%)	12 (11%)	0	100	100
35	e	125/127 (98%)	103 (82%)	22 (18%)	0	100	100
36	f	104/106 (98%)	90 (86%)	11 (11%)	3 (3%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	g	110/112 (98%)	98 (89%)	10 (9%)	2 (2%)	7	36
38	h	117/119 (98%)	100 (86%)	17 (14%)	0	100	100
39	i	97/99 (98%)	75 (77%)	21 (22%)	1 (1%)	13	47
40	j	85/87 (98%)	67 (79%)	16 (19%)	2 (2%)	5	31
41	k	75/77 (97%)	54 (72%)	19 (25%)	2 (3%)	4	29
42	l	48/50 (96%)	36 (75%)	11 (23%)	1 (2%)	5	33
43	m	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
44	n	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
45	o	103/105 (98%)	78 (76%)	25 (24%)	0	100	100
46	p	89/91 (98%)	78 (88%)	11 (12%)	0	100	100
48	q	204/206 (99%)	162 (79%)	39 (19%)	3 (2%)	8	40
49	r	212/214 (99%)	167 (79%)	41 (19%)	4 (2%)	6	35
50	s	215/217 (99%)	187 (87%)	27 (13%)	1 (0%)	25	61
51	t	221/223 (99%)	182 (82%)	37 (17%)	2 (1%)	14	49
52	u	258/260 (99%)	195 (76%)	61 (24%)	2 (1%)	16	53
53	v	204/206 (99%)	162 (79%)	41 (20%)	1 (0%)	25	61
54	w	221/223 (99%)	167 (76%)	47 (21%)	7 (3%)	3	26
55	x	182/184 (99%)	145 (80%)	34 (19%)	3 (2%)	8	38
56	y	184/199 (92%)	148 (80%)	36 (20%)	0	100	100
57	z	183/185 (99%)	147 (80%)	36 (20%)	0	100	100
58	AA	94/105 (90%)	76 (81%)	17 (18%)	1 (1%)	12	45
59	AB	151/153 (99%)	131 (87%)	18 (12%)	2 (1%)	10	42
60	AC	122/124 (98%)	93 (76%)	27 (22%)	2 (2%)	8	38
61	AD	148/150 (99%)	118 (80%)	27 (18%)	3 (2%)	6	34
62	AE	125/127 (98%)	104 (83%)	21 (17%)	0	100	100
63	AF	122/124 (98%)	89 (73%)	33 (27%)	0	100	100
64	AG	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	19	55
65	AH	116/125 (93%)	98 (84%)	17 (15%)	1 (1%)	14	49
66	AI	143/145 (99%)	117 (82%)	24 (17%)	2 (1%)	9	40
67	AJ	141/143 (99%)	126 (89%)	15 (11%)	0	100	100
68	AK	105/107 (98%)	90 (86%)	15 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	AL	85/87 (98%)	64 (75%)	19 (22%)	2 (2%)	5	31
70	AM	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	16	53
71	AN	142/144 (99%)	108 (76%)	34 (24%)	0	100	100
72	AO	132/134 (98%)	115 (87%)	17 (13%)	0	100	100
73	AP	68/70 (97%)	52 (76%)	15 (22%)	1 (2%)	8	40
74	AQ	95/97 (98%)	70 (74%)	25 (26%)	0	100	100
75	AR	79/81 (98%)	58 (73%)	21 (27%)	0	100	100
76	AS	61/63 (97%)	49 (80%)	12 (20%)	0	100	100
77	AT	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
78	AU	58/60 (97%)	42 (72%)	16 (28%)	0	100	100
79	AV	316/318 (99%)	252 (80%)	64 (20%)	0	100	100
80	AW	35/37 (95%)	21 (60%)	14 (40%)	0	100	100
81	AX	834/837 (100%)	676 (81%)	155 (19%)	3 (0%)	30	66
84	BA	202/204 (99%)	153 (76%)	47 (23%)	2 (1%)	13	47
All	All	12203/12421 (98%)	10189 (84%)	1938 (16%)	76 (1%)	24	58

5 of 76 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	i	98	ARG
40	j	65	ARG
42	l	30	ARG
48	q	113	ARG
54	w	68	LEU

5.3.2 Protein sidechains ⓘ

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	
4	P0	160/160 (100%)	157 (98%)	3 (2%)	52	70
5	P2	81/81 (100%)	78 (96%)	3 (4%)	29	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	A	193/194 (100%)	190 (98%)	3 (2%)	58	74
7	B	321/322 (100%)	314 (98%)	7 (2%)	47	65
8	C	288/288 (100%)	281 (98%)	7 (2%)	44	63
9	D	244/244 (100%)	241 (99%)	3 (1%)	67	78
10	E	134/152 (88%)	128 (96%)	6 (4%)	23	46
11	F	186/186 (100%)	179 (96%)	7 (4%)	28	51
12	G	187/191 (98%)	186 (100%)	1 (0%)	86	89
13	H	171/171 (100%)	168 (98%)	3 (2%)	54	71
14	I	177/186 (95%)	176 (99%)	1 (1%)	84	88
15	J	147/147 (100%)	140 (95%)	7 (5%)	21	45
16	L	154/154 (100%)	145 (94%)	9 (6%)	17	40
17	M	107/107 (100%)	103 (96%)	4 (4%)	29	52
18	N	175/175 (100%)	167 (95%)	8 (5%)	23	46
19	O	160/160 (100%)	155 (97%)	5 (3%)	35	56
20	P	140/145 (97%)	137 (98%)	3 (2%)	48	66
21	Q	150/150 (100%)	146 (97%)	4 (3%)	40	60
22	R	153/153 (100%)	144 (94%)	9 (6%)	16	40
23	S	156/156 (100%)	152 (97%)	4 (3%)	41	61
24	T	136/136 (100%)	132 (97%)	4 (3%)	37	58
25	U	87/87 (100%)	86 (99%)	1 (1%)	70	80
26	V	103/104 (99%)	99 (96%)	4 (4%)	27	50
27	W	54/54 (100%)	53 (98%)	1 (2%)	52	70
28	X	104/105 (99%)	102 (98%)	2 (2%)	52	70
29	Y	109/109 (100%)	109 (100%)	0	100	100
30	Z	115/115 (100%)	113 (98%)	2 (2%)	56	72
31	a	118/118 (100%)	117 (99%)	1 (1%)	79	84
32	b	46/46 (100%)	44 (96%)	2 (4%)	25	48
33	c	81/81 (100%)	79 (98%)	2 (2%)	42	62
34	d	94/96 (98%)	94 (100%)	0	100	100
35	e	109/109 (100%)	109 (100%)	0	100	100
36	f	90/90 (100%)	88 (98%)	2 (2%)	47	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	g	95/95 (100%)	94 (99%)	1 (1%)	70	80
38	h	104/104 (100%)	101 (97%)	3 (3%)	37	58
39	i	81/81 (100%)	78 (96%)	3 (4%)	29	52
40	j	70/70 (100%)	69 (99%)	1 (1%)	62	75
41	k	68/68 (100%)	67 (98%)	1 (2%)	60	75
42	l	45/45 (100%)	42 (93%)	3 (7%)	13	36
43	m	47/47 (100%)	45 (96%)	2 (4%)	25	48
44	n	23/23 (100%)	21 (91%)	2 (9%)	8	29
45	o	90/90 (100%)	89 (99%)	1 (1%)	70	80
46	p	71/71 (100%)	70 (99%)	1 (1%)	62	75
48	q	164/173 (95%)	158 (96%)	6 (4%)	29	52
49	r	191/191 (100%)	187 (98%)	4 (2%)	48	66
50	s	176/176 (100%)	174 (99%)	2 (1%)	70	80
51	t	182/182 (100%)	176 (97%)	6 (3%)	33	55
52	u	221/221 (100%)	215 (97%)	6 (3%)	40	60
53	v	173/173 (100%)	166 (96%)	7 (4%)	27	49
54	w	189/191 (99%)	183 (97%)	6 (3%)	34	55
55	x	165/165 (100%)	161 (98%)	4 (2%)	44	63
56	y	150/160 (94%)	144 (96%)	6 (4%)	27	49
57	z	158/158 (100%)	155 (98%)	3 (2%)	52	70
58	AA	77/98 (79%)	76 (99%)	1 (1%)	65	77
59	AB	133/134 (99%)	127 (96%)	6 (4%)	23	46
60	AC	88/100 (88%)	87 (99%)	1 (1%)	70	80
61	AD	127/127 (100%)	123 (97%)	4 (3%)	35	56
62	AE	81/96 (84%)	77 (95%)	4 (5%)	21	44
63	AF	101/104 (97%)	96 (95%)	5 (5%)	20	44
64	AG	117/117 (100%)	116 (99%)	1 (1%)	75	83
65	AH	94/113 (83%)	90 (96%)	4 (4%)	25	48
66	AI	128/128 (100%)	124 (97%)	4 (3%)	35	56
67	AJ	115/115 (100%)	112 (97%)	3 (3%)	41	61
68	AK	100/100 (100%)	99 (99%)	1 (1%)	73	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	AL	74/74 (100%)	71 (96%)	3 (4%)	26	49
70	AM	110/110 (100%)	108 (98%)	2 (2%)	54	71
71	AN	119/119 (100%)	115 (97%)	4 (3%)	32	54
72	AO	112/112 (100%)	108 (96%)	4 (4%)	30	52
73	AP	61/61 (100%)	59 (97%)	2 (3%)	33	55
74	AQ	83/83 (100%)	80 (96%)	3 (4%)	30	52
75	AR	70/70 (100%)	70 (100%)	0	100	100
76	AS	56/56 (100%)	54 (96%)	2 (4%)	30	52
77	AT	47/47 (100%)	45 (96%)	2 (4%)	25	48
78	AU	51/51 (100%)	47 (92%)	4 (8%)	10	33
79	AV	259/261 (99%)	255 (98%)	4 (2%)	60	75
80	AW	31/31 (100%)	30 (97%)	1 (3%)	34	55
81	AX	708/709 (100%)	687 (97%)	21 (3%)	36	57
84	BA	185/185 (100%)	179 (97%)	6 (3%)	34	55
All	All	10320/10457 (99%)	10042 (97%)	278 (3%)	41	60

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
72	AO	102	LYS
76	AS	49	ARG
81	AX	310	ASP
24	T	83	ARG
23	S	48	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
31	a	74	ASN
79	AV	17	ASN
48	q	140	ASN
78	AU	57	ASN
81	AX	186	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3220/3396 (94%)	1076 (33%)	33 (1%)
2	3	120/121 (99%)	28 (23%)	3 (2%)
3	4	157/158 (99%)	47 (29%)	5 (3%)
47	2	1774/1797 (98%)	779 (43%)	38 (2%)
82	AY	75/76 (98%)	29 (38%)	0
83	AZ	6/7 (85%)	5 (83%)	2 (33%)
All	All	5352/5555 (96%)	1964 (36%)	81 (1%)

5 of 1964 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	U
1	1	6	A
1	1	14	U
1	1	15	C
1	1	17	G

5 of 81 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	2	706	A
47	2	1481	C
47	2	740	A
47	2	1181	U
47	2	1680	G

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

1 non-standard protein/DNA/RNA residue is 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
81	DDE	AX	699	81	14,20,21	1.95	3 (21%)	14,28,30	1.82	5 (35%)

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
81	DDE	AX	699	81	-	6/20/21/23	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	AX	699	DDE	CBI-NAD	5.57	1.46	1.32
81	AX	699	DDE	CAT-CE1	3.11	1.54	1.50
81	AX	699	DDE	OAG-CBI	-2.23	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	AX	699	DDE	CAC-NCB-CAB	3.78	118.43	108.10
81	AX	699	DDE	OAG-CBI-NAD	-2.91	117.94	123.00
81	AX	699	DDE	CBW-CBI-NAD	2.64	118.64	115.28
81	AX	699	DDE	OAG-CBI-CBW	2.31	123.41	120.49
81	AX	699	DDE	CG-ND1-CE1	2.07	109.17	103.05

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	AX	699	DDE	N-CA-CB-CG
81	AX	699	DDE	C-CA-CB-CG
81	AX	699	DDE	CAU-CAT-CE1-ND1
81	AX	699	DDE	CAT-CAU-CBW-CBI
81	AX	699	DDE	OAG-CBI-CBW-CAU

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 8 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	GCP	AX	901	-	27,34,34	1.05	3 (11%)	34,54,54	2.18	8 (23%)

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	GCP	AX	901	-	-	5/15/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	AX	901	GCP	C6-N1	2.91	1.38	1.33
86	AX	901	GCP	PG-O1G	2.20	1.54	1.50
86	AX	901	GCP	PG-O3G	-2.11	1.50	1.54

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	AX	901	GCP	C5-C6-N1	-7.92	112.59	123.43
86	AX	901	GCP	C2-N1-C6	5.66	124.92	115.93
86	AX	901	GCP	O1B-PB-C3B	4.06	119.81	109.07
86	AX	901	GCP	N3-C2-N1	-3.06	123.14	127.22
86	AX	901	GCP	O1G-PG-C3B	-2.70	105.42	111.24

There are no chirality outliers.

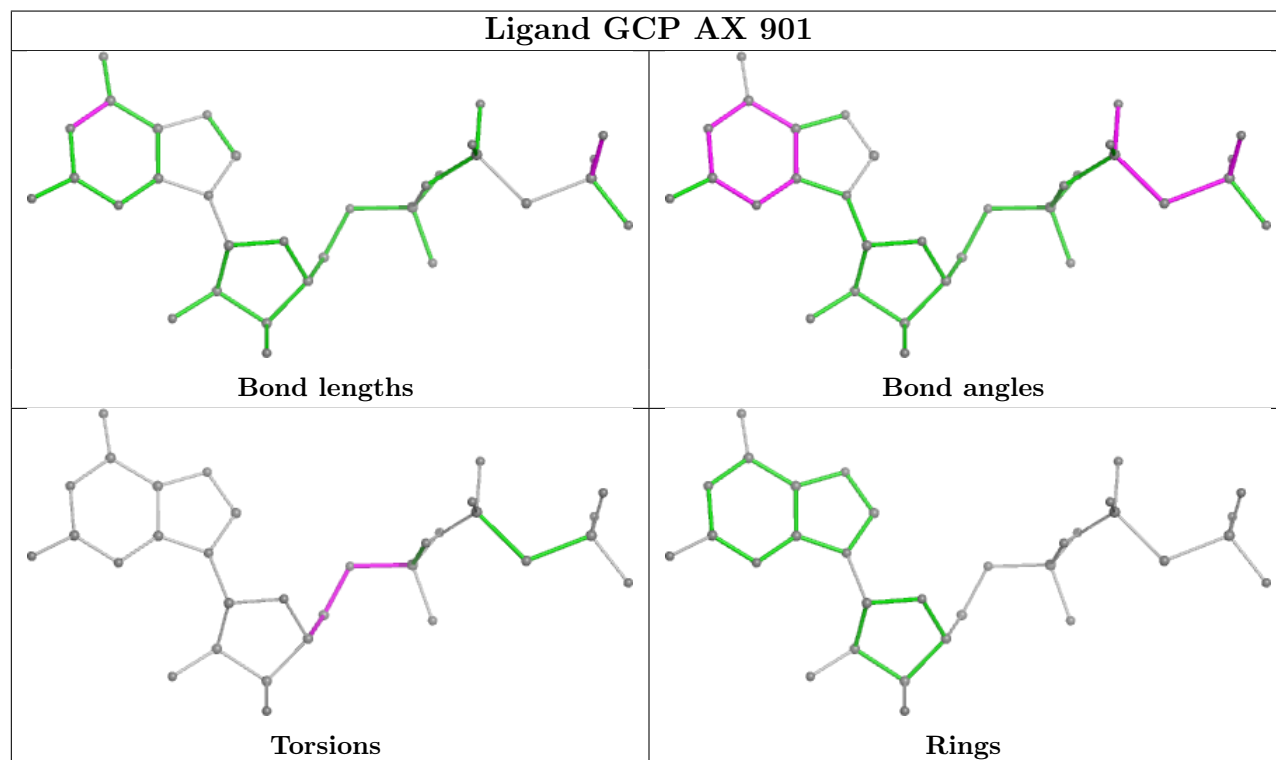
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	AX	901	GCP	C5'-O5'-PA-O1A
86	AX	901	GCP	C5'-O5'-PA-O2A
86	AX	901	GCP	C4'-C5'-O5'-PA
86	AX	901	GCP	C5'-O5'-PA-O3A
86	AX	901	GCP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

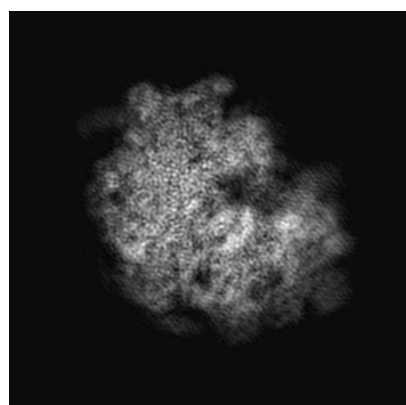
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0049. These allow visual inspection of the internal detail of the map and identification of artifacts.

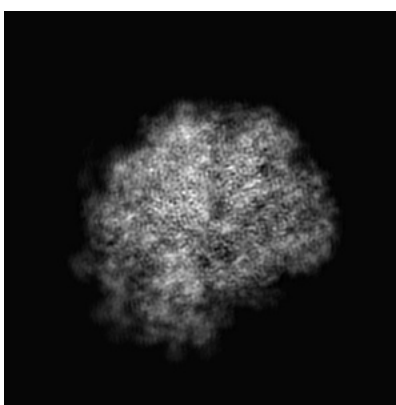
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

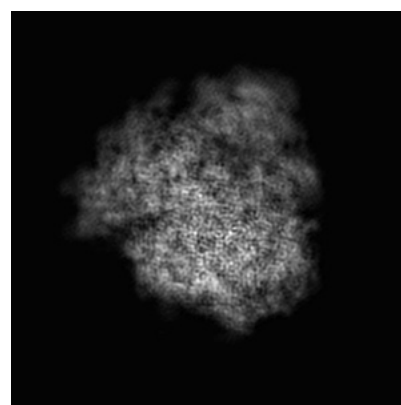
6.1.1 Primary map



X



Y

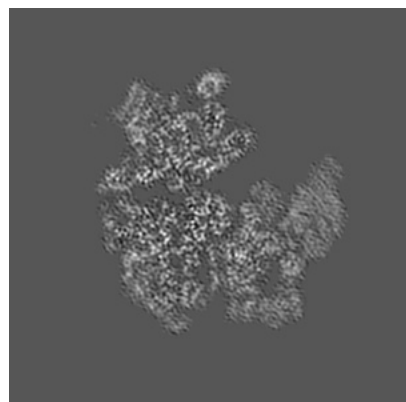


Z

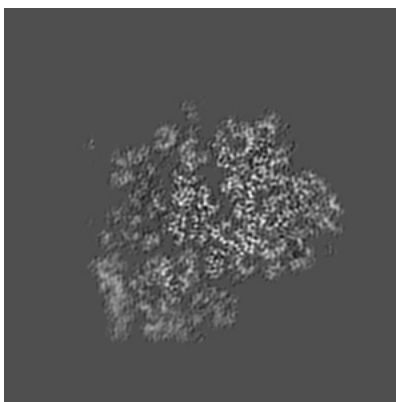
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

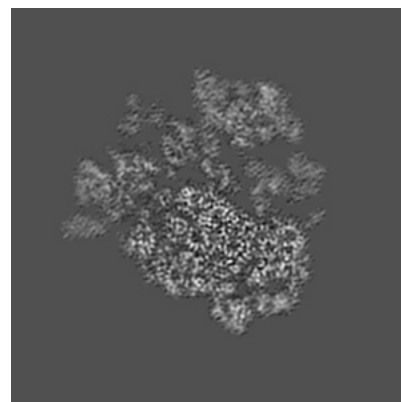
6.2.1 Primary map



X Index: 180



Y Index: 180

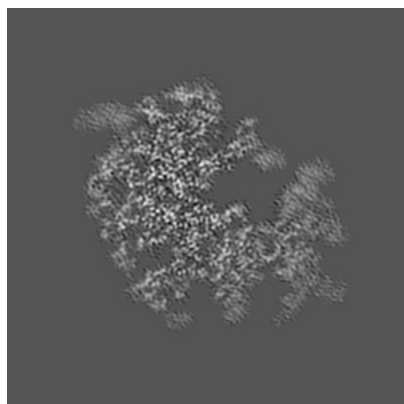


Z Index: 180

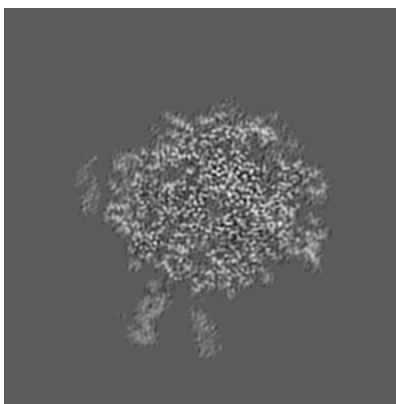
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

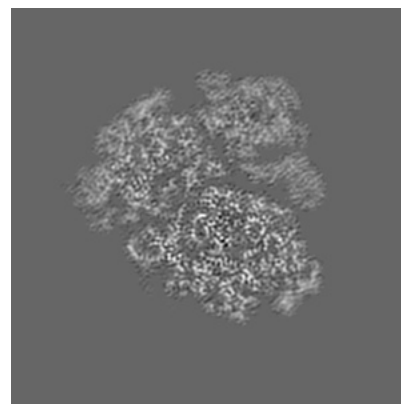
6.3.1 Primary map



X Index: 194



Y Index: 158

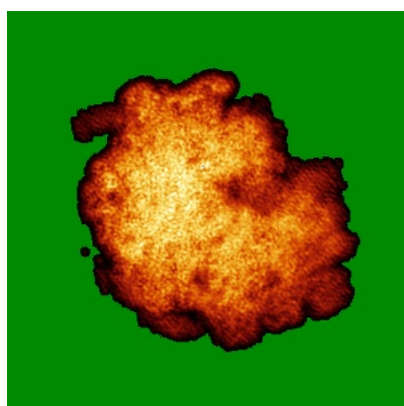


Z Index: 166

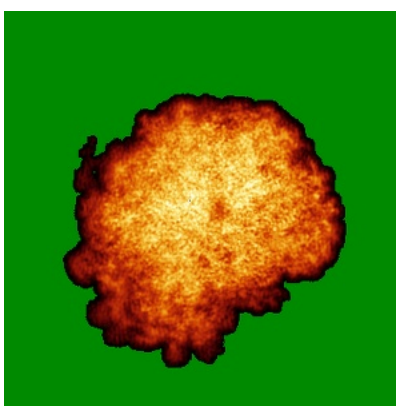
The images above show the largest variance slices of the map in three orthogonal directions.

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

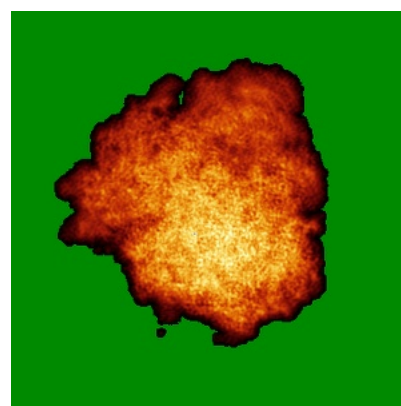
6.4.1 Primary map



X



Y

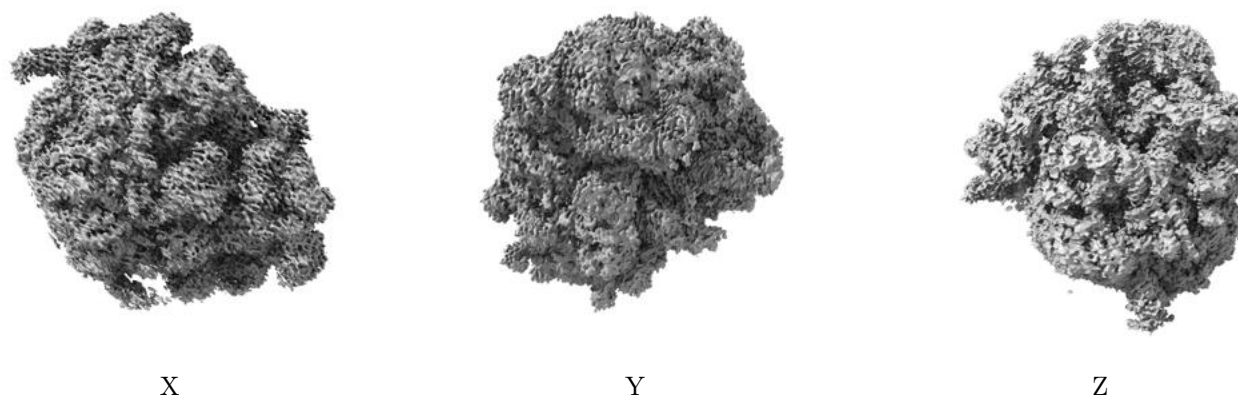


Z

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 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

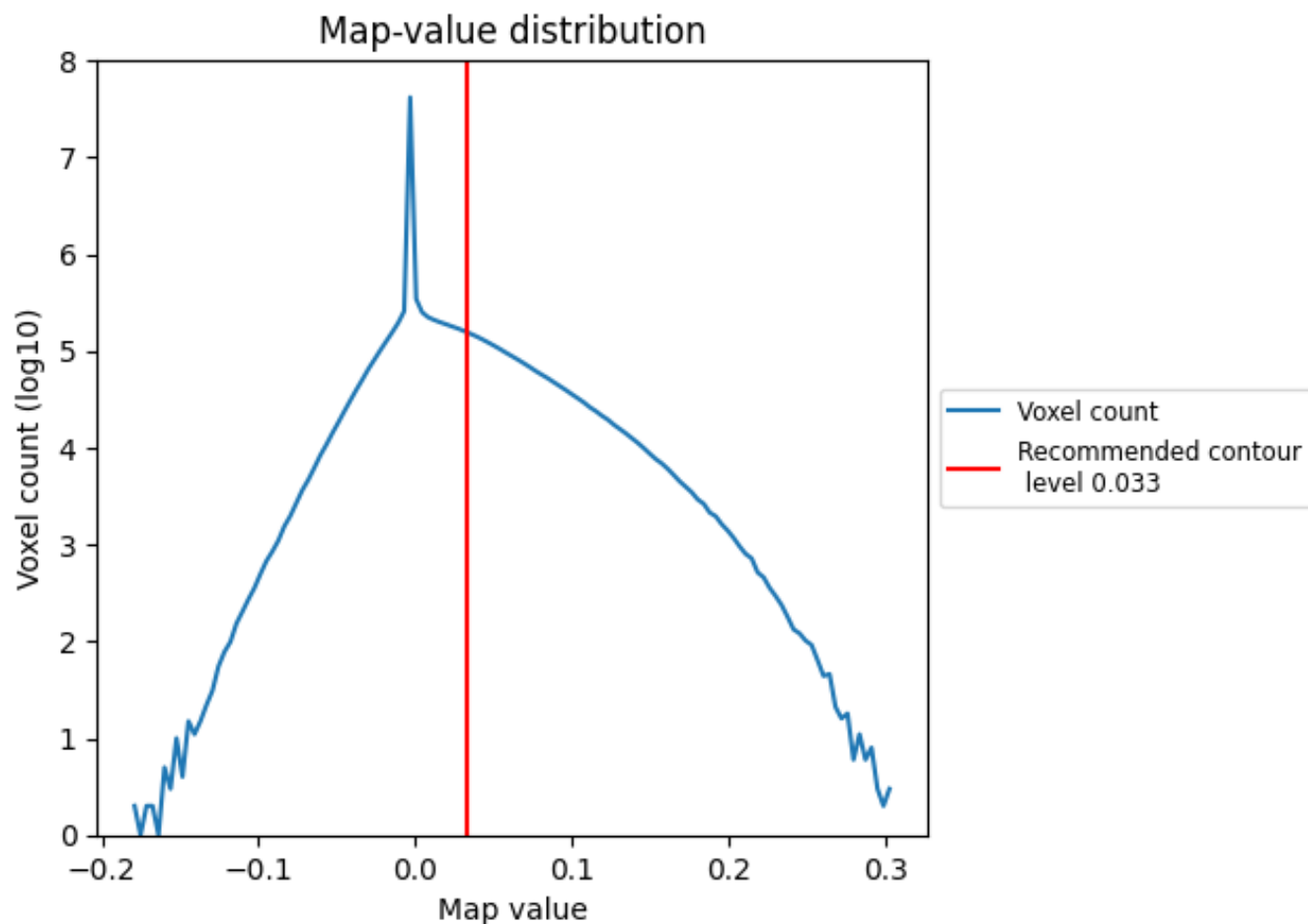
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

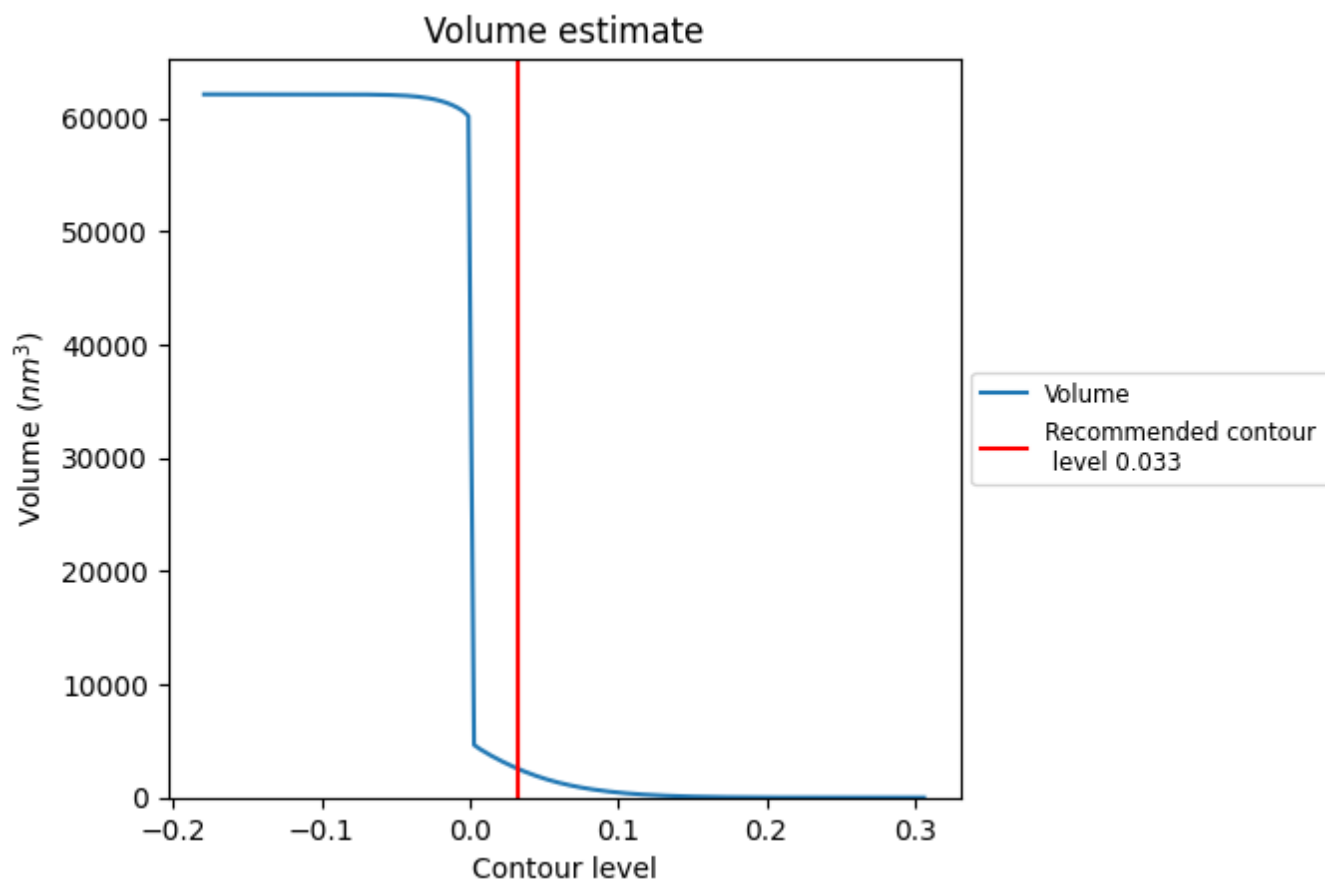
This section contains the results of statistical analysis of the map.

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.

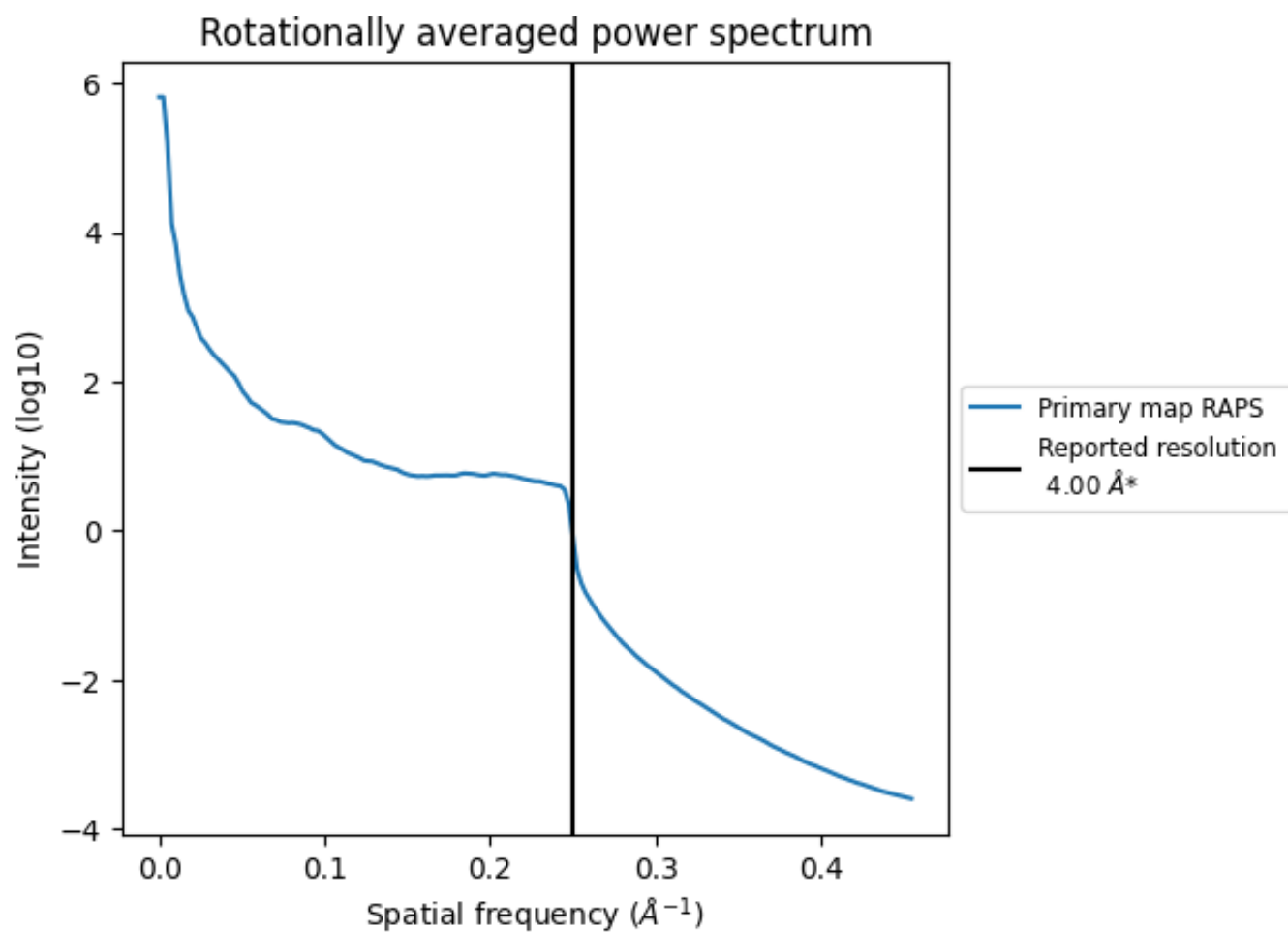
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2513 nm³; this corresponds to an approximate mass of 2270 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

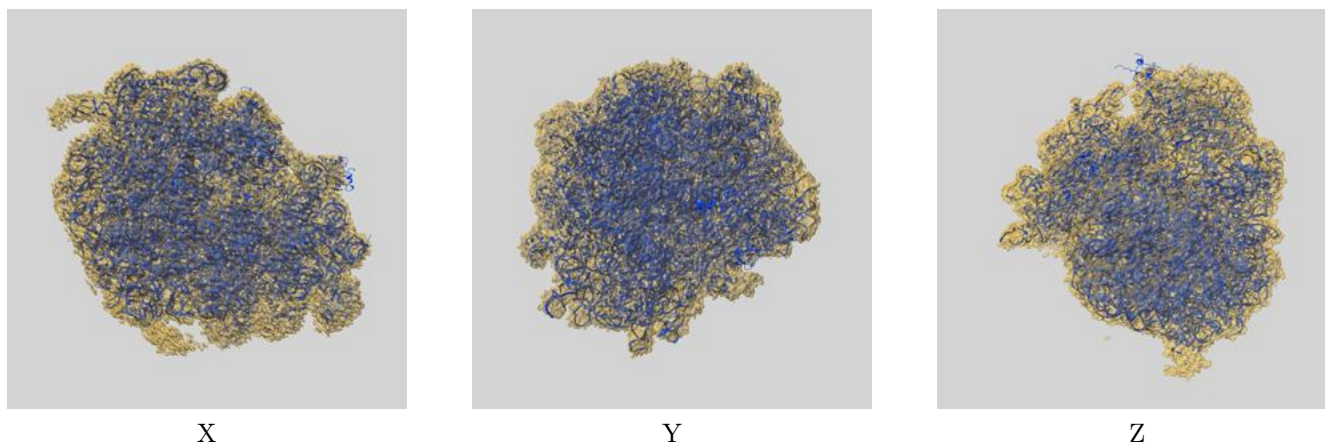
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

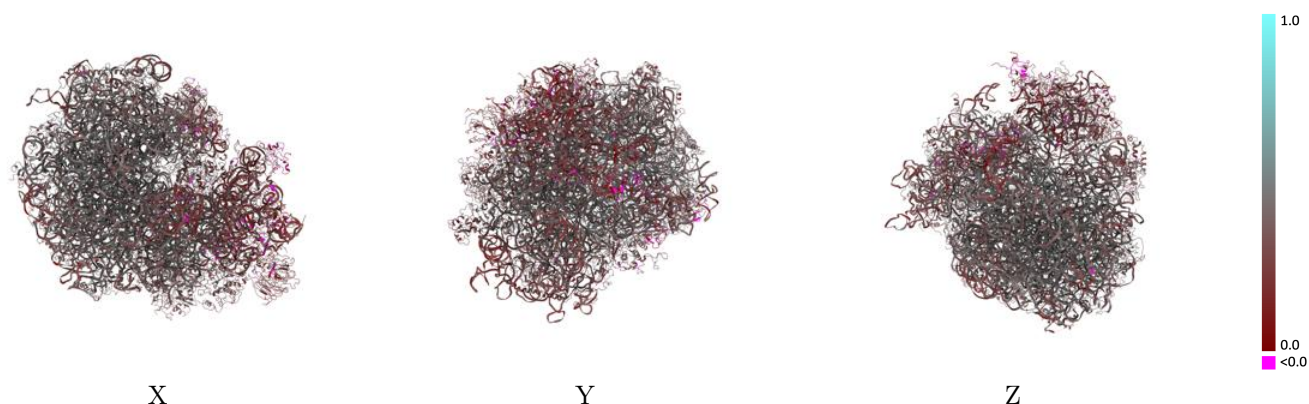
This section contains information regarding the fit between EMDB map EMD-0049 and PDB model 6GQV. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



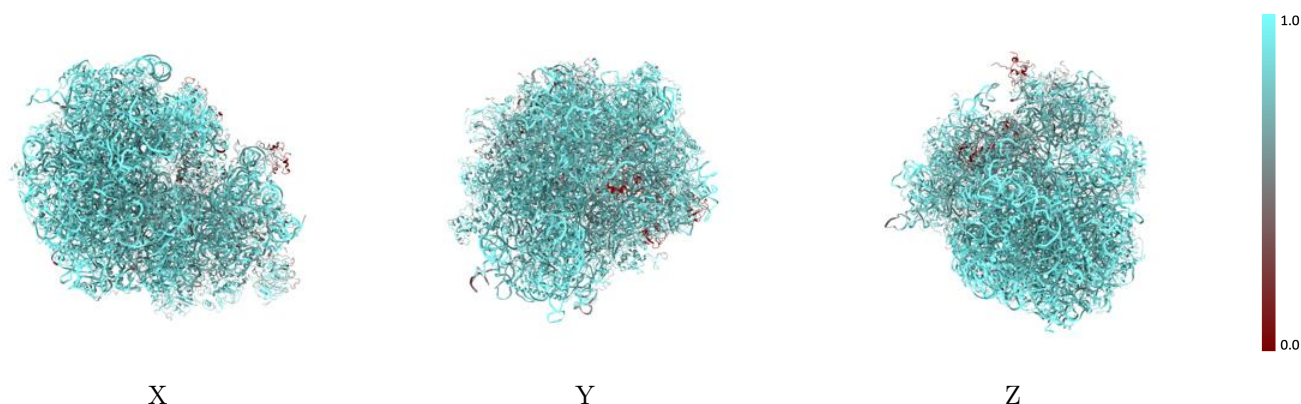
The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



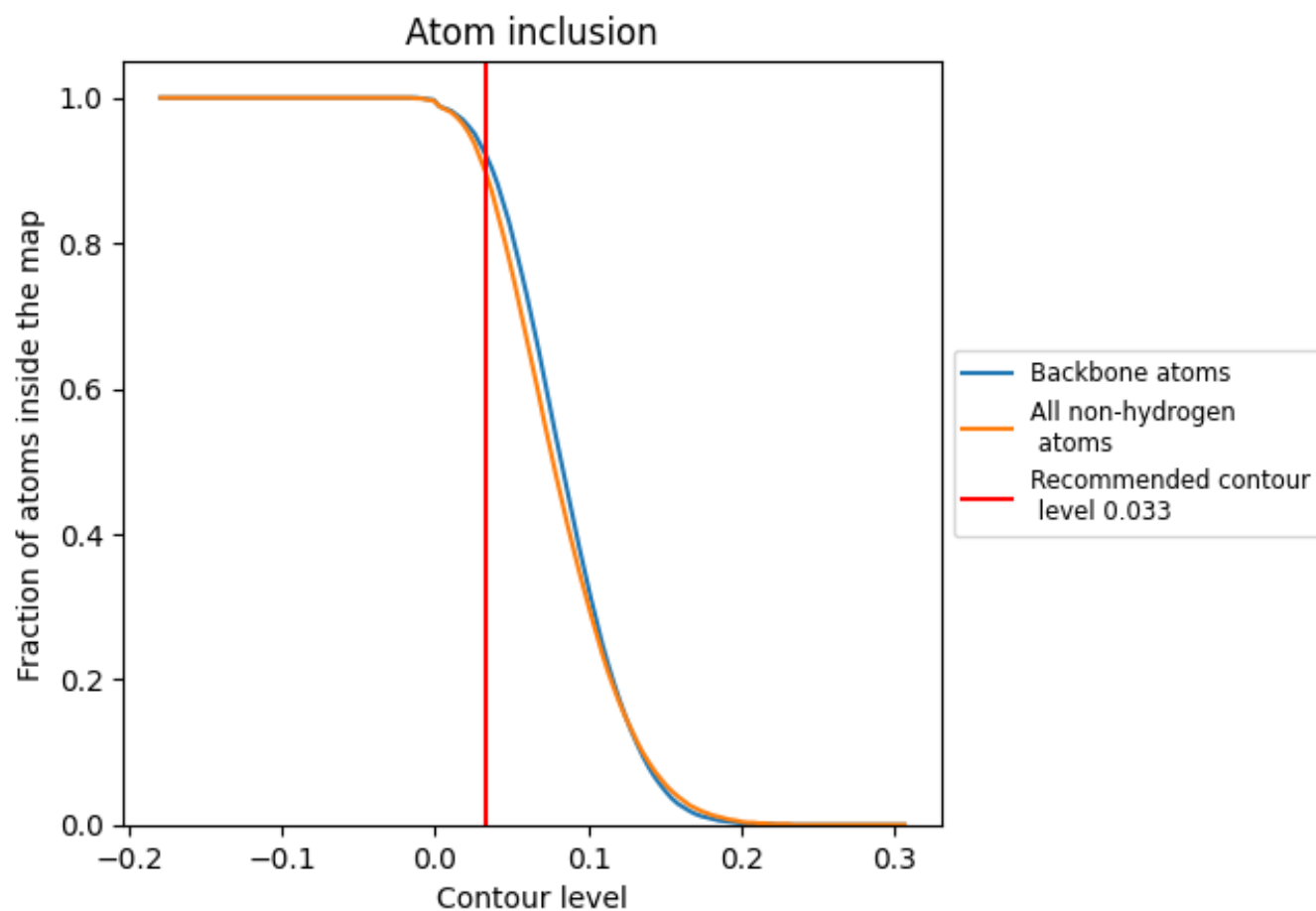
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.033).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8970	 0.3780
1	 0.9620	 0.4060
2	 0.9300	 0.3390
3	 0.9810	 0.3960
4	 0.9710	 0.4200
A	 0.8630	 0.4620
AA	 0.8670	 0.2720
AB	 0.7910	 0.3950
AC	 0.2450	 0.1250
AD	 0.8670	 0.3920
AE	 0.8890	 0.3890
AF	 0.8080	 0.2840
AG	 0.7620	 0.2500
AH	 0.7470	 0.2820
AI	 0.7790	 0.2900
AJ	 0.8080	 0.2680
AK	 0.6880	 0.2810
AL	 0.8280	 0.3480
AM	 0.8550	 0.4190
AN	 0.8110	 0.4140
AO	 0.8750	 0.3220
AP	 0.6250	 0.2320
AQ	 0.8550	 0.3750
AR	 0.8740	 0.3780
AS	 0.6370	 0.2470
AT	 0.8700	 0.3180
AU	 0.8100	 0.3710
AV	 0.7500	 0.2590
AW	 0.6640	 0.2630
AX	 0.7640	 0.3440
AY	 0.8380	 0.2940
AZ	 0.4440	 0.3240
B	 0.9000	 0.4470
BA	 0.6630	 0.2530
C	 0.9280	 0.4430



















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Chain	Atom inclusion	Q-score
D	 0.9010	 0.3750
E	 0.9090	 0.4020
F	 0.9020	 0.4280
G	 0.9020	 0.4100
H	 0.8780	 0.4080
I	 0.8960	 0.4300
J	 0.8660	 0.3700
L	 0.9230	 0.4270
M	 0.9100	 0.4030
N	 0.9070	 0.4580
O	 0.9000	 0.4250
P	 0.8980	 0.4500
P0	 0.2760	 0.1750
P2	 0.3050	 0.1930
Q	 0.9150	 0.4480
R	 0.9010	 0.4200
S	 0.9070	 0.4280
T	 0.8930	 0.4360
U	 0.8980	 0.3800
V	 0.8320	 0.4470
W	 0.8490	 0.4290
X	 0.8920	 0.4150
Y	 0.9170	 0.4220
Z	 0.9050	 0.4140
a	 0.9260	 0.4490
b	 0.8920	 0.4260
c	 0.8960	 0.4210
d	 0.8820	 0.4400
e	 0.8930	 0.4460
f	 0.9000	 0.4490
g	 0.8810	 0.4480
h	 0.8910	 0.4170
i	 0.9060	 0.4080
j	 0.9280	 0.4760
k	 0.8610	 0.3850
l	 0.8840	 0.4430
m	 0.8940	 0.4490
n	 0.7880	 0.4600
o	 0.8770	 0.4430
p	 0.8480	 0.4440
q	 0.8610	 0.3510
r	 0.8990	 0.3770

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Chain	Atom inclusion	Q-score
s	 0.8630	 0.4010
t	 0.7250	 0.2790
u	 0.8770	 0.3550
v	 0.7480	 0.2720
w	 0.8770	 0.3310
x	 0.8420	 0.3220
y	 0.8420	 0.3460
z	 0.8880	 0.3620