



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 01:46 PM UTC

PDB ID : 6TNU / pdb_00006tnu
EMDB ID : EMD-10537
Title : Yeast 80S ribosome in complex with eIF5A and decoding A-site and P-site tRNAs.
Authors : Buschauer, R.; Cheng, J.; Berninghausen, O.; Tesina, P.; Becker, T.; Beckmann, R.
Deposited on : 2019-12-10
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

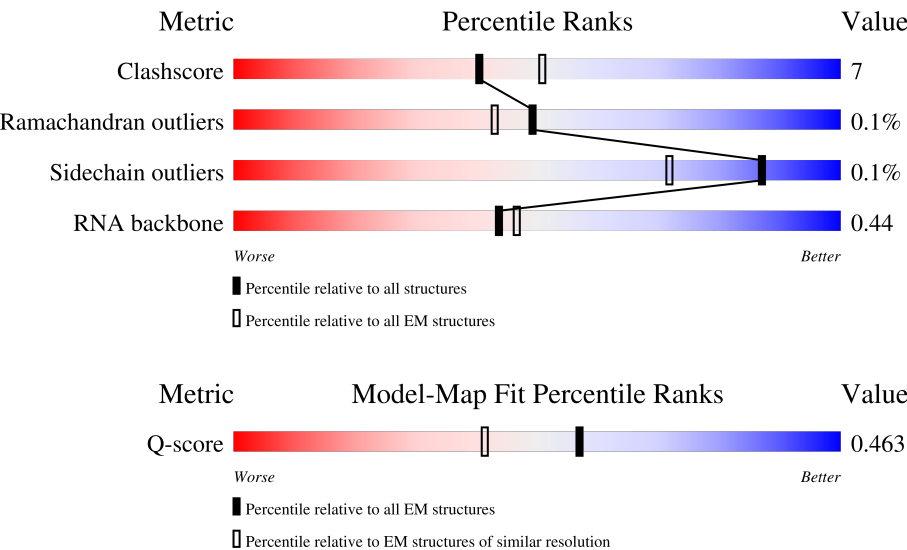
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	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	14724 (2.60 - 3.60)

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	2	1798	51% 34% 13%
2	1	6	67% 17% 17%
3	P	206	5% 77% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	Q	232	
5	E	117	
6	R	216	
7	A	222	
8	S	258	
9	B	206	
10	T	228	
11	U	184	
12	V	187	
13	W	184	
14	C	92	
15	X	142	
16	D	121	
17	Y	150	
18	Z	127	
19	F	141	
20	G	125	
21	H	145	
22	I	143	
23	J	100	
24	n	75	
25	a	87	
26	b	129	
27	c	144	
28	d	134	

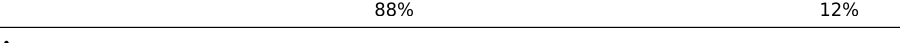
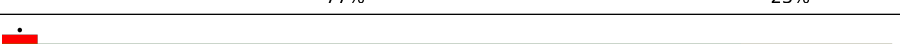
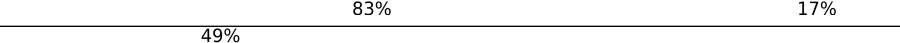
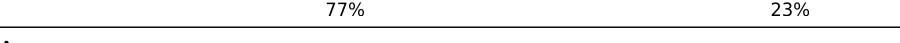
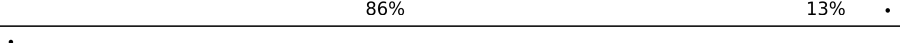
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	K	82	
30	e	97	
31	f	81	
32	M	53	
33	g	60	
34	N	73	
35	O	312	
36	L	63	
37	m	76	
38	BQ	3184	
39	BR	121	
40	BS	158	
41	AW	251	
42	BA	386	
43	BE	361	
44	BI	294	
45	BM	175	
46	BO	222	
47	AA	233	
48	AD	191	
49	BD	218	
50	AG	169	
51	AJ	193	
52	AM	136	
53	AQ	203	

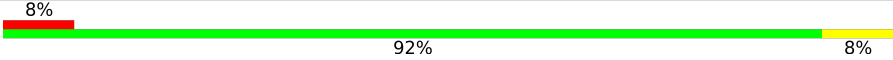
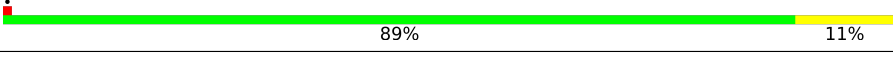
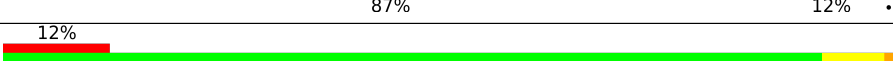
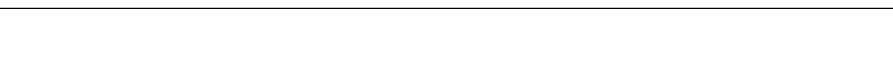
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	AU	197	
55	AX	183	
56	BB	185	
57	BF	188	
58	BH	171	
59	BJ	159	
60	BL	100	
61	AB	136	
62	AE	126	
63	AH	121	
64	AK	125	
65	AN	135	
66	AR	148	
67	AV	58	
68	AY	96	
69	BC	109	
70	BG	127	
71	BK	106	
72	BN	112	
73	BP	119	
74	AC	99	
75	AF	81	
76	AI	77	
77	AL	50	
78	AO	52	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	AS	25	
80	AP	103	
81	AT	91	
82	eI	154	
83	BT	210	

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 204962 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1771	Total	C	N	O	P	0	0
			37739	16872	6683	12413	1771		

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 3 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	206	Total	C	N	O	S	0	0
			1603	1030	284	287	2		

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	226	Total	C	N	O	S	0	0
			1798	1139	330	325	4		

- Molecule 5 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	117	Total	C	N	O	S	0	0
			916	583	171	155	7		

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	222	Total	C	N	O	S	0	0
			1729	1098	312	313	6		

- Molecule 8 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 9 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	206	Total	C	N	O	S	0	0
			1605	1005	299	298	3		

- Molecule 10 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	228	Total	C	N	O	S	0	0
			1815	1138	351	323	3		

- Molecule 11 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	184	Total	C	N	O	S	0	0
			1473	946	263	264			

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	V	187	Total	C	N	O	S	0	0
			1476	916	295	263	2		

- Molecule 13 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	184	Total	C	N	O	S	0	0
			1479	935	285	258	1		

- Molecule 14 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	92	Total	C	N	O	S	0	0
			752	487	122	141	2		

- Molecule 15 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	142	Total	C	N	O	S	0	0
			1142	733	217	189	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	121	Total	C	N	O	S	0	0
			875	551	153	169	2		

- Molecule 17 is a protein called 40S ribosomal protein S13.

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

- Molecule 18 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	127	Total	C	N	O	S	0	0
			923	568	185	167	3		

- Molecule 19 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 20 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 21 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	145	Total	C	N	O	S	0	0
			1188	741	237	208	2		

- Molecule 22 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 23 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 24 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	n	75	Total	C	N	O	P	0	0
			1624	728	298	523	75		

- Molecule 25 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	87	Total	C	N	O	S	0	0
			673	415	125	131	2		

- Molecule 26 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 27 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 28 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	d	134	Total	C	N	O	0	0
			1032	651	195	186		

- Molecule 29 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	K	82	Total	C	N	O	0	0
			651	416	123	112		

- Molecule 30 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	97	Total	C	N	O	S	0	0
			765	473	160	127	5		

- Molecule 31 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 32 is a protein called 40S ribosomal protein S29-A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	60	Total	C	N	O	S	0	0
			472	298	97	76	1		

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	N	73	Total	C	N	O	S	0	0
			556	352	105	95	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	97	ALA	LYS	conflict	UNP P05759

- Molecule 35 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	O	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		

- Molecule 36 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L	63	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 37 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	76	Total	C	N	O	P	0	0
			1611	721	281	534	75		

- Molecule 38 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BQ	3184	Total	C	N	O	P	0	0
			68091	30415	12259	22233	3184		

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

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

- Molecule 40 is a RNA chain called 5.8S rRNA.

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

- Molecule 41 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AW	251	Total	C	N	O	S	0	0
			1899	1182	385	331	1		

- Molecule 42 is a protein called 60S ribosomal protein L3.

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

- Molecule 43 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BI	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 45 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BM	167	Total	C	N	O	S	0	0
			1307	843	234	230			

- Molecule 46 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 47 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 48 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 49 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BD	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 50 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AG	169	Total	C	N	O	S	0	0
			1346	843	252	247	4		

- Molecule 51 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 52 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 53 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 54 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 55 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AX	183	Total	C	N	O	S	0	0
			1416	879	284	253			

- Molecule 56 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 57 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BF	188	Total	C	N	O	S	0	0
			1515	932	323	260			

- Molecule 58 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BH	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 59 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BJ	159	Total	C	N	O	S	0	0
			1272	802	245	221	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BL	100	Total	C	N	O	S	0	0
			796	516	131	149			

- Molecule 61 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AB	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 62 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	126	Total	C	N	O	S	0	0
			836	525	165	145	1		

- Molecule 63 is a protein called 60S ribosomal protein L25.

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

- Molecule 64 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AK	125	Total	C	N	O		0	0
			984	620	191	173			

- Molecule 65 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AN	135	Total	C	N	O		0	0
			1080	701	199	180			

- Molecule 66 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AR	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 67 is a protein called 60S ribosomal protein L29.

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

- Molecule 68 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AY	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 69 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	BC	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 70 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BG	127	Total	C	N	O	S	0	0
			1017	644	205	167	1		

- Molecule 71 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 72 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 73 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 74 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AC	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 75 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AF	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 76 is a protein called 60S ribosomal protein L38.

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

- Molecule 77 is a protein called 60S ribosomal protein L39.

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

- Molecule 78 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AO	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 79 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AS	25	Total	C	N	O	S	0	0
			229	139	62	27	1		

- Molecule 80 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AP	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 81 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 82 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	eI	154	Total	C	N	O	S	0	0
			1143	709	195	230	9		

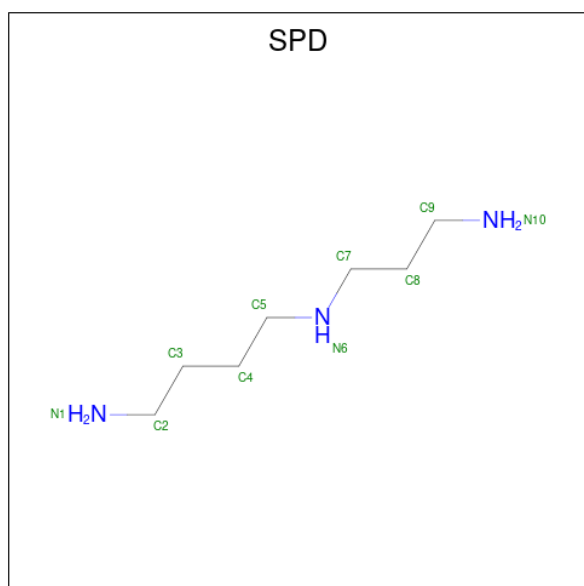
- Molecule 83 is a protein called 60S ribosomal protein L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	BT	210	Total	C	N	O	0	0
			1050	630	210	210		

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

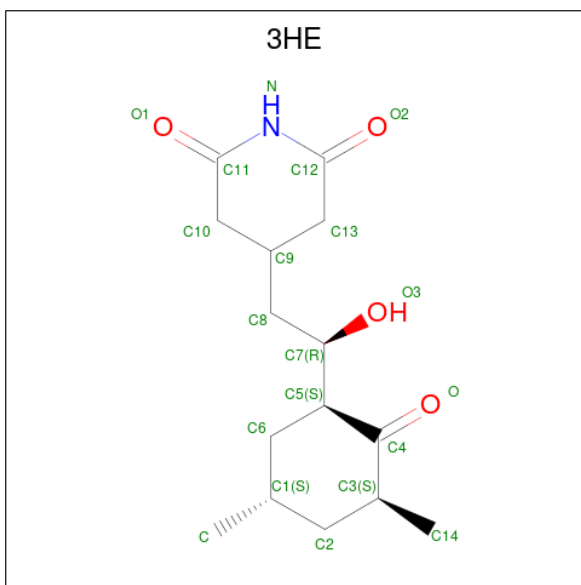
Mol	Chain	Residues	Atoms		AltConf
84	M	1	Total	Zn	0
			1	1	
84	N	1	Total	Zn	0
			1	1	
84	BN	1	Total	Zn	0
			1	1	
84	AF	1	Total	Zn	0
			1	1	
84	AO	1	Total	Zn	0
			1	1	
84	AP	1	Total	Zn	0
			1	1	
84	AT	1	Total	Zn	0
			1	1	

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
85	BQ	1	Total	C	N	0
			10	7	3	

- Molecule 86 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: $C_{15}H_{23}NO_4$).

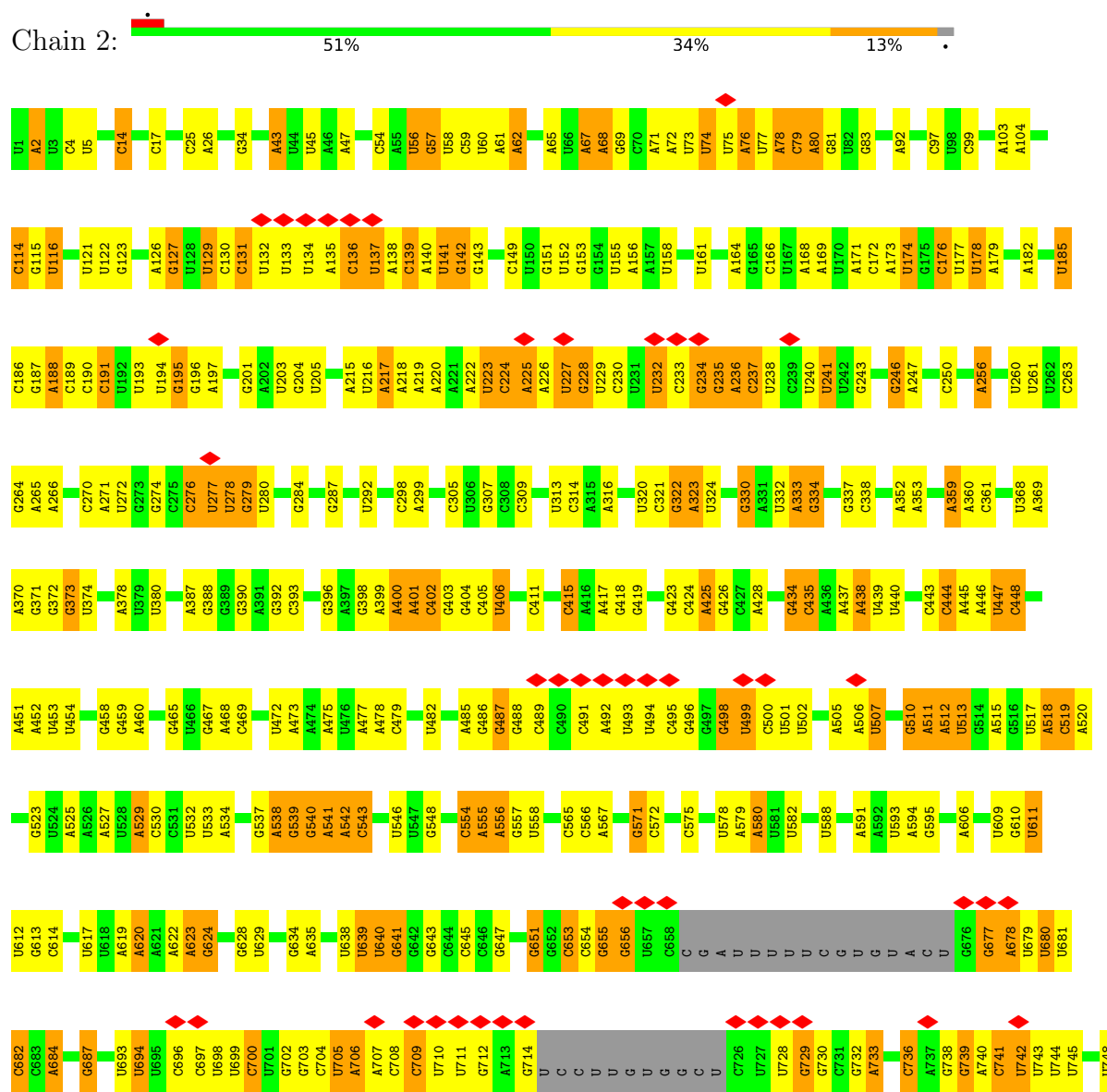


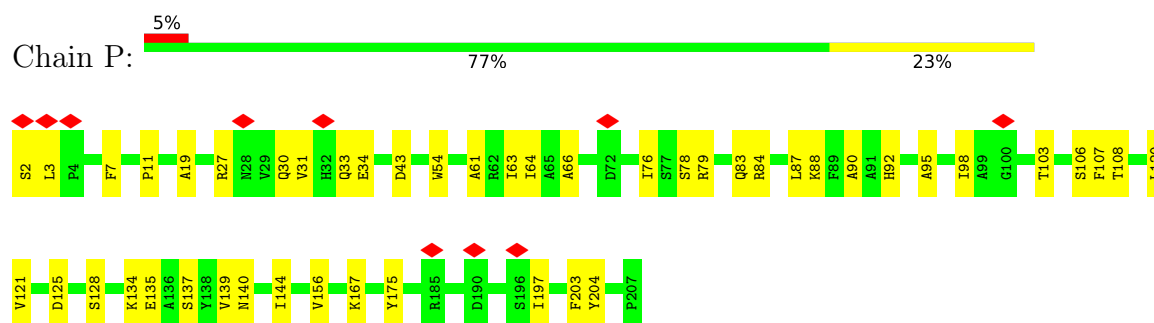
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
86	BQ	1	20	15	1	4	0

3 Residue-property plots

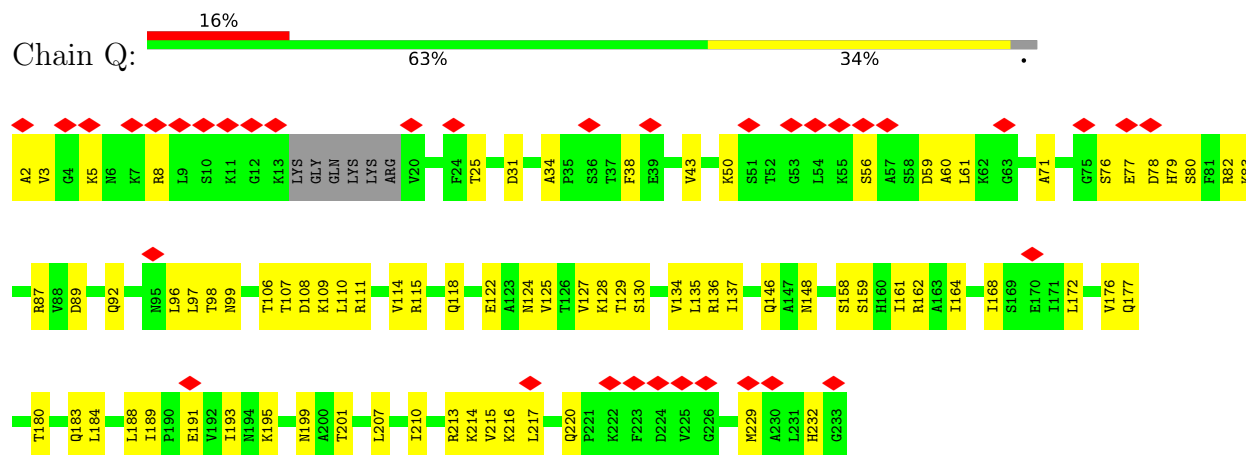
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

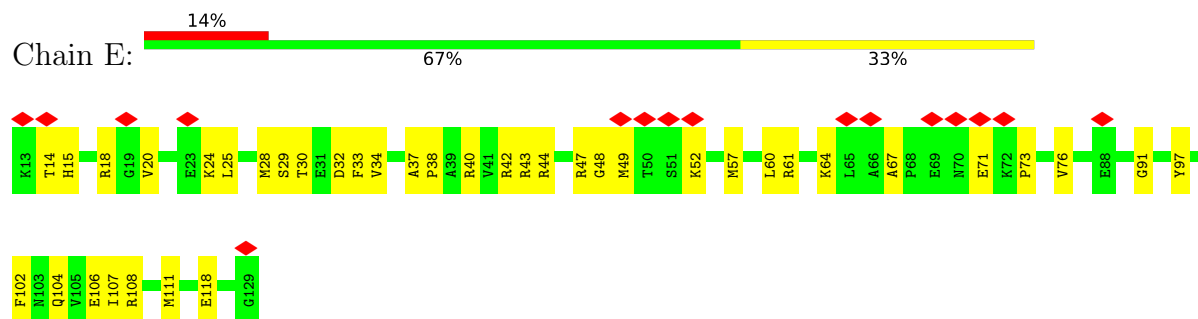




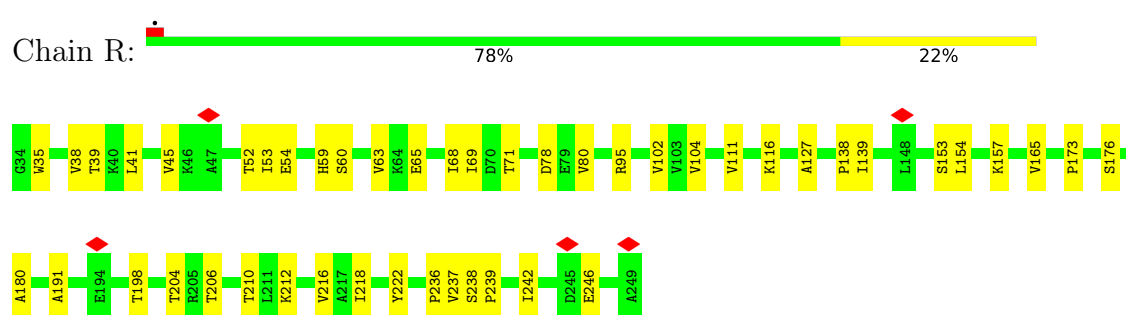
• Molecule 4: 40S ribosomal protein S1-A



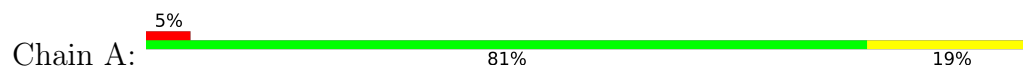
• Molecule 5: 40S ribosomal protein S15

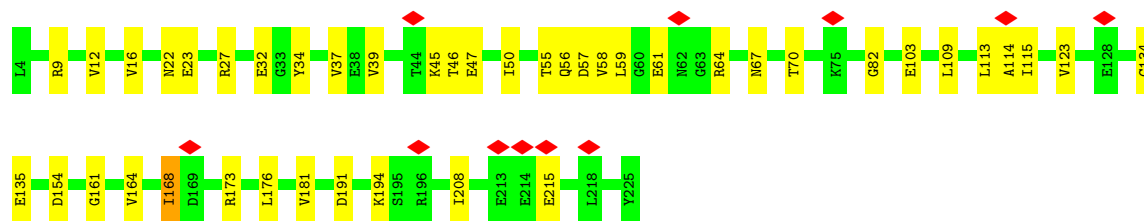


• Molecule 6: 40S ribosomal protein S2

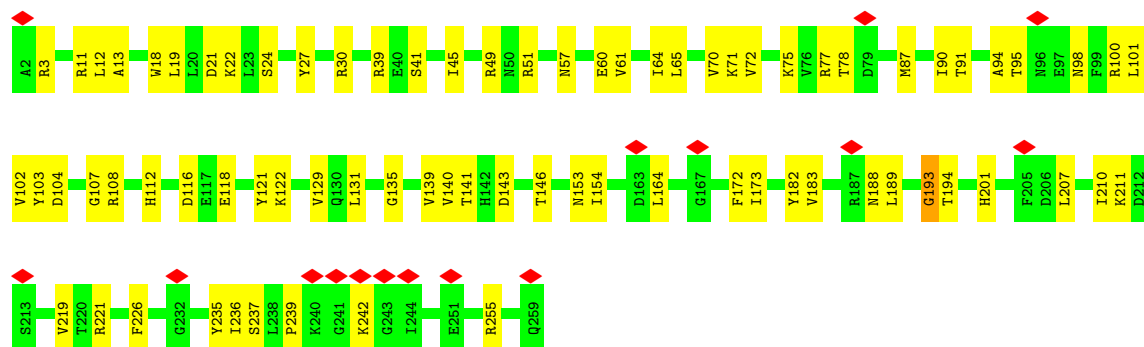


• Molecule 7: 40S ribosomal protein S3

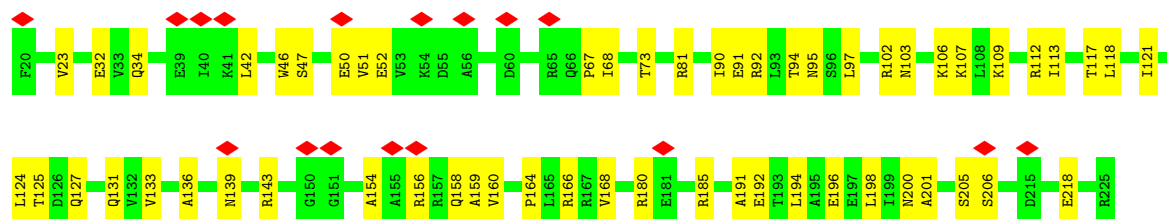
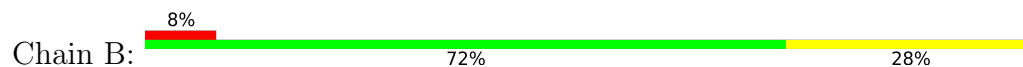




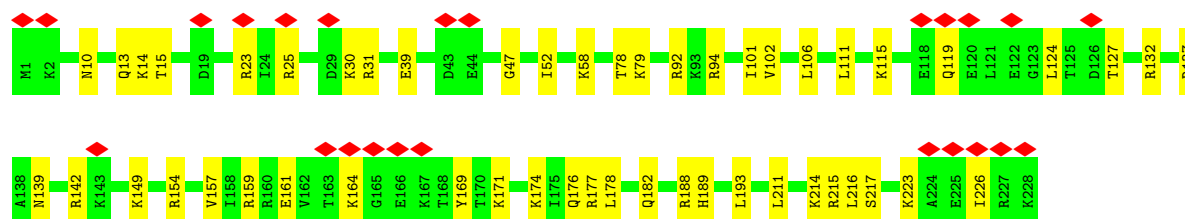
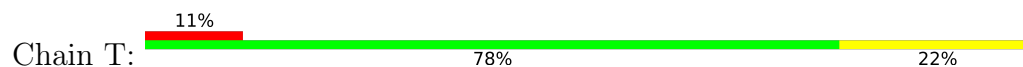
• Molecule 8: 40S ribosomal protein S4-A



• Molecule 9: Rps5p

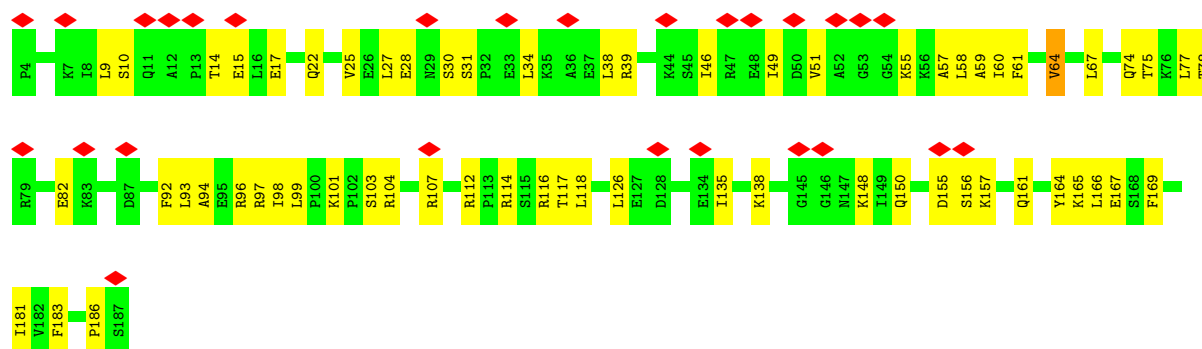


• Molecule 10: 40S ribosomal protein S6-A

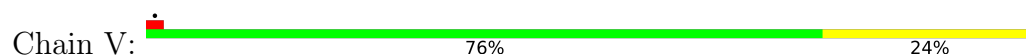


• Molecule 11: 40S ribosomal protein S7-A

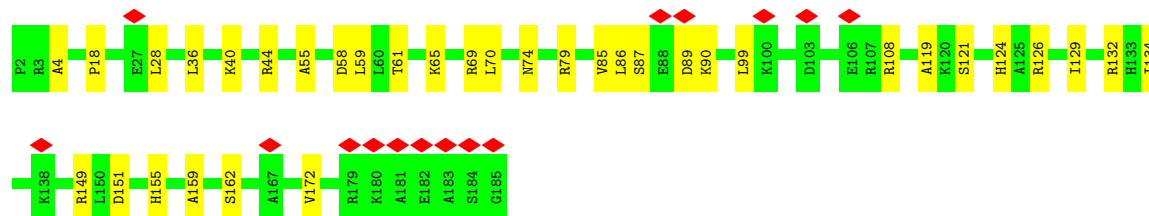
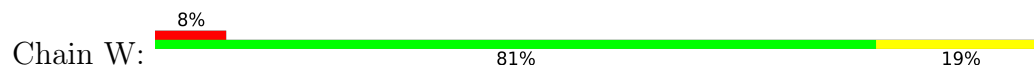




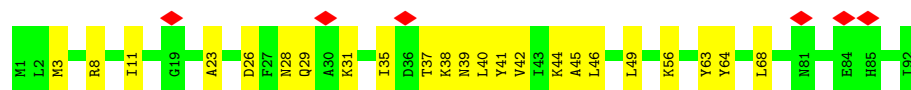
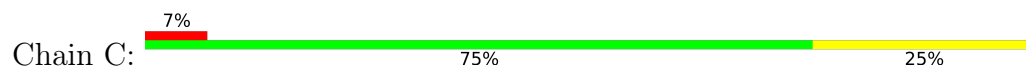
- Molecule 12: 40S ribosomal protein S8



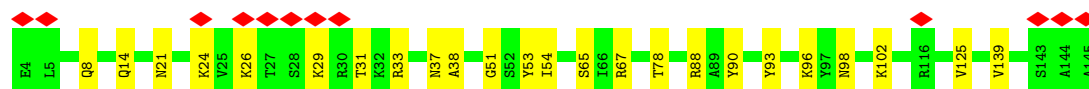
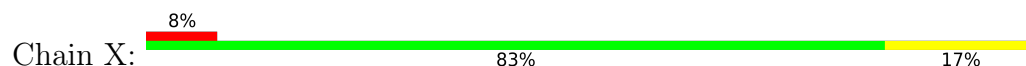
- Molecule 13: 40S ribosomal protein S9-A



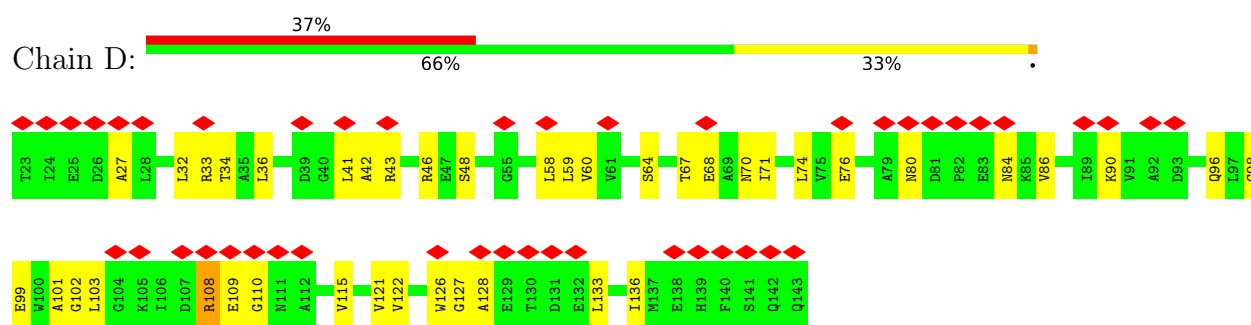
- Molecule 14: 40S ribosomal protein S10-A



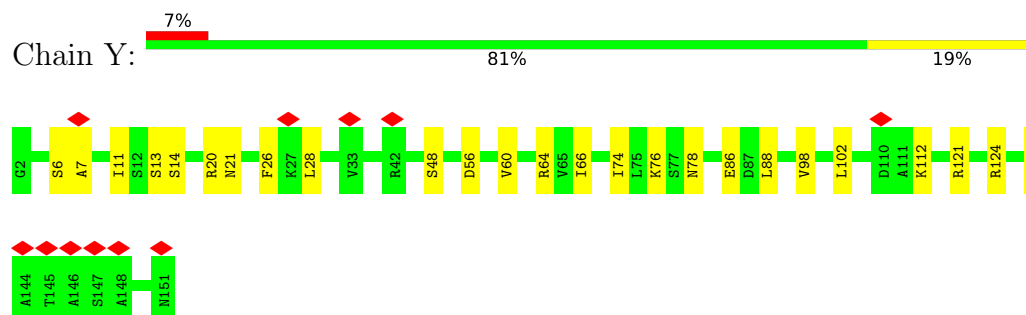
- Molecule 15: 40S ribosomal protein S11-A



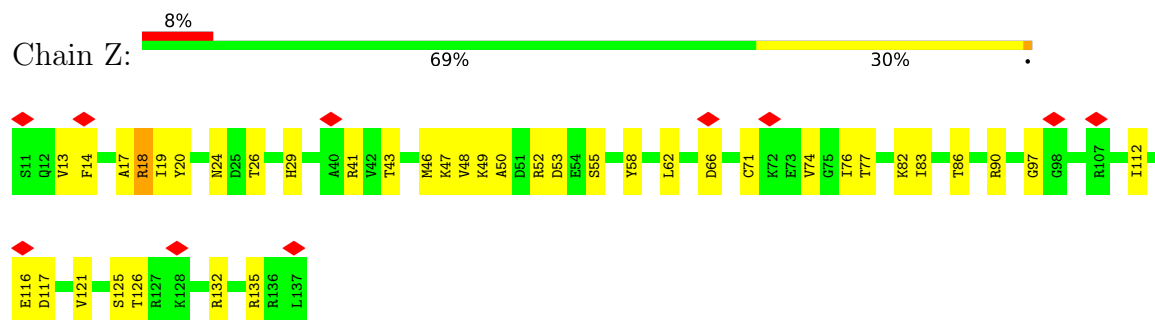
- Molecule 16: 40S ribosomal protein S12



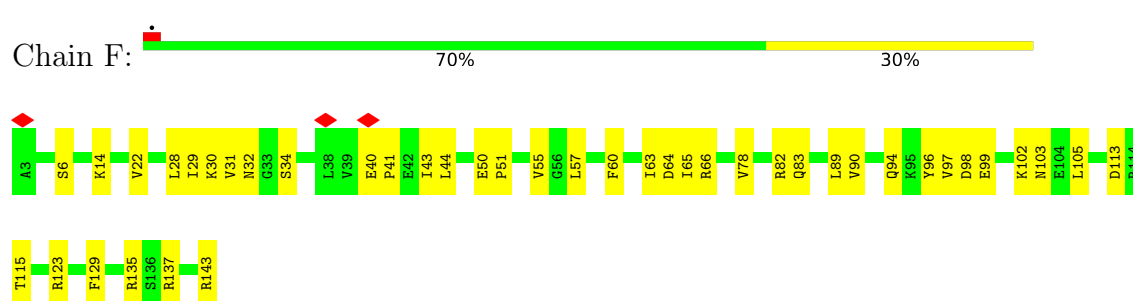
• Molecule 17: 40S ribosomal protein S13



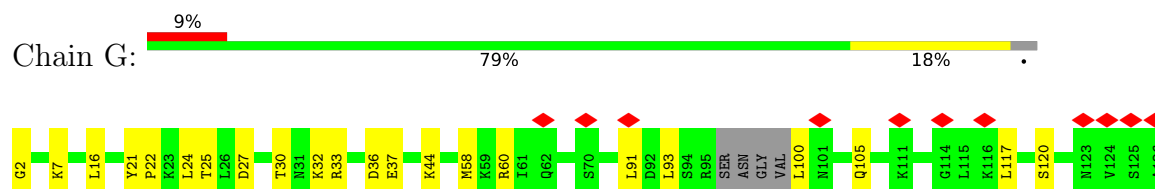
• Molecule 18: 40S ribosomal protein S14-B



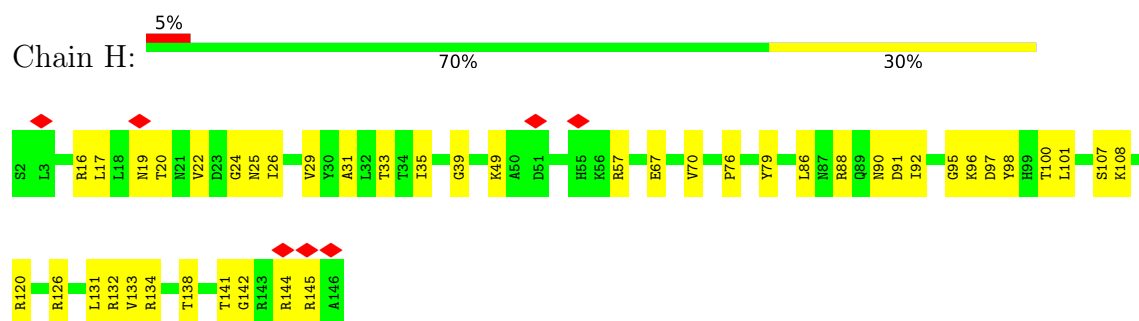
• Molecule 19: 40S ribosomal protein S16-A



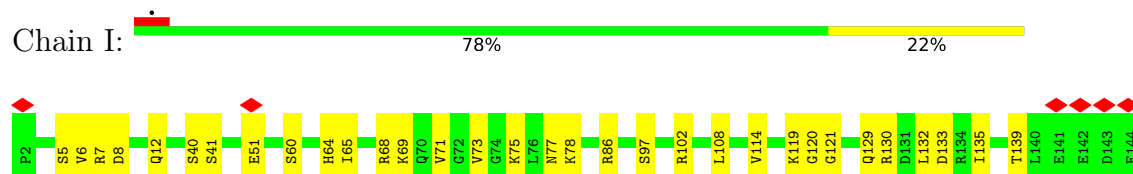
• Molecule 20: 40S ribosomal protein S17-B



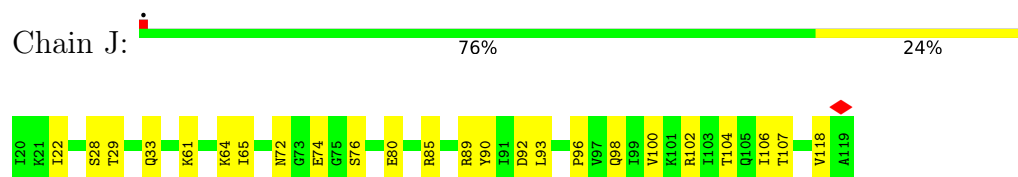
- Molecule 21: 40S ribosomal protein S18-A



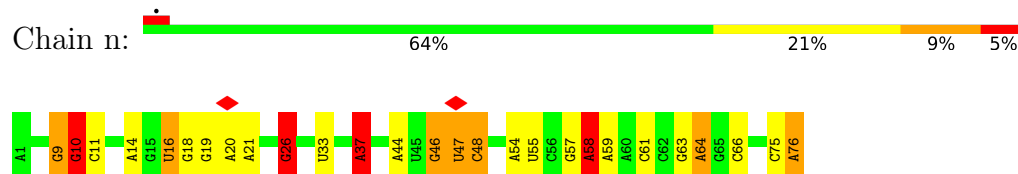
- Molecule 22: 40S ribosomal protein S19-A



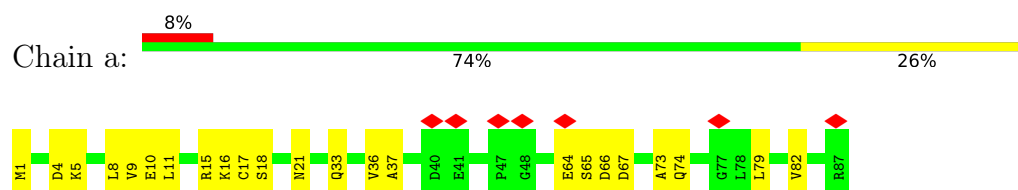
- Molecule 23: 40S ribosomal protein S20



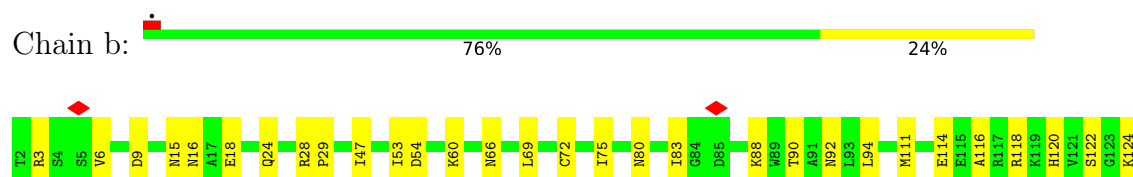
- Molecule 24: P-site tRNA



- Molecule 25: 40S ribosomal protein S21-A



- Molecule 26: 40S ribosomal protein S22-A





- Molecule 27: 40S ribosomal protein S23-A

Chain c: 79% 21%



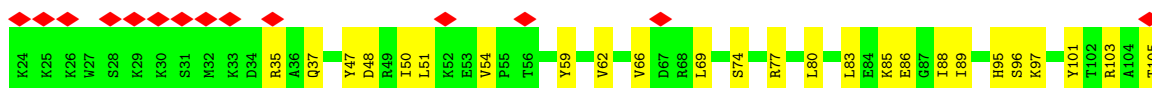
- Molecule 28: 40S ribosomal protein S24-A

Chain d: 10% 74% 26%



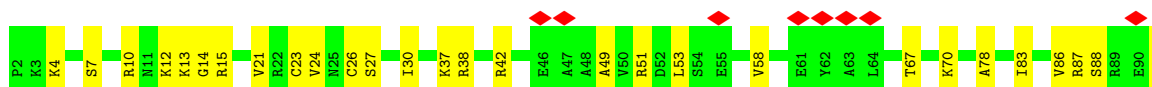
- Molecule 29: 40S ribosomal protein S25-A

Chain K: 17% 70% 30%



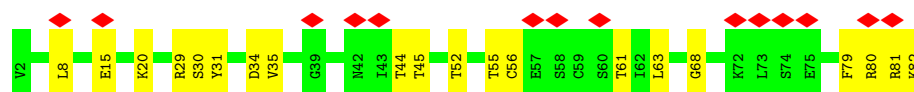
- Molecule 30: 40S ribosomal protein S26-B

Chain e: 8% 70% 30%



- Molecule 31: 40S ribosomal protein S27-A

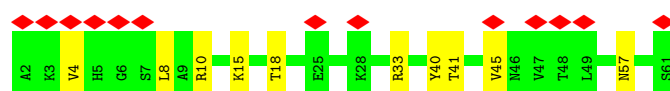
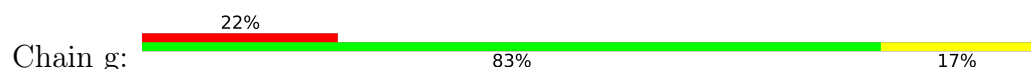
Chain f: 17% 75% 25%



- Molecule 32: 40S ribosomal protein S29-A



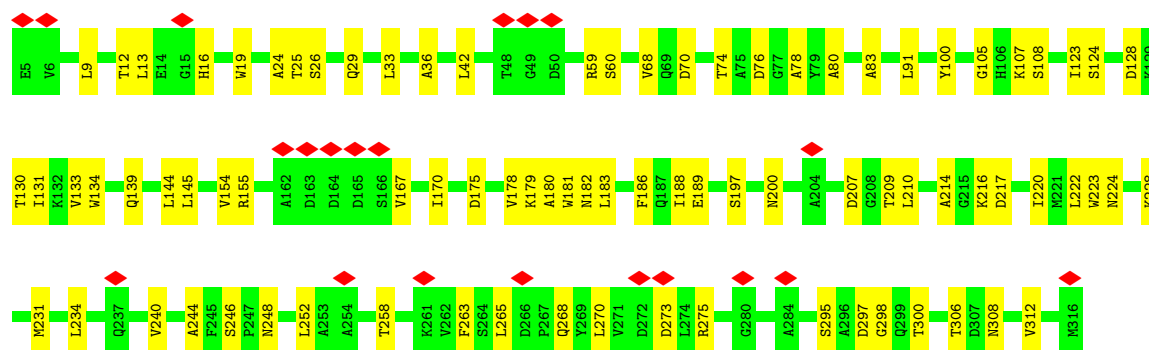
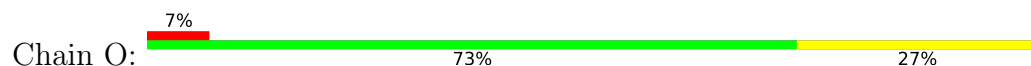
- Molecule 33: 40S ribosomal protein S30-A



- Molecule 34: Ubiquitin-40S ribosomal protein S31

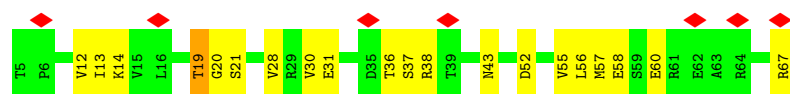


- Molecule 35: Guanine nucleotide-binding protein subunit beta-like protein

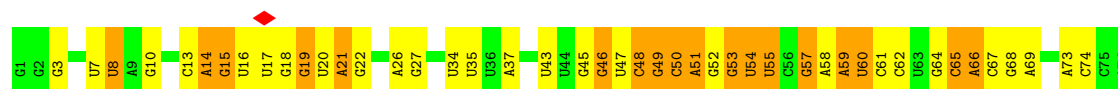


- Molecule 36: 40S ribosomal protein S28-A

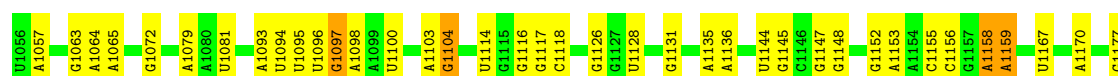
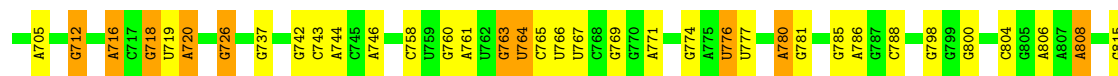
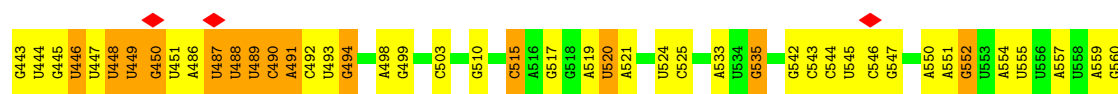
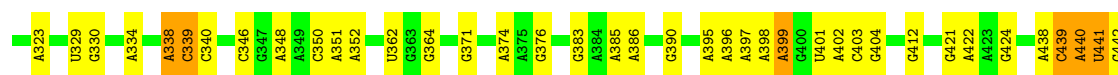




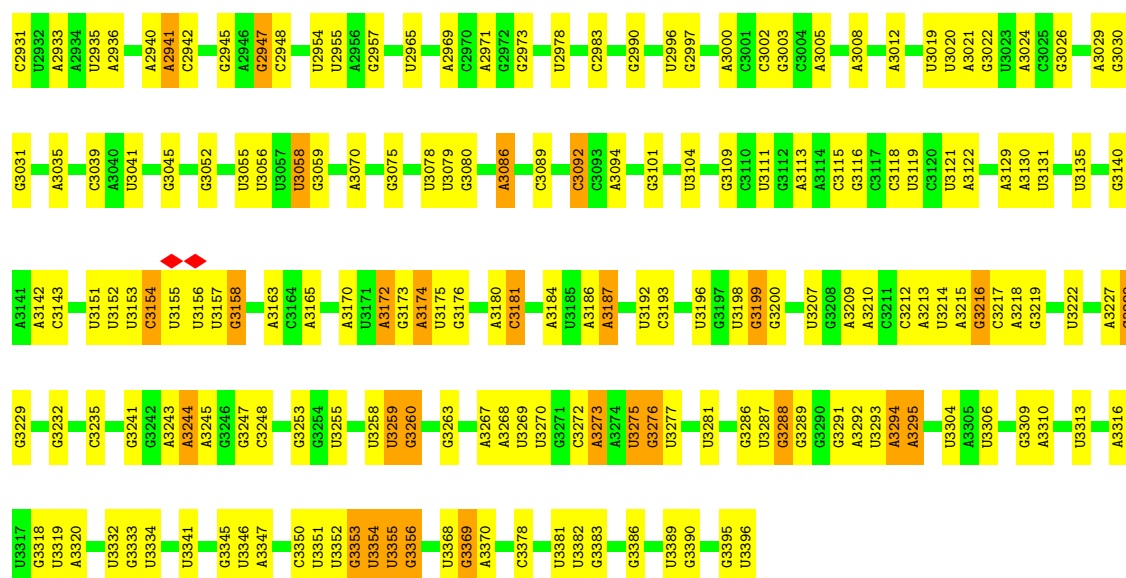
• Molecule 37: A-site tRNA



• Molecule 38: 25S rRNA



U2818	A2702	U2347	A2232	G1935	A1797	G1671	G1565	A1446	G1345	A1251	G1178
A2819	A2703	G2363	C2237	C1943	A1798	G1677	A1566	G1447	G1346	A1252	A1179
A2820	A2704	G2364	C2244	C1949	G1808	A1683	U1568	G1450	U1348	U1263	A1180
C2821	G2713	A2361	C2245	U1950	A1813	U1684	U1569	U1455	A1349	C1264	A1182
A2838	G2714	G2364	C2249	G1951	A1814	G1685	U1572	G1473	A1350	C1255	G1186
U2842	U2717	C2365	G2250	G1952	A1815	U1686	C1573	G1477	U1351	C1257	C1187
U2843	U2718	C2366	G2251	G1953	A1816	U1687	C1574	A1481	A1352	U1258	U1188
C2844	U2719	A2372	G2252	G1954	A1817	U1688	A1575	A1482	U1353	G1261	C1189
A2845	G2722	A2373	A2251	U1955	U1818	A1696	G1576	A1483	A1354	G1262	A1190
U2846	U2723	C2374	A2256	C2101	U1819	A1704	A1580	U1484	U1355	A1263	U1191
A2847	U2724	G2375	G2261	U2102	U1820	U1705	C1581	G1488	U1356	C1192	A1193
G2848	C2726	G2376	A2262	G2111	U1821	U1716	C1582	G1489	U1361	U1265	C1196
C2849	U2727	G2377	C2263	U2112	C1822	U1717	A1589	G1488	G1362	U1267	A1197
C2852	A2727	G2385	G2270	A2113	U1824	G1712	A1587	G1488	U1363	U1268	C1198
C2853	G2728	U2388	A2271	C2118	G1825	A1715	A1588	G1492	C1364	U1269	A1200
U2854	C2729	G2392	G2272	G2121	U1831	U1716	A1589	C1497	U1373	C1270	C1201
U2855	G2730	G2393	G2273	G2122	C1832	U1717	G1590	C1497	A1273	A1274	A1202
U2856	C2741	G2394	U2274	G2123	G1833	U1721	G1592	A1503	C1275	U1276	G1206
U2861	G2745	A2397	A2279	A2131	A1839	U1722	G1598	C1508	U1277	U1208	G1207
C2867	A2746	G2397	A2280	A2139	U1840	U1723	A1602	U1511	A1386	C1279	U1209
U2868	U2747	A2402	A2281	A2147	A1841	G1725	A1603	U1517	A1390	C1279	U1210
C2869	A2748	G2403	G2282	A2148	A1842	A1729	G1604	G1517	C1391	C1280	A1217
U2870	G2749	G2404	G2283	U2149	C1846	G1748	U1606	G1521	G1392	G1281	U1218
C2871	U2752	U2411	C2284	U2154	C1849	U1749	U1606	U1522	A1399	G1282	C1219
A2872	G2753	G2412	U2286	G2155	A1850	A1750	A1613	U1523	G1400	G1285	A1222
U2873	U2754	A2419	C2287	A2158	A1859	G1751	U1620	G1528	C1403	A1286	A1223
U2874	C2755	G2422	G2288	G2159	C1866	G1756	A1621	G1529	G1404	A1287	C1227
U2875	G2756	U2423	U2292	G2169	A1867	U1760	U1624	U1530	U1293	G1228	G1229
C2876	U2757	G2424	C2293	G2170	G1868	C1761	A1625	U1533	G1294	A1231	A1232
U2887	U2758	A2424	U2294	G2185	A1874	U1763	U1629	G1536	G1412	U1299	G1233
U2888	C2764	U2434	A2303	G2186	C1875	U1764	U1630	G1542	G1417	G1306	G1234
C2894	U2767	G2435	G2303	U2187	U1876	U1765	C1631	G1543	A1418	G1307	U1235
G2895	U2768	U2436	C2306	G2187	U1876	U1766	A1632	U1549	A1419	A1308	G1236
A2896	G2769	G2437	G2307	A2188	U1880	G1766	C1633	C1550	G1420	U1309	G1237
C2898	U2777	U2438	C2308	C2196	A1881	G1770	G1634	C1551	U1427	C1312	C1238
U2899	G2778	A2439	A2309	G2199	A1893	G1775	A1638	C1551	A1428	G1313	C1239
G2901	A2785	G2440	U2310	G2201	A1896	G1778	C1639	U1555	G1429	U1241	U1241
A2910	G2796	A2445	A2313	U2205	G1897	C1779	A1642	C1557	G1431	U1315	G1242
U2916	A2800	U2446	G2314	G2206	U1898	G1780	A1643	A1559	G1434	A1317	G1243
G2917	A2801	G2451	U2315	A2207	G1899	C1788	C1644	G1560	A1437	A1318	A1244
C2918	A2802	G2452	G2316	G2208	A1906	U1793	U1645	G1561	U1322	A1319	A1245
A2803	A2803	C2492	A2320	U2209	A1907	C1788	G1646	C1562	U1442	U1322	G1246
A2804	G2805	G2493	A2324	G2218	A1908	G1793	G1646	C1563	G1443	U1325	U1247
U2923	U2924	U2494	U2334	G2218	A1908	U1794	C1657	C1564	U1443	G1248	G1248
U2924	C2925	G2495	G2335	A2223	A1930	U1795	G1658	U1564		A1330	
C2925	C2928	U2496	C2339	C2231		G1796					
U2928		U2497									
C2928		U2498									



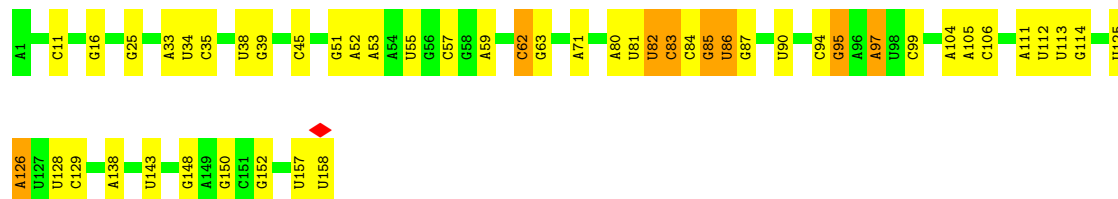
• Molecule 39: 5S rRNA

Chain BR: 71% 27%



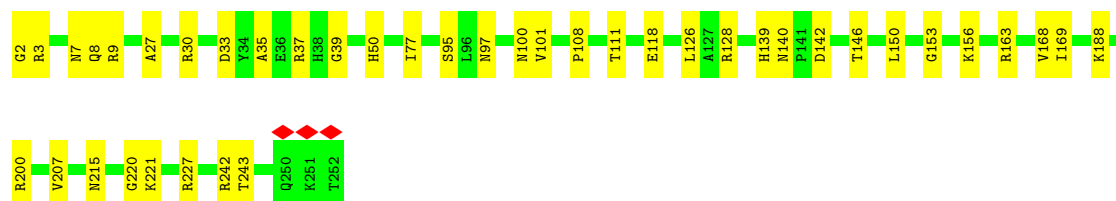
• Molecule 40: 5.8S rRNA

Chain BS: 69% 26% 5%



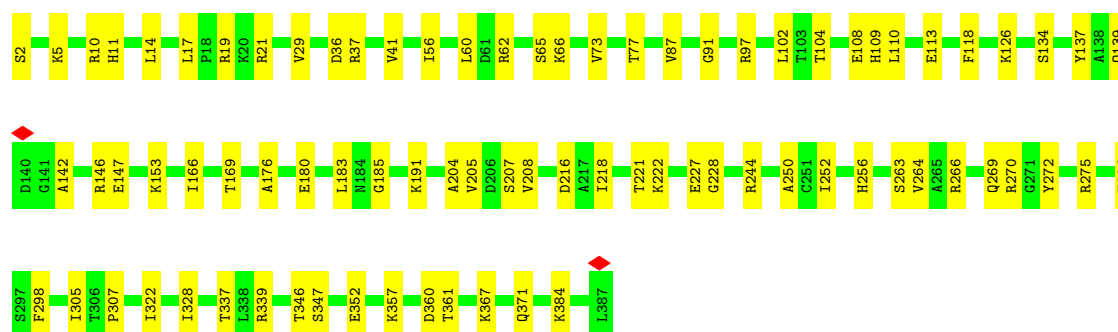
• Molecule 41: 60S ribosomal protein L2-A

Chain AW: 84% 16%

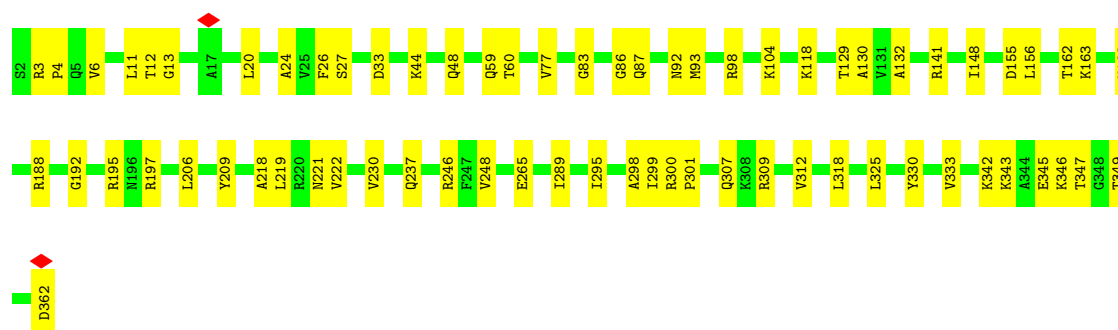
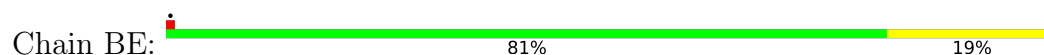


• Molecule 42: 60S ribosomal protein L3

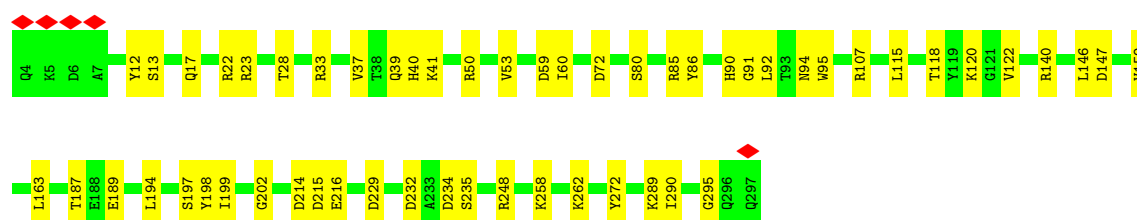
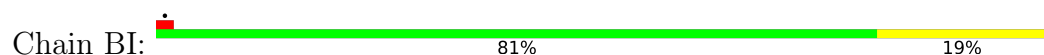
Chain BA: 79% 21%



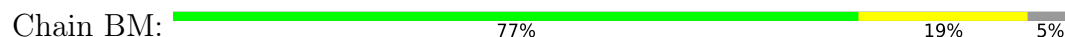
• Molecule 43: 60S ribosomal protein L4-A



• Molecule 44: 60S ribosomal protein L5

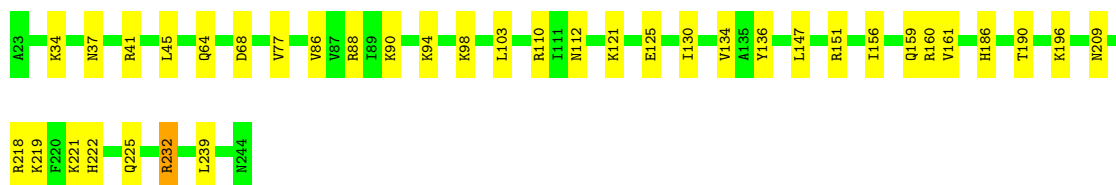


• Molecule 45: 60S ribosomal protein L6-B



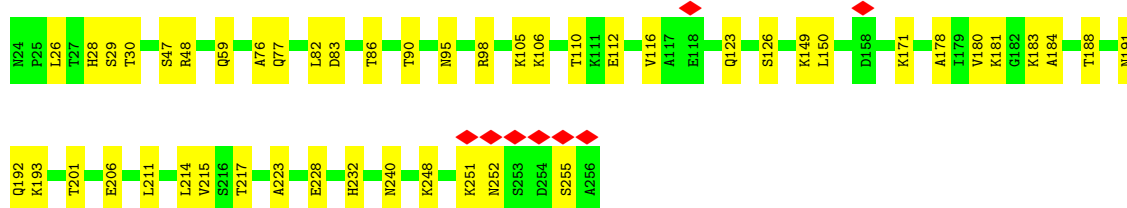
• Molecule 46: 60S ribosomal protein L7-A





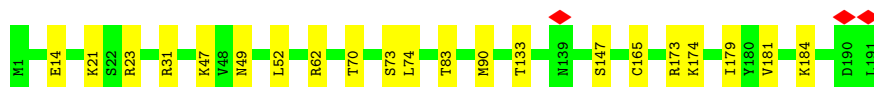
- Molecule 47: 60S ribosomal protein L8-A

Chain AA: 79% 21%



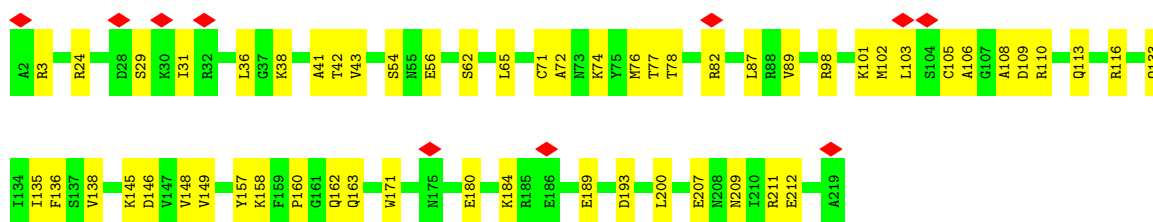
- Molecule 48: 60S ribosomal protein L9-A

Chain AD: 89% 11%



- Molecule 49: 60S ribosomal protein L10

Chain BD: 5% 74% 26%



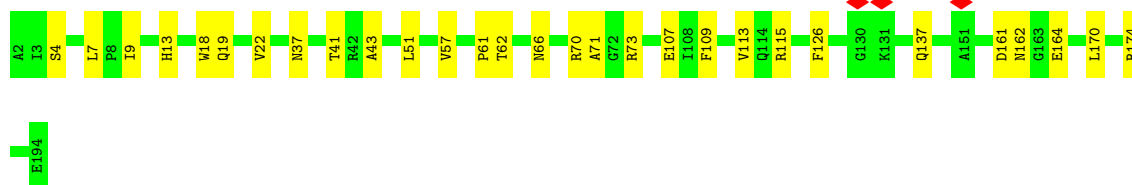
- Molecule 50: 60S ribosomal protein L11-B

Chain AG: 78% 22%



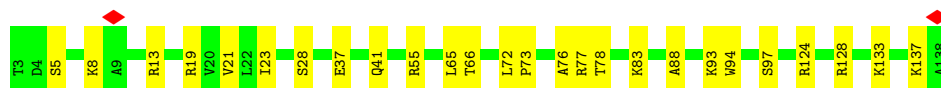
- Molecule 51: 60S ribosomal protein L13-A

Chain AJ:  85% 15%



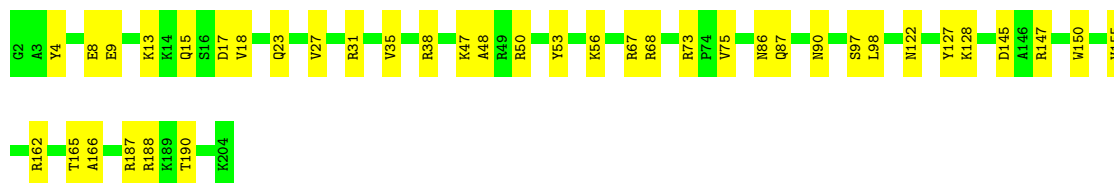
- Molecule 52: 60S ribosomal protein L14-A

Chain AM:  81% 19%



- Molecule 53: 60S ribosomal protein L15-A

Chain AQ:  81% 19%



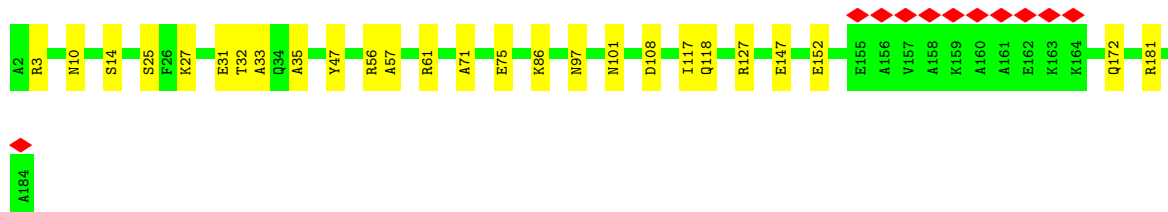
- Molecule 54: 60S ribosomal protein L16-A

Chain AU:  87% 13%



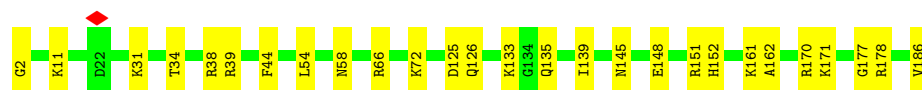
- Molecule 55: 60S ribosomal protein L17-A

Chain AX:  6% 86% 14%

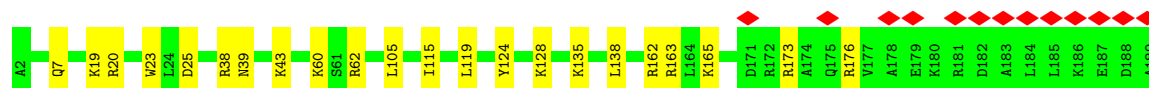
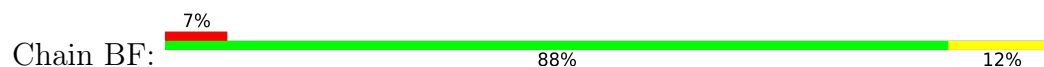


- Molecule 56: 60S ribosomal protein L18-A

Chain BB:  85% 15%



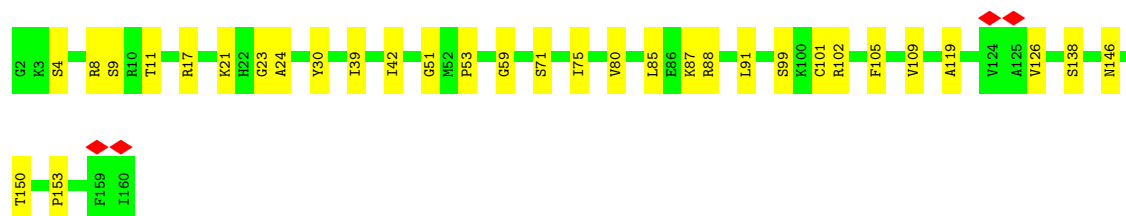
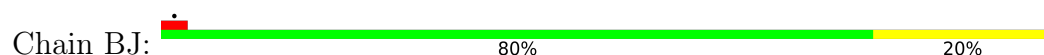
- Molecule 57: 60S ribosomal protein L19-A



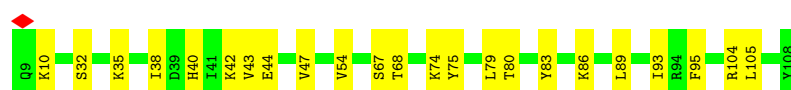
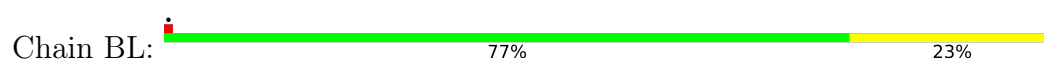
- Molecule 58: 60S ribosomal protein L20-A



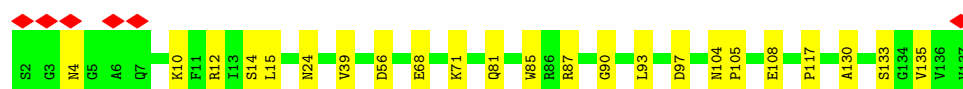
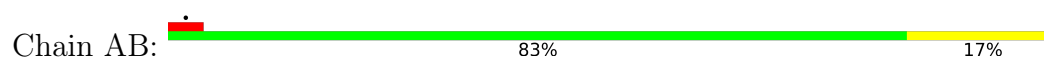
- Molecule 59: 60S ribosomal protein L21-A



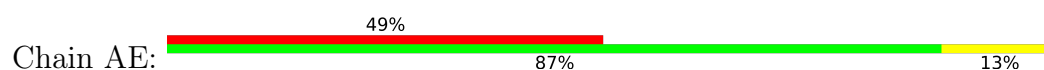
- Molecule 60: 60S ribosomal protein L22-A



- Molecule 61: 60S ribosomal protein L23-A



- Molecule 62: 60S ribosomal protein L24-A





- Molecule 63: 60S ribosomal protein L25

Chain AH: 88% 12%



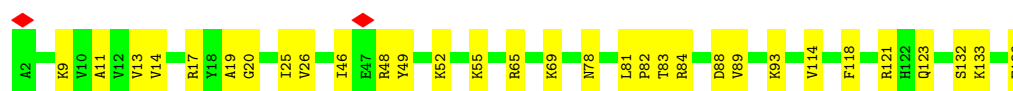
- Molecule 64: 60S ribosomal protein L26-A

Chain AK: 76% 24%



- Molecule 65: 60S ribosomal protein L27-A

Chain AN: 77% 23%



- Molecule 66: 60S ribosomal protein L28

Chain AR: 82% 18%



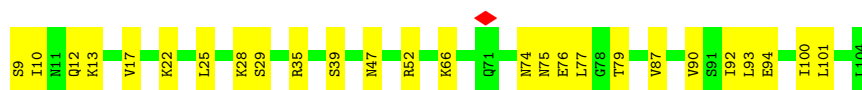
- Molecule 67: 60S ribosomal protein L29

Chain AV: 83% 16%

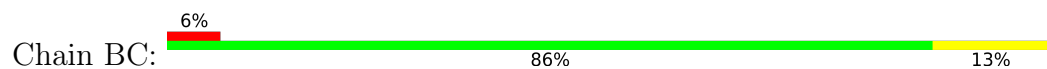


- Molecule 68: 60S ribosomal protein L30

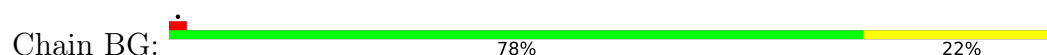
Chain AY: 73% 27%



- Molecule 69: 60S ribosomal protein L31-A



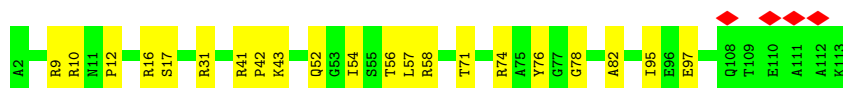
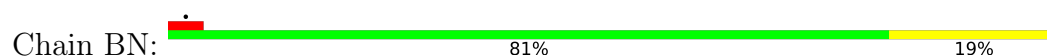
- Molecule 70: 60S ribosomal protein L32



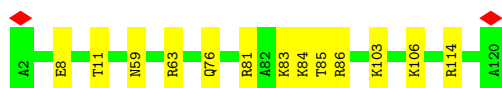
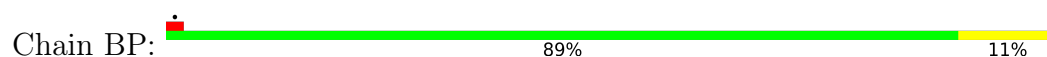
- Molecule 71: 60S ribosomal protein L33-A



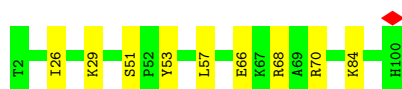
- Molecule 72: 60S ribosomal protein L34-A



- Molecule 73: 60S ribosomal protein L35-A

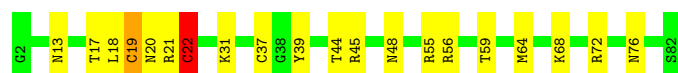


- Molecule 74: 60S ribosomal protein L36-A



- Molecule 75: 60S ribosomal protein L37-A

Chain AF:  75% 22% ..



- Molecule 76: 60S ribosomal protein L38

Chain AI:  6% 75% 25%



- Molecule 77: 60S ribosomal protein L39

Chain AL:  76% 24%



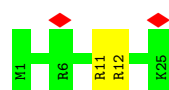
- Molecule 78: Ubiquitin-60S ribosomal protein L40

Chain AO:  67% 29% .



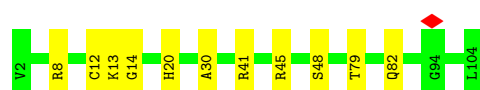
- Molecule 79: 60S ribosomal protein L41-A

Chain AS:  8% 92% 8%



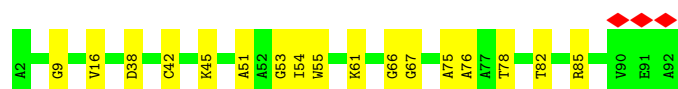
- Molecule 80: 60S ribosomal protein L42-A

Chain AP:  89% 11%

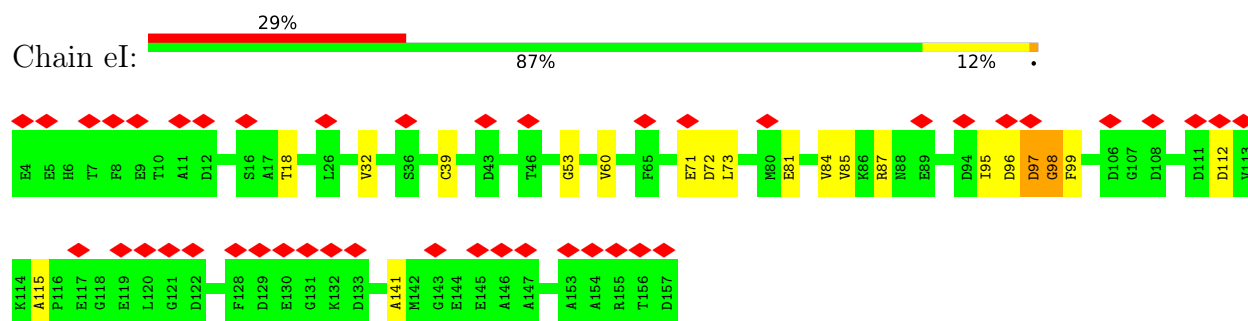


- Molecule 81: 60S ribosomal protein L43-A

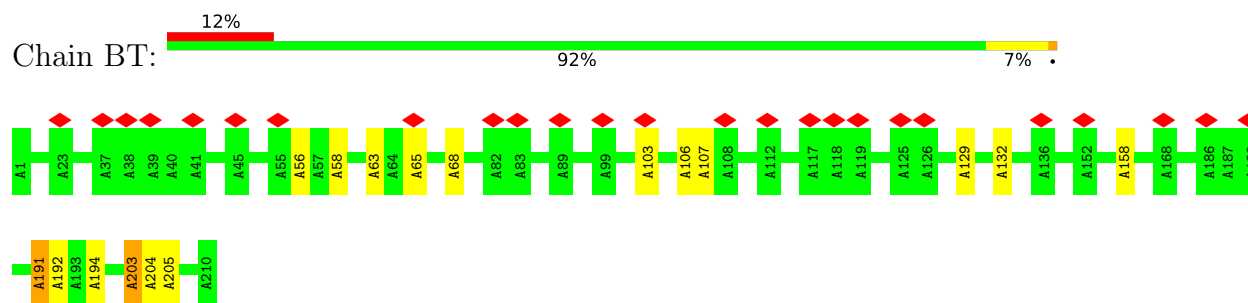
Chain AT:  81% 19%



- Molecule 82: Eukaryotic translation initiation factor 5A-1



- Molecule 83: 60S ribosomal protein L1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50989	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.374	Depositor
Minimum map value	-0.157	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.035	Depositor
Map size ($\text{\AA}$)	520.32, 520.32, 520.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, 1MG, M2G, 5MC, G7M, 5CT, SPD, T6A, ZN, 3HE, 1MA

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	2	0.33	0/42211	0.44	2/65773 (0.0%)
2	l	0.33	0/147	0.34	0/227
3	P	0.29	0/1644	0.51	0/2249
4	Q	0.29	0/1823	0.60	2/2447 (0.1%)
5	E	0.28	0/936	0.57	0/1259
6	R	0.38	0/1656	0.55	0/2251
7	A	0.33	0/1754	0.53	0/2361
8	S	0.32	0/2097	0.56	0/2823
9	B	0.29	0/1625	0.55	0/2197
10	T	0.29	0/1839	0.55	0/2460
11	U	0.27	0/1498	0.56	0/2019
12	V	0.35	0/1501	0.53	0/2006
13	W	0.30	0/1504	0.57	0/2016
14	C	0.25	0/769	0.50	0/1039
15	X	0.37	0/1168	0.48	0/1575
16	D	0.24	0/883	0.62	0/1199
17	Y	0.36	0/1215	0.58	0/1638
18	Z	0.32	0/934	0.58	0/1257
19	F	0.33	0/1125	0.54	0/1510
20	G	0.29	0/957	0.47	0/1283
21	H	0.27	0/1207	0.49	0/1623
22	I	0.31	0/1130	0.55	1/1517 (0.1%)
23	J	0.33	0/807	0.52	0/1091
24	n	0.61	6/1621 (0.4%)	0.42	0/2525
25	a	0.29	0/682	0.51	0/921
26	b	0.38	0/1038	0.56	1/1395 (0.1%)
27	c	0.42	0/1139	0.59	0/1518
28	d	0.26	0/1046	0.45	0/1401
29	K	0.25	0/661	0.52	0/888
30	e	0.39	0/778	0.58	0/1042
31	f	0.26	0/620	0.50	0/838
32	M	0.40	0/452	0.65	0/600

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.30	0/480	0.53	0/639
34	N	0.25	0/567	0.59	0/764
35	O	0.25	0/2436	0.51	0/3318
36	L	0.29	0/493	0.60	0/663
37	m	0.30	0/1799	0.50	0/2801
38	BQ	0.49	0/76214	0.46	0/118821
39	BR	0.38	0/2883	0.39	0/4491
40	BS	0.50	0/3746	0.46	0/5832
41	AW	0.64	0/1933	0.61	0/2598
42	BA	0.56	0/3146	0.57	0/4228
43	BE	0.55	0/2800	0.61	0/3790
44	BI	0.39	0/2400	0.51	0/3239
45	BM	0.43	0/1329	0.57	0/1794
46	BO	0.56	0/1821	0.59	0/2451
47	AA	0.42	0/1836	0.56	0/2481
48	AD	0.39	0/1529	0.50	0/2060
49	BD	0.44	0/1801	0.56	0/2416
50	AG	0.33	0/1367	0.51	0/1834
51	AJ	0.52	0/1568	0.56	0/2106
52	AM	0.43	0/1068	0.55	0/1438
53	AQ	0.66	0/1757	0.63	0/2354
54	AU	0.57	0/1585	0.53	0/2128
55	AX	0.61	0/1439	0.57	0/1938
56	BB	0.54	0/1465	0.57	0/1965
57	BF	0.50	0/1532	0.53	0/2043
58	BH	0.50	0/1473	0.56	0/1980
59	BJ	0.51	0/1296	0.53	0/1739
60	BL	0.36	0/812	0.48	0/1099
61	AB	0.56	0/1018	0.52	0/1369
62	AE	0.42	0/850	0.48	0/1152
63	AH	0.51	0/979	0.54	0/1321
64	AK	0.48	0/995	0.53	0/1329
65	AN	0.41	0/1106	0.53	0/1485
66	AR	0.60	0/1200	0.60	0/1607
67	AV	0.48	0/473	0.58	0/629
68	AY	0.44	0/745	0.47	0/1001
69	BC	0.55	0/890	0.54	0/1196
70	BG	0.59	0/1038	0.56	0/1390
71	BK	0.63	0/868	0.65	0/1168
72	BN	0.57	0/890	0.63	0/1189
73	BP	0.48	0/978	0.53	0/1301
74	AC	0.41	0/772	0.54	0/1026
75	AF	0.76	1/660 (0.2%)	0.88	2/875 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	AI	0.36	0/618	0.50	0/826
77	AL	0.64	0/443	0.58	0/588
78	AO	0.72	1/416 (0.2%)	0.95	2/553 (0.4%)
79	AS	0.49	0/230	0.78	0/296
80	AP	0.74	2/836 (0.2%)	0.75	3/1104 (0.3%)
81	AT	0.72	1/701 (0.1%)	0.80	1/934 (0.1%)
82	eI	0.33	0/1142	0.61	0/1537
83	BT	0.25	0/1049	0.57	0/1467
All	All	0.44	11/219939 (0.0%)	0.50	14/323301 (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
8	S	0	1
9	B	0	1
11	U	0	1
16	D	0	1
18	Z	0	1
19	F	0	1
22	I	0	1
26	b	0	1
34	N	0	1
36	L	0	1
43	BE	0	3
46	BO	0	1
47	AA	0	3
56	BB	0	1
66	AR	0	2
67	AV	0	2
68	AY	0	1
69	BC	0	1
73	BP	0	1
82	eI	0	2
83	BT	0	4
All	All	0	31

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	47	U	C5-C6	7.47	1.49	1.34
24	n	16	U	C5-C6	7.36	1.48	1.34
24	n	47	U	N1-C2	7.29	1.53	1.38
80	AP	14	GLY	C-N	7.22	1.43	1.33
24	n	16	U	N1-C2	7.19	1.52	1.38

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	AP	79	THR	N-CA-C	-7.90	96.42	108.67
78	AO	96	CYS	CA-C-N	6.94	129.46	120.44
78	AO	96	CYS	C-N-CA	6.94	129.46	120.44
75	AF	22	CYS	CA-C-N	6.00	133.17	121.41
75	AF	22	CYS	C-N-CA	6.00	133.17	121.41

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	B	42	LEU	Peptide
16	D	108	ARG	Peptide
8	S	193	GLY	Peptide
11	U	64	VAL	Peptide
18	Z	90	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	2	37739	0	18988	513	0
2	l	131	0	66	3	0
3	P	1603	0	1610	34	0
4	Q	1798	0	1890	62	0
5	E	916	0	941	30	0
6	R	1626	0	1715	39	0
7	A	1729	0	1812	29	0
8	S	2056	0	2140	66	0
9	B	1605	0	1669	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	T	1815	0	1894	41	0
11	U	1473	0	1555	51	0
12	V	1476	0	1501	34	0
13	W	1479	0	1556	26	0
14	C	752	0	719	17	0
15	X	1142	0	1209	19	0
16	D	875	0	878	24	0
17	Y	1192	0	1255	24	0
18	Z	923	0	948	26	0
19	F	1105	0	1166	32	0
20	G	948	0	990	20	0
21	H	1188	0	1218	33	0
22	I	1112	0	1124	25	0
23	J	797	0	863	19	0
24	n	1624	0	836	11	0
25	a	673	0	662	18	0
26	b	1021	0	1060	21	0
27	c	1121	0	1196	26	0
28	d	1032	0	1044	31	0
29	K	651	0	682	18	0
30	e	765	0	814	21	0
31	f	610	0	633	15	0
32	M	442	0	428	20	0
33	g	472	0	521	11	0
34	N	556	0	549	28	0
35	O	2383	0	2332	56	0
36	L	491	0	524	14	0
37	m	1611	0	817	24	0
38	BQ	68091	0	34217	530	0
39	BR	2579	0	1304	20	0
40	BS	3353	0	1695	26	0
41	AW	1899	0	1957	33	0
42	BA	3075	0	3142	60	0
43	BE	2748	0	2859	55	0
44	BI	2351	0	2294	41	0
45	BM	1307	0	1377	24	0
46	BO	1784	0	1862	28	0
47	AA	1804	0	1877	33	0
48	AD	1508	0	1572	17	0
49	BD	1764	0	1804	39	0
50	AG	1346	0	1370	27	0
51	AJ	1543	0	1608	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AM	1053	0	1149	22	0
53	AQ	1720	0	1779	27	0
54	AU	1555	0	1659	20	0
55	AX	1416	0	1433	19	0
56	BB	1441	0	1543	20	0
57	BF	1515	0	1606	20	0
58	BH	1437	0	1475	20	0
59	BJ	1272	0	1312	26	0
60	BL	796	0	812	15	0
61	AB	1003	0	1048	18	0
62	AE	836	0	706	12	0
63	AH	964	0	1025	11	0
64	AK	984	0	1075	20	0
65	AN	1080	0	1122	22	0
66	AR	1169	0	1211	21	0
67	AV	462	0	491	7	0
68	AY	737	0	792	17	0
69	BC	876	0	912	9	0
70	BG	1017	0	1081	21	0
71	BK	850	0	880	12	0
72	BN	880	0	942	20	0
73	BP	969	0	1078	9	0
74	AC	766	0	844	7	0
75	AF	645	0	645	16	0
76	AI	612	0	682	16	0
77	AL	436	0	475	12	0
78	AO	410	0	442	13	0
79	AS	229	0	273	2	0
80	AP	824	0	890	10	0
81	AT	694	0	734	14	0
82	eI	1143	0	1108	13	0
83	BT	1050	0	1052	8	0
84	AF	1	0	0	0	0
84	AO	1	0	0	0	0
84	AP	1	0	0	0	0
84	AT	1	0	0	0	0
84	BN	1	0	0	0	0
84	M	1	0	0	0	0
84	N	1	0	0	0	0
85	BQ	10	0	19	1	0
86	BQ	20	0	23	3	0
All	All	204962	0	151061	2358	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 7.

The worst 5 of 2358 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)
34:N:123:ASN:ND2	34:N:125:THR:OG1	1.81	1.13
81:AT:53:GLY:HA2	81:AT:66:GLY:O	1.61	1.00
1:2:219:A:H61	1:2:842:C:H42	1.03	0.96
38:BQ:383:G:N2	38:BQ:386:A:N7	2.15	0.93
37:m:7:U:O4	37:m:49:G:O6	1.89	0.91

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	
3	P	204/206 (99%)	181 (89%)	23 (11%)	0	100	100
4	Q	222/232 (96%)	196 (88%)	26 (12%)	0	100	100
5	E	115/117 (98%)	100 (87%)	15 (13%)	0	100	100
6	R	214/216 (99%)	189 (88%)	25 (12%)	0	100	100
7	A	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
8	S	256/258 (99%)	224 (88%)	32 (12%)	0	100	100
9	B	204/206 (99%)	189 (93%)	15 (7%)	0	100	100
10	T	226/228 (99%)	211 (93%)	15 (7%)	0	100	100
11	U	182/184 (99%)	160 (88%)	22 (12%)	0	100	100
12	V	183/187 (98%)	164 (90%)	19 (10%)	0	100	100
13	W	182/184 (99%)	162 (89%)	19 (10%)	1 (0%)	24	57
14	C	90/92 (98%)	77 (86%)	13 (14%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	X	140/142 (99%)	125 (89%)	15 (11%)	0	100	100
16	D	119/121 (98%)	89 (75%)	29 (24%)	1 (1%)	16	47
17	Y	148/150 (99%)	131 (88%)	17 (12%)	0	100	100
18	Z	125/127 (98%)	108 (86%)	16 (13%)	1 (1%)	16	47
19	F	139/141 (99%)	124 (89%)	15 (11%)	0	100	100
20	G	117/125 (94%)	112 (96%)	5 (4%)	0	100	100
21	H	143/145 (99%)	129 (90%)	14 (10%)	0	100	100
22	I	141/143 (99%)	128 (91%)	13 (9%)	0	100	100
23	J	98/100 (98%)	88 (90%)	10 (10%)	0	100	100
25	a	85/87 (98%)	72 (85%)	13 (15%)	0	100	100
26	b	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
27	c	142/144 (99%)	122 (86%)	20 (14%)	0	100	100
28	d	132/134 (98%)	123 (93%)	9 (7%)	0	100	100
29	K	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
30	e	95/97 (98%)	85 (90%)	10 (10%)	0	100	100
31	f	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
32	M	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
33	g	58/60 (97%)	48 (83%)	10 (17%)	0	100	100
34	N	71/73 (97%)	48 (68%)	23 (32%)	0	100	100
35	O	310/312 (99%)	265 (86%)	45 (14%)	0	100	100
36	L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
41	AW	249/251 (99%)	220 (88%)	29 (12%)	0	100	100
42	BA	384/386 (100%)	354 (92%)	30 (8%)	0	100	100
43	BE	359/361 (99%)	321 (89%)	37 (10%)	1 (0%)	36	67
44	BI	292/294 (99%)	268 (92%)	24 (8%)	0	100	100
45	BM	163/175 (93%)	146 (90%)	17 (10%)	0	100	100
46	BO	220/222 (99%)	205 (93%)	15 (7%)	0	100	100
47	AA	231/233 (99%)	209 (90%)	22 (10%)	0	100	100
48	AD	189/191 (99%)	172 (91%)	17 (9%)	0	100	100
49	BD	216/218 (99%)	188 (87%)	28 (13%)	0	100	100
50	AG	167/169 (99%)	155 (93%)	12 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	AJ	191/193 (99%)	169 (88%)	21 (11%)	1 (0%)	24	57
52	AM	134/136 (98%)	120 (90%)	14 (10%)	0	100	100
53	AQ	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
54	AU	195/197 (99%)	186 (95%)	9 (5%)	0	100	100
55	AX	181/183 (99%)	165 (91%)	16 (9%)	0	100	100
56	BB	183/185 (99%)	170 (93%)	13 (7%)	0	100	100
57	BF	186/188 (99%)	178 (96%)	8 (4%)	0	100	100
58	BH	169/171 (99%)	157 (93%)	12 (7%)	0	100	100
59	BJ	157/159 (99%)	142 (90%)	15 (10%)	0	100	100
60	BL	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
61	AB	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
62	AE	124/126 (98%)	106 (86%)	18 (14%)	0	100	100
63	AH	119/121 (98%)	109 (92%)	10 (8%)	0	100	100
64	AK	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
65	AN	133/135 (98%)	118 (89%)	15 (11%)	0	100	100
66	AR	146/148 (99%)	128 (88%)	18 (12%)	0	100	100
67	AV	56/58 (97%)	46 (82%)	10 (18%)	0	100	100
68	AY	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
69	BC	107/109 (98%)	92 (86%)	15 (14%)	0	100	100
70	BG	125/127 (98%)	114 (91%)	11 (9%)	0	100	100
71	BK	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
72	BN	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
73	BP	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
74	AC	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
75	AF	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
76	AI	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
77	AL	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
78	AO	50/52 (96%)	43 (86%)	7 (14%)	0	100	100
79	AS	23/25 (92%)	23 (100%)	0	0	100	100
80	AP	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
81	AT	89/91 (98%)	85 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
82	eI	151/154 (98%)	119 (79%)	31 (20%)	1 (1%)	18	49
83	BT	208/210 (99%)	177 (85%)	30 (14%)	1 (0%)	24	57
All	All	11337/11516 (98%)	10193 (90%)	1137 (10%)	7 (0%)	49	78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	D	109	GLU
82	eI	98	GLY
43	BE	4	PRO
83	BT	204	ALA
18	Z	18	ARG

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	
3	P	170/173 (98%)	170 (100%)	0	100	100
4	Q	200/205 (98%)	200 (100%)	0	100	100
5	E	95/98 (97%)	95 (100%)	0	100	100
6	R	175/175 (100%)	175 (100%)	0	100	100
7	A	182/182 (100%)	181 (100%)	1 (0%)	81	85
8	S	220/220 (100%)	220 (100%)	0	100	100
9	B	172/173 (99%)	172 (100%)	0	100	100
10	T	189/195 (97%)	189 (100%)	0	100	100
11	U	163/165 (99%)	163 (100%)	0	100	100
12	V	148/149 (99%)	148 (100%)	0	100	100
13	W	156/157 (99%)	156 (100%)	0	100	100
14	C	77/85 (91%)	77 (100%)	0	100	100
15	X	126/127 (99%)	126 (100%)	0	100	100
16	D	88/98 (90%)	88 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	127/127 (100%)	127 (100%)	0	100	100
18	Z	90/96 (94%)	90 (100%)	0	100	100
19	F	117/117 (100%)	117 (100%)	0	100	100
20	G	101/113 (89%)	101 (100%)	0	100	100
21	H	127/128 (99%)	127 (100%)	0	100	100
22	I	115/115 (100%)	115 (100%)	0	100	100
23	J	93/93 (100%)	93 (100%)	0	100	100
25	a	71/74 (96%)	71 (100%)	0	100	100
26	b	110/110 (100%)	110 (100%)	0	100	100
27	c	119/119 (100%)	119 (100%)	0	100	100
28	d	102/112 (91%)	102 (100%)	0	100	100
29	K	67/73 (92%)	67 (100%)	0	100	100
30	e	82/83 (99%)	82 (100%)	0	100	100
31	f	70/70 (100%)	70 (100%)	0	100	100
32	M	47/47 (100%)	46 (98%)	1 (2%)	47	71
33	g	50/51 (98%)	50 (100%)	0	100	100
34	N	56/63 (89%)	56 (100%)	0	100	100
35	O	250/257 (97%)	250 (100%)	0	100	100
36	L	55/56 (98%)	55 (100%)	0	100	100
41	AW	190/193 (98%)	190 (100%)	0	100	100
42	BA	318/322 (99%)	317 (100%)	1 (0%)	86	87
43	BE	288/288 (100%)	287 (100%)	1 (0%)	86	87
44	BI	241/243 (99%)	241 (100%)	0	100	100
45	BM	139/154 (90%)	139 (100%)	0	100	100
46	BO	186/186 (100%)	186 (100%)	0	100	100
47	AA	187/191 (98%)	187 (100%)	0	100	100
48	AD	168/171 (98%)	168 (100%)	0	100	100
49	BD	185/185 (100%)	185 (100%)	0	100	100
50	AG	145/147 (99%)	145 (100%)	0	100	100
51	AJ	154/154 (100%)	154 (100%)	0	100	100
52	AM	107/107 (100%)	107 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	AQ	175/175 (100%)	174 (99%)	1 (1%)	78	83
54	AU	160/160 (100%)	160 (100%)	0	100	100
55	AX	138/145 (95%)	138 (100%)	0	100	100
56	BB	150/150 (100%)	150 (100%)	0	100	100
57	BF	152/153 (99%)	152 (100%)	0	100	100
58	BH	155/155 (100%)	155 (100%)	0	100	100
59	BJ	135/136 (99%)	135 (100%)	0	100	100
60	BL	87/87 (100%)	87 (100%)	0	100	100
61	AB	104/104 (100%)	104 (100%)	0	100	100
62	AE	56/108 (52%)	56 (100%)	0	100	100
63	AH	104/105 (99%)	104 (100%)	0	100	100
64	AK	108/108 (100%)	108 (100%)	0	100	100
65	AN	112/115 (97%)	112 (100%)	0	100	100
66	AR	117/118 (99%)	117 (100%)	0	100	100
67	AV	46/46 (100%)	46 (100%)	0	100	100
68	AY	81/81 (100%)	81 (100%)	0	100	100
69	BC	92/96 (96%)	92 (100%)	0	100	100
70	BG	108/109 (99%)	108 (100%)	0	100	100
71	BK	90/90 (100%)	90 (100%)	0	100	100
72	BN	95/95 (100%)	95 (100%)	0	100	100
73	BP	104/104 (100%)	104 (100%)	0	100	100
74	AC	80/81 (99%)	80 (100%)	0	100	100
75	AF	67/67 (100%)	65 (97%)	2 (3%)	36	65
76	AI	68/68 (100%)	68 (100%)	0	100	100
77	AL	45/45 (100%)	45 (100%)	0	100	100
78	AO	45/47 (96%)	43 (96%)	2 (4%)	25	56
79	AS	22/23 (96%)	22 (100%)	0	100	100
80	AP	87/88 (99%)	87 (100%)	0	100	100
81	AT	71/71 (100%)	71 (100%)	0	100	100
82	eI	118/129 (92%)	118 (100%)	0	100	100
All	All	9290/9506 (98%)	9281 (100%)	9 (0%)	87	90

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
78	AO	112	LYS
78	AO	115	CYS
43	BE	12	THR
53	AQ	27	VAL
75	AF	19	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
46	BO	186	HIS
71	BK	106	ASN
48	AD	162	GLN
71	BK	88	ASN
82	eI	91	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1768/1798 (98%)	537 (30%)	53 (2%)
2	l	5/6 (83%)	1 (20%)	0
24	n	74/75 (98%)	19 (25%)	0
37	m	75/76 (98%)	35 (46%)	0
38	BQ	3180/3184 (99%)	722 (22%)	42 (1%)
39	BR	120/121 (99%)	15 (12%)	1 (0%)
40	BS	157/158 (99%)	32 (20%)	3 (1%)
All	All	5379/5418 (99%)	1361 (25%)	99 (1%)

5 of 1361 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	14	C
1	2	25	C
1	2	26	A

5 of 99 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	BQ	763	G
38	BQ	1716	U
38	BQ	873	C
38	BQ	1271	A
38	BQ	2231	C

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

8 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
24	1MG	n	9	24	23,26,27	2.94	8 (34%)	33,39,42	1.83	10 (30%)
82	5CT	eI	51	82	13,14,15	0.91	0	8,15,17	0.80	0
24	1MA	n	58	24	21,25,26	3.04	6 (28%)	30,37,40	2.68	9 (30%)
24	M2G	n	26	24	24,27,28	2.49	9 (37%)	33,40,43	1.84	9 (27%)
24	T6A	n	37	24	31,34,35	1.97	8 (25%)	43,49,52	2.30	11 (25%)
24	2MG	n	10	24	23,26,27	2.84	8 (34%)	33,38,41	1.94	8 (24%)
24	5MC	n	48	24	19,22,23	3.66	8 (42%)	26,32,35	0.90	1 (3%)
24	G7M	n	46	24	23,26,27	3.67	12 (52%)	34,39,42	1.69	6 (17%)

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
24	1MG	n	9	24	-	3/7/25/26	0/3/3/3
82	5CT	eI	51	82	-	7/13/14/16	-
24	1MA	n	58	24	-	2/7/25/26	0/3/3/3
24	M2G	n	26	24	-	2/11/29/30	0/3/3/3
24	T6A	n	37	24	-	8/23/41/42	0/3/3/3
24	2MG	n	10	24	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	5MC	n	48	24	-	2/7/25/26	0/2/2/2
24	G7M	n	46	24	-	3/7/25/26	0/3/3/3

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	46	G7M	C8-N7	10.73	1.51	1.33
24	n	48	5MC	C6-C5	9.08	1.49	1.34
24	n	58	1MA	C2-N3	8.89	1.46	1.30
24	n	9	1MG	C2-N3	7.96	1.46	1.33
24	n	10	2MG	C2-N3	7.55	1.46	1.32

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	58	1MA	C1'-N9-C8	-7.80	104.58	126.73
24	n	37	T6A	N6-C10-N11	7.65	124.29	113.77
24	n	58	1MA	C1'-N9-C4	6.93	146.96	126.49
24	n	10	2MG	C2-N3-C4	5.99	119.49	112.00
24	n	37	T6A	N3-C2-N1	-5.43	120.36	128.58

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	eI	51	5CT	NZ-C1-C2-C3
82	eI	51	5CT	NZ-C1-C2-O1
82	eI	51	5CT	C2-C3-C4-N1
24	n	37	T6A	C14-C12-C13-ODA
24	n	37	T6A	C14-C12-C13-ODB

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	n	58	1MA	1	0
24	n	26	M2G	1	0
24	n	37	T6A	2	0
24	n	10	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	$\# Z > 2$
85	SPD	BQ	3401	-	9,9,9	0.41	0	8,8,8	1.04	1 (12%)
86	3HE	BQ	3402	-	21,21,21	1.95	8 (38%)	23,30,30	1.87	7 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	SPD	BQ	3401	-	-	5/7/7/7	-
86	3HE	BQ	3402	-	-	4/8/36/36	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	BQ	3402	3HE	C-C1	-4.26	1.39	1.52
86	BQ	3402	3HE	C5-C4	2.86	1.55	1.51
86	BQ	3402	3HE	C11-N	2.78	1.42	1.37
86	BQ	3402	3HE	O2-C12	-2.59	1.18	1.23
86	BQ	3402	3HE	O1-C11	-2.44	1.18	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	BQ	3402	3HE	C9-C13-C12	-4.09	107.58	114.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	BQ	3402	3HE	C13-C12-N	-3.55	111.62	115.92
86	BQ	3402	3HE	O-C4-C3	2.69	126.04	122.11
86	BQ	3402	3HE	O2-C12-N	2.63	124.36	120.30
86	BQ	3402	3HE	C11-N-C12	-2.48	122.88	125.87

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

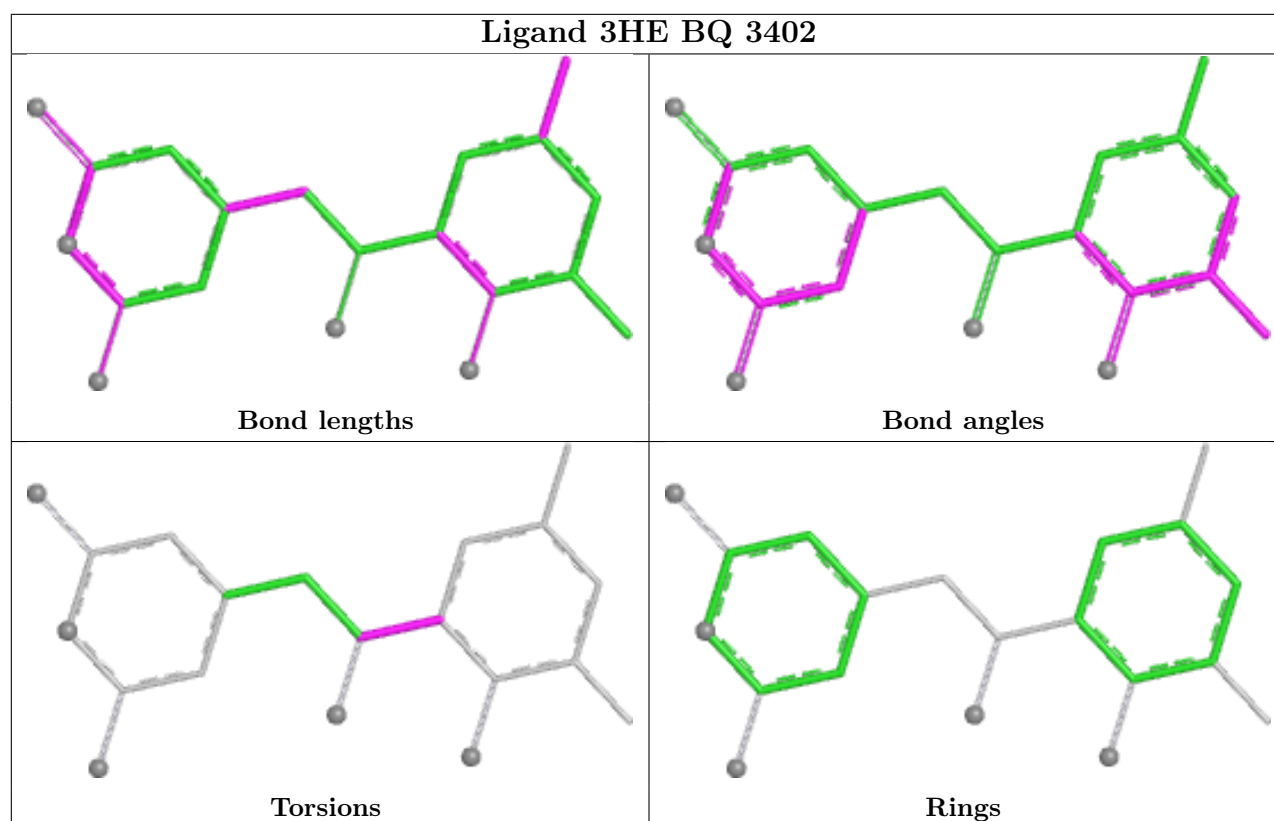
Mol	Chain	Res	Type	Atoms
86	BQ	3402	3HE	C4-C5-C7-C8
86	BQ	3402	3HE	C4-C5-C7-O3
86	BQ	3402	3HE	C6-C5-C7-C8
86	BQ	3402	3HE	C6-C5-C7-O3
85	BQ	3401	SPD	N6-C7-C8-C9

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	BQ	3401	SPD	1	0
86	BQ	3402	3HE	3	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	BQ	3
12	V	1
45	BM	1
68	AY	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BQ	1955:U	O3'	2093:A	P	29.09
1	V	123:LYS	C	135:LYS	N	21.25
1	BQ	2452:G	O3'	2492:C	P	17.28
1	BM	120:LYS	C	129:GLU	N	12.70
1	BQ	451:U	O3'	486:A	P	8.84

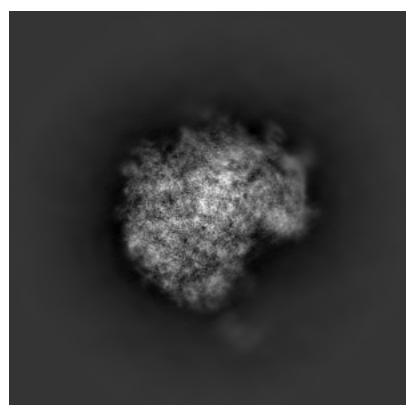
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10537. These allow visual inspection of the internal detail of the map and identification of artifacts.

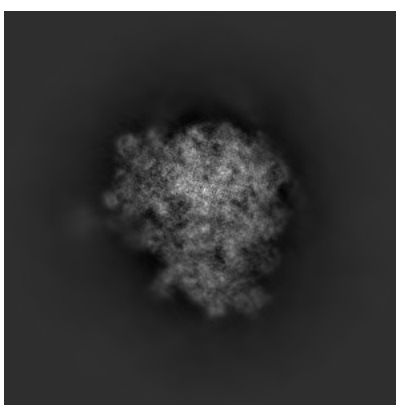
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

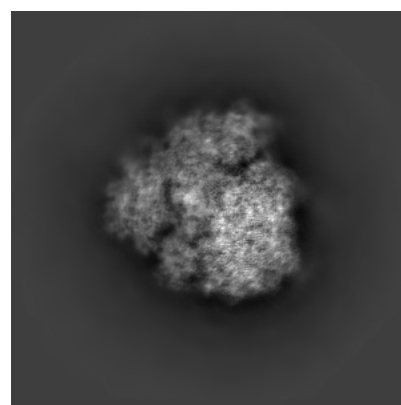
6.1.1 Primary map



X



Y

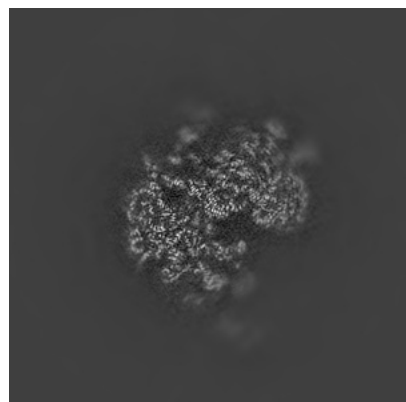


Z

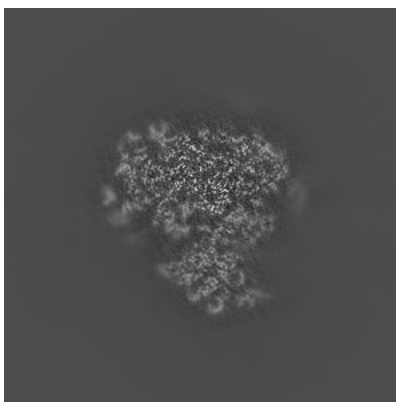
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

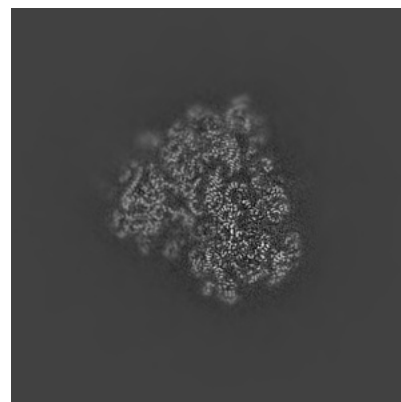
6.2.1 Primary map



X Index: 240



Y Index: 240

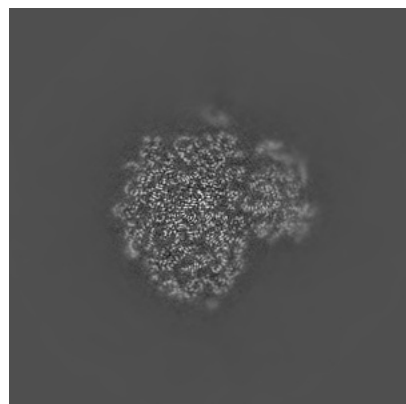


Z Index: 240

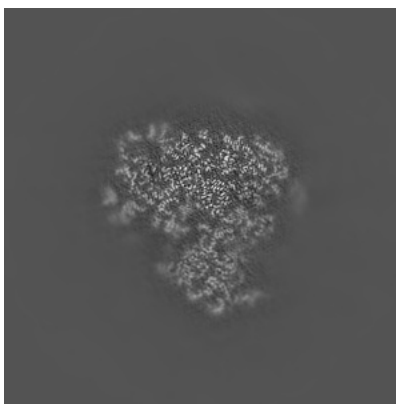
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

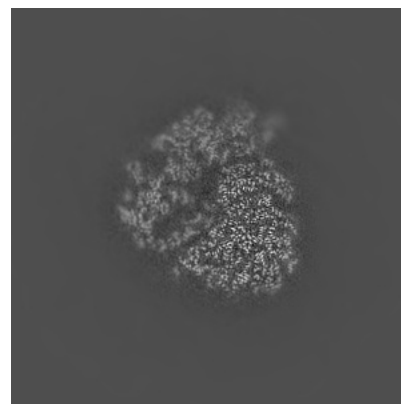
6.3.1 Primary map



X Index: 264



Y Index: 238

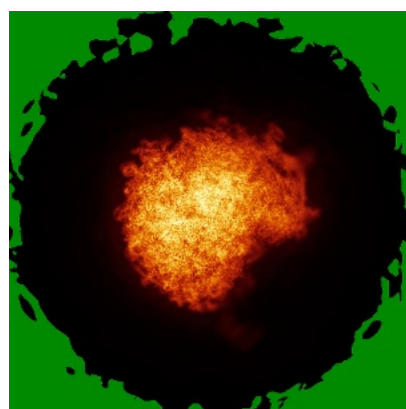


Z Index: 225

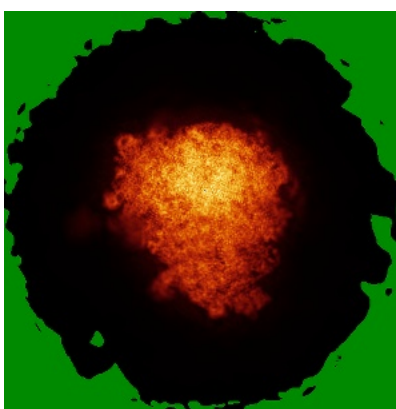
The images above show the largest variance slices of the map in three orthogonal directions.

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

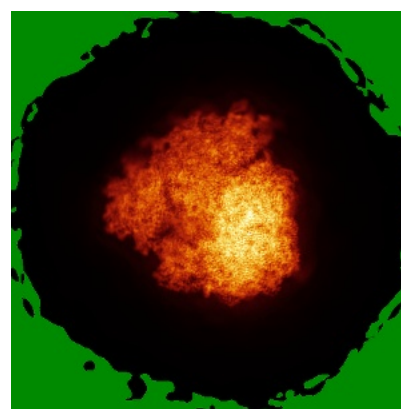
6.4.1 Primary map



X



Y

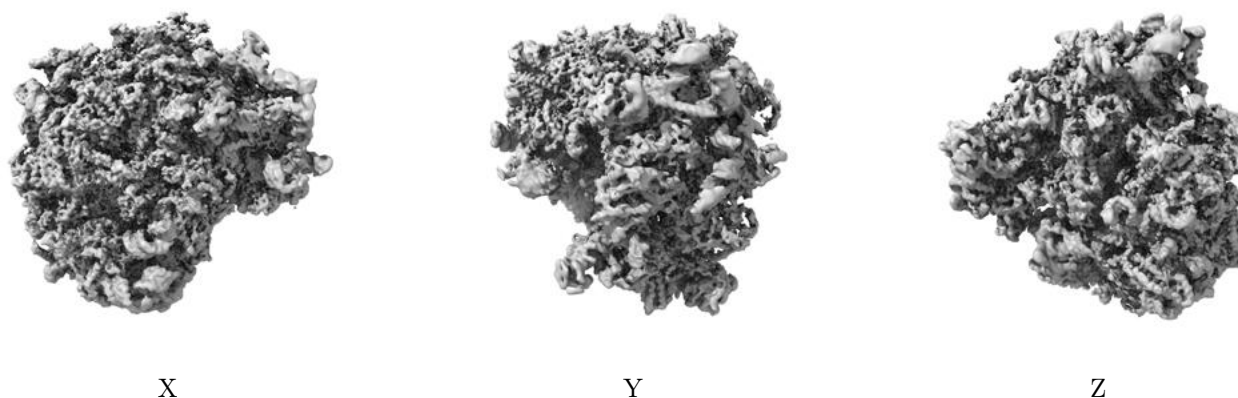


Z

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

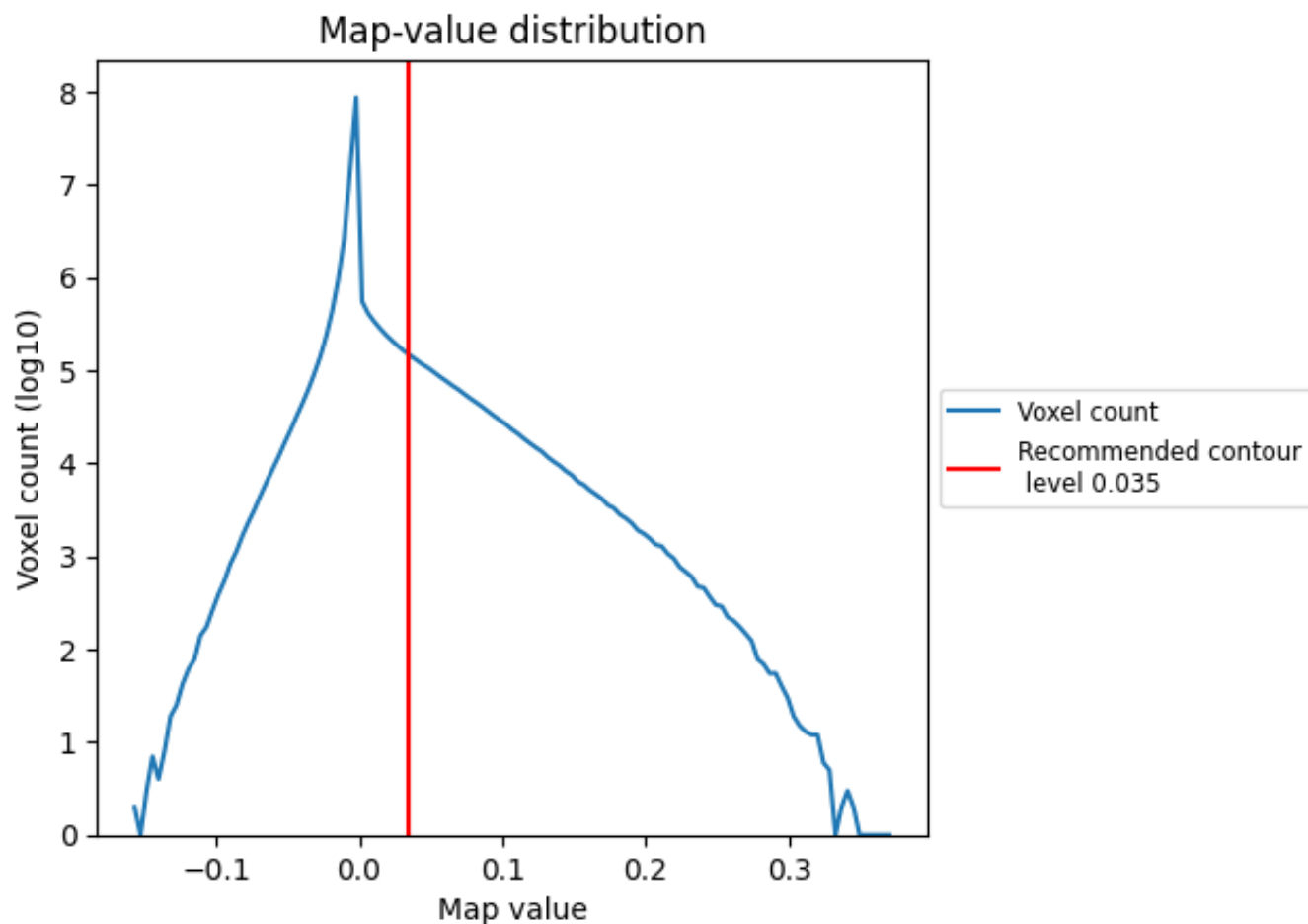
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

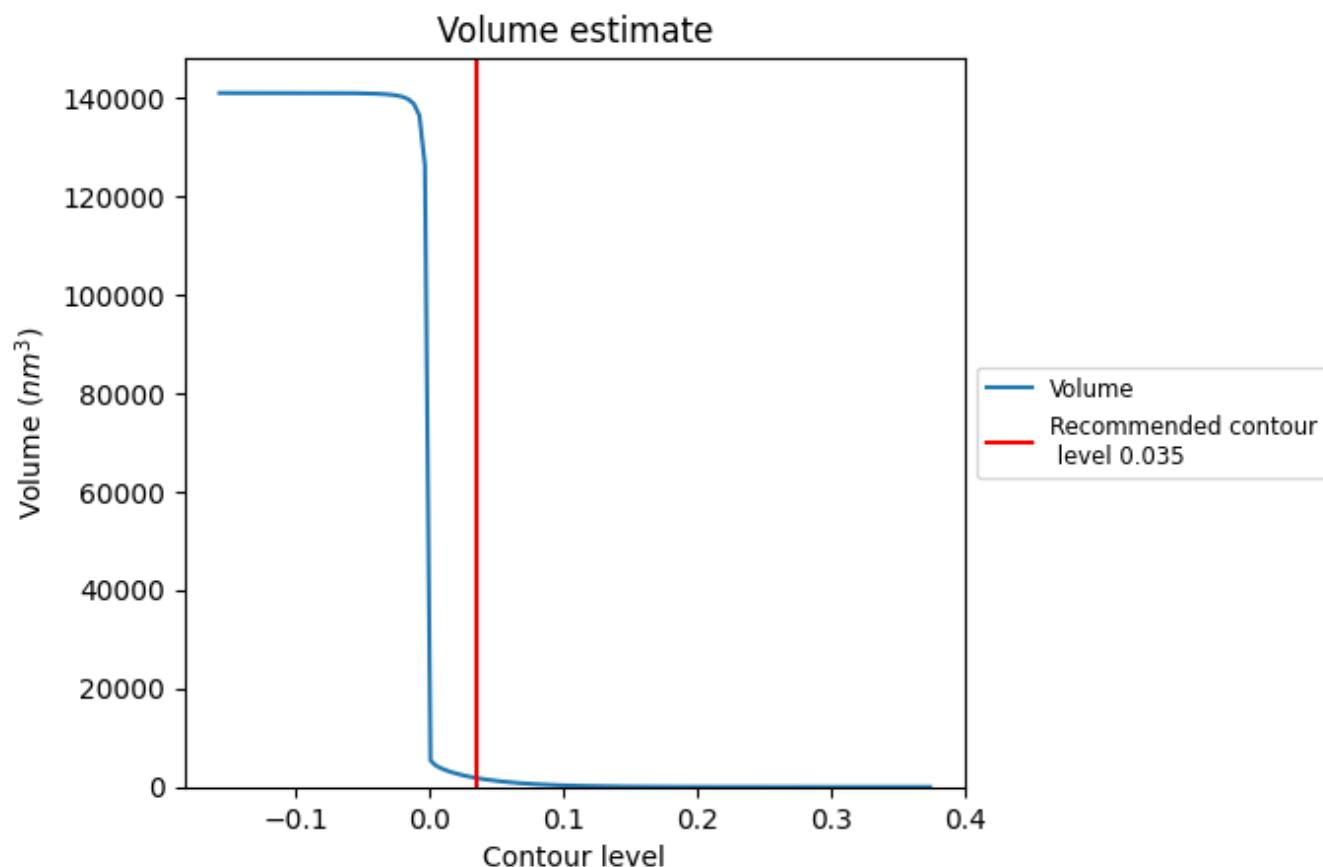
This section contains the results of statistical analysis of the map.

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.

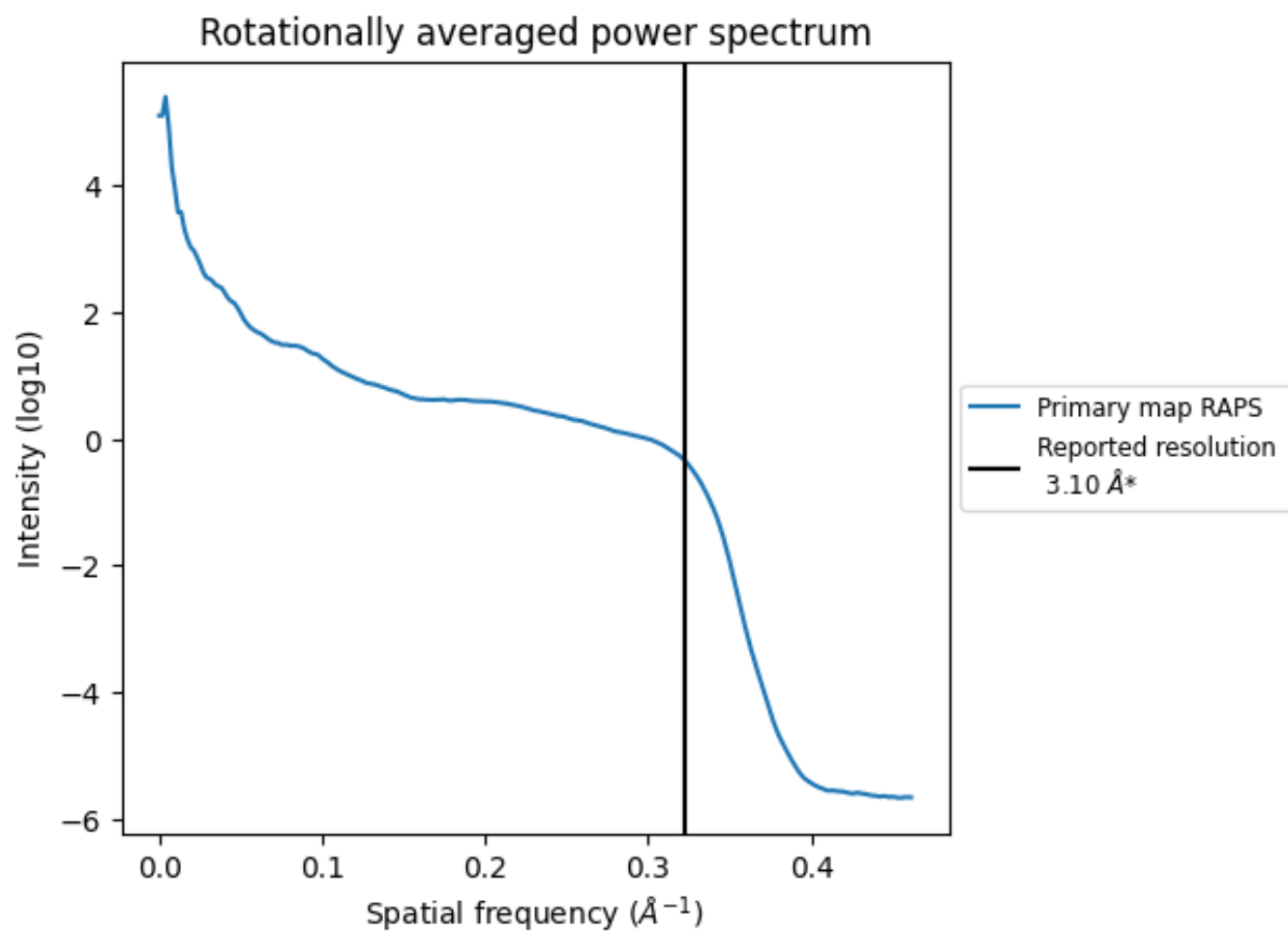
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1829 nm^3 ; this corresponds to an approximate mass of 1652 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 ⓘ

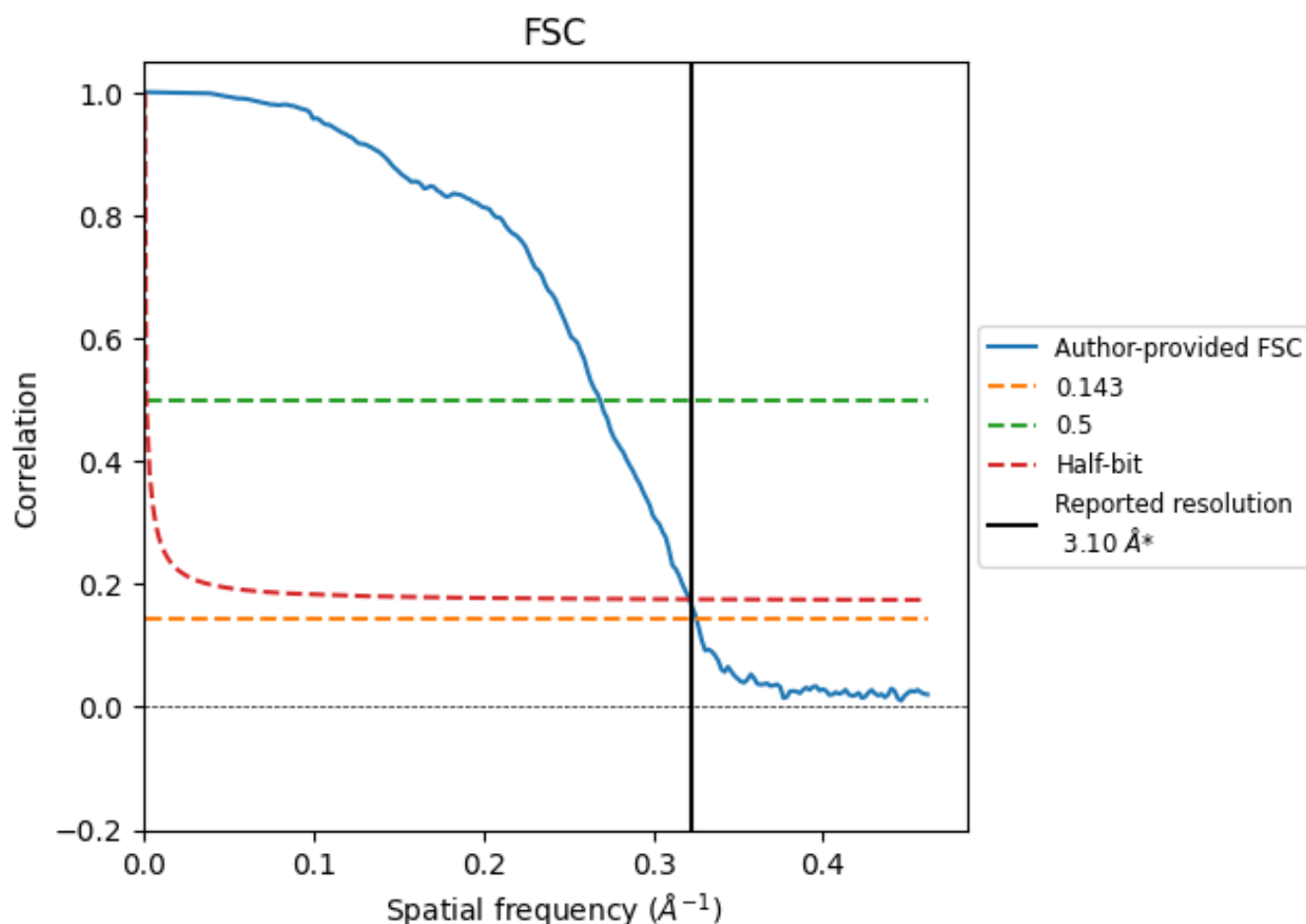


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

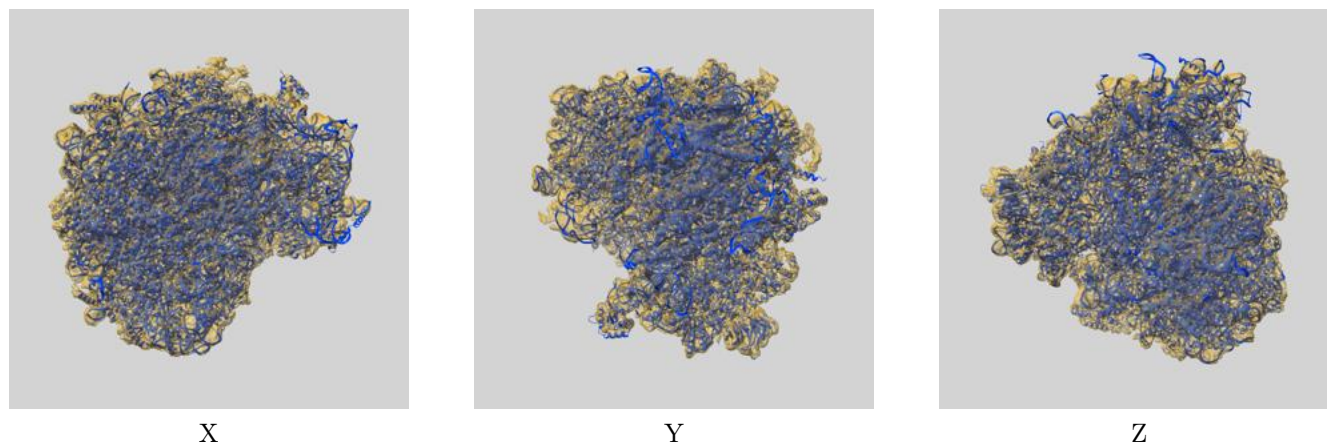
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.72	3.11
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

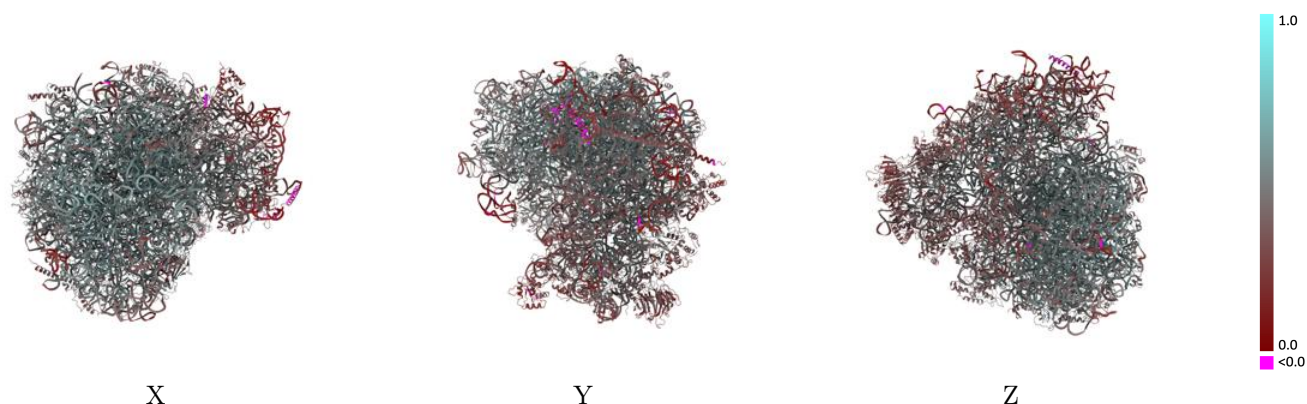
This section contains information regarding the fit between EMDB map EMD-10537 and PDB model 6TNU. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



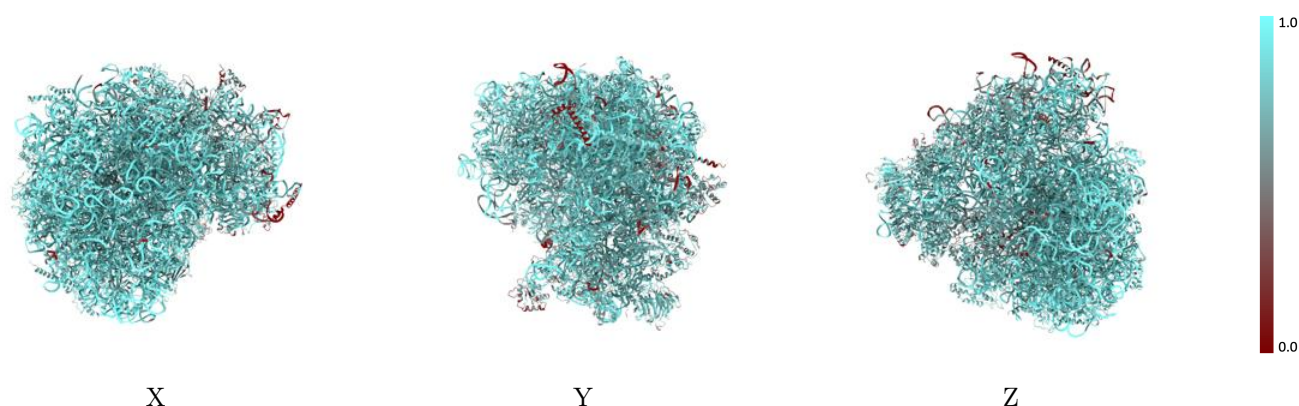
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



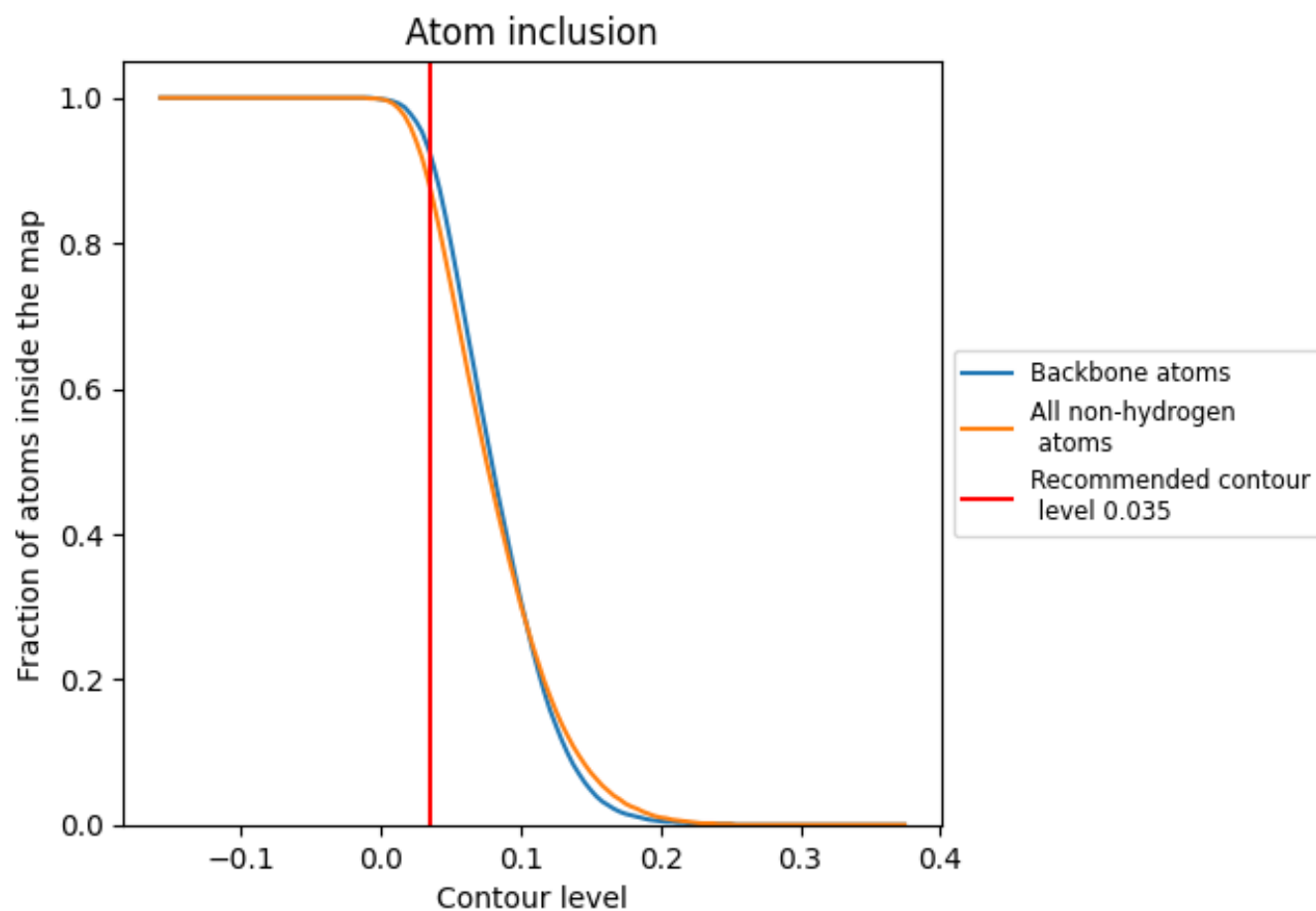
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8810	 0.4630
2	 0.9080	 0.4180
A	 0.7420	 0.3860
AA	 0.8340	 0.4490
AB	 0.8060	 0.5170
AC	 0.8350	 0.4590
AD	 0.8320	 0.4630
AE	 0.5280	 0.3380
AF	 0.9310	 0.5650
AG	 0.7870	 0.4030
AH	 0.8750	 0.5100
AI	 0.7650	 0.4330
AJ	 0.8670	 0.4890
AK	 0.8870	 0.5100
AL	 0.8990	 0.5470
AM	 0.8750	 0.4690
AN	 0.8460	 0.4590
AO	 0.8310	 0.4790
AP	 0.8340	 0.5300
AQ	 0.9060	 0.5520
AR	 0.8970	 0.5210
AS	 0.6920	 0.5140
AT	 0.8240	 0.5280
AU	 0.8720	 0.5090
AV	 0.8360	 0.4930
AW	 0.8560	 0.5470
AX	 0.8740	 0.5290
AY	 0.8250	 0.4670
B	 0.7090	 0.3510
BA	 0.8830	 0.5150
BB	 0.8750	 0.5170
BC	 0.8440	 0.5070
BD	 0.7860	 0.4520
BE	 0.8860	 0.5100
BF	 0.7830	 0.4540



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BG	 0.8860	 0.5430
BH	 0.8550	 0.5040
BI	 0.8440	 0.4190
BJ	 0.8590	 0.5120
BK	 0.9010	 0.5520
BL	 0.8360	 0.4270
BM	 0.8600	 0.4600
BN	 0.8420	 0.5080
BO	 0.8890	 0.5000
BP	 0.8600	 0.4890
BQ	 0.9630	 0.5150
BR	 0.9790	 0.4810
BS	 0.9720	 0.5410
BT	 0.7850	 0.3770
C	 0.7670	 0.3290
D	 0.5050	 0.2100
E	 0.7010	 0.3570
F	 0.7840	 0.3860
G	 0.7380	 0.3770
H	 0.7550	 0.3550
I	 0.8010	 0.3680
J	 0.7720	 0.3740
K	 0.6520	 0.3260
L	 0.6660	 0.3860
M	 0.8940	 0.4460
N	 0.5510	 0.2090
O	 0.7650	 0.3010
P	 0.7720	 0.3800
Q	 0.6610	 0.3530
R	 0.7640	 0.4340
S	 0.7610	 0.4160
T	 0.7380	 0.3800
U	 0.6660	 0.3300
V	 0.8250	 0.4480
W	 0.7470	 0.3810
X	 0.7580	 0.4730
Y	 0.7590	 0.4230
Z	 0.7230	 0.3860
a	 0.7270	 0.3930
b	 0.7660	 0.4520
c	 0.7760	 0.4850
d	 0.7500	 0.3790

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.7560	 0.4560
eI	 0.5380	 0.4210
f	 0.7160	 0.4080
g	 0.6400	 0.4080
l	 0.9540	 0.5140
m	 0.9150	 0.3620
n	 0.8920	 0.4120