



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 12:15 AM UTC

PDB ID : 8T2X / pdb_00008t2x
EMDB ID : EMD-40990
Title : Hypomethylated yeast 80S bound with cycloheximide, P-site tRNA, A-site tRNA, messenger RNA and eIF5A, PRE
Authors : Zhao, Y.; Li, H.
Deposited on : 2023-06-07
Resolution : 2.46 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

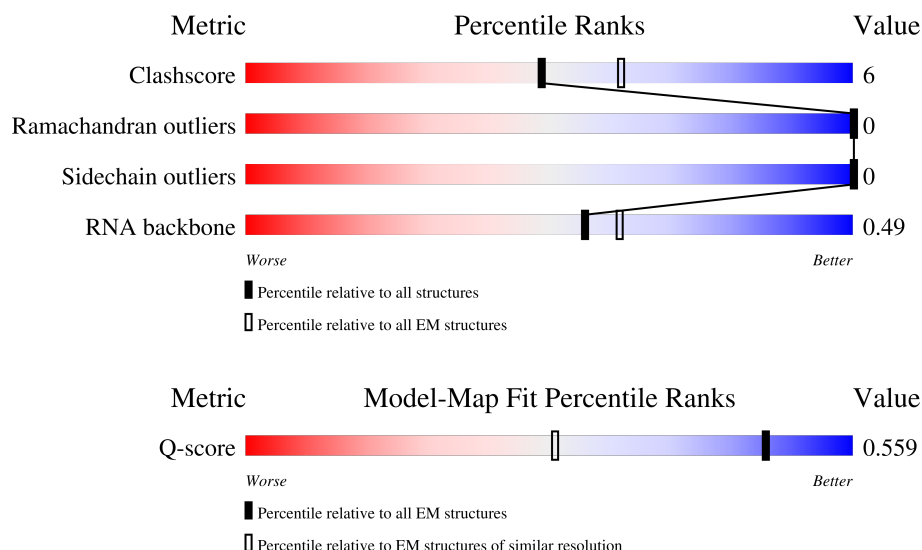
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.46 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	6014 (1.96 - 2.96)

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	BA	252	
2	BB	255	
3	BC	254	

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Mol	Chain	Length	Quality of chain
4	BE	261	
5	BG	236	
6	BH	190	
7	BI	200	
8	BJ	197	
9	BL	156	
10	BN	151	
11	BO	137	
12	BV	87	
13	BW	130	
14	BX	145	
15	BY	135	
16	Ba	119	
17	Bb	82	
18	Be	63	
19	BD	240	
20	BF	225	
21	BK	105	
22	BP	142	
23	BQ	143	
24	BR	136	
25	BS	146	
26	BT	144	
27	BU	121	
28	BZ	108	

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Mol	Chain	Length	Quality of chain
29	Bc	67	
30	Bd	56	
31	Bg	319	
32	Bf	152	
33	BM	143	
34	B5	1798	
35	AA	254	
36	AB	387	
37	AC	362	
38	A1	3395	
39	A3	121	
40	A4	158	
41	AD	297	
42	AE	176	
43	AF	244	
44	AG	256	
45	AH	191	
46	AI	221	
47	AJ	174	
48	AL	199	
49	AM	138	
50	AN	204	
51	AO	199	
52	AP	184	
53	AQ	186	

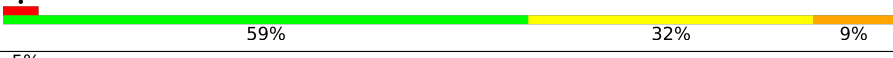
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Mol	Chain	Length	Quality of chain
54	AR	189	
55	AS	178	
56	AT	160	
57	AU	121	
58	AV	137	
59	AW	155	
60	AX	142	
61	AY	127	
62	AZ	136	
63	Aa	149	
64	Ab	59	
65	Ac	105	
66	Ad	113	
67	Ae	130	
68	Af	107	
69	Ag	121	
70	Ah	120	
71	Ai	100	
72	Aj	88	
73	Ak	78	
74	Al	51	
75	Am	128	
76	An	25	
77	Ao	106	
78	Ap	92	

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Mol	Chain	Length	Quality of chain
79	E	217	
80	tP	75	
81	tA	76	
82	MR	12	
83	eI	155	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 207315 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 protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BA	206	Total	C	N	O	S	0	0
			1612	1034	285	291	2		

- Molecule 2 is a protein called RPS1A isoform 1.

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

- Molecule 3 is a protein called RPS2 isoform 1.

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

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 5 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BG	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 6 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	BH	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 7 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 8 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 9 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BL	155	Total	C	N	O	S	0	0
			1244	798	235	208	3		

- Molecule 10 is a protein called 40S ribosomal protein S13.

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

- Molecule 11 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 12 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 13 is a protein called RPS22A isoform 1.

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

- Molecule 14 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 15 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BY	134	Total	C	N	O	S	0	0
			1073	676	208	189			

- Molecule 16 is a protein called RPS26B isoform 1.

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

- Molecule 17 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 18 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 19 is a protein called RPS3 isoform 1.

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

- Molecule 20 is a protein called Rps5p.

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

- Molecule 21 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BK	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 22 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BP	124	Total	C	N	O	S	0	0
			991	631	187	166	7		

- Molecule 23 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BQ	141	Total	C	N	O	S	0	0
			1105	708	203	194			

- Molecule 24 is a protein called 40S ribosomal protein S17-A.

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

- Molecule 25 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 26 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BT	141	Total	C	N	O	S	0	0
			1095	685	206	202	2		

- Molecule 27 is a protein called RPS20 isoform 1.

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

- Molecule 28 is a protein called RPS25A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BZ	102	Total	C	N	O	S	0	0
			804	511	153	139	1		

- Molecule 29 is a protein called RPS28A isoform 1.

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

- Molecule 30 is a protein called RPS29A isoform 1.

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

- Molecule 31 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bg	312	Total	C	N	O	S	0	0
			2401	1522	410	461	8		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bf	75	Total	C	N	O	S	0	0
			605	386	116	99	4		

- Molecule 33 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BM	124	Total	C	N	O	S	0	0
			935	587	165	181	2		

- Molecule 34 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B5	1782	Total	C	N	O	P	1	0
			37987	16988	6718	12499	1782		

- Molecule 35 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AA	247	Total	C	N	O	S	0	0
			1878	1170	381	326	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AB	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 37 is a protein called RPL4A isoform 1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A1	3216	Total	C	N	O	P	0	0
			68786	30729	12387	22454	3216		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 41 is a protein called RPL5 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AD	292	Total	C	N	O	S	0	0
			2341	1478	408	453	2		

- Molecule 42 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AE	167	Total	C	N	O	S	0	0
			1303	840	234	228	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	120	LYS	ASN	conflict	UNP Q02326

- Molecule 43 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AG	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 45 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 46 is a protein called RPL10 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AI	217	Total	C	N	O	S	0	0
			1759	1114	333	305	7		

- Molecule 47 is a protein called RPL11A isoform 1.

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

- Molecule 48 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	AL	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 49 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 50 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 51 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 52 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	AP	175	Total	C	N	O	0	0
			1388	862	277	249		

- Molecule 53 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 54 is a protein called 60S ribosomal protein L19-A.

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

- Molecule 55 is a protein called 60S ribosomal protein L20.

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

- Molecule 56 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 57 is a protein called 60S ribosomal protein L22-A.

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

- Molecule 58 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 59 is a protein called RPL24A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AW	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AX	121	Total	C	N	O	S	0	0
			968	623	170	173	2		

- Molecule 61 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AY	126	Total	C	N	O	S	0	0
			993	625	192	176			

- Molecule 62 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 63 is a protein called 60S ribosomal protein L28.

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

- Molecule 64 is a protein called RPL29 isoform 1.

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

- Molecule 65 is a protein called 60S ribosomal protein L30.

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

- Molecule 66 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ad	109	Total	C	N	O	S	0	0
			890	565	168	156	1		

- Molecule 67 is a protein called RPL32 isoform 1.

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

- Molecule 68 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 69 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 70 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 71 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 72 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 73 is a protein called RPL38 isoform 1.

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

- Molecule 74 is a protein called 60S ribosomal protein L39.

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

- Molecule 75 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 76 is a protein called 60S ribosomal protein L41-A.

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

- Molecule 77 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 78 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 79 is a protein called RPL1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	E	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

- Molecule 80 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	tP	75	Total	C	N	O	P	0	0
			1606	716	297	518	75		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
tP	10	A	G	conflict	GB 176433

- Molecule 81 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	tA	76	Total	C	N	O	P	0	0
			1628	726	302	524	76		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
tA	10	A	G	conflict	GB 176433

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Chain	Residue	Modelled	Actual	Comment	Reference
tA	17	A	-	insertion	GB 176433

- Molecule 82 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	MR	12	Total	C	N	O	P	0	0
			259	117	51	79	12		

- Molecule 83 is a protein called Eukaryotic translation initiation factor 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	eI	155	Total	C	N	O	S	0	0
			1148	712	196	231	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
eI	17	ALA	-	insertion	UNP A0A8H8ULI0

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
84	B5	39	Total	Mg	0
			39	39	
84	A1	139	Total	Mg	0
			139	139	
84	A4	1	Total	Mg	0
			1	1	
84	AP	1	Total	Mg	0
			1	1	
84	AV	1	Total	Mg	0
			1	1	

- Molecule 85 is POTASSIUM ION (CCD ID: K) (formula: K).

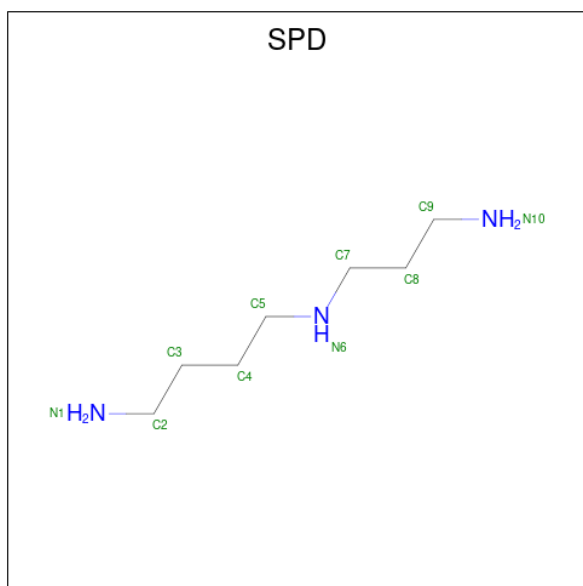
Mol	Chain	Residues	Atoms		AltConf
85	B5	10	Total	K	0
			10	10	
85	A1	12	Total	K	0
			12	12	

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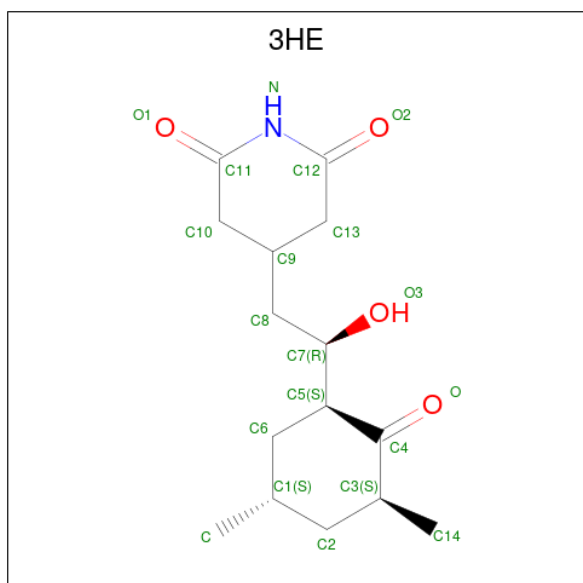
Mol	Chain	Residues	Atoms		AltConf
85	Ab	1	Total	K	0
			1	1	

- Molecule 86 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
86	A1	1	Total	C	N	0
			10	7	3	

- Molecule 87 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
87	A1	1	Total	C	N	O	0
			20	15	1	4	

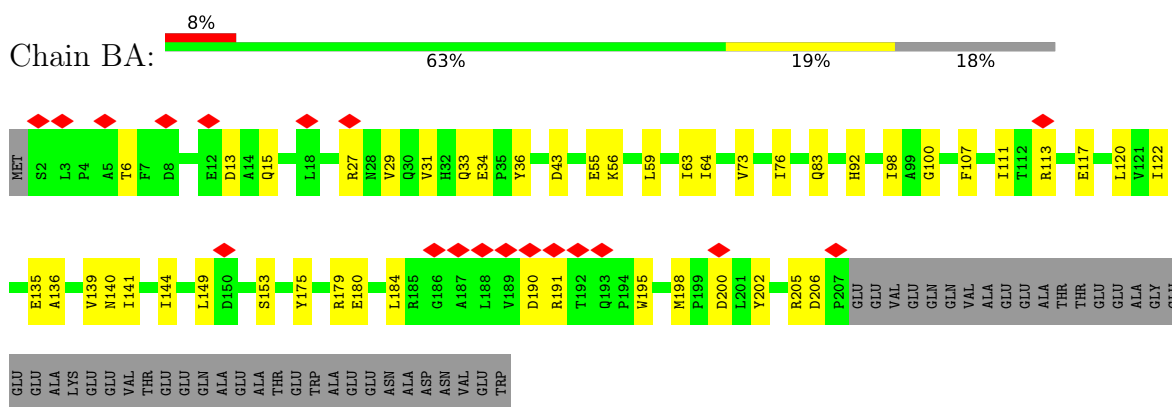
- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
88	Ao	1	Total	Zn	0
			1	1	

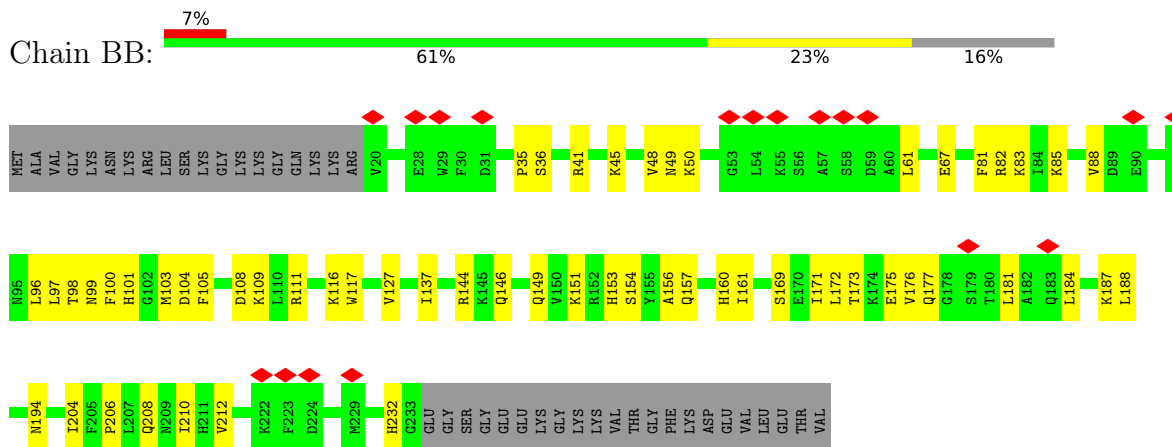
3 Residue-property plots

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.

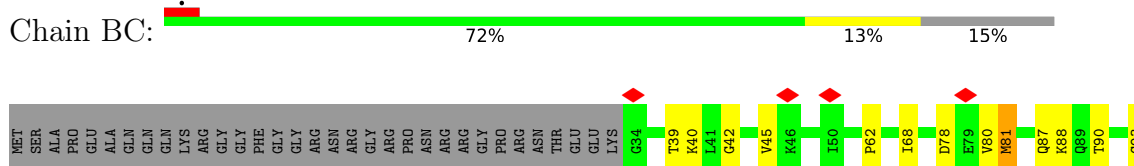
- Molecule 1: 40S ribosomal protein S0-A

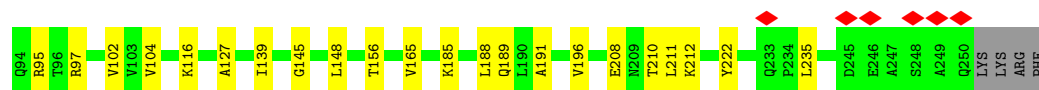


- Molecule 2: RPS1A isoform 1

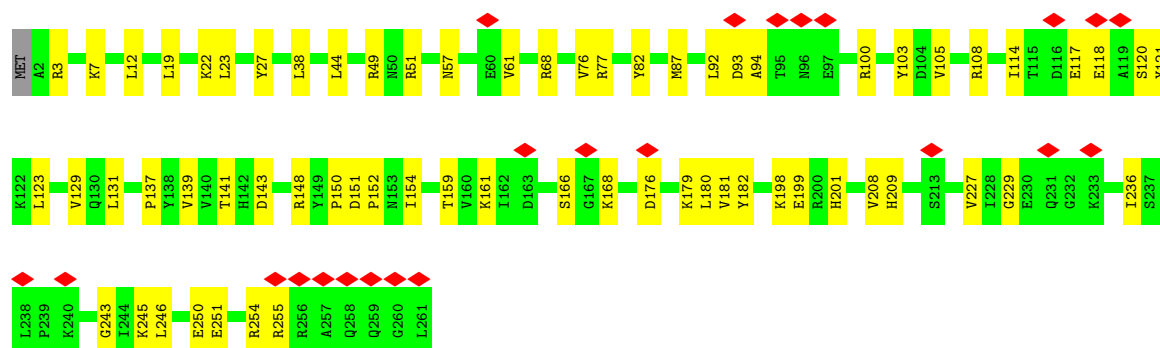
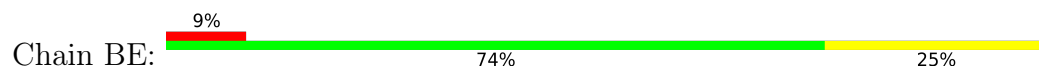


- Molecule 3: RPS2 isoform 1

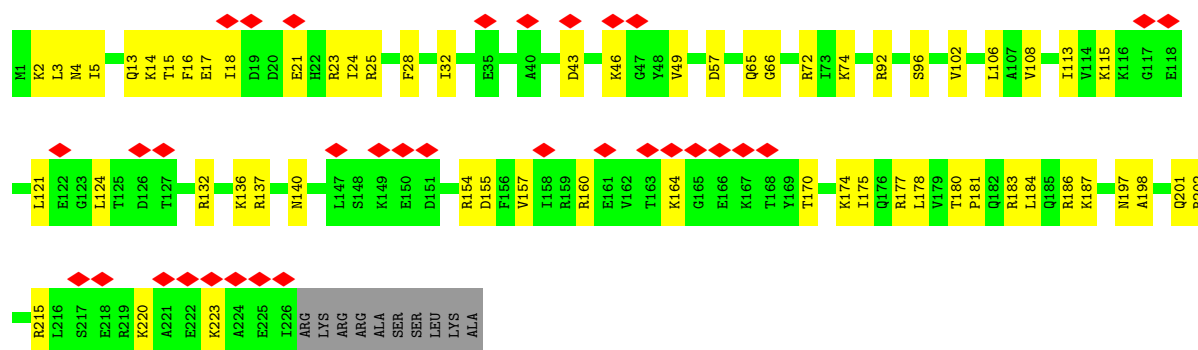
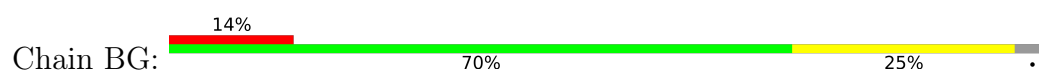




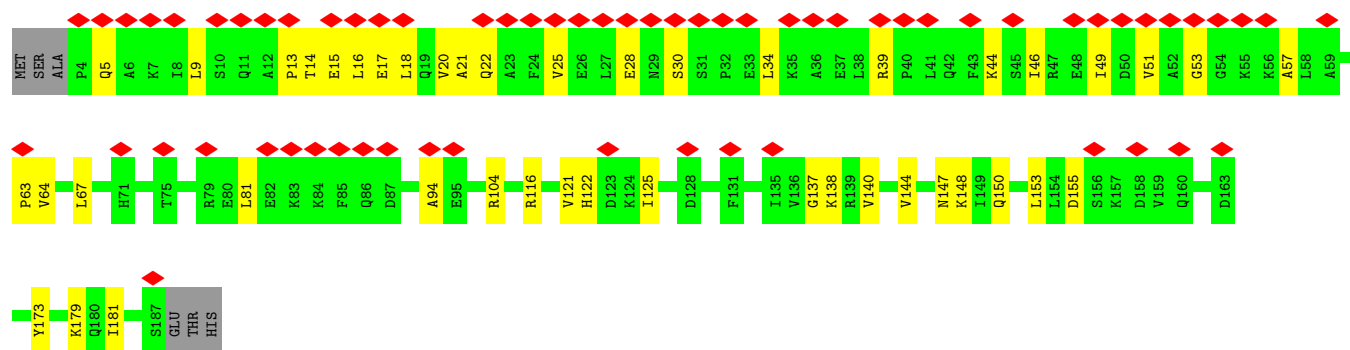
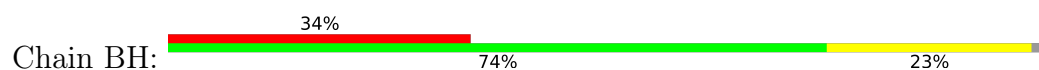
• Molecule 4: 40S ribosomal protein S4-A



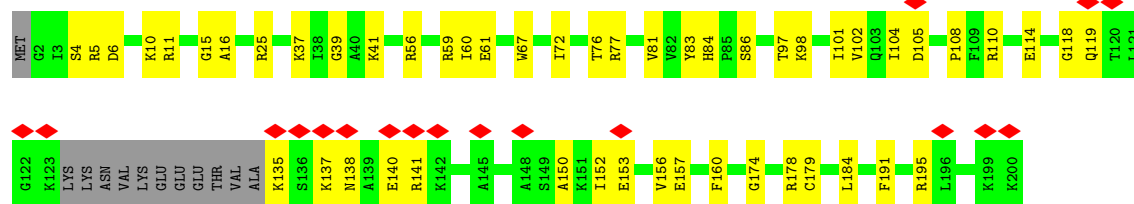
• Molecule 5: 40S ribosomal protein S6-A



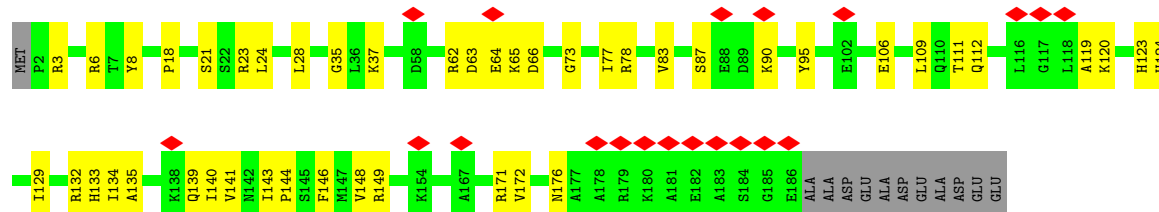
• Molecule 6: 40S ribosomal protein S7-A



• Molecule 7: 40S ribosomal protein S8-A



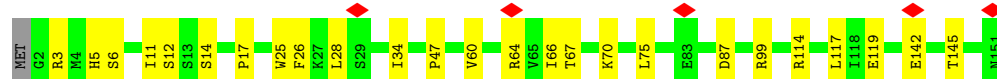
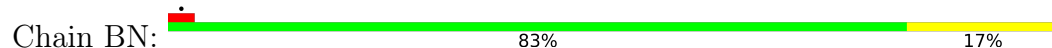
• Molecule 8: 40S ribosomal protein S9-A



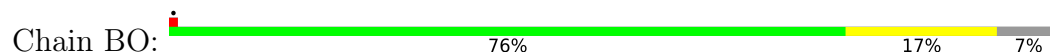
• Molecule 9: 40S ribosomal protein S11-A



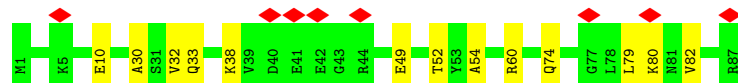
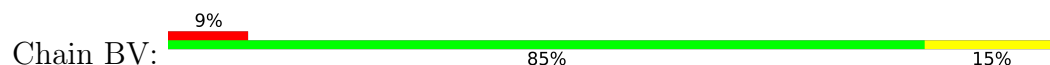
• Molecule 10: 40S ribosomal protein S13



• Molecule 11: 40S ribosomal protein S14-A

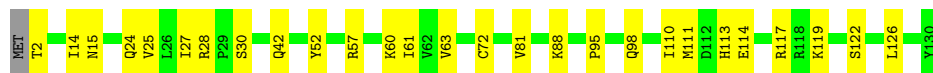


• Molecule 12: 40S ribosomal protein S21-A



- Molecule 13: RPS22A isoform 1

Chain BW:  78% 21%



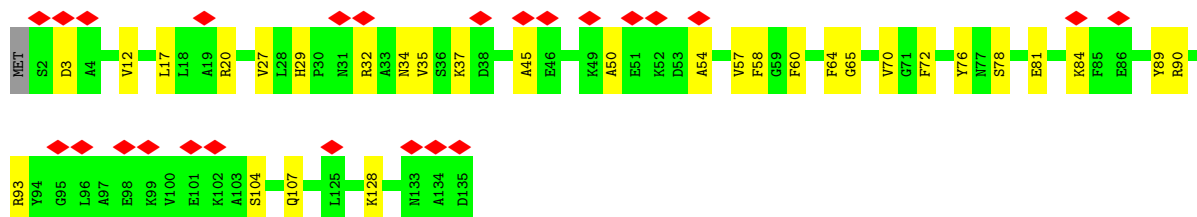
- Molecule 14: 40S ribosomal protein S23-A

Chain BX:  83% 16%



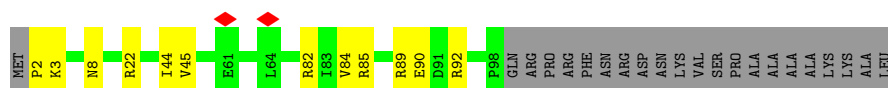
- Molecule 15: 40S ribosomal protein S24-A

Chain BY:  19% 77% 22%



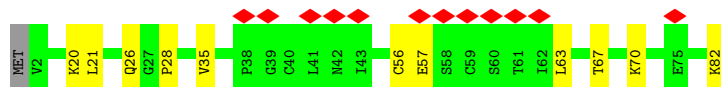
- Molecule 16: RPS26B isoform 1

Chain Ba:  71% 10% 18%



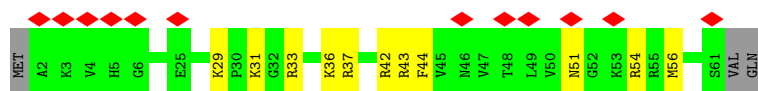
- Molecule 17: 40S ribosomal protein S27-A

Chain Bb:  15% 85% 13%

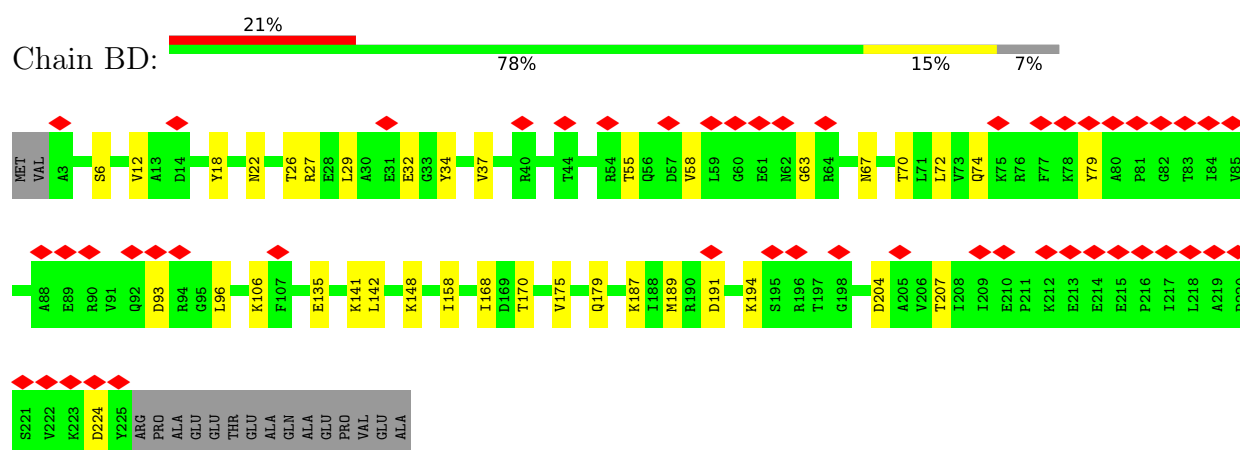


- Molecule 18: 40S ribosomal protein S30-A

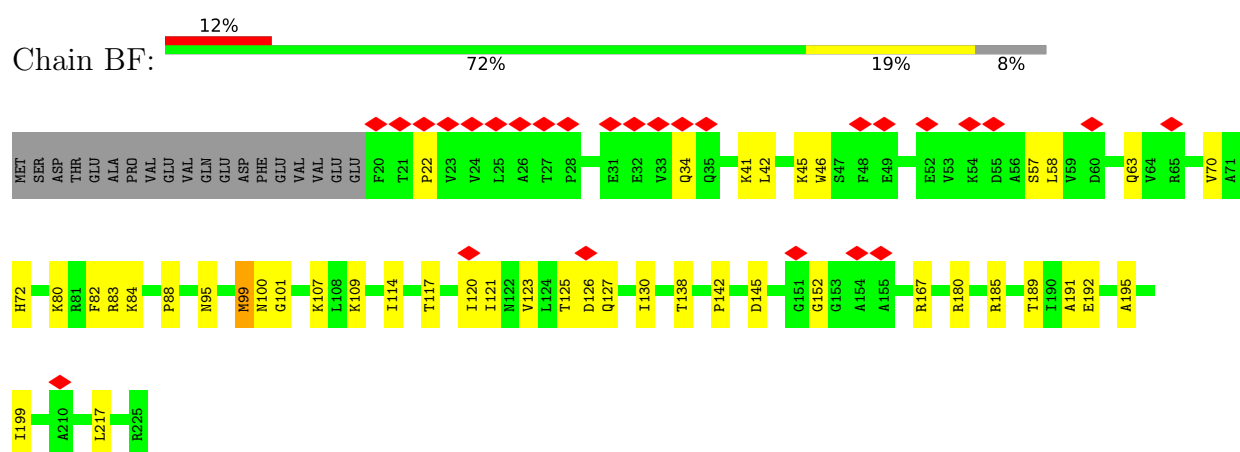
Chain Be:  19% 78% 17% 5%



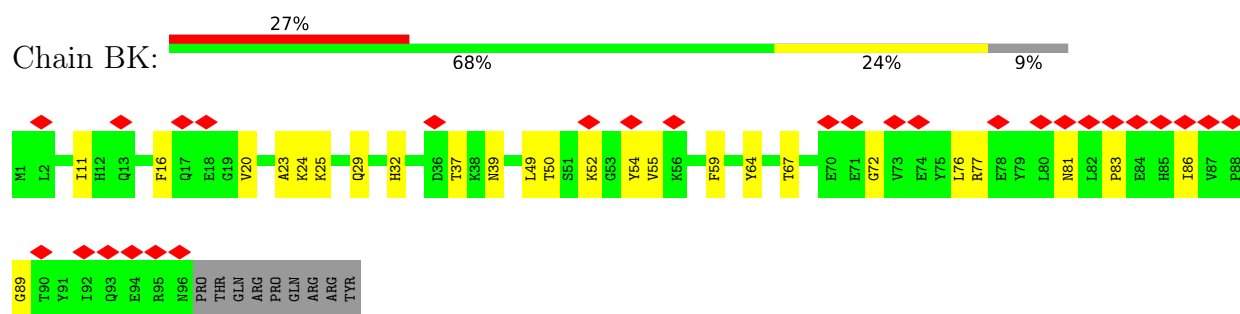
- Molecule 19: RPS3 isoform 1



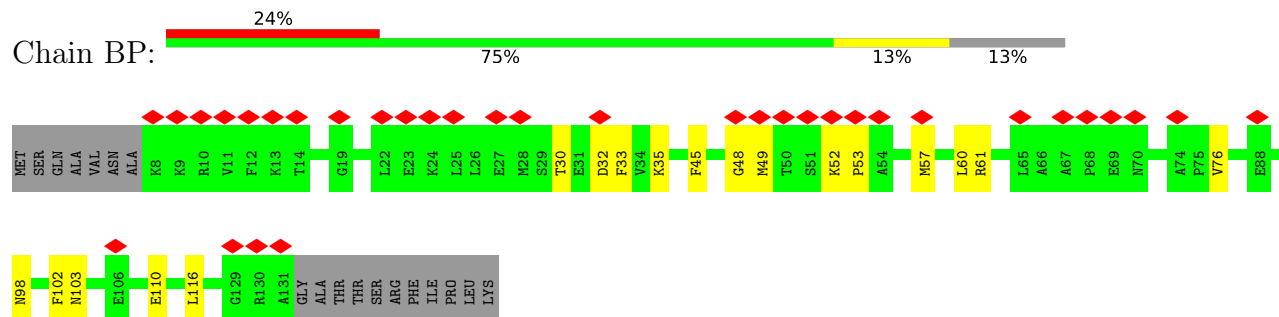
- Molecule 20: Rps5p



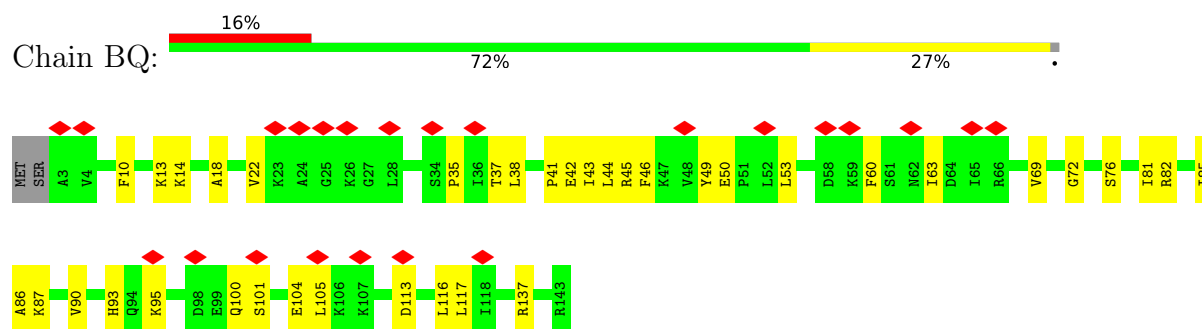
- Molecule 21: 40S ribosomal protein S10-A



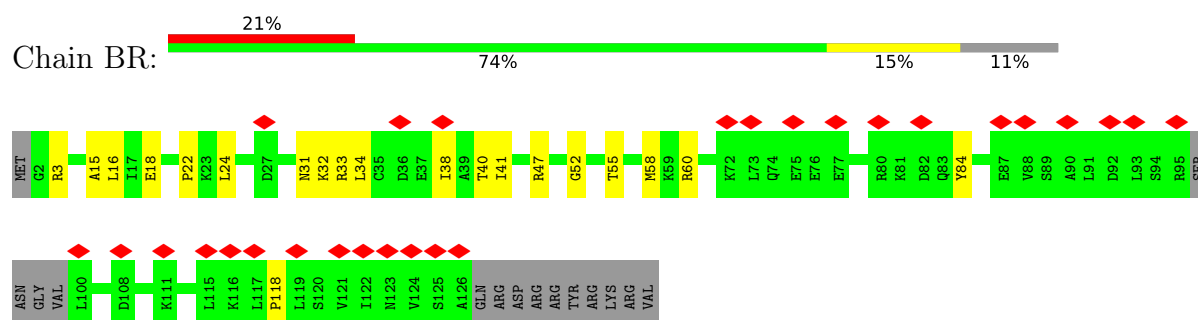
- Molecule 22: RPS15 isoform 1



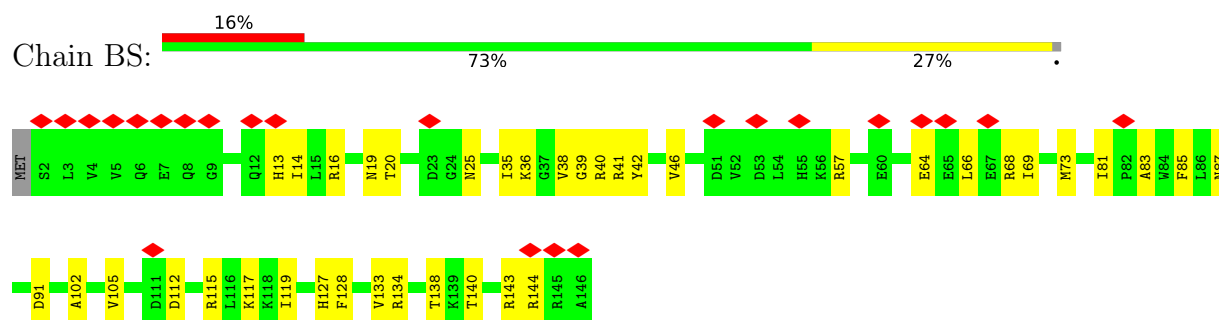
- Molecule 23: 40S ribosomal protein S16-A



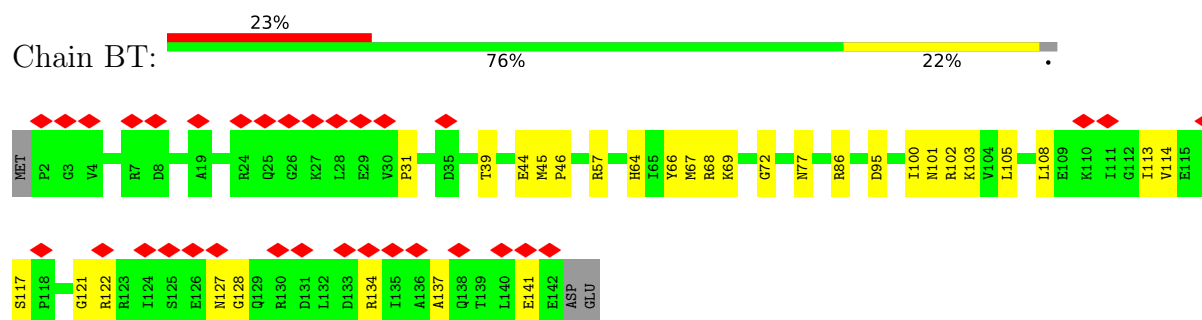
- Molecule 24: 40S ribosomal protein S17-A



- Molecule 25: 40S ribosomal protein S18-A

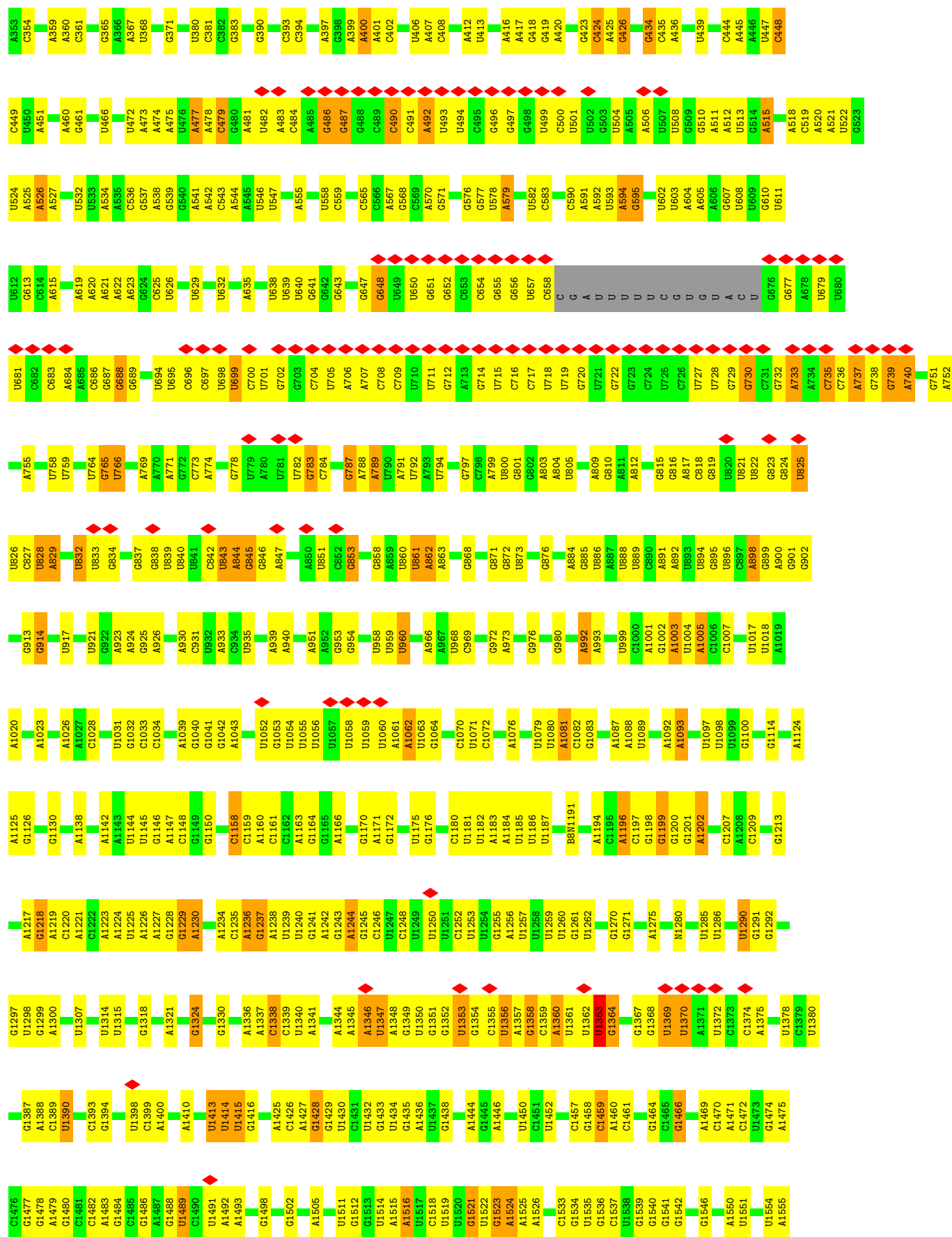


- Molecule 26: 40S ribosomal protein S19-A



- Molecule 27: RPS20 isoform 1

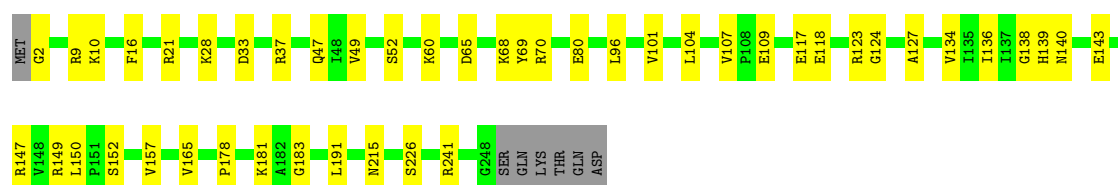






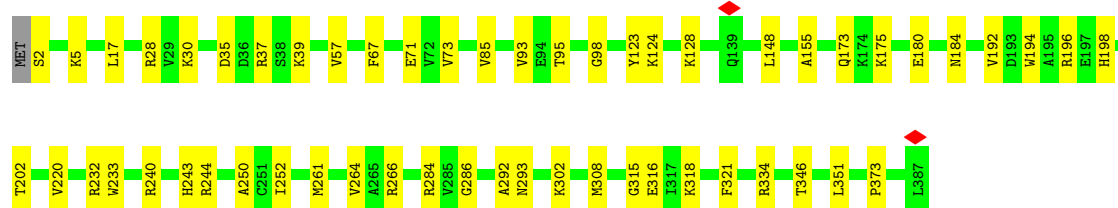
• Molecule 35: 60S ribosomal protein L2-A

Chain AA:  79% 18%



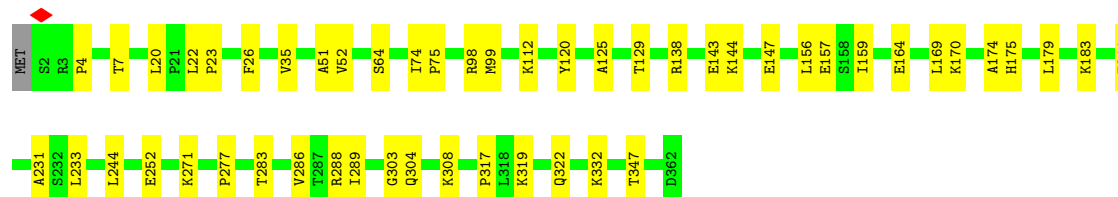
• Molecule 36: 60S ribosomal protein L3

Chain AB:  86% 14%



• Molecule 37: RPL4A isoform 1

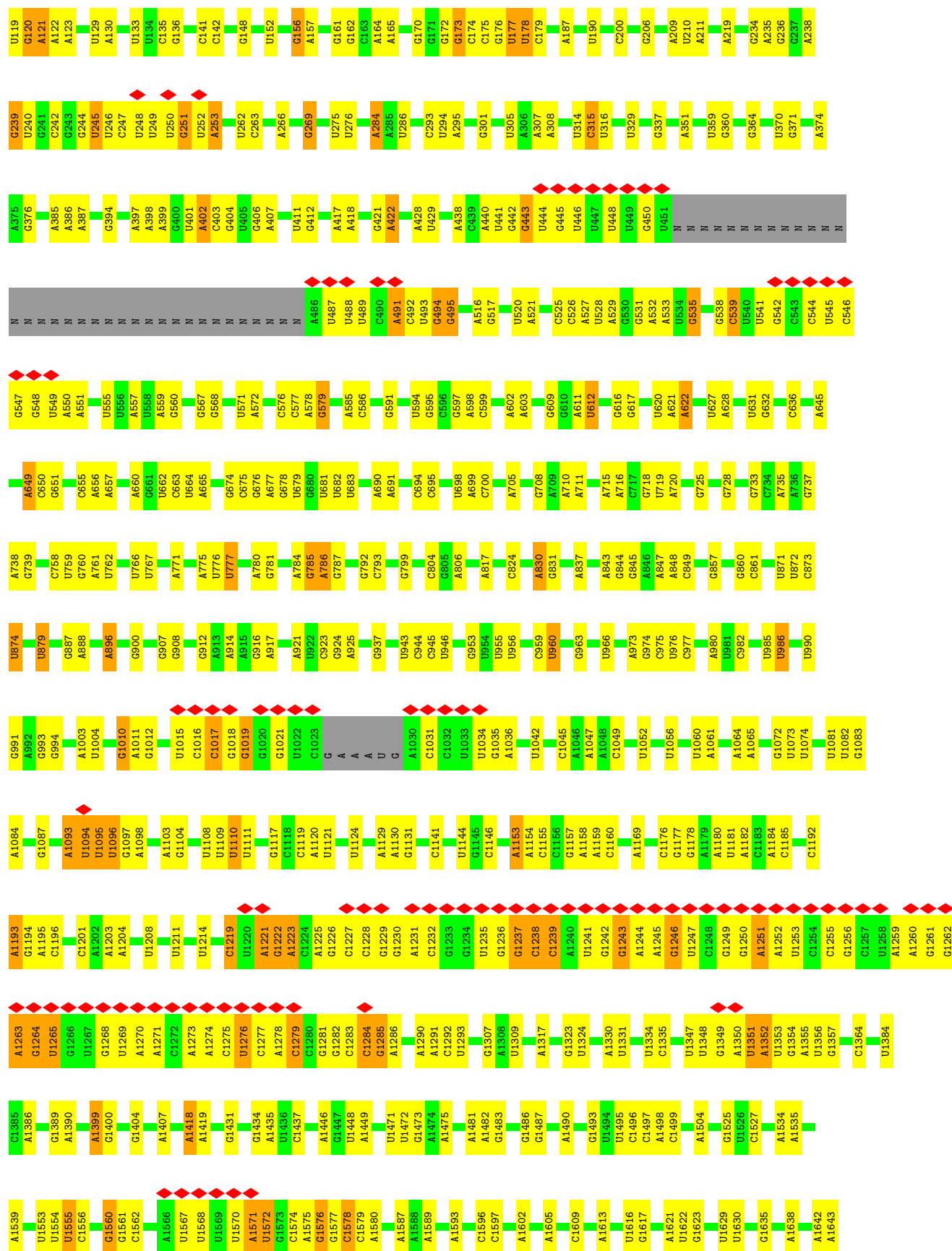
Chain AC:  86% 14%



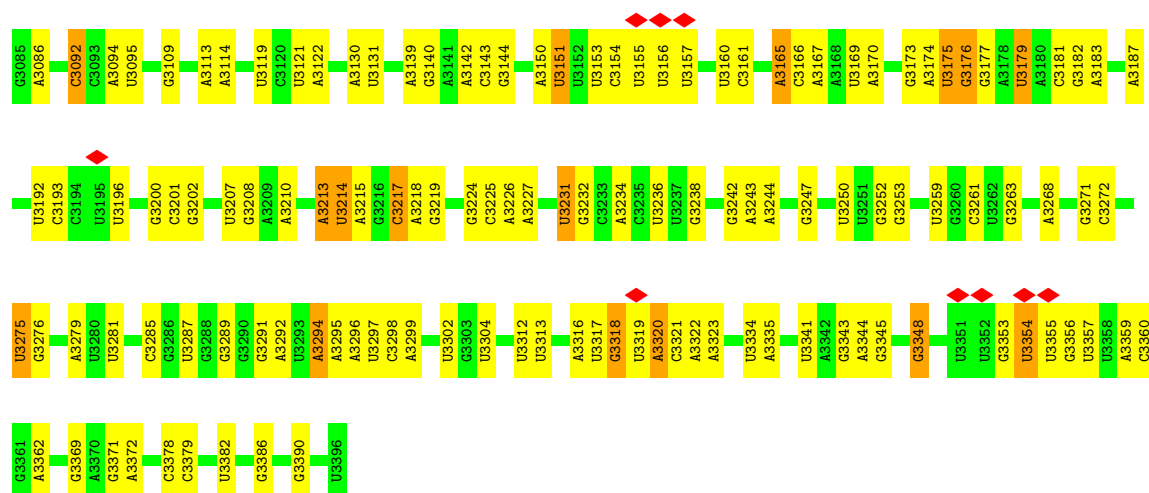
• Molecule 38: 25S rRNA

Chain A1:  60% 30% 5%

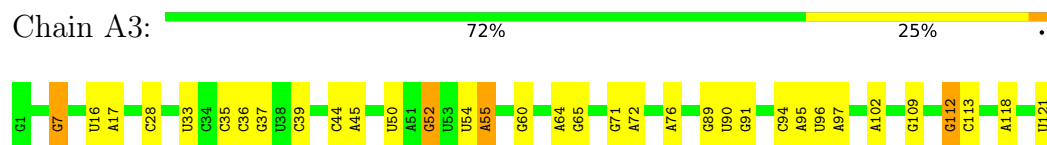




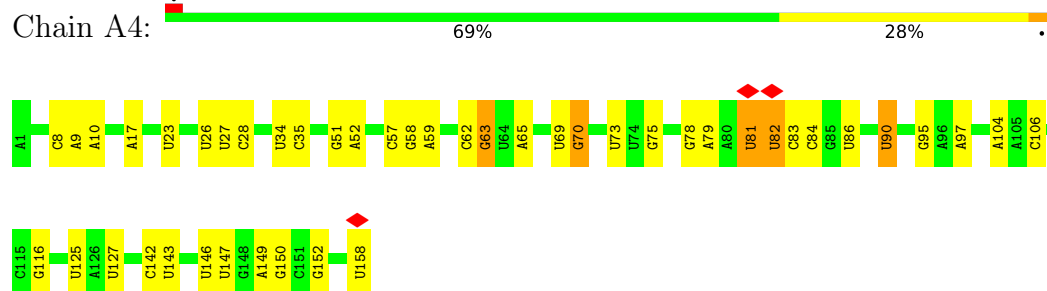




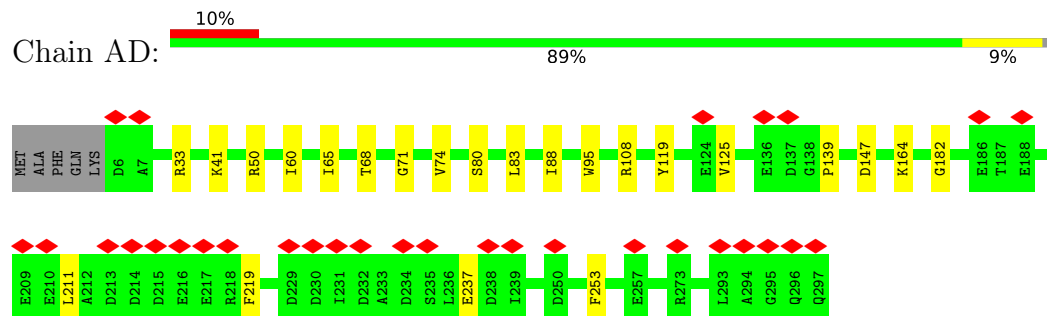
• Molecule 39: 5s rRNA



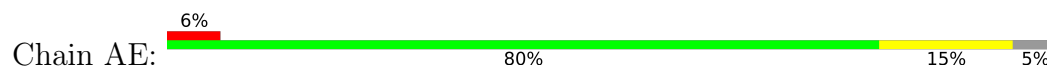
• Molecule 40: 5.8 S rRNA

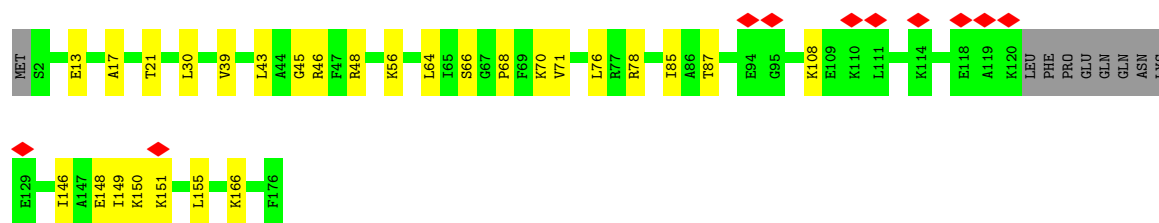


• Molecule 41: RPL5 isoform 1

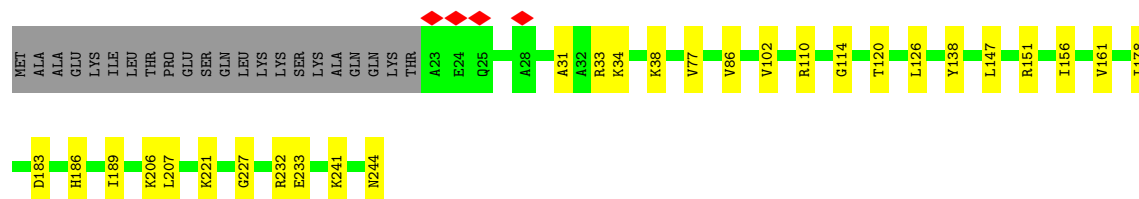
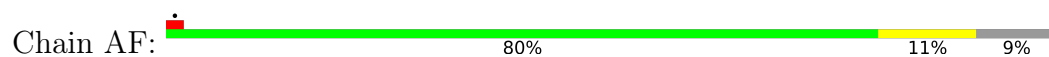


• Molecule 42: 60S ribosomal protein L6-A

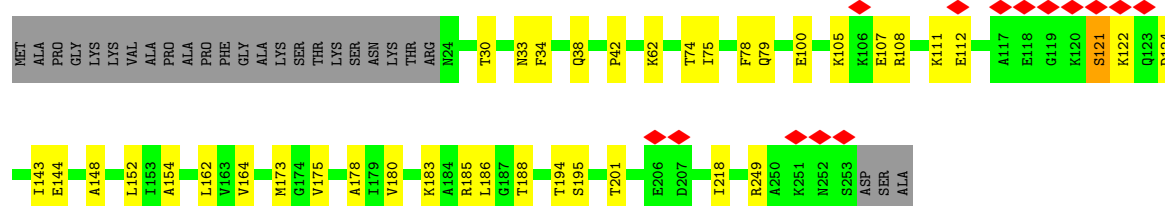
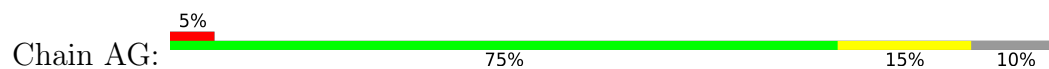




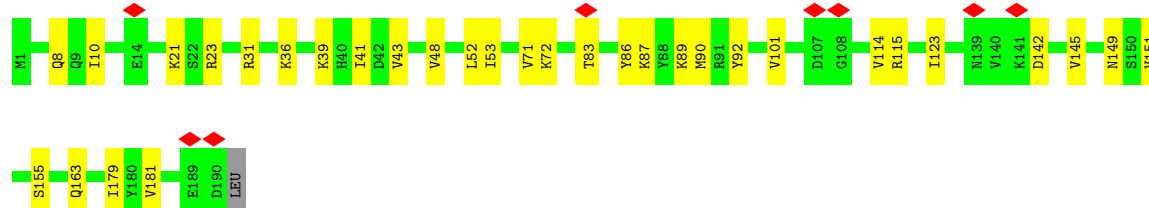
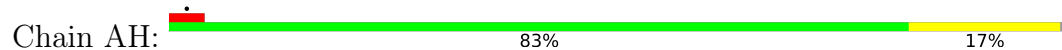
- Molecule 43: 60S ribosomal protein L7-A



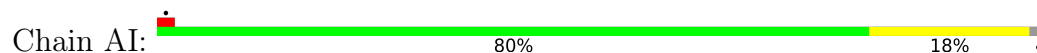
- Molecule 44: 60S ribosomal protein L8-A

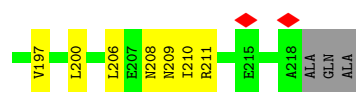


- Molecule 45: 60S ribosomal protein L9-A

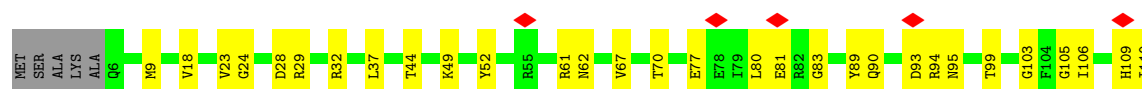
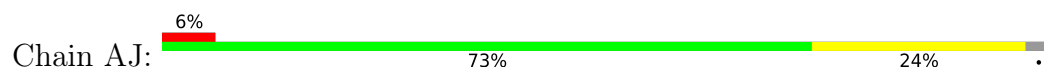


- Molecule 46: RPL10 isoform 1

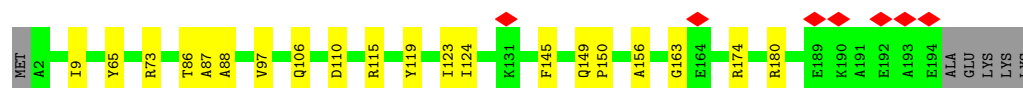




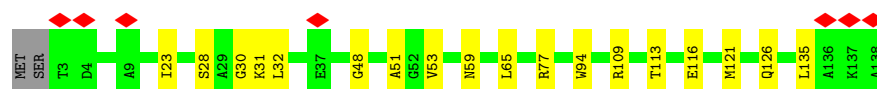
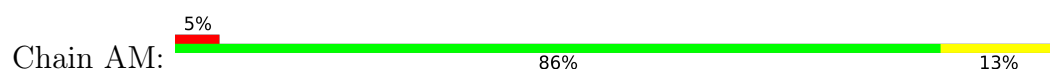
- Molecule 47: RPL11A isoform 1



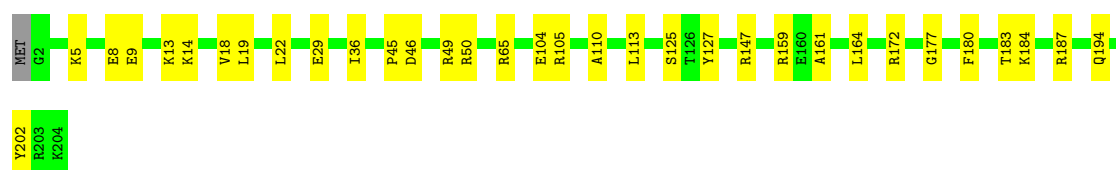
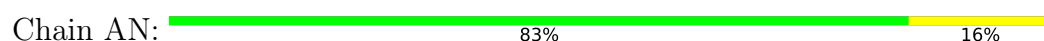
- Molecule 48: 60S ribosomal protein L13-A



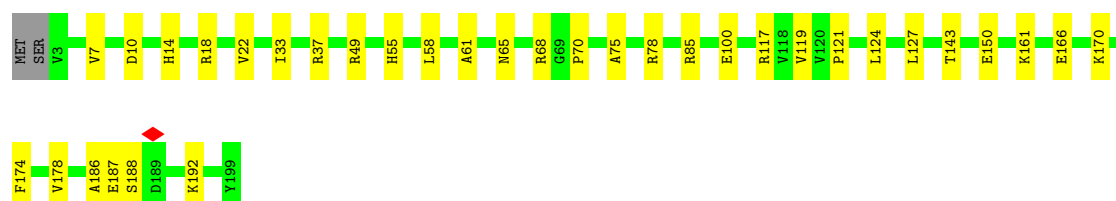
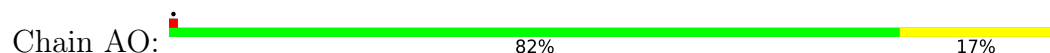
- Molecule 49: 60S ribosomal protein L14-A



- Molecule 50: 60S ribosomal protein L15-A



- Molecule 51: 60S ribosomal protein L16-A



- Molecule 52: 60S ribosomal protein L17-A

Chain AP:  82% 13% 5%



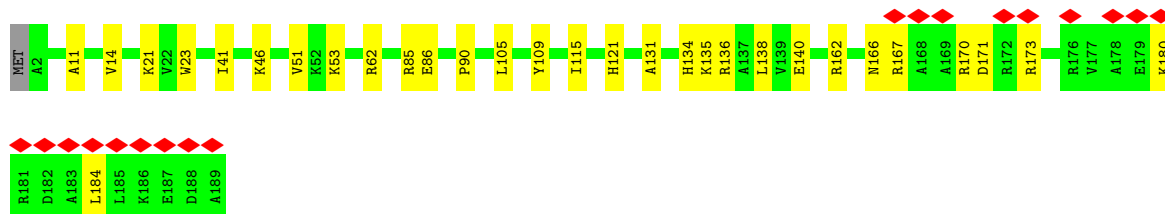
- Molecule 53: 60S ribosomal protein L18-A

Chain AQ:  88% 11%



- Molecule 54: 60S ribosomal protein L19-A

Chain AR:  10% 84% 16%



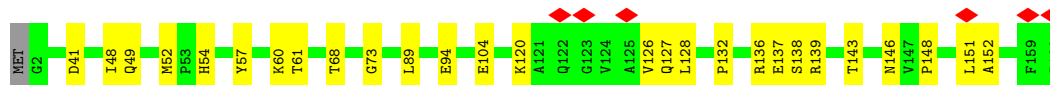
- Molecule 55: 60S ribosomal protein L20

Chain AS:  77% 20%



- Molecule 56: 60S ribosomal protein L21-A

Chain AT:  82% 17%

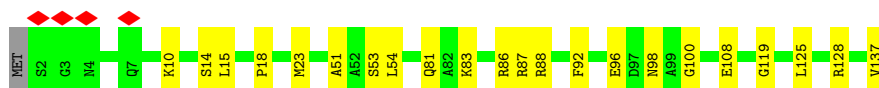
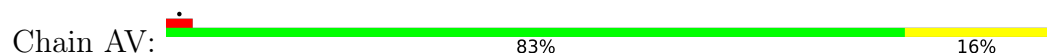


- Molecule 57: 60S ribosomal protein L22-A

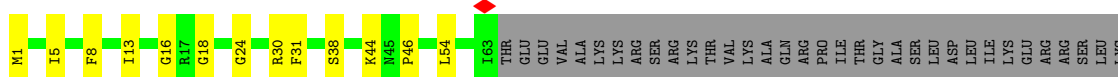
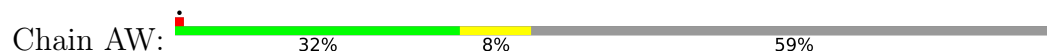
Chain AU:  74% 9% 17%



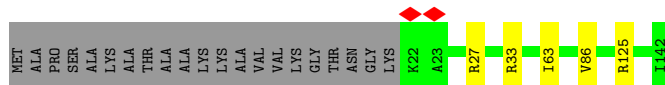
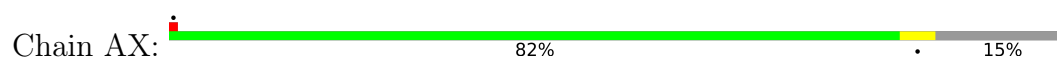
- Molecule 58: 60S ribosomal protein L23-A



- Molecule 59: RPL24A isoform 1



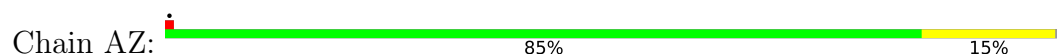
- Molecule 60: 60S ribosomal protein L25



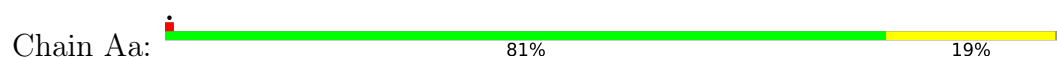
- Molecule 61: 60S ribosomal protein L26-A



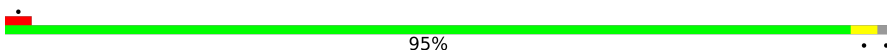
- Molecule 62: 60S ribosomal protein L27-A



- Molecule 63: 60S ribosomal protein L28



- Molecule 64: RPL29 isoform 1

Chain Ab:  95%



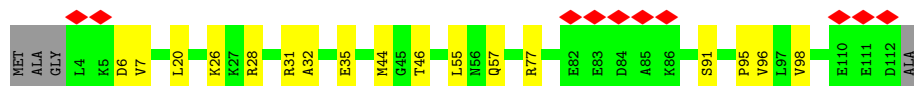
- Molecule 65: 60S ribosomal protein L30

Chain Ac:  76% 16% 8%

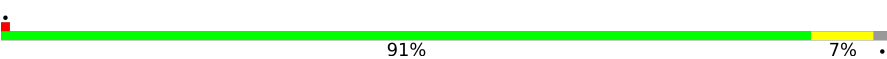


- Molecule 66: 60S ribosomal protein L31-A

Chain Ad:  9% 81% 15%



- Molecule 67: RPL32 isoform 1

Chain Ae:  91% 7%



- Molecule 68: 60S ribosomal protein L33-A

Chain Af:  91% 8%



- Molecule 69: 60S ribosomal protein L34-A

Chain Ag:  6% 81% 12% 7%



- Molecule 70: 60S ribosomal protein L35-A

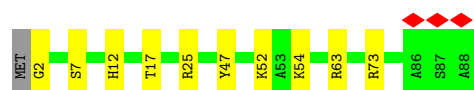
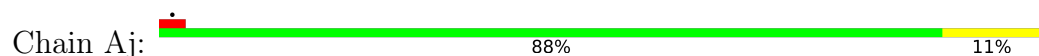
Chain Ah:  81% 18%



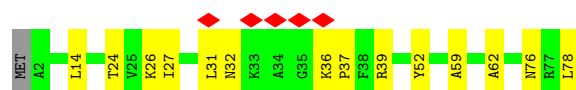
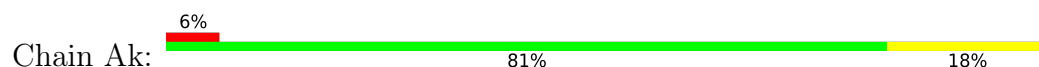
- Molecule 71: 60S ribosomal protein L36-A



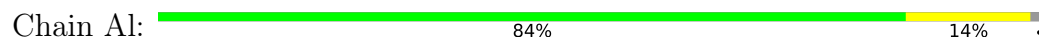
- Molecule 72: 60S ribosomal protein L37-A



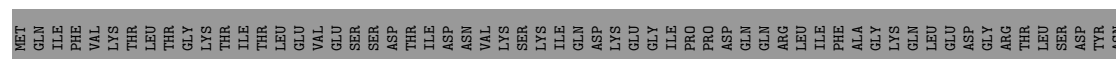
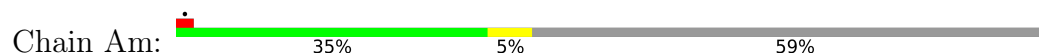
- Molecule 73: RPL38 isoform 1



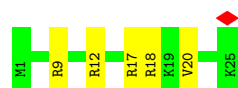
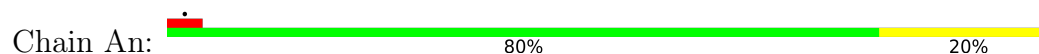
- Molecule 74: 60S ribosomal protein L39



- Molecule 75: Ubiquitin-60S ribosomal protein L40

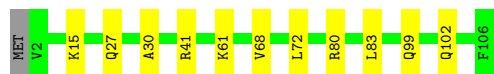


- Molecule 76: 60S ribosomal protein L41-A



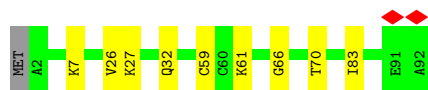
- Molecule 77: 60S ribosomal protein L42-A

Chain Ao:  89% 10%



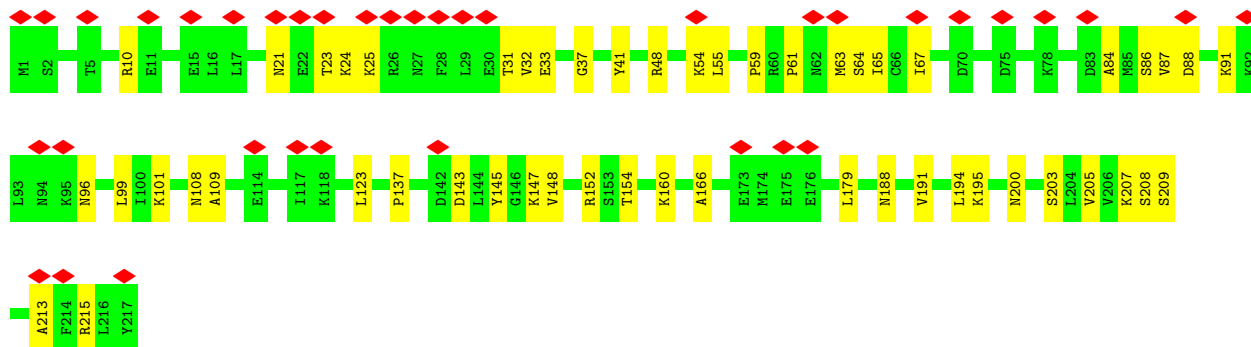
- Molecule 78: 60S ribosomal protein L43-A

Chain Ap:  89% 10%



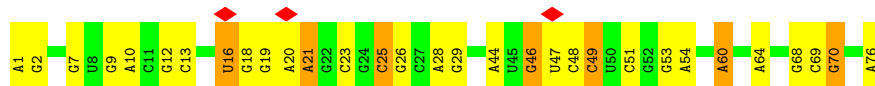
- Molecule 79: RPL1A isoform 1

Chain E:  17% 76% 24%



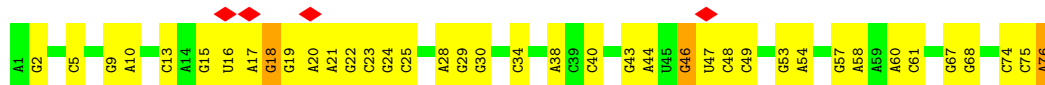
- Molecule 80: P site tRNA

Chain tP:  59% 32% 9%



- Molecule 81: A site tRNA

Chain tA:  5% 49% 47%

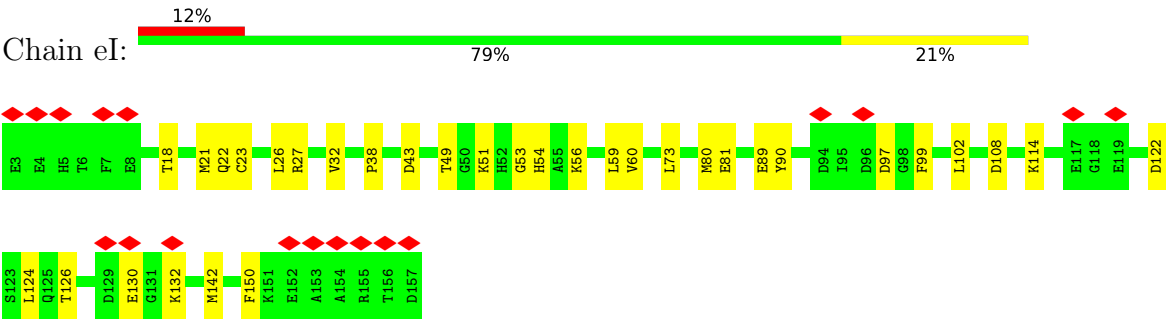


- Molecule 82: messenger RNA

Chain MR:  75% 25%



● Molecule 83: Eukaryotic translation initiation factor 5A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	295361	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	9.412	Depositor
Minimum map value	-4.108	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.255	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, G7M, 3HE, PSU, 1MA, 4AC, OMG, 5CT, 5MC, OMU, UR3, MA6, MG, B8N, K, HIC, 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	BA	0.23	0/1653	0.47	0/2261
2	BB	0.26	0/1735	0.55	0/2335
3	BC	0.26	0/1665	0.48	1/2263 (0.0%)
4	BE	0.20	0/2109	0.45	0/2839
5	BG	0.21	0/1844	0.45	0/2464
6	BH	0.22	0/1506	0.53	2/2028 (0.1%)
7	BI	0.27	0/1514	0.49	0/2021
8	BJ	0.21	0/1519	0.45	0/2035
9	BL	0.26	0/1272	0.45	0/1712
10	BN	0.28	0/1215	0.51	0/1638
11	BO	0.33	0/952	0.62	0/1279
12	BV	0.23	0/693	0.54	0/935
13	BW	0.27	0/1038	0.44	0/1395
14	BX	0.31	0/1139	0.50	0/1518
15	BY	0.21	0/1087	0.47	0/1449
16	Ba	0.30	0/782	0.58	0/1047
17	Bb	0.24	0/620	0.50	0/838
18	Be	0.22	0/483	0.44	0/643
19	BD	0.23	0/1759	0.51	0/2368
20	BF	0.22	0/1629	0.49	0/2202
21	BK	0.23	0/837	0.64	2/1131 (0.2%)
22	BP	0.22	0/1012	0.53	0/1356
23	BQ	0.23	0/1125	0.50	0/1510
24	BR	0.19	0/957	0.44	0/1283
25	BS	0.23	0/1211	0.52	0/1628
26	BT	0.23	0/1113	0.57	0/1494
27	BU	0.27	0/865	0.59	0/1169
28	BZ	0.19	0/814	0.49	2/1084 (0.2%)
29	Bc	0.25	0/499	0.56	0/670
30	Bd	0.22	0/452	0.66	2/600 (0.3%)
31	Bg	0.19	0/2454	0.49	0/3340
32	Bf	0.15	0/616	0.37	0/817

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BM	0.19	0/943	0.51	0/1274
34	B5	0.28	1/42034 (0.0%)	0.37	1/65493 (0.0%)
35	AA	0.40	0/1912	0.49	0/2569
36	AB	0.31	0/3139	0.46	0/4219
37	AC	0.31	0/2800	0.49	0/3790
38	A1	0.42	0/76161	0.41	1/118749 (0.0%)
39	A3	0.29	0/2861	0.32	0/4457
40	A4	0.40	0/3724	0.37	0/5798
41	AD	0.23	0/2390	0.42	0/3225
42	AE	0.22	0/1324	0.42	0/1782
43	AF	0.32	0/1821	0.47	0/2451
44	AG	0.30	0/1830	0.51	0/2469
45	AH	0.28	0/1531	0.49	0/2062
46	AI	0.30	0/1796	0.46	0/2409
47	AJ	0.25	0/1374	0.55	0/1842
48	AL	0.29	0/1568	0.42	0/2106
49	AM	0.24	0/1068	0.42	0/1438
50	AN	0.40	0/1757	0.52	0/2354
51	AO	0.32	0/1585	0.48	1/2128 (0.0%)
52	AP	0.33	0/1410	0.44	0/1893
53	AQ	0.31	0/1465	0.43	0/1965
54	AR	0.31	0/1538	0.46	0/2050
55	AS	0.31	0/1481	0.50	0/1990
56	AT	0.33	0/1300	0.50	1/1743 (0.1%)
57	AU	0.25	0/812	0.48	0/1099
58	AV	0.35	0/1018	0.50	0/1369
59	AW	0.31	0/533	0.42	0/707
60	AX	0.32	0/983	0.44	0/1325
61	AY	0.30	0/1004	0.44	0/1341
62	AZ	0.26	0/1118	0.45	0/1497
63	Aa	0.36	0/1204	0.47	0/1612
64	Ab	0.29	0/473	0.43	0/629
65	Ac	0.27	0/751	0.42	0/1008
66	Ad	0.30	0/904	0.42	0/1213
67	Ae	0.32	0/1041	0.42	0/1394
68	Af	0.30	0/868	0.40	0/1168
69	Ag	0.34	0/890	0.46	0/1189
70	Ah	0.28	0/978	0.45	0/1301
71	Ai	0.28	0/778	0.51	0/1034
72	Aj	0.41	0/696	0.50	0/923
73	Ak	0.27	0/618	0.51	0/826
74	Al	0.36	0/443	0.46	0/588
75	Am	0.28	0/423	0.54	0/562

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	An	0.30	0/234	0.60	0/300
77	Ao	0.34	0/860	0.45	0/1136
78	Ap	0.35	0/701	0.54	0/934
79	E	0.22	0/1745	0.52	0/2342
80	tP	0.30	0/1796	0.37	0/2799
81	tA	0.28	0/1821	0.38	0/2838
82	MR	0.32	0/291	0.35	0/451
83	eI	0.31	0/1147	0.62	0/1544
All	All	0.34	1/221111 (0.0%)	0.43	13/324737 (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
11	BO	0	1
14	BX	0	1
20	BF	0	1
43	AF	0	1
44	AG	0	2
54	AR	0	1
63	Aa	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	O3'-P	5.36	1.61	1.56

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Bd	4	GLU	CA-C-N	8.76	137.47	121.70
30	Bd	4	GLU	C-N-CA	8.76	137.47	121.70
21	BK	89	GLY	CA-C-N	6.63	133.63	121.70
21	BK	89	GLY	C-N-CA	6.63	133.63	121.70
6	BH	13	PRO	CA-C-N	5.93	132.38	121.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	AF	232	ARG	Peptide
44	AG	30	THR	Peptide
20	BF	99	MET	Peptide
11	BO	123	SER	Peptide
14	BX	88	PRO	Peptide

5.2 Too-close contacts

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	BA	1612	0	1623	33	0
2	BB	1709	0	1784	36	0
3	BC	1635	0	1723	24	0
4	BE	2068	0	2154	46	0
5	BG	1820	0	1918	44	0
6	BH	1481	0	1572	34	0
7	BI	1489	0	1525	37	0
8	BJ	1494	0	1573	36	0
9	BL	1244	0	1314	9	0
10	BN	1192	0	1255	16	0
11	BO	941	0	979	15	0
12	BV	684	0	672	10	0
13	BW	1021	0	1060	21	0
14	BX	1121	0	1196	15	0
15	BY	1073	0	1132	22	0
16	Ba	769	0	818	10	0
17	Bb	610	0	633	8	0
18	Be	475	0	525	9	0
19	BD	1734	0	1817	26	0
20	BF	1609	0	1675	34	0
21	BK	817	0	804	17	0
22	BP	991	0	1035	12	0
23	BQ	1105	0	1166	33	0
24	BR	948	0	990	18	0
25	BS	1192	0	1222	34	0
26	BT	1095	0	1114	25	0
27	BU	855	0	917	19	0
28	BZ	804	0	881	14	0
29	Bc	497	0	535	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Bd	442	0	432	12	0
31	Bg	2401	0	2356	61	0
32	Bf	605	0	654	11	0
33	BM	935	0	975	28	0
34	B5	37987	0	19105	418	0
35	AA	1878	0	1946	35	0
36	AB	3081	0	3162	39	0
37	AC	2748	0	2859	36	0
38	A1	68786	0	34573	501	0
39	A3	2579	0	1304	19	0
40	A4	3353	0	1695	20	0
41	AD	2341	0	2290	16	0
42	AE	1303	0	1376	19	0
43	AF	1784	0	1862	18	0
44	AG	1798	0	1894	25	0
45	AH	1510	0	1576	21	0
46	AI	1759	0	1799	23	0
47	AJ	1353	0	1383	30	0
48	AL	1543	0	1608	15	0
49	AM	1053	0	1149	13	0
50	AN	1720	0	1779	25	0
51	AO	1555	0	1659	21	0
52	AP	1388	0	1423	17	0
53	AQ	1441	0	1543	16	0
54	AR	1521	0	1617	26	0
55	AS	1445	0	1487	28	0
56	AT	1276	0	1323	18	0
57	AU	796	0	812	6	0
58	AV	1003	0	1048	15	0
59	AW	521	0	551	10	0
60	AX	968	0	1036	4	0
61	AY	993	0	1081	9	0
62	AZ	1092	0	1155	13	0
63	Aa	1173	0	1215	23	0
64	Ab	462	0	491	2	0
65	Ac	743	0	797	12	0
66	Ad	890	0	938	11	0
67	Ae	1020	0	1090	6	0
68	Af	850	0	880	8	0
69	Ag	880	0	945	12	0
70	Ah	969	0	1078	14	0
71	Ai	771	0	849	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	Aj	681	0	687	9	0
73	Ak	612	0	682	10	0
74	Al	436	0	475	5	0
75	Am	417	0	459	5	0
76	An	233	0	283	3	0
77	Ao	847	0	914	8	0
78	Ap	694	0	738	6	0
79	E	1718	0	1811	33	0
80	tP	1606	0	816	12	0
81	tA	1628	0	827	22	0
82	MR	259	0	130	2	0
83	eI	1148	0	1111	20	0
84	A1	139	0	0	0	0
84	A4	1	0	0	0	0
84	AP	1	0	0	0	0
84	AV	1	0	0	0	0
84	B5	39	0	0	0	0
85	A1	12	0	0	0	0
85	Ab	1	0	0	0	0
85	B5	10	0	0	0	0
86	A1	10	0	19	0	0
87	A1	20	0	23	0	0
88	Ao	1	0	0	0	0
All	All	207315	0	153382	2055	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 6.

The worst 5 of 2055 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:B5:898:A:C2	34:B5:914:G:N2	2.11	1.19
34:B5:898:A:H2	34:B5:914:G:N2	1.53	0.99
38:A1:2437:G:H1	38:A1:2510:U:H3	1.13	0.97
38:A1:172:G:H1	38:A1:246:U:H3	1.08	0.96
34:B5:515:A:H62	34:B5:537:G:H21	1.13	0.95

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
1	BA	204/252 (81%)	186 (91%)	18 (9%)	0	100	100
2	BB	212/255 (83%)	182 (86%)	30 (14%)	0	100	100
3	BC	215/254 (85%)	203 (94%)	12 (6%)	0	100	100
4	BE	258/261 (99%)	238 (92%)	20 (8%)	0	100	100
5	BG	224/236 (95%)	216 (96%)	8 (4%)	0	100	100
6	BH	182/190 (96%)	167 (92%)	15 (8%)	0	100	100
7	BI	184/200 (92%)	166 (90%)	18 (10%)	0	100	100
8	BJ	183/197 (93%)	171 (93%)	12 (7%)	0	100	100
9	BL	153/156 (98%)	140 (92%)	13 (8%)	0	100	100
10	BN	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
11	BO	125/137 (91%)	110 (88%)	15 (12%)	0	100	100
12	BV	85/87 (98%)	74 (87%)	11 (13%)	0	100	100
13	BW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
14	BX	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
15	BY	132/135 (98%)	122 (92%)	10 (8%)	0	100	100
16	Ba	95/119 (80%)	85 (90%)	10 (10%)	0	100	100
17	Bb	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
18	Be	58/63 (92%)	52 (90%)	6 (10%)	0	100	100
19	BD	221/240 (92%)	207 (94%)	14 (6%)	0	100	100
20	BF	204/225 (91%)	189 (93%)	15 (7%)	0	100	100
21	BK	94/105 (90%)	84 (89%)	10 (11%)	0	100	100
22	BP	122/142 (86%)	113 (93%)	9 (7%)	0	100	100
23	BQ	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
24	BR	117/136 (86%)	113 (97%)	4 (3%)	0	100	100
25	BS	143/146 (98%)	134 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BT	139/144 (96%)	128 (92%)	11 (8%)	0	100	100
27	BU	105/121 (87%)	97 (92%)	8 (8%)	0	100	100
28	BZ	100/108 (93%)	98 (98%)	2 (2%)	0	100	100
29	Bc	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
30	Bd	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
31	Bg	310/319 (97%)	284 (92%)	26 (8%)	0	100	100
32	Bf	73/152 (48%)	69 (94%)	4 (6%)	0	100	100
33	BM	122/143 (85%)	108 (88%)	14 (12%)	0	100	100
35	AA	245/254 (96%)	236 (96%)	9 (4%)	0	100	100
36	AB	383/387 (99%)	369 (96%)	14 (4%)	0	100	100
37	AC	359/362 (99%)	339 (94%)	20 (6%)	0	100	100
41	AD	290/297 (98%)	274 (94%)	16 (6%)	0	100	100
42	AE	163/176 (93%)	152 (93%)	11 (7%)	0	100	100
43	AF	220/244 (90%)	212 (96%)	8 (4%)	0	100	100
44	AG	228/256 (89%)	209 (92%)	19 (8%)	0	100	100
45	AH	188/191 (98%)	172 (92%)	16 (8%)	0	100	100
46	AI	215/221 (97%)	207 (96%)	8 (4%)	0	100	100
47	AJ	167/174 (96%)	156 (93%)	11 (7%)	0	100	100
48	AL	191/199 (96%)	183 (96%)	8 (4%)	0	100	100
49	AM	134/138 (97%)	126 (94%)	8 (6%)	0	100	100
50	AN	201/204 (98%)	190 (94%)	11 (6%)	0	100	100
51	AO	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
52	AP	171/184 (93%)	167 (98%)	4 (2%)	0	100	100
53	AQ	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
54	AR	186/189 (98%)	181 (97%)	5 (3%)	0	100	100
55	AS	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
56	AT	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
57	AU	98/121 (81%)	94 (96%)	4 (4%)	0	100	100
58	AV	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
59	AW	61/155 (39%)	61 (100%)	0	0	100	100
60	AX	119/142 (84%)	116 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	AY	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
62	AZ	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
63	Aa	146/149 (98%)	135 (92%)	11 (8%)	0	100	100
64	Ab	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
65	Ac	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
66	Ad	107/113 (95%)	102 (95%)	5 (5%)	0	100	100
67	Ae	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
68	Af	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
69	Ag	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
70	Ah	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
71	Ai	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
72	Aj	85/88 (97%)	84 (99%)	1 (1%)	0	100	100
73	Ak	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
74	Al	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
75	Am	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	103/106 (97%)	92 (89%)	11 (11%)	0	100	100
78	Ap	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
79	E	215/217 (99%)	199 (93%)	16 (7%)	0	100	100
83	eI	152/155 (98%)	131 (86%)	21 (14%)	0	100	100
All	All	11319/12258 (92%)	10641 (94%)	678 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	BA	173/210 (82%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BB	191/224 (85%)	191 (100%)	0	100	100
3	BC	176/205 (86%)	176 (100%)	0	100	100
4	BE	221/222 (100%)	221 (100%)	0	100	100
5	BG	193/201 (96%)	193 (100%)	0	100	100
6	BH	165/170 (97%)	165 (100%)	0	100	100
7	BI	150/161 (93%)	150 (100%)	0	100	100
8	BJ	158/166 (95%)	158 (100%)	0	100	100
9	BL	136/137 (99%)	136 (100%)	0	100	100
10	BN	127/128 (99%)	127 (100%)	0	100	100
11	BO	96/105 (91%)	96 (100%)	0	100	100
12	BV	74/74 (100%)	74 (100%)	0	100	100
13	BW	110/111 (99%)	110 (100%)	0	100	100
14	BX	119/120 (99%)	119 (100%)	0	100	100
15	BY	112/113 (99%)	112 (100%)	0	100	100
16	Ba	83/100 (83%)	83 (100%)	0	100	100
17	Bb	70/71 (99%)	70 (100%)	0	100	100
18	Be	51/54 (94%)	51 (100%)	0	100	100
19	BD	182/195 (93%)	182 (100%)	0	100	100
20	BF	173/191 (91%)	173 (100%)	0	100	100
21	BK	89/98 (91%)	89 (100%)	0	100	100
22	BP	104/118 (88%)	104 (100%)	0	100	100
23	BQ	117/119 (98%)	117 (100%)	0	100	100
24	BR	101/124 (82%)	101 (100%)	0	100	100
25	BS	128/129 (99%)	128 (100%)	0	100	100
26	BT	113/116 (97%)	113 (100%)	0	100	100
27	BU	100/114 (88%)	100 (100%)	0	100	100
28	BZ	84/89 (94%)	84 (100%)	0	100	100
29	Bc	56/60 (93%)	56 (100%)	0	100	100
30	Bd	47/49 (96%)	47 (100%)	0	100	100
31	Bg	256/262 (98%)	256 (100%)	0	100	100
32	Bf	66/135 (49%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BM	100/119 (84%)	100 (100%)	0	100	100
35	AA	189/196 (96%)	189 (100%)	0	100	100
36	AB	321/322 (100%)	321 (100%)	0	100	100
37	AC	288/289 (100%)	288 (100%)	0	100	100
41	AD	241/245 (98%)	241 (100%)	0	100	100
42	AE	137/153 (90%)	137 (100%)	0	100	100
43	AF	186/205 (91%)	186 (100%)	0	100	100
44	AG	189/208 (91%)	189 (100%)	0	100	100
45	AH	170/171 (99%)	170 (100%)	0	100	100
46	AI	185/187 (99%)	185 (100%)	0	100	100
47	AJ	147/150 (98%)	147 (100%)	0	100	100
48	AL	154/159 (97%)	154 (100%)	0	100	100
49	AM	107/109 (98%)	107 (100%)	0	100	100
50	AN	175/176 (99%)	175 (100%)	0	100	100
51	AO	160/162 (99%)	160 (100%)	0	100	100
52	AP	141/146 (97%)	141 (100%)	0	100	100
53	AQ	150/151 (99%)	150 (100%)	0	100	100
54	AR	153/154 (99%)	153 (100%)	0	100	100
55	AS	156/162 (96%)	156 (100%)	0	100	100
56	AT	136/137 (99%)	136 (100%)	0	100	100
57	AU	87/107 (81%)	87 (100%)	0	100	100
58	AV	104/105 (99%)	104 (100%)	0	100	100
59	AW	55/129 (43%)	55 (100%)	0	100	100
60	AX	105/118 (89%)	105 (100%)	0	100	100
61	AY	109/110 (99%)	109 (100%)	0	100	100
62	AZ	115/116 (99%)	115 (100%)	0	100	100
63	Aa	118/119 (99%)	118 (100%)	0	100	100
64	Ab	46/47 (98%)	46 (100%)	0	100	100
65	Ac	81/88 (92%)	81 (100%)	0	100	100
66	Ad	96/97 (99%)	96 (100%)	0	100	100
67	Ae	109/111 (98%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	Af	90/91 (99%)	90 (100%)	0	100	100
69	Ag	95/103 (92%)	95 (100%)	0	100	100
70	Ah	104/105 (99%)	104 (100%)	0	100	100
71	Ai	81/82 (99%)	81 (100%)	0	100	100
72	Aj	70/71 (99%)	70 (100%)	0	100	100
73	Ak	68/69 (99%)	68 (100%)	0	100	100
74	Al	45/46 (98%)	45 (100%)	0	100	100
75	Am	47/116 (40%)	47 (100%)	0	100	100
76	An	23/23 (100%)	23 (100%)	0	100	100
77	Ao	90/91 (99%)	90 (100%)	0	100	100
78	Ap	71/72 (99%)	71 (100%)	0	100	100
79	E	198/198 (100%)	198 (100%)	0	100	100
83	eI	118/129 (92%)	118 (100%)	0	100	100
All	All	9631/10315 (93%)	9631 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
33	BM	125	ASN
83	eI	88	ASN
47	AJ	43	GLN
83	eI	58	HIS
69	Ag	33	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1780/1798 (98%)	445 (25%)	22 (1%)
38	A1	3212/3395 (94%)	600 (18%)	23 (0%)
39	A3	120/121 (99%)	12 (10%)	0
40	A4	157/158 (99%)	26 (16%)	0
80	tP	74/75 (98%)	19 (25%)	0
81	tA	75/76 (98%)	16 (21%)	0
82	MR	11/12 (91%)	1 (9%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	5429/5635 (96%)	1119 (20%)	45 (0%)

5 of 1119 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	2	A
34	B5	4	C
34	B5	25	C
34	B5	26	A
34	B5	34	G

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	A1	1225	A
38	A1	2461	A
38	A1	1292	C
38	A1	1577	G
38	A1	2474	G

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

60 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
38	PSU	A1	2266	38	18,21,22	1.54	5 (27%)	21,30,33	2.21	4 (19%)
38	PSU	A1	2416	38,84	18,21,22	1.66	5 (27%)	21,30,33	2.07	4 (19%)
36	HIC	AB	243	36	10,11,12	1.30	1 (10%)	9,14,16	1.36	2 (22%)
38	PSU	A1	966	38	18,21,22	1.69	5 (27%)	21,30,33	2.09	5 (23%)
38	PSU	A1	2129	38	18,21,22	1.61	4 (22%)	21,30,33	2.15	3 (14%)
38	PSU	A1	990	38	18,21,22	1.47	4 (22%)	21,30,33	2.20	4 (19%)
38	PSU	A1	2880	38	18,21,22	1.62	5 (27%)	21,30,33	2.23	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PSU	B5	999	34	18,21,22	1.41	4 (22%)	21,30,33	2.17	5 (23%)
38	PSU	A1	776	38	18,21,22	1.50	4 (22%)	21,30,33	2.00	5 (23%)
38	PSU	A1	1004	38	18,21,22	1.48	4 (22%)	21,30,33	2.12	5 (23%)
38	PSU	A1	2191	38	18,21,22	1.55	4 (22%)	21,30,33	2.17	5 (23%)
38	PSU	A1	1052	38	18,21,22	1.43	4 (22%)	21,30,33	2.03	4 (19%)
40	PSU	A4	73	40	18,21,22	1.45	4 (22%)	21,30,33	2.02	3 (14%)
38	PSU	A1	1124	38	18,21,22	1.51	5 (27%)	21,30,33	2.27	4 (19%)
38	PSU	A1	2264	38	18,21,22	1.44	3 (16%)	21,30,33	2.17	5 (23%)
38	PSU	A1	2351	38	18,21,22	1.52	4 (22%)	21,30,33	2.16	4 (19%)
38	OMU	A1	2921	38,84	19,22,23	1.32	3 (15%)	25,31,34	1.89	6 (24%)
34	B8N	B5	1191	34	25,29,30	1.38	3 (12%)	28,42,45	3.04	6 (21%)
38	PSU	A1	2133	38	18,21,22	1.46	3 (16%)	21,30,33	2.20	5 (23%)
38	PSU	A1	2260	38	18,21,22	1.51	4 (22%)	21,30,33	2.15	3 (14%)
38	UR3	A1	2634	38	19,22,23	0.91	1 (5%)	26,32,35	1.74	4 (15%)
38	PSU	A1	2349	38,84	18,21,22	1.50	4 (22%)	21,30,33	1.97	4 (19%)
38	PSU	A1	2826	38	18,21,22	1.59	6 (33%)	21,30,33	2.26	6 (28%)
38	PSU	A1	2865	38	18,21,22	1.48	6 (33%)	21,30,33	2.19	4 (19%)
34	PSU	B5	302	34	18,21,22	1.48	4 (22%)	21,30,33	2.01	3 (14%)
34	PSU	B5	759	34	18,21,22	1.37	3 (16%)	21,30,33	2.00	3 (14%)
38	PSU	A1	2735	38	18,21,22	1.44	4 (22%)	21,30,33	2.16	4 (19%)
38	PSU	A1	2944	38,84	18,21,22	1.56	5 (27%)	21,30,33	2.23	4 (19%)
38	PSU	A1	1110	38	18,21,22	1.51	5 (27%)	21,30,33	2.01	5 (23%)
34	G7M	B5	1575	80,34	23,26,27	2.45	6 (26%)	34,39,42	3.29	15 (44%)
34	PSU	B5	1290	34	18,21,22	1.40	3 (16%)	21,30,33	2.02	3 (14%)
34	PSU	B5	632	34	18,21,22	1.45	4 (22%)	21,30,33	2.02	3 (14%)
34	4AC	B5	1773	34	21,24,25	1.02	2 (9%)	28,34,37	2.47	6 (21%)
34	MA6	B5	1781	34	23,26,27	1.45	5 (21%)	33,38,41	2.07	10 (30%)
38	PSU	A1	2340	38	18,21,22	1.57	4 (22%)	21,30,33	2.11	4 (19%)
83	5CT	eI	51	-	13,14,15	0.66	0	8,15,17	1.53	1 (12%)
34	PSU	B5	106	34	18,21,22	1.41	3 (16%)	21,30,33	2.08	4 (19%)
34	PSU	B5	1415	34	18,21,22	1.44	3 (16%)	21,30,33	2.04	4 (19%)
38	5MC	A1	2870	38	19,22,23	1.27	3 (15%)	26,32,35	1.39	4 (15%)
38	PSU	A1	986	38	18,21,22	1.45	4 (22%)	21,30,33	2.05	4 (19%)
38	5MC	A1	2278	38,84	19,22,23	1.51	3 (15%)	26,32,35	1.35	4 (15%)
34	PSU	B5	120	34	18,21,22	1.40	3 (16%)	21,30,33	2.13	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PSU	B5	1187	34	18,21,22	1.47	4 (22%)	21,30,33	2.07	3 (14%)
38	PSU	A1	2314	38	18,21,22	1.50	4 (22%)	21,30,33	2.12	4 (19%)
34	MA6	B5	1782	34	23,26,27	1.46	5 (21%)	33,38,41	2.14	10 (30%)
38	PSU	A1	2258	38	18,21,22	1.43	4 (22%)	21,30,33	2.11	4 (19%)
34	PSU	B5	466	34	18,21,22	1.40	3 (16%)	21,30,33	2.16	4 (19%)
34	4AC	B5	1280	34	21,24,25	1.06	1 (4%)	28,34,37	1.08	3 (10%)
34	PSU	B5	211	34	18,21,22	1.45	4 (22%)	21,30,33	2.10	4 (19%)
34	PSU	B5	1181	34	18,21,22	1.42	4 (22%)	21,30,33	2.15	4 (19%)
38	PSU	A1	1042	38	18,21,22	1.45	3 (16%)	21,30,33	2.12	4 (19%)
38	PSU	A1	1056	38	18,21,22	1.43	4 (22%)	21,30,33	2.07	4 (19%)
39	PSU	A3	50	39	18,21,22	1.38	3 (16%)	21,30,33	2.00	3 (14%)
38	OMG	A1	2922	38,81	23,26,27	1.19	4 (17%)	32,38,41	2.07	7 (21%)
38	PSU	A1	2975	38	18,21,22	1.57	5 (27%)	21,30,33	2.27	4 (19%)
38	1MA	A1	645	38,84	21,25,26	1.33	4 (19%)	30,37,40	1.69	6 (20%)
38	1MA	A1	2142	38	21,25,26	1.30	4 (19%)	30,37,40	1.81	4 (13%)
38	PSU	A1	960	38	18,21,22	1.55	5 (27%)	21,30,33	2.19	4 (19%)
34	PSU	B5	766	34	18,21,22	1.47	4 (22%)	21,30,33	2.09	5 (23%)
38	PSU	A1	2923	38,81	18,21,22	1.53	5 (27%)	21,30,33	2.14	3 (14%)

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
38	PSU	A1	2266	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2416	38,84	-	0/7/25/26	0/2/2/2
36	HIC	AB	243	36	-	0/5/6/8	0/1/1/1
38	PSU	A1	966	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2129	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	990	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2880	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	999	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	776	38	-	2/7/25/26	0/2/2/2
38	PSU	A1	1004	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2191	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1052	38	-	0/7/25/26	0/2/2/2
40	PSU	A4	73	40	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PSU	A1	1124	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2264	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2351	38	-	0/7/25/26	0/2/2/2
38	OMU	A1	2921	38,84	-	0/9/27/28	0/2/2/2
34	B8N	B5	1191	34	-	4/16/34/35	0/2/2/2
38	PSU	A1	2133	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2260	38	-	2/7/25/26	0/2/2/2
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2349	38,84	-	0/7/25/26	0/2/2/2
38	PSU	A1	2826	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2865	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	302	34	-	2/7/25/26	0/2/2/2
34	PSU	B5	759	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2735	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	2944	38,84	-	0/7/25/26	0/2/2/2
38	PSU	A1	1110	38	-	0/7/25/26	0/2/2/2
34	G7M	B5	1575	80,34	-	0/7/25/26	0/3/3/3
34	PSU	B5	1290	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	632	34	-	0/7/25/26	0/2/2/2
34	4AC	B5	1773	34	-	3/11/29/30	0/2/2/2
34	MA6	B5	1781	34	-	0/11/29/30	0/3/3/3
38	PSU	A1	2340	38	-	1/7/25/26	0/2/2/2
83	5CT	eI	51	-	-	7/13/14/16	-
34	PSU	B5	106	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	1415	34	-	0/7/25/26	0/2/2/2
38	5MC	A1	2870	38	-	4/7/25/26	0/2/2/2
38	PSU	A1	986	38	-	0/7/25/26	0/2/2/2
38	5MC	A1	2278	38,84	-	0/7/25/26	0/2/2/2
34	PSU	B5	120	34	-	0/7/25/26	0/2/2/2
34	PSU	B5	1187	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2314	38	-	1/7/25/26	0/2/2/2
34	MA6	B5	1782	34	-	3/11/29/30	0/3/3/3
38	PSU	A1	2258	38	-	2/7/25/26	0/2/2/2
34	PSU	B5	466	34	-	0/7/25/26	0/2/2/2
34	4AC	B5	1280	34	-	4/11/29/30	0/2/2/2
34	PSU	B5	211	34	-	2/7/25/26	0/2/2/2
34	PSU	B5	1181	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	1042	38	-	0/7/25/26	0/2/2/2
38	PSU	A1	1056	38	-	0/7/25/26	0/2/2/2
39	PSU	A3	50	39	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	OMG	A1	2922	38,81	-	0/9/27/28	0/3/3/3
38	PSU	A1	2975	38	-	0/7/25/26	0/2/2/2
38	1MA	A1	645	38,84	-	2/7/25/26	0/3/3/3
38	1MA	A1	2142	38	-	0/7/25/26	0/3/3/3
38	PSU	A1	960	38	-	0/7/25/26	0/2/2/2
34	PSU	B5	766	34	-	0/7/25/26	0/2/2/2
38	PSU	A1	2923	38,81	-	3/7/25/26	0/2/2/2

The worst 5 of 229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	C8-N7	7.10	1.45	1.33
34	B5	1575	G7M	C5-N7	-5.63	1.32	1.39
38	A1	2278	5MC	C5-C4	5.17	1.48	1.44
34	B5	1782	MA6	C5-C4	4.26	1.46	1.39
34	B5	1781	MA6	C5-C4	3.99	1.46	1.39

The worst 5 of 270 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B5	1191	B8N	C32-C31-N3	13.77	136.22	112.16
34	B5	1773	4AC	N4-C4-N3	9.03	128.52	113.87
34	B5	1575	G7M	CN7-N7-C8	-8.46	111.98	124.79
38	A1	1124	PSU	N1-C2-N3	7.27	122.83	115.17
38	A1	2826	PSU	N1-C2-N3	7.12	122.68	115.17

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	eI	51	5CT	C1-C2-C3-C4
83	eI	51	5CT	O1-C2-C3-C4
83	eI	51	5CT	C-CA-CB-CG
34	B5	1280	4AC	O7-C7-N4-C4
34	B5	1280	4AC	CM7-C7-N4-C4

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A1	2266	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A1	2880	PSU	1	0
38	A1	1110	PSU	1	0
34	B5	1575	G7M	2	0
34	B5	1290	PSU	1	0
38	A1	986	PSU	1	0
38	A1	2258	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 207 ligands modelled in this entry, 205 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	$\# Z > 2$
86	SPD	A1	3401	-	9,9,9	0.39	0	8,8,8	1.11	0
87	3HE	A1	3402	-	21,21,21	0.42	0	23,30,30	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	SPD	A1	3401	-	-	4/7/7/7	-
87	3HE	A1	3402	-	-	2/8/36/36	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

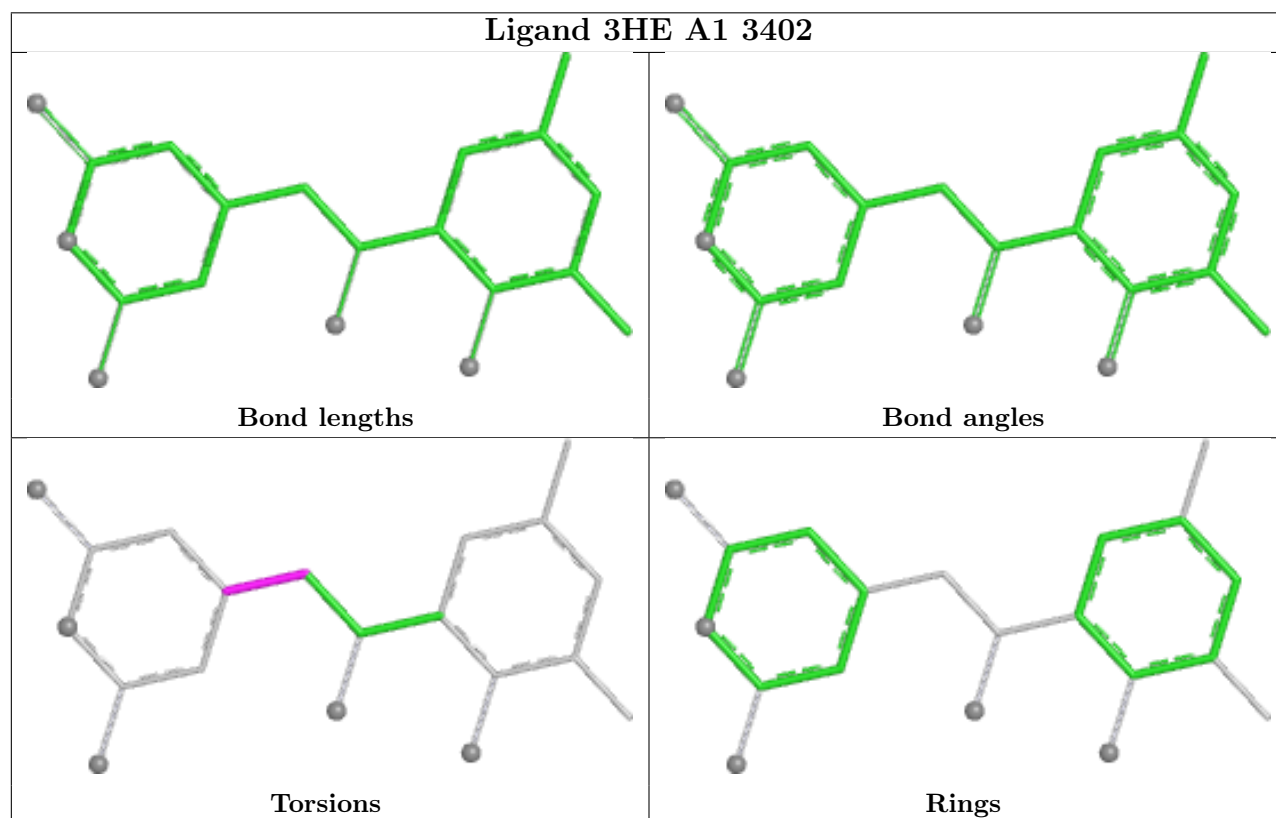
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	A1	3402	3HE	C7-C8-C9-C10
86	A1	3401	SPD	N6-C7-C8-C9
87	A1	3402	3HE	C7-C8-C9-C13
86	A1	3401	SPD	C2-C3-C4-C5
86	A1	3401	SPD	C4-C5-N6-C7

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.

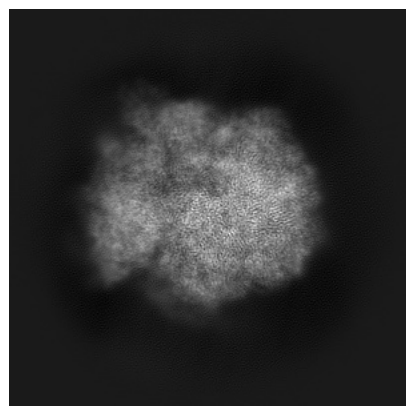
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40990. These allow visual inspection of the internal detail of the map and identification of artifacts.

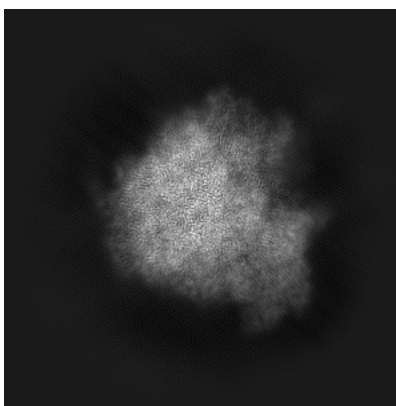
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

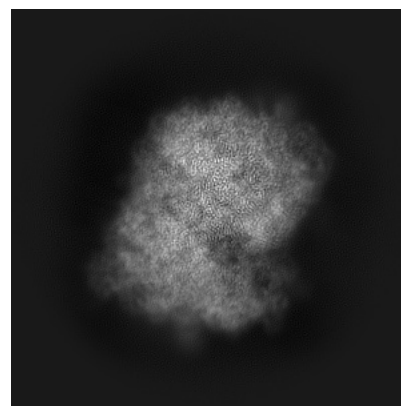
6.1.1 Primary map



X

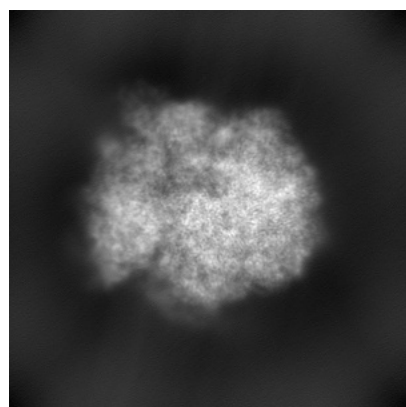


Y

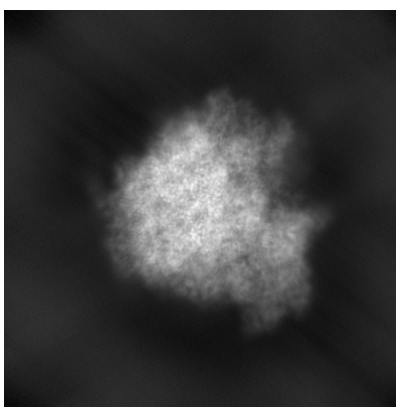


Z

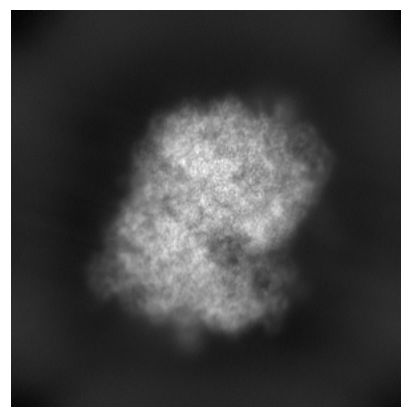
6.1.2 Raw map



X



Y

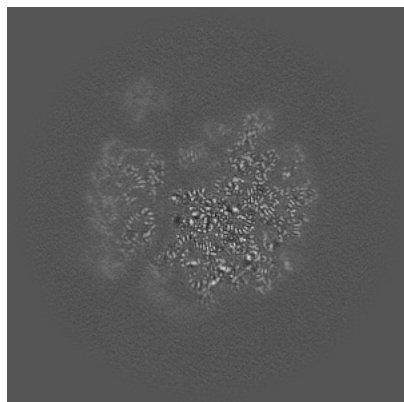


Z

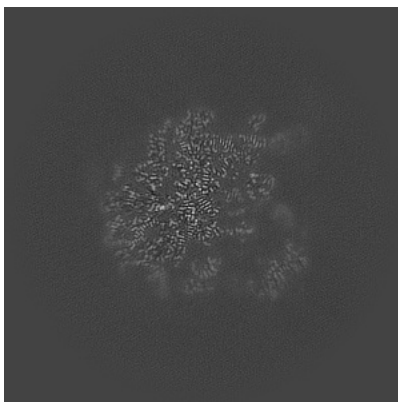
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

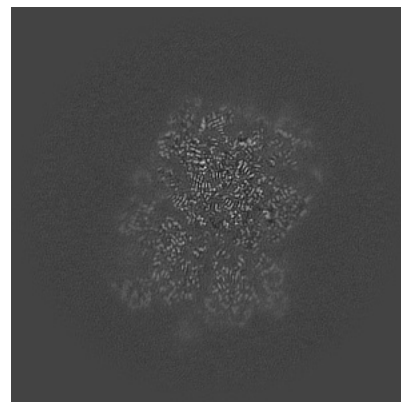
6.2.1 Primary map



X Index: 200

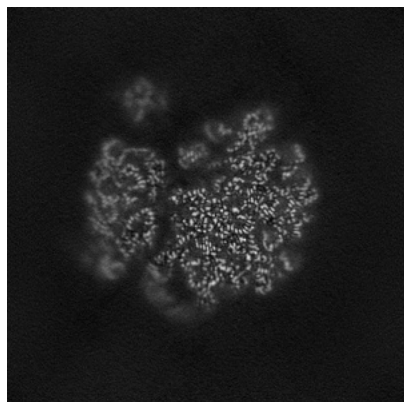


Y Index: 200

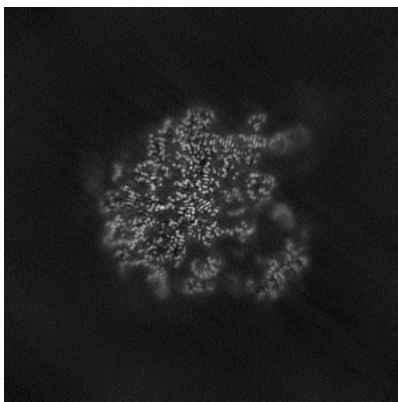


Z Index: 200

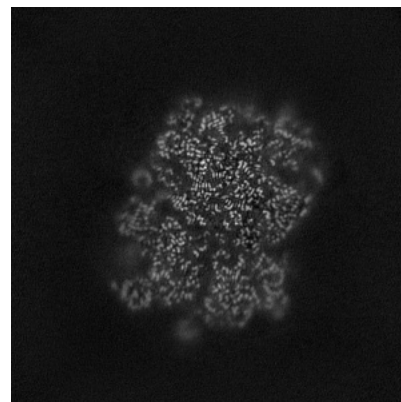
6.2.2 Raw map



X Index: 200



Y Index: 200

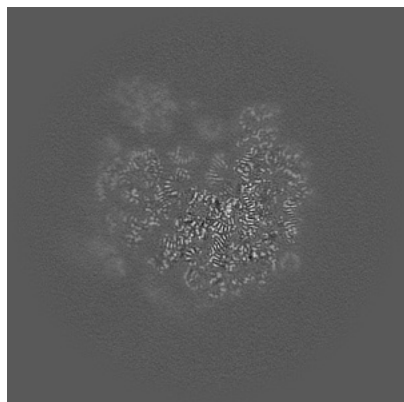


Z Index: 200

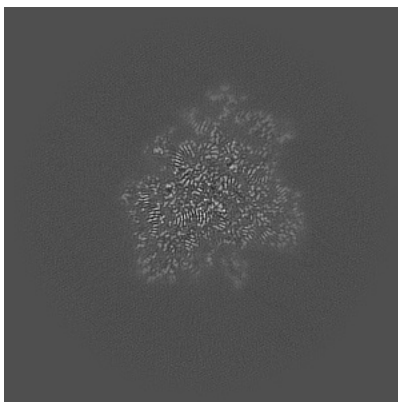
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

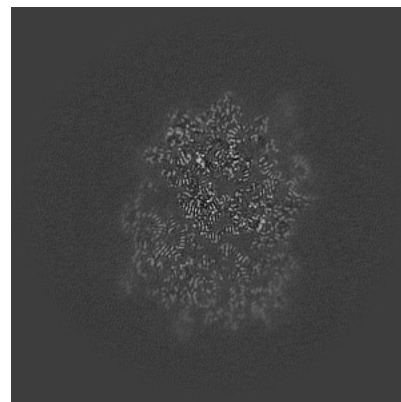
6.3.1 Primary map



X Index: 192

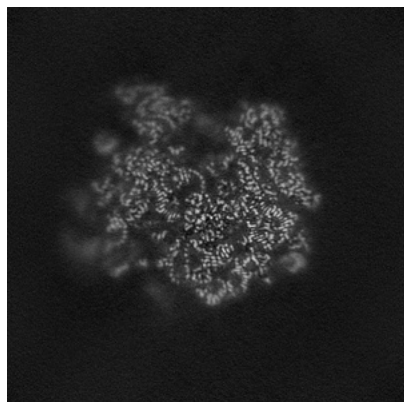


Y Index: 244

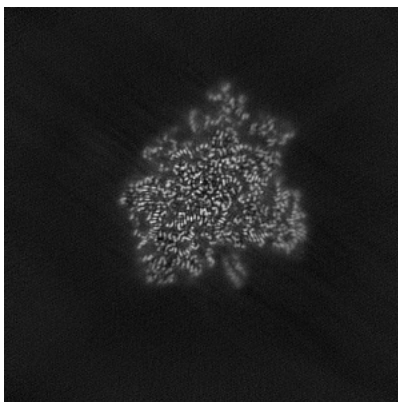


Z Index: 187

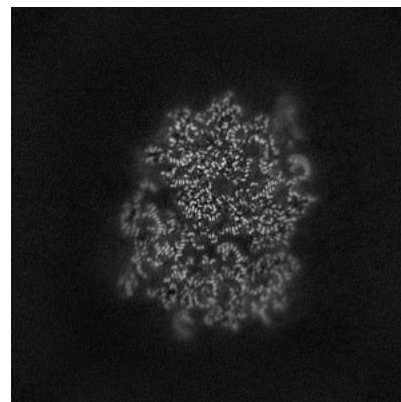
6.3.2 Raw map



X Index: 184



Y Index: 247

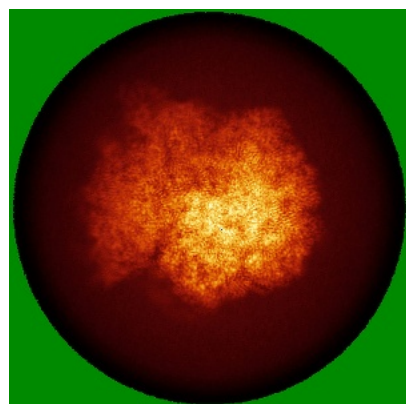


Z Index: 188

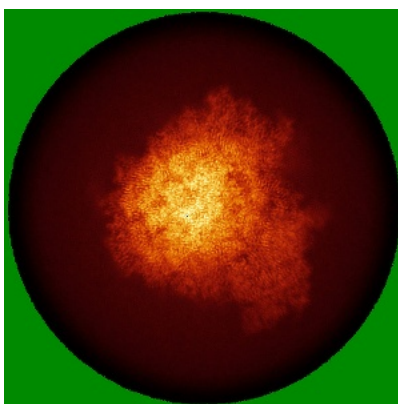
The images above show the largest variance slices of the map in three orthogonal directions.

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

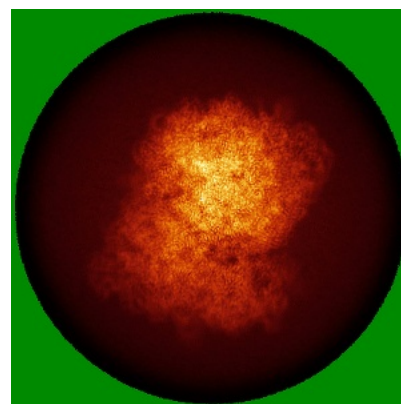
6.4.1 Primary map



X

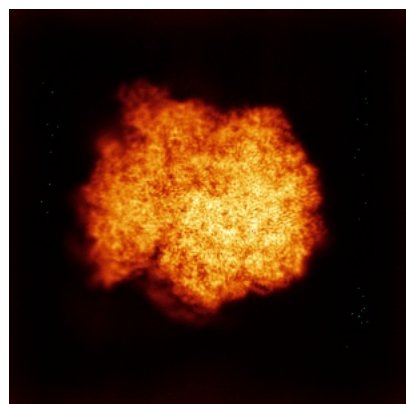


Y

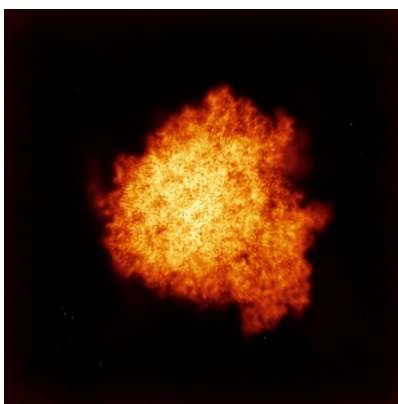


Z

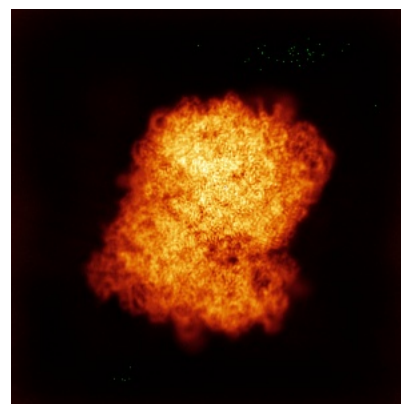
6.4.2 Raw map



X



Y

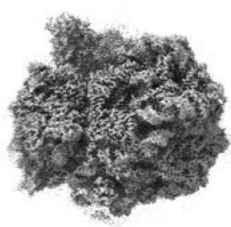


Z

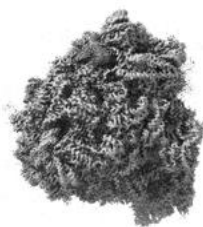
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

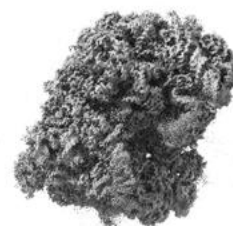
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

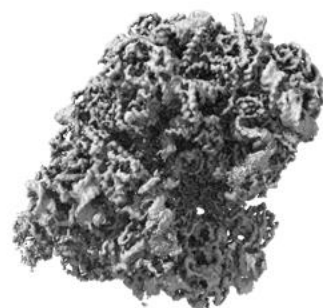
6.5.2 Raw map



X



Y



Z

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

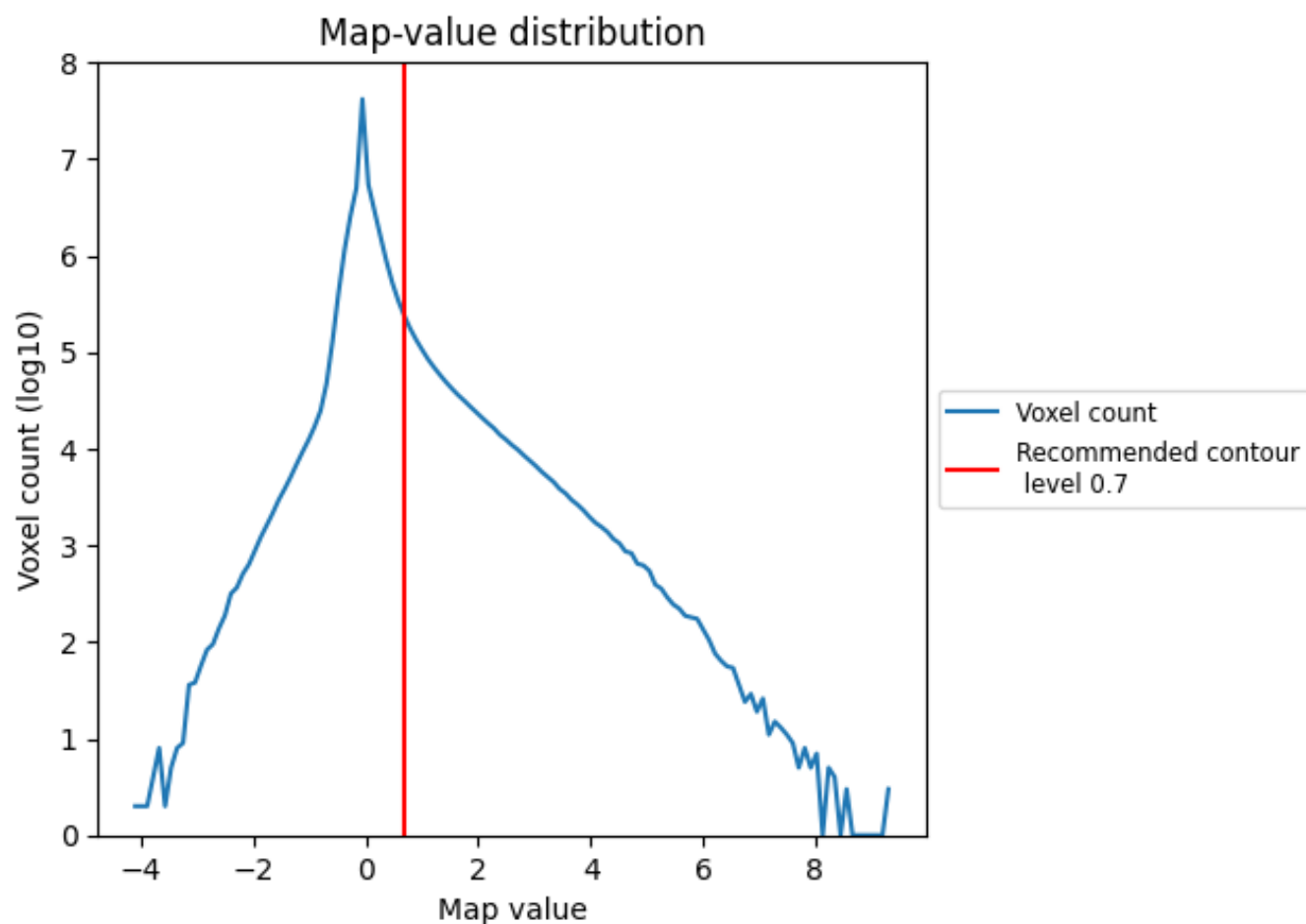
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

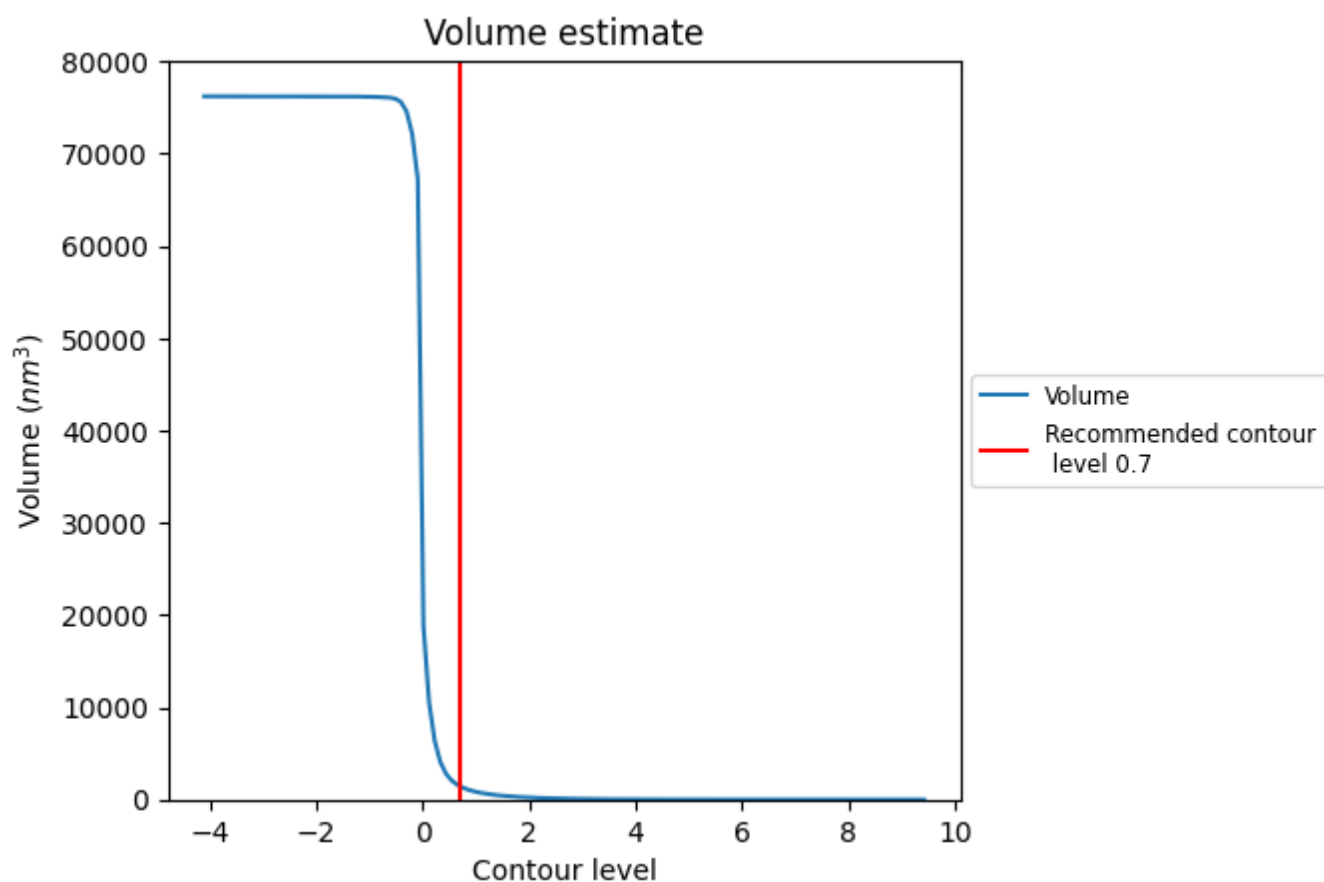
This section contains the results of statistical analysis of the map.

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.

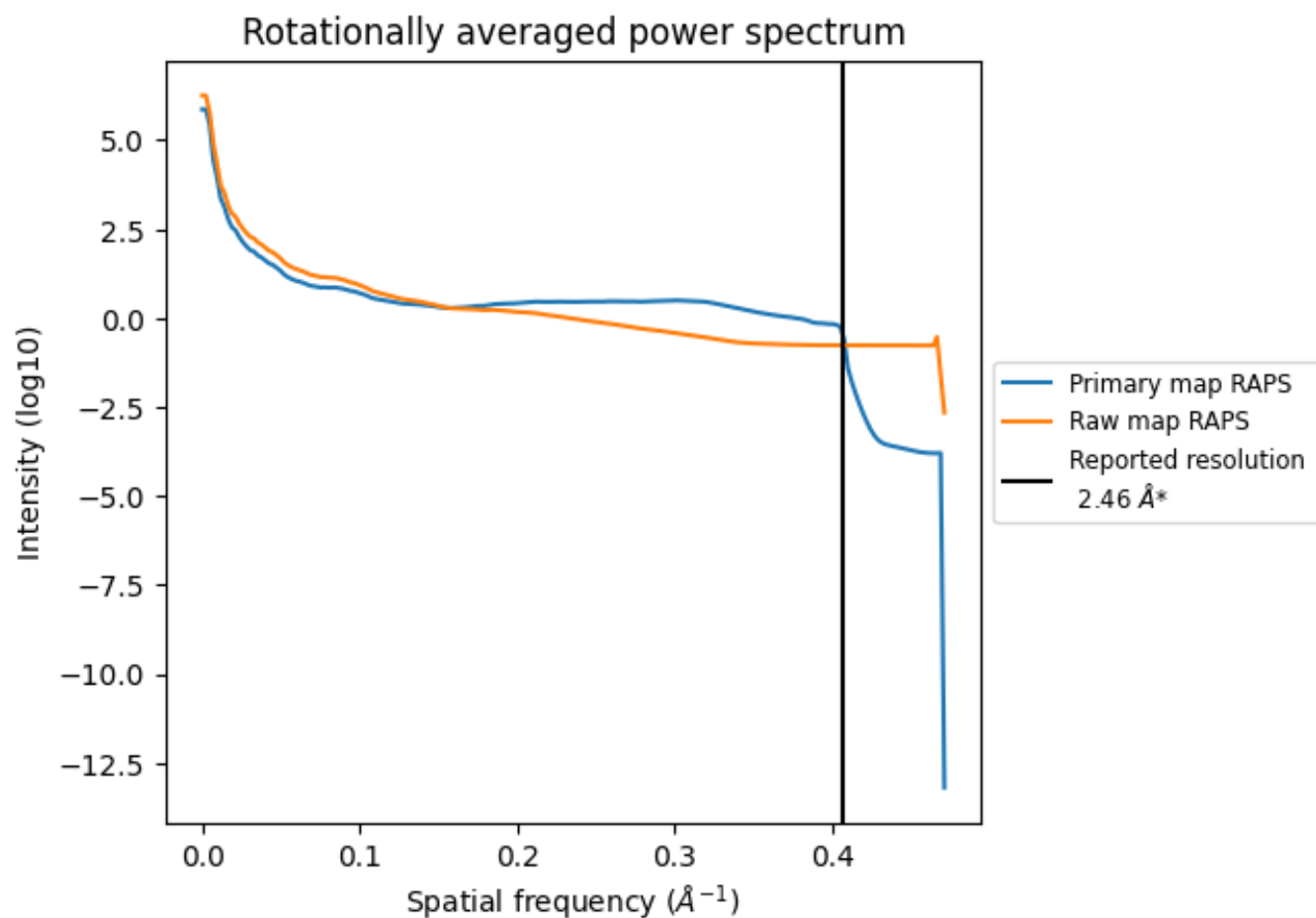
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1445 nm³; this corresponds to an approximate mass of 1305 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 ⓘ

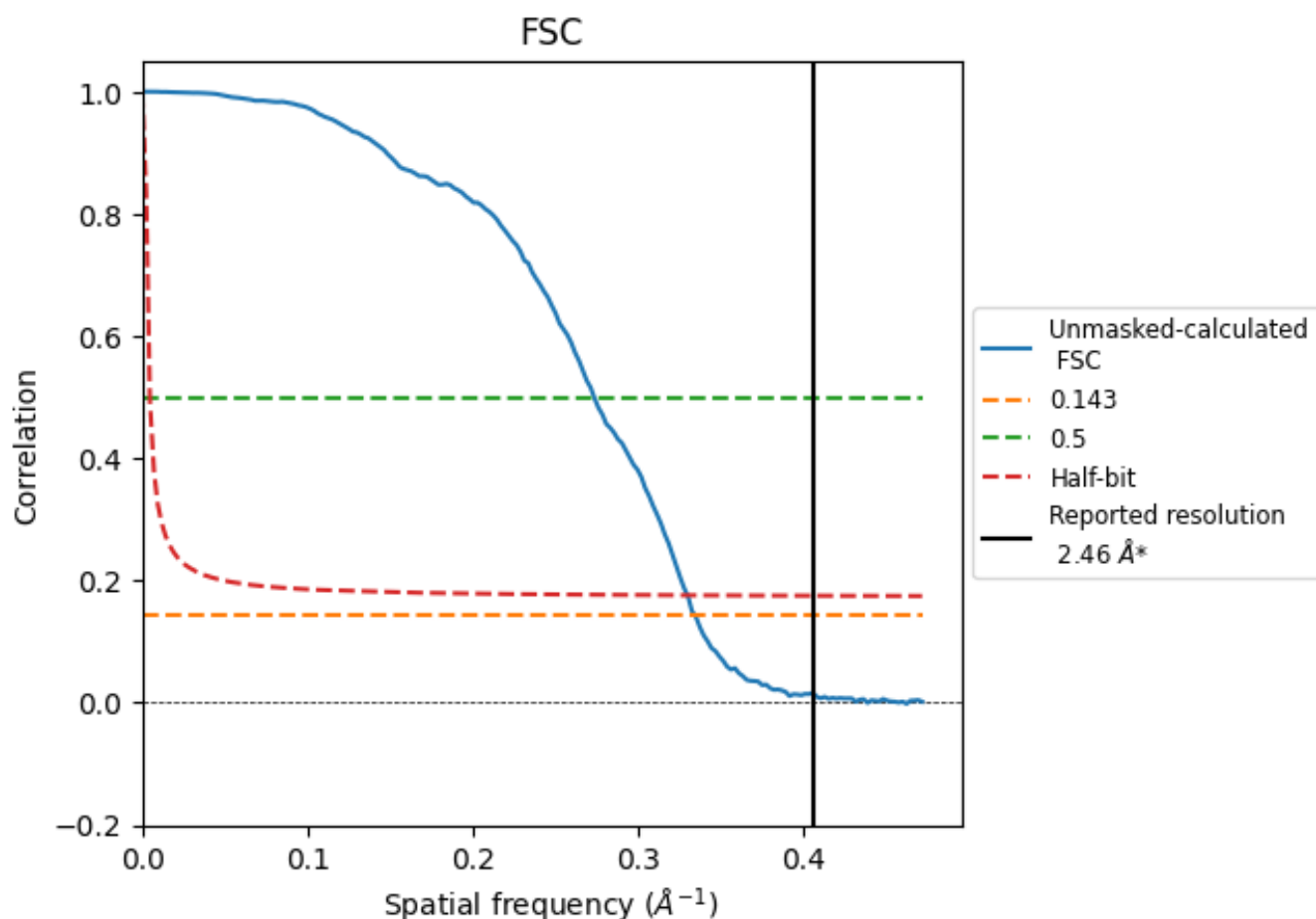


*Reported resolution corresponds to spatial frequency of 0.407 Å⁻¹

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 0.407 Å⁻¹

8.2 Resolution estimates [i](#)

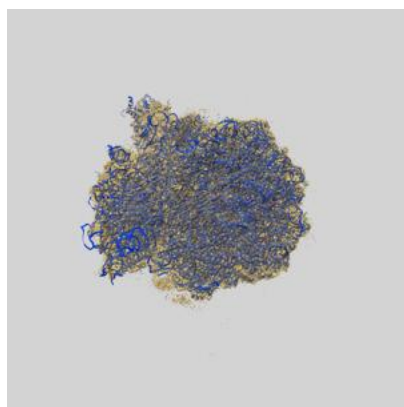
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.66	3.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.46 by more than 10 %

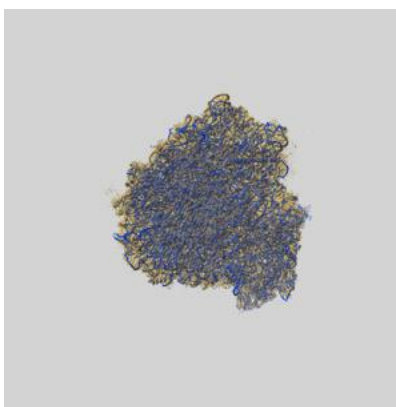
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40990 and PDB model 8T2X. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

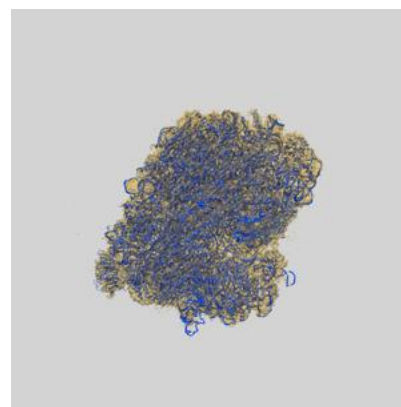
9.1 Map-model overlay [i](#)



X



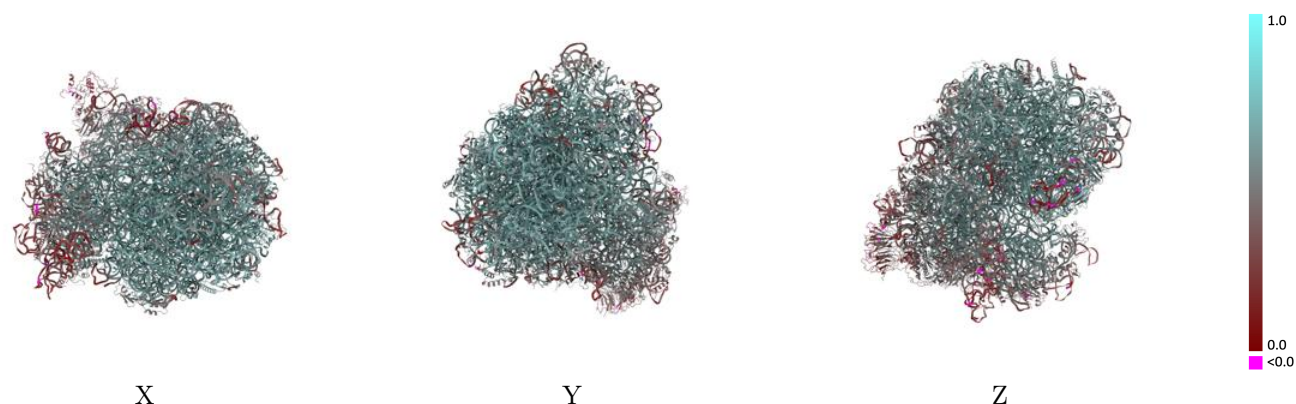
Y



Z

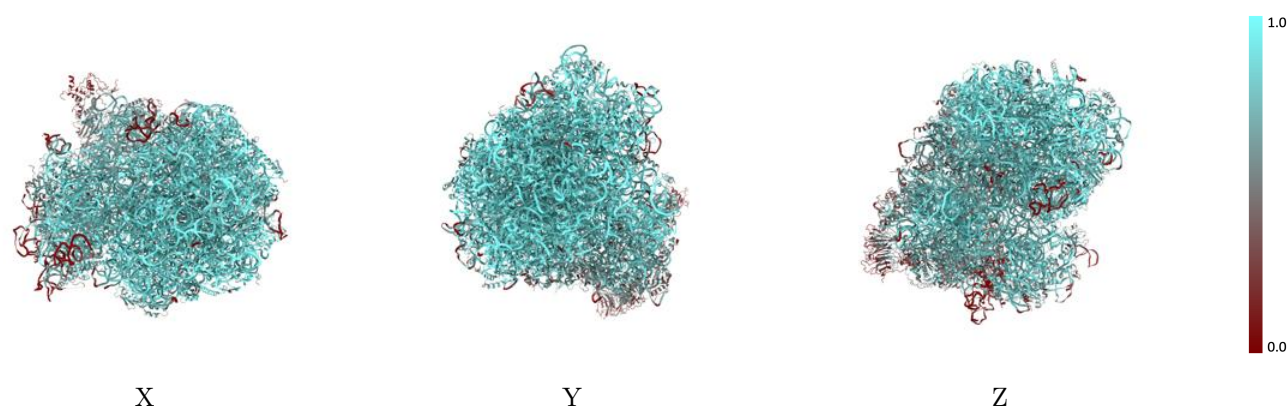
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



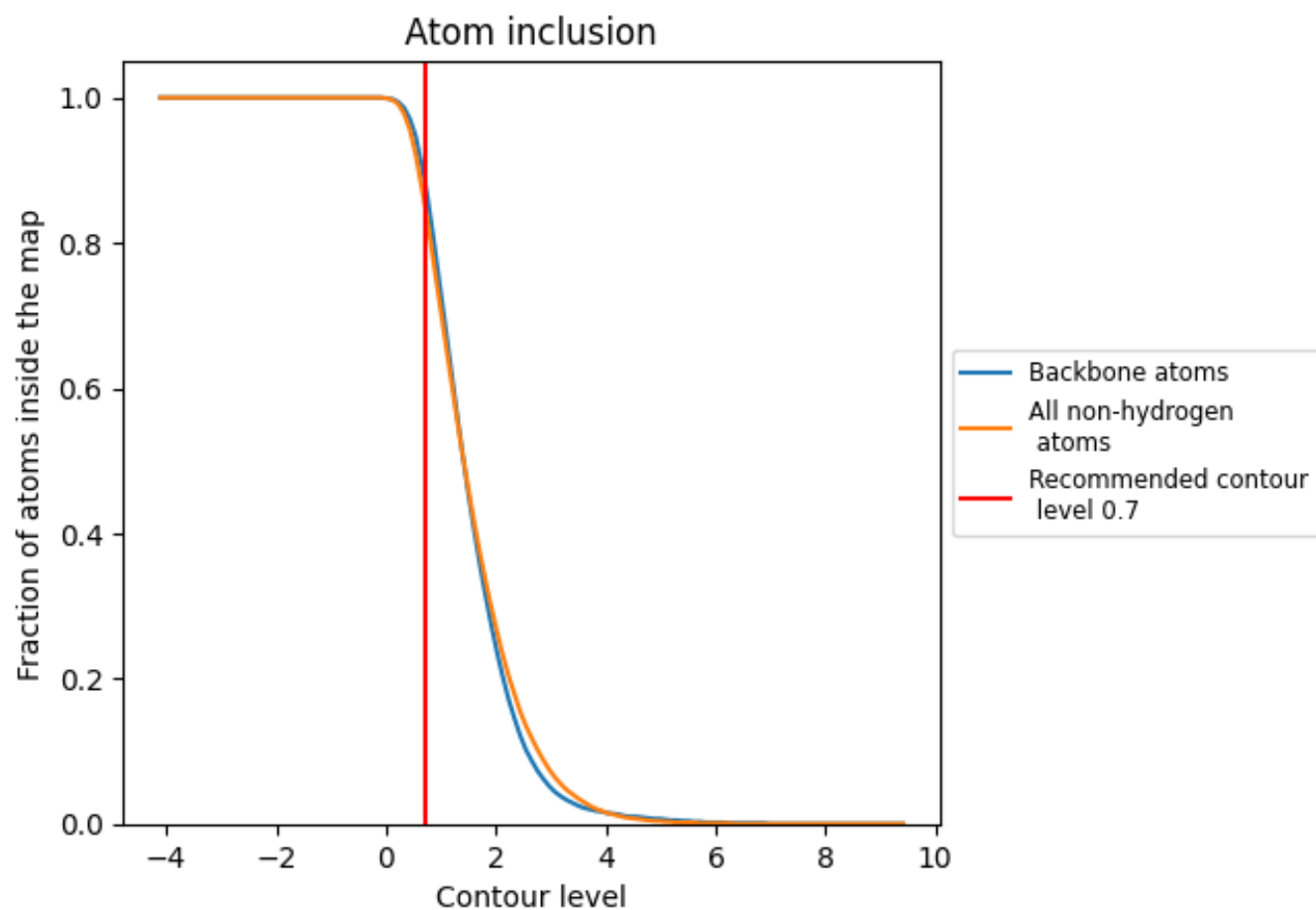
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.5590
A1	 0.9320	 0.6040
A3	 0.9650	 0.5760
A4	 0.9710	 0.6290
AA	 0.9830	 0.6780
AB	 0.9420	 0.6350
AC	 0.9310	 0.6200
AD	 0.7820	 0.5130
AE	 0.7990	 0.5210
AF	 0.9260	 0.6110
AG	 0.8400	 0.5510
AH	 0.8410	 0.5690
AI	 0.9160	 0.6210
AJ	 0.7540	 0.5000
AL	 0.9120	 0.6110
AM	 0.8460	 0.5470
AN	 0.9870	 0.6680
AO	 0.9440	 0.6250
AP	 0.9420	 0.6510
AQ	 0.9690	 0.6450
AR	 0.8430	 0.5790
AS	 0.9210	 0.6010
AT	 0.9150	 0.6100
AU	 0.7740	 0.5260
AV	 0.9390	 0.6470
AW	 0.9450	 0.6410
AX	 0.9350	 0.6210
AY	 0.9130	 0.6040
AZ	 0.8510	 0.5560
Aa	 0.9530	 0.6410
Ab	 0.9160	 0.6060
Ac	 0.8950	 0.5950
Ad	 0.8720	 0.6180
Ae	 0.9600	 0.6540
Af	 0.9720	 0.6480



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Chain	Atom inclusion	Q-score
Ag	 0.9120	 0.6310
Ah	 0.9300	 0.6000
Ai	 0.8860	 0.5740
Aj	 0.9680	 0.6740
Ak	 0.7380	 0.5240
Al	 0.9780	 0.6660
Am	 0.8860	 0.6150
An	 0.8540	 0.6240
Ao	 0.9350	 0.6410
Ap	 0.9430	 0.6550
B5	 0.8420	 0.5130
BA	 0.6740	 0.4580
BB	 0.7420	 0.4980
BC	 0.8070	 0.5290
BD	 0.5770	 0.4220
BE	 0.7440	 0.4790
BF	 0.6810	 0.4940
BG	 0.6770	 0.4280
BH	 0.5280	 0.4120
BI	 0.8040	 0.5340
BJ	 0.7050	 0.4560
BK	 0.5150	 0.3590
BL	 0.7920	 0.5520
BM	 0.1240	 0.2170
BN	 0.8450	 0.5560
BO	 0.8540	 0.5640
BP	 0.6080	 0.4390
BQ	 0.6360	 0.4520
BR	 0.5950	 0.4280
BS	 0.6730	 0.4640
BT	 0.6010	 0.4100
BU	 0.5260	 0.3880
BV	 0.7180	 0.4870
BW	 0.8920	 0.5700
BX	 0.9160	 0.6230
BY	 0.6390	 0.4240
BZ	 0.5150	 0.4410
Ba	 0.8690	 0.5840
Bb	 0.7210	 0.4840
Bc	 0.6920	 0.5220
Bd	 0.8230	 0.5140
Be	 0.6860	 0.4750

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Chain	Atom inclusion	Q-score
Bf	 0.2110	 0.2820
Bg	 0.3470	 0.3080
E	 0.6350	 0.4490
MR	 0.9420	 0.6060
eI	 0.7950	 0.5650
tA	 0.8760	 0.5540
tP	 0.9210	 0.5890