wwPDB EM Validation Summary Report

Dec 16, 2024 – 08:56 PM EST

PDB ID	:	8EVR
EMDB ID	:	EMD-28634
Title	:	Hypopseudouridylated yeast 80S bound with Taura syndrome virus (TSV) internal ribosome entry site (IRES), eEF2, GDP, and sordarin, Structure II
Authors	:	Zhao, Y.; Rai, J.; Li, H.
Deposited on	:	2022-10-20
Resolution	:	2.87 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:

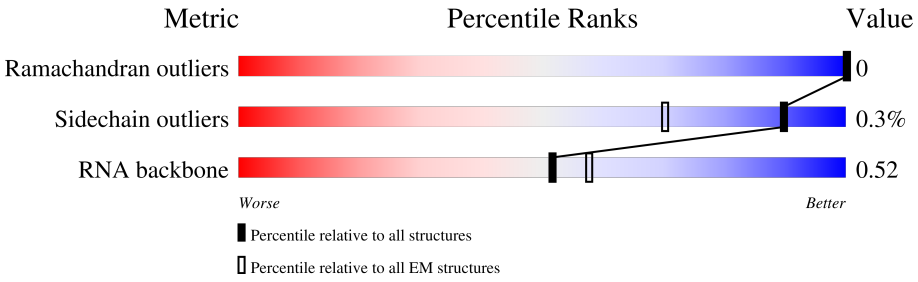
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.87 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	81% · 18%
2	BB	255	84% 16%
3	BC	254	84% · 15%
4	BE	261	99%
5	BG	236	96% ·
6	BH	190	12% 96% · ·
7	BI	200	94% 6%
8	BJ	197	94% 6%

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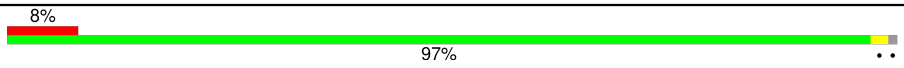
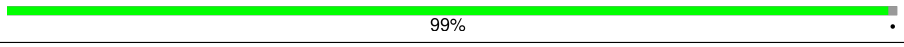
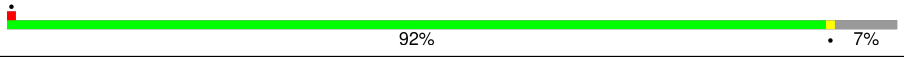
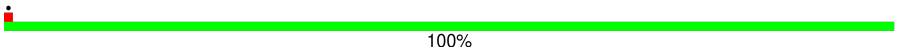
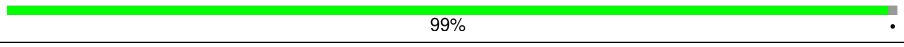
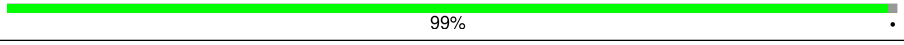
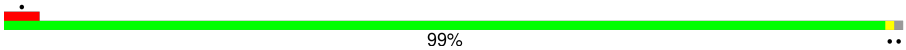
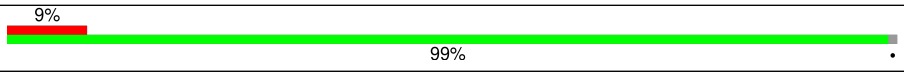
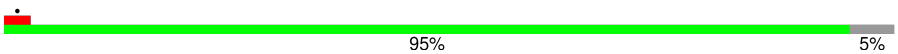
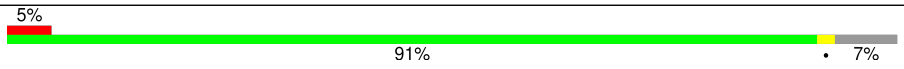
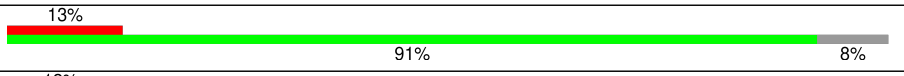
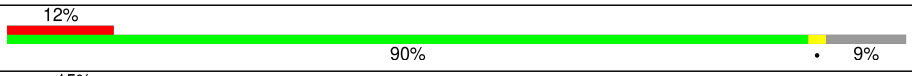
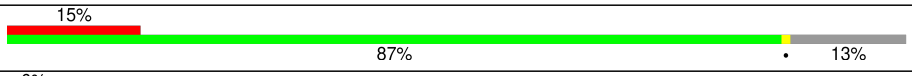
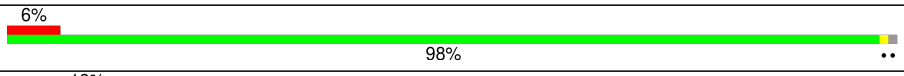
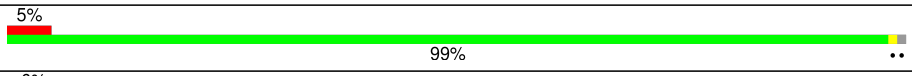
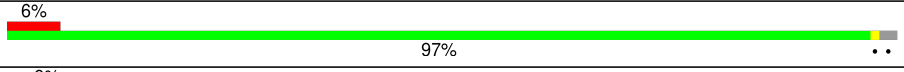
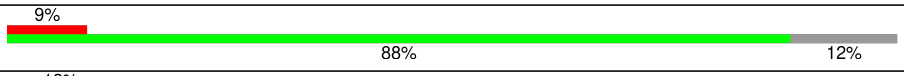
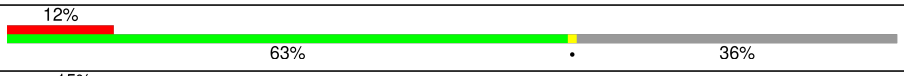
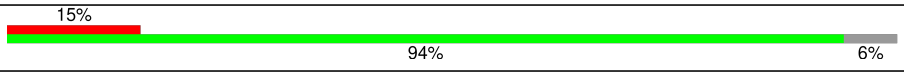
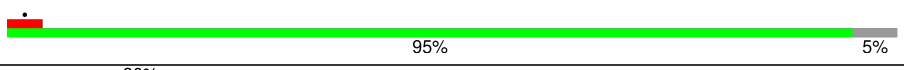
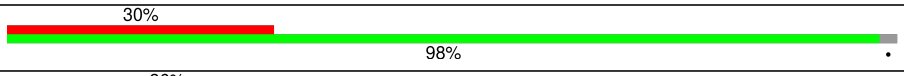
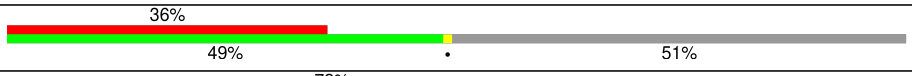
Mol	Chain	Length	Quality of chain
9	BL	156	
10	BN	151	
11	BO	137	
12	BV	87	
13	BW	130	
14	BX	145	
15	BY	135	
16	Ba	119	
17	Bb	82	
18	Be	63	
19	BD	240	
20	BF	225	
21	BK	105	
22	BP	142	
23	BQ	143	
24	BR	136	
25	BS	146	
26	BT	144	
27	BU	121	
28	BZ	108	
29	Bc	67	
30	Bd	56	
31	Bg	319	
32	Bf	152	
33	BM	143	

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Mol	Chain	Length	Quality of chain
34	B5	1798	73% 25%
35	AA	254	96%
36	AB	387	99%
37	AC	362	99%
38	A1	3360	76% 19% 5%
39	A3	121	89% 11%
40	A4	158	80% 20%
41	AD	297	98%
42	AE	176	88% 11%
43	AF	244	91% 9%
44	AG	256	89% 10%
45	AH	191	98%
46	AI	221	93% 7%
47	AJ	174	5% 97%
48	AL	199	97%
49	AM	138	99%
50	AN	204	100%
51	AO	199	98%
52	AP	184	95% 5%
53	AQ	186	99%
54	AR	189	16% 99%
55	AS	178	96%
56	AT	160	99%
57	AU	121	81% 17%
58	AV	137	99%

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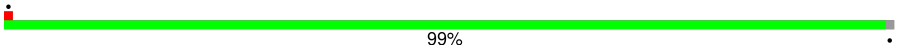
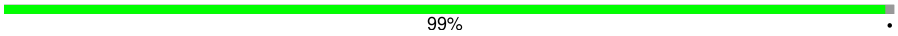
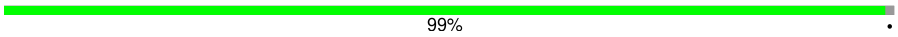
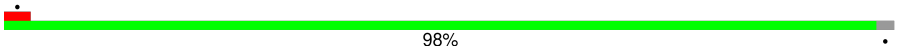
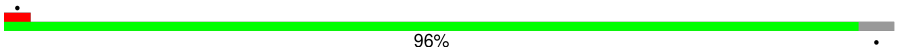
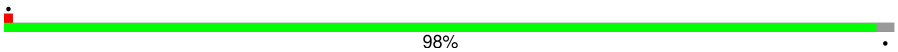
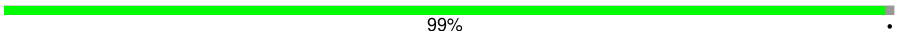
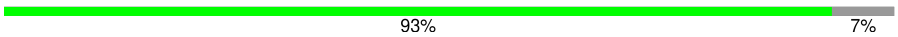
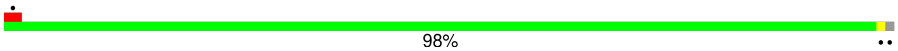
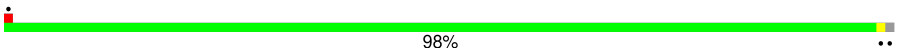
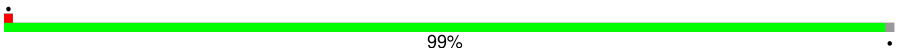
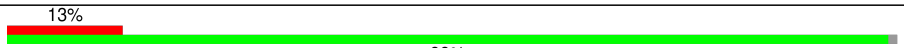
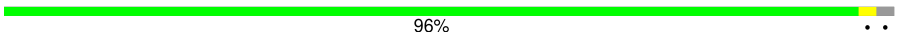
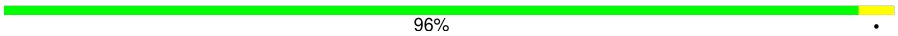
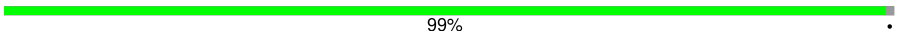
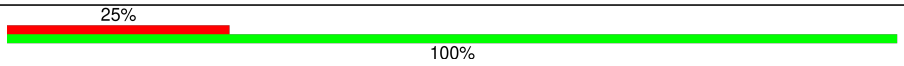
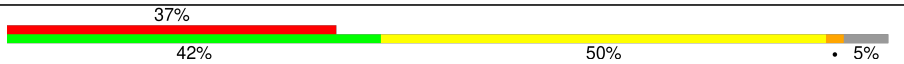
Mol	Chain	Length	Quality of chain
59	AW	155	
60	AX	142	
61	AY	127	
62	AZ	136	
63	Aa	149	
64	Ab	59	
65	Ac	105	
66	Ad	113	
67	Ae	130	
68	Af	107	
69	Ag	121	
70	Ah	120	
71	Ai	100	
72	Aj	88	
73	Ak	78	
74	Al	51	
75	Am	128	
76	An	25	
77	Ao	106	
78	Ap	92	
79	E	217	
80	DC	842	
81	V	312	
82	EC	202	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	W9C	DC	902	X	-	-	-

2 Entry composition (i)

There are 86 unique types of molecules in this entry. The entry contains 213962 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
			Total	C	N	O	S		
1	BA	206	1612	1034	285	291	2	0	0

- Molecule 2 is a protein called RPS1A isoform 1.

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

- Molecule 3 is a protein called RPS2 isoform 1.

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

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

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

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

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

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

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

- 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	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	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
			975	611	183	179	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	69	Total	C	N	O	0	0
			558	357	103	98		

- 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
			38004	17005	6718	12499	1782		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	1280	4AC	C	modified residue	GB 1329886537
B5	1773	4AC	C	modified residue	GB 1329886537

- 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	3198	Total	C	N	O	P	0	0
			68444	30595	12331	22320	3198		

- 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	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- 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	205	Total	C	N	O	S	0	0
			1672	1063	316	288	5		

- 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 1543	C 962	N 315	O 266	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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	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	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 1092	C 710	N 202	O 180	0	0

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

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

- Molecule 64 is a protein called RPL29 isoform 1.

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

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

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

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

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

- Molecule 67 is a protein called RPL32 isoform 1.

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

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

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

- 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 233	C 142	N 63	O 27	S 1	0	0

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

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

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

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

- Molecule 79 is a protein called RPL1A isoform 1.

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

- Molecule 80 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	DC	824	Total 6419	C 4085	N 1096	O 1208	S 30	0	0

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 82 is a RNA chain called TSV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	EC	191	Total 4045	C 1806	N 718	O 1330	P 191	0	0

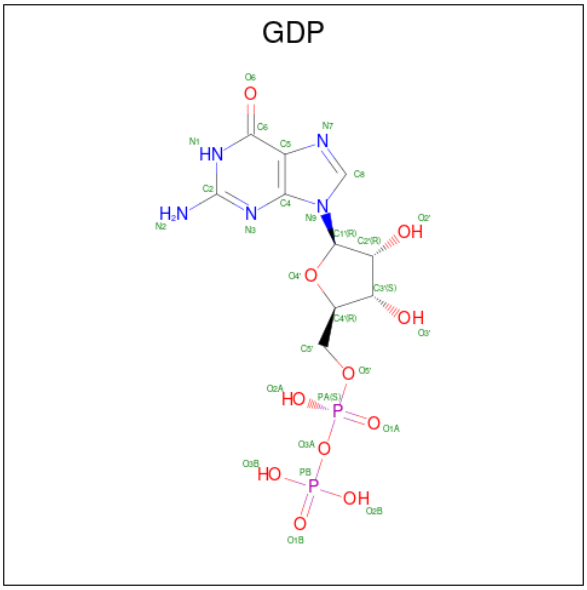
- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
83	Ba	1	Total Mg 1 1	0
83	B5	33	Total Mg 33 33	0
83	AB	1	Total Mg 1 1	0
83	A1	173	Total Mg 173 173	0
83	A3	2	Total Mg 2 2	0
83	A4	4	Total Mg 4 4	0
83	AL	1	Total Mg 1 1	0
83	AO	1	Total Mg 1 1	0
83	DC	1	Total Mg 1 1	0

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

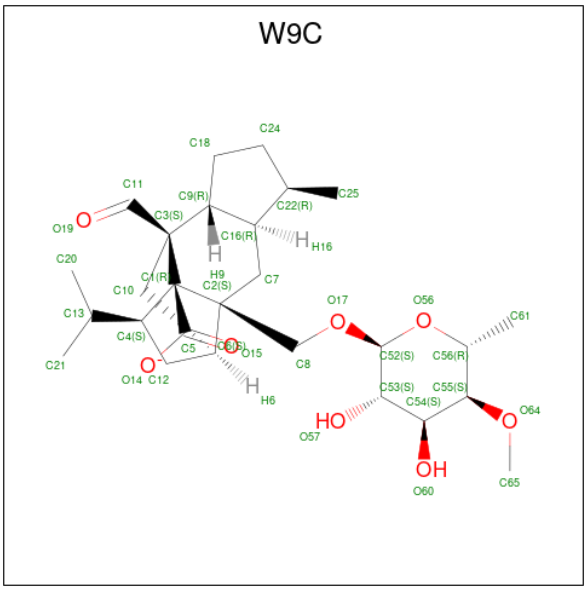
Mol	Chain	Residues	Atoms	AltConf
84	Ao	1	Total Zn 1 1	0

- Molecule 85 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
85	DC	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 86 is (1S,3S,3aR,4S,4aR,7R,7aR,8aS)-8a-{[(6-deoxy-4-O-methyl-alpha-D-altropyranosyl)oxy]methyl}-4-formyl-7-methyl-3-(propan-2-yl)decahydro-1,4-methano-s-indacene-3a(1H)-carboxylate (three-letter code: W9C) (formula: $C_{27}H_{41}O_8$).



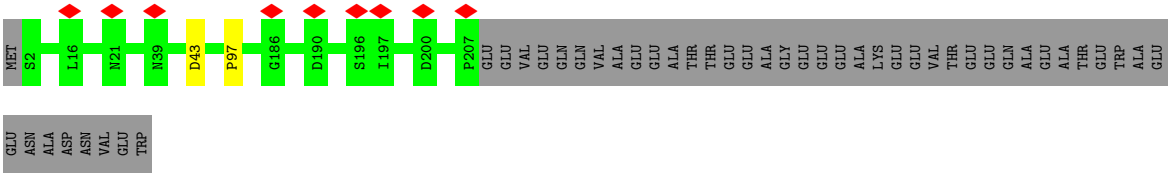
Mol	Chain	Residues	Atoms			AltConf
86	DC	1	Total	C	O	0
			35	27	8	

3 Residue-property plots (i)

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

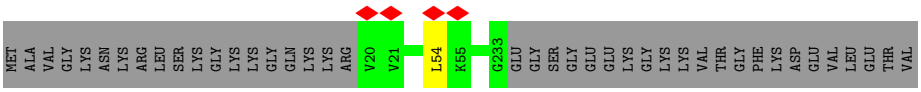
- Molecule 1: 40S ribosomal protein S0-A

Chain BA:



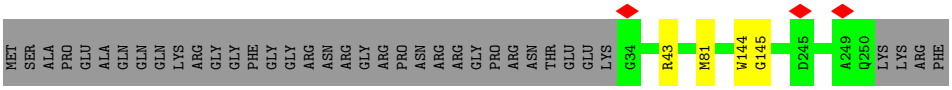
- Molecule 2: RPS1A isoform 1

Chain BB:



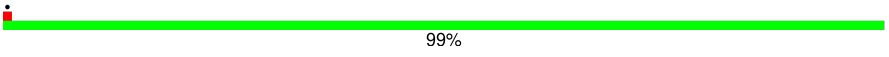
- Molecule 3: RPS2 isoform 1

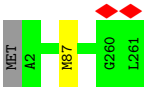
Chain BC:



- Molecule 4: 40S ribosomal protein S4-A

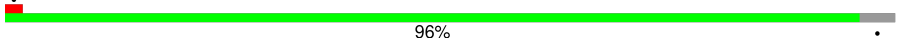
Chain BE:

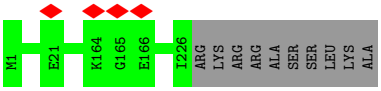




- Molecule 5: 40S ribosomal protein S6-A

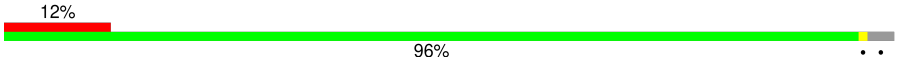
Chain BG:

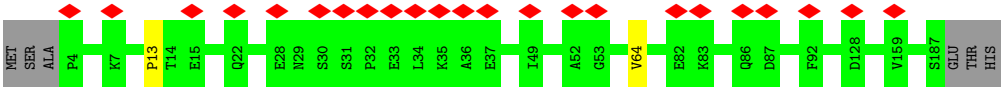




• Molecule 6: 40S ribosomal protein S7-A

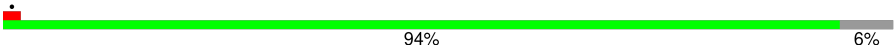
Chain BH:

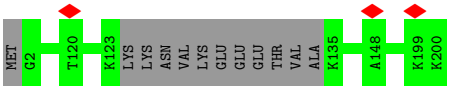




• Molecule 7: 40S ribosomal protein S8-A

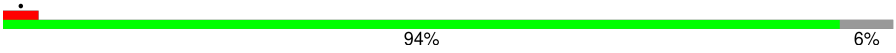
Chain BI:

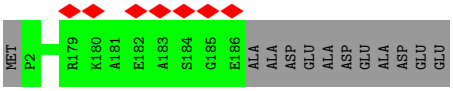




• Molecule 8: 40S ribosomal protein S9-A

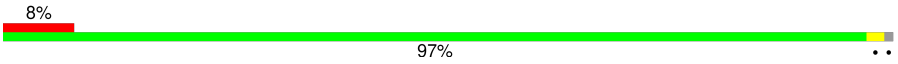
Chain BJ:

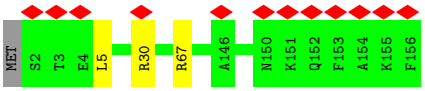




• Molecule 9: 40S ribosomal protein S11-A

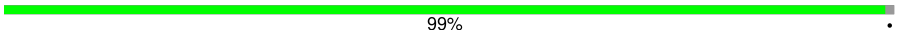
Chain BL:





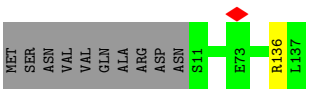
• Molecule 10: 40S ribosomal protein S13

Chain BN:



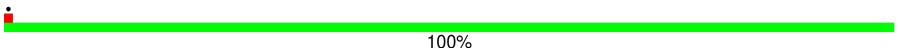
• Molecule 11: 40S ribosomal protein S14-A

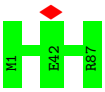
Chain BO:



• Molecule 12: 40S ribosomal protein S21-A

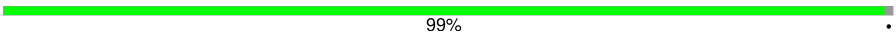
Chain BV:





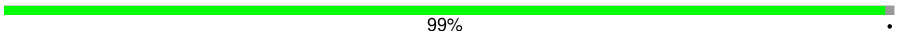
• Molecule 13: RPS22A isoform 1

Chain BW:



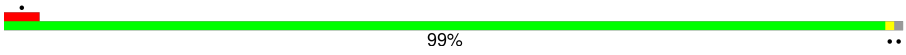
• Molecule 14: 40S ribosomal protein S23-A

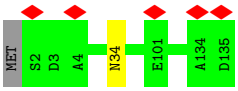
Chain BX:



• Molecule 15: 40S ribosomal protein S24-A

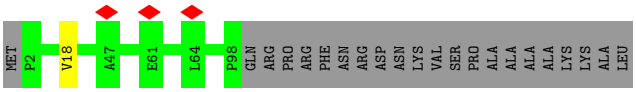
Chain BY:





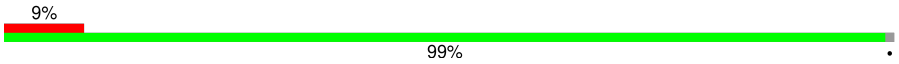
• Molecule 16: RPS26B isoform 1

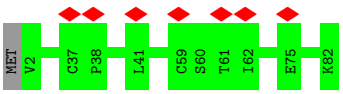
Chain Ba:



• Molecule 17: 40S ribosomal protein S27-A

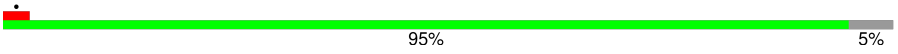
Chain Bb:

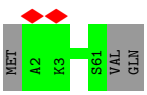




• Molecule 18: 40S ribosomal protein S30-A

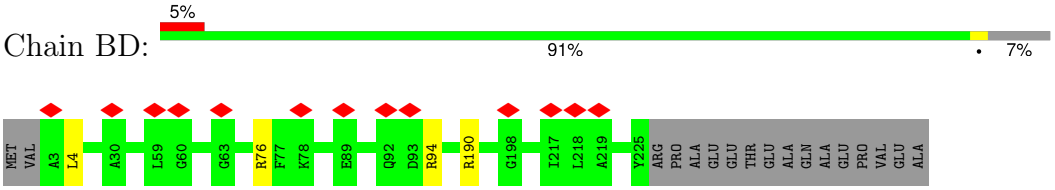
Chain Be:





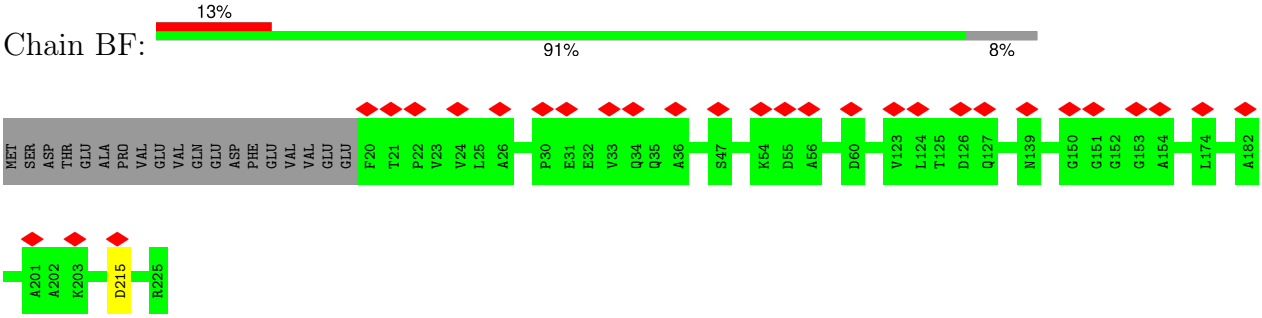
• Molecule 19: RPS3 isoform 1

Chain BD:



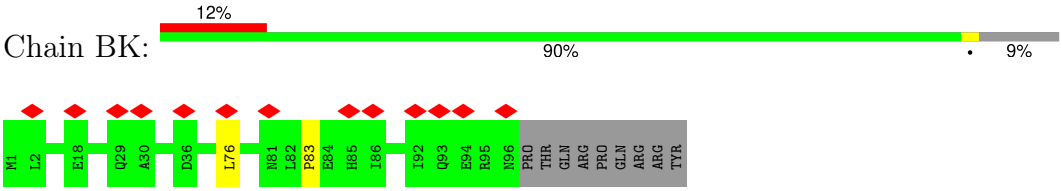
• Molecule 20: Rps5p

Chain BF:



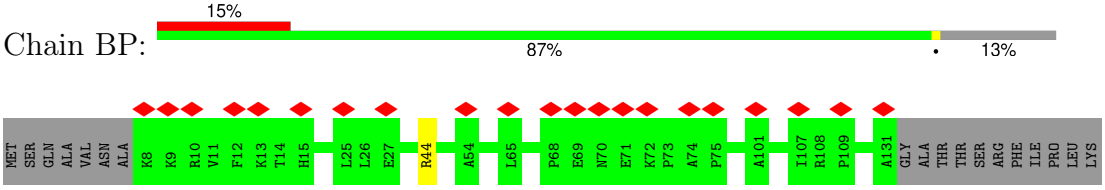
• Molecule 21: 40S ribosomal protein S10-A

Chain BK:



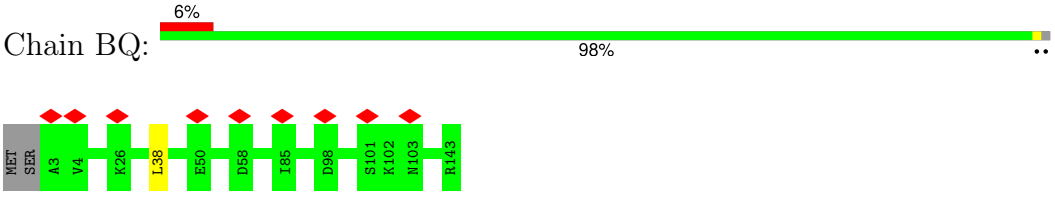
• Molecule 22: RPS15 isoform 1

Chain BP:



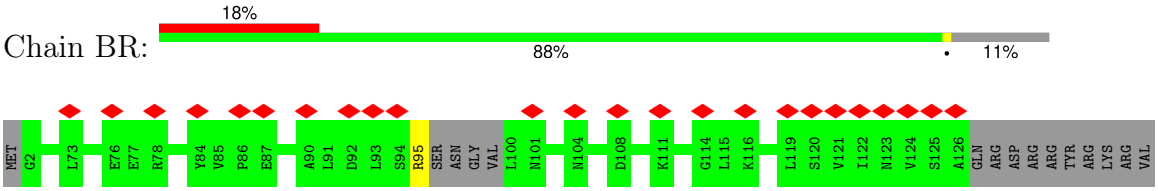
• Molecule 23: 40S ribosomal protein S16-A

Chain BQ:



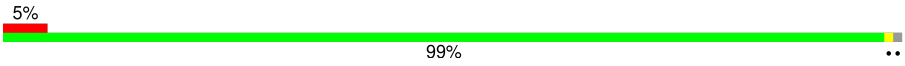
• Molecule 24: 40S ribosomal protein S17-A

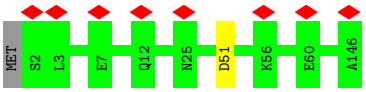
Chain BR:



• Molecule 25: 40S ribosomal protein S18-A

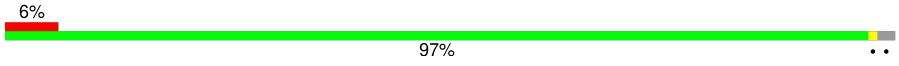
Chain BS:

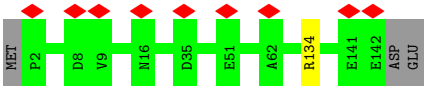




• Molecule 26: 40S ribosomal protein S19-A

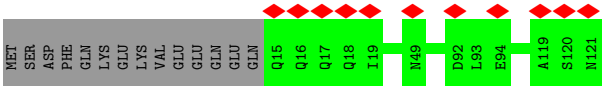
Chain BT:





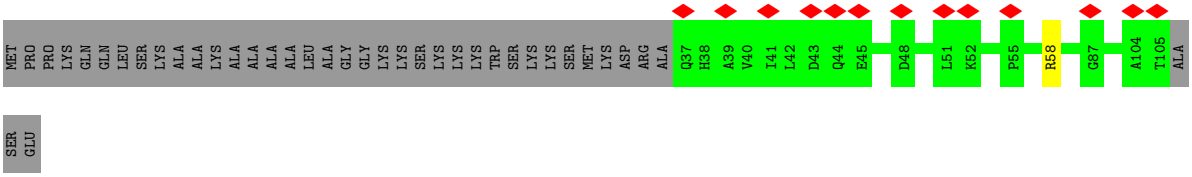
• Molecule 27: RPS20 isoform 1

Chain BU:



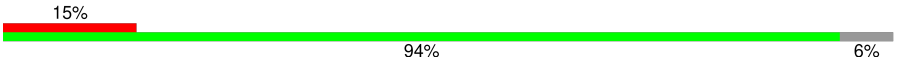
• Molecule 28: RPS25A isoform 1

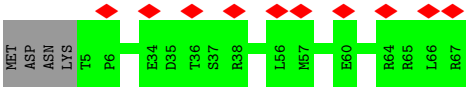
Chain BZ:



• Molecule 29: RPS28A isoform 1

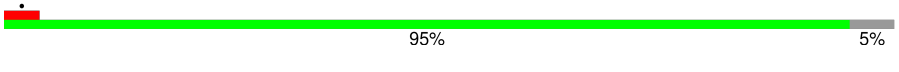
Chain Bc:

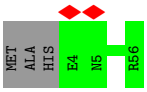




• Molecule 30: RPS29A isoform 1

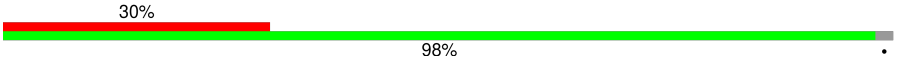
Chain Bd:

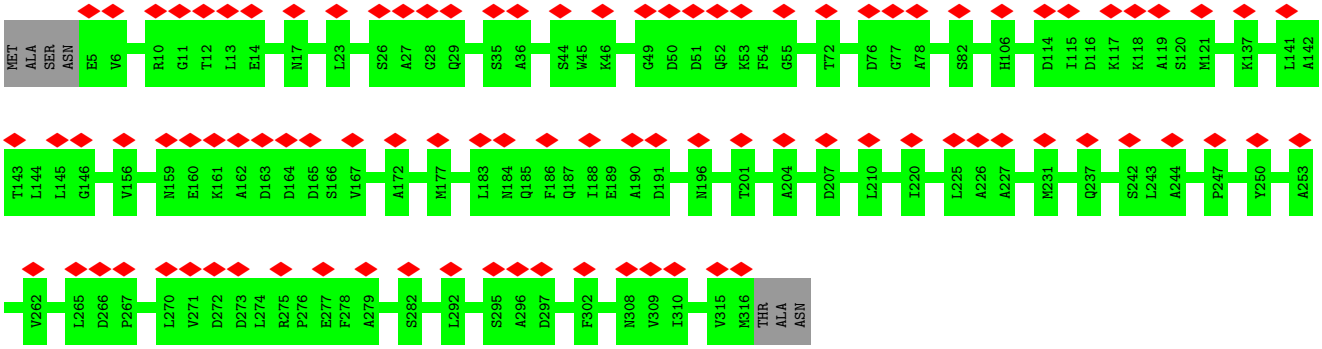




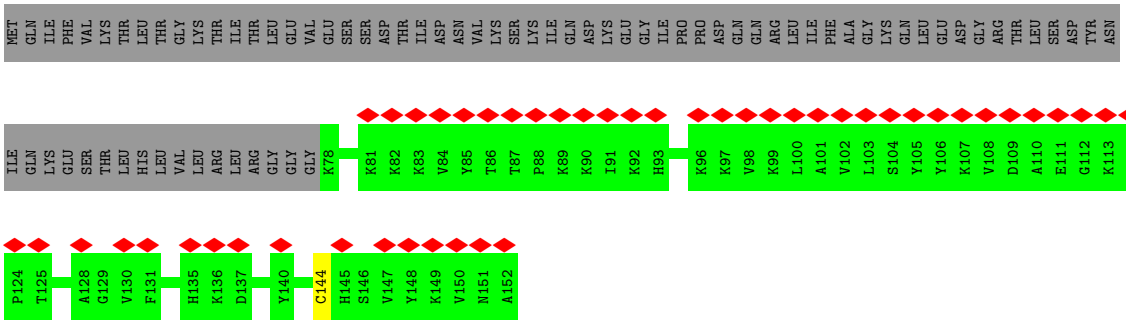
• Molecule 31: Guanine nucleotide-binding protein subunit beta-like protein

Chain Bg:

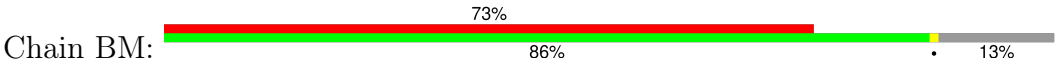


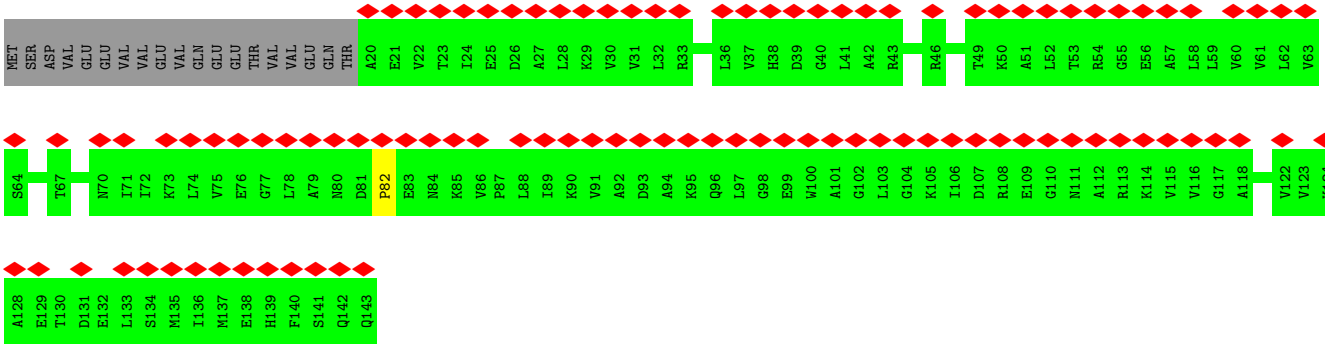


• Molecule 32: Ubiquitin-40S ribosomal protein S31

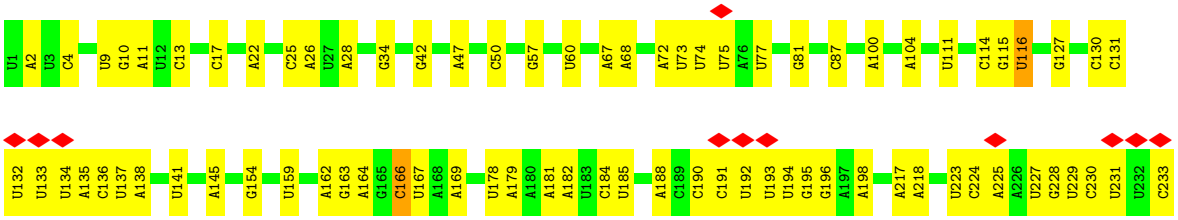


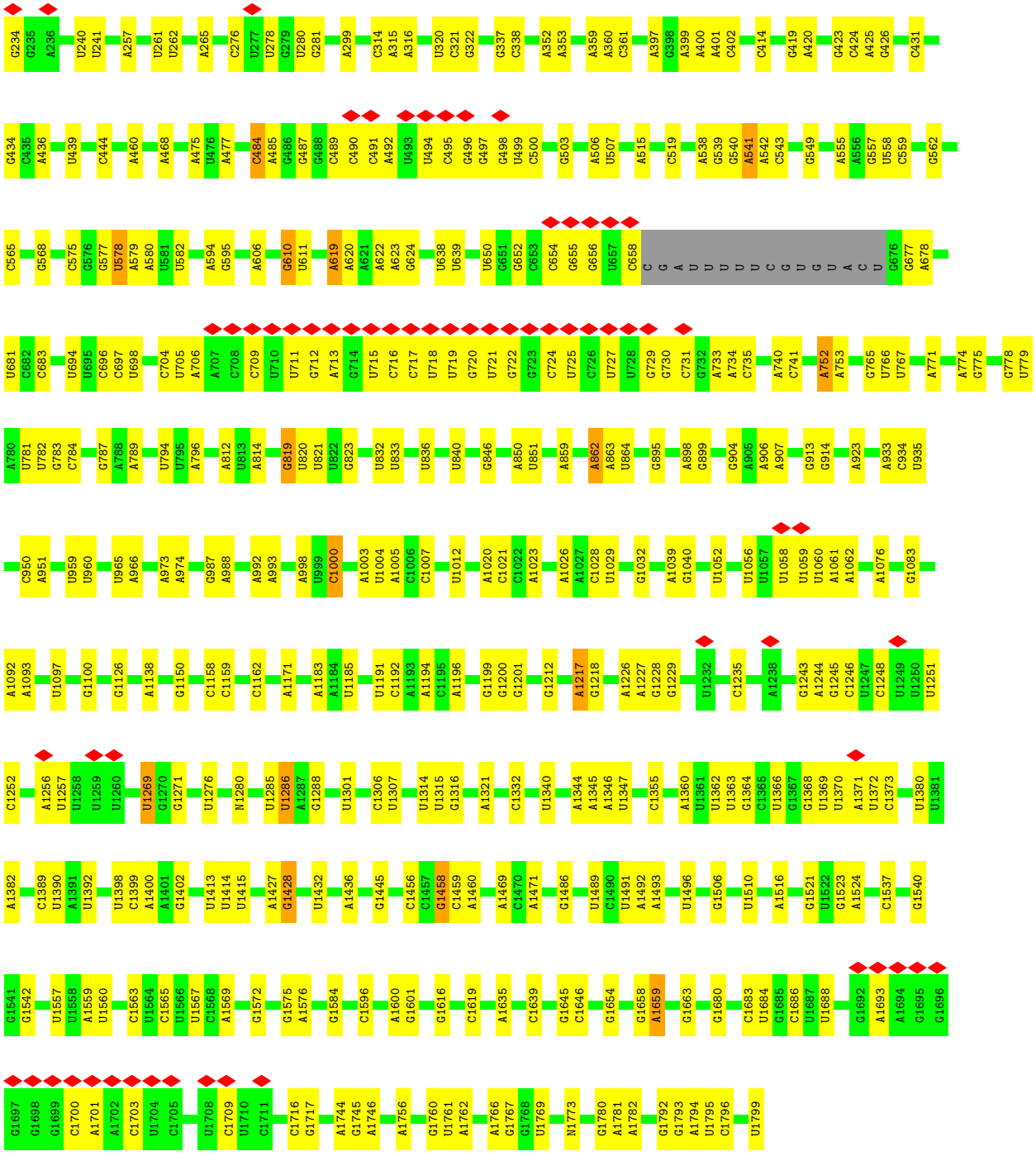
• Molecule 33: 40S ribosomal protein S12





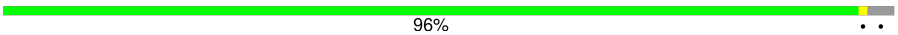
• Molecule 34: 18S rRNA

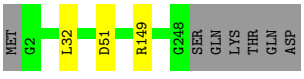




• Molecule 35: 60S ribosomal protein L2-A

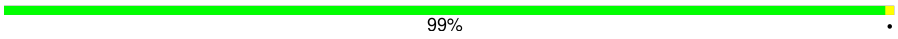
Chain AA:

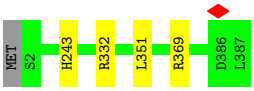




• Molecule 36: 60S ribosomal protein L3

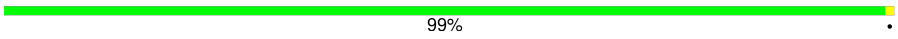
Chain AB:





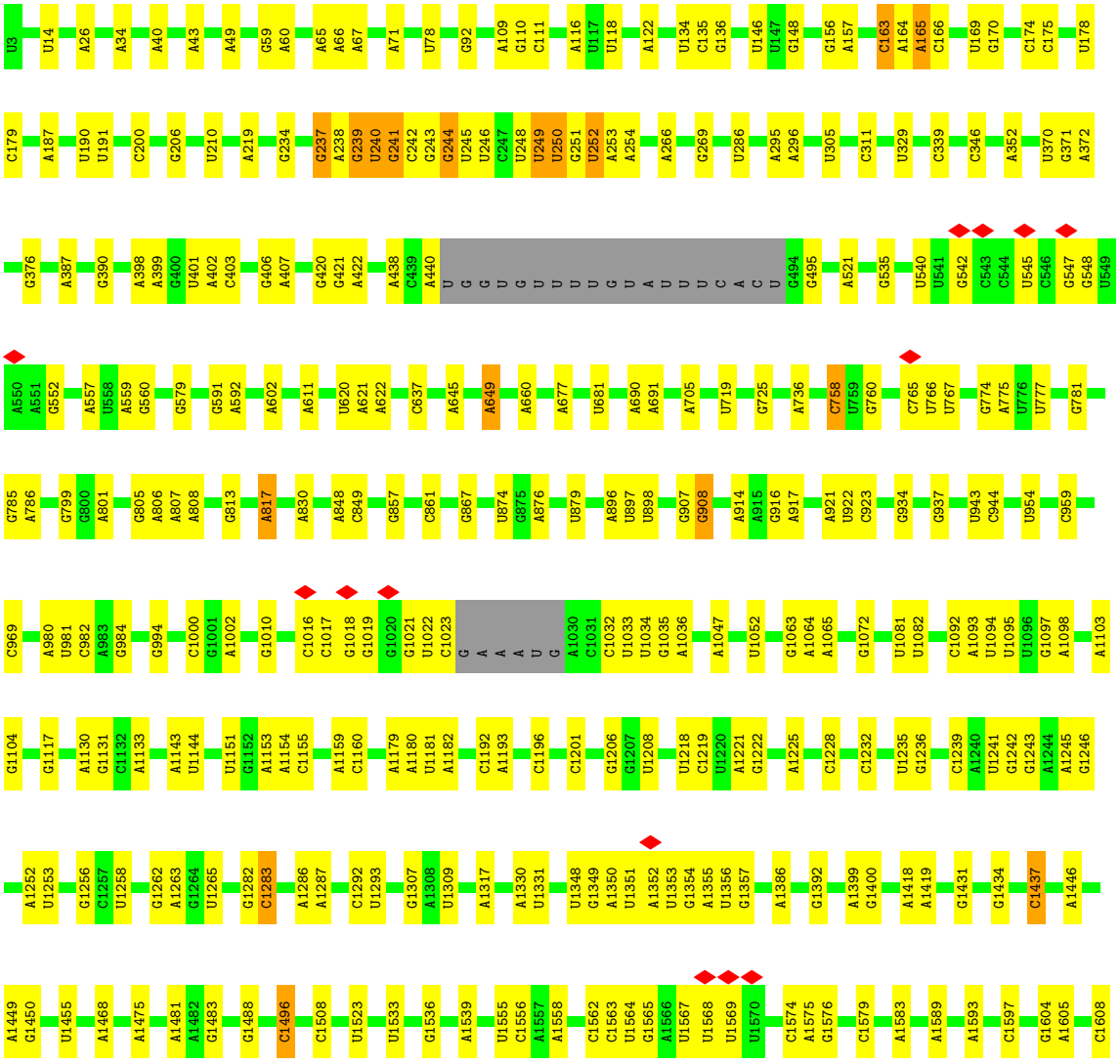
• Molecule 37: RPL4A isoform 1

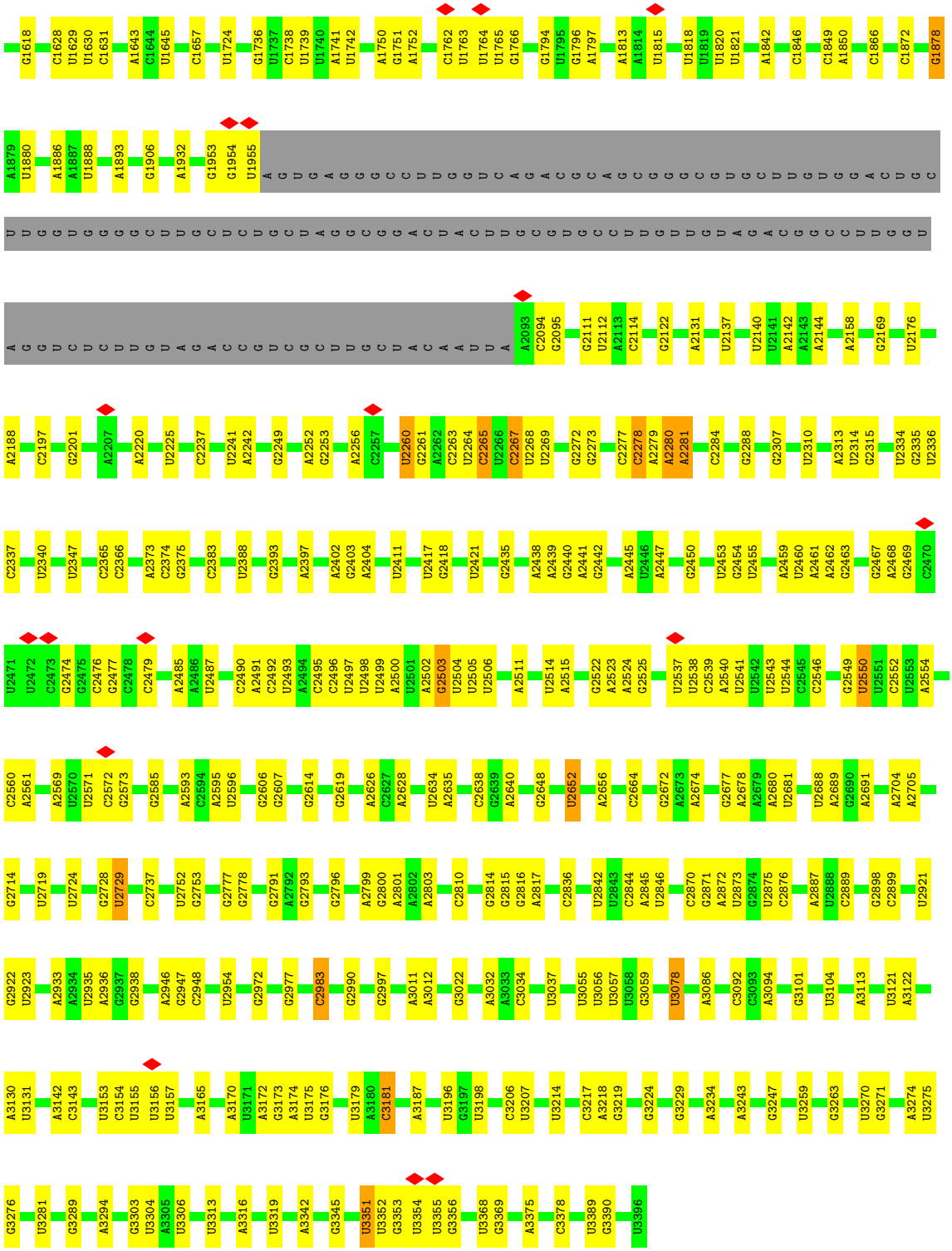
Chain AC:



• Molecule 38: 25S rRNA

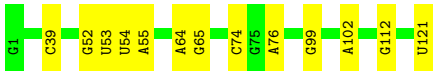
Chain A1:





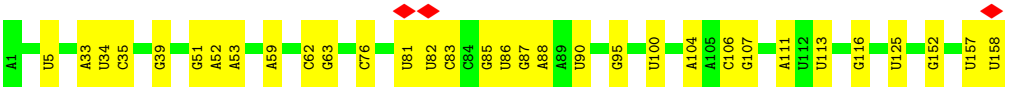
• Molecule 39: 5s rRNA

Chain A3:



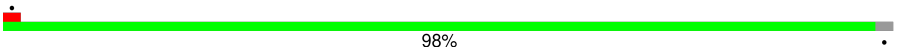
• Molecule 40: 5.8 S rRNA

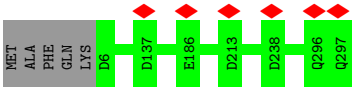
Chain A4:



• Molecule 41: RPL5 isoform 1

Chain AD:



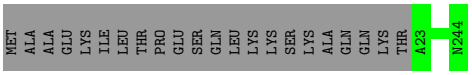


• Molecule 42: 60S ribosomal protein L6-A

Chain AE:

• Molecule 43: 60S ribosomal protein L7-A

Chain AF:

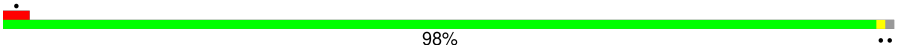


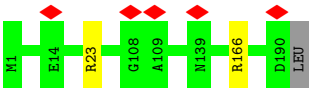
• Molecule 44: 60S ribosomal protein L8-A

Chain AG:

• Molecule 45: 60S ribosomal protein L9-A

Chain AH:



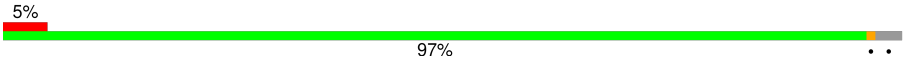


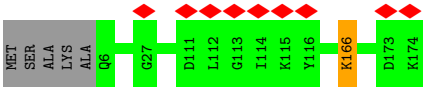
• Molecule 46: RPL10 isoform 1

Chain AI:

• Molecule 47: RPL11A isoform 1

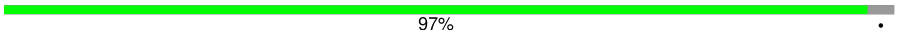
Chain AJ:

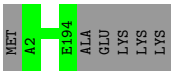




• Molecule 48: 60S ribosomal protein L13-A

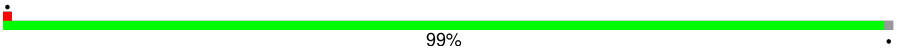
Chain AL:

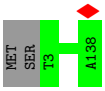




• Molecule 49: 60S ribosomal protein L14-A

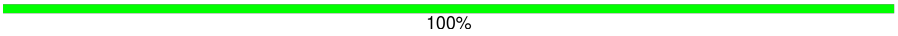
Chain AM:





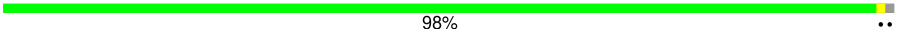
• Molecule 50: 60S ribosomal protein L15-A

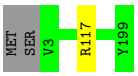
Chain AN:



• Molecule 51: 60S ribosomal protein L16-A

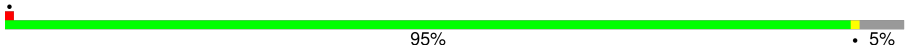
Chain AO:

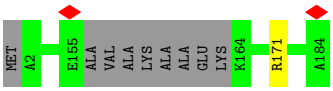




• Molecule 52: 60S ribosomal protein L17-A

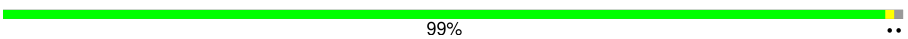
Chain AP:

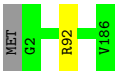




• Molecule 53: 60S ribosomal protein L18-A

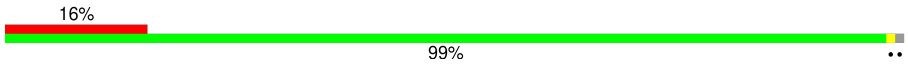
Chain AQ:

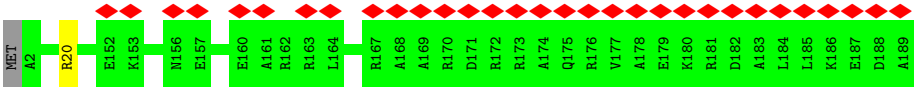




• Molecule 54: 60S ribosomal protein L19-A

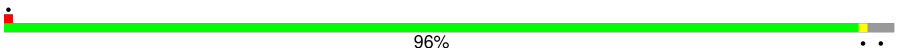
Chain AR:

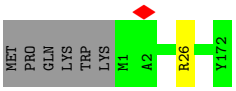




• Molecule 55: 60S ribosomal protein L20

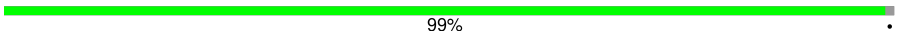
Chain AS:





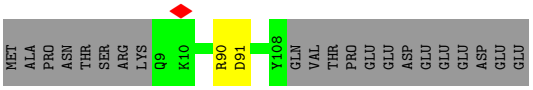
• Molecule 56: 60S ribosomal protein L21-A

Chain AT:



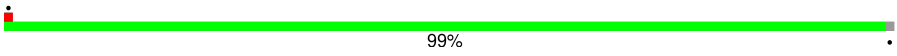
• Molecule 57: 60S ribosomal protein L22-A

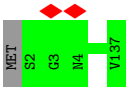
Chain AU:



• Molecule 58: 60S ribosomal protein L23-A

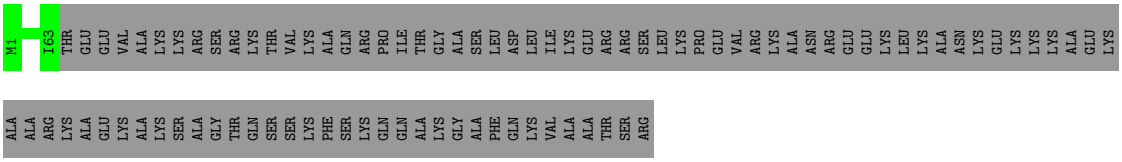
Chain AV:





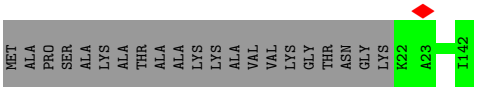
• Molecule 59: RPL24A isoform 1

Chain AW:



• Molecule 60: 60S ribosomal protein L25

Chain AX:

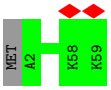


• Molecule 61: 60S ribosomal protein L26-A

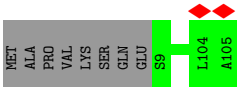
• Molecule 62: 60S ribosomal protein L27-A

• Molecule 63: 60S ribosomal protein L28

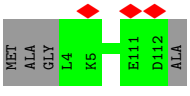
• Molecule 64: RPL29 isoform 1



• Molecule 65: 60S ribosomal protein L30

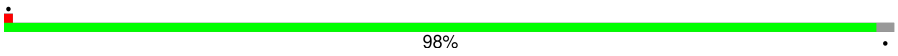


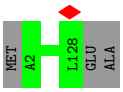
• Molecule 66: 60S ribosomal protein L31-A



• Molecule 67: RPL32 isoform 1

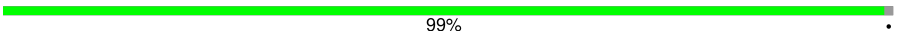
Chain Ae:





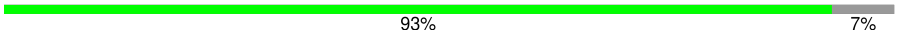
• Molecule 68: 60S ribosomal protein L33-A

Chain Af:



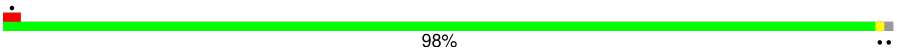
• Molecule 69: 60S ribosomal protein L34-A

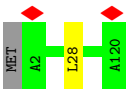
Chain Ag:



• Molecule 70: 60S ribosomal protein L35-A

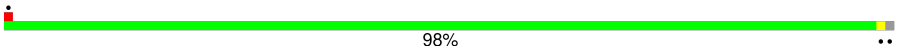
Chain Ah:

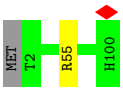




• Molecule 71: 60S ribosomal protein L36-A

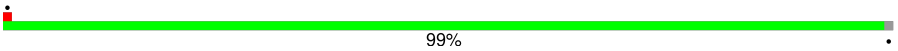
Chain Ai:

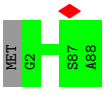




• Molecule 72: 60S ribosomal protein L37-A

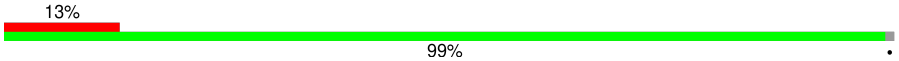
Chain Aj:

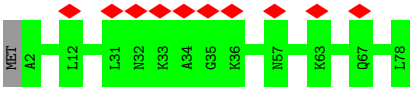




• Molecule 73: RPL38 isoform 1

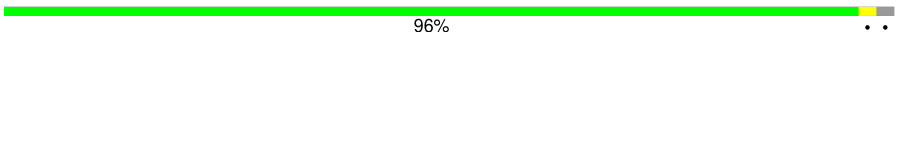
Chain Ak:





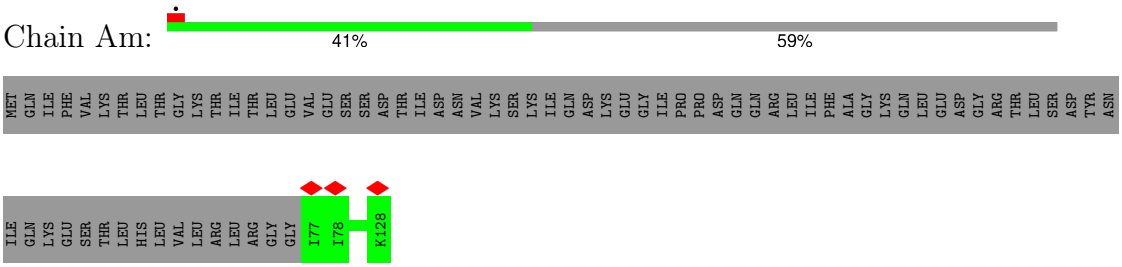
• Molecule 74: 60S ribosomal protein L39

Chain Al:



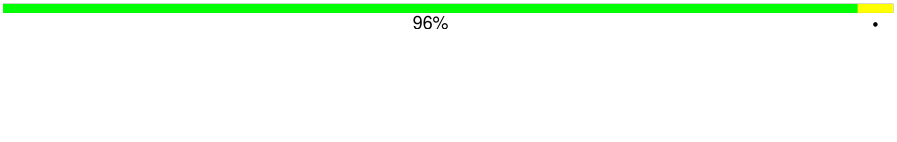
• Molecule 75: Ubiquitin-60S ribosomal protein L40

Chain Am:



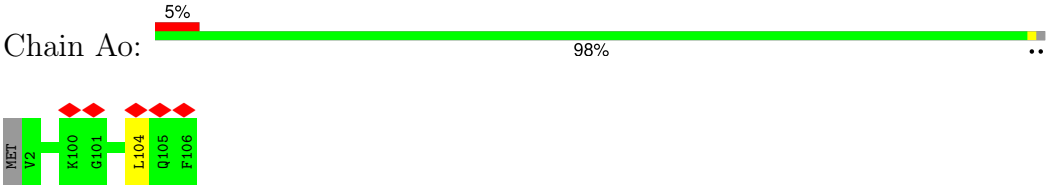
• Molecule 76: 60S ribosomal protein L41-A

Chain An:



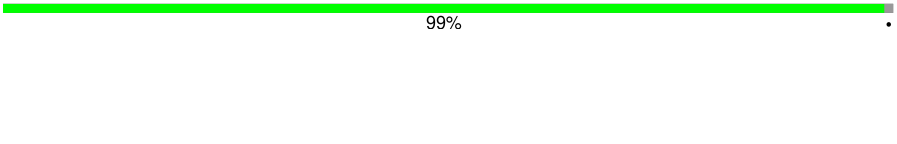
• Molecule 77: 60S ribosomal protein L42-A

Chain Ao:



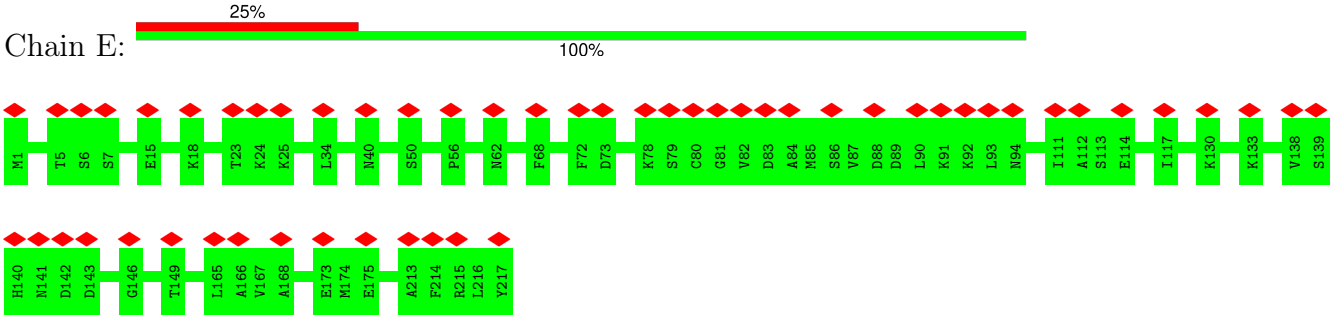
• Molecule 78: 60S ribosomal protein L43-A

Chain Ap:



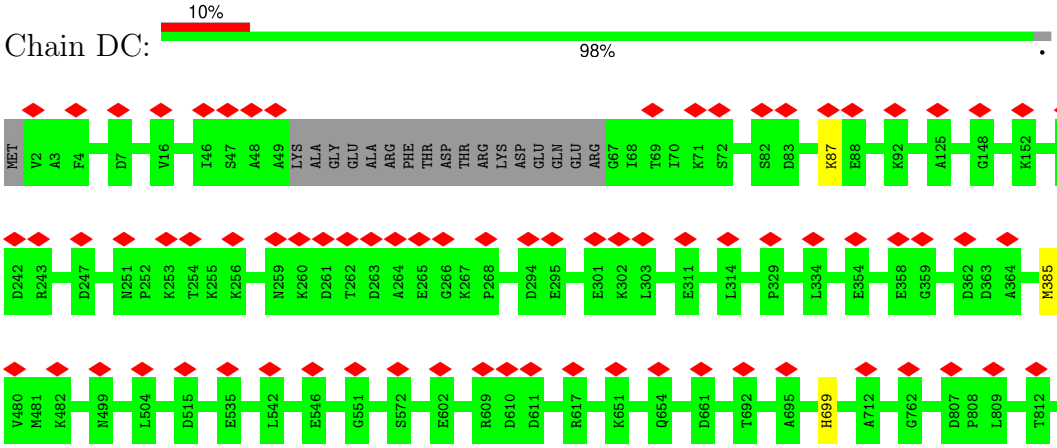
• Molecule 79: RPL1A isoform 1

Chain E:



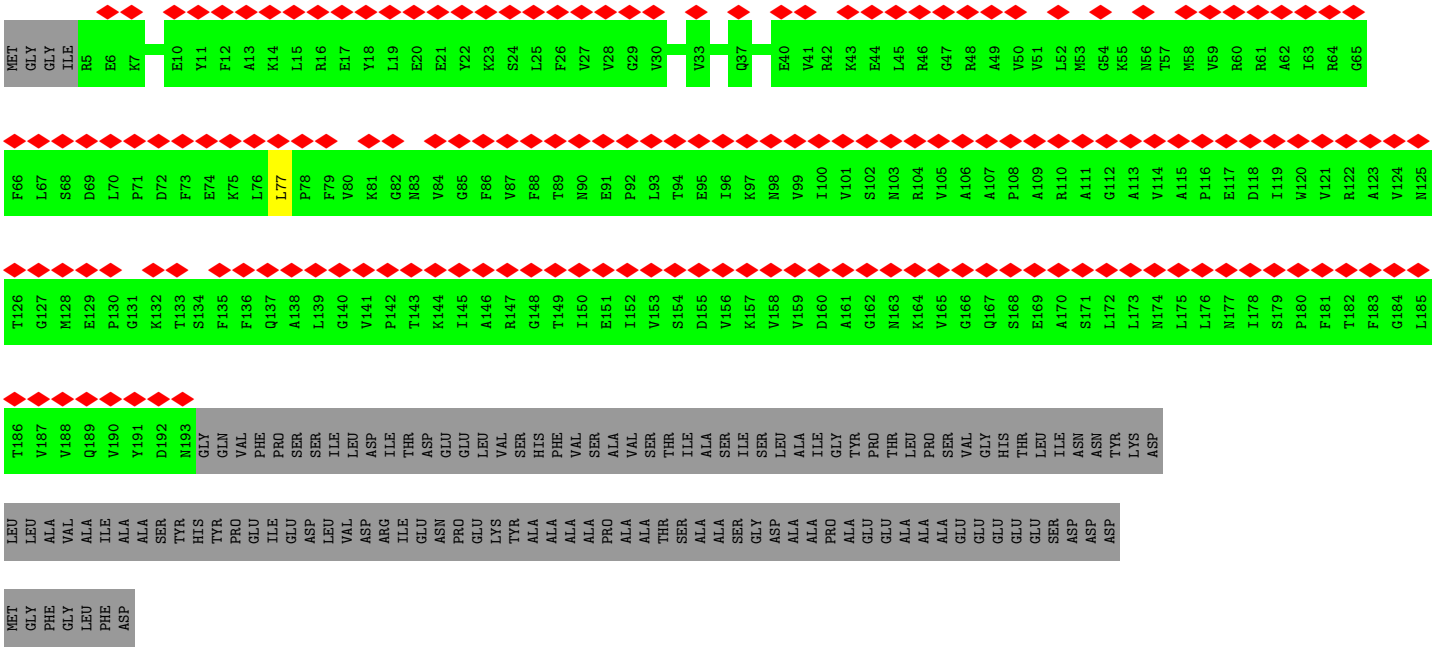
• Molecule 80: Elongation factor 2

Chain DC:



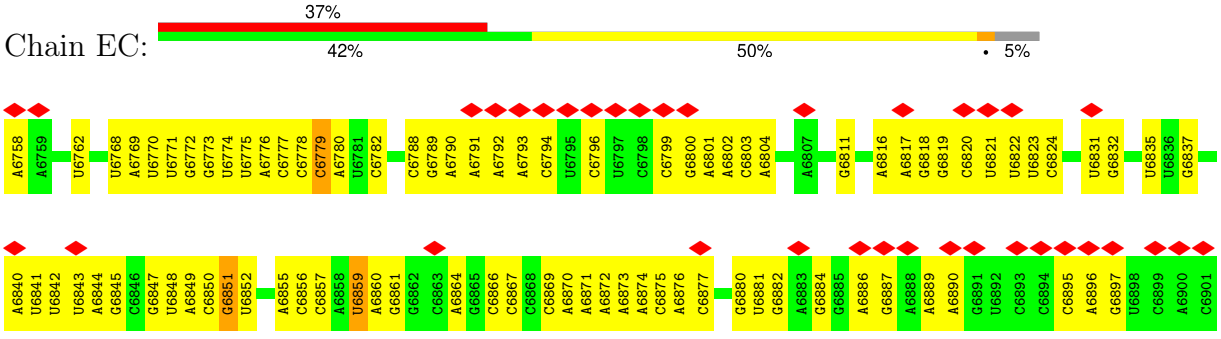
• Molecule 81: 60S acidic ribosomal protein P0

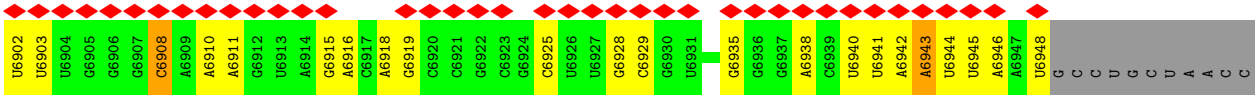
Chain V:



• Molecule 82: TSV IRES

Chain EC:




U6902
U6903
U6904
G6905
G6906
G6907
C6908
A6909
A6910
A6911
G6912
U6913
A6914
G6915
A6916
C6917
A6918
G6919
C6920
C6921
G6922
C6923
G6924
C6925
U6926
U6927
G6928
C6929
G6930
U6931
G6935
G6936
G6937
A6938
C6939
U6940
U6941
A6942
A6943
U6944
U6945
A6946
A6947
U6948
G
C
C
U
G
C
U
A
A
C
C

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47514	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.410	Depositor
Minimum map value	-1.730	Depositor
Average map value	0.058	Depositor
Map value standard deviation	0.237	Depositor
Recommended contour level	0.6	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: XSX, A2M, MA6, MG, ZN, 5MC, 4AC, GDP, OMC, UR3, G7M, 1MA, W9C, OMG, DDE, OMU, HIC

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	0.46	2/1653 (0.1%)	0.85	5/2261 (0.2%)
2	BB	0.28	0/1735	0.61	1/2335 (0.0%)
3	BC	0.32	0/1665	0.57	1/2263 (0.0%)
4	BE	0.29	0/2109	0.63	2/2839 (0.1%)
5	BG	0.27	0/1844	0.58	0/2464
6	BH	0.29	0/1506	0.62	1/2028 (0.0%)
7	BI	0.27	0/1514	0.61	0/2021
8	BJ	0.26	0/1519	0.57	0/2035
9	BL	0.28	0/1272	0.60	1/1712 (0.1%)
10	BN	0.31	0/1215	0.60	0/1638
11	BO	0.29	0/952	0.67	0/1279
12	BV	0.29	0/693	0.69	0/935
13	BW	0.27	0/1038	0.58	0/1395
14	BX	0.26	0/1139	0.57	0/1518
15	BY	0.29	0/1087	0.61	0/1449
16	Ba	0.29	0/782	0.76	1/1047 (0.1%)
17	Bb	0.27	0/620	0.65	0/838
18	Be	0.25	0/483	0.66	0/643
19	BD	0.28	0/1759	0.63	1/2368 (0.0%)
20	BF	0.34	0/1629	0.62	1/2202 (0.0%)
21	BK	0.63	2/837 (0.2%)	1.10	6/1131 (0.5%)
22	BP	0.28	0/1012	0.60	0/1356
23	BQ	0.28	0/1125	0.58	1/1510 (0.1%)
24	BR	0.26	0/984	0.62	0/1318
25	BS	0.26	0/1211	0.61	1/1628 (0.1%)
26	BT	0.28	0/1113	0.56	0/1494
27	BU	0.27	0/865	0.56	0/1169
28	BZ	0.28	0/566	0.62	0/761
29	Bc	0.30	0/499	0.78	0/670
30	Bd	0.28	0/452	0.61	0/600
31	Bg	0.27	0/2454	0.60	0/3340

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Bf	0.29	0/616	0.65	1/817 (0.1%)
33	BM	0.29	0/943	0.71	2/1274 (0.2%)
34	B5	0.31	0/41880	0.91	67/65248 (0.1%)
35	AA	0.31	0/1912	0.66	2/2569 (0.1%)
36	AB	0.29	0/3139	0.58	1/4219 (0.0%)
37	AC	0.28	0/2800	0.56	1/3790 (0.0%)
38	A1	0.39	0/75586	0.90	117/117845 (0.1%)
39	A3	0.35	0/2883	0.88	2/4491 (0.0%)
40	A4	0.36	0/3746	0.85	3/5832 (0.1%)
41	AD	0.29	0/2390	0.54	0/3225
42	AE	0.28	0/1260	0.54	0/1694
43	AF	0.29	0/1821	0.51	0/2451
44	AG	0.28	0/1830	0.53	0/2469
45	AH	0.34	0/1531	0.60	0/2062
46	AI	0.29	0/1708	0.56	0/2290
47	AJ	0.29	0/1374	0.65	0/1842
48	AL	0.28	0/1568	0.58	0/2106
49	AM	0.26	0/1068	0.53	0/1438
50	AN	0.29	0/1757	0.60	0/2354
51	AO	0.29	0/1585	0.53	0/2128
52	AP	0.30	0/1410	0.59	0/1893
53	AQ	0.28	0/1465	0.58	0/1965
54	AR	0.26	0/1538	0.58	0/2050
55	AS	0.32	0/1481	0.58	0/1990
56	AT	0.31	0/1300	0.55	0/1743
57	AU	0.30	0/812	0.62	2/1099 (0.2%)
58	AV	0.30	0/1018	0.60	0/1369
59	AW	0.32	0/533	0.59	0/707
60	AX	0.30	0/983	0.55	0/1325
61	AY	0.30	0/1004	0.62	0/1341
62	AZ	0.29	0/1118	0.54	0/1497
63	Aa	0.29	0/1204	0.58	0/1612
64	Ab	0.27	0/473	0.52	0/629
65	Ac	0.30	0/751	0.55	0/1008
66	Ad	0.28	0/904	0.57	0/1213
67	Ae	0.28	0/1041	0.55	0/1394
68	Af	0.31	0/868	0.59	0/1168
69	Ag	0.32	0/890	0.63	0/1189
70	Ah	0.26	0/978	0.53	1/1301 (0.1%)
71	Ai	0.29	0/778	0.62	0/1034
72	Aj	0.29	0/696	0.59	0/923
73	Ak	0.27	0/618	0.61	0/826
74	Al	0.29	0/443	0.67	1/588 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	Am	0.30	0/423	0.61	0/562
76	An	0.26	0/234	0.72	0/300
77	Ao	0.32	0/860	0.68	1/1136 (0.1%)
78	Ap	0.30	0/701	0.57	0/934
79	E	0.26	0/1745	0.58	0/2342
80	DC	0.29	0/6521	0.61	3/8830 (0.0%)
81	V	0.28	0/1498	0.61	1/2025 (0.0%)
82	EC	0.33	1/4521 (0.0%)	0.97	12/7039 (0.2%)
All	All	0.33	5/227538 (0.0%)	0.80	239/333423 (0.1%)

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
3	BC	0	2
6	BH	0	1
15	BY	0	1
44	AG	0	2
47	AJ	0	1
76	An	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	97	PRO	CB-CG	-11.35	0.93	1.50
21	BK	83	PRO	CB-CG	-11.28	0.93	1.50
82	EC	6758	A	OP3-P	-10.56	1.48	1.61
21	BK	83	PRO	CG-CD	-10.02	1.17	1.50
1	BA	97	PRO	CG-CD	-8.93	1.21	1.50

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BA	97	PRO	N-CD-CG	-18.30	75.76	103.20
21	BK	83	PRO	N-CD-CG	-17.68	76.67	103.20
1	BA	97	PRO	CA-CB-CG	-16.89	71.92	104.00
21	BK	83	PRO	CA-CB-CG	-16.53	72.59	104.00
21	BK	83	PRO	CB-CG-CD	14.33	162.40	106.50

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	AG	30	THR	Peptide
3	BC	144	TRP	Peptide
3	BC	145	GLY	Peptide
6	BH	64	VAL	Peptide
15	BY	34	ASN	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	204/252 (81%)	182 (89%)	22 (11%)	0	100	100
2	BB	212/255 (83%)	184 (87%)	28 (13%)	0	100	100
3	BC	215/254 (85%)	204 (95%)	11 (5%)	0	100	100
4	BE	258/261 (99%)	233 (90%)	25 (10%)	0	100	100
5	BG	224/236 (95%)	215 (96%)	9 (4%)	0	100	100
6	BH	182/190 (96%)	170 (93%)	12 (7%)	0	100	100
7	BI	184/200 (92%)	167 (91%)	17 (9%)	0	100	100
8	BJ	183/197 (93%)	172 (94%)	11 (6%)	0	100	100
9	BL	153/156 (98%)	138 (90%)	15 (10%)	0	100	100
10	BN	148/151 (98%)	140 (95%)	8 (5%)	0	100	100
11	BO	125/137 (91%)	111 (89%)	14 (11%)	0	100	100
12	BV	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
13	BW	127/130 (98%)	124 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	BX	142/145 (98%)	126 (89%)	16 (11%)	0	100	100
15	BY	132/135 (98%)	123 (93%)	9 (7%)	0	100	100
16	Ba	95/119 (80%)	80 (84%)	15 (16%)	0	100	100
17	Bb	79/82 (96%)	67 (85%)	12 (15%)	0	100	100
18	Be	58/63 (92%)	51 (88%)	7 (12%)	0	100	100
19	BD	221/240 (92%)	206 (93%)	15 (7%)	0	100	100
20	BF	204/225 (91%)	186 (91%)	18 (9%)	0	100	100
21	BK	94/105 (90%)	82 (87%)	12 (13%)	0	100	100
22	BP	122/142 (86%)	112 (92%)	10 (8%)	0	100	100
23	BQ	139/143 (97%)	134 (96%)	5 (4%)	0	100	100
24	BR	117/136 (86%)	109 (93%)	8 (7%)	0	100	100
25	BS	143/146 (98%)	126 (88%)	17 (12%)	0	100	100
26	BT	139/144 (96%)	126 (91%)	13 (9%)	0	100	100
27	BU	105/121 (87%)	97 (92%)	8 (8%)	0	100	100
28	BZ	67/108 (62%)	63 (94%)	4 (6%)	0	100	100
29	Bc	61/67 (91%)	56 (92%)	5 (8%)	0	100	100
30	Bd	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
31	Bg	310/319 (97%)	278 (90%)	32 (10%)	0	100	100
32	Bf	73/152 (48%)	64 (88%)	9 (12%)	0	100	100
33	BM	122/143 (85%)	115 (94%)	7 (6%)	0	100	100
35	AA	245/254 (96%)	228 (93%)	17 (7%)	0	100	100
36	AB	383/387 (99%)	361 (94%)	22 (6%)	0	100	100
37	AC	359/362 (99%)	337 (94%)	22 (6%)	0	100	100
41	AD	290/297 (98%)	274 (94%)	16 (6%)	0	100	100
42	AE	152/176 (86%)	141 (93%)	11 (7%)	0	100	100
43	AF	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
44	AG	228/256 (89%)	210 (92%)	18 (8%)	0	100	100
45	AH	188/191 (98%)	171 (91%)	17 (9%)	0	100	100
46	AI	201/221 (91%)	195 (97%)	6 (3%)	0	100	100
47	AJ	167/174 (96%)	150 (90%)	17 (10%)	0	100	100
48	AL	191/199 (96%)	178 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	AM	134/138 (97%)	127 (95%)	7 (5%)	0	100	100
50	AN	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
51	AO	195/199 (98%)	194 (100%)	1 (0%)	0	100	100
52	AP	171/184 (93%)	163 (95%)	8 (5%)	0	100	100
53	AQ	183/186 (98%)	177 (97%)	6 (3%)	0	100	100
54	AR	186/189 (98%)	178 (96%)	8 (4%)	0	100	100
55	AS	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
56	AT	157/160 (98%)	146 (93%)	11 (7%)	0	100	100
57	AU	98/121 (81%)	92 (94%)	6 (6%)	0	100	100
58	AV	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
59	AW	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
60	AX	119/142 (84%)	114 (96%)	5 (4%)	0	100	100
61	AY	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
62	AZ	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
63	Aa	146/149 (98%)	133 (91%)	13 (9%)	0	100	100
64	Ab	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
65	Ac	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
66	Ad	107/113 (95%)	100 (94%)	7 (6%)	0	100	100
67	Ae	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
68	Af	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
69	Ag	110/121 (91%)	105 (96%)	5 (4%)	0	100	100
70	Ah	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
71	Ai	97/100 (97%)	89 (92%)	8 (8%)	0	100	100
72	Aj	85/88 (97%)	81 (95%)	4 (5%)	0	100	100
73	Ak	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
74	Al	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
75	Am	50/128 (39%)	48 (96%)	2 (4%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	103/106 (97%)	91 (88%)	12 (12%)	0	100	100
78	Ap	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
79	E	215/217 (99%)	206 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	DC	819/842 (97%)	759 (93%)	60 (7%)	0	100	100
81	V	187/312 (60%)	176 (94%)	11 (6%)	0	100	100
All	All	12115/13257 (91%)	11288 (93%)	827 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	173/210 (82%)	173 (100%)	0	100	100
2	BB	191/224 (85%)	191 (100%)	0	100	100
3	BC	176/205 (86%)	175 (99%)	1 (1%)	84	94
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%)	134 (98%)	2 (2%)	60	84
10	BN	127/128 (99%)	127 (100%)	0	100	100
11	BO	96/105 (91%)	95 (99%)	1 (1%)	73	90
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%)	179 (98%)	3 (2%)	58	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	103 (99%)	1 (1%)	73	90
23	BQ	117/119 (98%)	117 (100%)	0	100	100
24	BR	110/124 (89%)	109 (99%)	1 (1%)	75	91
25	BS	128/129 (99%)	128 (100%)	0	100	100
26	BT	113/116 (97%)	112 (99%)	1 (1%)	75	91
27	BU	100/114 (88%)	100 (100%)	0	100	100
28	BZ	61/89 (68%)	60 (98%)	1 (2%)	58	82
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
33	BM	100/119 (84%)	100 (100%)	0	100	100
35	AA	189/196 (96%)	188 (100%)	1 (0%)	86	95
36	AB	321/322 (100%)	319 (99%)	2 (1%)	84	94
37	AC	288/289 (100%)	286 (99%)	2 (1%)	81	93
41	AD	241/245 (98%)	241 (100%)	0	100	100
42	AE	134/153 (88%)	133 (99%)	1 (1%)	81	93
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%)	168 (99%)	2 (1%)	67	87
46	AI	176/187 (94%)	176 (100%)	0	100	100
47	AJ	147/150 (98%)	146 (99%)	1 (1%)	81	93
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%)	159 (99%)	1 (1%)	84	94
52	AP	141/146 (97%)	140 (99%)	1 (1%)	81	93
53	AQ	150/151 (99%)	149 (99%)	1 (1%)	81	93
54	AR	153/154 (99%)	152 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	AS	156/162 (96%)	155 (99%)	1 (1%)	84 94
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
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%)	80 (99%)	1 (1%)	67 87
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
80	DC	699/714 (98%)	698 (100%)	1 (0%)	92 98
81	V	160/254 (63%)	160 (100%)	0	100 100
All	All	10346/11154 (93%)	10319 (100%)	27 (0%)	90 97

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	AC	138	ARG

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Mol	Chain	Res	Type
45	AH	23	ARG
55	AS	26	ARG
42	AE	77	ARG
45	AH	166	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
73	Ak	67	GLN
79	E	108	ASN
80	DC	355	GLN
23	BQ	100	GLN
23	BQ	94	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1775/1798 (98%)	415 (23%)	11 (0%)
38	A1	3194/3360 (95%)	595 (18%)	21 (0%)
39	A3	120/121 (99%)	11 (9%)	1 (0%)
40	A4	157/158 (99%)	30 (19%)	0
82	EC	188/202 (93%)	101 (53%)	7 (3%)
All	All	5434/5639 (96%)	1152 (21%)	40 (0%)

5 of 1152 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	2	A
34	B5	4	C
34	B5	9	U
34	B5	10	G
34	B5	11	A

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	A1	2241	U
82	EC	6844	A
38	A1	2280	A2M
39	A3	52	G

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Mol	Chain	Res	Type
82	EC	6876	A

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

67 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	$\#\|Z\| > 2$
34	G7M	B5	1575	34	20,26,27	2.75	5 (25%)	16,39,42	1.91	4 (25%)
38	OMU	A1	2417	38	19,22,23	1.25	3 (15%)	25,31,34	1.76	4 (16%)
38	A2M	A1	2281	38	18,25,26	0.79	0	20,36,39	1.60	4 (20%)
34	A2M	B5	28	34,83	18,25,26	0.87	0	20,36,39	1.20	2 (10%)
38	OMC	A1	2948	38	19,22,23	0.83	0	25,31,34	1.10	2 (8%)
34	A2M	B5	796	34	18,25,26	0.91	1 (5%)	20,36,39	1.48	3 (15%)
38	OMG	A1	2793	38	19,26,27	0.89	1 (5%)	21,38,41	1.00	1 (4%)
38	OMC	A1	2959	38	19,22,23	0.80	0	25,31,34	0.82	0
38	A2M	A1	649	38	18,25,26	0.82	0	20,36,39	1.18	2 (10%)
38	UR3	A1	2634	38	19,22,23	0.98	0	26,32,35	1.71	3 (11%)
38	5MC	A1	2870	38,83	19,22,23	1.48	3 (15%)	26,32,35	1.30	3 (11%)
38	A2M	A1	2640	38	18,25,26	0.85	0	20,36,39	1.19	2 (10%)
38	OMU	A1	2921	38	19,22,23	1.24	3 (15%)	25,31,34	1.84	5 (20%)
38	OMG	A1	2815	38	19,26,27	0.89	1 (5%)	21,38,41	1.05	2 (9%)
38	OMG	A1	805	38	19,26,27	0.89	1 (5%)	21,38,41	1.08	1 (4%)
38	A2M	A1	2946	38,83	18,25,26	0.85	0	20,36,39	1.61	4 (20%)
34	MA6	B5	1781	34	19,26,27	1.11	2 (10%)	18,38,41	1.92	3 (16%)
38	A2M	A1	817	38,83	18,25,26	0.88	0	20,36,39	1.37	3 (15%)
38	OMG	A1	908	38	19,26,27	0.94	1 (5%)	21,38,41	1.13	2 (9%)
38	OMG	A1	2288	38	19,26,27	0.90	1 (5%)	21,38,41	1.03	2 (9%)
38	OMG	A1	2922	38	19,26,27	0.89	1 (5%)	21,38,41	1.03	1 (4%)
38	A2M	A1	1133	38	18,25,26	0.84	0	20,36,39	1.39	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	A2M	B5	541	34	18,25,26	0.88	1 (5%)	20,36,39	1.27	2 (10%)
38	OMG	A1	867	38	19,26,27	0.87	1 (5%)	21,38,41	1.05	2 (9%)
38	A2M	A1	2280	38	18,25,26	0.84	0	20,36,39	1.39	3 (15%)
38	5MC	A1	2278	38,83	19,22,23	1.47	3 (15%)	26,32,35	1.27	3 (11%)
34	OMC	B5	1007	34	19,22,23	0.81	0	25,31,34	0.94	1 (4%)
34	A2M	B5	420	34	18,25,26	0.85	0	20,36,39	1.20	2 (10%)
34	MA6	B5	1782	34	19,26,27	0.96	2 (10%)	18,38,41	1.96	4 (22%)
34	OMG	B5	1271	34	19,26,27	0.88	1 (5%)	21,38,41	1.00	2 (9%)
34	4AC	B5	1280	34	21,24,25	1.04	1 (4%)	28,34,37	1.09	2 (7%)
36	HIC	AB	243	36	8,11,12	1.62	2 (25%)	5,14,16	0.97	0
38	OMG	A1	1450	38,83	19,26,27	0.87	1 (5%)	21,38,41	1.04	1 (4%)
38	OMC	A1	1437	38,83	19,22,23	0.84	0	25,31,34	1.24	3 (12%)
34	A2M	B5	436	34	18,25,26	0.87	1 (5%)	20,36,39	1.38	3 (15%)
38	OMU	A1	2724	38	19,22,23	1.23	3 (15%)	25,31,34	1.82	5 (20%)
38	OMC	A1	663	38	19,22,23	0.81	0	25,31,34	0.78	0
38	OMG	A1	2791	38	19,26,27	0.90	1 (5%)	21,38,41	1.03	1 (4%)
38	OMU	A1	2347	38	19,22,23	1.31	4 (21%)	25,31,34	1.81	6 (24%)
38	1MA	A1	2142	38,83	17,25,26	1.51	2 (11%)	17,37,40	1.23	2 (11%)
38	OMU	A1	2729	38	19,22,23	1.29	3 (15%)	25,31,34	1.72	5 (20%)
34	4AC	B5	1773	34	21,24,25	1.05	1 (4%)	28,34,37	1.38	5 (17%)
38	OMG	A1	2619	38	19,26,27	0.89	1 (5%)	21,38,41	1.01	2 (9%)
38	OMC	A1	650	38,83	19,22,23	0.79	0	25,31,34	0.80	0
38	OMC	A1	2337	38	19,22,23	0.80	0	25,31,34	0.90	1 (4%)
38	A2M	A1	1449	38,83	18,25,26	0.89	1 (5%)	20,36,39	1.15	2 (10%)
38	OMU	A1	2421	38	19,22,23	1.26	3 (15%)	25,31,34	1.84	5 (20%)
38	A2M	A1	807	38	18,25,26	0.82	0	20,36,39	1.33	3 (15%)
34	OMC	B5	1639	34	19,22,23	0.79	0	25,31,34	0.80	1 (4%)
38	A2M	A1	2220	38	18,25,26	0.81	0	20,36,39	1.29	2 (10%)
34	OMG	B5	562	34	19,26,27	0.89	1 (5%)	21,38,41	1.03	2 (9%)
34	A2M	B5	974	34	18,25,26	0.86	0	20,36,39	1.25	2 (10%)
80	DDE	DC	699	80	15,20,21	0.99	1 (6%)	11,28,30	1.12	1 (9%)
38	OMU	A1	1888	38	19,22,23	1.28	3 (15%)	25,31,34	1.85	4 (16%)
34	OMU	B5	1269	34	19,22,23	1.29	4 (21%)	25,31,34	1.90	8 (32%)
34	A2M	B5	100	34,83	18,25,26	0.88	1 (5%)	20,36,39	1.21	2 (10%)
34	OMG	B5	1126	34	19,26,27	0.88	1 (5%)	21,38,41	1.05	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	OMG	B5	1428	34	19,26,27	0.87	1 (5%)	21,38,41	1.02	2 (9%)
38	OMU	A1	898	38	19,22,23	1.25	3 (15%)	25,31,34	1.78	5 (20%)
34	OMU	B5	578	34	19,22,23	1.19	2 (10%)	25,31,34	1.80	5 (20%)
38	A2M	A1	876	38	18,25,26	0.84	0	20,36,39	1.17	2 (10%)
38	OMC	A1	2197	38	19,22,23	0.78	0	25,31,34	0.80	0
38	1MA	A1	645	38,83	17,25,26	1.49	2 (11%)	17,37,40	1.14	2 (11%)
34	OMG	B5	1572	34	19,26,27	0.89	1 (5%)	21,38,41	1.14	2 (9%)
34	A2M	B5	619	34,83	18,25,26	0.80	0	20,36,39	1.27	2 (10%)
34	OMC	B5	414	34	19,22,23	0.80	0	25,31,34	0.82	1 (4%)
34	XSX	B5	1191	34	24,28,29	1.00	1 (4%)	30,40,43	2.10	7 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	G7M	B5	1575	34	-	0/3/25/26	0/3/3/3
38	OMU	A1	2417	38	-	1/9/27/28	0/2/2/2
38	A2M	A1	2281	38	-	1/5/27/28	0/3/3/3
34	A2M	B5	28	34,83	-	0/5/27/28	0/3/3/3
38	OMC	A1	2948	38	-	1/9/27/28	0/2/2/2
34	A2M	B5	796	34	-	0/5/27/28	0/3/3/3
38	OMG	A1	2793	38	-	0/5/27/28	0/3/3/3
38	OMC	A1	2959	38	-	0/9/27/28	0/2/2/2
38	A2M	A1	649	38	-	1/5/27/28	0/3/3/3
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2
38	5MC	A1	2870	38,83	-	4/7/25/26	0/2/2/2
38	A2M	A1	2640	38	-	1/5/27/28	0/3/3/3
38	OMU	A1	2921	38	-	0/9/27/28	0/2/2/2
38	OMG	A1	2815	38	-	0/5/27/28	0/3/3/3
38	OMG	A1	805	38	-	0/5/27/28	0/3/3/3
38	A2M	A1	2946	38,83	-	1/5/27/28	0/3/3/3
34	MA6	B5	1781	34	-	2/7/29/30	0/3/3/3
38	A2M	A1	817	38,83	-	1/5/27/28	0/3/3/3
38	OMG	A1	908	38	-	0/5/27/28	0/3/3/3
38	OMG	A1	2288	38	-	0/5/27/28	0/3/3/3
38	OMG	A1	2922	38	-	0/5/27/28	0/3/3/3
38	A2M	A1	1133	38	-	0/5/27/28	0/3/3/3
34	A2M	B5	541	34	-	3/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	OMG	A1	867	38	-	1/5/27/28	0/3/3/3
38	A2M	A1	2280	38	-	2/5/27/28	0/3/3/3
38	5MC	A1	2278	38,83	-	0/7/25/26	0/2/2/2
34	OMC	B5	1007	34	-	1/9/27/28	0/2/2/2
34	A2M	B5	420	34	-	1/5/27/28	0/3/3/3
34	MA6	B5	1782	34	-	4/7/29/30	0/3/3/3
34	OMG	B5	1271	34	-	1/5/27/28	0/3/3/3
34	4AC	B5	1280	34	-	2/11/29/30	0/2/2/2
36	HIC	AB	243	36	-	0/5/6/8	0/1/1/1
38	OMG	A1	1450	38,83	-	1/5/27/28	0/3/3/3
38	OMC	A1	1437	38,83	-	2/9/27/28	0/2/2/2
34	A2M	B5	436	34	-	1/5/27/28	0/3/3/3
38	OMU	A1	2724	38	-	1/9/27/28	0/2/2/2
38	OMC	A1	663	38	-	1/9/27/28	0/2/2/2
38	OMG	A1	2791	38	-	1/5/27/28	0/3/3/3
38	OMU	A1	2347	38	-	0/9/27/28	0/2/2/2
38	1MA	A1	2142	38,83	-	1/3/25/26	0/3/3/3
38	OMU	A1	2729	38	-	3/9/27/28	0/2/2/2
34	4AC	B5	1773	34	-	4/11/29/30	0/2/2/2
38	OMG	A1	2619	38	-	1/5/27/28	0/3/3/3
38	OMC	A1	650	38,83	-	0/9/27/28	0/2/2/2
38	OMC	A1	2337	38	-	1/9/27/28	0/2/2/2
38	A2M	A1	1449	38,83	-	0/5/27/28	0/3/3/3
38	OMU	A1	2421	38	-	1/9/27/28	0/2/2/2
38	A2M	A1	807	38	-	0/5/27/28	0/3/3/3
34	OMC	B5	1639	34	-	0/9/27/28	0/2/2/2
38	A2M	A1	2220	38	-	0/5/27/28	0/3/3/3
34	OMG	B5	562	34	-	0/5/27/28	0/3/3/3
34	A2M	B5	974	34	-	0/5/27/28	0/3/3/3
80	DDE	DC	699	80	-	6/20/21/23	0/1/1/1
38	OMU	A1	1888	38	-	0/9/27/28	0/2/2/2
34	OMU	B5	1269	34	-	4/9/27/28	0/2/2/2
34	A2M	B5	100	34,83	-	2/5/27/28	0/3/3/3
34	OMG	B5	1126	34	-	2/5/27/28	0/3/3/3
34	OMG	B5	1428	34	-	4/5/27/28	0/3/3/3
38	OMU	A1	898	38	-	1/9/27/28	0/2/2/2
34	OMU	B5	578	34	-	4/9/27/28	0/2/2/2
38	A2M	A1	876	38	-	1/5/27/28	0/3/3/3
38	OMC	A1	2197	38	-	6/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	1MA	A1	645	38,83	-	0/3/25/26	0/3/3/3
34	OMG	B5	1572	34	-	0/5/27/28	0/3/3/3
34	A2M	B5	619	34,83	-	2/5/27/28	0/3/3/3
34	OMC	B5	414	34	-	1/9/27/28	0/2/2/2
34	XSX	B5	1191	34	-	4/16/34/35	0/2/2/2

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	1575	G7M	C8-N9	7.44	1.46	1.33
34	B5	1575	G7M	C8-N7	7.41	1.46	1.33
38	A1	2278	5MC	C5-C4	5.03	1.47	1.44
38	A1	2142	1MA	C2-N3	4.87	1.34	1.28
38	A1	2870	5MC	C5-C4	4.85	1.47	1.44

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A1	2634	UR3	C4-N3-C2	-6.76	119.14	124.58
34	B5	1781	MA6	C2-N1-C6	5.75	122.48	116.84
34	B5	1191	XSX	C3-C1-N3	-5.60	102.37	112.16
34	B5	1782	MA6	C2-N1-C6	5.54	122.27	116.84
34	B5	1191	XSX	C4-N3-C2	-5.33	118.41	124.66

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	B5	100	A2M	C1'-C2'-O2'-CM'
34	B5	414	OMC	C1'-C2'-O2'-CM2
34	B5	420	A2M	C1'-C2'-O2'-CM'
34	B5	436	A2M	C1'-C2'-O2'-CM'
34	B5	1007	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 220 ligands modelled in this entry, 218 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	GDP	DC	901	83	25,30,30	1.00	2 (8%)	30,47,47	1.51	4 (13%)
86	W9C	DC	902	-	34,39,39	0.68	2 (5%)	38,64,64	1.13	4 (10%)

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	GDP	DC	901	83	-	4/12/32/32	0/3/3/3
86	W9C	DC	902	-	1/1/15/16	3/21/104/104	0/7/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	DC	902	W9C	O14-C5	-2.90	1.20	1.30
85	DC	901	GDP	C6-N1	-2.56	1.33	1.37
85	DC	901	GDP	PA-O3A	2.16	1.61	1.59
86	DC	902	W9C	C1-C5	2.01	1.55	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	DC	901	GDP	C4'-O4'-C1'	-4.94	105.41	109.92
86	DC	902	W9C	C12-C6-C2	-4.32	98.40	105.09
85	DC	901	GDP	O4'-C1'-N9	3.27	113.08	108.75
86	DC	902	W9C	C20-C13-C4	2.95	120.27	112.41
85	DC	901	GDP	C8-N7-C5	2.50	106.81	102.55

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
86	DC	902	W9C	C52

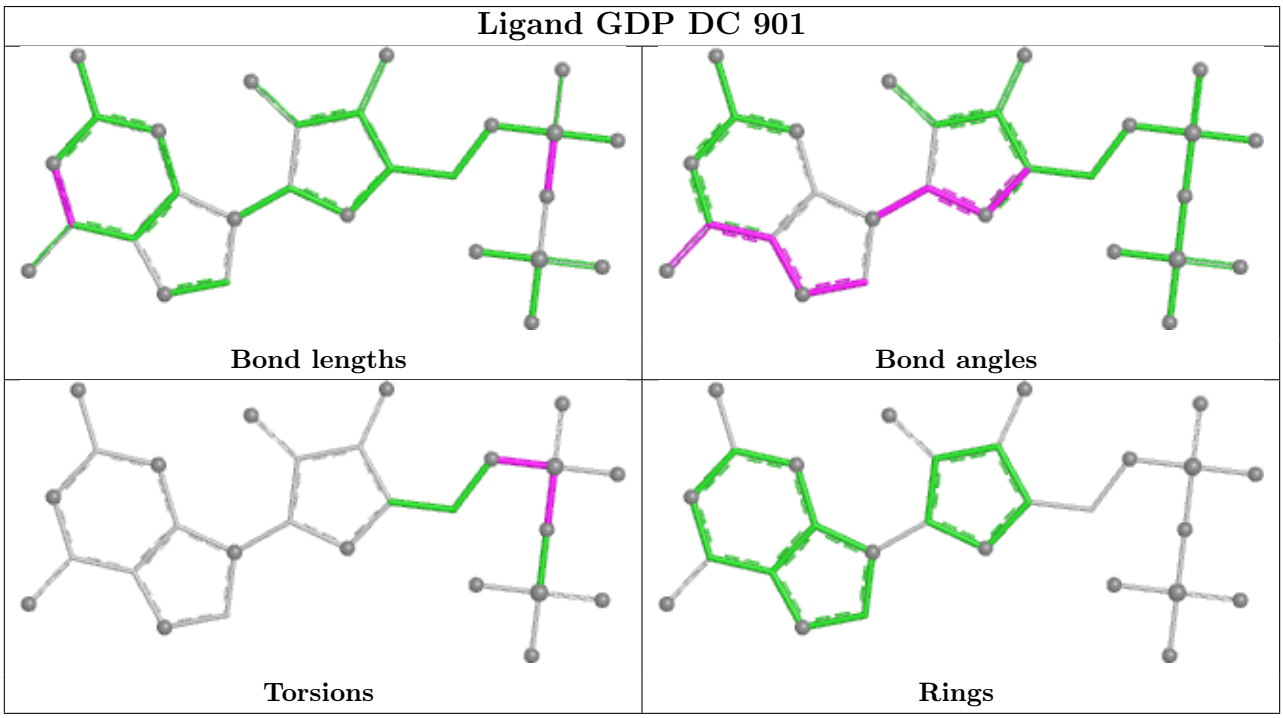
5 of 7 torsion outliers are listed below:

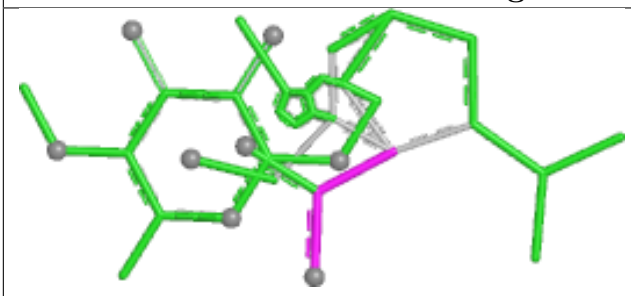
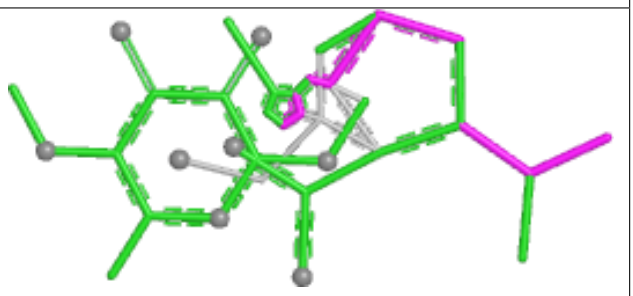
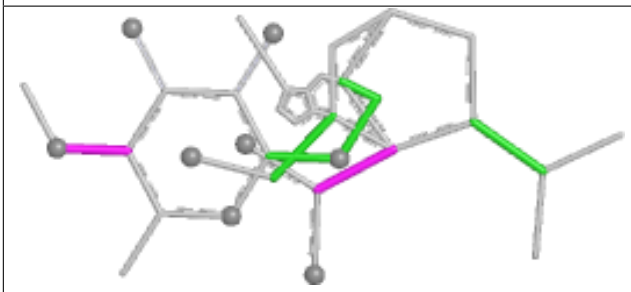
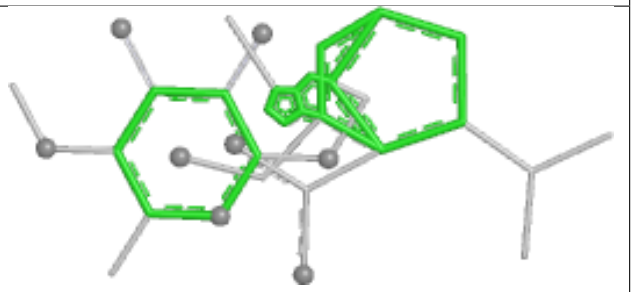
Mol	Chain	Res	Type	Atoms
85	DC	901	GDP	C5'-O5'-PA-O3A
85	DC	901	GDP	C5'-O5'-PA-O2A
86	DC	902	W9C	C2-C1-C5-O14
86	DC	902	W9C	C2-C1-C5-O15
86	DC	902	W9C	C54-C55-O64-C65

There are no ring outliers.

No monomer is involved in short contacts.

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



Ligand W9C DC 902	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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.

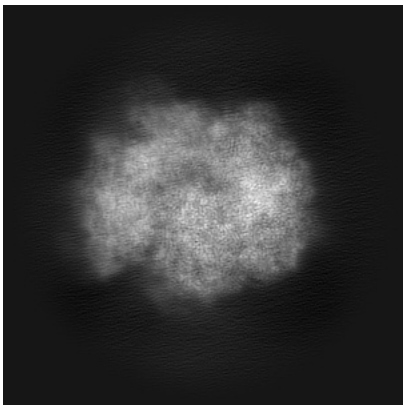
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28634. These allow visual inspection of the internal detail of the map and identification of artifacts.

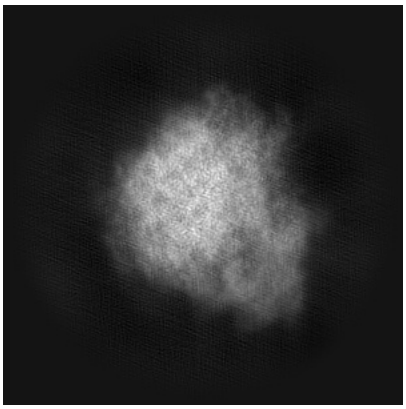
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

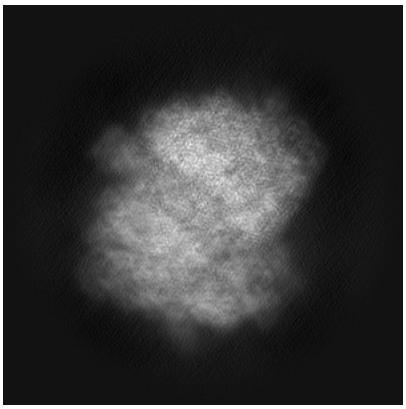
6.1.1 Primary map



X

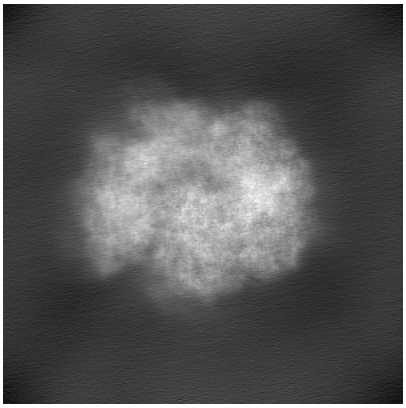


Y

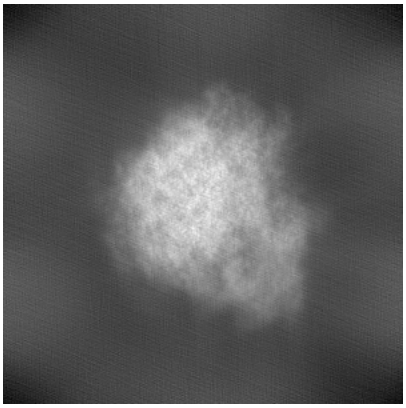


Z

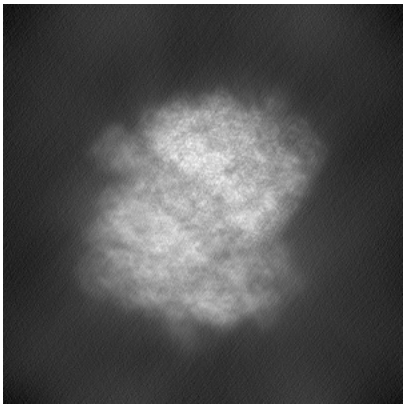
6.1.2 Raw map



X



Y

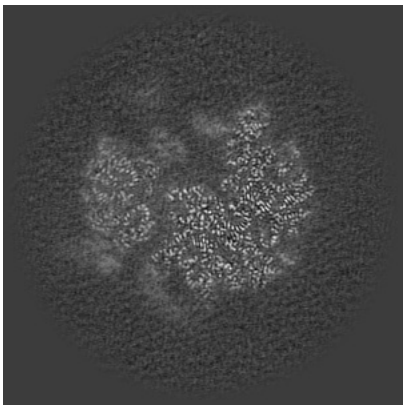


Z

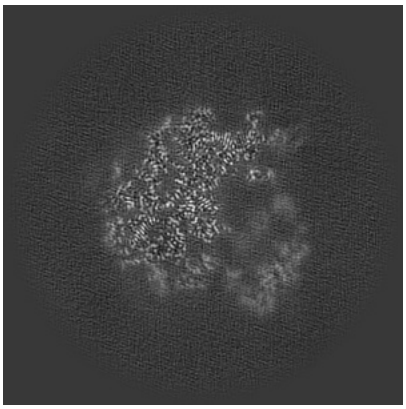
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 200



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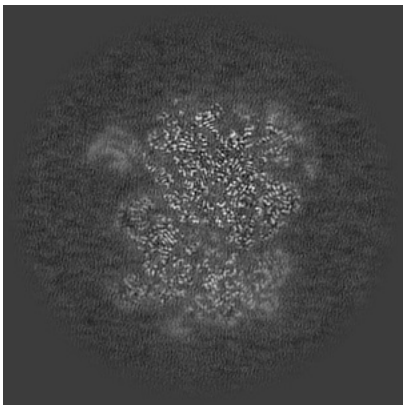
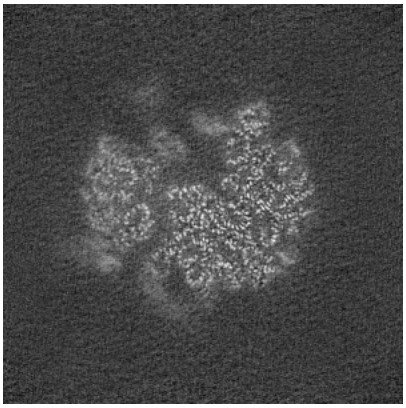


Z Index: 200

6.2.2 Raw map



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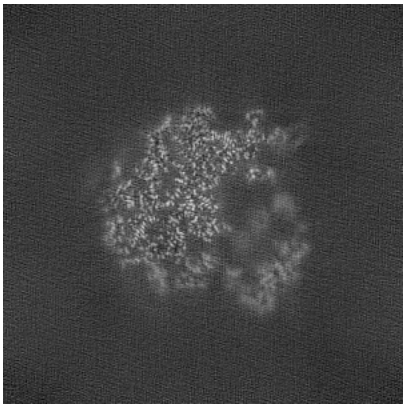
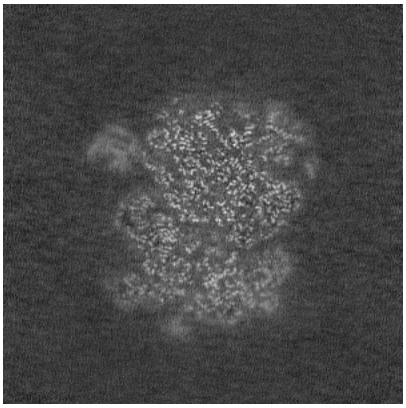


Y Index: 200

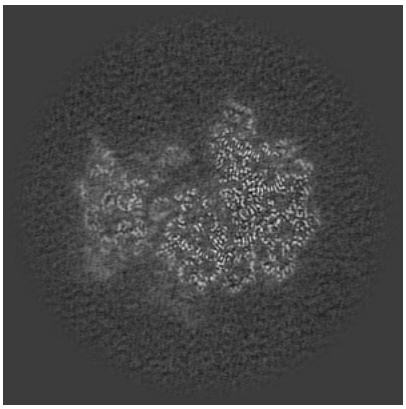


Z Index: 200

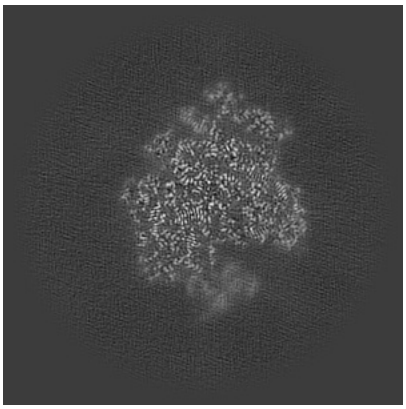
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

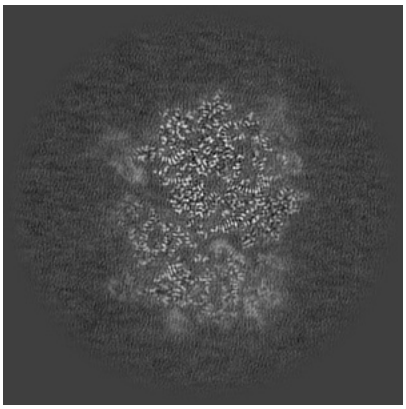
6.3.1 Primary map



X Index: 215

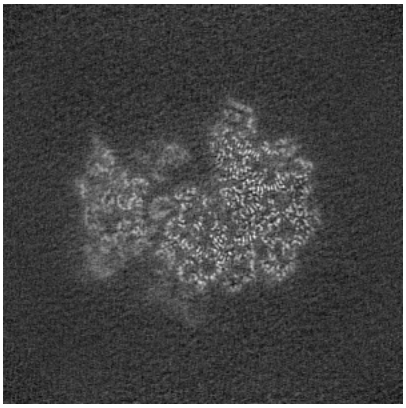


Y Index: 245

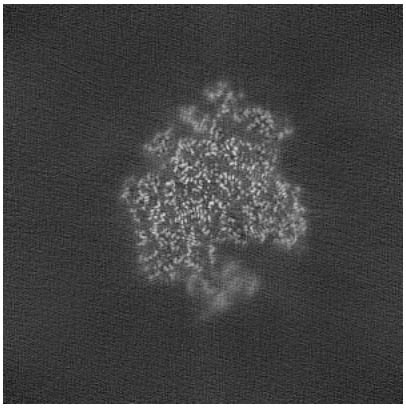


Z Index: 190

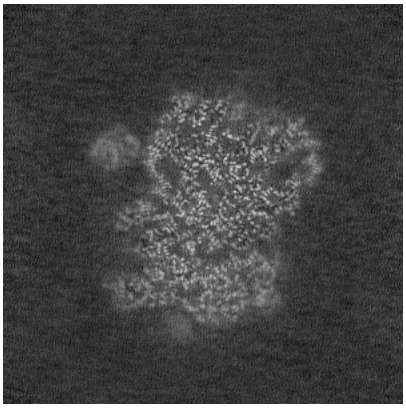
6.3.2 Raw map



X Index: 215



Y Index: 245

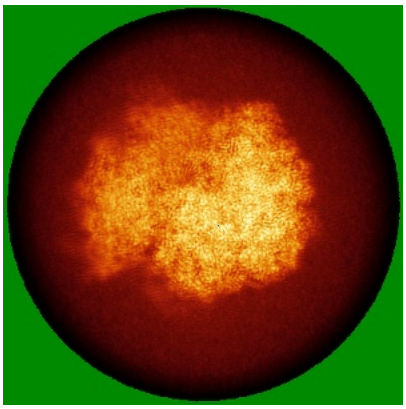


Z Index: 206

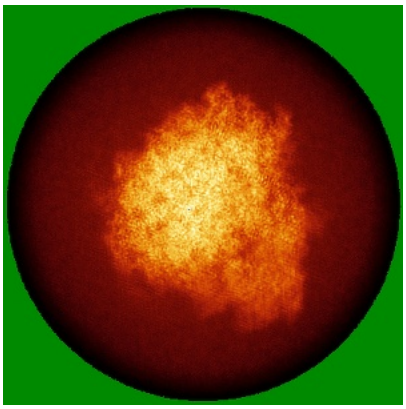
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

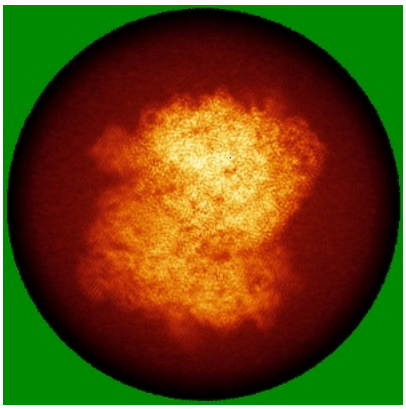
6.4.1 Primary map



X

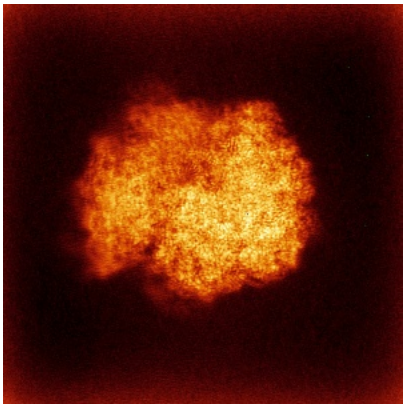


Y

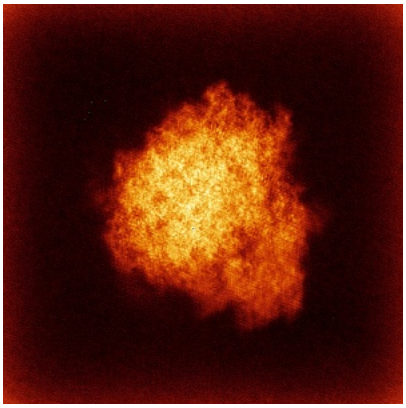


Z

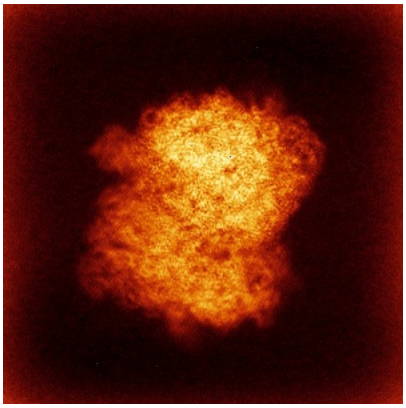
6.4.2 Raw map



X



Y

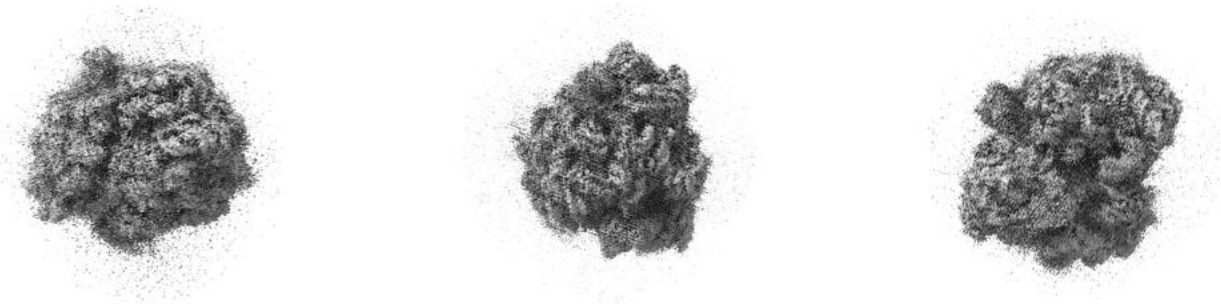


Z

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 0.6. 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.

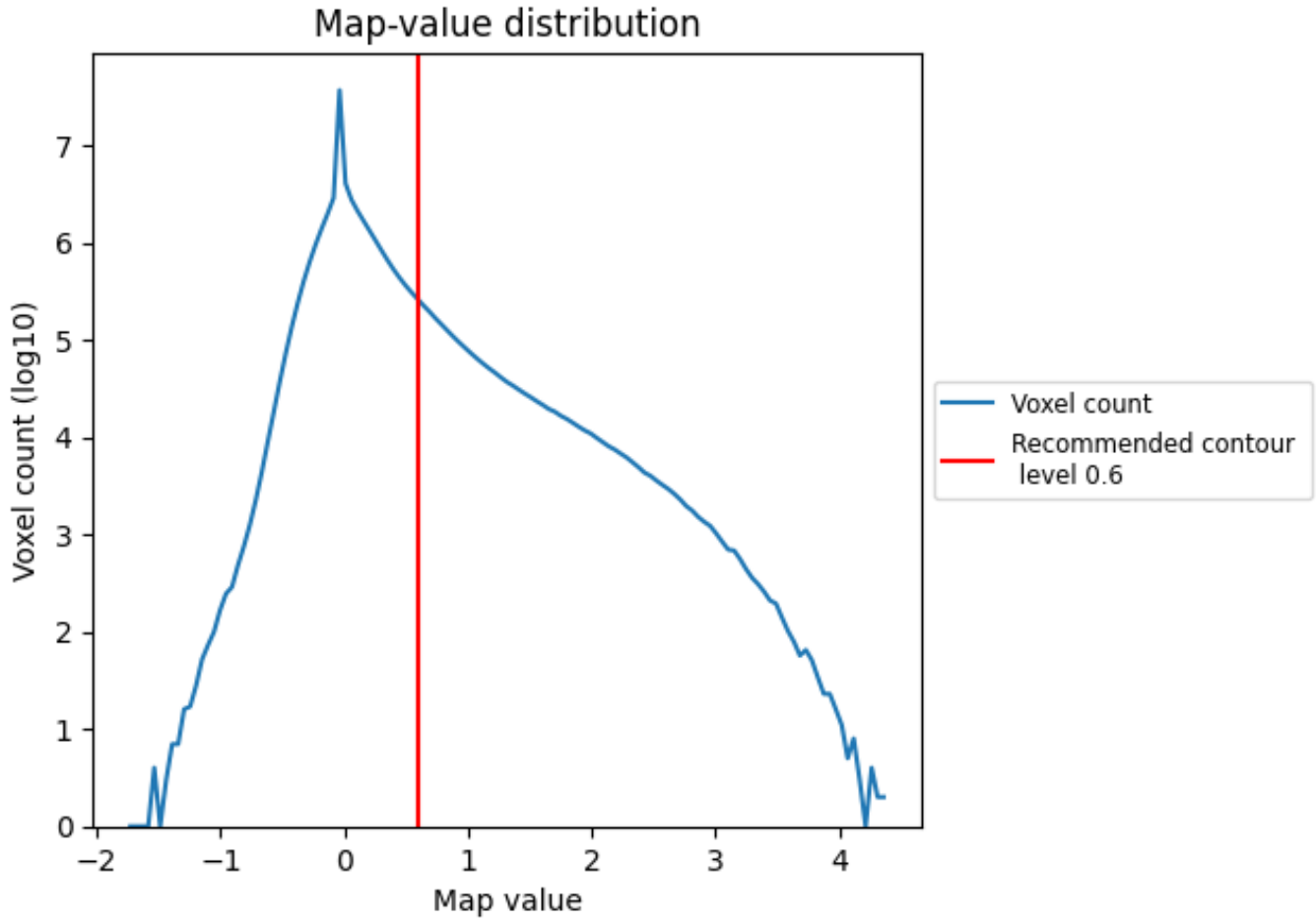
6.6 Mask visualisation (i)

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

7 Map analysis

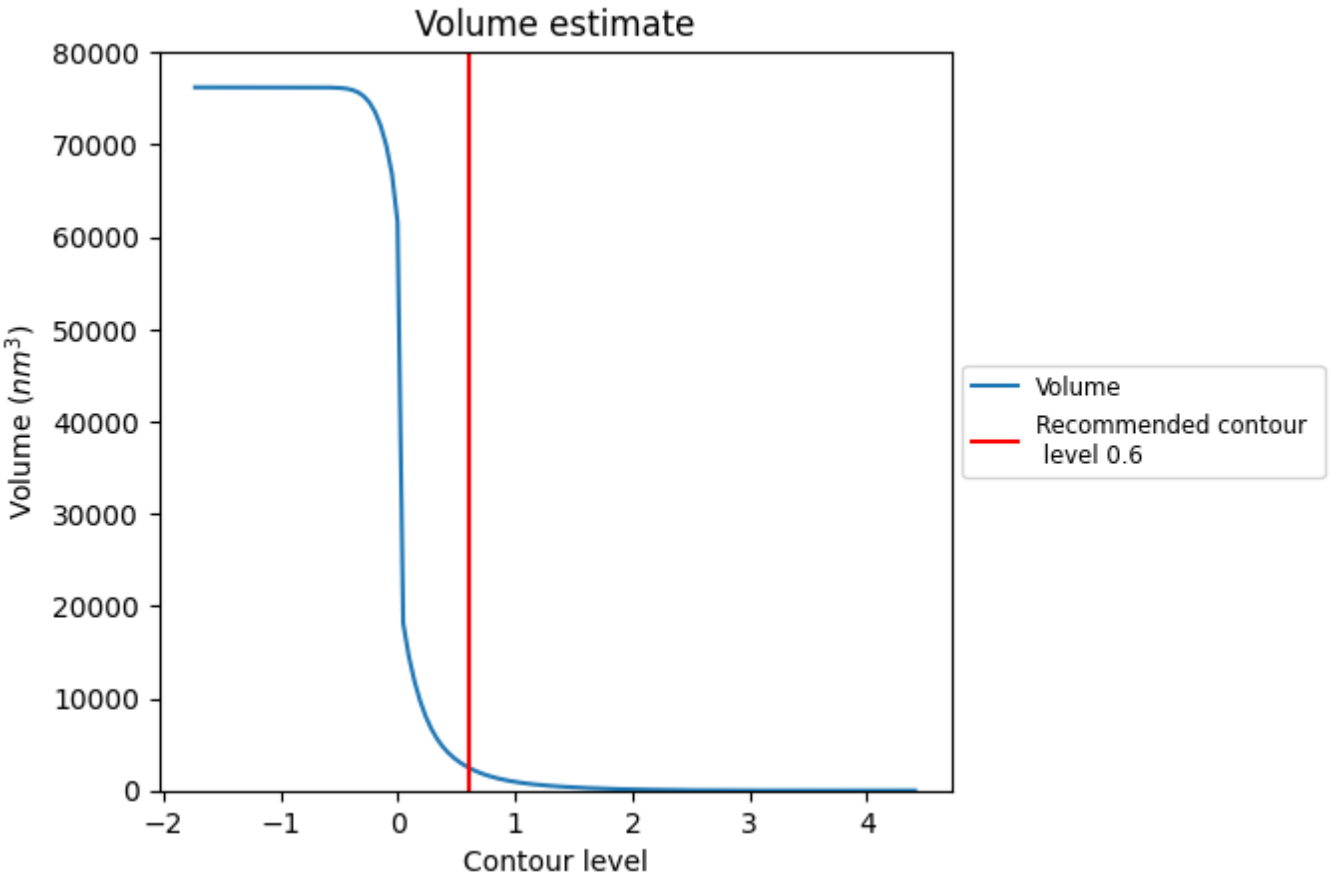
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

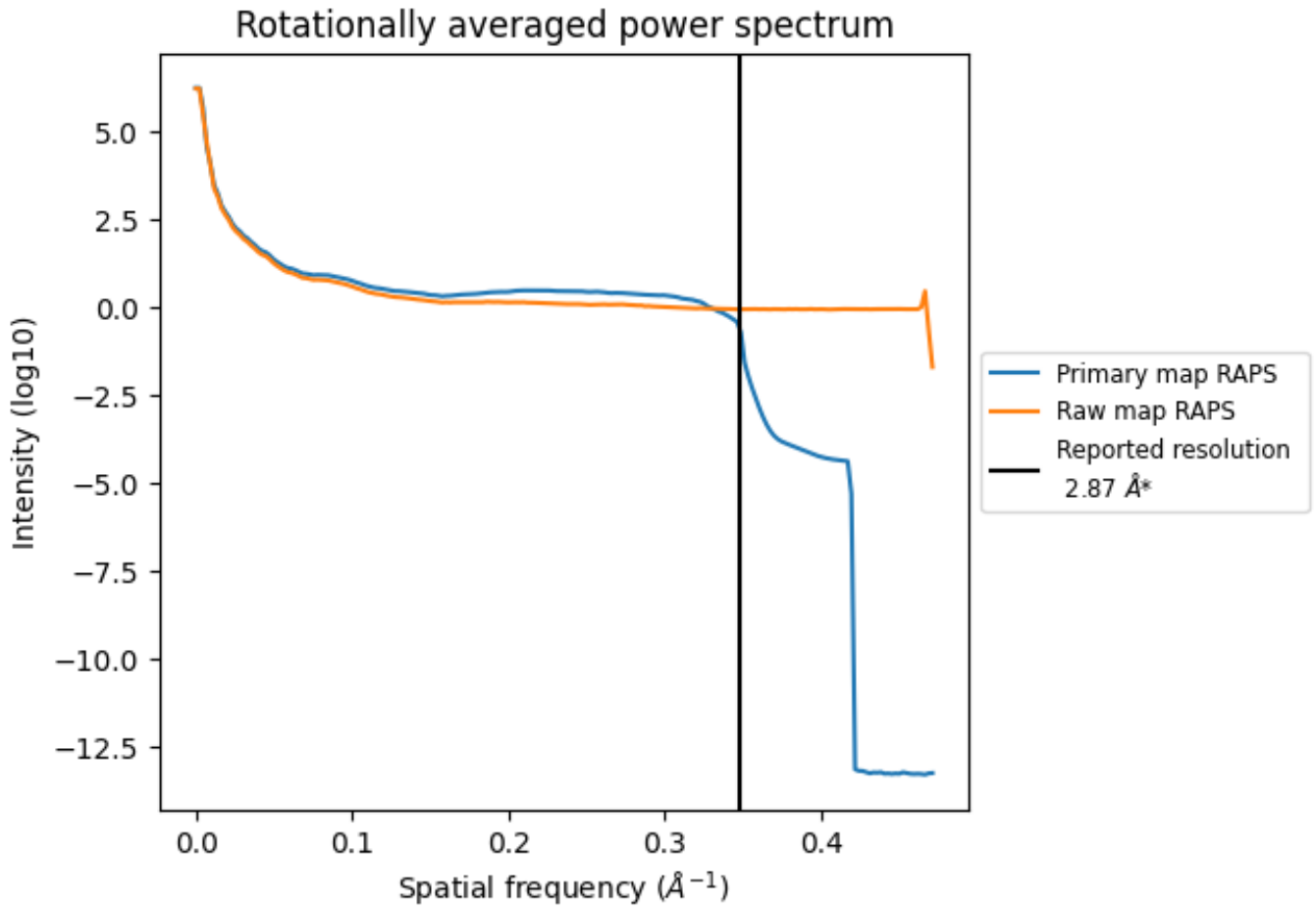
7.2 Volume estimate (i)



The volume at the recommended contour level is 2515 nm^3; this corresponds to an approximate mass of 2272 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

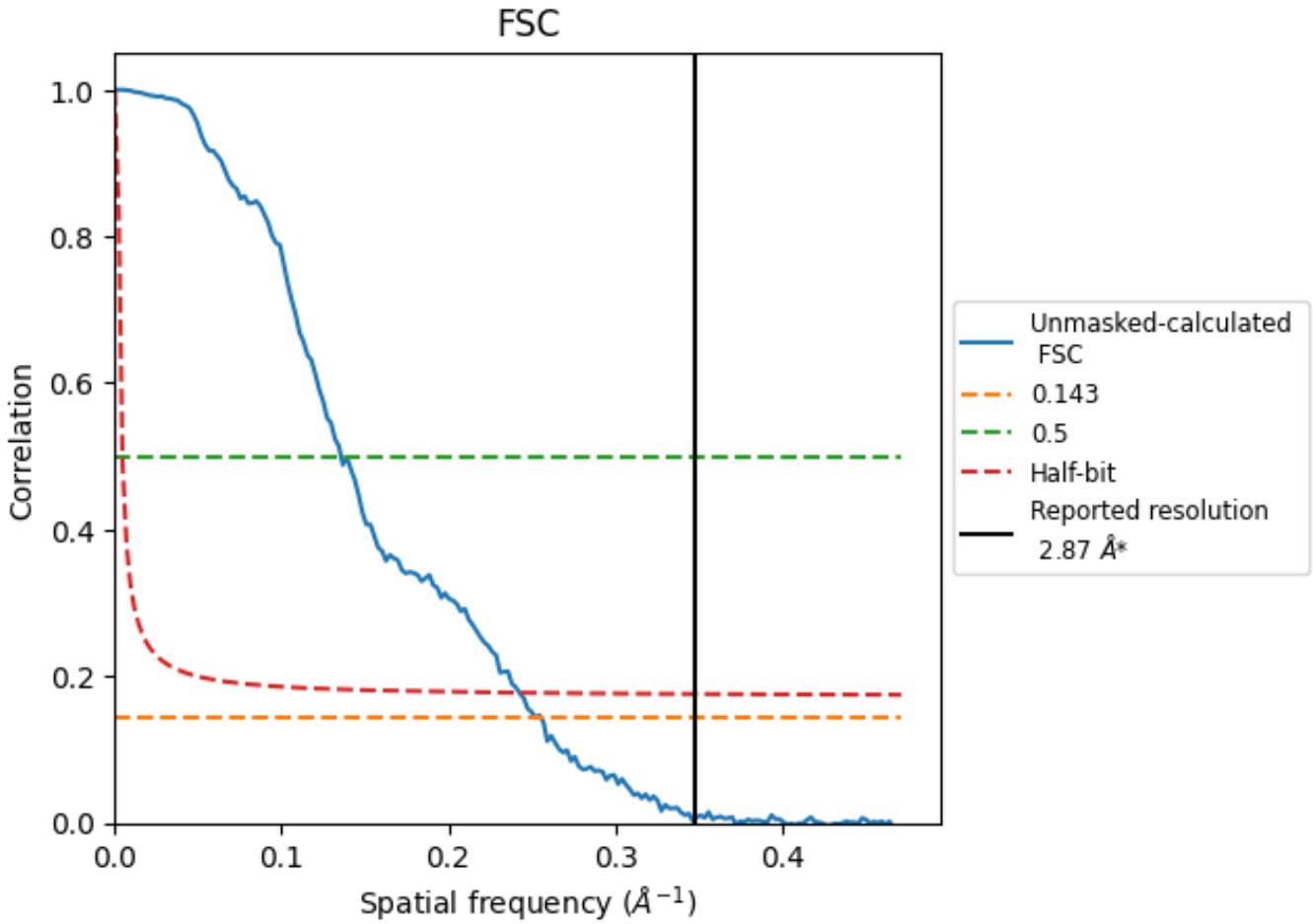


*Reported resolution corresponds to spatial frequency of 0.348 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.348 Å^{-1}

8.2 Resolution estimates (i)

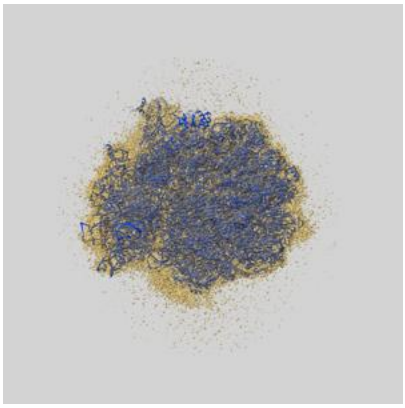
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	7.37	4.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 2.87 by more than 10 %

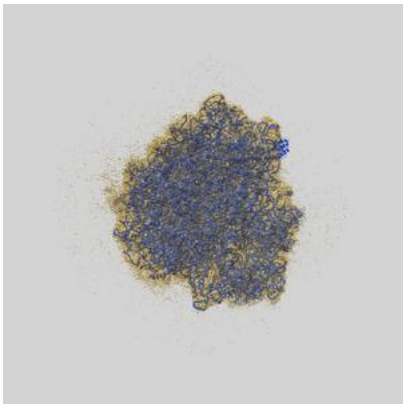
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28634 and PDB model 8EVR. Per-residue inclusion information can be found in section 3 on page 21.

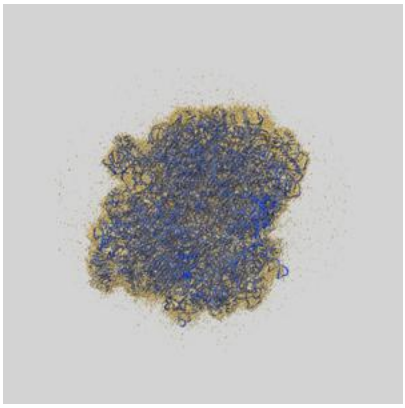
9.1 Map-model overlay



X



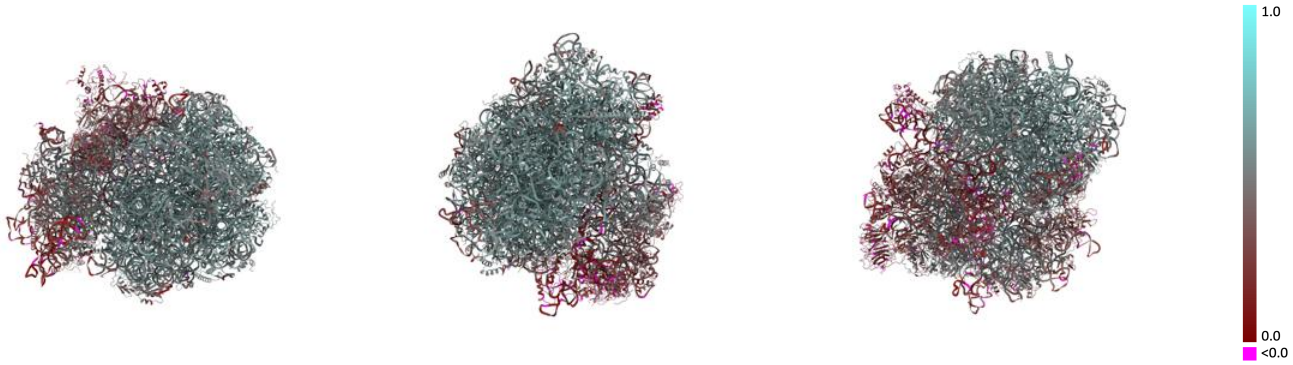
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

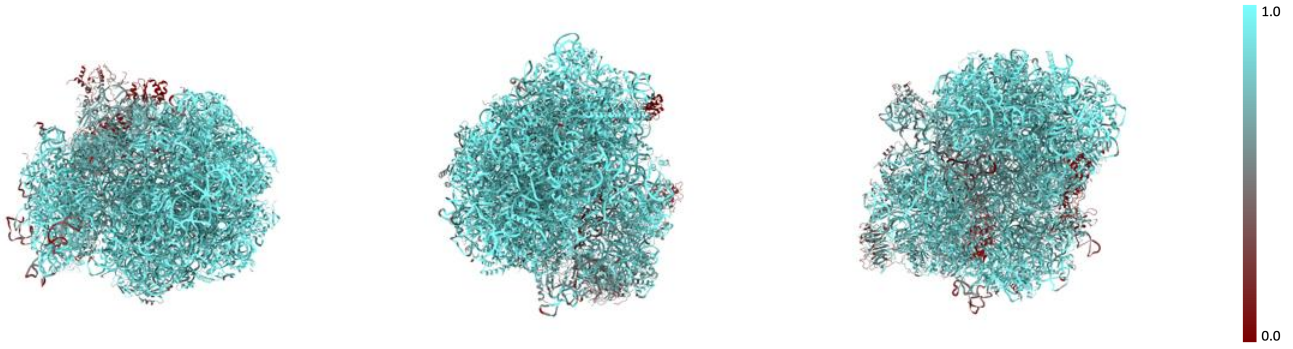
9.2 Q-score mapped to coordinate model



X Y Z

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

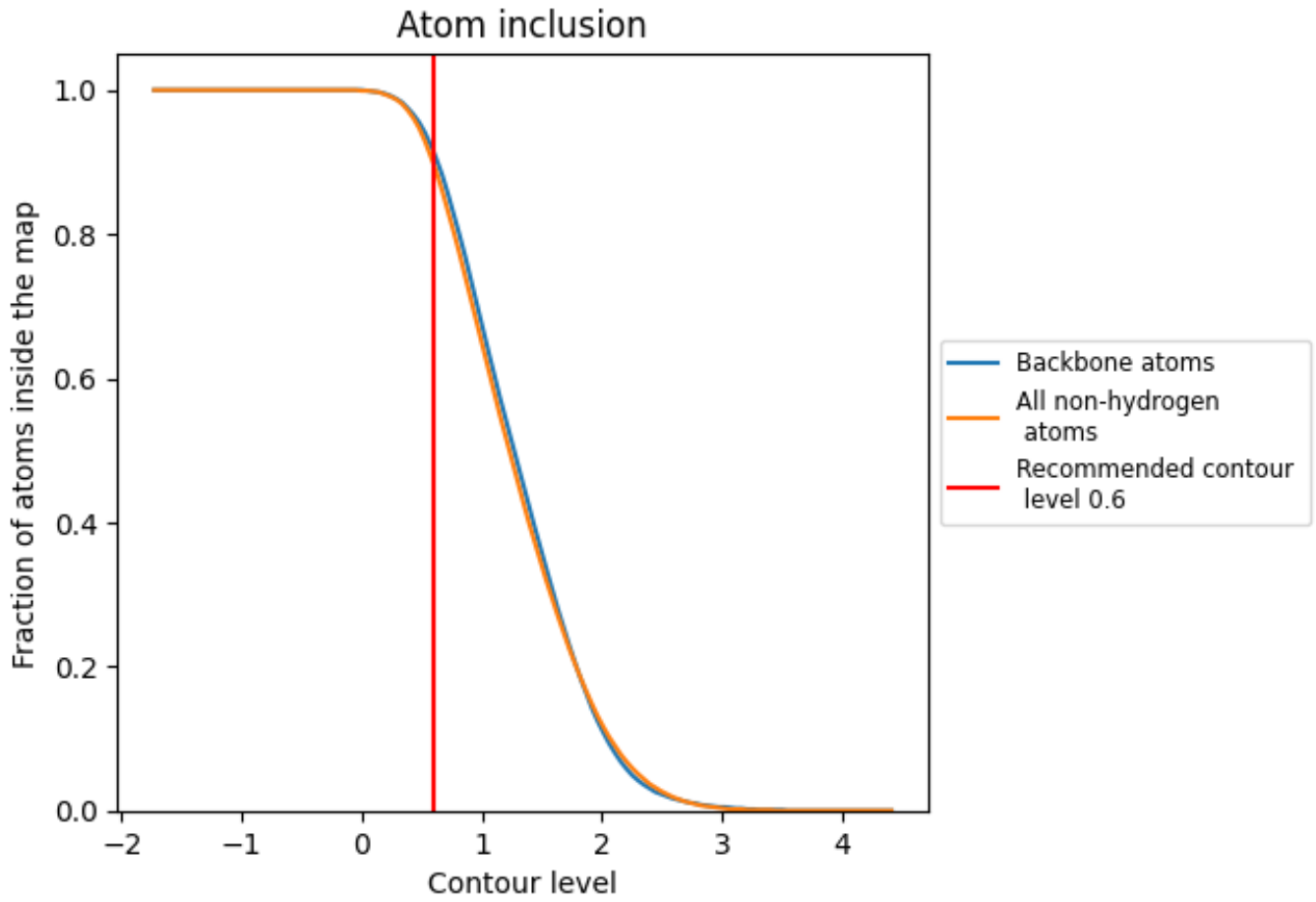
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8960	0.4700
A1	0.9690	0.5450
A3	0.9880	0.5370
A4	0.9820	0.5650
AA	0.9650	0.5960
AB	0.9610	0.5570
AC	0.9600	0.5680
AD	0.9000	0.4750
AE	0.9400	0.5160
AF	0.9770	0.5790
AG	0.9170	0.5240
AH	0.9140	0.5420
AI	0.9570	0.5560
AJ	0.8430	0.4180
AL	0.9560	0.5620
AM	0.9560	0.5510
AN	0.9900	0.6000
AO	0.9620	0.5680
AP	0.9530	0.5520
AQ	0.9790	0.5920
AR	0.8140	0.4660
AS	0.9640	0.5660
AT	0.9600	0.5490
AU	0.8950	0.4500
AV	0.9550	0.5720
AW	0.9720	0.5570
AX	0.9420	0.5390
AY	0.9600	0.5440
AZ	0.9270	0.5260
Aa	0.9740	0.5860
Ab	0.9430	0.5270
Ac	0.9000	0.5310
Ad	0.9360	0.5170
Ae	0.9740	0.5850
Af	0.9820	0.5850

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Chain	Atom inclusion	Q-score
Ag	0.9400	0.5430
Ah	0.9640	0.5500
Ai	0.9600	0.5280
Aj	0.9860	0.5960
Ak	0.6730	0.4290
Al	0.9810	0.5680
Am	0.9230	0.5480
An	0.9580	0.5180
Ao	0.9050	0.5520
Ap	0.9700	0.5790
B5	0.9140	0.4120
BA	0.8380	0.4370
BB	0.8270	0.4460
BC	0.9330	0.4880
BD	0.7970	0.3130
BE	0.9220	0.4430
BF	0.6910	0.2870
BG	0.8690	0.3610
BH	0.7220	0.3960
BI	0.9090	0.4430
BJ	0.9200	0.4600
BK	0.7000	0.2420
BL	0.8850	0.4680
BM	0.1780	0.1670
BN	0.8830	0.4760
BO	0.8790	0.4640
BP	0.6790	0.2990
BQ	0.7860	0.3070
BR	0.6850	0.3240
BS	0.7510	0.3010
BT	0.8030	0.3040
BU	0.7410	0.2740
BV	0.9050	0.4640
BW	0.9740	0.5400
BX	0.9580	0.5260
BY	0.8900	0.4040
BZ	0.6720	0.1990
Ba	0.9040	0.4920
Bb	0.8000	0.4400
Bc	0.6500	0.3000
Bd	0.9030	0.3510
Be	0.8840	0.4130

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Chain	Atom inclusion	Q-score
Bf	0.2720	0.1740
Bg	0.5550	0.2140
DC	0.7140	0.2960
E	0.5730	0.1810
EC	0.5020	0.1100
V	0.1250	0.2160