



## wwPDB EM Validation Summary Report ⓘ

Jun 27, 2026 – 11:10 AM EDT

PDB ID : 9E7F / pdb\_00009e7f  
EMDB ID : EMD-47668  
Title : Cryo-EM structure of the Pyrobaculum calidifontis 70S ribosome in complex with Dri  
Authors : Nissley, A.J.; Cate, J.H.D.  
Deposited on : 2024-11-01  
Resolution : 2.53 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

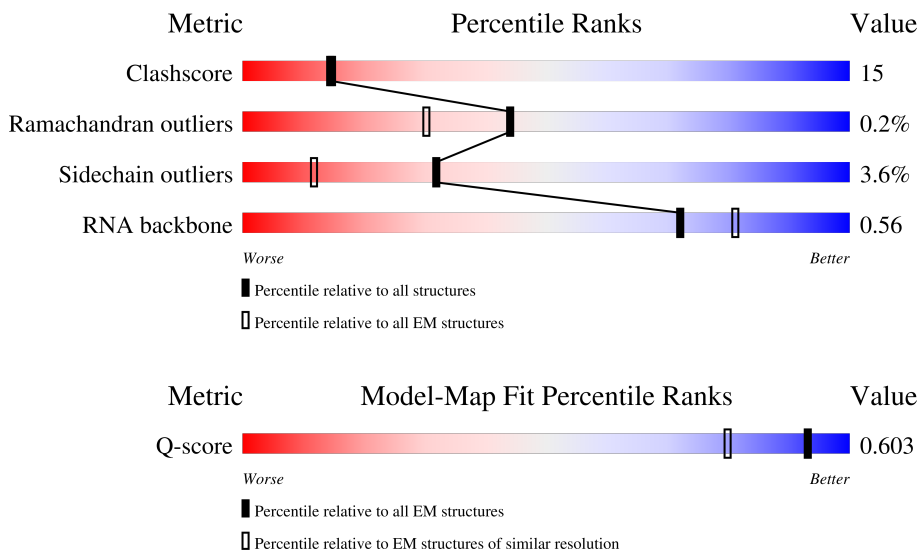
EMDB validation analysis : 0.0.1.dev133  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.53 Å.

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






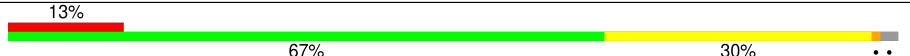

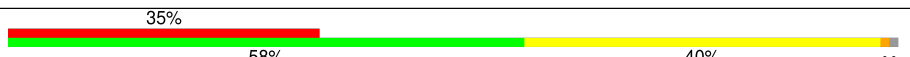
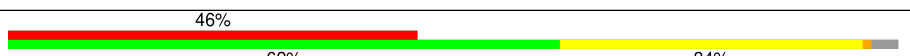
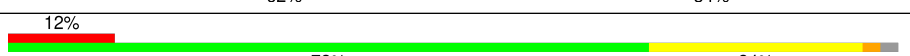
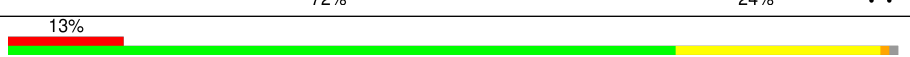


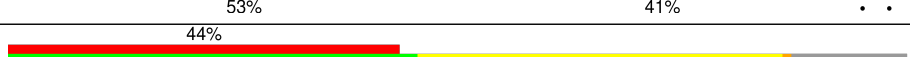

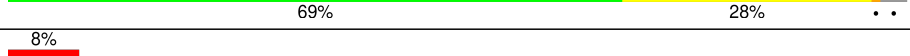
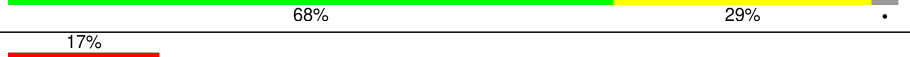




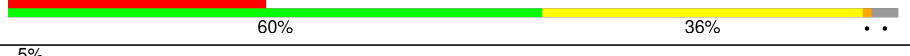

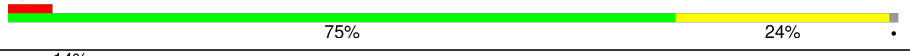



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7309 ( 2.03 - 3.03 )

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

Mol	Chain	Length	Quality of chain
1	2	129	
2	3	655	
3	1	3024	

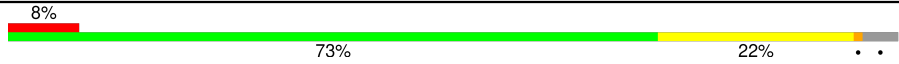
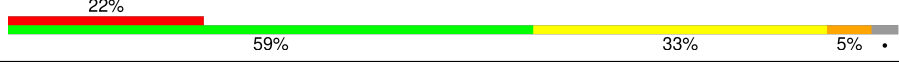
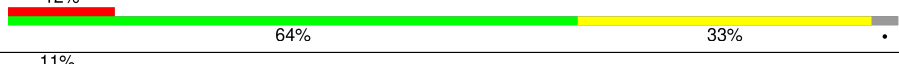



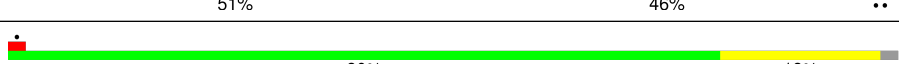
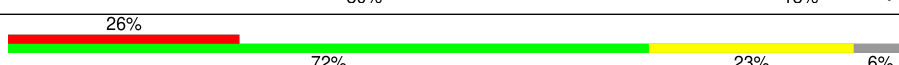
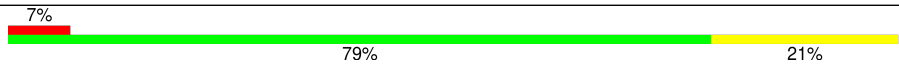


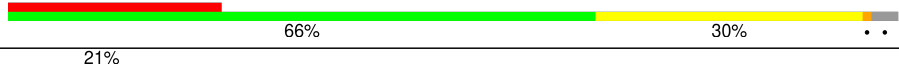
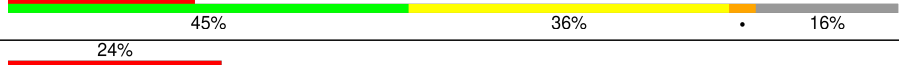

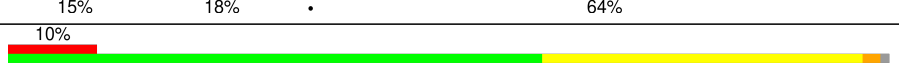










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Mol	Chain	Length	Quality of chain
4	4	1498	
5	AA	244	
6	AB	338	
7	AC	285	
8	AD	178	
9	AE	196	
10	AF	149	
11	AG	186	
12	AH	157	
13	AI	144	
14	AJ	103	
14	AK	103	
15	AL	156	
16	AM	189	
17	AN	178	
18	AO	205	
19	AP	122	
20	AQ	147	
21	AR	78	
22	AS	99	
23	AT	184	
24	AU	81	
25	AV	128	
26	AW	62	
27	AX	79	

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Mol	Chain	Length	Quality of chain
28	AY	179	
29	AZ	101	
30	Aa	91	
31	Ab	153	
32	Ac	84	
33	Ad	52	
34	Ae	67	
35	Af	51	
36	Ag	53	
37	Ah	91	
38	Ai	102	
39	Aj	184	
40	Ak	93	
41	BA	222	
42	BB	208	
43	BC	216	
44	BD	159	
45	BE	237	
46	BF	202	
47	BG	151	
48	BH	223	
49	BI	130	
50	BJ	131	
51	BK	142	
52	BL	106	

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Mol	Chain	Length	Quality of chain
53	BM	141	
54	BN	147	
55	BO	153	
56	BP	54	
57	BQ	151	
58	BR	147	
59	BS	71	
60	BT	158	
61	BU	158	
62	BV	128	
63	BW	110	
64	BX	100	
65	BY	67	
66	BZ	77	
67	Ba	54	
68	Bb	68	
69	Bc	65	

## 2 Entry composition i

There are 73 unique types of molecules in this entry. The entry contains 172182 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	129	2769	1231	512	897	129	0	0

- Molecule 2 is a protein called Putative signal-transduction protein with CBS domains.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	295	2251	1421	393	428	9	0	0

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	1	2849	61386	27335	11453	19749	2849	0	0

- Molecule 4 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	1430	30817	13730	5745	9912	1430	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	5	4AC	C	conflict	GB 343200235
4	1318	4AC	C	conflict	GB 343200235

- Molecule 5 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AA	239	1803	1136	354	308	5	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AB	336	2611	1681	476	450	4	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AC	278	2178	1406	395	371	6	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AD	178	1412	894	273	238	7	0	0

- Molecule 9 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AE	195	1520	990	254	272	4	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AF	145	1095	705	187	202	1	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AG	183	1510	979	278	246	7	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AH	155	1244	785	249	209	1	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AI	138	Total	C	N	O	S	0	0
			1068	682	202	181	3		

- Molecule 14 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AJ	101	Total	C	N	O	S	0	0
			788	500	143	144	1		
14	AK	90	Total	C	N	O	S	0	0
			700	441	130	128	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AL	152	Total	C	N	O	S	0	0
			1198	761	232	202	3		

- Molecule 16 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AM	184	Total	C	N	O	S	0	0
			1558	992	315	245	6		

- Molecule 17 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AN	169	Total	C	N	O	S	0	0
			1336	847	254	227	8		

- Molecule 18 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AO	200	Total	C	N	O	S	0	0
			1615	1027	309	278	1		

- Molecule 19 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AP	121	Total	C	N	O	S	0	0
			920	583	181	155	1		

- Molecule 20 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	AQ	146	1214	759	244	208	3	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	AR	76	603	382	109	109	3	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	AS	98	788	503	150	134	1	0	0

- Molecule 23 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	AT	183	1496	978	268	247	3	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	AU	81	651	417	115	117	2	0	0

- Molecule 25 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	AV	121	976	619	194	161	2	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	AW	56	449	287	86	70	6	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AX	67	Total	C	N	O	S	0	0
			554	343	117	92	2		

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AY	172	Total	C	N	O	S	0	0
			1374	888	245	235	6		

- Molecule 29 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AZ	98	Total	C	N	O	S	0	0
			742	481	128	132	1		

- Molecule 30 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Aa	88	Total	C	N	O	0	0
			726	460	146	120		

- Molecule 31 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ab	140	Total	C	N	O	S	0	0
			1183	757	239	186	1		

- Molecule 32 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ac	83	Total	C	N	O	S	0	0
			649	407	138	102	2		

- Molecule 33 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ad	52	Total	C	N	O	S	0	0
			429	265	93	65	6		

- Molecule 34 is a protein called LSU ribosomal protein L38E.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Ae	66	Total	C	N	O	0	0
			552	363	93	96		

- Molecule 35 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Af	50	Total	C	N	O	0	0
			415	260	96	59		

- Molecule 36 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ag	50	Total	C	N	O	S	0	0
			417	259	88	66	4		

- Molecule 37 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ah	91	Total	C	N	O	S	0	0
			739	467	142	123	7		

- Molecule 38 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ai	99	Total	C	N	O	S	0	0
			769	489	148	127	5		

- Molecule 39 is a protein called DJ-1/PfpI domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Aj	183	Total	C	N	O	S	0	0
			1469	954	248	265	2		

- Molecule 40 is a protein called PaREP1 domain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ak	90	Total	C	N	O	S	0	0
			743	478	127	136	2		

- Molecule 41 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BA	187	1487	965	263	256	3	0	0

- Molecule 42 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	BB	198	1600	1037	277	279	7	0	0

- Molecule 43 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BC	77	611	393	110	107	1	0	0

- Molecule 44 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BD	157	1284	831	240	209	4	0	0

- Molecule 45 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BE	236	1883	1223	336	322	2	0	0

- Molecule 46 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BF	194	1498	951	272	271	4	0	0

- Molecule 47 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	BG	140	1065	685	190	188	2	0	0

- Molecule 48 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	BH	220	1773	1128	325	313	7	0	0

- Molecule 49 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	BI	129	1036	676	177	180	3	0	0

- Molecule 50 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	BJ	130	1007	636	198	172	1	0	0

- Molecule 51 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	BK	134	1058	680	191	182	5	0	0

- Molecule 52 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	BL	38	315	201	64	49	1	0	0

- Molecule 53 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	BM	127	941	592	182	164	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	128	IAS	ASP	conflict	UNP A3MX63

- Molecule 54 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BN	144	Total	C	N	O	S	0	0
			1133	730	211	189	3		

- Molecule 55 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BO	143	Total	C	N	O	S	0	0
			1108	700	211	195	2		

- Molecule 56 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BP	29	Total	C	N	O	S	0	0
			241	150	51	36	4		

- Molecule 57 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BQ	149	Total	C	N	O	S	0	0
			1224	782	233	208	1		

- Molecule 58 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BR	144	Total	C	N	O	S	0	0
			1171	756	216	194	5		

- Molecule 59 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	BS	64	Total	C	N	O	0	0
			517	332	94	91		

- Molecule 60 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BT	135	Total	C	N	O	S	0	0
			1111	720	203	182	6		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	6	ALA	GLN	conflict	UNP A0A831L0N9
BT	19	THR	ALA	conflict	UNP A0A831L0N9
BT	28	SER	THR	conflict	UNP A0A831L0N9
BT	43	PRO	SER	conflict	UNP A0A831L0N9
BT	81	MET	ALA	conflict	UNP A0A831L0N9
BT	93	CYS	SER	conflict	UNP A0A831L0N9
BT	137	ARG	LYS	conflict	UNP A0A831L0N9

- Molecule 61 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	BU	155	1225	789	225	209	2	0	0

- Molecule 62 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
62	BV	115	950	597	185	168	0	0

- Molecule 63 is a protein called SSU ribosomal protein S25E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	BW	68	544	351	96	96	1	0	0

- Molecule 64 is a protein called SSU ribosomal protein S26E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	BX	95	772	490	150	128	4	0	0

- Molecule 65 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	BY	65	501	317	100	79	5	0	0

- Molecule 66 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	BZ	71	552	344	108	99	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BZ	37	ARG	LYS	conflict	UNP B1Y9V2

- Molecule 67 is a protein called SSU ribosomal protein S30E.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
67	Ba	43	357	222	80	55	0	0

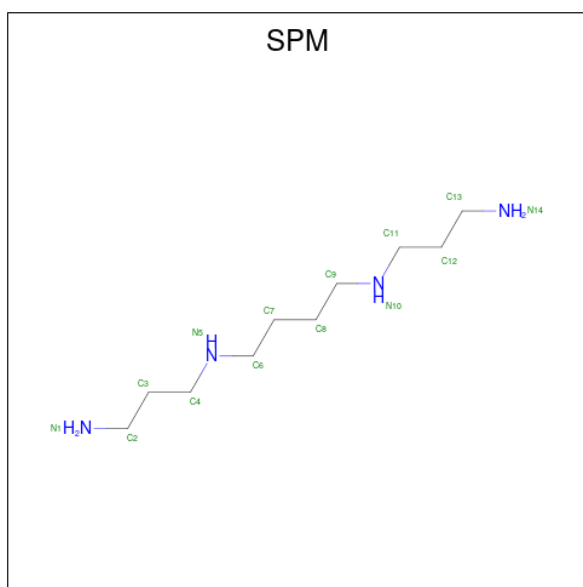
- Molecule 68 is a protein called aS35.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
68	Bb	60	479	301	95	83	0	0

- Molecule 69 is a protein called Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	Bc	64	477	301	90	82	4	0	0

- Molecule 70 is SPERMINE (CCD ID: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	
70	1	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	4	1	Total	C	N	0
			14	10	4	
70	AL	1	Total	C	N	0
			14	10	4	
70	AM	1	Total	C	N	0
			14	10	4	
70	Ah	1	Total	C	N	0
			14	10	4	

- Molecule 71 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
71	1	170	Total	Mg	0
			170	170	
71	4	77	Total	Mg	0
			77	77	
71	AA	1	Total	Mg	0
			1	1	
71	AL	2	Total	Mg	0
			2	2	
71	BK	1	Total	Mg	0
			1	1	

- Molecule 72 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
72	AW	1	Total	Zn	0
			1	1	
72	Ad	1	Total	Zn	0
			1	1	
72	Ag	1	Total	Zn	0
			1	1	
72	Ah	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
72	Ai	1	Total 1	Zn 1	0
72	BF	1	Total 1	Zn 1	0
72	BP	1	Total 1	Zn 1	0
72	BR	1	Total 1	Zn 1	0
72	BX	1	Total 1	Zn 1	0
72	BY	1	Total 1	Zn 1	0
72	Bc	1	Total 1	Zn 1	0

- Molecule 73 is water.

Mol	Chain	Residues	Atoms		AltConf
73	2	94	Total 94	O 94	0
73	3	4	Total 4	O 4	0
73	1	4730	Total 4730	O 4730	0
73	4	1186	Total 1186	O 1186	0
73	AA	13	Total 13	O 13	0
73	AB	4	Total 4	O 4	0
73	AC	7	Total 7	O 7	0
73	AE	1	Total 1	O 1	0
73	AG	1	Total 1	O 1	0
73	AH	1	Total 1	O 1	0
73	AL	11	Total 11	O 11	0
73	AM	5	Total 5	O 5	0

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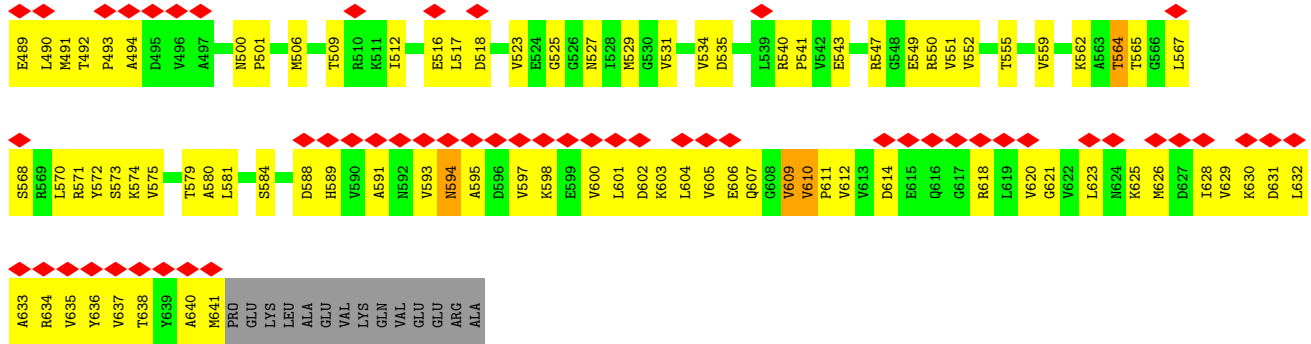
Mol	Chain	Residues	Atoms		AltConf
73	AN	1	Total 1	O 1	0
73	AQ	1	Total 1	O 1	0
73	AS	1	Total 1	O 1	0
73	AT	3	Total 3	O 3	0
73	AW	1	Total 1	O 1	0
73	AY	1	Total 1	O 1	0
73	Ab	7	Total 7	O 7	0
73	Ad	2	Total 2	O 2	0
73	Ag	1	Total 1	O 1	0
73	Ah	1	Total 1	O 1	0
73	BA	27	Total 27	O 27	0
73	BB	13	Total 13	O 13	0
73	BC	13	Total 13	O 13	0
73	BD	16	Total 16	O 16	0
73	BE	10	Total 10	O 10	0
73	BF	17	Total 17	O 17	0
73	BG	18	Total 18	O 18	0
73	BH	18	Total 18	O 18	0
73	BI	16	Total 16	O 16	0
73	BJ	11	Total 11	O 11	0
73	BK	15	Total 15	O 15	0

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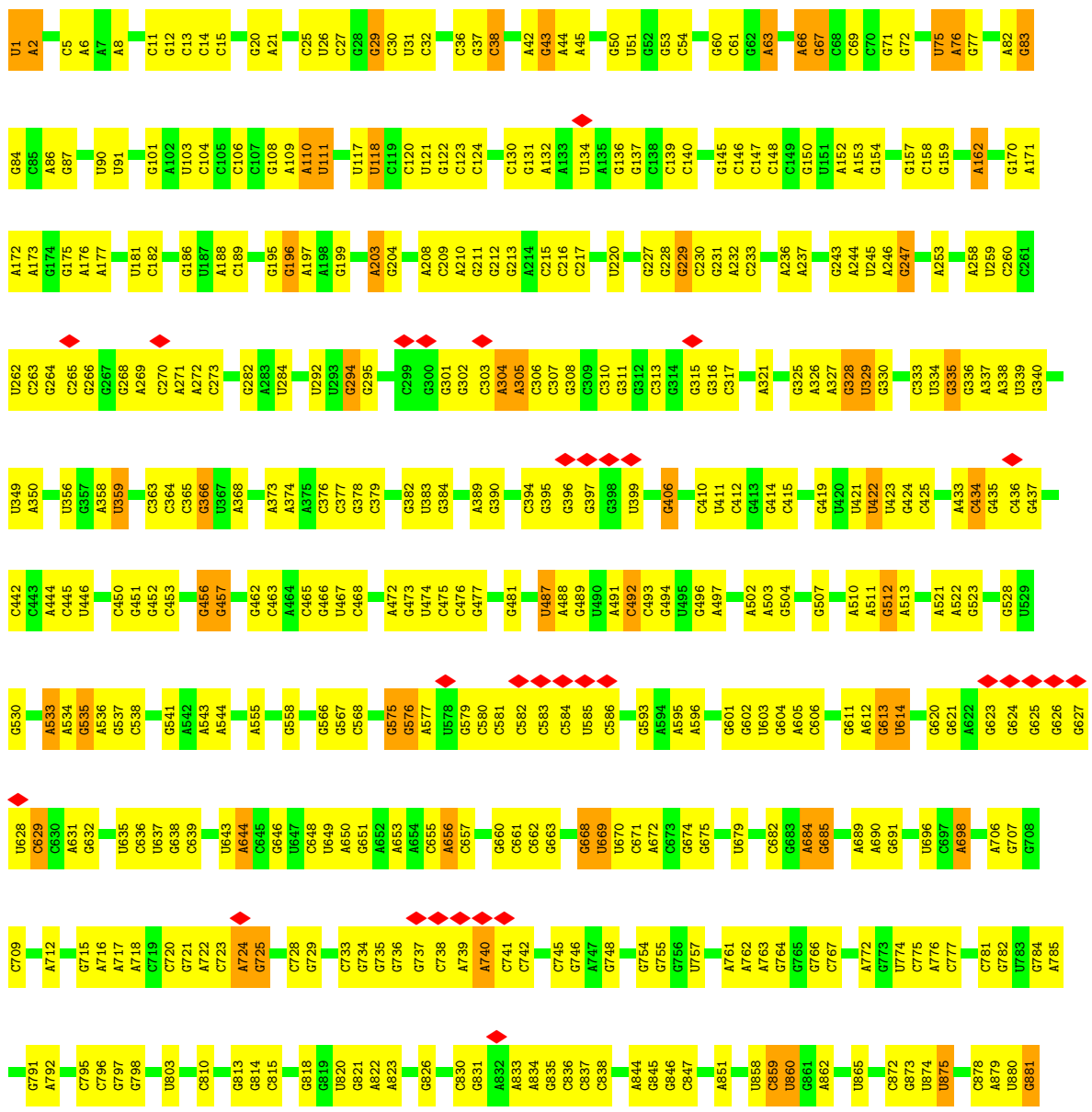
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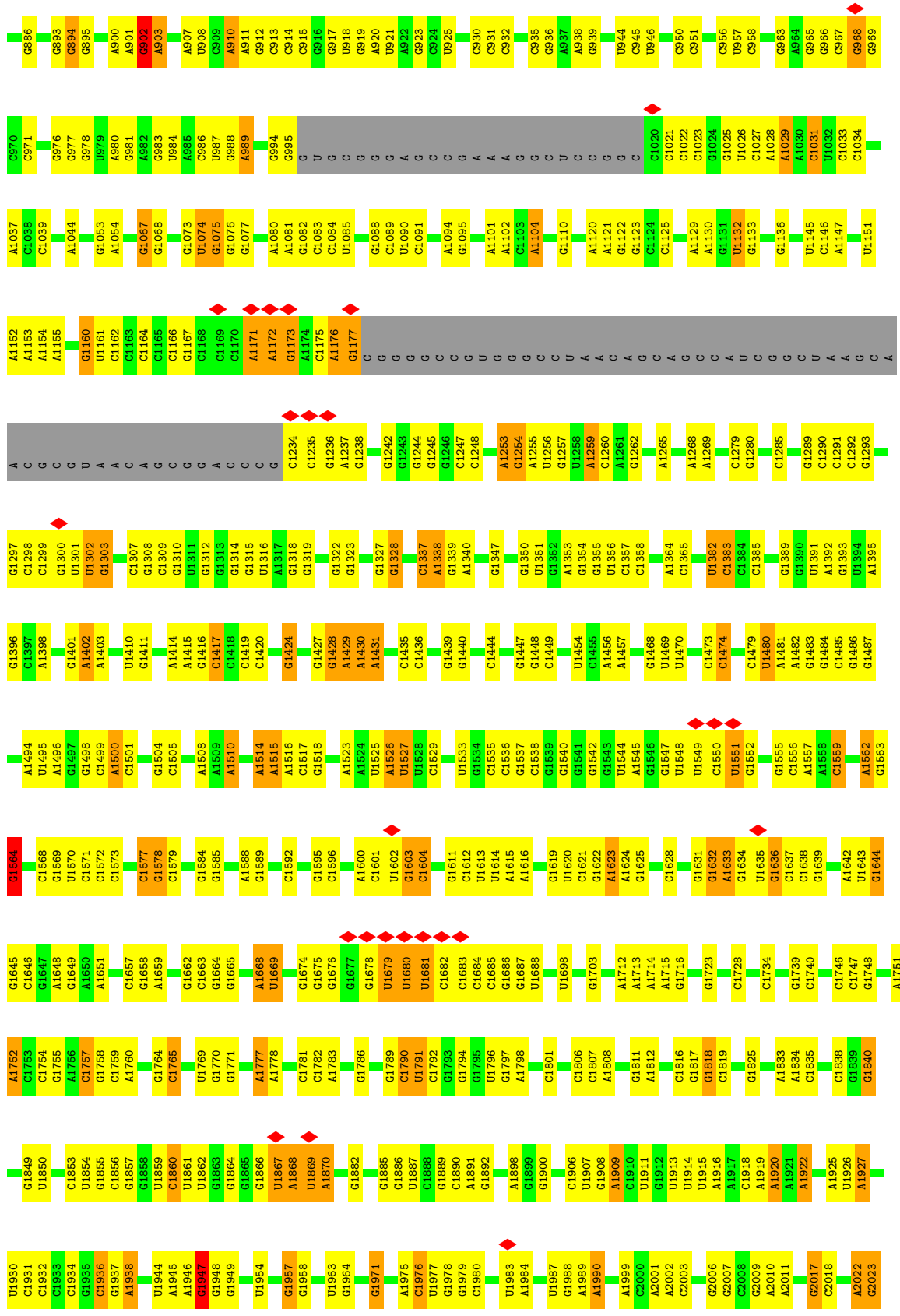
Mol	Chain	Residues	Atoms		AltConf
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73	BM	10	Total 10	O 10	0
73	BN	10	Total 10	O 10	0
73	BO	10	Total 10	O 10	0
73	BP	5	Total 5	O 5	0
73	BQ	6	Total 6	O 6	0
73	BR	9	Total 9	O 9	0
73	BS	4	Total 4	O 4	0
73	BT	12	Total 12	O 12	0
73	BU	11	Total 11	O 11	0
73	BV	3	Total 3	O 3	0
73	BW	11	Total 11	O 11	0
73	BX	7	Total 7	O 7	0
73	BY	6	Total 6	O 6	0
73	BZ	5	Total 5	O 5	0
73	Ba	4	Total 4	O 4	0
73	Bb	11	Total 11	O 11	0
73	Bc	9	Total 9	O 9	0



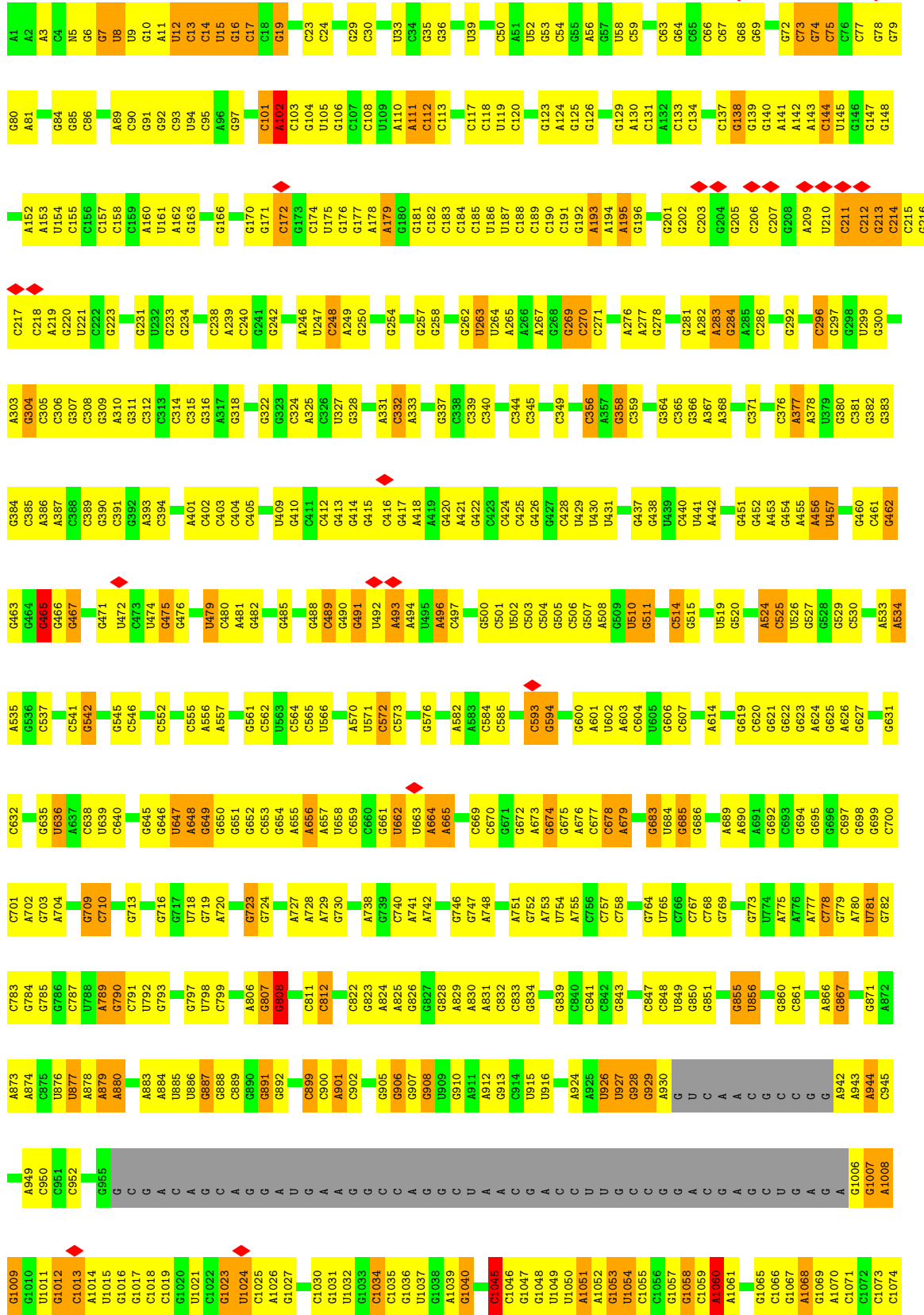


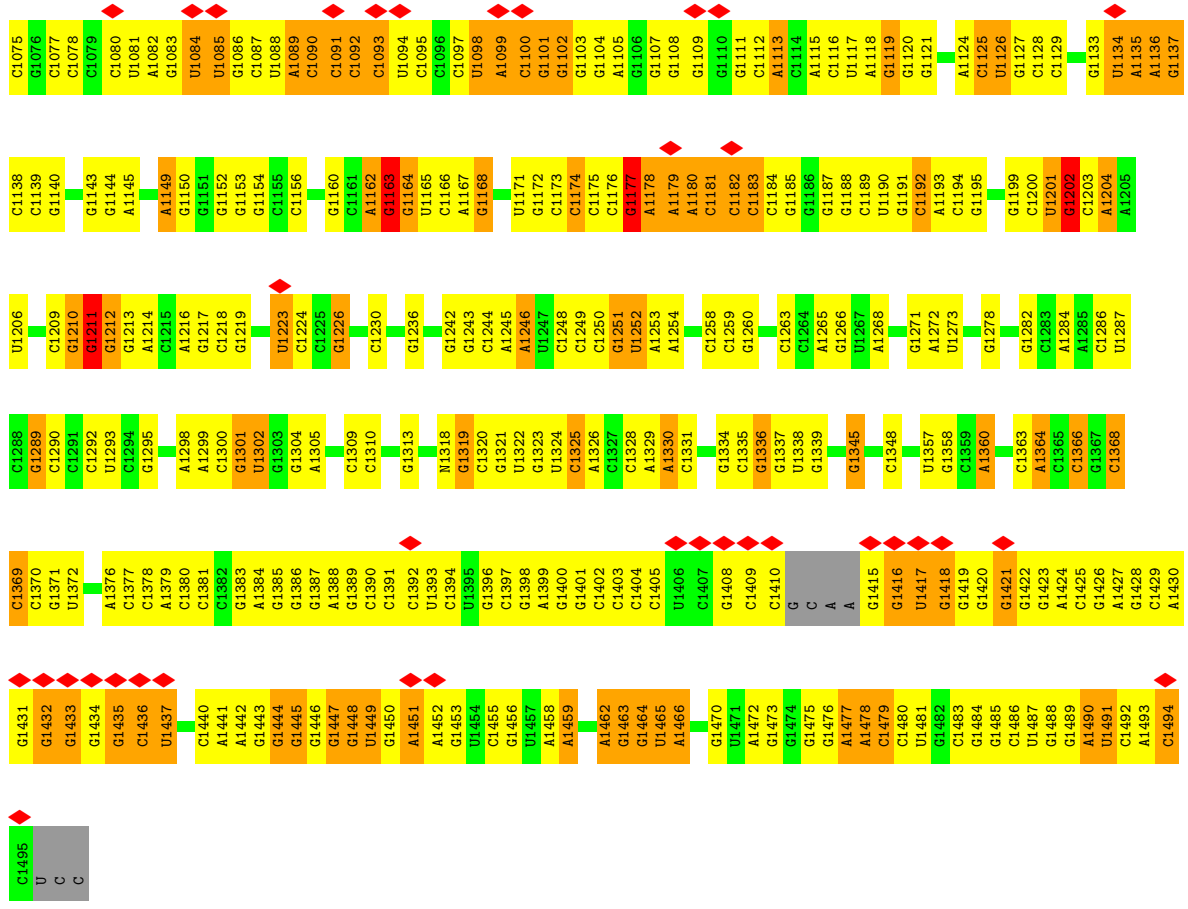
• Molecule 3: 23S rRNA



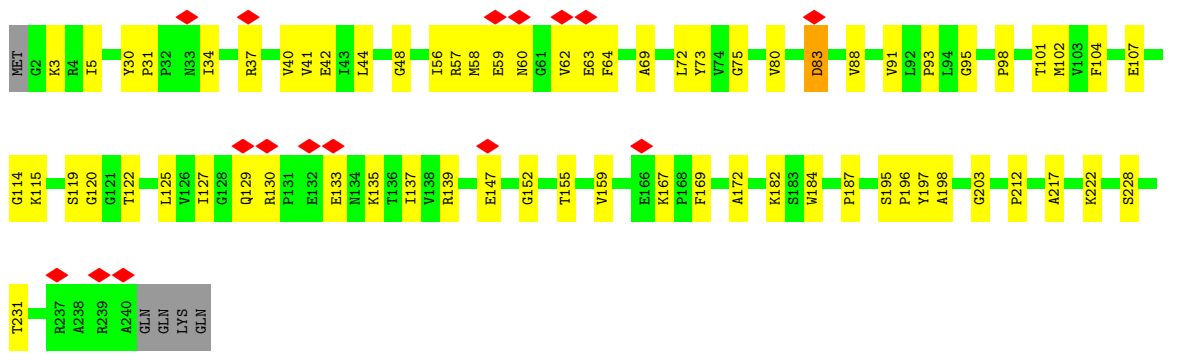
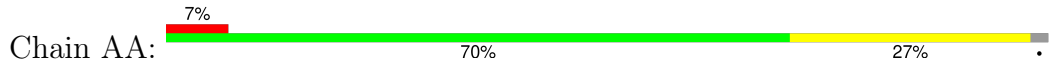




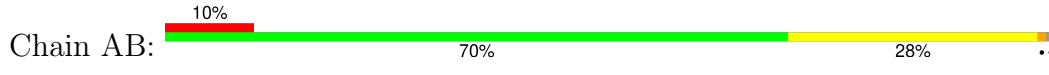


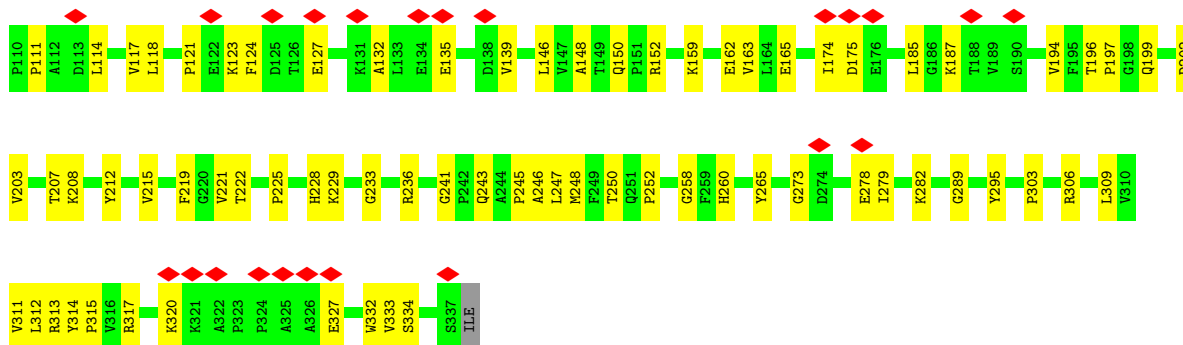


• Molecule 5: Large ribosomal subunit protein uL2

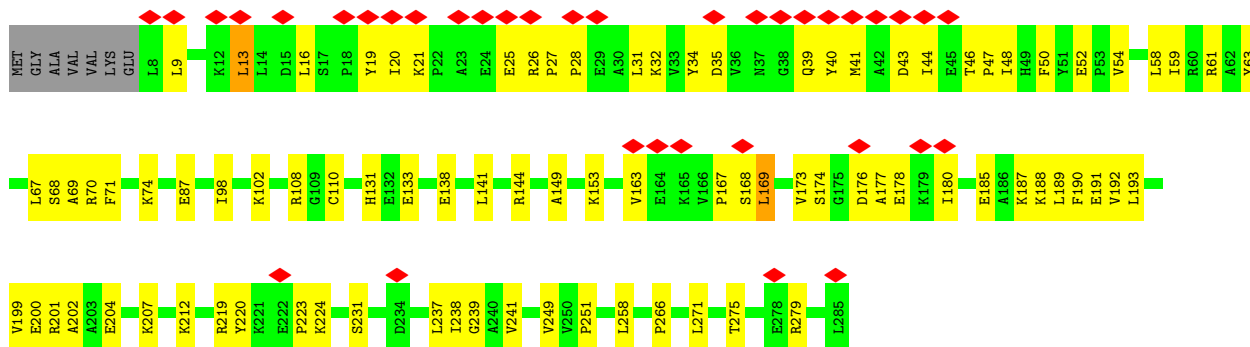


• Molecule 6: Large ribosomal subunit protein uL3

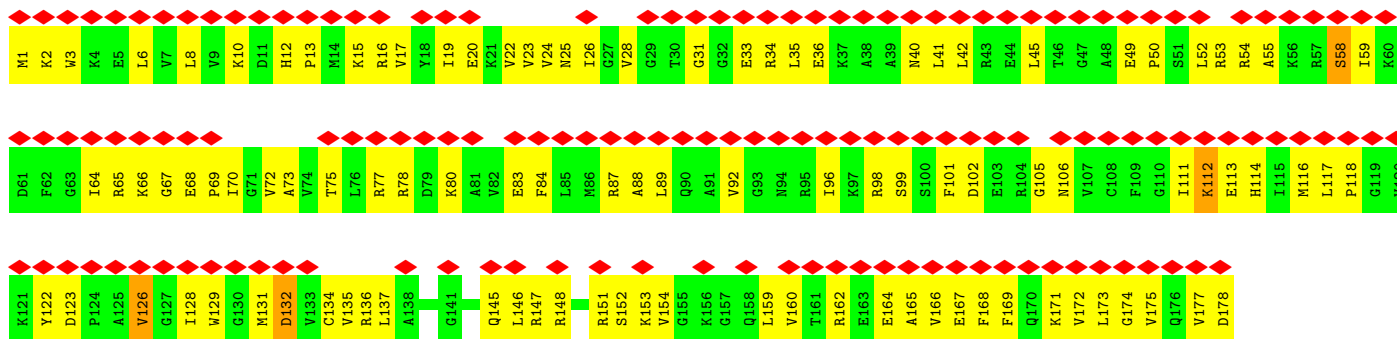
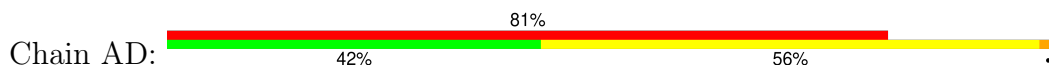




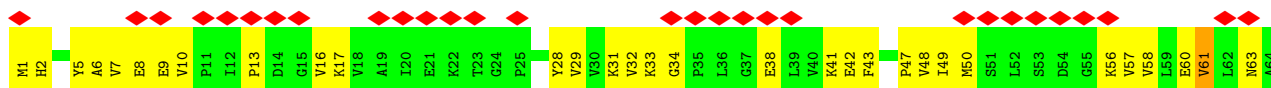
• Molecule 7: Large ribosomal subunit protein uL4

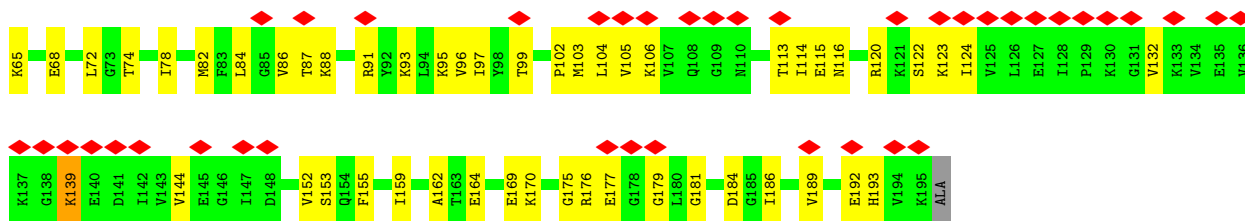


• Molecule 8: Large ribosomal subunit protein uL5

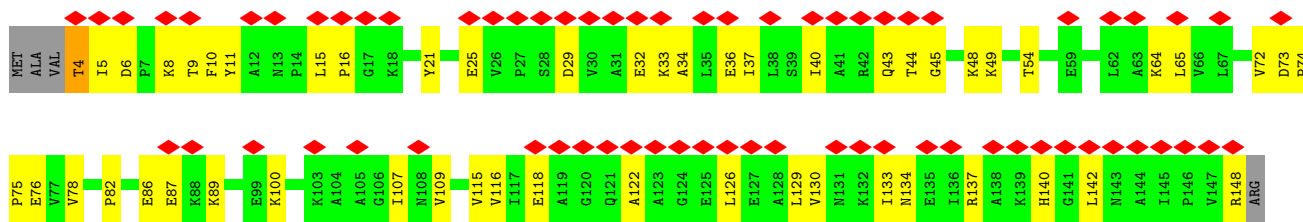


• Molecule 9: Large ribosomal subunit protein uL6

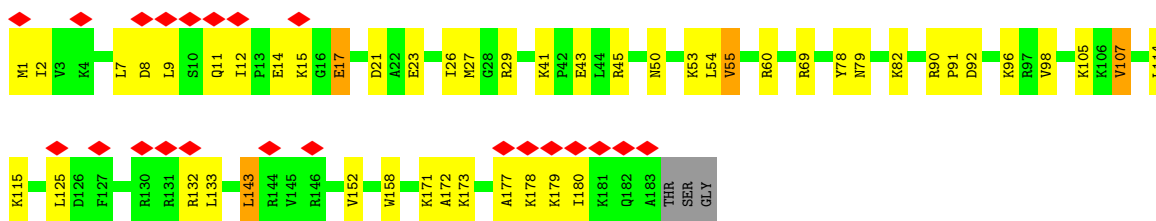
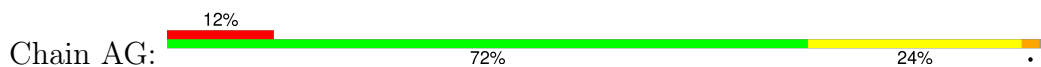




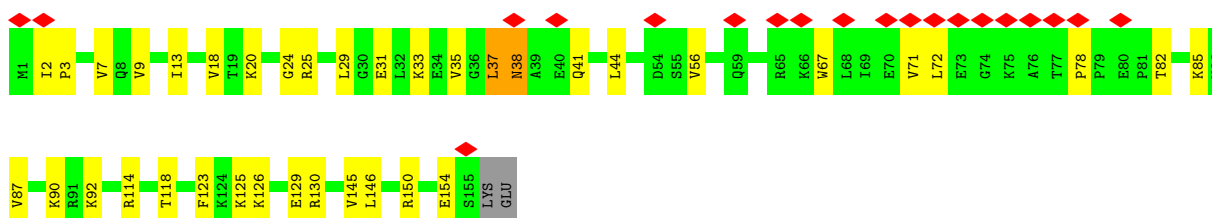
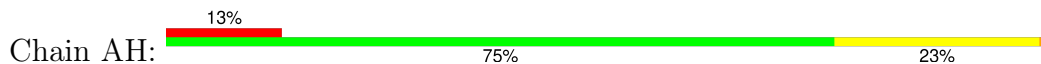
- Molecule 10: Large ribosomal subunit protein eL8



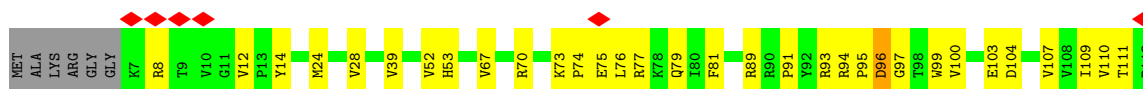
- Molecule 11: Large ribosomal subunit protein uL13



- Molecule 12: Large ribosomal subunit protein eL13

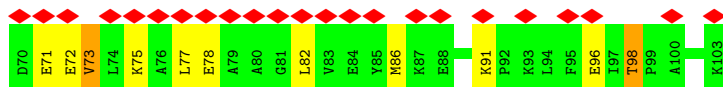
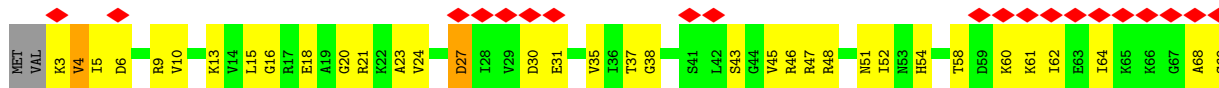
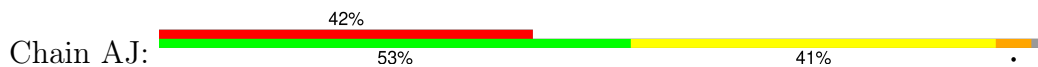


- Molecule 13: Large ribosomal subunit protein uL14

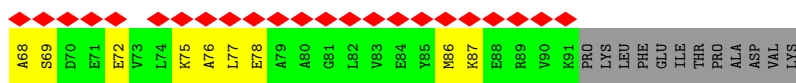
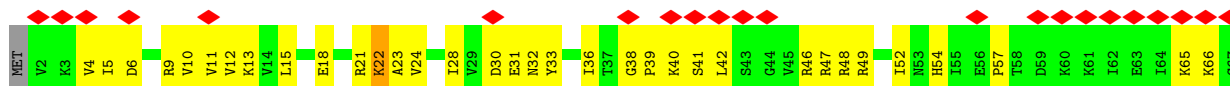
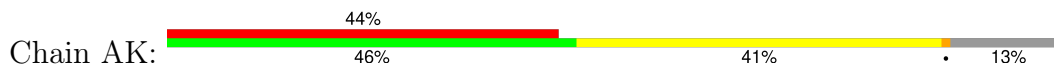




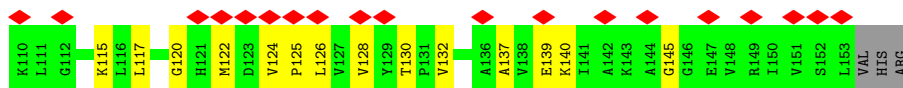
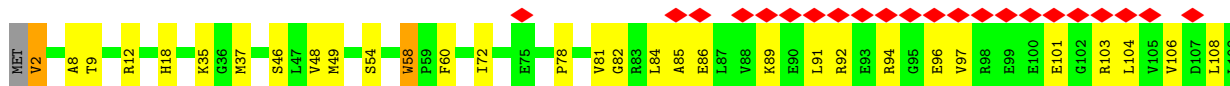
• Molecule 14: Large ribosomal subunit protein eL14



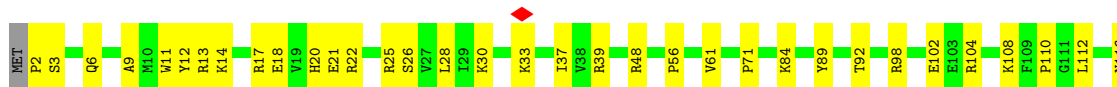
• Molecule 14: Large ribosomal subunit protein eL14



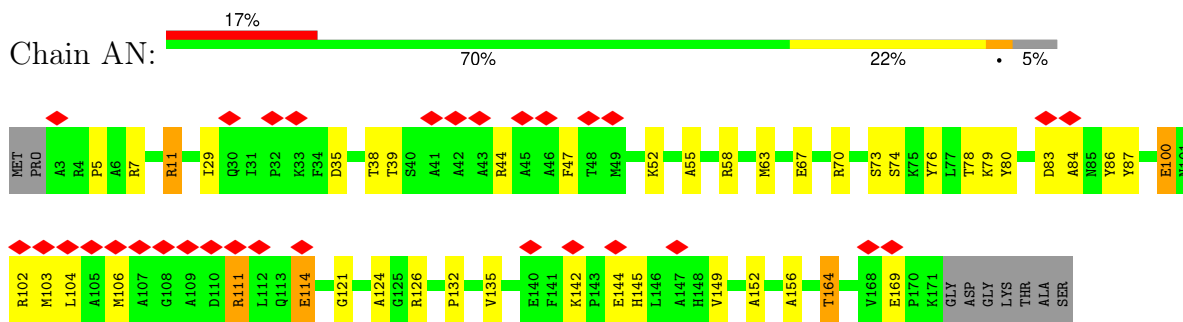
• Molecule 15: Large ribosomal subunit protein uL15



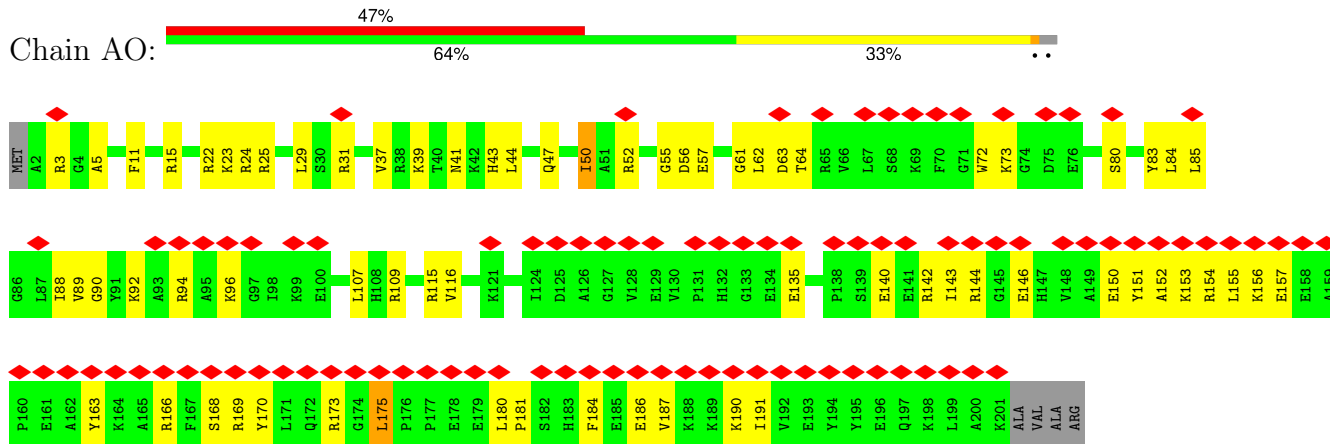
• Molecule 16: 50S ribosomal protein L15e



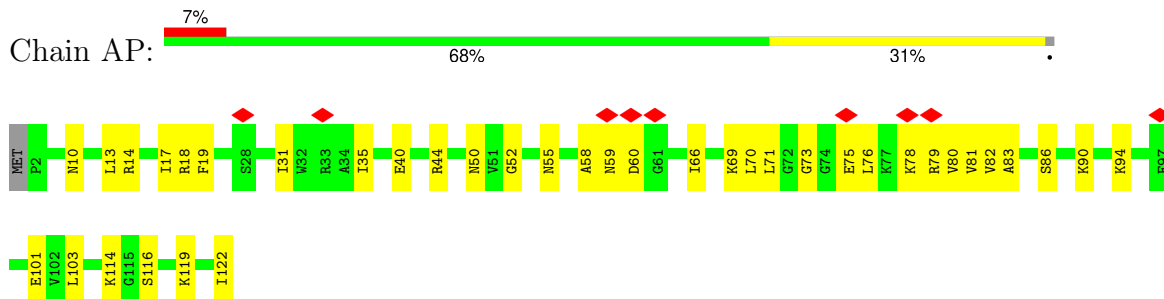
• Molecule 17: Large ribosomal subunit protein uL16



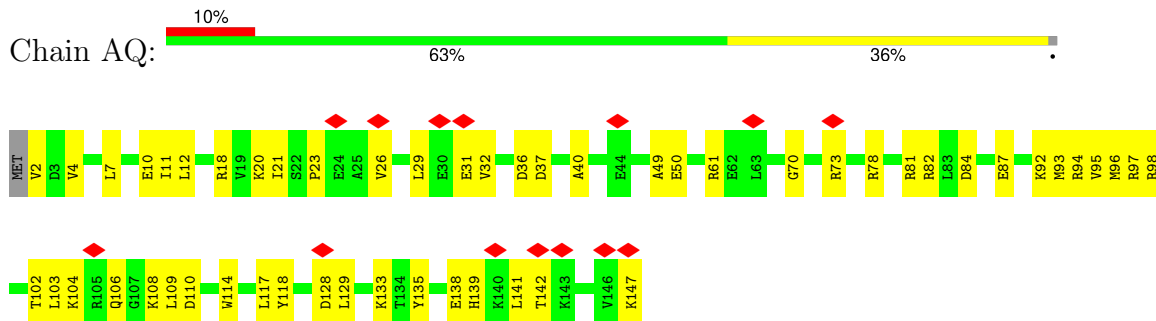
• Molecule 18: Large ribosomal subunit protein uL18



• Molecule 19: Large ribosomal subunit protein eL18

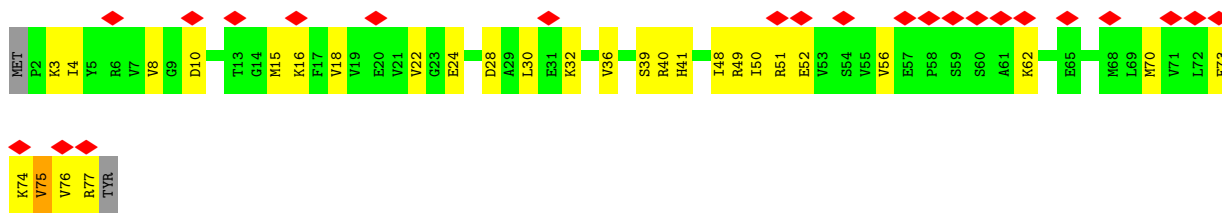


• Molecule 20: Large ribosomal subunit protein eL19

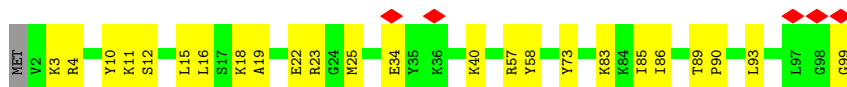
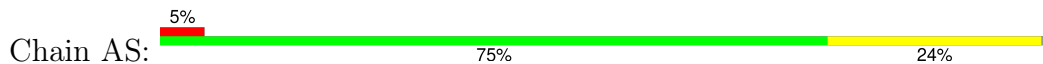


• Molecule 21: Large ribosomal subunit protein eL20

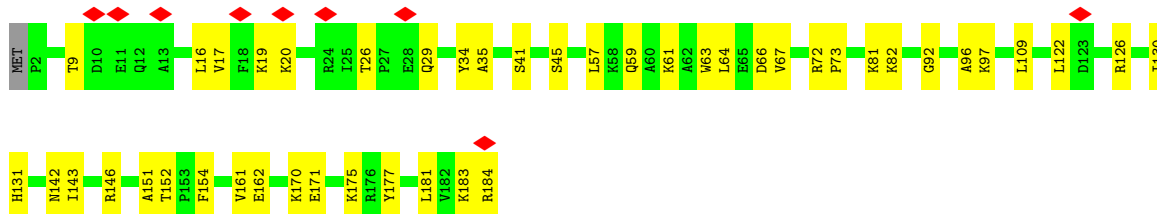
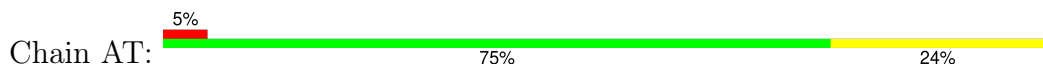




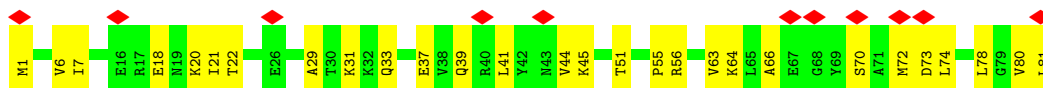
• Molecule 22: Large ribosomal subunit protein eL21



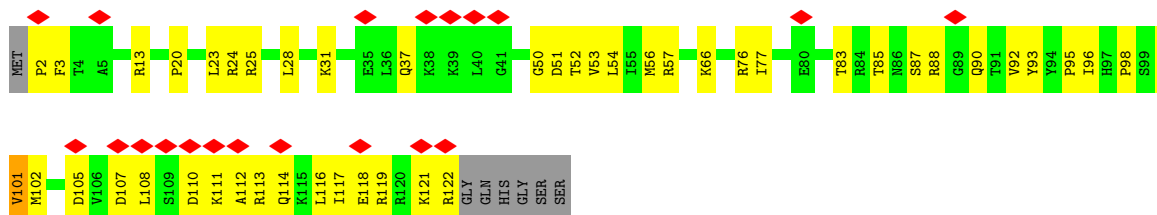
• Molecule 23: Large ribosomal subunit protein uL22



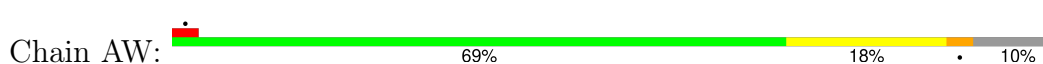
• Molecule 24: Large ribosomal subunit protein uL23



• Molecule 25: Large ribosomal subunit protein uL24

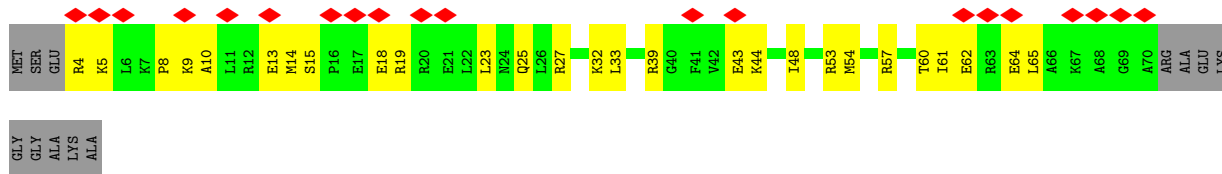


• Molecule 26: Large ribosomal subunit protein eL24

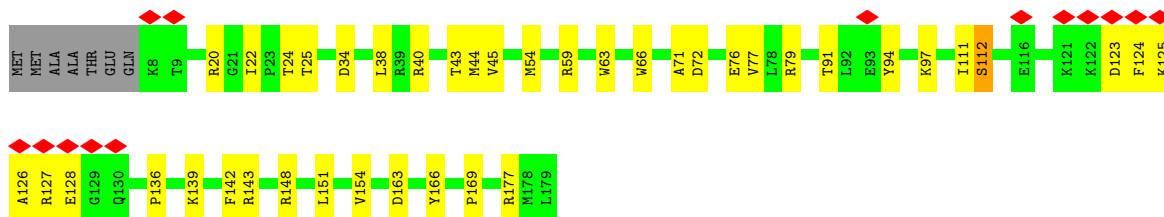
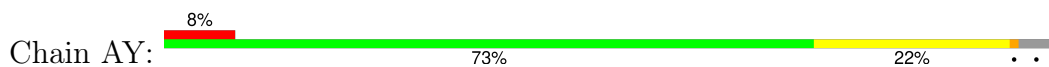




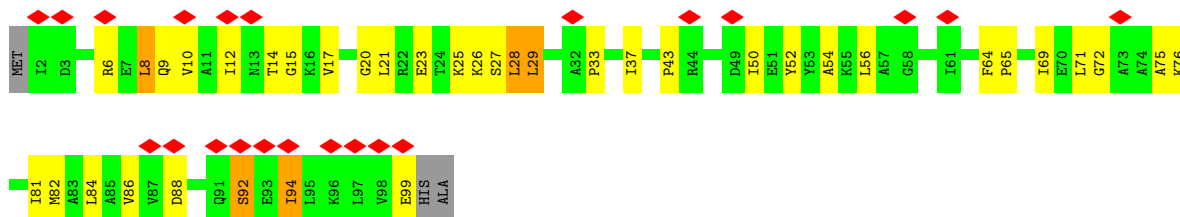
• Molecule 27: Large ribosomal subunit protein uL29



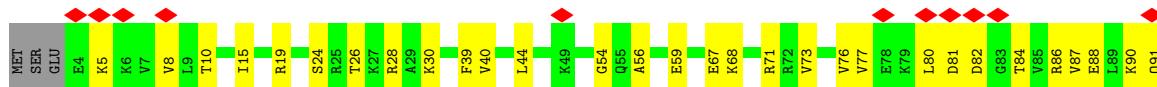
• Molecule 28: Large ribosomal subunit protein uL30



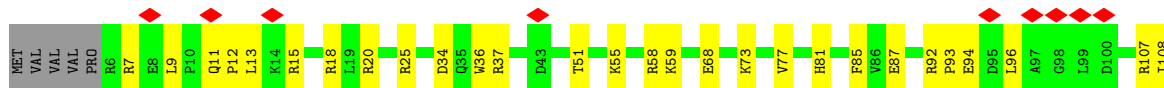
• Molecule 29: Large ribosomal subunit protein eL30



• Molecule 30: Large ribosomal subunit protein eL31



• Molecule 31: Large ribosomal subunit protein eL32

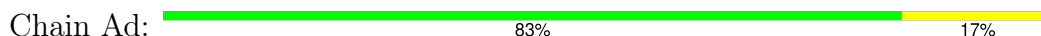




- Molecule 32: Large ribosomal subunit protein eL34



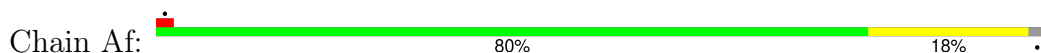
- Molecule 33: Large ribosomal subunit protein eL37



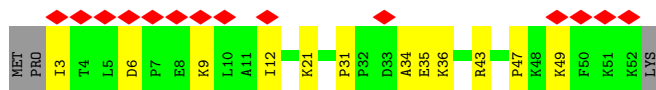
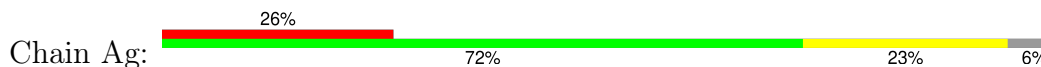
- Molecule 34: LSU ribosomal protein L38E



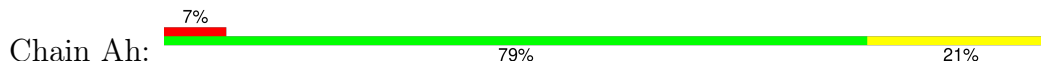
- Molecule 35: Large ribosomal subunit protein eL39



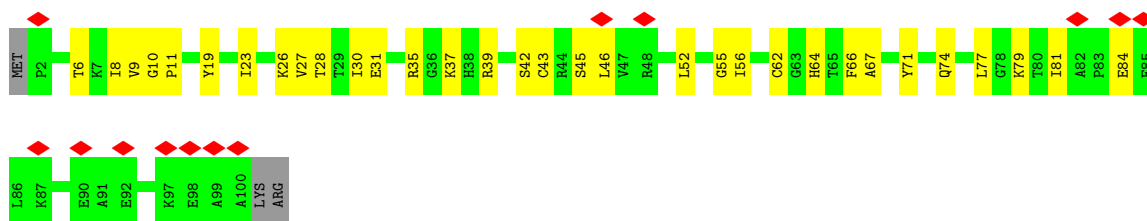
- Molecule 36: Large ribosomal subunit protein eL40



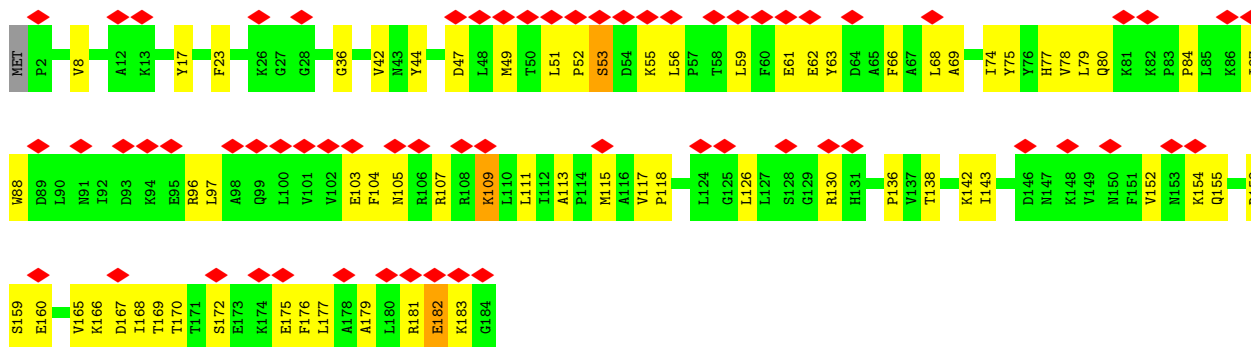
- Molecule 37: eL42



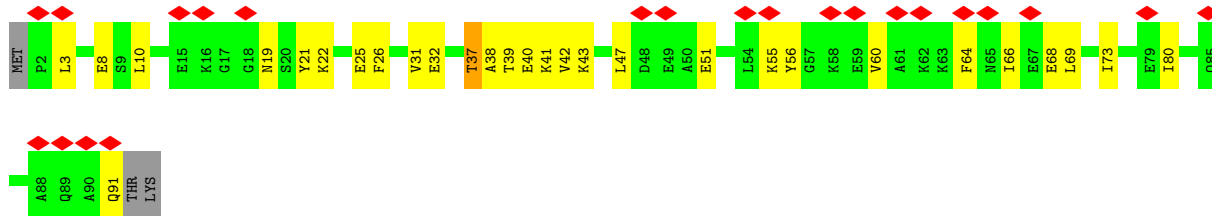
- Molecule 38: Large ribosomal subunit protein eL43



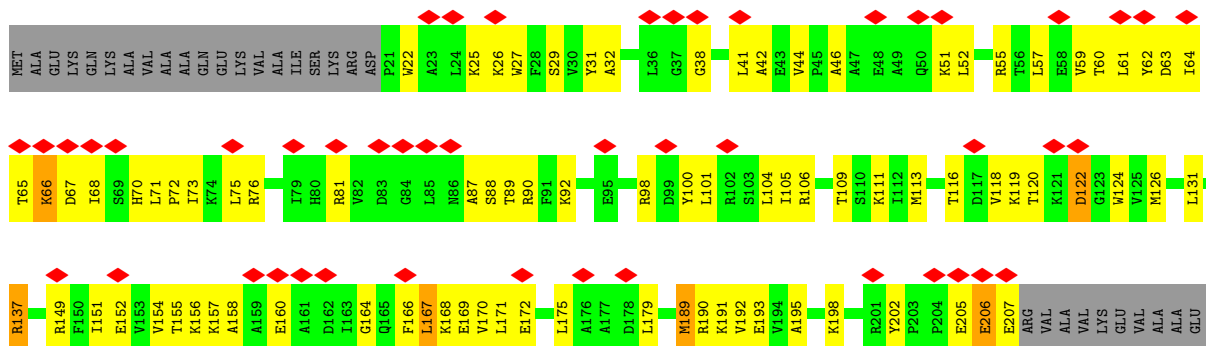
• Molecule 39: DJ-1/PfpI domain-containing protein



• Molecule 40: PaREP1 domain containing protein

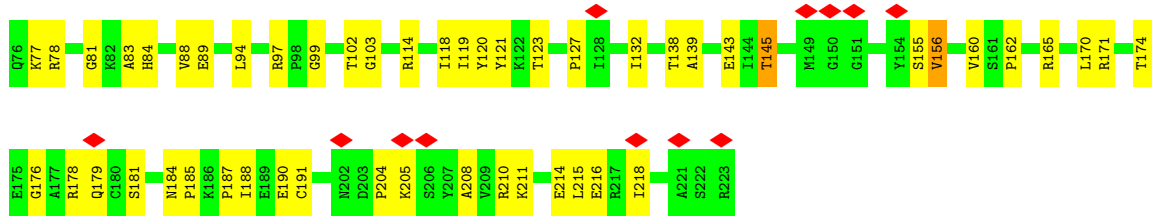


• Molecule 41: Small ribosomal subunit protein eS1

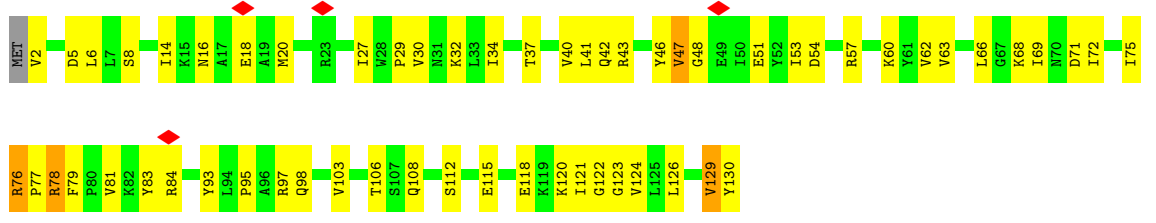




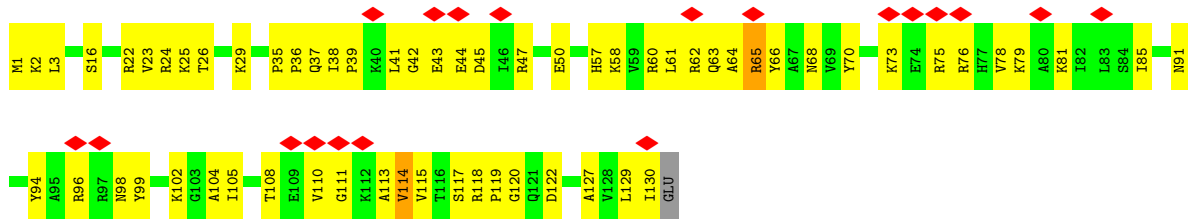




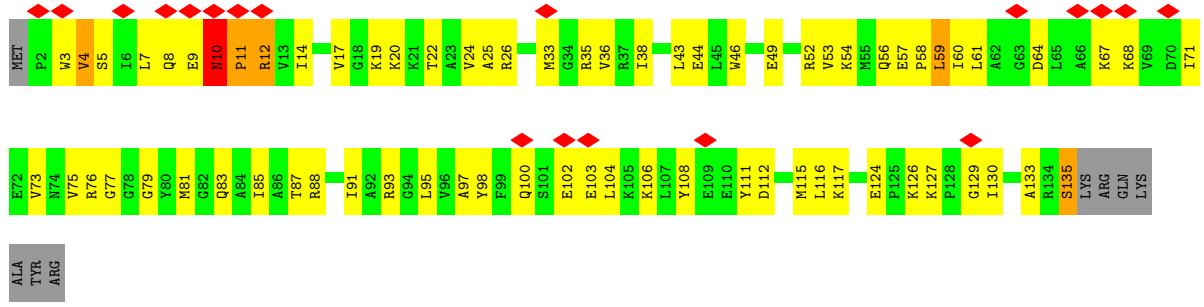
• Molecule 49: Small ribosomal subunit protein uS8



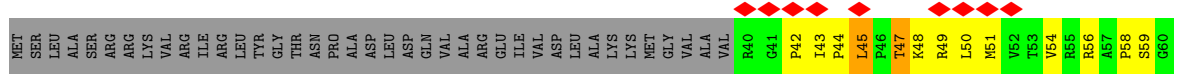
• Molecule 50: Small ribosomal subunit protein eS8

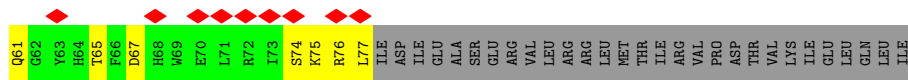


• Molecule 51: Small ribosomal subunit protein uS9

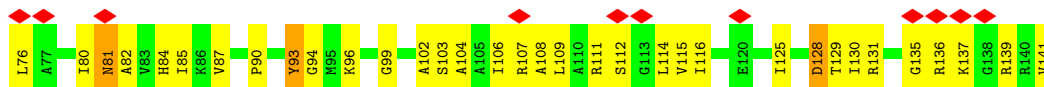
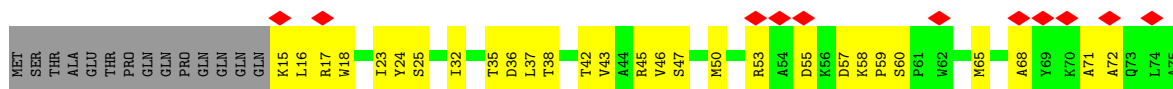


• Molecule 52: Small ribosomal subunit protein uS10





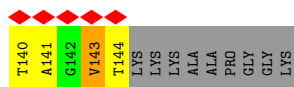
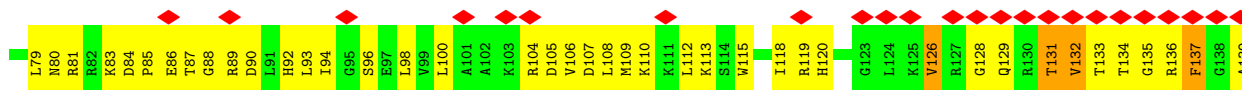
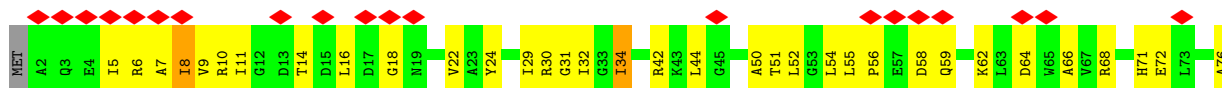
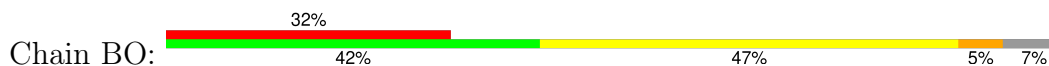
• Molecule 53: Small ribosomal subunit protein uS11



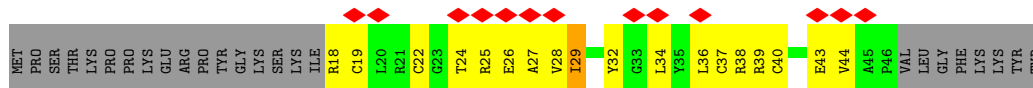
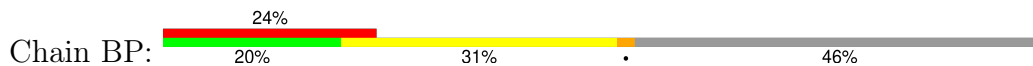
• Molecule 54: Small ribosomal subunit protein uS12



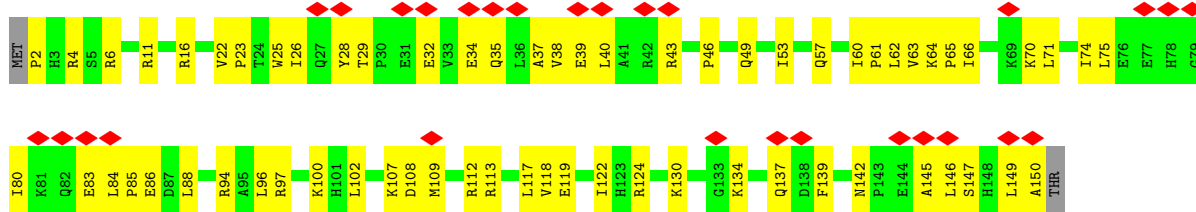
• Molecule 55: Small ribosomal subunit protein uS13



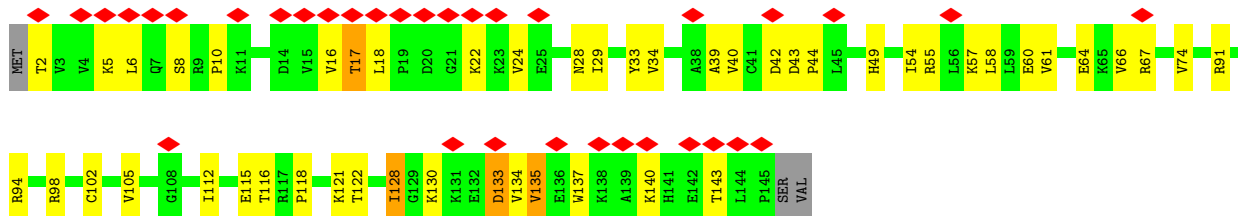
• Molecule 56: Small ribosomal subunit protein uS14



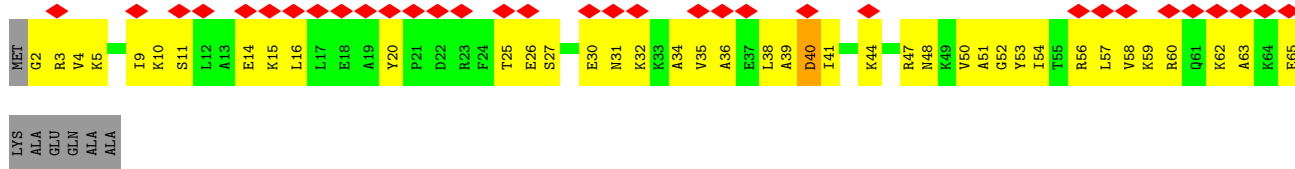
• Molecule 57: Small ribosomal subunit protein uS15



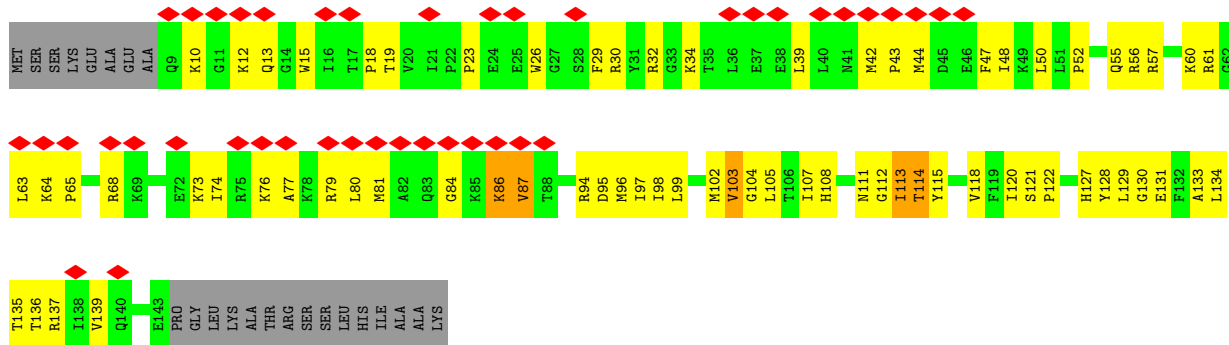
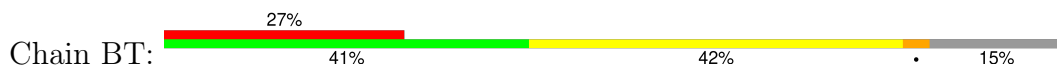
• Molecule 58: Small ribosomal subunit protein uS17



• Molecule 59: Small ribosomal subunit protein eS17

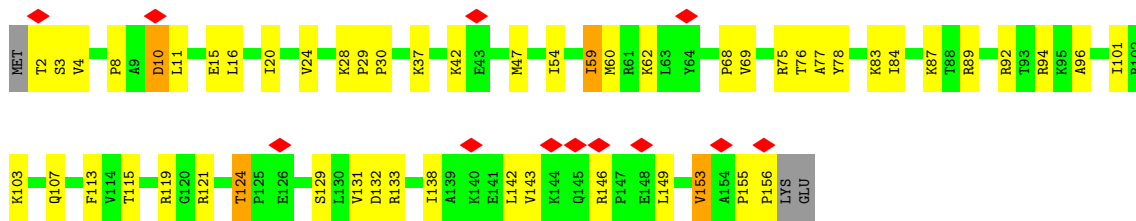


• Molecule 60: Small ribosomal subunit protein uS19

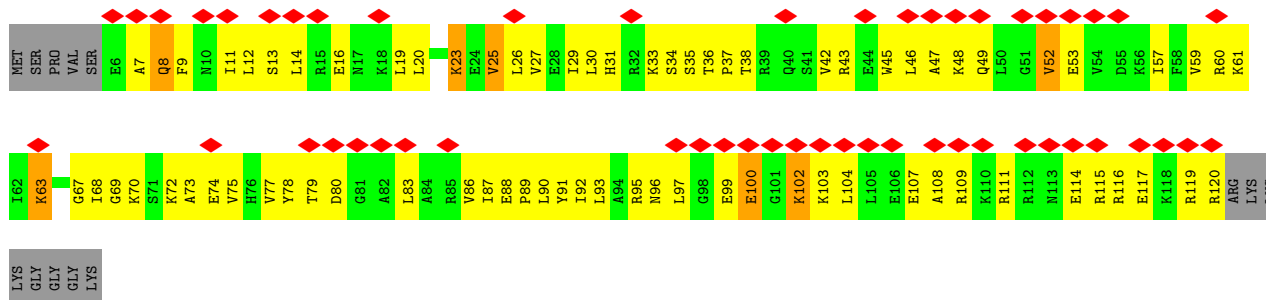


• Molecule 61: Small ribosomal subunit protein eS19

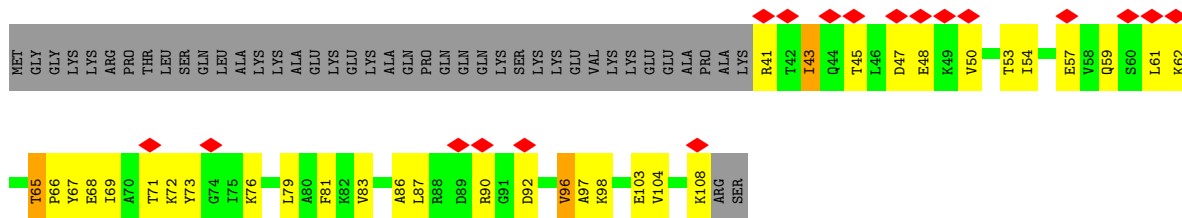




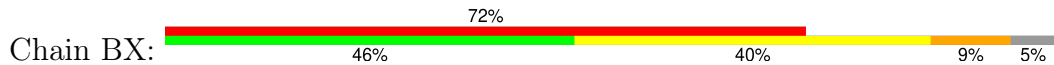
• Molecule 62: Small ribosomal subunit protein eS24



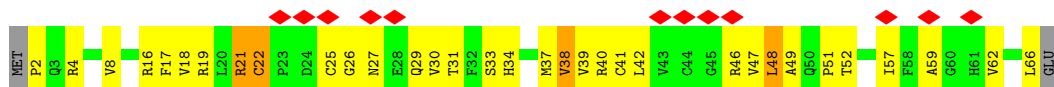
• Molecule 63: SSU ribosomal protein S25E



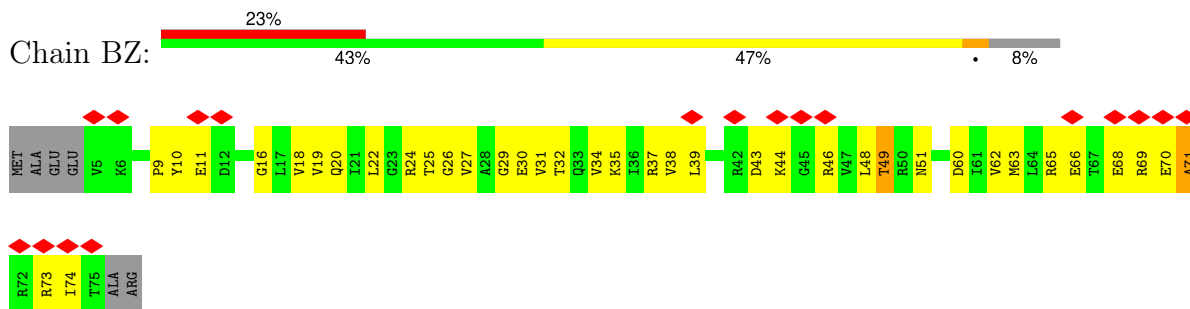
• Molecule 64: SSU ribosomal protein S26E



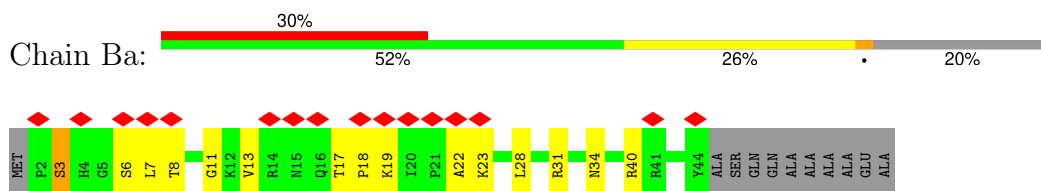
• Molecule 65: Small ribosomal subunit protein eS27



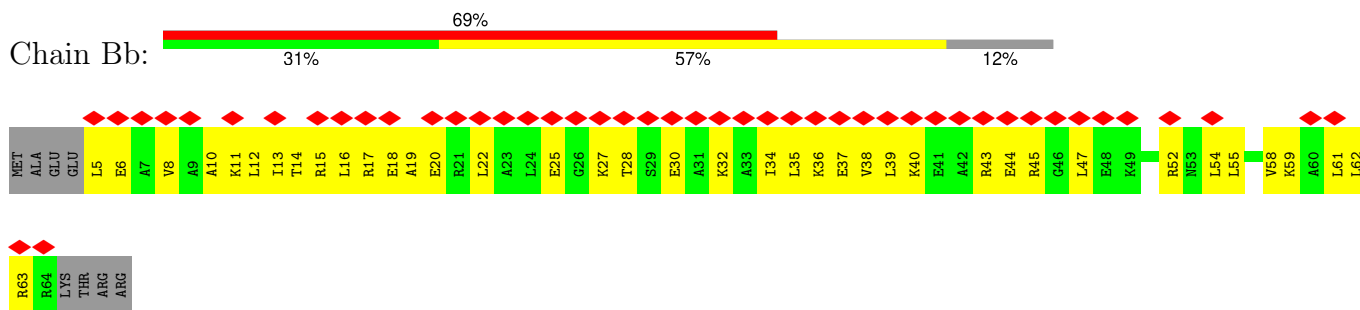
• Molecule 66: Small ribosomal subunit protein eS28



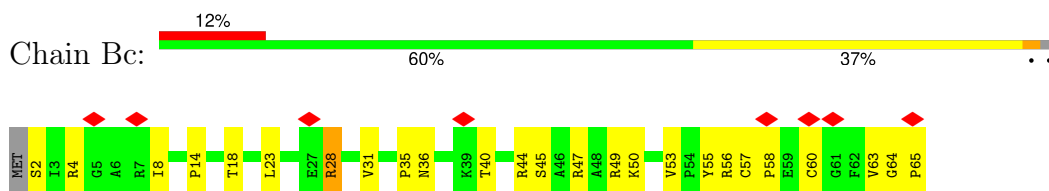
• Molecule 67: SSU ribosomal protein S30E



• Molecule 68: aS35



• Molecule 69: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.070	Depositor
Minimum map value	-0.389	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.188	Depositor
Map size ( $\text{\AA}$ )	504.2144, 504.2144, 504.2144	wwPDB
Map dimensions	608, 608, 608	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8293, 0.8293, 0.8293	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: PSU, G7M, IAS, OMC, SPM, 4AC, MG, 5MC, MA6, OMU, UR3, B8T, A2M, 6MZ, ZN, OMG, M7A

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	2	0.23	0/3096	0.36	2/4830 (0.0%)
2	3	0.28	0/2279	0.50	0/3084
3	1	0.32	1/67134 (0.0%)	0.35	11/104802 (0.0%)
4	4	0.34	2/33464 (0.0%)	0.39	15/52215 (0.0%)
5	AA	0.29	0/1847	0.44	0/2489
6	AB	0.27	0/2678	0.36	0/3643
7	AC	0.26	0/2234	0.40	0/3024
8	AD	0.19	0/1431	0.43	0/1913
9	AE	0.23	0/1548	0.41	1/2087 (0.0%)
10	AF	0.20	0/1114	0.38	0/1513
11	AG	0.26	0/1542	0.36	0/2076
12	AH	0.23	0/1265	0.35	0/1692
13	AI	0.29	0/1093	0.39	0/1487
14	AJ	0.25	0/795	0.48	0/1068
14	AK	0.27	0/704	0.44	0/944
15	AL	0.25	0/1225	0.40	0/1639
16	AM	0.24	0/1594	0.34	0/2138
17	AN	0.23	0/1365	0.34	0/1841
18	AO	0.20	0/1647	0.37	0/2212
19	AP	0.24	0/933	0.35	0/1263
20	AQ	0.25	0/1233	0.31	0/1645
21	AR	0.22	0/610	0.35	0/817
22	AS	0.25	0/805	0.36	0/1081
23	AT	0.24	0/1536	0.33	0/2075
24	AU	0.28	0/655	0.42	0/877
25	AV	0.25	0/990	0.39	0/1325
26	AW	0.27	0/460	0.33	0/613
27	AX	0.21	0/557	0.29	0/738
28	AY	0.29	0/1407	0.40	0/1905
29	AZ	0.24	0/754	0.42	0/1021
30	Aa	0.25	0/735	0.34	0/986

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	Ab	0.24	0/1209	0.39	0/1621
32	Ac	0.24	0/663	0.37	0/889
33	Ad	0.28	0/442	0.33	0/587
34	Ae	0.25	0/562	0.38	0/753
35	Af	0.24	0/423	0.31	0/566
36	Ag	0.23	0/424	0.40	0/564
37	Ah	0.24	0/753	0.32	0/1001
38	Ai	0.28	0/788	0.44	0/1057
39	Aj	0.24	0/1497	0.43	0/2029
40	Ak	0.22	0/754	0.36	0/1005
41	BA	0.26	0/1515	0.42	0/2043
42	BB	0.29	0/1638	0.47	2/2221 (0.1%)
43	BC	0.27	0/620	0.67	0/831
44	BD	0.25	0/1308	0.40	0/1755
45	BE	0.29	0/1929	0.44	0/2621
46	BF	0.28	0/1522	0.40	2/2059 (0.1%)
47	BG	0.23	0/1087	0.47	0/1465
48	BH	0.30	0/1809	0.45	0/2444
49	BI	0.37	0/1055	0.51	0/1425
50	BJ	0.26	0/1023	0.34	0/1370
51	BK	0.34	0/1079	0.56	1/1452 (0.1%)
52	BL	0.26	0/324	0.61	2/437 (0.5%)
53	BM	0.27	0/951	0.44	1/1288 (0.1%)
54	BN	0.30	0/1157	0.47	0/1551
55	BO	0.26	0/1125	0.45	1/1518 (0.1%)
56	BP	0.28	0/244	0.78	0/324
57	BQ	0.27	0/1254	0.36	0/1692
58	BR	0.29	0/1200	0.35	0/1629
59	BS	0.27	0/524	0.63	1/698 (0.1%)
60	BT	0.27	0/1139	0.47	0/1533
61	BU	0.30	0/1253	0.42	0/1695
62	BV	0.24	0/960	0.47	1/1280 (0.1%)
63	BW	0.28	0/551	0.48	0/741
64	BX	0.27	0/787	0.66	1/1054 (0.1%)
65	BY	0.27	0/511	0.36	0/689
66	BZ	0.30	0/555	0.67	0/745
67	Ba	0.24	0/364	0.38	0/486
68	Bb	0.24	0/478	0.61	0/634
69	Bc	0.24	0/491	0.41	0/670
All	All	0.30	3/174698 (0.0%)	0.39	41/257465 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
41	BA	0	1
43	BC	0	1
49	BI	0	2
51	BK	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	496	A2M	O3'-P	5.25	1.61	1.56
3	1	1990	A2M	O3'-P	5.23	1.61	1.56
4	4	880	A2M	O3'-P	5.12	1.61	1.56

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	101	C	OP1-P-O3'	-11.32	74.04	108.00
1	2	1	G	OP1-P-O3'	-9.21	80.38	108.00
4	4	1078	C	OP1-P-O3'	-9.19	80.44	108.00
3	1	2952	U	OP2-P-O3'	-9.06	80.82	108.00
4	4	808	G	OP1-P-O3'	-9.04	80.86	108.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	BA	66	LYS	Peptide
43	BC	184	GLY	Peptide
49	BI	76	ARG	Sidechain
49	BI	78	ARG	Sidechain
51	BK	12	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2769	0	1405	50	0
2	3	2251	0	2337	188	0
3	1	61386	0	31066	1027	0
4	4	30817	0	15598	768	0
5	AA	1803	0	1849	52	0
6	AB	2611	0	2737	75	0
7	AC	2178	0	2263	61	0
8	AD	1412	0	1511	106	0
9	AE	1520	0	1607	69	0
10	AF	1095	0	1156	44	0
11	AG	1510	0	1627	42	0
12	AH	1244	0	1346	42	0
13	AI	1068	0	1110	39	0
14	AJ	788	0	853	52	0
14	AK	700	0	760	40	0
15	AL	1198	0	1233	40	0
16	AM	1558	0	1641	45	0
17	AN	1336	0	1378	34	0
18	AO	1615	0	1688	66	0
19	AP	920	0	1010	24	0
20	AQ	1214	0	1272	40	0
21	AR	603	0	647	27	0
22	AS	788	0	832	16	0
23	AT	1496	0	1575	31	0
24	AU	651	0	720	28	0
25	AV	976	0	1073	32	0
26	AW	449	0	465	13	0
27	AX	554	0	613	21	0
28	AY	1374	0	1423	27	0
29	AZ	742	0	796	32	0
30	Aa	726	0	794	21	0
31	Ab	1183	0	1270	34	0
32	Ac	649	0	698	23	0
33	Ad	429	0	430	7	0
34	Ae	552	0	592	25	0
35	Af	415	0	464	9	0
36	Ag	417	0	440	11	0
37	Ah	739	0	782	18	0
38	Ai	769	0	792	30	0
39	Aj	1469	0	1535	56	0
40	Ak	743	0	775	20	0
41	BA	1487	0	1589	77	0
42	BB	1600	0	1645	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BC	611	0	648	47	0
44	BD	1284	0	1391	53	0
45	BE	1883	0	1968	72	0
46	BF	1498	0	1557	74	0
47	BG	1065	0	1139	80	0
48	BH	1773	0	1828	66	0
49	BI	1036	0	1090	45	0
50	BJ	1007	0	1086	53	0
51	BK	1058	0	1123	76	0
52	BL	315	0	329	23	0
53	BM	941	0	984	61	0
54	BN	1133	0	1203	38	0
55	BO	1108	0	1163	71	0
56	BP	241	0	251	21	0
57	BQ	1224	0	1287	52	0
58	BR	1171	0	1244	47	0
59	BS	517	0	560	37	0
60	BT	1111	0	1170	61	0
61	BU	1225	0	1301	43	0
62	BV	950	0	1013	81	0
63	BW	544	0	587	27	0
64	BX	772	0	827	54	0
65	BY	501	0	524	24	0
66	BZ	552	0	594	40	0
67	Ba	357	0	394	19	0
68	Bb	479	0	545	47	0
69	Bc	477	0	479	31	0
70	1	602	0	1117	19	0
70	4	252	0	468	9	0
70	AL	14	0	26	2	0
70	AM	14	0	26	0	0
70	Ah	14	0	26	0	0
71	1	170	0	0	0	0
71	4	77	0	0	0	0
71	AA	1	0	0	0	0
71	AL	2	0	0	0	0
71	BK	1	0	0	0	0
72	AW	1	0	0	0	0
72	Ad	1	0	0	0	0
72	Ag	1	0	0	0	0
72	Ah	1	0	0	0	0
72	Ai	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	BF	1	0	0	0	0
72	BP	1	0	0	0	0
72	BR	1	0	0	0	0
72	BX	1	0	0	0	0
72	BY	1	0	0	0	0
72	Bc	1	0	0	0	0
73	1	4730	0	0	153	0
73	2	94	0	0	3	0
73	3	4	0	0	3	0
73	4	1186	0	0	46	0
73	AA	13	0	0	0	0
73	AB	4	0	0	1	0
73	AC	7	0	0	0	0
73	AE	1	0	0	0	0
73	AG	1	0	0	0	0
73	AH	1	0	0	0	0
73	AL	11	0	0	1	0
73	AM	5	0	0	0	0
73	AN	1	0	0	0	0
73	AQ	1	0	0	0	0
73	AS	1	0	0	0	0
73	AT	3	0	0	0	0
73	AW	1	0	0	0	0
73	AY	1	0	0	0	0
73	Ab	7	0	0	0	0
73	Ad	2	0	0	0	0
73	Ag	1	0	0	0	0
73	Ah	1	0	0	0	0
73	BA	27	0	0	10	0
73	BB	13	0	0	1	0
73	BC	13	0	0	7	0
73	BD	16	0	0	1	0
73	BE	10	0	0	0	0
73	BF	17	0	0	0	0
73	BG	18	0	0	8	0
73	BH	18	0	0	2	0
73	BI	16	0	0	0	0
73	BJ	11	0	0	0	0
73	BK	15	0	0	3	0
73	BL	4	0	0	1	0
73	BM	10	0	0	5	0
73	BN	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	BO	10	0	0	1	0
73	BP	5	0	0	2	0
73	BQ	6	0	0	0	0
73	BR	9	0	0	0	0
73	BS	4	0	0	1	0
73	BT	12	0	0	2	0
73	BU	11	0	0	2	0
73	BV	3	0	0	0	0
73	BW	11	0	0	0	0
73	BX	7	0	0	2	0
73	BY	6	0	0	0	0
73	BZ	5	0	0	1	0
73	Ba	4	0	0	0	0
73	Bb	11	0	0	5	0
73	Bc	9	0	0	5	0
All	All	172182	0	123345	4352	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 4352 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BG:28:ARG:HA	73:BG:202:HOH:O	1.48	1.13
43:BC:171:ARG:HG3	73:BC:310:HOH:O	1.51	1.08
3:1:2326:C:H1'	73:1:5439:HOH:O	1.53	1.07
3:1:989:A:H1'	73:1:3936:HOH:O	1.56	1.05
3:1:101:G:H4'	73:1:6355:HOH:O	1.52	1.05

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3	291/655 (44%)	268 (92%)	22 (8%)	1 (0%)	36	53
5	AA	237/244 (97%)	229 (97%)	8 (3%)	0	100	100
6	AB	334/338 (99%)	324 (97%)	10 (3%)	0	100	100
7	AC	276/285 (97%)	269 (98%)	7 (2%)	0	100	100
8	AD	176/178 (99%)	167 (95%)	9 (5%)	0	100	100
9	AE	193/196 (98%)	187 (97%)	6 (3%)	0	100	100
10	AF	143/149 (96%)	140 (98%)	3 (2%)	0	100	100
11	AG	181/186 (97%)	179 (99%)	2 (1%)	0	100	100
12	AH	153/157 (98%)	151 (99%)	2 (1%)	0	100	100
13	AI	136/144 (94%)	134 (98%)	2 (2%)	0	100	100
14	AJ	99/103 (96%)	95 (96%)	4 (4%)	0	100	100
14	AK	88/103 (85%)	81 (92%)	5 (6%)	2 (2%)	5	7
15	AL	150/156 (96%)	144 (96%)	6 (4%)	0	100	100
16	AM	182/189 (96%)	179 (98%)	3 (2%)	0	100	100
17	AN	167/178 (94%)	161 (96%)	6 (4%)	0	100	100
18	AO	198/205 (97%)	193 (98%)	5 (2%)	0	100	100
19	AP	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
20	AQ	144/147 (98%)	143 (99%)	1 (1%)	0	100	100
21	AR	74/78 (95%)	74 (100%)	0	0	100	100
22	AS	96/99 (97%)	91 (95%)	5 (5%)	0	100	100
23	AT	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
24	AU	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
25	AV	119/128 (93%)	117 (98%)	1 (1%)	1 (1%)	16	29
26	AW	54/62 (87%)	52 (96%)	2 (4%)	0	100	100
27	AX	65/79 (82%)	65 (100%)	0	0	100	100
28	AY	170/179 (95%)	163 (96%)	6 (4%)	1 (1%)	21	36
29	AZ	96/101 (95%)	92 (96%)	4 (4%)	0	100	100
30	Aa	86/91 (94%)	84 (98%)	2 (2%)	0	100	100
31	Ab	138/153 (90%)	137 (99%)	1 (1%)	0	100	100
32	Ac	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
33	Ad	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
34	Ae	64/67 (96%)	63 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Af	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
36	Ag	48/53 (91%)	46 (96%)	2 (4%)	0	100	100
37	Ah	89/91 (98%)	89 (100%)	0	0	100	100
38	Ai	97/102 (95%)	90 (93%)	7 (7%)	0	100	100
39	Aj	181/184 (98%)	172 (95%)	9 (5%)	0	100	100
40	Ak	88/93 (95%)	87 (99%)	1 (1%)	0	100	100
41	BA	185/222 (83%)	181 (98%)	4 (2%)	0	100	100
42	BB	196/208 (94%)	188 (96%)	8 (4%)	0	100	100
43	BC	75/216 (35%)	59 (79%)	15 (20%)	1 (1%)	9	17
44	BD	155/159 (98%)	153 (99%)	2 (1%)	0	100	100
45	BE	234/237 (99%)	223 (95%)	11 (5%)	0	100	100
46	BF	192/202 (95%)	181 (94%)	11 (6%)	0	100	100
47	BG	138/151 (91%)	131 (95%)	7 (5%)	0	100	100
48	BH	218/223 (98%)	204 (94%)	14 (6%)	0	100	100
49	BI	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
50	BJ	128/131 (98%)	123 (96%)	5 (4%)	0	100	100
51	BK	132/142 (93%)	119 (90%)	11 (8%)	2 (2%)	8	15
52	BL	36/106 (34%)	31 (86%)	4 (11%)	1 (3%)	4	5
53	BM	123/141 (87%)	116 (94%)	7 (6%)	0	100	100
54	BN	142/147 (97%)	131 (92%)	10 (7%)	1 (1%)	18	32
55	BO	141/153 (92%)	134 (95%)	6 (4%)	1 (1%)	18	32
56	BP	27/54 (50%)	18 (67%)	8 (30%)	1 (4%)	2	3
57	BQ	147/151 (97%)	145 (99%)	2 (1%)	0	100	100
58	BR	142/147 (97%)	136 (96%)	6 (4%)	0	100	100
59	BS	62/71 (87%)	59 (95%)	3 (5%)	0	100	100
60	BT	133/158 (84%)	126 (95%)	5 (4%)	2 (2%)	8	15
61	BU	153/158 (97%)	147 (96%)	6 (4%)	0	100	100
62	BV	113/128 (88%)	110 (97%)	3 (3%)	0	100	100
63	BW	66/110 (60%)	61 (92%)	4 (6%)	1 (2%)	8	15
64	BX	93/100 (93%)	69 (74%)	19 (20%)	5 (5%)	1	1
65	BY	63/67 (94%)	57 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	BZ	69/77 (90%)	60 (87%)	8 (12%)	1 (1%)	9	16
67	Ba	41/54 (76%)	39 (95%)	2 (5%)	0	100	100
68	Bb	58/68 (85%)	58 (100%)	0	0	100	100
69	Bc	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
All	All	8622/9723 (89%)	8249 (96%)	352 (4%)	21 (0%)	44	62

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
51	BK	10	ASN
52	BL	59	SER
54	BN	6	SER
55	BO	112	LEU
64	BX	29	VAL

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3	249/552 (45%)	234 (94%)	15 (6%)	17	34
5	AA	181/186 (97%)	179 (99%)	2 (1%)	65	83
6	AB	280/282 (99%)	271 (97%)	9 (3%)	34	60
7	AC	226/231 (98%)	220 (97%)	6 (3%)	39	65
8	AD	149/149 (100%)	143 (96%)	6 (4%)	28	51
9	AE	165/165 (100%)	162 (98%)	3 (2%)	51	75
10	AF	115/118 (98%)	113 (98%)	2 (2%)	53	77
11	AG	163/165 (99%)	159 (98%)	4 (2%)	42	67
12	AH	133/135 (98%)	129 (97%)	4 (3%)	36	62
13	AI	115/118 (98%)	113 (98%)	2 (2%)	53	77
14	AJ	87/89 (98%)	83 (95%)	4 (5%)	24	45
14	AK	77/89 (86%)	75 (97%)	2 (3%)	40	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AL	121/125 (97%)	116 (96%)	5 (4%)	27	50
16	AM	161/165 (98%)	159 (99%)	2 (1%)	63	82
17	AN	134/140 (96%)	128 (96%)	6 (4%)	24	46
18	AO	166/169 (98%)	163 (98%)	3 (2%)	51	75
19	AP	99/100 (99%)	97 (98%)	2 (2%)	48	73
20	AQ	127/128 (99%)	125 (98%)	2 (2%)	55	78
21	AR	69/71 (97%)	67 (97%)	2 (3%)	37	63
22	AS	84/85 (99%)	82 (98%)	2 (2%)	43	69
23	AT	157/158 (99%)	154 (98%)	3 (2%)	50	74
24	AU	71/71 (100%)	70 (99%)	1 (1%)	59	80
25	AV	107/112 (96%)	101 (94%)	6 (6%)	19	37
26	AW	48/53 (91%)	43 (90%)	5 (10%)	7	13
27	AX	58/65 (89%)	56 (97%)	2 (3%)	32	57
28	AY	147/152 (97%)	144 (98%)	3 (2%)	48	73
29	AZ	77/79 (98%)	71 (92%)	6 (8%)	11	23
30	Aa	78/81 (96%)	74 (95%)	4 (5%)	21	41
31	Ab	125/137 (91%)	125 (100%)	0	100	100
32	Ac	67/68 (98%)	63 (94%)	4 (6%)	17	34
33	Ad	44/44 (100%)	44 (100%)	0	100	100
34	Ae	60/61 (98%)	56 (93%)	4 (7%)	15	29
35	Af	42/43 (98%)	42 (100%)	0	100	100
36	Ag	46/49 (94%)	46 (100%)	0	100	100
37	Ah	82/82 (100%)	82 (100%)	0	100	100
38	Ai	77/80 (96%)	77 (100%)	0	100	100
39	Aj	161/162 (99%)	155 (96%)	6 (4%)	30	54
40	Ak	79/82 (96%)	76 (96%)	3 (4%)	29	53
41	BA	157/181 (87%)	150 (96%)	7 (4%)	24	46
42	BB	174/182 (96%)	168 (97%)	6 (3%)	32	57
43	BC	63/183 (34%)	55 (87%)	8 (13%)	4	8
44	BD	136/138 (99%)	131 (96%)	5 (4%)	30	54
45	BE	203/204 (100%)	198 (98%)	5 (2%)	42	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BF	161/169 (95%)	151 (94%)	10 (6%)	16	32
47	BG	114/121 (94%)	107 (94%)	7 (6%)	17	33
48	BH	191/193 (99%)	187 (98%)	4 (2%)	47	72
49	BI	109/110 (99%)	104 (95%)	5 (5%)	24	45
50	BJ	105/106 (99%)	101 (96%)	4 (4%)	29	53
51	BK	110/117 (94%)	105 (96%)	5 (4%)	24	46
52	BL	34/94 (36%)	29 (85%)	5 (15%)	3	5
53	BM	93/106 (88%)	91 (98%)	2 (2%)	45	71
54	BN	117/120 (98%)	114 (97%)	3 (3%)	40	66
55	BO	113/119 (95%)	104 (92%)	9 (8%)	11	22
56	BP	25/48 (52%)	24 (96%)	1 (4%)	28	51
57	BQ	135/137 (98%)	129 (96%)	6 (4%)	25	47
58	BR	131/134 (98%)	125 (95%)	6 (5%)	24	45
59	BS	55/59 (93%)	54 (98%)	1 (2%)	51	75
60	BT	120/137 (88%)	115 (96%)	5 (4%)	26	49
61	BU	127/130 (98%)	121 (95%)	6 (5%)	23	44
62	BV	101/111 (91%)	93 (92%)	8 (8%)	11	22
63	BW	59/94 (63%)	55 (93%)	4 (7%)	14	28
64	BX	85/89 (96%)	80 (94%)	5 (6%)	18	35
65	BY	55/57 (96%)	48 (87%)	7 (13%)	4	8
66	BZ	59/63 (94%)	58 (98%)	1 (2%)	53	77
67	Ba	39/44 (89%)	38 (97%)	1 (3%)	40	66
68	Bb	49/56 (88%)	49 (100%)	0	100	100
69	Bc	51/52 (98%)	49 (96%)	2 (4%)	28	52
All	All	7398/8195 (90%)	7130 (96%)	268 (4%)	32	55

5 of 268 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
60	BT	113	ILE
61	BU	124	THR
65	BY	31	THR
26	AW	56	LYS
26	AW	5	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
51	BK	8	GLN
59	BS	48	ASN
51	BK	10	ASN
55	BO	120	HIS
66	BZ	20	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	128/129 (99%)	9 (7%)	1 (0%)
3	1	2844/3024 (94%)	353 (12%)	25 (0%)
4	4	1426/1498 (95%)	261 (18%)	32 (2%)
All	All	4398/4651 (94%)	623 (14%)	58 (1%)

5 of 623 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	8	A
1	2	25	G
1	2	28	G
1	2	59	U
1	2	60	A

5 of 58 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	4	101	C
4	4	1444	G
4	4	663	U
4	4	1421	G
4	4	1176	C

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

106 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
4	MA6	4	1478	4	23,26,27	0.35	0	33,38,41	0.81	1 (3%)
3	5MC	1	2056	71,3	19,22,23	1.53	3 (15%)	26,32,35	1.17	3 (11%)
3	OMU	1	2574	3	19,22,23	1.28	4 (21%)	25,31,34	1.80	4 (16%)
3	OMC	1	2704	3	19,22,23	0.81	0	25,31,34	0.81	0
4	OMG	4	1289	4,71	23,26,27	1.22	3 (13%)	32,38,41	2.00	5 (15%)
4	OMC	4	572	4	19,22,23	0.80	0	25,31,34	0.89	1 (4%)
3	OMG	1	2176	71,3	23,26,27	1.22	4 (17%)	32,38,41	1.98	6 (18%)
3	UR3	1	2698	3	19,22,23	0.94	1 (5%)	26,32,35	1.69	3 (11%)
3	PSU	1	2607	3	18,21,22	0.96	1 (5%)	21,30,33	0.75	0
3	OMC	1	2885	3	19,22,23	0.81	0	25,31,34	0.78	0
4	OMG	4	19	4	23,26,27	1.22	4 (17%)	32,38,41	2.01	5 (15%)
4	OMG	4	1211	4	23,26,27	1.24	3 (13%)	32,38,41	2.05	7 (21%)
3	OMU	1	2707	3	19,22,23	1.31	3 (15%)	25,31,34	1.88	5 (20%)
3	OMG	1	902	71,3	23,26,27	1.20	4 (17%)	32,38,41	1.98	6 (18%)
3	OMG	1	2066	3	23,26,27	1.25	4 (17%)	32,38,41	2.01	7 (21%)
53	IAS	BM	128	53	6,7,8	1.32	1 (16%)	3,8,10	1.21	0
4	MA6	4	1477	4	23,26,27	0.35	0	33,38,41	0.76	1 (3%)
4	M7A	4	508	4	19,25,26	0.29	0	25,37,40	0.59	0
4	OMC	4	514	4	19,22,23	0.83	0	25,31,34	0.92	1 (4%)
3	OMG	1	2366	3	23,26,27	1.19	3 (13%)	32,38,41	1.96	6 (18%)
3	PSU	1	2571	3	18,21,22	0.92	1 (5%)	21,30,33	0.68	0
3	OMG	1	2667	3	23,26,27	1.22	3 (13%)	32,38,41	2.04	6 (18%)
3	OMU	1	2408	3	19,22,23	1.25	3 (15%)	25,31,34	1.88	5 (20%)
3	A2M	1	2059	71,3	22,25,26	0.27	0	30,36,39	0.61	0
4	A2M	4	880	4	22,25,26	0.20	0	30,36,39	0.45	0
3	5MC	1	38	3	19,22,23	1.47	3 (15%)	26,32,35	1.33	5 (19%)
3	OMC	1	1816	3	19,22,23	0.79	0	25,31,34	0.74	0
3	OMG	1	2103	3	23,26,27	1.23	4 (17%)	32,38,41	1.99	5 (15%)
3	OMU	1	908	71,3	19,22,23	1.33	4 (21%)	25,31,34	2.00	7 (28%)
3	A2M	1	2011	3	22,25,26	0.21	0	30,36,39	0.45	0
4	OMC	4	1034	4	19,22,23	0.82	1 (5%)	25,31,34	0.83	0
3	OMG	1	1949	3	23,26,27	1.23	3 (13%)	32,38,41	1.96	6 (18%)
3	OMC	1	872	3	19,22,23	0.79	0	25,31,34	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	G7M	1	3023	3	23,26,27	1.84	2 (8%)	34,39,42	1.06	2 (5%)
3	PSU	1	2610	3	18,21,22	0.94	1 (5%)	21,30,33	0.73	0
3	A2M	1	1990	3	22,25,26	0.19	0	30,36,39	0.47	0
4	OMG	4	7	4	23,26,27	1.23	3 (13%)	32,38,41	2.01	6 (18%)
3	B8T	1	79	3	19,22,23	0.40	0	25,31,34	0.35	0
3	OMC	1	2624	3	19,22,23	0.83	1 (5%)	25,31,34	0.74	0
3	OMG	1	2608	3	23,26,27	1.19	4 (17%)	32,38,41	1.96	6 (18%)
4	OMG	4	465	4	23,26,27	1.22	4 (17%)	32,38,41	1.94	6 (18%)
4	OMG	4	462	4	23,26,27	1.21	3 (13%)	32,38,41	1.97	6 (18%)
4	PSU	4	263	4	18,21,22	0.92	1 (5%)	21,30,33	0.58	0
4	OMG	4	1210	4	23,26,27	1.23	3 (13%)	32,38,41	2.00	7 (21%)
3	OMC	1	2538	3	19,22,23	0.79	0	25,31,34	0.79	0
4	OMG	4	511	4	23,26,27	1.20	4 (17%)	32,38,41	1.96	6 (18%)
4	OMC	4	1368	4	19,22,23	0.83	1 (5%)	25,31,34	0.77	0
3	OMC	1	2116	3	19,22,23	0.83	0	25,31,34	0.64	0
3	B8T	1	2937	3	19,22,23	0.40	0	25,31,34	0.31	0
3	OMG	1	2537	3	23,26,27	1.19	3 (13%)	32,38,41	1.99	6 (18%)
4	OMU	4	15	4	19,22,23	1.37	4 (21%)	25,31,34	1.91	5 (20%)
4	OMG	4	674	4	23,26,27	1.22	3 (13%)	32,38,41	2.01	5 (15%)
3	OMG	1	2601	71,3	23,26,27	1.20	3 (13%)	32,38,41	2.02	7 (21%)
3	4AC	1	2016	3	21,24,25	0.39	0	28,34,37	0.57	0
3	OMG	1	1957	3	23,26,27	1.19	4 (17%)	32,38,41	2.00	6 (18%)
4	4AC	4	1318	4	21,24,25	0.39	0	28,34,37	0.73	0
4	A2M	4	496	4	22,25,26	0.21	0	30,36,39	0.46	0
4	A2M	4	879	4	22,25,26	0.22	0	30,36,39	0.38	0
3	PSU	1	2625	3	18,21,22	0.93	1 (5%)	21,30,33	0.70	0
3	OMU	1	2088	3	19,22,23	1.29	3 (15%)	25,31,34	1.81	5 (20%)
3	PSU	1	2044	3	18,21,22	0.94	1 (5%)	21,30,33	0.57	0
3	OMC	1	2143	3	19,22,23	0.29	0	25,31,34	0.35	0
3	OMU	1	2155	3	19,22,23	1.27	3 (15%)	25,31,34	1.88	5 (20%)
3	OMU	1	875	3	19,22,23	1.31	4 (21%)	25,31,34	1.91	5 (20%)
4	B8T	4	1469	4	19,22,23	0.44	0	25,31,34	0.39	0
3	OMC	1	2884	3	19,22,23	0.81	0	25,31,34	0.83	1 (4%)
3	OMC	1	493	3	19,22,23	0.79	0	25,31,34	0.83	0
3	OMC	1	1976	3	19,22,23	0.84	2 (10%)	25,31,34	0.80	0
4	A2M	4	569	4,71	22,25,26	0.20	0	30,36,39	0.48	0
3	OMG	1	2104	3	23,26,27	1.21	4 (17%)	32,38,41	2.00	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMU	1	2666	3	19,22,23	1.28	3 (15%)	25,31,34	1.89	5 (20%)
3	OMC	1	2720	3	19,22,23	0.78	0	25,31,34	0.89	0
4	OMG	4	908	4	23,26,27	1.21	4 (17%)	32,38,41	2.02	6 (18%)
3	OMG	1	1971	3	23,26,27	1.22	3 (13%)	32,38,41	2.01	7 (21%)
4	OMG	4	1212	4	23,26,27	1.20	4 (17%)	32,38,41	2.03	7 (21%)
3	OMG	1	2071	3	23,26,27	1.20	4 (17%)	32,38,41	1.89	6 (18%)
4	OMU	4	877	4	19,22,23	1.29	4 (21%)	25,31,34	1.90	5 (20%)
4	OMG	4	467	4	23,26,27	1.25	4 (17%)	32,38,41	1.93	5 (15%)
4	OMG	4	1202	4,71	23,26,27	1.23	3 (13%)	32,38,41	2.08	7 (21%)
3	OMC	1	2115	3	19,22,23	0.81	0	25,31,34	0.76	0
3	OMU	1	2623	3	19,22,23	1.27	4 (21%)	25,31,34	1.87	4 (16%)
4	OMC	4	1184	4	19,22,23	0.78	0	25,31,34	0.73	0
4	OMG	4	1163	4	23,26,27	1.26	3 (13%)	32,38,41	2.10	6 (18%)
3	OMG	1	2017	3	23,26,27	1.24	3 (13%)	32,38,41	2.00	6 (18%)
3	OMC	1	673	3	19,22,23	0.79	0	25,31,34	0.79	0
3	OMG	1	1947	3	23,26,27	1.20	4 (17%)	32,38,41	2.04	7 (21%)
3	OMU	1	2851	3	19,22,23	1.28	4 (21%)	25,31,34	1.82	5 (20%)
3	OMU	1	2628	3	19,22,23	1.25	3 (15%)	25,31,34	1.84	6 (24%)
4	OMG	4	475	4	23,26,27	1.21	3 (13%)	32,38,41	2.00	7 (21%)
3	OMU	1	2077	3	19,22,23	1.34	4 (21%)	25,31,34	1.83	5 (20%)
4	4AC	4	5	4	21,24,25	0.41	0	28,34,37	0.70	0
3	PSU	1	1911	3	18,21,22	0.94	1 (5%)	21,30,33	0.76	0
3	PSU	1	1987	3	18,21,22	0.91	1 (5%)	21,30,33	0.70	0
4	OMC	4	1045	4	19,22,23	0.82	0	25,31,34	0.85	1 (4%)
3	OMG	1	2388	3	23,26,27	1.21	4 (17%)	32,38,41	2.03	7 (21%)
4	OMG	4	906	4	23,26,27	1.23	3 (13%)	32,38,41	2.03	7 (21%)
4	A2M	4	1060	4	22,25,26	0.23	0	30,36,39	0.72	2 (6%)
3	A2M	1	2691	71,3	22,25,26	0.20	0	30,36,39	0.36	0
3	OMC	1	492	3	19,22,23	0.76	0	25,31,34	0.82	1 (4%)
4	OMC	4	489	4	19,22,23	0.85	1 (5%)	25,31,34	1.03	2 (8%)
4	6MZ	4	1459	4,71	22,25,26	1.45	5 (22%)	29,36,39	2.18	8 (27%)
3	OMC	1	2555	3	19,22,23	0.83	0	25,31,34	1.01	1 (4%)
4	B8T	4	1035	4	19,22,23	0.44	0	25,31,34	0.53	0
4	A2M	4	40	4	22,25,26	0.18	0	30,36,39	0.39	0
3	OMG	1	2362	3	23,26,27	1.22	3 (13%)	32,38,41	2.05	6 (18%)
3	OMC	1	2018	3	19,22,23	0.80	0	25,31,34	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MA6	4	1478	4	-	2/11/29/30	0/3/3/3
3	5MC	1	2056	71,3	-	1/7/25/26	0/2/2/2
3	OMU	1	2574	3	-	0/9/27/28	0/2/2/2
3	OMC	1	2704	3	-	0/9/27/28	0/2/2/2
4	OMG	4	1289	4,71	-	0/9/27/28	0/3/3/3
4	OMC	4	572	4	-	0/9/27/28	0/2/2/2
3	OMG	1	2176	71,3	-	0/9/27/28	0/3/3/3
3	UR3	1	2698	3	-	0/7/25/26	0/2/2/2
3	PSU	1	2607	3	-	0/7/25/26	0/2/2/2
3	OMC	1	2885	3	-	0/9/27/28	0/2/2/2
4	OMG	4	19	4	-	2/9/27/28	0/3/3/3
4	OMG	4	1211	4	-	3/9/27/28	0/3/3/3
3	OMU	1	2707	3	-	0/9/27/28	0/2/2/2
3	OMG	1	902	71,3	-	0/9/27/28	0/3/3/3
3	OMG	1	2066	3	-	0/9/27/28	0/3/3/3
53	IAS	BM	128	53	-	1/7/7/8	-
4	MA6	4	1477	4	-	0/11/29/30	0/3/3/3
4	M7A	4	508	4	-	4/7/37/38	0/3/3/3
4	OMC	4	514	4	-	0/9/27/28	0/2/2/2
3	OMG	1	2366	3	-	1/9/27/28	0/3/3/3
3	PSU	1	2571	3	-	0/7/25/26	0/2/2/2
3	OMG	1	2667	3	-	0/9/27/28	0/3/3/3
3	OMU	1	2408	3	-	0/9/27/28	0/2/2/2
3	A2M	1	2059	71,3	-	1/9/27/28	0/3/3/3
4	A2M	4	880	4	-	0/9/27/28	0/3/3/3
3	5MC	1	38	3	-	1/7/25/26	0/2/2/2
3	OMC	1	1816	3	-	0/9/27/28	0/2/2/2
3	OMG	1	2103	3	-	0/9/27/28	0/3/3/3
3	OMU	1	908	71,3	-	4/9/27/28	0/2/2/2
3	A2M	1	2011	3	-	1/9/27/28	0/3/3/3
4	OMC	4	1034	4	-	0/9/27/28	0/2/2/2
3	OMG	1	1949	3	-	0/9/27/28	0/3/3/3
3	OMC	1	872	3	-	0/9/27/28	0/2/2/2
3	G7M	1	3023	3	-	2/7/25/26	0/3/3/3
3	PSU	1	2610	3	-	0/7/25/26	0/2/2/2
3	A2M	1	1990	3	-	0/9/27/28	0/3/3/3
4	OMG	4	7	4	-	0/9/27/28	0/3/3/3
3	B8T	1	79	3	-	0/7/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	1	2624	3	-	0/9/27/28	0/2/2/2
3	OMG	1	2608	3	-	2/9/27/28	0/3/3/3
4	OMG	4	465	4	-	2/9/27/28	0/3/3/3
4	OMG	4	462	4	-	0/9/27/28	0/3/3/3
4	PSU	4	263	4	-	0/7/25/26	0/2/2/2
4	OMG	4	1210	4	-	1/9/27/28	0/3/3/3
3	OMC	1	2538	3	-	0/9/27/28	0/2/2/2
4	OMG	4	511	4	-	3/9/27/28	0/3/3/3
4	OMC	4	1368	4	-	2/9/27/28	0/2/2/2
3	OMC	1	2116	3	-	2/9/27/28	0/2/2/2
3	B8T	1	2937	3	-	2/7/27/28	0/2/2/2
3	OMG	1	2537	3	-	2/9/27/28	0/3/3/3
4	OMU	4	15	4	-	0/9/27/28	0/2/2/2
4	OMG	4	674	4	-	0/9/27/28	0/3/3/3
3	OMG	1	2601	71,3	-	0/9/27/28	0/3/3/3
3	4AC	1	2016	3	-	0/11/29/30	0/2/2/2
3	OMG	1	1957	3	-	0/9/27/28	0/3/3/3
4	4AC	4	1318	4	-	0/11/29/30	0/2/2/2
4	A2M	4	496	4	-	3/9/27/28	0/3/3/3
4	A2M	4	879	4	-	4/9/27/28	0/3/3/3
3	PSU	1	2625	3	-	0/7/25/26	0/2/2/2
3	OMU	1	2088	3	-	1/9/27/28	0/2/2/2
3	PSU	1	2044	3	-	2/7/25/26	0/2/2/2
3	OMC	1	2143	3	-	0/9/27/28	0/2/2/2
3	OMU	1	2155	3	-	2/9/27/28	0/2/2/2
3	OMU	1	875	3	-	0/9/27/28	0/2/2/2
4	B8T	4	1469	4	-	0/7/27/28	0/2/2/2
3	OMC	1	2884	3	-	0/9/27/28	0/2/2/2
3	OMC	1	493	3	-	1/9/27/28	0/2/2/2
3	OMC	1	1976	3	-	0/9/27/28	0/2/2/2
4	A2M	4	569	4,71	-	0/9/27/28	0/3/3/3
3	OMG	1	2104	3	-	1/9/27/28	0/3/3/3
3	OMU	1	2666	3	-	0/9/27/28	0/2/2/2
3	OMC	1	2720	3	-	0/9/27/28	0/2/2/2
4	OMG	4	908	4	-	3/9/27/28	0/3/3/3
3	OMG	1	1971	3	-	0/9/27/28	0/3/3/3
4	OMG	4	1212	4	-	0/9/27/28	0/3/3/3
3	OMG	1	2071	3	-	0/9/27/28	0/3/3/3
4	OMU	4	877	4	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	4	467	4	-	1/9/27/28	0/3/3/3
4	OMG	4	1202	4,71	-	2/9/27/28	0/3/3/3
3	OMC	1	2115	3	-	0/9/27/28	0/2/2/2
3	OMU	1	2623	3	-	0/9/27/28	0/2/2/2
4	OMC	4	1184	4	-	0/9/27/28	0/2/2/2
4	OMG	4	1163	4	-	4/9/27/28	0/3/3/3
3	OMG	1	2017	3	-	1/9/27/28	0/3/3/3
3	OMC	1	673	3	-	0/9/27/28	0/2/2/2
3	OMG	1	1947	3	-	2/9/27/28	0/3/3/3
3	OMU	1	2851	3	-	0/9/27/28	0/2/2/2
3	OMU	1	2628	3	-	2/9/27/28	0/2/2/2
4	OMG	4	475	4	-	0/9/27/28	0/3/3/3
3	OMU	1	2077	3	-	1/9/27/28	0/2/2/2
4	4AC	4	5	4	-	0/11/29/30	0/2/2/2
3	PSU	1	1911	3	-	0/7/25/26	0/2/2/2
3	PSU	1	1987	3	-	0/7/25/26	0/2/2/2
4	OMC	4	1045	4	-	3/9/27/28	0/2/2/2
3	OMG	1	2388	3	-	1/9/27/28	0/3/3/3
4	OMG	4	906	4	-	0/9/27/28	0/3/3/3
4	A2M	4	1060	4	-	4/9/27/28	0/3/3/3
3	A2M	1	2691	71,3	-	1/9/27/28	0/3/3/3
3	OMC	1	492	3	-	1/9/27/28	0/2/2/2
4	OMC	4	489	4	-	0/9/27/28	0/2/2/2
4	6MZ	4	1459	4,71	-	0/9/27/28	0/3/3/3
3	OMC	1	2555	3	-	1/9/27/28	0/2/2/2
4	B8T	4	1035	4	-	2/7/27/28	0/2/2/2
4	A2M	4	40	4	-	0/9/27/28	0/3/3/3
3	OMG	1	2362	3	-	3/9/27/28	0/3/3/3
3	OMC	1	2018	3	-	0/9/27/28	0/2/2/2

The worst 5 of 197 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	3023	G7M	C8-N7	7.56	1.45	1.33
3	1	2056	5MC	C5-C4	5.41	1.48	1.44
3	1	38	5MC	C5-C4	5.06	1.47	1.44
3	1	3023	G7M	C8-N9	4.03	1.46	1.35
4	4	1459	6MZ	C5-C4	4.03	1.46	1.39

The worst 5 of 314 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	1163	OMG	C5-C4-N3	-6.70	117.72	128.39
3	1	2698	UR3	C4-N3-C2	-6.47	119.38	124.58
3	1	2017	OMG	C5-C4-N3	-6.45	118.13	128.39
3	1	2667	OMG	C5-C4-N3	-6.44	118.14	128.39
4	4	1459	6MZ	C5-C4-N3	-6.37	117.94	126.72

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	4	496	A2M	C1'-C2'-O2'-CM'
4	4	879	A2M	C3'-C4'-C5'-O5'
4	4	879	A2M	C1'-C2'-O2'-CM'
4	4	1045	OMC	O4'-C4'-C5'-O5'
4	4	1060	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

80 monomers are involved in 128 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	4	1478	MA6	2	0
3	1	2056	5MC	1	0
3	1	2704	OMC	3	0
4	4	1289	OMG	3	0
4	4	572	OMC	2	0
3	1	2698	UR3	1	0
3	1	2607	PSU	1	0
3	1	2885	OMC	3	0
4	4	1211	OMG	4	0
3	1	2707	OMU	1	0
3	1	902	OMG	3	0
53	BM	128	IAS	1	0
4	4	1477	MA6	2	0
4	4	514	OMC	1	0
3	1	2366	OMG	2	0
3	1	2667	OMG	2	0
3	1	2408	OMU	2	0
3	1	2059	A2M	1	0
4	4	880	A2M	4	0
3	1	1816	OMC	1	0
3	1	2103	OMG	1	0
3	1	2011	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	4	1034	OMC	1	0
3	1	872	OMC	1	0
3	1	3023	G7M	1	0
3	1	2610	PSU	1	0
3	1	1990	A2M	4	0
4	4	7	OMG	3	0
3	1	2624	OMC	2	0
3	1	2608	OMG	1	0
4	4	465	OMG	2	0
4	4	462	OMG	1	0
4	4	263	PSU	2	0
4	4	1210	OMG	4	0
3	1	2538	OMC	2	0
4	4	1368	OMC	1	0
3	1	2537	OMG	1	0
4	4	15	OMU	1	0
4	4	674	OMG	1	0
3	1	1957	OMG	1	0
4	4	1318	4AC	1	0
4	4	879	A2M	3	0
3	1	2088	OMU	2	0
3	1	2044	PSU	2	0
3	1	2155	OMU	1	0
3	1	875	OMU	3	0
3	1	2884	OMC	1	0
3	1	493	OMC	1	0
3	1	1976	OMC	1	0
3	1	2104	OMG	3	0
3	1	2720	OMC	1	0
4	4	908	OMG	1	0
3	1	1971	OMG	1	0
4	4	1212	OMG	2	0
3	1	2071	OMG	1	0
4	4	877	OMU	2	0
4	4	467	OMG	1	0
4	4	1202	OMG	2	0
3	1	2115	OMC	1	0
3	1	2623	OMU	2	0
4	4	1184	OMC	3	0
4	4	1163	OMG	2	0
3	1	2017	OMG	1	0
3	1	1947	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	2851	OMU	4	0
3	1	2628	OMU	3	0
4	4	475	OMG	5	0
3	1	2077	OMU	1	0
4	4	5	4AC	1	0
4	4	1045	OMC	1	0
3	1	2388	OMG	1	0
4	4	906	OMG	1	0
4	4	1060	A2M	1	0
3	1	492	OMC	2	0
4	4	489	OMC	1	0
4	4	1459	6MZ	2	0
3	1	2555	OMC	2	0
4	4	1035	B8T	1	0
3	1	2362	OMG	1	0
3	1	2018	OMC	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 326 ligands modelled in this entry, 262 are monoatomic - leaving 64 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	$\# Z  > 2$
70	SPM	1	3131	-	13,13,13	0.17	0	12,12,12	0.23	0
70	SPM	1	3114	-	13,13,13	0.17	0	12,12,12	0.47	0
70	SPM	4	3014	-	13,13,13	0.16	0	12,12,12	0.44	0
70	SPM	4	3015	-	13,13,13	0.15	0	12,12,12	0.37	0
70	SPM	Ah	101	-	13,13,13	0.17	0	12,12,12	0.20	0
70	SPM	1	3116	-	13,13,13	0.16	0	12,12,12	0.31	0
70	SPM	1	3107	-	13,13,13	0.17	0	12,12,12	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
70	SPM	1	3130	-	13,13,13	0.15	0	12,12,12	0.13	0
70	SPM	1	3142	-	13,13,13	0.16	0	12,12,12	0.38	0
70	SPM	1	3127	-	13,13,13	0.16	0	12,12,12	0.35	0
70	SPM	1	3120	-	13,13,13	0.17	0	12,12,12	0.23	0
70	SPM	1	3132	-	13,13,13	0.14	0	12,12,12	0.20	0
70	SPM	1	3140	-	13,13,13	0.15	0	12,12,12	0.32	0
70	SPM	4	3004	-	13,13,13	0.17	0	12,12,12	0.16	0
70	SPM	4	3018	-	13,13,13	0.16	0	12,12,12	0.34	0
70	SPM	4	3016	-	13,13,13	0.15	0	12,12,12	0.20	0
70	SPM	4	3013	-	13,13,13	0.16	0	12,12,12	0.26	0
70	SPM	1	3102	-	13,13,13	0.18	0	12,12,12	0.42	0
70	SPM	1	3103	-	13,13,13	0.17	0	12,12,12	0.49	0
70	SPM	1	3115	-	13,13,13	0.17	0	12,12,12	0.42	0
70	SPM	4	3005	-	13,13,13	0.14	0	12,12,12	0.23	0
70	SPM	1	3109	-	13,13,13	0.18	0	12,12,12	0.31	0
70	SPM	1	3129	-	13,13,13	0.16	0	12,12,12	0.39	0
70	SPM	1	3134	-	13,13,13	0.19	0	12,12,12	0.38	0
70	SPM	1	3123	-	13,13,13	0.16	0	12,12,12	0.39	0
70	SPM	1	3125	-	13,13,13	0.16	0	12,12,12	0.28	0
70	SPM	1	3137	-	13,13,13	0.16	0	12,12,12	0.34	0
70	SPM	AL	201	-	13,13,13	0.16	0	12,12,12	0.32	0
70	SPM	AM	201	-	13,13,13	0.17	0	12,12,12	0.43	0
70	SPM	1	3117	-	13,13,13	0.17	0	12,12,12	0.32	0
70	SPM	1	3112	-	13,13,13	0.17	0	12,12,12	0.29	0
70	SPM	1	3139	-	13,13,13	0.16	0	12,12,12	0.23	0
70	SPM	1	3122	-	13,13,13	0.18	0	12,12,12	0.28	0
70	SPM	1	3105	-	13,13,13	0.15	0	12,12,12	0.18	0
70	SPM	4	3003	-	13,13,13	0.18	0	12,12,12	0.20	0
70	SPM	1	3104	-	13,13,13	0.18	0	12,12,12	0.27	0
70	SPM	1	3128	-	13,13,13	0.16	0	12,12,12	0.22	0
70	SPM	1	3106	3	13,13,13	0.15	0	12,12,12	0.34	0
70	SPM	4	3012	-	13,13,13	0.17	0	12,12,12	0.10	0
70	SPM	1	3108	-	13,13,13	0.18	0	12,12,12	0.53	0
70	SPM	1	3121	-	13,13,13	0.24	0	12,12,12	0.27	0
70	SPM	1	3133	-	13,13,13	0.17	0	12,12,12	0.29	0
70	SPM	4	3011	-	13,13,13	0.15	0	12,12,12	0.42	0
70	SPM	1	3135	-	13,13,13	0.16	0	12,12,12	0.60	0
70	SPM	4	3006	-	13,13,13	0.15	0	12,12,12	0.27	0
70	SPM	4	3010	-	13,13,13	0.16	0	12,12,12	0.65	0
70	SPM	1	3113	-	13,13,13	0.16	0	12,12,12	0.29	0
70	SPM	1	3126	-	13,13,13	0.16	0	12,12,12	0.50	0
70	SPM	4	3001	-	13,13,13	0.16	0	12,12,12	0.35	0
70	SPM	4	3009	-	13,13,13	0.19	0	12,12,12	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
70	SPM	1	3141	-	13,13,13	0.17	0	12,12,12	0.59	0
70	SPM	1	3138	-	13,13,13	0.18	0	12,12,12	0.65	0
70	SPM	1	3110	-	13,13,13	0.16	0	12,12,12	0.18	0
70	SPM	1	3119	-	13,13,13	0.19	0	12,12,12	0.31	0
70	SPM	4	3002	-	13,13,13	0.18	0	12,12,12	0.41	0
70	SPM	4	3007	-	13,13,13	0.21	0	12,12,12	0.55	0
70	SPM	1	3111	-	13,13,13	0.16	0	12,12,12	0.26	0
70	SPM	4	3017	-	13,13,13	0.24	0	12,12,12	1.59	1 (8%)
70	SPM	1	3124	-	13,13,13	0.15	0	12,12,12	0.26	0
70	SPM	4	3008	-	13,13,13	0.15	0	12,12,12	0.18	0
70	SPM	1	3143	-	13,13,13	0.18	0	12,12,12	0.42	0
70	SPM	1	3101	-	13,13,13	0.17	0	12,12,12	0.45	0
70	SPM	1	3118	-	13,13,13	0.16	0	12,12,12	0.20	0
70	SPM	1	3136	-	13,13,13	0.15	0	12,12,12	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	SPM	1	3131	-	-	0/11/11/11	-
70	SPM	1	3114	-	-	2/11/11/11	-
70	SPM	4	3014	-	-	3/11/11/11	-
70	SPM	4	3015	-	-	1/11/11/11	-
70	SPM	Ah	101	-	-	2/11/11/11	-
70	SPM	1	3116	-	-	2/11/11/11	-
70	SPM	1	3107	-	-	1/11/11/11	-
70	SPM	1	3130	-	-	0/11/11/11	-
70	SPM	1	3142	-	-	1/11/11/11	-
70	SPM	1	3127	-	-	0/11/11/11	-
70	SPM	1	3120	-	-	2/11/11/11	-
70	SPM	1	3132	-	-	5/11/11/11	-
70	SPM	1	3140	-	-	1/11/11/11	-
70	SPM	4	3004	-	-	0/11/11/11	-
70	SPM	4	3018	-	-	0/11/11/11	-
70	SPM	4	3016	-	-	1/11/11/11	-
70	SPM	4	3013	-	-	1/11/11/11	-
70	SPM	1	3102	-	-	0/11/11/11	-
70	SPM	1	3103	-	-	0/11/11/11	-
70	SPM	1	3115	-	-	1/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	SPM	4	3005	-	-	1/11/11/11	-
70	SPM	1	3109	-	-	1/11/11/11	-
70	SPM	1	3129	-	-	1/11/11/11	-
70	SPM	1	3134	-	-	2/11/11/11	-
70	SPM	1	3123	-	-	2/11/11/11	-
70	SPM	1	3125	-	-	1/11/11/11	-
70	SPM	1	3137	-	-	2/11/11/11	-
70	SPM	AL	201	-	-	1/11/11/11	-
70	SPM	AM	201	-	-	1/11/11/11	-
70	SPM	1	3117	-	-	2/11/11/11	-
70	SPM	1	3112	-	-	1/11/11/11	-
70	SPM	1	3139	-	-	0/11/11/11	-
70	SPM	1	3122	-	-	0/11/11/11	-
70	SPM	1	3105	-	-	1/11/11/11	-
70	SPM	4	3003	-	-	4/11/11/11	-
70	SPM	1	3104	-	-	2/11/11/11	-
70	SPM	1	3128	-	-	1/11/11/11	-
70	SPM	1	3106	3	-	2/11/11/11	-
70	SPM	4	3012	-	-	2/11/11/11	-
70	SPM	1	3108	-	-	3/11/11/11	-
70	SPM	1	3121	-	-	1/11/11/11	-
70	SPM	1	3133	-	-	3/11/11/11	-
70	SPM	4	3011	-	-	2/11/11/11	-
70	SPM	1	3135	-	-	0/11/11/11	-
70	SPM	4	3006	-	-	2/11/11/11	-
70	SPM	4	3010	-	-	3/11/11/11	-
70	SPM	1	3113	-	-	2/11/11/11	-
70	SPM	1	3126	-	-	3/11/11/11	-
70	SPM	4	3001	-	-	0/11/11/11	-
70	SPM	4	3009	-	-	2/11/11/11	-
70	SPM	1	3141	-	-	4/11/11/11	-
70	SPM	1	3138	-	-	5/11/11/11	-
70	SPM	1	3110	-	-	0/11/11/11	-
70	SPM	1	3119	-	-	3/11/11/11	-
70	SPM	4	3002	-	-	2/11/11/11	-
70	SPM	4	3007	-	-	5/11/11/11	-
70	SPM	1	3111	-	-	0/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	SPM	4	3017	-	-	5/11/11/11	-
70	SPM	1	3124	-	-	0/11/11/11	-
70	SPM	4	3008	-	-	0/11/11/11	-
70	SPM	1	3143	-	-	2/11/11/11	-
70	SPM	1	3101	-	-	4/11/11/11	-
70	SPM	1	3118	-	-	1/11/11/11	-
70	SPM	1	3136	-	-	1/11/11/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	4	3017	SPM	C7-C8-C9	5.12	137.21	113.56

There are no chirality outliers.

5 of 103 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	4	3017	SPM	C6-C7-C8-C9
70	1	3138	SPM	N5-C6-C7-C8
70	4	3007	SPM	C7-C8-C9-N10
70	AL	201	SPM	N10-C11-C12-C13
70	1	3134	SPM	N5-C6-C7-C8

There are no ring outliers.

22 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	1	3114	SPM	2	0
70	4	3014	SPM	2	0
70	1	3116	SPM	1	0
70	1	3107	SPM	1	0
70	1	3120	SPM	1	0
70	1	3140	SPM	1	0
70	1	3102	SPM	1	0
70	1	3103	SPM	1	0
70	4	3005	SPM	2	0
70	1	3134	SPM	1	0
70	1	3125	SPM	1	0
70	AL	201	SPM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	1	3117	SPM	1	0
70	1	3139	SPM	1	0
70	1	3128	SPM	2	0
70	1	3106	SPM	2	0
70	4	3012	SPM	2	0
70	1	3108	SPM	1	0
70	1	3121	SPM	1	0
70	1	3126	SPM	1	0
70	4	3017	SPM	2	0
70	4	3008	SPM	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

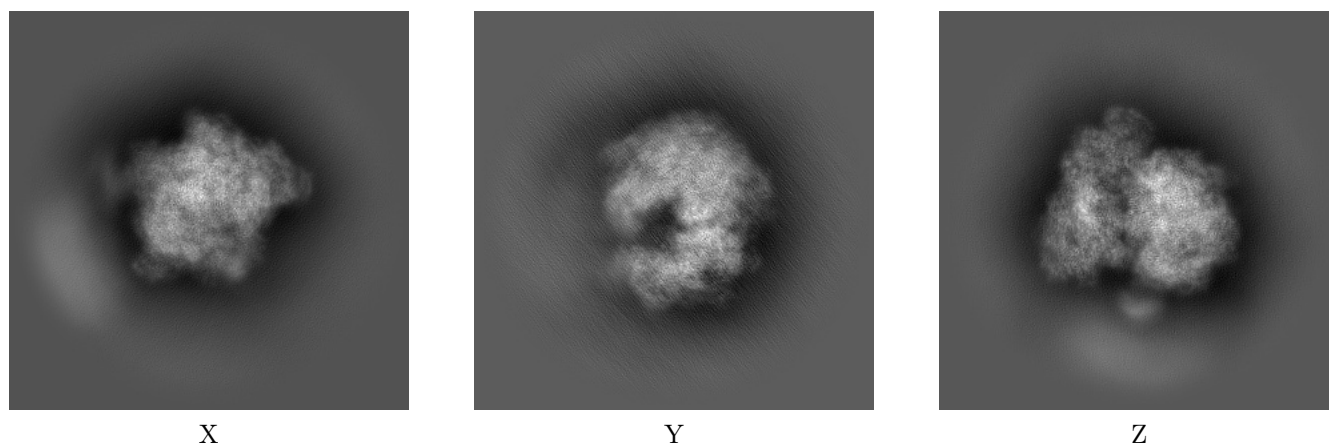
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47668. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

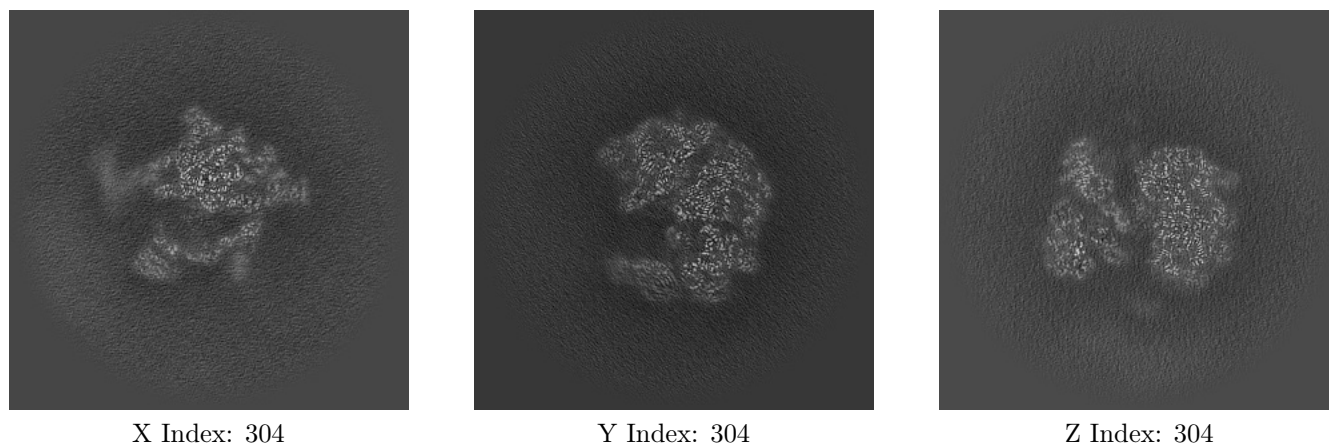
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

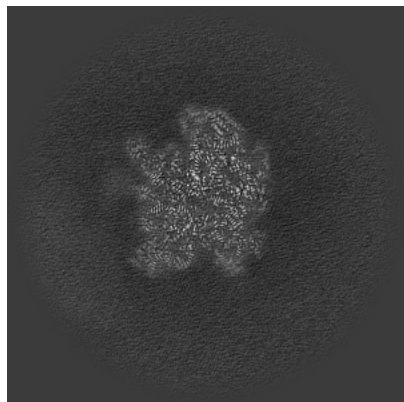
#### 6.2.1 Primary map



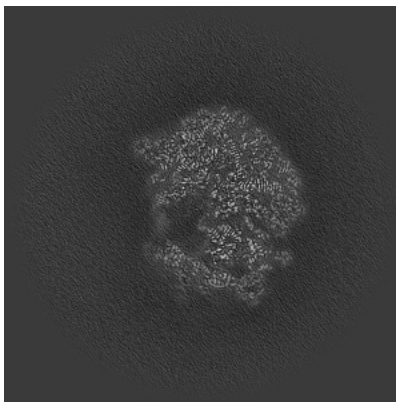
The images above show central slices of the map in three orthogonal directions.

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

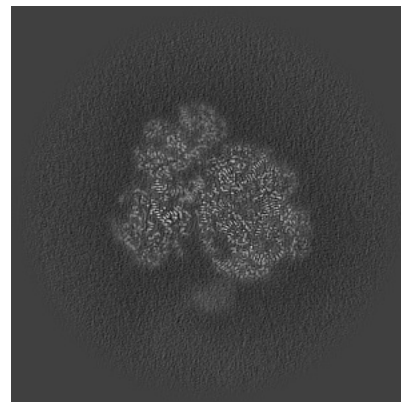
### 6.3.1 Primary map



X Index: 334



Y Index: 288

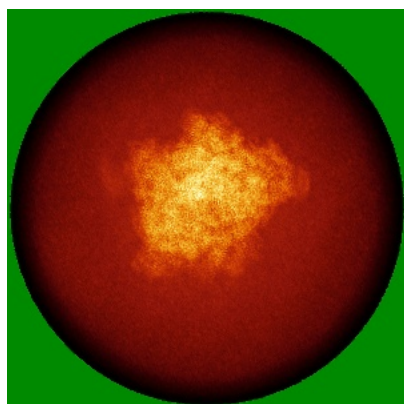


Z Index: 326

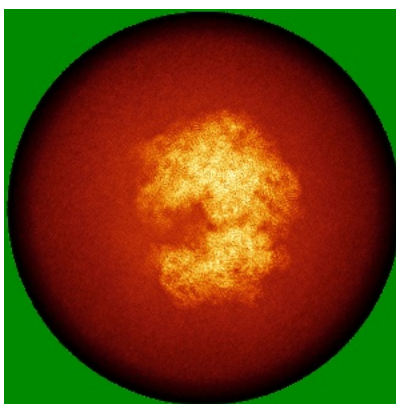
The images above show the largest variance slices of the map in three orthogonal directions.

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

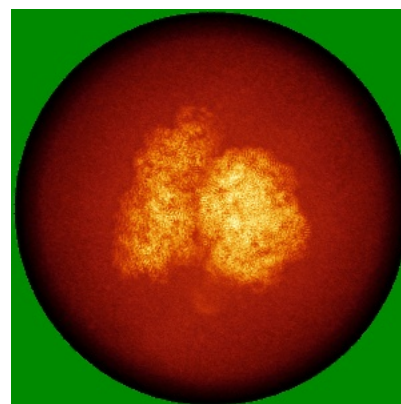
### 6.4.1 Primary map



X



Y

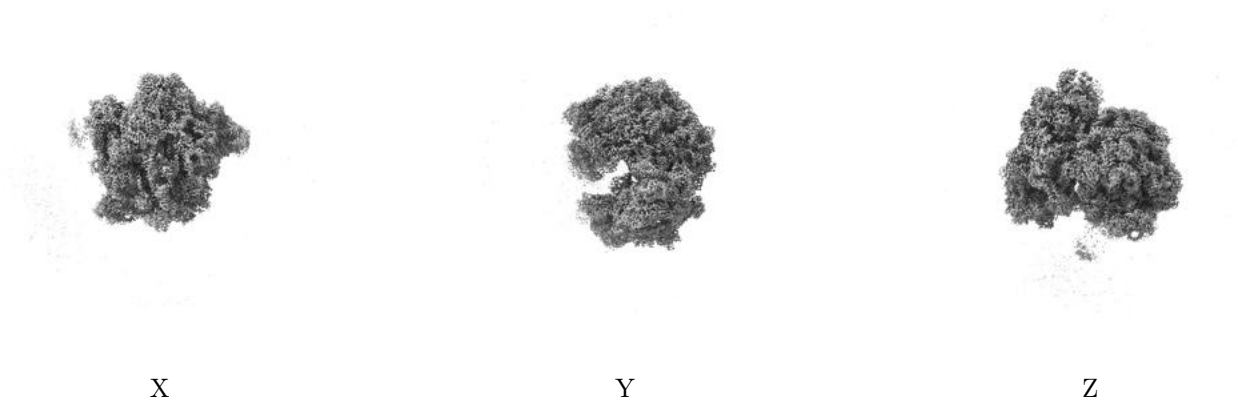


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.188. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

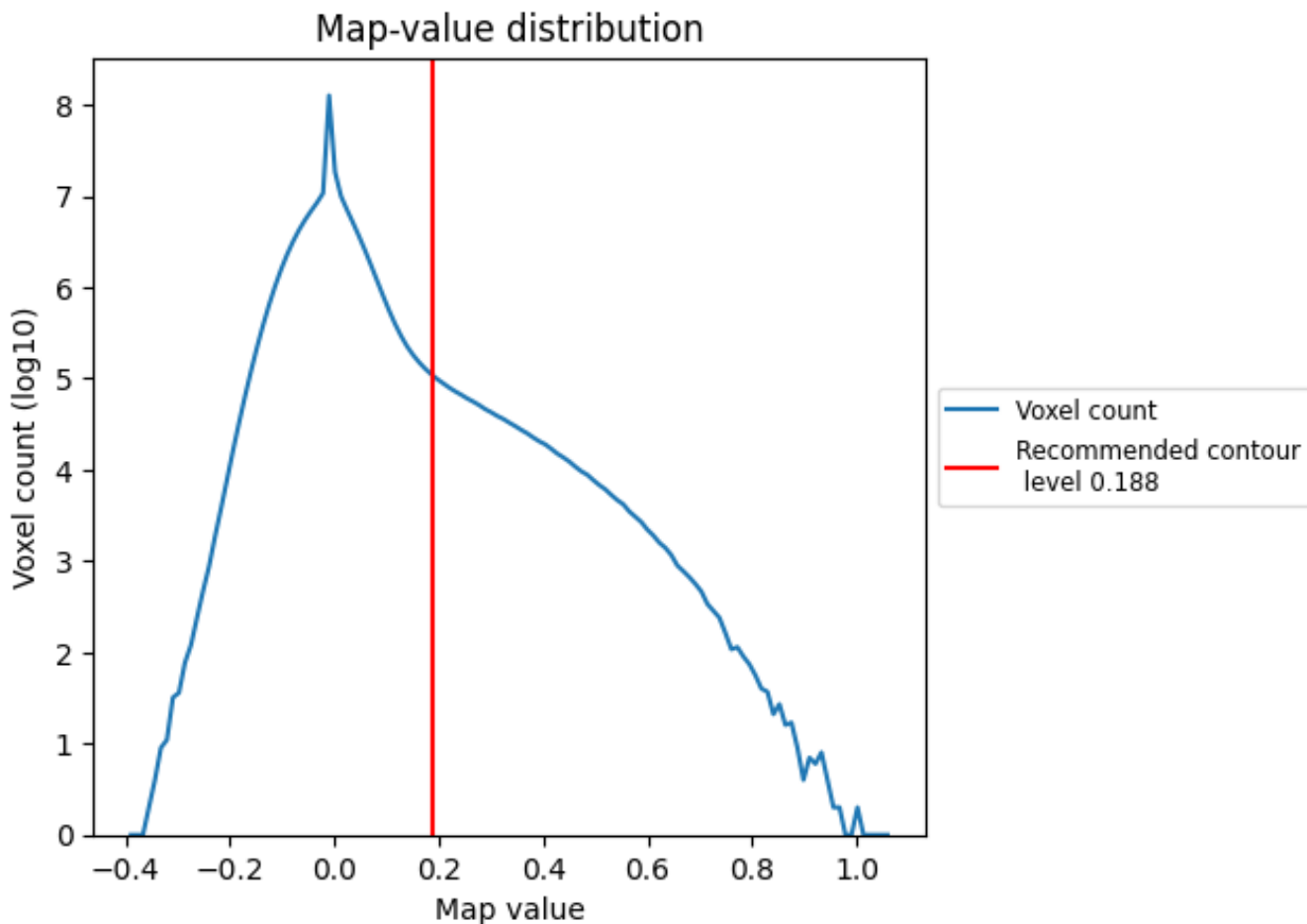
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

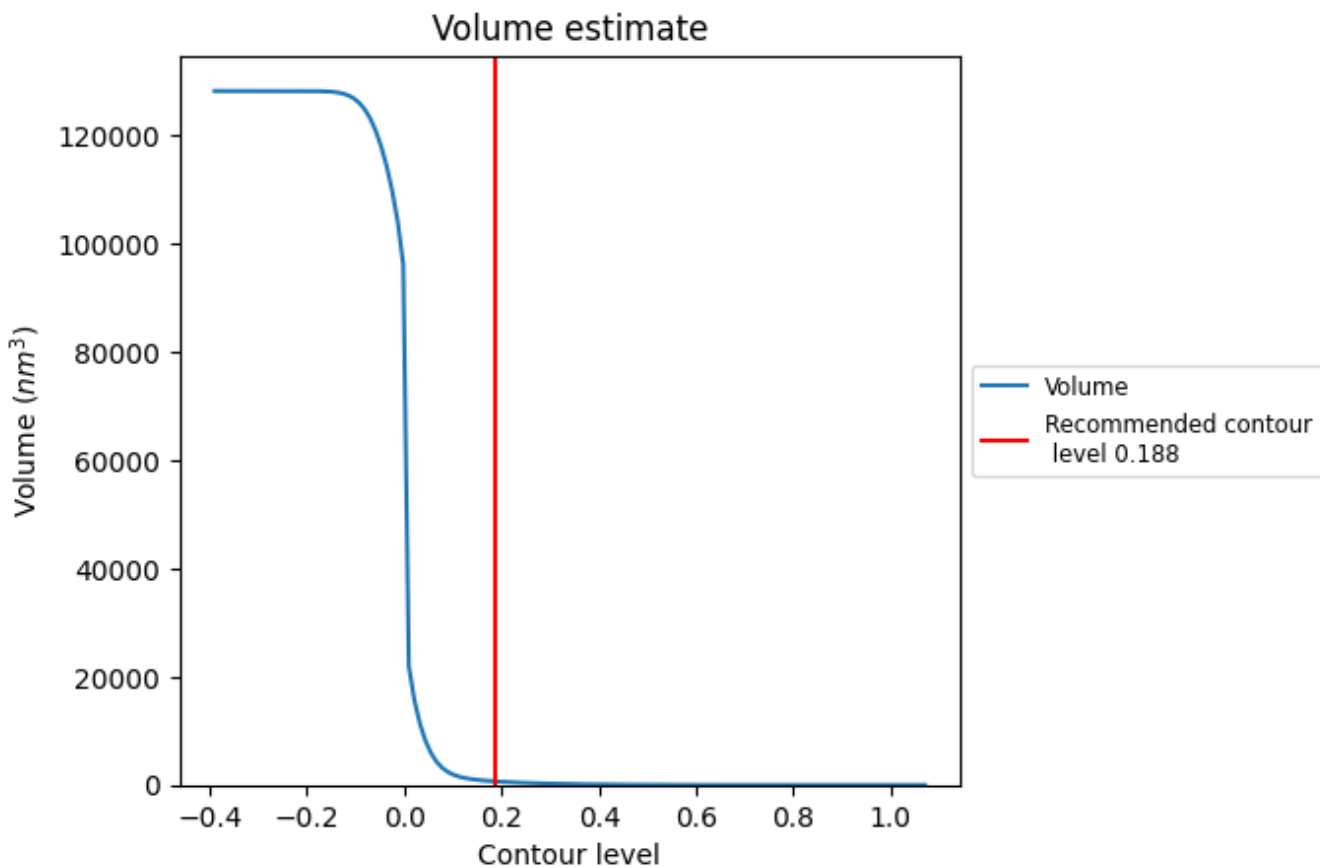
This section contains the results of statistical analysis of the map.

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



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

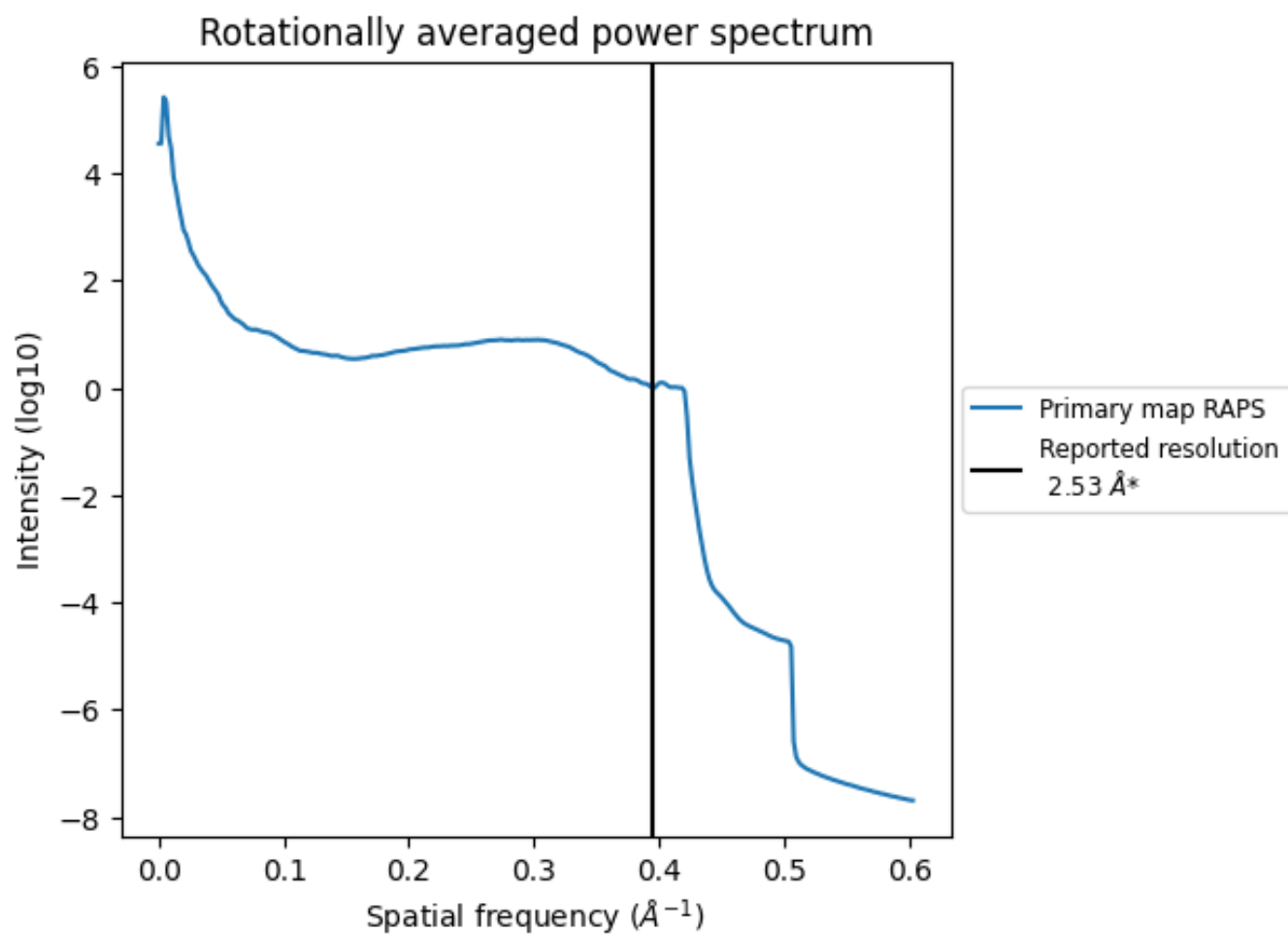
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $654 \text{ nm}^3$ ; this corresponds to an approximate mass of 590 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  $0.395 \text{\AA}^{-1}$

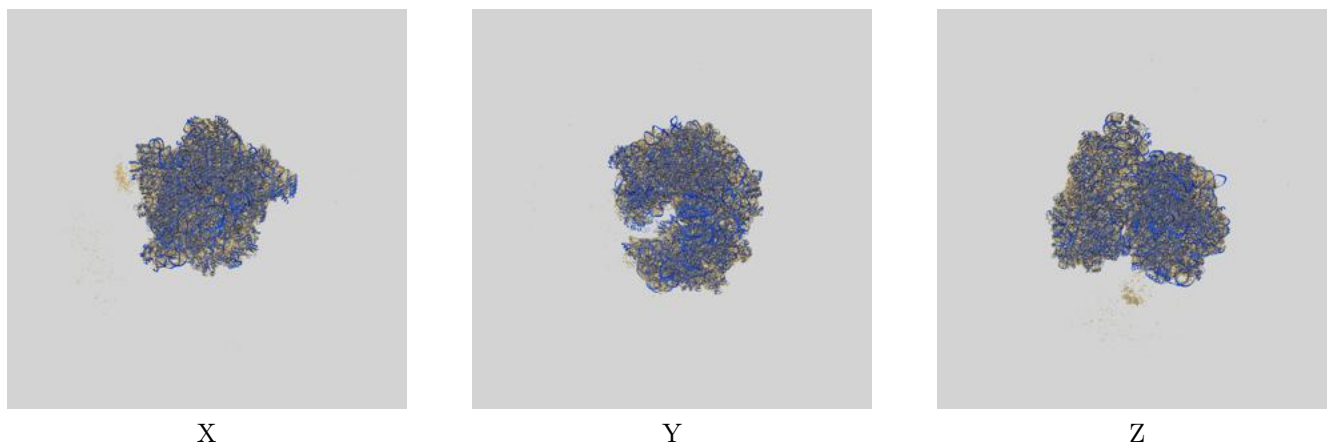
## 8 Fourier-Shell correlation

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

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

This section contains information regarding the fit between EMDB map EMD-47668 and PDB model 9E7F. Per-residue inclusion information can be found in section 3 on page 24.

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



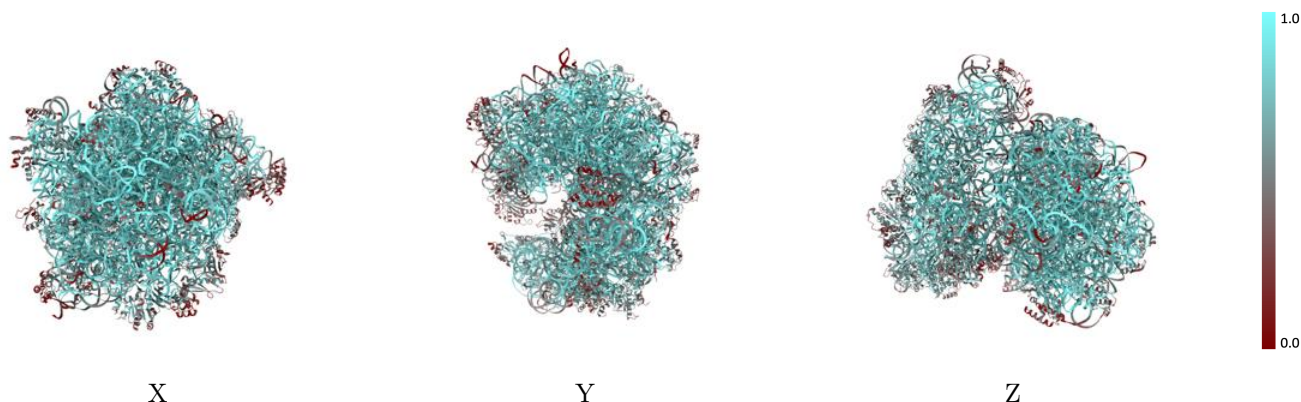
The images above show the 3D surface view of the map at the recommended contour level 0.188 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



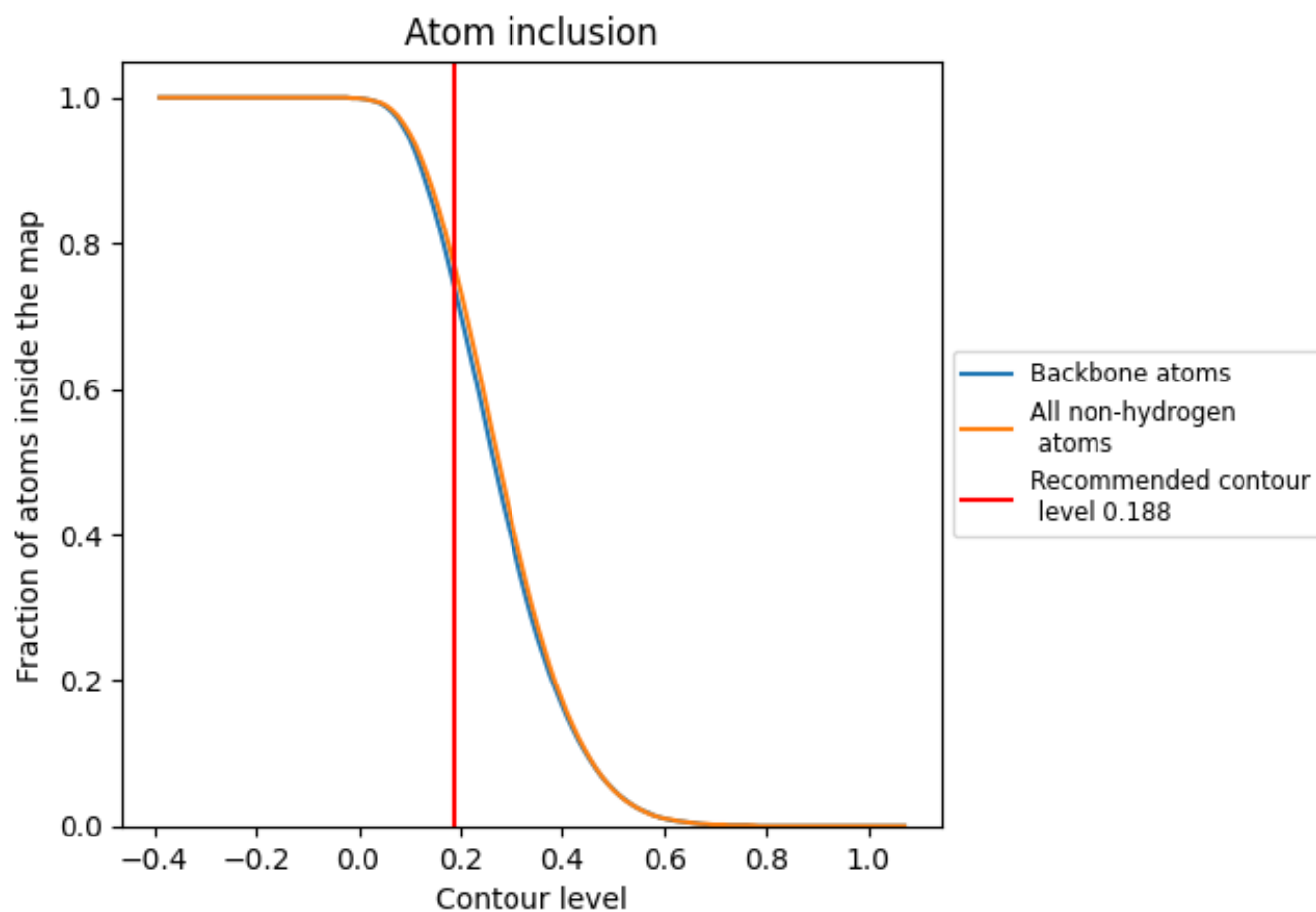
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.188).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 77% 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 (0.188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7700	 0.6030
1	 0.8910	 0.6350
2	 0.6920	 0.5650
3	 0.4220	 0.4750
4	 0.8440	 0.5760
AA	 0.8280	 0.6530
AB	 0.7950	 0.6530
AC	 0.7410	 0.6350
AD	 0.2020	 0.4570
AE	 0.5100	 0.5950
AF	 0.4580	 0.5650
AG	 0.7480	 0.6370
AH	 0.7520	 0.6410
AI	 0.7720	 0.6440
AJ	 0.4840	 0.5610
AK	 0.4310	 0.5540
AL	 0.6600	 0.6120
AM	 0.8060	 0.6480
AN	 0.6810	 0.6320
AO	 0.4550	 0.5580
AP	 0.7480	 0.6370
AQ	 0.7460	 0.6310
AR	 0.5790	 0.6000
AS	 0.8260	 0.6540
AT	 0.8300	 0.6600
AU	 0.7370	 0.6420
AV	 0.7000	 0.6210
AW	 0.7970	 0.6430
AX	 0.6020	 0.5970
AY	 0.7730	 0.6370
AZ	 0.6060	 0.5870
Aa	 0.7480	 0.6340
Ab	 0.7570	 0.6390
Ac	 0.8410	 0.6380
Ad	 0.9560	 0.6920



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Chain	Atom inclusion	Q-score
Ae	 0.6530	 0.6210
Af	 0.8930	 0.6670
Ag	 0.5960	 0.6070
Ah	 0.7760	 0.6480
Ai	 0.7470	 0.6250
Aj	 0.5370	 0.5970
Ak	 0.6110	 0.6030
BA	 0.5380	 0.5450
BB	 0.5530	 0.5340
BC	 0.3510	 0.4920
BD	 0.6750	 0.5850
BE	 0.6780	 0.5920
BF	 0.6970	 0.5820
BG	 0.3110	 0.4760
BH	 0.6850	 0.5780
BI	 0.7840	 0.5970
BJ	 0.6580	 0.5920
BK	 0.6830	 0.5600
BL	 0.4290	 0.5440
BM	 0.6520	 0.5560
BN	 0.6300	 0.5750
BO	 0.5240	 0.5370
BP	 0.4430	 0.4860
BQ	 0.6230	 0.5750
BR	 0.6240	 0.5800
BS	 0.3820	 0.4680
BT	 0.5620	 0.5480
BU	 0.7270	 0.5880
BV	 0.4530	 0.5290
BW	 0.5990	 0.5550
BX	 0.2620	 0.4780
BY	 0.6170	 0.5730
BZ	 0.5740	 0.5300
Ba	 0.5430	 0.5440
Bb	 0.2580	 0.4540
Bc	 0.6290	 0.5630