



wwPDB EM Validation Summary Report ⓘ

Jun 1, 2026 – 05:30 pm BST

PDB ID : 28LN / pdb_000028ln
EMDB ID : EMD-56598
Title : XBP1u-stalled RPL4 RNC in complex with NAC
Authors : Santos, J.; Guennigmann, M.; Gora, R.J.; Iljina, M.; Predin, M.; Kotan, I.E.;
De, P.; Choudhary, D.; Jang, J.; Tippmann, F.; Hins, C.; Ban, N.; Tans, S.J.;
Shan, S.; Kramer, G.; Bukau, B.
Deposited on : 2026-02-05
Resolution : 2.70 Å (reported)
Based on initial models : 6r7q, 7qwr, 8qoi

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

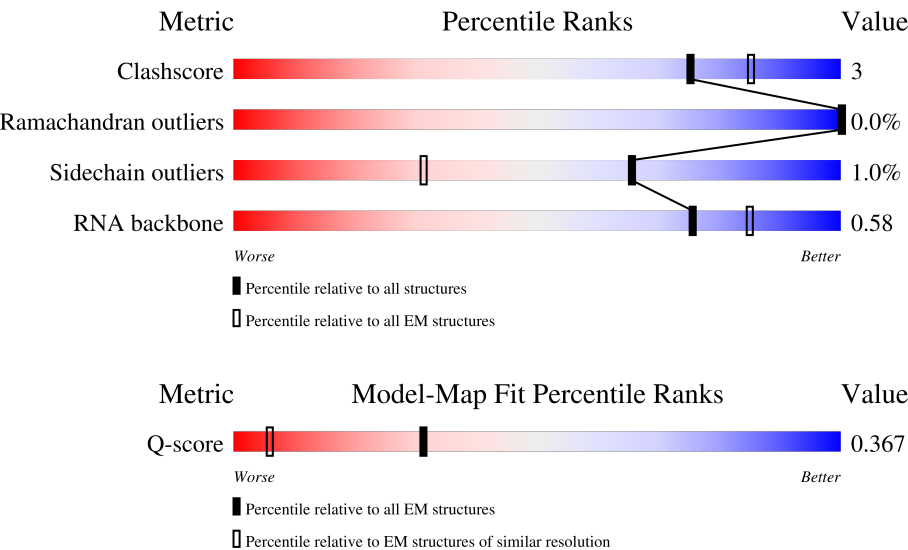
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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

Mol	Chain	Length	Quality of chain
1	B1	184	
2	B2	76	
3	B4	6	

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Mol	Chain	Length	Quality of chain
4	B5	5069	
5	B7	120	
6	B8	157	
7	BA	257	
8	BB	403	
9	BC	427	
10	BD	297	
11	BE	288	
12	BF	248	
13	BG	266	
14	BH	192	
15	BI	214	
16	BJ	178	
17	BL	211	
18	BM	215	
19	BN	204	
20	BO	203	
21	BP	184	
22	BQ	188	
23	BR	196	
24	BS	176	
25	BT	160	
26	BU	128	
27	BV	140	
28	BW	157	

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Mol	Chain	Length	Quality of chain
29	BX	156	
30	BY	145	
31	BZ	136	
32	Ba	148	
33	Bb	159	
34	Bc	115	
35	Bd	125	
36	Be	135	
37	Bf	110	
38	Bg	117	
39	Bh	123	
40	Bi	105	
41	Bj	97	
42	Bk	70	
43	Bl	51	
44	Bm	128	
45	Bo	106	
46	Bp	92	
47	Br	137	
48	Bs	317	
49	Bt	165	
50	Bu	215	
51	Bv	206	
52	A2	1869	
53	AA	295	

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Mol	Chain	Length	Quality of chain
54	AB	264	
55	AC	293	
56	AD	243	
57	AE	263	
58	AF	204	
59	AG	249	
60	AH	194	
61	AI	208	
62	AJ	194	
63	AK	165	
64	AL	158	
65	AM	132	
66	AN	151	
67	AO	151	
68	AP	145	
69	AQ	146	
70	AR	135	
71	AS	152	
72	AT	145	
73	AU	119	
74	AV	84	
75	AW	130	
76	AX	143	
77	AY	133	
78	AZ	125	

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Mol	Chain	Length	Quality of chain
79	Aa	115	
80	Ab	84	
81	Ac	69	
82	Ad	56	
83	Ae	133	
84	Af	156	
85	Ag	317	
86	Ah	25	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 220645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein uL4,X-box-binding protein 1, luminal form,X-box-binding protein 1, luminal form,X-box-binding protein 1, luminal form.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B1	34	Total	C	N	O	S	0	0
			283	187	48	45	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	178	CYS	PRO	conflict	UNP P17861
B1	179	ALA	SER	conflict	UNP P17861

- Molecule 2 is a RNA chain called tRNA-Met-CAT.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B2	76	Total	C	N	O	P	0	0
			1638	736	288	538	76		

- Molecule 3 is a RNA chain called mRNA fragment (6-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B4	6	Total	C	N	O	P	0	0
			127	57	21	43	6		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B5	3638	Total	C	N	O	P	0	0
			78039	34791	14254	25356	3638		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B7	120	Total	C	N	O	P	0	0
			2570	1141	456	851	122		

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B8	156	Total	C	N	O	P	0	0
			3320	1482	585	1097	156		

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BA	248	Total	C	N	O	S	0	0
			1899	1189	389	315	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 9 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BC	367	Total	C	N	O	S	0	0
			2919	1835	582	488	14		

- Molecule 10 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BD	293	Total	C	N	O	S	0	0
			2386	1510	435	427	14		

- Molecule 11 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BE	221	Total	C	N	O	S	0	0
			1773	1142	335	292	4		

- Molecule 12 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BF	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 13 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BG	240	Total	C	N	O	S	0	0
			1927	1229	370	324	4		

- Molecule 14 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 15 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BI	205	Total	C	N	O	S	0	0
			1660	1054	319	274	13		

- Molecule 16 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BJ	171	Total	C	N	O	S	0	0
			1371	867	256	242	6		

- Molecule 17 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 18 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 19 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 20 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 21 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 22 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 23 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 24 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BS	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 25 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 26 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BU	104	Total	C	N	O	S	0	0
			851	544	150	155	2		

- Molecule 27 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 28 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BW	122	Total	C	N	O	S	0	0
			997	622	203	168	4		

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BX	126	Total	C	N	O	S	0	0
			1031	658	196	176	1		

- Molecule 30 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BY	132	Total	C	N	O	S	0	0
			1102	692	223	184	3		

- Molecule 31 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 32 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ba	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 33 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bb	99	Total	C	N	O	S	0	0
			809	503	177	125	4		

- Molecule 34 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bc	106	Total	C	N	O	S	0	0
			824	523	146	148	7		

- Molecule 35 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bd	107	Total	C	N	O	S	0	0
			883	558	171	152	2		

- Molecule 36 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Be	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 37 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 38 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bg	109	Total	C	N	O	S	0	0
			868	544	179	139	6		

- Molecule 39 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 40 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bi	99	Total	C	N	O	S	0	0
			813	509	173	126	5		

- Molecule 41 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 42 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bk	68	Total	C	N	O	S	0	0
			559	360	101	97	1		

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bl	50	Total	C	N	O	S	1	0
			451	286	100	64	1		

- Molecule 44 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bm	51	Total	C	N	O	S	0	0
			419	260	88	65	6		

- Molecule 45 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bo	102	Total	C	N	O	S	1	0
			843	528	174	135	6		

- Molecule 46 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bp	88	Total	C	N	O	S	0	0
			681	430	131	113	7		

- Molecule 47 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Br	124	Total	C	N	O	S	0	0
			990	614	205	167	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Br	2	ACE	-	acetylation	UNP P46779

- Molecule 48 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bs	196	Total	C	N	O	S	0	0
			1506	958	263	276	9		

- Molecule 49 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bt	156	Total	C	N	O	S	0	0
			1178	733	221	220	4		

- Molecule 50 is a protein called Nascent polypeptide-associated complex subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bu	66	Total	C	N	O	S	0	0
			522	330	95	96	1		

- Molecule 51 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bv	109	Total	C	N	O	S	0	0
			846	528	157	157	4		

- Molecule 52 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	A2	1779	Total	C	N	O	P	0	0
			38027	16999	6818	12431	1779		

- Molecule 53 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AA	217	Total	C	N	O	S	0	0
			1708	1085	299	316	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	2	ACE	-	acetylation	UNP P08865

- Molecule 54 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AB	223	Total	C	N	O	S	0	0
			1806	1146	326	320	14		

- Molecule 55 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AC	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 56 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AD	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 57 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 58 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AF	192	Total	C	N	O	S	0	0
			1517	948	287	275	7		

- Molecule 59 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AG	240	Total	C	N	O	S	0	0
			1945	1212	393	333	7		

- Molecule 60 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AH	188	Total	C	N	O	S	0	0
			1515	966	279	269	1		

- Molecule 61 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AI	203	Total	C	N	O	S	0	0
			1670	1048	329	288	5		

- Molecule 62 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AJ	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 63 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AK	97	Total	C	N	O	S	0	0
			816	533	144	133	6		

- Molecule 64 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AL	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 65 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AM	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 66 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 67 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	138	IAS	ASP	modified residue	UNP P62263

- Molecule 68 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AP	127	Total	C	N	O	S	0	0
			1044	663	197	177	7		

- Molecule 69 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AQ	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 70 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AR	134	Total	C	N	O	S	0	0
			1082	680	201	197	4		

- Molecule 71 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AS	146	Total	C	N	O	S	0	0
			1200	753	242	204	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	2	ACE	-	acetylation	UNP P62269

- Molecule 72 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AT	144	Total	C	N	O	S	0	0
			1123	704	217	199	3		

- Molecule 73 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 74 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AV	84	Total	C	N	O	S	0	0
			639	395	117	122	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	0	ACE	-	acetylation	UNP P63220

- Molecule 75 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 76 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AX	141	Total	C	N	O	S	1	0
			1105	698	220	184	3		

- Molecule 77 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AY	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 78 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AZ	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 79 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 80 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ab	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 81 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Ac	65	Total	C	N	O	S	0	0
			512	311	103	96	2		

- Molecule 82 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Ad	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 83 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Ae	57	Total	C	N	O	S	0	0
			451	279	99	72	1		

- Molecule 84 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Af	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 85 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Ag	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 86 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ah	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	B5	285	Total 285	Mg 285	0
87	B7	4	Total 4	Mg 4	0
87	B8	6	Total 6	Mg 6	0
87	BA	3	Total 3	Mg 3	0
87	BB	1	Total 1	Mg 1	0
87	BN	1	Total 1	Mg 1	0
87	BV	1	Total 1	Mg 1	0
87	Ba	1	Total 1	Mg 1	0
87	Be	1	Total 1	Mg 1	0
87	Bf	2	Total 2	Mg 2	0
87	Bg	1	Total 1	Mg 1	0
87	Bj	1	Total 1	Mg 1	0
87	A2	123	Total 123	Mg 123	0
87	AI	1	Total 1	Mg 1	0
87	AX	1	Total 1	Mg 1	0

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

Mol	Chain	Residues	Atoms		AltConf
88	Bg	1	Total 1	Zn 1	0
88	Bj	1	Total 1	Zn 1	0
88	Bm	1	Total 1	Zn 1	0
88	Bo	1	Total 1	Zn 1	0
88	Bp	1	Total 1	Zn 1	0

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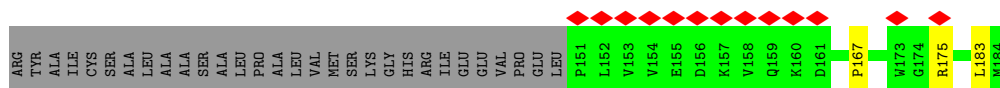
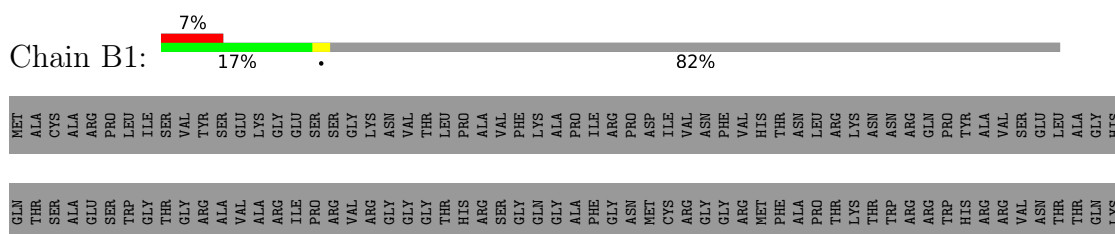
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Mol	Chain	Residues	Atoms		AltConf
88	Aa	1	Total 1	Zn 1	0
88	Ad	1	Total 1	Zn 1	0
88	Af	1	Total 1	Zn 1	0

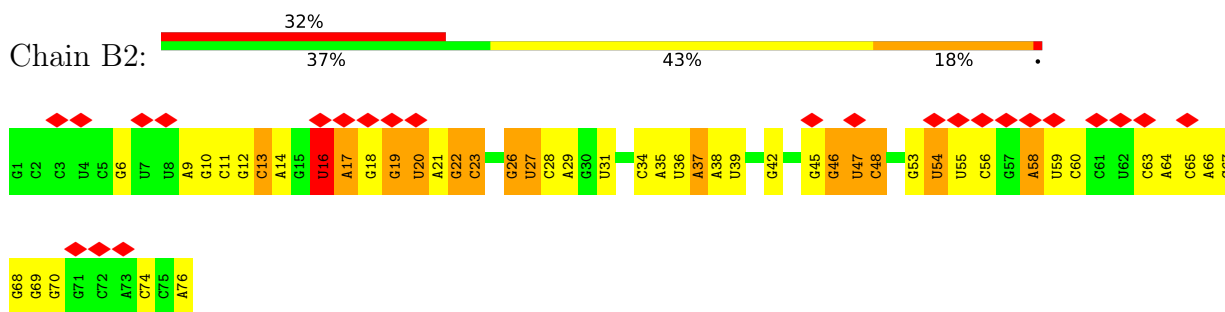
3 Residue-property plots

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

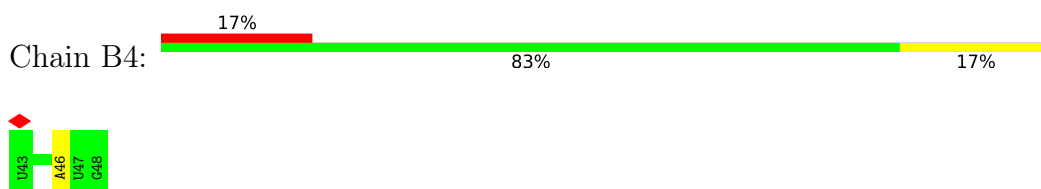
- Molecule 1: Large ribosomal subunit protein uL4,X-box-binding protein 1, luminal form,X-box-binding protein 1, luminal form,X-box-binding protein 1, luminal form



- Molecule 2: tRNA-Met-CAT



- Molecule 3: mRNA fragment (6-MER)



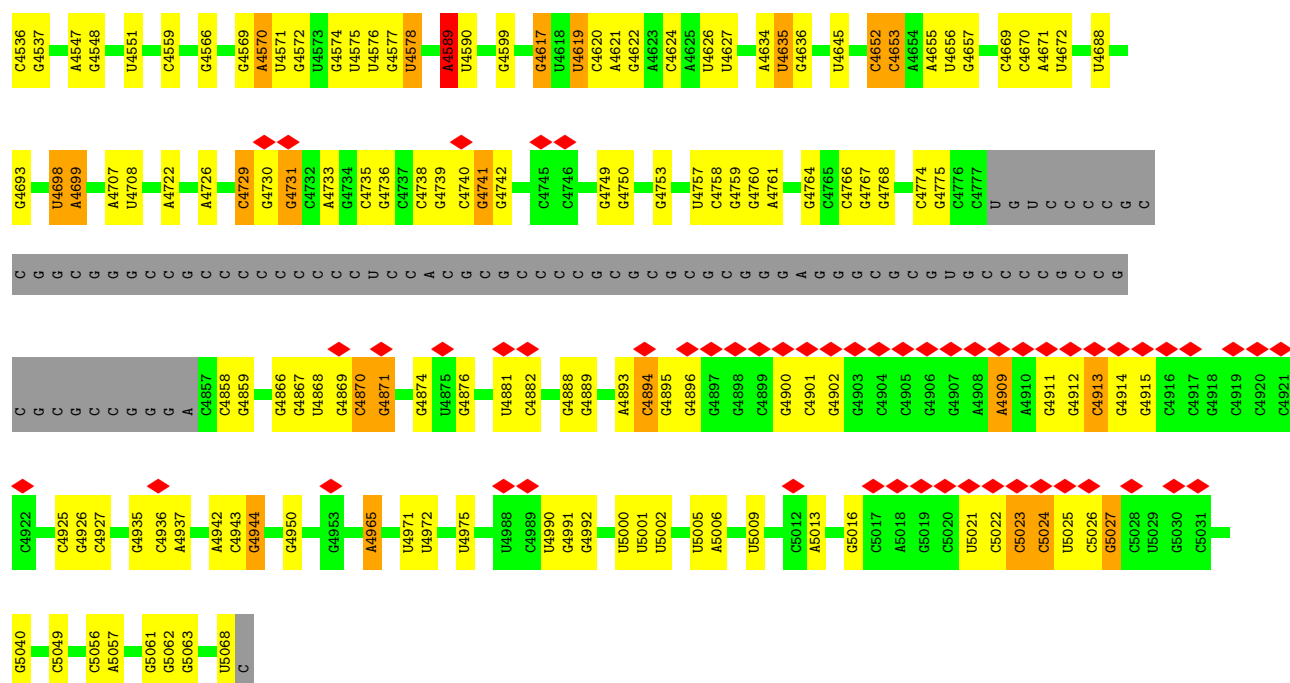
- Molecule 4: 28S rRNA



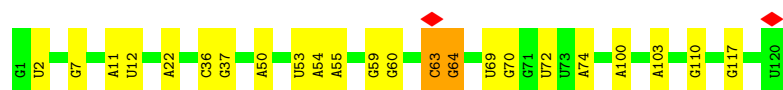
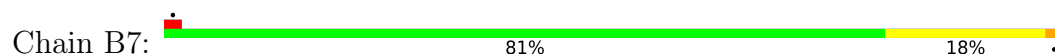


U2825	A2675	A2385	C	A2001	C1919	U1778	U1682	A1502	G1393
G2826	G2685	A2373	A	G2002	C1920	A1779	U1690	G1503	A1396
U2827	U2618	G2394	C	U2003	G1921	U1780	G1690	U1513	A1397
G2828	U2666	G2394	C	G2004	C1930	U1781	G1696	A1514	G1398
G2829	G2687	U2397	C	U2005	A1931	C1784	G1697	A1517	C1401
U2836	G2693	A2400	C	U2006	C1934	A1785	A1697	G1521	G1402
G2837	A2694	G2400	C	U2007	G1939	A1786	A1699	A1522	G1403
U2838	A2695	U2409	C	A2008	A1940	A1787	A1700	A1523	C1406
G2842	A2696	C2409	U	A2009	A1941	U1791	C1701	A1533	G1407
A2843	G2702	G2413	C	C2010	A1944	A1792	G1702	C1534	C1408
A2844	C2703	U2414	C	A2011	G1944	A1793	C1703	U1535	U1409
G2854	G2704	G2420	C	A2012	G1945	A1801	G1704	U1536	C1410
C2855	U2705	G2420	C	A2013	U1946	A1802	C1705	U1537	G1411
A2856	U2706	C2421	C	U2014	U1953	A1803	C1706	G1538	G1414
U2707	A2422	A2422	C	C2015	G1954	A1804	C1707	C1539	G1415
G2708	G2423	U2424	C	A2016	U1958	C1811	A1708	A1540	G1418
C2709	U2424	G2433	C	C2017	A1959	C1819	C1711	A1546	A1419
G2710	G2563	G2436	C	U2018	G1960	A1820	C1712	A1559	A1418
G2711	A2564	U2436	C	C2019	C1965	C1827	C1713	G1560	C1438
G2715	G2565	G2461	C	U2020	A1966	G1828	A1718	G1573	A1442
G2716	G2566	G2462	C	C2021	G1967	U1832	C1719	A1576	A1451
G2723	U2567	C2462	C	C2022	G1968	U1833	G1720	U1577	G1452
A2724	G2568	G2468	C	A2023	A1969	G1834	U1729	U1581	G1456
G2725	G2569	C2469	C	A2024	C1970	G1835	G1740	C1589	C1457
U2740	U2574	G2470	C	A2025	G1971	A1836	A1741	A1458	A1459
G2741	G2575	G2473	C	A2032	G1972	G1841	A1742	U1590	G1474
A2742	C2582	G2474	C	G2033	U1973	G1854	U1743	U1595	C1475
G2753	G2585	U2477	C	G2038	G1974	G1854	A1748	A1612	C1476
G2758	A2586	C2477	C	G2045	G1975	C1858	A1750	G1616	G1478
G2759	C2587	G2482	C	A2046	C1976	U1859	C1754	G1623	G1481
U2760	C2588	A2483	C	U2047	C1977	U1860	U1755	C1624	C1482
G2761	A2600	U2484	C	G2054	A1978	U1861	U1756	A1630	C1483
U2762	C2612	G2485	C	G2055	U1979	G1868	U1757	A1631	C1484
A2763	C2626	U2489	C	A2068	G1980	C1869	G1760	G1632	G1485
U2768	U2631	C2490	C	C2072	G1981	A1870	C1761	G1487	G1488
C2769	U2632	G2492	C	G2075	A1982	G1871	C1762	G1640	G1491
G2770	G2639	U2493	C	C2082	A1983	C1874	G1763	G1653	G1492
G2776	A2646	U2494	C	G2084	U1985	G1884	A1764	C1660	U1493
A2786	G2651	U2494	C	G2088	C2082	G1884	A1765	U1675	G1494
U2787	G2657	G2500	C	U2089	G2082	A1896	A1766	C1676	A1496
A2788	G2657	G2502	C	G2089	G1987	C1913	G1767	U1676	G1497
U2789	G2661	C2503	C	C2090	G1988	C1914	G1768	G1679	C1500
C2803	G2668	G2504	C	G2091	A1989	G1915	A1769	G1501	G1501
C2804	U2507	U2363	C	A2092	A1990	U1917	U1770		
C2813	A2512	G2363	C	G2093	U1991	G1918	C1771		
A2814		C2364	C	A2094	C1992		U1772		
			C	G2095	C1993		C1773		
			C	U2096	G1994				
			C	G2097	C1995				
			C	G2108	U1996				
			C		A1997				
			C		A1998				
			C		G2000				

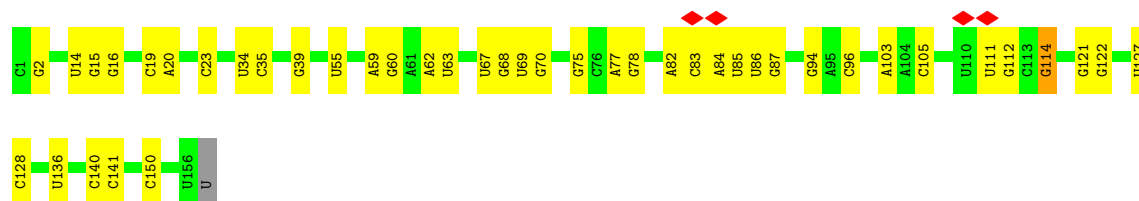




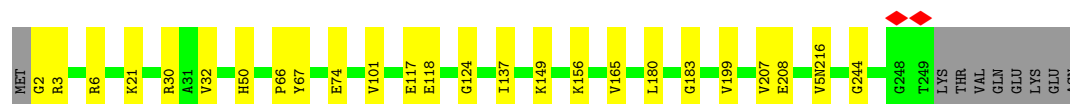
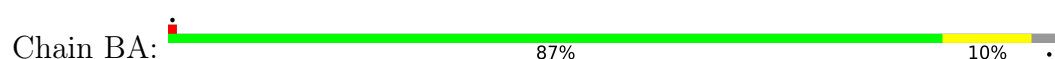
- Molecule 5: 5S rRNA



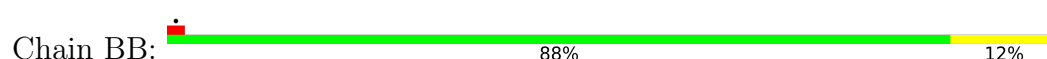
- Molecule 6: 5.8S rRNA

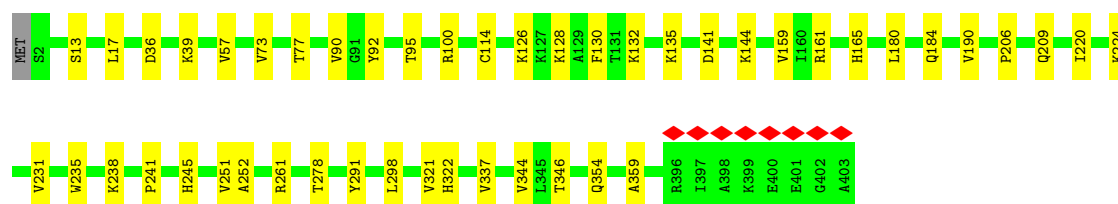


- Molecule 7: Large ribosomal subunit protein uL2

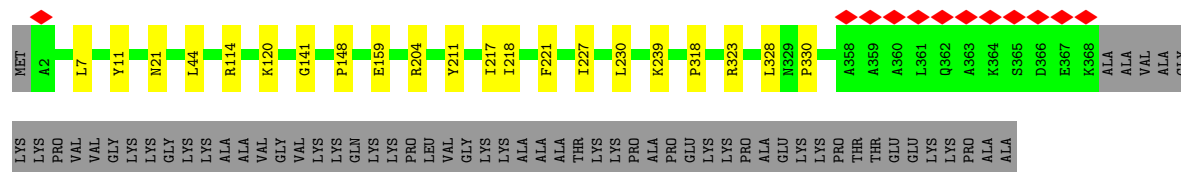
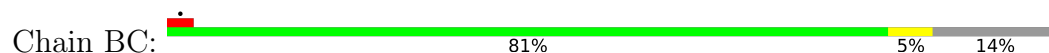


- Molecule 8: Large ribosomal subunit protein uL3

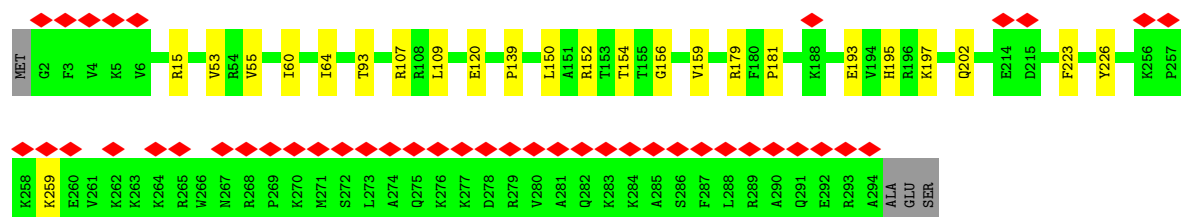




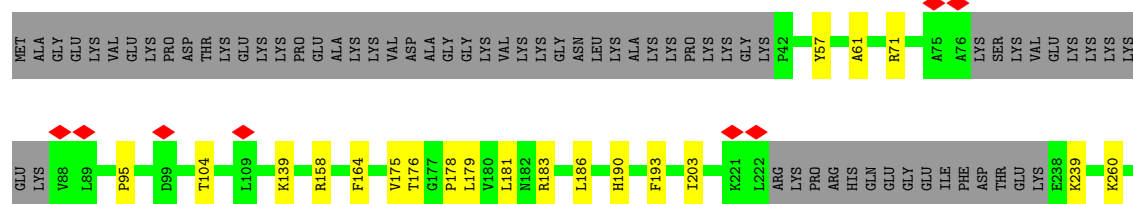
• Molecule 9: 60S ribosomal protein L4



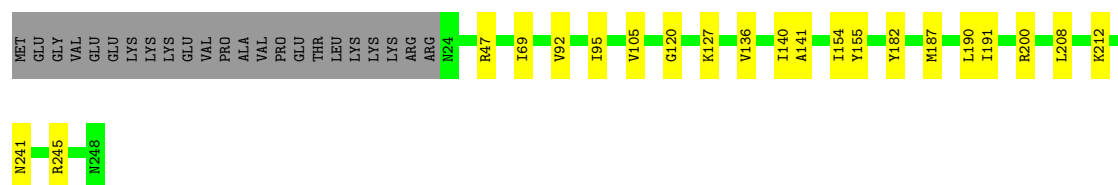
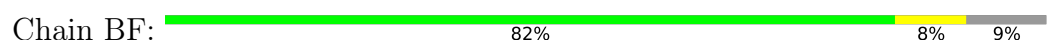
• Molecule 10: 60S ribosomal protein L5



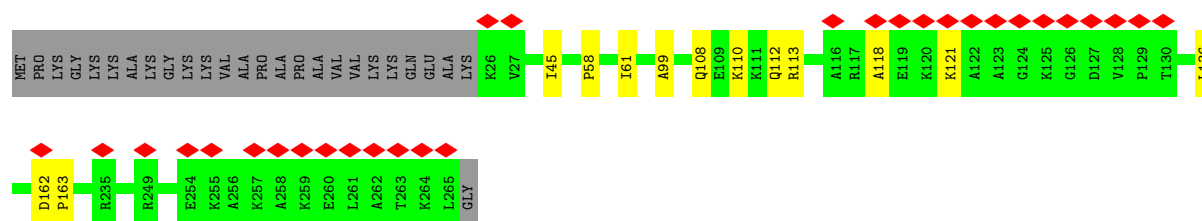
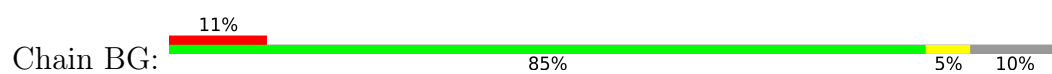
• Molecule 11: Large ribosomal subunit protein eL6



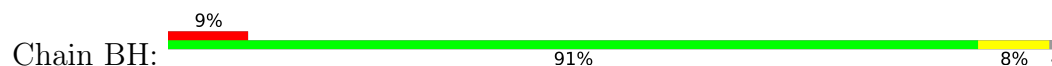
• Molecule 12: Large ribosomal subunit protein uL30



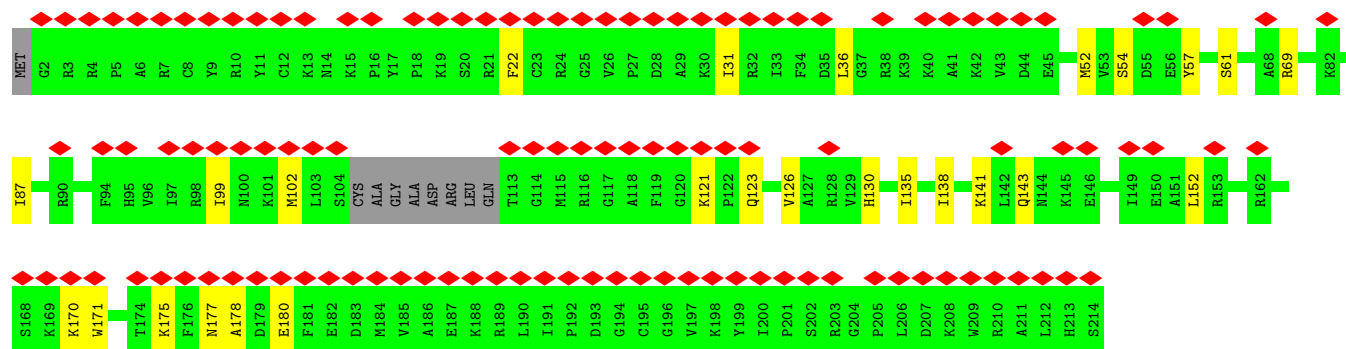
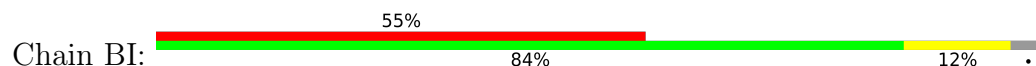
• Molecule 13: 60S ribosomal protein L7a



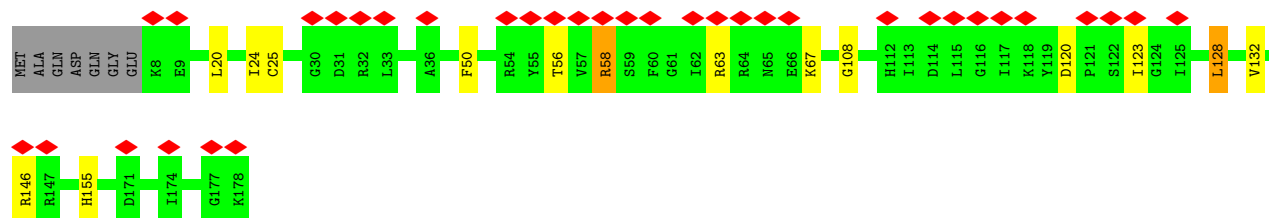
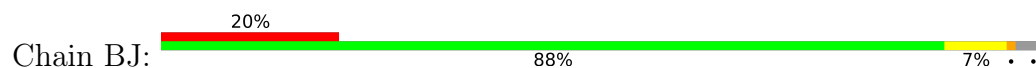
• Molecule 14: 60S ribosomal protein L9



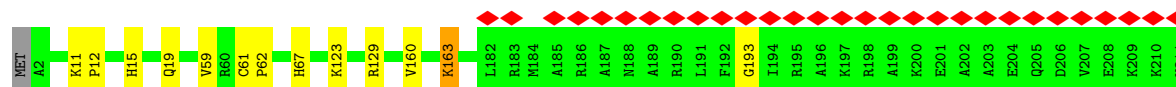
• Molecule 15: 60S ribosomal protein L10



• Molecule 16: 60S ribosomal protein L11

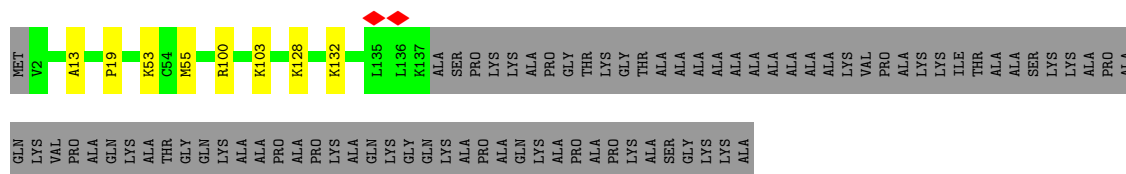


• Molecule 17: 60S ribosomal protein L13



- Molecule 18: 60S ribosomal protein L14

Chain BM:  60% 37%



- Molecule 19: 60S ribosomal protein L15

Chain BN:  90% 10%




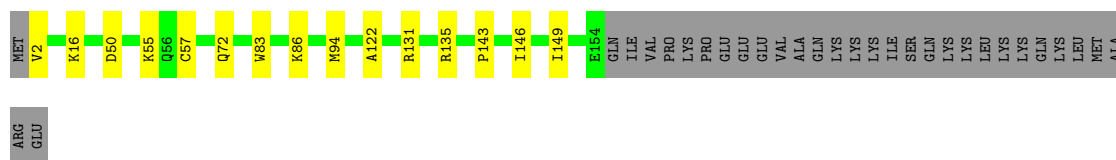
- Molecule 20: 60S ribosomal protein L13a

Chain BO:  92% 7%



- Molecule 21: 60S ribosomal protein L17

Chain BP:  75% 8% 17%




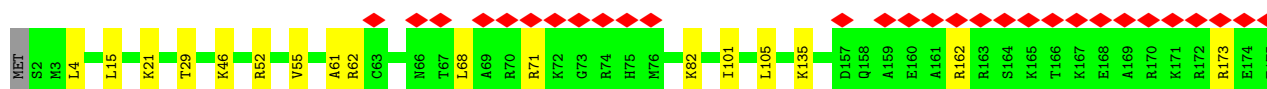
- Molecule 22: 60S ribosomal protein L18

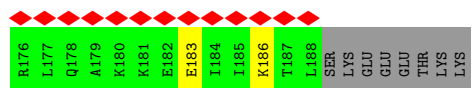
Chain BQ:  94% 6%



- Molecule 23: 60S ribosomal protein L19

Chain BR:  21% 86% 10% 5%





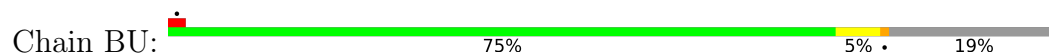
- Molecule 24: 60S ribosomal protein L18a



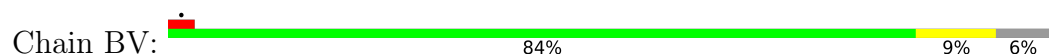
- Molecule 25: 60S ribosomal protein L21



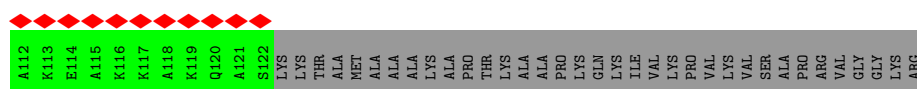
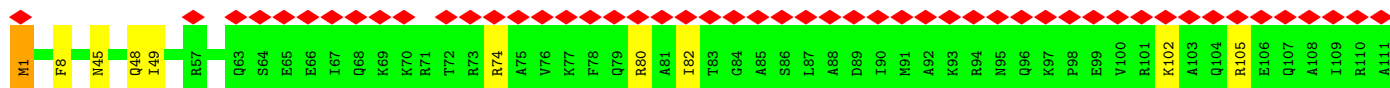
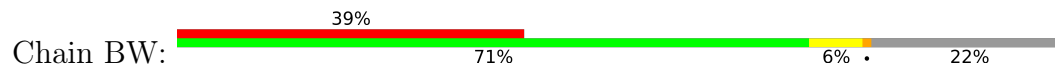
- Molecule 26: 60S ribosomal protein L22



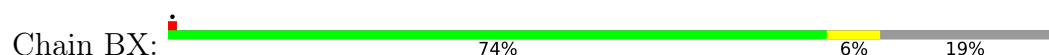
- Molecule 27: 60S ribosomal protein L23

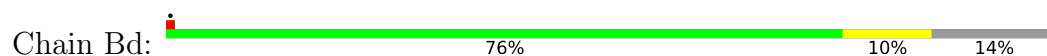


- Molecule 28: 60S ribosomal protein L24

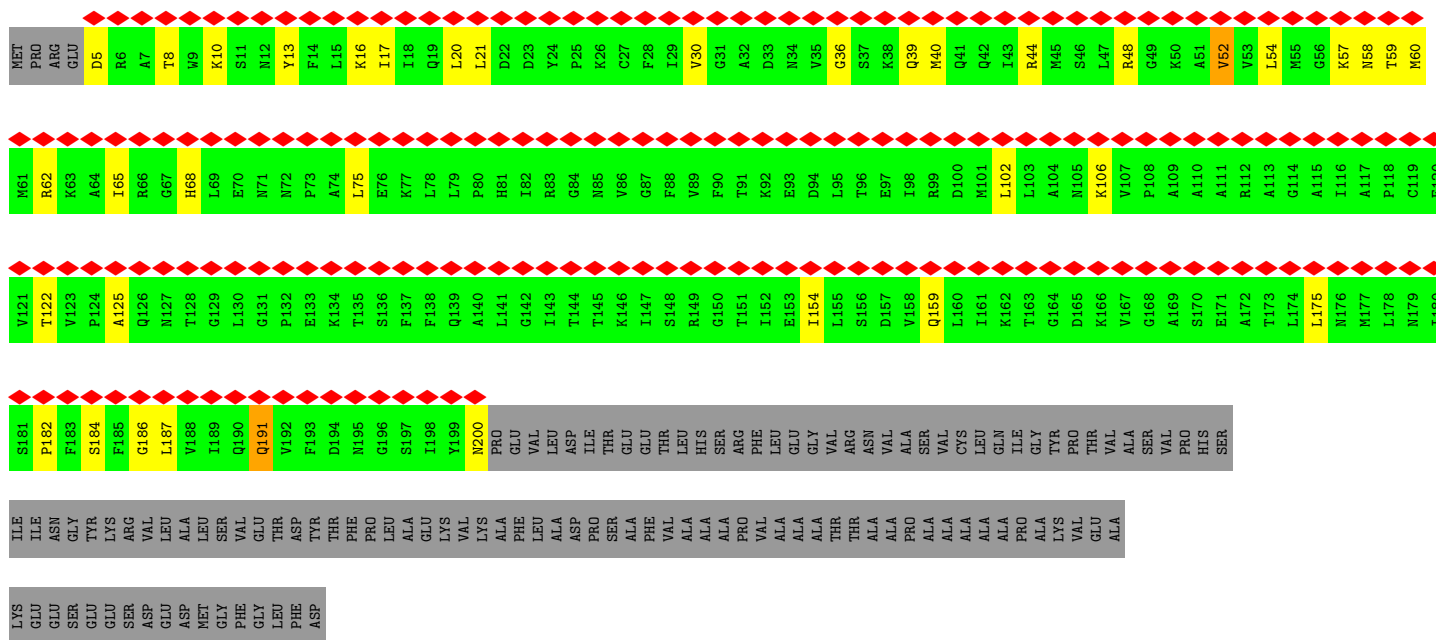


- Molecule 29: 60S ribosomal protein L23a

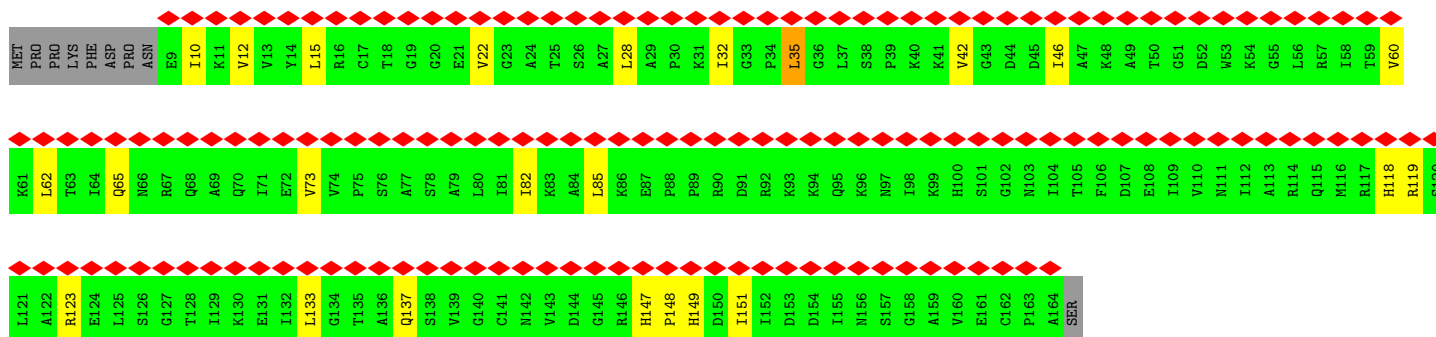
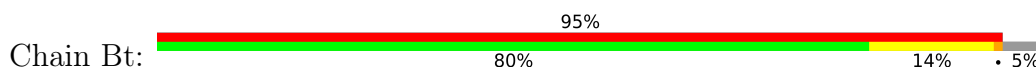




- Molecule 48: 60S acidic ribosomal protein P0

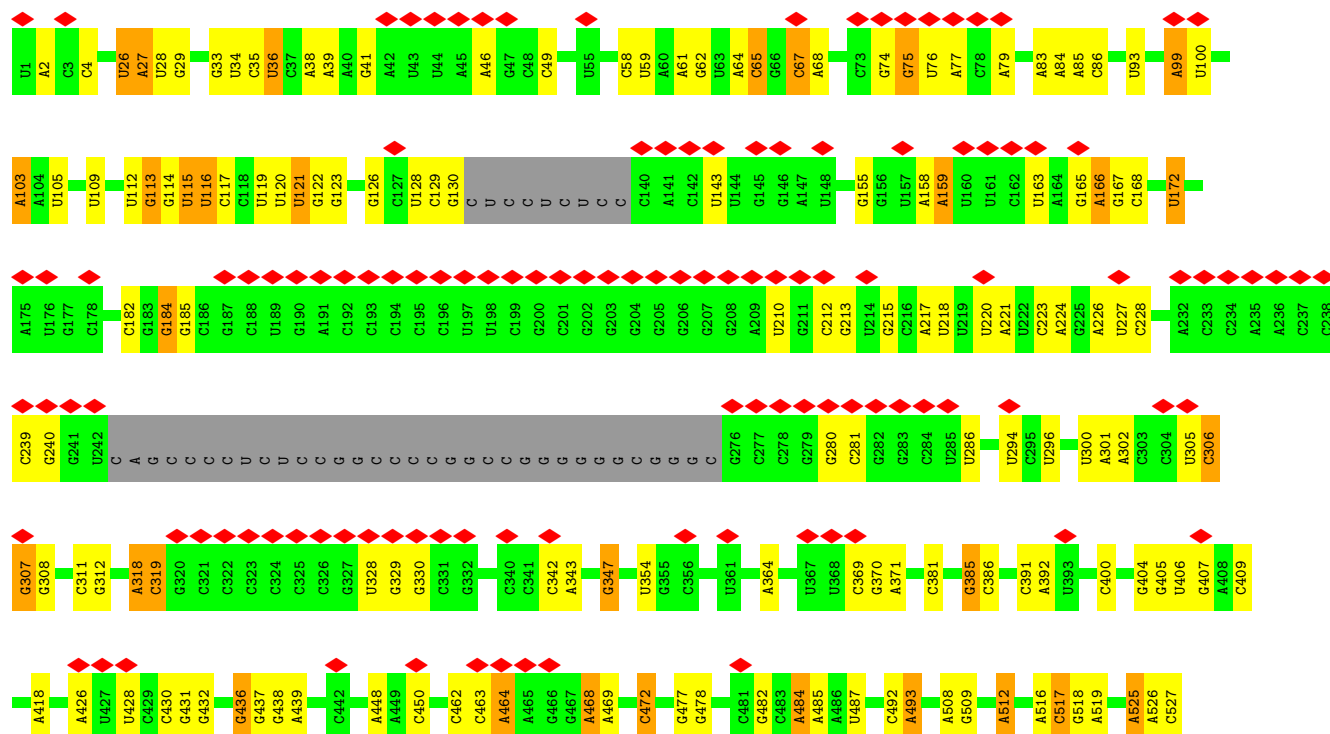


- Molecule 49: Large ribosomal subunit protein uL11

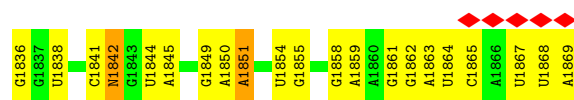


- Molecule 50: Nascent polypeptide-associated complex subunit alpha

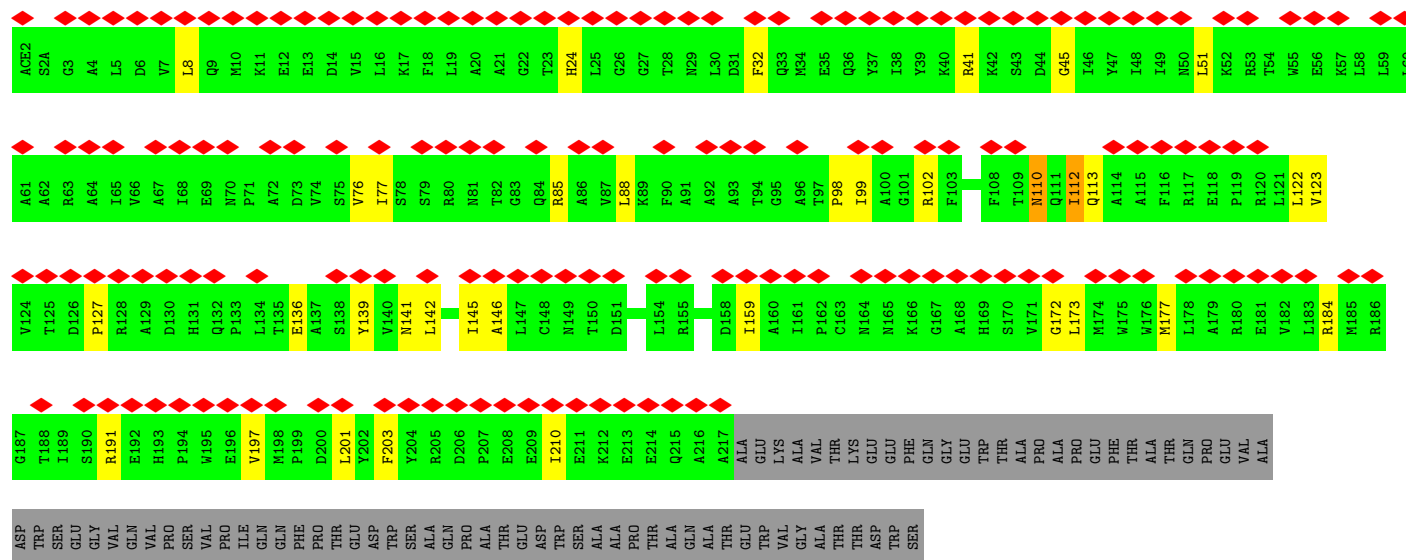


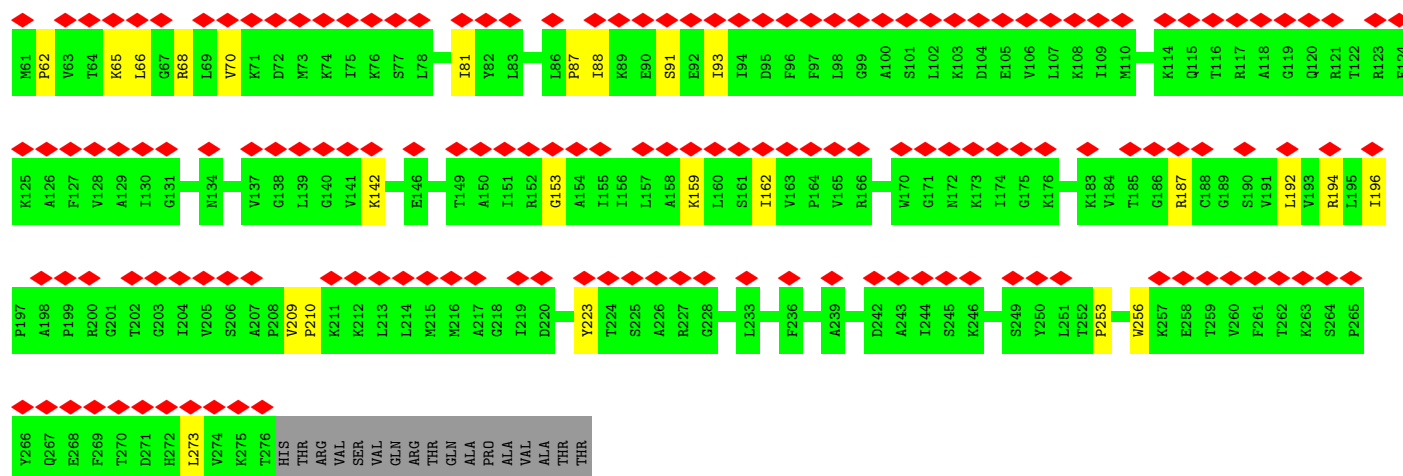


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U1520	C1521	A1522	G1536	A1537	U1543	G1552	C1553	C1554	C1557	G1558	C1559	U1560	A1561	G1570	C1574	G1575	A1579	A1580	G1584	U1585	U1586	G1587	C1593	A1594	C1597	G1600	A1601	G1606	G1610	G1611	G1612	G1613	U1621	U1622	A1623	U1624	U1625	A1630	U1631	G1632	G1639	U1643	U1647	G1748	G1749	C1750	C1751	A1822	A1823	A1824	A1825	G1829	U1830	A1831	A1832	A1835																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
G1413	A1414	C1415	C1416	C1417	C1418	C1419	A1421	C1422	C1423	C1424	C1427	G1428	C1433	C1434	C1435	C1436	A1437	A1438	A1439	U1442	U1445	U1446	G1447	A1448	A1454	A1455	G1456	C1460	G1461	U1462	U1463	G1466	C1467	C1468	A1469	U1477	U1478	U1479	A1480	A1489	U1490	G1491	G1497	U1504	G1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	U1901	U1902	U1903	U1904	U1905	U1906	U1907	U1908	U1909	U1910	U1911	U1912	U1913	U1914	U1915	U1916	U1917	U1918	U1919	U1920	U1921	U1922	U1923	U1924	U1925	U1926	U1927	U1928	U1929	U1930	U1931	U1932	U1933	U1934	U1935	U1936	U1937	U1938	U1939	U1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	U2000	U2001	U2002	U2003	U2004	U2005	U2006	U2007	U2008	U2009	U2010	U2011	U2012	U2013	U2014	U2015	U2016	U2017	U2018	U2019	U2020	U2021	U2022	U2023	U2024	U2025	U2026	U2027	U2028	U2029	U2030	U2031	U2032	U2033	U2034	U2035	U2036	U2037	U2038	U2039	U2040	U2041	U2042	U2043	U2044	U2045	U2046	U2047	U2048	U2049	U2050	U2051	U2052	U2053	U2054	U2055	U2056	U2057	U2058	U2059	U2060	U2061	U2062	U2063	U2064	U2065	U2066	U2067	U2068	U2069	U2070	U2071	U2072	U2073	U2074	U2075	U2076	U2077	U2078	U2079	U2080	U2081	U2082	U2083	U2084	U2085	U2086	U2087	U2088	U2089	U2090	U2091	U2092	U2093	U2094	U2095	U2096	U2097	U2098	U2099	U2100	U2101	U2102	U2103	U2104	U2105	U2106	U2107	U2108	U2109	U2110	U2111	U2112	U2113	U2114	U2115	U2116	U2117	U2118	U2119	U2120	U2121	U2122	U2123	U2124	U2125	U2126	U2127	U2128	U2129	U2130	U2131	U2132	U2133	U2134	U2135	U2136	U2137	U2138	U2139	U2140	U2141	U2142	U2143	U2144	U2145	U2146	U2147	U2148	U2149	U2150	U2151	U2152	U2153	U2154	U2155	U2156	U2157	U2158	U2159	U2160	U2161	U2162	U2163	U2164	U2165	U2166	U2167	U2168	U2169	U2170	U2171	U2172	U2173	U2174	U2175	U2176	U2177	U2178	U2179	U2180	U2181	U2182	U2183	U2184	U2185	U2186	U2187	U2188	U2189	U2190	U2191	U2192	U2193	U2194	U2195	U2196	U2197	U2198	U2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	U2230	U2231	U2232	U2233	U2234	U2235	U2236	U2237	U2238	U2239	U2240	U2241	U2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	U2250	U2251	U2252	U2253	U2254	U2255	U2256	U2257	U2258	U2259	U2260	U2261	U2262	U2263	U2264	U2265	U2266	U2267	U2268	U2269	U2270	U2271	U2272	U2273	U2274	U2275	U2276	U2277	U2278	U2279	U2280	U2281	U2282	U2283	U2284	U2285	U2286	U2287	U2288	U2289	U2290	U2291	U2292	U2293	U2294	U2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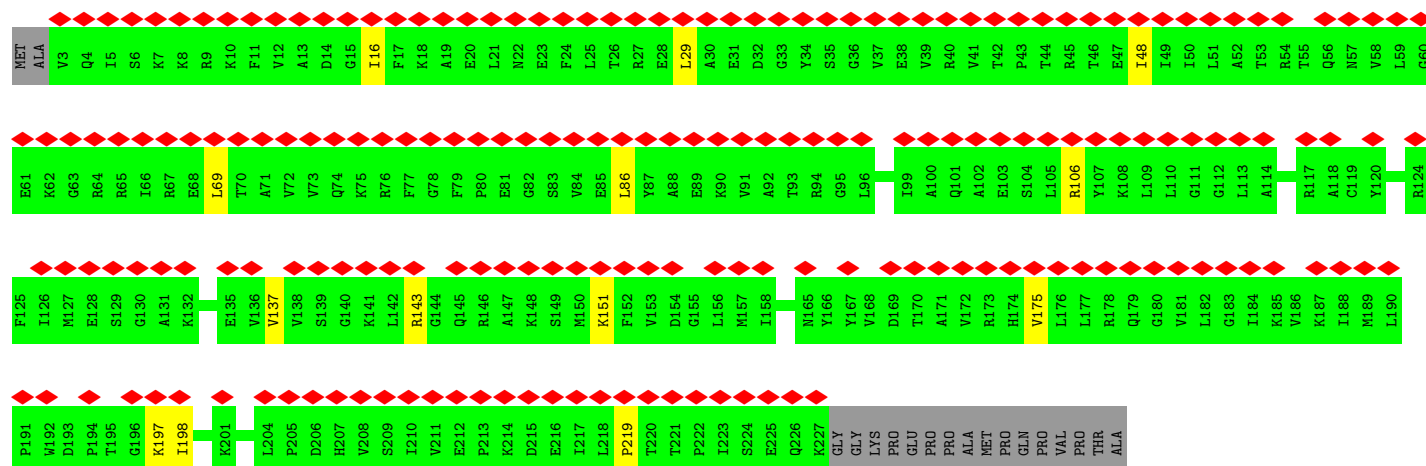
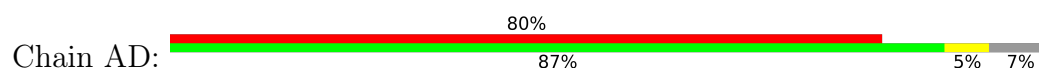


• Molecule 53: Small ribosomal subunit protein uS2

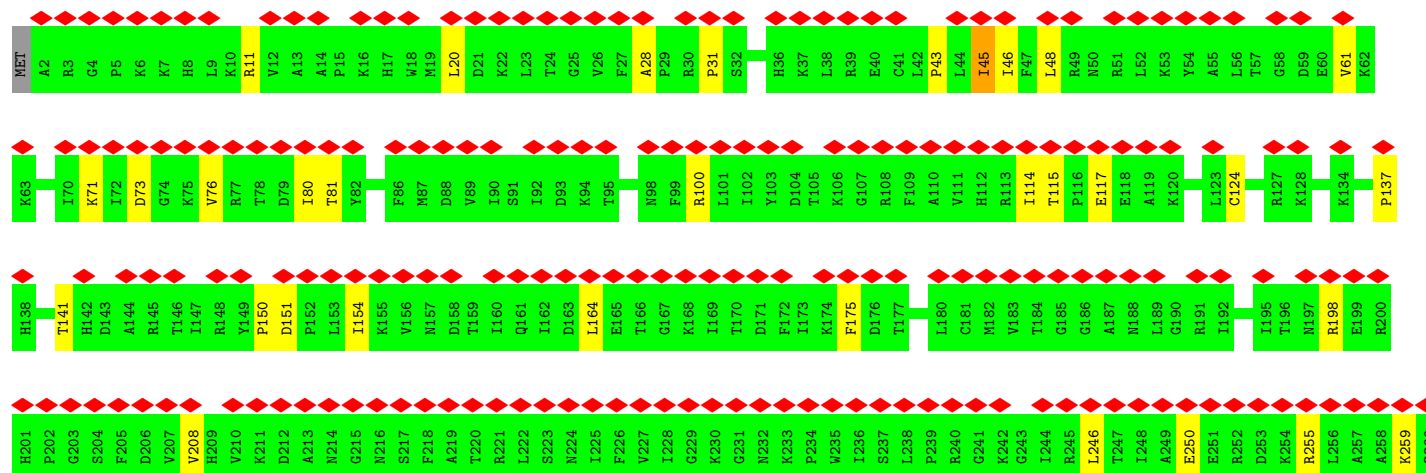
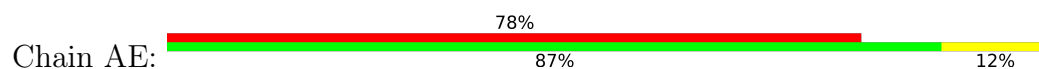




• Molecule 56: 40S ribosomal protein S3



• Molecule 57: Small ribosomal subunit protein eS4, X isoform





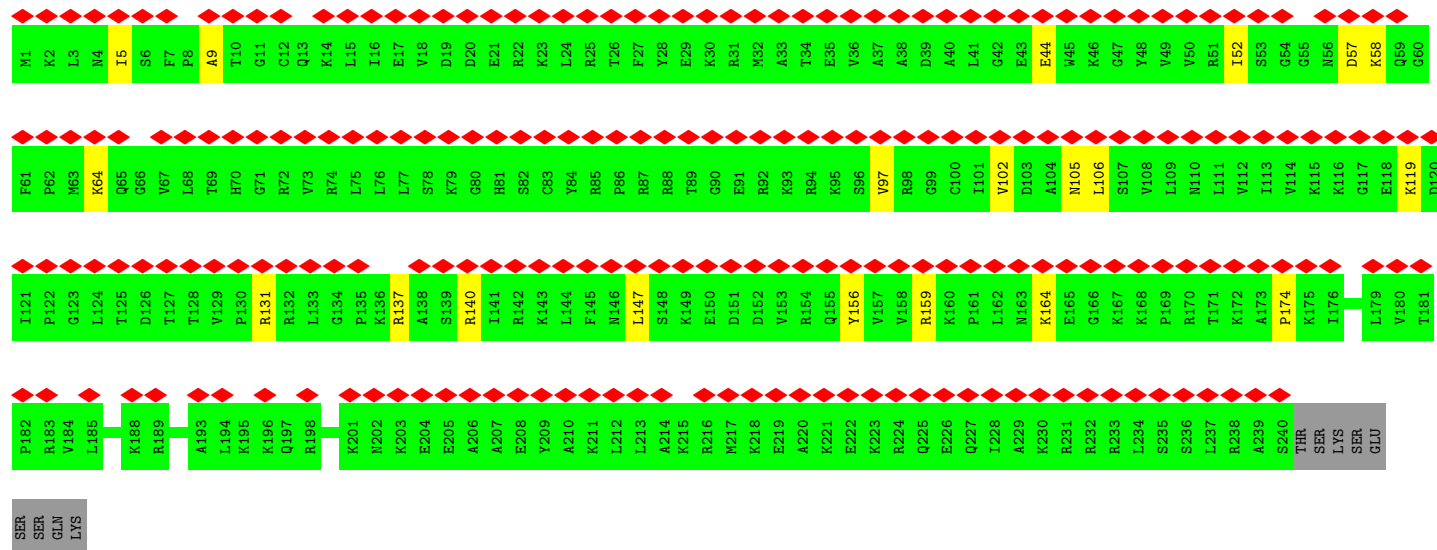
• Molecule 58: 40S ribosomal protein S5

Chain AF:



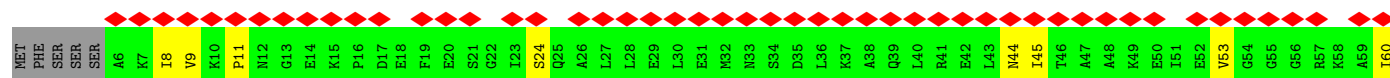
• Molecule 59: 40S ribosomal protein S6

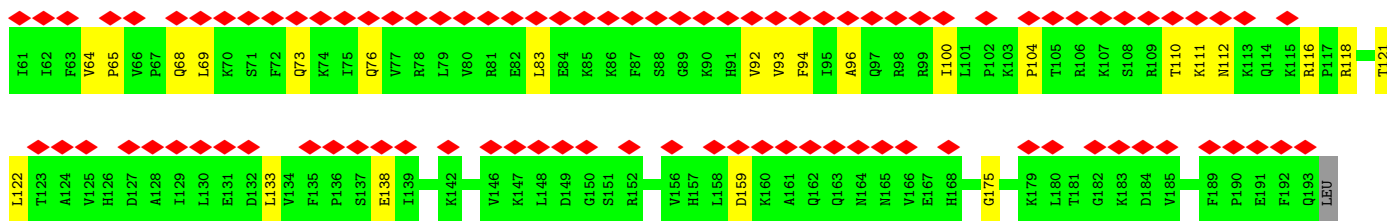
Chain AG:



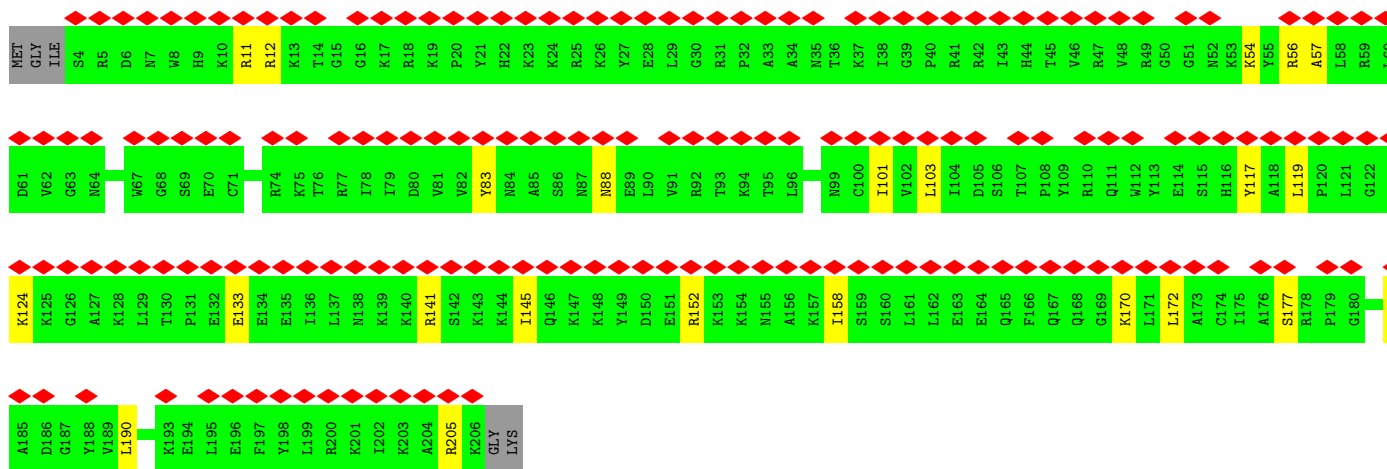
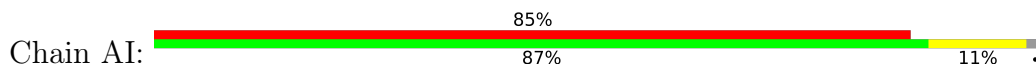
• Molecule 60: 40S ribosomal protein S7

Chain AH:

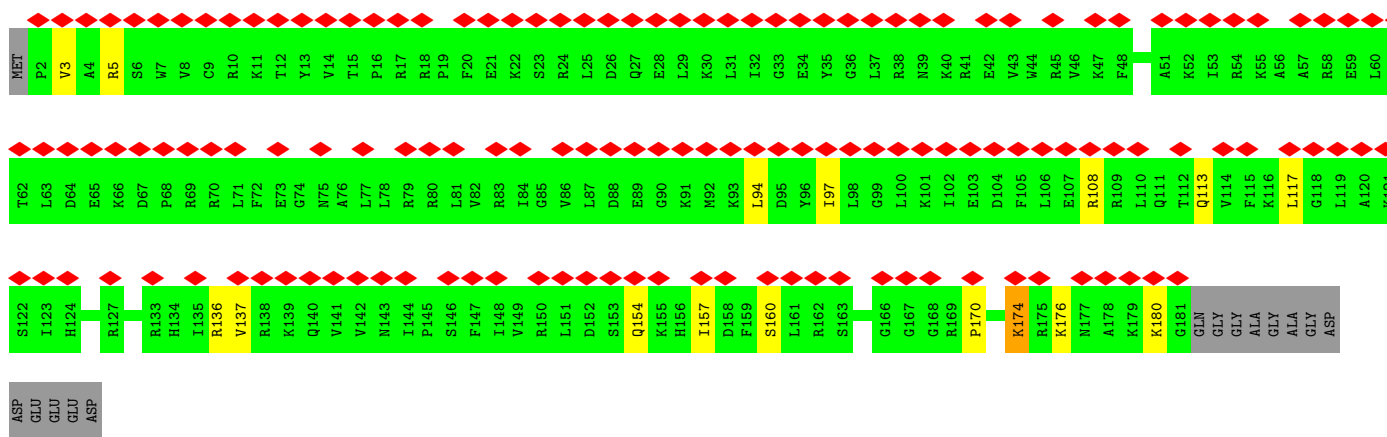
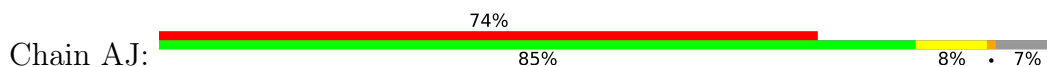




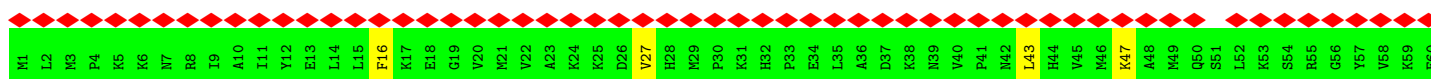
• Molecule 61: 40S ribosomal protein S8

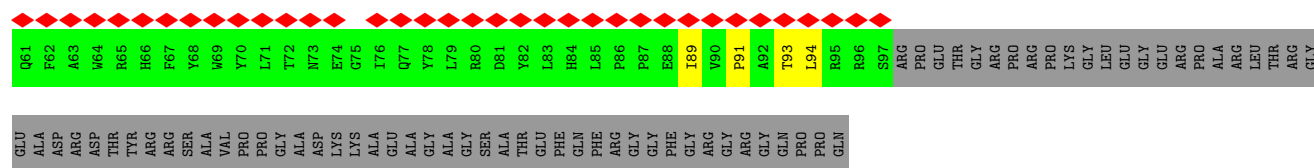


• Molecule 62: 40S ribosomal protein S9

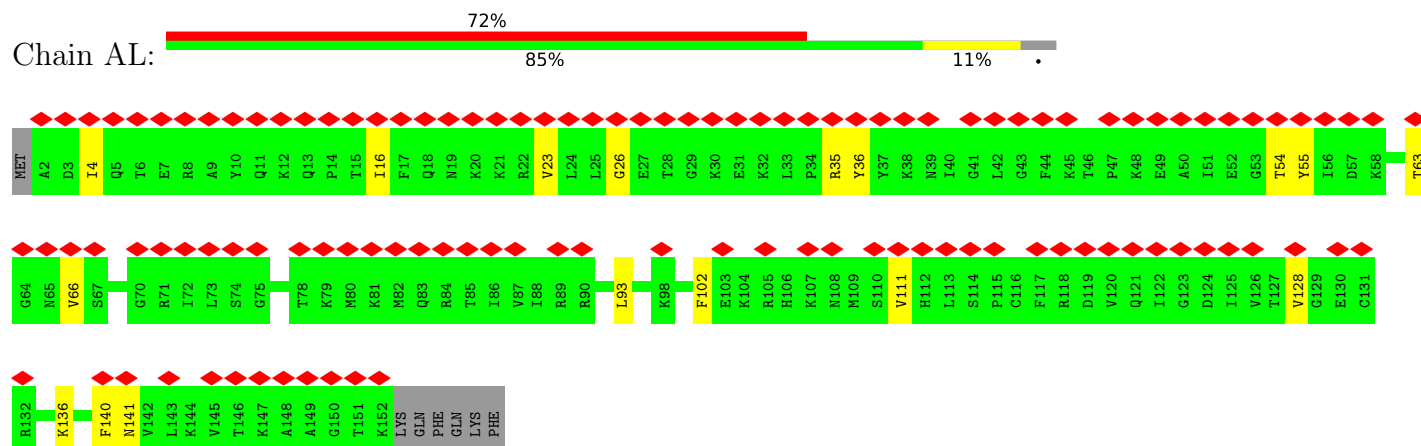


• Molecule 63: 40S ribosomal protein S10

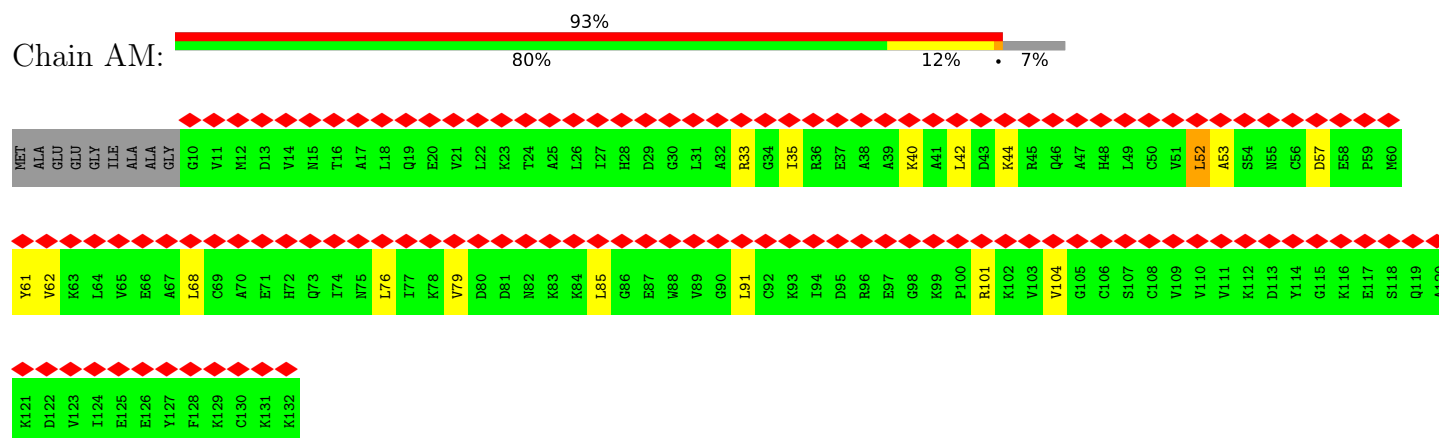




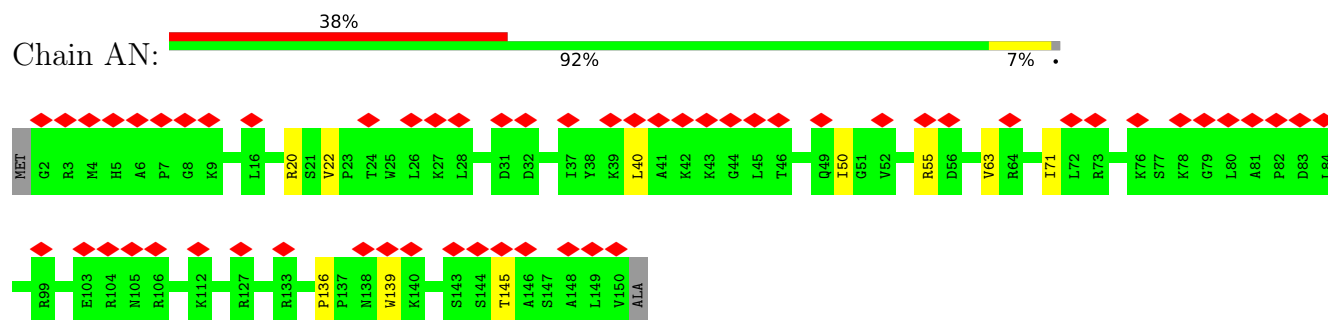
- Molecule 64: Small ribosomal subunit protein uS17



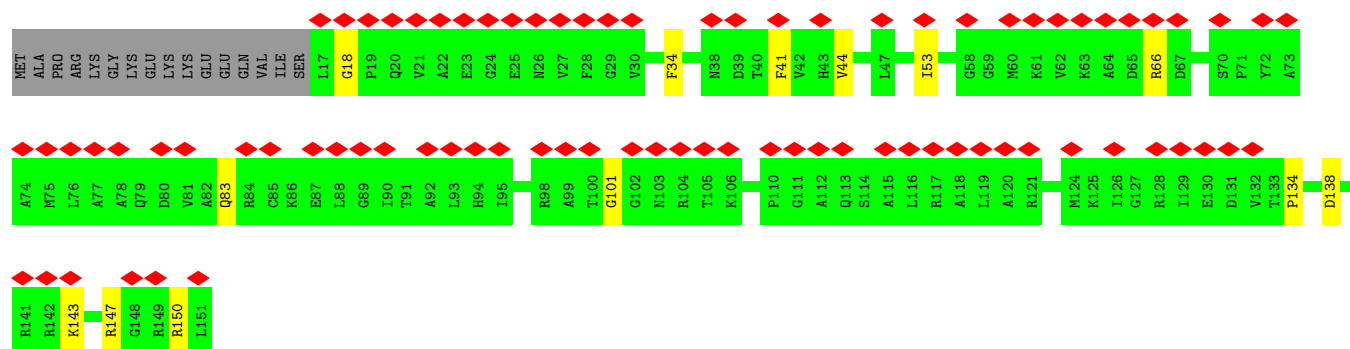
- Molecule 65: 40S ribosomal protein S12



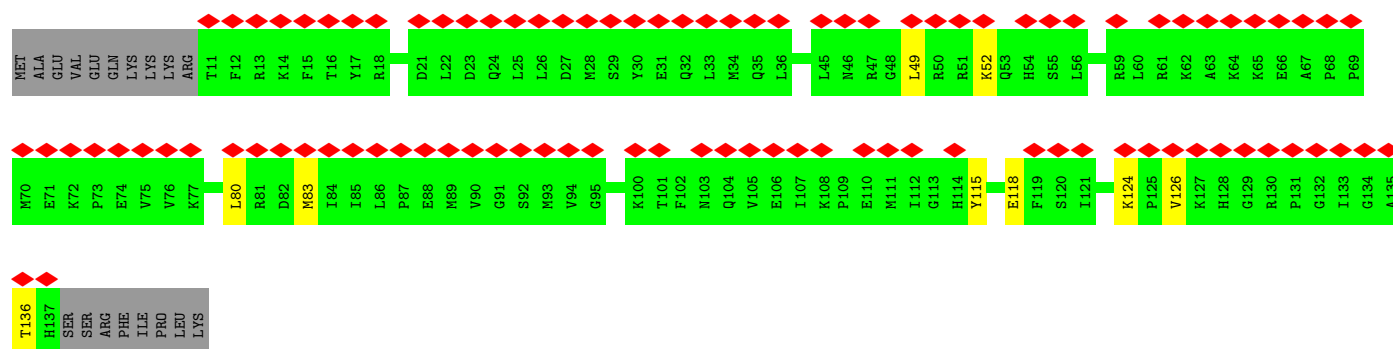
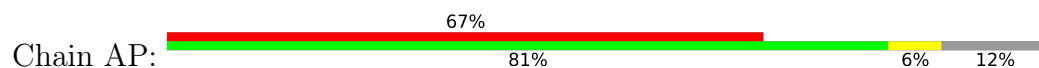
- Molecule 66: 40S ribosomal protein S13



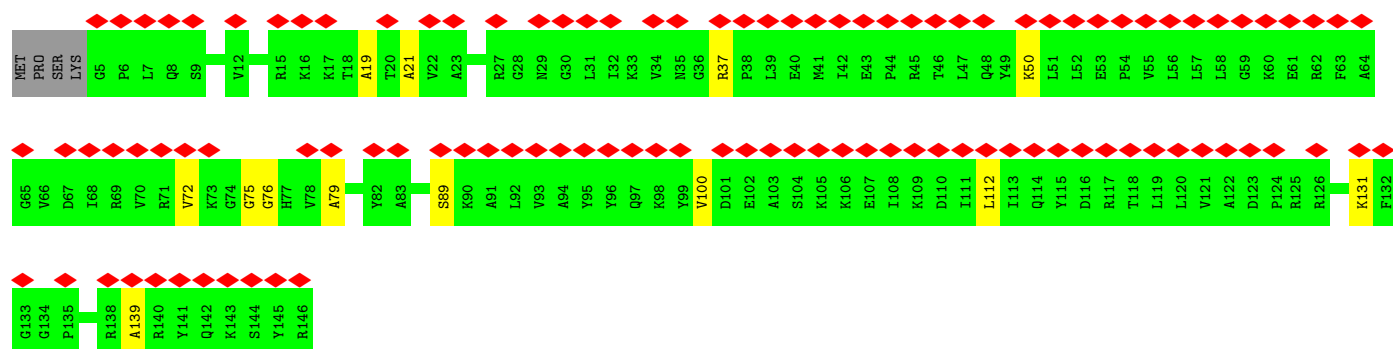
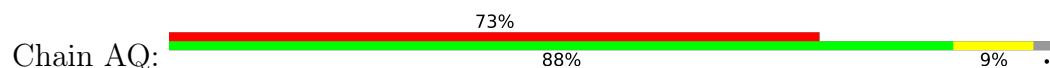
- Molecule 67: 40S ribosomal protein S14



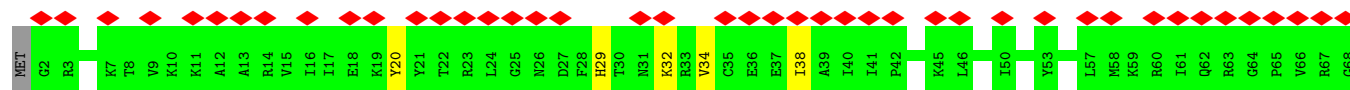
• Molecule 68: 40S ribosomal protein S15

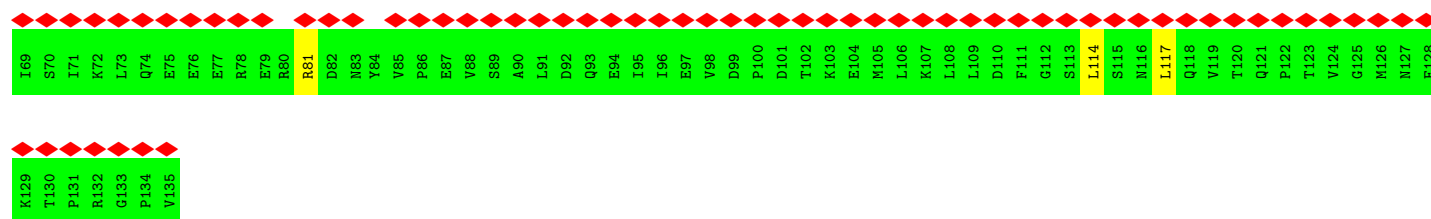


• Molecule 69: 40S ribosomal protein S16



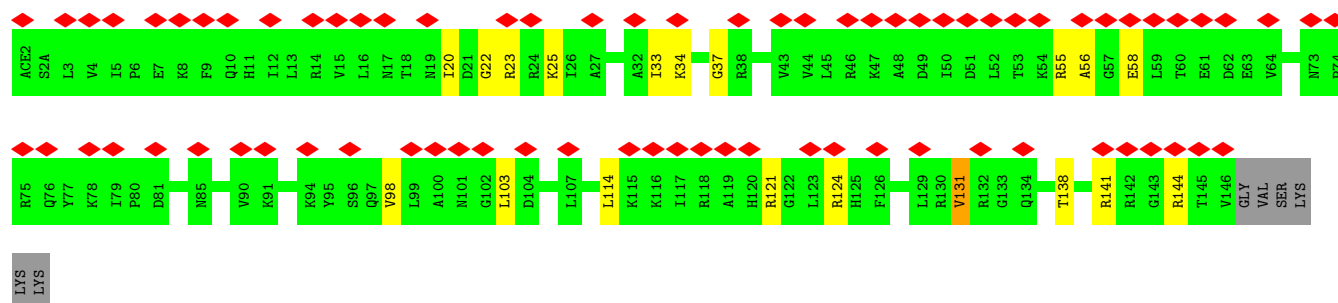
• Molecule 70: 40S ribosomal protein S17





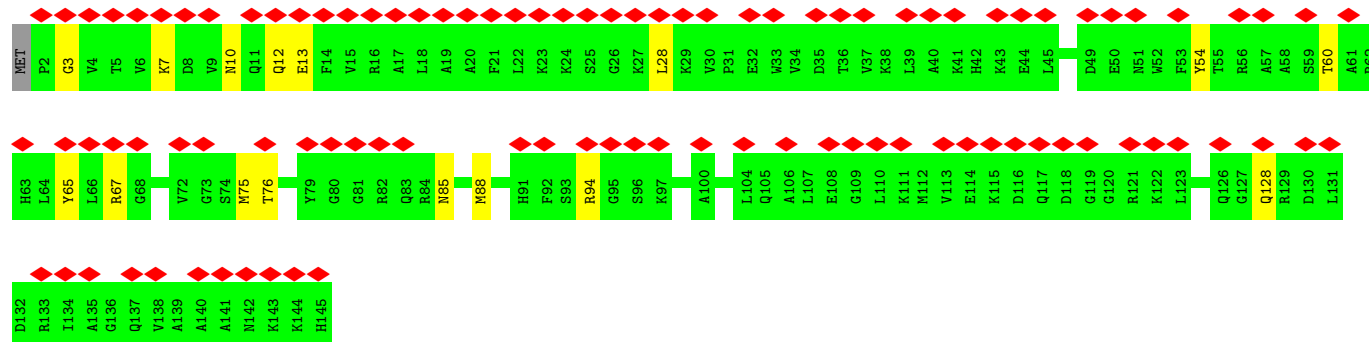
• Molecule 71: Small ribosomal subunit protein uS13

Chain AS: 49% 84% 12%



• Molecule 72: Small ribosomal subunit protein eS19

Chain AT: 68% 88% 11%



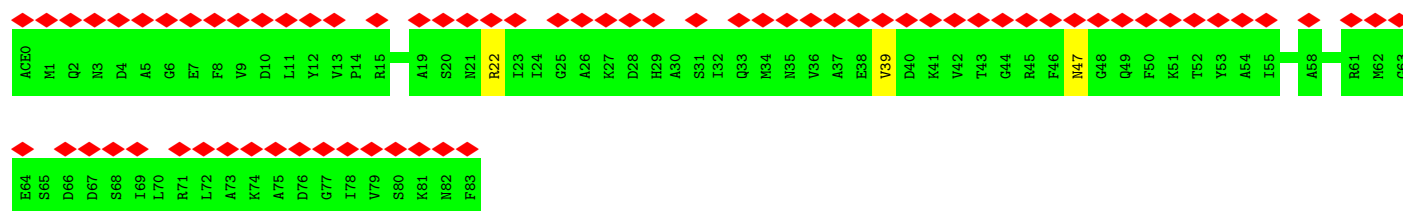
• Molecule 73: 40S ribosomal protein S20

Chain AU: 71% 76% 9% 15%

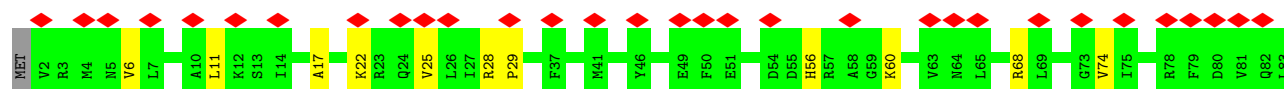
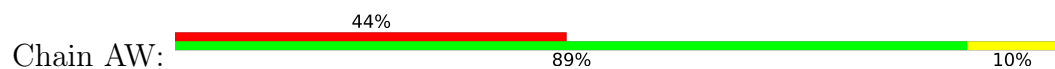


• Molecule 74: Small ribosomal subunit protein eS21

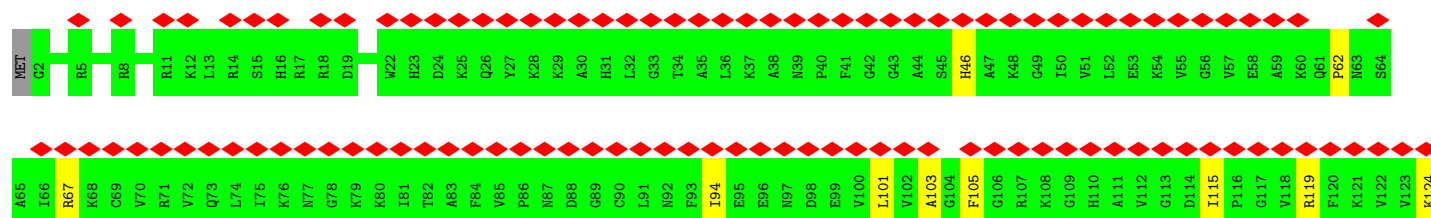
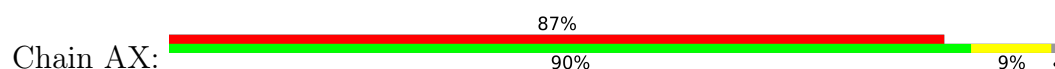
Chain AV: 85% 96% 1%



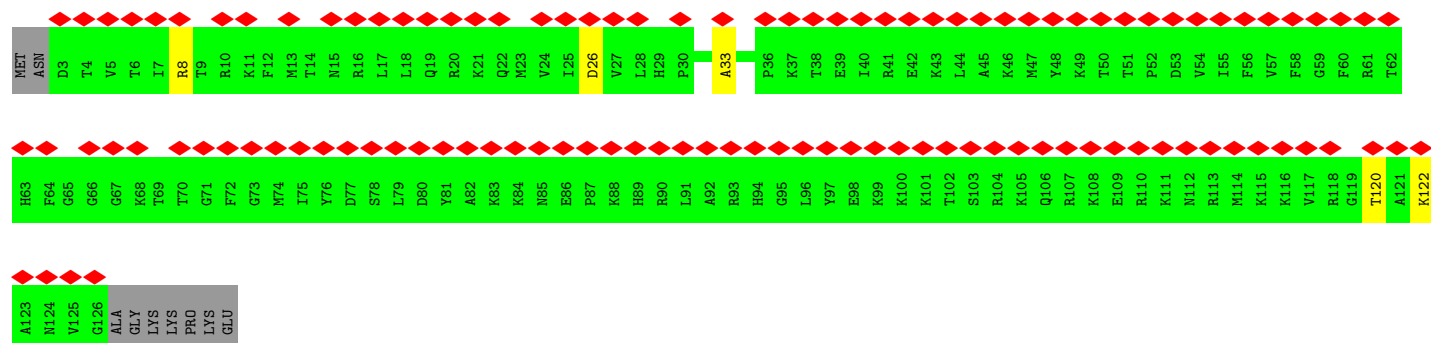
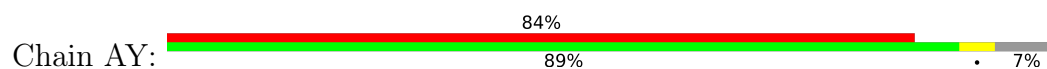
• Molecule 75: 40S ribosomal protein S15a



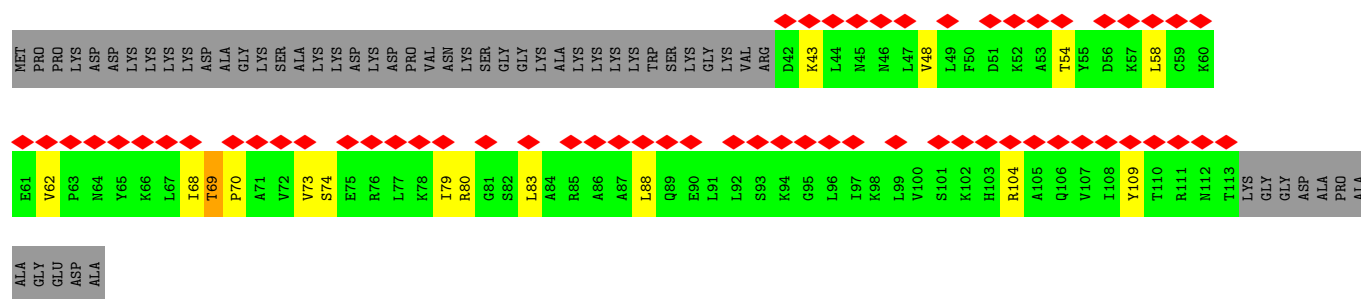
• Molecule 76: Small ribosomal subunit protein uS12



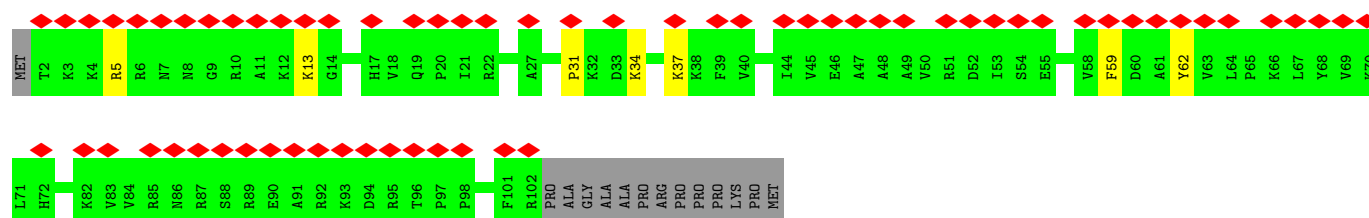
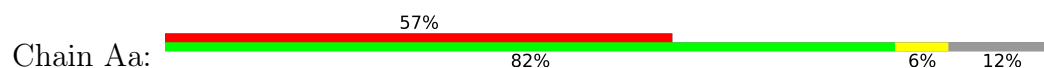
• Molecule 77: 40S ribosomal protein S24



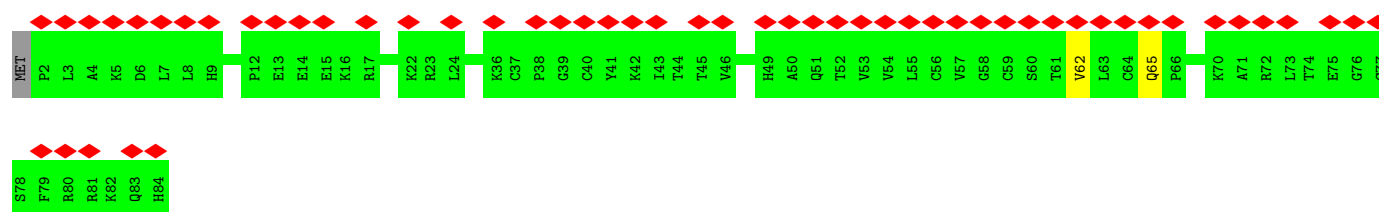
• Molecule 78: Small ribosomal subunit protein eS25



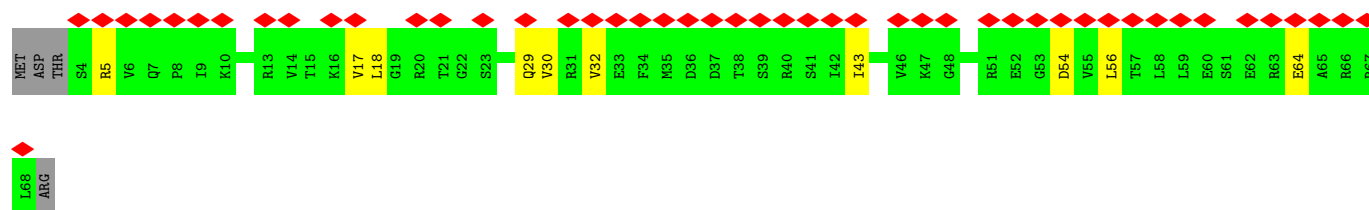
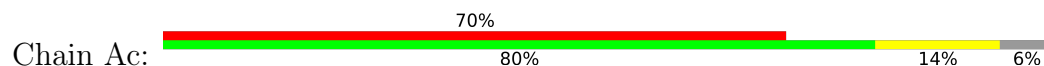
- Molecule 79: 40S ribosomal protein S26



- Molecule 80: 40S ribosomal protein S27

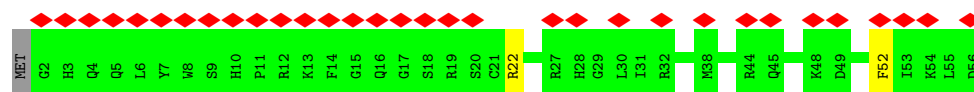


- Molecule 81: 40S ribosomal protein S28

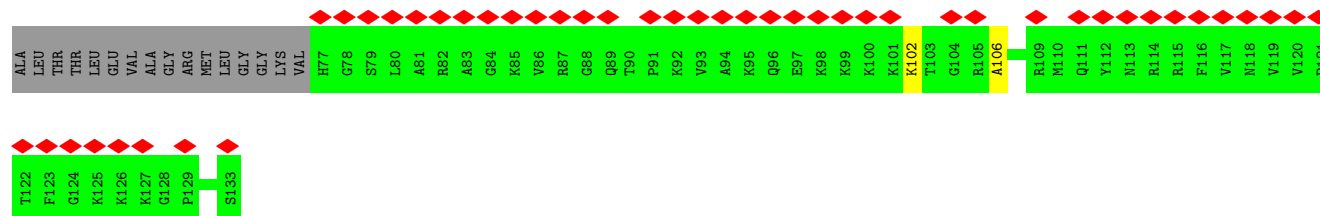
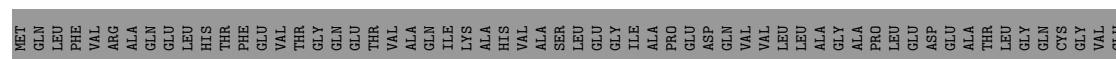
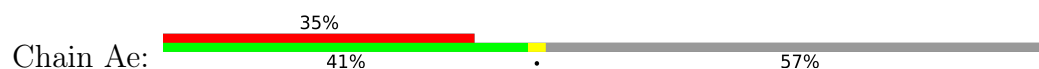


- Molecule 82: 40S ribosomal protein S29

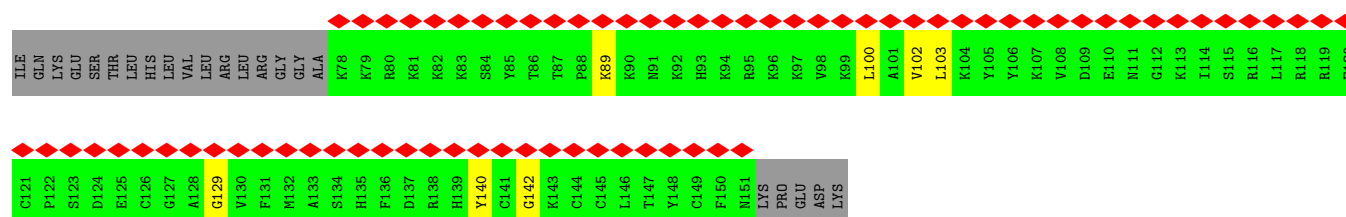
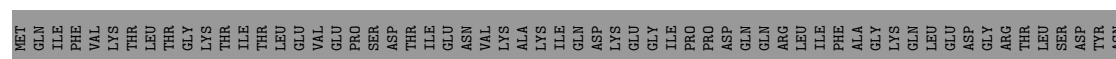
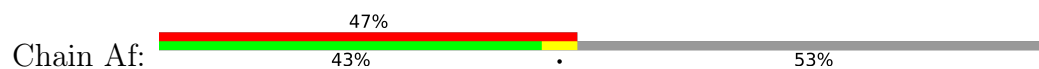




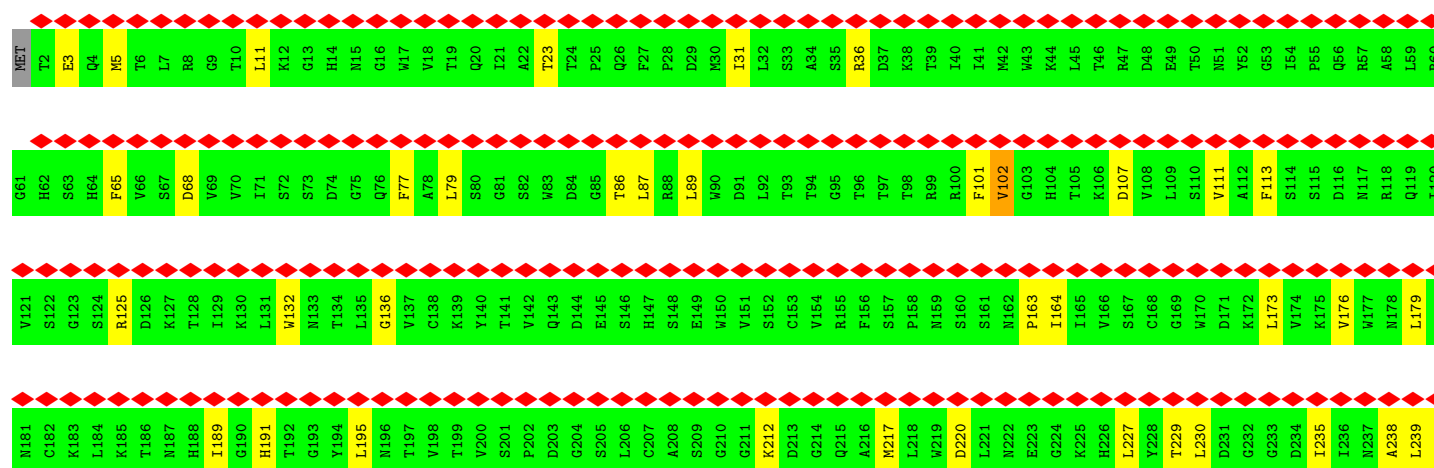
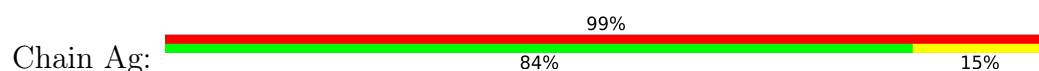
- Molecule 83: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein

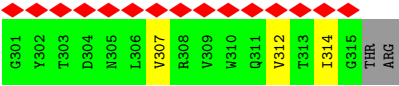
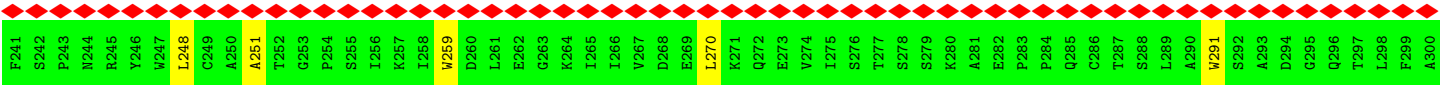


- Molecule 84: Ubiquitin

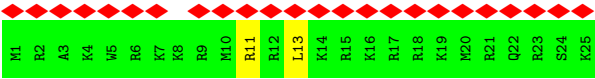
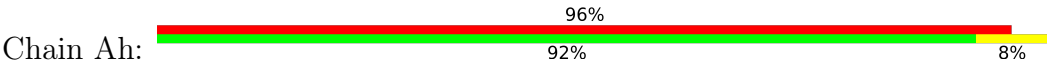


- Molecule 85: Receptor of activated protein C kinase 1





● Molecule 86: 60S ribosomal protein L41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104588	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.263	Depositor
Minimum map value	-0.461	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.149	Depositor
Map size (Å)	586.32, 586.32, 586.32	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, T6A, 5MC, IAS, ACE, MG, UR3, 5MU, A2M, OMC, B8N, HY3, NMM, UY1, MLZ, V5N, MA6, 4AC, G7M, PSU, GTP, 1MA, HIC, M2G, ZN, H2U, 6MZ, 2MG, OMU

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	B1	0.10	0/295	0.25	0/403
2	B2	0.25	1/1434 (0.1%)	0.29	0/2232
3	B4	0.09	0/141	0.25	0/217
4	B5	0.14	0/84341	0.19	0/131575
5	B7	0.08	0/2835	0.16	0/4418
6	B8	0.14	0/3613	0.16	0/5627
7	BA	0.12	0/1924	0.24	0/2578
8	BB	0.11	0/3294	0.24	0/4406
9	BC	0.12	0/2973	0.23	0/3992
10	BD	0.08	0/2432	0.20	0/3256
11	BE	0.09	0/1807	0.22	0/2425
12	BF	0.11	0/1916	0.22	0/2553
13	BG	0.10	0/1960	0.23	0/2639
14	BH	0.07	0/1537	0.19	0/2066
15	BI	0.07	0/1698	0.20	0/2266
16	BJ	0.07	0/1394	0.19	0/1863
17	BL	0.11	0/1732	0.24	0/2315
18	BM	0.21	0/1142	0.30	0/1527
19	BN	0.12	0/1746	0.23	0/2338
20	BO	0.11	0/1682	0.23	0/2250
21	BP	0.10	0/1268	0.23	0/1701
22	BQ	0.11	0/1537	0.25	0/2052
23	BR	0.09	0/1582	0.18	0/2091
24	BS	0.09	0/1501	0.20	0/2013
25	BT	0.09	0/1326	0.19	0/1770
26	BU	0.08	0/865	0.22	0/1160
27	BV	0.11	0/993	0.24	0/1332
28	BW	0.08	0/1012	0.20	0/1342
29	BX	0.10	0/1050	0.21	0/1409
30	BY	0.10	0/1119	0.21	0/1488
31	BZ	0.09	0/1130	0.20	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ba	0.10	0/1179	0.24	0/1573
33	Bb	0.07	0/811	0.19	0/1070
34	Bc	0.09	0/835	0.22	0/1118
35	Bd	0.10	0/898	0.22	0/1210
36	Be	0.12	0/1071	0.22	0/1429
37	Bf	0.13	0/895	0.23	0/1198
38	Bg	0.10	0/878	0.22	0/1170
39	Bh	0.08	0/1023	0.18	0/1351
40	Bi	0.07	0/824	0.20	0/1090
41	Bj	0.11	0/720	0.26	0/952
42	Bk	0.06	0/565	0.17	0/750
43	Bl	0.10	0/465	0.19	0/614
44	Bm	0.06	0/425	0.20	0/564
45	Bo	0.08	0/848	0.21	0/1116
46	Bp	0.10	0/691	0.22	0/919
47	Br	0.12	0/1003	0.23	0/1346
48	Bs	0.07	0/1529	0.20	0/2063
49	Bt	0.08	0/1193	0.22	0/1609
50	Bu	0.07	0/527	0.22	0/703
51	Bv	0.10	0/854	0.29	0/1144
52	A2	0.14	4/40445 (0.0%)	0.16	0/63039
53	AA	0.08	0/1743	0.21	0/2369
54	AB	0.08	0/1832	0.21	0/2448
55	AC	0.08	0/1726	0.22	0/2332
56	AD	0.07	0/1780	0.20	0/2397
57	AE	0.08	0/2118	0.22	0/2849
58	AF	0.08	0/1539	0.24	0/2071
59	AG	0.07	0/1968	0.20	0/2619
60	AH	0.08	0/1538	0.22	0/2060
61	AI	0.08	0/1699	0.21	0/2266
62	AJ	0.06	0/1524	0.19	0/2035
63	AK	0.07	0/840	0.21	0/1133
64	AL	0.07	0/1250	0.20	0/1673
65	AM	0.09	0/963	0.27	0/1291
66	AN	0.07	0/1226	0.19	0/1649
67	AO	0.08	0/1014	0.21	0/1358
68	AP	0.07	0/1065	0.19	0/1424
69	AQ	0.08	0/1146	0.22	0/1534
70	AR	0.07	0/1097	0.20	0/1474
71	AS	0.09	0/1216	0.25	0/1630
72	AT	0.07	0/1130	0.20	0/1513
73	AU	0.07	0/813	0.21	0/1092
74	AV	0.08	0/644	0.19	0/862

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	AW	0.07	0/1051	0.20	0/1406
76	AX	0.08	0/1116	0.23	0/1486
77	AY	0.07	0/1031	0.20	0/1370
78	AZ	0.10	0/580	0.29	0/780
79	Aa	0.08	0/828	0.23	0/1109
80	Ab	0.07	0/664	0.21	0/891
81	Ac	0.06	0/514	0.17	0/688
82	Ad	0.07	0/469	0.20	0/623
83	Ae	0.07	0/457	0.20	0/602
84	Af	0.08	0/622	0.26	0/822
85	Ag	0.07	0/2497	0.23	0/3399
86	Ah	0.06	0/240	0.15	0/305
All	All	0.12	5/230898 (0.0%)	0.20	0/338399

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B2	37	T6A	O3'-P	5.11	1.61	1.56
52	A2	799	OMU	O3'-P	5.06	1.61	1.56
52	A2	512	A2M	O3'-P	5.04	1.61	1.56
52	A2	172	OMU	O3'-P	5.01	1.61	1.56
52	A2	484	A2M	O3'-P	5.01	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B1	283	0	281	3	0
2	B2	1638	0	850	21	0
3	B4	127	0	64	0	0
4	B5	78039	0	39528	403	0
5	B7	2570	0	1295	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B8	3320	0	1686	12	0
7	BA	1899	0	1986	15	0
8	BB	3239	0	3376	29	0
9	BC	2919	0	3092	14	0
10	BD	2386	0	2421	14	0
11	BE	1773	0	1928	11	0
12	BF	1878	0	2009	14	0
13	BG	1927	0	2080	7	0
14	BH	1518	0	1601	8	0
15	BI	1660	0	1710	13	0
16	BJ	1371	0	1412	11	0
17	BL	1701	0	1818	11	0
18	BM	1120	0	1187	6	0
19	BN	1701	0	1749	14	0
20	BO	1650	0	1794	9	0
21	BP	1242	0	1267	9	0
22	BQ	1513	0	1628	8	0
23	BR	1566	0	1729	13	0
24	BS	1461	0	1502	5	0
25	BT	1298	0	1366	8	0
26	BU	851	0	877	4	0
27	BV	979	0	1039	10	0
28	BW	997	0	1053	8	0
29	BX	1031	0	1110	5	0
30	BY	1102	0	1189	7	0
31	BZ	1107	0	1182	7	0
32	Ba	1163	0	1206	9	0
33	Bb	809	0	875	4	0
34	Bc	824	0	874	8	0
35	Bd	883	0	923	8	0
36	Be	1053	0	1147	8	0
37	Bf	876	0	912	4	0
38	Bg	868	0	959	4	0
39	Bh	1015	0	1148	9	0
40	Bi	813	0	894	9	0
41	Bj	705	0	737	4	0
42	Bk	559	0	624	4	0
43	Bl	451	0	490	2	0
44	Bm	419	0	452	2	0
45	Bo	843	0	914	6	0
46	Bp	681	0	731	6	0
47	Br	990	0	1054	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Bs	1506	0	1562	22	0
49	Bt	1178	0	1235	10	0
50	Bu	522	0	565	7	0
51	Bv	846	0	891	13	0
52	A2	38027	0	19276	230	0
53	AA	1708	0	1710	22	0
54	AB	1806	0	1895	19	0
55	AC	1690	0	1777	14	0
56	AD	1752	0	1848	7	0
57	AE	2076	0	2177	17	0
58	AF	1517	0	1569	11	0
59	AG	1945	0	2112	12	0
60	AH	1515	0	1611	19	0
61	AI	1670	0	1755	13	0
62	AJ	1499	0	1618	9	0
63	AK	816	0	841	3	0
64	AL	1229	0	1302	10	0
65	AM	953	0	990	11	0
66	AN	1202	0	1289	4	0
67	AO	1010	0	1033	9	0
68	AP	1044	0	1089	6	0
69	AQ	1128	0	1195	9	0
70	AR	1082	0	1137	5	0
71	AS	1200	0	1262	10	0
72	AT	1123	0	1152	11	0
73	AU	803	0	873	6	0
74	AV	639	0	638	1	0
75	AW	1034	0	1080	6	0
76	AX	1105	0	1175	6	0
77	AY	1014	0	1082	4	0
78	AZ	574	0	627	11	0
79	Aa	814	0	863	5	0
80	Ab	650	0	672	1	0
81	Ac	512	0	541	6	0
82	Ad	458	0	448	2	0
83	Ae	451	0	494	1	0
84	Af	610	0	634	8	0
85	Ag	2440	0	2396	26	0
86	Ah	239	0	289	2	0
87	A2	123	0	0	0	0
87	AI	1	0	0	0	0
87	AX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	B5	285	0	0	0	0
87	B7	4	0	0	0	0
87	B8	6	0	0	0	0
87	BA	3	0	0	0	0
87	BB	1	0	0	0	0
87	BN	1	0	0	0	0
87	BV	1	0	0	0	0
87	Ba	1	0	0	0	0
87	Be	1	0	0	0	0
87	Bf	2	0	0	0	0
87	Bg	1	0	0	0	0
87	Bj	1	0	0	0	0
88	Aa	1	0	0	0	0
88	Ad	1	0	0	0	0
88	Af	1	0	0	0	0
88	Bg	1	0	0	0	0
88	Bj	1	0	0	0	0
88	Bm	1	0	0	0	0
88	Bo	1	0	0	0	0
88	Bp	1	0	0	0	0
All	All	220645	0	164452	1202	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 3.

The worst 5 of 1202 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)
18:BM:128:LYS:O	18:BM:132:LYS:HG3	1.44	1.18
5:B7:72:U:H3	5:B7:103:A:H61	1.15	0.94
4:B5:1858:C:H42	4:B5:1874:C:H42	1.32	0.77
16:BJ:56:THR:HG22	16:BJ:58:ARG:HH12	1.50	0.77
52:A2:84:A:H5''	77:AY:122:LYS:HD2	1.66	0.76

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B1	32/184 (17%)	31 (97%)	1 (3%)	0	100	100
7	BA	245/257 (95%)	235 (96%)	10 (4%)	0	100	100
8	BB	399/403 (99%)	396 (99%)	3 (1%)	0	100	100
9	BC	365/427 (86%)	360 (99%)	5 (1%)	0	100	100
10	BD	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
11	BE	215/288 (75%)	210 (98%)	5 (2%)	0	100	100
12	BF	224/248 (90%)	218 (97%)	6 (3%)	0	100	100
13	BG	238/266 (90%)	237 (100%)	1 (0%)	0	100	100
14	BH	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
15	BI	201/214 (94%)	198 (98%)	3 (2%)	0	100	100
16	BJ	169/178 (95%)	168 (99%)	1 (1%)	0	100	100
17	BL	208/211 (99%)	202 (97%)	6 (3%)	0	100	100
18	BM	134/215 (62%)	130 (97%)	4 (3%)	0	100	100
19	BN	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
20	BO	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
21	BP	151/184 (82%)	149 (99%)	2 (1%)	0	100	100
22	BQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
23	BR	185/196 (94%)	185 (100%)	0	0	100	100
24	BS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
25	BT	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
26	BU	102/128 (80%)	100 (98%)	2 (2%)	0	100	100
27	BV	129/140 (92%)	127 (98%)	2 (2%)	0	100	100
28	BW	120/157 (76%)	116 (97%)	4 (3%)	0	100	100
29	BX	124/156 (80%)	124 (100%)	0	0	100	100
30	BY	130/145 (90%)	129 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
32	Ba	144/148 (97%)	139 (96%)	4 (3%)	1 (1%)	18	41
33	Bb	94/159 (59%)	92 (98%)	2 (2%)	0	100	100
34	Bc	104/115 (90%)	104 (100%)	0	0	100	100
35	Bd	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
36	Be	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
37	Bf	107/110 (97%)	107 (100%)	0	0	100	100
38	Bg	107/117 (92%)	107 (100%)	0	0	100	100
39	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
40	Bi	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
41	Bj	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
42	Bk	66/70 (94%)	66 (100%)	0	0	100	100
43	Bl	49/51 (96%)	49 (100%)	0	0	100	100
44	Bm	49/128 (38%)	49 (100%)	0	0	100	100
45	Bo	100/106 (94%)	97 (97%)	3 (3%)	0	100	100
46	Bp	86/92 (94%)	85 (99%)	1 (1%)	0	100	100
47	Br	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
48	Bs	194/317 (61%)	188 (97%)	6 (3%)	0	100	100
49	Bt	154/165 (93%)	153 (99%)	1 (1%)	0	100	100
50	Bu	64/215 (30%)	61 (95%)	3 (5%)	0	100	100
51	Bv	107/206 (52%)	102 (95%)	5 (5%)	0	100	100
53	AA	215/295 (73%)	213 (99%)	2 (1%)	0	100	100
54	AB	219/264 (83%)	218 (100%)	1 (0%)	0	100	100
55	AC	216/293 (74%)	216 (100%)	0	0	100	100
56	AD	223/243 (92%)	222 (100%)	1 (0%)	0	100	100
57	AE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
58	AF	190/204 (93%)	182 (96%)	8 (4%)	0	100	100
59	AG	238/249 (96%)	237 (100%)	1 (0%)	0	100	100
60	AH	186/194 (96%)	183 (98%)	3 (2%)	0	100	100
61	AI	201/208 (97%)	198 (98%)	3 (2%)	0	100	100
62	AJ	178/194 (92%)	177 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	AK	95/165 (58%)	94 (99%)	1 (1%)	0	100	100
64	AL	149/158 (94%)	147 (99%)	2 (1%)	0	100	100
65	AM	121/132 (92%)	118 (98%)	3 (2%)	0	100	100
66	AN	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
67	AO	131/151 (87%)	129 (98%)	2 (2%)	0	100	100
68	AP	125/145 (86%)	124 (99%)	1 (1%)	0	100	100
69	AQ	140/146 (96%)	138 (99%)	2 (1%)	0	100	100
70	AR	132/135 (98%)	132 (100%)	0	0	100	100
71	AS	144/152 (95%)	141 (98%)	3 (2%)	0	100	100
72	AT	141/145 (97%)	141 (100%)	0	0	100	100
73	AU	99/119 (83%)	98 (99%)	1 (1%)	0	100	100
74	AV	82/84 (98%)	82 (100%)	0	0	100	100
75	AW	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
76	AX	139/143 (97%)	138 (99%)	1 (1%)	0	100	100
77	AY	122/133 (92%)	122 (100%)	0	0	100	100
78	AZ	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
79	Aa	99/115 (86%)	99 (100%)	0	0	100	100
80	Ab	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
81	Ac	63/69 (91%)	62 (98%)	1 (2%)	0	100	100
82	Ad	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
83	Ae	55/133 (41%)	53 (96%)	2 (4%)	0	100	100
84	Af	72/156 (46%)	68 (94%)	4 (6%)	0	100	100
85	Ag	312/317 (98%)	301 (96%)	11 (4%)	0	100	100
86	Ah	23/25 (92%)	23 (100%)	0	0	100	100
All	All	11826/13850 (85%)	11645 (98%)	180 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	Ba	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B1	32/151 (21%)	32 (100%)	0	100	100
7	BA	189/198 (96%)	187 (99%)	2 (1%)	65	85
8	BB	347/348 (100%)	344 (99%)	3 (1%)	70	87
9	BC	305/348 (88%)	305 (100%)	0	100	100
10	BD	247/250 (99%)	245 (99%)	2 (1%)	73	88
11	BE	195/252 (77%)	193 (99%)	2 (1%)	68	86
12	BF	195/215 (91%)	195 (100%)	0	100	100
13	BG	205/223 (92%)	205 (100%)	0	100	100
14	BH	169/171 (99%)	169 (100%)	0	100	100
15	BI	175/181 (97%)	173 (99%)	2 (1%)	65	85
16	BJ	144/149 (97%)	142 (99%)	2 (1%)	59	82
17	BL	176/177 (99%)	174 (99%)	2 (1%)	65	85
18	BM	116/161 (72%)	116 (100%)	0	100	100
19	BN	171/172 (99%)	171 (100%)	0	100	100
20	BO	173/174 (99%)	172 (99%)	1 (1%)	78	91
21	BP	134/163 (82%)	132 (98%)	2 (2%)	57	81
22	BQ	164/165 (99%)	163 (99%)	1 (1%)	78	91
23	BR	166/175 (95%)	165 (99%)	1 (1%)	78	91
24	BS	157/157 (100%)	153 (98%)	4 (2%)	42	71
25	BT	139/140 (99%)	138 (99%)	1 (1%)	76	90
26	BU	94/115 (82%)	92 (98%)	2 (2%)	47	75
27	BV	101/107 (94%)	100 (99%)	1 (1%)	68	86
28	BW	101/126 (80%)	100 (99%)	1 (1%)	68	86
29	BX	113/133 (85%)	111 (98%)	2 (2%)	51	78
30	BY	123/135 (91%)	123 (100%)	0	100	100
31	BZ	117/118 (99%)	116 (99%)	1 (1%)	70	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Ba	119/120 (99%)	118 (99%)	1 (1%)	73	88
33	Bb	82/125 (66%)	82 (100%)	0	100	100
34	Bc	90/97 (93%)	87 (97%)	3 (3%)	33	63
35	Bd	96/110 (87%)	96 (100%)	0	100	100
36	Be	114/121 (94%)	114 (100%)	0	100	100
37	Bf	88/89 (99%)	88 (100%)	0	100	100
38	Bg	94/100 (94%)	91 (97%)	3 (3%)	34	64
39	Bh	109/110 (99%)	109 (100%)	0	100	100
40	Bi	85/89 (96%)	83 (98%)	2 (2%)	43	72
41	Bj	73/80 (91%)	72 (99%)	1 (1%)	59	82
42	Bk	63/65 (97%)	62 (98%)	1 (2%)	55	80
43	Bl	48/48 (100%)	47 (98%)	1 (2%)	47	75
44	Bm	47/116 (40%)	47 (100%)	0	100	100
45	Bo	90/93 (97%)	89 (99%)	1 (1%)	65	85
46	Bp	71/75 (95%)	69 (97%)	2 (3%)	38	68
47	Br	107/120 (89%)	105 (98%)	2 (2%)	50	77
48	Bs	164/258 (64%)	159 (97%)	5 (3%)	36	66
49	Bt	128/137 (93%)	122 (95%)	6 (5%)	23	51
50	Bu	59/183 (32%)	58 (98%)	1 (2%)	53	79
51	Bv	93/165 (56%)	86 (92%)	7 (8%)	12	31
53	AA	180/242 (74%)	178 (99%)	2 (1%)	65	85
54	AB	202/231 (87%)	201 (100%)	1 (0%)	81	92
55	AC	184/225 (82%)	183 (100%)	1 (0%)	81	92
56	AD	189/202 (94%)	188 (100%)	1 (0%)	81	92
57	AE	224/225 (100%)	223 (100%)	1 (0%)	84	93
58	AF	162/170 (95%)	160 (99%)	2 (1%)	63	84
59	AG	209/218 (96%)	208 (100%)	1 (0%)	81	92
60	AH	168/174 (97%)	168 (100%)	0	100	100
61	AI	177/180 (98%)	173 (98%)	4 (2%)	44	73
62	AJ	160/168 (95%)	158 (99%)	2 (1%)	61	83
63	AK	88/136 (65%)	86 (98%)	2 (2%)	44	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	AL	135/142 (95%)	135 (100%)	0	100	100
65	AM	104/108 (96%)	101 (97%)	3 (3%)	37	67
66	AN	130/131 (99%)	127 (98%)	3 (2%)	44	73
67	AO	104/118 (88%)	104 (100%)	0	100	100
68	AP	113/130 (87%)	113 (100%)	0	100	100
69	AQ	117/121 (97%)	116 (99%)	1 (1%)	70	87
70	AR	121/122 (99%)	121 (100%)	0	100	100
71	AS	126/131 (96%)	123 (98%)	3 (2%)	43	72
72	AT	113/114 (99%)	113 (100%)	0	100	100
73	AU	93/107 (87%)	92 (99%)	1 (1%)	65	85
74	AV	67/67 (100%)	65 (97%)	2 (3%)	36	66
75	AW	112/113 (99%)	109 (97%)	3 (3%)	39	69
76	AX	113/114 (99%)	110 (97%)	3 (3%)	39	69
77	AY	108/115 (94%)	108 (100%)	0	100	100
78	AZ	64/103 (62%)	63 (98%)	1 (2%)	55	80
79	Aa	88/98 (90%)	88 (100%)	0	100	100
80	Ab	75/76 (99%)	75 (100%)	0	100	100
81	Ac	58/62 (94%)	58 (100%)	0	100	100
82	Ad	48/49 (98%)	48 (100%)	0	100	100
83	Ae	46/104 (44%)	46 (100%)	0	100	100
84	Af	67/140 (48%)	67 (100%)	0	100	100
85	Ag	272/275 (99%)	269 (99%)	3 (1%)	65	85
86	Ah	24/24 (100%)	24 (100%)	0	100	100
All	All	10309/11740 (88%)	10201 (99%)	108 (1%)	65	86

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	Bt	35	LEU
55	AC	91	SER
75	AW	105	THR
49	Bt	73	VAL
51	Bv	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
75	AW	70	ASN
80	Ab	9	HIS
85	Ag	188	HIS
34	Bc	33	GLN
33	Bb	11	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B2	75/76 (98%)	16 (21%)	0
3	B4	5/6 (83%)	1 (20%)	0
4	B5	3628/5069 (71%)	553 (15%)	21 (0%)
5	B7	118/120 (98%)	9 (7%)	1 (0%)
52	A2	1773/1869 (94%)	233 (13%)	4 (0%)
6	B8	155/157 (98%)	21 (13%)	1 (0%)
All	All	5754/7297 (78%)	833 (14%)	27 (0%)

5 of 833 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B2	13	C
2	B2	16	H2U
2	B2	17	A
2	B2	18	G
2	B2	19	G

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	B5	4056	C
4	B5	4347	A
52	A2	688	U
4	B5	4255	A
4	B5	4652	C

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

240 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
52	4AC	A2	1842	52	21,24,25	1.06	1 (4%)	29,34,37	1.26	3 (10%)
4	PSU	B5	5000	4	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
4	PSU	B5	4575	4	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
4	PSU	B5	4352	4	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
4	OMG	B5	4227	4	23,26,27	1.18	3 (13%)	33,38,41	1.92	6 (18%)
4	OMG	B5	1521	4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
4	OMG	B5	3791	4	23,26,27	1.19	3 (13%)	33,38,41	1.94	6 (18%)
52	OMG	A2	1328	87,52	23,26,27	1.18	3 (13%)	33,38,41	1.96	6 (18%)
52	PSU	A2	822	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
4	PSU	B5	4470	4	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
4	A2M	B5	3723	4	22,25,26	1.45	4 (18%)	31,36,39	2.10	9 (29%)
4	PSU	B5	1859	4	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
4	OMG	B5	1315	87,4	23,26,27	1.21	3 (13%)	33,38,41	1.91	6 (18%)
4	OMG	B5	4498	4	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
52	PSU	A2	218	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	OMU	A2	172	52	19,22,23	1.22	3 (15%)	26,31,34	1.74	5 (19%)
4	PSU	B5	4972	4	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
52	A2M	A2	1383	52	22,25,26	1.48	4 (18%)	31,36,39	2.12	10 (32%)
4	PSU	B5	3769	4	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
52	PSU	A2	1004	52	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	PSU	A2	1692	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
52	OMU	A2	1804	52	19,22,23	1.24	3 (15%)	26,31,34	1.66	5 (19%)
52	PSU	A2	1643	52	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
4	OMG	B5	3626	4	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
4	OMC	B5	4455	4	19,22,23	0.80	0	26,31,34	0.75	0
4	OMG	B5	3743	4	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
52	PSU	A2	1367	52	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
4	PSU	B5	4292	4	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
52	OMC	A2	517	52	19,22,23	0.83	0	26,31,34	0.93	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2M	B5	2400	4	22,25,26	1.44	4 (18%)	31,36,39	2.13	10 (32%)
5	GTP	B7	1	5	30,34,34	0.50	0	46,54,54	0.51	0
4	PSU	B5	3883	4	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	681	52	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
4	OMG	B5	2423	4	23,26,27	1.19	3 (13%)	33,38,41	1.95	7 (21%)
4	A2M	B5	400	4	22,25,26	1.46	4 (18%)	31,36,39	2.05	8 (25%)
52	OMG	A2	1447	52	23,26,27	1.19	3 (13%)	33,38,41	1.97	6 (18%)
52	OMG	A2	509	87,52	23,26,27	1.20	3 (13%)	33,38,41	1.97	6 (18%)
52	A2M	A2	166	52	22,25,26	1.47	4 (18%)	31,36,39	2.19	10 (32%)
4	PSU	B5	4402	4	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
52	OMU	A2	116	52	19,22,23	1.21	2 (10%)	26,31,34	1.69	4 (15%)
2	H2U	B2	16	2	18,21,22	1.07	2 (11%)	21,30,33	2.07	1 (4%)
52	PSU	A2	609	52	18,21,22	1.34	2 (11%)	22,30,33	1.83	3 (13%)
2	1MA	B2	58	2	21,25,26	1.40	4 (19%)	31,37,40	1.73	5 (16%)
4	PSU	B5	1791	4	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
4	A2M	B5	3866	4	22,25,26	1.45	4 (18%)	31,36,39	2.11	10 (32%)
4	OMG	B5	3943	4	23,26,27	1.19	3 (13%)	33,38,41	1.95	6 (18%)
52	PSU	A2	36	52	18,21,22	1.36	2 (11%)	22,30,33	1.82	3 (13%)
52	PSU	A2	210	52	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
4	PSU	B5	4422	4	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	PSU	A2	34	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	OMU	A2	1288	52	19,22,23	1.22	3 (15%)	26,31,34	1.66	5 (19%)
4	PSU	B5	4295	4	18,21,22	1.32	2 (11%)	22,30,33	1.89	3 (13%)
4	PSU	B5	4311	4	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
4	PSU	B5	2842	4	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
52	PSU	A2	866	52	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
52	PSU	A2	1445	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
4	A2M	B5	4522	87,4	22,25,26	1.43	4 (18%)	31,36,39	2.19	10 (32%)
2	H2U	B2	20	2	18,21,22	1.00	2 (11%)	21,30,33	2.34	1 (4%)
4	OMU	B5	2414	4	19,22,23	1.24	3 (15%)	26,31,34	1.72	4 (15%)
2	2MG	B2	6	2	23,26,27	1.27	4 (17%)	32,38,41	2.19	6 (18%)
52	OMU	A2	627	52	19,22,23	1.19	3 (15%)	26,31,34	1.71	5 (19%)
2	PSU	B2	27	2	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
8	HIC	BB	245	8	10,11,12	0.60	0	8,14,16	0.40	0
52	MA6	A2	1850	52	23,26,27	2.25	5 (21%)	34,38,41	3.72	14 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	MLZ	Bo	53	45	8,9,10	0.50	0	4,9,11	0.11	0
52	OMG	A2	644	52	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
6	PSU	B8	69	6	18,21,22	1.34	2 (11%)	22,30,33	1.88	4 (18%)
4	PSU	B5	2507	4	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
4	PSU	B5	3761	4	18,21,22	1.33	2 (11%)	22,30,33	1.90	5 (22%)
4	PSU	B5	4635	4	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
52	PSU	A2	966	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
4	A2M	B5	3784	4	22,25,26	1.42	4 (18%)	31,36,39	2.24	11 (35%)
4	A2M	B5	2786	87,4	22,25,26	1.43	4 (18%)	31,36,39	2.20	8 (25%)
2	OMC	B2	34	2,3	19,22,23	0.27	0	26,31,34	0.37	0
4	PSU	B5	4360	4	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	3636	4	18,21,22	1.36	3 (16%)	22,30,33	1.89	3 (13%)
52	OMC	A2	462	52	19,22,23	0.82	0	26,31,34	0.81	0
52	PSU	A2	572	52	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
4	PSU	B5	4578	4	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
4	OMU	B5	2836	4	19,22,23	1.23	2 (10%)	26,31,34	1.72	4 (15%)
4	OMC	B5	2421	87,4	19,22,23	0.81	0	26,31,34	0.85	1 (3%)
4	OMG	B5	3898	87,4	23,26,27	1.19	3 (13%)	33,38,41	1.97	7 (21%)
4	OMU	B5	4226	4	19,22,23	1.25	3 (15%)	26,31,34	1.71	4 (15%)
52	A2M	A2	668	87,52	22,25,26	1.47	4 (18%)	31,36,39	2.11	9 (29%)
52	PSU	A2	1177	52	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
52	4AC	A2	1337	52	21,24,25	1.08	2 (9%)	29,34,37	1.20	3 (10%)
2	5MC	B2	48	2	18,22,23	0.95	2 (11%)	26,32,35	1.16	2 (7%)
4	OMU	B5	4305	4	19,22,23	1.24	3 (15%)	26,31,34	1.67	4 (15%)
4	1MA	B5	1321	87,4	21,25,26	1.37	4 (19%)	31,37,40	1.69	6 (19%)
52	A2M	A2	1031	52	22,25,26	1.47	4 (18%)	31,36,39	2.09	9 (29%)
4	A2M	B5	4589	4	22,25,26	1.46	4 (18%)	31,36,39	2.08	9 (29%)
4	PSU	B5	1743	4	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
4	OMC	B5	2860	4	19,22,23	0.81	0	26,31,34	0.83	1 (3%)
33	MLZ	Bb	5	33	8,9,10	0.50	0	4,9,11	0.13	0
4	PSU	B5	4688	4	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
4	OMG	B5	4369	4	23,26,27	1.20	3 (13%)	33,38,41	1.90	6 (18%)
4	PSU	B5	1781	4	18,21,22	1.34	2 (11%)	22,30,33	1.89	4 (18%)
4	PSU	B5	3638	4	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
52	A2M	A2	27	52	22,25,26	1.48	4 (18%)	31,36,39	2.13	10 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	A2M	A2	512	52	22,25,26	1.47	4 (18%)	31,36,39	2.12	9 (29%)
52	PSU	A2	105	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
52	MA6	A2	1851	52	23,26,27	2.25	5 (21%)	34,38,41	3.67	13 (38%)
52	OMG	A2	601	52	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
52	PSU	A2	651	52	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
52	A2M	A2	468	52	22,25,26	1.48	4 (18%)	31,36,39	2.09	9 (29%)
2	T6A	B2	37	2	31,34,35	0.47	0	44,49,52	0.60	1 (2%)
52	OMC	A2	1272	52	19,22,23	0.82	0	26,31,34	0.80	0
52	OMG	A2	867	52	23,26,27	1.19	3 (13%)	33,38,41	1.97	7 (21%)
4	PSU	B5	1861	4	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
4	OMG	B5	4636	4	23,26,27	1.19	3 (13%)	33,38,41	1.92	6 (18%)
52	PSU	A2	1056	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	863	52	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
4	OMC	B5	2350	87,4	19,22,23	0.82	0	26,31,34	0.96	2 (7%)
4	OMG	B5	4195	2,4	23,26,27	1.20	3 (13%)	33,38,41	1.98	7 (21%)
4	A2M	B5	2362	87,4	22,25,26	1.45	4 (18%)	31,36,39	2.11	9 (29%)
4	PSU	B5	3694	4	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
4	OMC	B5	3886	4	19,22,23	0.81	0	26,31,34	0.88	0
4	A2M	B5	1325	4	22,25,26	1.44	4 (18%)	31,36,39	2.11	10 (32%)
4	PSU	B5	4551	4	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
52	PSU	A2	815	52	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
52	PSU	A2	1625	52	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
52	A2M	A2	484	52	22,25,26	1.48	4 (18%)	31,36,39	2.16	9 (29%)
4	OMC	B5	2364	4	19,22,23	0.80	0	26,31,34	0.77	0
4	PSU	B5	4520	87,4	18,21,22	1.35	2 (11%)	22,30,33	1.94	4 (18%)
6	OMU	B8	14	6,4	19,22,23	1.23	3 (15%)	26,31,34	1.72	5 (19%)
52	PSU	A2	1046	52	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
2	M2G	B2	26	2	24,27,28	1.31	4 (16%)	35,40,43	1.85	6 (17%)
4	OMG	B5	1624	4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
52	OMC	A2	797	52	19,22,23	0.81	0	26,31,34	0.81	0
2	PSU	B2	55	2	18,21,22	1.34	2 (11%)	22,30,33	1.82	3 (13%)
52	OMC	A2	174	52	19,22,23	0.82	0	26,31,34	0.82	0
4	OMC	B5	3700	87,4	19,22,23	0.79	0	26,31,34	0.75	0
4	OMU	B5	3924	4	19,22,23	1.23	2 (10%)	26,31,34	1.71	4 (15%)
4	PSU	B5	4441	4	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
4	PSU	B5	4430	4	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	6MZ	B5	4219	4	22,25,26	1.46	4 (18%)	30,36,39	2.26	9 (30%)
4	PSU	B5	2631	4	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
2	H2U	B2	47	2	18,21,22	1.01	2 (11%)	21,30,33	1.94	1 (4%)
4	A2M	B5	1870	4	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
52	A2M	A2	99	87,52	22,25,26	1.48	4 (18%)	31,36,39	2.17	8 (25%)
52	A2M	A2	576	52	22,25,26	1.46	4 (18%)	31,36,39	2.12	10 (32%)
6	OMG	B8	75	6	23,26,27	1.20	3 (13%)	33,38,41	1.95	6 (18%)
52	OMC	A2	1391	52	19,22,23	0.82	0	26,31,34	0.81	0
52	PSU	A2	1174	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
4	UY1	B5	3817	87,4	19,22,23	1.35	3 (15%)	22,31,34	1.79	4 (18%)
4	OMG	B5	4617	4	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
4	A2M	B5	1523	4	22,25,26	1.45	4 (18%)	31,36,39	2.08	9 (29%)
52	PSU	A2	1136	52	18,21,22	1.33	2 (11%)	22,30,33	1.90	4 (18%)
52	A2M	A2	590	52	22,25,26	1.48	4 (18%)	31,36,39	2.19	7 (22%)
4	PSU	B5	1778	4	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
4	A2M	B5	3824	4	22,25,26	1.46	4 (18%)	31,36,39	2.11	10 (32%)
4	OMC	B5	2823	4	19,22,23	0.81	0	26,31,34	0.82	0
4	PSU	B5	3714	4	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	4971	4	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
52	OMU	A2	1326	87,52	19,22,23	1.18	2 (10%)	26,31,34	1.71	5 (19%)
52	PSU	A2	1232	52	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
4	OMC	B5	1880	87,4	19,22,23	0.80	0	26,31,34	0.80	0
4	OMC	B5	3807	4	19,22,23	0.81	0	26,31,34	0.81	1 (3%)
4	PSU	B5	1682	4	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
4	PSU	B5	3767	4	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
52	OMU	A2	354	52	19,22,23	1.21	4 (21%)	26,31,34	1.68	5 (19%)
2	G7M	B2	46	2	23,26,27	3.09	8 (34%)	35,39,42	3.35	15 (42%)
4	PSU	B5	1535	4	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
4	A2M	B5	3829	4	22,25,26	1.46	4 (18%)	31,36,39	2.11	9 (29%)
52	PSU	A2	1045	52	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
4	PSU	B5	4627	4	18,21,22	1.35	2 (11%)	22,30,33	1.94	3 (13%)
4	5MC	B5	3781	87,4	18,22,23	0.95	2 (11%)	26,32,35	1.19	3 (11%)
4	PSU	B5	3843	4	18,21,22	1.39	2 (11%)	22,30,33	1.86	3 (13%)
67	IAS	AO	138	67	6,7,8	0.95	0	6,8,10	1.32	1 (16%)
52	PSU	A2	93	52	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	PSU	A2	109	52	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
4	PSU	B5	4492	87,4	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
76	HY3	AX	62	76	6,8,9	8.06	4 (66%)	5,10,12	1.09	0
52	PSU	A2	649	52	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	1244	87,52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
2	PSU	B2	39	2	18,21,22	0.90	1 (5%)	22,30,33	0.63	0
52	PSU	A2	1081	52	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	5009	4	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
52	OMU	A2	121	52	19,22,23	1.21	3 (15%)	26,31,34	1.64	4 (15%)
4	PSU	B5	3729	4	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
52	PSU	A2	814	52	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
4	OMG	B5	2875	4	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)
4	PSU	B5	1780	4	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
4	OMU	B5	4497	87,4	19,22,23	1.19	2 (10%)	26,31,34	1.74	5 (19%)
4	OMG	B5	4622	4	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
52	G7M	A2	1639	2,52	23,26,27	3.13	9 (39%)	35,39,42	3.31	13 (37%)
52	6MZ	A2	1832	87,52	22,25,26	1.48	4 (18%)	30,36,39	2.22	9 (30%)
4	OMG	B5	4493	4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
4	OMC	B5	4535	4	19,22,23	0.82	0	26,31,34	0.83	0
52	PSU	A2	1347	52	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
52	B8N	A2	1248	52	24,29,30	1.30	3 (12%)	29,42,45	1.30	3 (10%)
6	PSU	B8	55	6	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
52	OMU	A2	799	52	19,22,23	1.21	4 (21%)	26,31,34	1.69	5 (19%)
52	OMG	A2	1490	87,52	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
52	PSU	A2	686	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
4	PSU	B5	3919	87,4	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
4	OMC	B5	3868	4	19,22,23	0.81	0	26,31,34	0.77	0
4	PSU	B5	4531	4	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
7	V5N	BA	216	7	9,11,12	2.07	2 (22%)	9,14,16	1.73	2 (22%)
4	PSU	B5	3821	4	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
4	PSU	B5	4456	4	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
32	V5N	Ba	39	32	9,11,12	2.07	2 (22%)	9,14,16	1.81	2 (22%)
4	A2M	B5	4570	4	22,25,26	1.46	4 (18%)	31,36,39	2.14	9 (29%)
4	OMG	B5	2363	87,4	23,26,27	1.18	3 (13%)	33,38,41	1.95	6 (18%)
52	A2M	A2	159	52	22,25,26	1.48	4 (18%)	31,36,39	2.09	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	OMG	A2	436	52	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
52	OMU	A2	428	52	19,22,23	1.21	3 (15%)	26,31,34	1.72	5 (19%)
72	NMM	AT	67	72	9,11,12	0.60	0	6,12,14	0.48	0
2	5MU	B2	54	2	19,22,23	1.44	6 (31%)	28,32,35	2.00	6 (21%)
4	PSU	B5	1676	4	18,21,22	1.37	2 (11%)	22,30,33	1.85	4 (18%)
4	PSU	B5	3852	87,4	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
4	PSU	B5	2838	4	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
4	5MC	B5	4446	87,4	18,22,23	1.00	2 (11%)	26,32,35	1.21	2 (7%)
4	A2M	B5	2814	87,4	22,25,26	1.46	4 (18%)	31,36,39	2.13	9 (29%)
52	OMG	A2	683	52	23,26,27	1.19	3 (13%)	33,38,41	1.93	6 (18%)
4	PSU	B5	4298	4	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
4	A2M	B5	1322	4	22,25,26	1.46	4 (18%)	31,36,39	2.12	8 (25%)
4	PSU	B5	3850	4	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)
4	PSU	B5	4499	4	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
4	PSU	B5	4672	4	18,21,22	1.39	2 (11%)	22,30,33	1.88	3 (13%)
52	OMU	A2	1442	87,52	19,22,23	1.21	3 (15%)	26,31,34	1.68	5 (19%)
4	OMC	B5	1339	4	19,22,23	0.82	0	26,31,34	0.78	0
4	OMG	B5	4391	4	23,26,27	1.20	3 (13%)	33,38,41	1.92	6 (18%)
52	PSU	A2	801	52	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
4	A2M	B5	1533	87,4	22,25,26	1.46	4 (18%)	31,36,39	2.08	8 (25%)
52	PSU	A2	406	52	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
4	PSU	B5	1581	4	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
4	A2M	B5	3717	4	22,25,26	1.48	4 (18%)	31,36,39	2.07	9 (29%)
2	PSU	B2	31	2	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
4	UR3	B5	4529	4	19,22,23	0.99	1 (5%)	26,32,35	1.43	1 (3%)
52	A2M	A2	1678	52	22,25,26	1.46	4 (18%)	31,36,39	2.26	10 (32%)
4	OMC	B5	3840	4	19,22,23	0.81	0	26,31,34	0.83	0
52	PSU	A2	296	52	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
52	OMC	A2	1703	52	19,22,23	0.82	0	26,31,34	0.83	1 (3%)
52	PSU	A2	119	52	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
52	PSU	A2	1238	52	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
4	A2M	B5	398	4	22,25,26	1.45	4 (18%)	31,36,39	2.16	9 (29%)
2	2MG	B2	10	2	23,26,27	1.27	4 (17%)	32,38,41	2.25	6 (18%)
4	OMC	B5	2803	4	19,22,23	0.83	0	26,31,34	0.81	0
4	OMU	B5	4619	4	19,22,23	1.22	3 (15%)	26,31,34	1.70	4 (15%)

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
52	4AC	A2	1842	52	-	4/11/29/30	0/2/2/2
4	PSU	B5	5000	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4575	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4352	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	4227	4	-	0/9/27/28	0/3/3/3
4	OMG	B5	1521	4	-	0/9/27/28	0/3/3/3
4	OMG	B5	3791	4	-	0/9/27/28	0/3/3/3
52	OMG	A2	1328	87,52	-	0/9/27/28	0/3/3/3
52	PSU	A2	822	52	-	1/7/25/26	0/2/2/2
4	PSU	B5	4470	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	3723	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	1859	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	1315	87,4	-	2/9/27/28	0/3/3/3
4	OMG	B5	4498	4	-	0/9/27/28	0/3/3/3
52	PSU	A2	218	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	172	52	-	0/9/27/28	0/2/2/2
4	PSU	B5	4972	4	-	0/7/25/26	0/2/2/2
52	A2M	A2	1383	52	-	0/9/27/28	0/3/3/3
4	PSU	B5	3769	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	1004	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1692	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	1804	52	-	0/9/27/28	0/2/2/2
52	PSU	A2	1643	52	-	0/7/25/26	0/2/2/2
4	OMG	B5	3626	4	-	0/9/27/28	0/3/3/3
4	OMC	B5	4455	4	-	0/9/27/28	0/2/2/2
4	OMG	B5	3743	4	-	0/9/27/28	0/3/3/3
52	PSU	A2	1367	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	4292	4	-	0/7/25/26	0/2/2/2
52	OMC	A2	517	52	-	1/9/27/28	0/2/2/2
4	A2M	B5	2400	4	-	0/9/27/28	0/3/3/3
5	GTP	B7	1	5	-	3/22/38/38	0/3/3/3
4	PSU	B5	3883	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	681	52	-	0/7/25/26	0/2/2/2
4	OMG	B5	2423	4	-	0/9/27/28	0/3/3/3
4	A2M	B5	400	4	-	0/9/27/28	0/3/3/3
52	OMG	A2	1447	52	-	2/9/27/28	0/3/3/3
52	OMG	A2	509	87,52	-	3/9/27/28	0/3/3/3
52	A2M	A2	166	52	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	B5	4402	4	-	0/7/25/26	0/2/2/2
52	OMU	A2	116	52	-	1/9/27/28	0/2/2/2
2	H2U	B2	16	2	-	7/7/38/39	0/2/2/2
52	PSU	A2	609	52	-	0/7/25/26	0/2/2/2
2	1MA	B2	58	2	-	0/7/25/26	0/3/3/3
4	PSU	B5	1791	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	3866	4	-	2/9/27/28	0/3/3/3
4	OMG	B5	3943	4	-	0/9/27/28	0/3/3/3
52	PSU	A2	36	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	210	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	4422	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	34	52	-	0/7/25/26	0/2/2/2
52	OMU	A2	1288	52	-	0/9/27/28	0/2/2/2
4	PSU	B5	4295	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4311	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	2842	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	866	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1445	52	-	0/7/25/26	0/2/2/2
4	A2M	B5	4522	87,4	-	2/9/27/28	0/3/3/3
2	H2U	B2	20	2	-	5/7/38/39	0/2/2/2
4	OMU	B5	2414	4	-	0/9/27/28	0/2/2/2
2	2MG	B2	6	2	-	0/9/27/28	0/3/3/3
52	OMU	A2	627	52	-	2/9/27/28	0/2/2/2
2	PSU	B2	27	2	-	0/7/25/26	0/2/2/2
8	HIC	BB	245	8	-	2/5/6/8	0/1/1/1
52	MA6	A2	1850	52	-	3/11/29/30	0/3/3/3
45	MLZ	Bo	53	45	-	0/7/8/10	-
52	OMG	A2	644	52	-	4/9/27/28	0/3/3/3
6	PSU	B8	69	6	-	0/7/25/26	0/2/2/2
4	PSU	B5	2507	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3761	4	-	2/7/25/26	0/2/2/2
4	PSU	B5	4635	4	-	2/7/25/26	0/2/2/2
52	PSU	A2	966	52	-	0/7/25/26	0/2/2/2
4	A2M	B5	3784	4	-	2/9/27/28	0/3/3/3
4	A2M	B5	2786	87,4	-	3/9/27/28	0/3/3/3
2	OMC	B2	34	2,3	-	0/9/27/28	0/2/2/2
4	PSU	B5	4360	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3636	4	-	0/7/25/26	0/2/2/2
52	OMC	A2	462	52	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	A2	572	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	4578	4	-	0/7/25/26	0/2/2/2
4	OMU	B5	2836	4	-	1/9/27/28	0/2/2/2
4	OMC	B5	2421	87,4	-	3/9/27/28	0/2/2/2
4	OMG	B5	3898	87,4	-	0/9/27/28	0/3/3/3
4	OMU	B5	4226	4	-	0/9/27/28	0/2/2/2
52	A2M	A2	668	87,52	-	2/9/27/28	0/3/3/3
52	PSU	A2	1177	52	-	0/7/25/26	0/2/2/2
52	4AC	A2	1337	52	-	4/11/29/30	0/2/2/2
2	5MC	B2	48	2	-	3/7/25/26	0/2/2/2
4	OMU	B5	4305	4	-	0/9/27/28	0/2/2/2
4	1MA	B5	1321	87,4	-	1/7/25/26	0/3/3/3
52	A2M	A2	1031	52	-	0/9/27/28	0/3/3/3
4	A2M	B5	4589	4	-	3/9/27/28	0/3/3/3
4	PSU	B5	1743	4	-	0/7/25/26	0/2/2/2
4	OMC	B5	2860	4	-	0/9/27/28	0/2/2/2
33	MLZ	Bb	5	33	-	0/7/8/10	-
4	PSU	B5	4688	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	4369	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	1781	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3638	4	-	0/7/25/26	0/2/2/2
52	A2M	A2	27	52	-	1/9/27/28	0/3/3/3
52	A2M	A2	512	52	-	3/9/27/28	0/3/3/3
52	PSU	A2	105	52	-	0/7/25/26	0/2/2/2
52	MA6	A2	1851	52	-	2/11/29/30	0/3/3/3
52	OMG	A2	601	52	-	0/9/27/28	0/3/3/3
52	PSU	A2	651	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	468	52	-	2/9/27/28	0/3/3/3
2	T6A	B2	37	2	-	8/23/41/42	0/3/3/3
52	OMC	A2	1272	52	-	1/9/27/28	0/2/2/2
52	OMG	A2	867	52	-	1/9/27/28	0/3/3/3
4	PSU	B5	1861	4	-	0/7/25/26	0/2/2/2
4	OMG	B5	4636	4	-	0/9/27/28	0/3/3/3
52	PSU	A2	1056	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	863	52	-	0/7/25/26	0/2/2/2
4	OMC	B5	2350	87,4	-	2/9/27/28	0/2/2/2
4	OMG	B5	4195	2,4	-	0/9/27/28	0/3/3/3
4	A2M	B5	2362	87,4	-	0/9/27/28	0/3/3/3
4	PSU	B5	3694	4	-	0/7/25/26	0/2/2/2
4	OMC	B5	3886	4	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A2M	B5	1325	4	-	2/9/27/28	0/3/3/3
4	PSU	B5	4551	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	815	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1625	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	484	52	-	0/9/27/28	0/3/3/3
4	OMC	B5	2364	4	-	0/9/27/28	0/2/2/2
4	PSU	B5	4520	87,4	-	0/7/25/26	0/2/2/2
6	OMU	B8	14	6,4	-	0/9/27/28	0/2/2/2
52	PSU	A2	1046	52	-	0/7/25/26	0/2/2/2
2	M2G	B2	26	2	-	0/11/29/30	0/3/3/3
4	OMG	B5	1624	4	-	1/9/27/28	0/3/3/3
52	OMC	A2	797	52	-	0/9/27/28	0/2/2/2
2	PSU	B2	55	2	-	0/7/25/26	0/2/2/2
52	OMC	A2	174	52	-	0/9/27/28	0/2/2/2
4	OMC	B5	3700	87,4	-	4/9/27/28	0/2/2/2
4	OMU	B5	3924	4	-	0/9/27/28	0/2/2/2
4	PSU	B5	4441	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4430	4	-	0/7/25/26	0/2/2/2
4	6MZ	B5	4219	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	2631	4	-	0/7/25/26	0/2/2/2
2	H2U	B2	47	2	-	7/7/38/39	0/2/2/2
4	A2M	B5	1870	4	-	1/9/27/28	0/3/3/3
52	A2M	A2	99	87,52	-	2/9/27/28	0/3/3/3
52	A2M	A2	576	52	-	2/9/27/28	0/3/3/3
6	OMG	B8	75	6	-	0/9/27/28	0/3/3/3
52	OMC	A2	1391	52	-	2/9/27/28	0/2/2/2
52	PSU	A2	1174	52	-	0/7/25/26	0/2/2/2
4	UY1	B5	3817	87,4	-	2/9/27/28	0/2/2/2
4	OMG	B5	4617	4	-	0/9/27/28	0/3/3/3
4	A2M	B5	1523	4	-	0/9/27/28	0/3/3/3
52	PSU	A2	1136	52	-	0/7/25/26	0/2/2/2
52	A2M	A2	590	52	-	3/9/27/28	0/3/3/3
4	PSU	B5	1778	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	3824	4	-	0/9/27/28	0/3/3/3
4	OMC	B5	2823	4	-	1/9/27/28	0/2/2/2
4	PSU	B5	3714	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4971	4	-	0/7/25/26	0/2/2/2
52	OMU	A2	1326	87,52	-	0/9/27/28	0/2/2/2
52	PSU	A2	1232	52	-	0/7/25/26	0/2/2/2
4	OMC	B5	1880	87,4	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMC	B5	3807	4	-	2/9/27/28	0/2/2/2
4	PSU	B5	1682	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3767	4	-	0/7/25/26	0/2/2/2
52	OMU	A2	354	52	-	0/9/27/28	0/2/2/2
2	G7M	B2	46	2	-	3/7/25/26	0/3/3/3
4	PSU	B5	1535	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	3829	4	-	0/9/27/28	0/3/3/3
52	PSU	A2	1045	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	4627	4	-	0/7/25/26	0/2/2/2
4	5MC	B5	3781	87,4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3843	4	-	1/7/25/26	0/2/2/2
67	IAS	AO	138	67	-	1/7/7/8	-
52	PSU	A2	93	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	109	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	4492	87,4	-	0/7/25/26	0/2/2/2
76	HY3	AX	62	76	-	1/1/12/14	0/1/1/1
52	PSU	A2	649	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1244	87,52	-	0/7/25/26	0/2/2/2
2	PSU	B2	39	2	-	0/7/25/26	0/2/2/2
52	PSU	A2	1081	52	-	1/7/25/26	0/2/2/2
4	PSU	B5	5009	4	-	0/7/25/26	0/2/2/2
52	OMU	A2	121	52	-	0/9/27/28	0/2/2/2
4	PSU	B5	3729	4	-	0/7/25/26	0/2/2/2
52	PSU	A2	814	52	-	0/7/25/26	0/2/2/2
4	OMG	B5	2875	4	-	0/9/27/28	0/3/3/3
4	PSU	B5	1780	4	-	2/7/25/26	0/2/2/2
4	OMU	B5	4497	87,4	-	0/9/27/28	0/2/2/2
4	OMG	B5	4622	4	-	2/9/27/28	0/3/3/3
52	G7M	A2	1639	2,52	-	2/7/25/26	0/3/3/3
52	6MZ	A2	1832	87,52	-	0/9/27/28	0/3/3/3
4	OMG	B5	4493	4	-	0/9/27/28	0/3/3/3
4	OMC	B5	4535	4	-	0/9/27/28	0/2/2/2
52	PSU	A2	1347	52	-	0/7/25/26	0/2/2/2
52	B8N	A2	1248	52	-	0/16/34/35	0/2/2/2
6	PSU	B8	55	6	-	0/7/25/26	0/2/2/2
52	OMU	A2	799	52	-	3/9/27/28	0/2/2/2
52	OMG	A2	1490	87,52	-	0/9/27/28	0/3/3/3
52	PSU	A2	686	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	3919	87,4	-	0/7/25/26	0/2/2/2
4	OMC	B5	3868	4	-	0/9/27/28	0/2/2/2
4	PSU	B5	4531	4	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	V5N	BA	216	7	-	3/9/10/12	0/1/1/1
4	PSU	B5	3821	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4456	4	-	0/7/25/26	0/2/2/2
32	V5N	Ba	39	32	-	0/9/10/12	0/1/1/1
4	A2M	B5	4570	4	-	0/9/27/28	0/3/3/3
4	OMG	B5	2363	87,4	-	4/9/27/28	0/3/3/3
52	A2M	A2	159	52	-	0/9/27/28	0/3/3/3
52	OMG	A2	436	52	-	0/9/27/28	0/3/3/3
52	OMU	A2	428	52	-	2/9/27/28	0/2/2/2
72	NMM	AT	67	72	-	0/9/11/13	-
2	5MU	B2	54	2	-	0/7/25/26	0/2/2/2
4	PSU	B5	1676	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	3852	87,4	-	0/7/25/26	0/2/2/2
4	PSU	B5	2838	4	-	0/7/25/26	0/2/2/2
4	5MC	B5	4446	87,4	-	4/7/25/26	0/2/2/2
4	A2M	B5	2814	87,4	-	1/9/27/28	0/3/3/3
52	OMG	A2	683	52	-	0/9/27/28	0/3/3/3
4	PSU	B5	4298	4	-	0/7/25/26	0/2/2/2
4	A2M	B5	1322	4	-	2/9/27/28	0/3/3/3
4	PSU	B5	3850	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4499	4	-	0/7/25/26	0/2/2/2
4	PSU	B5	4672	4	-	0/7/25/26	0/2/2/2
52	OMU	A2	1442	87,52	-	0/9/27/28	0/2/2/2
4	OMC	B5	1339	4	-	0/9/27/28	0/2/2/2
4	OMG	B5	4391	4	-	1/9/27/28	0/3/3/3
52	PSU	A2	801	52	-	0/7/25/26	0/2/2/2
4	A2M	B5	1533	87,4	-	1/9/27/28	0/3/3/3
52	PSU	A2	406	52	-	0/7/25/26	0/2/2/2
4	PSU	B5	1581	4	-	2/7/25/26	0/2/2/2
4	A2M	B5	3717	4	-	0/9/27/28	0/3/3/3
2	PSU	B2	31	2	-	0/7/25/26	0/2/2/2
4	UR3	B5	4529	4	-	0/7/25/26	0/2/2/2
52	A2M	A2	1678	52	-	1/9/27/28	0/3/3/3
4	OMC	B5	3840	4	-	1/9/27/28	0/2/2/2
52	PSU	A2	296	52	-	0/7/25/26	0/2/2/2
52	OMC	A2	1703	52	-	3/9/27/28	0/2/2/2
52	PSU	A2	119	52	-	0/7/25/26	0/2/2/2
52	PSU	A2	1238	52	-	0/7/25/26	0/2/2/2
4	A2M	B5	398	4	-	2/9/27/28	0/3/3/3
2	2MG	B2	10	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMC	B5	2803	4	-	0/9/27/28	0/2/2/2
4	OMU	B5	4619	4	-	0/9/27/28	0/2/2/2

The worst 5 of 571 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	AX	62	HY3	C3-CA	-18.71	1.36	1.55
52	A2	1639	G7M	C4-N9	7.83	1.58	1.38
2	B2	46	G7M	O6-C6	7.72	1.38	1.23
52	A2	1639	G7M	O6-C6	7.65	1.38	1.23
2	B2	46	G7M	C4-N9	7.46	1.57	1.38

The worst 5 of 1039 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A2	1850	MA6	C4-N9-C8	14.75	121.72	105.73
52	A2	1851	MA6	C4-N9-C8	14.40	121.33	105.73
2	B2	46	G7M	C8-N7-C5	11.45	122.10	107.78
52	A2	1639	G7M	C8-N7-C5	11.45	122.09	107.78
2	B2	20	H2U	C4-N3-C2	-9.87	117.60	125.79

There are no chirality outliers.

5 of 165 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B7	1	GTP	C5'-O5'-PA-O3A
7	BA	216	V5N	O-C-CA-CB
76	AX	62	HY3	O-C-CA-C3
2	B2	16	H2U	O4'-C1'-N1-C6
2	B2	16	H2U	C2'-C1'-N1-C6

There are no ring outliers.

76 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	A2	1842	4AC	1	0
4	B5	3791	OMG	1	0
52	A2	1328	OMG	1	0
4	B5	3723	A2M	1	0
4	B5	1315	OMG	1	0
52	A2	172	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B5	3769	PSU	1	0
52	A2	1804	OMU	1	0
4	B5	4455	OMC	2	0
52	A2	1447	OMG	2	0
52	A2	166	A2M	2	0
52	A2	116	OMU	3	0
2	B2	16	H2U	2	0
2	B2	58	1MA	1	0
4	B5	3943	OMG	1	0
52	A2	36	PSU	1	0
4	B5	4295	PSU	2	0
4	B5	4311	PSU	1	0
4	B5	4522	A2M	1	0
4	B5	2414	OMU	1	0
2	B2	27	PSU	1	0
8	BB	245	HIC	1	0
2	B2	34	OMC	2	0
52	A2	462	OMC	1	0
4	B5	4578	PSU	1	0
4	B5	4226	OMU	1	0
52	A2	1337	4AC	2	0
52	A2	1031	A2M	1	0
4	B5	4589	A2M	1	0
4	B5	2860	OMC	1	0
52	A2	27	A2M	1	0
52	A2	601	OMG	1	0
52	A2	468	A2M	3	0
2	B2	37	T6A	2	0
52	A2	1272	OMC	1	0
4	B5	2350	OMC	1	0
4	B5	2362	A2M	1	0
4	B5	3886	OMC	1	0
4	B5	1325	A2M	1	0
52	A2	484	A2M	1	0
4	B5	2364	OMC	1	0
2	B2	26	M2G	1	0
4	B5	4219	6MZ	1	0
4	B5	1870	A2M	2	0
52	A2	99	A2M	2	0
52	A2	576	A2M	1	0
52	A2	1391	OMC	1	0
4	B5	4617	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	A2	1136	PSU	1	0
4	B5	1778	PSU	2	0
4	B5	3824	A2M	1	0
4	B5	3807	OMC	1	0
4	B5	3829	A2M	2	0
52	A2	121	OMU	1	0
4	B5	2875	OMG	1	0
52	A2	1832	6MZ	1	0
4	B5	4535	OMC	1	0
52	A2	1248	B8N	1	0
52	A2	799	OMU	1	0
52	A2	1490	OMG	1	0
4	B5	4456	PSU	1	0
4	B5	4570	A2M	2	0
52	A2	159	A2M	4	0
52	A2	436	OMG	1	0
72	AT	67	NMM	2	0
2	B2	54	5MU	1	0
4	B5	4446	5MC	1	0
4	B5	2814	A2M	1	0
4	B5	4391	OMG	2	0
4	B5	3717	A2M	2	0
52	A2	1678	A2M	1	0
4	B5	3840	OMC	1	0
52	A2	1703	OMC	1	0
4	B5	398	A2M	1	0
4	B5	2803	OMC	1	0
4	B5	4619	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 440 ligands modelled in this entry, 440 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

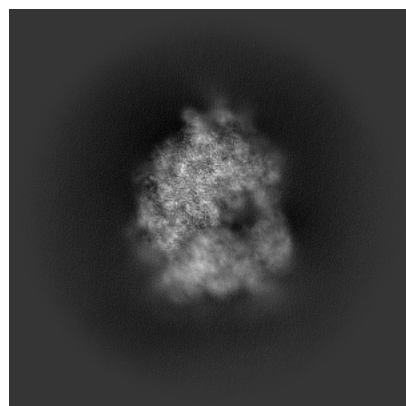
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56598. These allow visual inspection of the internal detail of the map and identification of artifacts.

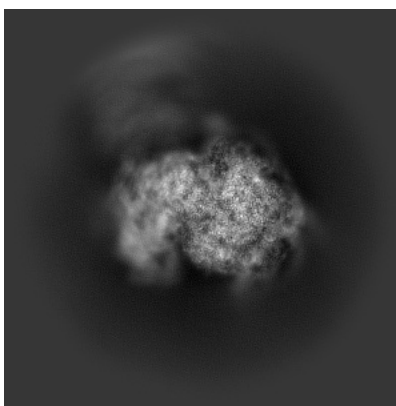
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

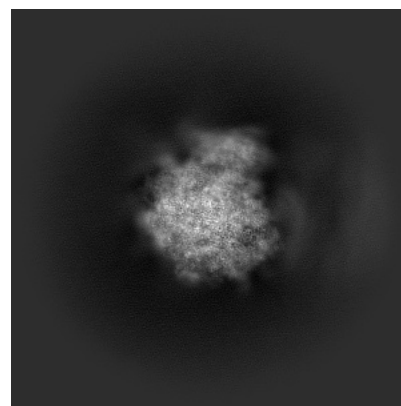
6.1.1 Primary map



X

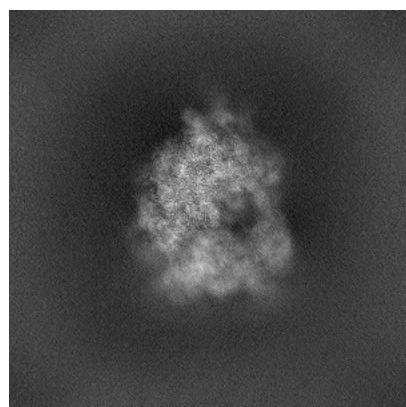


Y

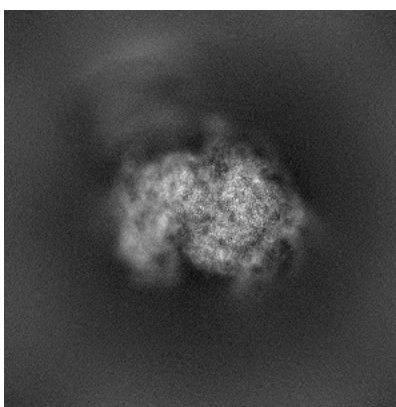


Z

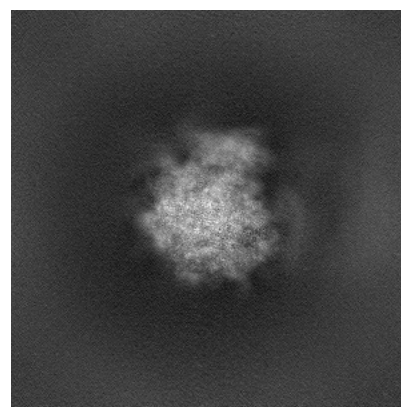
6.1.2 Raw map



X



Y

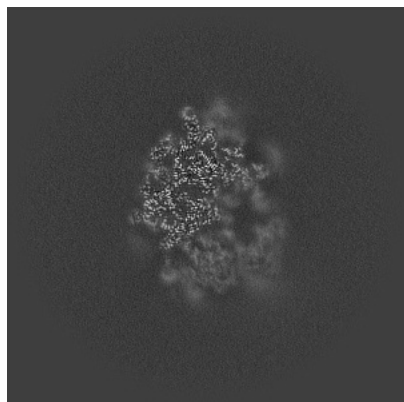


Z

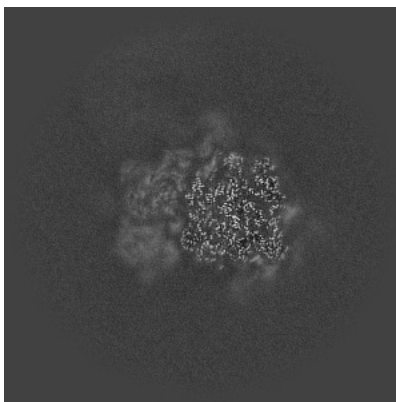
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

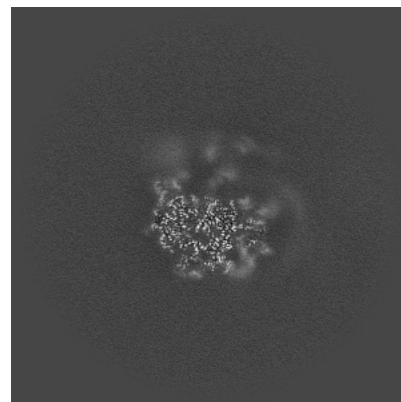
6.2.1 Primary map



X Index: 280

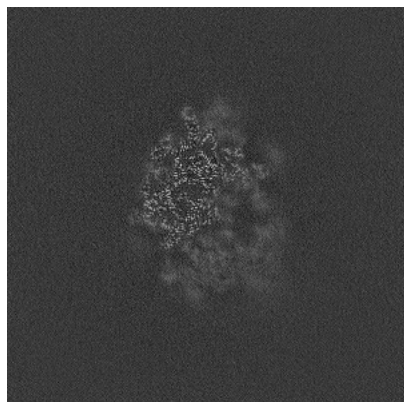


Y Index: 280

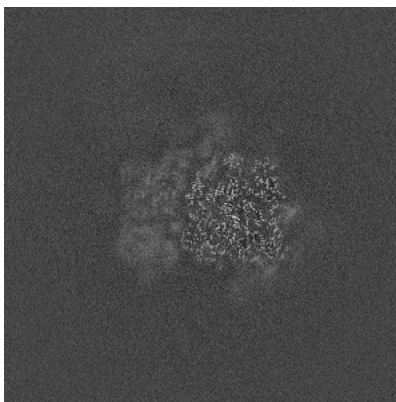


Z Index: 280

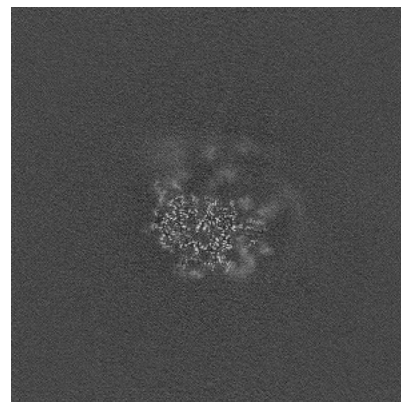
6.2.2 Raw map



X Index: 280



Y Index: 280

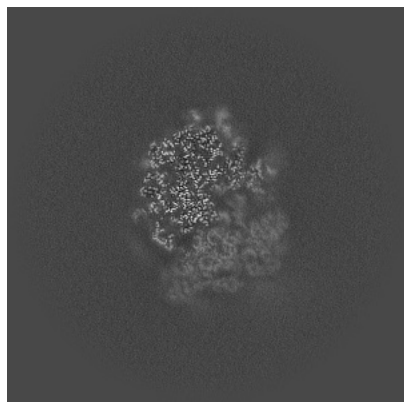


Z Index: 280

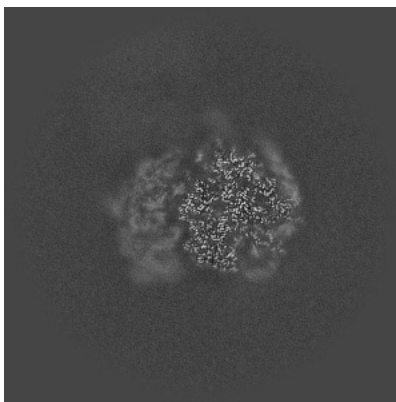
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

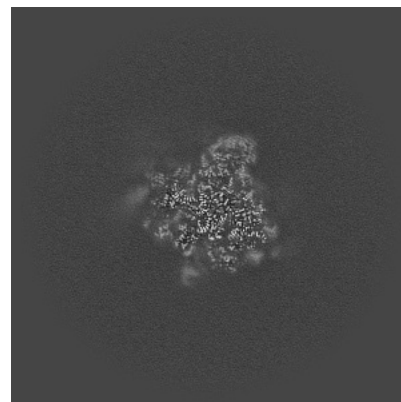
6.3.1 Primary map



X Index: 294

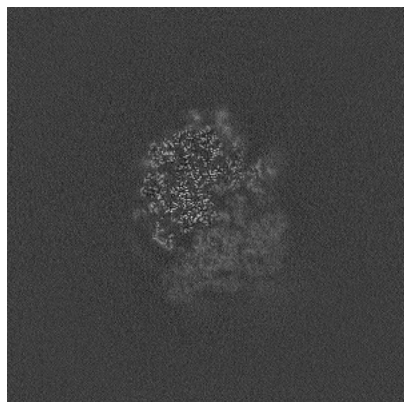


Y Index: 264

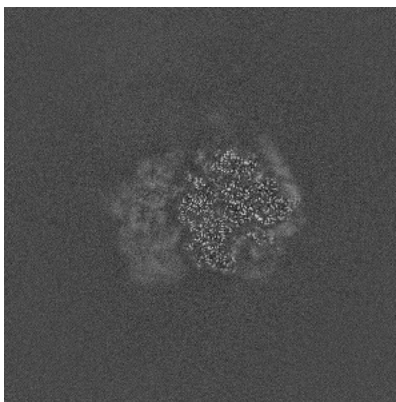


Z Index: 327

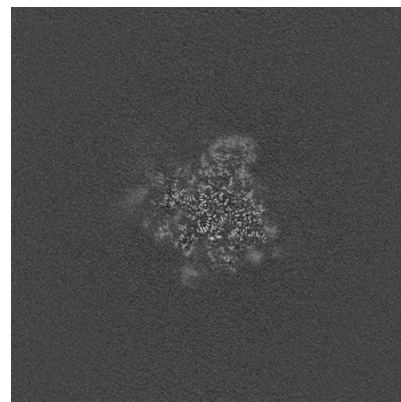
6.3.2 Raw map



X Index: 294



Y Index: 262

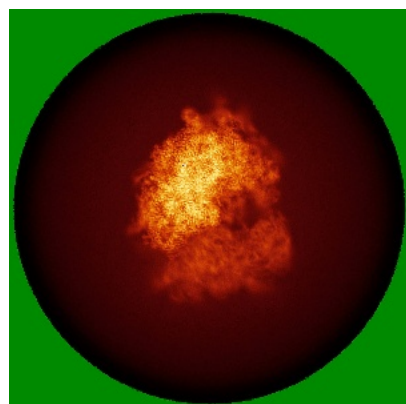


Z Index: 327

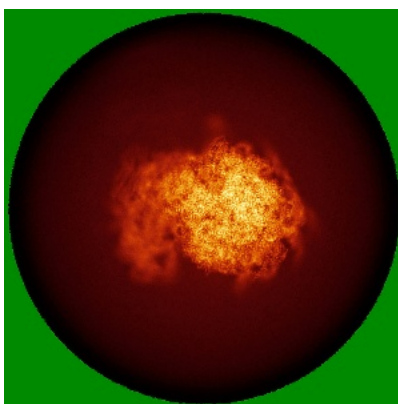
The images above show the largest variance slices of the map in three orthogonal directions.

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

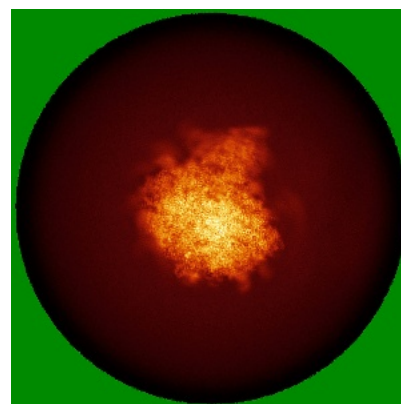
6.4.1 Primary map



X

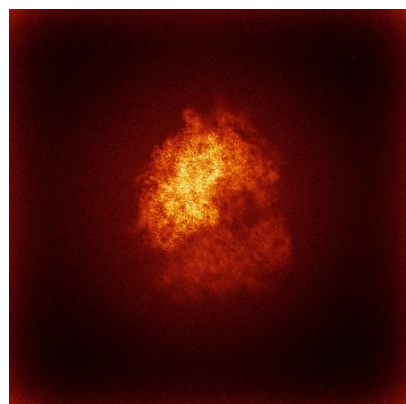


Y

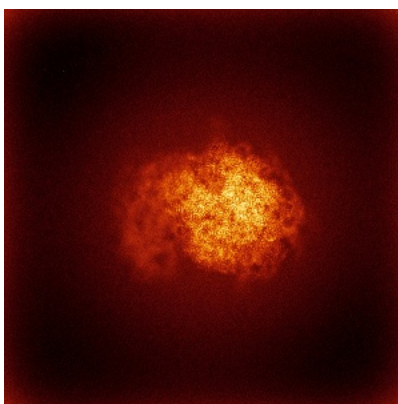


Z

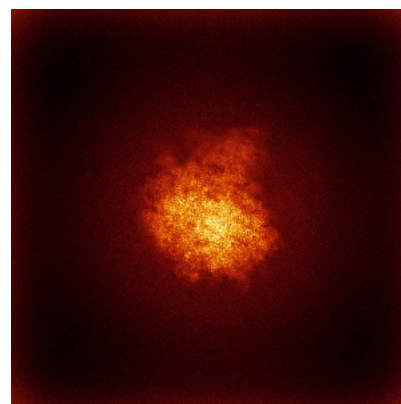
6.4.2 Raw map



X



Y

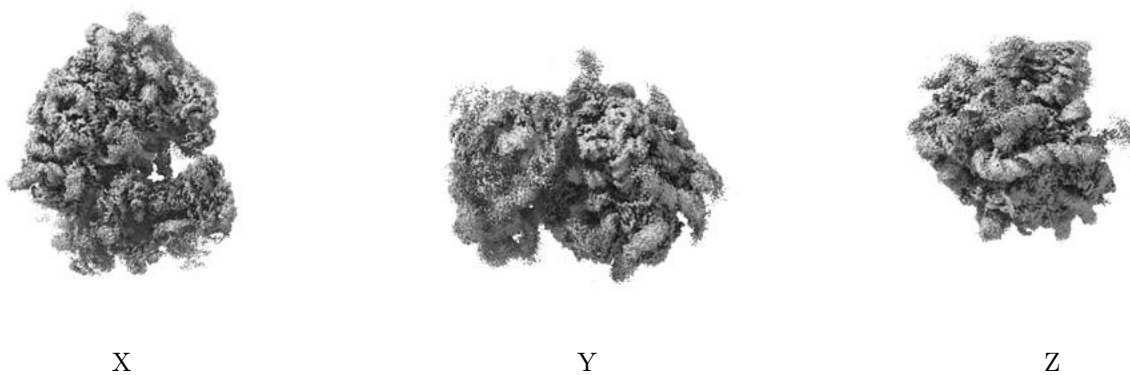


Z

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

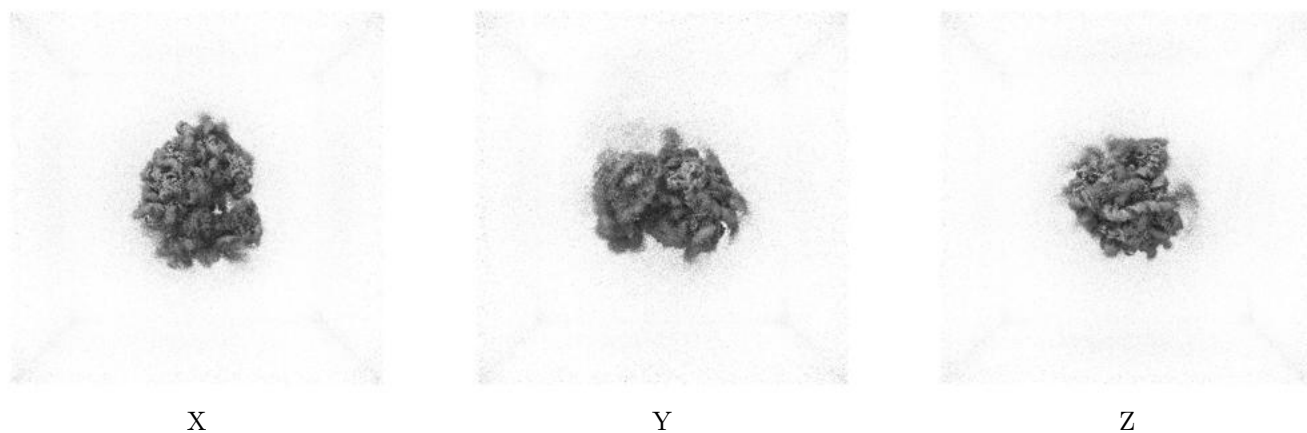
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.149. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

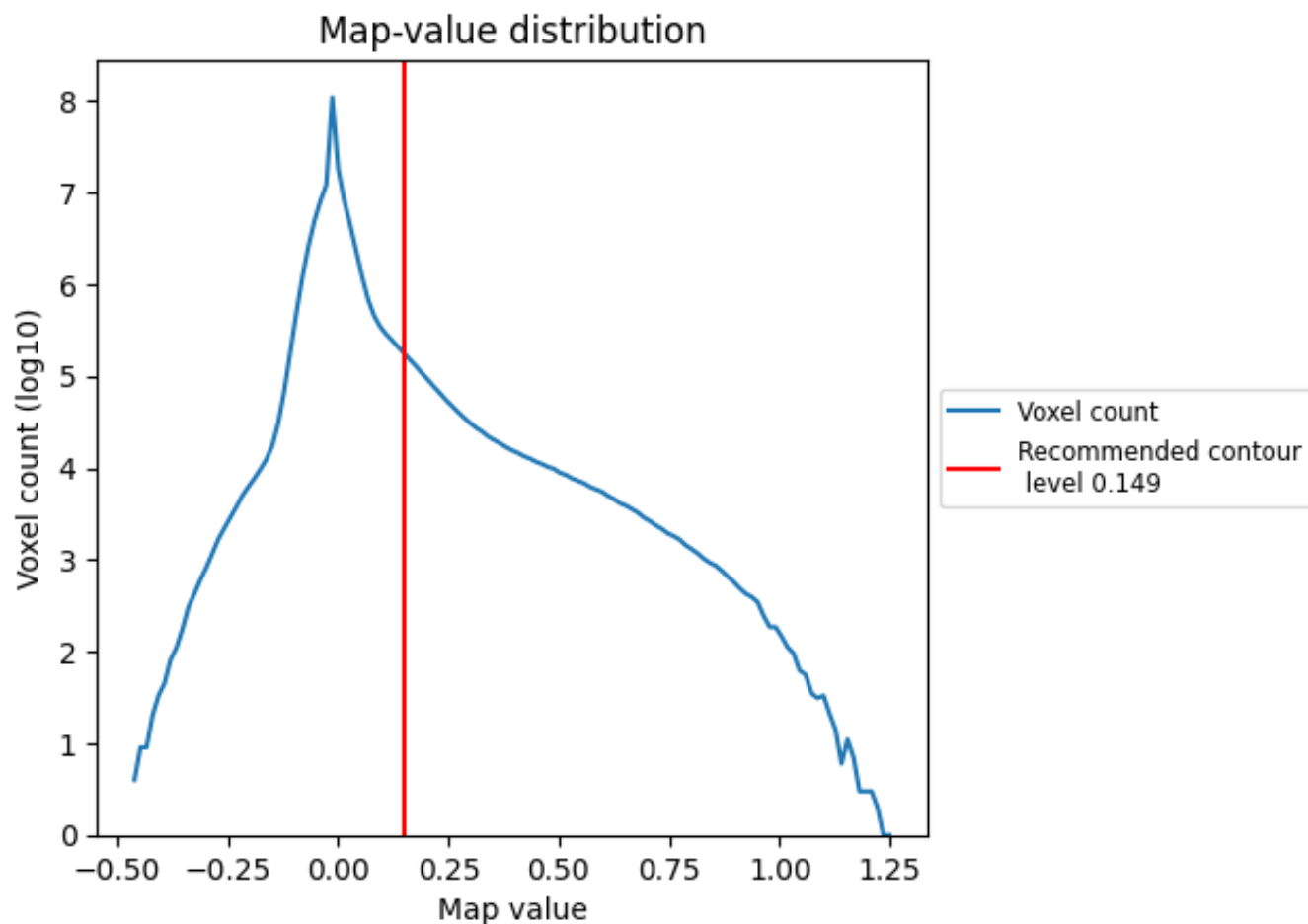
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

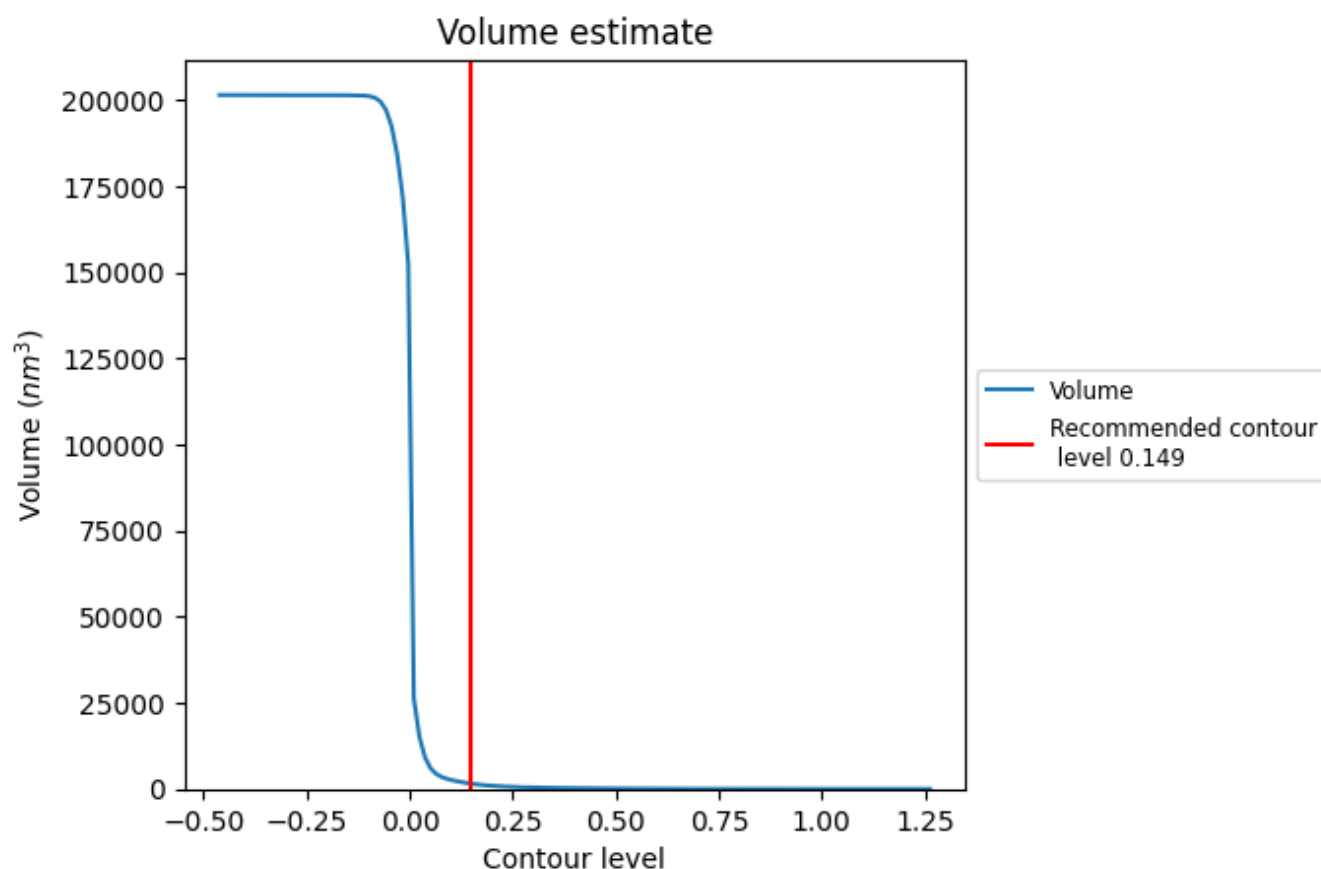
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

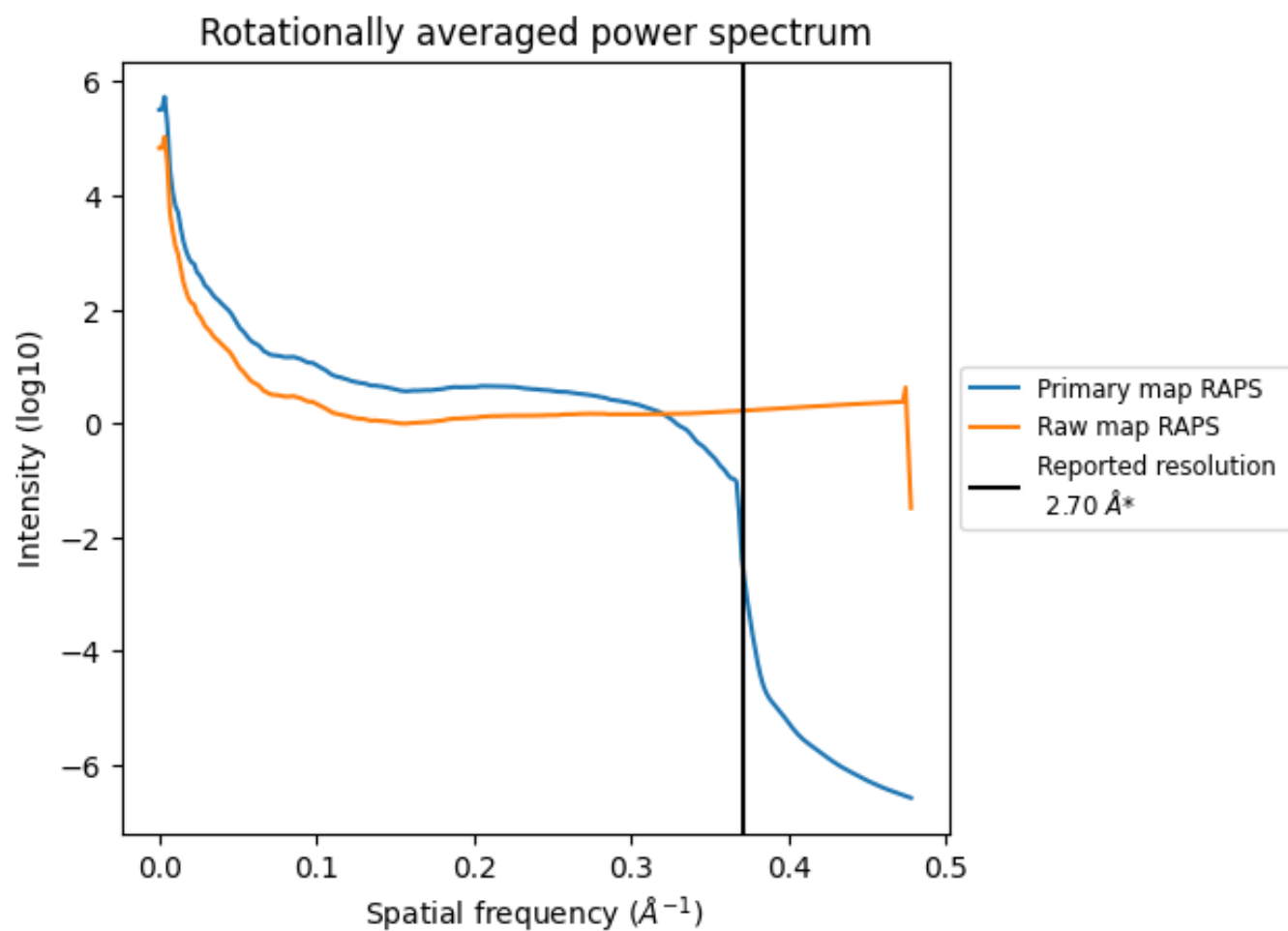
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1547 nm^3 ; this corresponds to an approximate mass of 1397 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

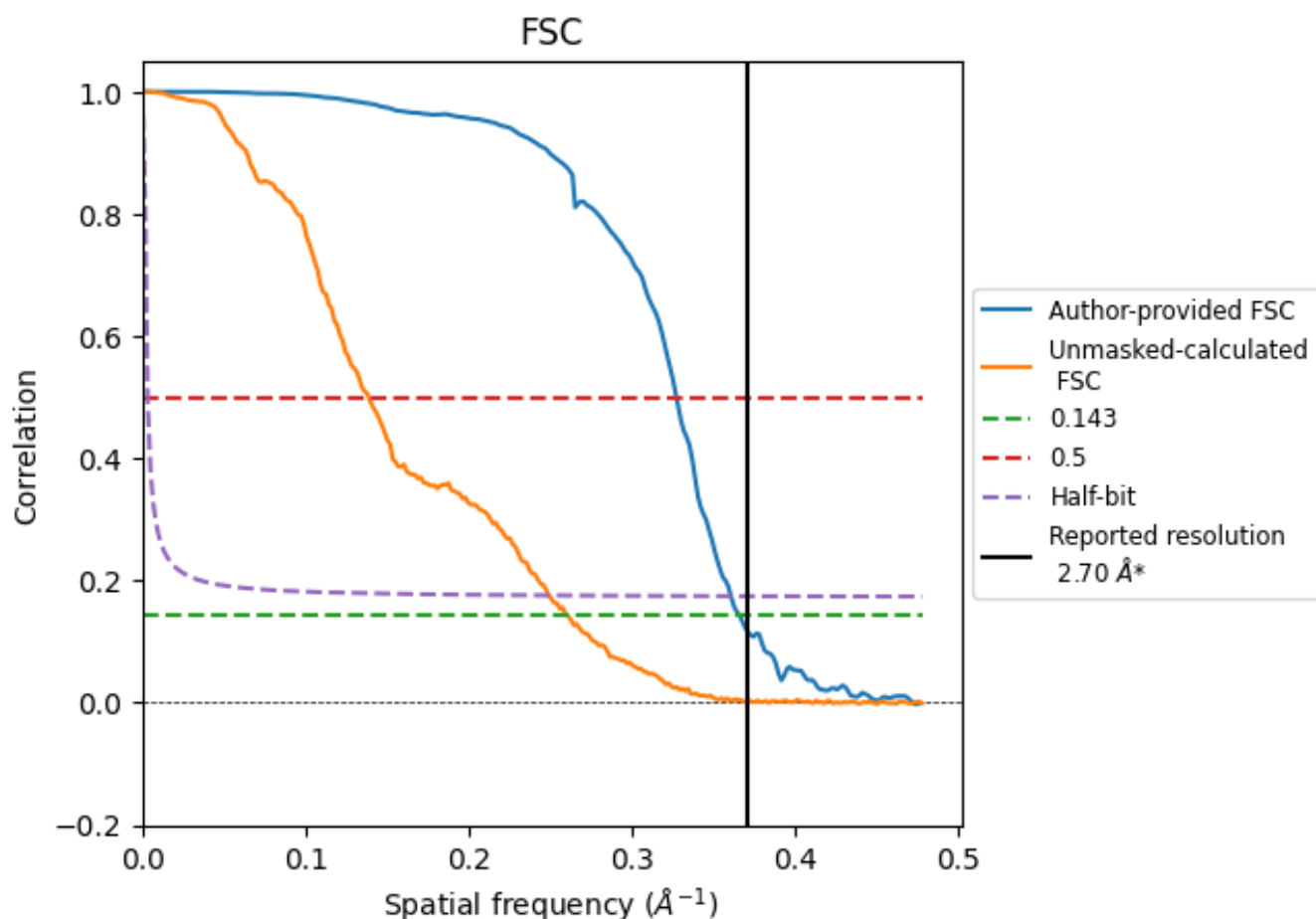


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

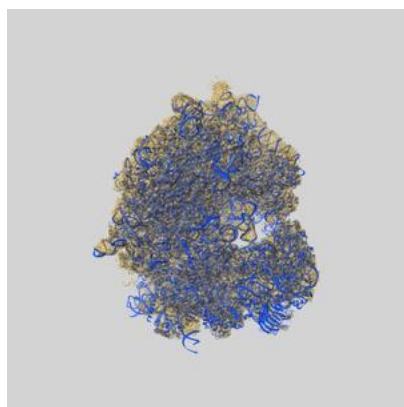
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.73	3.06	2.77
Unmasked-calculated*	3.84	7.21	4.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.84 differs from the reported value 2.7 by more than 10 %

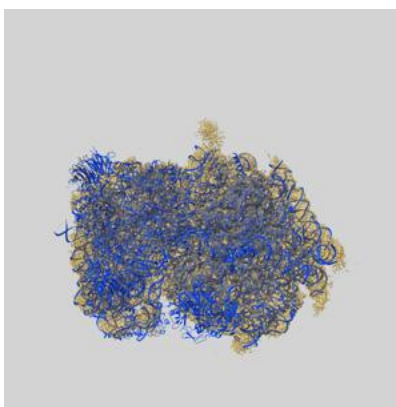
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56598 and PDB model 28LN. Per-residue inclusion information can be found in section [3](#) on page [22](#).

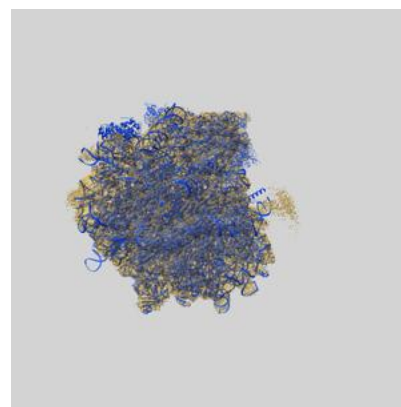
9.1 Map-model overlay [i](#)



X



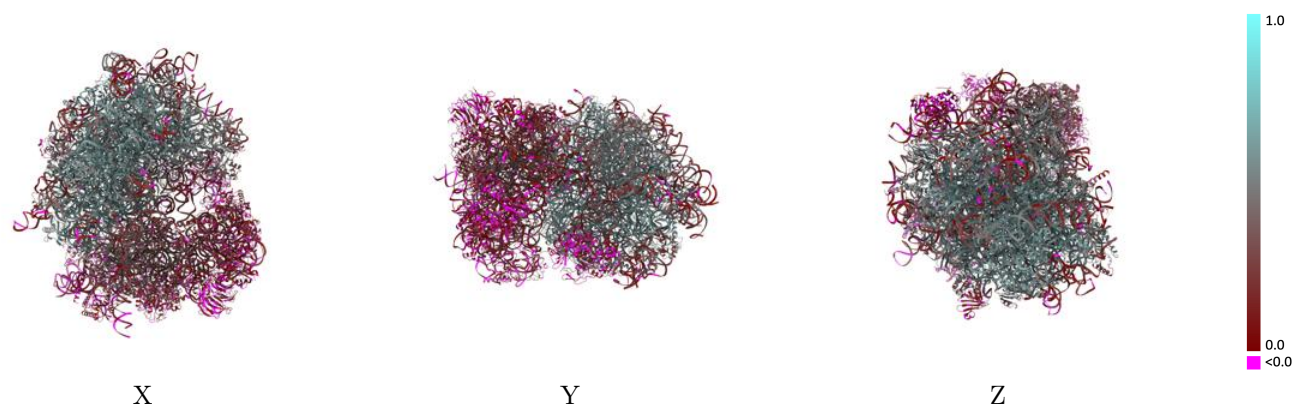
Y



Z

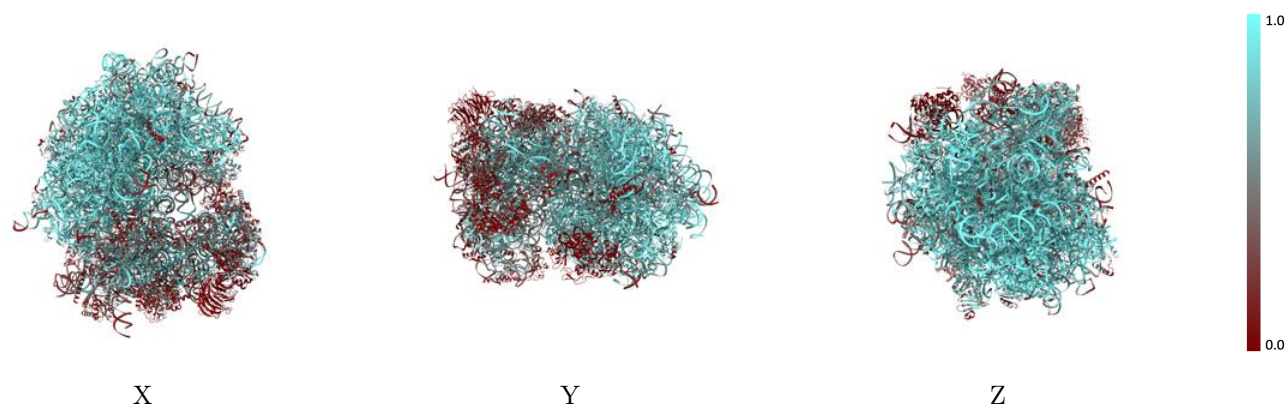
The images above show the 3D surface view of the map at the recommended contour level 0.149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



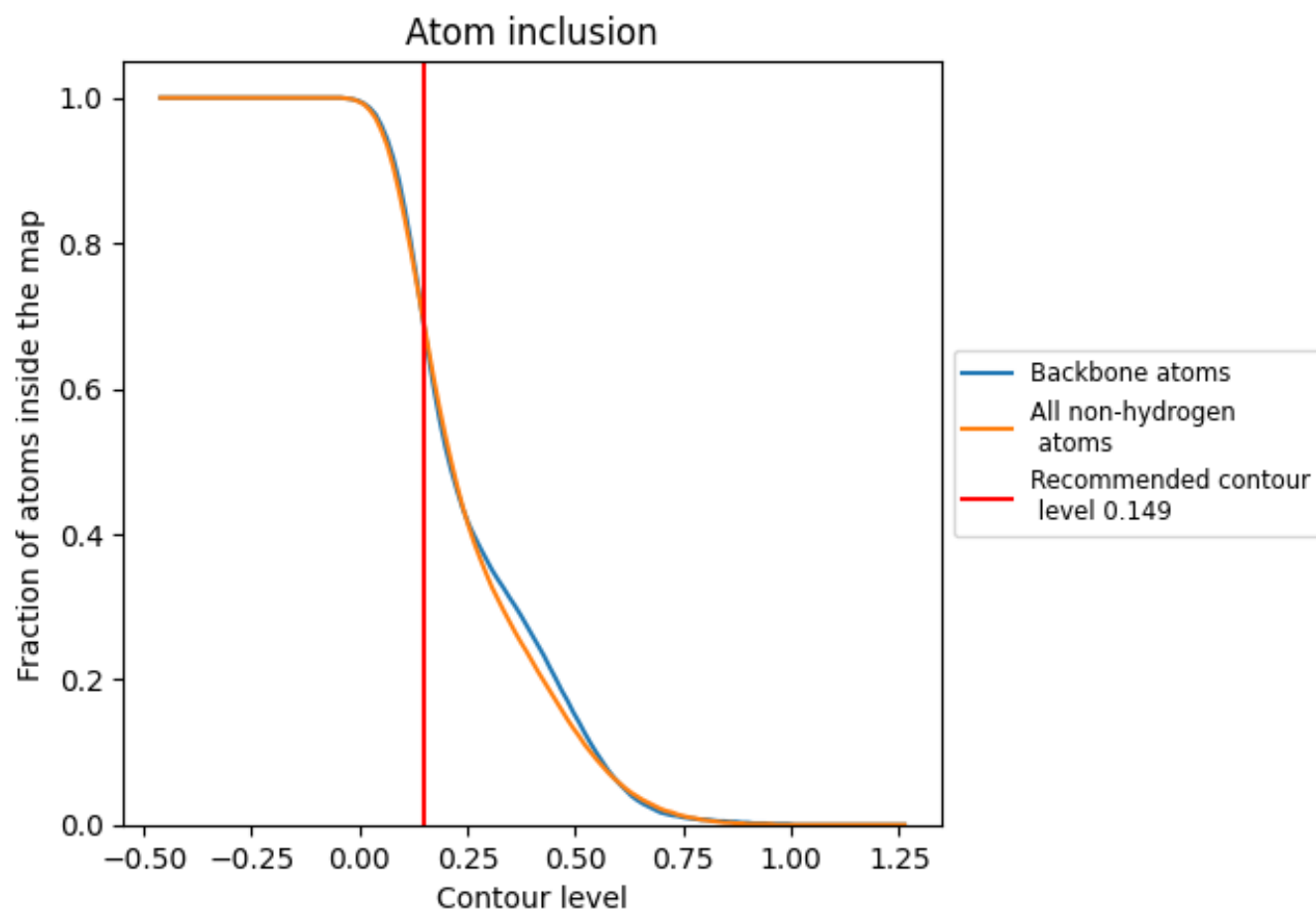
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.149).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 69% 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 (0.149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6880	 0.3670
A2	 0.6480	 0.2030
AA	 0.2520	 0.2150
AB	 0.2870	 0.2610
AC	 0.2830	 0.2190
AD	 0.1750	 0.1620
AE	 0.2260	 0.1080
AF	 0.2650	 0.1620
AG	 0.1030	 0.0790
AH	 0.2430	 0.1730
AI	 0.1560	 0.1390
AJ	 0.2410	 0.1090
AK	 0.0850	 0.0810
AL	 0.2480	 0.1940
AM	 0.0050	 0.0240
AN	 0.4530	 0.3710
AO	 0.3660	 0.2830
AP	 0.2460	 0.1290
AQ	 0.2460	 0.1380
AR	 0.1770	 0.1480
AS	 0.3990	 0.1560
AT	 0.3160	 0.1500
AU	 0.2070	 0.1670
AV	 0.2400	 0.2100
AW	 0.4480	 0.2960
AX	 0.1430	 0.1550
AY	 0.1360	 0.0790
AZ	 0.1910	 0.1450
Aa	 0.3500	 0.2610
Ab	 0.3260	 0.2450
Ac	 0.2400	 0.1910
Ad	 0.3470	 0.1370
Ae	 0.1810	 0.1040
Af	 0.0100	 0.0210
Ag	 0.0150	 0.0660























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Chain	Atom inclusion	Q-score
Ah	 0.0830	 0.2060
B1	 0.4890	 0.3790
B2	 0.5400	 0.2290
B4	 0.7320	 0.2860
B5	 0.8690	 0.4610
B7	 0.9510	 0.4820
B8	 0.9450	 0.5280
BA	 0.9230	 0.5970
BB	 0.8910	 0.5620
BC	 0.9270	 0.5820
BD	 0.7060	 0.4140
BE	 0.8450	 0.5030
BF	 0.9120	 0.5670
BG	 0.7700	 0.4910
BH	 0.6950	 0.4190
BI	 0.3520	 0.2650
BJ	 0.6060	 0.3560
BL	 0.7610	 0.4970
BM	 0.8480	 0.5010
BN	 0.9340	 0.6040
BO	 0.8900	 0.5580
BP	 0.9100	 0.5750
BQ	 0.9150	 0.5900
BR	 0.7010	 0.4460
BS	 0.8500	 0.5340
BT	 0.8340	 0.5290
BU	 0.7890	 0.4720
BV	 0.8780	 0.5710
BW	 0.4310	 0.3030
BX	 0.8680	 0.5370
BY	 0.8870	 0.5530
BZ	 0.8550	 0.5230
Ba	 0.9060	 0.5710
Bb	 0.6100	 0.4200
Bc	 0.7550	 0.4600
Bd	 0.8840	 0.5490
Be	 0.9170	 0.5910
Bf	 0.9400	 0.5990
Bg	 0.8720	 0.5560
Bh	 0.8650	 0.5480
Bi	 0.6370	 0.4660
Bj	 0.8990	 0.5820

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Chain	Atom inclusion	Q-score
Bk	 0.6560	 0.4540
Bl	 0.8680	 0.5530
Bm	 0.0170	 0.0730
Bo	 0.4940	 0.4260
Bp	 0.8720	 0.5520
Br	 0.9450	 0.5800
Bs	 0.0070	 0.0400
Bt	 0.0010	 0.0380
Bu	 0.4550	 0.1120
Bv	 0.5520	 0.2470