wwPDB EM Validation Summary Report (i)

Mar 4, 2025 – 04:04 am GMT

PDB ID	:	8Q87
EMDB ID	:	EMD-18169
Title	:	Structure of the G. gallus 80S rotated ribosome in complex with eEF2 and SERBP1
Authors	:	Nurullina, L.; Jenner, L.; Yusupov, M.
Deposited on	:	2023-08-18
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

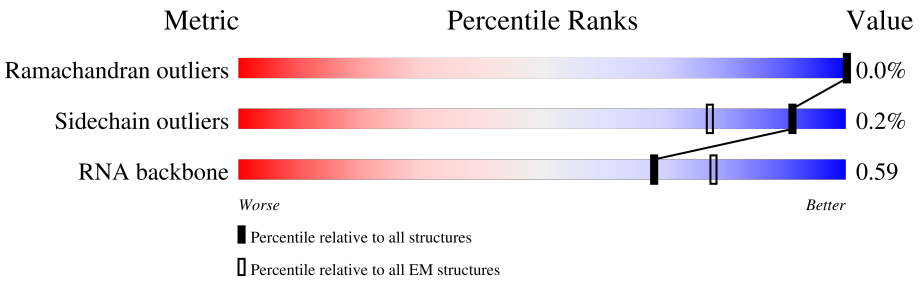
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 2.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	B5	4441	9% 68% 14% 18%
2	B8	157	6% 85% 15%
3	B7	119	92% 8%
4	Az	25	12% 100%
5	BA	257	96%
6	BB	403	99%
7	BC	421	86% 14%
8	BD	297	8% 100%

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Mol	Chain	Length	Quality of chain
9	BE	298	5% 76% 24%
10	BF	246	95% 5%
11	BG	266	9% 79% 21%
12	BH	192	100%
13	BI	214	5% 99%
14	BJ	178	18% 95%
15	BL	211	6% 98%
16	BM	131	99%
17	BN	204	100%
18	BO	203	99%
19	BP	184	84% 16%
20	BQ	187	100%
21	BR	196	10% 85% 15%
22	BS	176	100%
23	BT	160	99%
24	BU	128	19% 78% 22%
25	BV	140	99%
26	BW	157	39% 61%
27	BX	155	77% 23%
28	BY	145	92% 8%
29	BZ	136	99%
30	Ba	148	99%
31	Bb	71	14% 99%
32	Bc	115	7% 83% 17%
33	Bd	176	5% 60% 40%

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Mol	Chain	Length	Quality of chain
34	Be	135	96%
35	Bf	110	100%
36	Bg	117	92% 8%
37	Bh	123	99%
38	Bi	105	95% 5%
39	Bj	97	89% 11%
40	Bk	70	23% 99%
41	Bl	51	98%
42	Bm	128	41% 59%
43	Bo	105	100%
44	Bp	92	8% 99%
45	Br	138	90% 10%
46	A2	1823	9% 77% 16% 7%
47	Aa	264	9% 80% 19%
48	AA	84	14% 99%
49	AB	69	20% 88% 12%
50	Ab	264	83% 17%
51	AC	156	15% 40% 60%
52	Ac	243	6% 93% 7%
53	Ad	263	99%
54	AD	133	10% 43% 57%
55	AE	115	8% 86% 14%
56	Ae	204	93% 6%
57	Af	249	9% 91% 9%
58	AF	317	98%

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Mol	Chain	Length	Quality of chain
59	Ag	194	21% 96%
60	AG	171	32% 68%
61	Ah	207	9% 98%
62	Ai	194	92% 8%
63	Aj	165	58% 42%
64	Ak	158	10% 94% 5%
65	Al	132	30% 83% 16%
66	Am	151	6% 99%
67	An	151	11% 89% 10%
68	Ao	145	8% 88% 12%
69	Aq	135	17% 95%
70	Ar	152	95% 5%
71	As	145	98%
72	At	119	87% 13%
73	Au	84	100%
74	Av	130	99%
75	Aw	143	99%
76	Ax	131	95% 5%
77	Ay	125	55% 44%
78	AZ	296	70% 30%
79	Ap	146	97%
80	V	76	17% 80% 20%
81	S	404	10% 90%
82	A	858	32% 100%
83	Bs	316	58% 63% 37%

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Mol	Chain	Length	Quality of chain
84	Bt	165	91% 92% 8%
85	Bv	217	99% 98% ••

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 228127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	B5	3638	78070	34789	14272	25371	3638	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3295	UY1	U	modified residue	GB KT445934.2

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B8	157	3338	1490	588	1103	157	0	0

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B7	119	2536	1130	449	838	119	0	0

- Molecule 4 is a protein called 60S ribosomal protein L41.

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

- Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BA	246	1887	1185	385	311	6	0	0

- Molecule 6 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	BB	398	3209	2042	603	550	14	0	0

- Molecule 7 is a protein called 60S ribosomal protein L4 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	BC	361	2888	1816	574	484	14	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	BD	296	2388	1506	437	433	12	0	0

- Molecule 9 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BE	225	1820	1167	355	296	2	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	BF	234	1939	1245	377	309	8	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	BG	210	1704	1089	326	284	5	0	0

- Molecule 12 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	BH	192	1533	962	288	277	6	0	0

- Molecule 13 is a protein called Ribosomal protein uL16,Large ribosomal subunit protein uL16,Large ribosomal subunit protein uL16,Large ribosomal subunit protein uL16,Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	BI	213	1710	1082	334	279	15	0	0

- Molecule 14 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	BJ	170	1362	861	255	241	5	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	BL	208	1691	1060	350	276	5	0	0

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	BM	130	1077	688	209	172	8	0	0

- Molecule 17 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BN	203	1700	1071	359	266	4	0	0

- Molecule 18 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	BO	201	1642	1058	321	258	5	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	BP	155	1259	788	244	218	9	0	0

- Molecule 20 is a protein called Ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	BQ	187	1502	939	314	244	5	0	0

- Molecule 21 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	BR	166	1378	856	295	217	10	0	0

- Molecule 22 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	BS	176	1463	931	286	235	11	0	0

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	BT	159	1299	825	252	216	6	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	BU	100	817	523	143	149	2	0	0

- Molecule 25 is a protein called Ribosomal protei uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	BV	139	1033	648	199	181	5	0	0

- Molecule 26 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	BW	62	519	332	101	83	3	0	0

- Molecule 27 is a protein called Ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	BX	119	976	624	183	168	1	0	0

- Molecule 28 is a protein called Ribosomal protein L26 like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BY	133	1106	694	224	185	3	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein eL27.

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

- Molecule 30 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Ba	147	1179	748	240	187	4	0	0

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Bb	70	582	360	126	94	2	0	0

- Molecule 32 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Bc	95	738	468	131	133	6	0	0

- Molecule 33 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Bd	105	867	549	168	148	2	0	0

- Molecule 34 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Be	130	1074	681	219	169	5	0	0

- Molecule 35 is a protein called Ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Bf	110	886	559	178	144	5	0	0

- Molecule 36 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Bg	108	860	540	178	137	5	0	0

- Molecule 37 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Bh	122	1023	646	208	168	1	1	0

- Molecule 38 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Bi	100	821	515	173	127	6	0	0

- Molecule 39 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Bj	86	704	432	155	112	5	0	0

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Bk	69	569	366	103	99	1	0	0

- Molecule 41 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Bl	50	442	281	96	64	1	0	0

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Bm	52	429	266	90	67	6	0	0

- Molecule 43 is a protein called Ribosomal protein L36a like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Bo	105	861	540	177	138	6	0	0

- Molecule 44 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Bp	91	706	445	134	120	7	0	0

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Br	124	1007	624	213	167	3	0	0

- Molecule 46 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	A2	1697	36242	16199	6484	11862	1697	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1206	B8N	U	modified residue	GB KT445934.2
A2	1295	4AC	C	modified residue	GB KT445934.2
A2	1796	4AC	C	modified residue	GB KT445934.2

- Molecule 47 is a protein called Ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Aa	213	1730	1098	309	309	14	0	0

- Molecule 48 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	AA	83	657	410	125	115	7	0	0

- Molecule 49 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	AB	61	476	290	93	91	2	0	0

- Molecule 50 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Ab	219	1698	1099	291	299	9	0	0

- Molecule 51 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	AC	63	516	325	98	86	7	0	0

- Molecule 52 is a protein called DNA-(apurinic or apyrimidinic site) lyase.

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

- Molecule 53 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Ad	262	2076	1324	387	357	8	0	0

- Molecule 54 is a protein called Ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	AD	57	452	279	99	73	1	0	0

- Molecule 55 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	AE	99	793	492	165	131	5	0	0

- Molecule 56 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	Ae	191	1508	943	286	272	7	0	0

- Molecule 57 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	Af	227	1838	1144	367	320	7	0	0

- Molecule 58 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	AF	311	2420	1526	422	460	12	0	0

- Molecule 59 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	Ag	187	1500	956	276	267	1	0	0

- Molecule 60 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	AG	55	459	286	94	74	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	Ah	203	1669	1050	328	286	5	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	Ai	179	1495	953	299	241	2	0	0

- Molecule 63 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	Aj	96	812	532	143	131	6	0	0

- Molecule 64 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	Ak	150	1218	773	229	210	6	0	0

- Molecule 65 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	Al	111	860	540	151	161	8	0	0

- Molecule 66 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	Am	150	1208	773	229	205	1	0	0

- Molecule 67 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	An	136	1016	621	199	190	6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	IAS	ASP	modified residue	UNP Q5ZHW8

- Molecule 68 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	Ao	128	1050	666	198	179	7	0	0

- Molecule 69 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	Aq	133	1073	673	200	196	4	0	0

- Molecule 70 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	Ar	144	1191	748	241	201	1	0	0

- Molecule 71 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	As	143	1115	698	216	199	2	0	0

- Molecule 72 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	At	103	815	511	154	146	4	0	0

- Molecule 73 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	Au	84	640	394	118	124	4	0	0

- Molecule 74 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	Av	129	1035	659	193	177	6	0	0

- Molecule 75 is a protein called Ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	Aw	142	1104	696	220	185	3	0	0

- Molecule 76 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	Ax	125	1015	642	199	169	5	0	0

- Molecule 77 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	Ay	70	555	357	101	96	1	0	0

- Molecule 78 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	AZ	207	1626	1036	287	295	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	2	ACE	-	acetylation	UNP P50890

- Molecule 79 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	Ap	141	1123	715	212	193	3	0	0

- Molecule 80 is a RNA chain called Phe tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
80	V	76	1628	727	302	524	75	0	0

- Molecule 81 is a protein called SERPINE1 mRNA binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
81	S	42	325	190	69	66	0	0

- Molecule 82 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	A	857	6690	4244	1151	1249	46	0	0

- Molecule 83 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	Bs	199	1527	972	266	279	10	0	0

- Molecule 84 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	Bt	152	1135	704	210	217	4	0	0

- Molecule 85 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	Bv	215	1722	1107	303	305	7	0	0

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
86	B5	337	337	337	0
86	B8	8	8	8	0
86	B7	6	6	6	0

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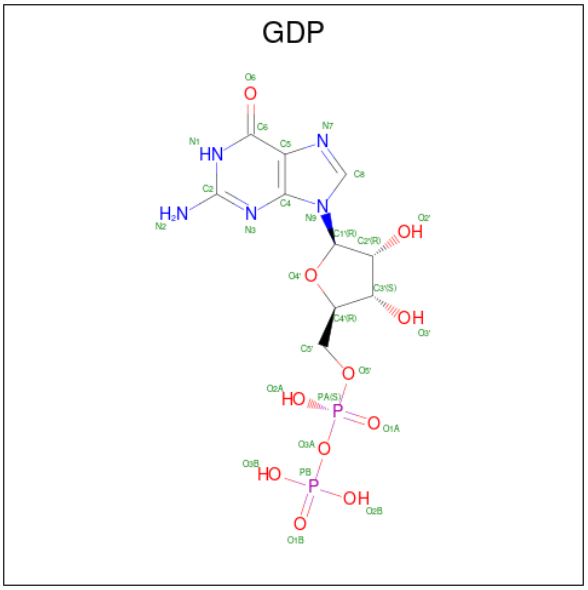
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
86	BA	3	3	3	0
86	BB	1	1	1	0
86	BH	1	1	1	0
86	BI	1	1	1	0
86	BN	2	2	2	0
86	BP	2	2	2	0
86	BV	1	1	1	0
86	Ba	1	1	1	0
86	Bb	2	2	2	0
86	Be	2	2	2	0
86	Bf	1	1	1	0
86	Bg	1	1	1	0
86	Bo	1	1	1	0
86	A2	116	116	116	0
86	AG	1	1	1	0
86	Ak	1	1	1	0
86	An	1	1	1	0
86	As	1	1	1	0
86	At	1	1	1	0
86	A	1	1	1	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
87	Bg	1	1	1	0
87	Bj	1	1	1	0
87	Bm	1	1	1	0
87	Bo	1	1	1	0
87	Bp	1	1	1	0
87	AC	1	1	1	0
87	AE	1	1	1	0
87	AG	1	1	1	0

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 89 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
89	B5	2982	2982	2982	0
89	B8	81	81	81	0
89	B7	69	69	69	0
89	Az	1	1	1	0
89	BA	18	18	18	0
89	BB	21	21	21	0
89	BC	30	30	30	0
89	BD	25	25	25	0
89	BE	10	10	10	0
89	BF	9	9	9	0
89	BG	1	1	1	0
89	BH	11	11	11	0
89	BI	21	21	21	0
89	BL	24	24	24	0
89	BM	10	10	10	0
89	BN	32	32	32	0
89	BO	24	24	24	0
89	BP	22	22	22	0
89	BQ	28	28	28	0
89	BR	8	8	8	0
89	BS	14	14	14	0
89	BT	16	16	16	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
89	BV	7	7	7	0
			Total	O	
89	BW	3	3	3	0
			Total	O	
89	BX	6	6	6	0
			Total	O	
89	BY	10	10	10	0
			Total	O	
89	Ba	25	25	25	0
			Total	O	
89	Bb	7	7	7	0
			Total	O	
89	Bc	1	1	1	0
			Total	O	
89	Bd	5	5	5	0
			Total	O	
89	Be	29	29	29	0
			Total	O	
89	Bf	24	24	24	0
			Total	O	
89	Bg	14	14	14	0
			Total	O	
89	Bh	7	7	7	0
			Total	O	
89	Bi	12	12	12	0
			Total	O	
89	Bj	9	9	9	0
			Total	O	
89	Bl	4	4	4	0
			Total	O	
89	Bm	12	12	12	0
			Total	O	
89	Bo	15	15	15	0
			Total	O	
89	Bp	9	9	9	0
			Total	O	
89	Br	7	7	7	0
			Total	O	
89	A2	197	197	197	0
			Total	O	
89	Ab	8	8	8	0

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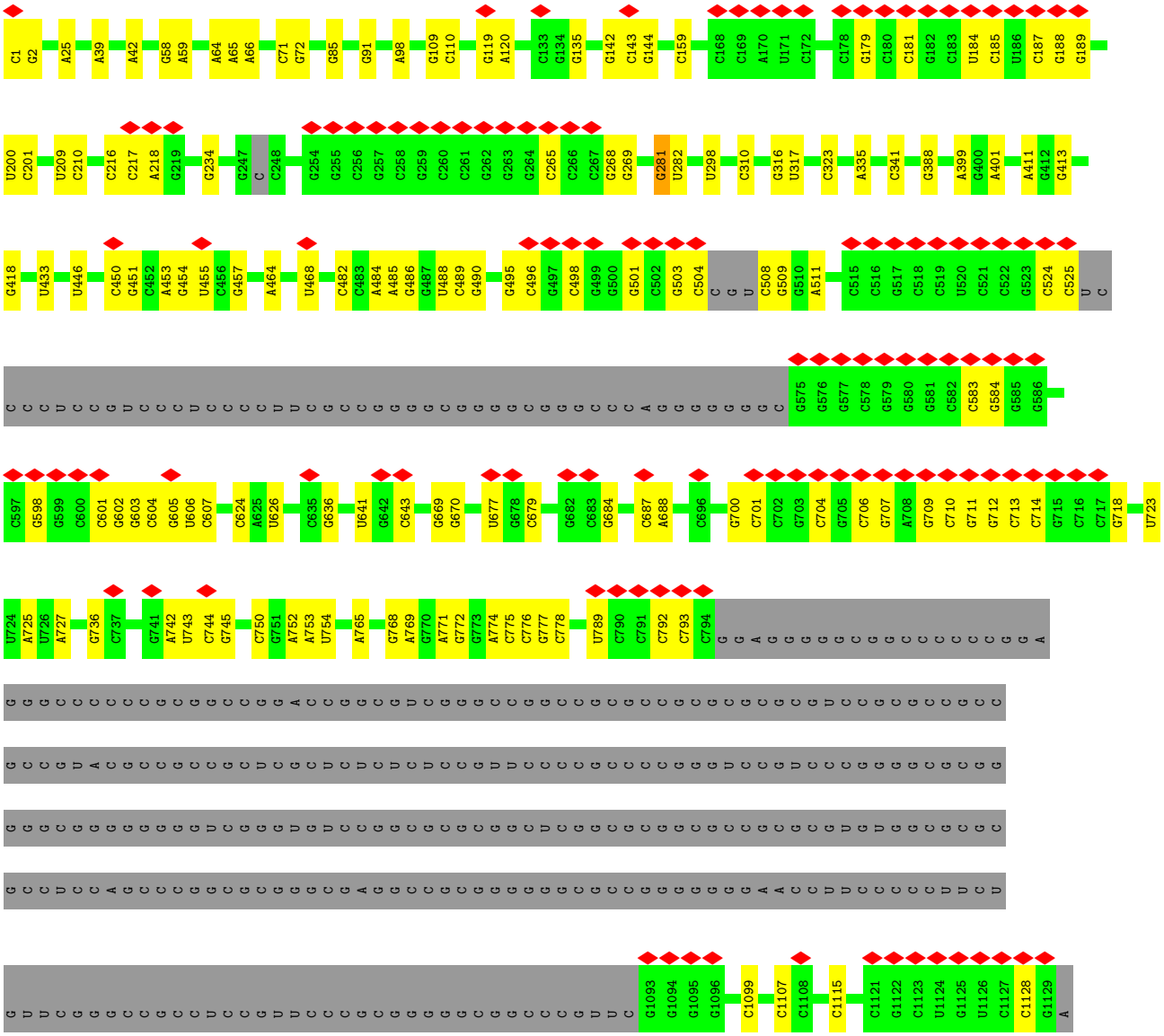
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
89	Ad	1	1	1	0
			Total	O	
89	AE	2	2	2	0
			Total	O	
89	Ae	1	1	1	0
			Total	O	
89	AG	1	1	1	0
			Total	O	
89	Ak	1	1	1	0
			Total	O	
89	Am	1	1	1	0
			Total	O	
89	An	1	1	1	0
			Total	O	
89	Ar	2	2	2	0
			Total	O	
89	As	1	1	1	0
			Total	O	
89	Au	1	1	1	0
			Total	O	
89	Av	2	2	2	0
			Total	O	
89	Ax	1	1	1	0
			Total	O	
89	AZ	1	1	1	0
			Total	O	
89	V	9	9	9	0
			Total	O	
89	A	2	2	2	0

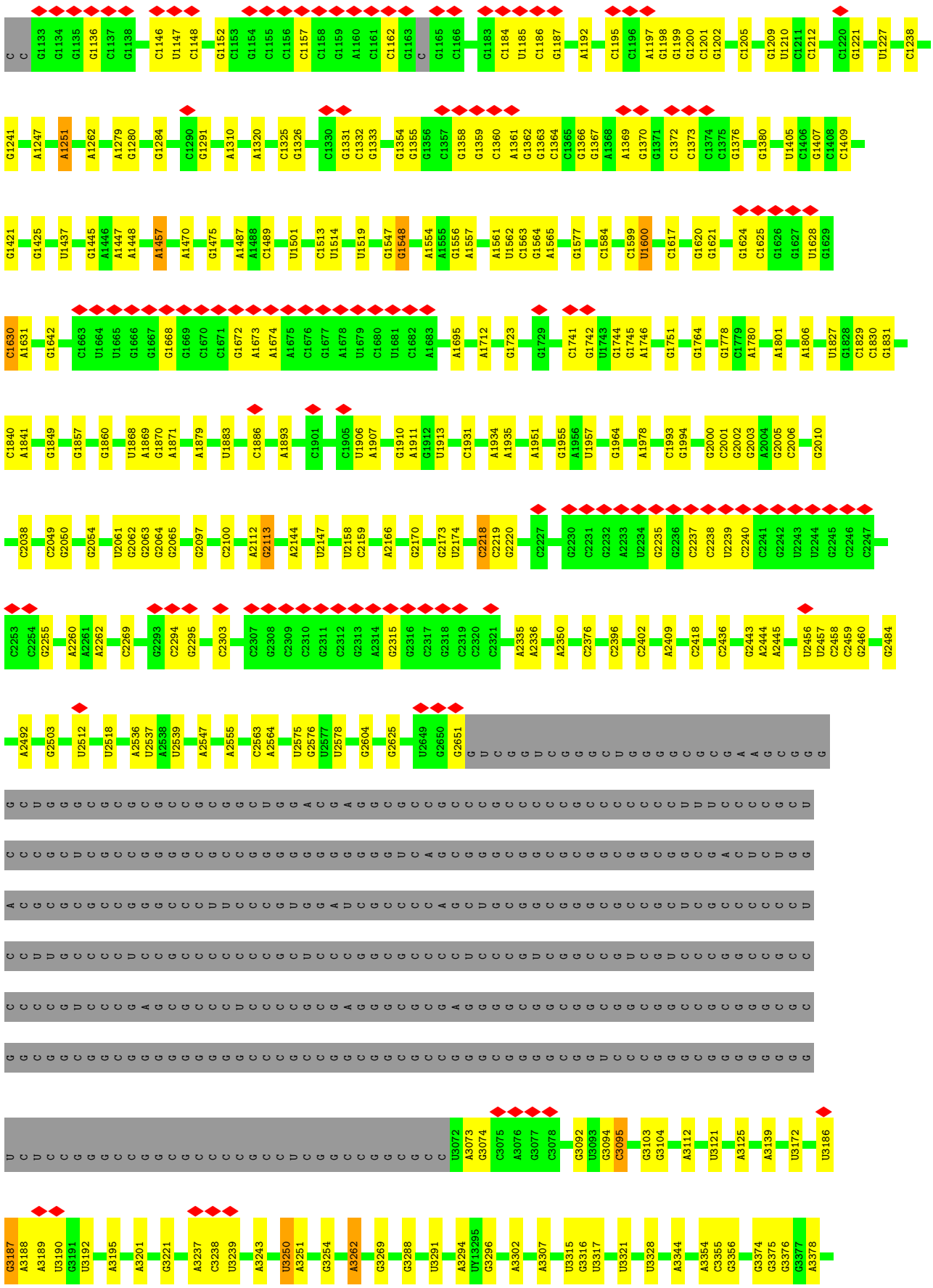
3 Residue-property plots (i)

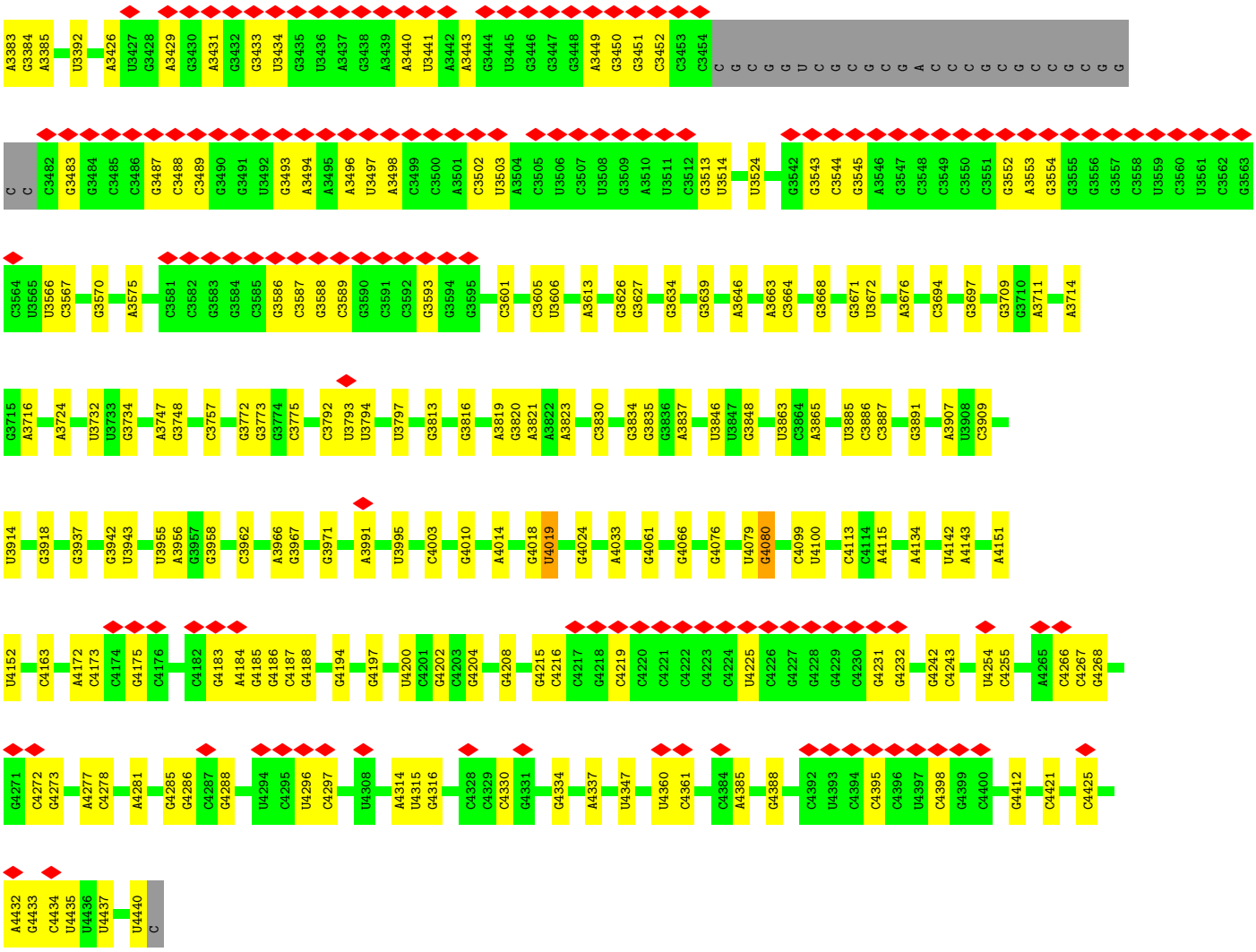
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 28S rRNA

Chain B5:

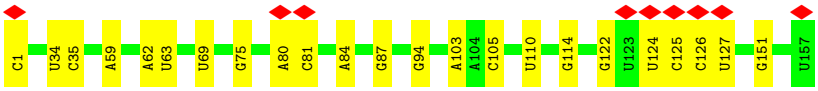



C C G1133 G1134 G1135 G1136 C1137 G1138 C1146 U1147 C1148 G1152 C1153 G1154 C1155 C1156 C1157 C1158 G1159 A1160 C1161 C1162 G1163 C G1165 C1166 G1183 C1184 U1185 C1186 G1187 A1192 C1195 C1196 A1197 G1198 G1199 G1200 C1201 G1202 C1205 G1209 U1210 C1211 C1212 C1220 G1221 U1227 C1238
G1241 A1247 A1251 A1262 A1279 G1280 G1284 C1290 G1291 A1310 A1320 C1325 G1326 C1330 G1331 C1332 G1333 G1354 G1355 G1356 C1357 G1358 G1359 C1360 A1361 G1362 G1363 C1364 C1365 G1366 G1367 A1368 A1369 G1370 G1371 C1372 C1373 C1374 C1375 G1376 G1380 U1405 C1406 G1407 C1408 C1409
G1421 G1425 U1437 G1445 A1446 A1447 A1448 A1457 A1470 G1475 A1487 A1488 C1489 U1501 C1513 U1514 U1519 G1547 G1548 A1554 A1555 G1556 A1557 A1561 U1562 C1563 G1564 A1565 G1577 C1584 C1599 U1600 C1617 G1620 G1621 G1624 C1625 G1626 G1627 U1628 G1629
C1630 A1631 G1642 C1663 U1664 U1665 G1666 G1667 G1668 G1669 C1670 C1671 G1672 A1673 A1674 A1675 C1676 G1677 A1678 U1679 C1680 U1681 C1682 A1683 A1695 A1712 G1723 G1729 C1741 G1742 U1743 G1744 G1745 A1746 G1751 G1764 G1778 C1779 A1780 A1801 A1806 U1827 G1828 C1829 C1830 G1831
C1840 A1841 G1849 G1857 G1860 U1868 A1869 G1870 A1871 A1879 U1883 C1886 A1893 C1901 C1905 U1906 A1907 G1910 A1911 G1912 U1913 C1931 A1934 A1935 A1951 G1955 A1956 U1957 G1964 A1978 C1993 G1994 G2000 C2001 G2002 G2003 A2004 G2005 C2006 G2010
C2038 C2049 G2050 G2054 U2061 G2062 G2063 G2064 G2065 G2097 C2100 A2112 G2113 A2144 U2147 U2158 C2159 A2166 G2170 G2173 U2174 C2218 C2219 G2220 C2227 G2230 C2231 G2232 A2233 U2234 G2235 G2236 C2237 C2238 U2239 C2240 C2241 G2242 U2243 U2244 G2245 C2246 C2247
C2253 C2254 G2255 A2260 A2261 A2262 C2269 G2293 C2294 G2295 C2303 C2307 G2308 C2309 C2310 G2311 C2312 G2313 A2314 G2315 G2316 C2317 G2318 C2319 C2320 C2321 A2335 A2336 A2350 C2376 C2396 C2402 A2409 C2418 C2436 G2443 A2444 A2445 U2456 U2457 C2458 C2459 G2460 G2484
A2492 G2503 U2512 U2518 A2536 U2537 A2538 U2539 A2547 A2555 C2563 A2564 U2575 G2576 U2577 U2578 G2604 G2625 U2649 G2650 G2651 G U C G G U C G G G C U G G G G C U U C C G A A G C G C G G G C C C G C C C G C C C



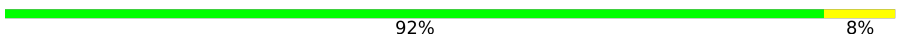
- Molecule 2: 5.8S rRNA

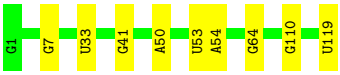
Chain B8:



- Molecule 3: 5S rRNA

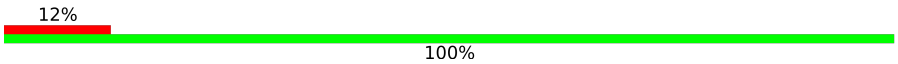
Chain B7:

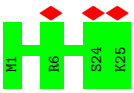




- Molecule 4: 60S ribosomal protein L41

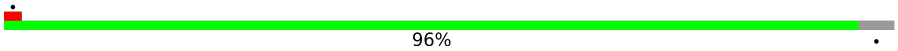
Chain Az:

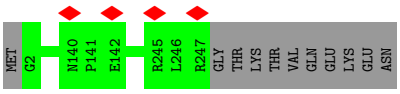




• Molecule 5: 60S ribosomal protein L8

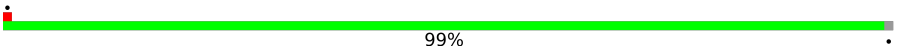
Chain BA:

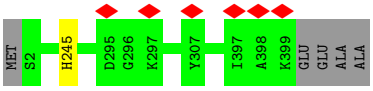




• Molecule 6: Ribosomal protein uL3

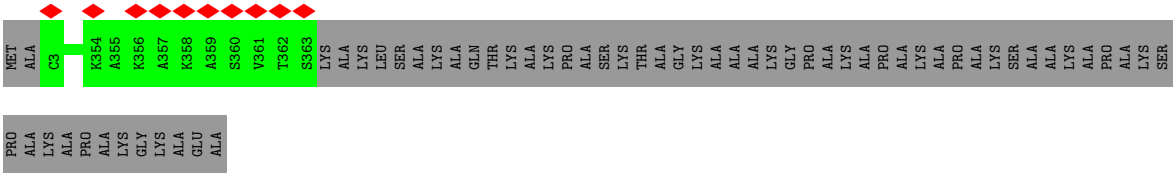
Chain BB:





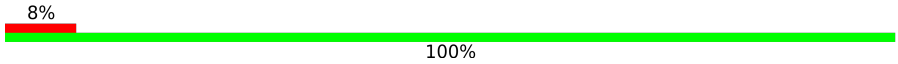
• Molecule 7: 60S ribosomal protein L4 C-terminal domain-containing protein

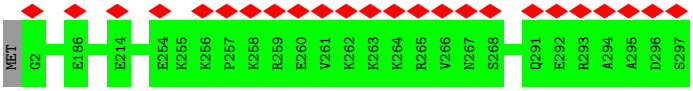
Chain BC:



• Molecule 8: Large ribosomal subunit protein uL18

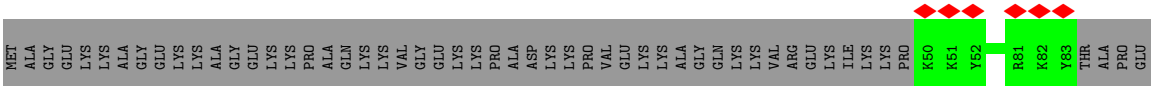
Chain BD:

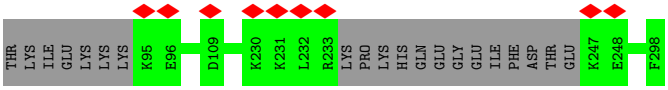




• Molecule 9: 60S ribosomal protein L6

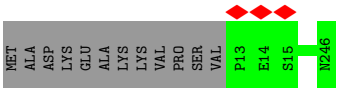
Chain BE:





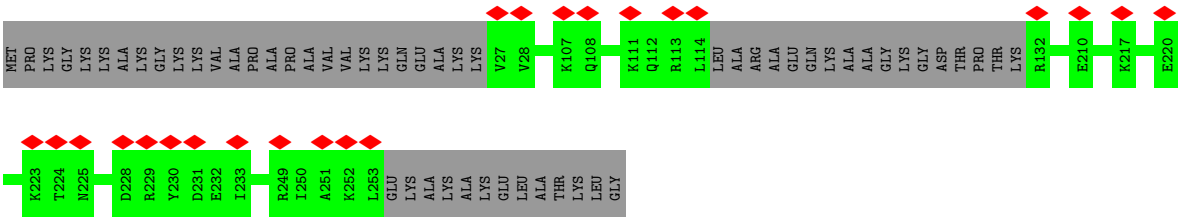
• Molecule 10: Large ribosomal subunit protein uL30

Chain BF: 95% 5%



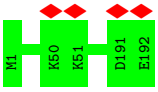
• Molecule 11: Large ribosomal subunit protein eL8

Chain BG: 9% 79% 21%



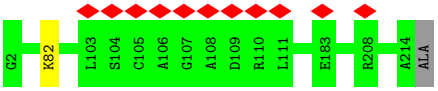
• Molecule 12: 60S ribosomal protein L9

Chain BH: 100%



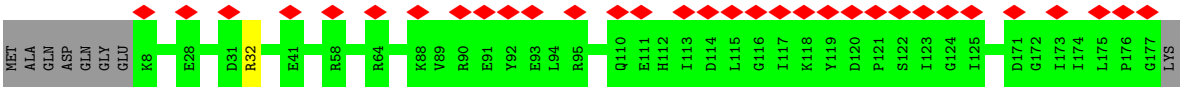
• Molecule 13: Ribosomal protein uL16,Large ribosomal subunit protein uL16,Large ribosomal subunit protein uL16,Large ribosomal subunit protein uL16,Large ribosomal subunit protein uL16

Chain BI: 5% 99%



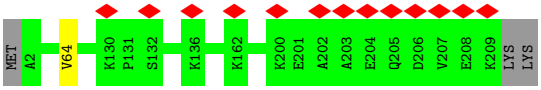
• Molecule 14: 60S ribosomal protein L11

Chain BJ: 18% 95%



• Molecule 15: Large ribosomal subunit protein eL13

Chain BL: 6% 98%



• Molecule 16: 60S ribosomal protein L14

Chain BM: 99%

• Molecule 17: Ribosomal protein L15

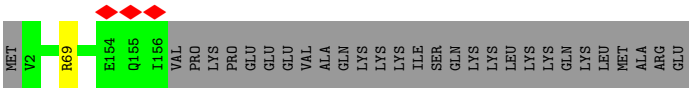
Chain BN: 100%

• Molecule 18: Ribosomal protein uL13

Chain BO: 99%

• Molecule 19: Large ribosomal subunit protein uL22

Chain BP: 84% 16%



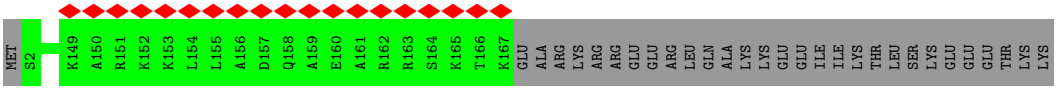
• Molecule 20: Ribosomal protein eL18

Chain BQ: 100%

There are no outlier residues recorded for this chain.

• Molecule 21: Ribosomal protein L19

Chain BR: 10% 85% 15%



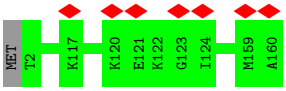
• Molecule 22: Ribosomal protein eL20

Chain BS: 100%

There are no outlier residues recorded for this chain.

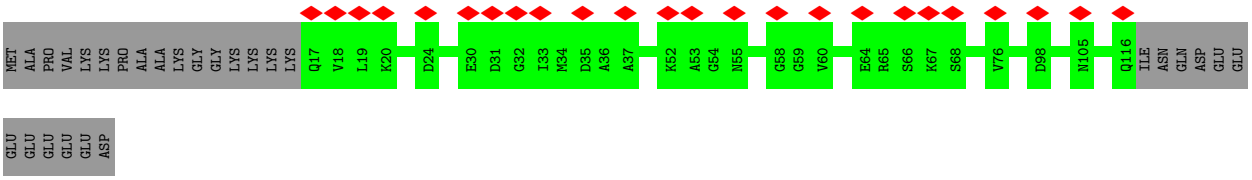
• Molecule 23: 60S ribosomal protein L21

Chain BT: 99%



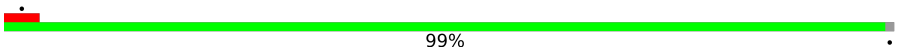
• Molecule 24: Large ribosomal subunit protein eL22

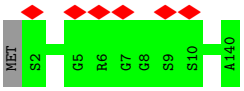
Chain BU:



• Molecule 25: Ribosomal protei uL14

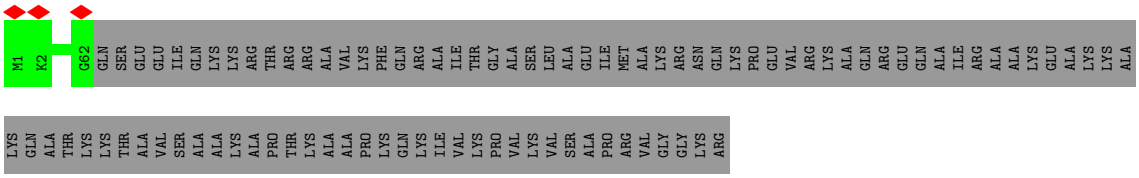
Chain BV:





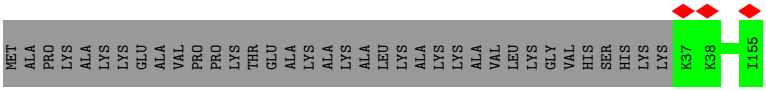
• Molecule 26: Ribosomal protein L24

Chain BW:



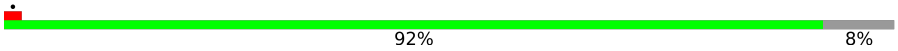
• Molecule 27: Ribosomal protein uL23

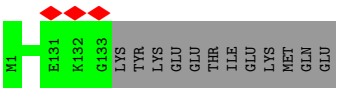
Chain BX:



• Molecule 28: Ribosomal protein L26 like 1

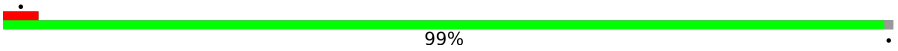
Chain BY:

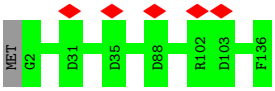




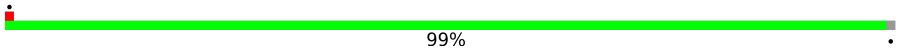
• Molecule 29: Large ribosomal subunit protein eL27

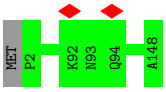
Chain BZ:



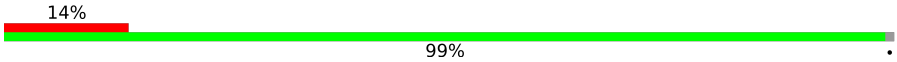


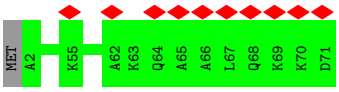
• Molecule 30: Ribosomal protein uL15

Chain Ba: 



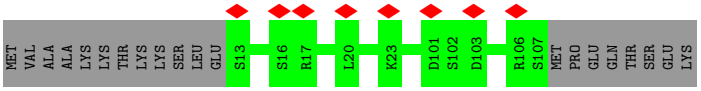
• Molecule 31: 60S ribosomal protein L29

Chain Bb: 



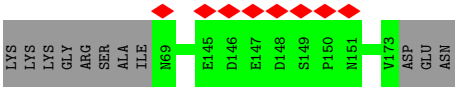
• Molecule 32: Large ribosomal subunit protein eL30

Chain Bc:

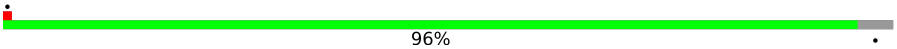


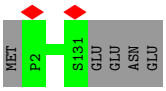
• Molecule 33: 60S ribosomal protein L31

Chain Bd:

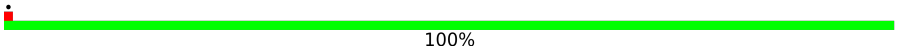


• Molecule 34: Ribosomal protein L32

Chain Be: 

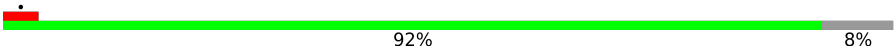


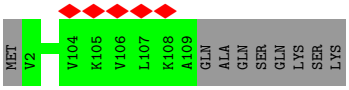
• Molecule 35: Ribosomal protein eL33

Chain Bf: 

• Molecule 36: 60S ribosomal protein L34

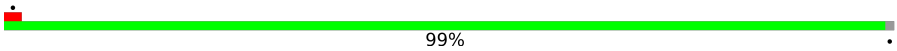
Chain Bg:





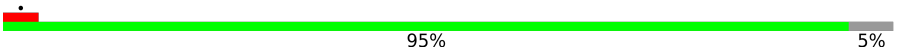
• Molecule 37: Large ribosomal subunit protein uL29

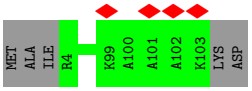
Chain Bh:



• Molecule 38: Large ribosomal subunit protein eL36

Chain Bi:



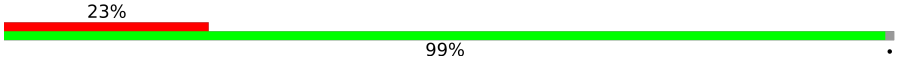


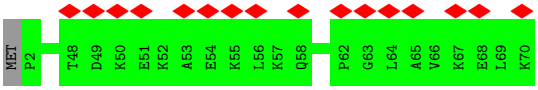
• Molecule 39: Ribosomal protein L37

Chain Bj:

• Molecule 40: 60S ribosomal protein L38

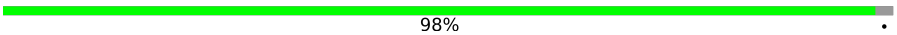
Chain Bk:





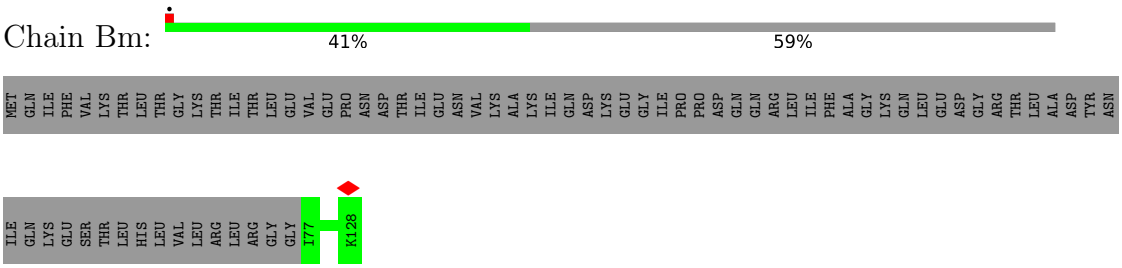
• Molecule 41: Large ribosomal subunit protein eL39

Chain Bl:



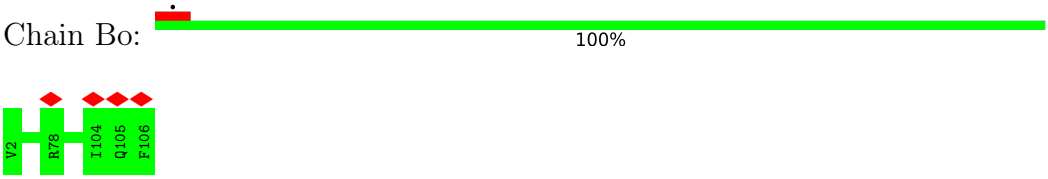
• Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain Bm:



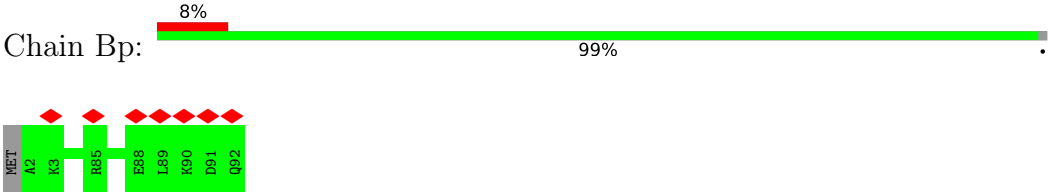
- Molecule 43: Ribosomal protein L36a like

Chain Bo:



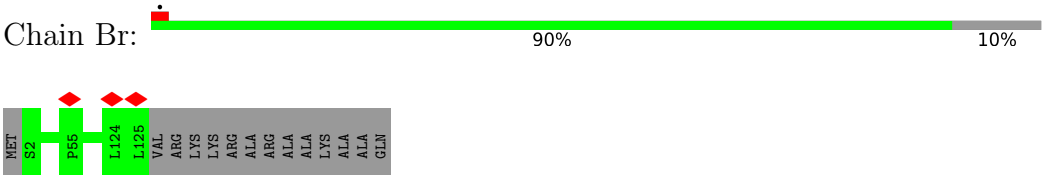
- Molecule 44: Large ribosomal subunit protein eL43

Chain Bp:



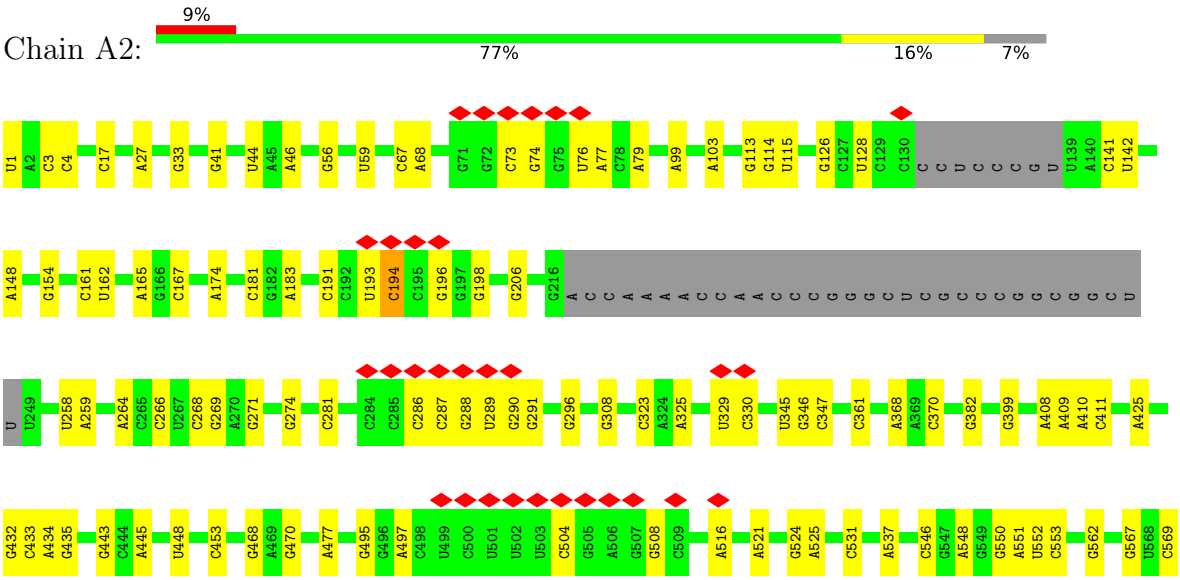
- Molecule 45: 60S ribosomal protein L28

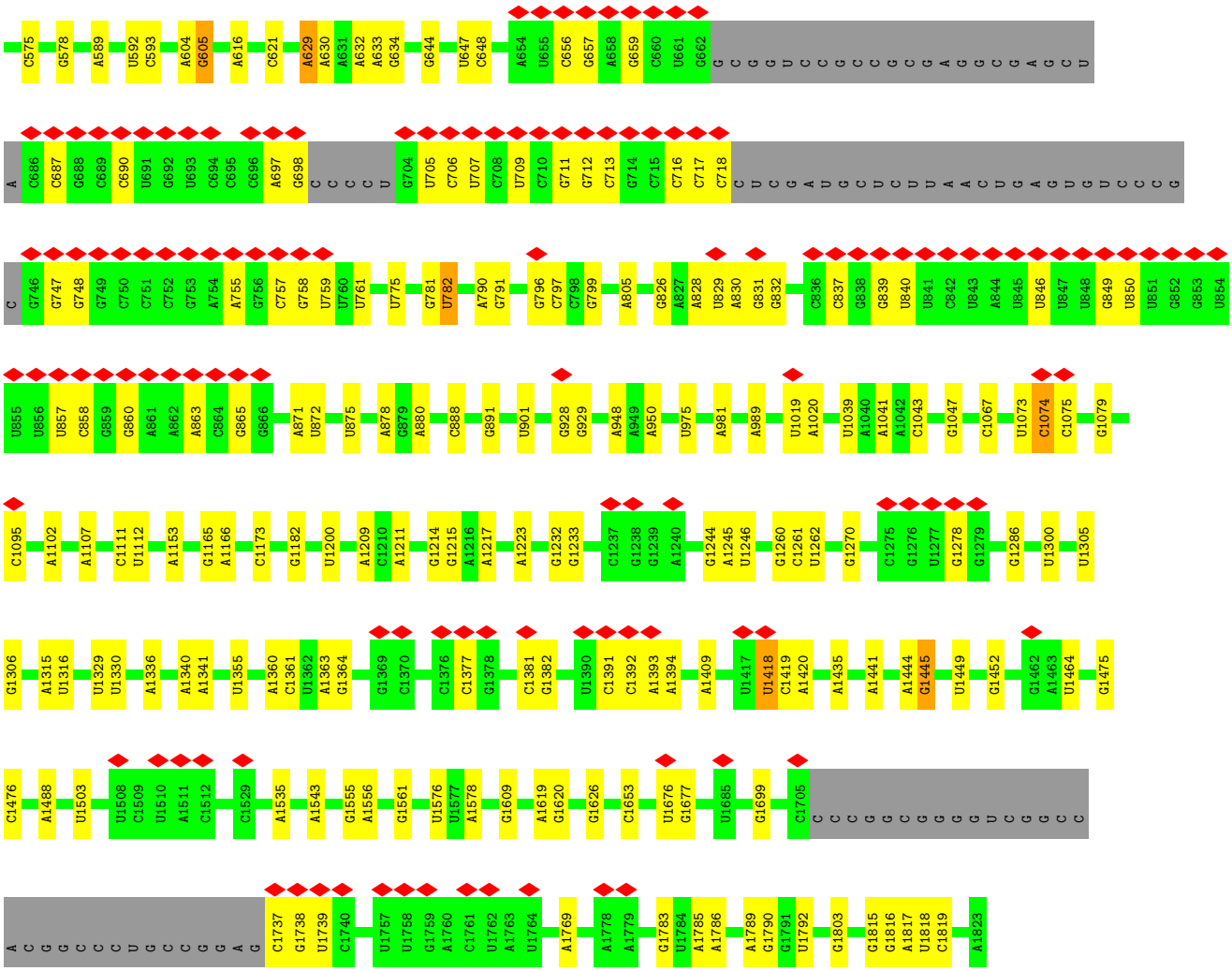
Chain Br:



- Molecule 46: 18S rRNA

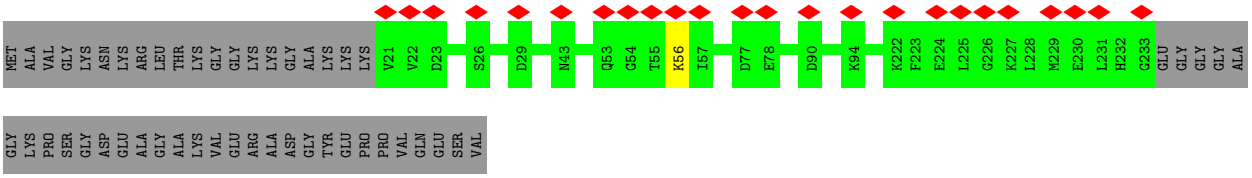
Chain A2:





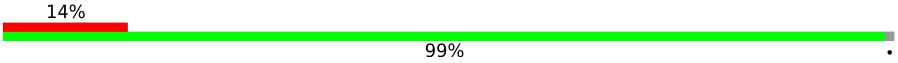
- Molecule 47: Ribosomal protein eS1

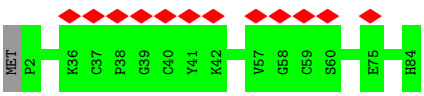
Chain Aa:



- Molecule 48: 40S ribosomal protein S27

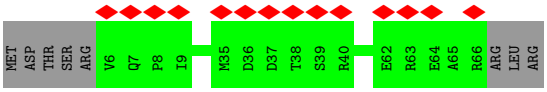
Chain AA:





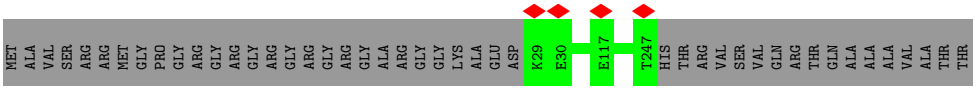
- Molecule 49: 40S ribosomal protein S28

Chain AB:



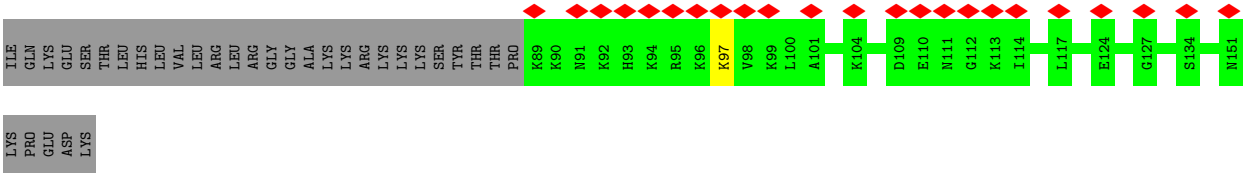
- Molecule 50: 40S ribosomal protein S2

Chain Ab:



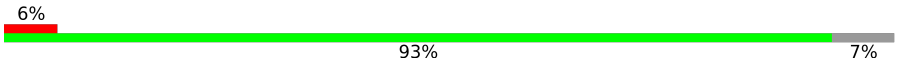
- Molecule 51: Ubiquitin

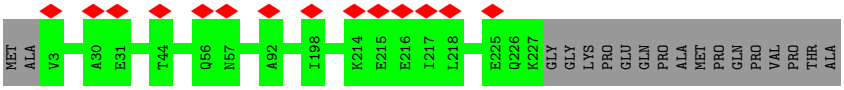
Chain AC:



- Molecule 52: DNA-(apurinic or apyrimidinic site) lyase

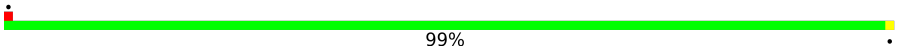
Chain Ac:

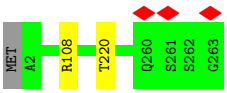




- Molecule 53: Small ribosomal subunit protein eS4

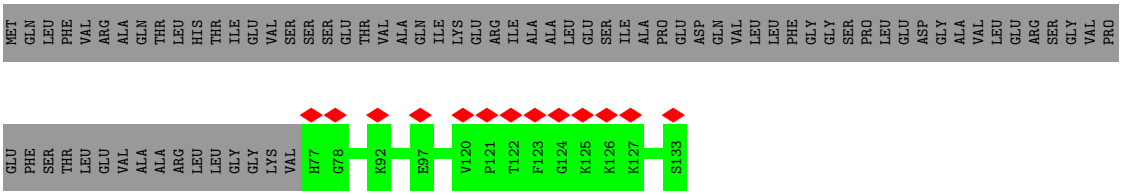
Chain Ad:





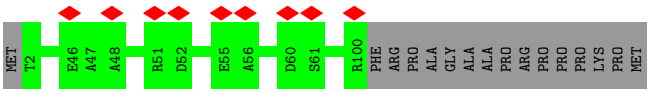
- Molecule 54: Ribosomal protein eS30

Chain AD:



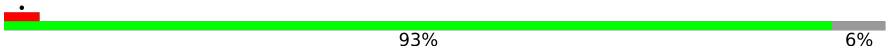
- Molecule 55: 40S ribosomal protein S26

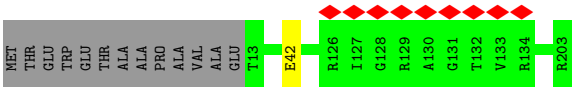
Chain AE:



- Molecule 56: Ribosomal protein S5

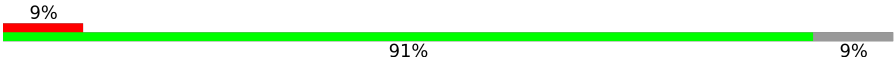
Chain Ae:

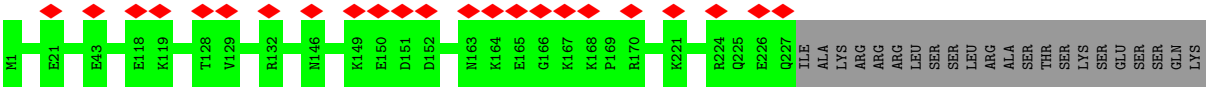




- Molecule 57: Small ribosomal subunit protein eS6

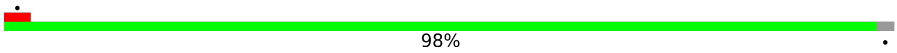
Chain Af:

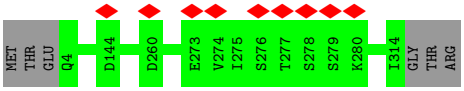




- Molecule 58: Small ribosomal subunit protein RACK1

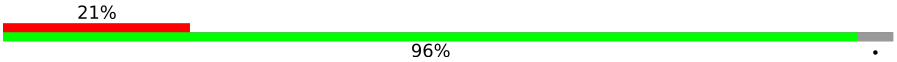
Chain AF:

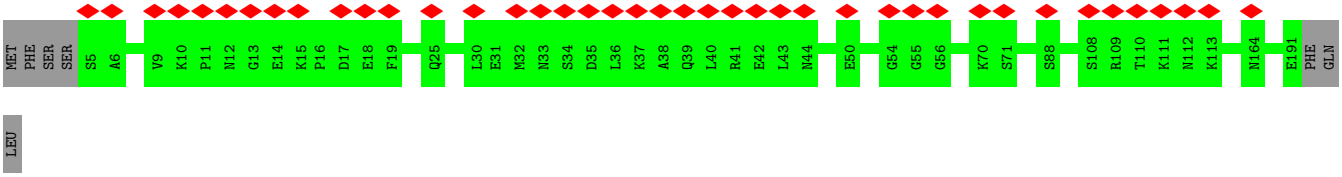




- Molecule 59: 40S ribosomal protein S7

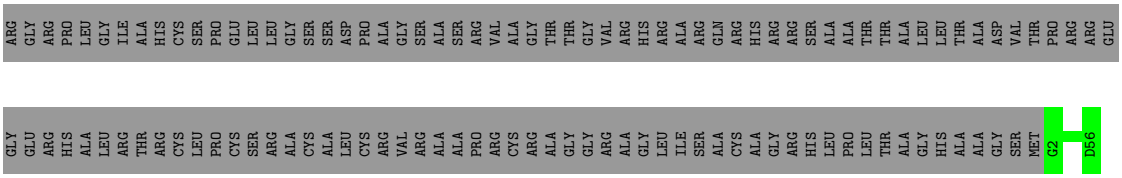
Chain Ag:





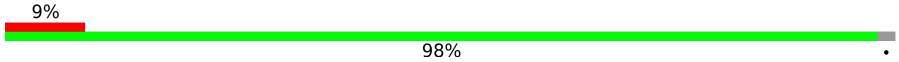
- Molecule 60: 40S ribosomal protein S29

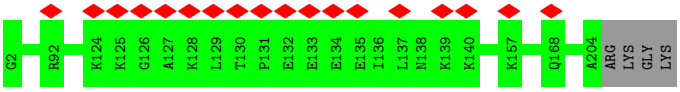
Chain AG:



- Molecule 61: 40S ribosomal protein S8

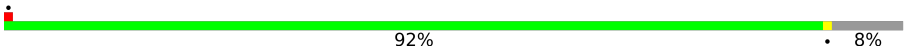
Chain Ah:

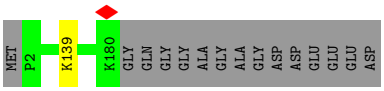




- Molecule 62: 40S ribosomal protein S9

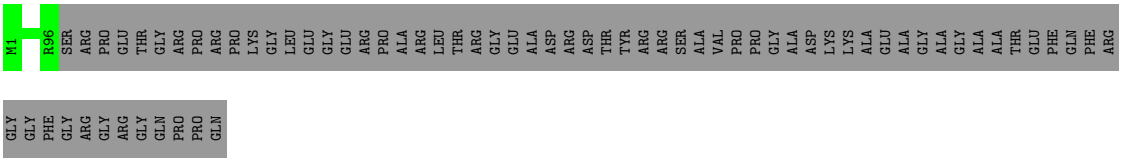
Chain Ai:





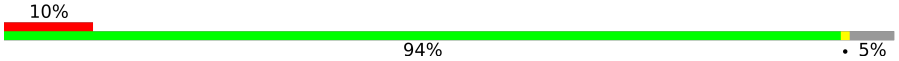
- Molecule 63: Ribosomal protein S10

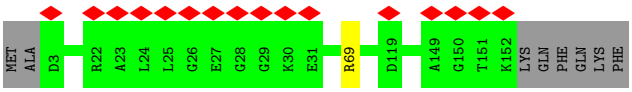
Chain Aj:



- Molecule 64: 40S ribosomal protein S11

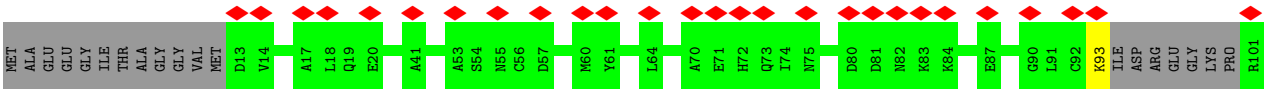
Chain Ak:

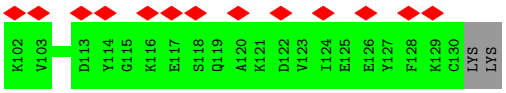




- Molecule 65: Small ribosomal subunit protein eS12

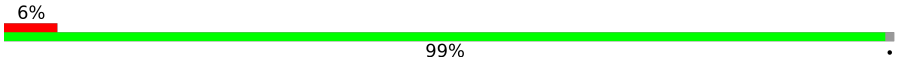
Chain Al:

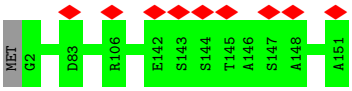




- Molecule 66: Small ribosomal subunit protein uS15

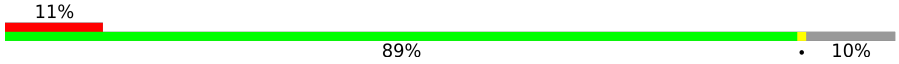
Chain Am:

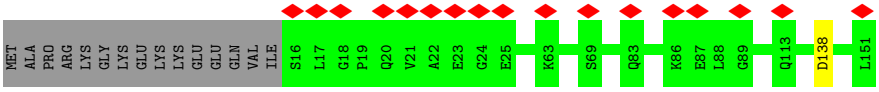




- Molecule 67: Ribosomal protein S14

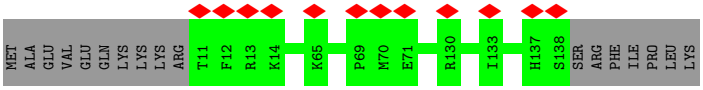
Chain An:





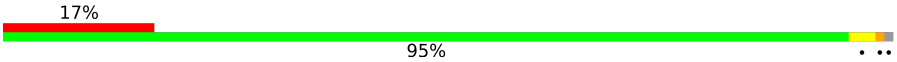
- Molecule 68: Small ribosomal subunit protein uS19

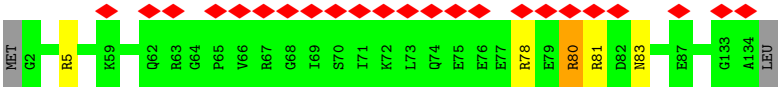
Chain Ao:



- Molecule 69: Small ribosomal subunit protein eS17

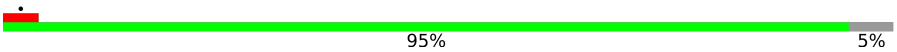
Chain Aq:

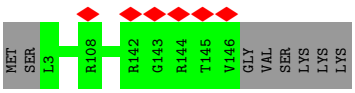




- Molecule 70: 40S ribosomal protein S18

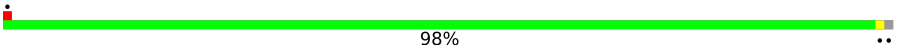
Chain Ar:

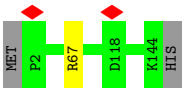




- Molecule 71: Ribosomal protein eS19

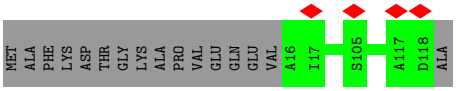
Chain As:





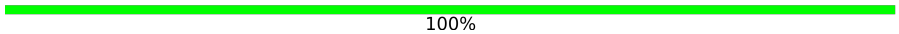
- Molecule 72: 40S ribosomal protein S20

Chain At:



- Molecule 73: Small ribosomal subunit protein eS21

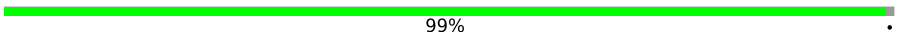
Chain Au:



There are no outlier residues recorded for this chain.

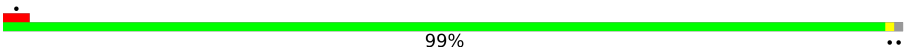
• Molecule 74: 40S ribosomal protein S15a

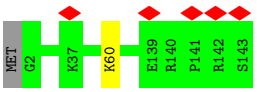
Chain Av:



• Molecule 75: Ribosomal protein uS12

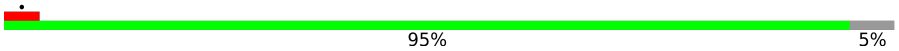
Chain Aw:

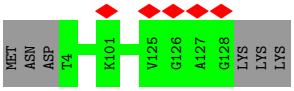




• Molecule 76: 40S ribosomal protein S24

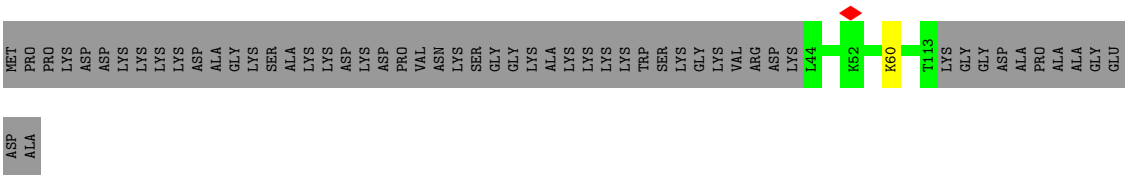
Chain Ax:





• Molecule 77: 40S ribosomal protein S25

Chain Ay:

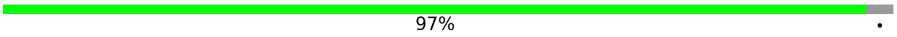


• Molecule 78: Small ribosomal subunit protein uS2

Chain AZ:

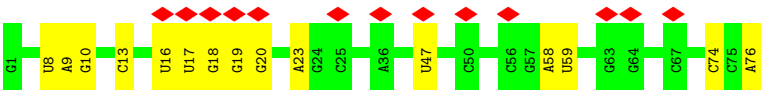
• Molecule 79: Ribosomal protein S16

Chain Ap:



• Molecule 80: Phe tRNA

Chain V:

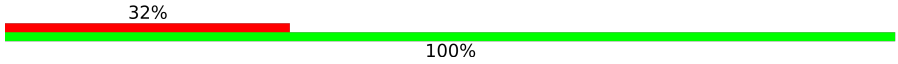


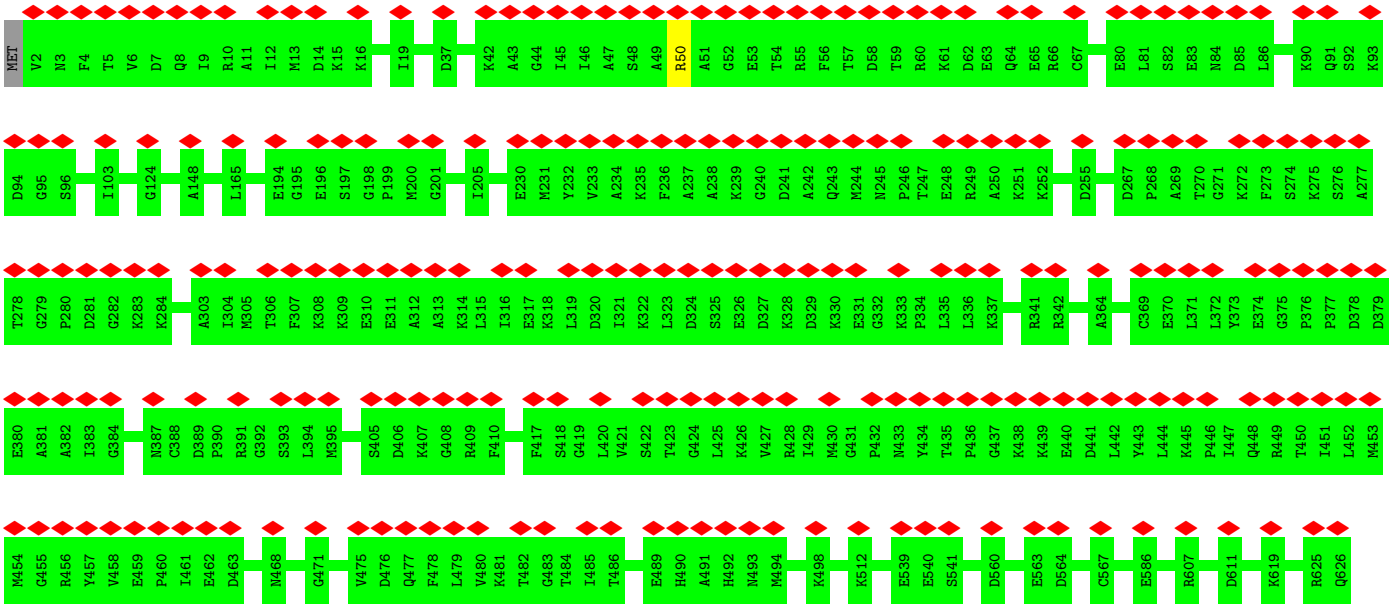
• Molecule 81: SERPINE1 mRNA binding protein 1

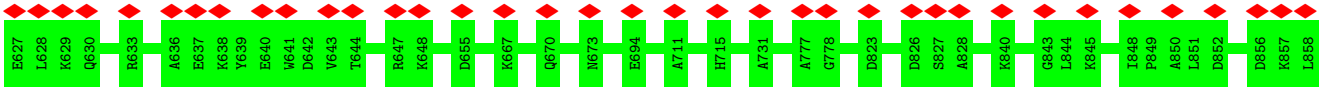
Chain S:

• Molecule 82: Elongation factor 2

Chain A:

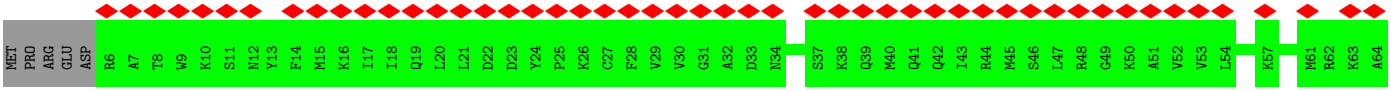


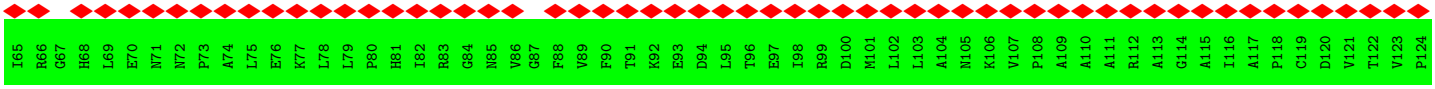


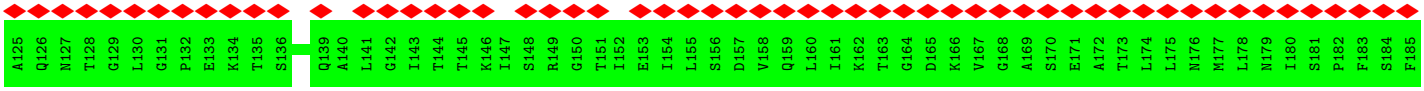


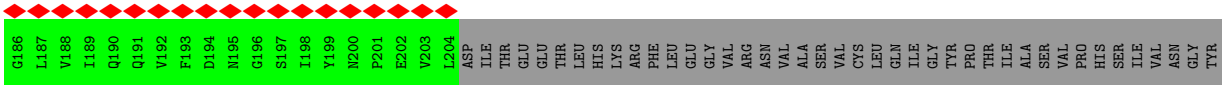
- Molecule 83: Large ribosomal subunit protein uL10

Chain Bs:



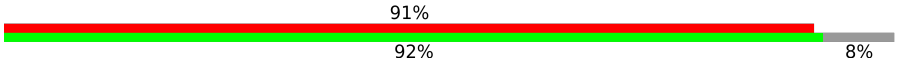


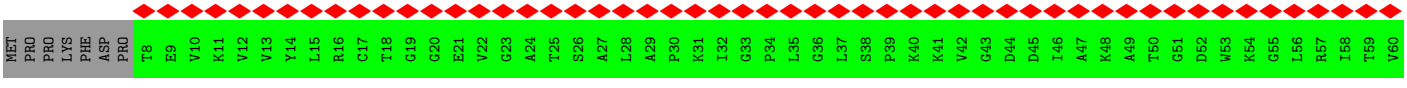


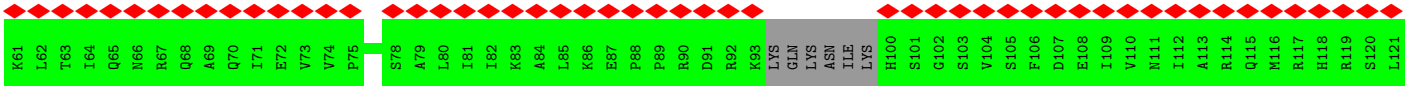


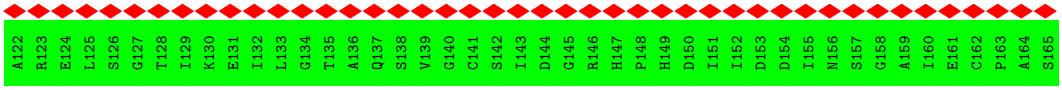
- Molecule 84: 60S ribosomal protein L12

Chain Bt:



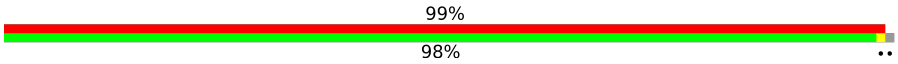






- Molecule 85: Ribosomal protein

Chain Bv:



P61 K62 F63 S64 V65 C66 L67 L68 G69 D70 Q71 Q72 H73 C74 D75 E76 A77 K78 A79 V80 E81 I82 P83 H84 M85 D86 I87 E88 A89 L90 K91 K92 L93 N94 K95 N96 K97 K98 L99 V100 K101 K102 L103 A104 K105 K106 Y107 D108 A109 F110 L111 A112 S113 E114 S115 L116 I117 K118 Q119 I120

P121 R122 I123 L124 G125 P126 G127 L128 N129 K130 A131 G132 K133 F134 P135 S136 L137 L138 T139 H140 N141 E142 N143 L144 V145 A146 K147 V148 D149 E150 V151 K152 S153 T154 I155 K156 F157 Q158 M159 K160 K161 V162 L163 C164 L165 A166 V167 A168 V169 G170 H171 V172 K173 M174 T175 E176 D177 E178 L179 V180

Y181 N182 I183 H184 L185 A186 I187 N188 F189 L190 V191 S192 L193 L194 K195 K196 N197 W198 Q199 N200 V201 R202 A203 L204 Y205 I206 K207 S208 T209 M210 G211 K212 P213 Q214 R215 L216 Y217

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100204	Depositor
Resolution determination method	FSC 3 SIGMA CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	35.598	Depositor
Minimum map value	-17.913	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	1.080	Depositor
Recommended contour level	3	Depositor
Map size (Å)	465.74, 465.74, 465.74	wwPDB
Map dimensions	580, 580, 580	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.803, 0.803, 0.803	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, 5MC, A2M, OMU, PSU, 4AC, OMG, DDE, ACE, MLZ, 6MZ, MG, ZN, GDP, MA6, B8N, IAS, UY1, NMM, OMC, UR3, HIC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	B5	0.38	1/85039 (0.0%)	0.79	29/132680 (0.0%)
2	B8	0.40	1/3656 (0.0%)	0.74	1/5693 (0.0%)
3	B7	0.36	0/2832	0.77	0/4413
4	Az	0.22	0/240	0.68	0/305
5	BA	0.28	0/1926	0.57	0/2582
6	BB	0.29	0/3264	0.53	0/4363
7	BC	0.27	0/2942	0.53	0/3950
8	BD	0.28	0/2431	0.50	0/3255
9	BE	0.27	0/1854	0.52	0/2477
10	BF	0.27	0/1975	0.52	0/2634
11	BG	0.26	0/1736	0.51	0/2342
12	BH	0.27	0/1552	0.52	0/2086
13	BI	0.27	0/1751	0.54	0/2342
14	BJ	0.27	0/1385	0.54	0/1852
15	BL	0.26	0/1723	0.55	0/2302
16	BM	0.26	0/1097	0.50	0/1460
17	BN	0.27	0/1745	0.56	0/2337
18	BO	0.27	0/1674	0.52	0/2239
19	BP	0.27	0/1285	0.51	0/1723
20	BQ	0.28	0/1526	0.59	0/2038
21	BR	0.24	0/1394	0.54	0/1845
22	BS	0.29	0/1502	0.55	0/2016
23	BT	0.28	0/1327	0.50	0/1771
24	BU	0.25	0/831	0.49	0/1115
25	BV	0.28	0/1047	0.53	0/1402
26	BW	0.28	0/532	0.51	0/708
27	BX	0.26	0/993	0.51	0/1334
28	BY	0.28	0/1123	0.56	0/1493
29	BZ	0.28	0/1130	0.51	0/1507
30	Ba	0.28	0/1209	0.52	0/1615
31	Bb	0.26	0/593	0.49	0/782

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Bc	0.27	0/748	0.47	0/1004
33	Bd	0.26	0/882	0.55	0/1187
34	Be	0.27	0/1093	0.54	0/1457
35	Bf	0.29	0/905	0.57	0/1211
36	Bg	0.26	0/870	0.57	0/1159
37	Bh	0.27	0/1034	0.52	0/1365
38	Bi	0.26	0/832	0.55	0/1100
39	Bj	0.28	0/718	0.58	0/948
40	Bk	0.26	0/575	0.49	0/761
41	Bl	0.25	0/452	0.54	0/596
42	Bm	0.26	0/435	0.54	0/575
43	Bo	0.28	0/864	0.52	0/1139
44	Bp	0.26	0/716	0.51	0/950
45	Br	0.26	0/1024	0.57	0/1374
46	A2	0.36	1/39536 (0.0%)	0.78	12/61603 (0.0%)
47	Aa	0.27	0/1757	0.50	0/2352
48	AA	0.28	0/670	0.53	0/897
49	AB	0.28	0/478	0.62	0/641
50	Ab	0.28	0/1734	0.48	0/2342
51	AC	0.29	0/526	0.55	0/696
52	Ac	0.28	0/1780	0.52	0/2396
53	Ad	0.32	0/2118	0.55	0/2848
54	AD	0.26	0/458	0.54	0/602
55	AE	0.26	0/806	0.56	0/1080
56	Ae	0.29	0/1530	0.53	0/2059
57	Af	0.27	0/1861	0.55	0/2481
58	AF	0.28	0/2477	0.52	0/3372
59	Ag	0.26	0/1522	0.51	0/2039
60	AG	0.29	0/470	0.54	0/623
61	Ah	0.29	0/1702	0.55	0/2273
62	Ai	0.33	0/1520	0.56	0/2030
63	Aj	0.29	0/836	0.48	0/1128
64	Ak	0.31	0/1239	0.55	0/1657
65	Al	0.25	0/868	0.48	0/1165
66	Am	0.26	0/1232	0.50	0/1656
67	An	0.27	0/1020	0.56	0/1366
68	Ao	0.30	0/1071	0.53	0/1432
69	Aq	0.27	0/1087	0.52	0/1459
70	Ar	0.28	0/1209	0.58	0/1620
71	As	0.28	0/1120	0.48	0/1499
72	At	0.26	0/825	0.57	0/1108
73	Au	0.28	0/644	0.51	0/863
74	Av	0.30	0/1052	0.54	0/1408

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	Aw	0.30	0/1122	0.54	0/1498
76	Ax	0.30	0/1032	0.54	0/1371
77	Ay	0.29	0/561	0.52	0/755
78	AZ	0.30	0/1661	0.51	0/2259
79	Ap	0.29	0/1141	0.55	0/1527
80	V	0.25	0/1822	0.76	0/2841
81	S	0.25	0/331	0.55	0/436
82	A	0.26	0/6798	0.51	0/9181
83	Bs	0.25	0/1551	0.50	0/2094
84	Bt	0.24	0/1149	0.54	0/1549
85	Bv	0.25	0/1749	0.54	0/2344
All	All	0.33	3/236527 (0.0%)	0.69	42/346037 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A2	1	U	OP3-P	-10.88	1.48	1.61
2	B8	1	C	OP3-P	-10.59	1.48	1.61
1	B5	1	C	OP3-P	-10.56	1.48	1.61

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	A2	194	C	C2-N1-C1'	9.27	129.00	118.80
1	B5	3250	U	C2-N1-C1'	8.71	128.15	117.70
1	B5	3095	C	C2-N1-C1'	8.69	128.36	118.80
46	A2	194	C	N1-C2-O2	8.54	124.02	118.90
1	B5	3095	C	N1-C2-O2	8.36	123.92	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Az	23/25 (92%)	23 (100%)	0	0	100	100
5	BA	244/257 (95%)	235 (96%)	9 (4%)	0	100	100
6	BB	395/403 (98%)	387 (98%)	8 (2%)	0	100	100
7	BC	359/421 (85%)	354 (99%)	5 (1%)	0	100	100
8	BD	294/297 (99%)	282 (96%)	12 (4%)	0	100	100
9	BE	219/298 (74%)	211 (96%)	8 (4%)	0	100	100
10	BF	232/246 (94%)	225 (97%)	7 (3%)	0	100	100
11	BG	206/266 (77%)	198 (96%)	8 (4%)	0	100	100
12	BH	190/192 (99%)	188 (99%)	2 (1%)	0	100	100
13	BI	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
14	BJ	168/178 (94%)	164 (98%)	4 (2%)	0	100	100
15	BL	206/211 (98%)	200 (97%)	5 (2%)	1 (0%)	25	38
16	BM	128/131 (98%)	126 (98%)	2 (2%)	0	100	100
17	BN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
18	BO	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
19	BP	153/184 (83%)	150 (98%)	3 (2%)	0	100	100
20	BQ	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
21	BR	164/196 (84%)	164 (100%)	0	0	100	100
22	BS	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
23	BT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
24	BU	98/128 (77%)	97 (99%)	1 (1%)	0	100	100
25	BV	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
26	BW	60/157 (38%)	59 (98%)	1 (2%)	0	100	100
27	BX	117/155 (76%)	114 (97%)	3 (3%)	0	100	100
28	BY	131/145 (90%)	130 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
30	Ba	145/148 (98%)	140 (97%)	5 (3%)	0	100	100
31	Bb	68/71 (96%)	68 (100%)	0	0	100	100
32	Bc	93/115 (81%)	93 (100%)	0	0	100	100
33	Bd	103/176 (58%)	101 (98%)	2 (2%)	0	100	100
34	Be	128/135 (95%)	128 (100%)	0	0	100	100
35	Bf	108/110 (98%)	108 (100%)	0	0	100	100
36	Bg	106/117 (91%)	105 (99%)	1 (1%)	0	100	100
37	Bh	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
38	Bi	98/105 (93%)	98 (100%)	0	0	100	100
39	Bj	84/97 (87%)	84 (100%)	0	0	100	100
40	Bk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
41	Bl	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
42	Bm	50/128 (39%)	50 (100%)	0	0	100	100
43	Bo	102/105 (97%)	99 (97%)	3 (3%)	0	100	100
44	Bp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
45	Br	122/138 (88%)	119 (98%)	3 (2%)	0	100	100
47	Aa	211/264 (80%)	204 (97%)	7 (3%)	0	100	100
48	AA	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
49	AB	59/69 (86%)	58 (98%)	1 (2%)	0	100	100
50	Ab	217/264 (82%)	216 (100%)	1 (0%)	0	100	100
51	AC	61/156 (39%)	58 (95%)	3 (5%)	0	100	100
52	Ac	223/243 (92%)	216 (97%)	7 (3%)	0	100	100
53	Ad	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
54	AD	55/133 (41%)	55 (100%)	0	0	100	100
55	AE	97/115 (84%)	97 (100%)	0	0	100	100
56	Ae	189/204 (93%)	180 (95%)	8 (4%)	1 (0%)	25	38
57	Af	225/249 (90%)	221 (98%)	4 (2%)	0	100	100
58	AF	309/317 (98%)	290 (94%)	19 (6%)	0	100	100
59	Ag	185/194 (95%)	173 (94%)	12 (6%)	0	100	100
60	AG	53/171 (31%)	53 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	Ah	202/207 (98%)	194 (96%)	8 (4%)	0	100	100
62	Ai	177/194 (91%)	175 (99%)	2 (1%)	0	100	100
63	Aj	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
64	Ak	148/158 (94%)	141 (95%)	7 (5%)	0	100	100
65	Al	107/132 (81%)	96 (90%)	11 (10%)	0	100	100
66	Am	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
67	An	132/151 (87%)	128 (97%)	4 (3%)	0	100	100
68	Ao	126/145 (87%)	121 (96%)	5 (4%)	0	100	100
69	Aq	131/135 (97%)	122 (93%)	7 (5%)	2 (2%)	8	12
70	Ar	142/152 (93%)	132 (93%)	10 (7%)	0	100	100
71	As	140/145 (97%)	137 (98%)	3 (2%)	0	100	100
72	At	101/119 (85%)	94 (93%)	7 (7%)	0	100	100
73	Au	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
74	Av	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
75	Aw	140/143 (98%)	137 (98%)	3 (2%)	0	100	100
76	Ax	123/131 (94%)	123 (100%)	0	0	100	100
77	Ay	68/125 (54%)	66 (97%)	2 (3%)	0	100	100
78	AZ	205/296 (69%)	202 (98%)	3 (2%)	0	100	100
79	Ap	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
81	S	40/404 (10%)	37 (92%)	3 (8%)	0	100	100
82	A	854/858 (100%)	813 (95%)	41 (5%)	0	100	100
83	Bs	197/316 (62%)	194 (98%)	3 (2%)	0	100	100
84	Bt	148/165 (90%)	132 (89%)	16 (11%)	0	100	100
85	Bv	213/217 (98%)	192 (90%)	20 (9%)	1 (0%)	25	38
All	All	12525/14686 (85%)	12158 (97%)	362 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	BL	64	VAL
56	Ae	42	GLU
69	Aq	80	ARG
85	Bv	28	PHE
69	Aq	81	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Az	24/24 (100%)	24 (100%)	0	100	100
5	BA	189/199 (95%)	189 (100%)	0	100	100
6	BB	346/349 (99%)	346 (100%)	0	100	100
7	BC	305/338 (90%)	305 (100%)	0	100	100
8	BD	248/249 (100%)	248 (100%)	0	100	100
9	BE	196/256 (77%)	196 (100%)	0	100	100
10	BF	201/211 (95%)	201 (100%)	0	100	100
11	BG	186/225 (83%)	186 (100%)	0	100	100
12	BH	171/171 (100%)	171 (100%)	0	100	100
13	BI	178/178 (100%)	177 (99%)	1 (1%)	84	92
14	BJ	142/148 (96%)	141 (99%)	1 (1%)	81	91
15	BL	175/178 (98%)	175 (100%)	0	100	100
16	BM	112/113 (99%)	112 (100%)	0	100	100
17	BN	171/172 (99%)	171 (100%)	0	100	100
18	BO	172/173 (99%)	172 (100%)	0	100	100
19	BP	136/163 (83%)	135 (99%)	1 (1%)	81	91
20	BQ	159/159 (100%)	159 (100%)	0	100	100
21	BR	147/175 (84%)	147 (100%)	0	100	100
22	BS	157/157 (100%)	157 (100%)	0	100	100
23	BT	139/140 (99%)	139 (100%)	0	100	100
24	BU	90/113 (80%)	90 (100%)	0	100	100
25	BV	106/107 (99%)	106 (100%)	0	100	100
26	BW	54/127 (42%)	54 (100%)	0	100	100
27	BX	107/134 (80%)	107 (100%)	0	100	100
28	BY	123/135 (91%)	123 (100%)	0	100	100
29	BZ	117/118 (99%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Ba	121/122 (99%)	121 (100%)	0	100	100
31	Bb	61/62 (98%)	61 (100%)	0	100	100
32	Bc	80/98 (82%)	80 (100%)	0	100	100
33	Bd	95/148 (64%)	95 (100%)	0	100	100
34	Be	118/123 (96%)	118 (100%)	0	100	100
35	Bf	89/89 (100%)	89 (100%)	0	100	100
36	Bg	93/101 (92%)	93 (100%)	0	100	100
37	Bh	110/110 (100%)	110 (100%)	0	100	100
38	Bi	85/89 (96%)	85 (100%)	0	100	100
39	Bj	73/80 (91%)	73 (100%)	0	100	100
40	Bk	64/65 (98%)	64 (100%)	0	100	100
41	Bl	47/48 (98%)	47 (100%)	0	100	100
42	Bm	48/115 (42%)	48 (100%)	0	100	100
43	Bo	92/92 (100%)	92 (100%)	0	100	100
44	Bp	74/75 (99%)	74 (100%)	0	100	100
45	Br	109/118 (92%)	109 (100%)	0	100	100
47	Aa	194/228 (85%)	193 (100%)	1 (0%)	86	94
48	AA	75/76 (99%)	75 (100%)	0	100	100
49	AB	54/62 (87%)	54 (100%)	0	100	100
50	Ab	185/214 (86%)	185 (100%)	0	100	100
51	AC	56/140 (40%)	55 (98%)	1 (2%)	54	73
52	Ac	189/202 (94%)	189 (100%)	0	100	100
53	Ad	223/224 (100%)	221 (99%)	2 (1%)	75	88
54	AD	46/108 (43%)	46 (100%)	0	100	100
55	AE	87/99 (88%)	87 (100%)	0	100	100
56	Ae	161/170 (95%)	161 (100%)	0	100	100
57	Af	199/219 (91%)	199 (100%)	0	100	100
58	AF	270/275 (98%)	270 (100%)	0	100	100
59	Ag	167/174 (96%)	167 (100%)	0	100	100
60	AG	48/130 (37%)	48 (100%)	0	100	100
61	Ah	176/178 (99%)	176 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	Ai	160/168 (95%)	159 (99%)	1 (1%)	84	92
63	Aj	88/136 (65%)	88 (100%)	0	100	100
64	Ak	133/140 (95%)	132 (99%)	1 (1%)	79	90
65	Al	94/109 (86%)	93 (99%)	1 (1%)	70	84
66	Am	130/131 (99%)	130 (100%)	0	100	100
67	An	105/118 (89%)	105 (100%)	0	100	100
68	Ao	114/130 (88%)	114 (100%)	0	100	100
69	Aq	119/121 (98%)	115 (97%)	4 (3%)	32	52
70	Ar	125/132 (95%)	125 (100%)	0	100	100
71	As	112/114 (98%)	112 (100%)	0	100	100
72	At	94/106 (89%)	94 (100%)	0	100	100
73	Au	69/69 (100%)	69 (100%)	0	100	100
74	Av	112/113 (99%)	112 (100%)	0	100	100
75	Aw	114/115 (99%)	113 (99%)	1 (1%)	75	88
76	Ax	107/113 (95%)	107 (100%)	0	100	100
77	Ay	61/102 (60%)	60 (98%)	1 (2%)	58	76
78	AZ	172/245 (70%)	171 (99%)	1 (1%)	84	92
79	Ap	116/119 (98%)	116 (100%)	0	100	100
81	S	33/312 (11%)	33 (100%)	0	100	100
82	A	729/730 (100%)	728 (100%)	1 (0%)	92	97
83	Bs	167/259 (64%)	167 (100%)	0	100	100
84	Bt	124/137 (90%)	124 (100%)	0	100	100
85	Bv	194/196 (99%)	192 (99%)	2 (1%)	73	86
All	All	10912/12461 (88%)	10892 (100%)	20 (0%)	91	97

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
75	Aw	60	LYS
82	A	50	ARG
85	Bv	27	LYS
85	Bv	26	ARG
53	Ad	220	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
49	AB	29	GLN
49	AB	45	ASN
85	Bv	171	HIS
83	Bs	68	HIS
83	Bs	159	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B5	3630/4441 (81%)	562 (15%)	30 (0%)
2	B8	156/157 (99%)	19 (12%)	0
3	B7	118/119 (99%)	9 (7%)	0
46	A2	1685/1823 (92%)	277 (16%)	4 (0%)
80	V	75/76 (98%)	13 (17%)	2 (2%)
All	All	5664/6616 (85%)	880 (15%)	36 (0%)

5 of 880 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B5	2	G
1	B5	25	A
1	B5	39	A
1	B5	42	A
1	B5	58	G

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B5	4142	U
80	V	58	A
1	B5	4432	A
46	A2	1418	U
1	B5	1197	A

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

143 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	$\#\|Z\| > 2$
46	PSU	A2	93	46	18,21,22	0.52	0	22,30,33	0.56	0
1	A2M	B5	3966	86,1	18,25,26	0.67	0	18,36,39	0.87	1 (5%)
1	A2M	B5	1251	1	18,25,26	0.64	0	18,36,39	0.74	1 (5%)
1	PSU	B5	4116	1	18,21,22	0.52	0	22,30,33	0.57	0
46	OMG	A2	470	86,46	18,26,27	0.97	3 (16%)	19,38,41	0.63	0
46	B8N	A2	1206	46	24,29,30	0.57	0	29,42,45	0.64	0
1	PSU	B5	1700	1	18,21,22	0.46	0	22,30,33	0.68	0
1	OMC	B5	3346	1	19,22,23	0.30	0	26,31,34	0.41	0
46	OMU	A2	1284	86,46	19,22,23	0.24	0	26,31,34	0.48	0
1	OMG	B5	3835	1	18,26,27	0.93	3 (16%)	19,38,41	0.57	0
1	PSU	B5	3755	1	18,21,22	0.49	0	22,30,33	0.58	0
46	A2M	A2	551	46	18,25,26	0.65	0	18,36,39	0.78	1 (5%)
1	PSU	B5	3172	1	18,21,22	0.48	0	22,30,33	0.63	0
1	PSU	B5	3975	1	18,21,22	0.56	0	22,30,33	0.55	0
1	OMG	B5	3813	1	18,26,27	0.95	3 (16%)	19,38,41	0.60	0
1	PSU	B5	3995	1	18,21,22	0.50	0	22,30,33	0.64	0
46	PSU	A2	774	46	18,21,22	0.53	0	22,30,33	0.55	0
1	PSU	B5	4343	86,1	18,21,22	0.50	0	22,30,33	0.57	0
46	A2M	A2	1341	46	18,25,26	0.66	0	18,36,39	0.82	1 (5%)
46	A2M	A2	99	86,46	18,25,26	0.65	0	18,36,39	0.77	1 (5%)
1	A2M	B5	2564	1	18,25,26	0.66	0	18,36,39	0.70	1 (5%)
1	OMG	B5	3639	1	18,26,27	0.99	3 (16%)	19,38,41	0.60	0
1	PSU	B5	3900	1	18,21,22	0.53	0	22,30,33	0.58	0
1	OMC	B5	3318	1	19,22,23	0.30	0	26,31,34	0.40	0
1	OMC	B5	1790	86,1	19,22,23	0.30	0	26,31,34	0.63	0
1	PSU	B5	3736	1	18,21,22	0.53	0	22,30,33	0.57	0
1	PSU	B5	3885	1	18,21,22	0.45	0	22,30,33	0.89	0
46	PSU	A2	782	46	18,21,22	0.63	1 (5%)	22,30,33	0.67	1 (4%)
1	OMC	B5	3178	86,1	19,22,23	0.26	0	26,31,34	0.50	0
1	A2M	B5	399	1	18,25,26	0.65	0	18,36,39	0.74	1 (5%)
1	OMG	B5	1445	1	18,26,27	0.95	3 (16%)	19,38,41	0.63	0
1	PSU	B5	3114	86,1	18,21,22	0.47	0	22,30,33	0.59	0
1	A2M	B5	2536	1	18,25,26	0.66	0	18,36,39	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	A2M	B5	1447	1	18,25,26	0.65	0	18,36,39	0.76	1 (5%)
1	OMG	B5	2113	86,1	18,26,27	0.93	3 (16%)	19,38,41	0.64	0
46	PSU	A2	258	46	18,21,22	0.53	0	22,30,33	0.61	0
82	DDE	A	715	82	14,20,21	0.48	0	14,28,30	0.57	0
1	PSU	B5	3804	1	18,21,22	0.49	0	22,30,33	0.61	0
1	OMG	B5	4066	1	18,26,27	0.96	3 (16%)	19,38,41	0.70	0
1	5MC	B5	3259	86,1	18,22,23	0.31	0	26,32,35	0.42	0
1	OMG	B5	3671	1	18,26,27	0.94	2 (11%)	19,38,41	0.74	0
1	OMC	B5	2610	1	19,22,23	0.28	0	26,31,34	0.34	0
46	A2M	A2	27	86,46	18,25,26	0.66	0	18,36,39	0.74	1 (5%)
1	OMG	B5	3269	1	18,26,27	0.94	2 (11%)	19,38,41	0.58	0
2	PSU	B8	69	86,2	18,21,22	0.54	0	22,30,33	0.63	1 (4%)
1	1MA	B5	1247	86,1	16,25,26	0.84	1 (6%)	18,37,40	0.62	0
46	6MZ	A2	1786	86,46	18,25,26	0.71	0	16,36,39	0.83	1 (6%)
46	OMU	A2	315	46	19,22,23	0.32	0	26,31,34	0.58	0
1	PSU	B5	1606	86,1	18,21,22	0.52	0	22,30,33	0.61	0
1	PSU	B5	2257	1	18,21,22	0.47	0	22,30,33	0.61	0
1	PSU	B5	3739	1	18,21,22	0.47	0	22,30,33	0.62	0
1	PSU	B5	4022	1	18,21,22	0.53	0	22,30,33	0.59	0
46	PSU	A2	642	46	18,21,22	0.52	0	22,30,33	0.62	0
6	HIC	BB	245	6	8,11,12	1.59	2 (25%)	6,14,16	1.03	0
1	PSU	B5	4071	1	18,21,22	0.53	0	22,30,33	0.56	0
1	A2M	B5	1780	86,1	18,25,26	0.65	0	18,36,39	0.88	1 (5%)
1	OMU	B5	3941	86,1	19,22,23	0.30	0	26,31,34	0.44	0
46	OMU	A2	389	46	19,22,23	0.28	0	26,31,34	0.46	0
46	A2M	A2	629	86,46	18,25,26	0.63	0	18,36,39	0.79	1 (5%)
2	OMG	B8	75	2	18,26,27	0.96	3 (16%)	19,38,41	0.62	0
1	OMU	B5	2586	1	19,22,23	0.33	0	26,31,34	0.55	0
1	OMC	B5	3899	1	19,22,23	0.30	0	26,31,34	0.40	0
46	OMG	A2	1286	46	18,26,27	0.92	1 (5%)	19,38,41	0.63	0
1	5MC	B5	3890	86,1	18,22,23	0.36	0	26,32,35	0.65	0
1	PSU	B5	3742	1	18,21,22	0.53	0	22,30,33	0.57	0
46	OMU	A2	116	46	19,22,23	0.28	0	26,31,34	0.42	0
46	PSU	A2	610	46	18,21,22	0.49	0	22,30,33	0.61	0
46	PSU	A2	1132	86,46	18,21,22	0.50	0	22,30,33	0.59	0
46	A2M	A2	165	46	18,25,26	0.66	0	18,36,39	0.90	2 (11%)
1	OMC	B5	3364	1	19,22,23	0.34	0	26,31,34	0.46	0
46	A2M	A2	445	46	18,25,26	0.64	0	18,36,39	0.72	1 (5%)
1	PSU	B5	3874	1	18,21,22	0.50	0	22,30,33	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
46	OMG	A2	562	46	18,26,27	0.97	3 (16%)	19,38,41	0.59	0
46	4AC	A2	1796	46	21,24,25	0.30	0	29,34,37	0.30	0
1	PSU	B5	3397	86,1	18,21,22	0.51	0	22,30,33	0.59	0
1	A2M	B5	3302	1	18,25,26	0.66	0	18,36,39	0.78	1 (5%)
1	OMC	B5	2100	1	19,22,23	0.34	0	26,31,34	0.42	0
46	4AC	A2	1295	46	21,24,25	0.34	0	29,34,37	0.41	0
1	A2M	B5	3307	1	18,25,26	0.66	0	18,36,39	0.78	1 (5%)
1	A2M	B5	1457	86,1	18,25,26	0.67	0	18,36,39	0.82	1 (5%)
1	PSU	B5	1771	1	18,21,22	0.47	0	22,30,33	0.58	0
1	PSU	B5	4372	86,1	18,21,22	0.50	0	22,30,33	0.57	0
1	PSU	B5	3192	1	18,21,22	0.55	0	22,30,33	0.59	0
1	OMC	B5	2171	86,1	19,22,23	0.31	0	26,31,34	0.45	0
1	OMU	B5	3402	1	19,22,23	0.33	0	26,31,34	0.53	0
1	PSU	B5	4132	1	18,21,22	0.52	0	22,30,33	0.62	0
1	A2M	B5	401	1	18,25,26	0.65	0	18,36,39	0.71	1 (5%)
46	OMG	A2	605	46	18,26,27	0.94	2 (11%)	19,38,41	0.72	0
1	OMC	B5	3979	86,1	19,22,23	0.31	0	26,31,34	0.44	0
1	OMG	B5	4080	1	18,26,27	0.98	2 (11%)	19,38,41	0.62	0
1	PSU	B5	1652	1	18,21,22	0.48	0	22,30,33	0.58	0
1	A2M	B5	3201	1	18,25,26	0.66	0	18,36,39	0.72	1 (5%)
67	IAS	An	138	67	6,7,8	1.04	0	6,8,10	1.29	1 (16%)
1	6MZ	B5	3663	1	18,25,26	0.72	0	16,36,39	0.71	1 (6%)
1	OMC	B5	2553	1	19,22,23	0.30	0	26,31,34	0.39	0
1	PSU	B5	3964	86,1	18,21,22	0.53	0	22,30,33	0.59	0
2	PSU	B8	55	2	18,21,22	0.49	0	22,30,33	0.60	0
46	PSU	A2	821	46	18,21,22	0.54	0	22,30,33	0.54	0
1	A2M	B5	3262	1	18,25,26	0.64	0	18,36,39	0.85	1 (5%)
1	PSU	B5	3796	1	18,21,22	0.50	0	22,30,33	0.56	0
1	OMU	B5	4063	1	19,22,23	0.33	0	26,31,34	0.67	0
46	PSU	A2	109	86,46	18,21,22	0.54	0	22,30,33	0.56	0
46	A2M	A2	989	46	18,25,26	0.65	0	18,36,39	0.80	1 (5%)
1	OMG	B5	2625	1	18,26,27	0.94	2 (11%)	19,38,41	0.58	0
1	OMG	B5	1548	86,1	18,26,27	0.98	2 (11%)	19,38,41	0.63	0
1	PSU	B5	1690	1	18,21,22	0.49	0	22,30,33	0.58	0
1	A2M	B5	4014	1	18,25,26	0.65	0	18,36,39	0.70	1 (5%)
46	PSU	A2	647	46	18,21,22	1.50	5 (27%)	22,30,33	2.11	5 (22%)
1	UY1	B5	3295	86,1	19,22,23	0.49	0	22,31,34	0.56	0
1	OMG	B5	3942	1	18,26,27	0.98	3 (16%)	19,38,41	0.63	0
46	OMU	A2	121	46	19,22,23	0.31	0	26,31,34	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
46	PSU	A2	1039	46	18,21,22	0.66	1 (5%)	22,30,33	0.66	0
1	PSU	B5	4019	1	18,21,22	0.75	1 (5%)	22,30,33	0.55	0
1	PSU	B5	3866	1	18,21,22	0.52	0	22,30,33	0.56	0
46	OMU	A2	171	46	19,22,23	0.27	0	26,31,34	0.63	0
71	NMM	As	67	71	9,11,12	1.56	1 (11%)	6,12,14	4.10	2 (33%)
1	OMC	B5	1265	1	19,22,23	0.29	0	26,31,34	0.45	0
1	A2M	B5	3344	1	18,25,26	0.66	0	18,36,39	0.74	1 (5%)
46	MA6	A2	1805	46	18,26,27	0.75	0	19,38,41	0.73	0
1	OMU	B5	3749	1	19,22,23	0.31	0	26,31,34	0.48	0
1	OMG	B5	2173	1	18,26,27	0.97	2 (11%)	19,38,41	0.57	0
43	MLZ	Bo	53	43	8,9,10	0.70	0	4,9,11	0.57	0
1	OMG	B5	3221	1	18,26,27	0.96	3 (16%)	19,38,41	0.63	0
46	PSU	A2	775	46	18,21,22	0.54	0	22,30,33	0.61	0
1	A2M	B5	3195	1	18,25,26	0.67	0	18,36,39	0.75	1 (5%)
1	PSU	B5	3846	1	18,21,22	0.56	0	22,30,33	0.61	1 (4%)
46	OMC	A2	478	46	19,22,23	0.31	0	26,31,34	0.39	0
1	PSU	B5	1600	86,1	18,21,22	0.85	1 (5%)	22,30,33	0.62	0
1	OMG	B5	4061	1	18,26,27	0.93	3 (16%)	19,38,41	0.67	0
1	PSU	B5	3116	1	18,21,22	0.51	0	22,30,33	0.57	0
1	OMG	B5	3376	86,1	18,26,27	1.00	3 (16%)	19,38,41	0.68	0
1	OMG	B5	3937	1	18,26,27	1.00	3 (16%)	19,38,41	0.60	0
1	OMG	B5	1241	86,1	18,26,27	1.03	3 (16%)	19,38,41	0.71	0
1	A2M	B5	2112	86,1	18,25,26	0.65	0	18,36,39	0.72	1 (5%)
1	OMG	B5	3104	1	18,26,27	0.96	3 (16%)	19,38,41	0.67	0
1	UR3	B5	3973	1	19,22,23	0.31	0	26,32,35	0.30	0
46	MA6	A2	1804	46	18,26,27	0.75	0	19,38,41	0.71	0
46	OMG	A2	1445	86,46	18,26,27	0.95	2 (11%)	19,38,41	0.57	0
1	PSU	B5	1769	1	18,21,22	0.50	0	22,30,33	0.59	0
46	OMG	A2	644	46	18,26,27	0.96	3 (16%)	19,38,41	0.68	0
46	OMC	A2	1658	46	19,22,23	0.27	0	26,31,34	0.43	0
1	OMU	B5	3670	1	19,22,23	0.33	0	26,31,34	0.46	0
1	OMC	B5	3285	1	19,22,23	0.31	0	26,31,34	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PSU	A2	93	46	-	0/7/25/26	0/2/2/2
1	A2M	B5	3966	86,1	-	0/5/27/28	0/3/3/3
1	A2M	B5	1251	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	4116	1	-	0/7/25/26	0/2/2/2
46	OMG	A2	470	86,46	-	1/5/27/28	0/3/3/3
46	B8N	A2	1206	46	-	3/16/34/35	0/2/2/2
1	PSU	B5	1700	1	-	1/7/25/26	0/2/2/2
1	OMC	B5	3346	1	-	0/9/27/28	0/2/2/2
46	OMU	A2	1284	86,46	-	0/9/27/28	0/2/2/2
1	OMG	B5	3835	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3755	1	-	0/7/25/26	0/2/2/2
46	A2M	A2	551	46	-	0/5/27/28	0/3/3/3
1	PSU	B5	3172	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3975	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3813	1	-	2/5/27/28	0/3/3/3
1	PSU	B5	3995	1	-	0/7/25/26	0/2/2/2
46	PSU	A2	774	46	-	0/7/25/26	0/2/2/2
1	PSU	B5	4343	86,1	-	0/7/25/26	0/2/2/2
46	A2M	A2	1341	46	-	0/5/27/28	0/3/3/3
46	A2M	A2	99	86,46	-	0/5/27/28	0/3/3/3
1	A2M	B5	2564	1	-	0/5/27/28	0/3/3/3
1	OMG	B5	3639	1	-	1/5/27/28	0/3/3/3
1	PSU	B5	3900	1	-	0/7/25/26	0/2/2/2
1	OMC	B5	3318	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	1790	86,1	-	0/9/27/28	0/2/2/2
1	PSU	B5	3736	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3885	1	-	0/7/25/26	0/2/2/2
46	PSU	A2	782	46	-	0/7/25/26	0/2/2/2
1	OMC	B5	3178	86,1	-	4/9/27/28	0/2/2/2
1	A2M	B5	399	1	-	1/5/27/28	0/3/3/3
1	OMG	B5	1445	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3114	86,1	-	0/7/25/26	0/2/2/2
1	A2M	B5	2536	1	-	1/5/27/28	0/3/3/3
1	A2M	B5	1447	1	-	0/5/27/28	0/3/3/3
1	OMG	B5	2113	86,1	-	2/5/27/28	0/3/3/3
46	PSU	A2	258	46	-	2/7/25/26	0/2/2/2
82	DDE	A	715	82	-	6/20/21/23	0/1/1/1
1	PSU	B5	3804	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4066	1	-	0/5/27/28	0/3/3/3
1	5MC	B5	3259	86,1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3671	1	-	1/5/27/28	0/3/3/3
1	OMC	B5	2610	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	A2M	A2	27	86,46	-	0/5/27/28	0/3/3/3
1	OMG	B5	3269	1	-	0/5/27/28	0/3/3/3
2	PSU	B8	69	86,2	-	0/7/25/26	0/2/2/2
1	1MA	B5	1247	86,1	-	0/3/25/26	0/3/3/3
46	6MZ	A2	1786	86,46	-	0/5/27/28	0/3/3/3
46	OMU	A2	315	46	-	0/9/27/28	0/2/2/2
1	PSU	B5	1606	86,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	2257	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3739	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4022	1	-	0/7/25/26	0/2/2/2
46	PSU	A2	642	46	-	0/7/25/26	0/2/2/2
6	HIC	BB	245	6	-	0/5/6/8	0/1/1/1
1	PSU	B5	4071	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	1780	86,1	-	0/5/27/28	0/3/3/3
1	OMU	B5	3941	86,1	-	0/9/27/28	0/2/2/2
46	OMU	A2	389	46	-	4/9/27/28	0/2/2/2
46	A2M	A2	629	86,46	-	3/5/27/28	0/3/3/3
2	OMG	B8	75	2	-	0/5/27/28	0/3/3/3
1	OMU	B5	2586	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	3899	1	-	0/9/27/28	0/2/2/2
46	OMG	A2	1286	46	-	0/5/27/28	0/3/3/3
1	5MC	B5	3890	86,1	-	3/7/25/26	0/2/2/2
1	PSU	B5	3742	1	-	0/7/25/26	0/2/2/2
46	OMU	A2	116	46	-	0/9/27/28	0/2/2/2
46	PSU	A2	610	46	-	0/7/25/26	0/2/2/2
46	PSU	A2	1132	86,46	-	0/7/25/26	0/2/2/2
46	A2M	A2	165	46	-	0/5/27/28	0/3/3/3
1	OMC	B5	3364	1	-	0/9/27/28	0/2/2/2
46	A2M	A2	445	46	-	0/5/27/28	0/3/3/3
1	PSU	B5	3874	1	-	0/7/25/26	0/2/2/2
46	OMG	A2	562	46	-	0/5/27/28	0/3/3/3
46	4AC	A2	1796	46	-	0/11/29/30	0/2/2/2
1	PSU	B5	3397	86,1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3302	1	-	0/5/27/28	0/3/3/3
1	OMC	B5	2100	1	-	3/9/27/28	0/2/2/2
46	4AC	A2	1295	46	-	2/11/29/30	0/2/2/2
1	A2M	B5	3307	1	-	0/5/27/28	0/3/3/3
1	A2M	B5	1457	86,1	-	2/5/27/28	0/3/3/3
1	PSU	B5	1771	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	4372	86,1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3192	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	B5	2171	86,1	-	2/9/27/28	0/2/2/2
1	OMU	B5	3402	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	4132	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	401	1	-	0/5/27/28	0/3/3/3
46	OMG	A2	605	46	-	3/5/27/28	0/3/3/3
1	OMC	B5	3979	86,1	-	0/9/27/28	0/2/2/2
1	OMG	B5	4080	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	1652	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3201	1	-	1/5/27/28	0/3/3/3
67	IAS	An	138	67	-	2/7/7/8	-
1	6MZ	B5	3663	1	-	0/5/27/28	0/3/3/3
1	OMC	B5	2553	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	3964	86,1	-	2/7/25/26	0/2/2/2
2	PSU	B8	55	2	-	0/7/25/26	0/2/2/2
46	PSU	A2	821	46	-	0/7/25/26	0/2/2/2
1	A2M	B5	3262	1	-	1/5/27/28	0/3/3/3
1	PSU	B5	3796	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	4063	1	-	0/9/27/28	0/2/2/2
46	PSU	A2	109	86,46	-	0/7/25/26	0/2/2/2
46	A2M	A2	989	46	-	0/5/27/28	0/3/3/3
1	OMG	B5	2625	1	-	0/5/27/28	0/3/3/3
1	OMG	B5	1548	86,1	-	1/5/27/28	0/3/3/3
1	PSU	B5	1690	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	4014	1	-	0/5/27/28	0/3/3/3
46	PSU	A2	647	46	-	0/7/25/26	0/2/2/2
1	UY1	B5	3295	86,1	-	2/9/27/28	0/2/2/2
1	OMG	B5	3942	1	-	0/5/27/28	0/3/3/3
46	OMU	A2	121	46	-	0/9/27/28	0/2/2/2
46	PSU	A2	1039	46	-	1/7/25/26	0/2/2/2
1	PSU	B5	4019	1	-	2/7/25/26	0/2/2/2
1	PSU	B5	3866	1	-	0/7/25/26	0/2/2/2
46	OMU	A2	171	46	-	0/9/27/28	0/2/2/2
71	NMM	As	67	71	-	4/9/11/13	-
1	OMC	B5	1265	1	-	0/9/27/28	0/2/2/2
1	A2M	B5	3344	1	-	1/5/27/28	0/3/3/3
46	MA6	A2	1805	46	-	1/7/29/30	0/3/3/3
1	OMU	B5	3749	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	2173	1	-	0/5/27/28	0/3/3/3
43	MLZ	Bo	53	43	-	1/7/8/10	-
1	OMG	B5	3221	1	-	0/5/27/28	0/3/3/3

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PSU	A2	775	46	-	2/7/25/26	0/2/2/2
1	A2M	B5	3195	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3846	1	-	0/7/25/26	0/2/2/2
46	OMC	A2	478	46	-	0/9/27/28	0/2/2/2
1	PSU	B5	1600	86,1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4061	1	-	0/5/27/28	0/3/3/3
1	PSU	B5	3116	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3376	86,1	-	0/5/27/28	0/3/3/3
1	OMG	B5	3937	1	-	1/5/27/28	0/3/3/3
1	OMG	B5	1241	86,1	-	0/5/27/28	0/3/3/3
1	A2M	B5	2112	86,1	-	1/5/27/28	0/3/3/3
1	OMG	B5	3104	1	-	0/5/27/28	0/3/3/3
1	UR3	B5	3973	1	-	0/7/25/26	0/2/2/2
46	MA6	A2	1804	46	-	0/7/29/30	0/3/3/3
46	OMG	A2	1445	86,46	-	1/5/27/28	0/3/3/3
1	PSU	B5	1769	1	-	0/7/25/26	0/2/2/2
46	OMG	A2	644	46	-	1/5/27/28	0/3/3/3
46	OMC	A2	1658	46	-	0/9/27/28	0/2/2/2
1	OMU	B5	3670	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	3285	1	-	0/9/27/28	0/2/2/2

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	As	67	NMM	CZ-NH2	4.16	1.44	1.34
6	BB	245	HIC	CD2-CG	3.40	1.41	1.36
46	A2	647	PSU	C4-N3	-3.24	1.32	1.38
1	B5	1600	PSU	O4'-C1'	-3.21	1.39	1.43
1	B5	1241	OMG	C5-C6	-2.53	1.42	1.47

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
71	As	67	NMM	NE-CZ-NH2	-8.97	111.26	119.48
46	A2	647	PSU	N1-C2-N3	6.48	122.47	115.13
46	A2	647	PSU	C4-N3-C2	-4.44	119.95	126.34
71	As	67	NMM	NE-CZ-NH1	4.25	128.22	120.26
46	A2	647	PSU	O2-C2-N1	-3.64	118.78	122.79

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B5	399	A2M	C1'-C2'-O2'-CM'
1	B5	2536	A2M	C1'-C2'-O2'-CM'
1	B5	3178	OMC	C2'-C1'-N1-C6
1	B5	3192	PSU	C3'-C4'-C5'-O5'
1	B5	3201	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 501 ligands modelled in this entry, 500 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
88	GDP	A	901	-	24,30,30	0.87	1 (4%)	30,47,47	0.89	1 (3%)

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
88	GDP	A	901	-	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	A	901	GDP	C5-C6	-2.11	1.43	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	A	901	GDP	PA-O3A-PB	3.35	144.33	132.83

There are no chirality outliers.

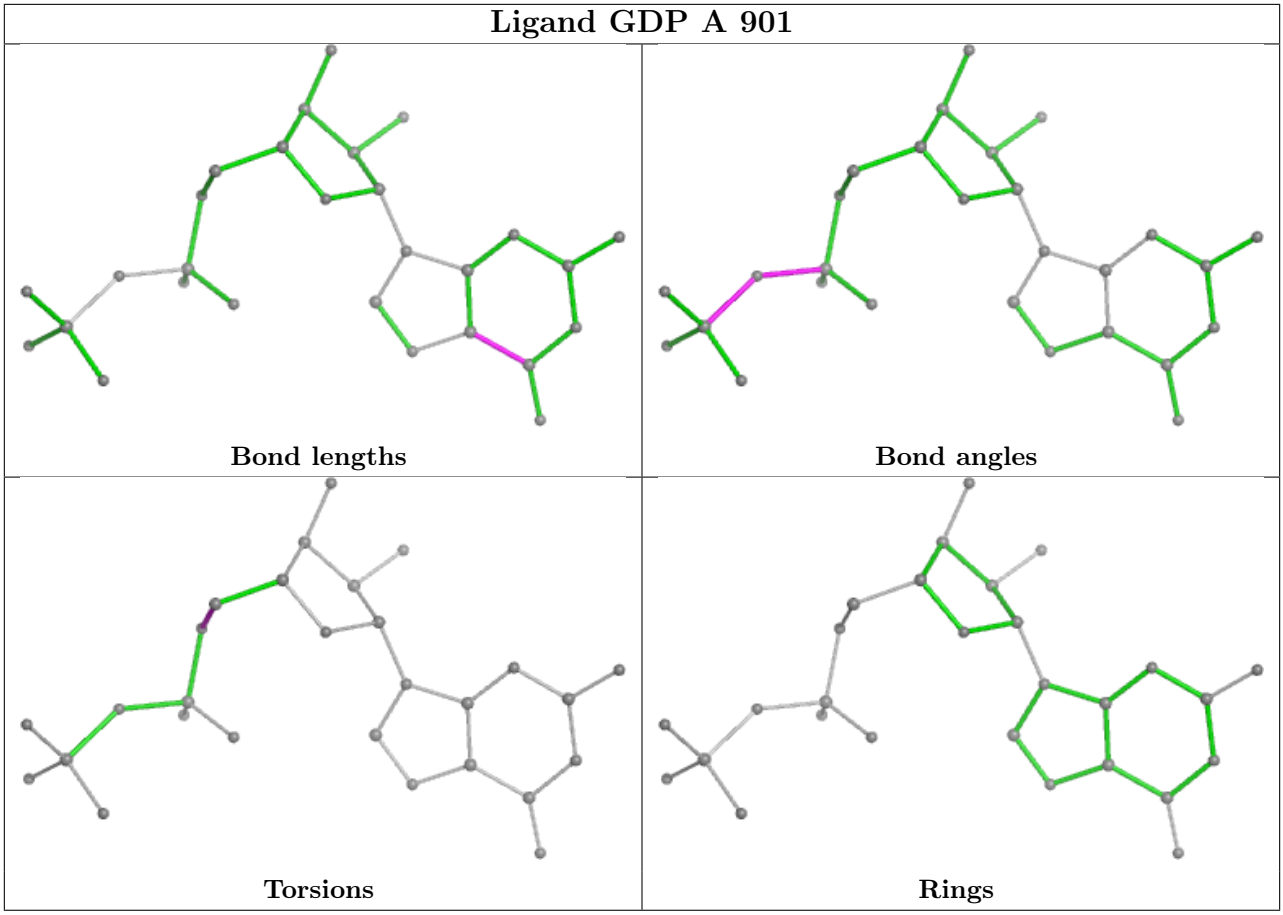
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	A	901	GDP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

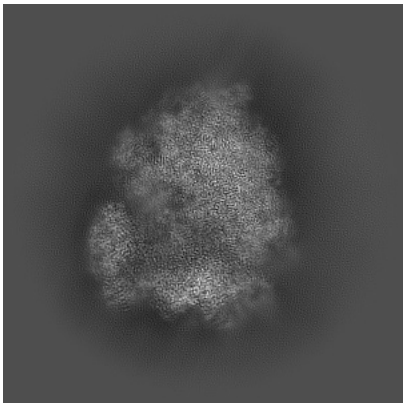
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-18169. These allow visual inspection of the internal detail of the map and identification of artifacts.

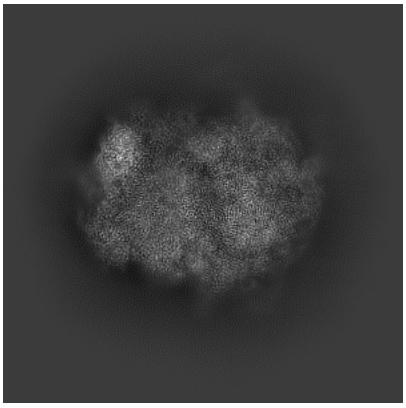
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

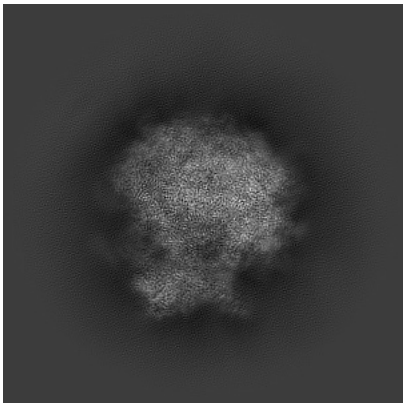
6.1.1 Primary map



X



Y

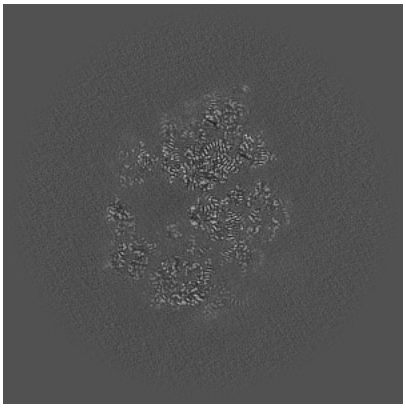


Z

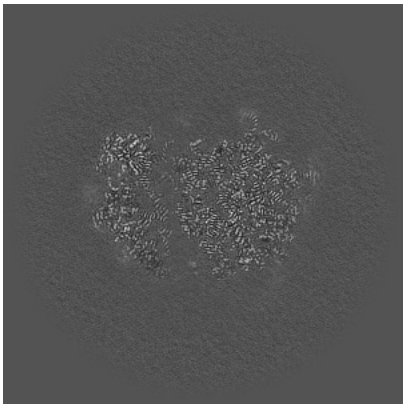
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

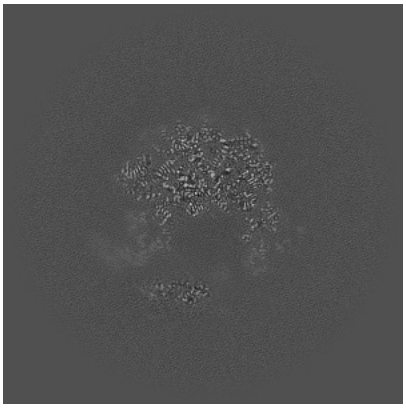
6.2.1 Primary map



X Index: 290



Y Index: 290

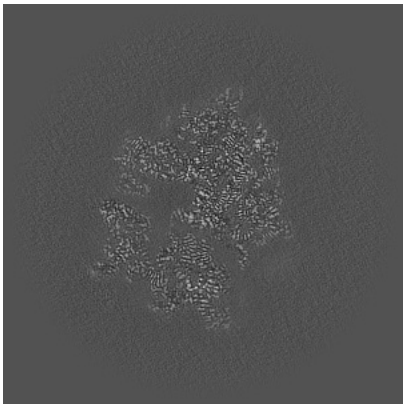


Z Index: 290

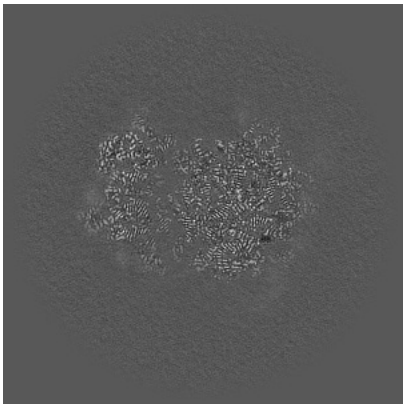
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

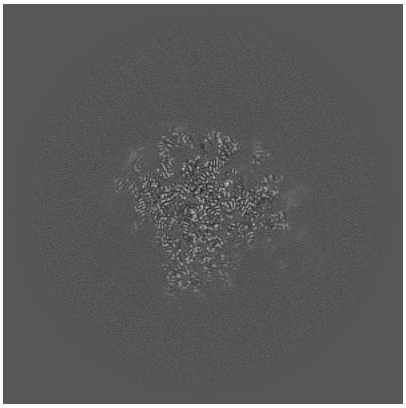
6.3.1 Primary map



X Index: 270



Y Index: 298

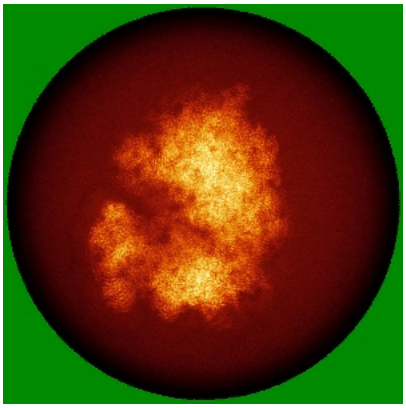


Z Index: 348

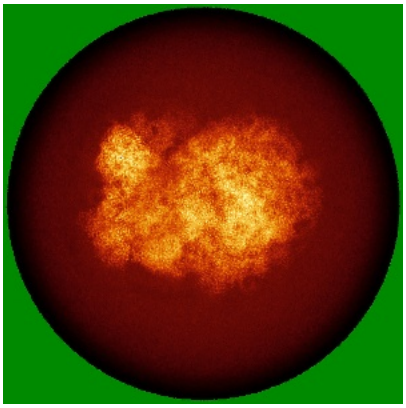
The images above show the largest variance slices of the map in three orthogonal directions.

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

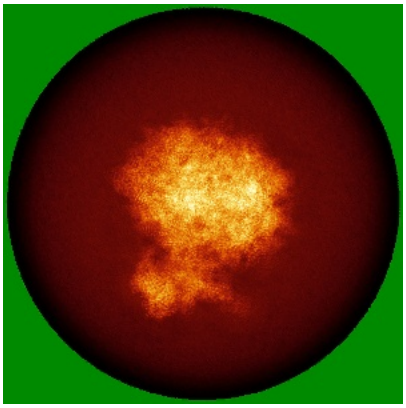
6.4.1 Primary map



X



Y

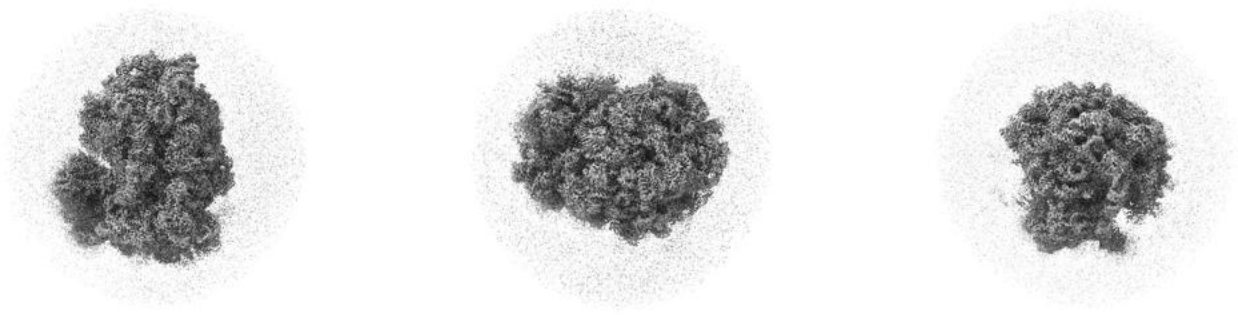


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

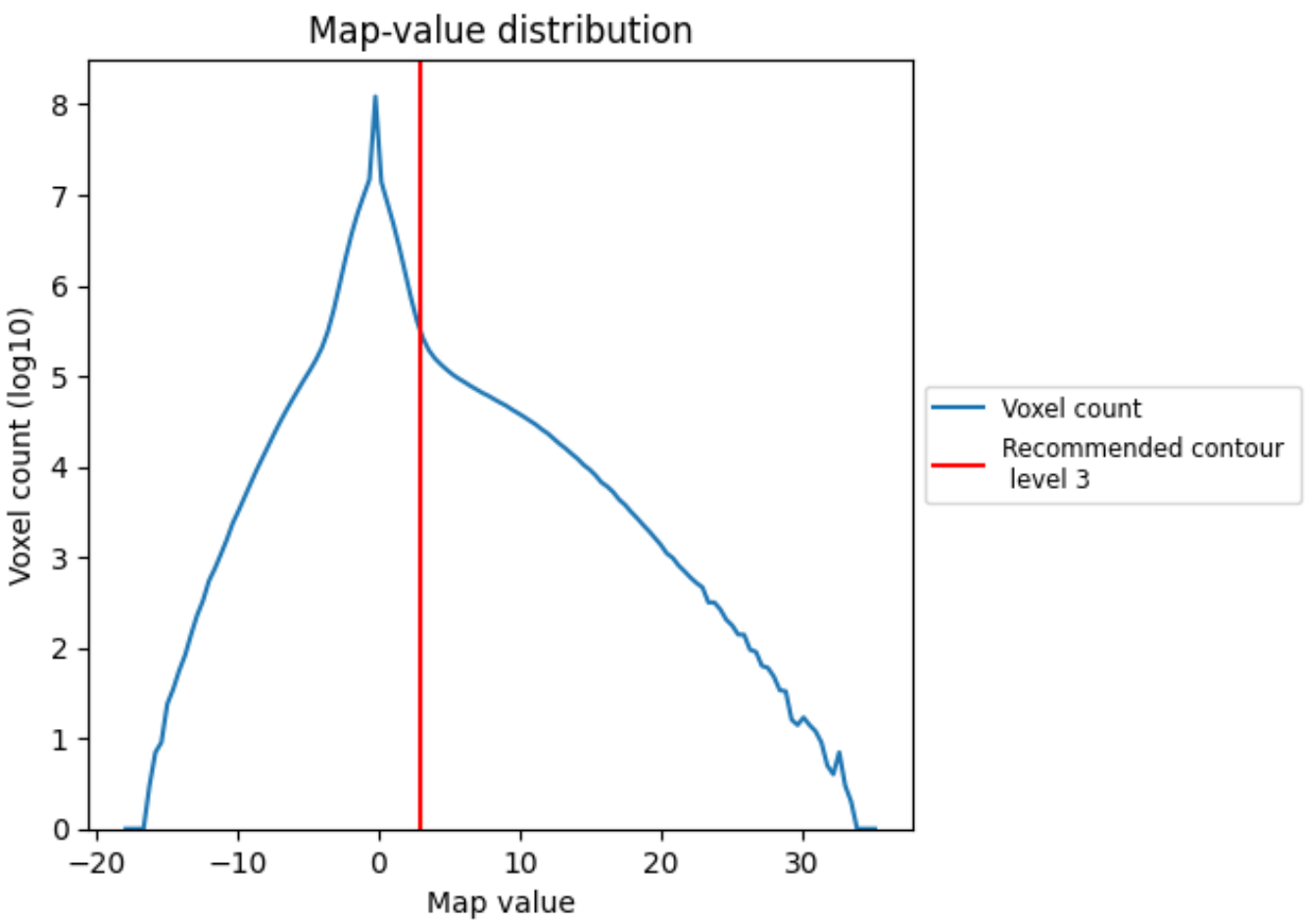
6.6 Mask visualisation (i)

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

7 Map analysis (i)

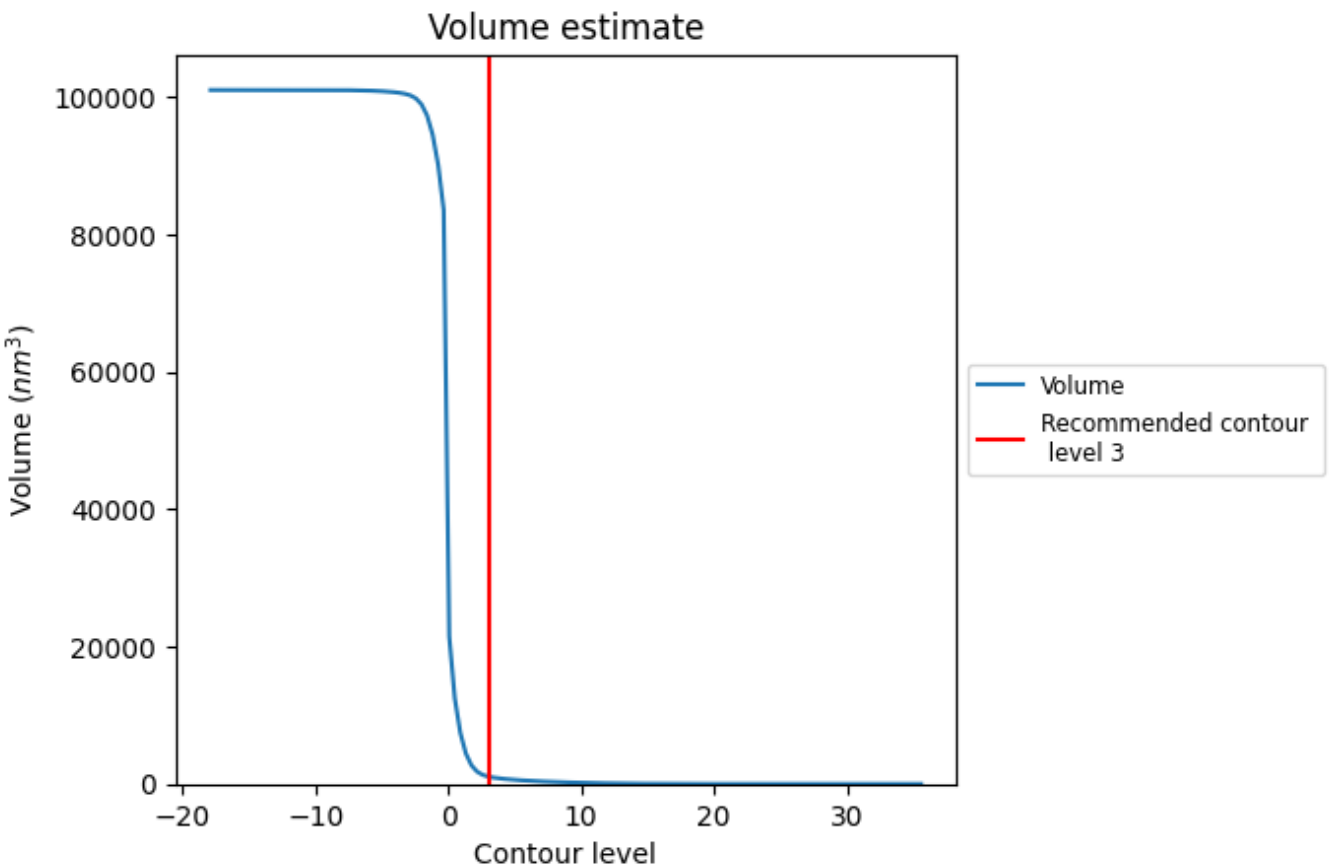
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

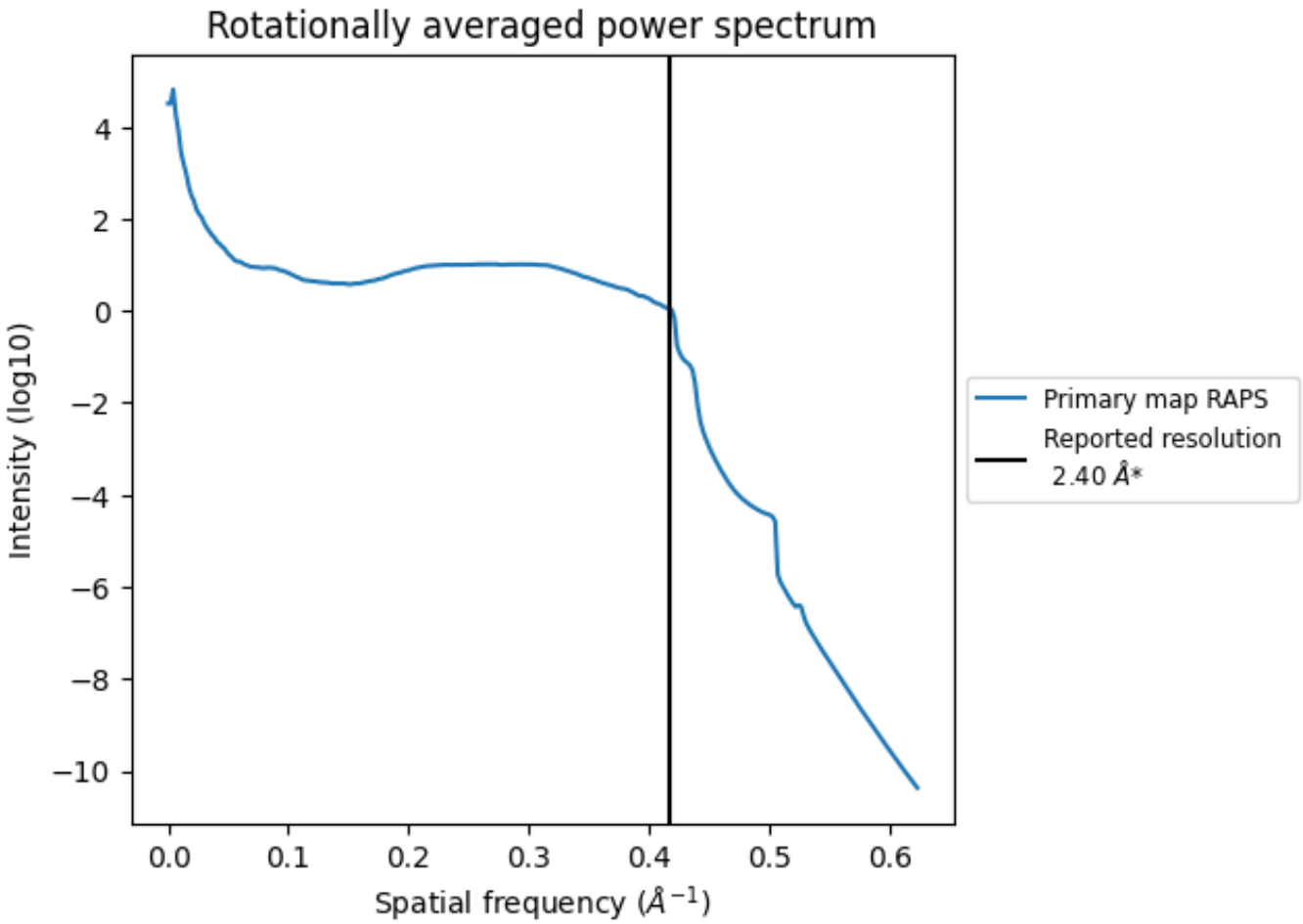
7.2 Volume estimate (i)



The volume at the recommended contour level is 1075 nm^3; this corresponds to an approximate mass of 971 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

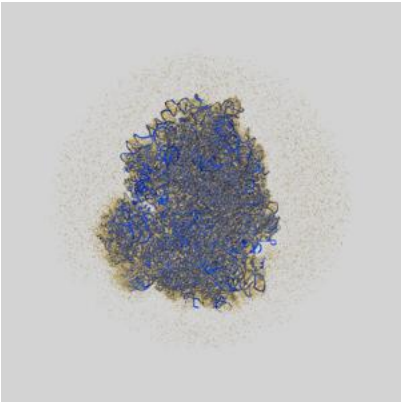
8 Fourier-Shell correlation (i)

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

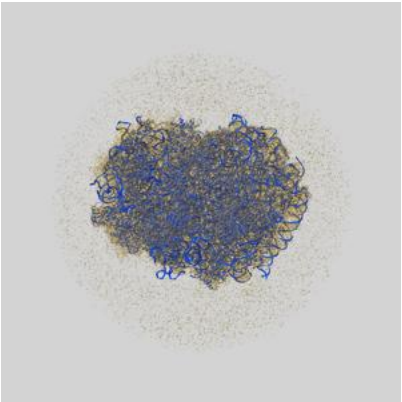
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-18169 and PDB model 8Q87. Per-residue inclusion information can be found in section 3 on page 25.

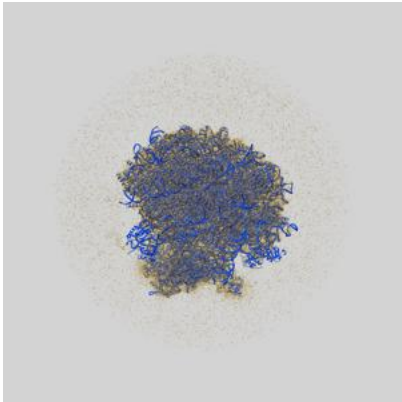
9.1 Map-model overlay (i)



X



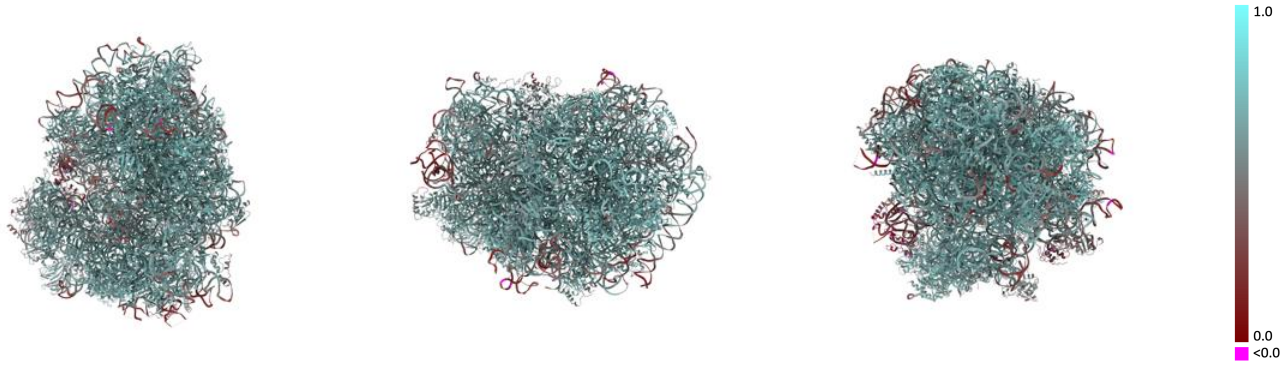
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

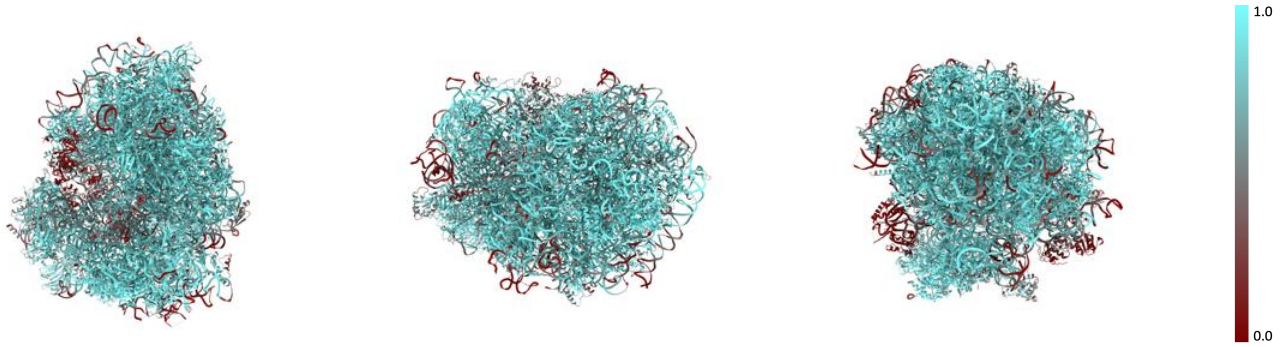
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

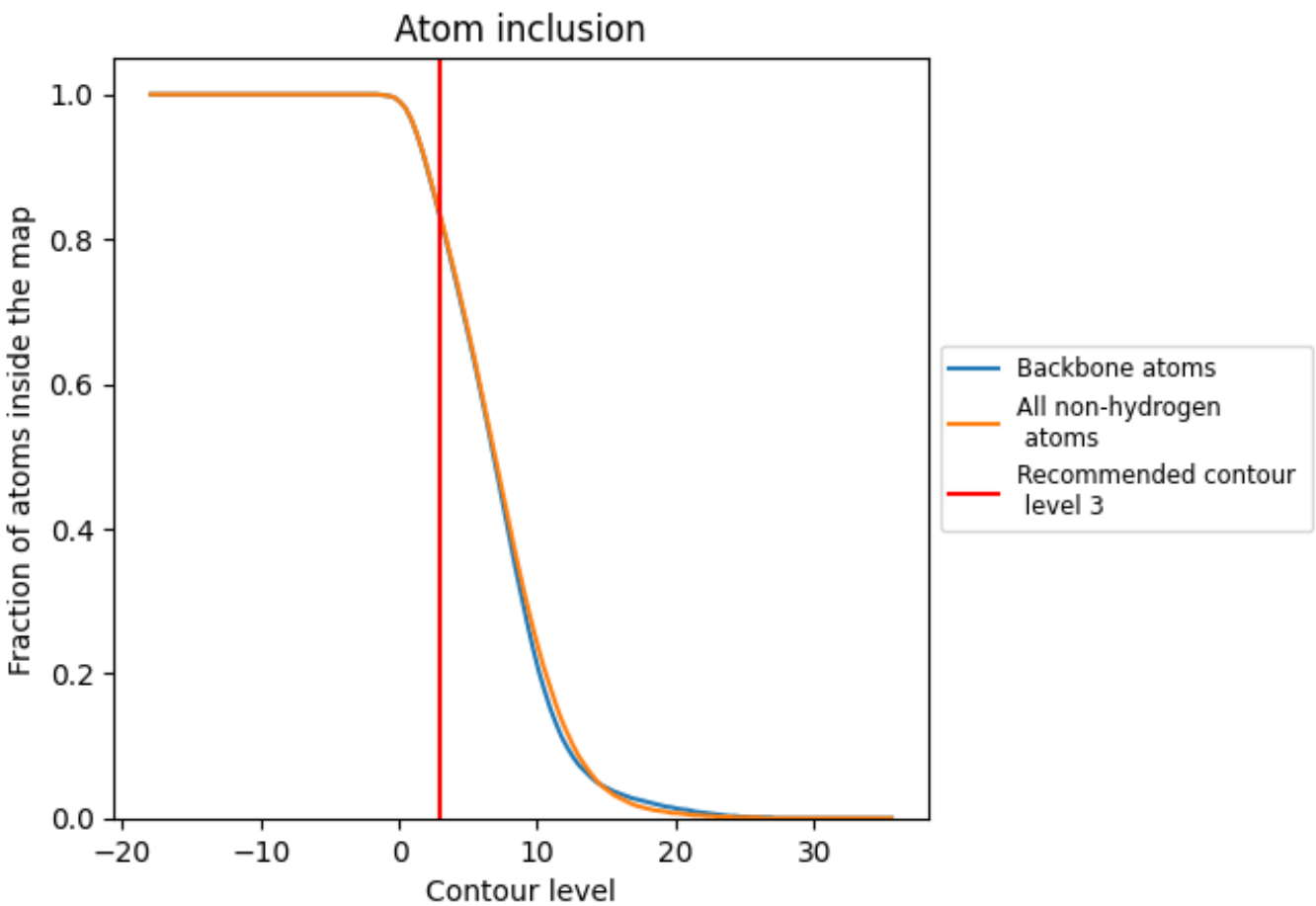
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8320	0.6210
A	0.5550	0.5490
A2	0.8430	0.6100
AA	0.7770	0.5950
AB	0.6130	0.5490
AC	0.5290	0.4900
AD	0.6680	0.5920
AE	0.7950	0.6360
AF	0.8910	0.6120
AG	0.9460	0.6720
AZ	0.9240	0.6550
Aa	0.7530	0.5970
Ab	0.9070	0.6600
Ac	0.8050	0.6120
Ad	0.9730	0.6610
Ae	0.8900	0.6330
Af	0.7970	0.5950
Ag	0.6480	0.5430
Ah	0.8140	0.6110
Ai	0.9560	0.6540
Aj	0.9380	0.6270
Ak	0.8510	0.6340
Al	0.5210	0.4410
Am	0.8190	0.6330
An	0.7150	0.6000
Ao	0.8360	0.6320
Ap	0.9520	0.6600
Aq	0.7090	0.5810
Ar	0.8930	0.6360
As	0.9510	0.6630
At	0.8530	0.5940
Au	0.9390	0.6510
Av	0.9770	0.6730
Aw	0.8600	0.6540
Ax	0.9240	0.6420

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Chain	Atom inclusion	Q-score
Ay	0.9150	0.6300
Az	0.7250	0.6440
B5	0.8480	0.6160
B7	0.9710	0.6670
B8	0.8960	0.6430
BA	0.9500	0.6980
BB	0.9380	0.6910
BC	0.9400	0.6880
BD	0.8500	0.6400
BE	0.8610	0.6510
BF	0.9430	0.6940
BG	0.7900	0.6220
BH	0.9170	0.6810
BI	0.8870	0.6640
BJ	0.6850	0.5990
BL	0.8750	0.6540
BM	0.9460	0.6900
BN	0.9930	0.7100
BO	0.9520	0.6890
BP	0.9350	0.6860
BQ	0.9700	0.7020
BR	0.8430	0.6510
BS	0.9710	0.6970
BT	0.8890	0.6670
BU	0.5960	0.5680
BV	0.8720	0.6810
BW	0.8760	0.6750
BX	0.8990	0.6610
BY	0.9050	0.6640
BZ	0.8600	0.6500
Ba	0.9590	0.7010
Bb	0.7950	0.6340
Bc	0.8290	0.6570
Bd	0.8780	0.6650
Be	0.9620	0.6960
Bf	0.9650	0.7040
Bg	0.9220	0.6730
Bh	0.8900	0.6600
Bi	0.8690	0.6590
Bj	0.9780	0.7000
Bk	0.6550	0.5910
Bl	0.9050	0.6660

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Chain	Atom inclusion	Q-score
Bm	0.9380	0.6810
Bo	0.8970	0.6760
Bp	0.8640	0.6760
Br	0.9360	0.6780
Bs	0.1530	0.4360
Bt	0.0510	0.2570
Bv	0.0170	0.2360
S	0.6620	0.6280
V	0.6090	0.5160