



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 08:42 PM UTC

PDB ID : 8IFD / pdb_00008ifd
EMDB ID : EMD-35413
Title : Dibekacin-added human 80S ribosome
Authors : Tomono, J.; Asano, K.; Chiashi, T.; Tanaka, Y.; Yokoyama, T.
Deposited on : 2023-02-17
Resolution : 2.59 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

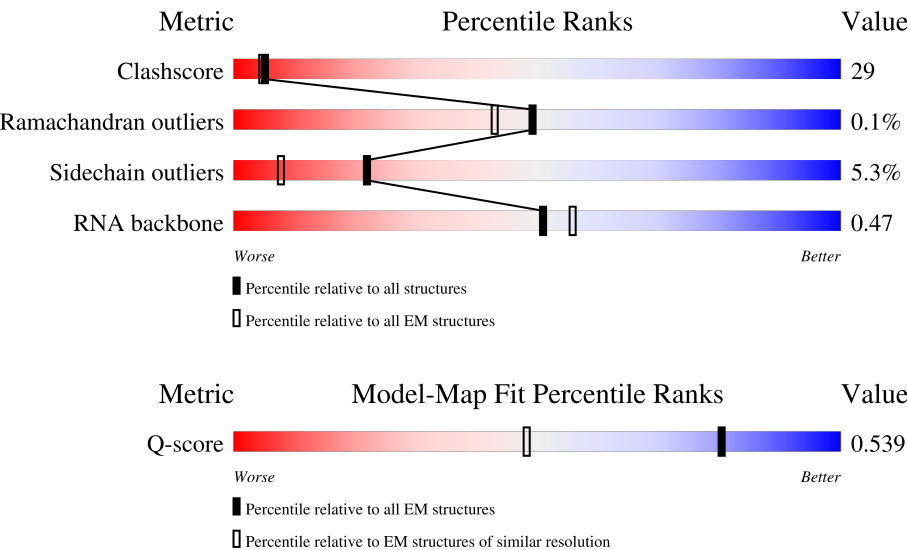
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.59 Å.

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



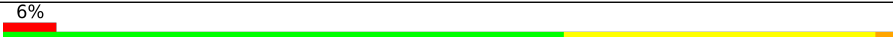
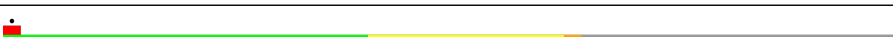
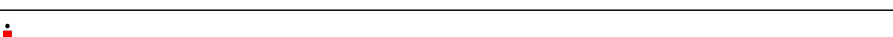
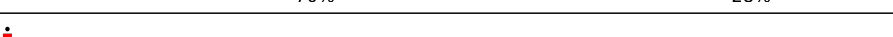
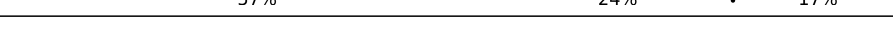
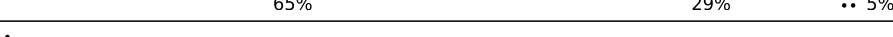
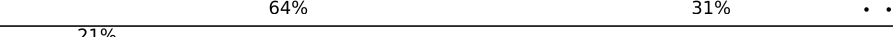
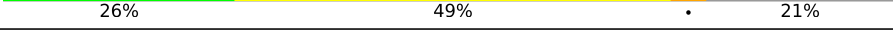
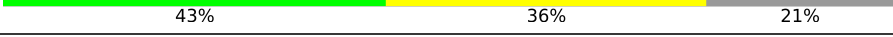
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7741 (2.09 - 3.09)

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

Mol	Chain	Length	Quality of chain
1	1A	5070	9% 20% 41% 12% 27%
2	1B	121	40% 50% 8%
3	1C	157	7% 26% 61% 12%

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Mol	Chain	Length	Quality of chain
4	1D	257	
5	1E	403	
6	1F	427	
7	1G	297	
8	1H	288	
9	2A	248	
10	2B	266	
11	2C	192	
12	2D	214	
13	2E	178	
14	2F	211	
15	2G	215	
16	2H	204	
17	2I	203	
18	2J	184	
19	2K	188	
20	2L	196	
21	2M	176	
22	2N	160	
23	2O	128	
24	2P	140	
25	2Q	157	
26	2R	156	
27	2S	145	
28	2T	136	

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Mol	Chain	Length	Quality of chain
29	2U	148	
30	2V	159	
31	2W	115	
32	2X	125	
33	2Y	135	
34	2Z	110	
35	2a	117	
36	2b	123	
37	2c	105	
38	2d	97	
39	2e	70	
40	2f	51	
41	2g	128	
42	2h	25	
43	2i	106	
44	2j	92	
45	2k	137	
46	2l	217	
47	2m	1869	
48	2n	295	
49	2o	264	
50	2p	243	
51	2q	263	
52	2r	204	
53	2s	194	

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Mol	Chain	Length	Quality of chain
54	2t	208	
55	2u	165	
56	2v	158	
57	2w	145	
58	2x	146	
59	2y	135	
60	2z	152	
61	20	145	
62	21	119	
63	3A	83	
64	3B	143	
65	3C	115	
66	3D	69	
67	3E	56	
68	3F	317	
69	3G	293	
70	3H	249	
71	3I	194	
72	3J	132	
73	3K	151	
74	3L	151	
75	3M	130	
76	3N	133	
77	3O	125	
78	3P	84	

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Mol	Chain	Length	Quality of chain
79	3Q	59	54% 53% 44% ••
80	3R	156	43% 22% 19% • 57%

2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 218821 atoms, of which 888 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	3717	Total	C	N	O	P	0	0
			79674	35479	14585	25894	3716		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	2113	C	G	conflict	GB 86475748

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	156	Total	C	N	O	P	0	0
			3310	1477	585	1093	155		

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1E	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2A	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2B	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2C	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 12 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2D	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2E	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2F	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2G	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2H	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2I	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2J	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	2K	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2L	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2M	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	2N	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2O	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 24 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2P	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2Q	124	Total	C	N	O	S	0	0
			1015	634	207	170	4		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2R	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2S	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2T	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 29 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2U	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2V	109	Total	C	N	O	S	0	0
			882	549	192	137	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2W	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 32 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	2X	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2Y	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2Z	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2a	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 36 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2b	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	2c	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 38 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2d	86	Total	C	N	O	S	1	0
			713	439	158	111	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	2e	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	2f	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 41 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	2g	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	2h	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	2i	105	Total	C	N	O	S	1	0
			870	547	178	139	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	2j	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2k	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 46 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2l	217	Total	C	N	O	S	0	0
			1740	1113	312	306	9		

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2m	1742	Total	C	N	O	P	0	0
			36900	16458	6595	12106	1741		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2m	582	C	U	conflict	GB 36162
2m	583	C	A	conflict	GB 36162
2m	584	G	A	conflict	GB 36162
2m	798	A	G	conflict	GB 36162
2m	1095	U	C	conflict	GB 36162

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	2n	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 49 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2o	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 50 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2p	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 51 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	2q	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 52 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2r	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 53 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	2s	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 54 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2t	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 55 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	2u	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 56 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	2v	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 57 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	2w	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 58 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	2x	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 59 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	2y	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 60 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	2z	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 61 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	20	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 62 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	21	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 63 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	3A	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 64 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	3B	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 65 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	3C	102	Total	C	N	O	S	1	0
			829	517	174	133	5		

- Molecule 66 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	3D	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 67 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	3E	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 68 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	3F	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 69 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	3G	222	Total	C	N	O	S	1	0
			1733	1120	301	302	10		

- Molecule 70 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	3H	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 71 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	3I	185	Total	C	N	O	S	1	0
			1533	974	309	248	2		

- Molecule 72 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	3J	122	Total	C	N	O	S	0	0
			942	590	165	179	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3J	52	GLN	LEU	conflict	UNP P25398
3J	69	LEU	CYS	conflict	UNP P25398
3J	99	ASN	LYS	conflict	UNP P25398

- Molecule 73 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	3K	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 74 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	3L	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
75	3M	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
76	3N	131	Total	C	N	O	S	1	0
			1073	678	212	178	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
77	3O	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 78 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	3P	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

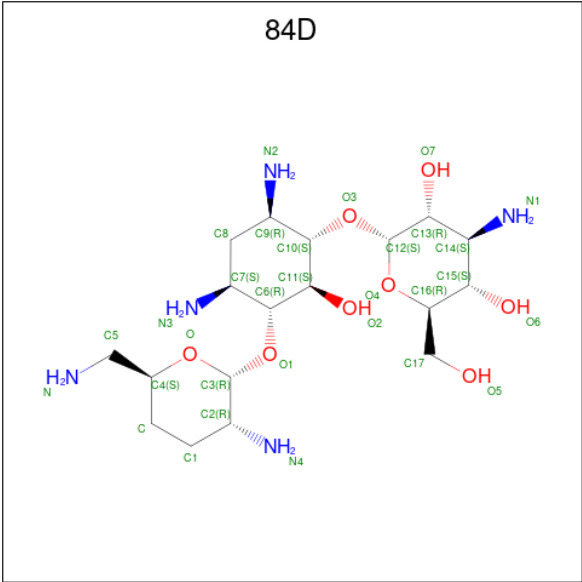
- Molecule 79 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	3Q	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	3R	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 81 is Dibekacin (CCD ID: 84D) (formula: C₁₈H₃₇N₅O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	

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Mol	Chain	Residues	Atoms					AltConf
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	1A	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	2m	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	2m	1	Total	C	H	N	O	0
			68	18	37	5	8	
81	2m	1	Total	C	H	N	O	0
			68	18	37	5	8	

- Molecule 82 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
82	1A	270	Total	Mg	0
			270	270	
82	1B	2	Total	Mg	0
			2	2	
82	1C	5	Total	Mg	0
			5	5	
82	1D	1	Total	Mg	0
			1	1	
82	2H	1	Total	Mg	0
			1	1	
82	2J	1	Total	Mg	0
			1	1	
82	2K	1	Total	Mg	0
			1	1	
82	2M	1	Total	Mg	0
			1	1	
82	2P	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
82	2V	1	Total 1	Mg 1	0
82	2Y	1	Total 1	Mg 1	0
82	2Z	1	Total 1	Mg 1	0
82	2a	1	Total 1	Mg 1	0
82	2d	1	Total 1	Mg 1	0
82	2m	105	Total 105	Mg 105	0
82	2o	1	Total 1	Mg 1	0
82	3H	1	Total 1	Mg 1	0
82	3K	1	Total 1	Mg 1	0
82	3L	1	Total 1	Mg 1	0

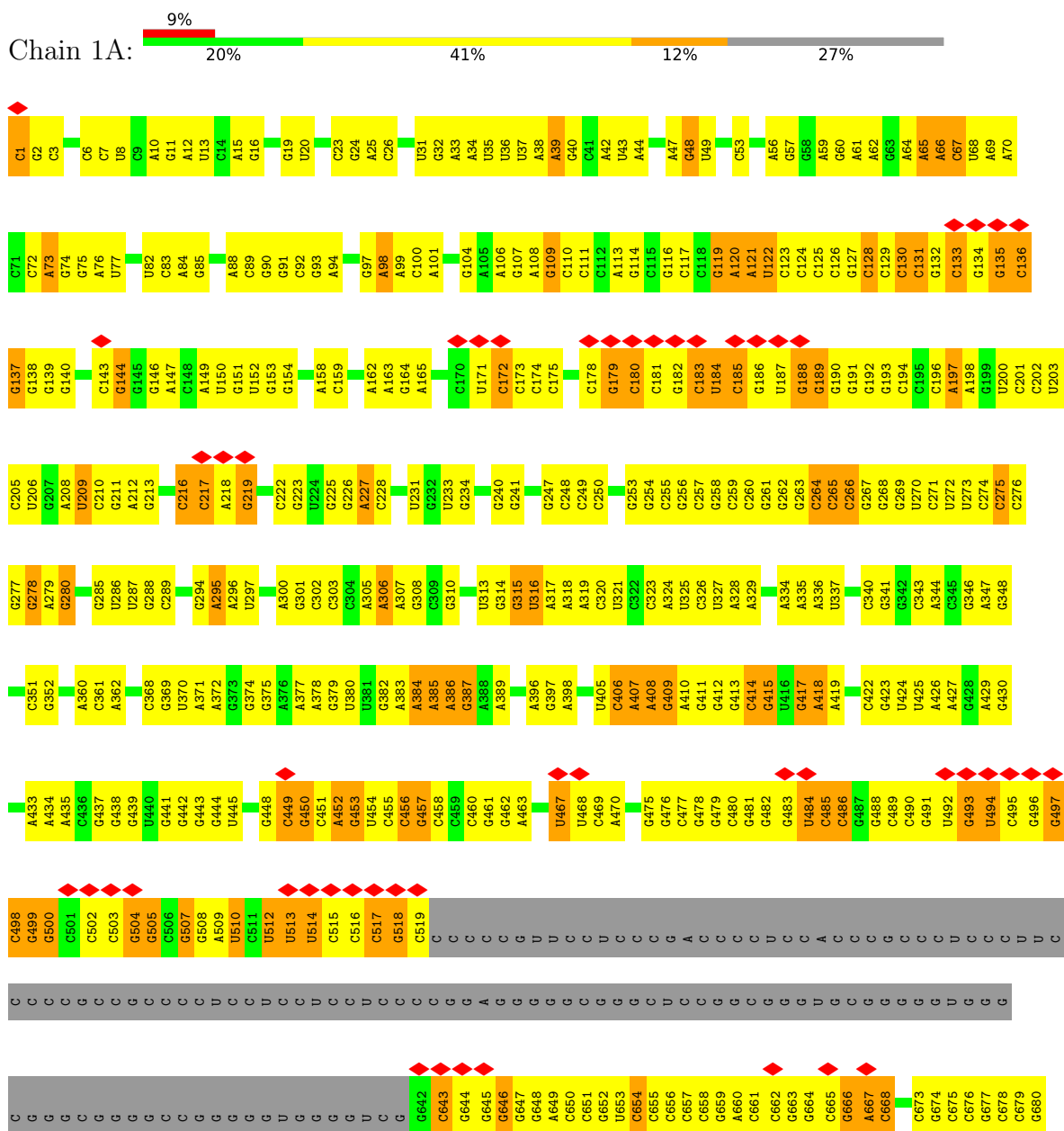
- Molecule 83 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
83	2d	1	Total 1	Zn 1	0
83	2g	1	Total 1	Zn 1	0
83	2j	1	Total 1	Zn 1	0
83	3C	1	Total 1	Zn 1	0

3 Residue-property plots

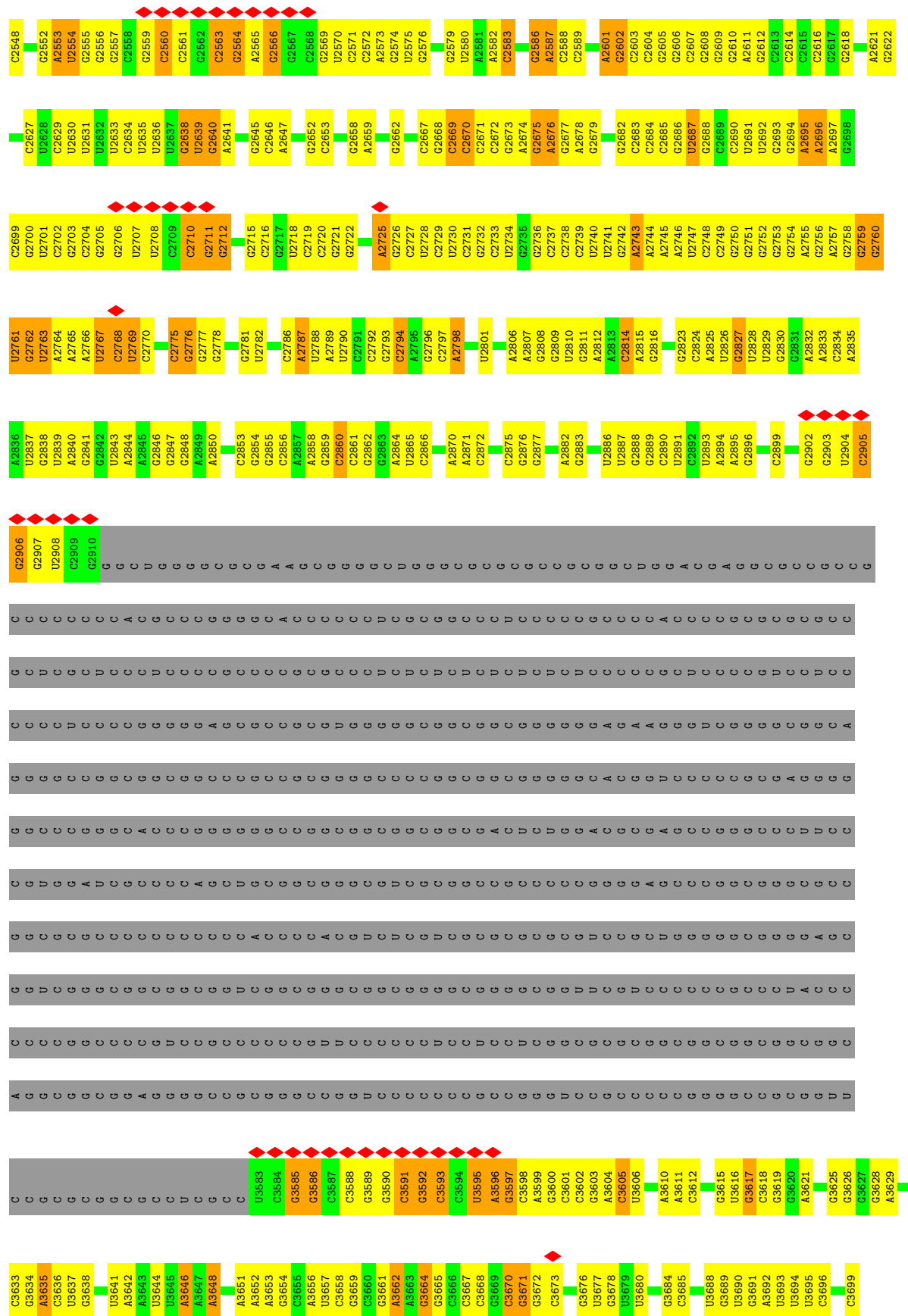
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 28S ribosomal RNA

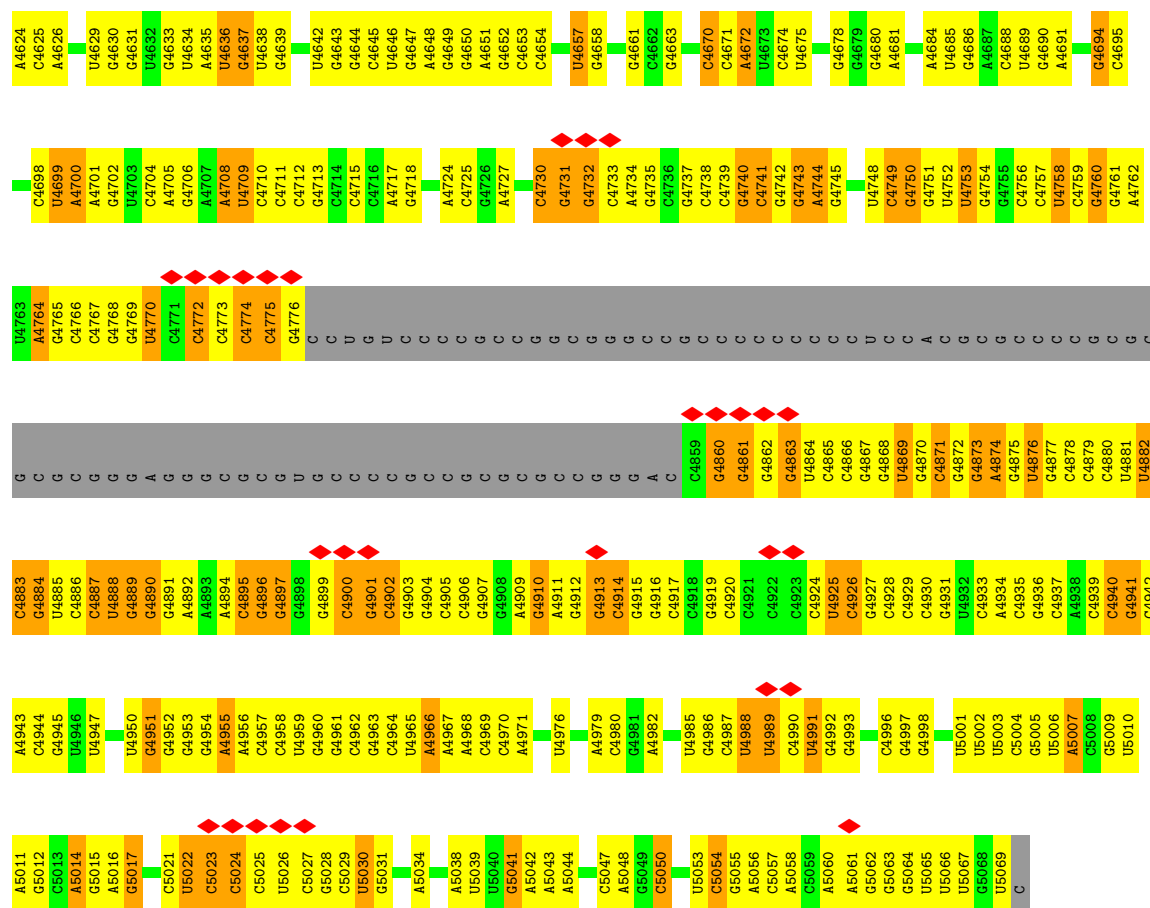




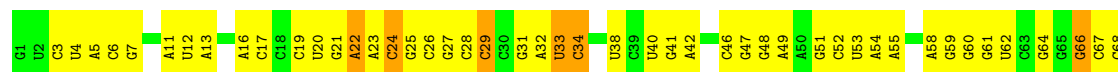




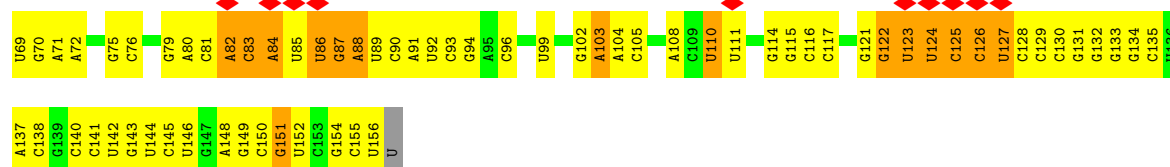
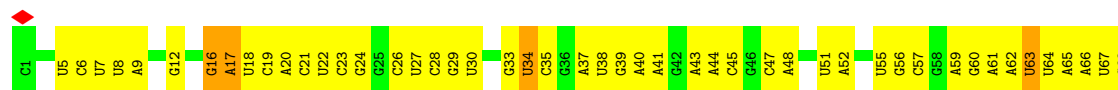
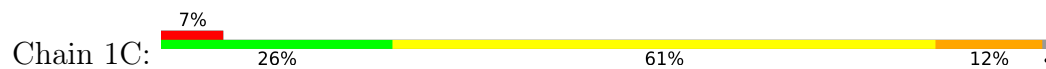
C4560	C4485	G4418	C4349	A4281	U4218	G4151	G4090	C	G3969	A3908	G3839	C3771	C3700
A4487	C4486	U4419	C4350	A4282	A4219	G4152	G4091	C	G3970	C3909	U3840	U3772	G3701
U4492	A4487	C4420	U4351	C4283	A4220	C4153	G4092	U	G3971	C3910	A3845	A3773	A3702
U4492	A4487	C4421	U4352	C4284	A4221	C4154	G4093	G	A3972	C3911	A3846	A3774	C3706
U4492	A4487	C4422	U4353	U4285	G4222	C4155	G4094	C	G3973	U3912	C3847	A3775	U3707
U4423	A4423	U4423	G4356	C4288	G4226	C4157	G4095	G4034	G3974	U3914	U3848	G3777	C3708
A4424	A4424	A4424	G4357	U4289	U4227	C4158	G4096	G4035	G3975	U3915	A3849	U3778	U3709
G4425	U4290	U4290	U4358	U4289	G4228	C4159	G4097	G4036	C3976	G3916	A3850	G3710	A3711
A4428	G4291	G4291	C4162	U4229	U4229	U4163	A4098	C4037	C3977	A3917	C3781	A3712	A3712
C4429	U4296	U4296	C4164	C4230	C4230	C4164	G4099	C4038	C	C3918	C3855	U3713	U3713
G4430	G4297	G4297	C4165	C4231	C4231	C4165	C4100	G4039	C	U3920	C3857	G3714	G3714
	U4300	U4300	G4166	U4232	U4232	G4166	C4101	C4040	C	U3921	C3858	U3715	U3715
	U4301	U4301	C4167	A4233	A4233	C4167	C4102	C4041	C	A3922	G3859	A3716	A3716
	U4302	U4302	G4168	G4236	G4236	G4168	C4103	C4042	C	A3923	C3860	A3717	A3717
	U4303	U4303	C4169	C4237	C4237	C4169	G4104	G4043	C	C3924	A3861	A3718	A3718
	U4304	U4304	A4170	G4238	G4238	A4170	C4105	G4044	C	U3925	A3862	A3719	A3719
	G4305	G4305	G4173	C4240	C4240	G4173	A4106	U4045	C	A3928	A3865	G3720	G3720
	U4306	U4306	U4174	C4241	C4241	U4174	G4107	A4046	C	G3929	C3866	U3721	U3721
	A4307	A4307	G4175	U4242	U4242	G4175	C4108	A4047	C	U3930	C3867	G3722	G3722
				C4243	C4243		A4108	U4048	C	C3931	A3868	A3723	A3723
				G4245	G4245		G4109	U4049	C	U3932	C3869	A3724	A3724
				G4246	G4246		C4110	U4050	C	G3933	C3870	G3725	G3725
				U4247	U4247		U4111	A4051	C	C3934	A3871	A3726	A3726
				G4248	G4248		C4112	C4052	C	A3935	A3872	A3727	A3727
				G4249	G4249		U4113	A4053	C	C3936	C3873	A3728	A3728
				G4250	G4250		C4114	C4054	C	A3937	C3874		
				A4251	A4251		G4115	U4054	C	G3938	A3877	A3732	A3732
				C4252	C4252		C4116	U4055	C	G3939	C3878	A3733	A3733
				G4253	G4253			U4056	C	U3940	C3879	A3734	A3734
				U4189	U4189		U4120	A4057	C	G3941	C3880	G3735	G3735
				G4191	G4191		G4121	C4057	C	A3942	C3881	A3736	A3736
				A4192	A4192		C4122	U4058	C	A3943	C3882	A3737	A3737
				C4193	C4193		G4123	C4059	C	G3944	C3883	G3738	G3738
				U4194	U4194		U4124	U4060	C	A3945	U3884	A3746	A3746
							C4125	G4061	C	G3946	G3885	A3747	A3747
							C4126	A4062	C	C3947	A3815	A3748	A3748
							A4127	U4063	C	A3948	G3816	G3751	G3751
							G4128	U4064	C	A3949	C3888	G3752	G3752
							C4129	C4065	C	U3950	A3817	G3753	G3753
							G4130	U4066	C	G3951	U3818	G3754	G3754
							C4131	U4067	C	C3952	A3819	G3755	G3755
							C4132	U4068	C	U3953	U3820	A3756	A3756
							C4133	U4069	C	A3954	A3821	G3757	G3757
							G4134	U4070	C	G3955	G3823	U3758	U3758
							G4135	U4071	C	G3956	A3824	A3759	A3759
							C4136	C4072	C	U3957	G3825	A3760	A3760
							C4137	U4073	C	G3958	G3826	G3761	G3761
							C4138	A4074	C	U3959	C3827	U3762	U3762
							C4139	U4075	C	A3960	C3833	U3763	U3763
							C4140	G4076	C	G3961	C3834	G3764	G3764
							G4141	U4079	C	A3962	C3835	A3765	A3765
							C4142	C4080	C	A3963	A3836	G3766	G3766
							C4143	G4081	C	U3964	C3837	A3767	A3767
							C4144	U4082	C	A3965	U3838	U3770	U3770
							C4145	U4083	C	G3966	A3839		
							G4146	A4084	C	U3967	A3840		
							C4147	U4085	C	U3968	A3841		
							C4148	G4086	C				
							C4149	U4087	C				
							G4150	G4088	C				
								C4089	C				
								G4090	C				
								C4091	C				
								U4092	C				
								G4093	C				
								C4094	C				
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								G4104	C				
								A4105	C				
								G4106	C				
								C4107	C				
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								G4109	C				
								C4110	C				
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								U4117	C				
								A4118	C				
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								C4120	C				
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								U4173	C				
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								C4178	C				



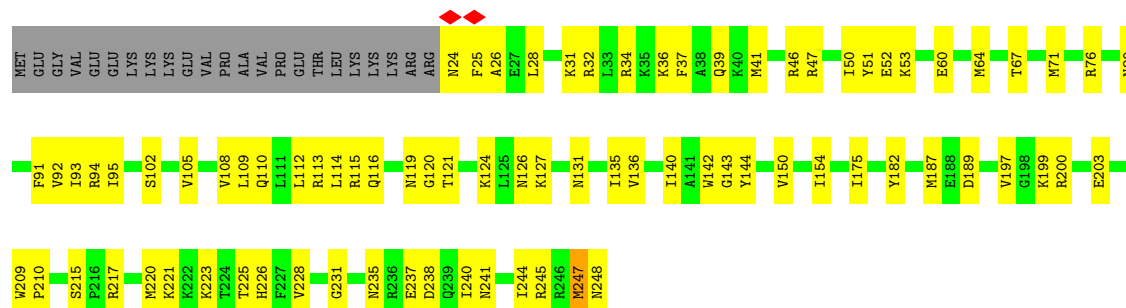
• Molecule 2: 5S ribosomal RNA



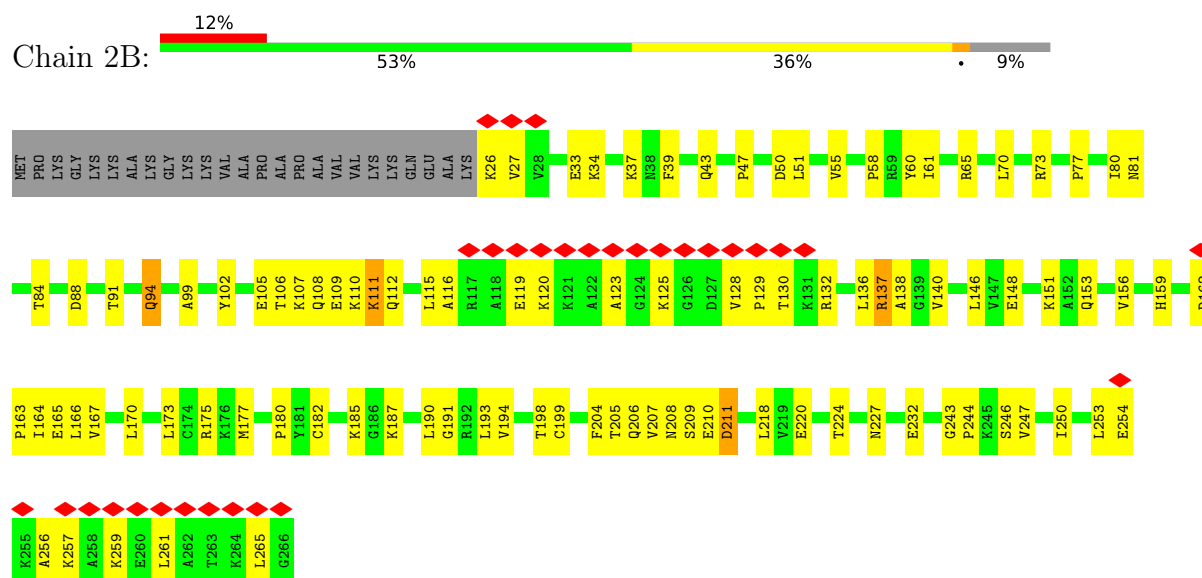
• Molecule 3: 5.8S ribosomal RNA



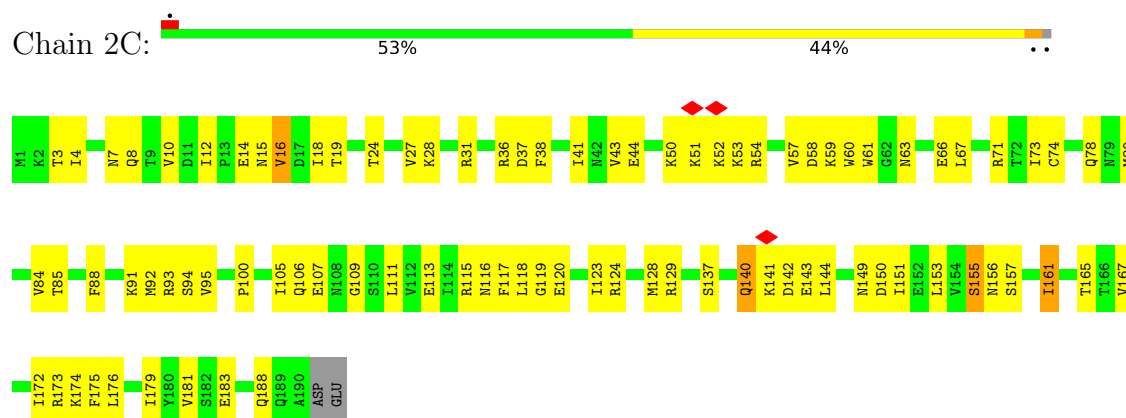
Chain 1G:



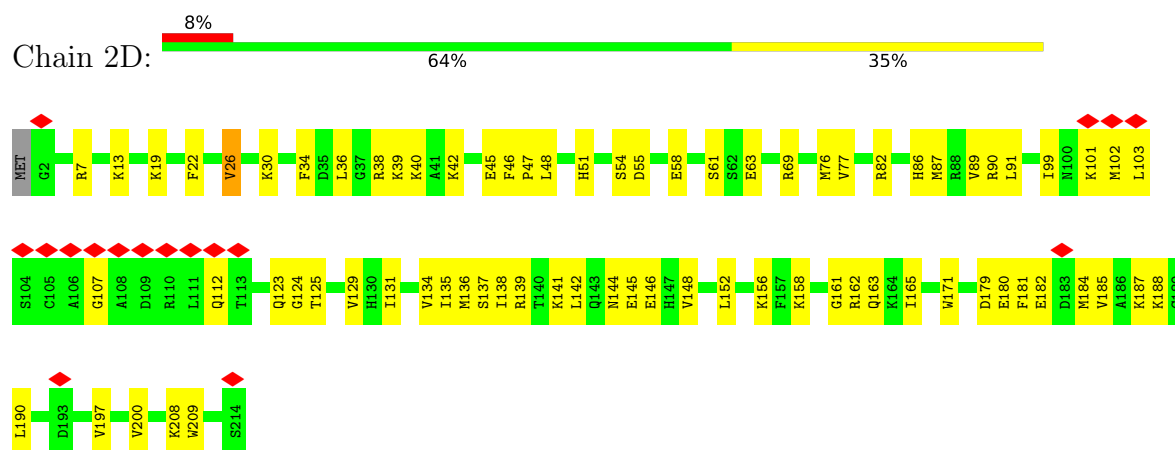
- Molecule 10: 60S ribosomal protein L7a



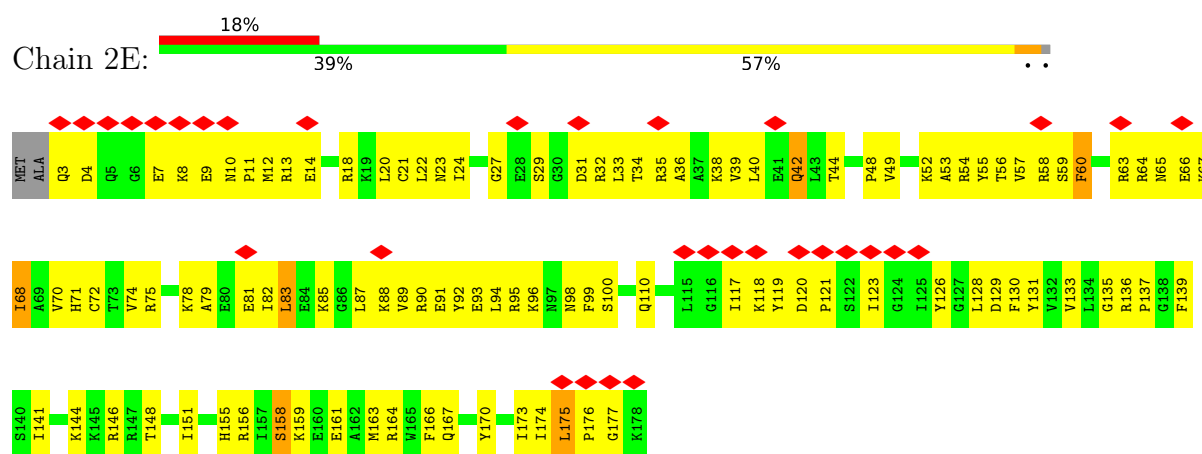
- Molecule 11: 60S ribosomal protein L9



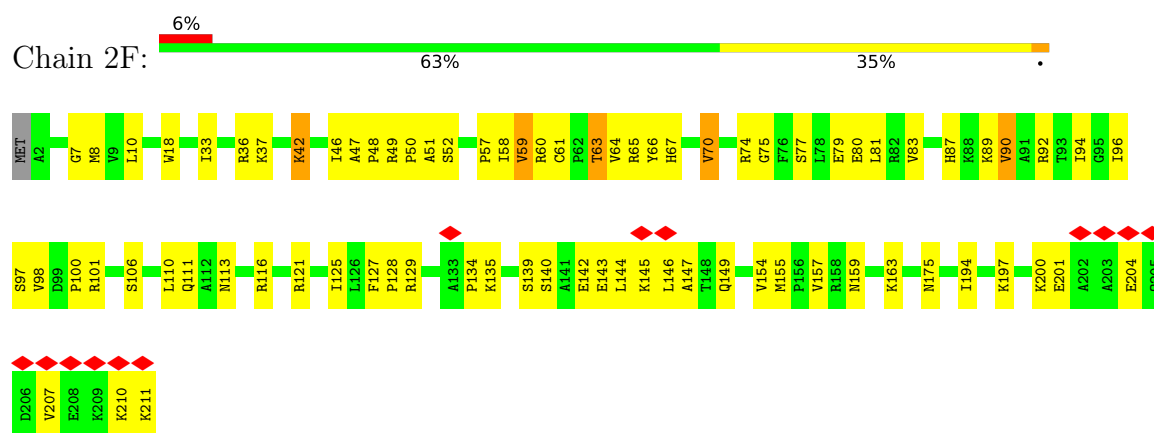
- Molecule 12: 60S ribosomal protein L10-like



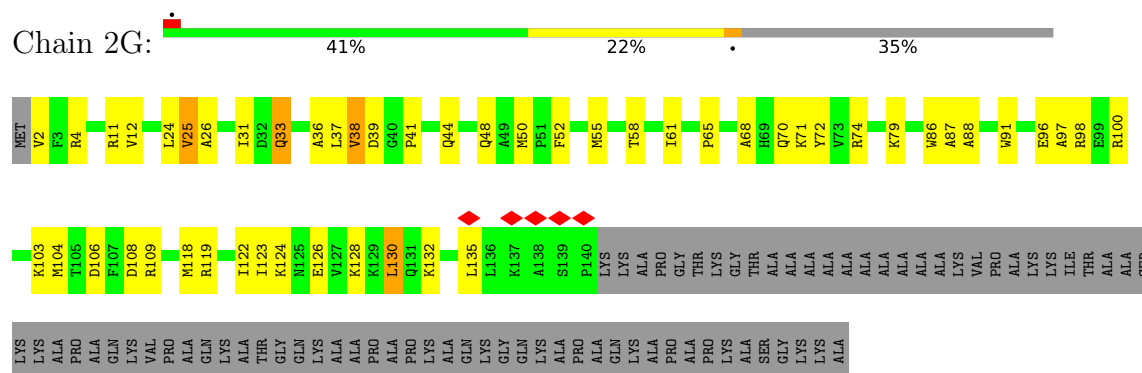
- Molecule 13: 60S ribosomal protein L11



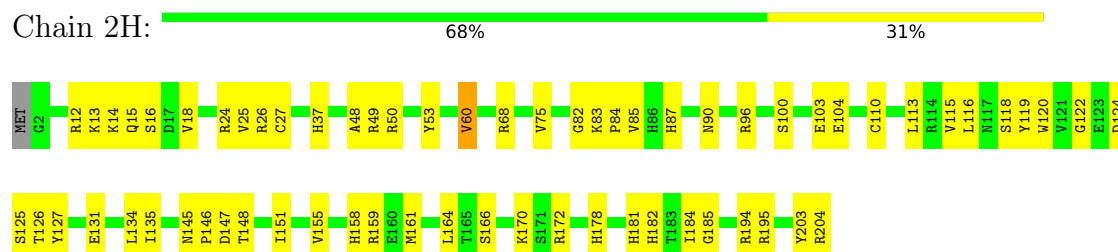
• Molecule 14: 60S ribosomal protein L13



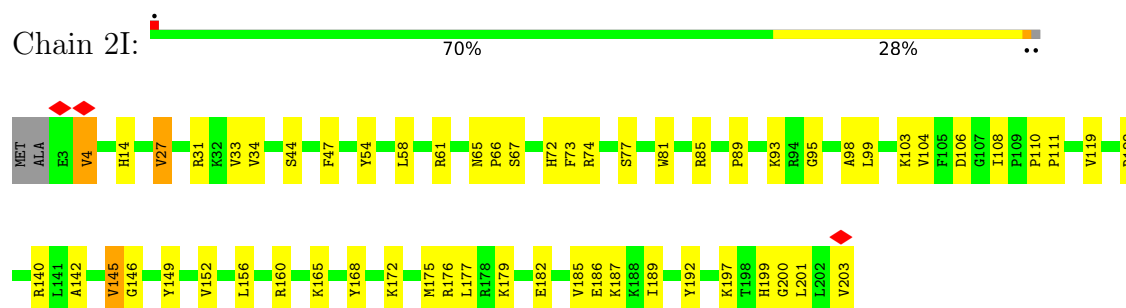
• Molecule 15: 60S ribosomal protein L14



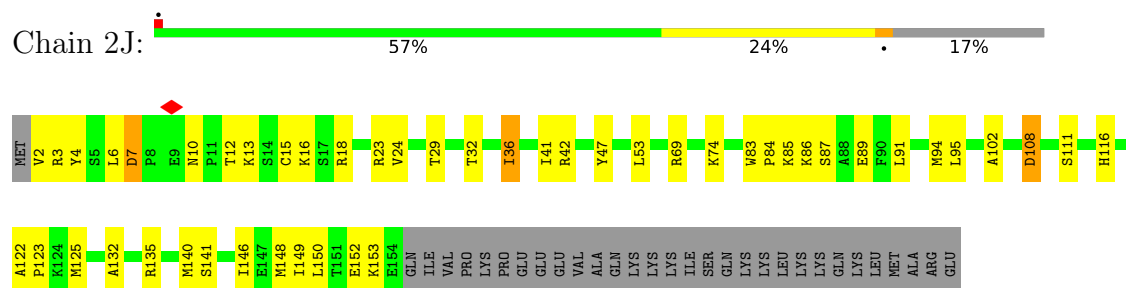
• Molecule 16: 60S ribosomal protein L15



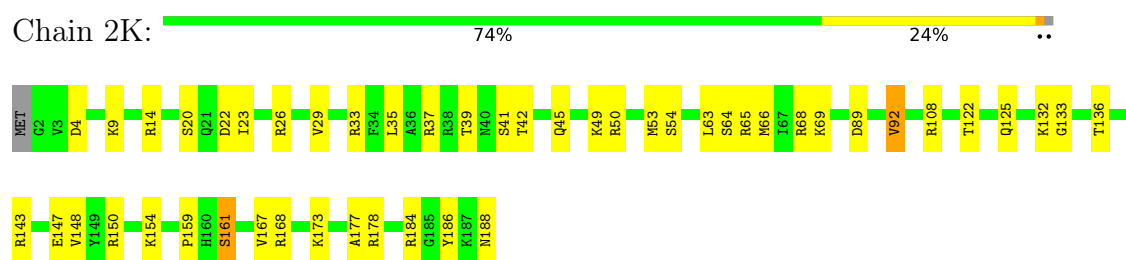
- Molecule 17: 60S ribosomal protein L13a



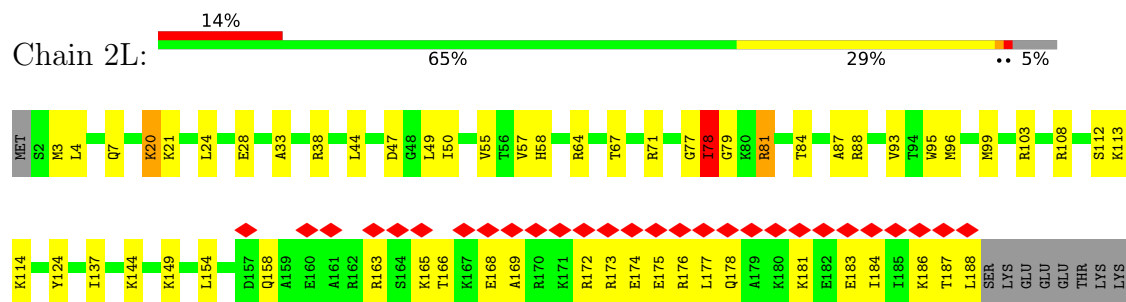
- Molecule 18: 60S ribosomal protein L17



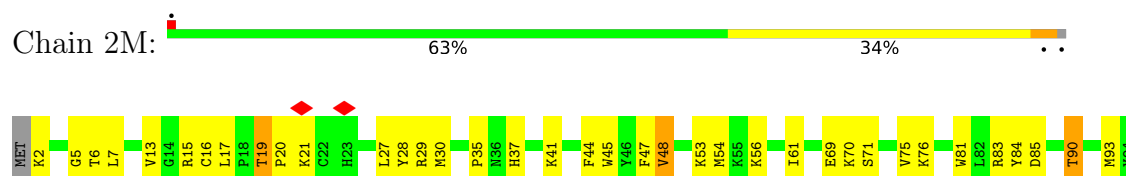
- Molecule 19: 60S ribosomal protein L18



- Molecule 20: 60S ribosomal protein L19

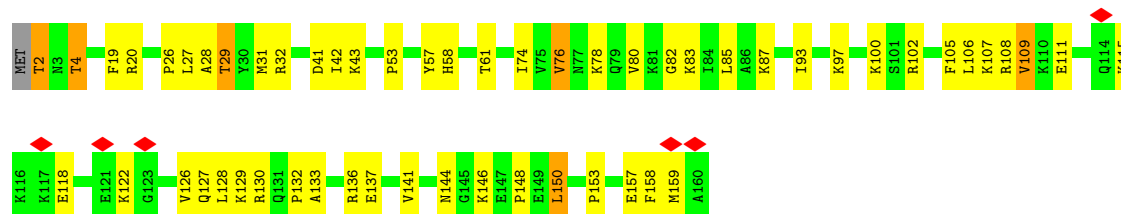


- Molecule 21: 60S ribosomal protein L18a

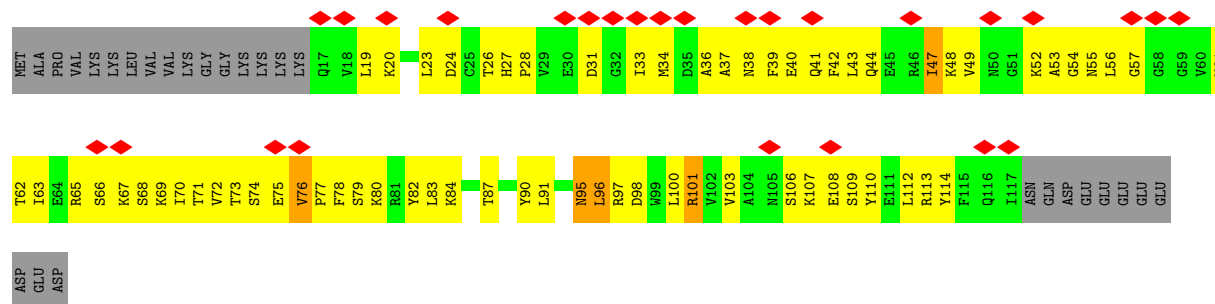




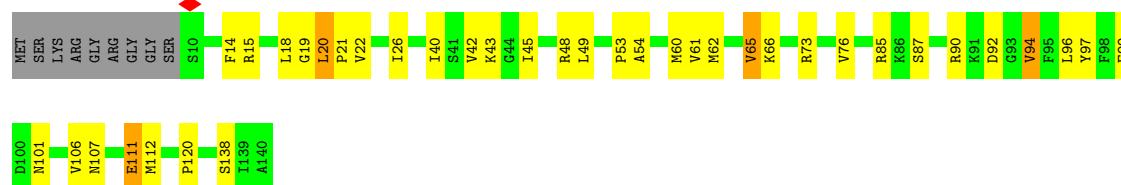
- Molecule 22: 60S ribosomal protein L21



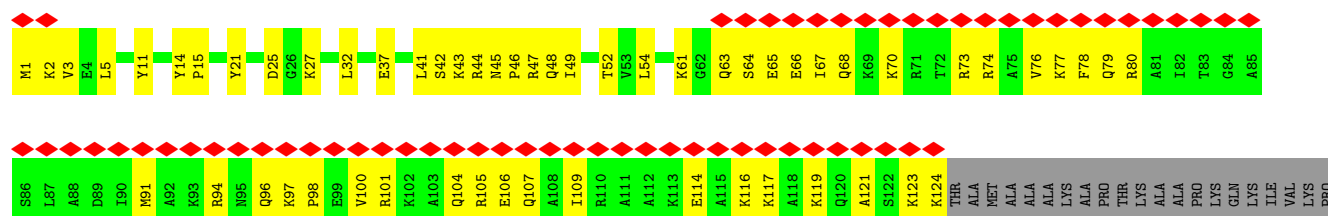
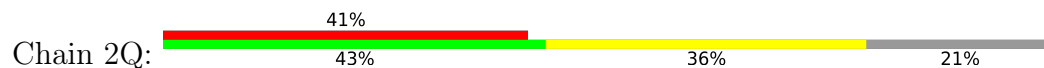
- Molecule 23: 60S ribosomal protein L22



- Molecule 24: 60S ribosomal protein L23



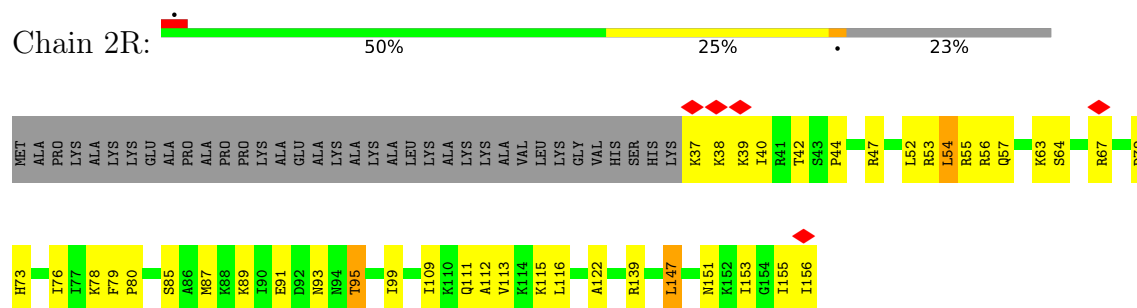
- Molecule 25: 60S ribosomal protein L24



VAL
LYS
VAL
SER
ALA
PRO
ARG
VAL
GLY
LYS
ARG

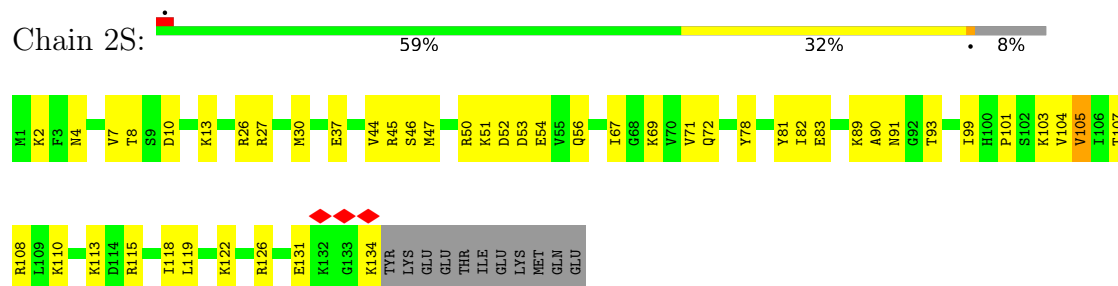
• Molecule 26: 60S ribosomal protein L23a

Chain 2R:



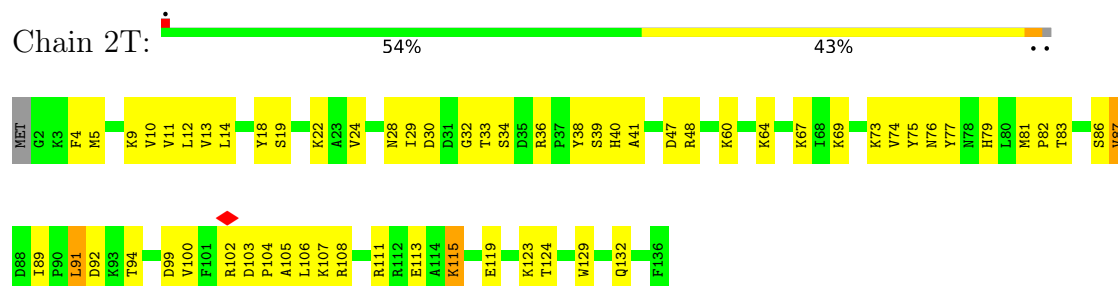
• Molecule 27: 60S ribosomal protein L26

Chain 2S:



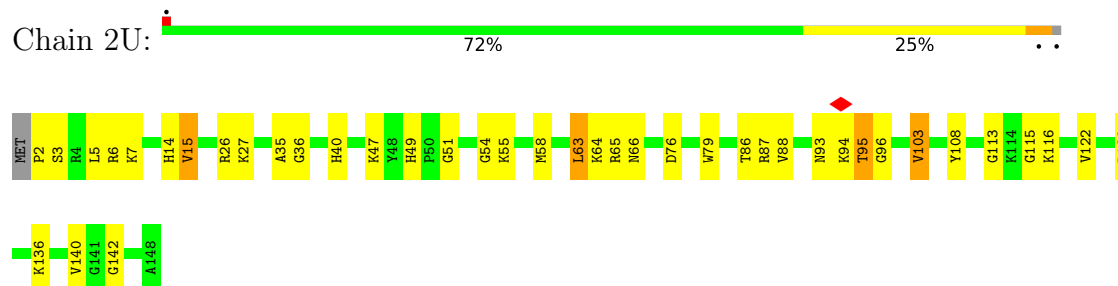
• Molecule 28: 60S ribosomal protein L27

Chain 2T:



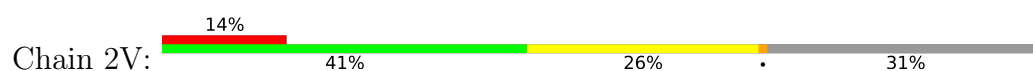
• Molecule 29: 60S ribosomal protein L27a

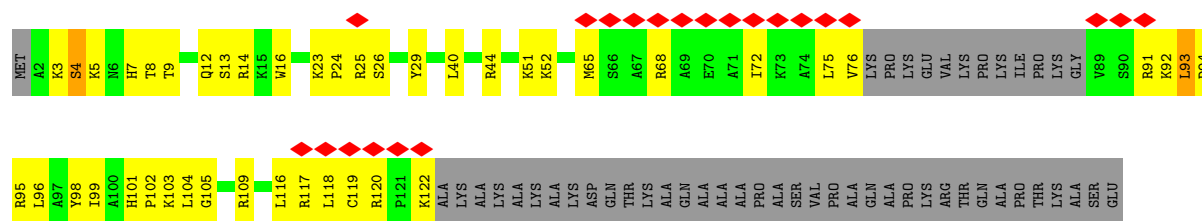
Chain 2U:



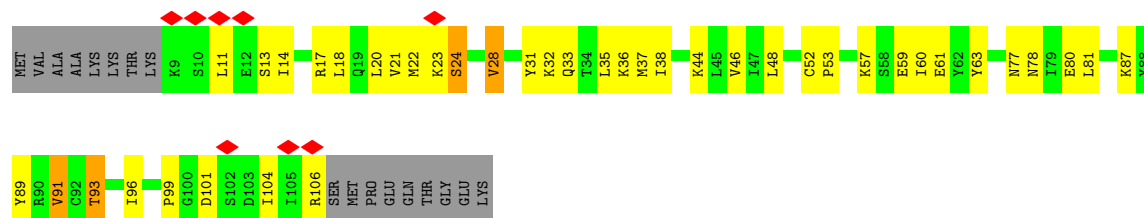
• Molecule 30: 60S ribosomal protein L29

Chain 2V:

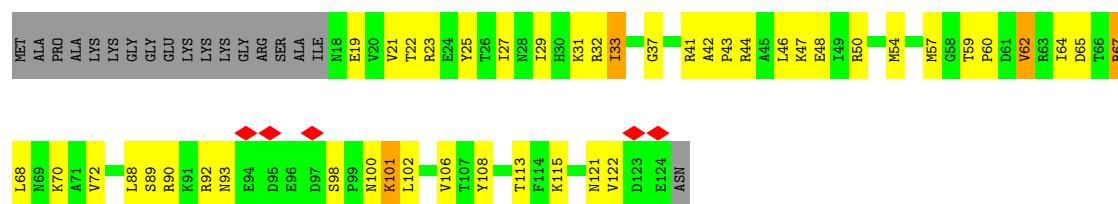




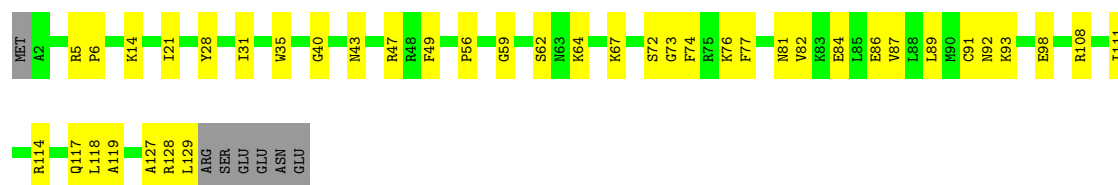
- Molecule 31: 60S ribosomal protein L30



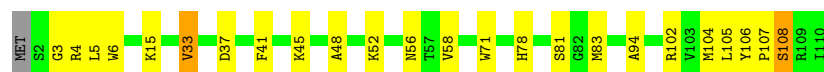
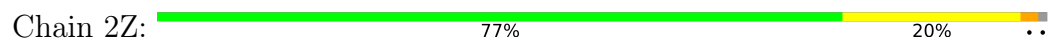
- Molecule 32: 60S ribosomal protein L31



- Molecule 33: 60S ribosomal protein L32

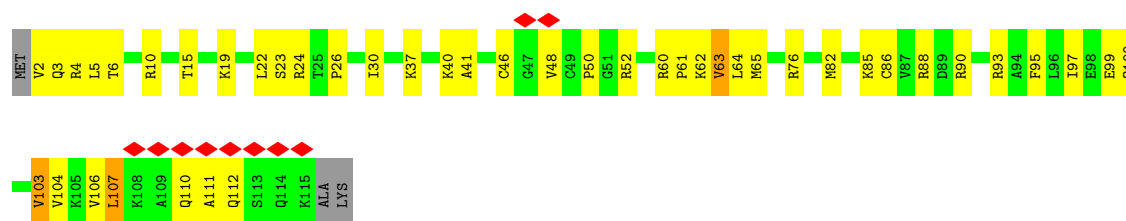


- Molecule 34: 60S ribosomal protein L35a

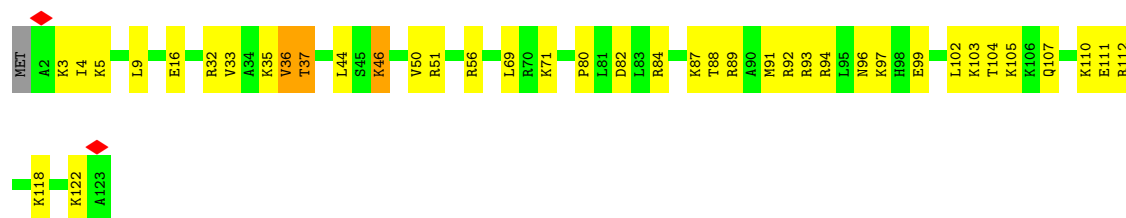


- Molecule 35: 60S ribosomal protein L34

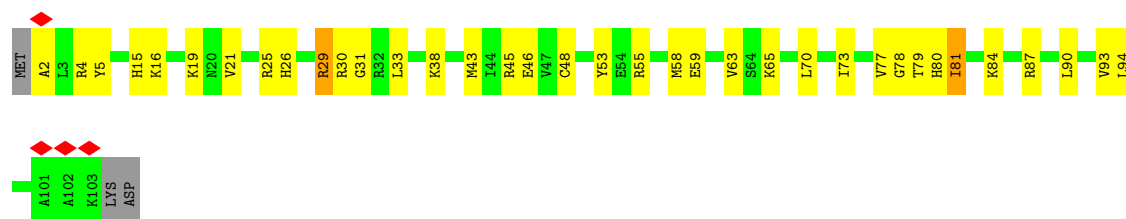




- Molecule 36: 60S ribosomal protein L35



- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37



- Molecule 39: 60S ribosomal protein L38

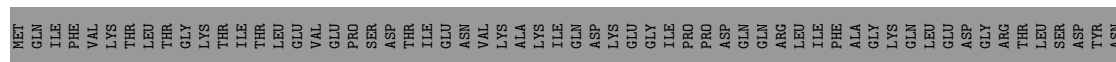


- Molecule 40: 60S ribosomal protein L39





- Molecule 41: Large ribosomal subunit protein eL40



- Molecule 42: 60S ribosomal protein L41



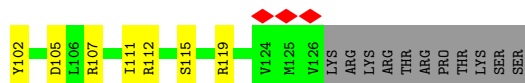
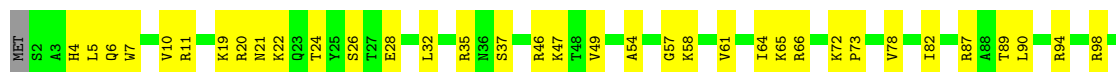
- Molecule 43: 60S ribosomal protein L36a



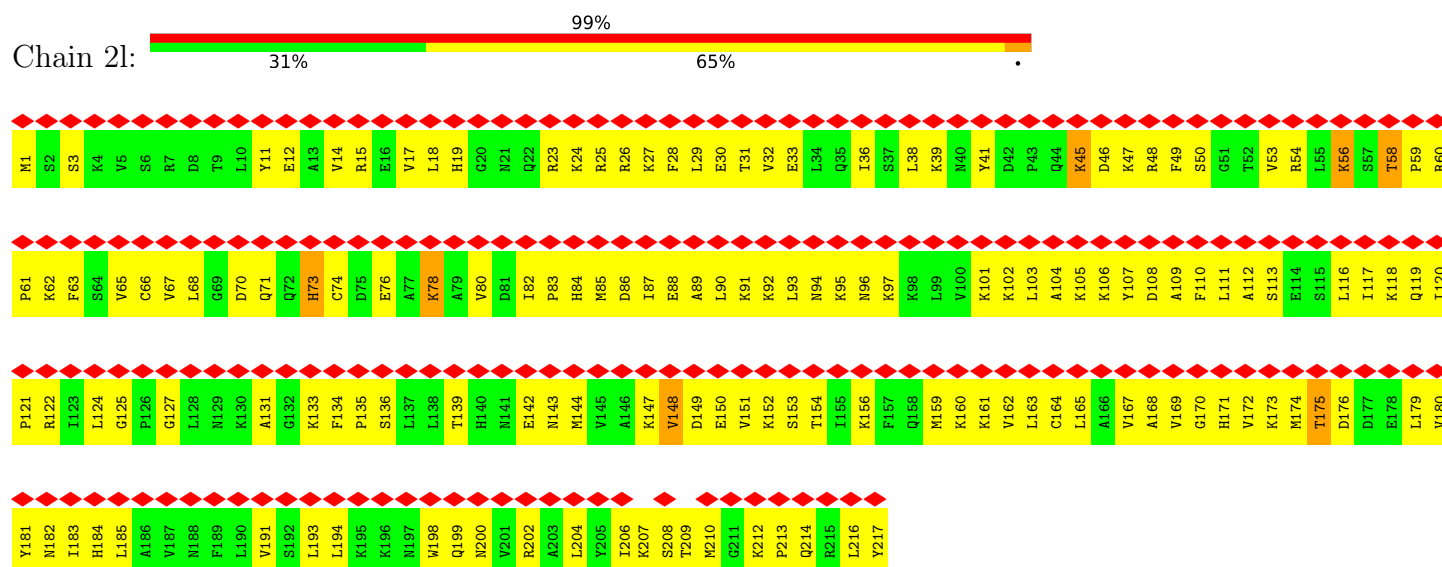
- Molecule 44: 60S ribosomal protein L37a



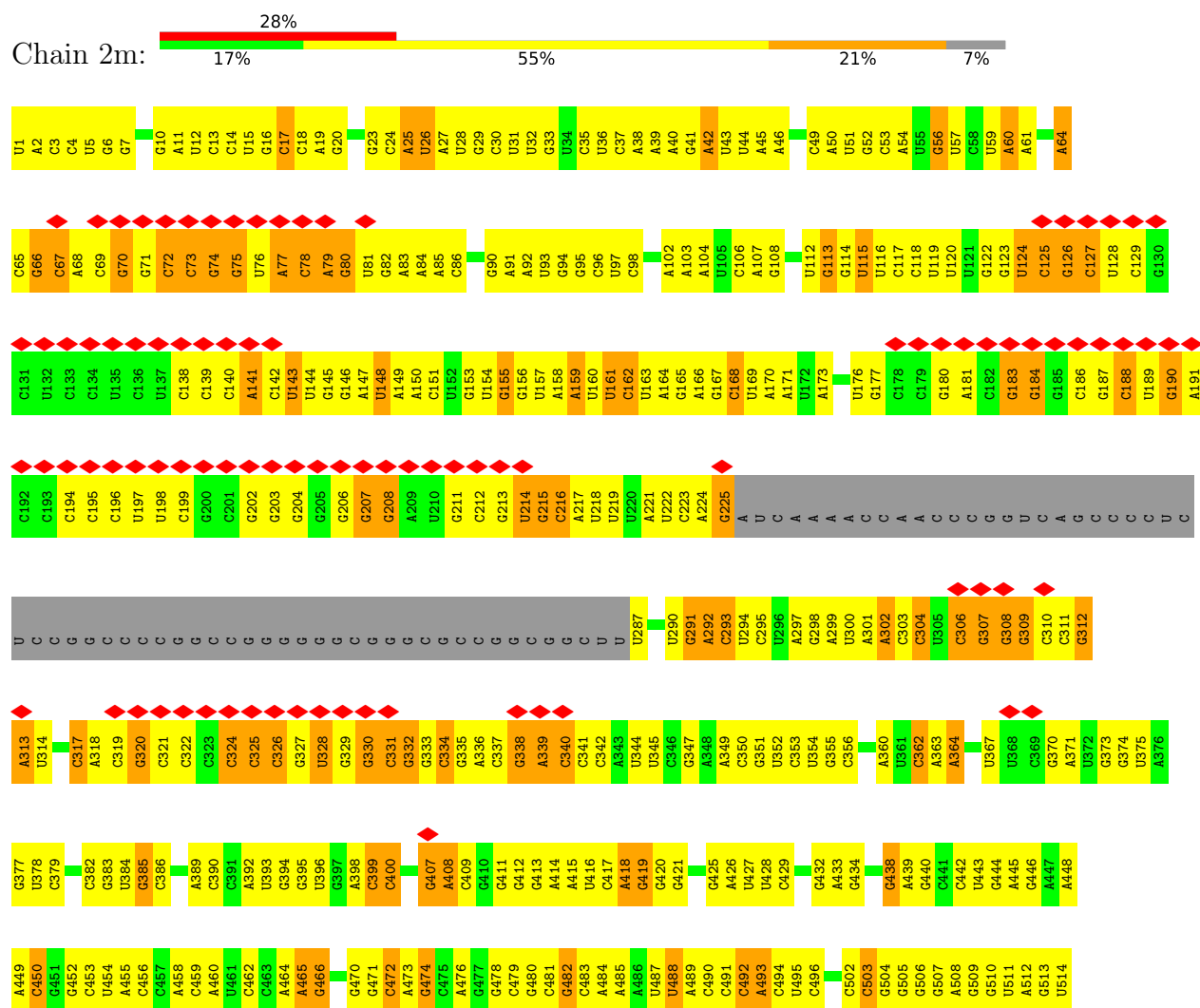
- Molecule 45: 60S ribosomal protein L28

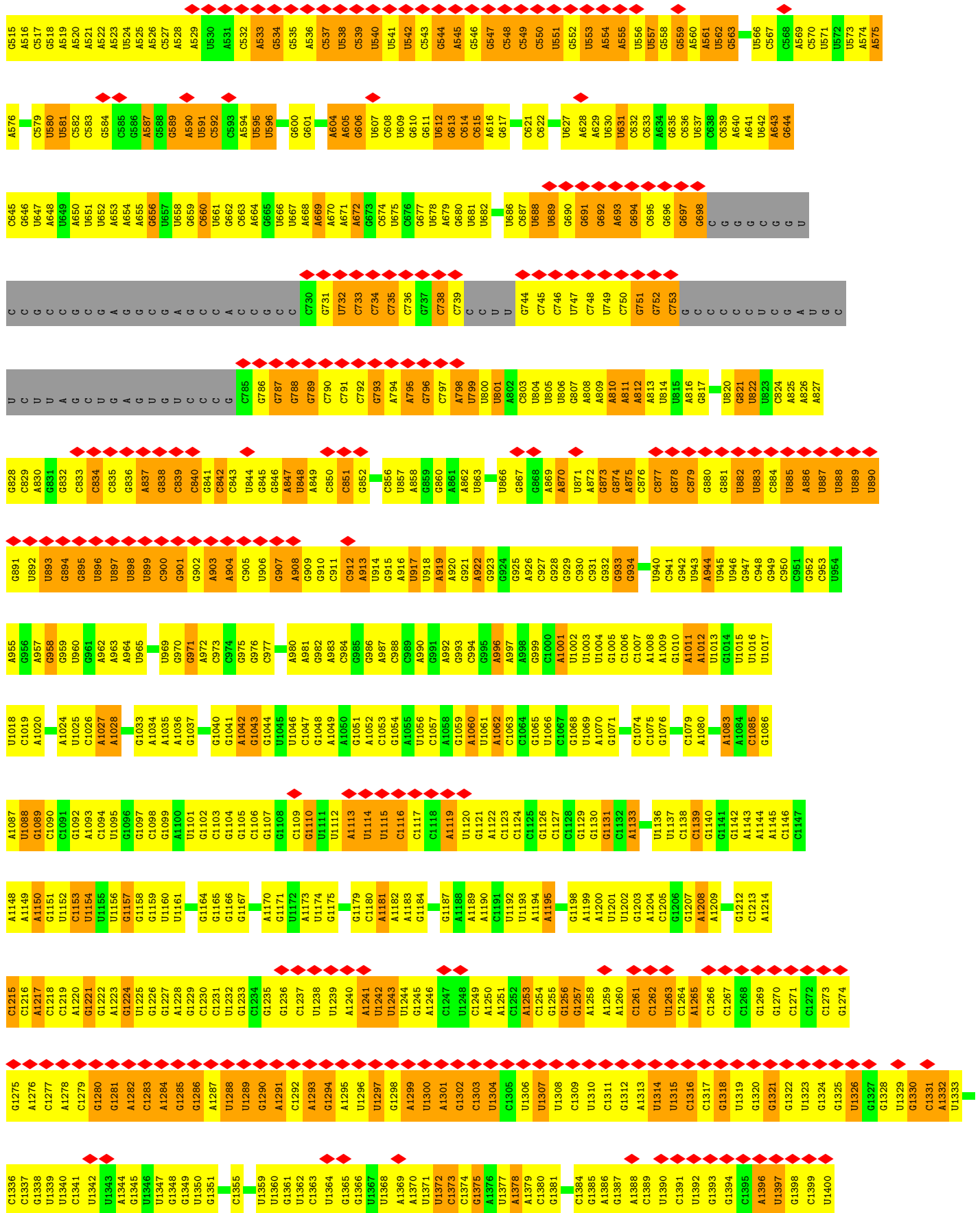


• Molecule 46: 60S ribosomal protein L10a



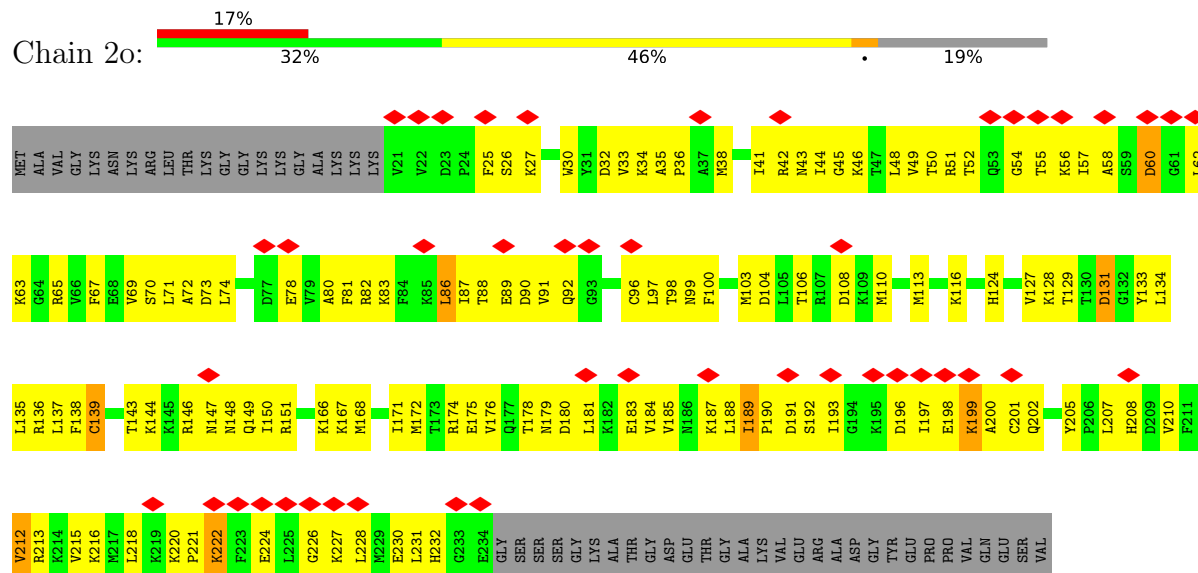
• Molecule 47: 18S ribosomal RNA



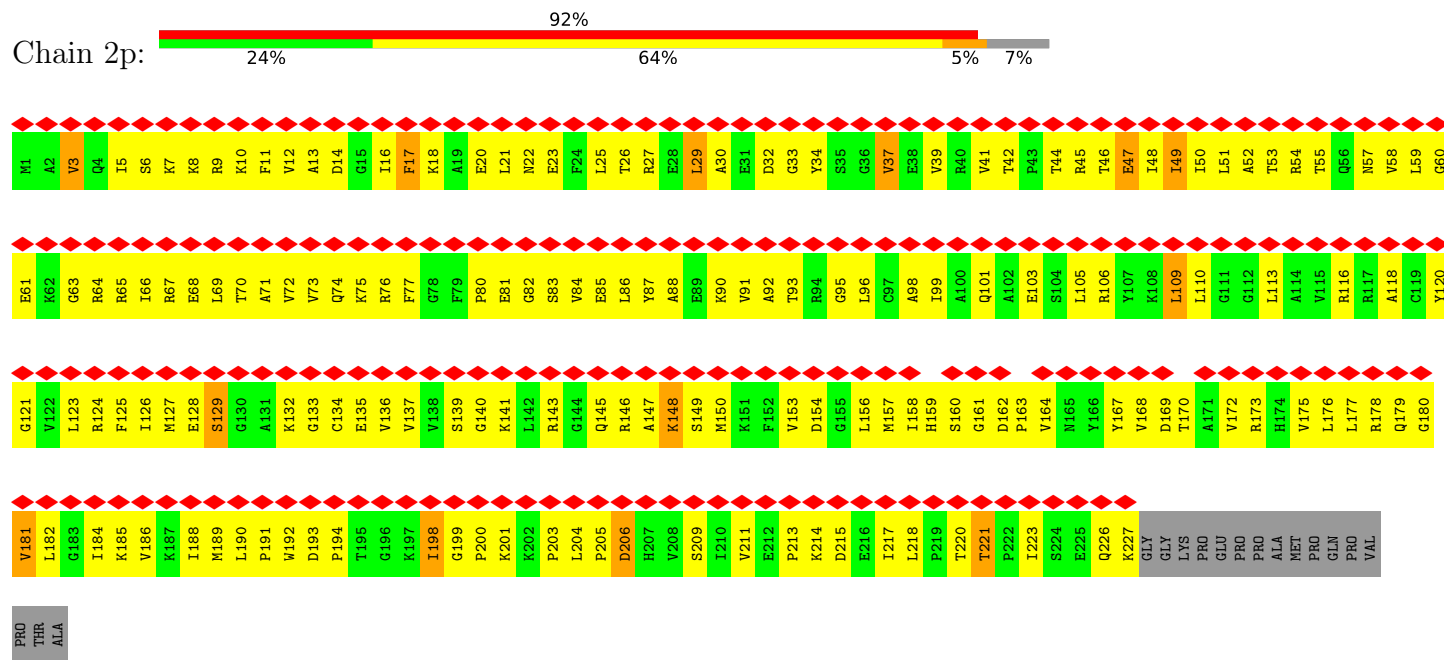




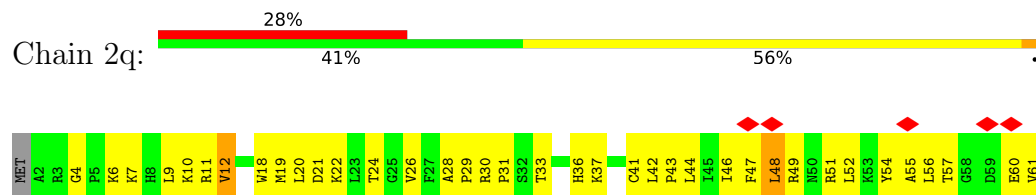
- Molecule 49: 40S ribosomal protein S3a

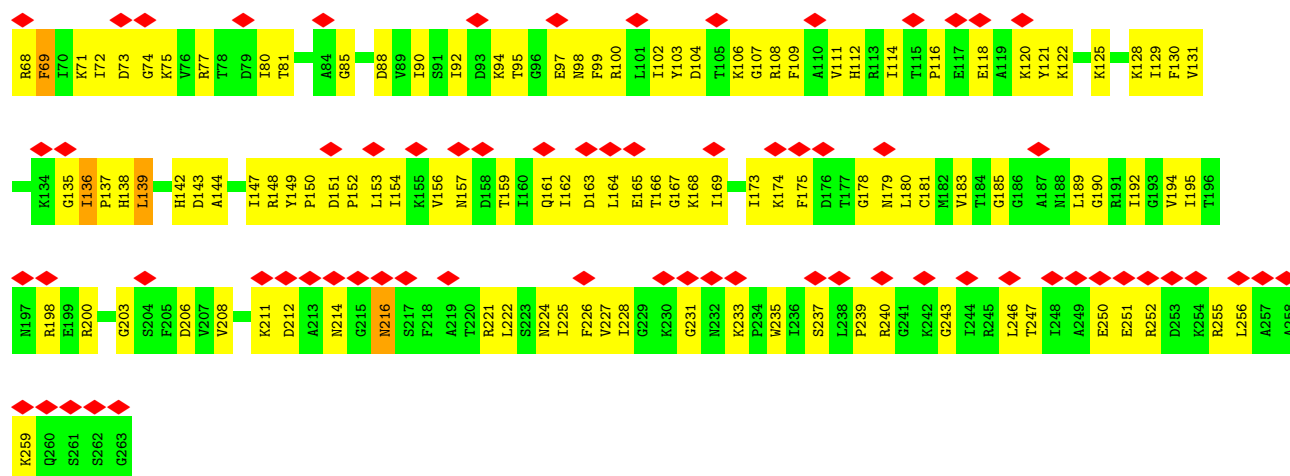


- Molecule 50: 40S ribosomal protein S3

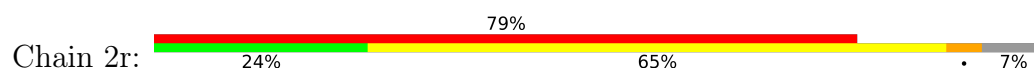


- Molecule 51: 40S ribosomal protein S4, X isoform





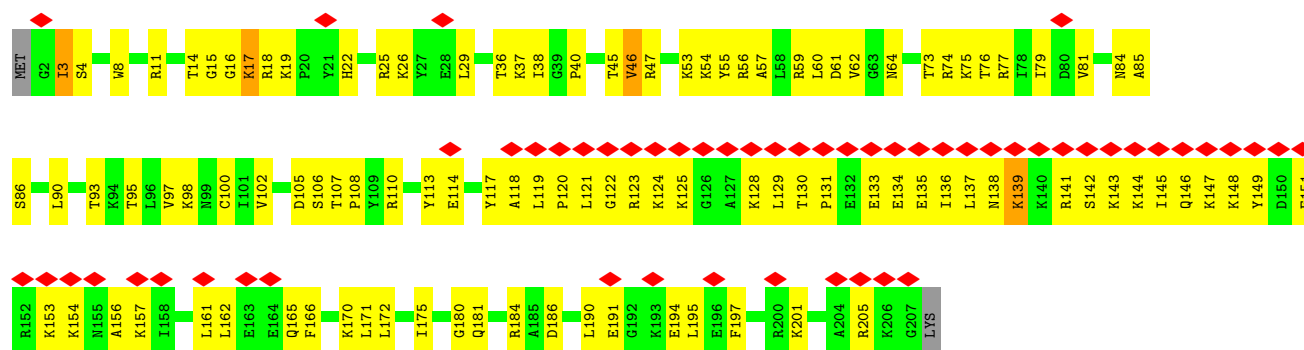
• Molecule 52: 40S ribosomal protein S5



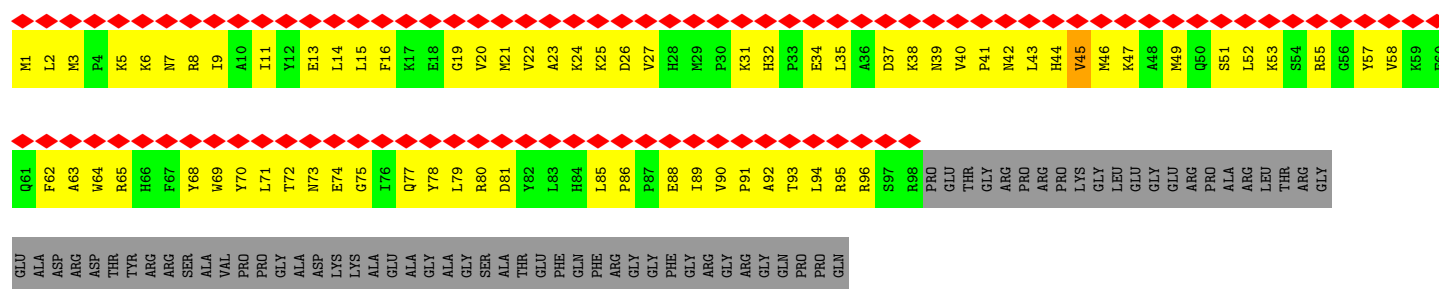
• Molecule 53: 40S ribosomal protein S7



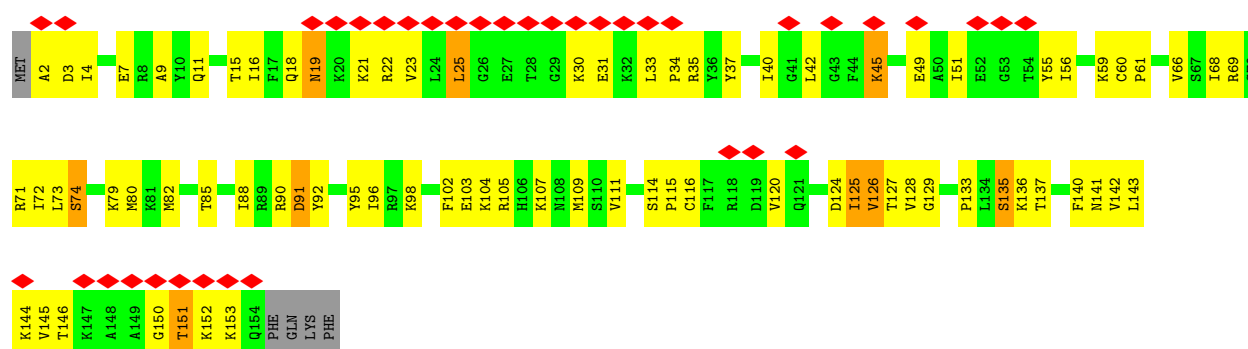
Chain 2t: 27% 47% 50%



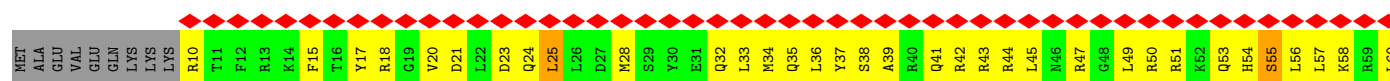
Chain 2u:

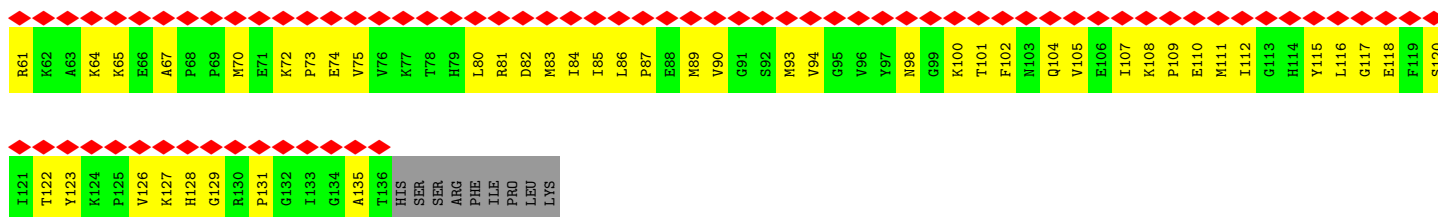


Chain 2v:

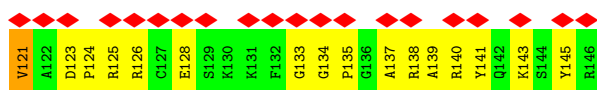
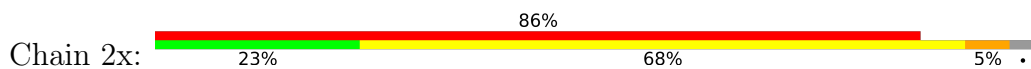


Chain 2w: 32% 88% 54% 12%

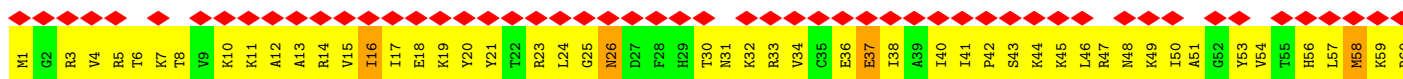




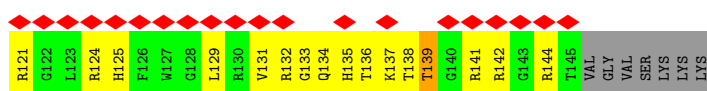
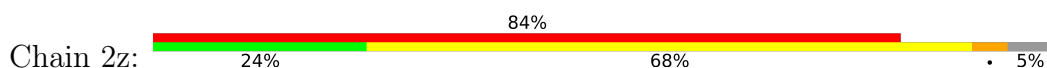
• Molecule 58: 40S ribosomal protein S16



• Molecule 59: 40S ribosomal protein S17

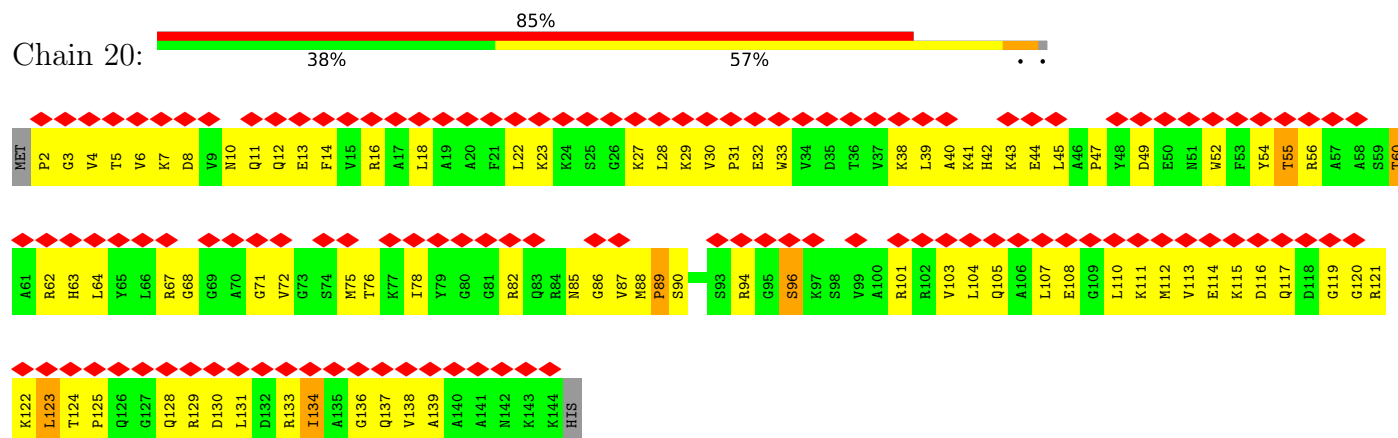


• Molecule 60: 40S ribosomal protein S18



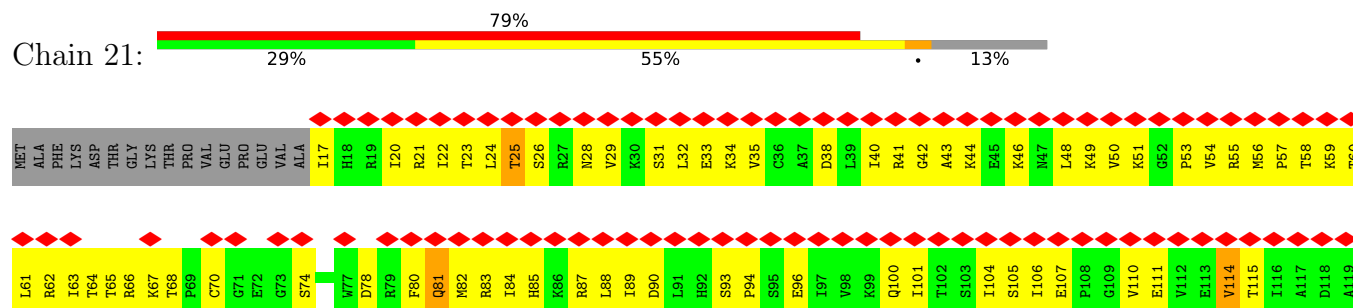
- Molecule 61: 40S ribosomal protein S19

Chain 20:



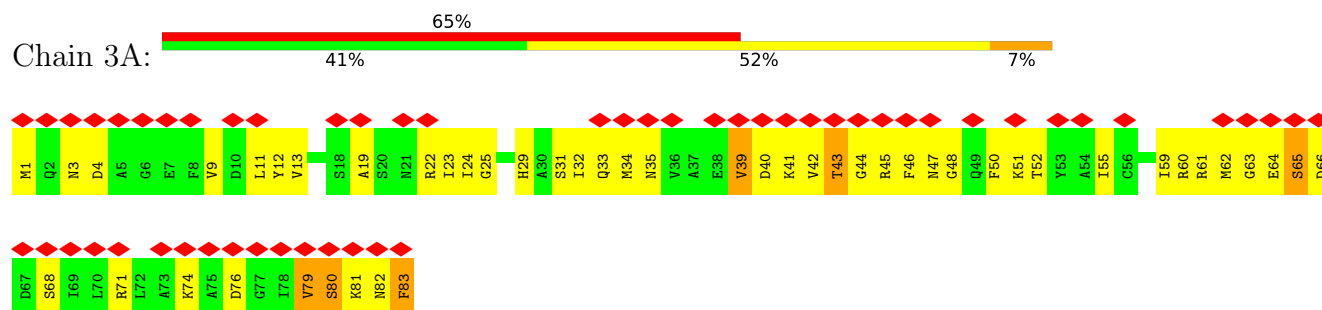
- Molecule 62: 40S ribosomal protein S20

Chain 21:



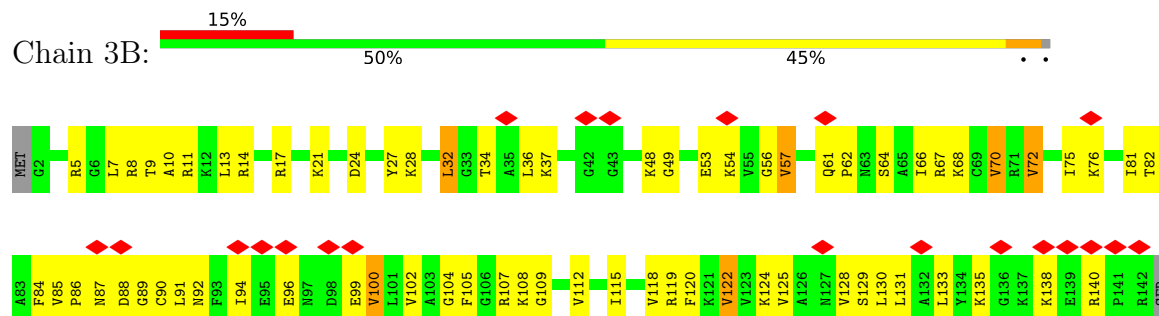
- Molecule 63: 40S ribosomal protein S21

Chain 3A:

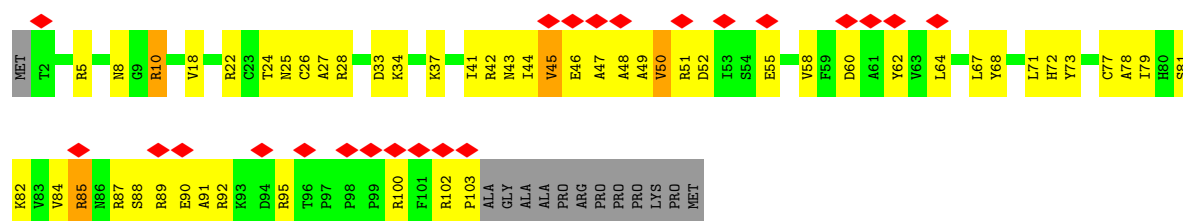
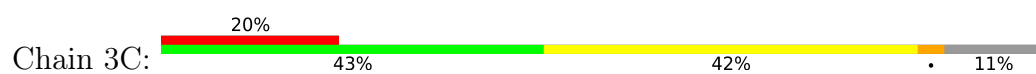


- Molecule 64: 40S ribosomal protein S23

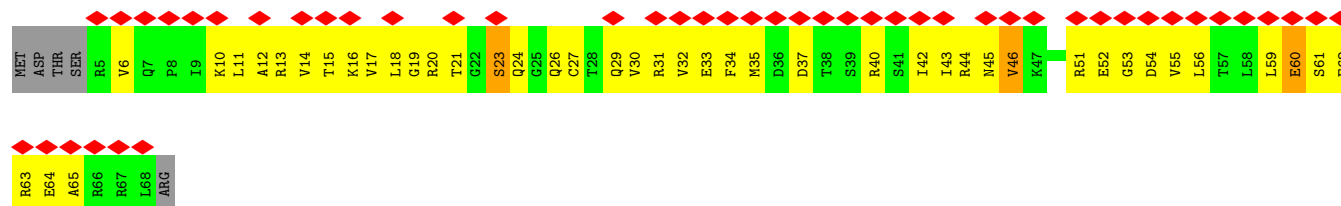
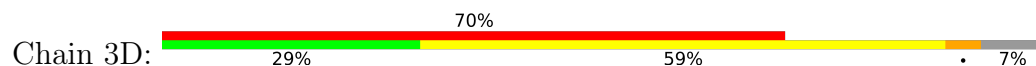
Chain 3B:



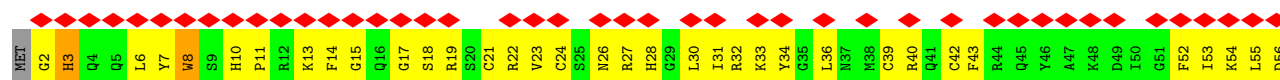
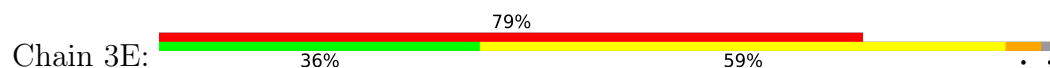
- Molecule 65: 40S ribosomal protein S26



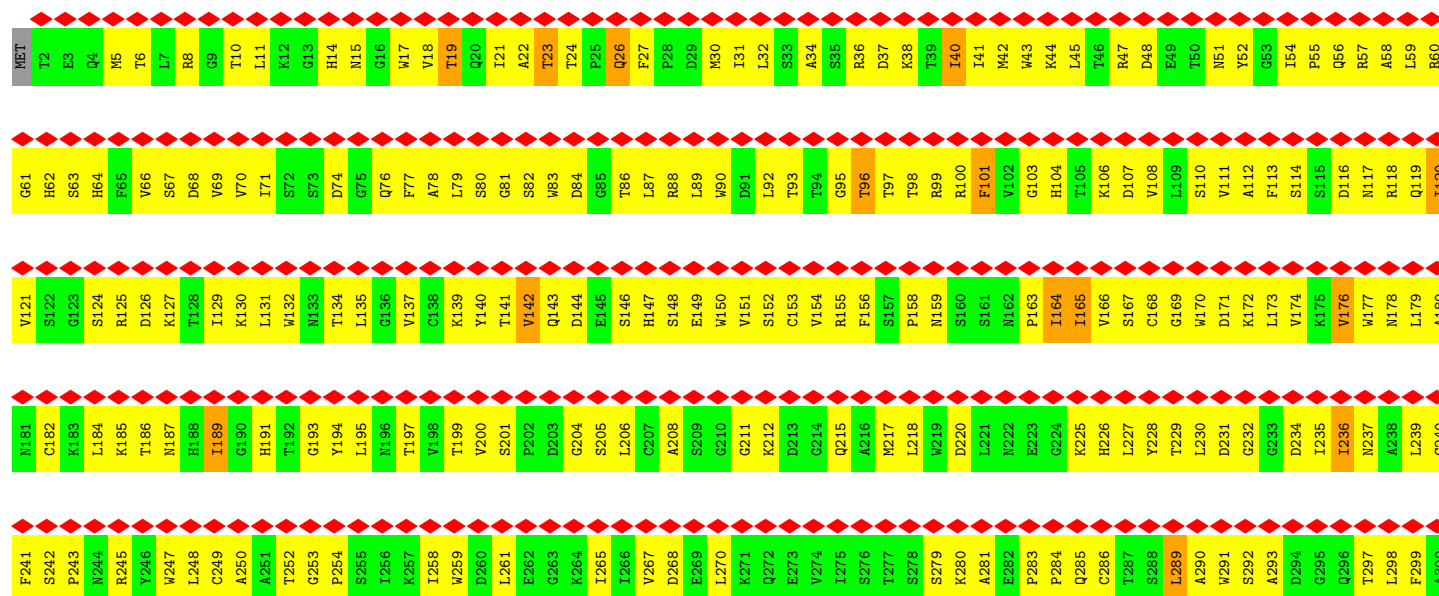
• Molecule 66: 40S ribosomal protein S28



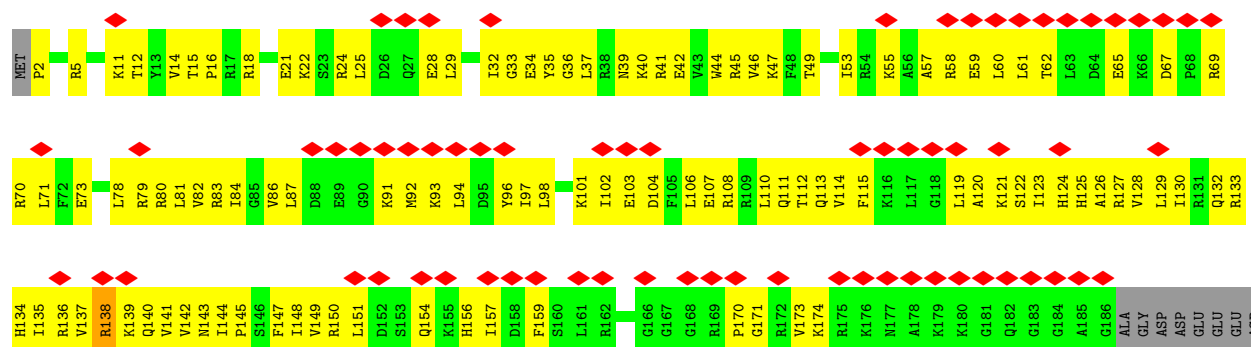
• Molecule 67: 40S ribosomal protein S29

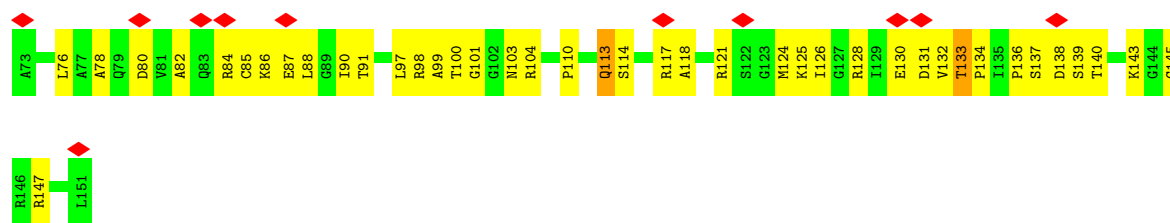


• Molecule 68: Receptor of activated protein C kinase 1

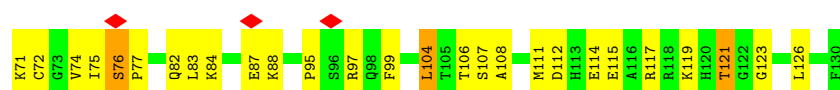
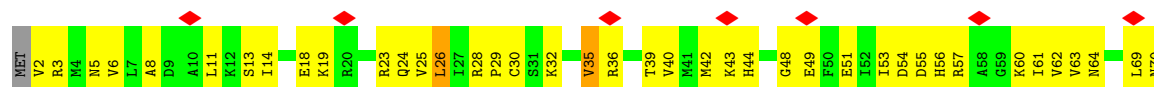




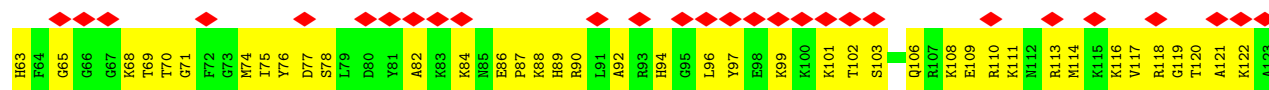
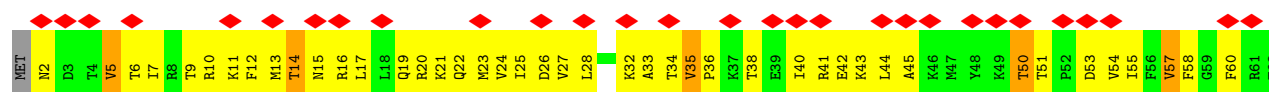




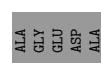
- Molecule 75: 40S ribosomal protein S15a



- Molecule 76: 40S ribosomal protein S24



- Molecule 77: 40S ribosomal protein S25



- Molecule 78: 40S ribosomal protein S27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28291	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.025	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	504.32, 504.32, 504.32	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.788, 0.788, 0.788	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, MG, ZN, 84D

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	1A	0.10	0/89127	0.25	0/139035
2	1B	0.09	0/2858	0.24	0/4455
3	1C	0.09	0/3696	0.25	0/5758
4	1D	0.09	0/1936	0.26	0/2596
5	1E	0.09	0/3306	0.25	0/4424
6	1F	0.11	0/2981	0.29	0/4002
7	1G	0.10	0/2428	0.29	0/3252
8	1H	0.10	0/1942	0.27	0/2606
9	2A	0.11	0/1916	0.28	0/2553
10	2B	0.10	0/1971	0.27	0/2651
11	2C	0.09	0/1537	0.27	0/2066
12	2D	0.09	0/1751	0.24	0/2340
13	2E	0.09	0/1433	0.29	0/1915
14	2F	0.11	0/1732	0.27	0/2315
15	2G	0.11	0/1161	0.29	0/1554
16	2H	0.10	0/1746	0.26	0/2338
17	2I	0.11	0/1682	0.25	0/2250
18	2J	0.10	0/1268	0.27	0/1701
19	2K	0.10	0/1537	0.25	0/2052
20	2L	0.09	0/1582	0.24	1/2091 (0.0%)
21	2M	0.11	0/1493	0.30	0/2003
22	2N	0.10	0/1326	0.24	0/1770
23	2O	0.10	0/839	0.30	0/1126
24	2P	0.10	0/993	0.25	0/1332
25	2Q	0.09	0/1030	0.26	0/1364
26	2R	0.09	0/1002	0.24	0/1345
27	2S	0.10	0/1132	0.26	0/1504
28	2T	0.10	0/1130	0.28	0/1507
29	2U	0.09	0/1191	0.23	0/1591
30	2V	0.09	0/895	0.25	0/1182
31	2W	0.10	0/774	0.24	0/1038
32	2X	0.10	0/903	0.26	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	2Y	0.10	0/1071	0.26	0/1429
34	2Z	0.10	0/895	0.28	0/1198
35	2a	0.09	0/916	0.25	0/1220
36	2b	0.08	0/1023	0.20	0/1351
37	2c	0.08	0/843	0.21	0/1115
38	2d	0.10	0/731	0.27	0/966
39	2e	0.10	0/575	0.26	0/761
40	2f	0.10	0/454	0.22	0/599
41	2g	0.10	0/425	0.26	0/561
42	2h	0.08	0/231	0.15	0/294
43	2i	0.09	0/887	0.25	0/1170
44	2j	0.08	0/718	0.22	0/953
45	2k	0.11	0/1017	0.25	0/1364
46	2l	0.09	0/1768	0.29	0/2371
47	2m	0.08	0/41243	0.22	0/64257
48	2n	0.08	0/1778	0.26	0/2416
49	2o	0.08	0/1765	0.24	0/2362
50	2p	0.10	0/1793	0.29	0/2414
51	2q	0.08	0/2118	0.26	0/2849
52	2r	0.08	0/1516	0.26	0/2037
53	2s	0.11	0/1519	0.28	0/2033
54	2t	0.09	0/1715	0.25	0/2287
55	2u	0.09	0/851	0.27	0/1147
56	2v	0.08	0/1268	0.27	0/1696
57	2w	0.08	0/1065	0.23	0/1423
58	2x	0.12	0/1142	0.31	0/1528
59	2y	0.09	0/1105	0.29	0/1484
60	2z	0.10	0/1216	0.28	0/1628
61	20	0.21	0/1131	0.40	2/1515 (0.1%)
62	21	0.08	0/827	0.23	0/1110
63	3A	0.08	0/643	0.26	0/860
64	3B	0.07	0/1116	0.23	0/1490
65	3C	0.10	0/847	0.28	0/1135
66	3D	0.10	0/508	0.29	0/680
67	3E	0.07	0/470	0.24	0/623
68	3F	0.08	0/2493	0.28	0/3394
69	3G	0.09	0/1773	0.30	0/2395
70	3H	0.08	0/1946	0.24	0/2590
71	3I	0.10	0/1561	0.27	0/2083
72	3J	0.09	0/952	0.23	0/1279
73	3K	0.10	0/1232	0.23	0/1656
74	3L	0.11	0/1062	0.31	0/1425
75	3M	0.09	0/1051	0.26	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	3N	0.10	0/1094	0.28	0/1452
77	3O	0.11	0/604	0.36	0/810
78	3P	0.09	0/665	0.27	0/891
79	3Q	0.14	0/465	0.26	0/612
80	3R	0.08	0/560	0.27	0/745
All	All	0.10	0/232946	0.25	3/341996 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	20	89	PRO	N-CD-CG	-7.51	91.94	103.20
61	20	89	PRO	CA-N-CD	-7.00	102.21	112.00
20	2L	78	ILE	N-CA-C	-5.51	108.13	113.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	79674	0	40254	3068	0
2	1B	2558	0	1296	72	0
3	1C	3310	0	1680	131	0
4	1D	1898	0	1993	96	0
5	1E	3238	0	3376	119	0
6	1F	2927	0	3104	97	0
7	1G	2382	0	2410	113	0
8	1H	1904	0	2055	116	0
9	2A	1878	0	2009	70	0
10	2B	1935	0	2087	85	0
11	2C	1518	0	1601	95	0
12	2D	1711	0	1749	75	0
13	2E	1410	0	1441	122	0
14	2F	1701	0	1818	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	2G	1138	0	1204	59	0
16	2H	1701	0	1749	62	0
17	2I	1650	0	1794	66	0
18	2J	1242	0	1269	40	0
19	2K	1513	0	1628	45	0
20	2L	1566	0	1729	57	0
21	2M	1453	0	1490	58	0
22	2N	1298	0	1366	57	0
23	2O	825	0	850	74	0
24	2P	979	0	1039	27	0
25	2Q	1015	0	1079	78	0
26	2R	985	0	1066	42	0
27	2S	1115	0	1205	48	0
28	2T	1107	0	1182	55	0
29	2U	1162	0	1213	38	0
30	2V	882	0	959	52	0
31	2W	764	0	804	43	0
32	2X	888	0	930	36	0
33	2Y	1053	0	1147	31	0
34	2Z	876	0	912	26	0
35	2a	906	0	1002	51	0
36	2b	1015	0	1148	43	0
37	2c	832	0	917	32	0
38	2d	713	0	750	19	0
39	2e	569	0	637	36	0
40	2f	444	0	483	17	0
41	2g	430	0	465	21	0
42	2h	230	0	276	9	0
43	2i	870	0	946	44	0
44	2j	708	0	756	25	0
45	2k	1002	0	1068	35	0
46	2l	1740	0	1854	215	0
47	2m	36900	0	18597	2048	0
48	2n	1741	0	1746	201	0
49	2o	1738	0	1809	137	0
50	2p	1765	0	1865	252	0
51	2q	2076	0	2177	171	0
52	2r	1495	0	1549	218	0
53	2s	1497	0	1590	174	0
54	2t	1686	0	1772	142	0
55	2u	827	0	854	112	0
56	2v	1247	0	1323	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2w	1045	0	1095	152	0
58	2x	1124	0	1193	204	0
59	2y	1090	0	1149	160	0
60	2z	1198	0	1261	177	0
61	20	1112	0	1146	135	0
62	21	817	0	882	105	0
63	3A	636	0	637	58	0
64	3B	1098	0	1167	75	0
65	3C	829	0	883	73	0
66	3D	506	0	536	75	0
67	3E	459	0	450	61	0
68	3F	2436	0	2393	292	0
69	3G	1733	0	1826	159	0
70	3H	1923	0	2089	238	0
71	3I	1533	0	1653	148	0
72	3J	942	0	961	97	0
73	3K	1208	0	1294	85	0
74	3L	1049	0	1073	79	0
75	3M	1034	0	1080	76	0
76	3N	1073	0	1155	144	0
77	3O	598	0	656	151	0
78	3P	651	0	672	47	0
79	3Q	459	0	503	34	0
80	3R	548	0	555	61	0
81	1A	651	777	0	20	0
81	2m	93	111	0	6	0
82	1A	270	0	0	0	0
82	1B	2	0	0	0	0
82	1C	5	0	0	0	0
82	1D	1	0	0	0	0
82	20	1	0	0	0	0
82	2H	1	0	0	0	0
82	2J	1	0	0	0	0
82	2K	1	0	0	0	0
82	2M	1	0	0	0	0
82	2P	1	0	0	0	0
82	2V	1	0	0	0	0
82	2Y	1	0	0	0	0
82	2Z	1	0	0	0	0
82	2a	1	0	0	0	0
82	2d	1	0	0	0	0
82	2m	105	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	3H	1	0	0	0	0
82	3K	1	0	0	0	0
82	3L	1	0	0	0	0
83	2d	1	0	0	0	0
83	2g	1	0	0	0	0
83	2j	1	0	0	0	0
83	3C	1	0	0	0	0
All	All	217933	888	161381	10895	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 10895 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:2x:72:VAL:HG21	58:2x:84:ILE:HD11	1.20	1.18
65:3C:44:ILE:HG21	65:3C:67:LEU:HD13	1.19	1.17
68:3F:32:LEU:HD21	68:3F:71:ILE:HD11	1.22	1.15
77:3O:99:LEU:HD21	77:3O:102:LYS:HB3	1.19	1.15
55:2u:25:LYS:HD3	55:2u:46:MET:HE1	1.18	1.15

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1D	246/257 (96%)	227 (92%)	19 (8%)	0	100	100
5	1E	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
6	1F	366/427 (86%)	344 (94%)	22 (6%)	0	100	100
7	1G	291/297 (98%)	277 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	1H	232/288 (81%)	210 (90%)	22 (10%)	0	100	100
9	2A	224/248 (90%)	212 (95%)	12 (5%)	0	100	100
10	2B	240/266 (90%)	227 (95%)	13 (5%)	0	100	100
11	2C	188/192 (98%)	176 (94%)	12 (6%)	0	100	100
12	2D	211/214 (99%)	198 (94%)	13 (6%)	0	100	100
13	2E	174/178 (98%)	166 (95%)	7 (4%)	1 (1%)	21	42
14	2F	208/211 (99%)	192 (92%)	16 (8%)	0	100	100
15	2G	137/215 (64%)	129 (94%)	8 (6%)	0	100	100
16	2H	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
17	2I	199/203 (98%)	193 (97%)	6 (3%)	0	100	100
18	2J	151/184 (82%)	144 (95%)	7 (5%)	0	100	100
19	2K	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
20	2L	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
21	2M	173/176 (98%)	159 (92%)	14 (8%)	0	100	100
22	2N	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
23	2O	99/128 (77%)	85 (86%)	14 (14%)	0	100	100
24	2P	129/140 (92%)	124 (96%)	5 (4%)	0	100	100
25	2Q	122/157 (78%)	109 (89%)	13 (11%)	0	100	100
26	2R	118/156 (76%)	113 (96%)	4 (3%)	1 (1%)	16	34
27	2S	132/145 (91%)	127 (96%)	5 (4%)	0	100	100
28	2T	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
29	2U	145/148 (98%)	141 (97%)	4 (3%)	0	100	100
30	2V	105/159 (66%)	100 (95%)	5 (5%)	0	100	100
31	2W	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
32	2X	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
33	2Y	126/135 (93%)	119 (94%)	6 (5%)	1 (1%)	16	34
34	2Z	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
35	2a	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
36	2b	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
37	2c	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
38	2d	85/97 (88%)	82 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	2e	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
40	2f	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
41	2g	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
42	2h	22/25 (88%)	22 (100%)	0	0	100	100
43	2i	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
44	2j	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	2k	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
46	2l	215/217 (99%)	173 (80%)	42 (20%)	0	100	100
48	2n	219/295 (74%)	199 (91%)	19 (9%)	1 (0%)	24	46
49	2o	212/264 (80%)	204 (96%)	8 (4%)	0	100	100
50	2p	225/243 (93%)	204 (91%)	21 (9%)	0	100	100
51	2q	260/263 (99%)	247 (95%)	13 (5%)	0	100	100
52	2r	187/204 (92%)	169 (90%)	18 (10%)	0	100	100
53	2s	182/194 (94%)	159 (87%)	22 (12%)	1 (0%)	24	46
54	2t	204/208 (98%)	193 (95%)	11 (5%)	0	100	100
55	2u	96/165 (58%)	85 (88%)	11 (12%)	0	100	100
56	2v	151/158 (96%)	138 (91%)	12 (8%)	1 (1%)	18	38
57	2w	125/145 (86%)	116 (93%)	9 (7%)	0	100	100
58	2x	139/146 (95%)	127 (91%)	12 (9%)	0	100	100
59	2y	133/135 (98%)	118 (89%)	15 (11%)	0	100	100
60	2z	143/152 (94%)	131 (92%)	12 (8%)	0	100	100
61	20	141/145 (97%)	129 (92%)	12 (8%)	0	100	100
62	2l	101/119 (85%)	95 (94%)	6 (6%)	0	100	100
63	3A	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
64	3B	139/143 (97%)	130 (94%)	9 (6%)	0	100	100
65	3C	101/115 (88%)	95 (94%)	6 (6%)	0	100	100
66	3D	62/69 (90%)	51 (82%)	11 (18%)	0	100	100
67	3E	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
68	3F	311/317 (98%)	283 (91%)	28 (9%)	0	100	100
69	3G	221/293 (75%)	204 (92%)	17 (8%)	0	100	100
70	3H	235/249 (94%)	228 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	3I	184/194 (95%)	167 (91%)	17 (9%)	0	100	100
72	3J	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
73	3K	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
74	3L	138/151 (91%)	125 (91%)	13 (9%)	0	100	100
75	3M	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
76	3N	130/133 (98%)	127 (98%)	3 (2%)	0	100	100
77	3O	73/125 (58%)	61 (84%)	12 (16%)	0	100	100
78	3P	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
79	3Q	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
80	3R	65/156 (42%)	61 (94%)	4 (6%)	0	100	100
All	All	11562/12905 (90%)	10818 (94%)	738 (6%)	6 (0%)	49	70

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	2R	38	LYS
33	2Y	92	ASN
53	2s	15	LYS
48	2n	28	THR
13	2E	175	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	1D	190/199 (96%)	184 (97%)	6 (3%)	34	62
5	1E	348/349 (100%)	336 (97%)	12 (3%)	32	60
6	1F	306/348 (88%)	296 (97%)	10 (3%)	33	61
7	1G	246/250 (98%)	235 (96%)	11 (4%)	24	50
8	1H	209/252 (83%)	193 (92%)	16 (8%)	12	27
9	2A	195/215 (91%)	191 (98%)	4 (2%)	47	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	2B	204/223 (92%)	195 (96%)	9 (4%)	25	50
11	2C	169/171 (99%)	159 (94%)	10 (6%)	18	38
12	2D	180/181 (99%)	174 (97%)	6 (3%)	33	61
13	2E	148/149 (99%)	141 (95%)	7 (5%)	23	48
14	2F	176/177 (99%)	166 (94%)	10 (6%)	18	40
15	2G	118/161 (73%)	112 (95%)	6 (5%)	21	45
16	2H	171/172 (99%)	165 (96%)	6 (4%)	32	59
17	2I	173/174 (99%)	169 (98%)	4 (2%)	44	71
18	2J	134/163 (82%)	128 (96%)	6 (4%)	24	50
19	2K	164/165 (99%)	160 (98%)	4 (2%)	43	70
20	2L	166/175 (95%)	160 (96%)	6 (4%)	31	58
21	2M	156/157 (99%)	148 (95%)	8 (5%)	21	45
22	2N	139/140 (99%)	131 (94%)	8 (6%)	18	39
23	2O	91/115 (79%)	82 (90%)	9 (10%)	7	16
24	2P	101/107 (94%)	96 (95%)	5 (5%)	22	46
25	2Q	103/126 (82%)	103 (100%)	0	100	100
26	2R	108/133 (81%)	104 (96%)	4 (4%)	30	57
27	2S	124/135 (92%)	122 (98%)	2 (2%)	55	79
28	2T	117/118 (99%)	110 (94%)	7 (6%)	17	37
29	2U	120/121 (99%)	114 (95%)	6 (5%)	22	46
30	2V	89/126 (71%)	84 (94%)	5 (6%)	19	40
31	2W	83/97 (86%)	78 (94%)	5 (6%)	17	37
32	2X	98/110 (89%)	90 (92%)	8 (8%)	10	24
33	2Y	114/121 (94%)	111 (97%)	3 (3%)	40	68
34	2Z	88/89 (99%)	86 (98%)	2 (2%)	44	71
35	2a	98/100 (98%)	93 (95%)	5 (5%)	21	45
36	2b	109/110 (99%)	104 (95%)	5 (5%)	24	49
37	2c	86/89 (97%)	82 (95%)	4 (5%)	23	48
38	2d	74/80 (92%)	69 (93%)	5 (7%)	14	32
39	2e	64/65 (98%)	58 (91%)	6 (9%)	8	18
40	2f	47/48 (98%)	45 (96%)	2 (4%)	26	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	2g	47/115 (41%)	46 (98%)	1 (2%)	47	73
42	2h	23/24 (96%)	22 (96%)	1 (4%)	26	51
43	2i	94/94 (100%)	91 (97%)	3 (3%)	34	62
44	2j	74/75 (99%)	67 (90%)	7 (10%)	8	18
45	2k	109/121 (90%)	103 (94%)	6 (6%)	19	41
46	2l	195/196 (100%)	186 (95%)	9 (5%)	24	49
48	2n	183/243 (75%)	163 (89%)	20 (11%)	6	13
49	2o	195/231 (84%)	181 (93%)	14 (7%)	13	30
50	2p	190/202 (94%)	173 (91%)	17 (9%)	9	20
51	2q	224/225 (100%)	214 (96%)	10 (4%)	24	50
52	2r	159/170 (94%)	148 (93%)	11 (7%)	14	32
53	2s	166/174 (95%)	153 (92%)	13 (8%)	11	26
54	2t	178/180 (99%)	172 (97%)	6 (3%)	32	60
55	2u	89/136 (65%)	86 (97%)	3 (3%)	32	60
56	2v	137/142 (96%)	129 (94%)	8 (6%)	18	39
57	2w	113/130 (87%)	111 (98%)	2 (2%)	51	76
58	2x	117/121 (97%)	108 (92%)	9 (8%)	12	27
59	2y	122/122 (100%)	110 (90%)	12 (10%)	7	17
60	2z	126/132 (96%)	119 (94%)	7 (6%)	19	40
61	20	113/115 (98%)	105 (93%)	8 (7%)	13	31
62	21	94/107 (88%)	87 (93%)	7 (7%)	13	29
63	3A	67/67 (100%)	58 (87%)	9 (13%)	4	7
64	3B	113/115 (98%)	104 (92%)	9 (8%)	11	25
65	3C	90/98 (92%)	84 (93%)	6 (7%)	15	33
66	3D	57/62 (92%)	53 (93%)	4 (7%)	14	31
67	3E	48/49 (98%)	46 (96%)	2 (4%)	26	52
68	3F	272/275 (99%)	252 (93%)	20 (7%)	13	29
69	3G	189/225 (84%)	182 (96%)	7 (4%)	30	57
70	3H	207/218 (95%)	193 (93%)	14 (7%)	14	32
71	3I	162/168 (96%)	158 (98%)	4 (2%)	42	69
72	3J	102/108 (94%)	97 (95%)	5 (5%)	22	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	3K	130/131 (99%)	122 (94%)	8 (6%)	16	36
74	3L	110/119 (92%)	102 (93%)	8 (7%)	13	29
75	3M	112/113 (99%)	104 (93%)	8 (7%)	13	31
76	3N	114/115 (99%)	109 (96%)	5 (4%)	25	50
77	3O	66/103 (64%)	57 (86%)	9 (14%)	3	7
78	3P	75/76 (99%)	69 (92%)	6 (8%)	11	25
79	3Q	47/48 (98%)	43 (92%)	4 (8%)	10	22
80	3R	60/140 (43%)	57 (95%)	3 (5%)	22	46
All	All	10075/10996 (92%)	9538 (95%)	537 (5%)	22	43

5 of 537 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	3H	15	LEU
70	3H	217	MET
69	3G	264	SER
77	3O	79	ILE
32	2X	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
46	2l	19	HIS
52	2r	203	ASN
48	2n	36	GLN
49	2o	147	ASN
56	2v	11	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	3704/5070 (73%)	810 (21%)	54 (1%)
2	1B	119/121 (98%)	14 (11%)	2 (1%)
3	1C	155/157 (98%)	28 (18%)	2 (1%)
47	2m	1714/1869 (91%)	492 (28%)	0
All	All	5692/7217 (78%)	1344 (23%)	58 (1%)

5 of 1344 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	6	C
1	1A	13	U
1	1A	39	A
1	1A	42	A
1	1A	48	G

5 of 58 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2695	A
2	1B	109	U
1	1A	3888	G
2	1B	33	U
1	1A	4731	G

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
41	MLZ	2g	98	41	8,9,10	0.88	1 (12%)	4,9,11	0.57	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
41	MLZ	2g	98	41	-	2/7/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2g	98	MLZ	O-C	2.04	1.27	1.20

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	2g	98	MLZ	CD-CE-NZ-CM
41	2g	98	MLZ	C-CA-CB-CG

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 425 ligands modelled in this entry, 401 are monoatomic - leaving 24 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
81	84D	2m	1902	-	32,33,33	1.55	7 (21%)	40,48,48	1.13	4 (10%)
81	84D	1A	5114	-	32,33,33	1.56	7 (21%)	40,48,48	1.15	5 (12%)
81	84D	1A	5118	-	32,33,33	1.56	7 (21%)	40,48,48	1.00	3 (7%)
81	84D	1A	5119	-	32,33,33	1.54	6 (18%)	40,48,48	1.11	3 (7%)
81	84D	1A	5104	-	32,33,33	1.61	9 (28%)	40,48,48	1.81	4 (10%)
81	84D	1A	5102	-	32,33,33	1.57	7 (21%)	40,48,48	1.28	4 (10%)
81	84D	1A	5117	-	32,33,33	1.57	7 (21%)	40,48,48	1.21	4 (10%)
81	84D	1A	5112	-	32,33,33	1.60	7 (21%)	40,48,48	1.32	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	84D	2m	1901	-	32,33,33	1.54	6 (18%)	40,48,48	1.13	7 (17%)
81	84D	1A	5110	-	32,33,33	1.55	7 (21%)	40,48,48	1.16	4 (10%)
81	84D	2m	1903	-	32,33,33	1.56	6 (18%)	40,48,48	1.13	6 (15%)
81	84D	1A	5116	-	32,33,33	1.53	6 (18%)	40,48,48	1.07	2 (5%)
81	84D	1A	5106	-	32,33,33	1.55	7 (21%)	40,48,48	1.15	5 (12%)
81	84D	1A	5109	-	32,33,33	1.68	7 (21%)	40,48,48	1.83	8 (20%)
81	84D	1A	5121	-	32,33,33	1.54	7 (21%)	40,48,48	1.04	3 (7%)
81	84D	1A	5120	-	32,33,33	1.54	6 (18%)	40,48,48	1.12	3 (7%)
81	84D	1A	5108	-	32,33,33	1.55	6 (18%)	40,48,48	1.20	3 (7%)
81	84D	1A	5107	-	32,33,33	1.59	7 (21%)	40,48,48	1.14	4 (10%)
81	84D	1A	5111	-	32,33,33	1.56	7 (21%)	40,48,48	1.00	2 (5%)
81	84D	1A	5105	-	32,33,33	1.61	7 (21%)	40,48,48	1.38	6 (15%)
81	84D	1A	5115	-	32,33,33	1.57	7 (21%)	40,48,48	1.08	4 (10%)
81	84D	1A	5113	-	32,33,33	1.57	7 (21%)	40,48,48	1.25	6 (15%)
81	84D	1A	5101	-	32,33,33	1.56	7 (21%)	40,48,48	1.06	3 (7%)
81	84D	1A	5103	-	32,33,33	1.52	6 (18%)	40,48,48	1.21	4 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	84D	2m	1902	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5114	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5118	-	-	6/12/65/65	0/3/3/3
81	84D	1A	5119	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5104	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5102	-	-	2/12/65/65	0/3/3/3
81	84D	1A	5117	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5112	-	-	2/12/65/65	0/3/3/3
81	84D	2m	1901	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5110	-	-	3/12/65/65	1/3/3/3
81	84D	2m	1903	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5116	-	-	5/12/65/65	0/3/3/3
81	84D	1A	5106	-	-	7/12/65/65	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	84D	1A	5109	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5121	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5120	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5108	-	-	6/12/65/65	0/3/3/3
81	84D	1A	5107	-	-	2/12/65/65	0/3/3/3
81	84D	1A	5111	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5105	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5115	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5113	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5101	-	-	5/12/65/65	0/3/3/3
81	84D	1A	5103	-	-	3/12/65/65	0/3/3/3

The worst 5 of 163 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	1A	5109	84D	C15-C14	-5.13	1.47	1.53
81	1A	5112	84D	C15-C14	-4.86	1.47	1.53
81	1A	5102	84D	C15-C14	-4.70	1.47	1.53
81	1A	5104	84D	C15-C14	-4.62	1.47	1.53
81	1A	5113	84D	C15-C14	-4.58	1.47	1.53

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	1A	5104	84D	O-C4-C	8.07	118.40	109.91
81	1A	5109	84D	C3-O-C4	4.66	118.30	113.13
81	1A	5104	84D	C3-O-C4	4.14	117.72	113.13
81	1A	5109	84D	O4-C12-C13	4.08	118.76	110.37
81	1A	5105	84D	C16-C15-C14	4.06	115.16	110.67

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	1A	5101	84D	O-C4-C5-N
81	1A	5101	84D	C-C4-C5-N
81	1A	5104	84D	O-C4-C5-N
81	1A	5105	84D	O-C4-C5-N
81	1A	5105	84D	C-C4-C5-N

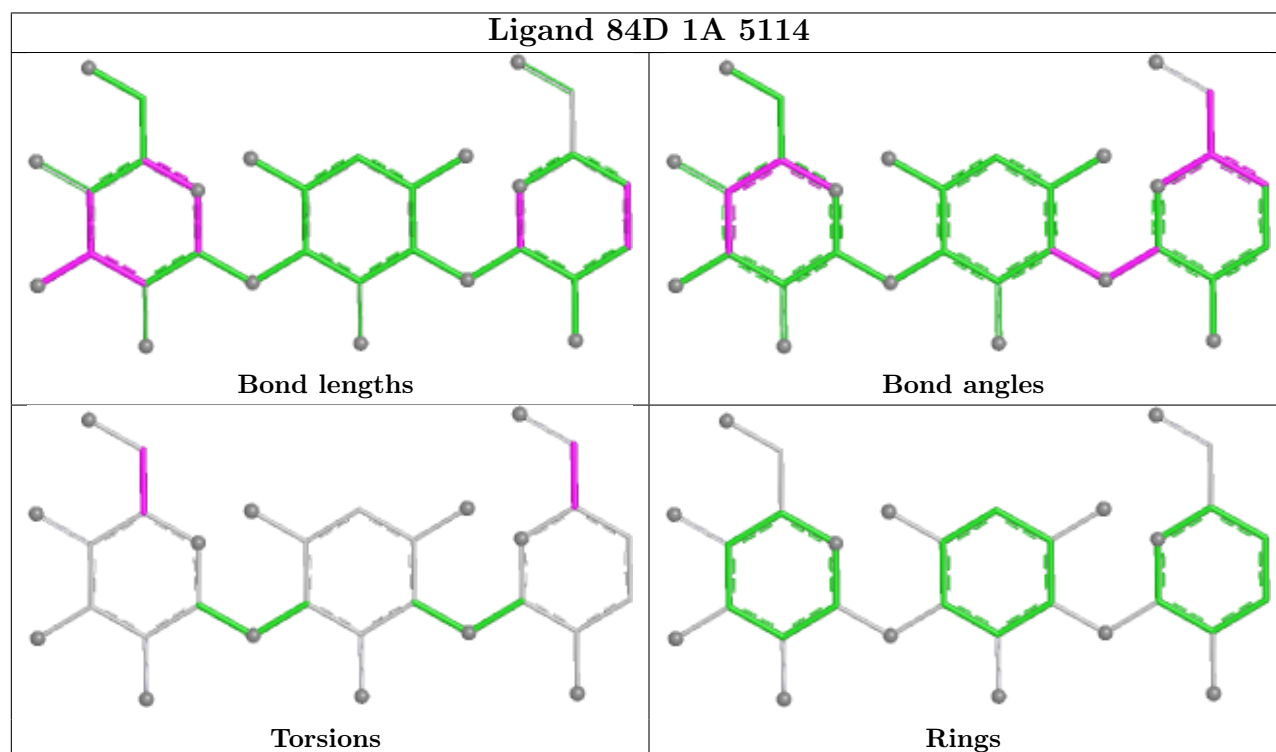
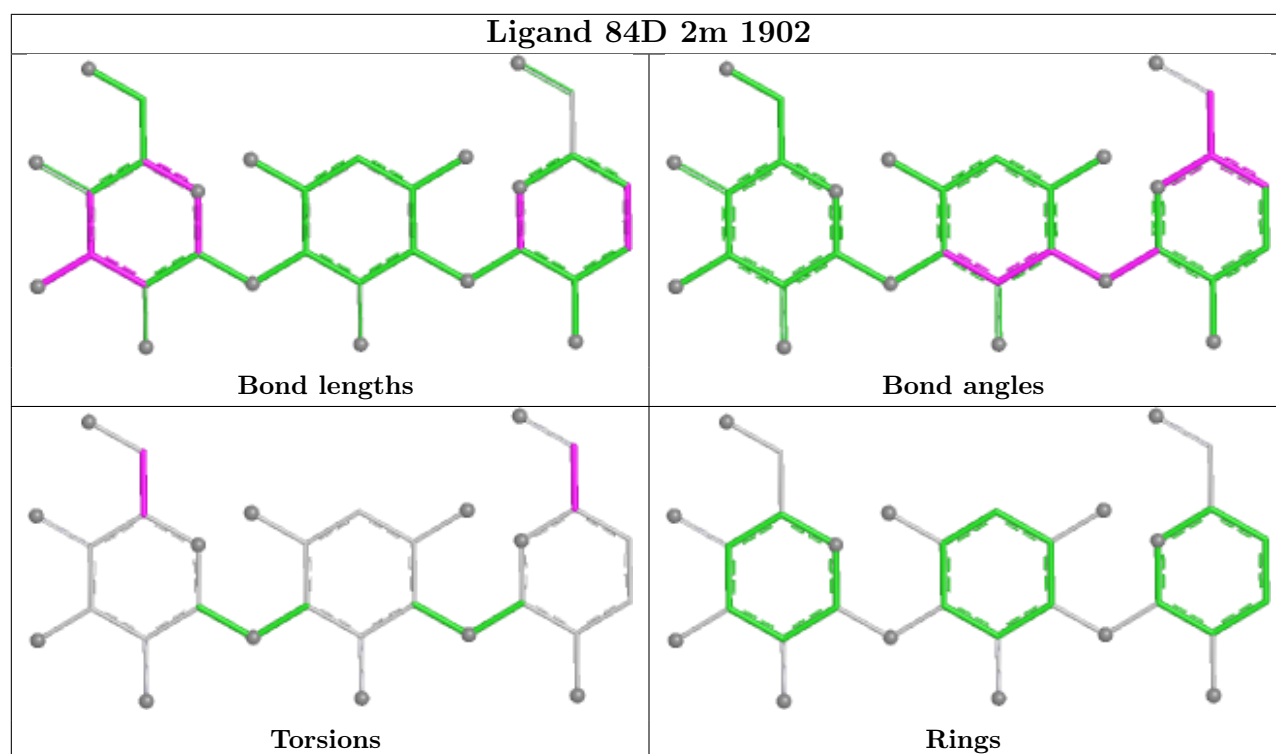
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	1A	5110	84D	C-C1-C2-C3-C4-O

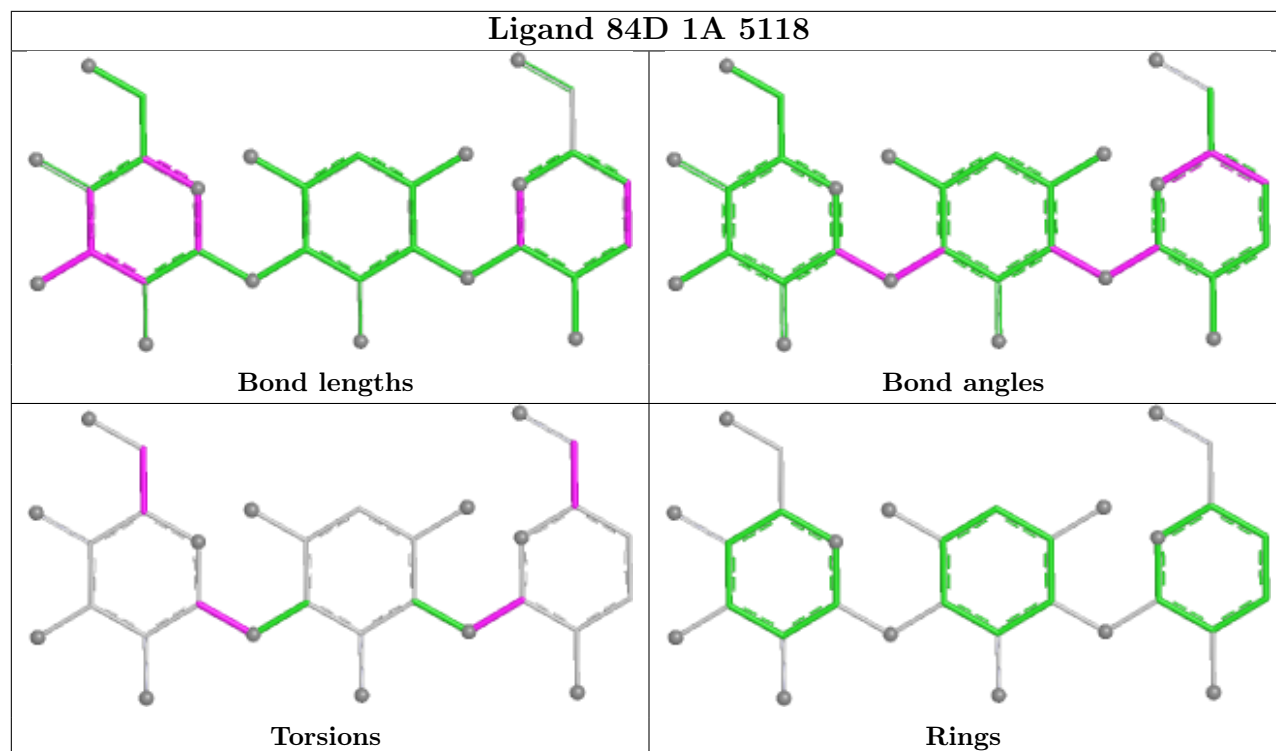
15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	2m	1902	84D	2	0
81	1A	5118	84D	2	0
81	1A	5119	84D	1	0
81	1A	5104	84D	3	0
81	2m	1901	84D	3	0
81	1A	5110	84D	4	0
81	2m	1903	84D	1	0
81	1A	5116	84D	1	0
81	1A	5106	84D	1	0
81	1A	5109	84D	1	0
81	1A	5107	84D	1	0
81	1A	5105	84D	2	0
81	1A	5115	84D	2	0
81	1A	5101	84D	1	0
81	1A	5103	84D	1	0

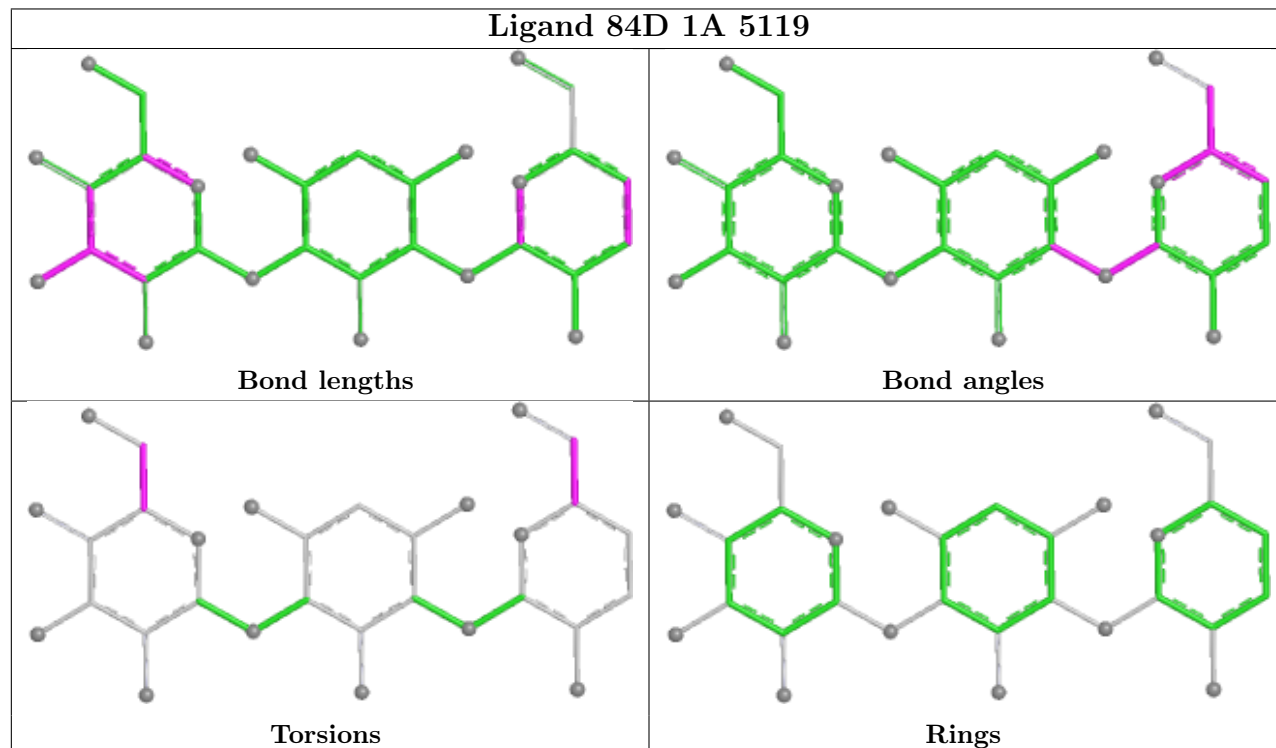
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

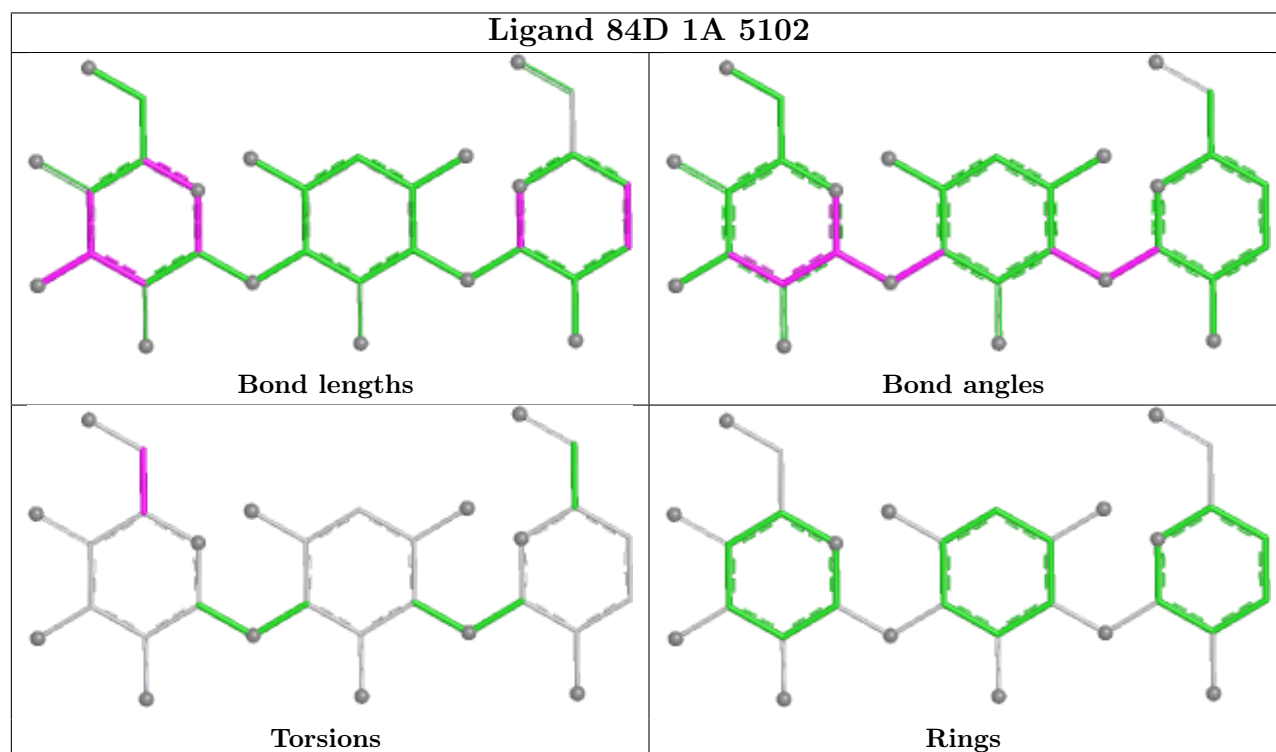
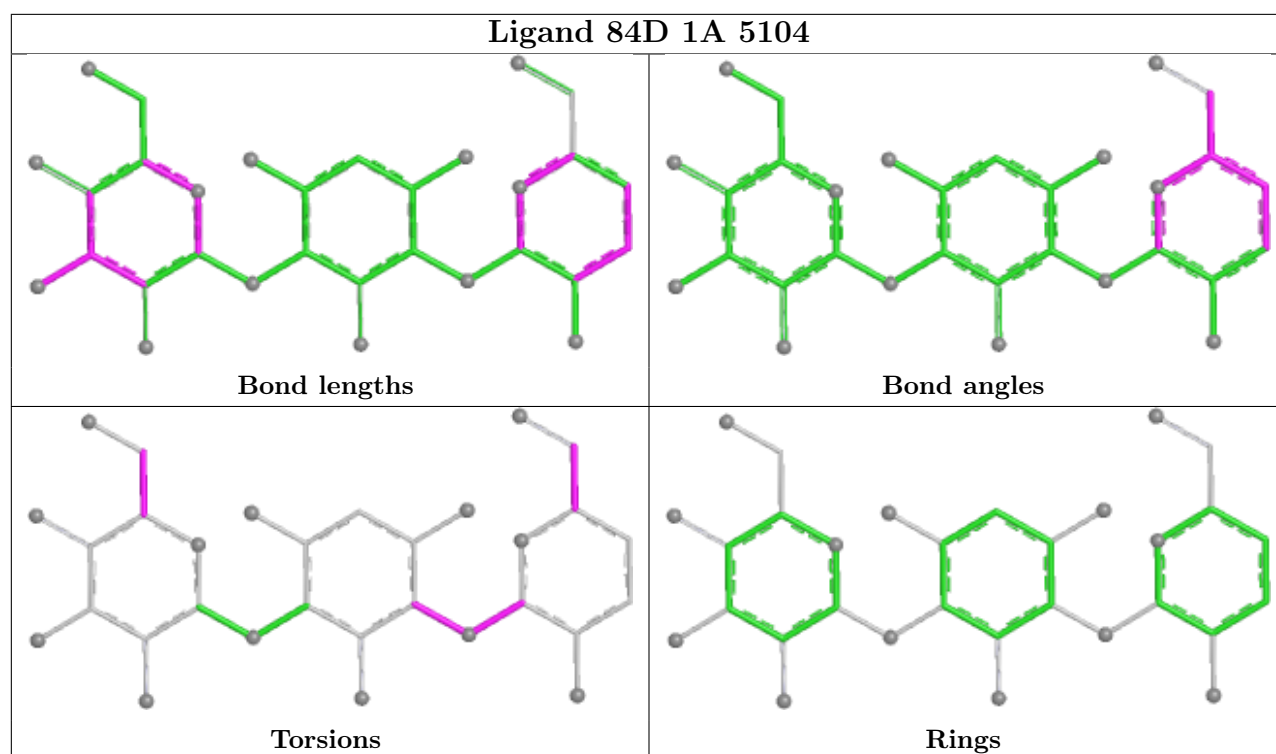


Ligand 84D 1A 5118

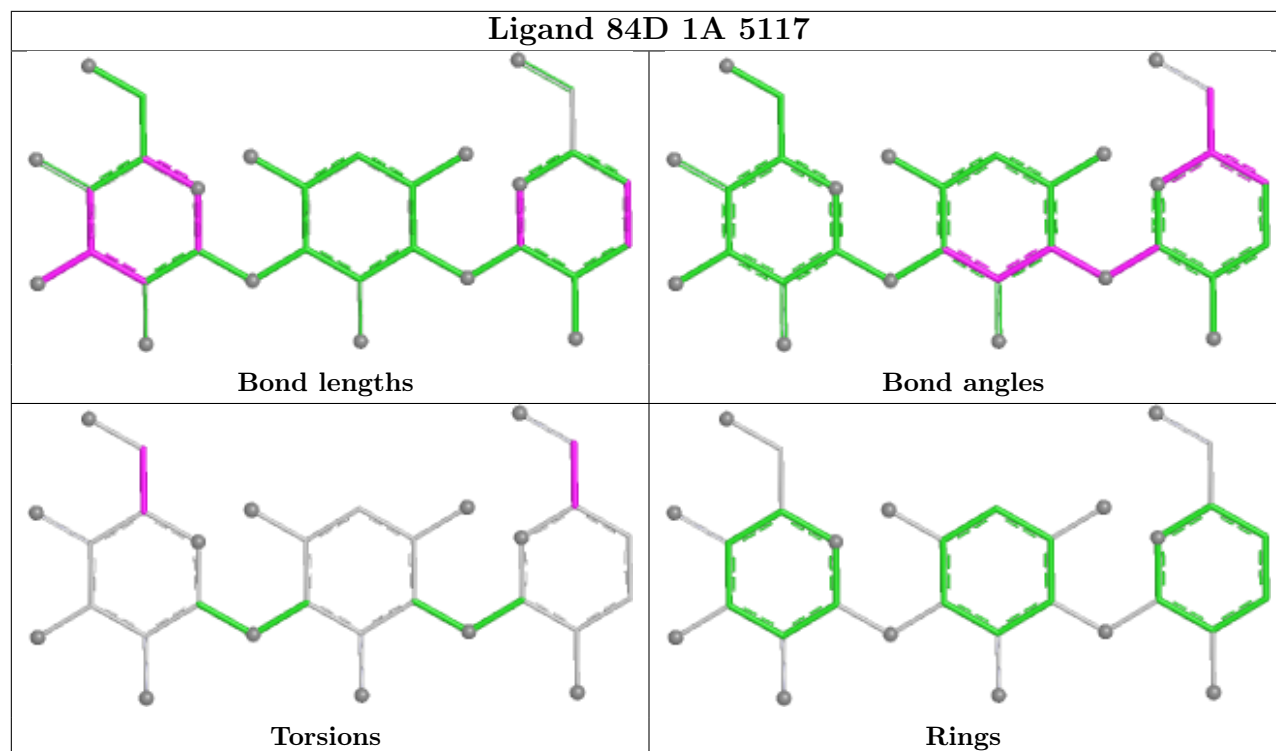


Ligand 84D 1A 5119

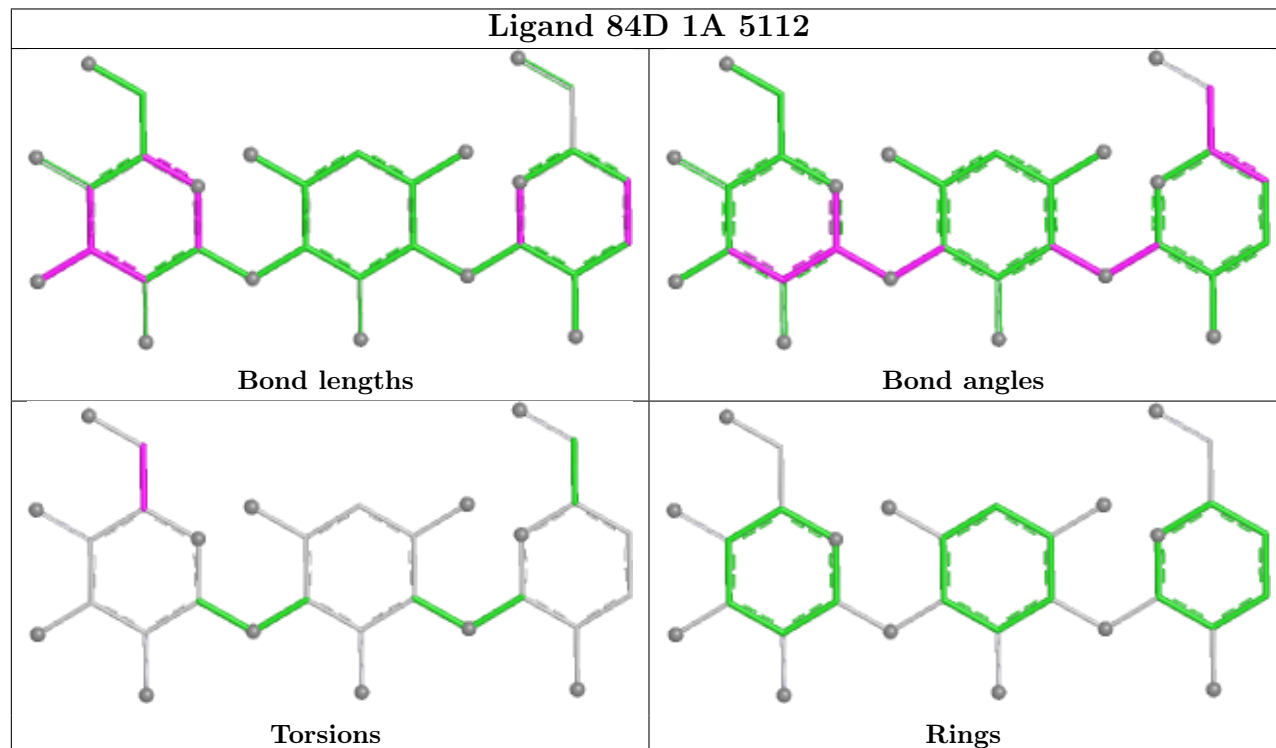


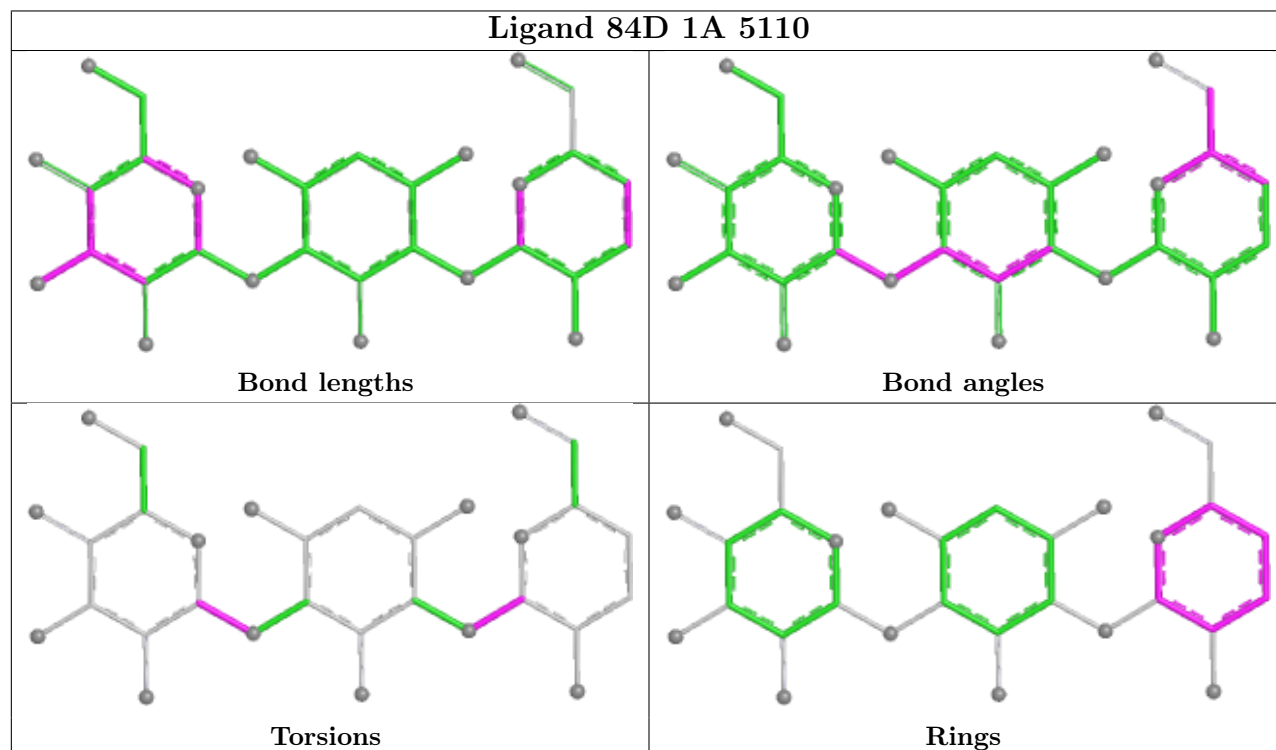
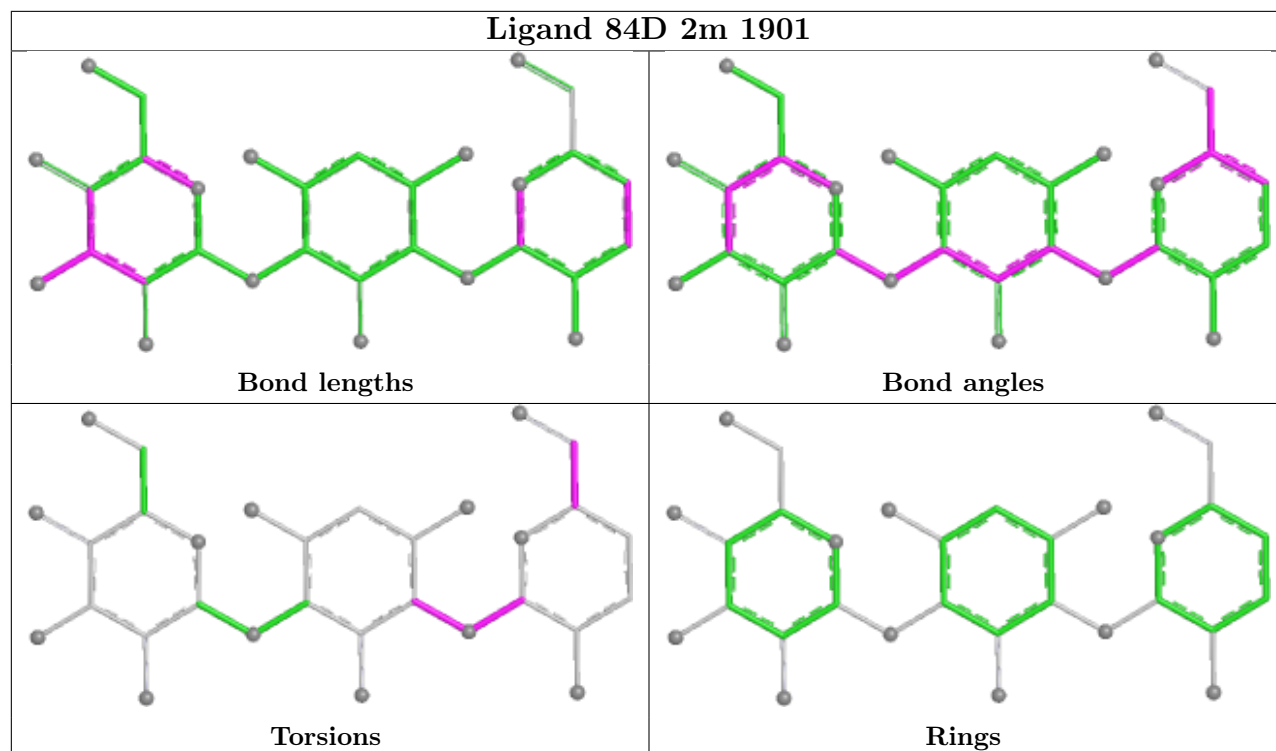


Ligand 84D 1A 5117

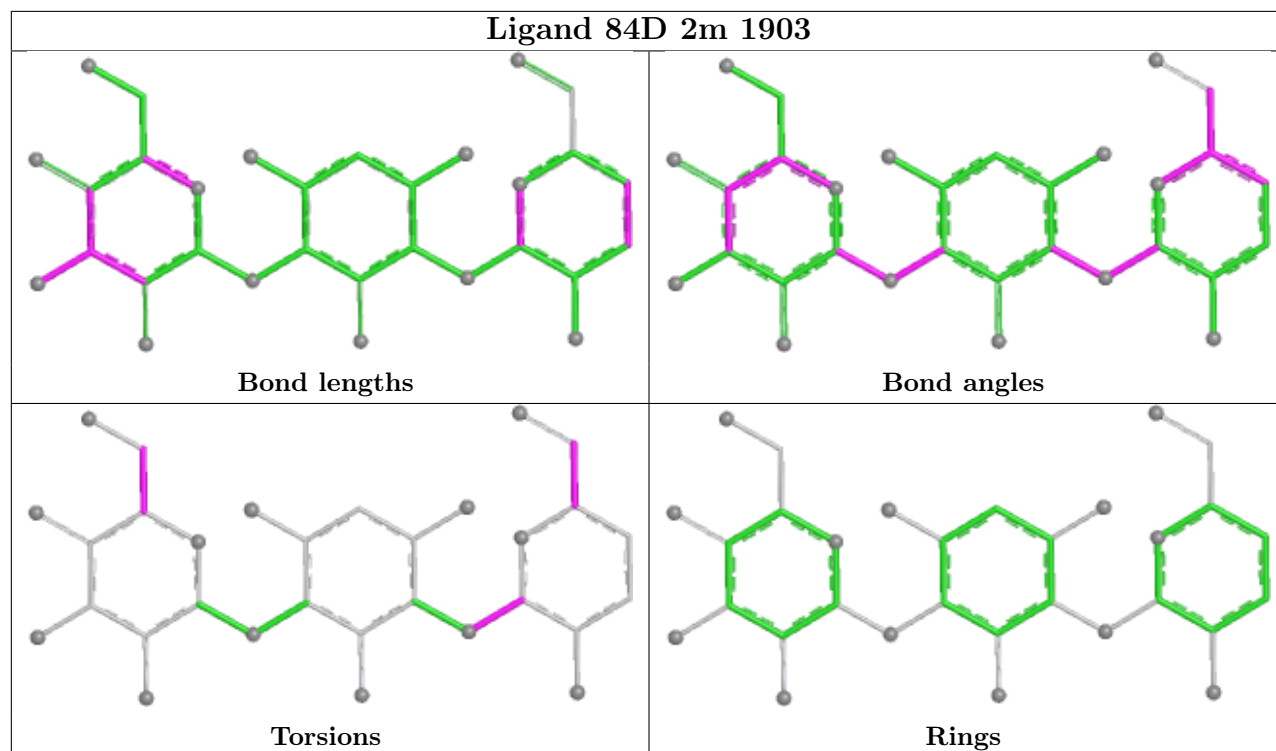


Ligand 84D 1A 5112

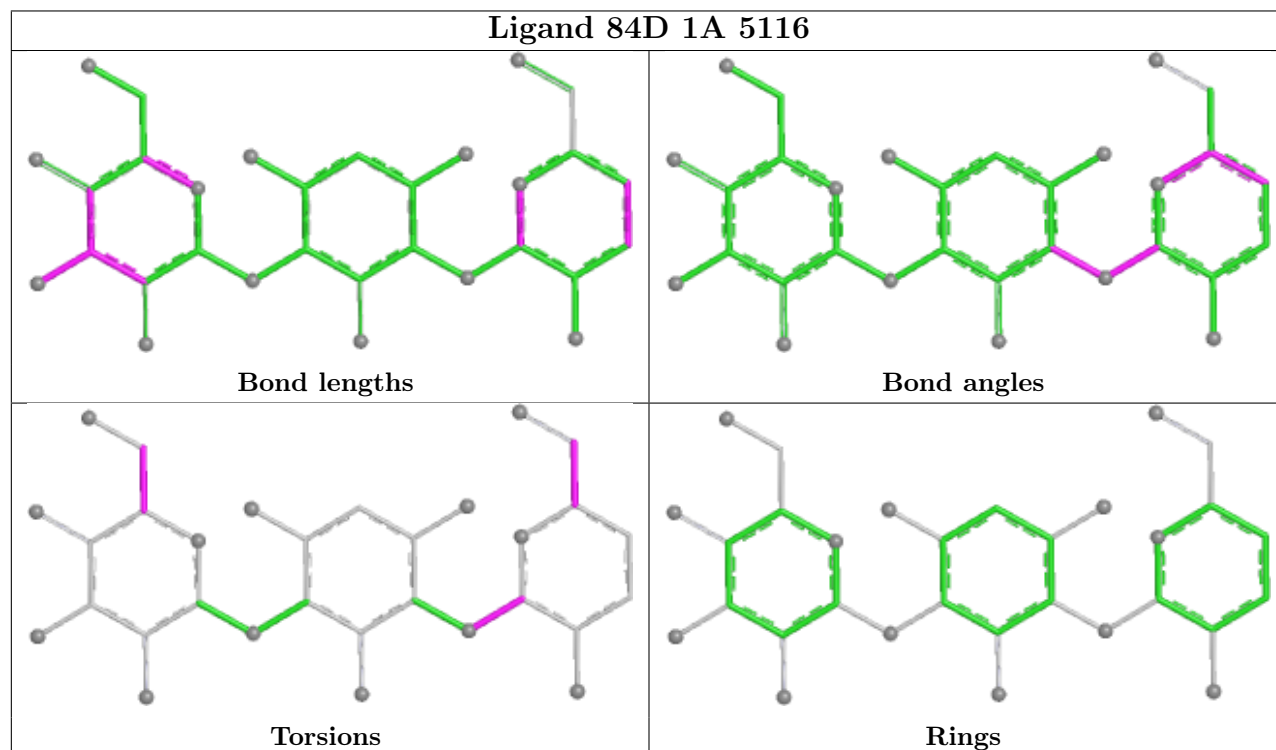




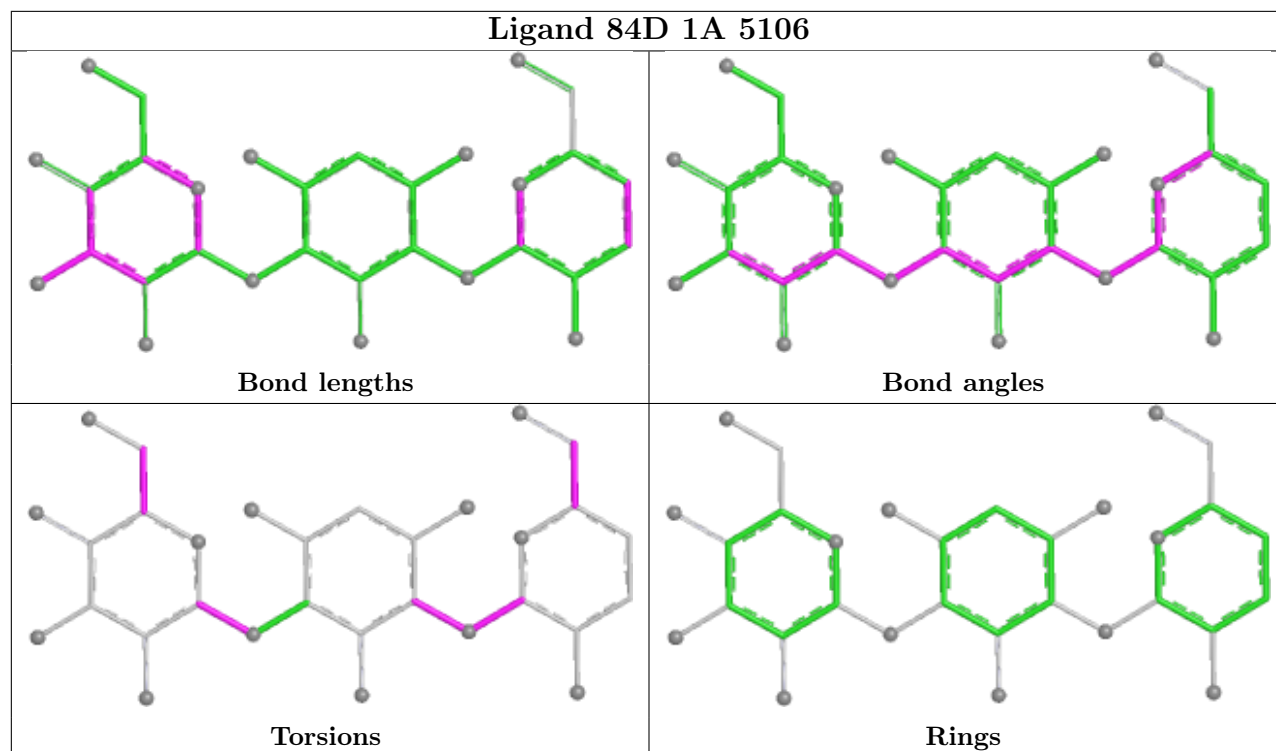
Ligand 84D 2m 1903



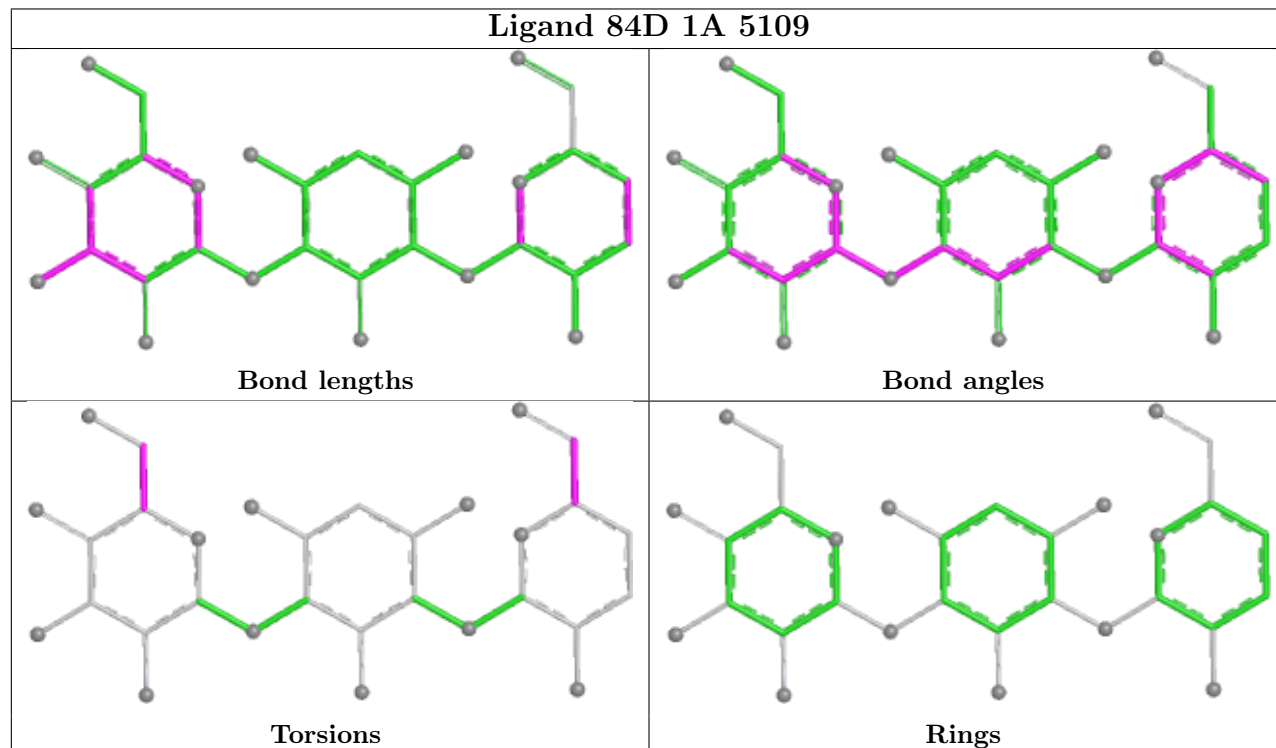
Ligand 84D 1A 5116



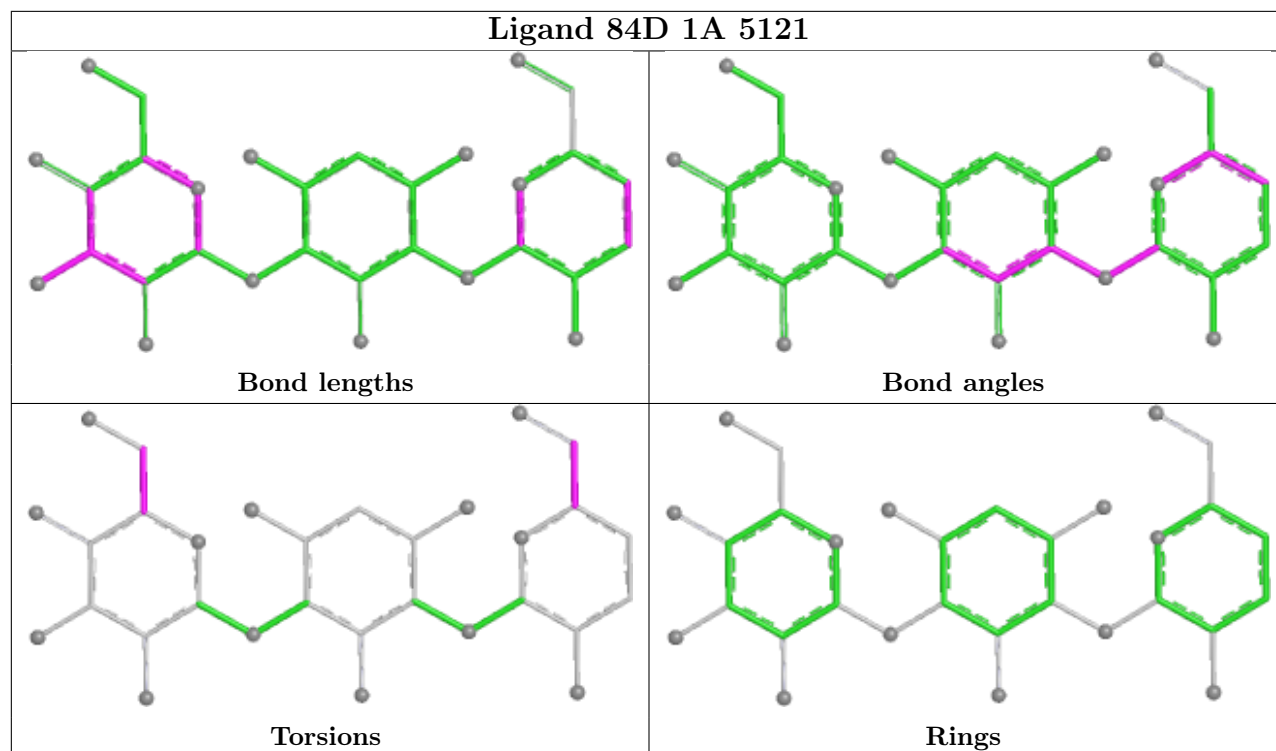
Ligand 84D 1A 5106



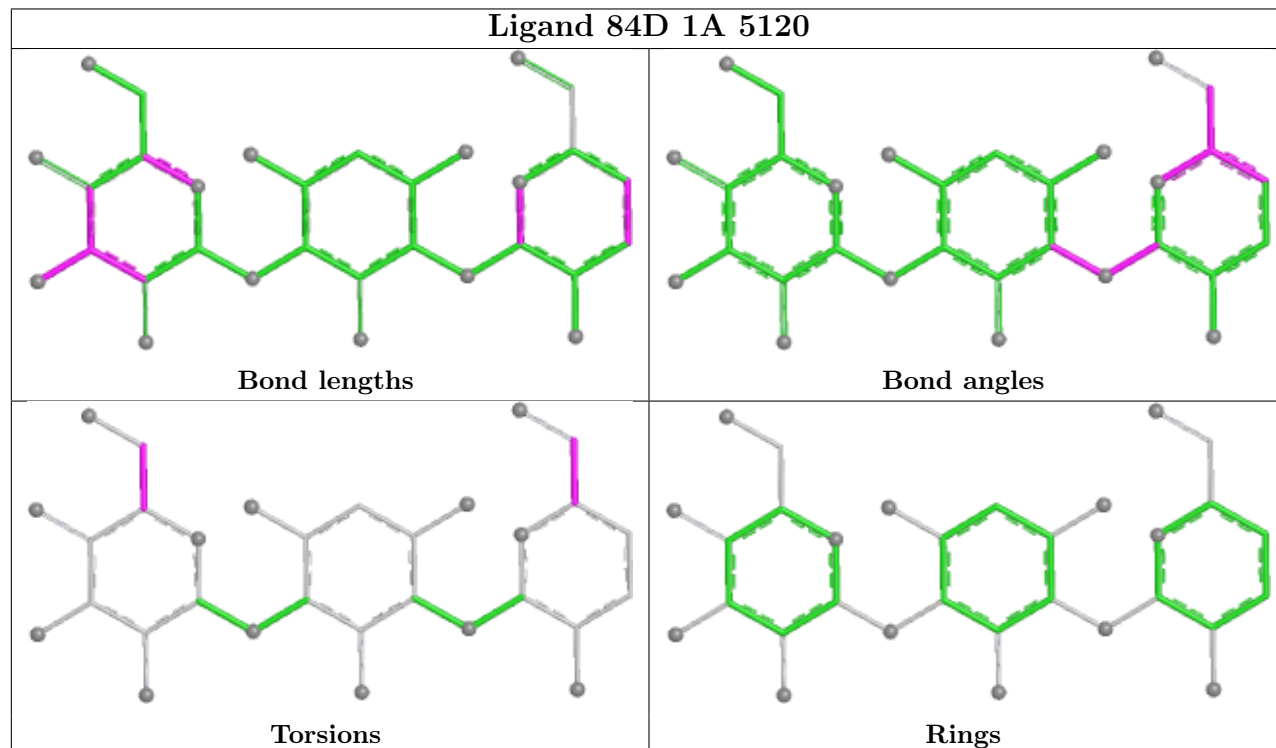
Ligand 84D 1A 5109

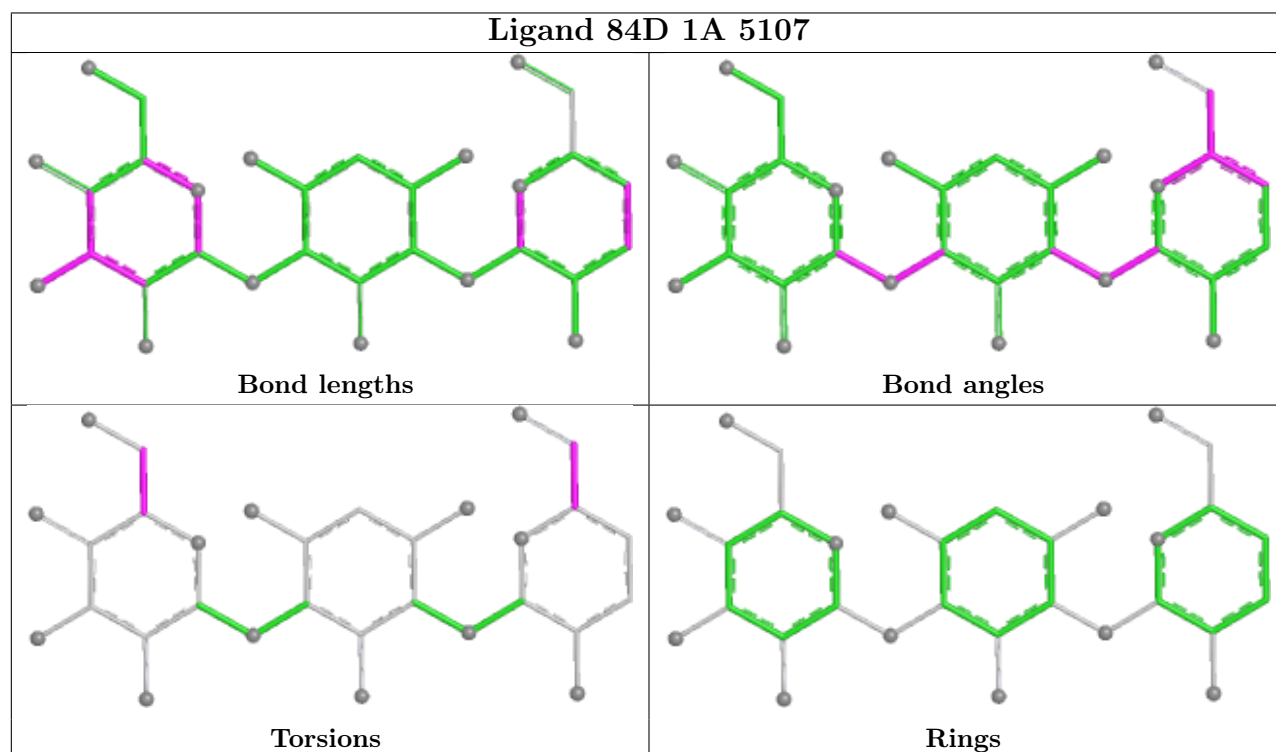
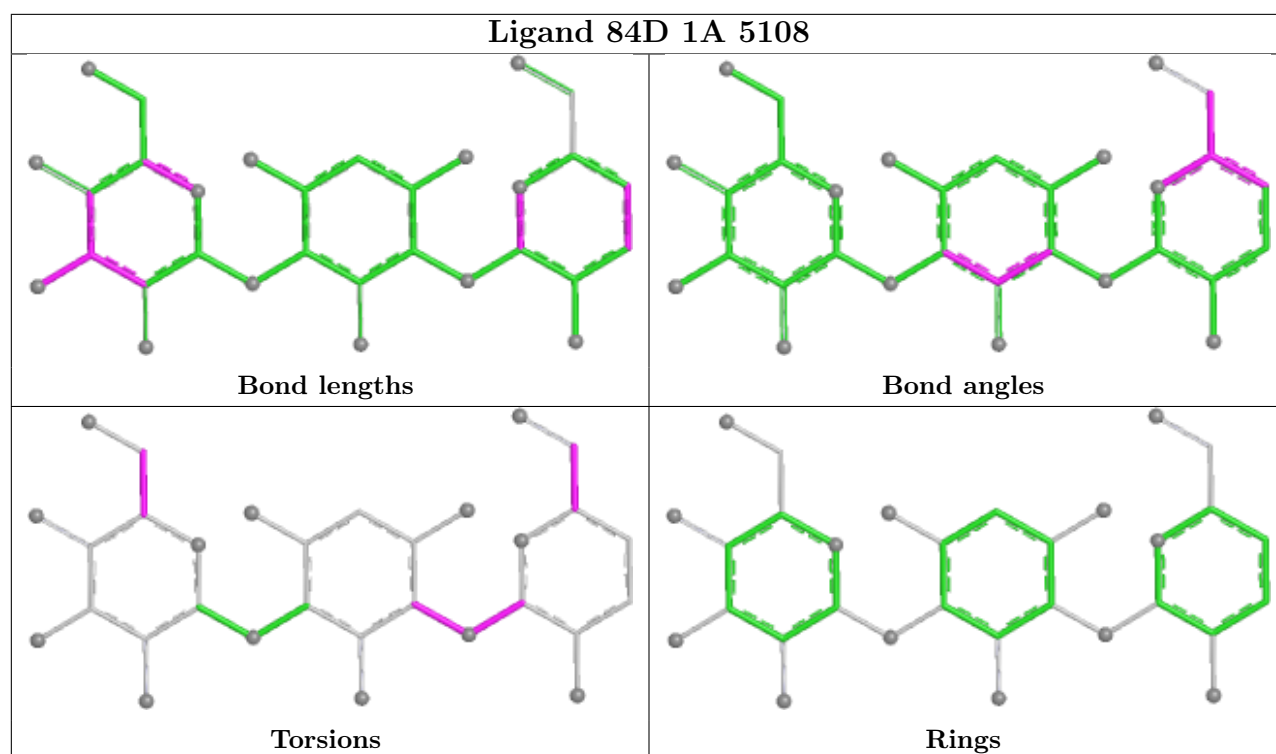


Ligand 84D 1A 5121

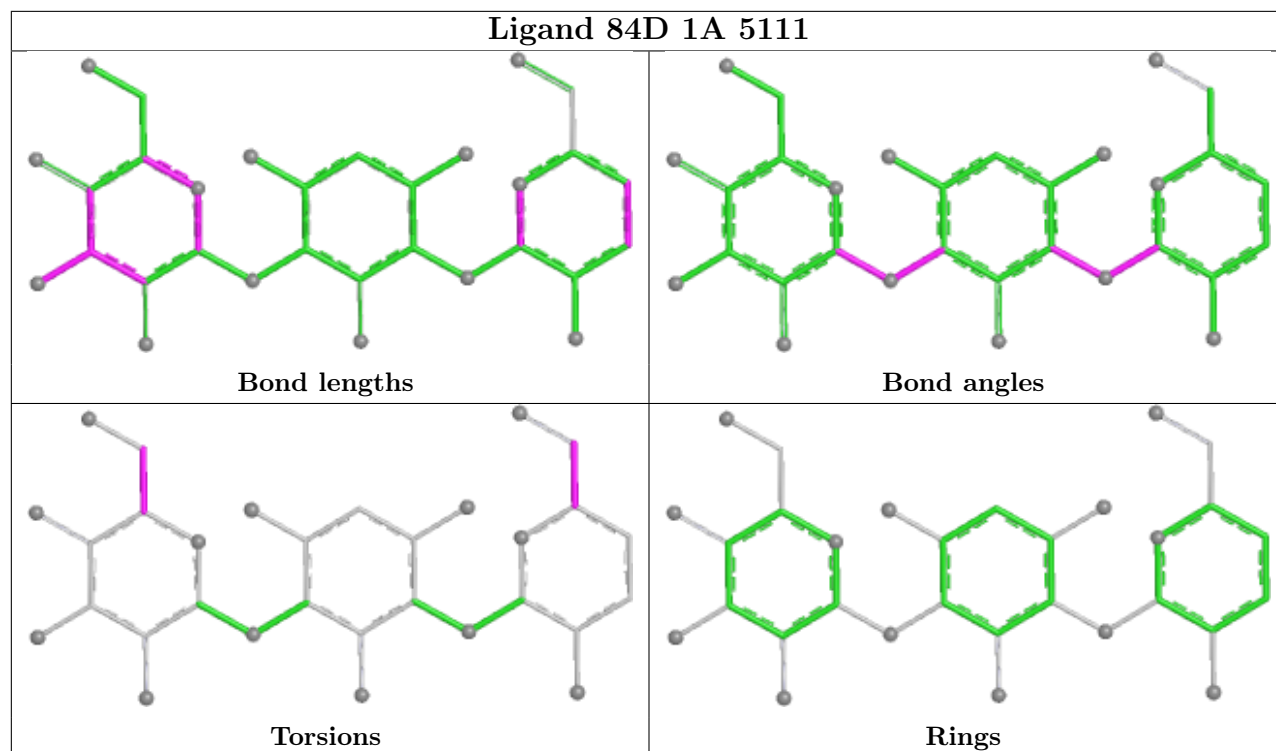


Ligand 84D 1A 5120

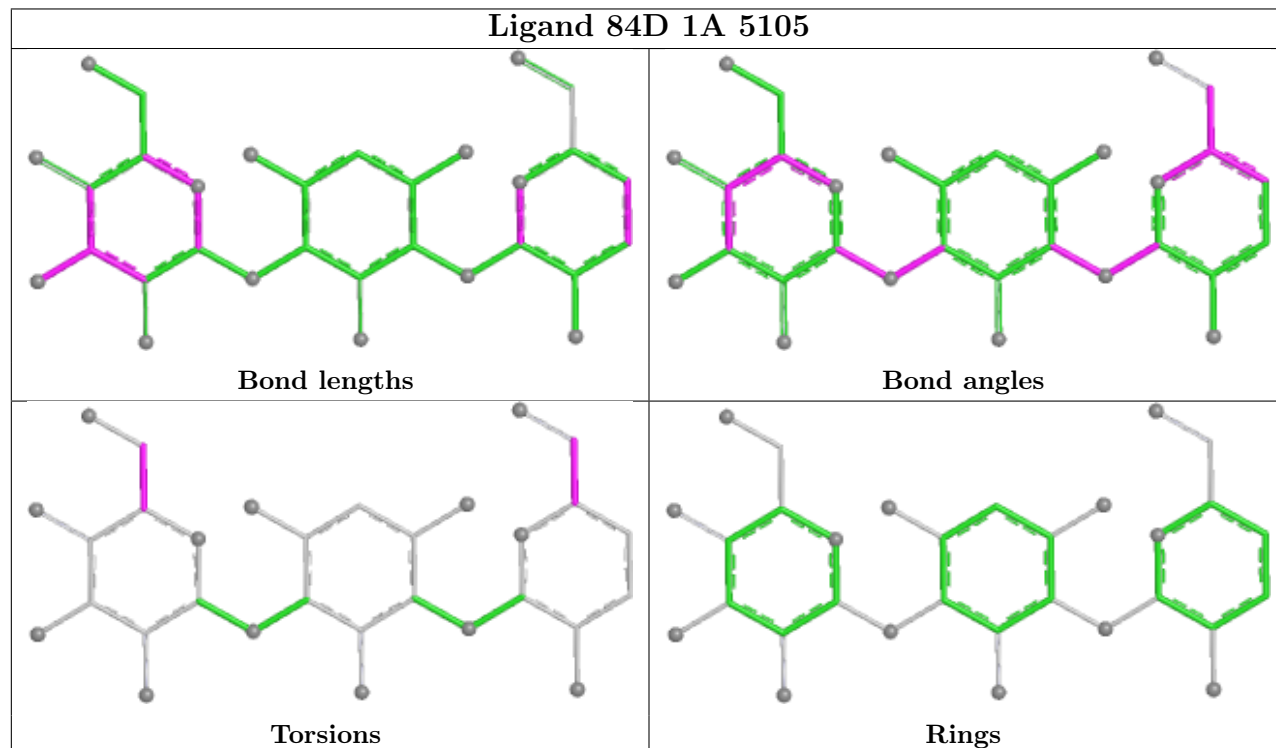


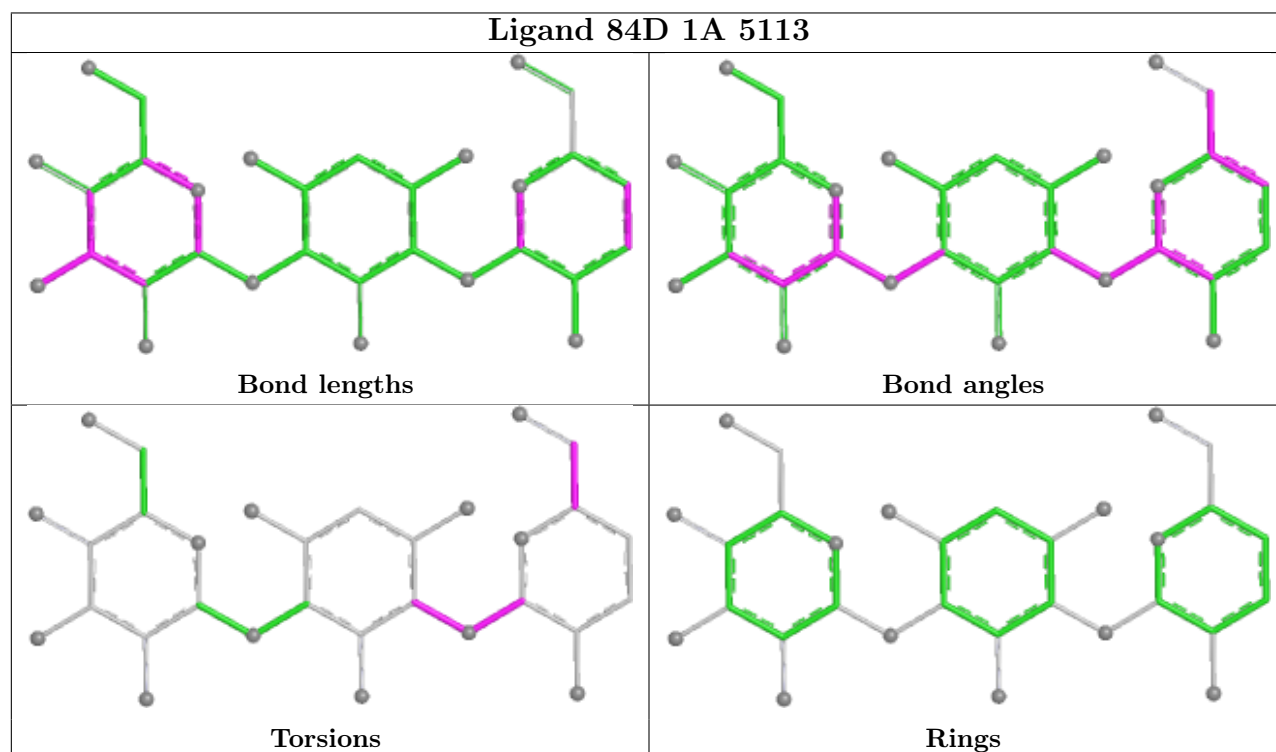
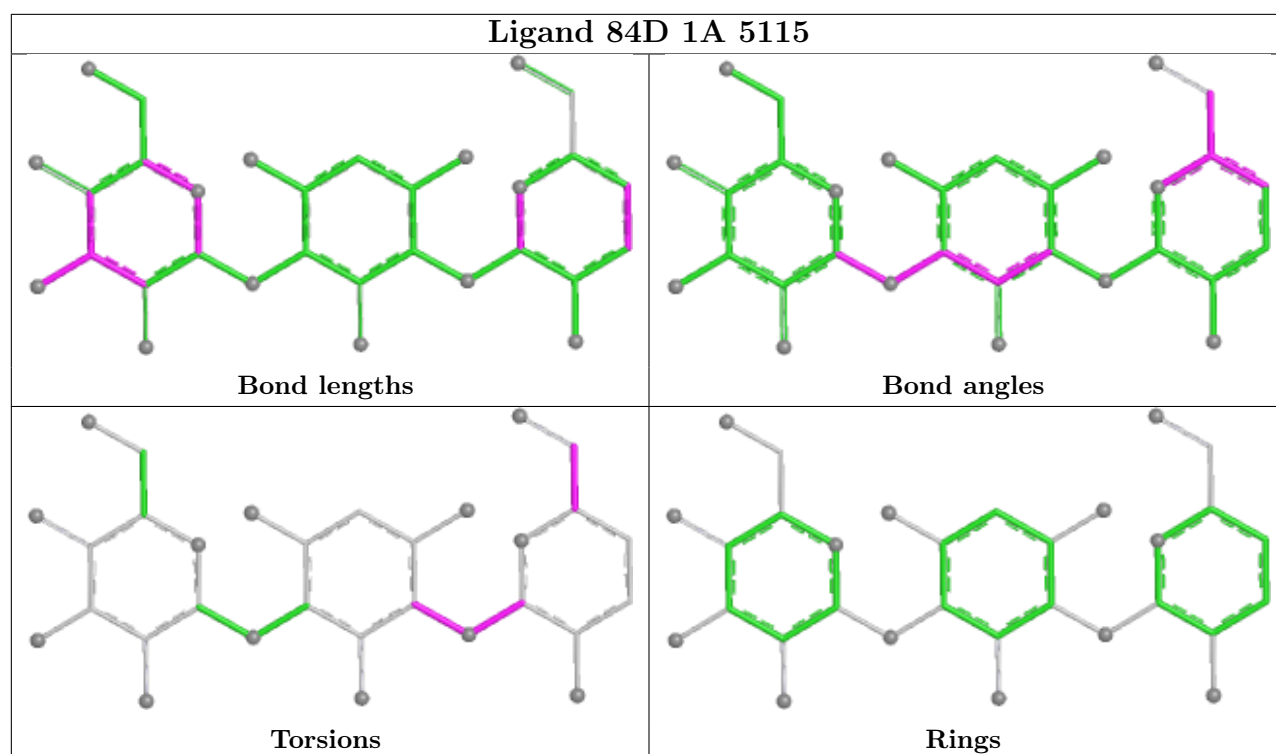


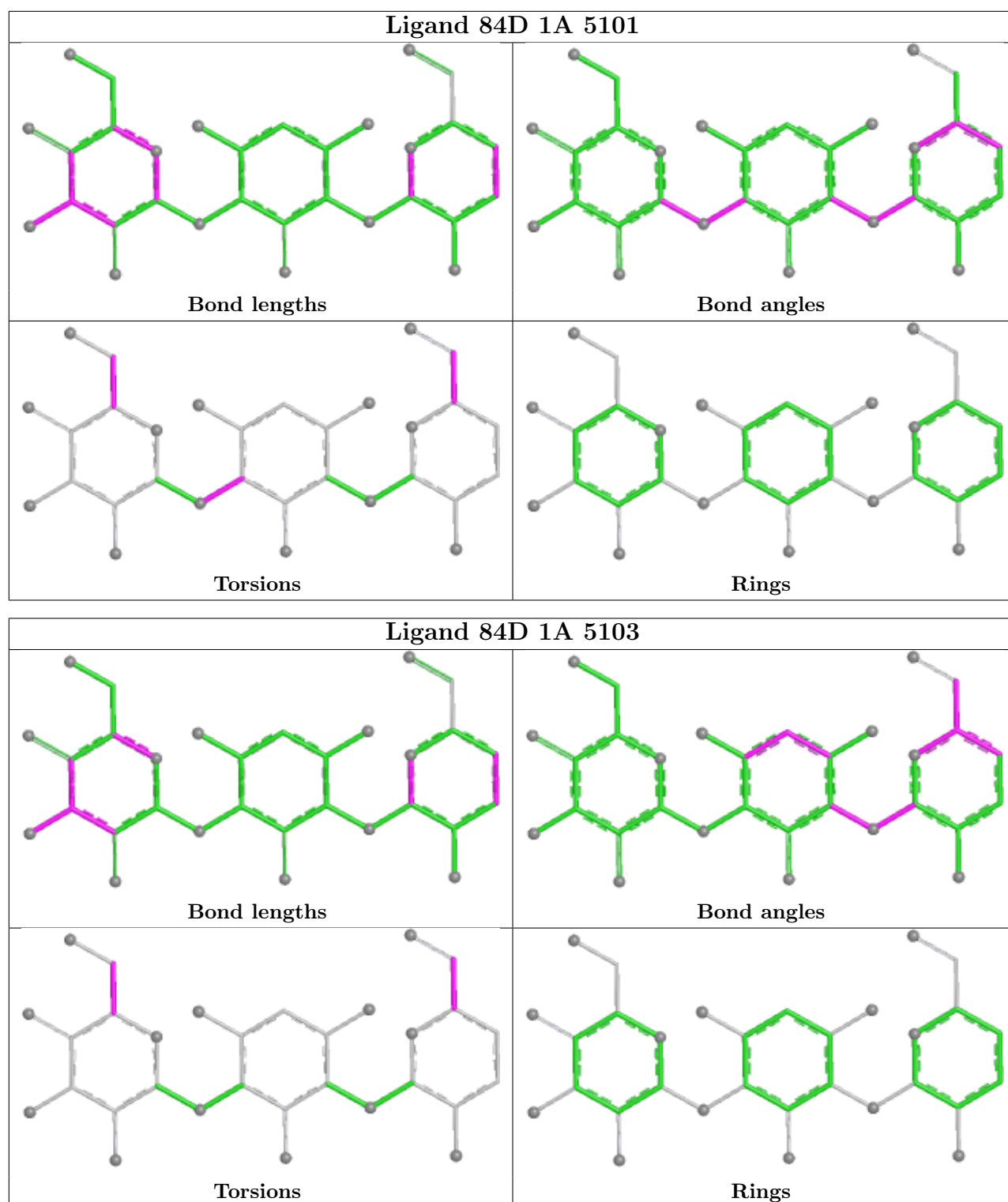
Ligand 84D 1A 5111



Ligand 84D 1A 5105







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

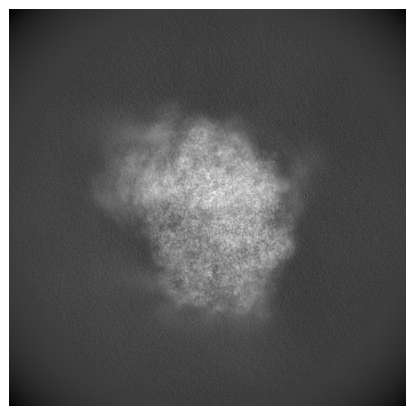
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35413. These allow visual inspection of the internal detail of the map and identification of artifacts.

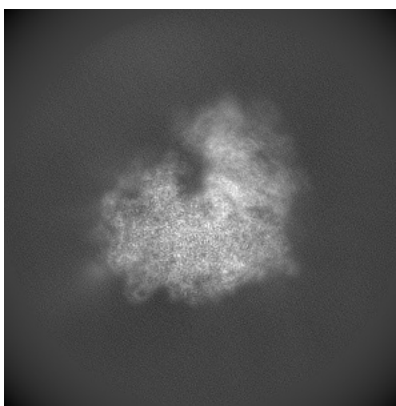
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

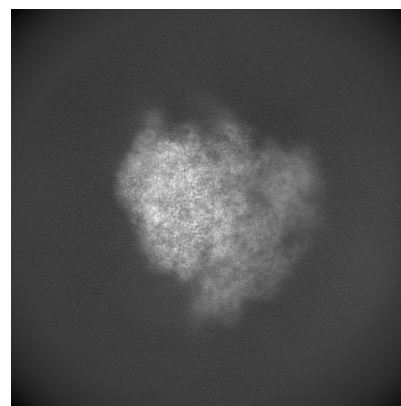
6.1.1 Primary map



X

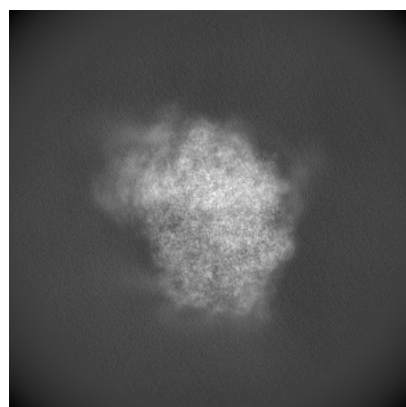


Y

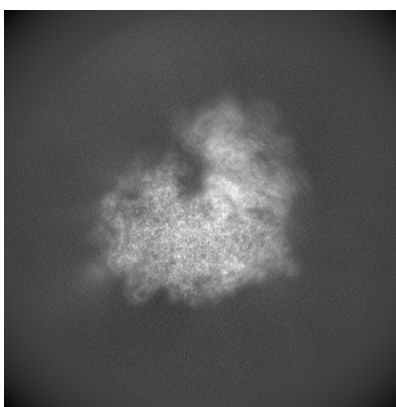


Z

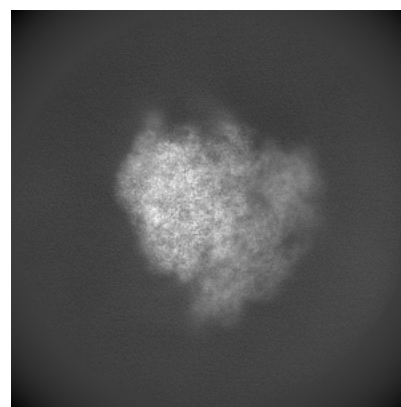
6.1.2 Raw map



X



Y

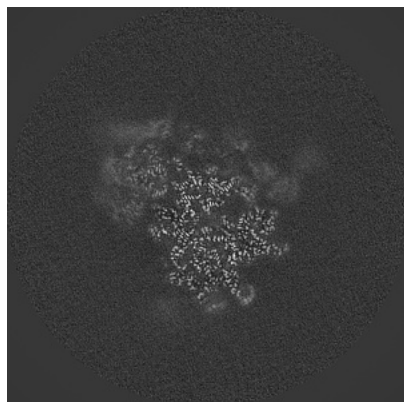


Z

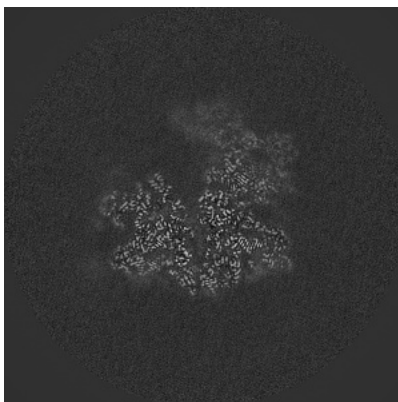
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

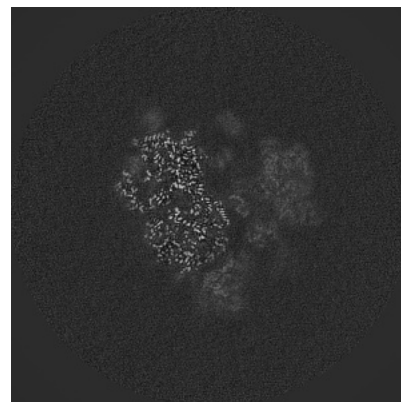
6.2.1 Primary map



X Index: 320

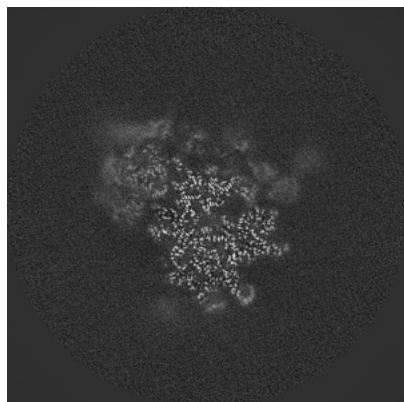


Y Index: 320

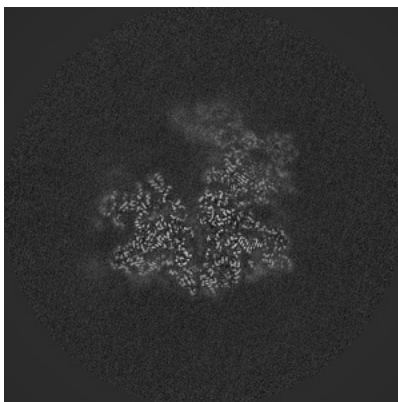


Z Index: 320

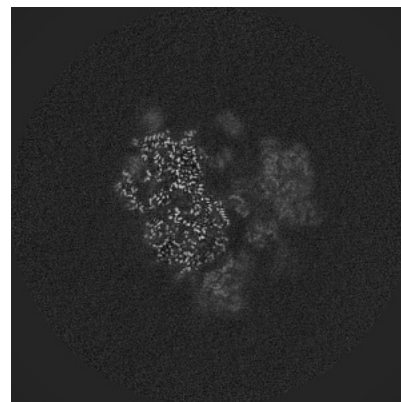
6.2.2 Raw map



X Index: 320



Y Index: 320

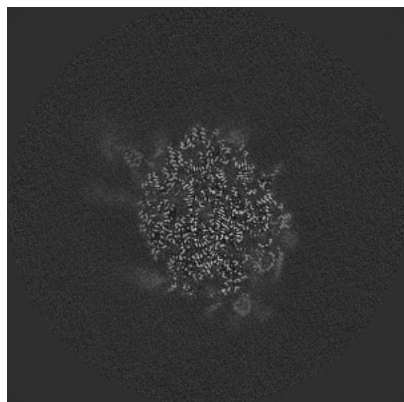


Z Index: 320

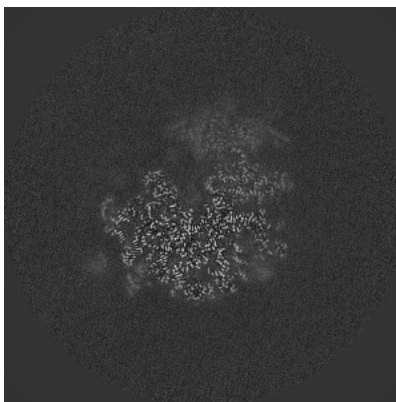
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

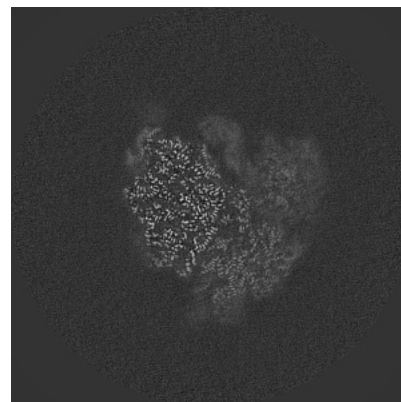
6.3.1 Primary map



X Index: 288

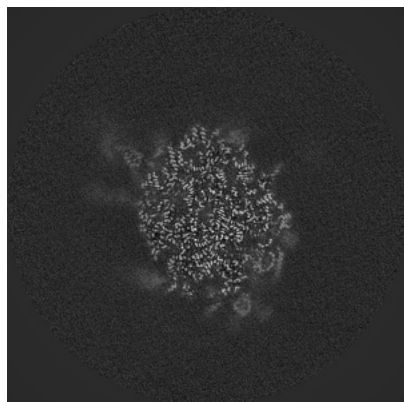


Y Index: 339

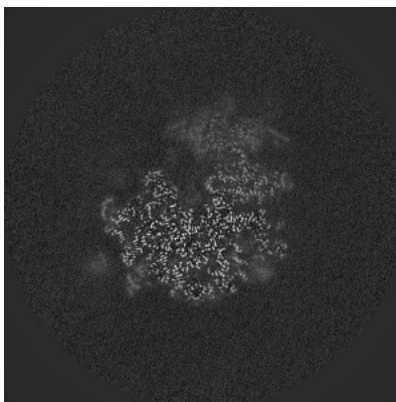


Z Index: 350

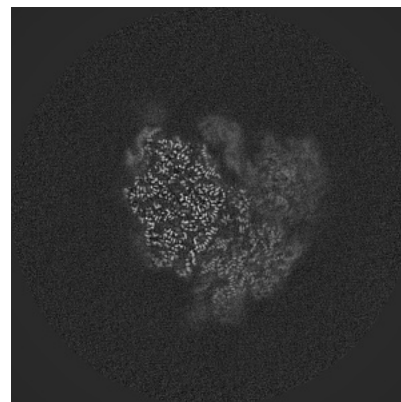
6.3.2 Raw map



X Index: 288



Y Index: 339

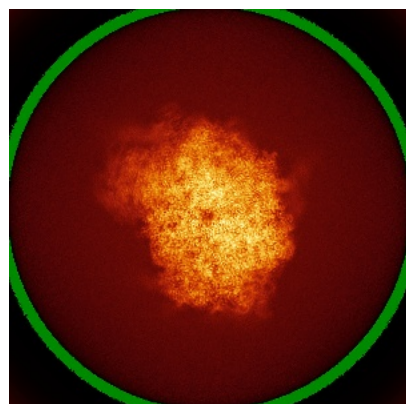


Z Index: 350

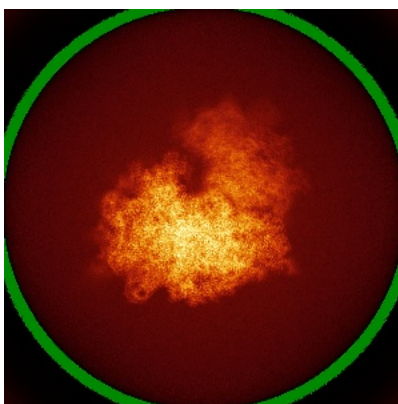
The images above show the largest variance slices of the map in three orthogonal directions.

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

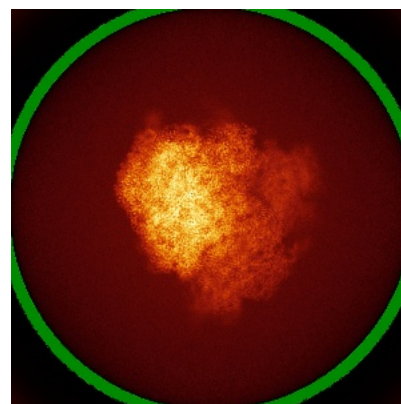
6.4.1 Primary map



X

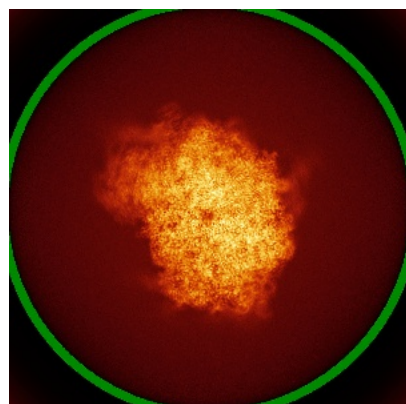


Y

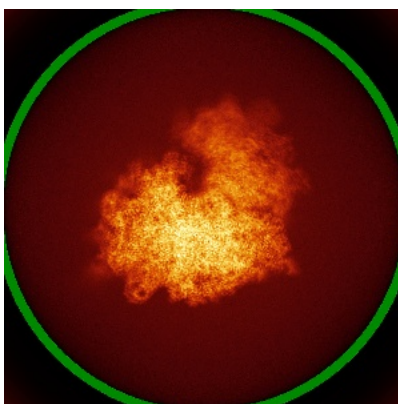


Z

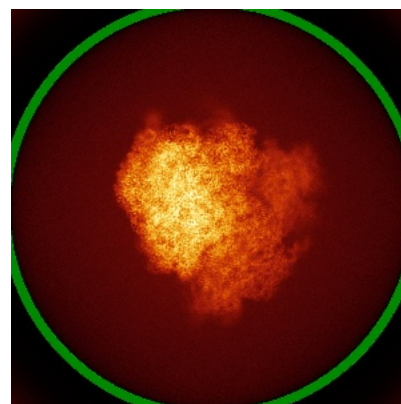
6.4.2 Raw map



X



Y

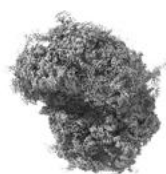


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



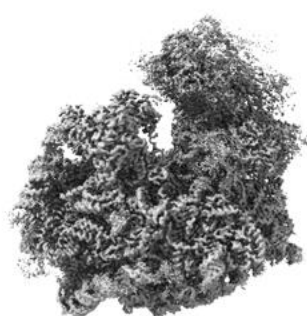
Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

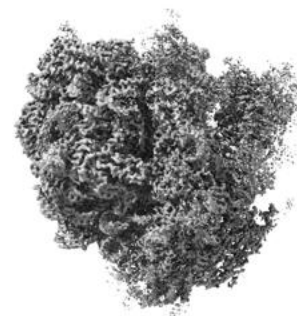
6.5.2 Raw map



X



Y



Z

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

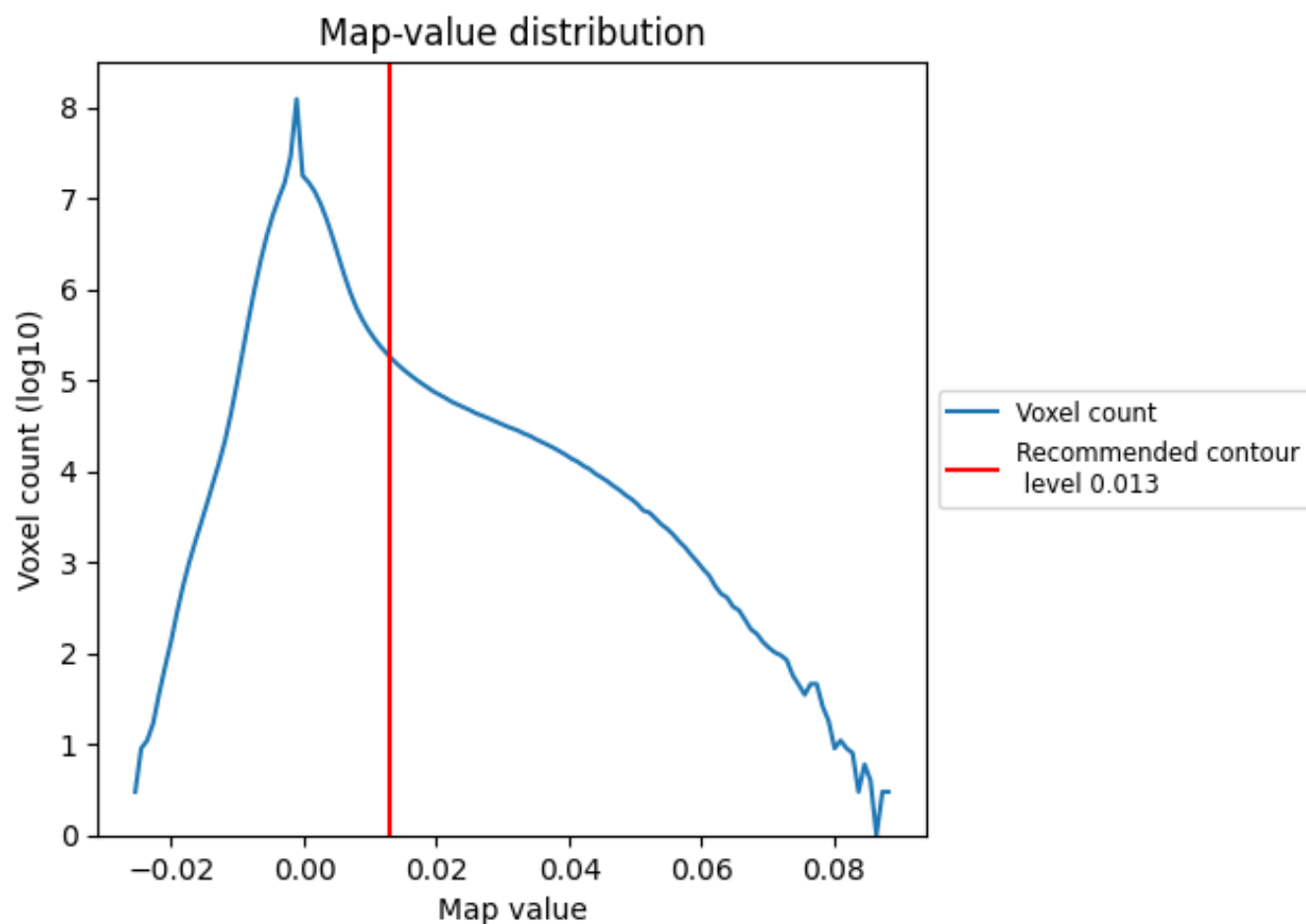
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

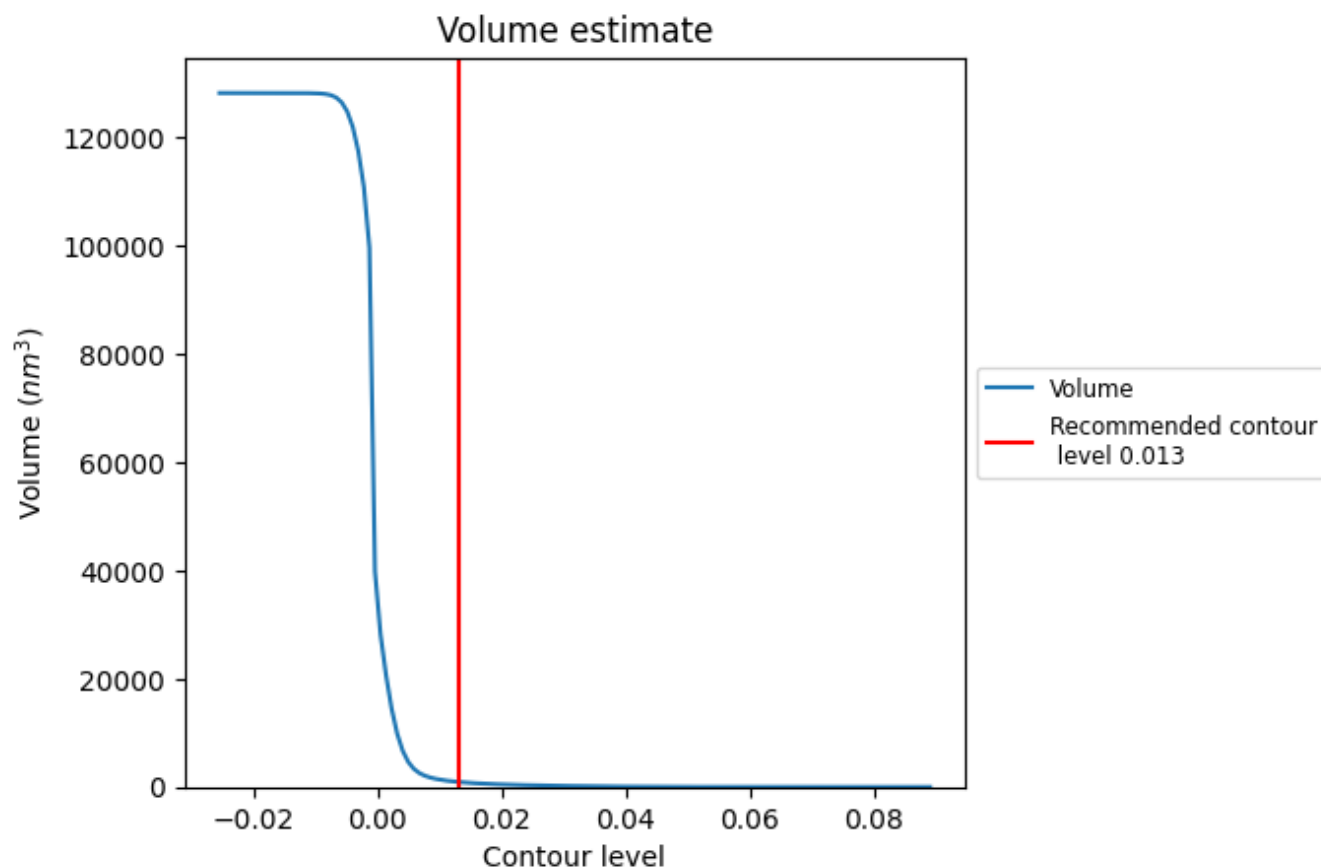
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

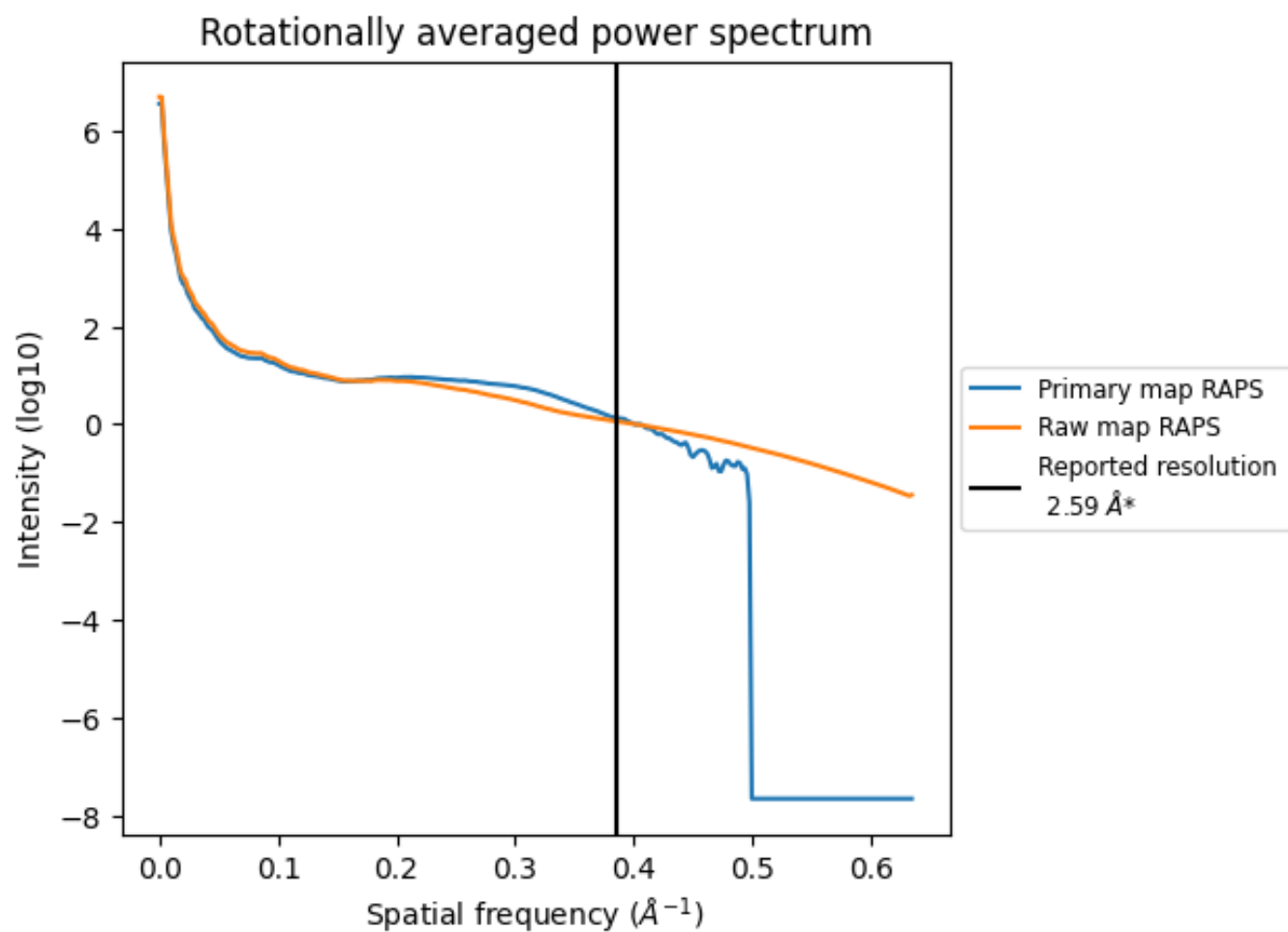
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 927 nm^3 ; this corresponds to an approximate mass of 837 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

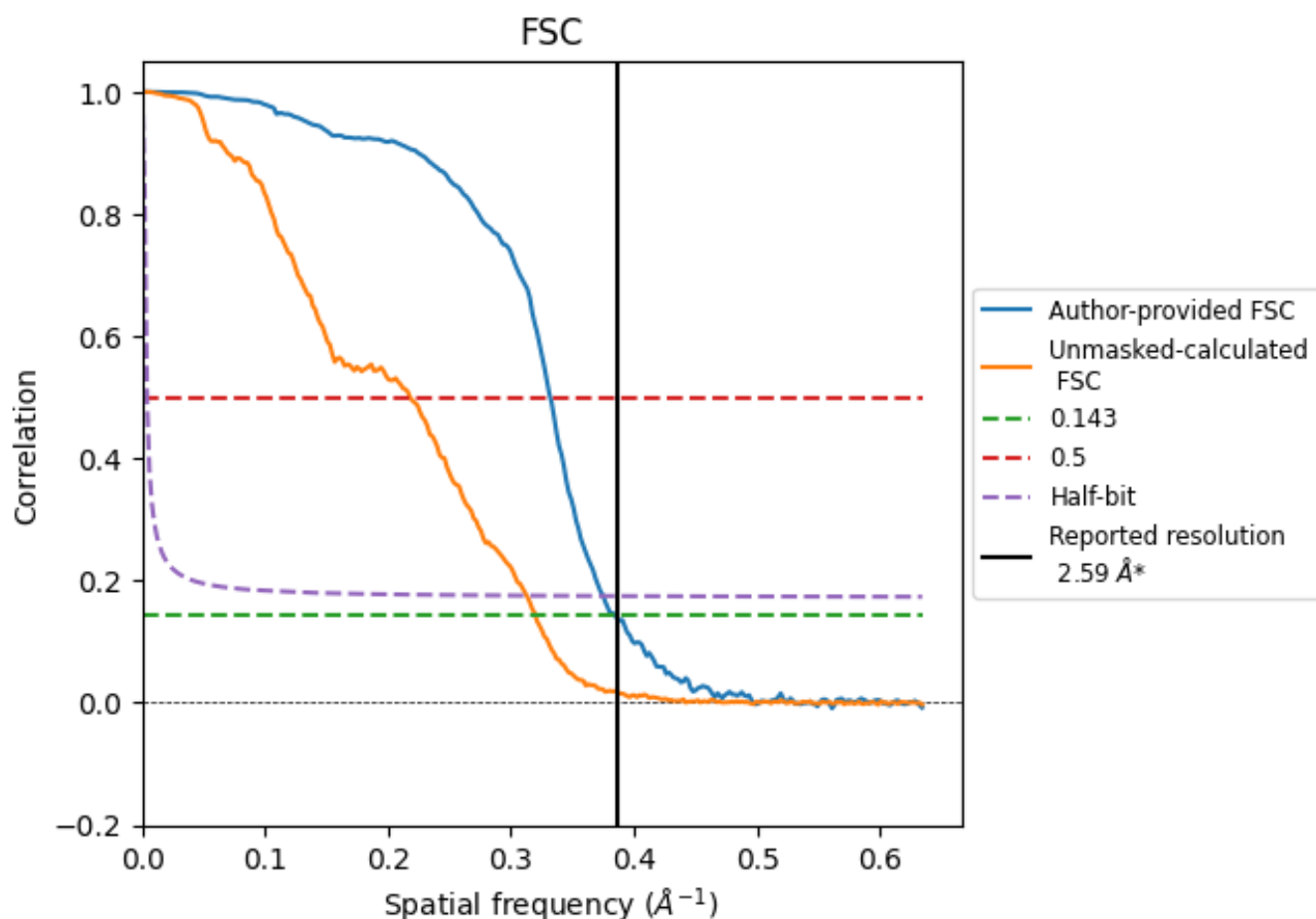


*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.386 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

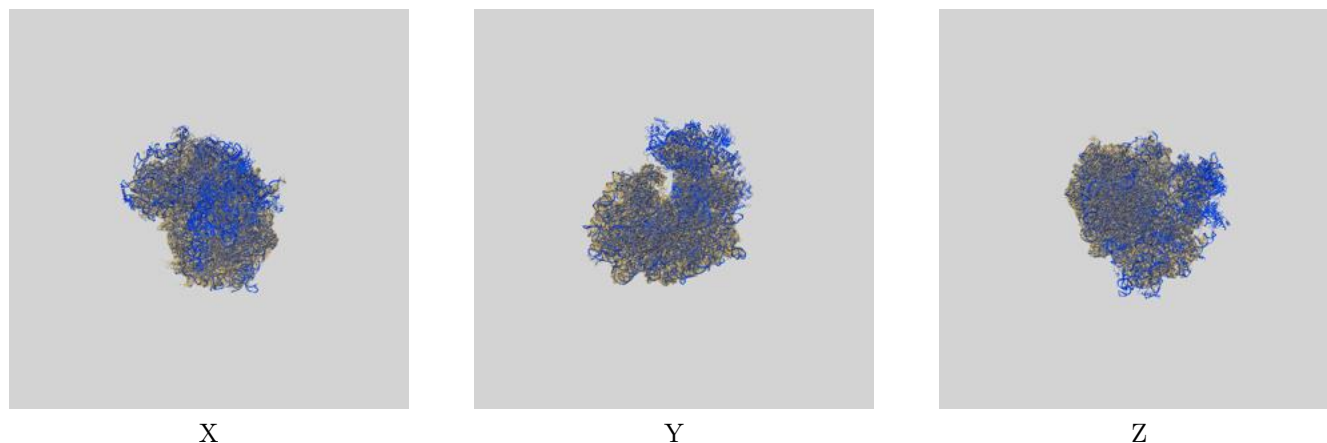
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.60	3.01	2.67
Unmasked-calculated*	3.13	4.59	3.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.13 differs from the reported value 2.59 by more than 10 %

9 Map-model fit [i](#)

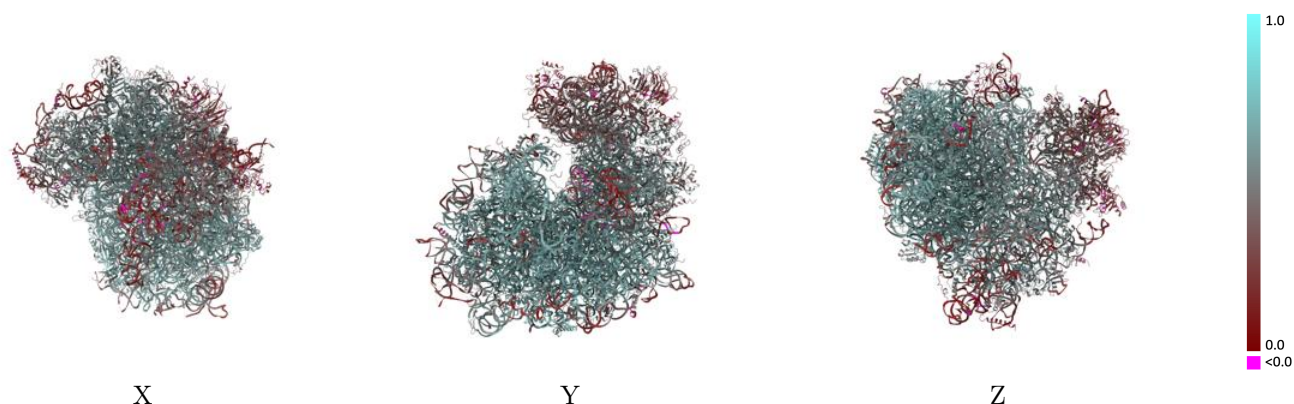
This section contains information regarding the fit between EMDB map EMD-35413 and PDB model 8IFD. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



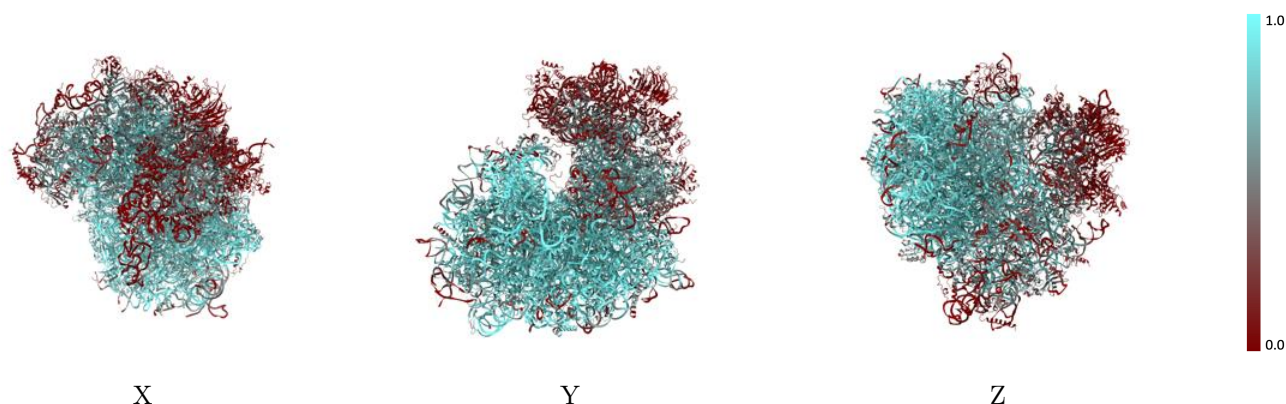
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



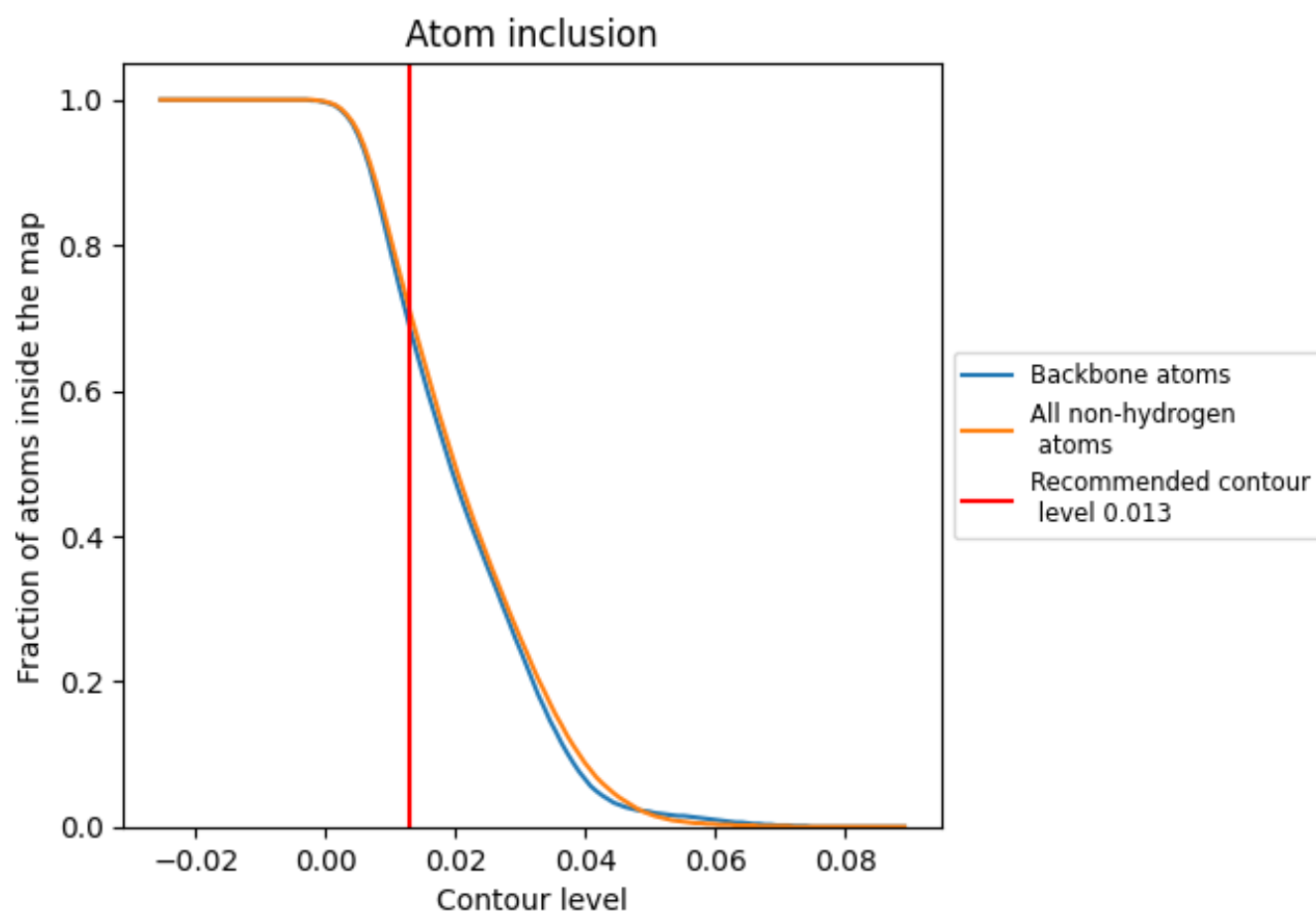
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7070	 0.5390
1A	 0.8460	 0.5680
1B	 0.9720	 0.6270
1C	 0.9160	 0.6050
1D	 0.9430	 0.6630
1E	 0.8880	 0.6400
1F	 0.8960	 0.6400
1G	 0.8470	 0.6080
1H	 0.7790	 0.5820
20	 0.1950	 0.3740
21	 0.0930	 0.3710
2A	 0.9050	 0.6480
2B	 0.7670	 0.5710
2C	 0.8430	 0.6240
2D	 0.7950	 0.6080
2E	 0.6190	 0.5400
2F	 0.8490	 0.6090
2G	 0.8810	 0.6200
2H	 0.9640	 0.6690
2I	 0.9020	 0.6420
2J	 0.9170	 0.6590
2K	 0.9380	 0.6630
2L	 0.7650	 0.5980
2M	 0.9190	 0.6490
2N	 0.8640	 0.6350
2O	 0.5730	 0.5180
2P	 0.8870	 0.6480
2Q	 0.4210	 0.4260
2R	 0.8570	 0.6310
2S	 0.8770	 0.6360
2T	 0.8580	 0.6170
2U	 0.9430	 0.6620
2V	 0.7380	 0.5730
2W	 0.8170	 0.6040
2X	 0.8550	 0.6300



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Chain	Atom inclusion	Q-score
2Y	 0.9230	 0.6550
2Z	 0.9400	 0.6610
2a	 0.8370	 0.6250
2b	 0.8650	 0.6260
2c	 0.8380	 0.6180
2d	 0.9440	 0.6570
2e	 0.7310	 0.5850
2f	 0.8860	 0.6430
2g	 0.8440	 0.6350
2h	 0.8570	 0.6500
2i	 0.8290	 0.6240
2j	 0.8680	 0.6390
2k	 0.9320	 0.6430
2l	 0.0230	 0.2010
2m	 0.6130	 0.4610
2n	 0.2280	 0.4800
2o	 0.5730	 0.5480
2p	 0.0620	 0.3760
2q	 0.5490	 0.5290
2r	 0.2010	 0.4160
2s	 0.2490	 0.4530
2t	 0.5740	 0.5480
2u	 0.0160	 0.2680
2v	 0.6040	 0.5660
2w	 0.0400	 0.3410
2x	 0.1680	 0.3880
2y	 0.0740	 0.3900
2z	 0.1530	 0.3740
3A	 0.3220	 0.5070
3B	 0.6160	 0.5670
3C	 0.6130	 0.5550
3D	 0.2080	 0.4050
3E	 0.2000	 0.3870
3F	 0.0100	 0.2940
3G	 0.5510	 0.5230
3H	 0.3120	 0.4270
3I	 0.4990	 0.4940
3J	 0.0000	 0.1750
3K	 0.5830	 0.5680
3L	 0.6190	 0.5560
3M	 0.6840	 0.5720
3N	 0.4140	 0.4690

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Chain	Atom inclusion	Q-score
3O	 0.0960	 0.3310
3P	 0.2890	 0.4970
3Q	 0.3580	 0.4730
3R	 0.0000	 0.1770