wwPDB EM Validation Summary Report

Jun 9, 2024 – 04:03 AM JST

PDB ID	:	8IFD
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:

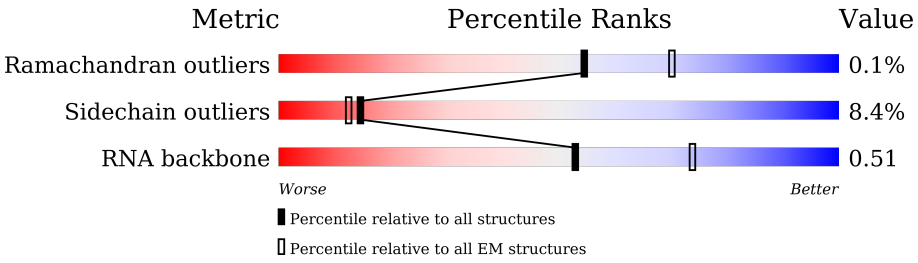
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.59 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.



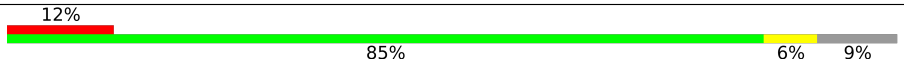
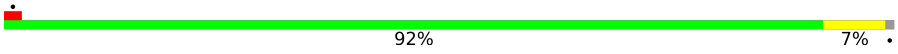
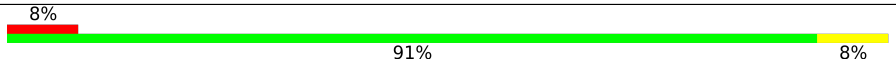
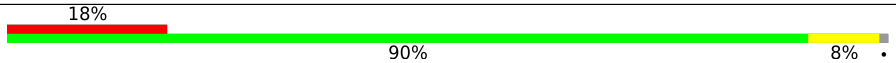
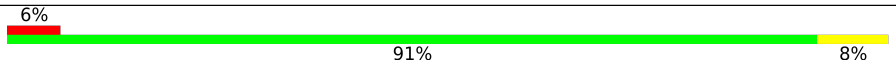
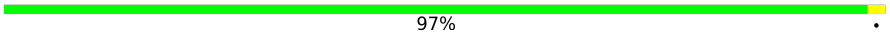
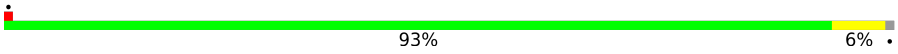
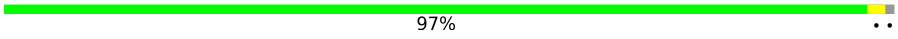
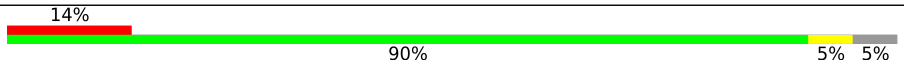
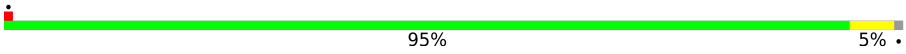
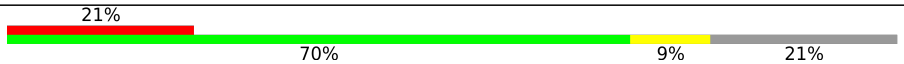
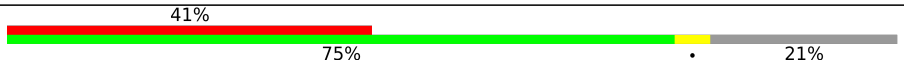
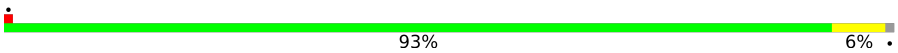
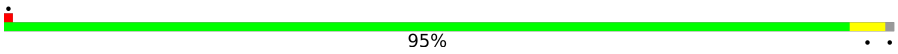
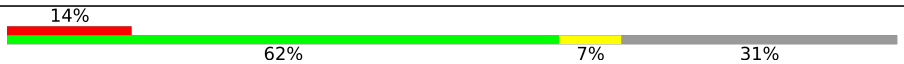
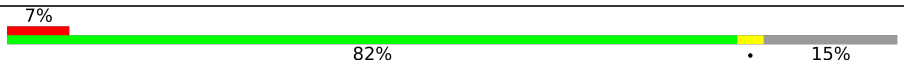
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1A	5070	9% 57% 16% 27%
2	1B	121	87% 12%
3	1C	157	7% 81% 18%
4	1D	257	93%
5	1E	403	95% 5%
6	1F	427	82% 14%
7	1G	297	5% 93% 6%
8	1H	288	9% 75% 7% 18%

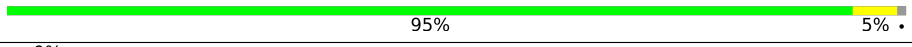
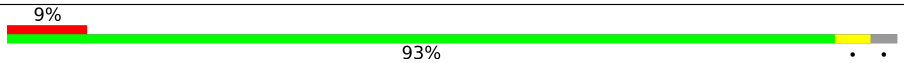
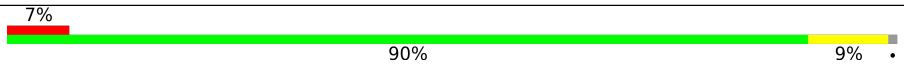
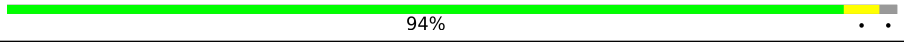
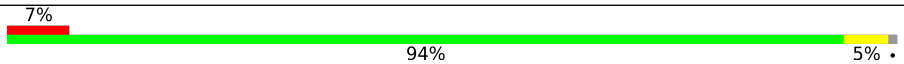
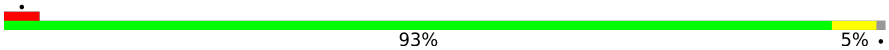
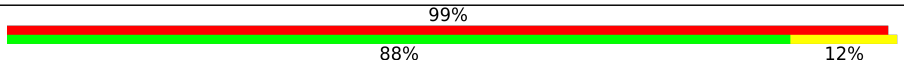
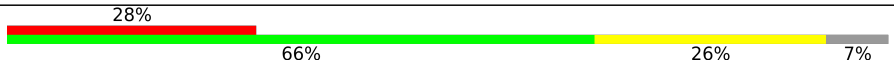
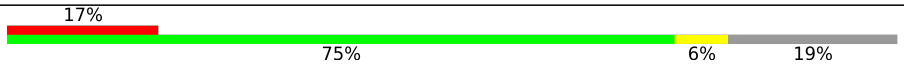
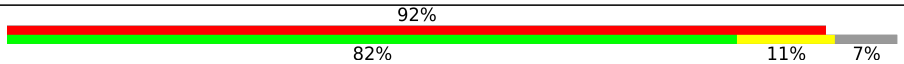
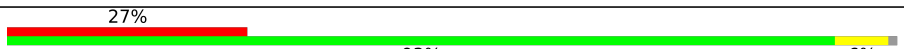
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
29	2U	148	
30	2V	159	
31	2W	115	
32	2X	125	
33	2Y	135	

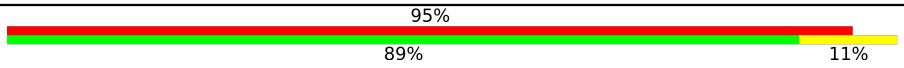
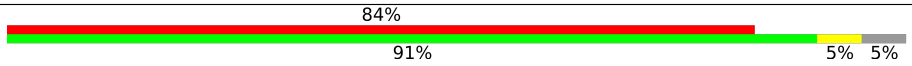
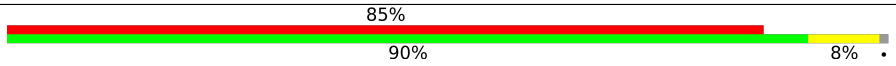
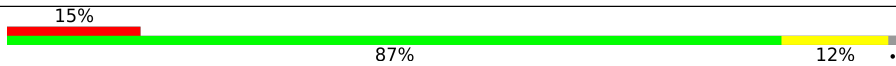
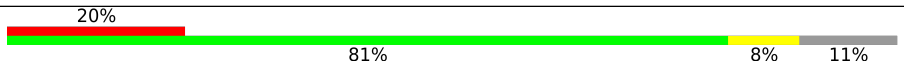
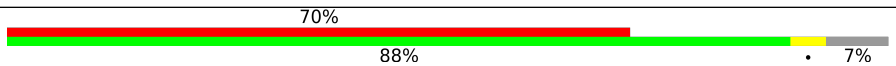
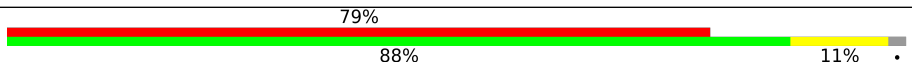
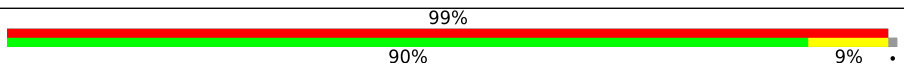
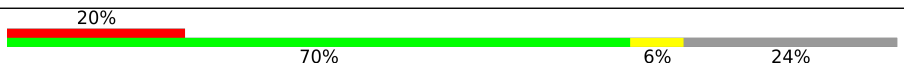
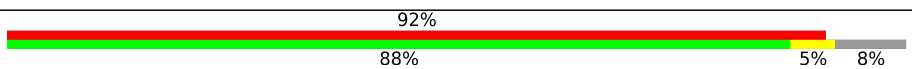
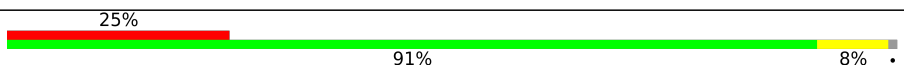
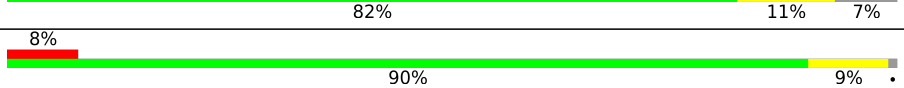
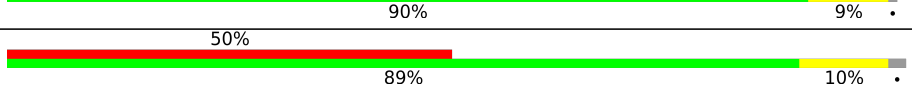
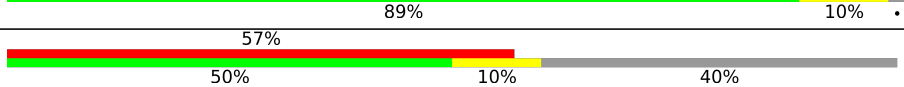
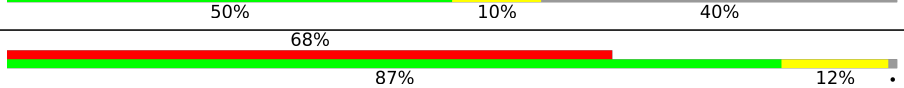
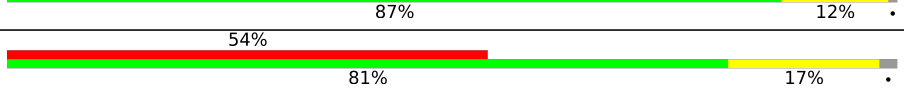
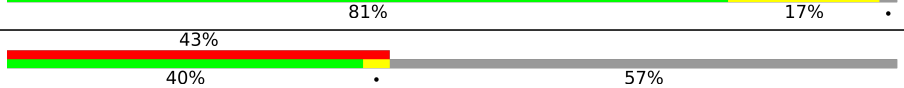
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
54	2t	208	
55	2u	165	
56	2v	158	
57	2w	145	
58	2x	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
79	3Q	59	
80	3R	156	

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
			Total	C	N	O	P		
1	1A	3717	79674	35479	14585	25894	3716	0	0

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
			Total	C	N	O	P		
2	1B	120	2558	1141	456	842	119	0	0

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

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

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

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

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

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

- 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		

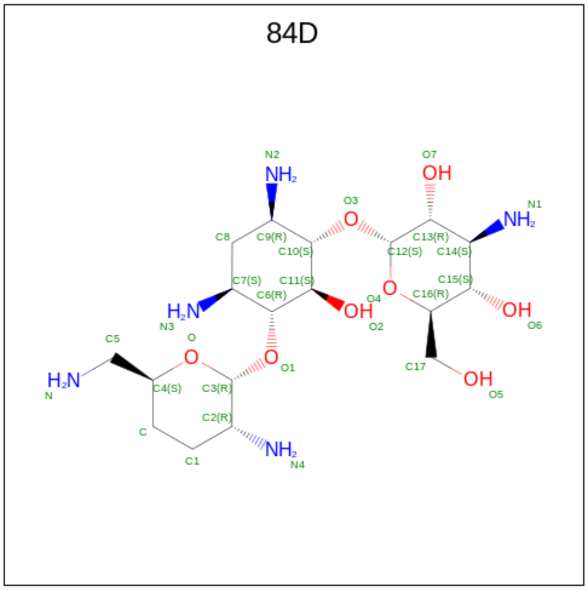
- Molecule 79 is a protein called 40S ribosomal protein S30.

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 (three-letter code: 84D) (formula: $C_{18}H_{37}N_5O_8$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
82	2V	1	Total Mg 1 1	0
82	2Y	1	Total Mg 1 1	0
82	2Z	1	Total Mg 1 1	0
82	2a	1	Total Mg 1 1	0
82	2d	1	Total Mg 1 1	0
82	2m	105	Total Mg 105 105	0
82	20	1	Total Mg 1 1	0
82	3H	1	Total Mg 1 1	0
82	3K	1	Total Mg 1 1	0
82	3L	1	Total Mg 1 1	0

- Molecule 83 is ZINC ION (three-letter code: ZN) (formula: Zn).

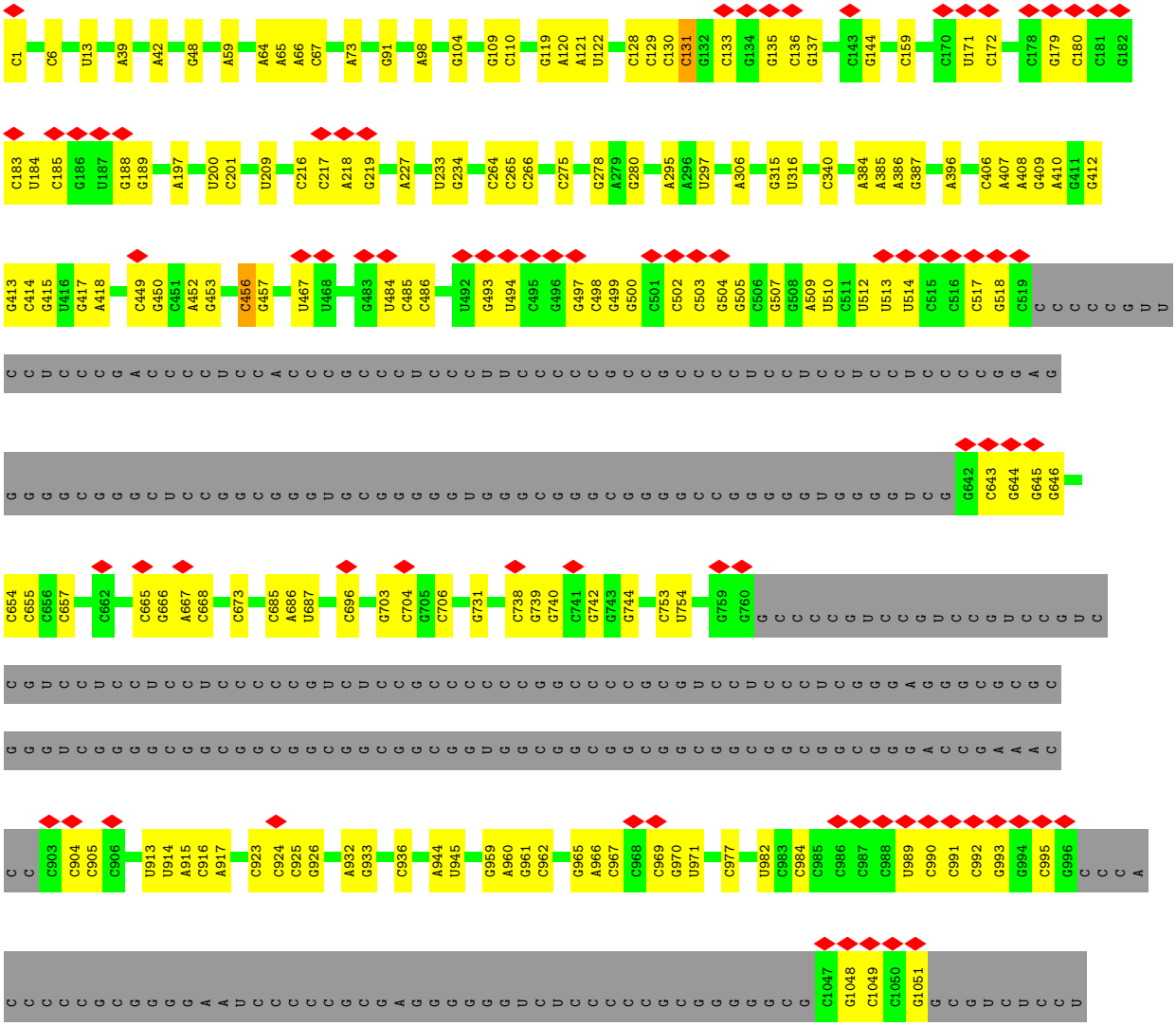
Mol	Chain	Residues	Atoms	AltConf
83	2d	1	Total Zn 1 1	0
83	2g	1	Total Zn 1 1	0
83	2j	1	Total Zn 1 1	0
83	3C	1	Total Zn 1 1	0

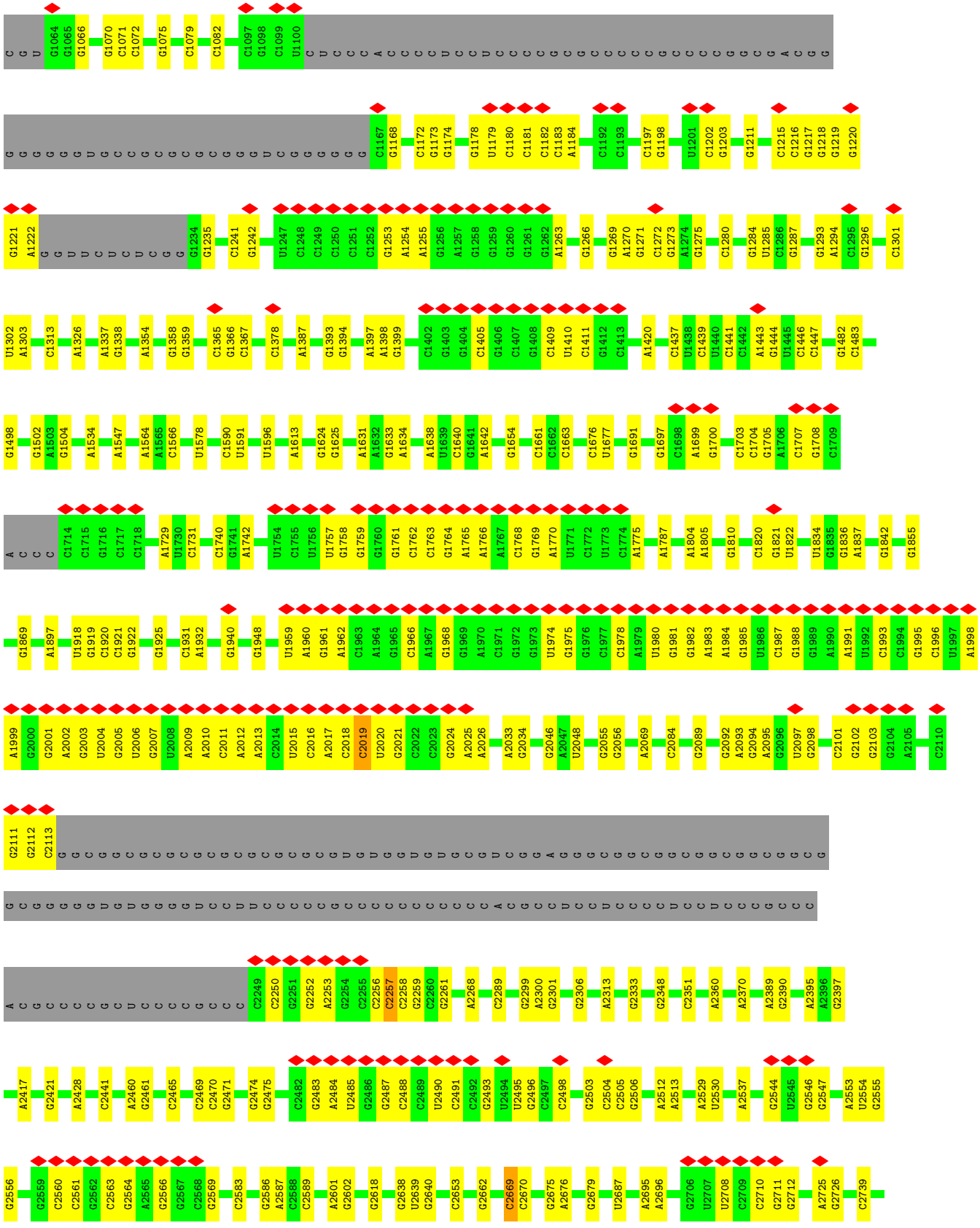
3 Residue-property plots (i)

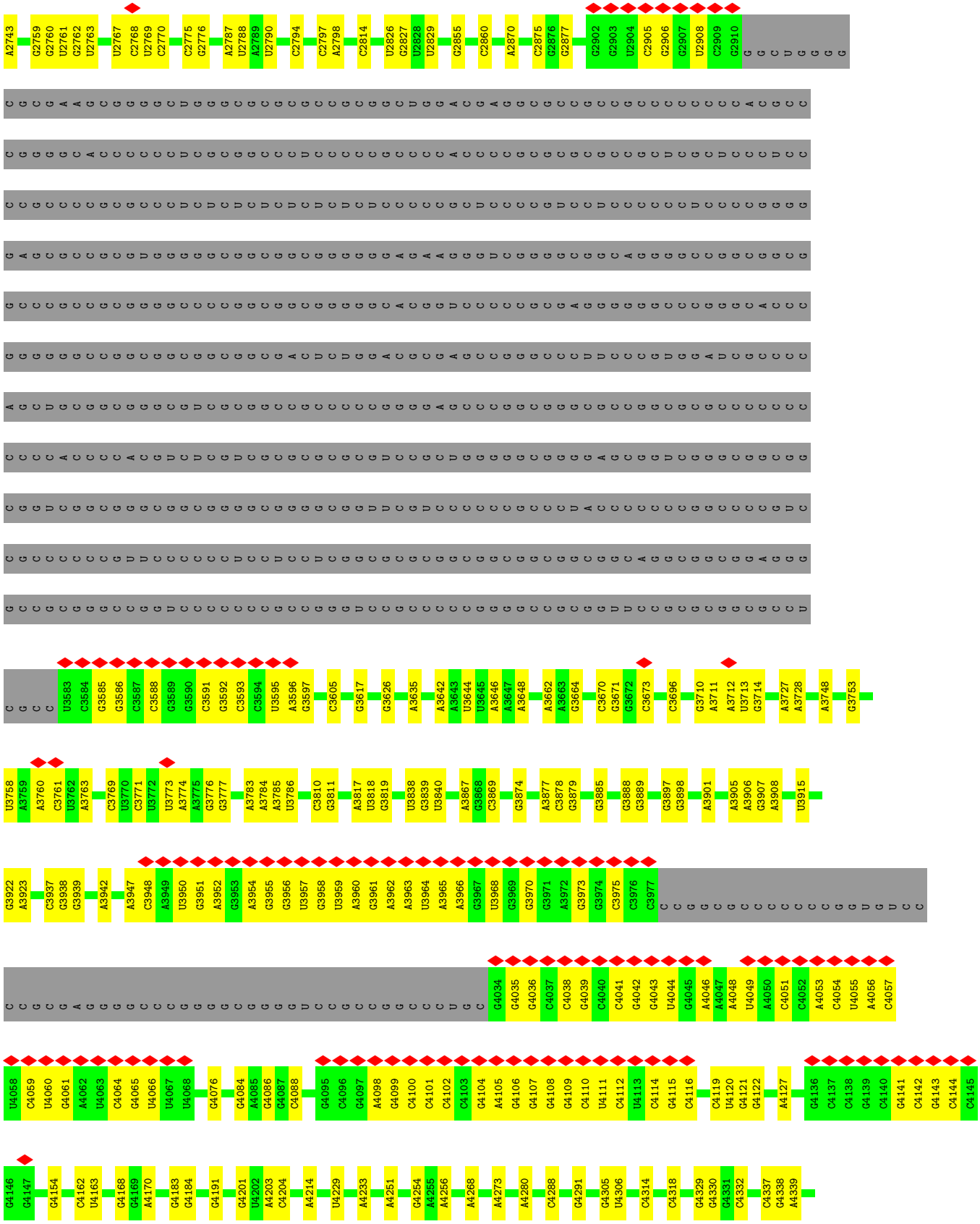
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

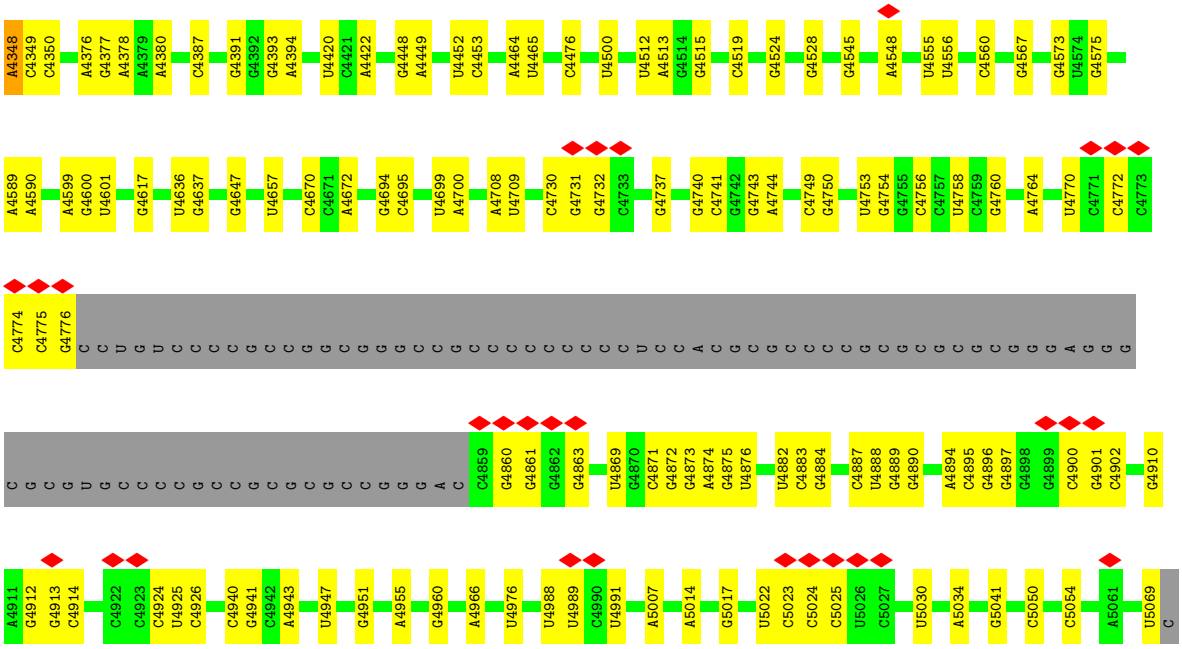
- Molecule 1: 28S ribosomal RNA

Chain 1A:



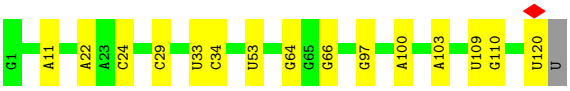






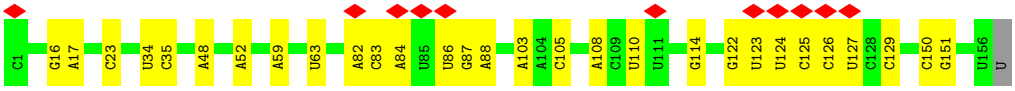
• Molecule 2: 5S ribosomal RNA

Chain 1B:



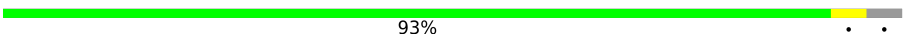
• Molecule 3: 5.8S ribosomal RNA

Chain 1C:



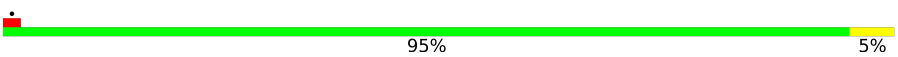
• Molecule 4: 60S ribosomal protein L8

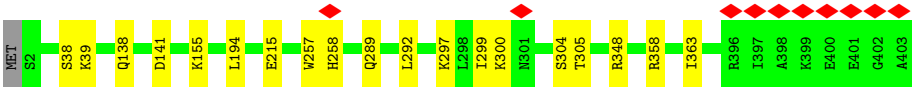
Chain 1D:



• Molecule 5: 60S ribosomal protein L3

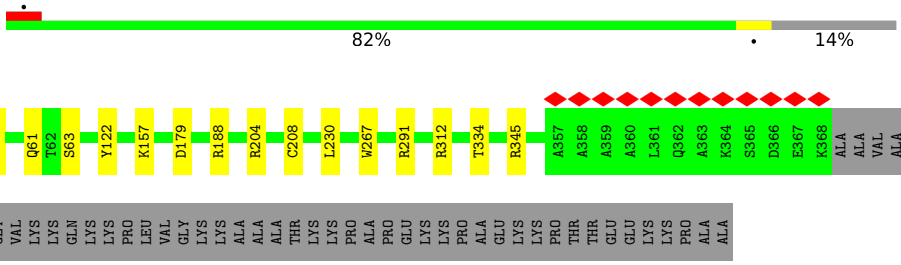
Chain 1E:





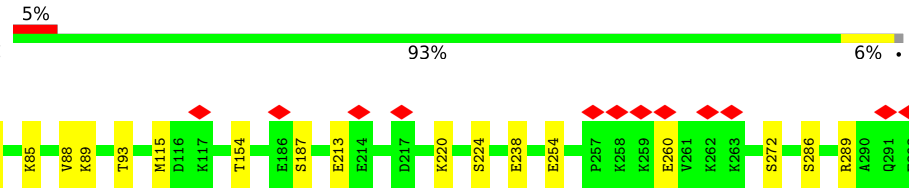
• Molecule 6: 60S ribosomal protein L4

Chain 1F:



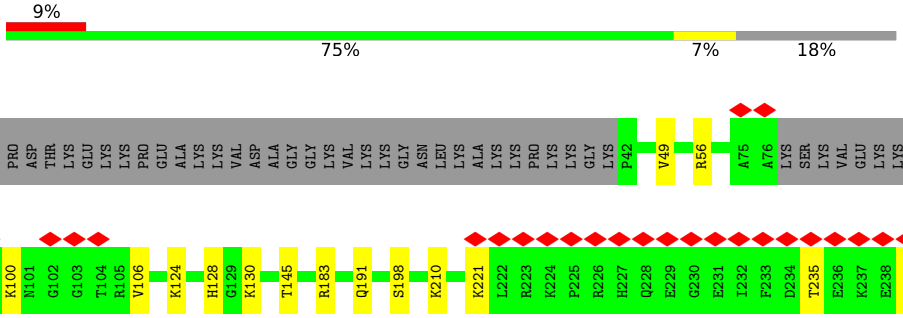
• Molecule 7: 60S ribosomal protein L5

Chain 1G:



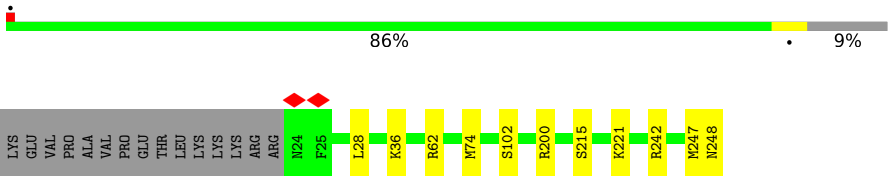
• Molecule 8: 60S ribosomal protein L6

Chain 1H:



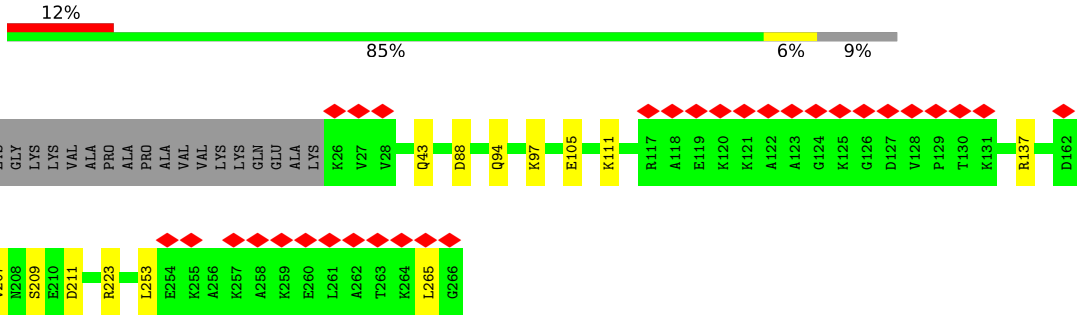
• Molecule 9: 60S ribosomal protein L7

Chain 2A:



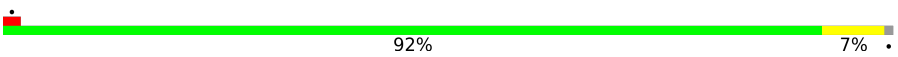
• Molecule 10: 60S ribosomal protein L7a

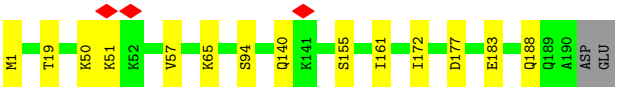
Chain 2B:



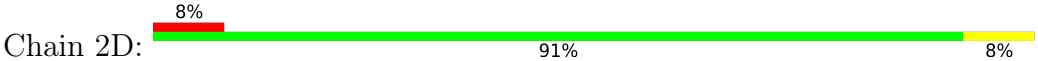
• Molecule 11: 60S ribosomal protein L9

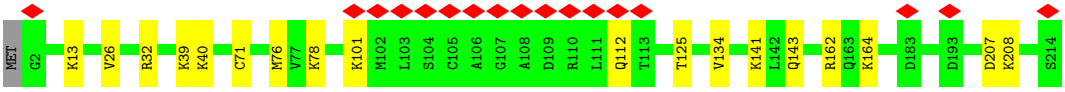
Chain 2C:



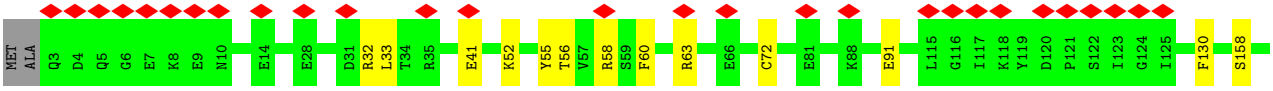


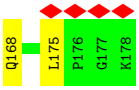
• Molecule 12: 60S ribosomal protein L10-like



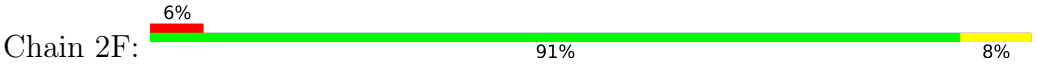


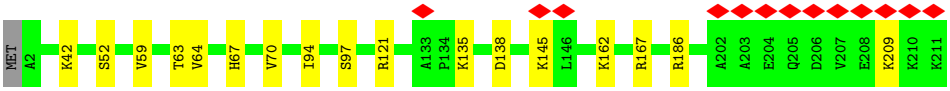
• Molecule 13: 60S ribosomal protein L11



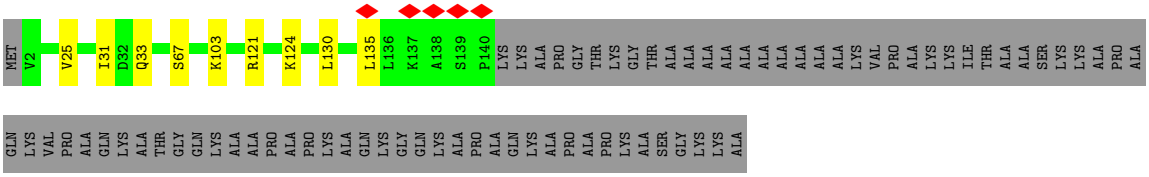


• Molecule 14: 60S ribosomal protein L13



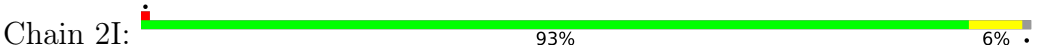


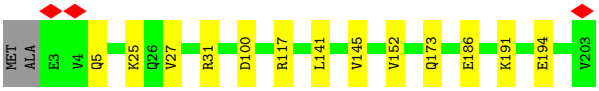
• Molecule 15: 60S ribosomal protein L14



• Molecule 16: 60S ribosomal protein L15

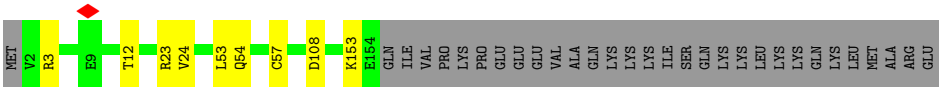
• Molecule 17: 60S ribosomal protein L13a





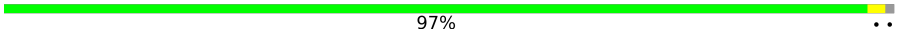
• Molecule 18: 60S ribosomal protein L17

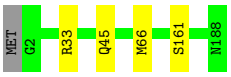
Chain 2J:



• Molecule 19: 60S ribosomal protein L18

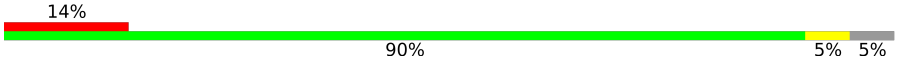
Chain 2K:





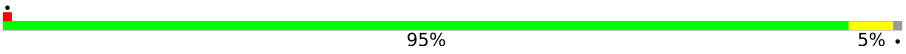
• Molecule 20: 60S ribosomal protein L19

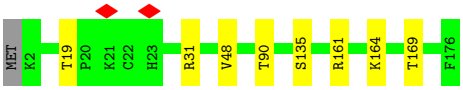
Chain 2L:



• Molecule 21: 60S ribosomal protein L18a

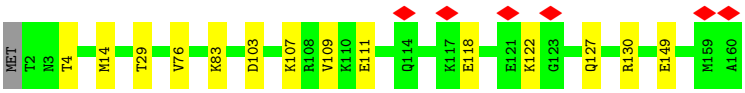
Chain 2M:





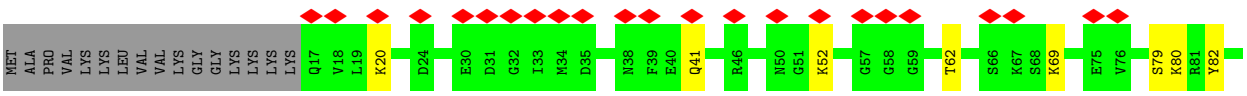
• Molecule 22: 60S ribosomal protein L21

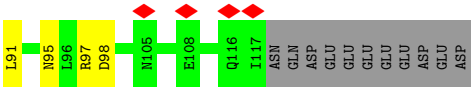
Chain 2N:



• Molecule 23: 60S ribosomal protein L22

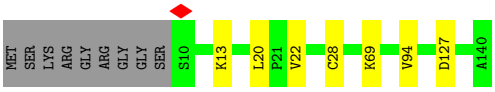
Chain 2O:





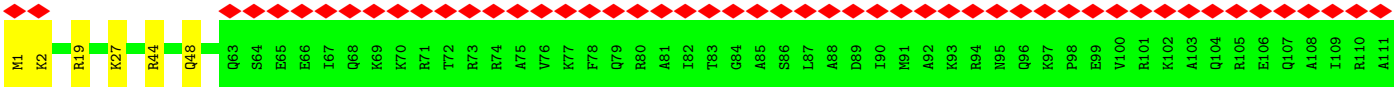
• Molecule 24: 60S ribosomal protein L23

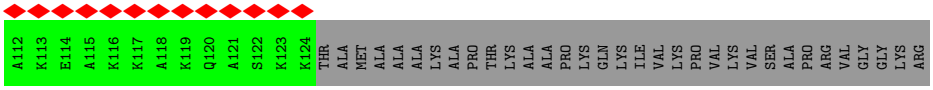
Chain 2P:



• Molecule 25: 60S ribosomal protein L24

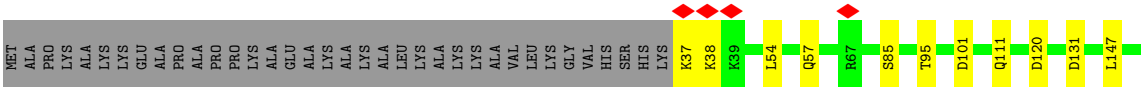
Chain 2Q:





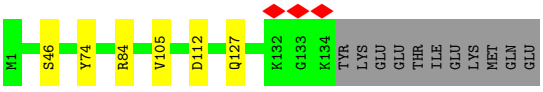
• Molecule 26: 60S ribosomal protein L23a

Chain 2R:



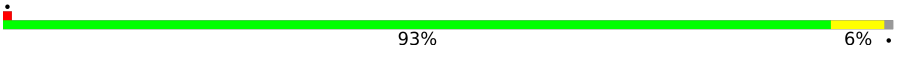
• Molecule 27: 60S ribosomal protein L26

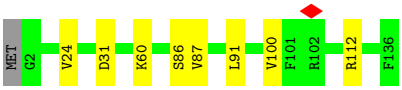
Chain 2S:



• Molecule 28: 60S ribosomal protein L27

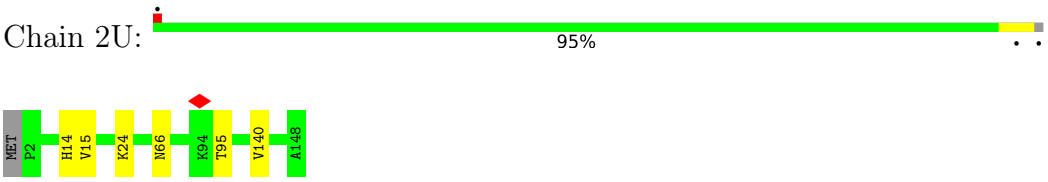
Chain 2T:





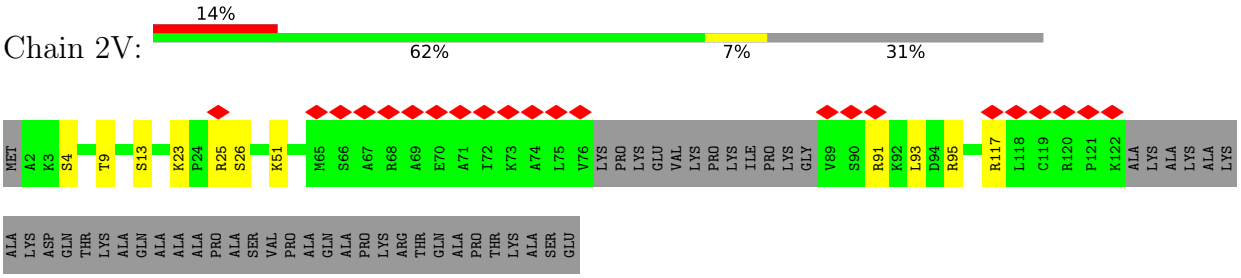
• Molecule 29: 60S ribosomal protein L27a

Chain 2U:



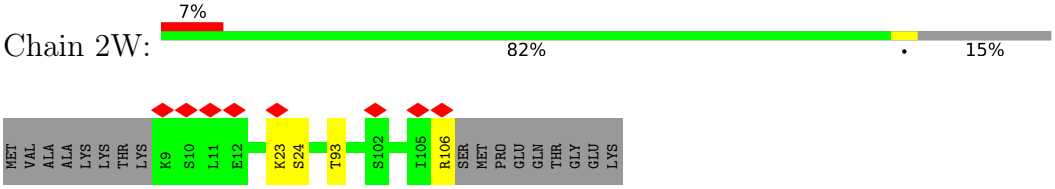
• Molecule 30: 60S ribosomal protein L29

Chain 2V:



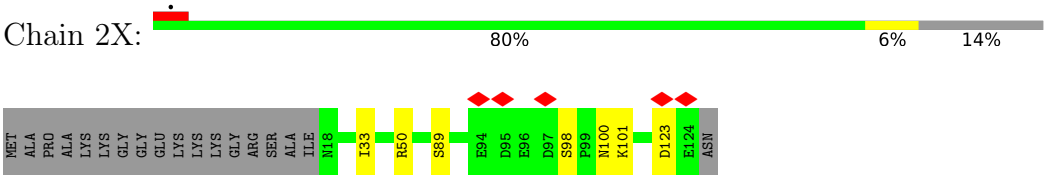
• Molecule 31: 60S ribosomal protein L30

Chain 2W:



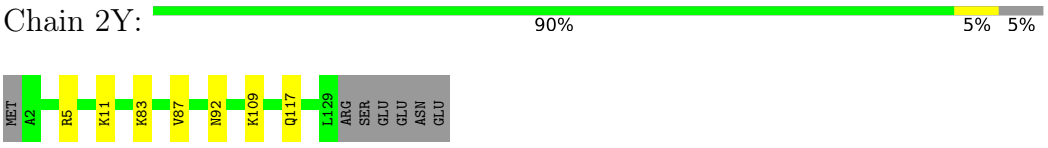
• Molecule 32: 60S ribosomal protein L31

Chain 2X:



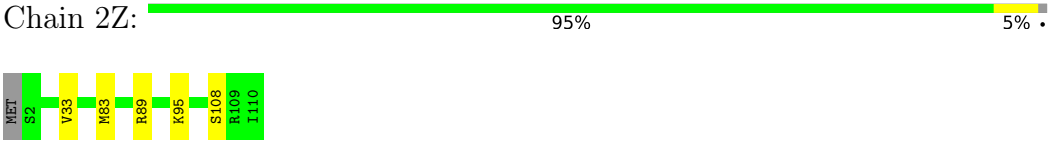
• Molecule 33: 60S ribosomal protein L32

Chain 2Y:



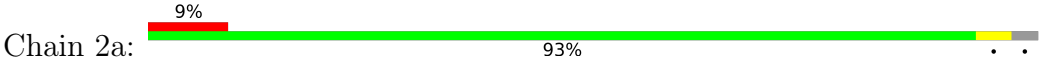
• Molecule 34: 60S ribosomal protein L35a

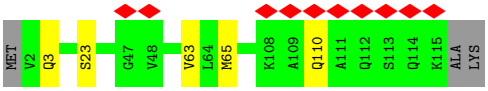
Chain 2Z:



• Molecule 35: 60S ribosomal protein L34

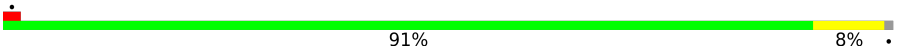
Chain 2a:

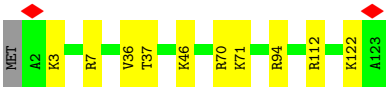




• Molecule 36: 60S ribosomal protein L35

Chain 2b:



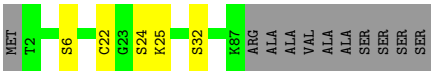


• Molecule 37: 60S ribosomal protein L36

Chain 2c:

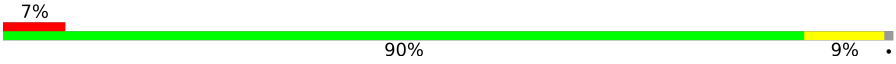
• Molecule 38: 60S ribosomal protein L37

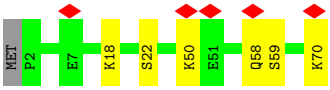
Chain 2d:



• Molecule 39: 60S ribosomal protein L38

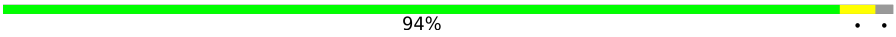
Chain 2e:





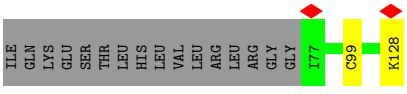
• Molecule 40: 60S ribosomal protein L39

Chain 2f:



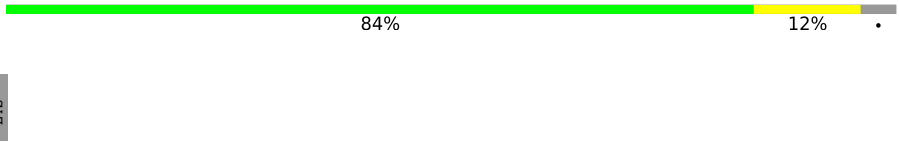
• Molecule 41: Large ribosomal subunit protein eL40

Chain 2g:



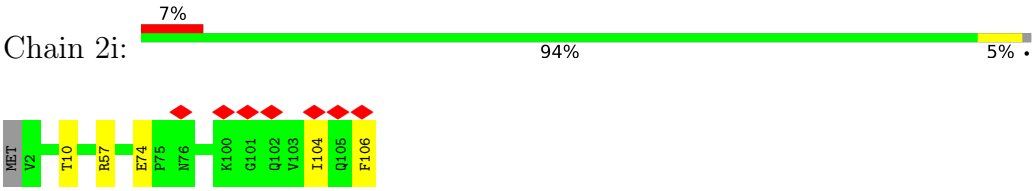
• Molecule 42: 60S ribosomal protein L41

Chain 2h:



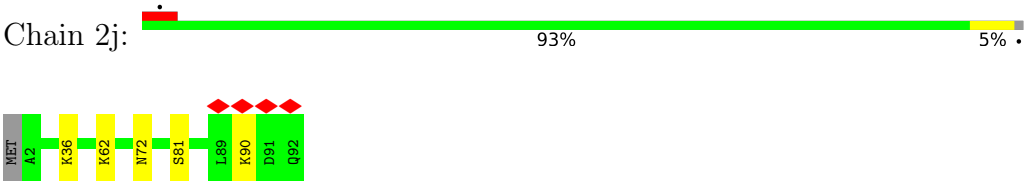
• Molecule 43: 60S ribosomal protein L36a

Chain 2i:



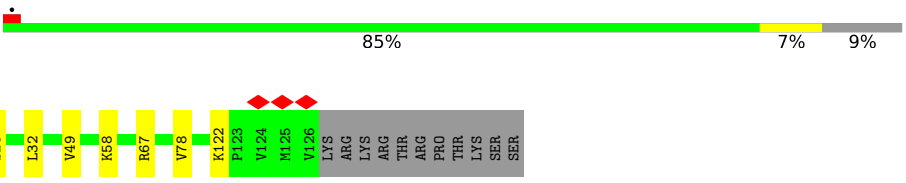
• Molecule 44: 60S ribosomal protein L37a

Chain 2j:



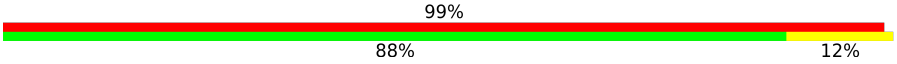
• Molecule 45: 60S ribosomal protein L28

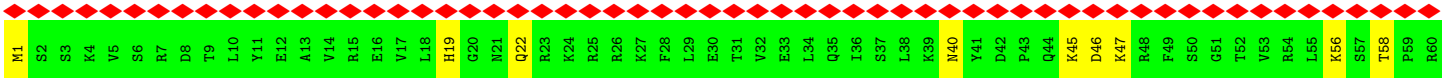
Chain 2k:

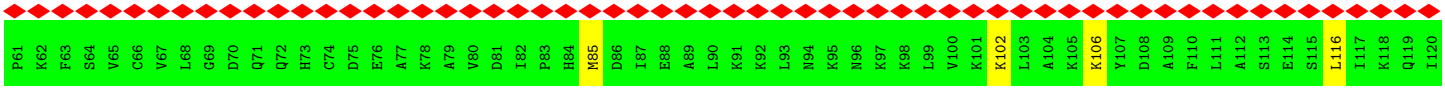


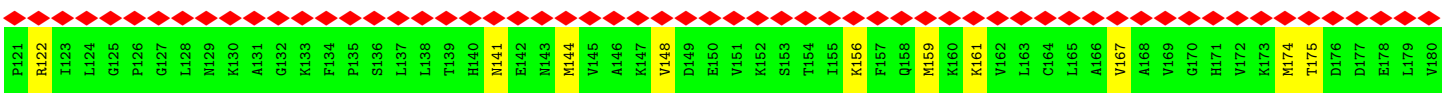
• Molecule 46: 60S ribosomal protein L10a

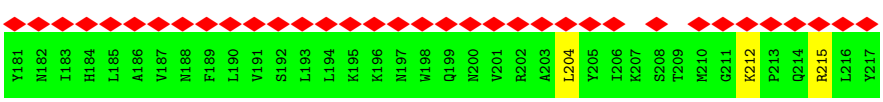
Chain 2l:





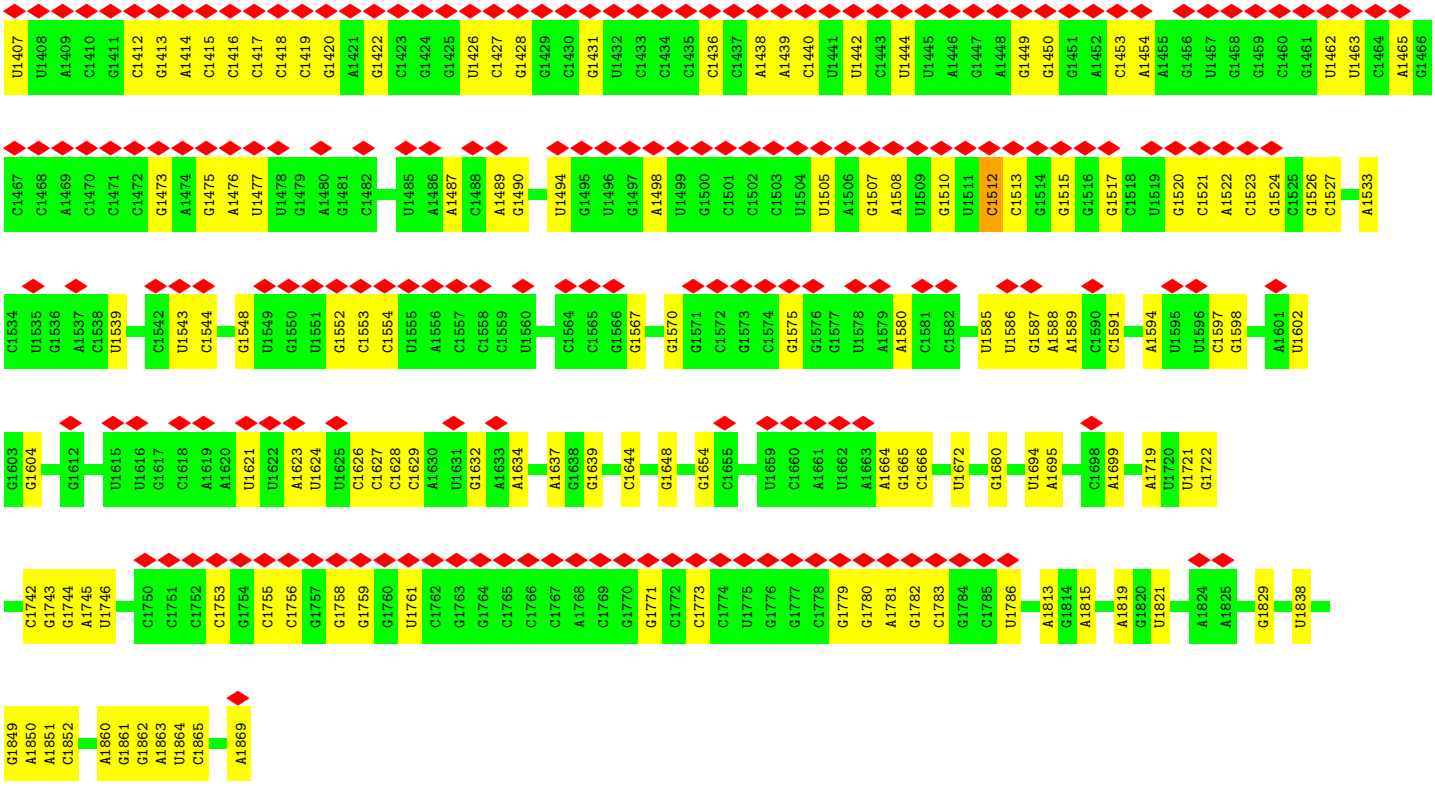






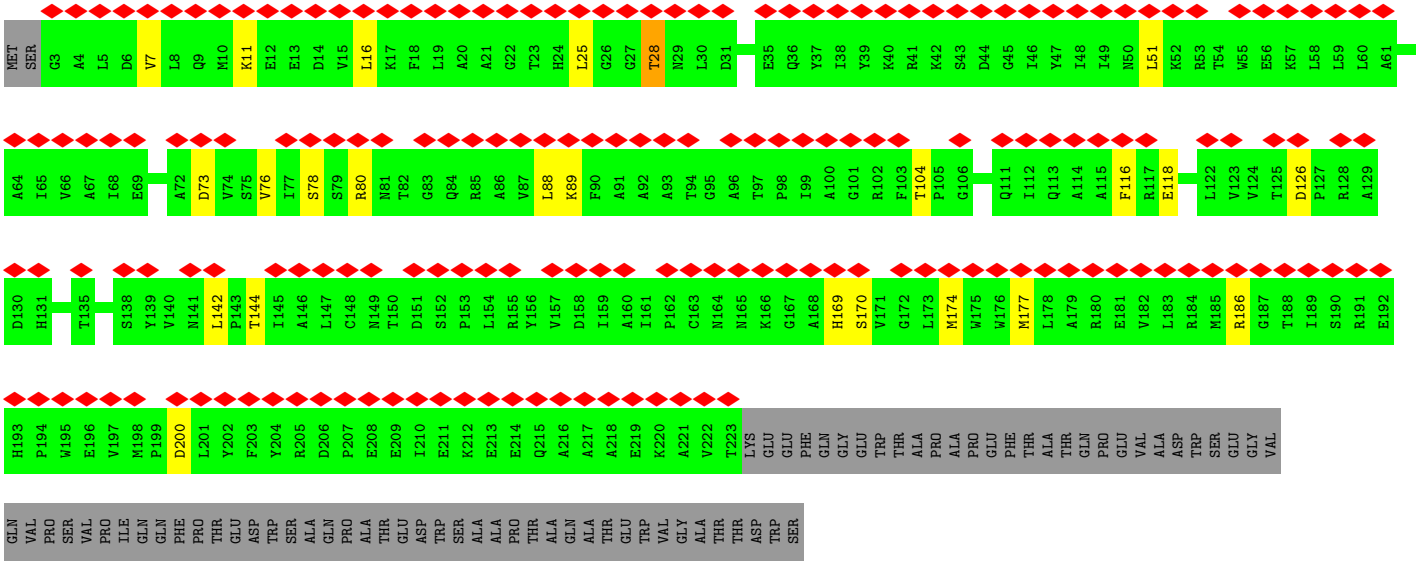
• Molecule 47: 18S ribosomal RNA

Chain 2m:



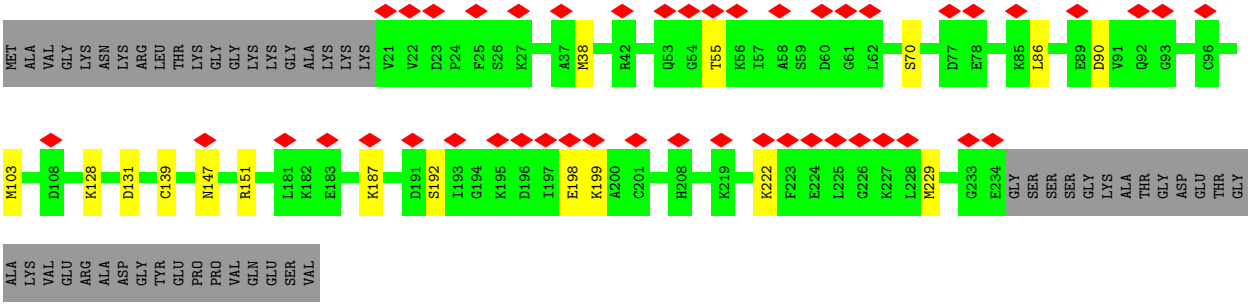
• Molecule 48: 40S ribosomal protein SA

Chain 2n:



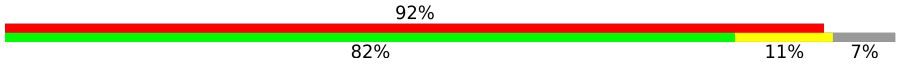
• Molecule 49: 40S ribosomal protein S3a

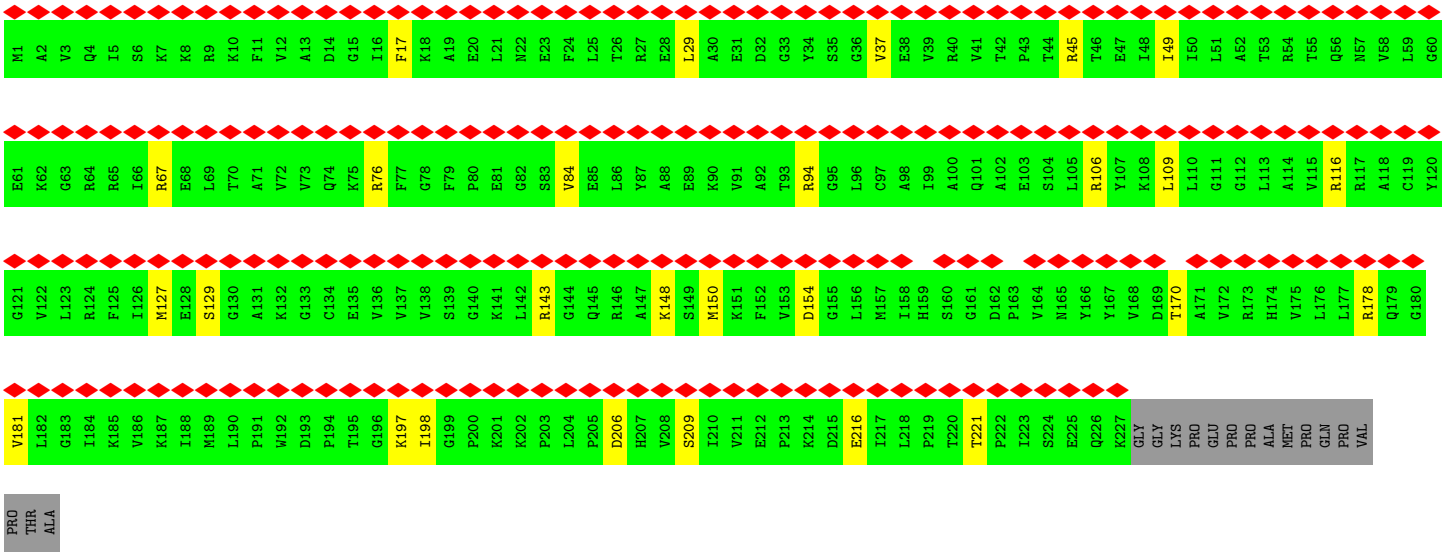
Chain 2o:



• Molecule 50: 40S ribosomal protein S3

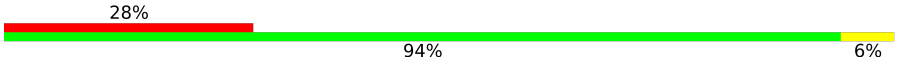
Chain 2p:

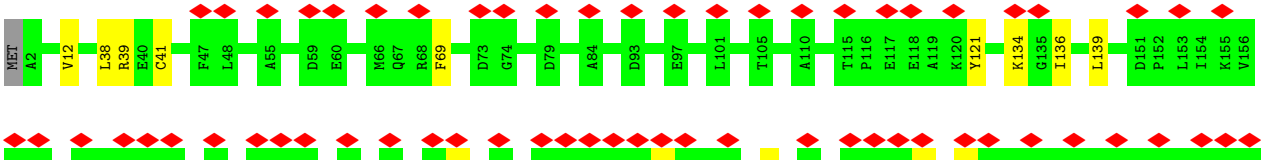


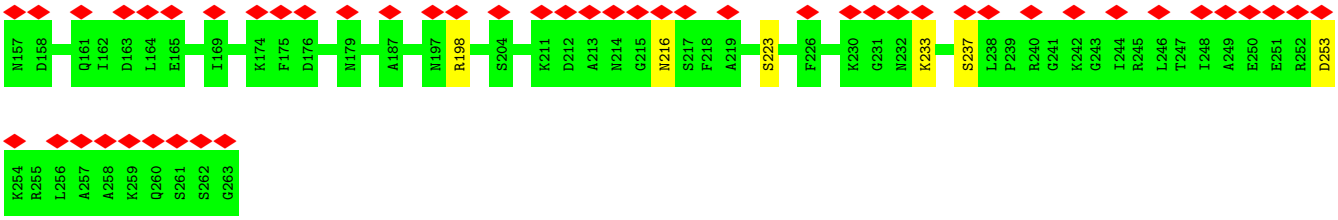


• Molecule 51: 40S ribosomal protein S4, X isoform

Chain 2q:

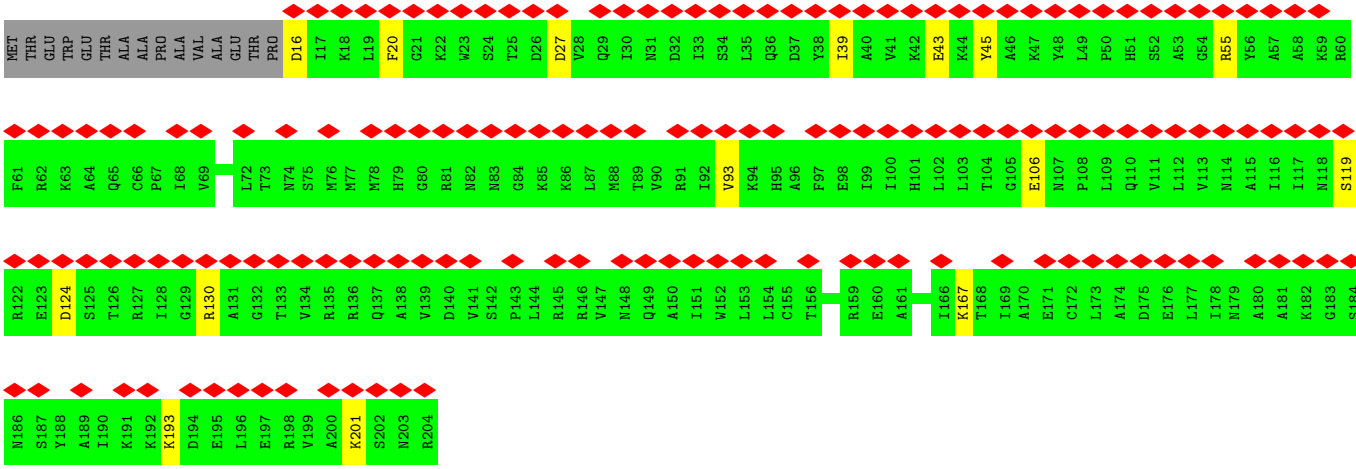






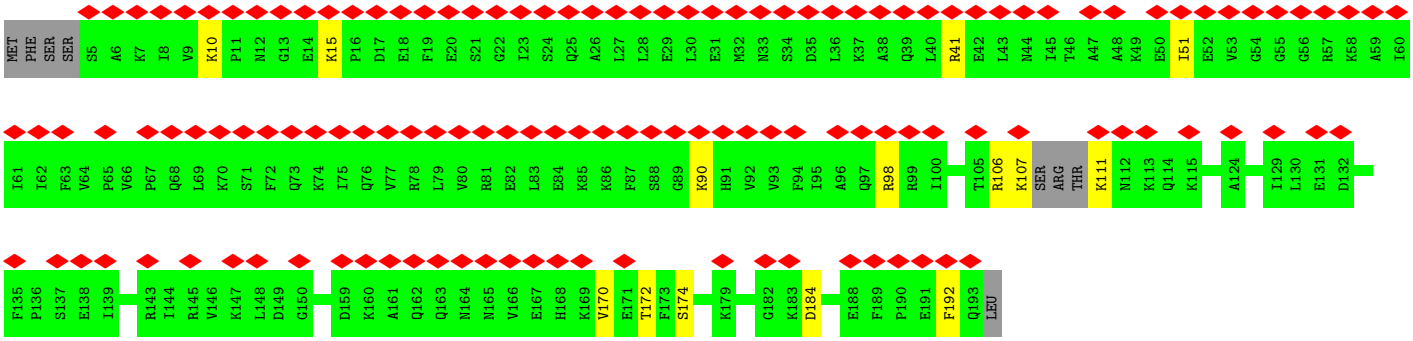
• Molecule 52: 40S ribosomal protein S5

Chain 2r:



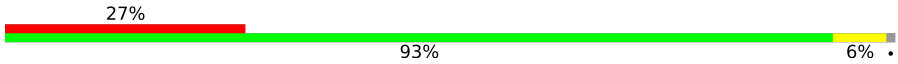
• Molecule 53: 40S ribosomal protein S7

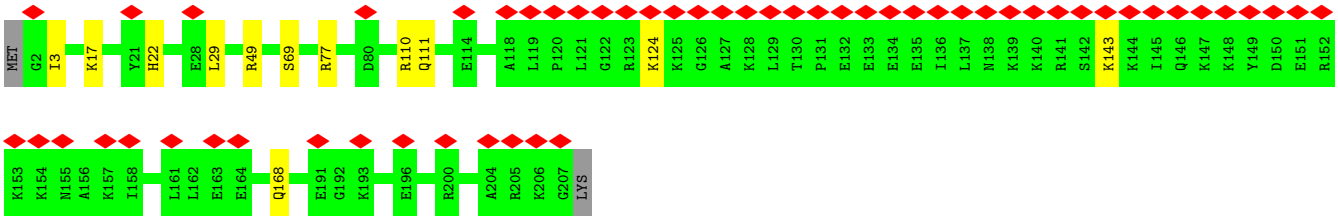
Chain 2s:



• Molecule 54: 40S ribosomal protein S8

Chain 2t:



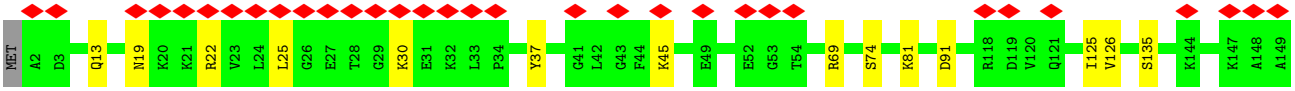


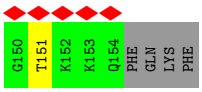
• Molecule 55: 40S ribosomal protein S10

Chain 2u:

• Molecule 56: 40S ribosomal protein S11

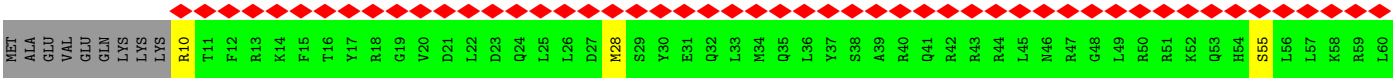
Chain 2v:

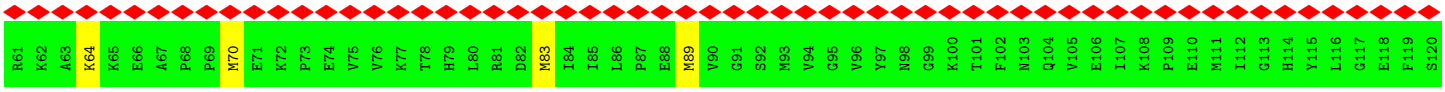


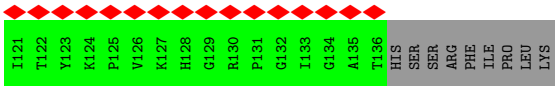


• Molecule 57: 40S ribosomal protein S15

Chain 2w:

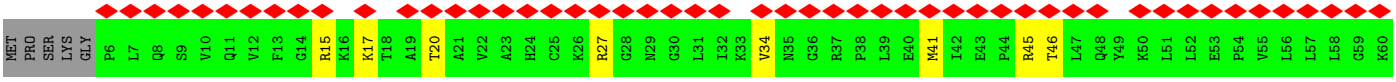


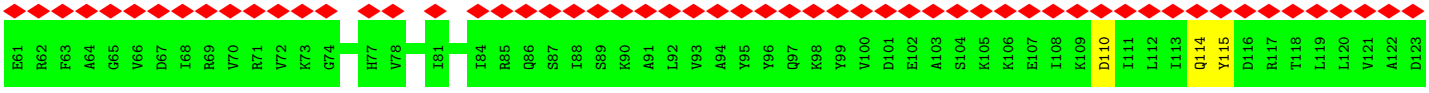


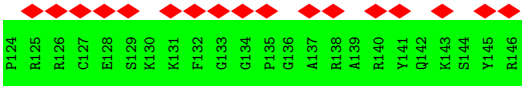


• Molecule 58: 40S ribosomal protein S16

Chain 2x:

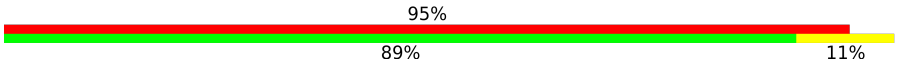


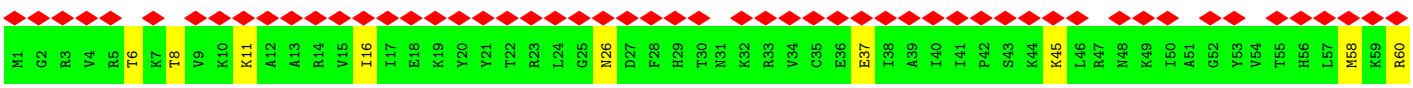


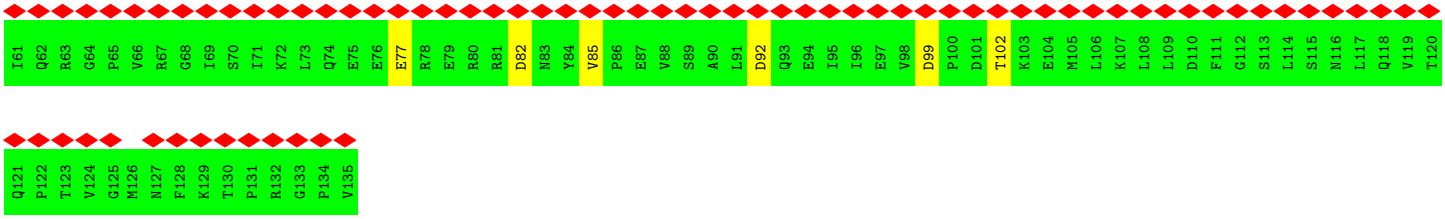


• Molecule 59: 40S ribosomal protein S17

Chain 2y:

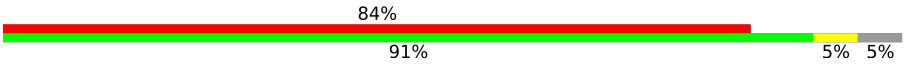


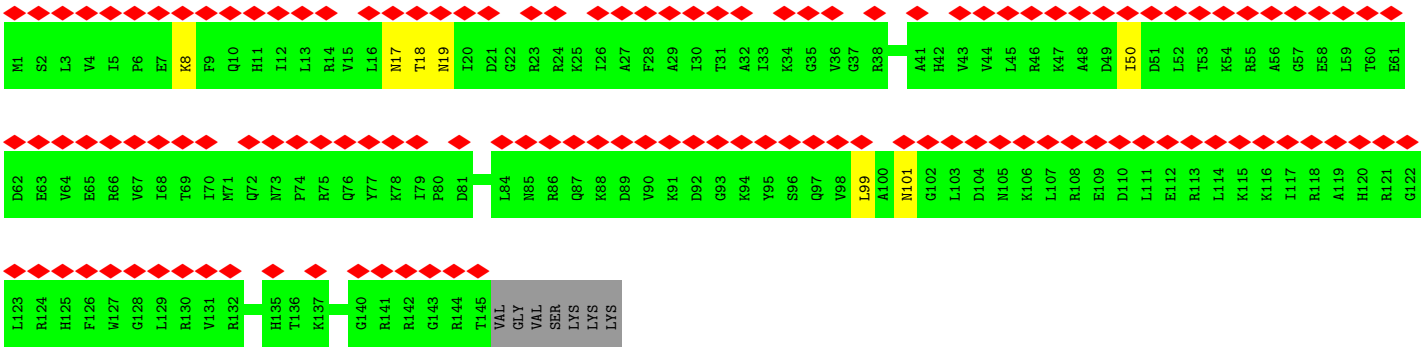




• Molecule 60: 40S ribosomal protein S18

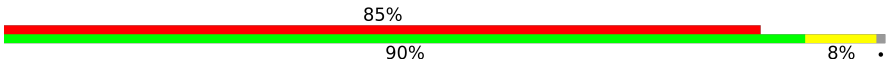
Chain 2z:

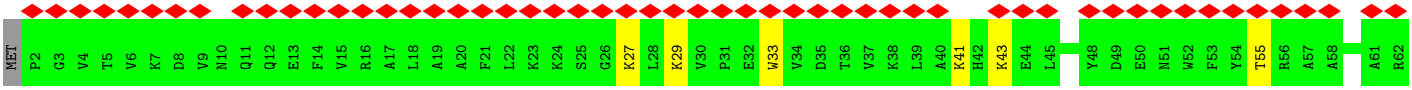


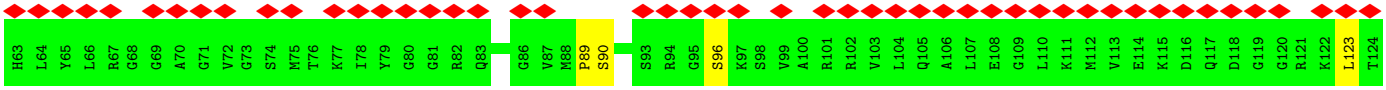


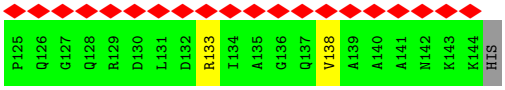
• Molecule 61: 40S ribosomal protein S19

Chain 20:



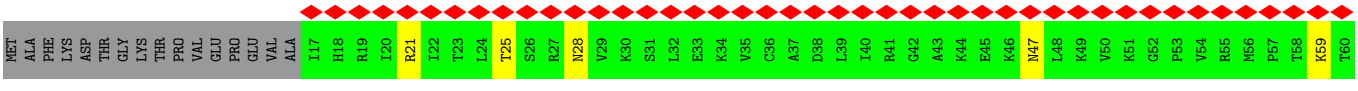






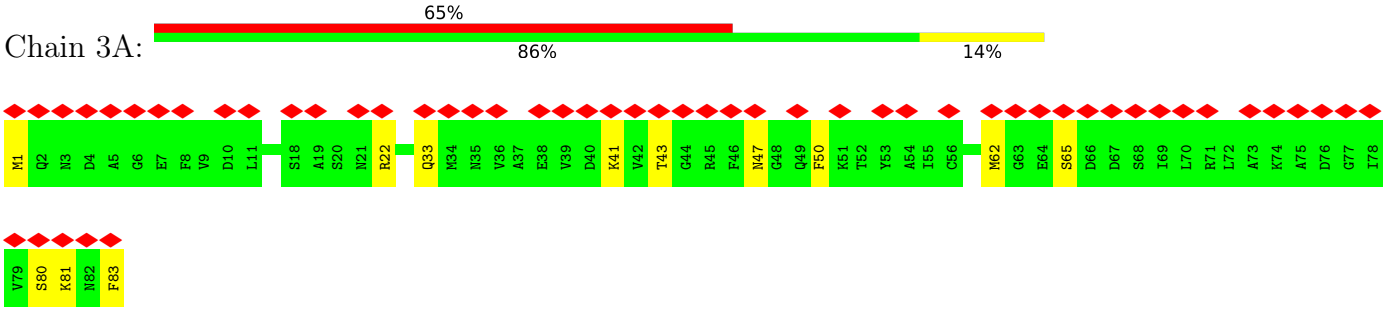
• Molecule 62: 40S ribosomal protein S20

Chain 21:



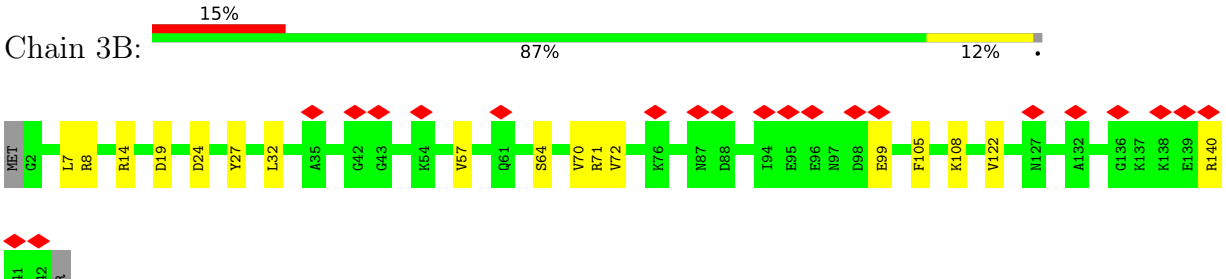
• Molecule 63: 40S ribosomal protein S21

Chain 3A:



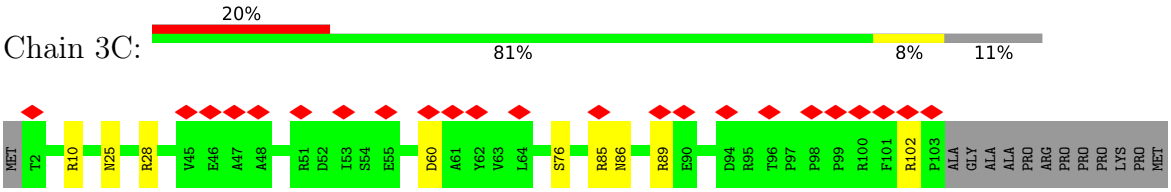
• Molecule 64: 40S ribosomal protein S23

Chain 3B:



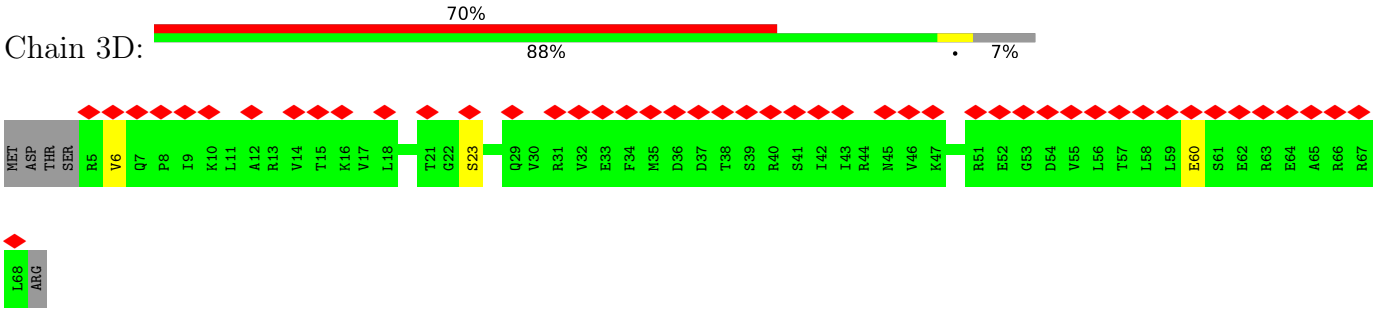
• Molecule 65: 40S ribosomal protein S26

Chain 3C:



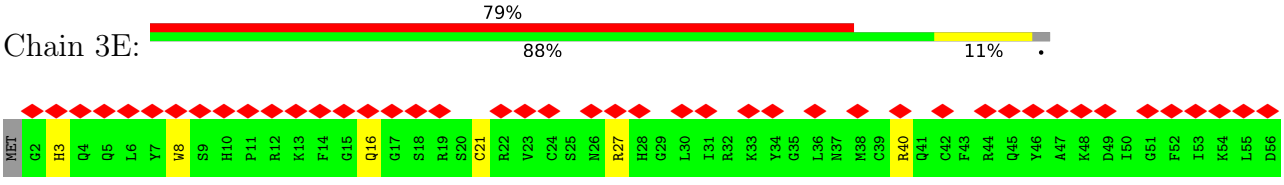
• Molecule 66: 40S ribosomal protein S28

Chain 3D:



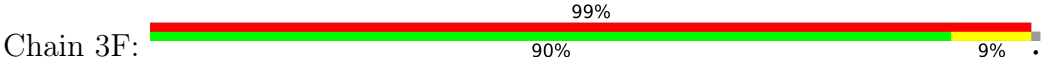
• Molecule 67: 40S ribosomal protein S29

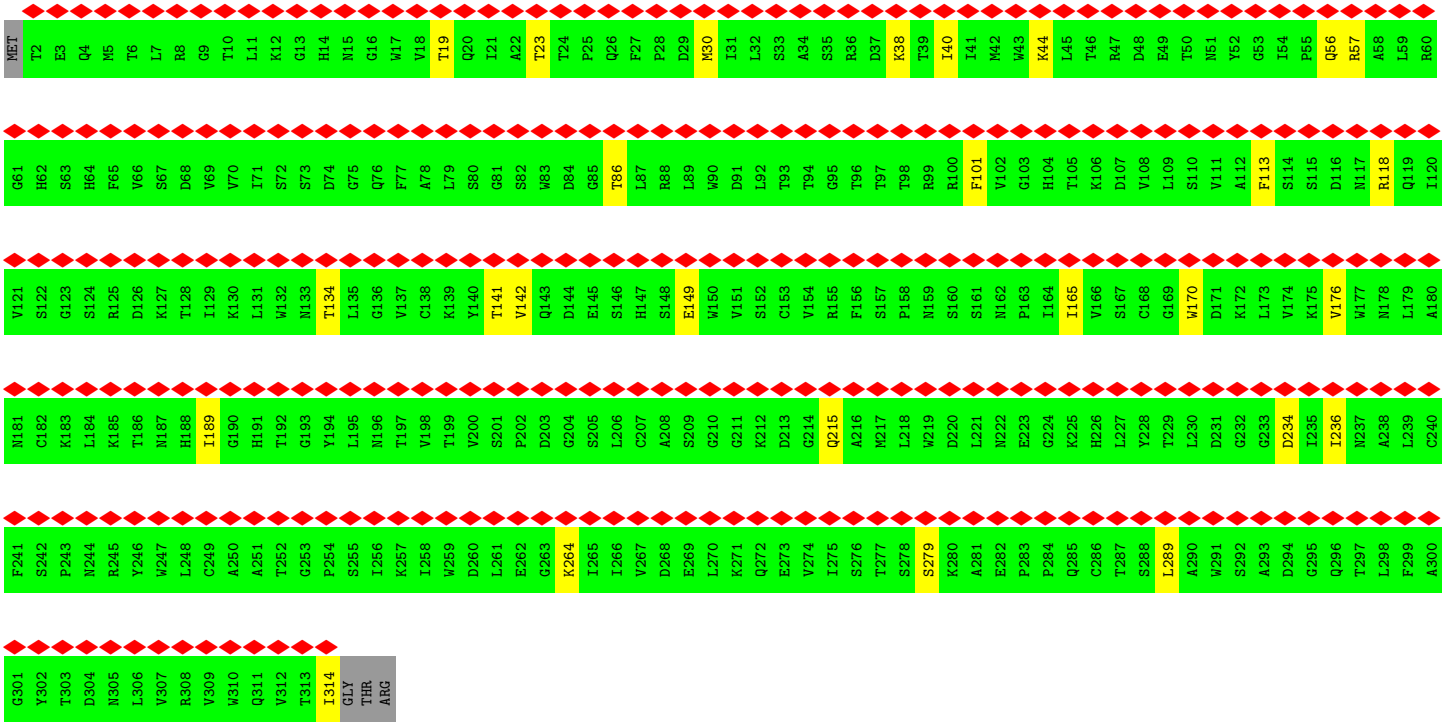
Chain 3E:



• Molecule 68: Receptor of activated protein C kinase 1

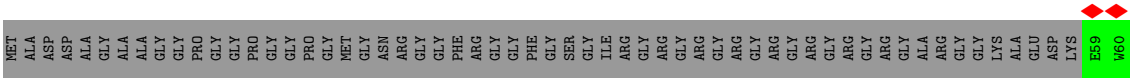
Chain 3F:

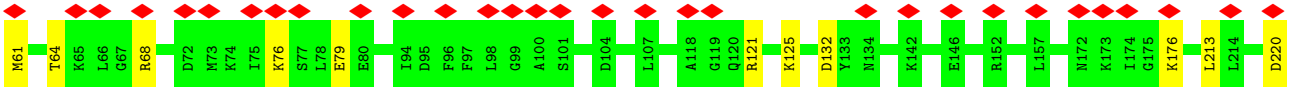


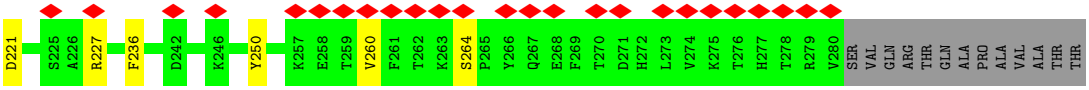


• Molecule 69: 40S ribosomal protein S2

Chain 3G:

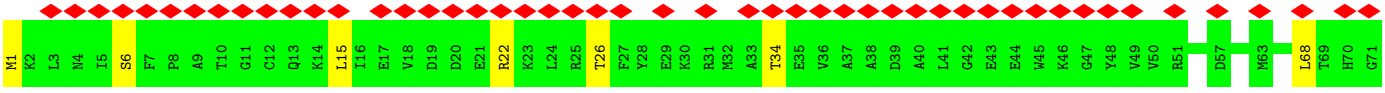


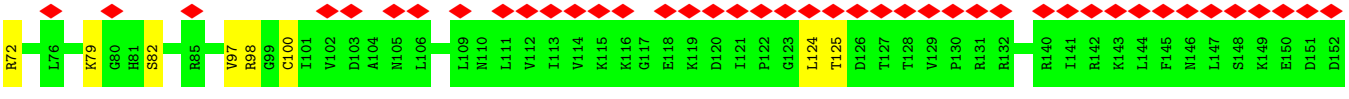


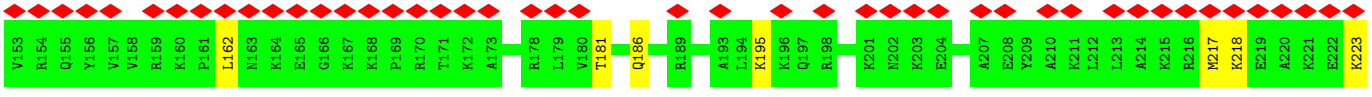


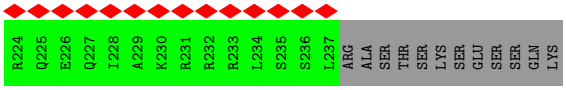
• Molecule 70: 40S ribosomal protein S6

Chain 3H:



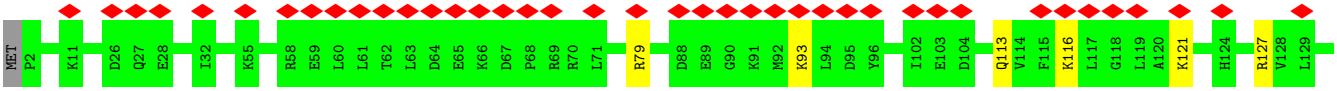


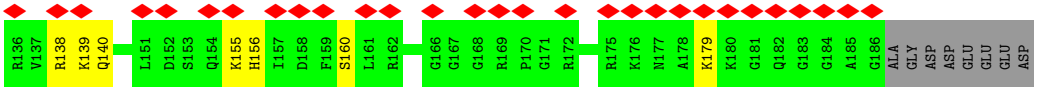




• Molecule 71: 40S ribosomal protein S9

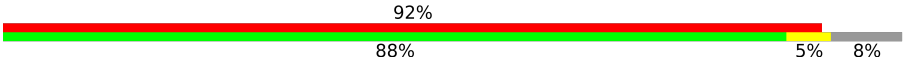
Chain 3I:

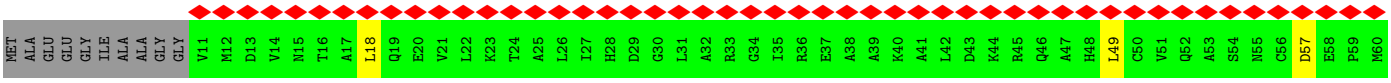


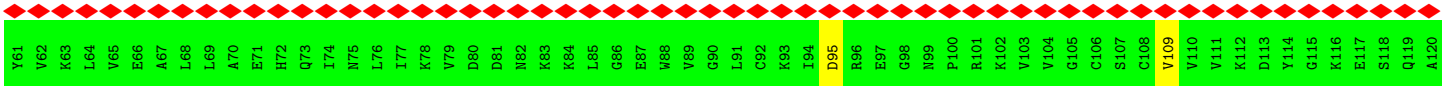


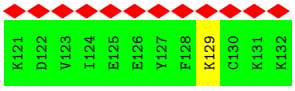
• Molecule 72: 40S ribosomal protein S12

Chain 3J:



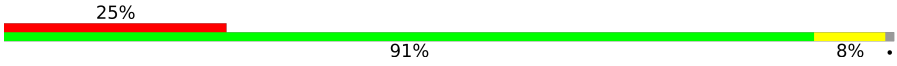


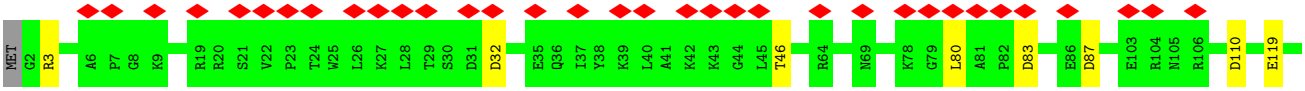


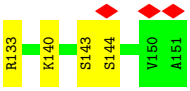


• Molecule 73: 40S ribosomal protein S13

Chain 3K:

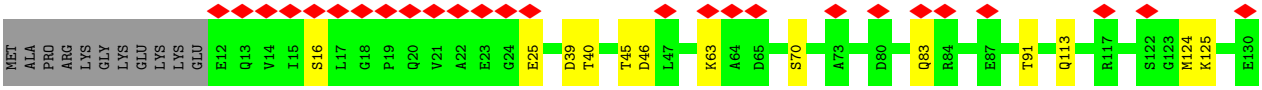


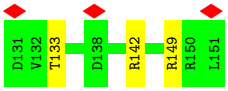




• Molecule 74: 40S ribosomal protein S14

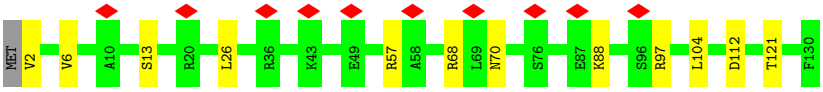
Chain 3L:





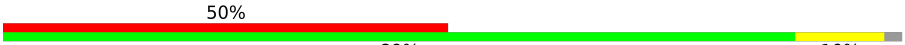
• Molecule 75: 40S ribosomal protein S15a

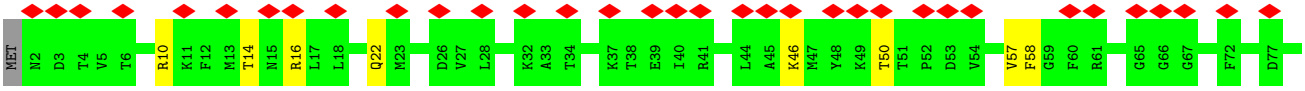
Chain 3M:

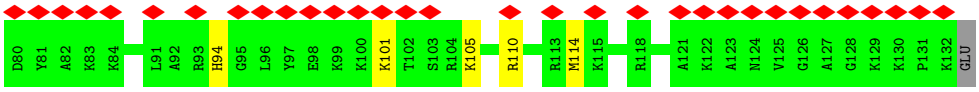


• Molecule 76: 40S ribosomal protein S24

Chain 3N:

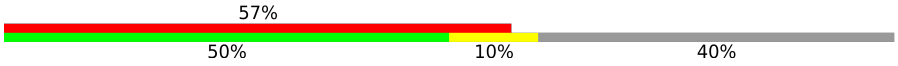


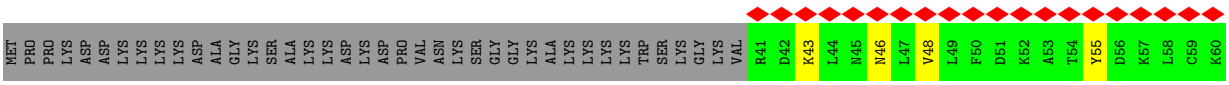


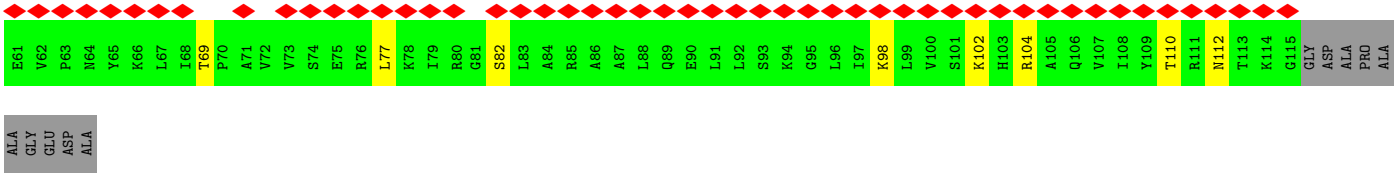


• Molecule 77: 40S ribosomal protein S25

Chain 3O:

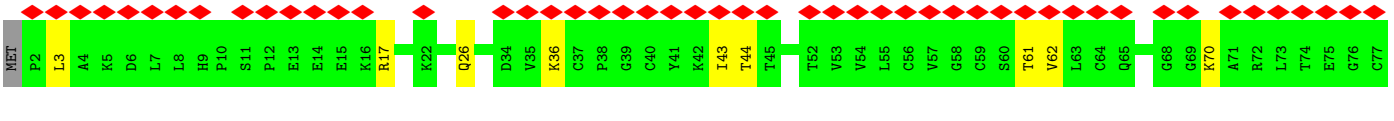


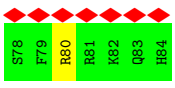




• Molecule 78: 40S ribosomal protein S27

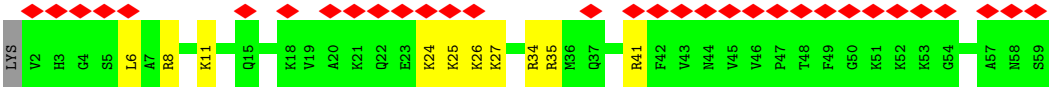
Chain 3P:



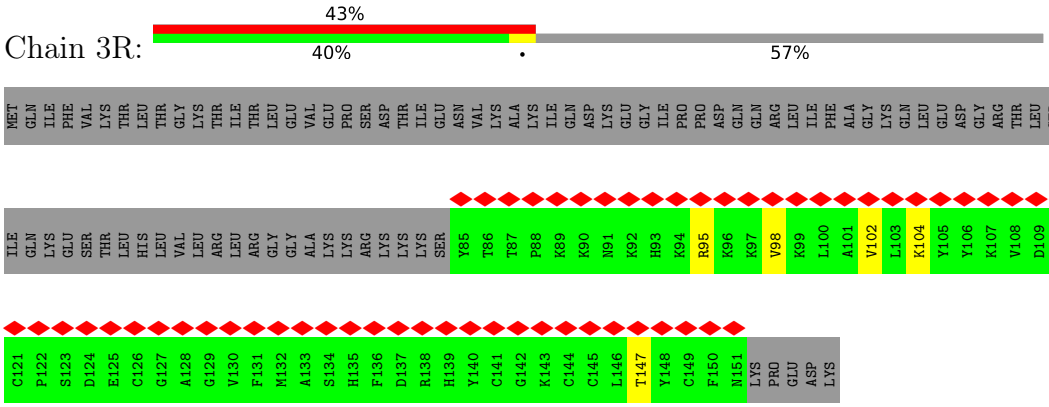


• Molecule 79: 40S ribosomal protein S30

Chain 3Q:



• Molecule 80: Ubiquitin-40S ribosomal protein S27a



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (i)

5.1 Standard geometry (i)

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

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	0.21	0/89127	0.77	11/139035 (0.0%)
2	1B	0.19	0/2858	0.75	0/4455
3	1C	0.19	0/3696	0.75	0/5758
4	1D	0.25	0/1936	0.54	0/2596
5	1E	0.25	0/3306	0.51	0/4424
6	1F	0.25	0/2981	0.53	0/4002
7	1G	0.26	0/2428	0.50	0/3252
8	1H	0.25	0/1942	0.52	0/2606
9	2A	0.26	0/1916	0.51	0/2553
10	2B	0.25	0/1971	0.50	0/2651
11	2C	0.24	0/1537	0.51	0/2066
12	2D	0.25	0/1751	0.51	0/2340
13	2E	0.25	0/1433	0.52	0/1915
14	2F	0.25	0/1732	0.55	0/2315
15	2G	0.26	0/1161	0.50	0/1554
16	2H	0.24	0/1746	0.56	0/2338
17	2I	0.25	0/1682	0.51	0/2250
18	2J	0.25	0/1268	0.50	0/1701
19	2K	0.25	0/1537	0.57	0/2052
20	2L	0.23	0/1582	0.54	0/2091
21	2M	0.26	0/1493	0.54	0/2003
22	2N	0.25	0/1326	0.50	0/1770
23	2O	0.26	0/839	0.50	0/1126
24	2P	0.25	0/993	0.50	0/1332
25	2Q	0.24	0/1030	0.53	0/1364
26	2R	0.24	0/1002	0.51	0/1345
27	2S	0.25	0/1132	0.53	0/1504
28	2T	0.26	0/1130	0.51	0/1507
29	2U	0.25	0/1191	0.50	0/1591
30	2V	0.24	0/895	0.53	0/1182
31	2W	0.25	0/774	0.46	0/1038
32	2X	0.24	0/903	0.52	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	2Y	0.25	0/1071	0.53	0/1429
34	2Z	0.26	0/895	0.57	0/1198
35	2a	0.25	0/916	0.55	0/1220
36	2b	0.24	0/1023	0.50	0/1351
37	2c	0.24	0/843	0.54	0/1115
38	2d	0.24	0/731	0.57	0/966
39	2e	0.25	0/575	0.50	0/761
40	2f	0.24	0/454	0.54	0/599
41	2g	0.25	0/425	0.51	0/561
42	2h	0.23	0/231	0.66	0/294
43	2i	0.25	0/887	0.54	0/1170
44	2j	0.24	0/718	0.51	0/953
45	2k	0.24	0/1017	0.55	0/1364
46	2l	0.24	0/1768	0.48	0/2371
47	2m	0.17	0/41243	0.75	18/64257 (0.0%)
48	2n	0.24	0/1778	0.47	0/2416
49	2o	0.24	0/1765	0.48	0/2362
50	2p	0.25	0/1793	0.51	0/2414
51	2q	0.24	0/2118	0.51	0/2849
52	2r	0.23	0/1516	0.49	0/2037
53	2s	0.25	0/1519	0.49	0/2033
54	2t	0.24	0/1715	0.52	0/2287
55	2u	0.24	0/851	0.46	0/1147
56	2v	0.24	0/1268	0.52	0/1696
57	2w	0.24	0/1065	0.52	0/1423
58	2x	0.25	0/1142	0.53	0/1528
59	2y	0.24	0/1105	0.51	0/1484
60	2z	0.24	0/1216	0.55	0/1628
61	20	0.30	0/1131	0.55	2/1515 (0.1%)
62	21	0.23	0/827	0.51	0/1110
63	3A	0.25	0/643	0.50	0/860
64	3B	0.24	0/1116	0.50	0/1490
65	3C	0.24	0/847	0.57	0/1135
66	3D	0.23	0/508	0.59	0/680
67	3E	0.24	0/470	0.51	0/623
68	3F	0.23	0/2493	0.48	0/3394
69	3G	0.24	0/1773	0.48	0/2395
70	3H	0.24	0/1946	0.55	0/2590
71	3I	0.25	0/1561	0.55	0/2083
72	3J	0.24	0/952	0.44	0/1279
73	3K	0.24	0/1232	0.49	0/1656
74	3L	0.25	0/1062	0.56	0/1425
75	3M	0.25	0/1051	0.51	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	3N	0.24	0/1094	0.54	0/1452
77	3O	0.24	0/604	0.52	0/810
78	3P	0.24	0/665	0.47	0/891
79	3Q	0.26	0/465	0.53	0/612
80	3R	0.23	0/560	0.48	0/745
All	All	0.22	0/232946	0.68	31/341996 (0.0%)

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	4924	C	N3-C2-O2	-7.73	116.49	121.90
61	20	89	PRO	N-CD-CG	-7.51	91.94	103.20
47	2m	549	C	N1-C2-O2	7.05	123.13	118.90
61	20	89	PRO	CA-N-CD	-6.64	102.21	111.50
1	1A	456	C	O4'-C1'-N1	6.53	113.42	108.20

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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	1G	291/297 (98%)	277 (95%)	14 (5%)	0	100	100
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%)	25	47
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%)	19	39
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%)	19	39
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	2d	85/97 (88%)	82 (96%)	3 (4%)	0	100	100
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%)	29	52
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%)	29	52
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%)	22	43
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	21	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	3H	235/249 (94%)	228 (97%)	7 (3%)	0	100	100
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%)	54	75

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 (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	1D	190/199 (96%)	180 (95%)	10 (5%)	22	45
5	1E	348/349 (100%)	329 (94%)	19 (6%)	21	43
6	1F	306/348 (88%)	289 (94%)	17 (6%)	21	42
7	1G	246/250 (98%)	228 (93%)	18 (7%)	14	28
8	1H	209/252 (83%)	190 (91%)	19 (9%)	9	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	2A	195/215 (91%)	184 (94%)	11 (6%)	21 42
10	2B	204/223 (92%)	187 (92%)	17 (8%)	11 22
11	2C	169/171 (99%)	155 (92%)	14 (8%)	11 22
12	2D	180/181 (99%)	162 (90%)	18 (10%)	7 14
13	2E	148/149 (99%)	134 (90%)	14 (10%)	8 16
14	2F	176/177 (99%)	159 (90%)	17 (10%)	8 15
15	2G	118/161 (73%)	109 (92%)	9 (8%)	13 26
16	2H	171/172 (99%)	166 (97%)	5 (3%)	42 68
17	2I	173/174 (99%)	160 (92%)	13 (8%)	13 27
18	2J	134/163 (82%)	125 (93%)	9 (7%)	16 33
19	2K	164/165 (99%)	160 (98%)	4 (2%)	49 74
20	2L	166/175 (95%)	156 (94%)	10 (6%)	19 39
21	2M	156/157 (99%)	148 (95%)	8 (5%)	24 46
22	2N	139/140 (99%)	125 (90%)	14 (10%)	7 14
23	2O	91/115 (79%)	79 (87%)	12 (13%)	4 7
24	2P	101/107 (94%)	94 (93%)	7 (7%)	15 31
25	2Q	103/126 (82%)	97 (94%)	6 (6%)	20 40
26	2R	108/133 (81%)	98 (91%)	10 (9%)	9 17
27	2S	124/135 (92%)	118 (95%)	6 (5%)	25 49
28	2T	117/118 (99%)	109 (93%)	8 (7%)	16 32
29	2U	120/121 (99%)	114 (95%)	6 (5%)	24 47
30	2V	89/126 (71%)	78 (88%)	11 (12%)	4 8
31	2W	83/97 (86%)	79 (95%)	4 (5%)	25 49
32	2X	98/110 (89%)	91 (93%)	7 (7%)	14 29
33	2Y	114/121 (94%)	108 (95%)	6 (5%)	22 45
34	2Z	88/89 (99%)	83 (94%)	5 (6%)	20 41
35	2a	98/100 (98%)	93 (95%)	5 (5%)	24 46
36	2b	109/110 (99%)	99 (91%)	10 (9%)	9 17
37	2c	86/89 (97%)	78 (91%)	8 (9%)	9 17
38	2d	74/80 (92%)	69 (93%)	5 (7%)	16 32
39	2e	64/65 (98%)	58 (91%)	6 (9%)	8 17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	2f	47/48 (98%)	45 (96%)	2 (4%)	29 54
41	2g	47/115 (41%)	45 (96%)	2 (4%)	29 54
42	2h	23/24 (96%)	20 (87%)	3 (13%)	4 7
43	2i	94/94 (100%)	89 (95%)	5 (5%)	22 45
44	2j	74/75 (99%)	69 (93%)	5 (7%)	16 32
45	2k	109/121 (90%)	100 (92%)	9 (8%)	11 22
46	2l	195/196 (100%)	169 (87%)	26 (13%)	4 7
48	2n	183/243 (75%)	159 (87%)	24 (13%)	4 7
49	2o	195/231 (84%)	178 (91%)	17 (9%)	10 20
50	2p	190/202 (94%)	163 (86%)	27 (14%)	3 5
51	2q	224/225 (100%)	209 (93%)	15 (7%)	16 33
52	2r	159/170 (94%)	144 (91%)	15 (9%)	8 17
53	2s	166/174 (95%)	153 (92%)	13 (8%)	12 25
54	2t	178/180 (99%)	166 (93%)	12 (7%)	16 33
55	2u	89/136 (65%)	82 (92%)	7 (8%)	12 24
56	2v	137/142 (96%)	123 (90%)	14 (10%)	7 14
57	2w	113/130 (87%)	106 (94%)	7 (6%)	18 37
58	2x	117/121 (97%)	106 (91%)	11 (9%)	8 17
59	2y	122/122 (100%)	107 (88%)	15 (12%)	4 9
60	2z	126/132 (96%)	119 (94%)	7 (6%)	21 42
61	20	113/115 (98%)	102 (90%)	11 (10%)	8 15
62	21	94/107 (88%)	82 (87%)	12 (13%)	4 8
63	3A	67/67 (100%)	55 (82%)	12 (18%)	2 2
64	3B	113/115 (98%)	96 (85%)	17 (15%)	3 5
65	3C	90/98 (92%)	80 (89%)	10 (11%)	6 11
66	3D	57/62 (92%)	54 (95%)	3 (5%)	22 45
67	3E	48/49 (98%)	42 (88%)	6 (12%)	4 8
68	3F	272/275 (99%)	245 (90%)	27 (10%)	8 15
69	3G	189/225 (84%)	172 (91%)	17 (9%)	9 18
70	3H	207/218 (95%)	185 (89%)	22 (11%)	6 12
71	3I	162/168 (96%)	148 (91%)	14 (9%)	10 20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
72	3J	102/108 (94%)	96 (94%)	6 (6%)	19 39
73	3K	130/131 (99%)	118 (91%)	12 (9%)	9 17
74	3L	110/119 (92%)	94 (86%)	16 (14%)	3 5
75	3M	112/113 (99%)	100 (89%)	12 (11%)	6 12
76	3N	114/115 (99%)	101 (89%)	13 (11%)	5 10
77	3O	66/103 (64%)	54 (82%)	12 (18%)	1 2
78	3P	75/76 (99%)	65 (87%)	10 (13%)	4 7
79	3Q	47/48 (98%)	37 (79%)	10 (21%)	1 1
80	3R	60/140 (43%)	55 (92%)	5 (8%)	11 22
All	All	10075/10996 (92%)	9224 (92%)	851 (8%)	14 21

5 of 851 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	2p	37	VAL
58	2x	20	THR
75	3M	112	ASP
50	2p	148	LYS
50	2p	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
73	3K	13	GLN
74	3L	20	GLN
76	3N	106	GLN
46	2l	19	HIS
45	2k	4	HIS

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	1716/1869 (91%)	494 (28%)	0
All	All	5694/7217 (78%)	1346 (23%)	58 (1%)

5 of 1346 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	0.86	0	4,9,11	0.56	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	-	1/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	2g	98	MLZ	CD-CE-NZ-CM

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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	1A	5106	-	32,33,33	1.56	7 (21%)	40,48,48	1.13	5 (12%)
81	84D	1A	5119	-	32,33,33	1.54	6 (18%)	40,48,48	1.08	3 (7%)
81	84D	1A	5112	-	32,33,33	1.61	7 (21%)	40,48,48	1.27	5 (12%)
81	84D	1A	5105	-	32,33,33	1.61	7 (21%)	40,48,48	1.21	5 (12%)
81	84D	1A	5104	-	32,33,33	1.61	9 (28%)	40,48,48	1.81	4 (10%)
81	84D	1A	5113	-	32,33,33	1.57	7 (21%)	40,48,48	1.23	5 (12%)
81	84D	2m	1901	-	32,33,33	1.55	7 (21%)	40,48,48	1.07	7 (17%)
81	84D	1A	5121	-	32,33,33	1.54	6 (18%)	40,48,48	1.00	3 (7%)
81	84D	1A	5116	-	32,33,33	1.53	6 (18%)	40,48,48	1.01	2 (5%)
81	84D	1A	5118	-	32,33,33	1.56	7 (21%)	40,48,48	0.98	3 (7%)
81	84D	1A	5103	-	32,33,33	1.52	6 (18%)	40,48,48	1.17	3 (7%)
81	84D	1A	5108	-	32,33,33	1.55	6 (18%)	40,48,48	1.15	3 (7%)
81	84D	2m	1902	-	32,33,33	1.55	6 (18%)	40,48,48	1.10	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
81	84D	1A	5109	-	32,33,33	1.68	7 (21%)	40,48,48	1.80	8 (20%)
81	84D	1A	5114	-	32,33,33	1.56	7 (21%)	40,48,48	1.09	4 (10%)
81	84D	1A	5120	-	32,33,33	1.54	6 (18%)	40,48,48	1.10	3 (7%)
81	84D	1A	5107	-	32,33,33	1.59	7 (21%)	40,48,48	1.11	4 (10%)
81	84D	1A	5110	-	32,33,33	1.56	6 (18%)	40,48,48	1.14	4 (10%)
81	84D	1A	5101	-	32,33,33	1.56	7 (21%)	40,48,48	1.04	3 (7%)
81	84D	1A	5102	-	32,33,33	1.57	7 (21%)	40,48,48	1.24	4 (10%)
81	84D	1A	5117	-	32,33,33	1.57	7 (21%)	40,48,48	1.17	4 (10%)
81	84D	2m	1903	-	32,33,33	1.56	6 (18%)	40,48,48	1.07	5 (12%)
81	84D	1A	5115	-	32,33,33	1.57	7 (21%)	40,48,48	1.07	5 (12%)
81	84D	1A	5111	-	32,33,33	1.56	6 (18%)	40,48,48	0.99	1 (2%)

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	1A	5106	-	-	5/12/65/65	0/3/3/3
81	84D	1A	5119	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5112	-	-	2/12/65/65	0/3/3/3
81	84D	1A	5105	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5104	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5113	-	-	2/12/65/65	0/3/3/3
81	84D	2m	1901	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5121	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5116	-	-	5/12/65/65	0/3/3/3
81	84D	1A	5118	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5103	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5108	-	-	6/12/65/65	0/3/3/3
81	84D	2m	1902	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5109	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5114	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5120	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5107	-	-	2/12/65/65	0/3/3/3
81	84D	1A	5110	-	-	3/12/65/65	1/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	84D	1A	5101	-	-	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	2m	1903	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5115	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5111	-	-	4/12/65/65	0/3/3/3

The worst 5 of 160 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 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	1A	5104	84D	O-C4-C	7.95	118.40	109.86
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	3.97	118.76	110.35
81	1A	5109	84D	C12-C13-C14	3.85	115.58	110.40

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

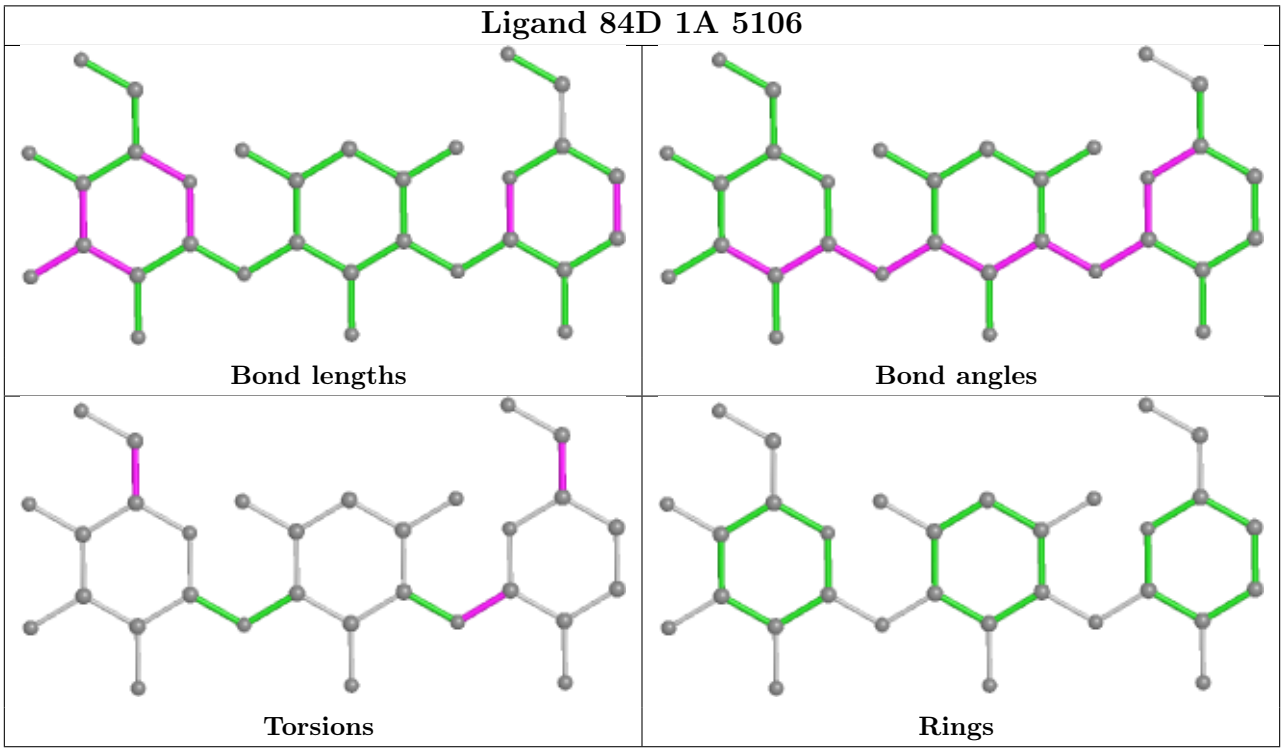
Mol	Chain	Res	Type	Atoms
81	1A	5101	84D	O-C4-C5-N
81	1A	5101	84D	C-C4-C5-N
81	1A	5104	84D	O-C4-C5-N
81	1A	5105	84D	O-C4-C5-N
81	1A	5105	84D	C-C4-C5-N

All (1) ring outliers are listed below:

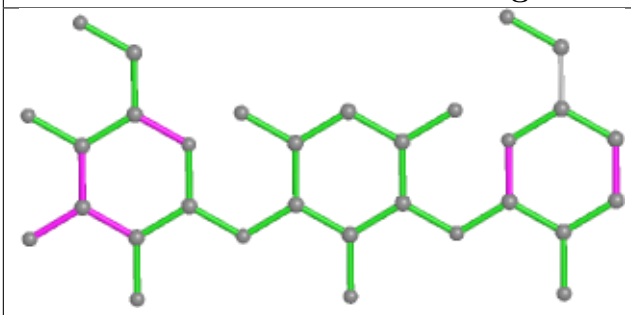
Mol	Chain	Res	Type	Atoms
81	1A	5110	84D	C-C1-C2-C3-C4-O

No monomer is involved in short contacts.

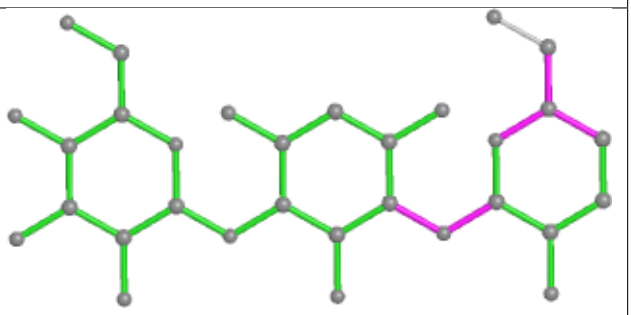
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



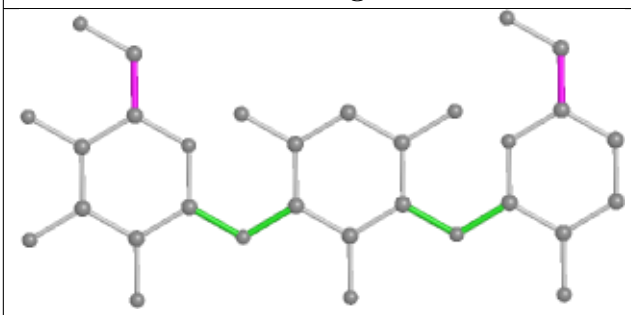
Ligand 84D 1A 5119



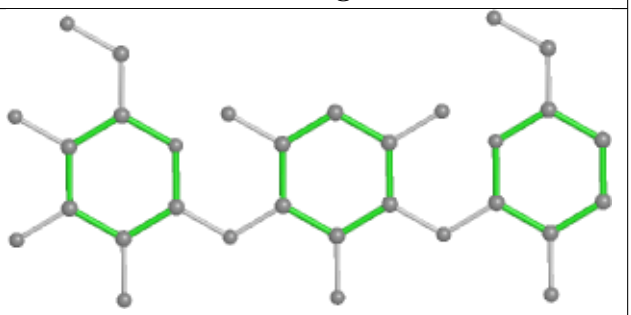
Bond lengths



Bond angles

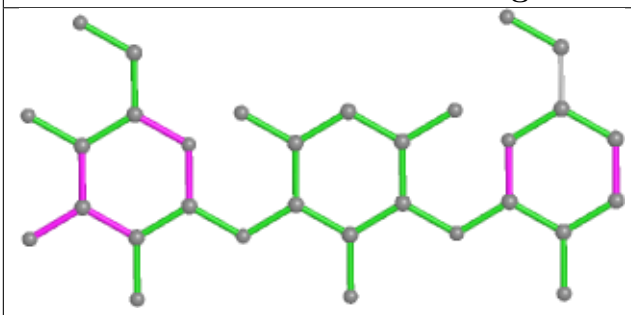


Torsions

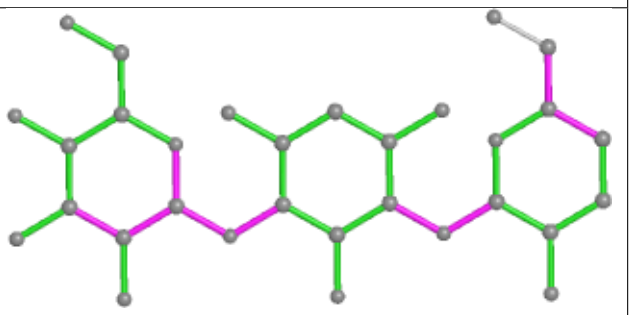


Rings

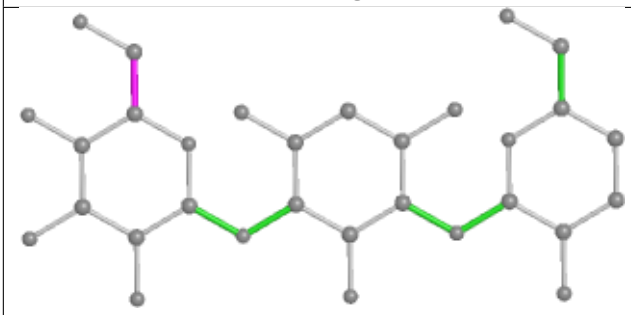
Ligand 84D 1A 5112



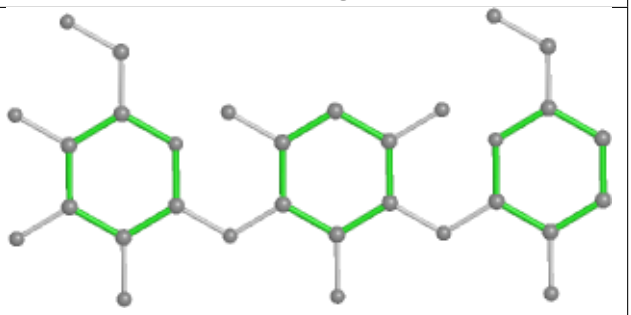
Bond lengths



Bond angles

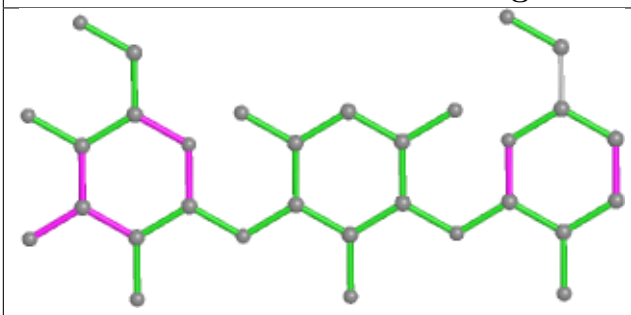


Torsions

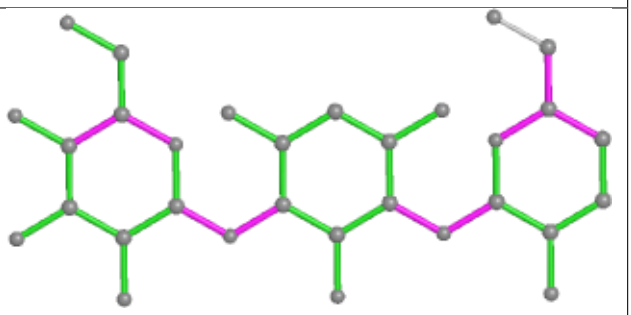


Rings

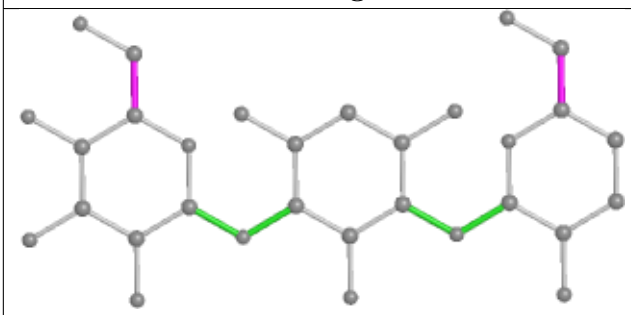
Ligand 84D 1A 5105



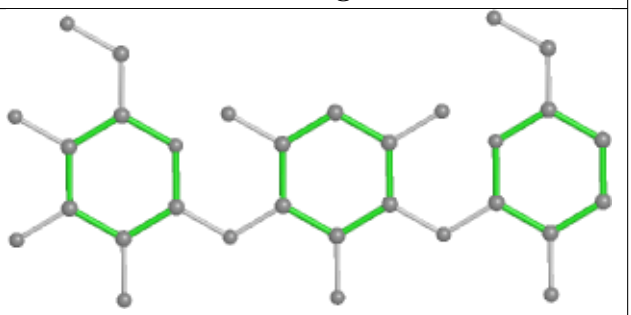
Bond lengths



Bond angles

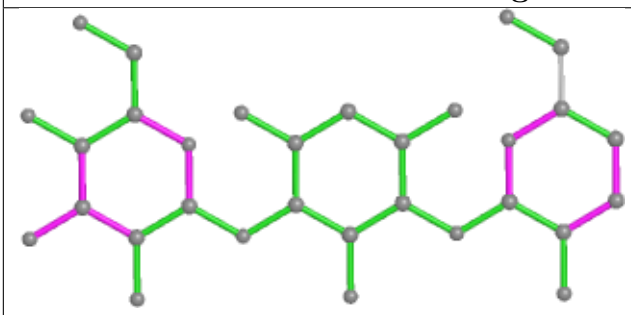


Torsions

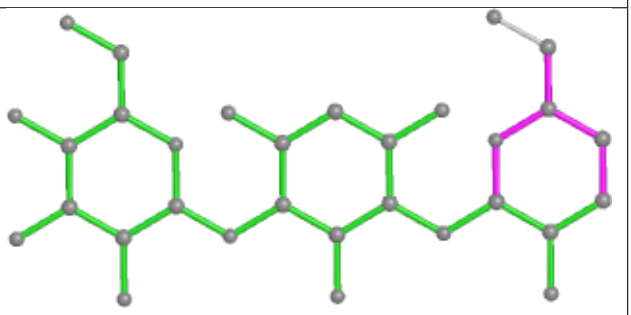


Rings

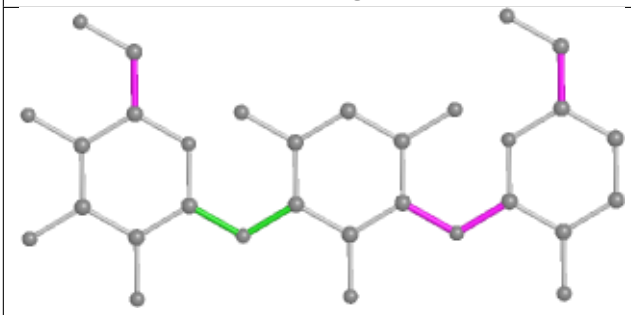
Ligand 84D 1A 5104



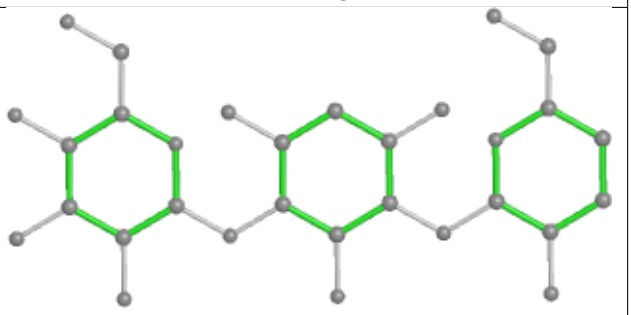
Bond lengths



Bond angles

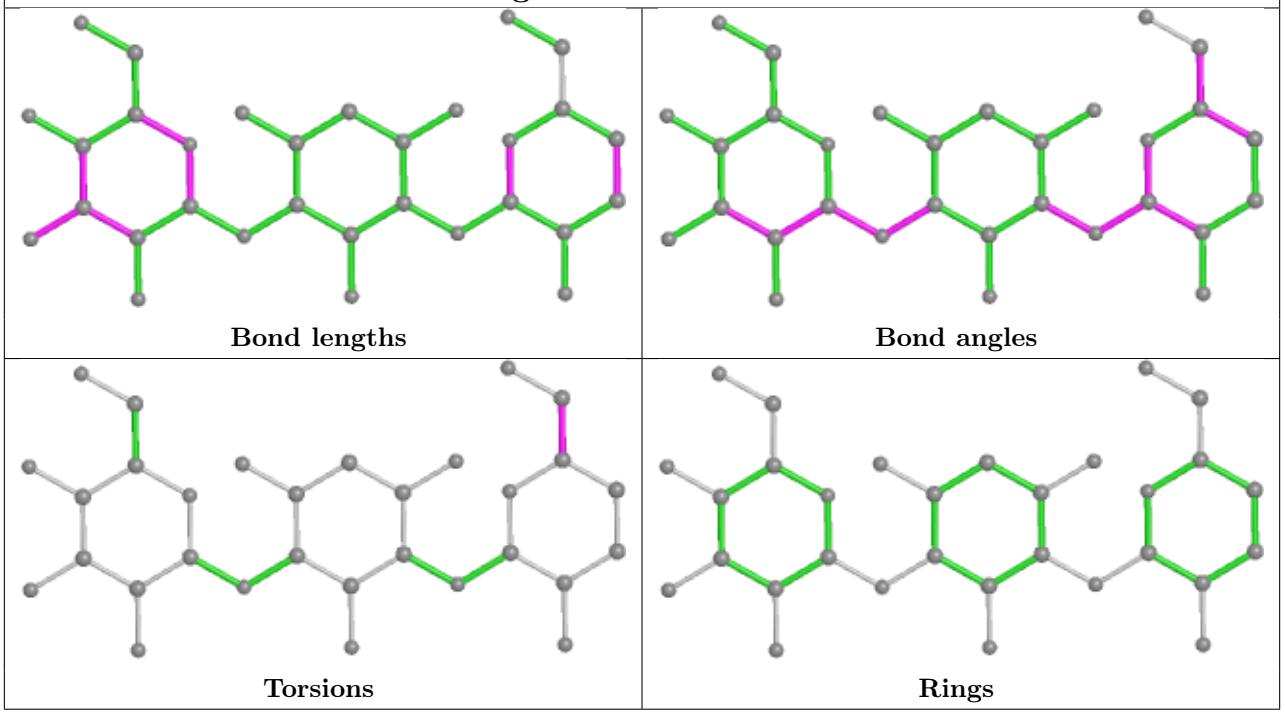


Torsions

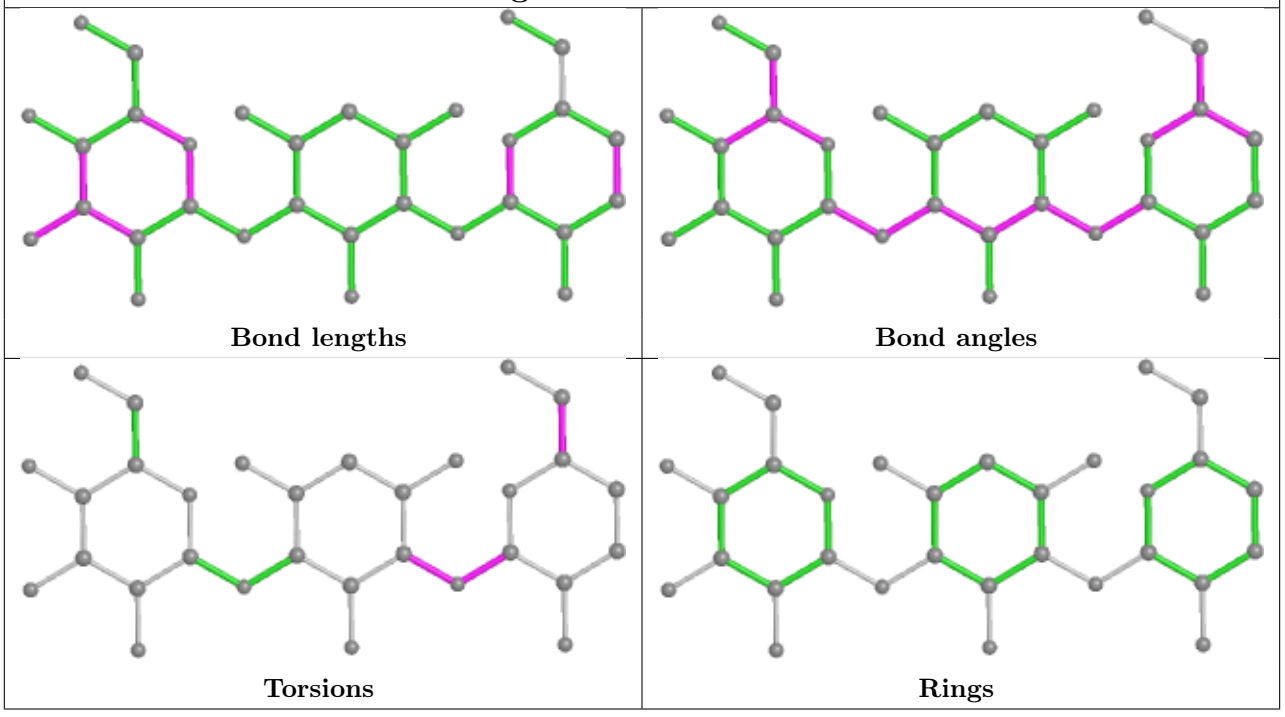


Rings

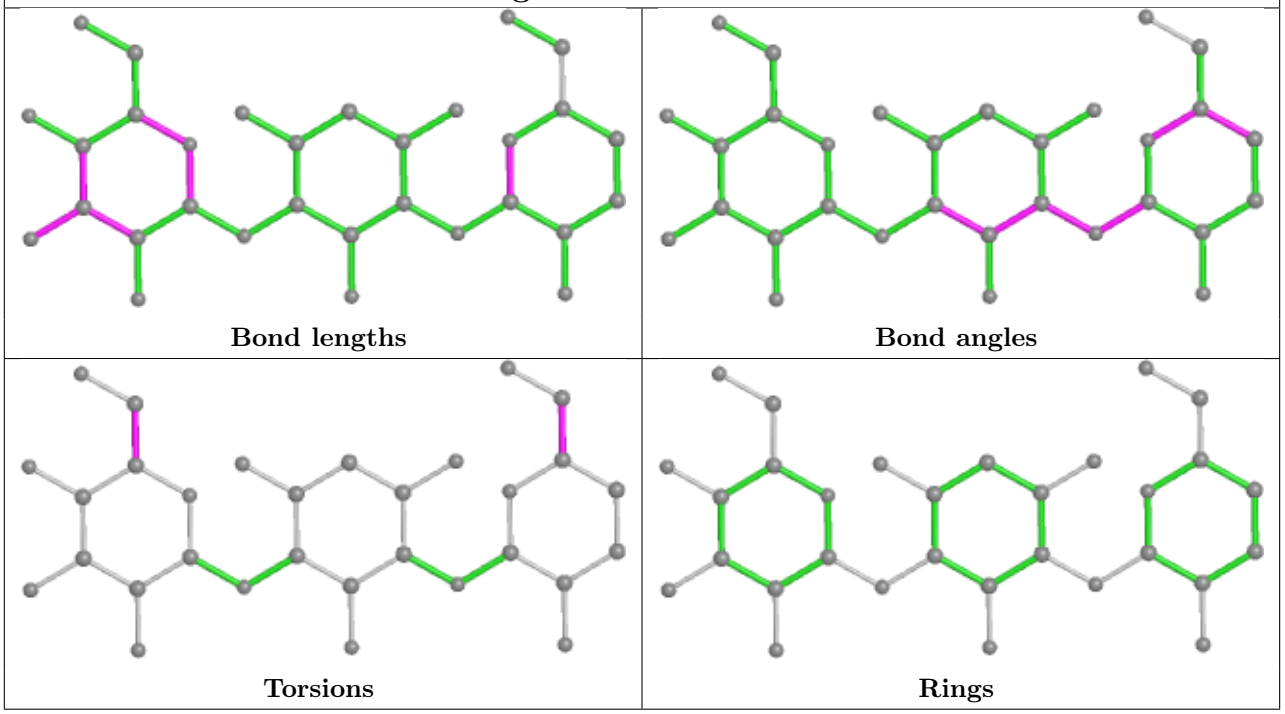
Ligand 84D 1A 5113



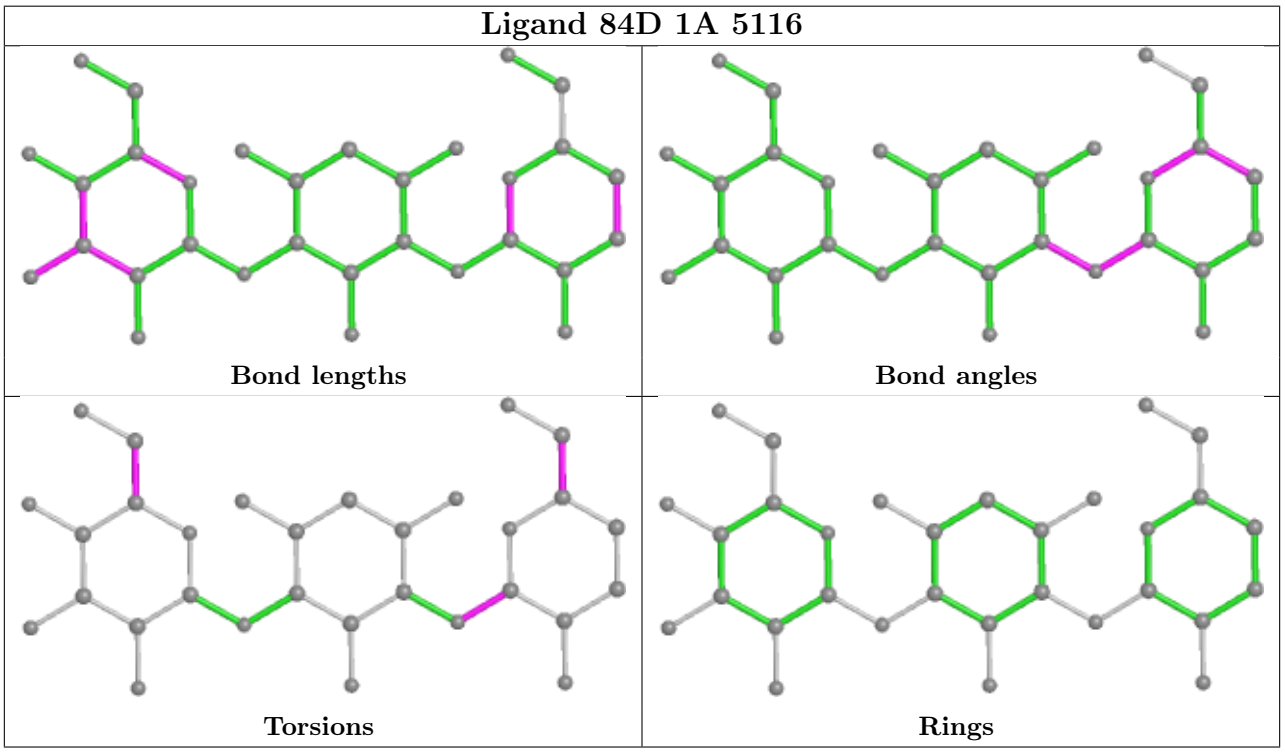
Ligand 84D 2m 1901



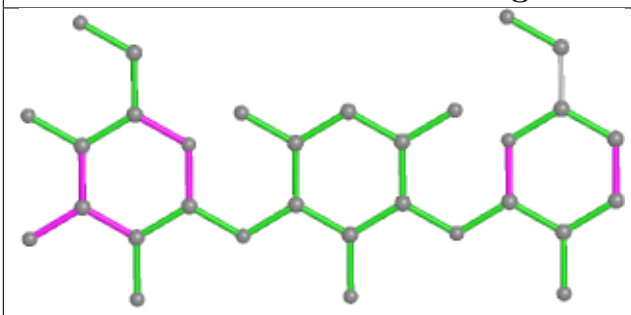
Ligand 84D 1A 5121



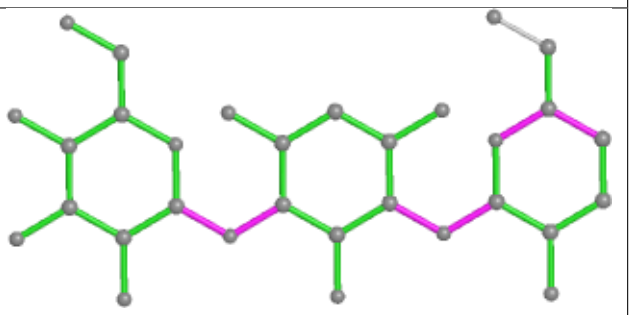
Ligand 84D 1A 5116



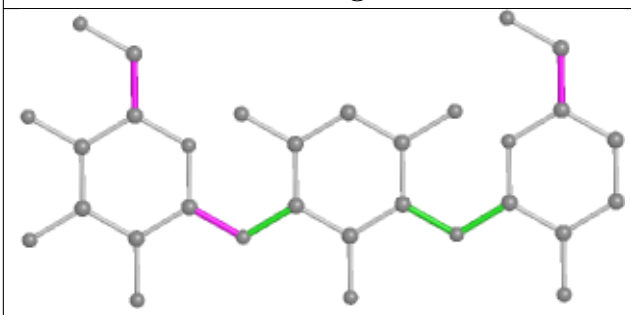
Ligand 84D 1A 5118



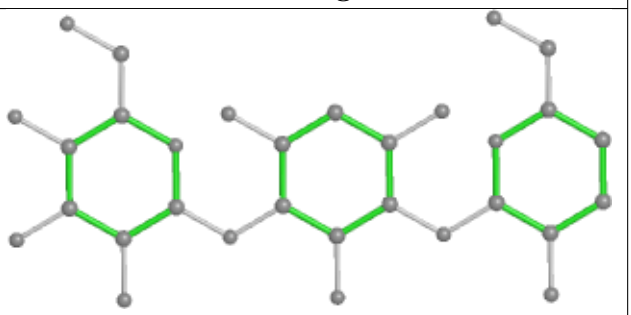
Bond lengths



Bond angles

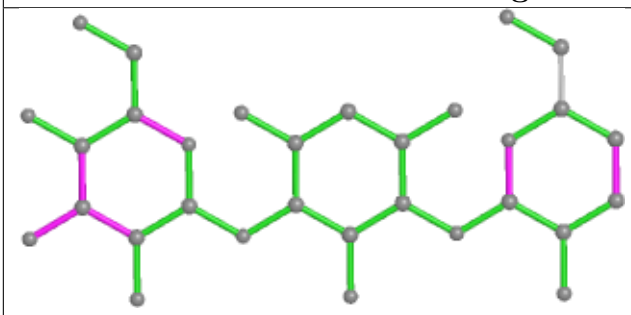


Torsions

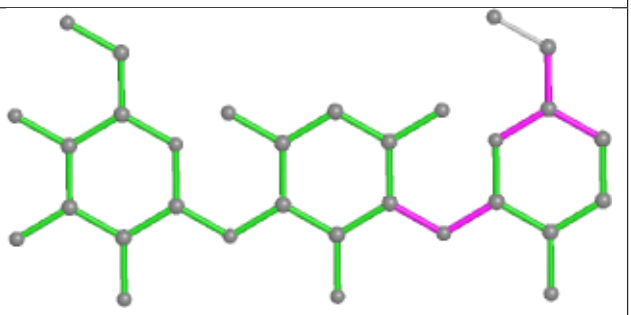


Rings

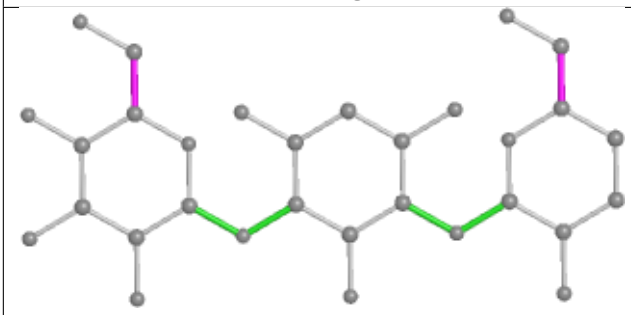
Ligand 84D 1A 5103



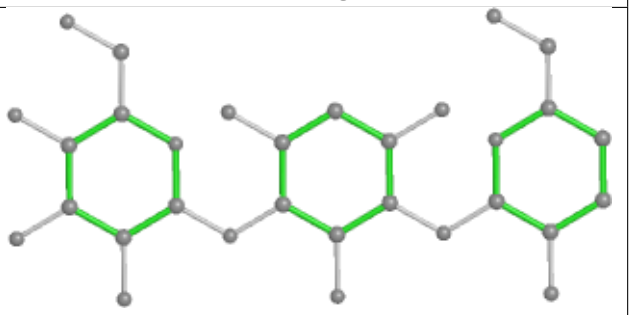
Bond lengths



Bond angles

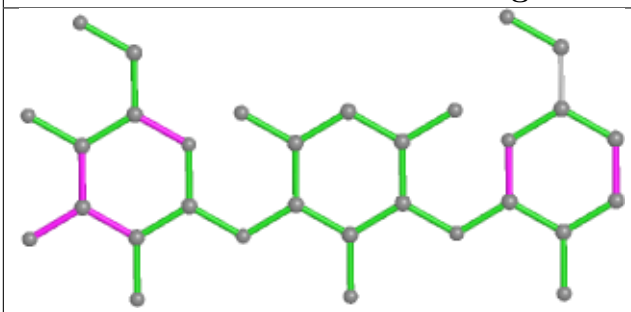


Torsions

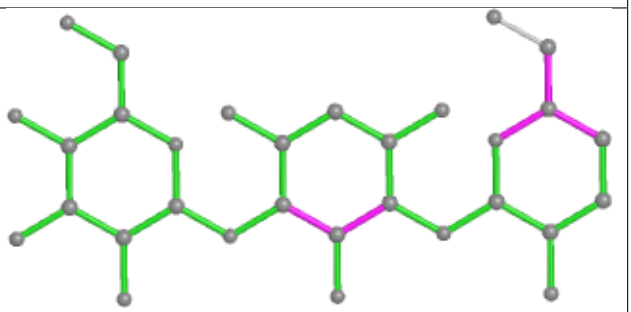


Rings

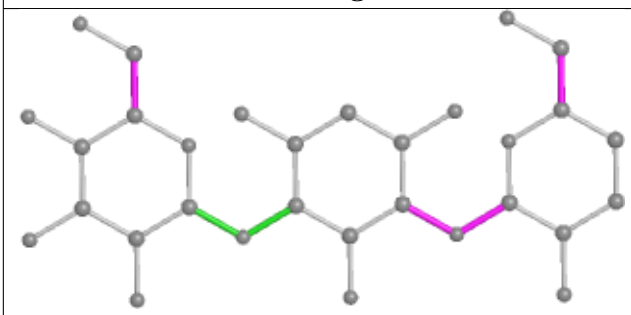
Ligand 84D 1A 5108



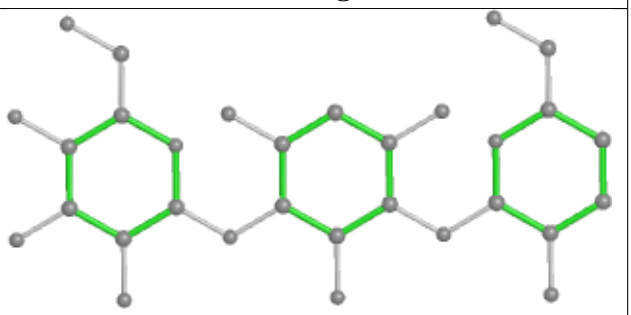
Bond lengths



Bond angles

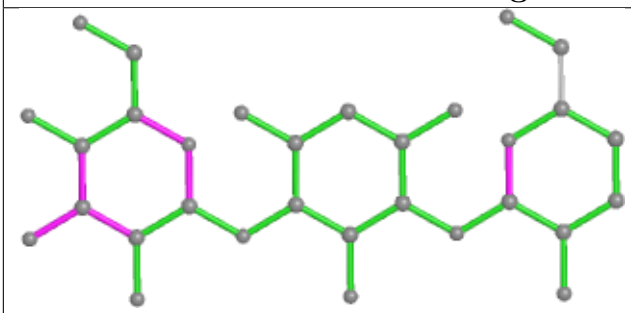


Torsions

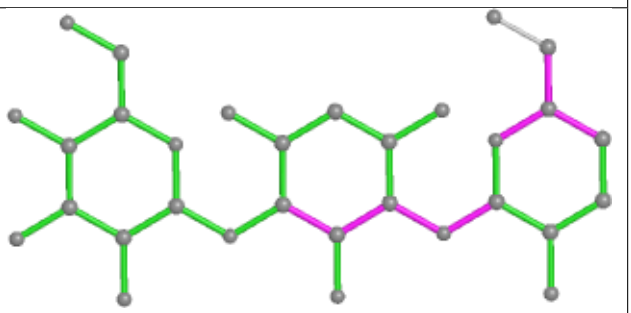


Rings

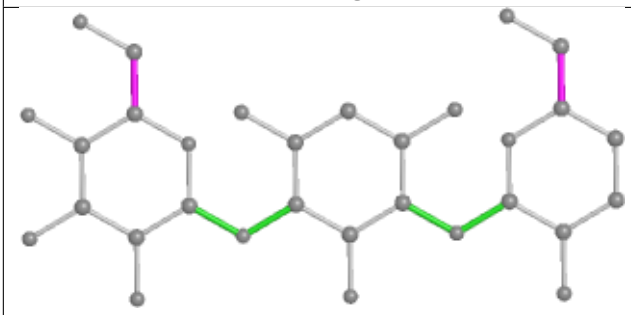
Ligand 84D 2m 1902



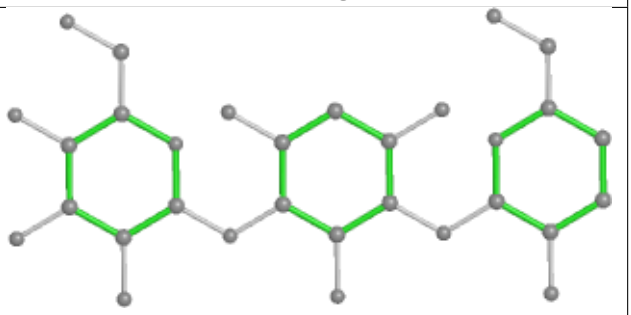
Bond lengths



Bond angles

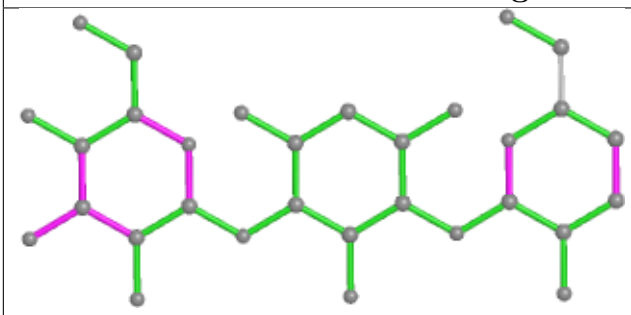


Torsions

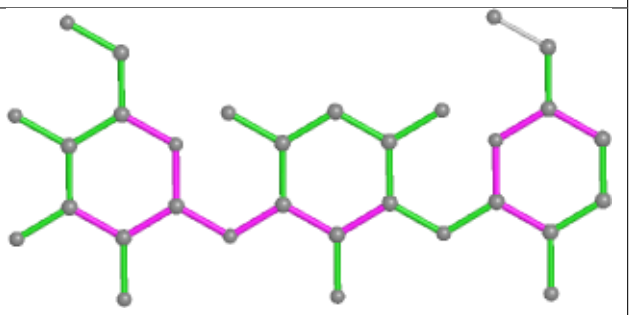


Rings

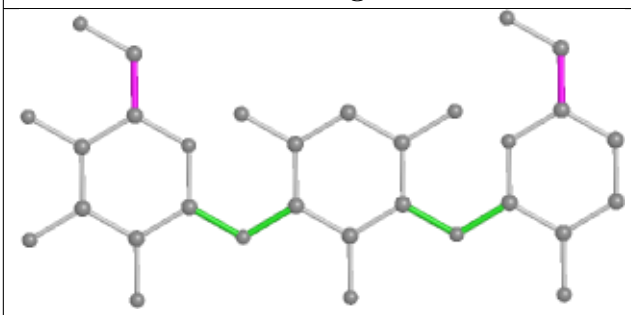
Ligand 84D 1A 5109



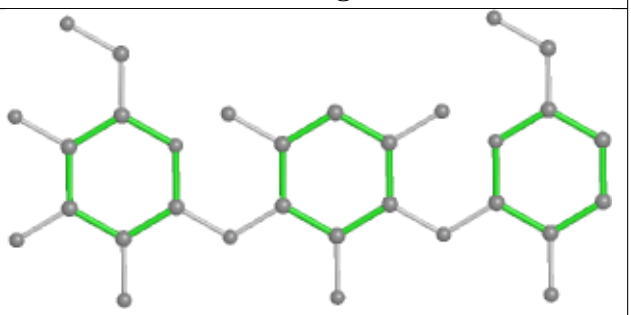
Bond lengths



Bond angles

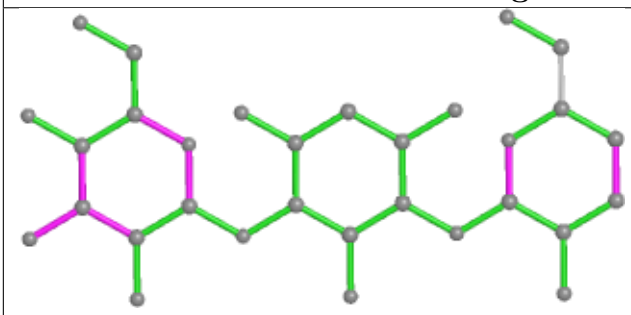


Torsions

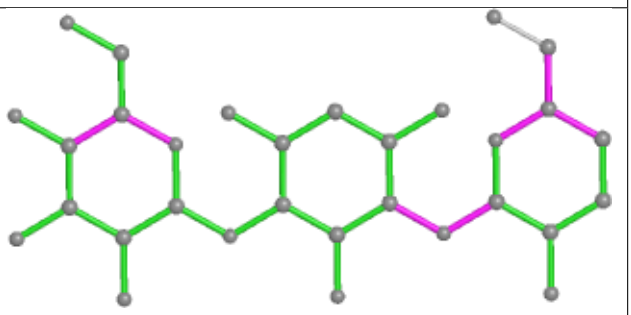


Rings

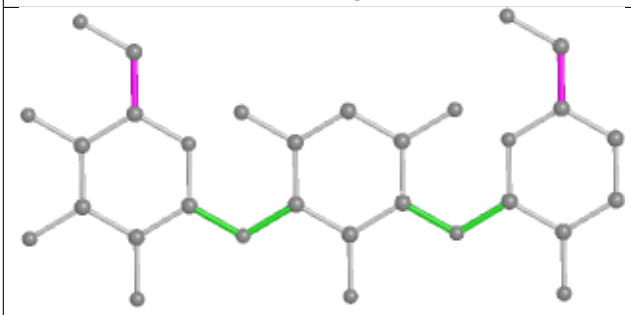
Ligand 84D 1A 5114



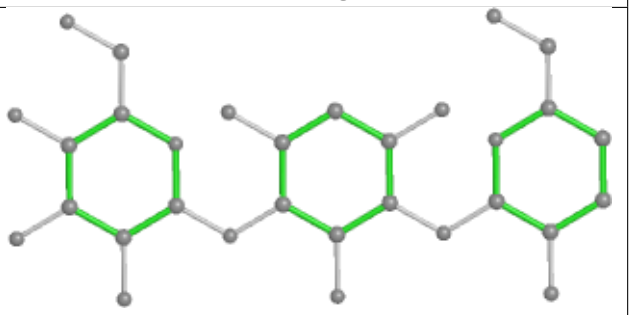
Bond lengths



Bond angles

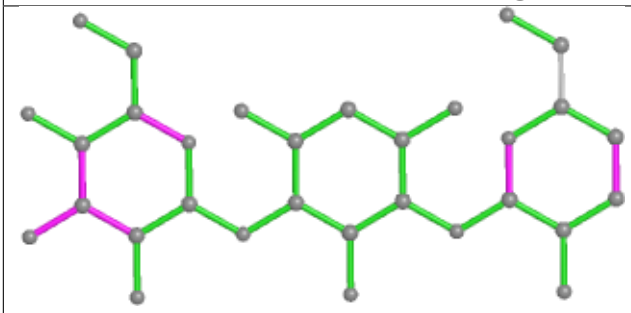


Torsions

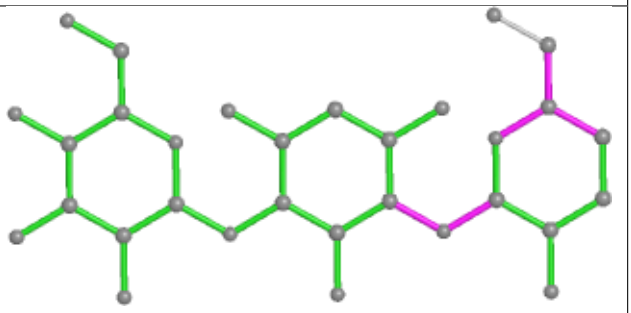


Rings

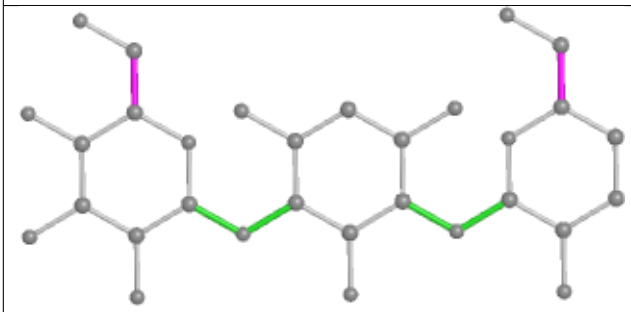
Ligand 84D 1A 5120



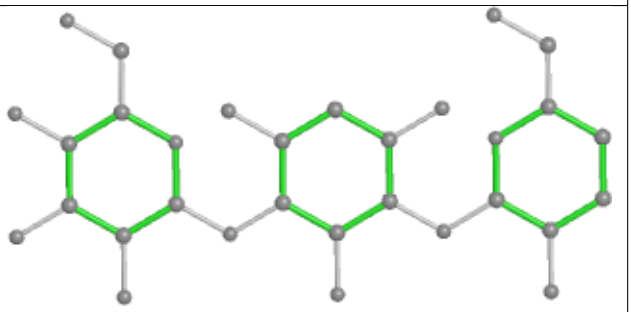
Bond lengths



Bond angles

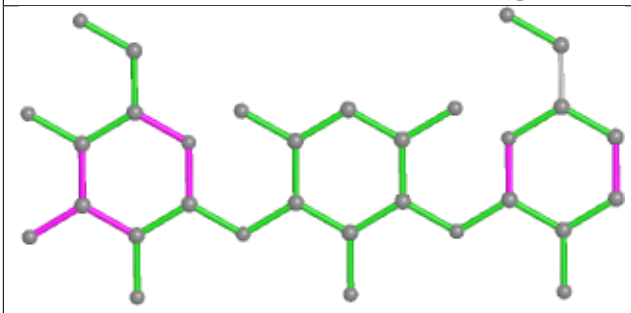


Torsions

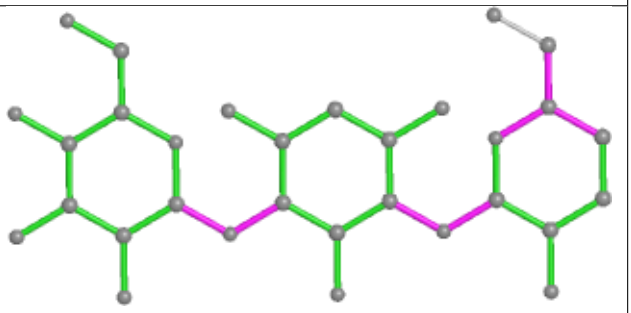


Rings

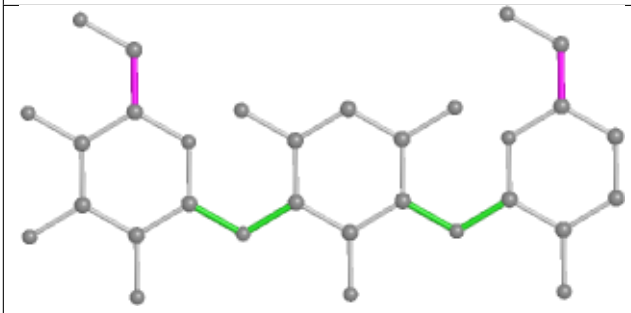
Ligand 84D 1A 5107



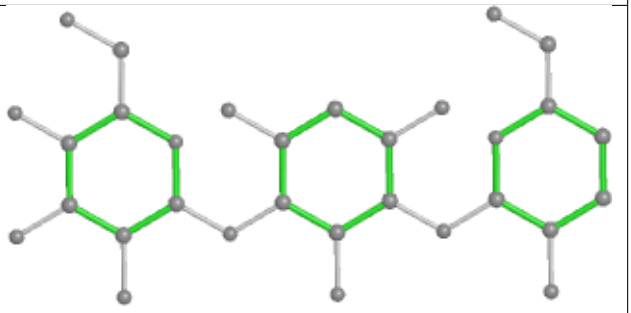
Bond lengths



Bond angles

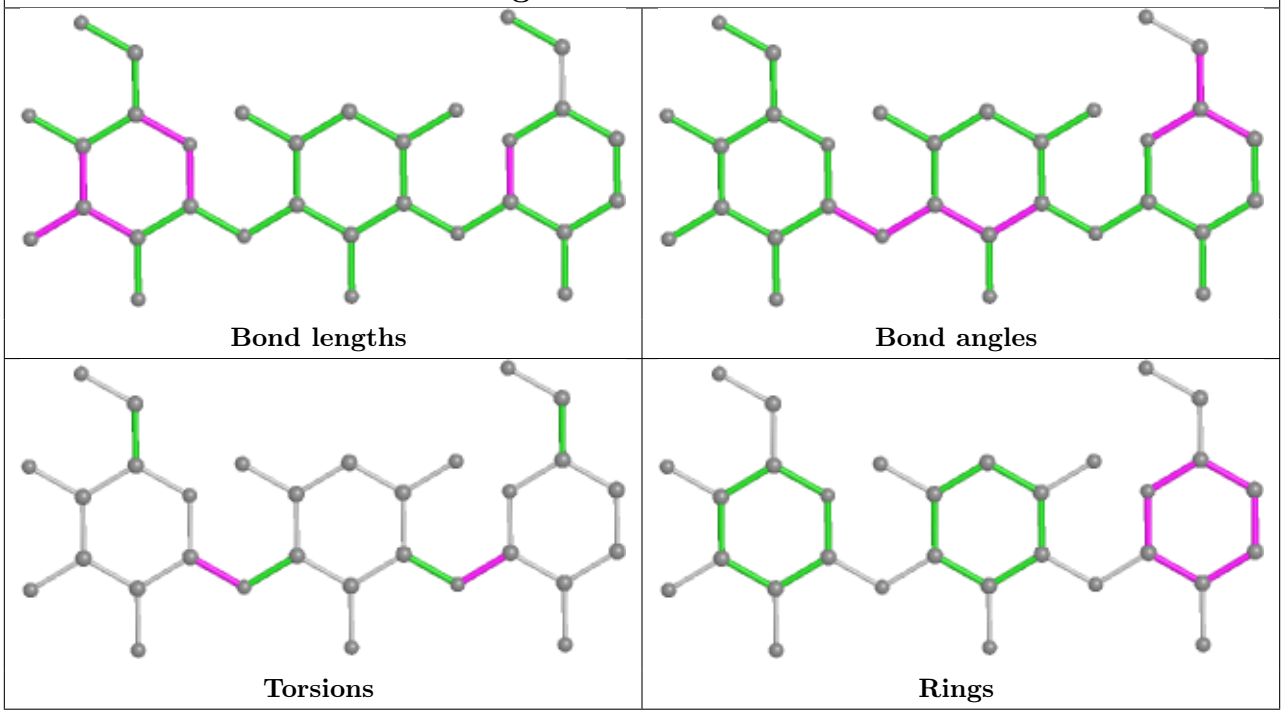


Torsions

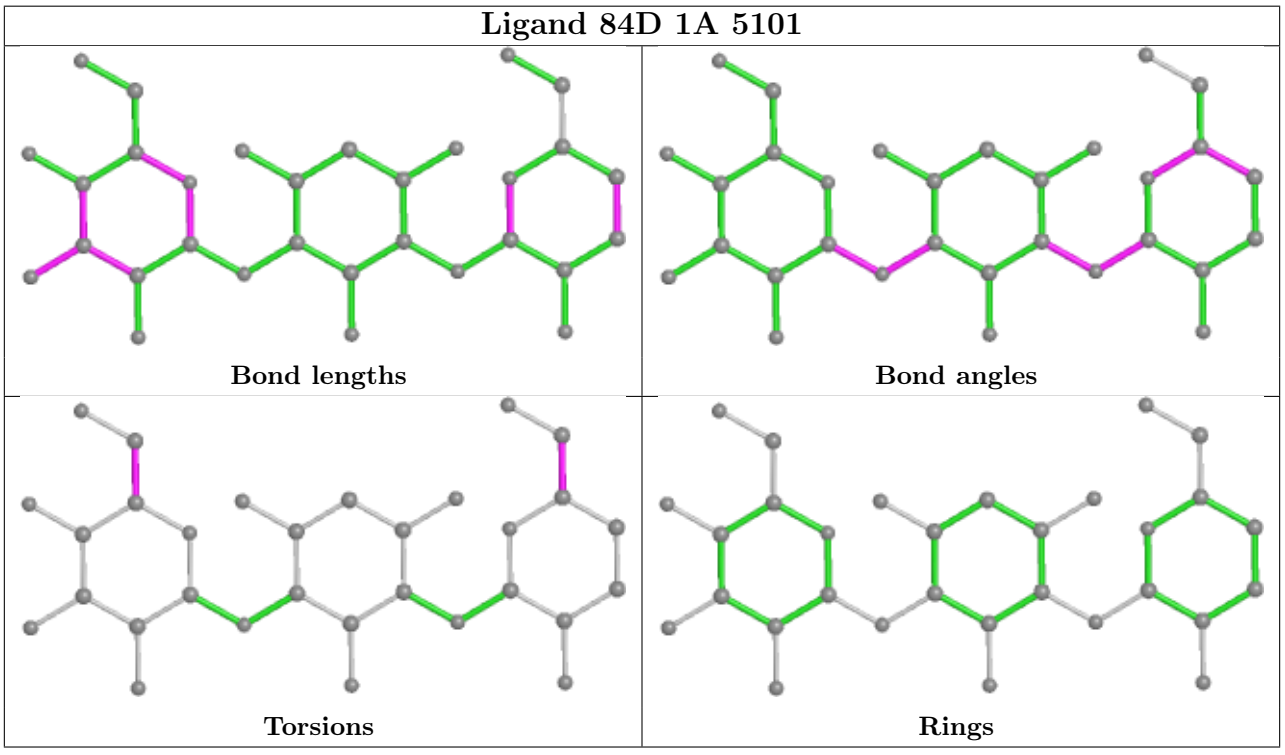


Rings

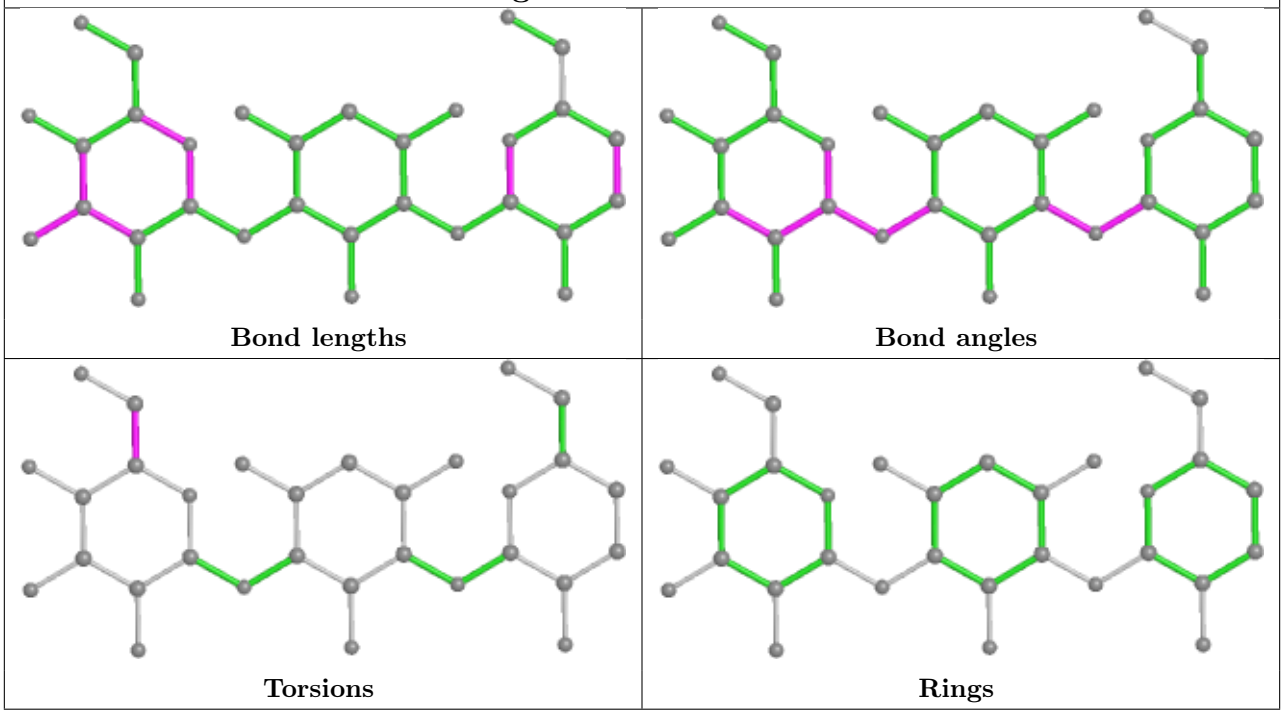
Ligand 84D 1A 5110



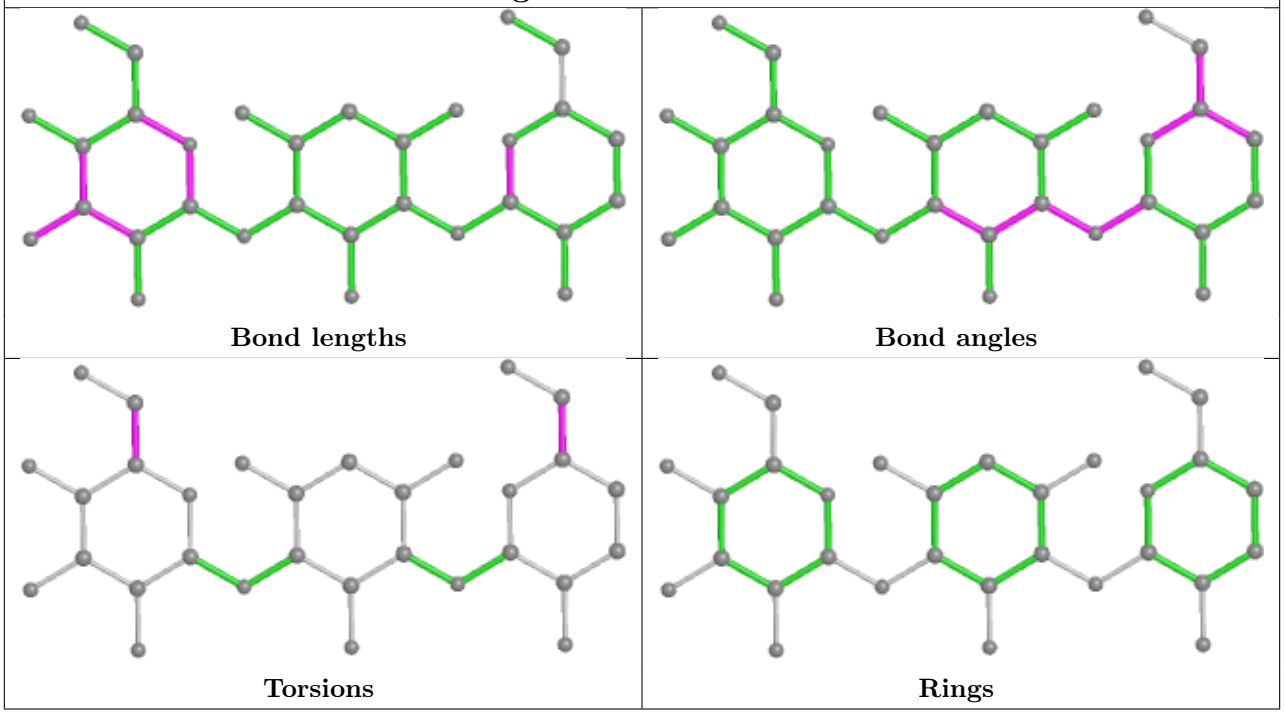
Ligand 84D 1A 5101



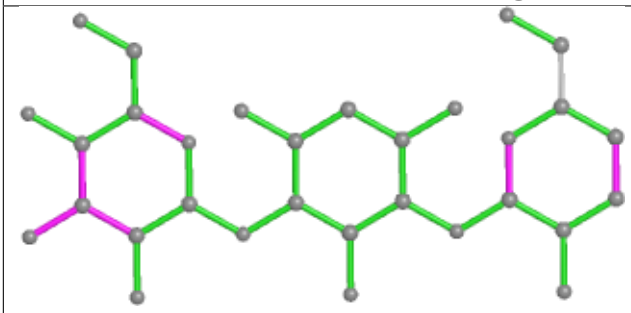
Ligand 84D 1A 5102



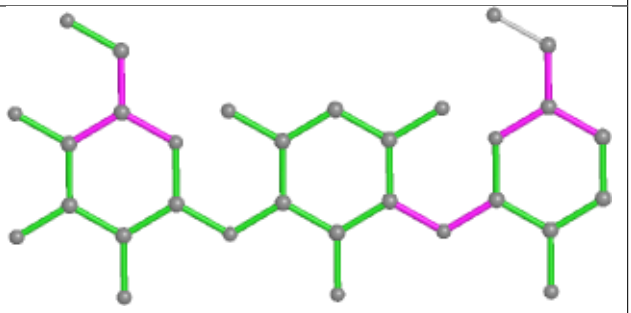
Ligand 84D 1A 5117



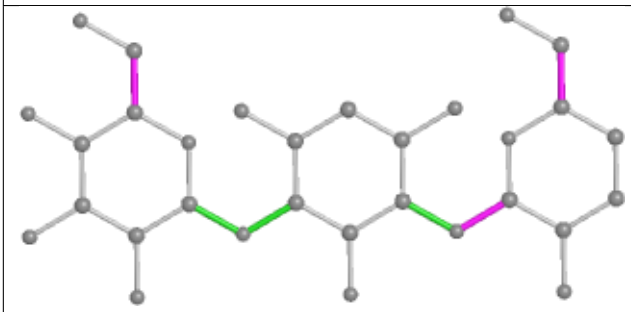
Ligand 84D 2m 1903



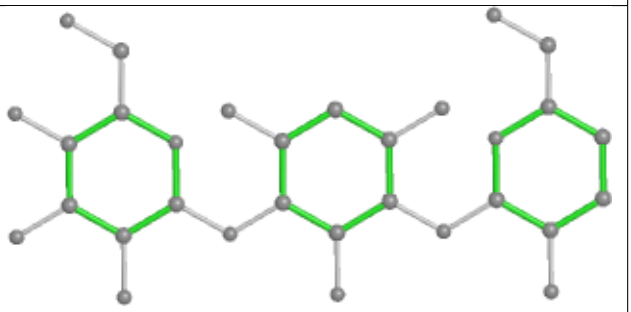
Bond lengths



Bond angles

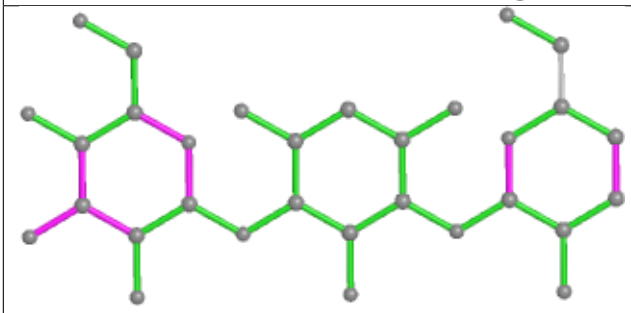


Torsions

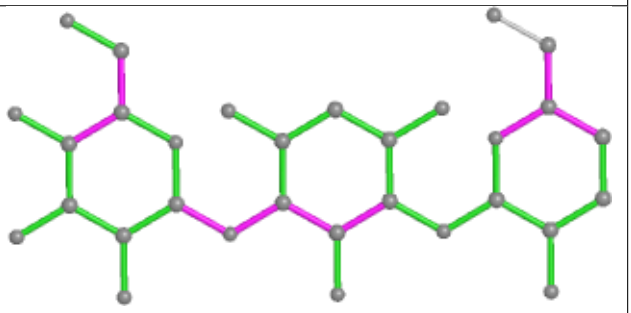


Rings

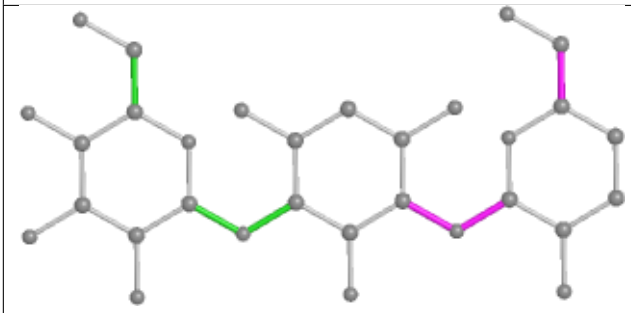
Ligand 84D 1A 5115



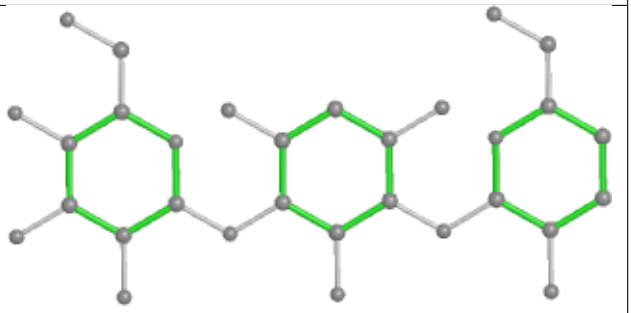
Bond lengths



Bond angles

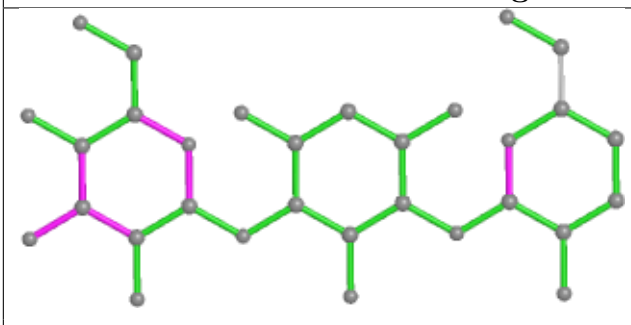


Torsions

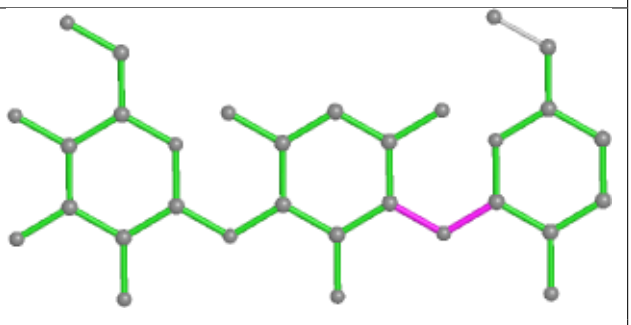


Rings

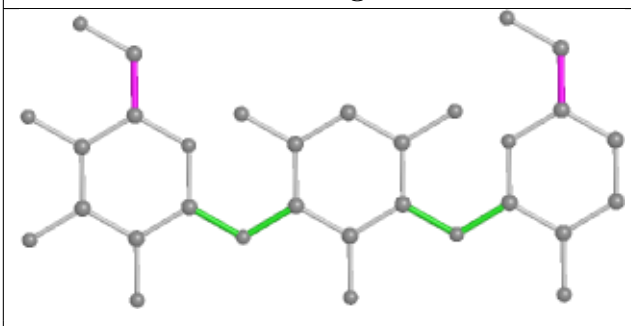
Ligand 84D 1A 5111



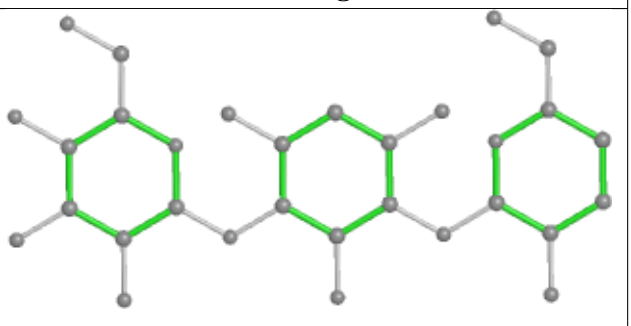
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

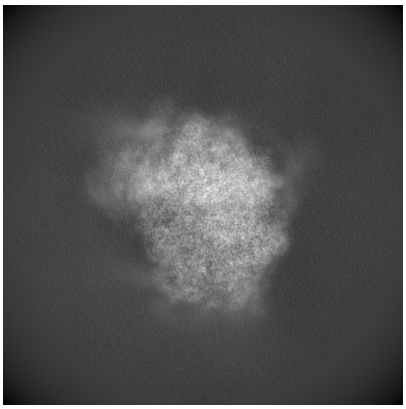
6 Map visualisation

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.

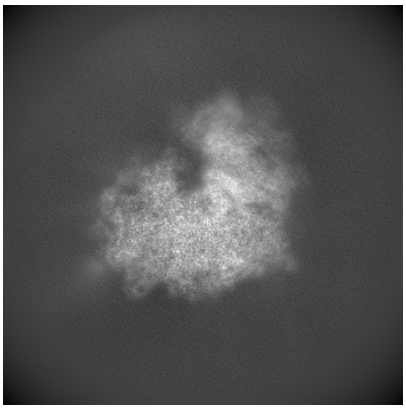
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

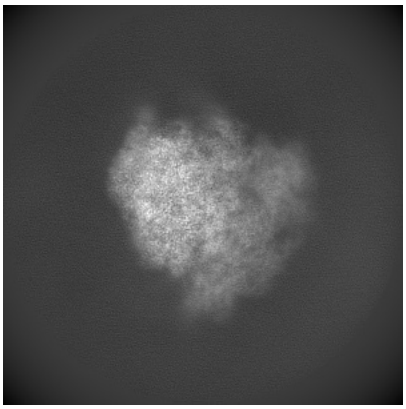
6.1.1 Primary map



X

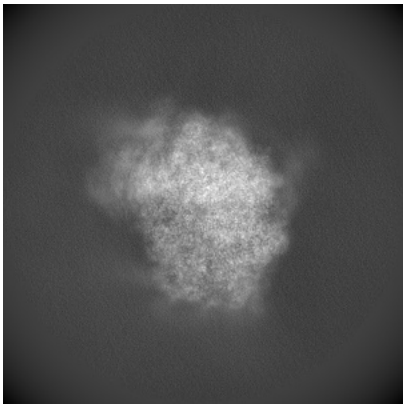


Y

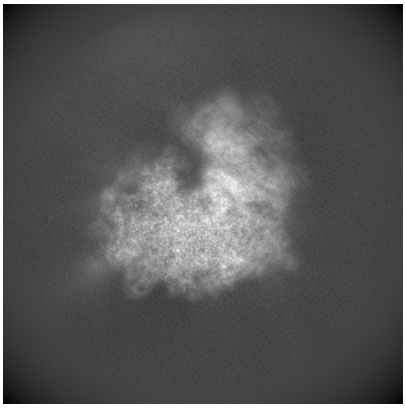


Z

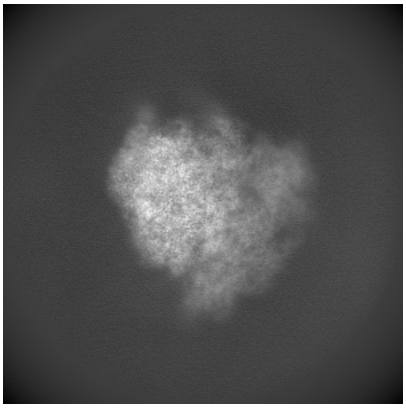
6.1.2 Raw map



X



Y

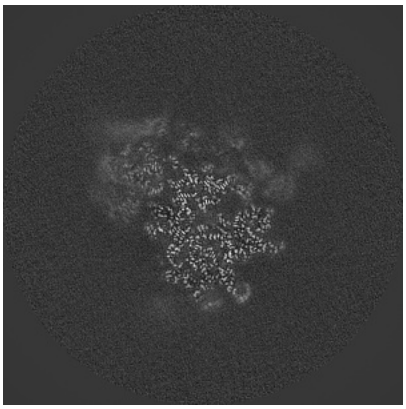


Z

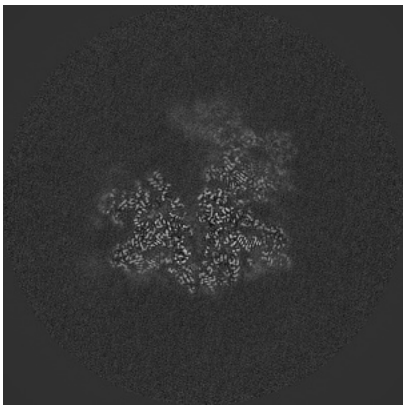
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

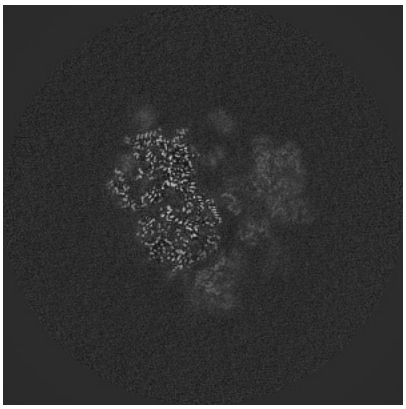
6.2.1 Primary map



X Index: 320

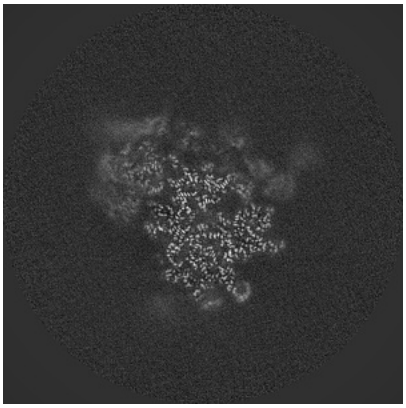


Y Index: 320

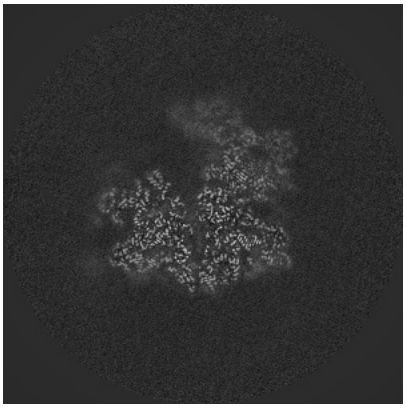


Z Index: 320

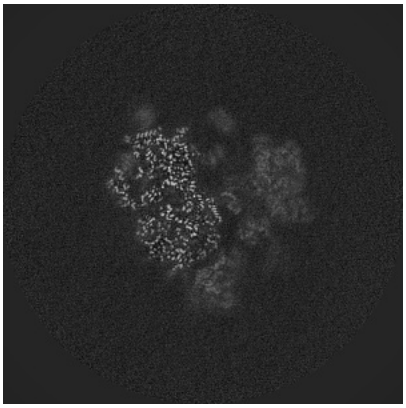
6.2.2 Raw map



X Index: 320



Y Index: 320

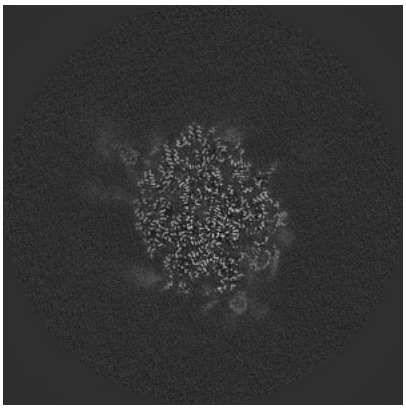


Z Index: 320

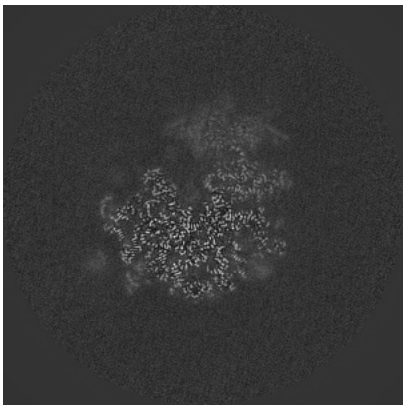
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

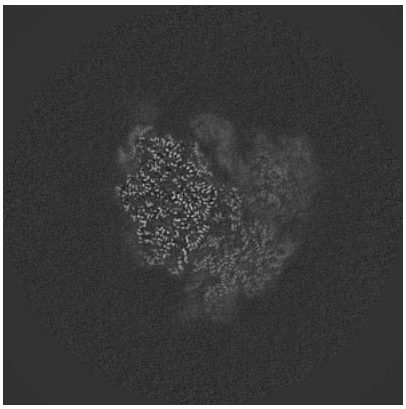
6.3.1 Primary map



X Index: 288

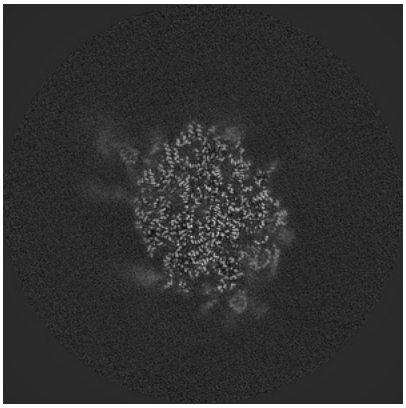


Y Index: 339

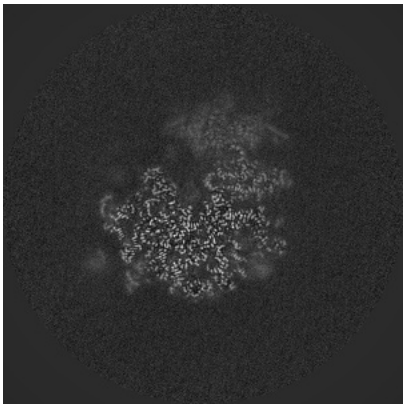


Z Index: 350

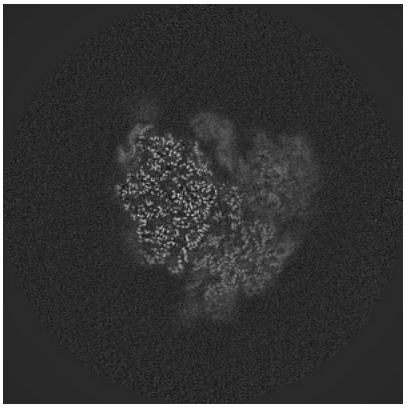
6.3.2 Raw map



X Index: 288



Y Index: 339

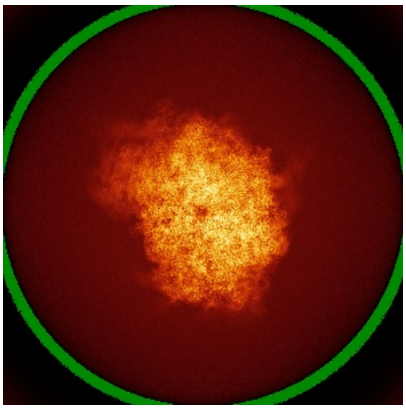


Z Index: 350

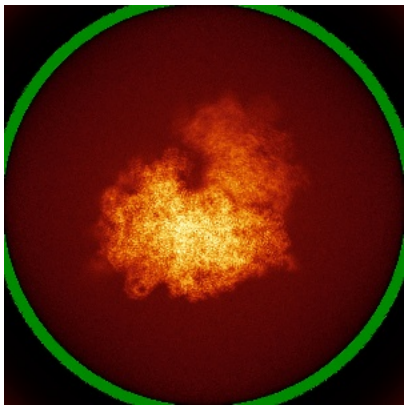
The images above show the largest variance slices of the map in three orthogonal directions.

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

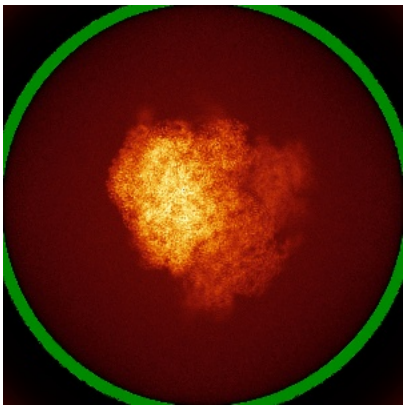
6.4.1 Primary map



X

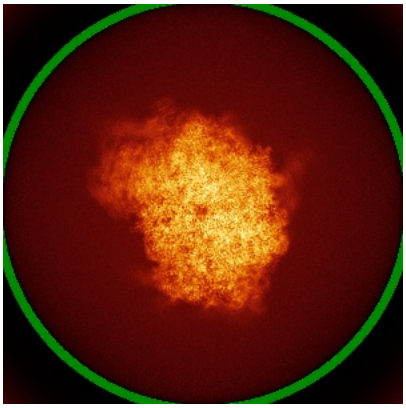


Y

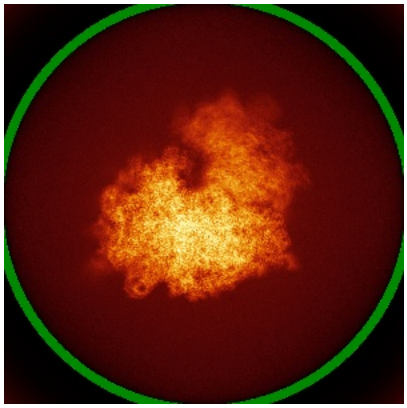


Z

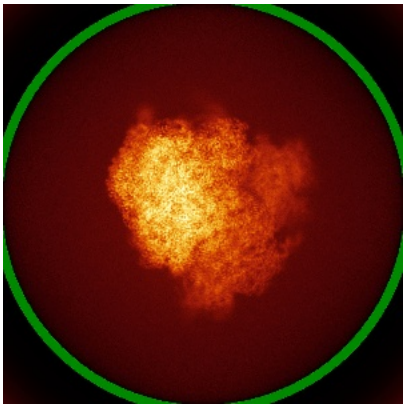
6.4.2 Raw map



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.

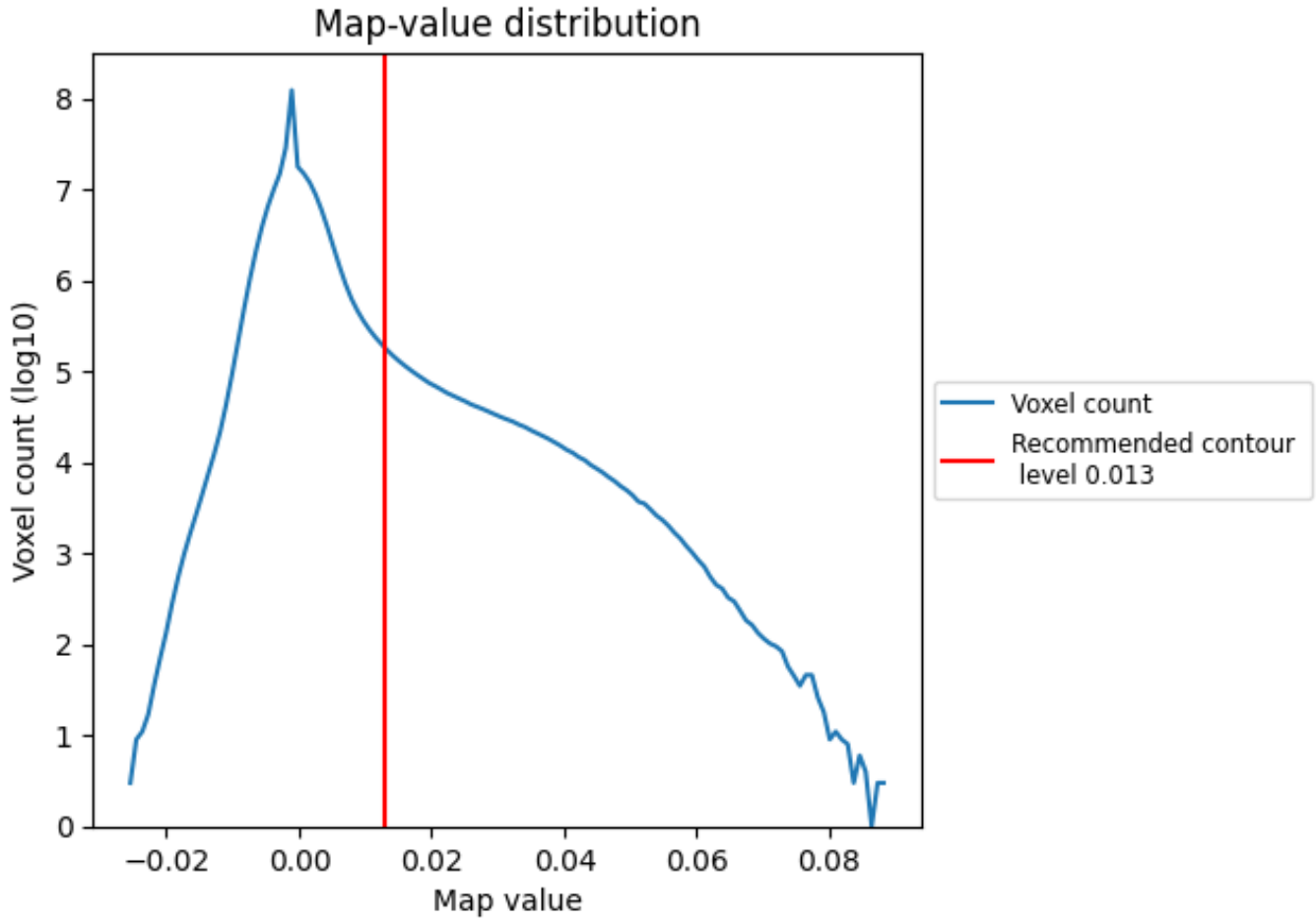
6.6 Mask visualisation (i)

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

7 Map analysis

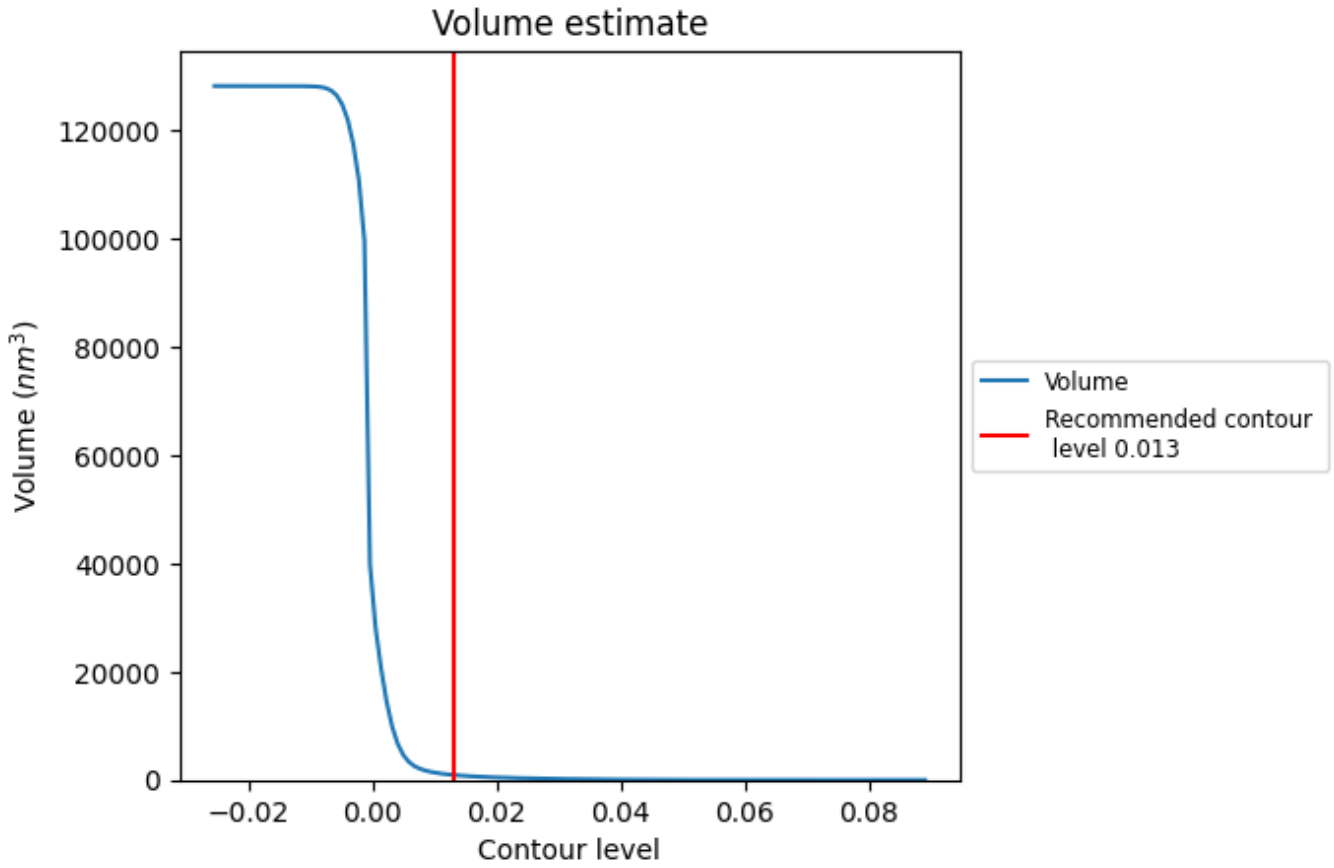
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

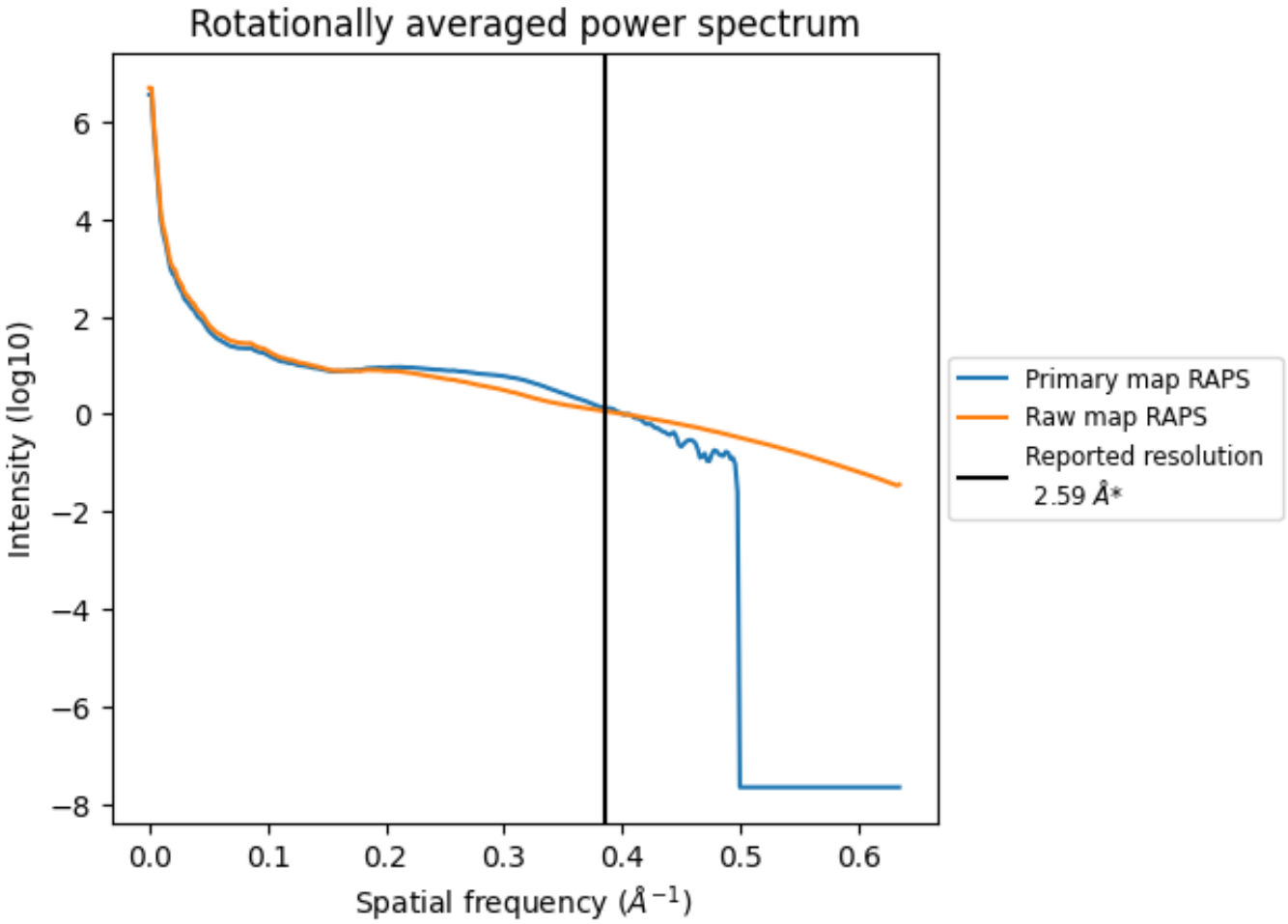
7.2 Volume estimate (i)



The volume at the recommended contour level is 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 (i)

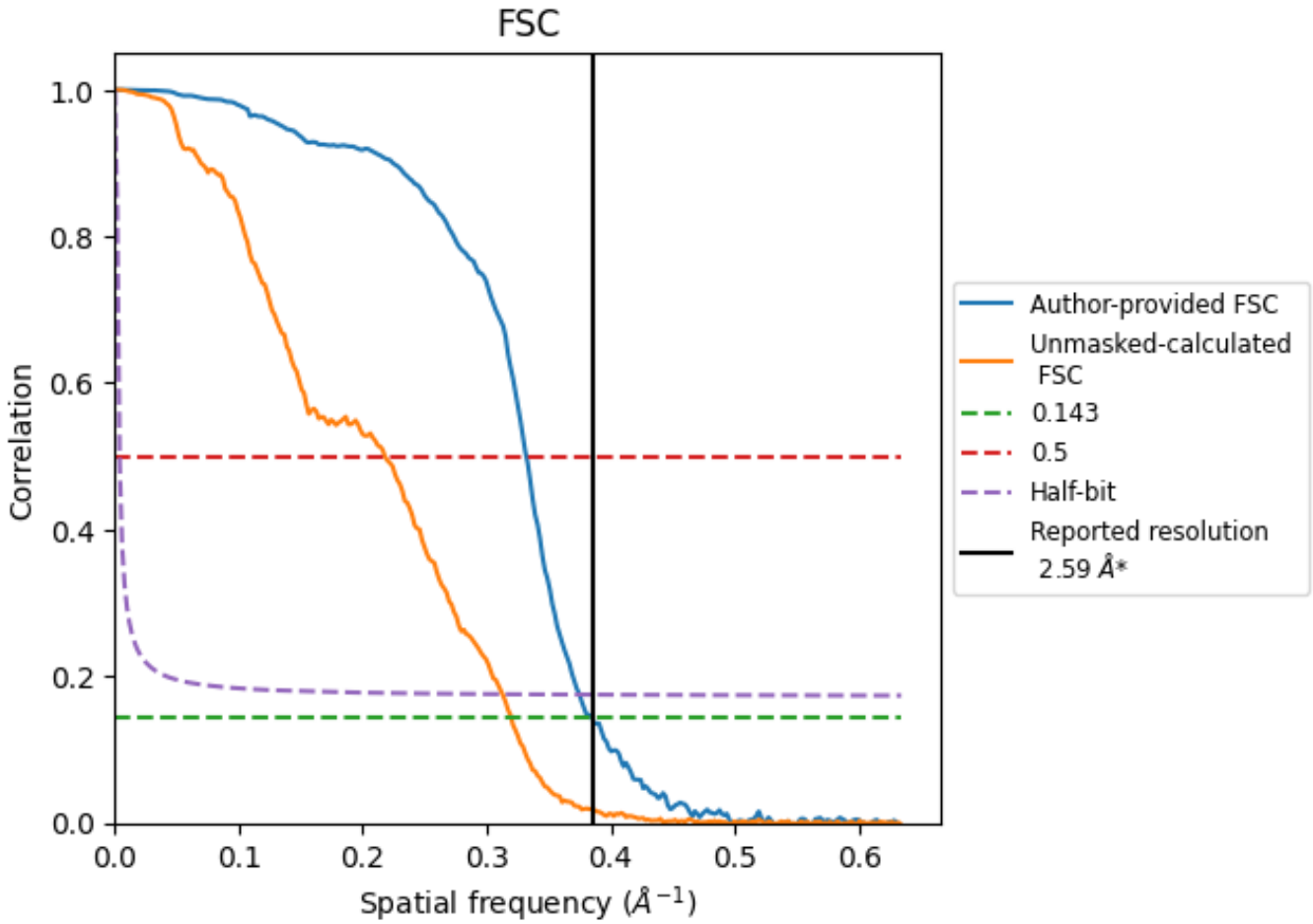


*Reported resolution corresponds to spatial frequency of 0.386 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.386 Å^{-1}

8.2 Resolution estimates (i)

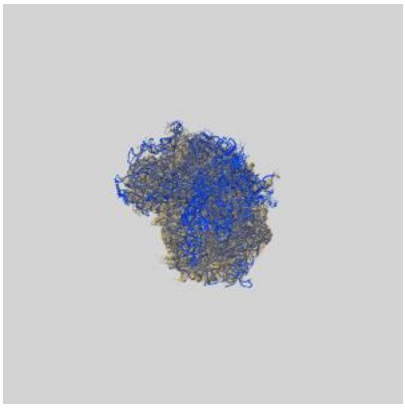
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.60	3.01	2.67
Unmasked-calculated*	3.13	4.59	3.20

*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 %

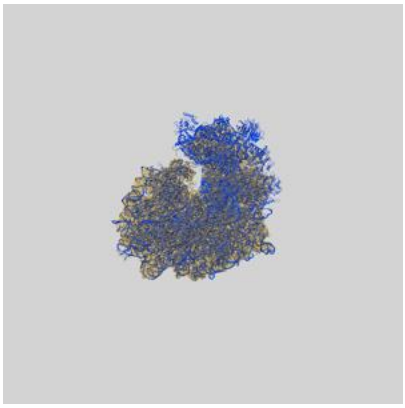
9 Map-model fit

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 21.

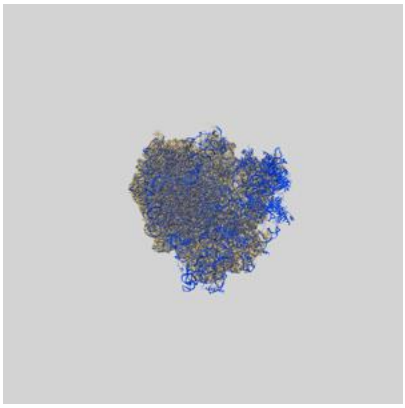
9.1 Map-model overlay



X



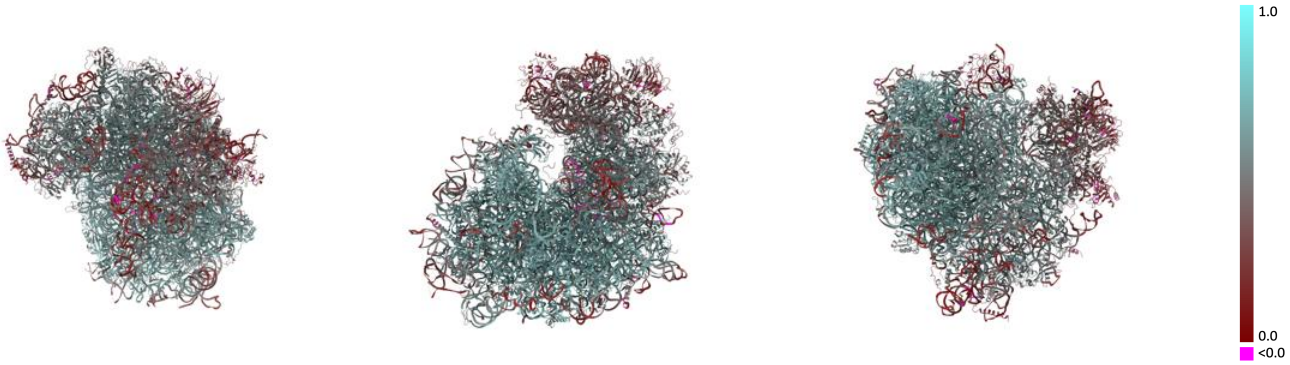
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

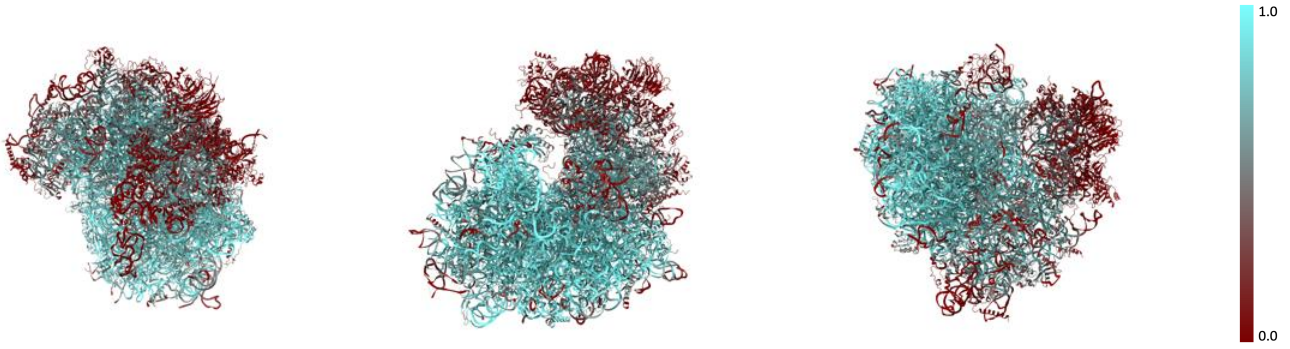
9.2 Q-score mapped to coordinate model (i)



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.

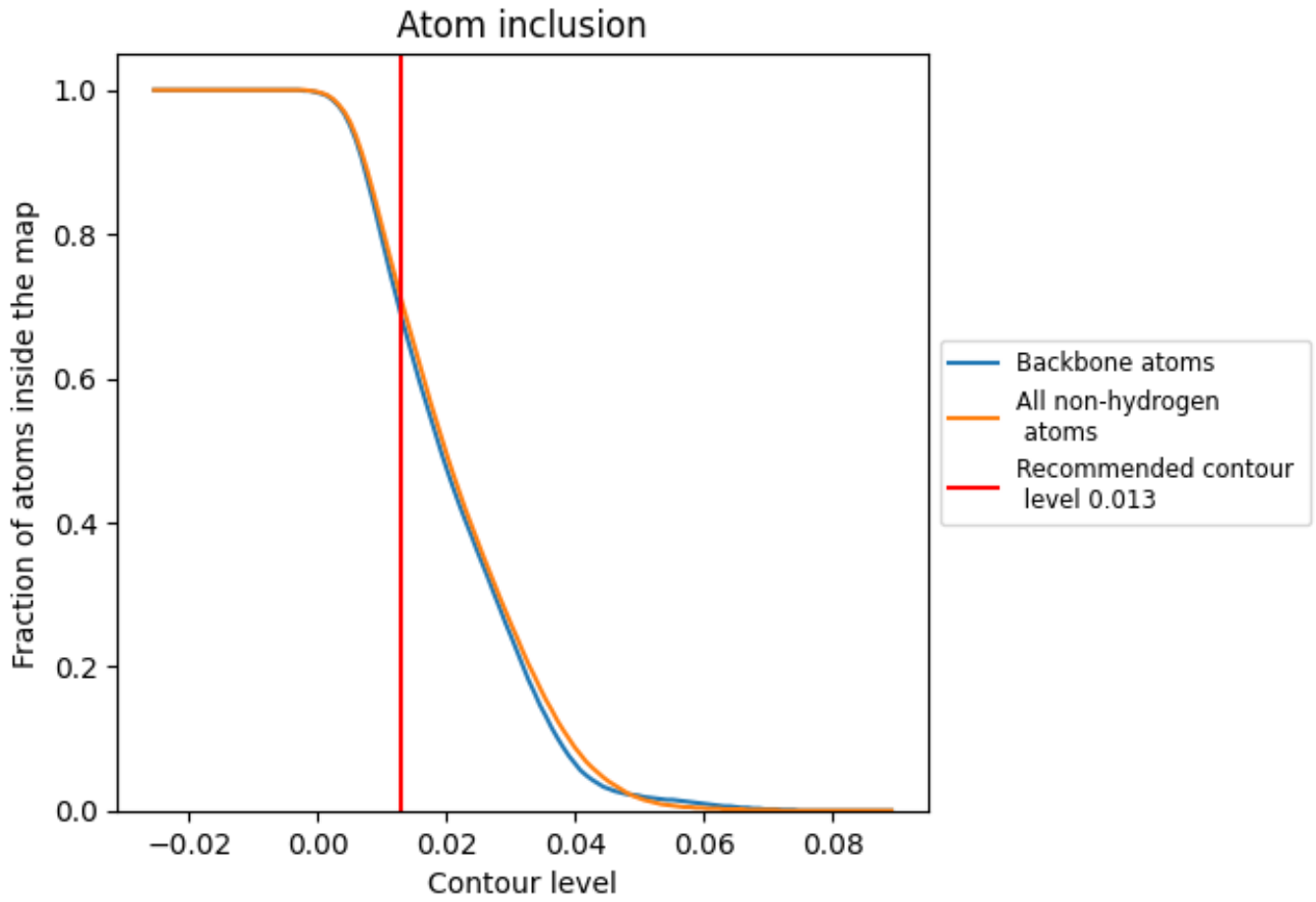
9.3 Atom inclusion mapped to coordinate model (i)



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 (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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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