



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 03:51 AM UTC

PDB ID : 8IFE / pdb_00008ife
EMDB ID : EMD-35414
Title : Arbekacin-added human 80S ribosome
Authors : Tomono, J.; Asano, K.; Chiashi, T.; Tanaka, Y.; Yokoyama, T.
Deposited on : 2023-02-17
Resolution : 2.57 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

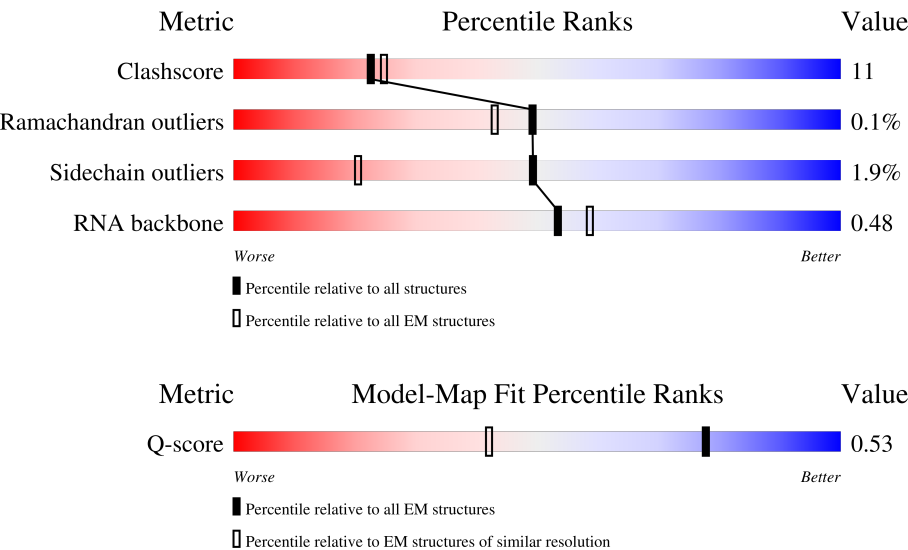
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.57 Å.

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



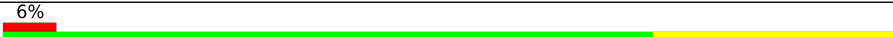
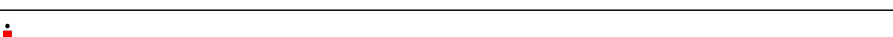
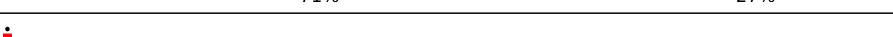
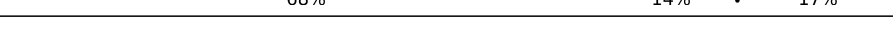
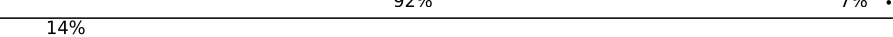
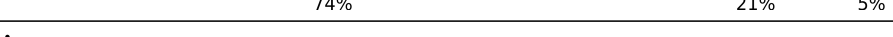
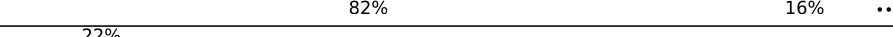
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7615 (2.07 - 3.07)

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

Mol	Chain	Length	Quality of chain
1	1A	5070	
2	1B	121	
3	1C	157	

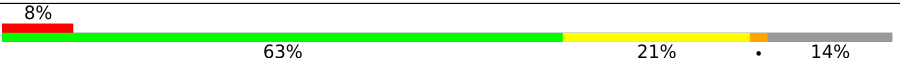
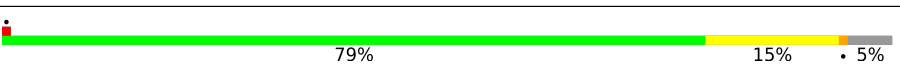
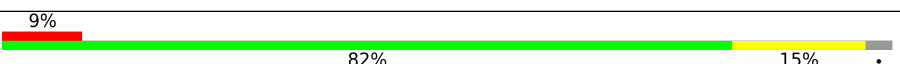
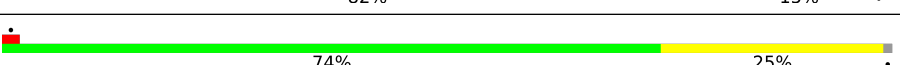
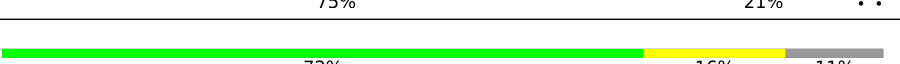
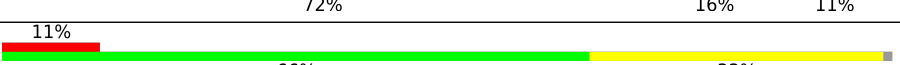
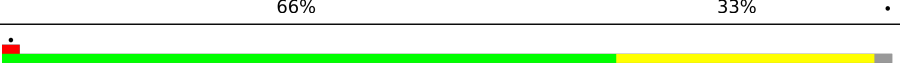
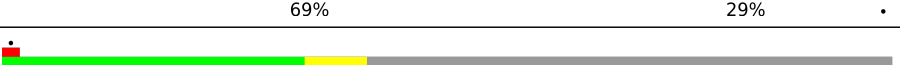
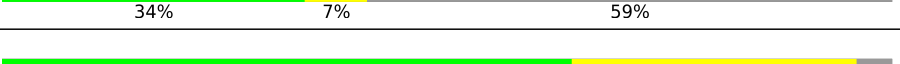
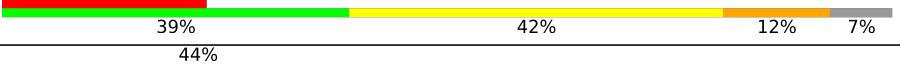
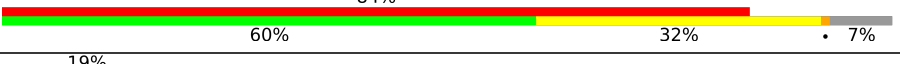
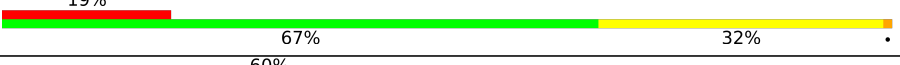
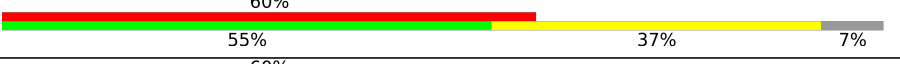
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Mol	Chain	Length	Quality of chain
4	1D	257	
5	1E	403	
6	1F	427	
7	1G	297	
8	1H	288	
9	2A	248	
10	2B	266	
11	2C	192	
12	2D	214	
13	2E	178	
14	2F	211	
15	2G	215	
16	2H	204	
17	2I	203	
18	2J	184	
19	2K	188	
20	2L	196	
21	2M	176	
22	2N	160	
23	2O	128	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

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

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

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Mol	Chain	Length	Quality of chain
79	3Q	59	53% 78% 20%
80	3R	156	43% 31% 12% 57%

2 Entry composition

There are 83 unique types of molecules in this entry. The entry contains 219097 atoms, of which 1012 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	3717	Total	C	N	O	P	0	0
			79676	35480	14585	25895	3716		

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

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
			1741	1113	312	307	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		

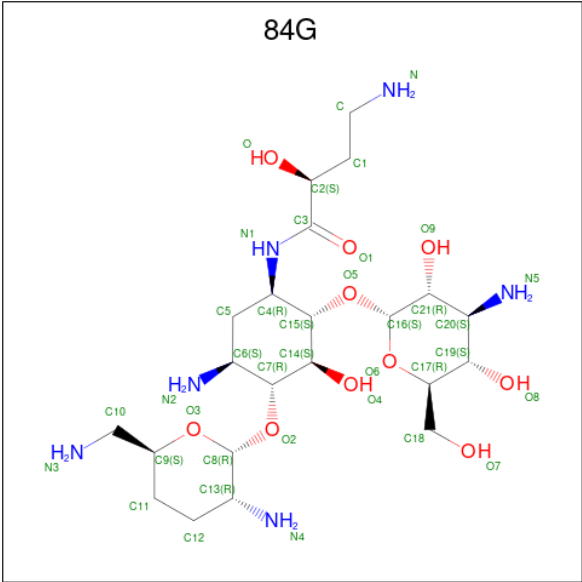
- Molecule 79 is a protein called 40S ribosomal protein S30.

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 Arbekacin (CCD ID: 84G) (formula: C₂₂H₄₄N₆O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	

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Mol	Chain	Residues	Atoms					AltConf
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	1A	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	2D	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	2i	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	2m	1	Total	C	H	N	O	0
			82	22	44	6	10	
81	2m	1	Total	C	H	N	O	0
			82	22	44	6	10	

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

Mol	Chain	Residues	Atoms		AltConf
82	1A	268	Total	Mg	0
			268	268	
82	1B	3	Total	Mg	0
			3	3	
82	1C	5	Total	Mg	0
			5	5	
82	1D	1	Total	Mg	0
			1	1	
82	1E	1	Total	Mg	0
			1	1	
82	2H	1	Total	Mg	0
			1	1	
82	2J	1	Total	Mg	0
			1	1	
82	2L	1	Total	Mg	0
			1	1	
82	2M	2	Total	Mg	0
			2	2	
82	2P	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
82	2Y	1	Total 1	Mg 1	0
82	2Z	1	Total 1	Mg 1	0
82	2a	1	Total 1	Mg 1	0
82	2d	1	Total 1	Mg 1	0
82	2m	120	Total 120	Mg 120	0
82	20	1	Total 1	Mg 1	0
82	3H	1	Total 1	Mg 1	0

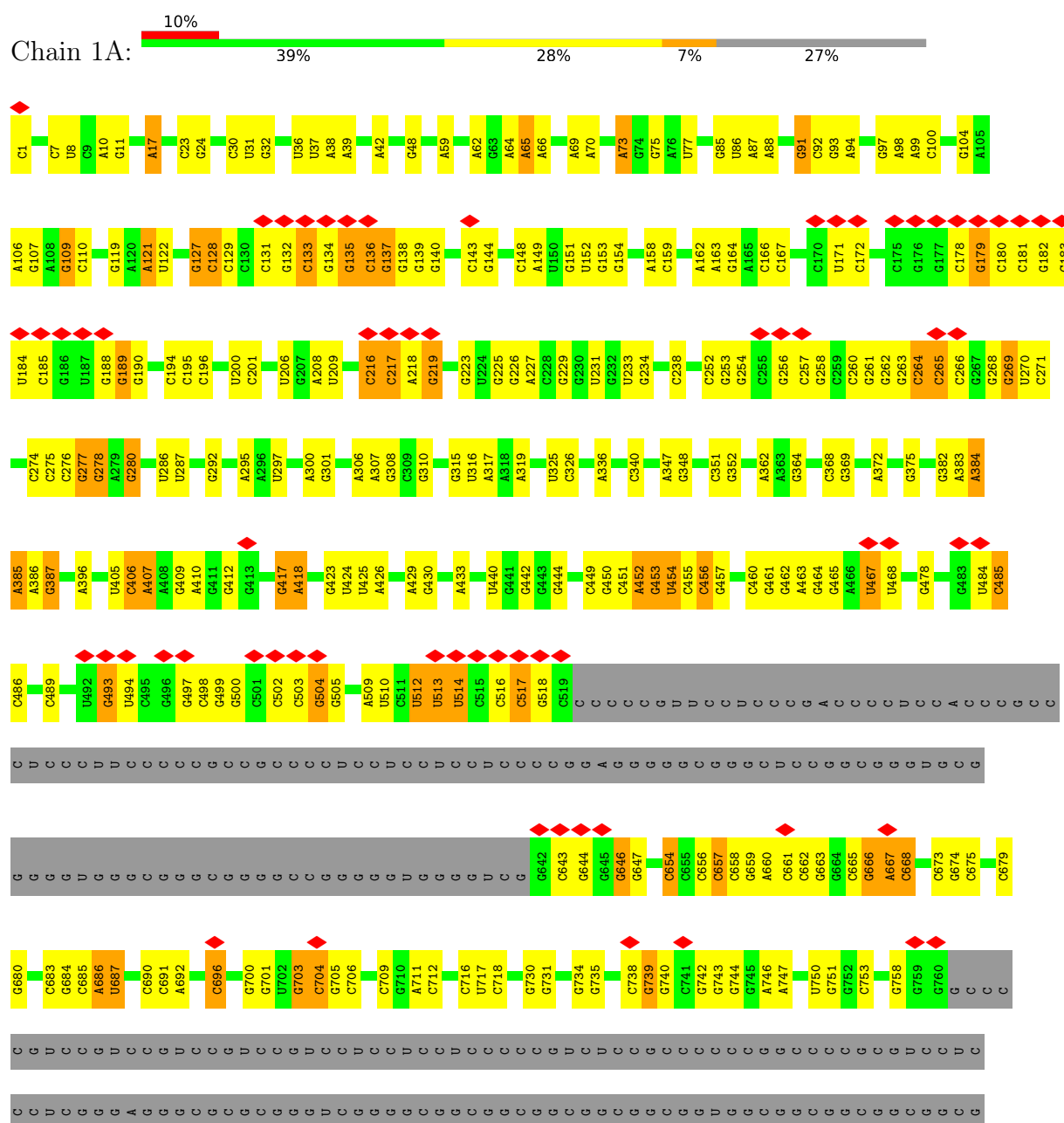
- Molecule 83 is ZINC ION (CCD ID: ZN) (formula: Zn).

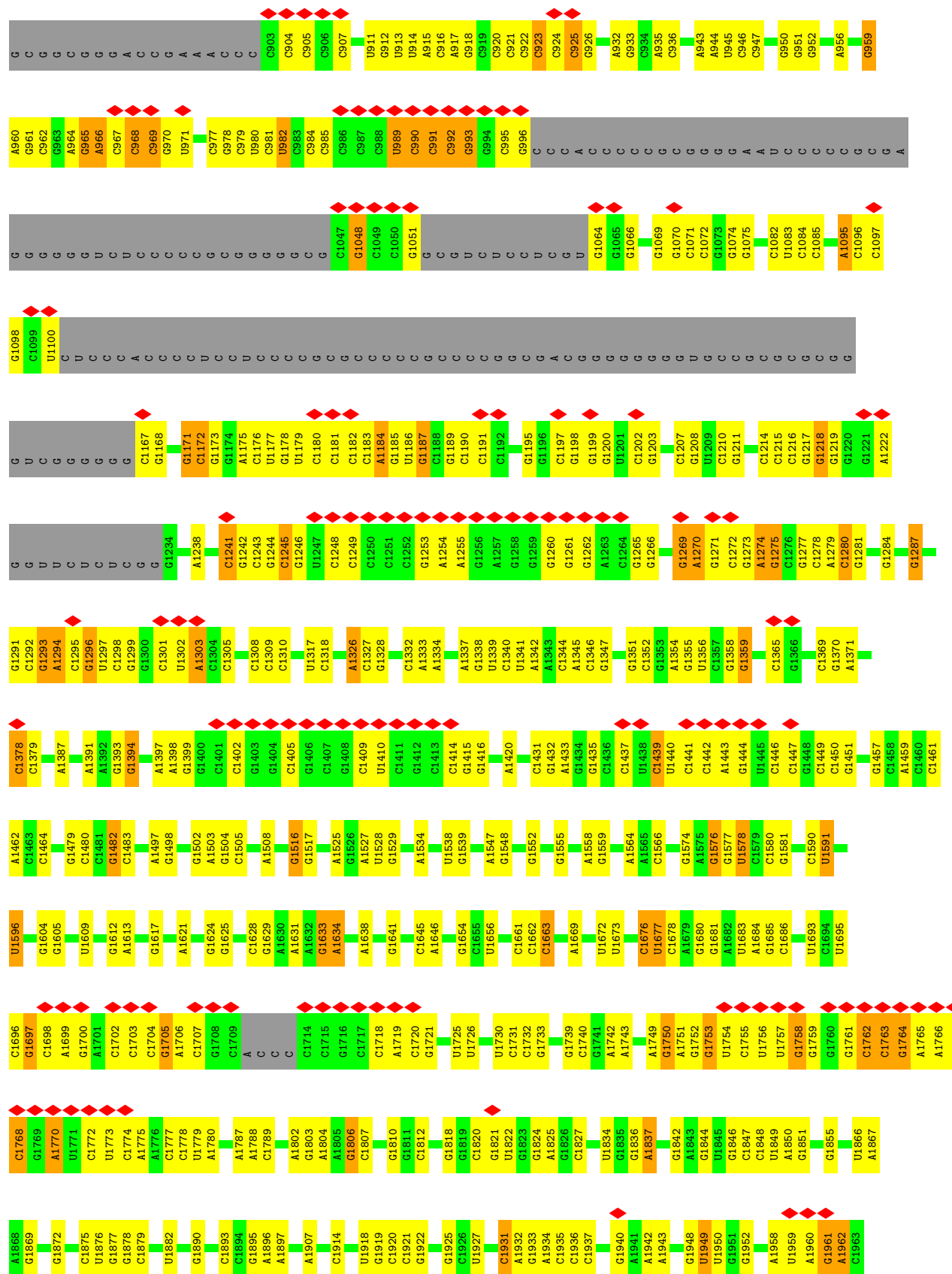
Mol	Chain	Residues	Atoms		AltConf
83	2d	1	Total 1	Zn 1	0
83	2g	1	Total 1	Zn 1	0
83	2i	1	Total 1	Zn 1	0
83	2j	1	Total 1	Zn 1	0
83	3C	1	Total 1	Zn 1	0
83	3E	1	Total 1	Zn 1	0

3 Residue-property plots

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

• Molecule 1: 28S ribosomal RNA





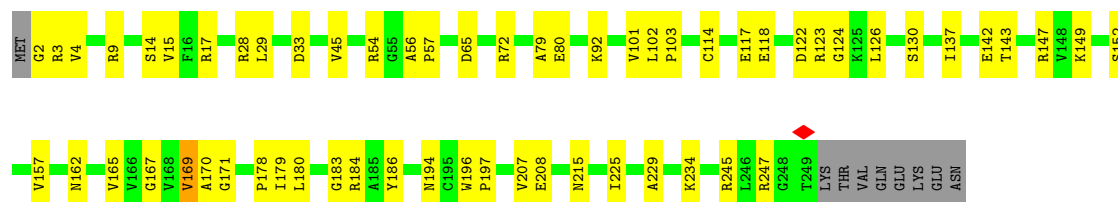






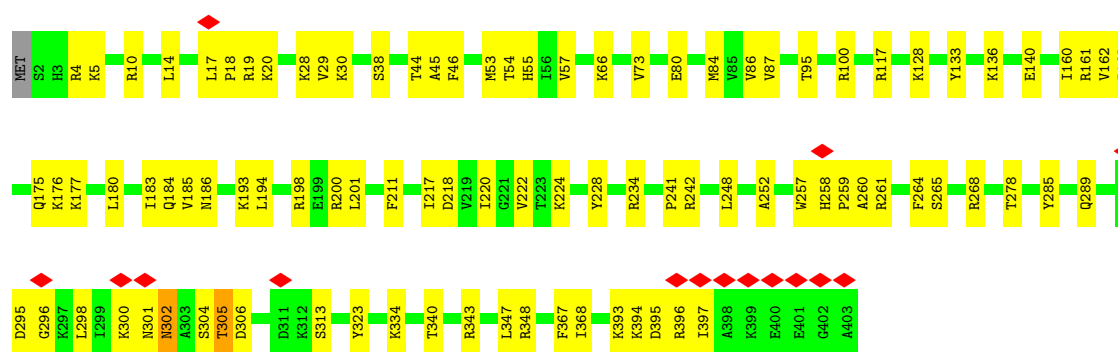
- Molecule 4: 60S ribosomal protein L8

Chain 1D:  73% 23%



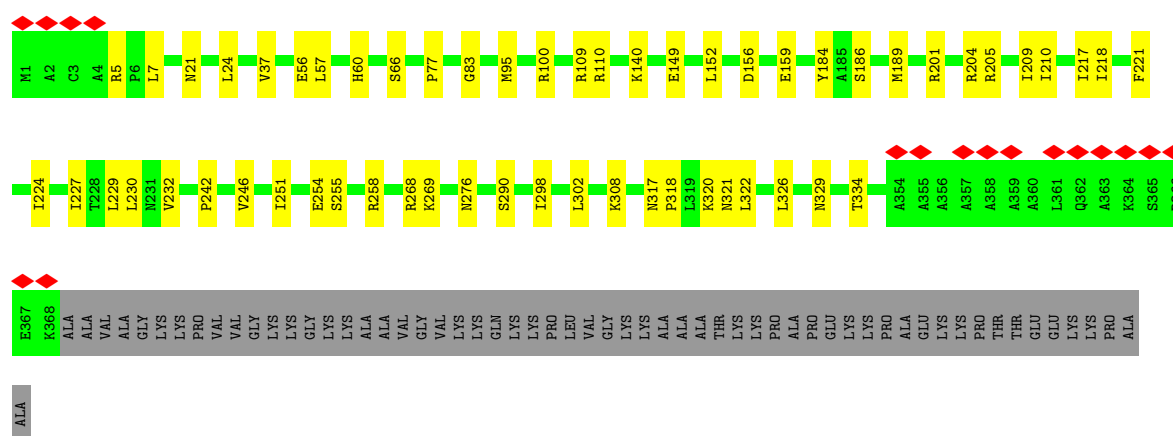
- Molecule 5: 60S ribosomal protein L3

Chain 1E:  76% 23%



- Molecule 6: 60S ribosomal protein L4

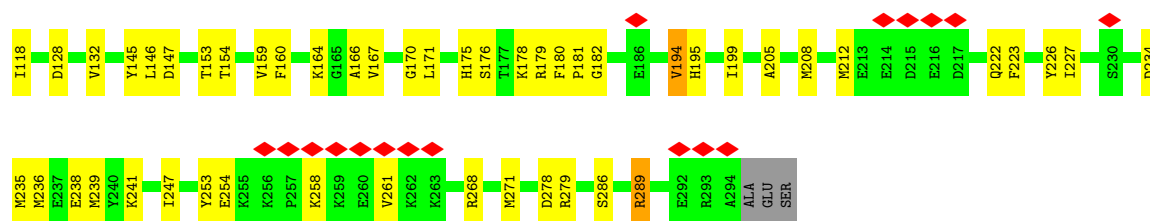
Chain 1F:  73% 13% 14%



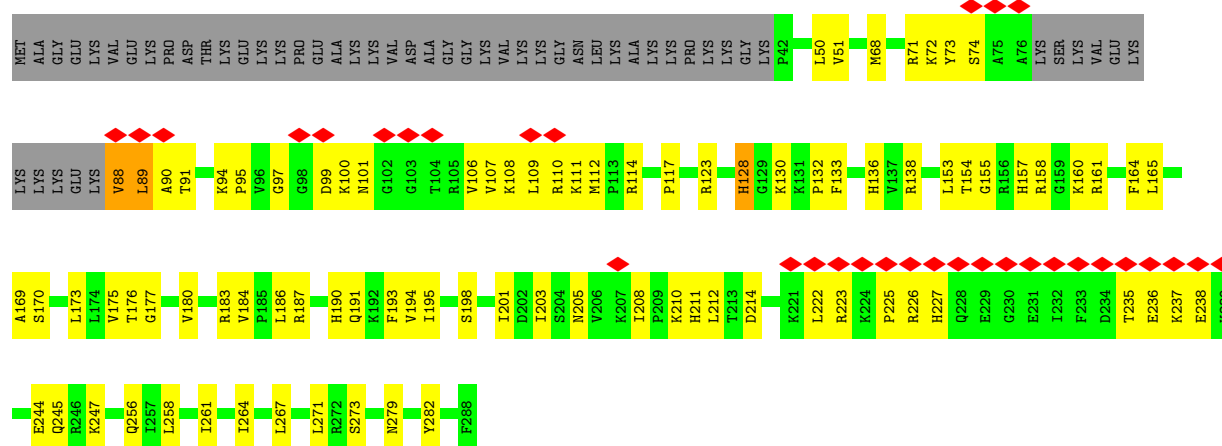
- Molecule 7: 60S ribosomal protein L5

Chain 1G:  7% 71% 27%

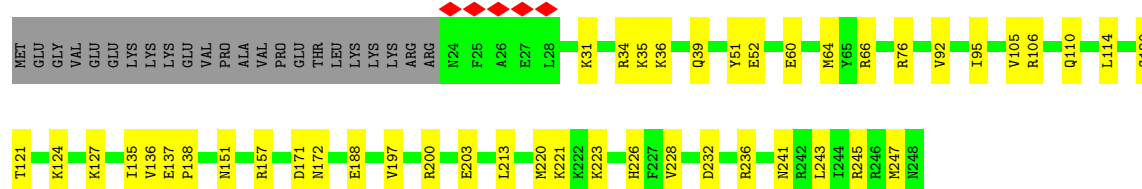
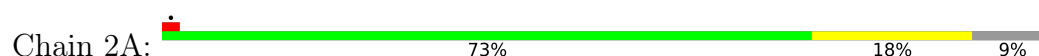




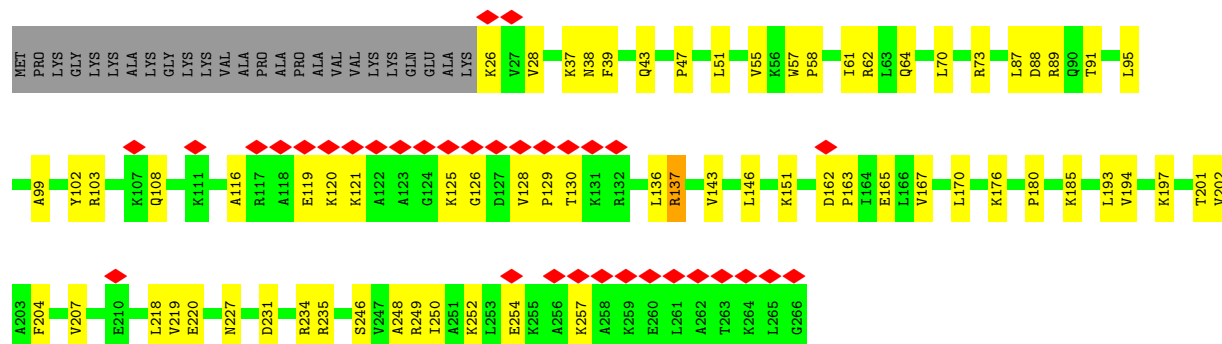
• Molecule 8: 60S ribosomal protein L6



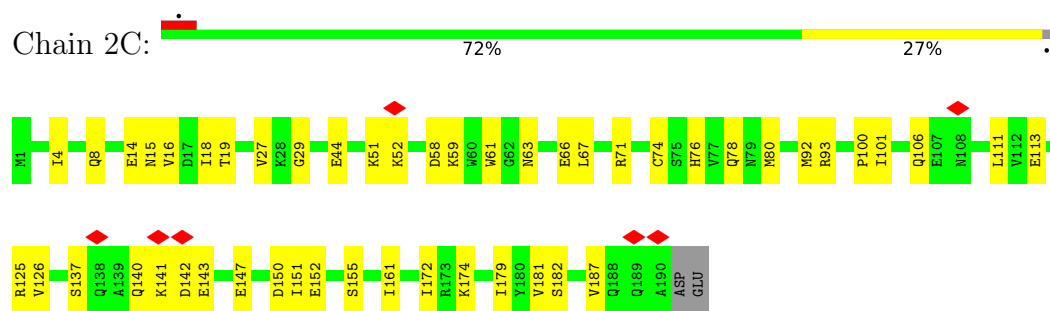
• Molecule 9: 60S ribosomal protein L7



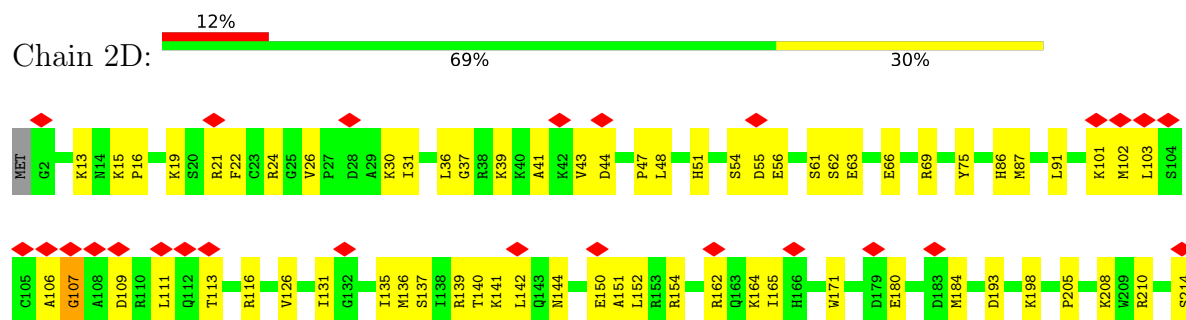
• Molecule 10: 60S ribosomal protein L7a



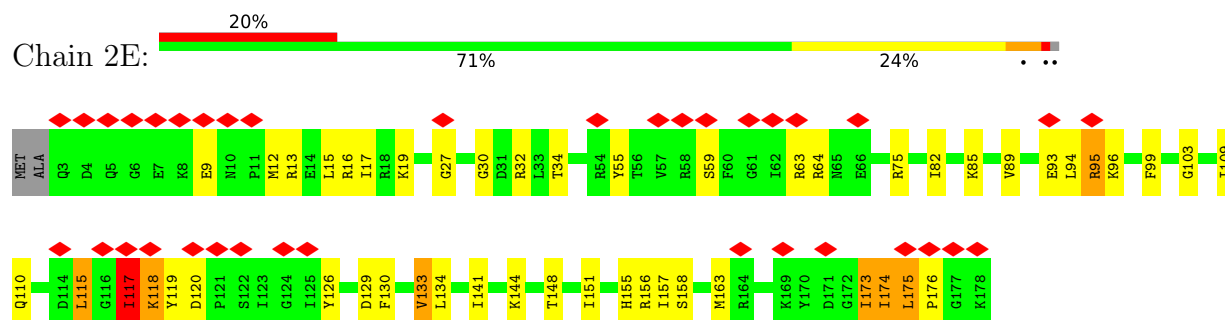
- Molecule 11: 60S ribosomal protein L9



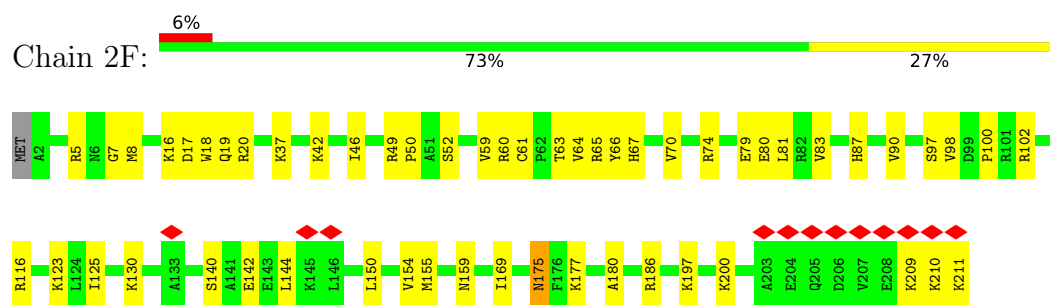
- Molecule 12: 60S ribosomal protein L10-like



- Molecule 13: 60S ribosomal protein L11

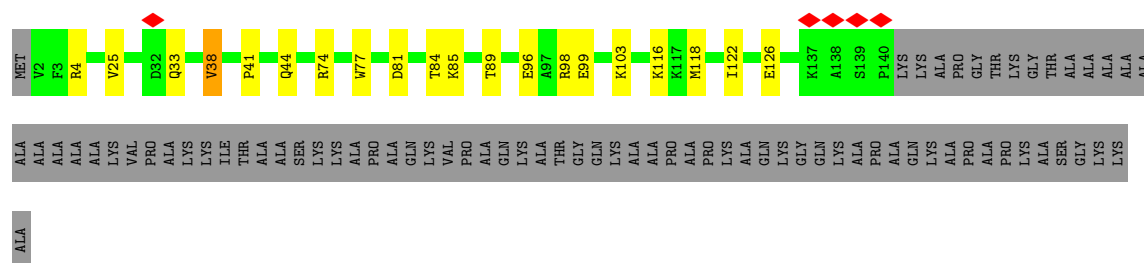


- Molecule 14: 60S ribosomal protein L13



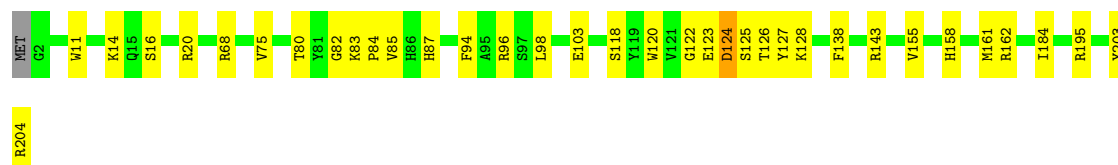
- Molecule 15: 60S ribosomal protein L14





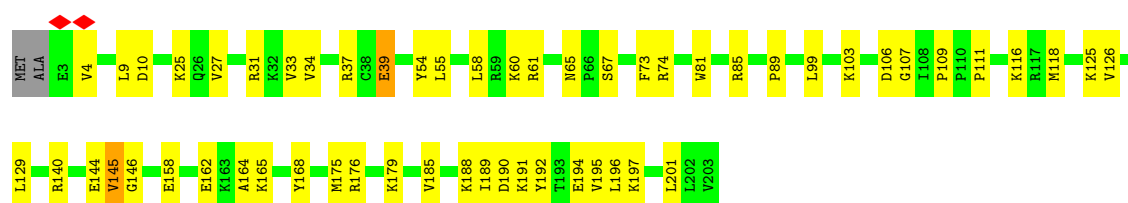
- Molecule 16: 60S ribosomal protein L15

Chain 2H: 82% 17%



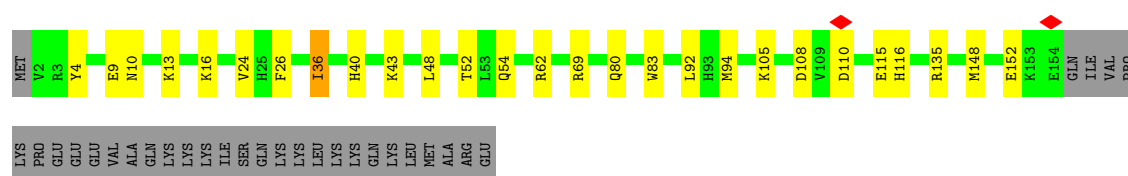
- Molecule 17: 60S ribosomal protein L13a

Chain 2I: 71% 27% ..



- Molecule 18: 60S ribosomal protein L17

Chain 2J: 68% 14% 17%



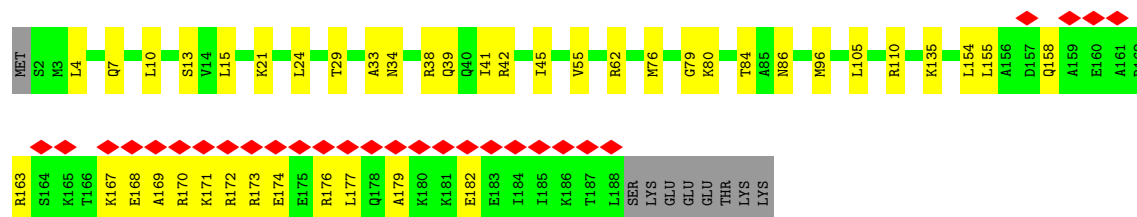
- Molecule 19: 60S ribosomal protein L18

Chain 2K: 92% 7%

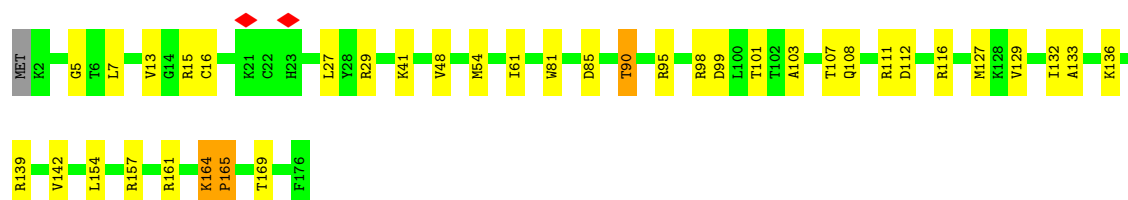
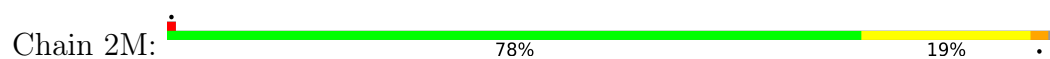


- Molecule 20: 60S ribosomal protein L19

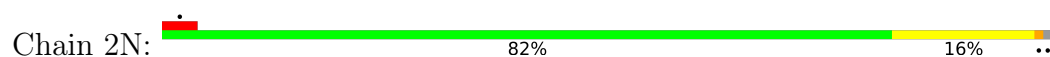
Chain 2L: 14% 74% 21% 5%



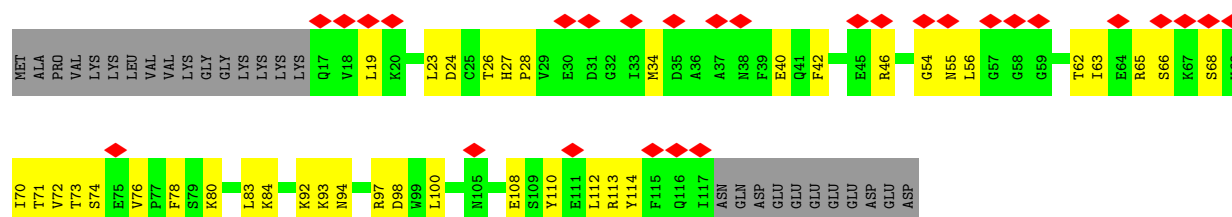
- Molecule 21: 60S ribosomal protein L18a



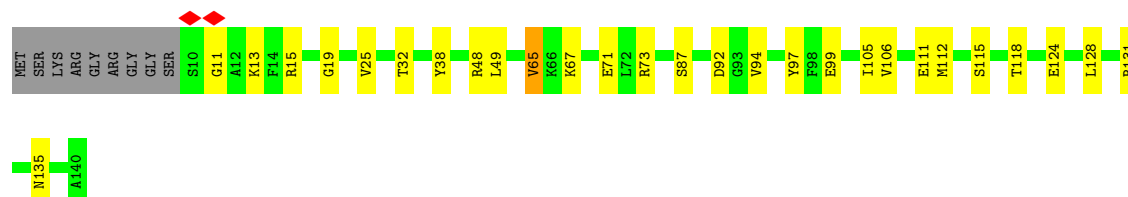
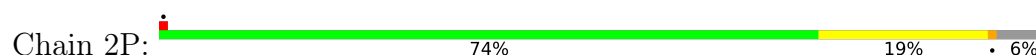
- Molecule 22: 60S ribosomal protein L21



- Molecule 23: 60S ribosomal protein L22

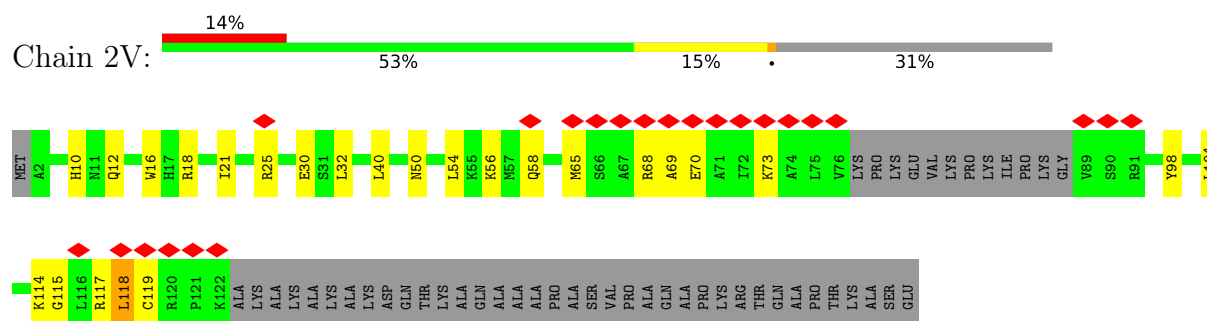


- Molecule 24: 60S ribosomal protein L23

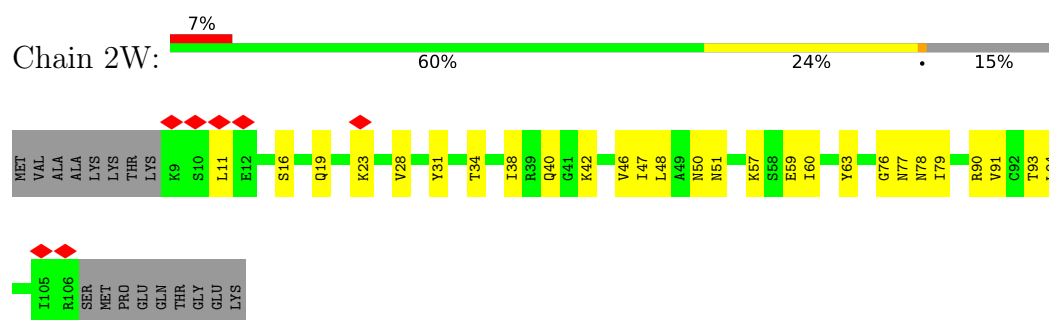


- Molecule 25: 60S ribosomal protein L24

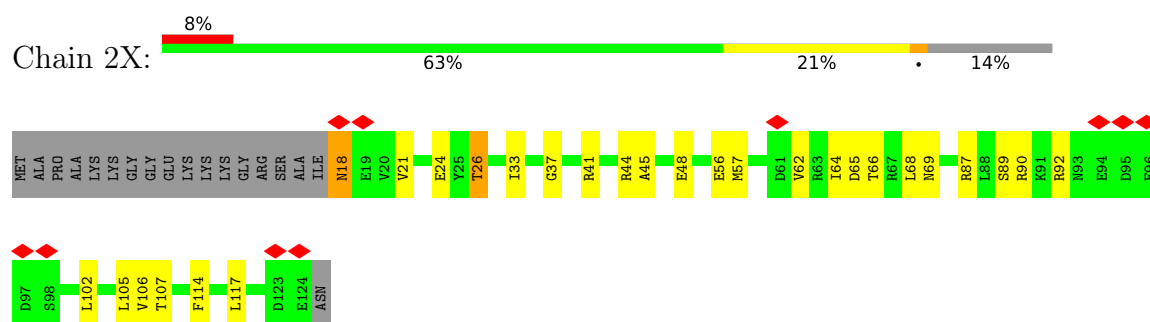
- Molecule 30: 60S ribosomal protein L29



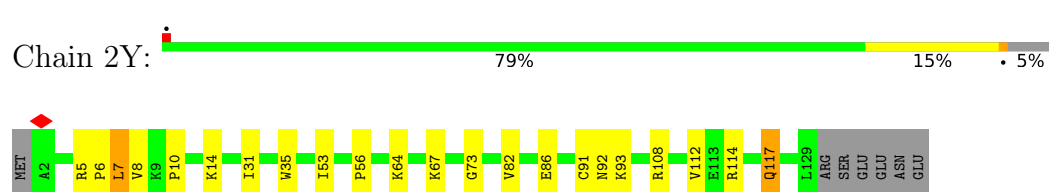
- Molecule 31: 60S ribosomal protein L30



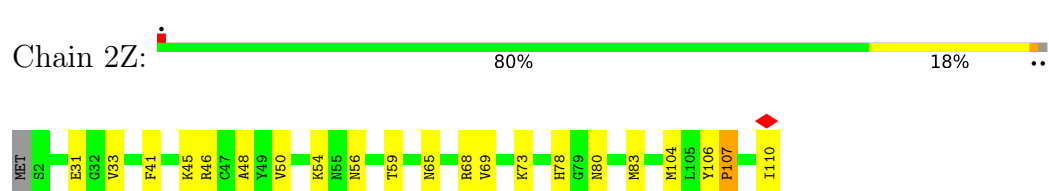
- Molecule 32: 60S ribosomal protein L31



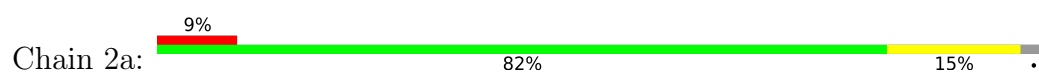
- Molecule 33: 60S ribosomal protein L32



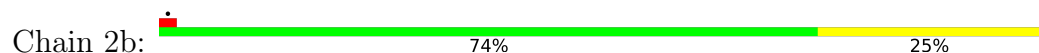
- Molecule 34: 60S ribosomal protein L35a



- Molecule 35: 60S ribosomal protein L34



- Molecule 36: 60S ribosomal protein L35



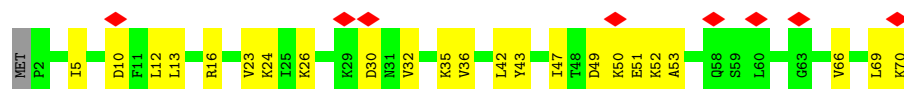
- Molecule 37: 60S ribosomal protein L36



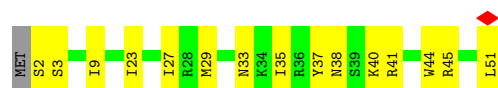
- Molecule 38: 60S ribosomal protein L37



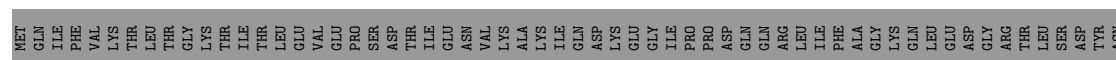
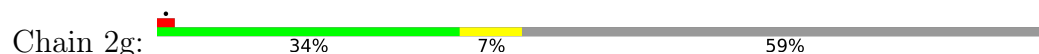
- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39



- Molecule 41: Ubiquitin-60S ribosomal protein L40





- Molecule 42: 60S ribosomal protein L41

Chain 2h: 64% 32% .



- Molecule 43: 60S ribosomal protein L36a

Chain 2i: 7% 81% 17% ..



- Molecule 44: 60S ribosomal protein L37a

Chain 2j: 84% 15% .



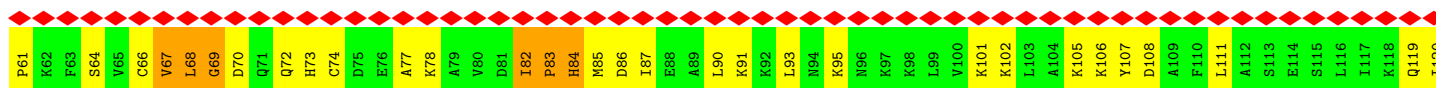
- Molecule 45: 60S ribosomal protein L28

Chain 2k: 66% 25% 9%



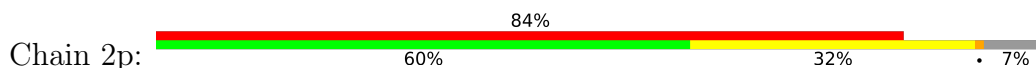
- Molecule 46: 60S ribosomal protein L10a

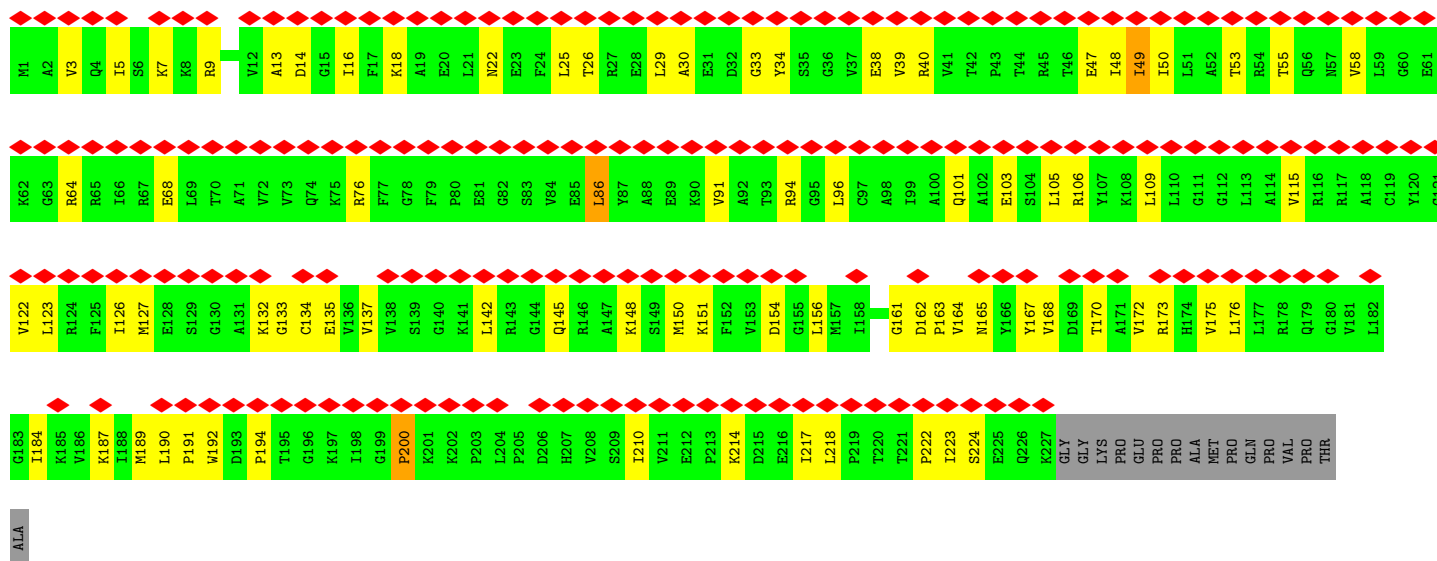
Chain 2l: 100% 64% 33%



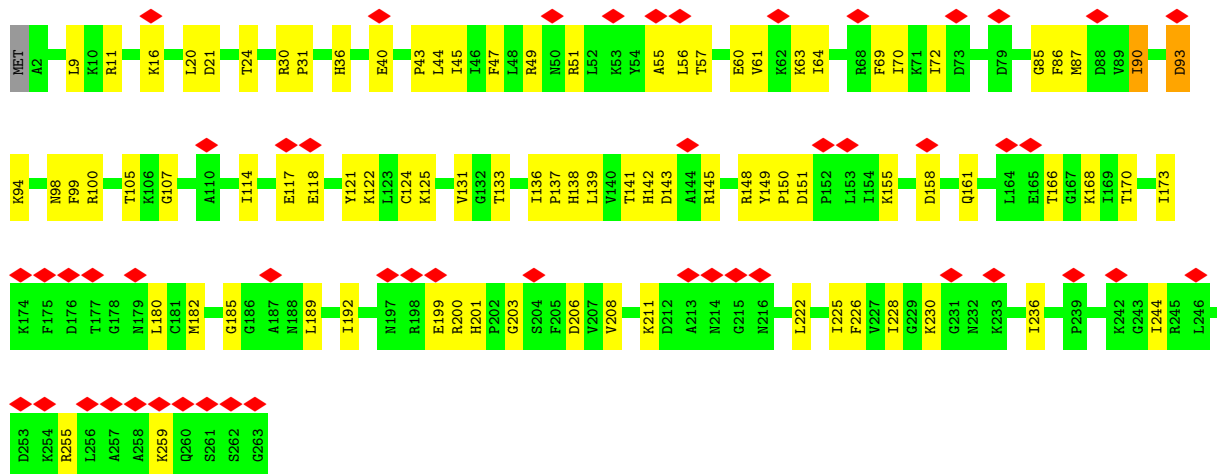


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U1616	U1617	U1618	U1619	A1620	U1621	U1622	A1623	U1624	C1628	C1629	A1630	U1631	C1632	A1633	U1634	C1635	U1639	U1643	C1644	C1645	U1648	U1649	A1650	U1654	U1658	U1659	C1660	A1661	U1662	A1663	A1664	U1665	C1666	U1667	U1668	U1669	C1670	U1671	U1672	U1673	U1674	A1675	U1676	U1677	U1678	U1679	U1680	U1681	C1682	C1683	U1684	U1690					
U1549	U1550	U1551	U1552	C1553	C1554	U1555	A1556	C1557	C1558	C1559	U1560	A1561	C1562	C1563	C1564	C1565	U1566	C1567	C1568	A1569	C1570	C1571	C1572	C1573	C1574	C1575	U1579	A1580	U1585	U1586	C1587	A1588	A1589	C1590	C1591	C1592	C1593	A1594	U1595	U1598	A1601	U1602	C1603	C1604	C1605	C1606	A1607	U1608	C1609	C1610	C1611	C1612	C1613	A1614	U1615		
A1487	C1488	A1489	C1490	G1491	U1492	U1495	U1496	U1497	A1498	U1499	C1502	C1503	U1504	U1505	A1506	C1507	A1508	U1509	C1510	U1511	C1512	C1513	U1514	U1515	U1516	C1517	C1518	U1519	U1520	C1521	A1522	U1524	C1525	U1526	C1527	U1528	C1529	U1530	A1531	C1532	A1533	C1534	U1535	C1536	U1537	C1538	U1539	A1540	U1541	C1542	U1543	C1544	A1545	U1546	C1547	U1548	
C1419	G1420	A1421	G1422	C1423	G1424	G1425	U1426	C1427	A1428	G1429	C1430	G1431	U1432	C1433	C1434	C1435	C1436	C1437	A1438	A1439	U1442	C1443	U1444	U1445	A1446	G1447	A1448	G1449	G1450	A1451	A1452	C1453	A1454	A1455	C1456	U1457	G1458	G1459	C1460	G1461	U1462	U1463	C1464	A1465	G1466	U1470	C1471	C1472	G1473	A1474	G1475	A1476	U1477	U1478	G1479	A1480	
G1338	U1342	U1347	G1348	G1349	G1354	C1355	G1356	C1363	U1364	G1365	G1366	U1371	U1372	C1373	C1374	G1375	A1376	U1377	A1378	C1379	G1380	G1381	A1386	G1387	A1388	U1392	G1393	C1394	C1395	U1396	U1397	G1398	C1399	A1401	A1402	C1403	U1404	A1405	G1406	U1407	U1408	A1409	C1410	G1411	C1412	G1413	A1414	C1415	C1416	C1417	C1418						
C1273	G1274	G1275	A1276	C1277	A1278	C1279	G1280	G1281	A1282	C1283	A1284	G1285	G1286	A1287	U1288	U1289	G1290	A1291	C1292	A1293	G1294	A1295	U1296	U1297	G1298	A1299	U1300	A1301	C1302	C1303	U1304	C1305	U1306	U1307	U1308	C1309	U1310	C1311	G1312	A1313	U1314	U1315	C1316	C1317	G1318	U1319	G1320	G1321	C1322	U1323	G1324	U1325	U1326	G1330	C1331	A1332	U1333
G1207	A1208	A1209	C1215	C1216	A1217	C1218	C1219	A1220	G1221	G1224	U1225	G1226	G1227	A1228	G1229	U1232	G1233	C1234	G1235	C1236	C1237	U1238	U1239	A1240	A1241	U1242	U1243	U1244	G1245	A1246	C1247	U1248	C1249	A1250	A1251	C1252	A1253	C1254	G1255	G1256	G1257	A1258	A1259	A1260	C1261	C1262	U1263	C1264	A1265	C1266	C1267	C1268	G1269	G1270	C1271	C1272	
C1124	C1125	C1126	G1129	G1130	G1131	C1132	A1133	U1136	U1137	C1138	G1139	G1140	A1144	A1145	A1148	A1149	A1150	C1153	U1154	U1155	U1156	G1157	G1158	C1159	U1160	G1171	U1172	U1173	G1174	G1175	U1178	A1181	A1182	A1183	G1184	G1187	A1188	A1189	A1190	A1195	A1199	A1200	U1201	U1202	G1203	A1204	C1205	G1206									
A1024	U1025	C1026	A1027	G1033	A1036	G1037	G1041	U1042	G1043	C1047	G1048	A1055	A1060	U1061	A1062	U1069	A1070	G1071	A1080	A1083	A1084	C1085	U1088	G1089	A1093	C1094	C1098	G1099	A1100	U1101	G1102	C1103	G1104	C1109	G1110	U1111	U1112	A1113	U1114	U1115	C1116	C1117	C1118	A1119	U1120												
G952	C953	U954	U955	C956	A957	C958	C959	A962	A963	A964	U965	G970	G971	A972	C973	A980	A981	C982	A983	C984	C985	C986	A987	C988	C989	A990	C991	A992	C993	A996	A998	C999	C1000	A1001	U1002	U1003	U1004	G1005	C1006	C1007	A1008	A1012	U1013	G1014	U1015	U1016	U1017	U1018	C1019	A1020	A1023						
U882	U883	C884	U885	C886	U887	U888	U889	U890	C891	U892	U893	G894	G895	U896	U897	U898	C899	C900	G901	C902	A903	A904	C905	U906	C907	A908	C909	G910	C911	C912	C913	U914	G915	U916	U917	U918	A919	C920	G921	G924	G925	G928	C929	C930	C931	G932	C933	C934	U939	U940	C941	G942	U943	U944	U945	U946	
A811	A812	A813	U814	U815	A816	C817	U821	U822	A825	A826	A827	A830	C834	C835	G836	A837	G838	C839	C840	C841	C842	C843	U844	G845	G846	U847	U848	A849	C850	C851	C852	C853	A854	C855	C856	A858	C859	G860	G867	C868	A869	A870	U871	A872	G873	C874	A875	C876	C877	C878	C879	G880	G881				

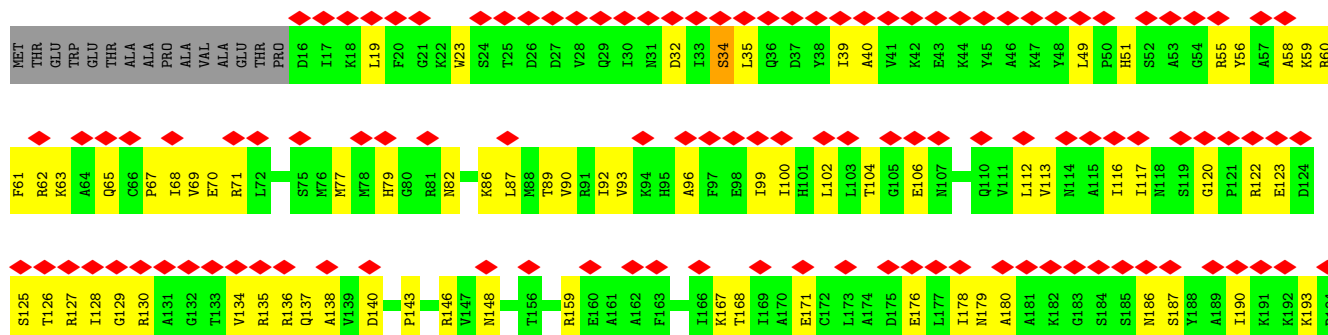


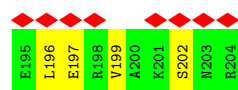


• Molecule 51: 40S ribosomal protein S4, X isoform

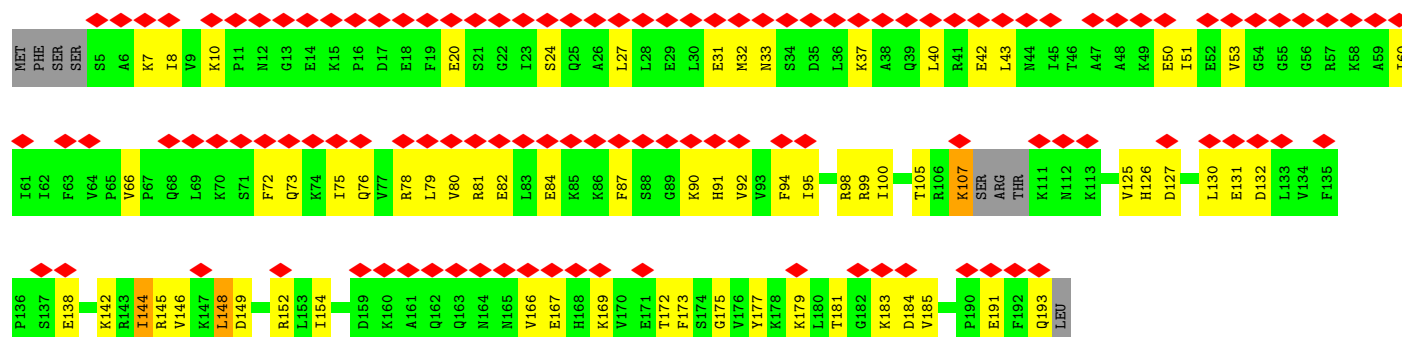


• Molecule 52: 40S ribosomal protein S5

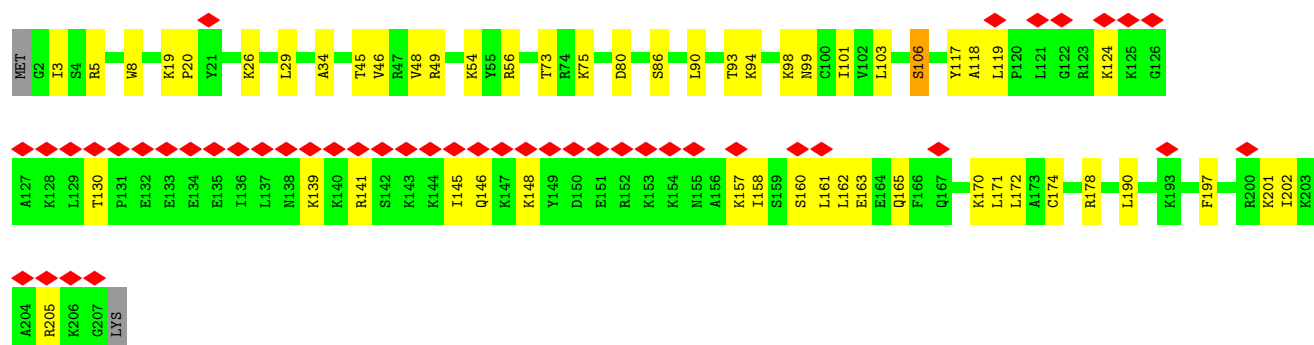
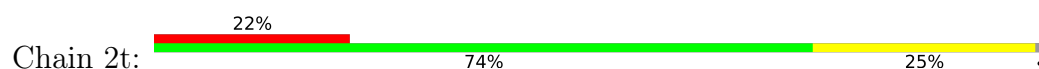




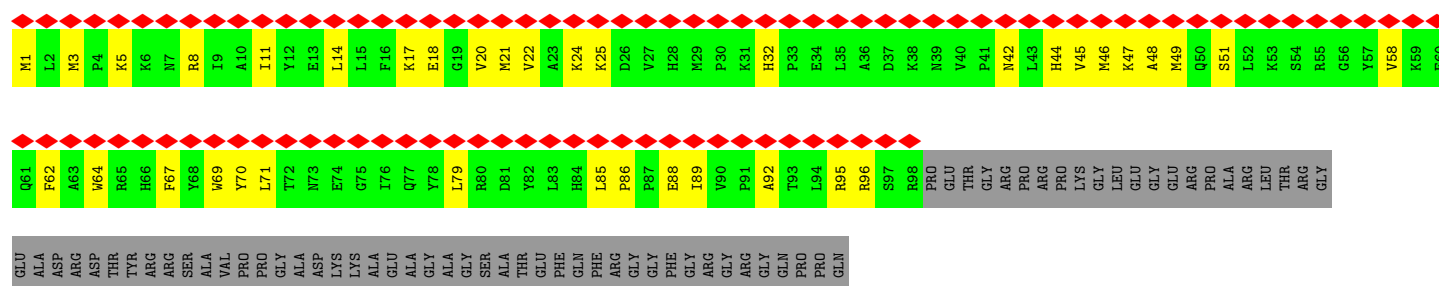
• Molecule 53: 40S ribosomal protein S7



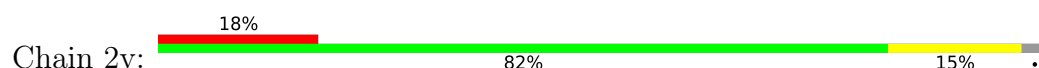
• Molecule 54: 40S ribosomal protein S8



• Molecule 55: 40S ribosomal protein S10

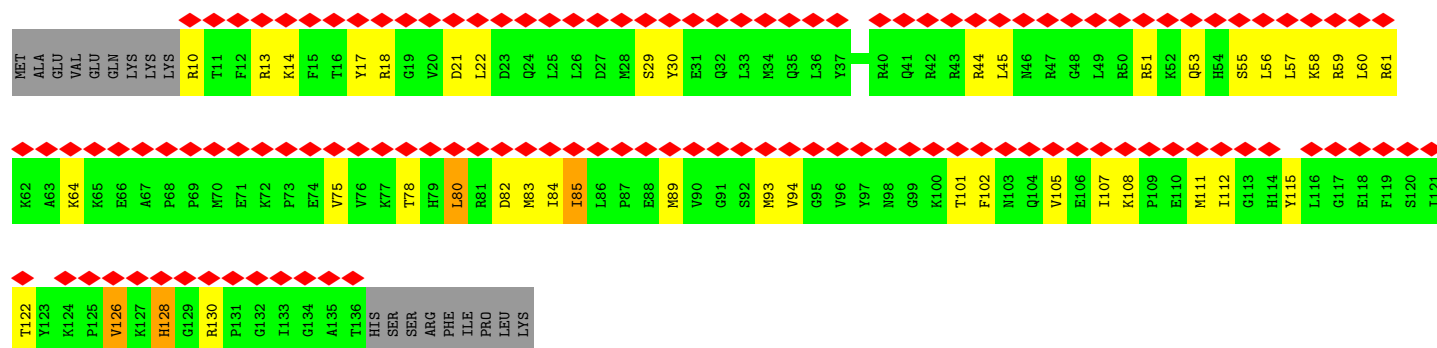
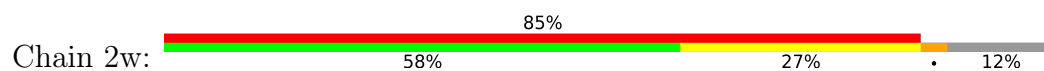


• Molecule 56: 40S ribosomal protein S11

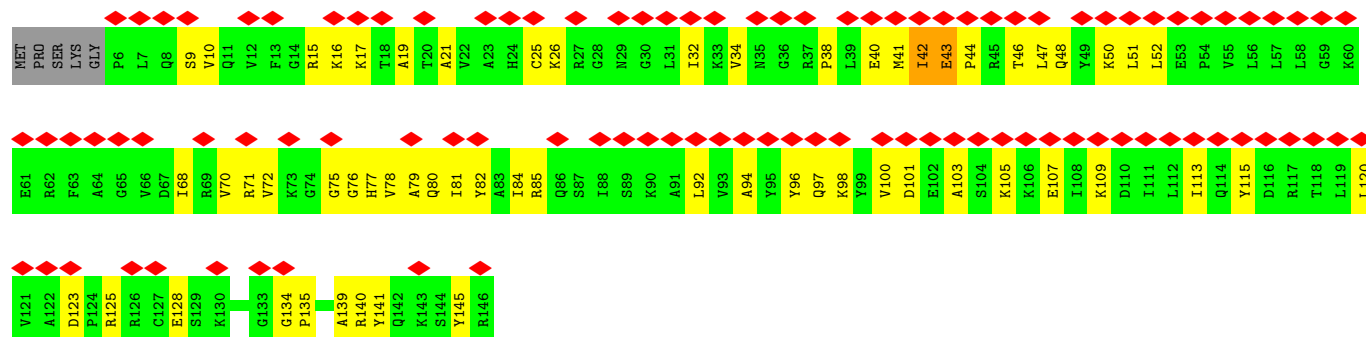




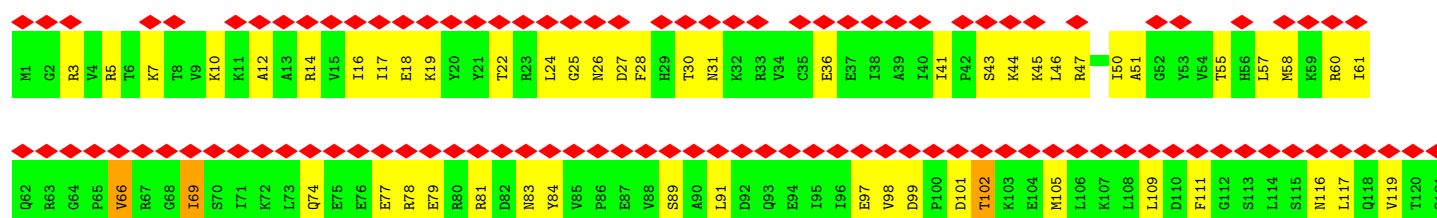
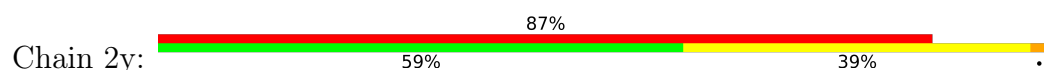
• Molecule 57: 40S ribosomal protein S15



• Molecule 58: 40S ribosomal protein S16

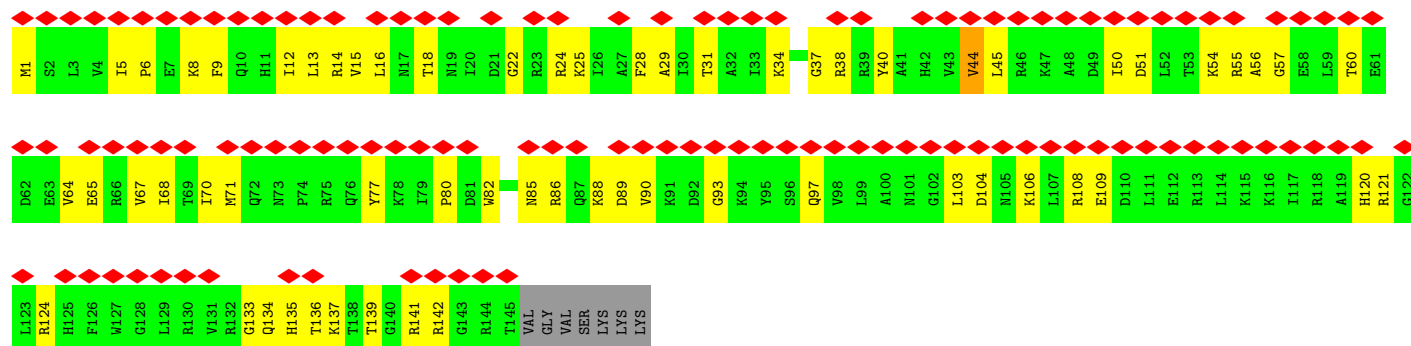
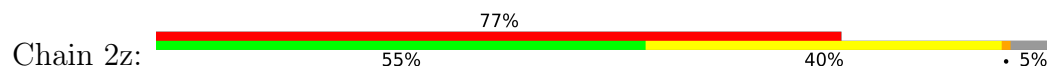


• Molecule 59: 40S ribosomal protein S17

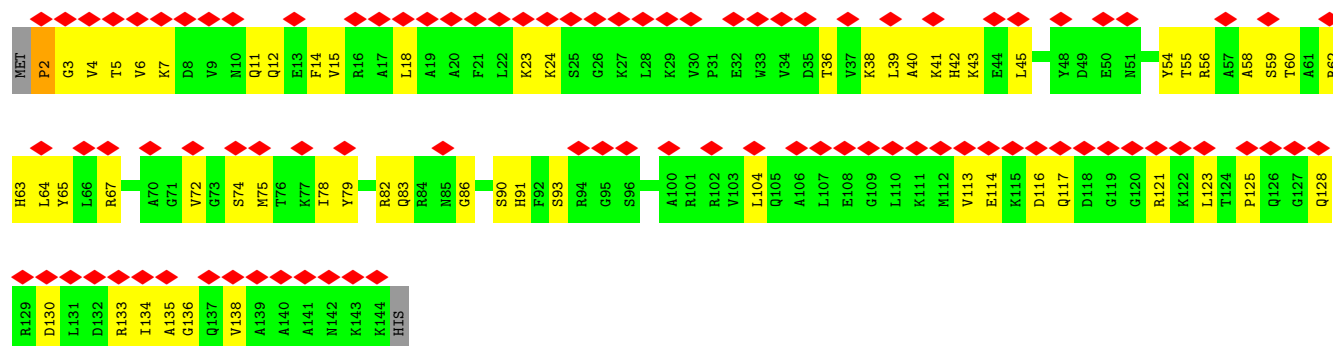




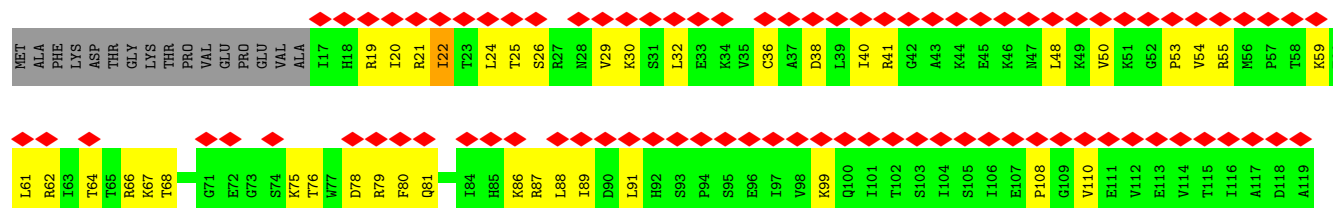
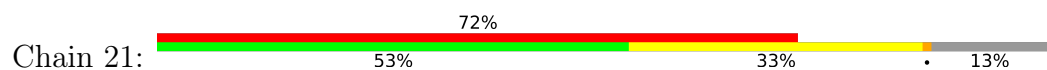
• Molecule 60: 40S ribosomal protein S18



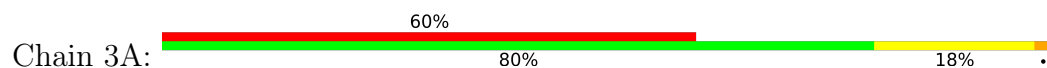
• Molecule 61: 40S ribosomal protein S19

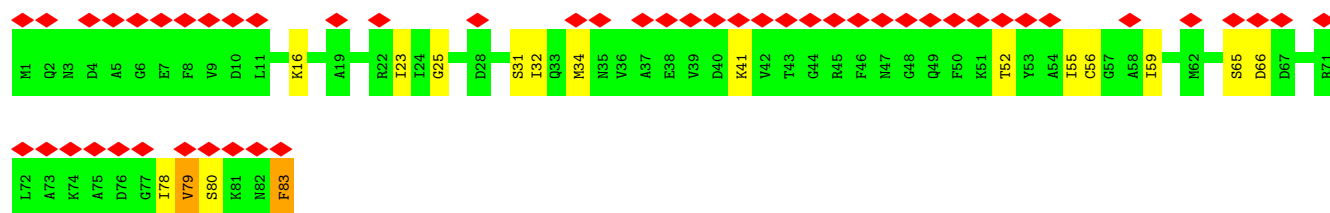


• Molecule 62: 40S ribosomal protein S20

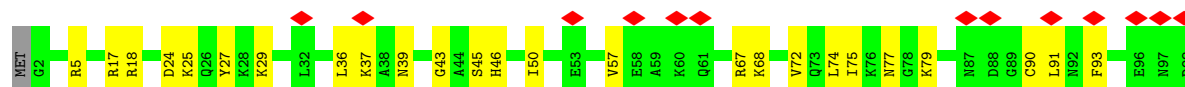


• Molecule 63: 40S ribosomal protein S21

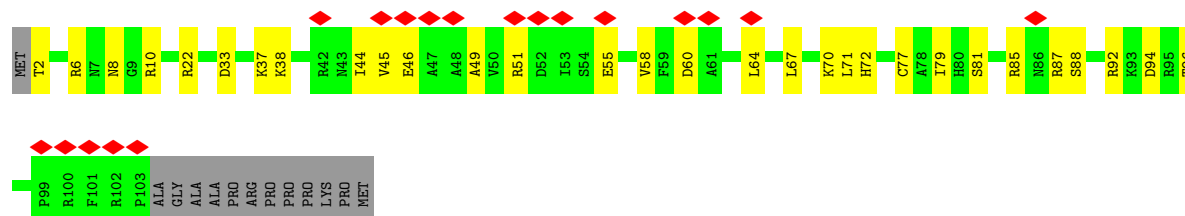




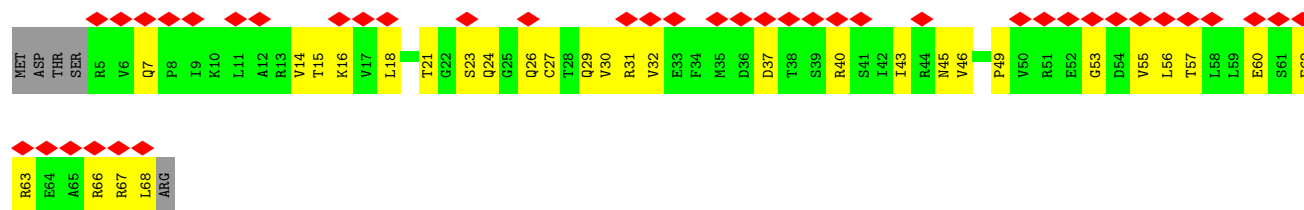
- Molecule 64: 40S ribosomal protein S23



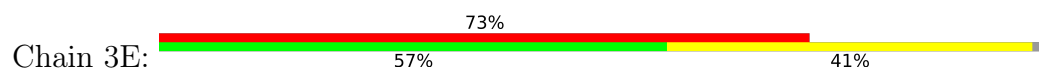
- Molecule 65: 40S ribosomal protein S26



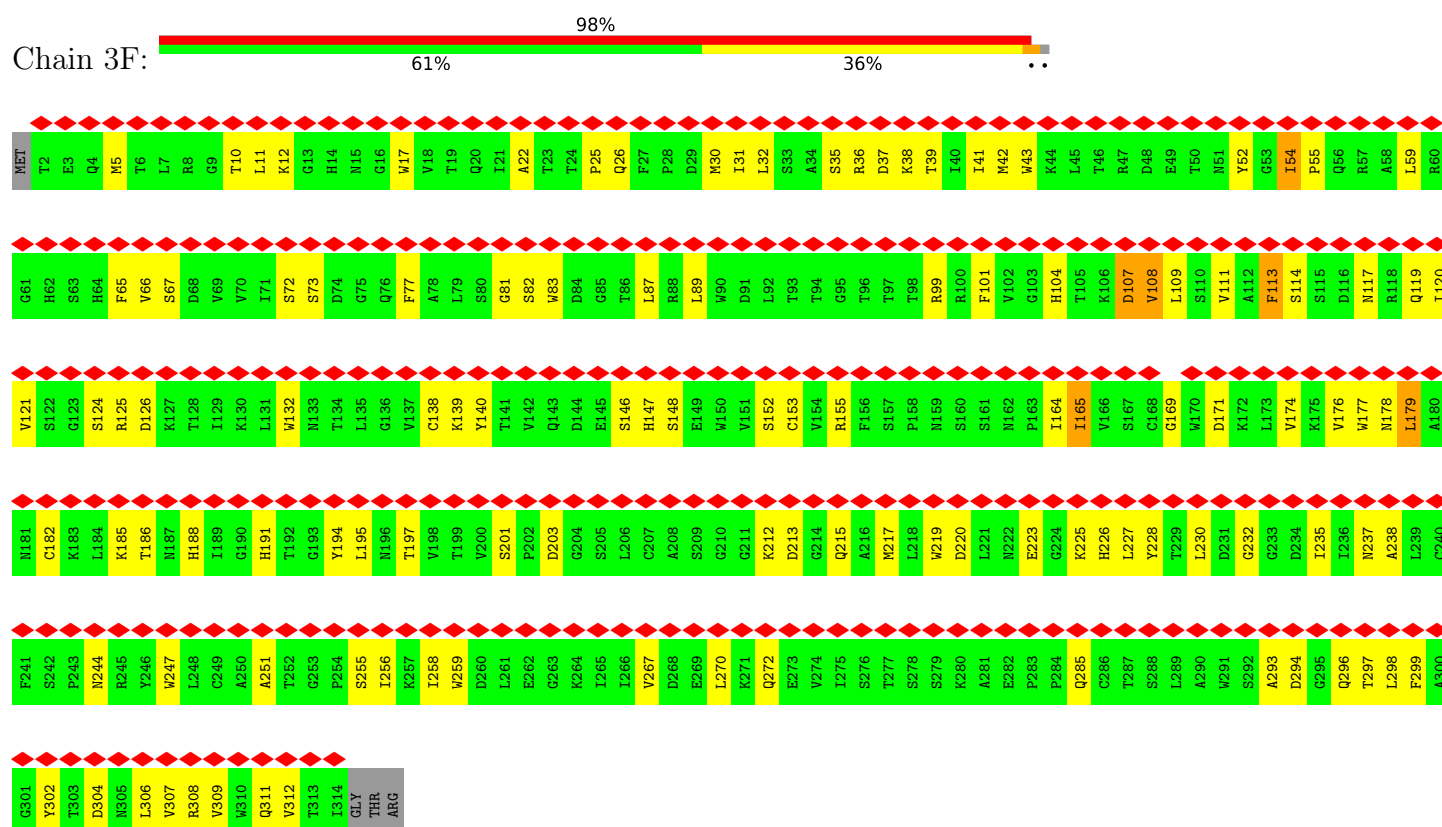
- Molecule 66: 40S ribosomal protein S28

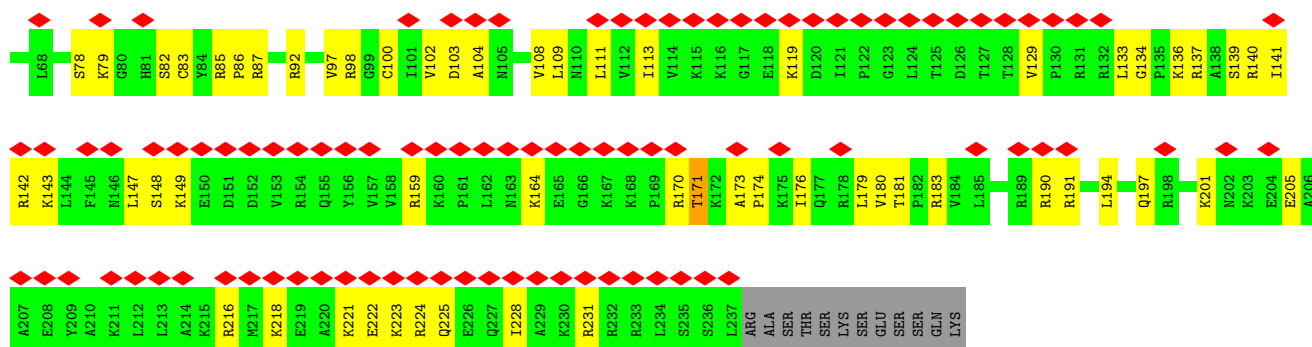


- Molecule 67: 40S ribosomal protein S29

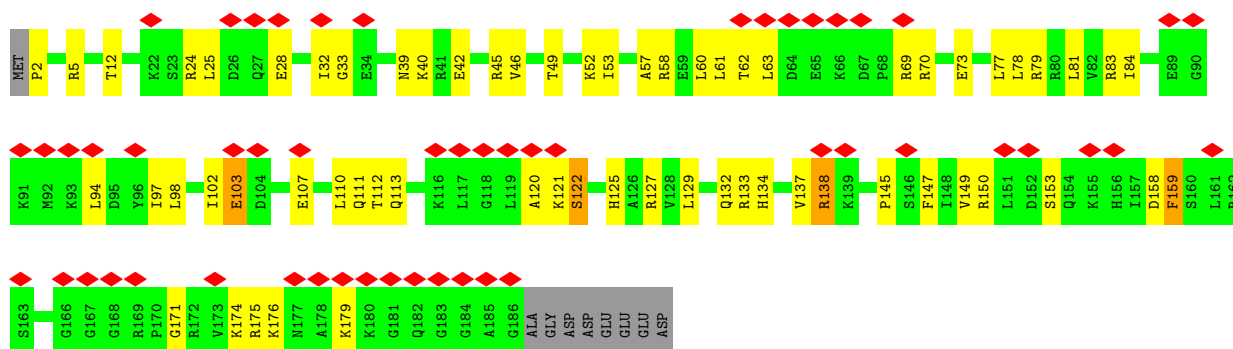


- Molecule 68: Receptor of activated protein C kinase 1

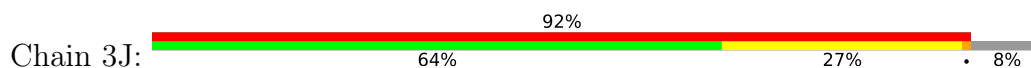




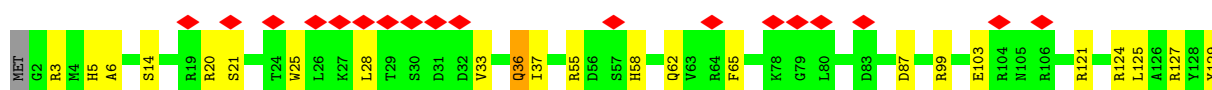
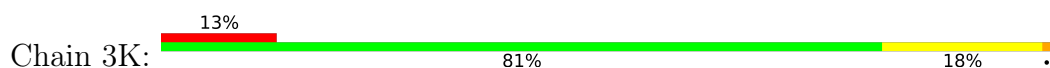
• Molecule 71: 40S ribosomal protein S9



• Molecule 72: 40S ribosomal protein S12

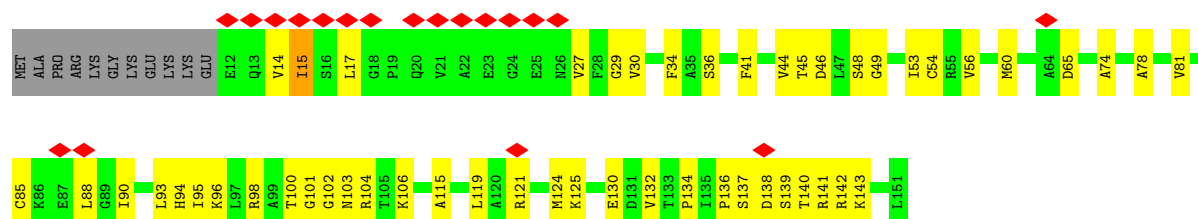


• Molecule 73: 40S ribosomal protein S13

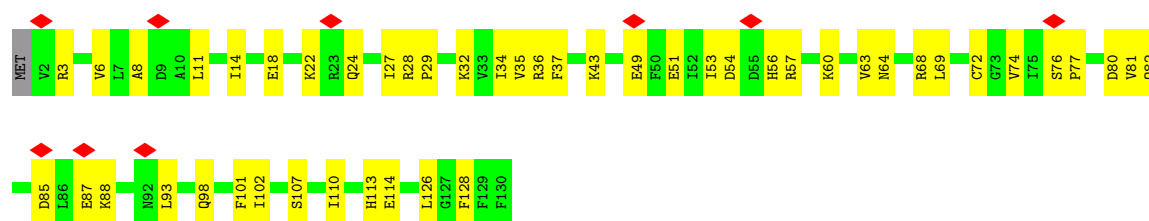




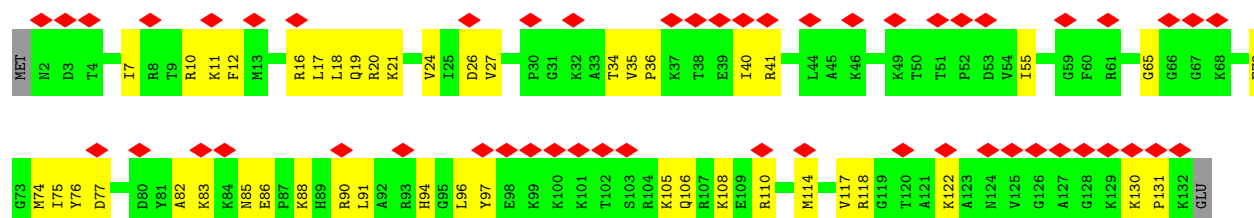
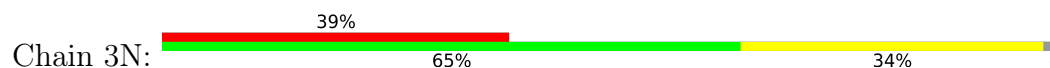
• Molecule 74: 40S ribosomal protein S14



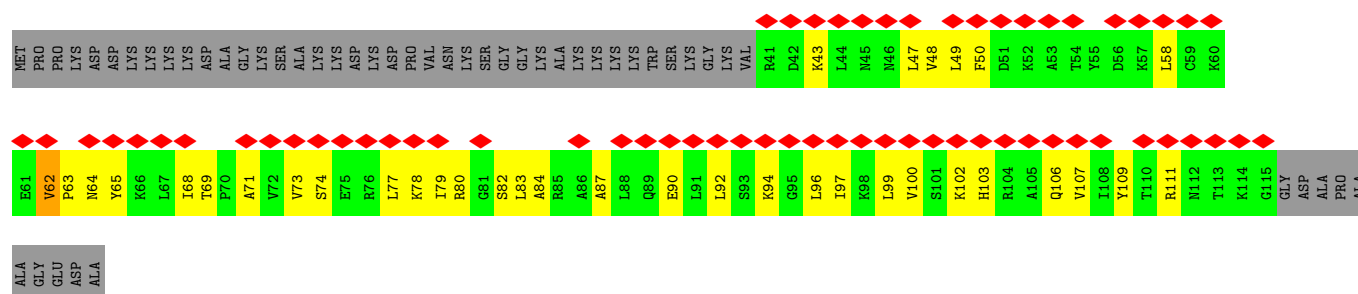
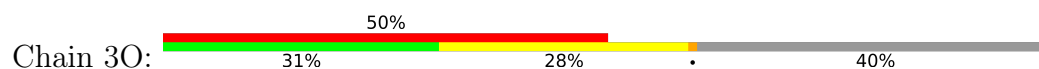
• Molecule 75: 40S ribosomal protein S15a



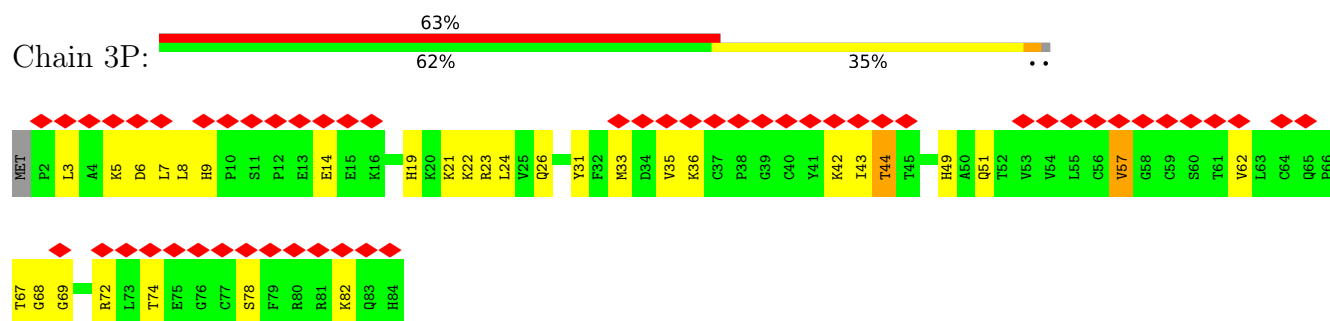
• Molecule 76: 40S ribosomal protein S24



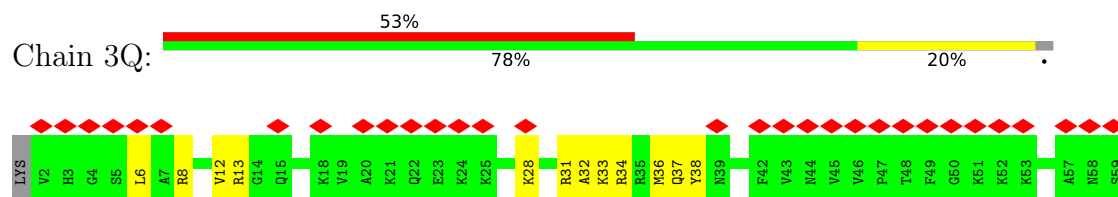
• Molecule 77: 40S ribosomal protein S25



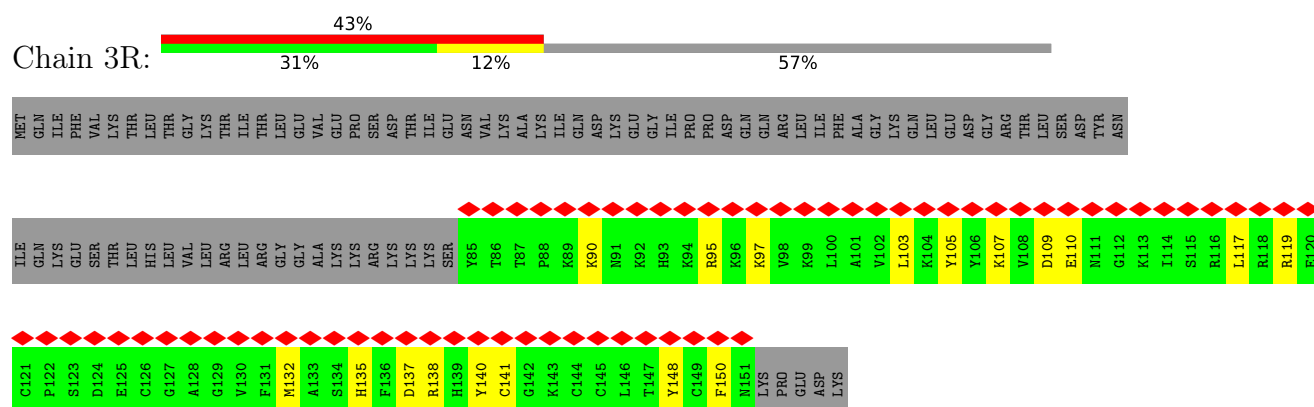
- Molecule 78: 40S ribosomal protein S27



- Molecule 79: 40S ribosomal protein S30



- Molecule 80: Ubiquitin-40S ribosomal protein S27a



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29424	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size ($\text{\AA}$)	504.32, 504.32, 504.32	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.788, 0.788, 0.788	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 84G, ZN, 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	0/89129	0.26	0/139038
2	1B	0.20	0/2858	0.25	0/4455
3	1C	0.21	0/3701	0.25	0/5766
4	1D	0.18	0/1936	0.32	0/2596
5	1E	0.19	0/3306	0.33	0/4424
6	1F	0.17	0/2981	0.31	0/4002
7	1G	0.16	0/2428	0.35	0/3252
8	1H	0.17	0/1942	0.36	0/2606
9	2A	0.18	0/1916	0.31	0/2553
10	2B	0.17	0/1971	0.33	0/2651
11	2C	0.16	0/1537	0.36	0/2066
12	2D	0.15	0/1751	0.39	0/2340
13	2E	0.17	0/1433	0.40	0/1915
14	2F	0.16	0/1732	0.30	0/2315
15	2G	0.17	0/1161	0.31	0/1554
16	2H	0.19	0/1746	0.33	0/2338
17	2I	0.18	0/1682	0.30	0/2250
18	2J	0.18	0/1268	0.32	0/1701
19	2K	0.18	0/1537	0.31	0/2052
20	2L	0.15	0/1582	0.27	0/2091
21	2M	0.19	0/1493	0.40	3/2003 (0.1%)
22	2N	0.17	0/1326	0.29	0/1770
23	2O	0.14	0/839	0.41	0/1126
24	2P	0.17	0/993	0.32	0/1332
25	2Q	0.14	0/1030	0.31	0/1364
26	2R	0.15	0/1002	0.29	0/1345
27	2S	0.18	0/1132	0.33	0/1504
28	2T	0.18	0/1130	0.36	0/1507
29	2U	0.18	0/1191	0.28	0/1591
30	2V	0.20	0/895	0.38	0/1182
31	2W	0.18	0/774	0.33	0/1038
32	2X	0.17	0/903	0.33	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	2Y	0.18	0/1071	0.31	0/1429
34	2Z	0.20	0/895	0.35	0/1198
35	2a	0.14	0/916	0.26	0/1220
36	2b	0.17	0/1023	0.30	0/1351
37	2c	0.14	0/843	0.27	0/1115
38	2d	0.20	0/731	0.36	0/966
39	2e	0.16	0/575	0.35	0/761
40	2f	0.17	0/454	0.28	0/599
41	2g	0.14	0/425	0.28	0/561
42	2h	0.15	0/231	0.24	0/294
43	2i	0.21	0/887	0.36	0/1170
44	2j	0.17	0/718	0.26	0/953
45	2k	0.18	0/1017	0.32	0/1364
46	2l	0.45	7/1769 (0.4%)	0.49	3/2371 (0.1%)
47	2m	0.19	6/41243 (0.0%)	0.26	0/64257
48	2n	0.12	0/1778	0.32	0/2416
49	2o	0.12	0/1765	0.30	0/2362
50	2p	0.22	1/1793 (0.1%)	0.52	3/2414 (0.1%)
51	2q	0.17	1/2118 (0.0%)	0.33	0/2849
52	2r	0.14	0/1516	0.38	0/2037
53	2s	1.23	1/1519 (0.1%)	0.44	2/2033 (0.1%)
54	2t	0.13	0/1715	0.34	0/2287
55	2u	0.13	0/851	0.36	0/1147
56	2v	0.15	0/1268	0.30	0/1696
57	2w	0.13	0/1065	0.37	0/1423
58	2x	0.13	0/1142	0.39	0/1528
59	2y	0.18	0/1105	0.45	0/1484
60	2z	0.13	0/1216	0.37	2/1628 (0.1%)
61	20	0.27	1/1131 (0.1%)	0.40	0/1515
62	21	0.17	0/827	0.40	0/1110
63	3A	0.12	0/643	0.33	0/860
64	3B	0.13	0/1116	0.30	0/1490
65	3C	0.16	0/847	0.35	0/1135
66	3D	0.12	0/508	0.38	0/680
67	3E	0.17	0/470	0.39	0/623
68	3F	0.11	0/2493	0.36	0/3394
69	3G	0.15	0/1773	0.37	0/2395
70	3H	0.12	0/1946	0.32	0/2590
71	3I	0.13	0/1561	0.33	0/2083
72	3J	0.24	0/952	0.31	0/1279
73	3K	0.18	0/1232	0.28	0/1656
74	3L	0.14	0/1062	0.35	0/1425
75	3M	0.16	0/1051	0.35	0/1406

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	3N	0.17	0/1094	0.40	0/1452
77	3O	0.16	0/604	0.52	0/810
78	3P	0.09	0/665	0.30	0/891
79	3Q	0.10	0/465	0.30	0/612
80	3R	0.11	0/560	0.37	0/745
All	All	0.22	17/232954 (0.0%)	0.30	13/342007 (0.0%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	2s	107	LYS	CD-CE	47.63	2.95	1.52
47	2m	744	G	C6-N1	12.48	1.64	1.39
47	2m	744	G	N1-C2	12.31	1.62	1.37
47	2m	744	G	C2-N3	9.86	1.52	1.32
47	2m	744	G	C5-C6	9.66	1.61	1.42

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	2p	200	PRO	N-CD-CG	-13.47	83.00	103.20
50	2p	200	PRO	CA-CB-CG	-11.27	83.10	104.50
46	2l	84	HIS	CG-CD2-NE2	9.12	116.32	107.20
53	2s	107	LYS	CG-CD-CE	7.37	128.26	111.30
53	2s	107	LYS	CD-CE-NZ	6.47	132.60	111.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	79676	0	40260	1021	0
2	1B	2558	0	1296	23	0
3	1C	3314	0	1683	35	0
4	1D	1898	0	1993	51	0
5	1E	3238	0	3376	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	1F	2927	0	3104	42	0
7	1G	2382	0	2410	68	0
8	1H	1904	0	2055	92	0
9	2A	1878	0	2009	35	0
10	2B	1935	0	2087	54	0
11	2C	1518	0	1601	45	0
12	2D	1711	0	1749	57	0
13	2E	1410	0	1441	84	0
14	2F	1701	0	1818	49	0
15	2G	1138	0	1204	20	0
16	2H	1701	0	1749	34	0
17	2I	1650	0	1794	46	0
18	2J	1242	0	1269	22	0
19	2K	1513	0	1628	11	0
20	2L	1566	0	1729	38	0
21	2M	1453	0	1490	30	0
22	2N	1298	0	1366	23	0
23	2O	825	0	850	29	0
24	2P	979	0	1039	16	0
25	2Q	1015	0	1079	22	0
26	2R	985	0	1066	24	0
27	2S	1115	0	1205	40	0
28	2T	1107	0	1182	30	0
29	2U	1162	0	1213	21	0
30	2V	882	0	959	33	0
31	2W	764	0	804	23	0
32	2X	888	0	930	16	0
33	2Y	1053	0	1147	14	0
34	2Z	876	0	912	21	0
35	2a	906	0	1002	15	0
36	2b	1015	0	1148	24	0
37	2c	832	0	917	18	0
38	2d	713	0	750	14	0
39	2e	569	0	637	24	0
40	2f	444	0	483	13	0
41	2g	430	0	466	9	0
42	2h	230	0	276	7	0
43	2i	870	0	944	28	0
44	2j	708	0	756	11	0
45	2k	1002	0	1068	28	0
46	2l	1741	0	1854	101	0
47	2m	36900	0	18596	763	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	2n	1741	0	1746	74	0
49	2o	1738	0	1809	41	0
50	2p	1765	0	1865	68	0
51	2q	2076	0	2177	62	0
52	2r	1495	0	1549	69	0
53	2s	1497	0	1590	84	0
54	2t	1686	0	1772	37	0
55	2u	827	0	854	32	0
56	2v	1247	0	1323	22	0
57	2w	1045	0	1095	57	0
58	2x	1124	0	1193	75	0
59	2y	1090	0	1149	72	0
60	2z	1198	0	1261	54	0
61	20	1112	0	1146	82	0
62	21	817	0	882	47	0
63	3A	636	0	637	21	0
64	3B	1098	0	1167	37	0
65	3C	829	0	883	21	0
66	3D	506	0	536	28	0
67	3E	459	0	448	32	0
68	3F	2436	0	2393	89	0
69	3G	1733	0	1826	57	0
70	3H	1923	0	2089	79	0
71	3I	1533	0	1653	61	0
72	3J	942	0	961	41	0
73	3K	1208	0	1294	20	0
74	3L	1049	0	1073	44	0
75	3M	1034	0	1080	47	0
76	3N	1073	0	1155	44	0
77	3O	598	0	656	35	0
78	3P	651	0	672	23	0
79	3Q	459	0	503	20	0
80	3R	548	0	555	16	0
81	1A	722	836	0	25	0
81	2D	38	44	0	3	0
81	2i	38	44	0	3	0
81	2m	76	88	0	2	0
82	1A	268	0	0	0	0
82	1B	3	0	0	0	0
82	1C	5	0	0	0	0
82	1D	1	0	0	0	0
82	1E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	20	1	0	0	0	0
82	2H	1	0	0	0	0
82	2J	1	0	0	0	0
82	2L	1	0	0	0	0
82	2M	2	0	0	0	0
82	2P	1	0	0	0	0
82	2Y	1	0	0	0	0
82	2Z	1	0	0	0	0
82	2a	1	0	0	0	0
82	2d	1	0	0	0	0
82	2m	120	0	0	0	0
82	3H	1	0	0	0	0
83	2d	1	0	0	0	0
83	2g	1	0	0	0	0
83	2i	1	0	0	0	0
83	2j	1	0	0	0	0
83	3C	1	0	0	0	0
83	3E	1	0	0	0	0
All	All	218085	1012	161386	4220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 4220 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2m:1421:A:H2'	61:20:2:PRO:N	1.17	1.48
58:2x:43:GLU:CG	58:2x:44:PRO:HD3	1.47	1.44
13:2E:93:GLU:OE1	13:2E:173:ILE:CG1	1.70	1.40
47:2m:744:G:C2	53:2s:107:LYS:CE	2.06	1.38
46:2l:69:GLY:CA	46:2l:84:HIS:NE2	1.71	1.38

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1D	246/257 (96%)	223 (91%)	23 (9%)	0	100	100
5	1E	400/403 (99%)	384 (96%)	16 (4%)	0	100	100
6	1F	366/427 (86%)	342 (93%)	24 (7%)	0	100	100
7	1G	291/297 (98%)	279 (96%)	12 (4%)	0	100	100
8	1H	232/288 (81%)	209 (90%)	23 (10%)	0	100	100
9	2A	224/248 (90%)	215 (96%)	9 (4%)	0	100	100
10	2B	240/266 (90%)	227 (95%)	13 (5%)	0	100	100
11	2C	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
12	2D	211/214 (99%)	192 (91%)	18 (8%)	1 (0%)	24	44
13	2E	174/178 (98%)	163 (94%)	9 (5%)	2 (1%)	11	24
14	2F	208/211 (99%)	190 (91%)	18 (9%)	0	100	100
15	2G	137/215 (64%)	132 (96%)	5 (4%)	0	100	100
16	2H	201/204 (98%)	191 (95%)	9 (4%)	1 (0%)	24	44
17	2I	199/203 (98%)	193 (97%)	6 (3%)	0	100	100
18	2J	151/184 (82%)	143 (95%)	8 (5%)	0	100	100
19	2K	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
20	2L	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
21	2M	173/176 (98%)	160 (92%)	12 (7%)	1 (1%)	21	39
22	2N	157/160 (98%)	150 (96%)	7 (4%)	0	100	100
23	2O	99/128 (77%)	87 (88%)	12 (12%)	0	100	100
24	2P	129/140 (92%)	123 (95%)	6 (5%)	0	100	100
25	2Q	122/157 (78%)	110 (90%)	12 (10%)	0	100	100
26	2R	118/156 (76%)	113 (96%)	4 (3%)	1 (1%)	16	32
27	2S	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
28	2T	133/136 (98%)	124 (93%)	9 (7%)	0	100	100
29	2U	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
30	2V	105/159 (66%)	95 (90%)	10 (10%)	0	100	100
31	2W	96/115 (84%)	92 (96%)	4 (4%)	0	100	100
32	2X	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
33	2Y	126/135 (93%)	118 (94%)	7 (6%)	1 (1%)	16	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	2Z	107/110 (97%)	102 (95%)	4 (4%)	1 (1%)	14	29
35	2a	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
36	2b	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
37	2c	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
38	2d	85/97 (88%)	83 (98%)	2 (2%)	0	100	100
39	2e	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
40	2f	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
41	2g	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
42	2h	22/25 (88%)	22 (100%)	0	0	100	100
43	2i	104/106 (98%)	96 (92%)	8 (8%)	0	100	100
44	2j	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
45	2k	123/137 (90%)	115 (94%)	8 (6%)	0	100	100
46	2l	215/217 (99%)	171 (80%)	42 (20%)	2 (1%)	14	29
48	2n	219/295 (74%)	205 (94%)	13 (6%)	1 (0%)	24	44
49	2o	212/264 (80%)	205 (97%)	7 (3%)	0	100	100
50	2p	225/243 (93%)	199 (88%)	26 (12%)	0	100	100
51	2q	260/263 (99%)	245 (94%)	15 (6%)	0	100	100
52	2r	187/204 (92%)	164 (88%)	23 (12%)	0	100	100
53	2s	182/194 (94%)	162 (89%)	20 (11%)	0	100	100
54	2t	204/208 (98%)	199 (98%)	5 (2%)	0	100	100
55	2u	96/165 (58%)	87 (91%)	9 (9%)	0	100	100
56	2v	151/158 (96%)	137 (91%)	14 (9%)	0	100	100
57	2w	125/145 (86%)	118 (94%)	7 (6%)	0	100	100
58	2x	139/146 (95%)	127 (91%)	10 (7%)	2 (1%)	9	18
59	2y	133/135 (98%)	120 (90%)	11 (8%)	2 (2%)	8	16
60	2z	143/152 (94%)	126 (88%)	17 (12%)	0	100	100
61	20	141/145 (97%)	127 (90%)	14 (10%)	0	100	100
62	21	101/119 (85%)	94 (93%)	7 (7%)	0	100	100
63	3A	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
64	3B	139/143 (97%)	129 (93%)	10 (7%)	0	100	100
65	3C	101/115 (88%)	92 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	3D	62/69 (90%)	50 (81%)	12 (19%)	0	100	100
67	3E	53/56 (95%)	49 (92%)	3 (6%)	1 (2%)	6	12
68	3F	311/317 (98%)	284 (91%)	27 (9%)	0	100	100
69	3G	221/293 (75%)	209 (95%)	12 (5%)	0	100	100
70	3H	235/249 (94%)	221 (94%)	14 (6%)	0	100	100
71	3I	184/194 (95%)	164 (89%)	20 (11%)	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%)	122 (88%)	15 (11%)	1 (1%)	18	36
75	3M	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
76	3N	130/133 (98%)	122 (94%)	8 (6%)	0	100	100
77	3O	73/125 (58%)	62 (85%)	11 (15%)	0	100	100
78	3P	81/84 (96%)	70 (86%)	11 (14%)	0	100	100
79	3Q	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
80	3R	65/156 (42%)	55 (85%)	10 (15%)	0	100	100
All	All	11562/12905 (90%)	10759 (93%)	786 (7%)	17 (0%)	49	69

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	2Y	92	ASN
34	2Z	107	PRO
48	2n	28	THR
58	2x	42	ILE
58	2x	43	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	1D	190/199 (96%)	185 (97%)	5 (3%)	40	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	1E	348/349 (100%)	341 (98%)	7 (2%)	48	72
6	1F	306/348 (88%)	304 (99%)	2 (1%)	76	88
7	1G	246/250 (98%)	240 (98%)	6 (2%)	43	68
8	1H	209/252 (83%)	201 (96%)	8 (4%)	29	54
9	2A	195/215 (91%)	195 (100%)	0	100	100
10	2B	204/223 (92%)	200 (98%)	4 (2%)	48	72
11	2C	169/171 (99%)	166 (98%)	3 (2%)	51	74
12	2D	180/181 (99%)	178 (99%)	2 (1%)	65	83
13	2E	148/149 (99%)	138 (93%)	10 (7%)	14	31
14	2F	176/177 (99%)	169 (96%)	7 (4%)	28	52
15	2G	118/161 (73%)	117 (99%)	1 (1%)	73	87
16	2H	171/172 (99%)	170 (99%)	1 (1%)	78	89
17	2I	173/174 (99%)	170 (98%)	3 (2%)	53	76
18	2J	134/163 (82%)	131 (98%)	3 (2%)	45	70
19	2K	164/165 (99%)	164 (100%)	0	100	100
20	2L	166/175 (95%)	165 (99%)	1 (1%)	78	89
21	2M	156/157 (99%)	153 (98%)	3 (2%)	50	73
22	2N	139/140 (99%)	136 (98%)	3 (2%)	45	70
23	2O	91/115 (79%)	89 (98%)	2 (2%)	45	70
24	2P	101/107 (94%)	97 (96%)	4 (4%)	28	52
25	2Q	103/126 (82%)	102 (99%)	1 (1%)	68	84
26	2R	108/133 (81%)	102 (94%)	6 (6%)	19	38
27	2S	124/135 (92%)	123 (99%)	1 (1%)	73	87
28	2T	117/118 (99%)	116 (99%)	1 (1%)	70	85
29	2U	120/121 (99%)	119 (99%)	1 (1%)	73	87
30	2V	89/126 (71%)	88 (99%)	1 (1%)	65	83
31	2W	83/97 (86%)	79 (95%)	4 (5%)	23	45
32	2X	98/110 (89%)	93 (95%)	5 (5%)	21	43
33	2Y	114/121 (94%)	111 (97%)	3 (3%)	40	66
34	2Z	88/89 (99%)	87 (99%)	1 (1%)	65	83
35	2a	98/100 (98%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2b	109/110 (99%)	108 (99%)	1 (1%)	70	85
37	2c	86/89 (97%)	85 (99%)	1 (1%)	63	82
38	2d	74/80 (92%)	74 (100%)	0	100	100
39	2e	64/65 (98%)	63 (98%)	1 (2%)	55	77
40	2f	47/48 (98%)	47 (100%)	0	100	100
41	2g	47/115 (41%)	47 (100%)	0	100	100
42	2h	23/24 (96%)	23 (100%)	0	100	100
43	2i	94/94 (100%)	92 (98%)	2 (2%)	47	71
44	2j	74/75 (99%)	72 (97%)	2 (3%)	39	65
45	2k	109/121 (90%)	108 (99%)	1 (1%)	70	85
46	2l	195/196 (100%)	194 (100%)	1 (0%)	81	91
48	2n	183/243 (75%)	177 (97%)	6 (3%)	33	59
49	2o	195/231 (84%)	195 (100%)	0	100	100
50	2p	190/202 (94%)	185 (97%)	5 (3%)	40	66
51	2q	224/225 (100%)	220 (98%)	4 (2%)	51	74
52	2r	159/170 (94%)	155 (98%)	4 (2%)	42	67
53	2s	166/174 (95%)	160 (96%)	6 (4%)	31	56
54	2t	178/180 (99%)	173 (97%)	5 (3%)	38	64
55	2u	89/136 (65%)	87 (98%)	2 (2%)	45	70
56	2v	137/142 (96%)	136 (99%)	1 (1%)	76	88
57	2w	113/130 (87%)	108 (96%)	5 (4%)	25	48
58	2x	117/121 (97%)	117 (100%)	0	100	100
59	2y	122/122 (100%)	120 (98%)	2 (2%)	55	77
60	2z	126/132 (96%)	122 (97%)	4 (3%)	34	59
61	20	113/115 (98%)	111 (98%)	2 (2%)	51	74
62	21	94/107 (88%)	92 (98%)	2 (2%)	47	71
63	3A	67/67 (100%)	64 (96%)	3 (4%)	24	47
64	3B	113/115 (98%)	111 (98%)	2 (2%)	51	74
65	3C	90/98 (92%)	86 (96%)	4 (4%)	25	48
66	3D	57/62 (92%)	56 (98%)	1 (2%)	51	74
67	3E	48/49 (98%)	47 (98%)	1 (2%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	3F	272/275 (99%)	265 (97%)	7 (3%)	40	66
69	3G	189/225 (84%)	187 (99%)	2 (1%)	65	83
70	3H	207/218 (95%)	205 (99%)	2 (1%)	68	84
71	3I	162/168 (96%)	157 (97%)	5 (3%)	35	60
72	3J	102/108 (94%)	101 (99%)	1 (1%)	68	84
73	3K	130/131 (99%)	127 (98%)	3 (2%)	44	69
74	3L	110/119 (92%)	110 (100%)	0	100	100
75	3M	112/113 (99%)	110 (98%)	2 (2%)	51	74
76	3N	114/115 (99%)	113 (99%)	1 (1%)	70	85
77	3O	66/103 (64%)	64 (97%)	2 (3%)	36	62
78	3P	75/76 (99%)	70 (93%)	5 (7%)	15	31
79	3Q	47/48 (98%)	46 (98%)	1 (2%)	47	71
80	3R	60/140 (43%)	60 (100%)	0	100	100
All	All	10075/10996 (92%)	9877 (98%)	198 (2%)	49	72

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	2p	49	ILE
57	2w	85	ILE
51	2q	40	GLU
53	2s	148	LEU
60	2z	44	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
31	2W	72	HIS
73	3K	36	GLN
49	2o	92	GLN
73	3K	13	GLN
79	3Q	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	3704/5070 (73%)	833 (22%)	30 (0%)
2	1B	119/121 (98%)	18 (15%)	2 (1%)
3	1C	155/157 (98%)	29 (18%)	2 (1%)
47	2m	1714/1869 (91%)	478 (27%)	0
All	All	5692/7217 (78%)	1358 (23%)	34 (0%)

5 of 1358 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	17	A
1	1A	30	C
1	1A	39	A
1	1A	42	A
1	1A	48	G

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	4896	G
1	1A	4913	G
3	1C	86	U
1	1A	2389	A
1	1A	2299	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	0.80	0	4,9,11	0.59	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 439 ligands modelled in this entry, 416 are monoatomic - leaving 23 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	84G	1A	5112	-	39,40,40	1.84	7 (17%)	48,57,57	1.27	4 (8%)
81	84G	1A	5117	-	39,40,40	1.85	9 (23%)	48,57,57	1.23	5 (10%)
81	84G	1A	5114	-	39,40,40	1.85	7 (17%)	48,57,57	1.21	4 (8%)
81	84G	1A	5108	-	39,40,40	1.85	8 (20%)	48,57,57	1.14	3 (6%)
81	84G	1A	5102	-	39,40,40	1.89	7 (17%)	48,57,57	1.32	6 (12%)
81	84G	1A	5106	-	39,40,40	1.86	9 (23%)	48,57,57	1.10	5 (10%)
81	84G	1A	5115	-	39,40,40	1.86	8 (20%)	48,57,57	1.25	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	84G	1A	5105	-	39,40,40	1.85	7 (17%)	48,57,57	1.18	5 (10%)
81	84G	2i	201	-	39,40,40	1.97	9 (23%)	48,57,57	1.29	5 (10%)
81	84G	1A	5107	-	39,40,40	1.85	8 (20%)	48,57,57	1.16	3 (6%)
81	84G	1A	5101	-	39,40,40	1.87	6 (15%)	48,57,57	1.51	8 (16%)
81	84G	1A	5109	-	39,40,40	1.86	7 (17%)	48,57,57	1.25	4 (8%)
81	84G	2m	1901	-	39,40,40	1.80	7 (17%)	48,57,57	2.32	12 (25%)
81	84G	2D	301	-	39,40,40	1.84	7 (17%)	48,57,57	1.32	6 (12%)
81	84G	1A	5104	82	39,40,40	1.87	8 (20%)	48,57,57	1.24	3 (6%)
81	84G	1A	5113	-	39,40,40	1.85	8 (20%)	48,57,57	1.13	3 (6%)
81	84G	1A	5103	-	39,40,40	1.84	8 (20%)	48,57,57	1.12	4 (8%)
81	84G	1A	5110	-	39,40,40	1.89	7 (17%)	48,57,57	1.08	4 (8%)
81	84G	2m	1902	-	39,40,40	1.85	7 (17%)	48,57,57	1.29	5 (10%)
81	84G	1A	5119	-	39,40,40	1.86	8 (20%)	48,57,57	1.13	3 (6%)
81	84G	1A	5116	-	39,40,40	1.84	7 (17%)	48,57,57	1.25	4 (8%)
81	84G	1A	5111	-	39,40,40	1.84	7 (17%)	48,57,57	1.33	4 (8%)
81	84G	1A	5118	-	39,40,40	1.83	7 (17%)	48,57,57	1.19	4 (8%)

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	84G	1A	5112	-	-	8/23/76/76	0/3/3/3
81	84G	1A	5117	-	-	6/23/76/76	0/3/3/3
81	84G	1A	5114	-	-	9/23/76/76	0/3/3/3
81	84G	1A	5108	-	-	8/23/76/76	0/3/3/3
81	84G	1A	5102	-	-	8/23/76/76	0/3/3/3
81	84G	1A	5106	-	-	10/23/76/76	0/3/3/3
81	84G	1A	5115	-	-	6/23/76/76	0/3/3/3
81	84G	1A	5105	-	-	6/23/76/76	0/3/3/3
81	84G	2i	201	-	-	9/23/76/76	0/3/3/3
81	84G	1A	5107	-	-	10/23/76/76	0/3/3/3
81	84G	1A	5101	-	-	9/23/76/76	1/3/3/3
81	84G	1A	5109	-	-	5/23/76/76	0/3/3/3
81	84G	2m	1901	-	-	3/23/76/76	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	84G	2D	301	-	-	7/23/76/76	0/3/3/3
81	84G	1A	5104	82	-	7/23/76/76	0/3/3/3
81	84G	1A	5113	-	-	5/23/76/76	0/3/3/3
81	84G	1A	5103	-	-	7/23/76/76	0/3/3/3
81	84G	1A	5110	-	-	10/23/76/76	0/3/3/3
81	84G	2m	1902	-	-	6/23/76/76	0/3/3/3
81	84G	1A	5119	-	-	7/23/76/76	0/3/3/3
81	84G	1A	5116	-	-	4/23/76/76	0/3/3/3
81	84G	1A	5111	-	-	12/23/76/76	1/3/3/3
81	84G	1A	5118	-	-	5/23/76/76	1/3/3/3

The worst 5 of 173 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	1A	5111	84G	C3-N1	6.76	1.48	1.34
81	1A	5109	84G	C3-N1	6.68	1.48	1.34
81	1A	5119	84G	C3-N1	6.66	1.48	1.34
81	1A	5112	84G	C3-N1	6.65	1.48	1.34
81	1A	5102	84G	C3-N1	6.65	1.48	1.34

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	2m	1901	84G	C17-C19-C20	7.78	119.28	110.67
81	2m	1901	84G	C16-C21-C20	6.30	118.86	110.40
81	1A	5111	84G	C16-O5-C15	-4.63	107.00	117.98
81	2m	1901	84G	O6-C17-C19	4.52	117.84	109.70
81	2m	1901	84G	C16-O6-C17	4.39	122.29	113.72

There are no chirality outliers.

5 of 167 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	1A	5101	84G	C-C1-C2-O
81	1A	5101	84G	O-C2-C3-O1
81	1A	5102	84G	C-C1-C2-O
81	1A	5102	84G	C1-C2-C3-O1
81	1A	5102	84G	C1-C2-C3-N1

All (3) ring outliers are listed below:

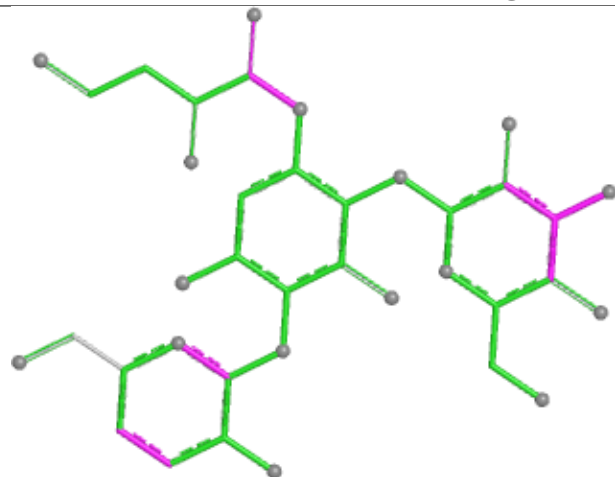
Mol	Chain	Res	Type	Atoms
81	1A	5118	84G	C11-C12-C13-C8-C9-O3
81	1A	5111	84G	C11-C12-C13-C8-C9-O3
81	1A	5101	84G	C11-C12-C13-C8-C9-O3

17 monomers are involved in 33 short contacts:

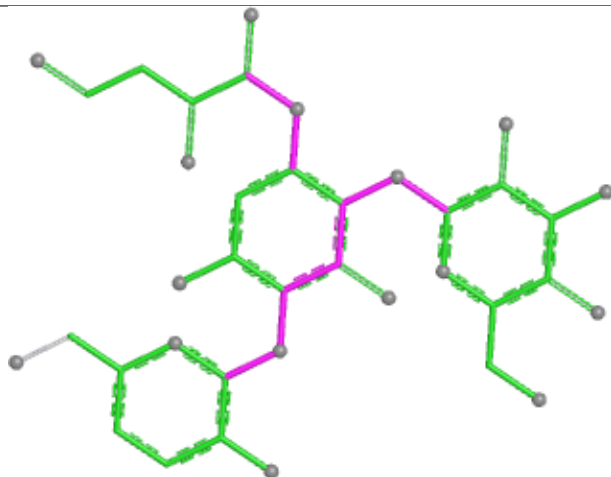
Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	1A	5112	84G	1	0
81	1A	5102	84G	2	0
81	1A	5106	84G	1	0
81	1A	5115	84G	1	0
81	1A	5105	84G	1	0
81	2i	201	84G	3	0
81	1A	5107	84G	2	0
81	1A	5101	84G	1	0
81	2m	1901	84G	1	0
81	2D	301	84G	3	0
81	1A	5113	84G	6	0
81	1A	5103	84G	3	0
81	1A	5110	84G	2	0
81	2m	1902	84G	1	0
81	1A	5119	84G	1	0
81	1A	5111	84G	2	0
81	1A	5118	84G	2	0

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

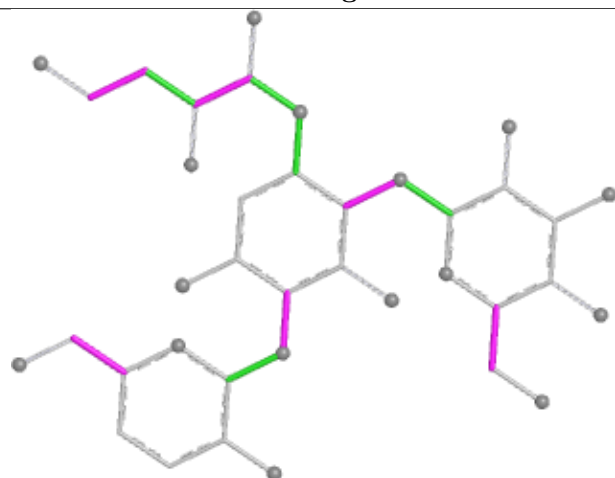
Ligand 84G 1A 5112



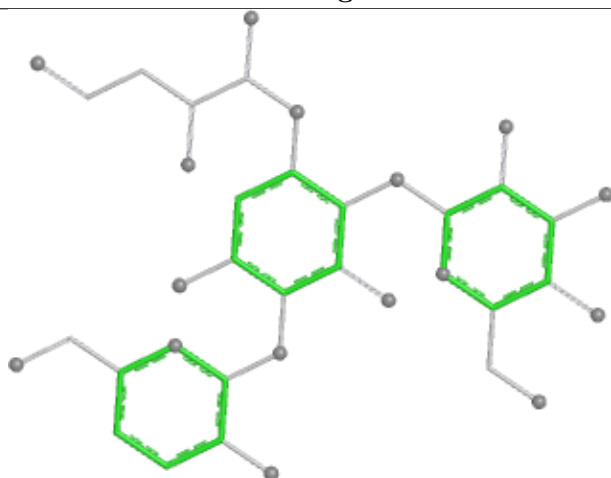
Bond lengths



Bond angles

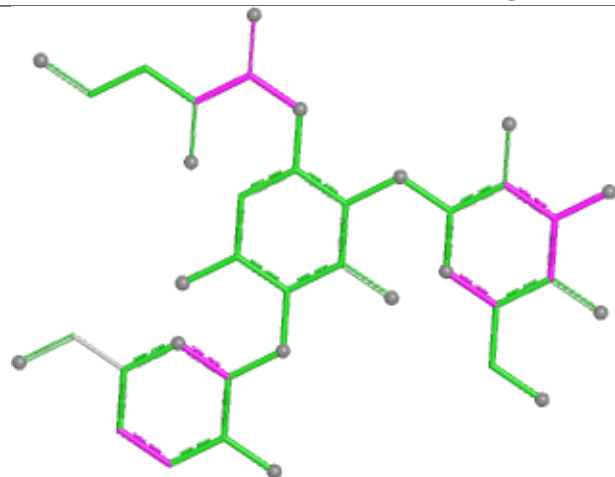


Torsions

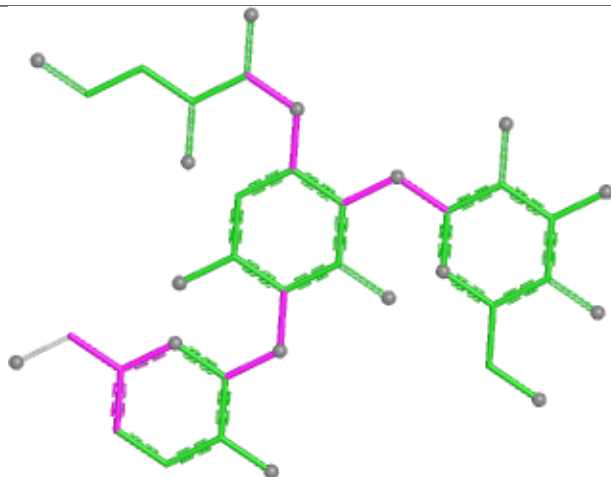


Rings

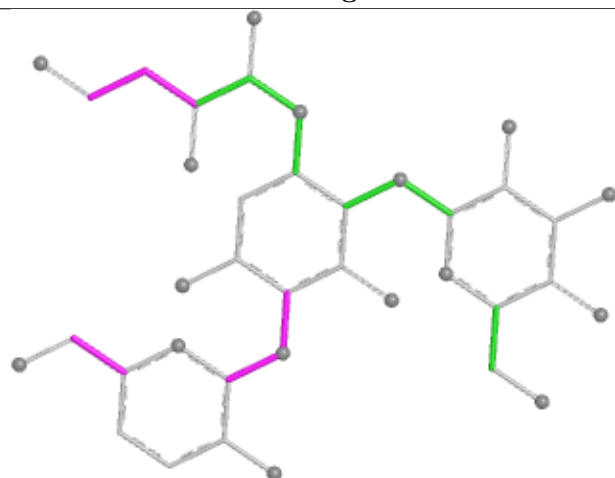
Ligand 84G 1A 5117



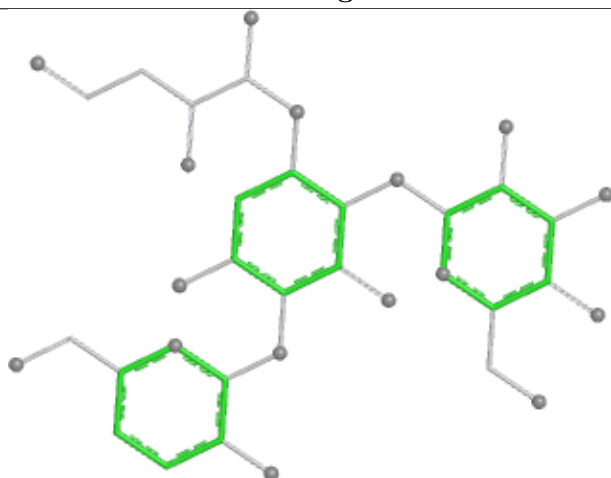
Bond lengths



Bond angles

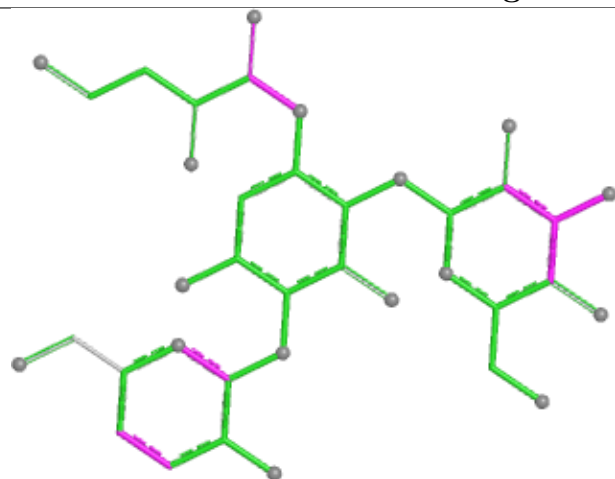


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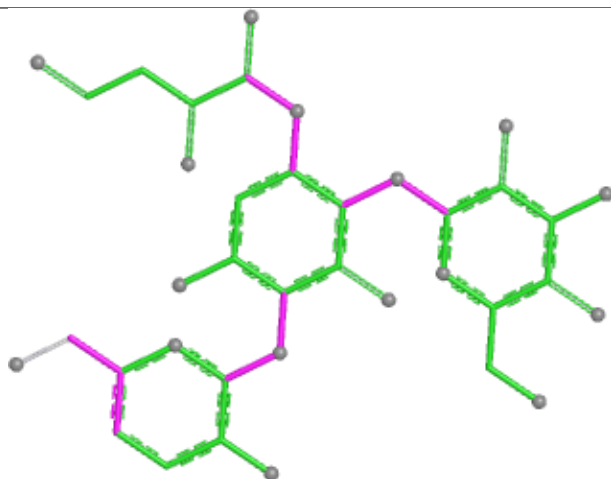


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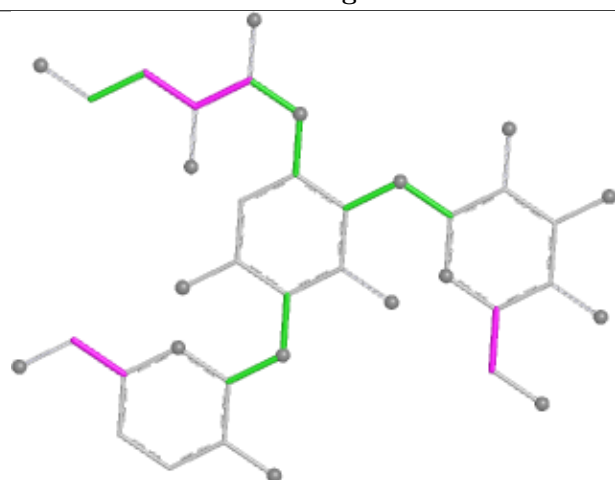
Ligand 84G 1A 5114



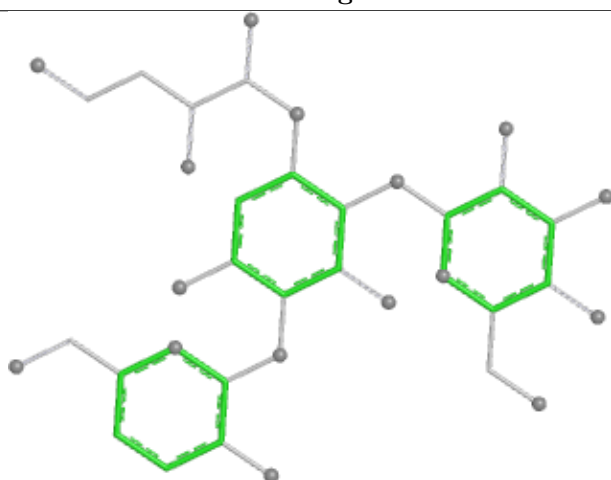
Bond lengths



Bond angles

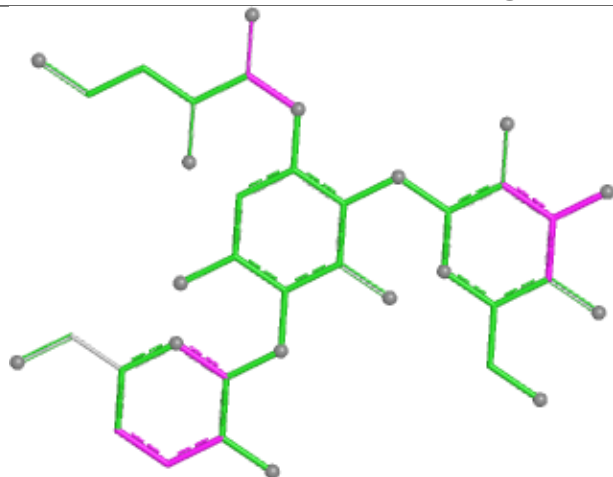


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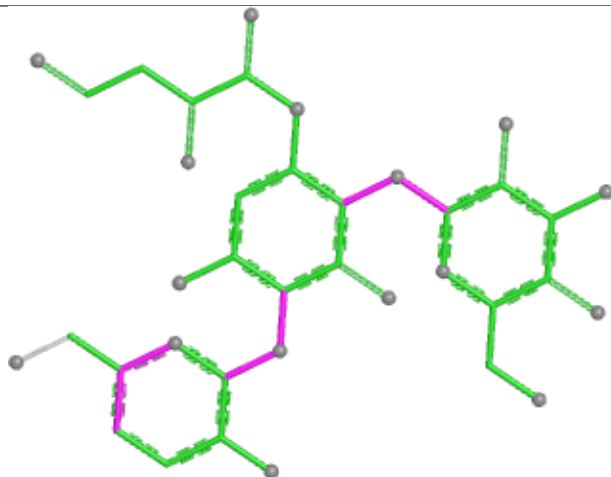


Rings

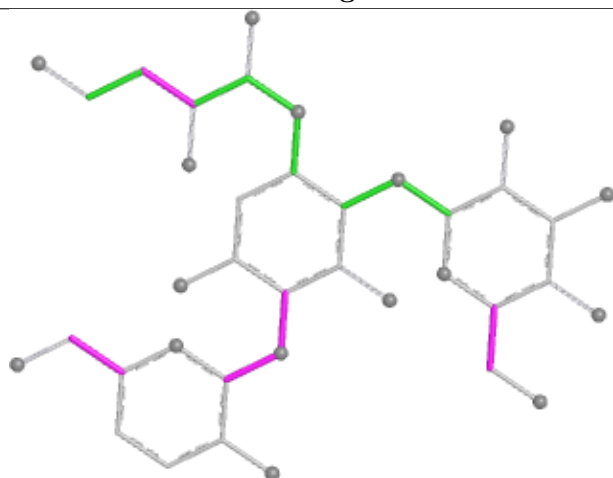
Ligand 84G 1A 5108



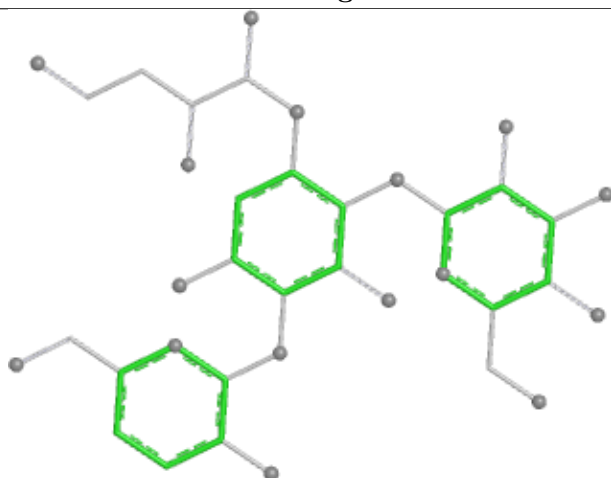
Bond lengths



Bond angles

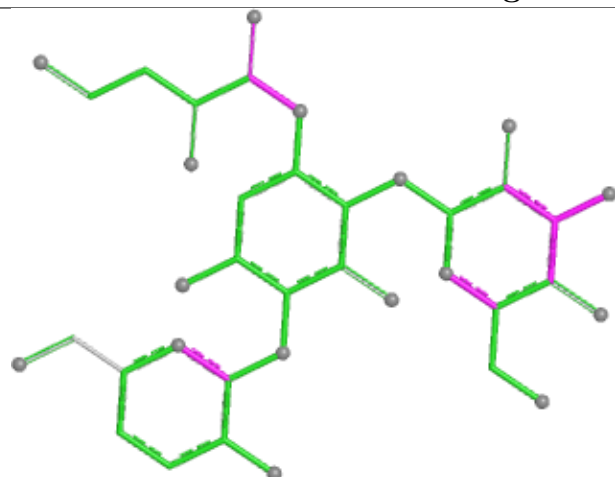


Torsions

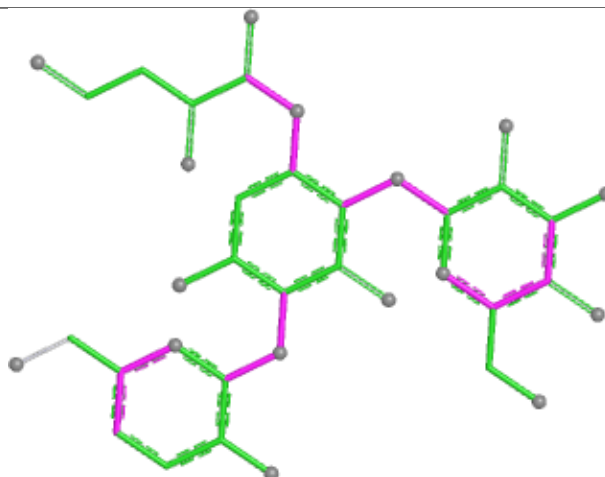


Rings

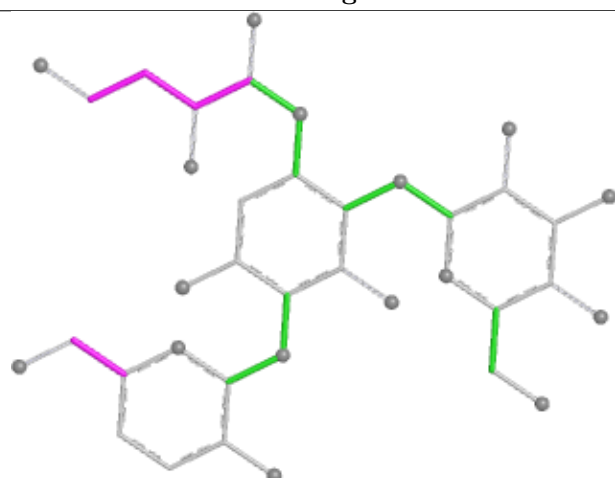
Ligand 84G 1A 5102



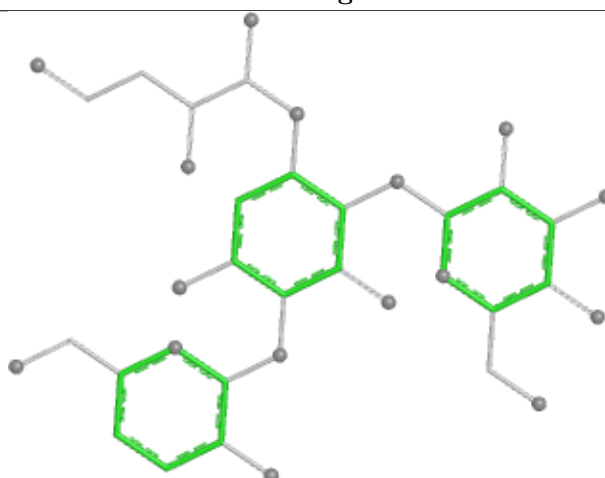
Bond lengths



Bond angles

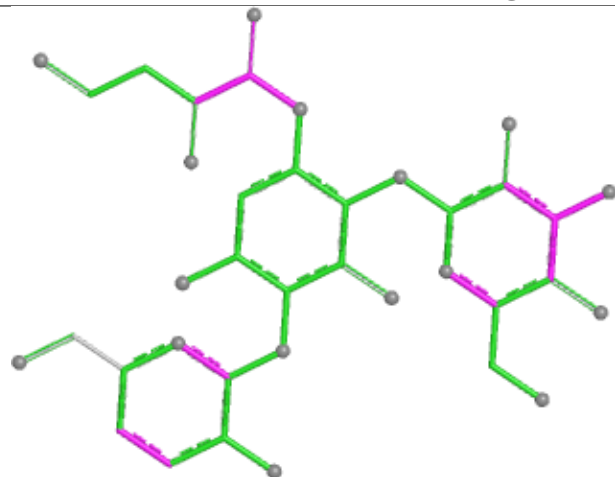


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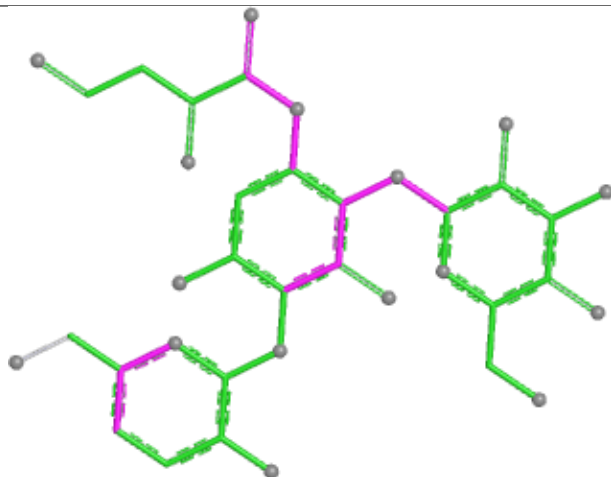


Rings

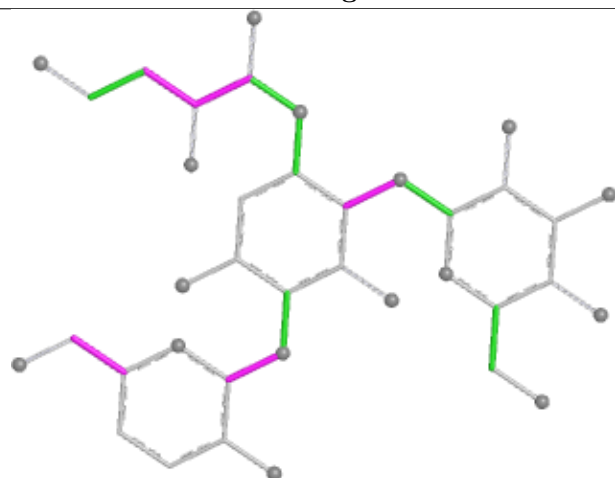
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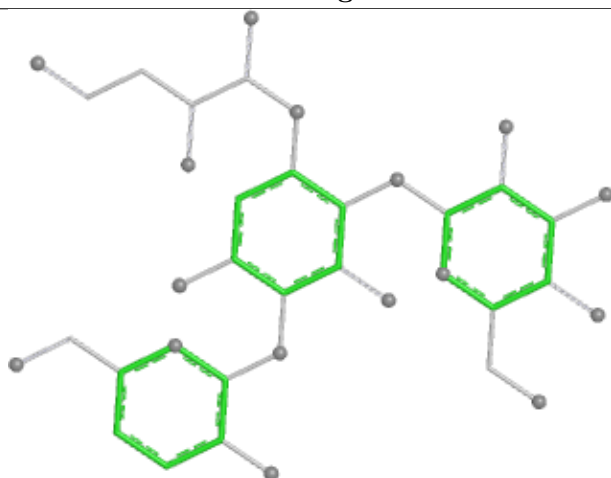
Bond lengths



Bond angles

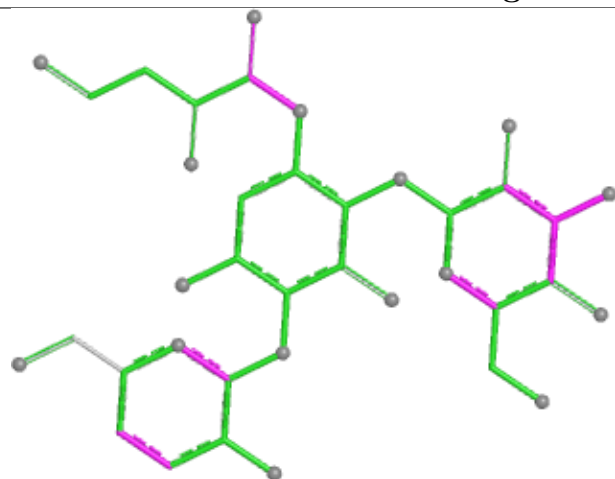


Torsions

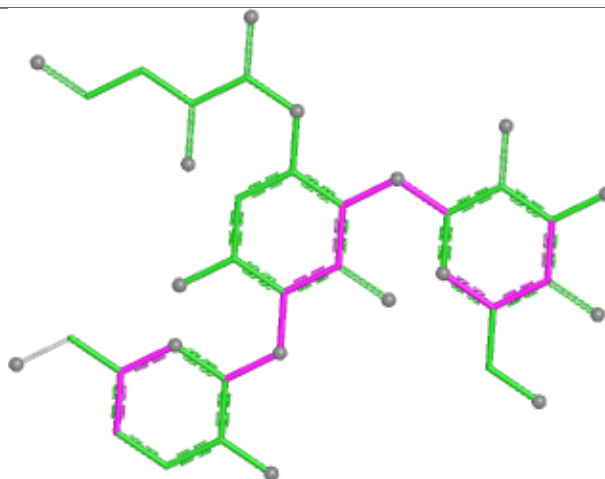


Rings

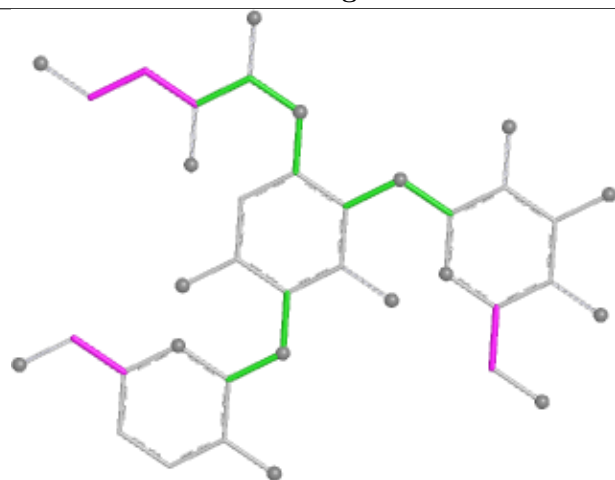
Ligand 84G 1A 5115



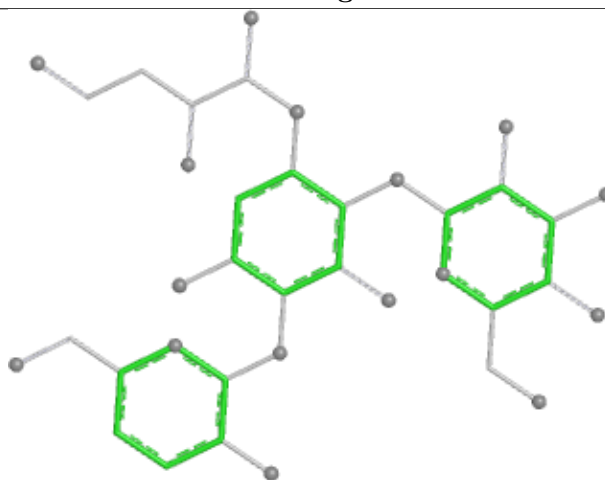
Bond lengths



Bond angles

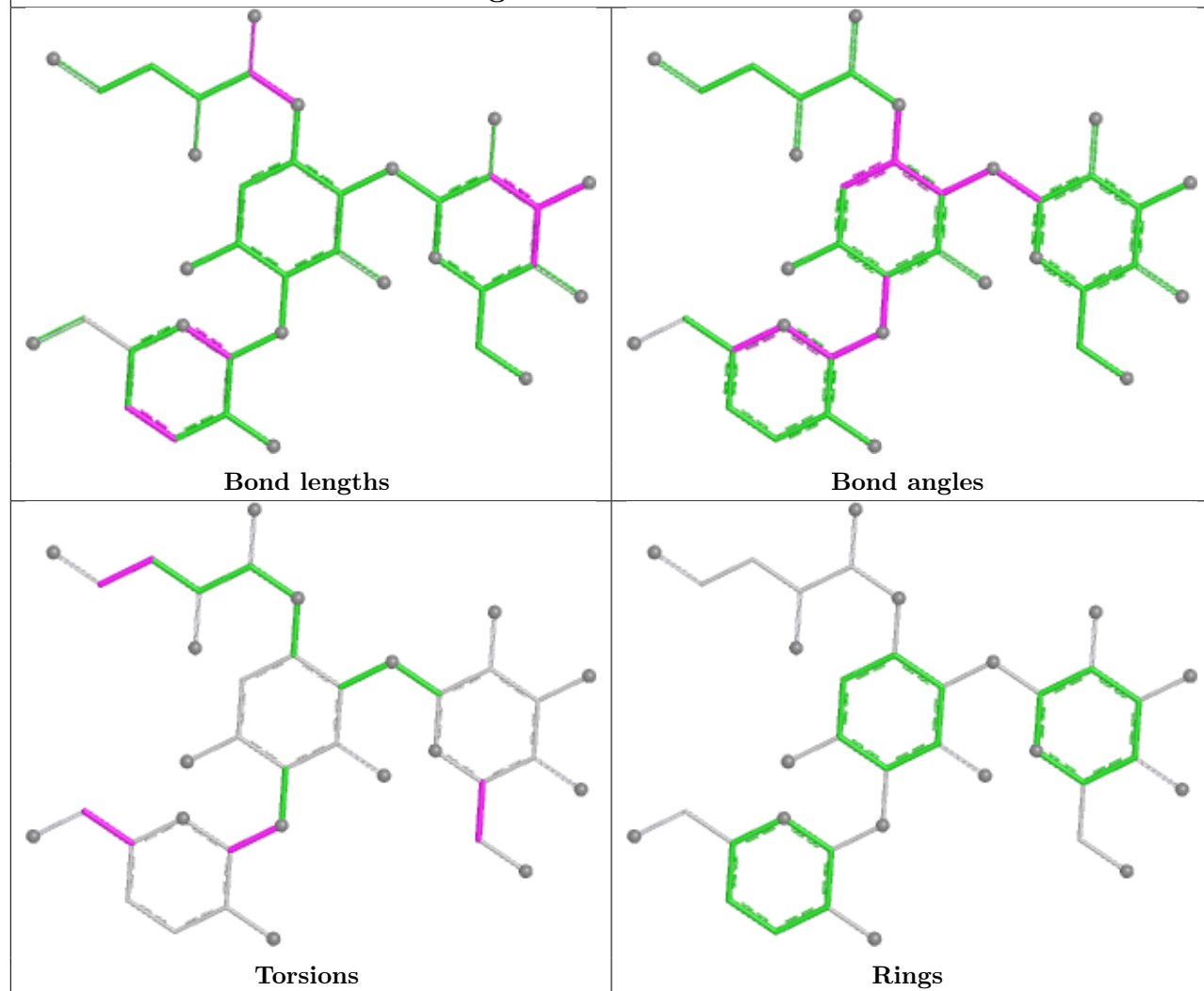


Torsions

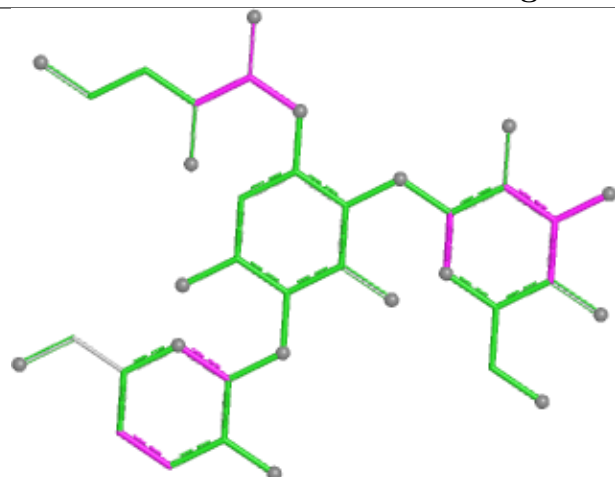


Rings

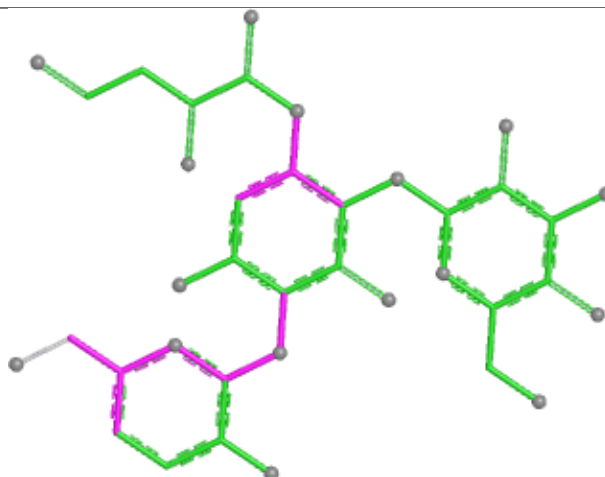
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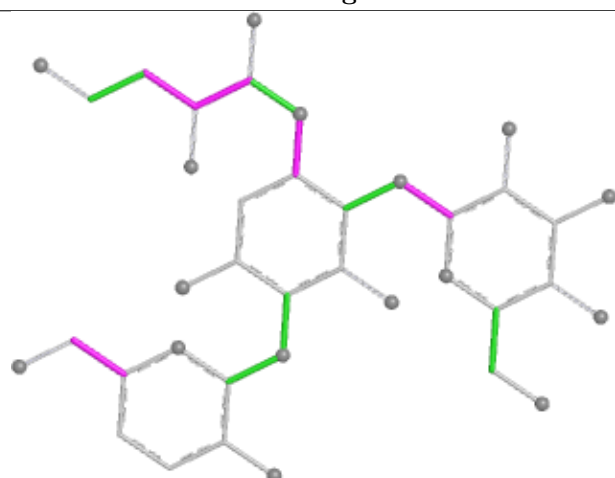
Ligand 84G 2i 201



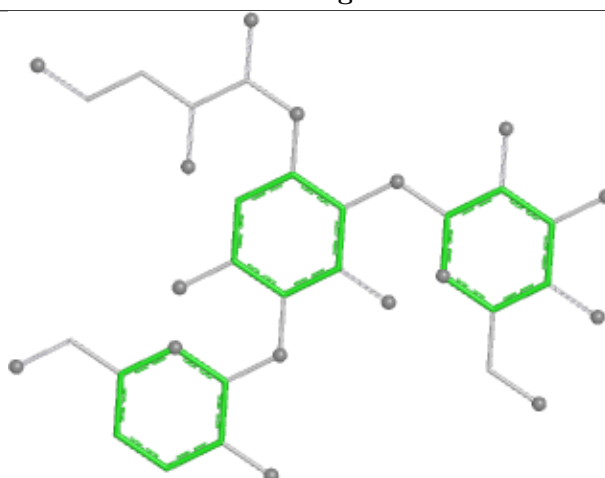
Bond lengths



Bond angles

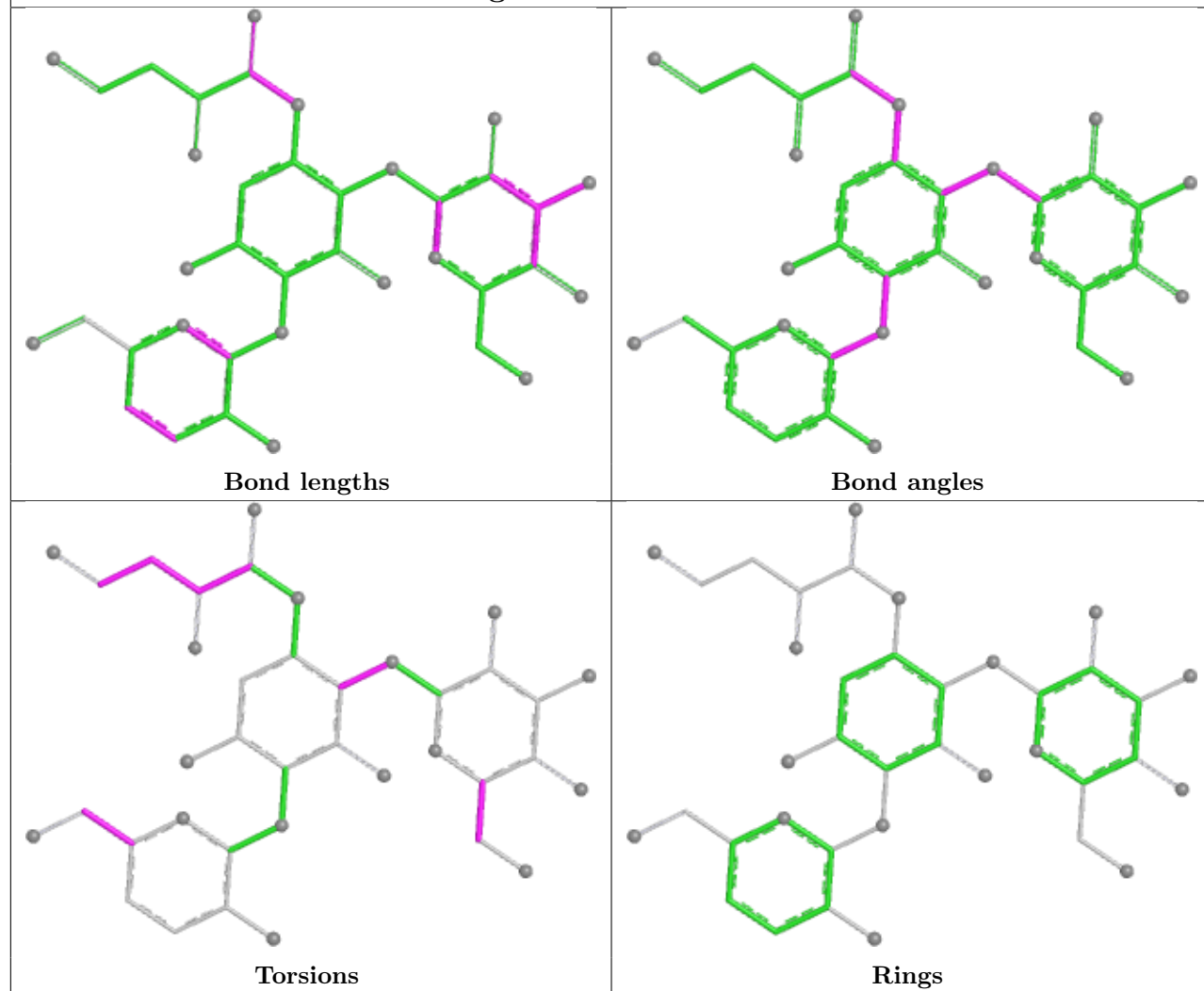


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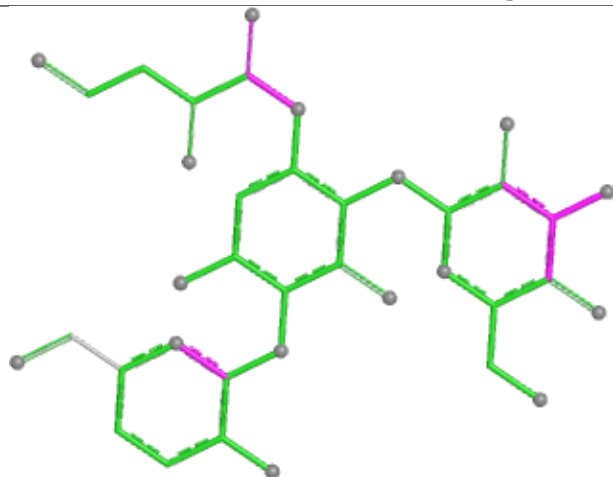


Rings

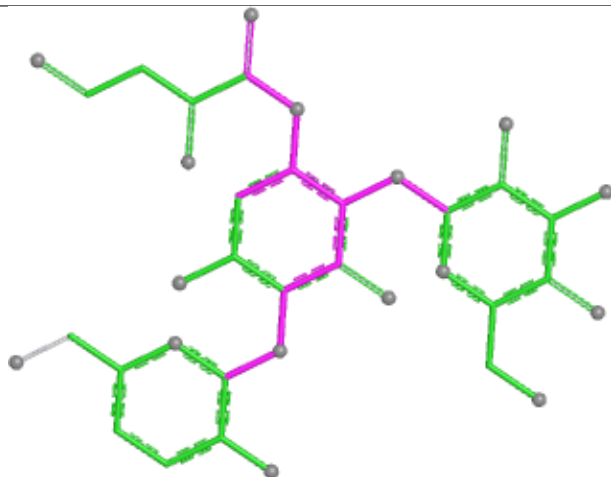
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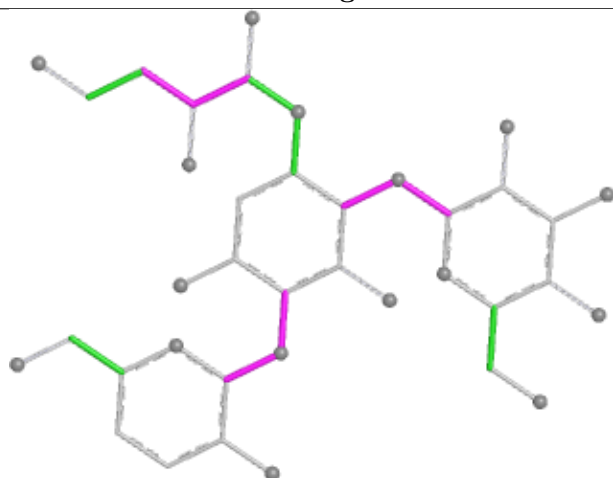
Ligand 84G 1A 5101



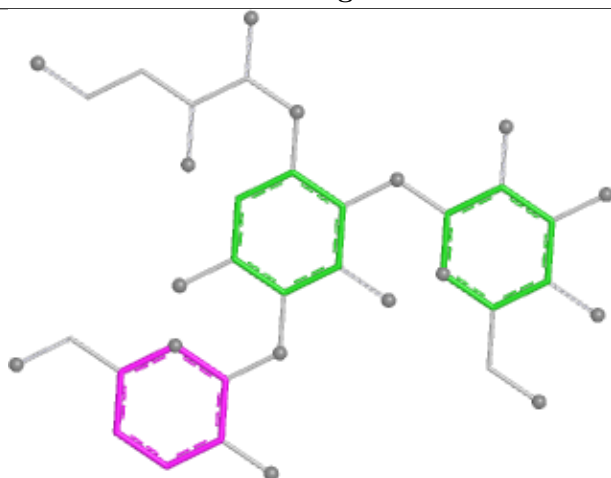
Bond lengths



Bond angles

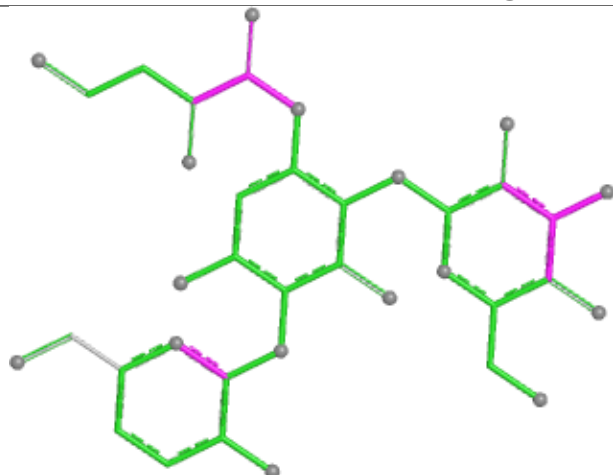


Torsions

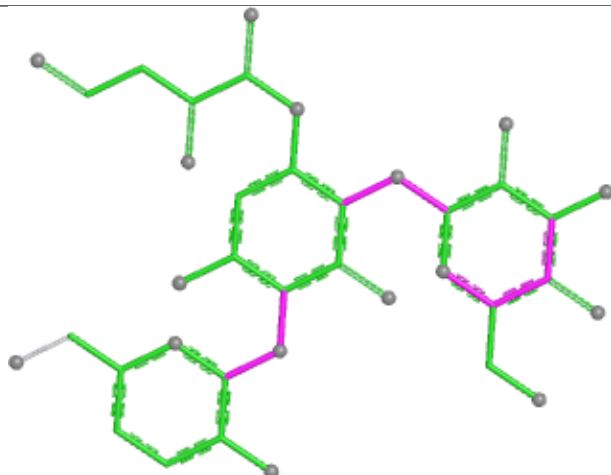


Rings

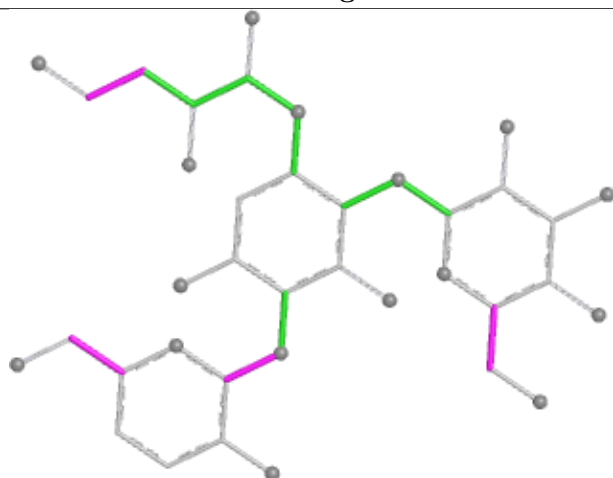
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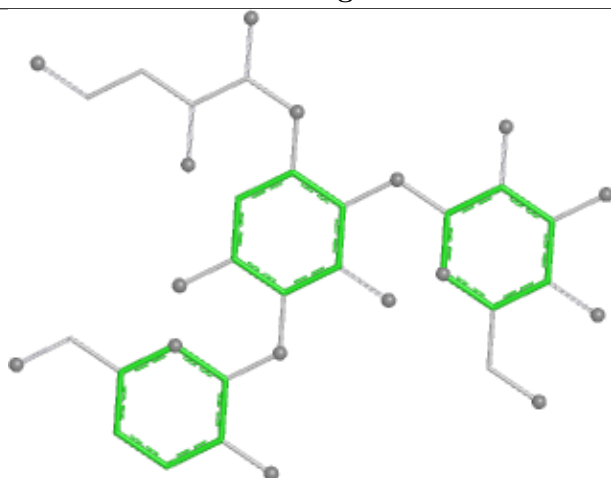
Bond lengths



Bond angles

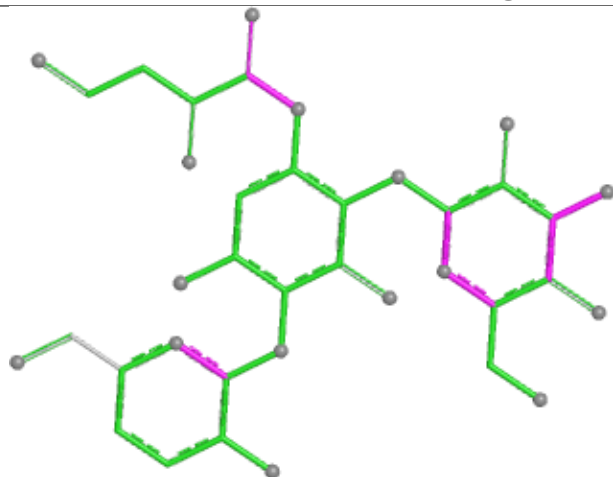


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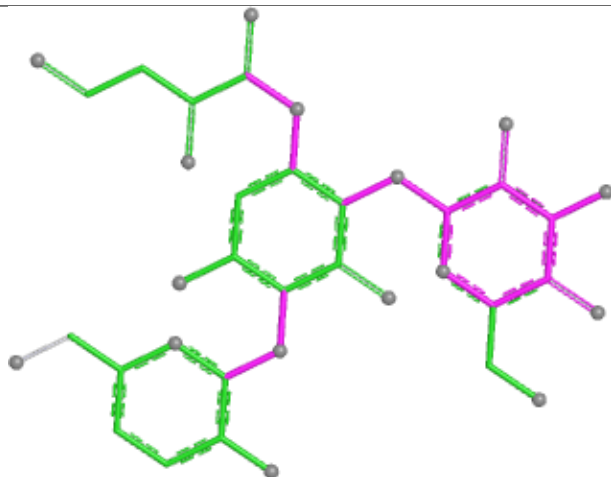


Rings

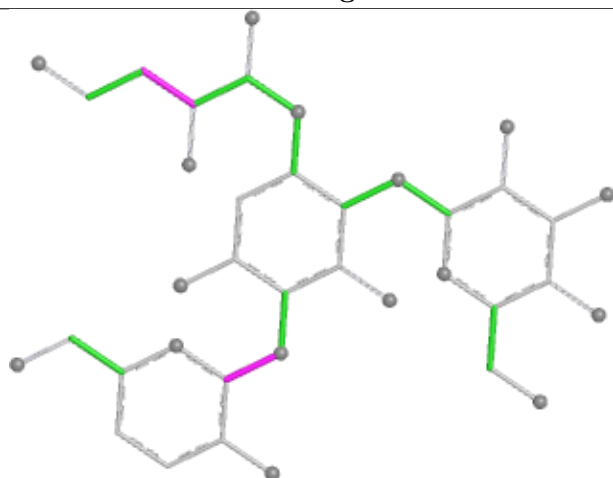
Ligand 84G 2m 1901



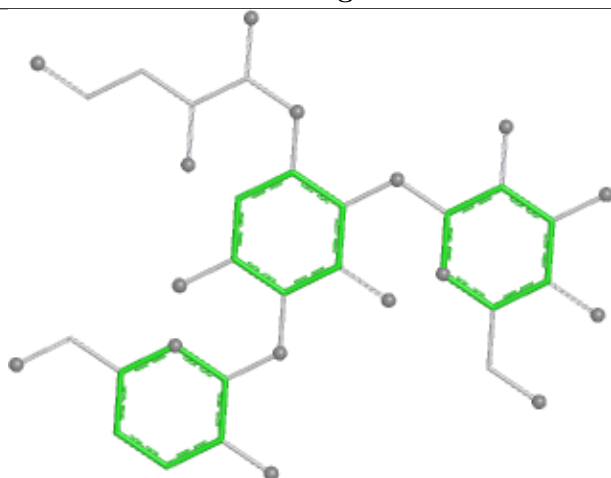
Bond lengths



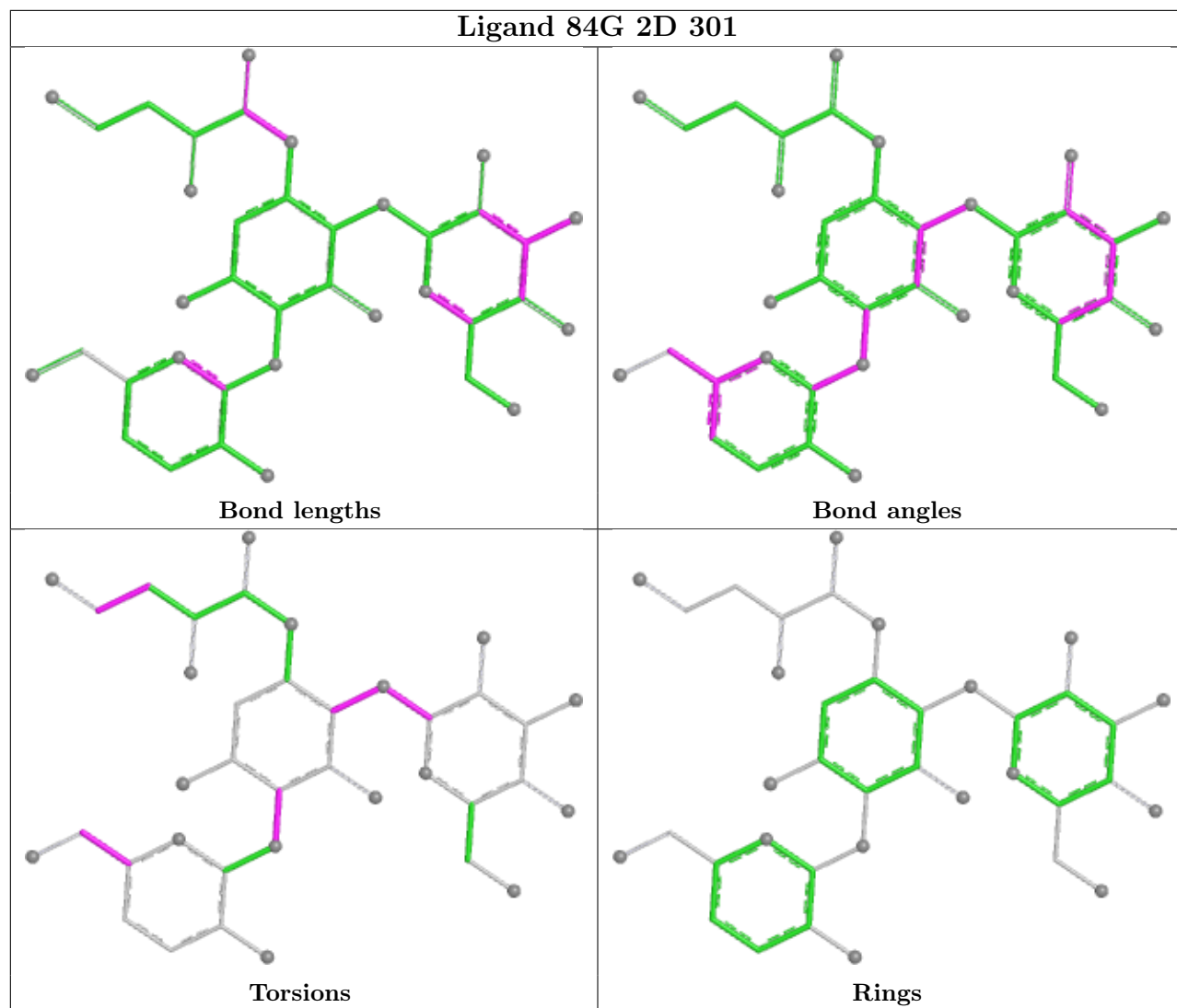
Bond angles



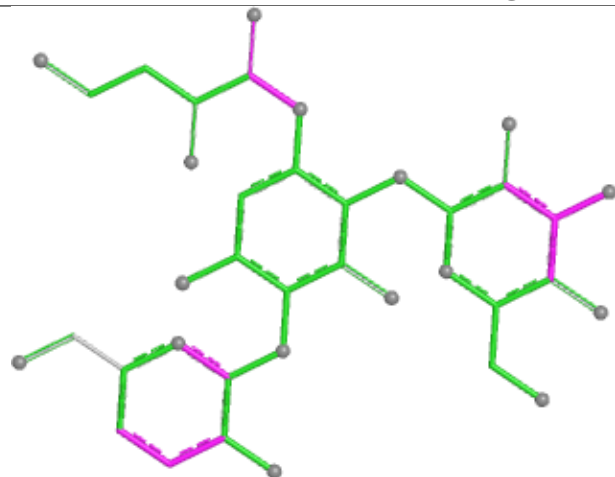
Torsions



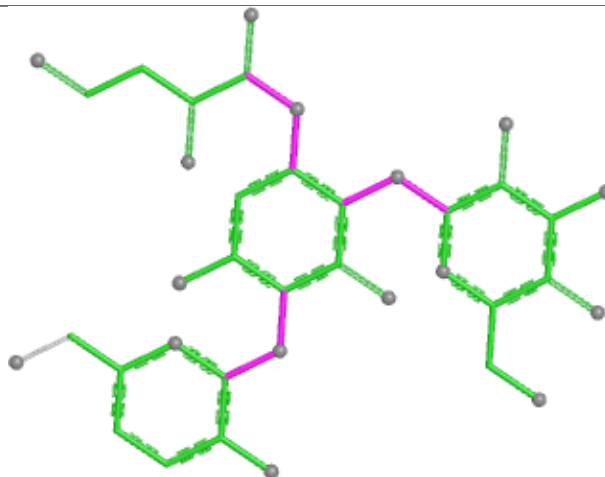
Rings



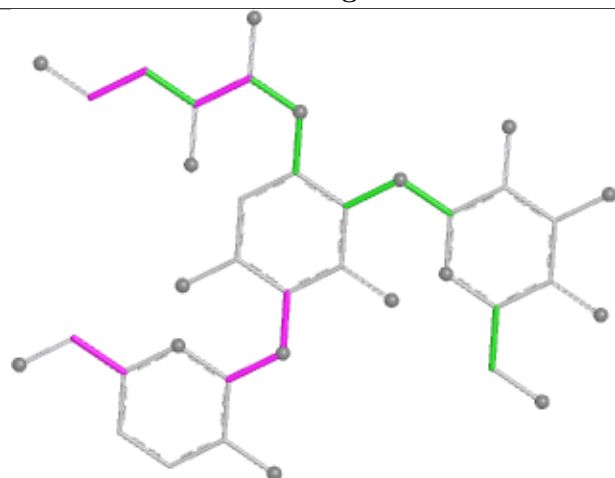
Ligand 84G 1A 5104



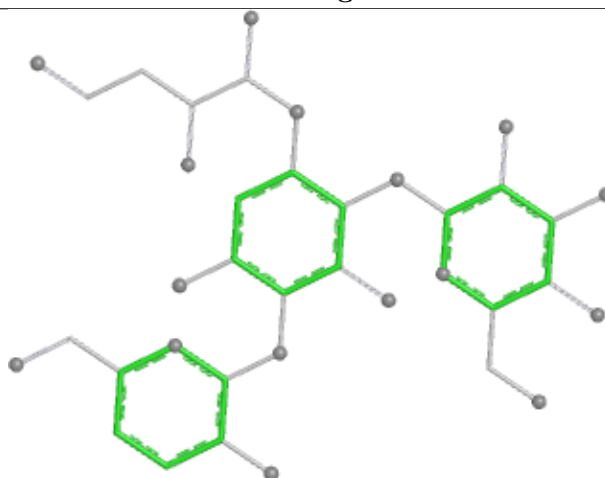
Bond lengths



Bond angles

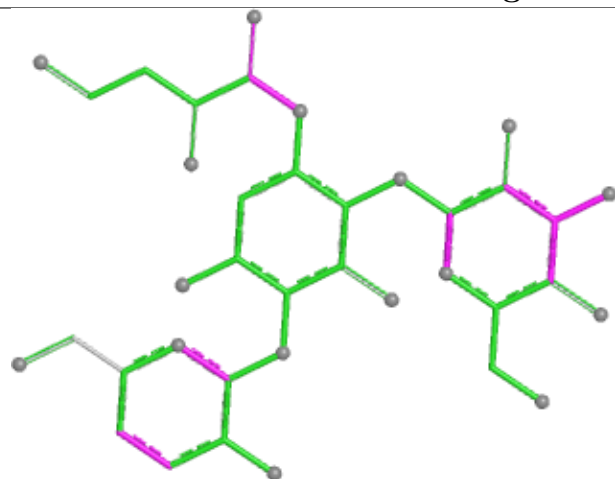


Torsions

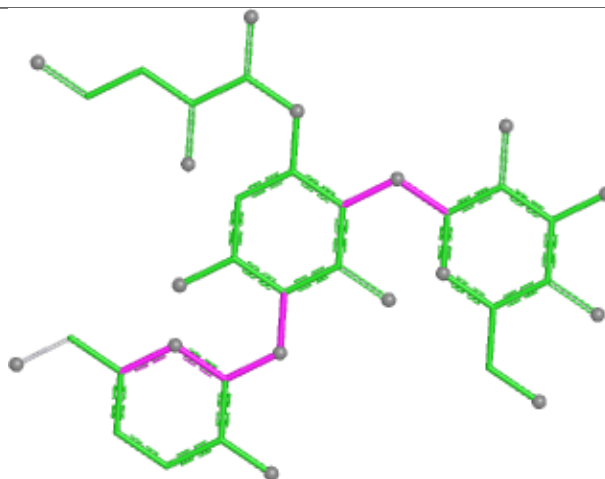


Rings

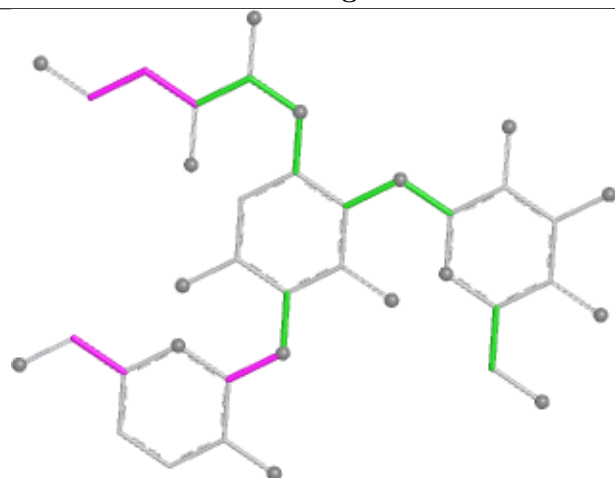
Ligand 84G 1A 5113



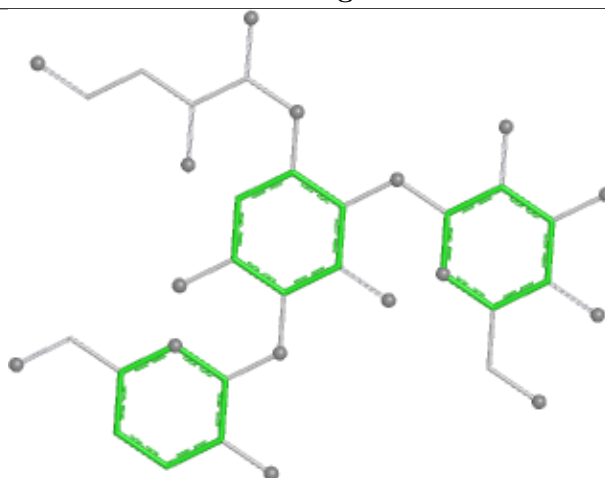
Bond lengths



Bond angles

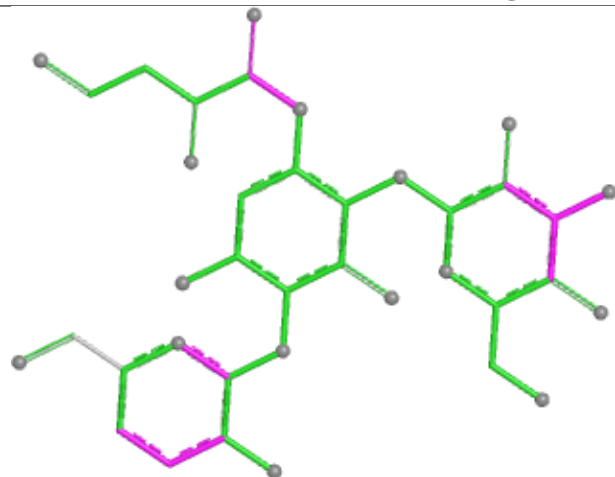


Torsions

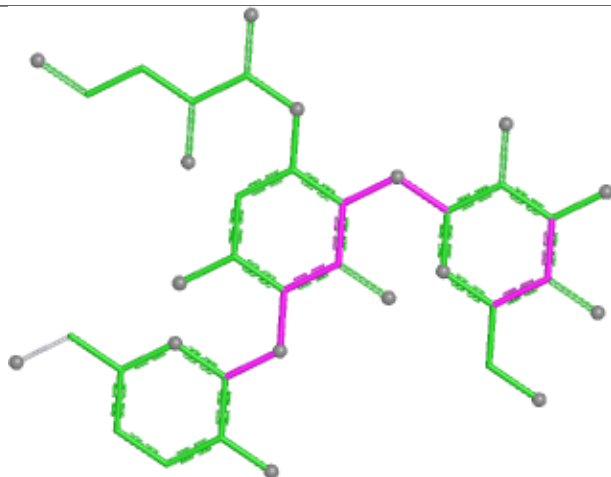


Rings

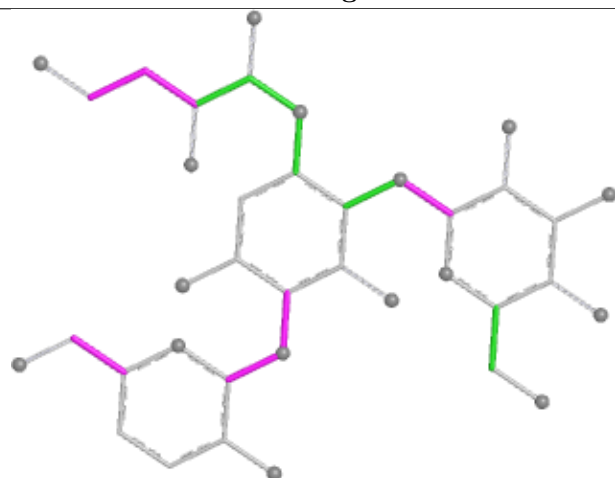
Ligand 84G 1A 5103



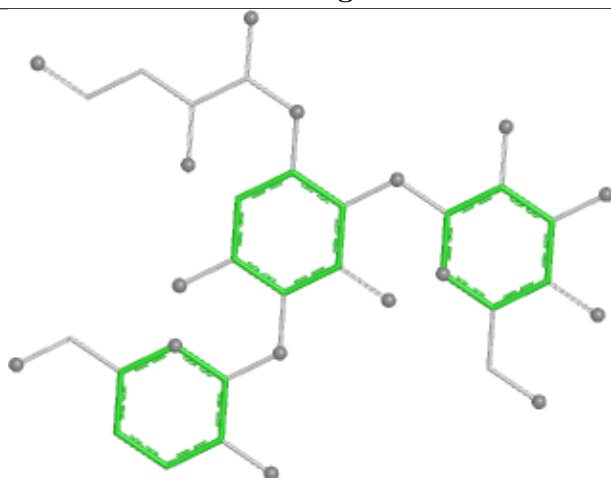
Bond lengths



Bond angles

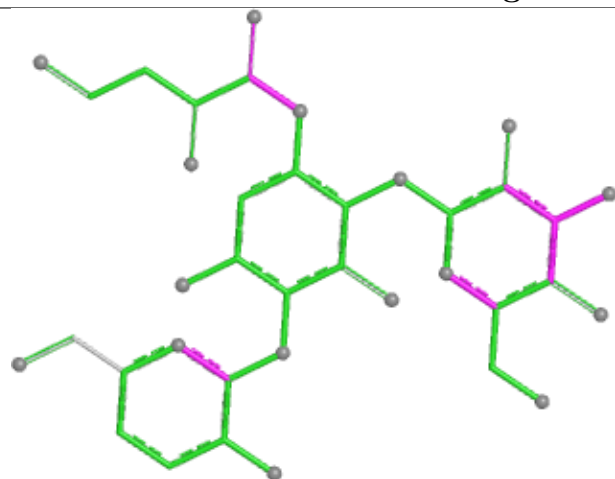


Torsions

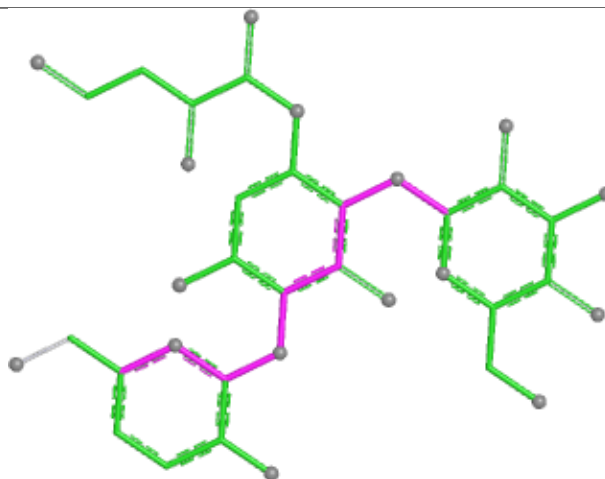


Rings

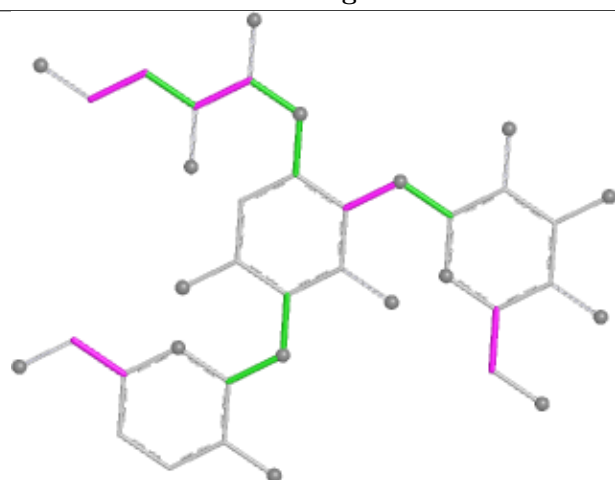
Ligand 84G 1A 5110



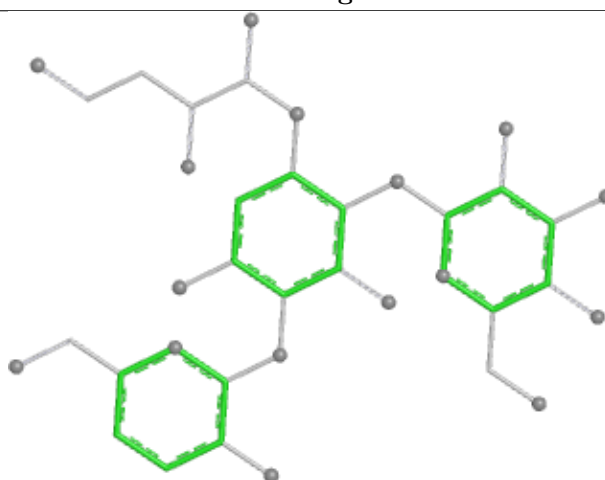
Bond lengths



Bond angles

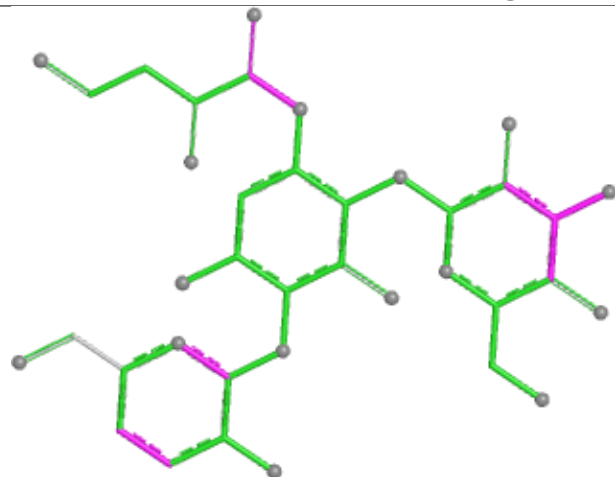


Torsions

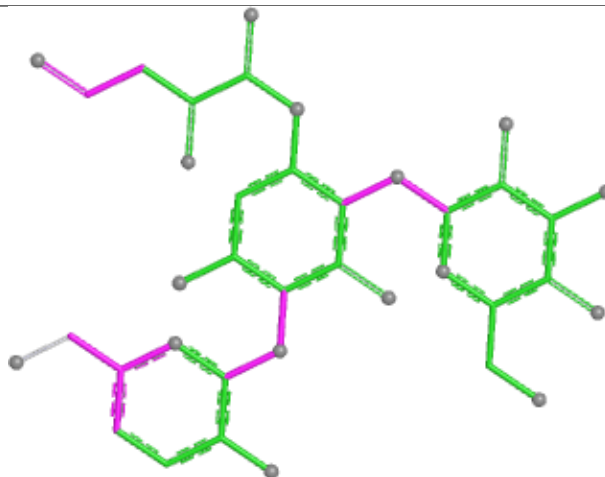


Rings

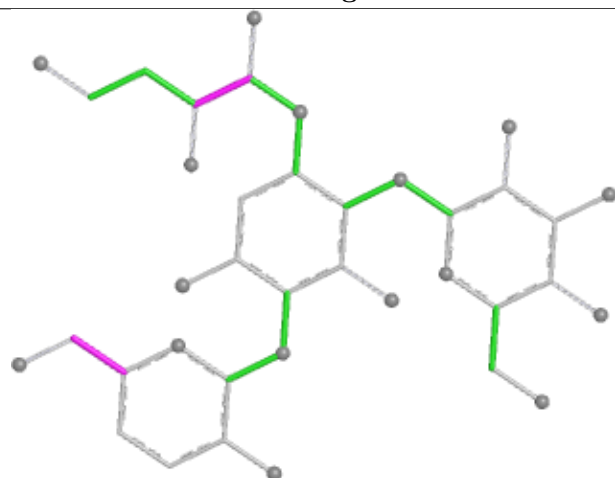
Ligand 84G 2m 1902



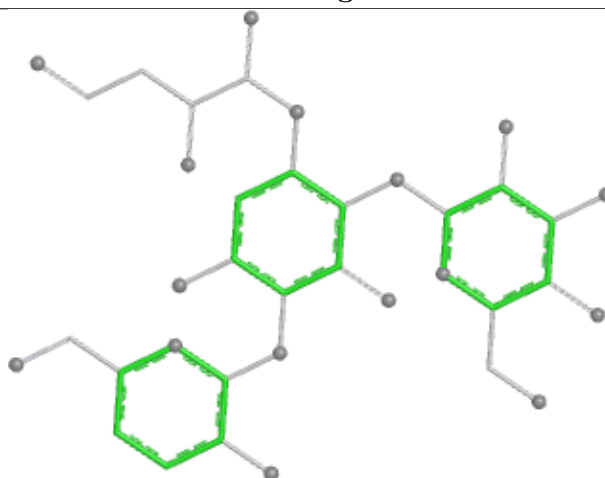
Bond lengths



Bond angles

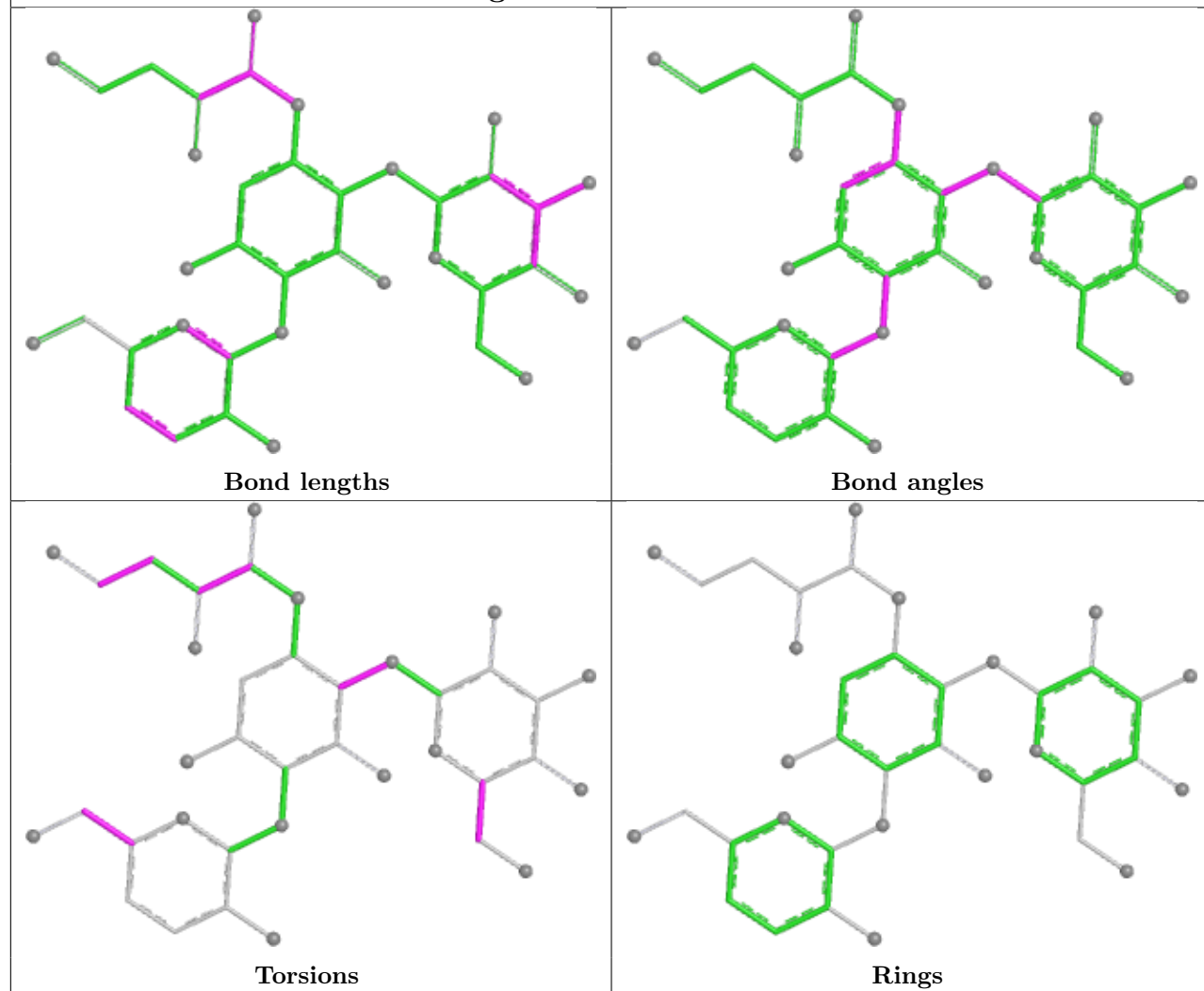


Torsions

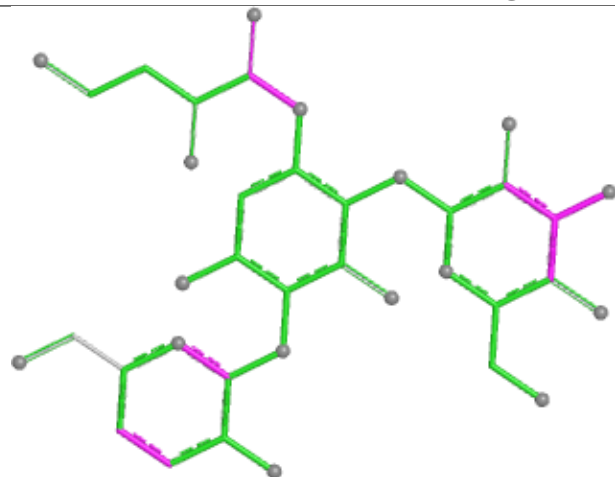


Rings

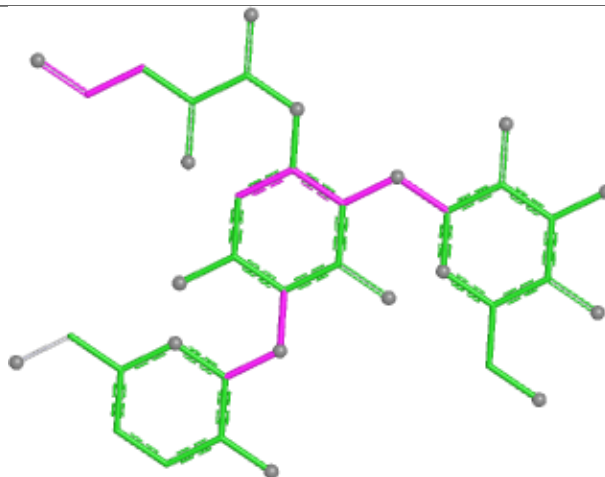
Ligand 84G 1A 5119



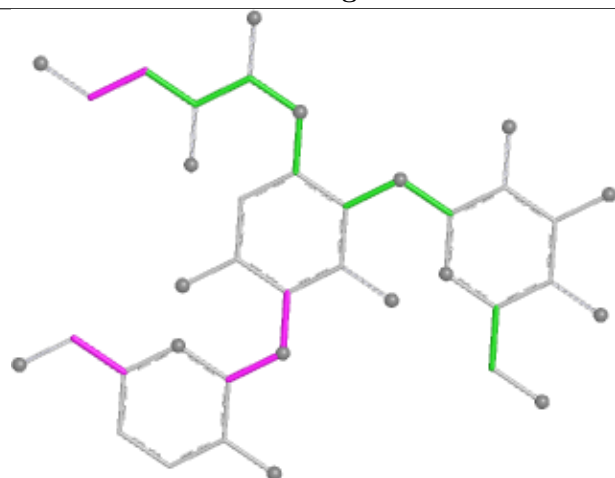
Ligand 84G 1A 5116



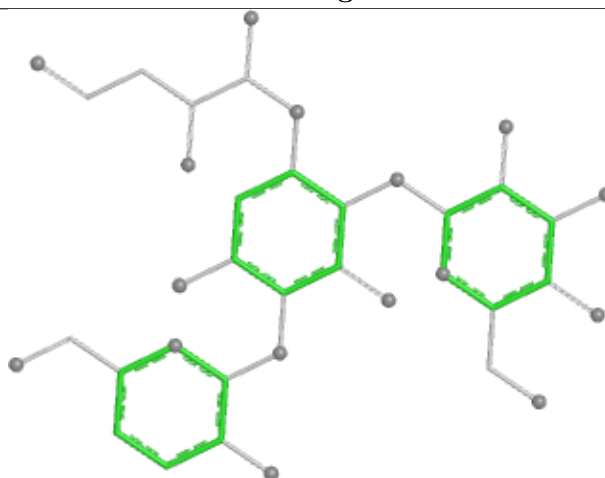
Bond lengths



Bond angles

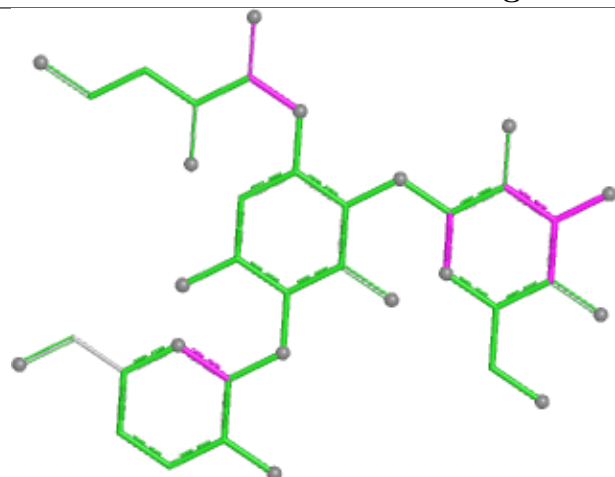


Torsions

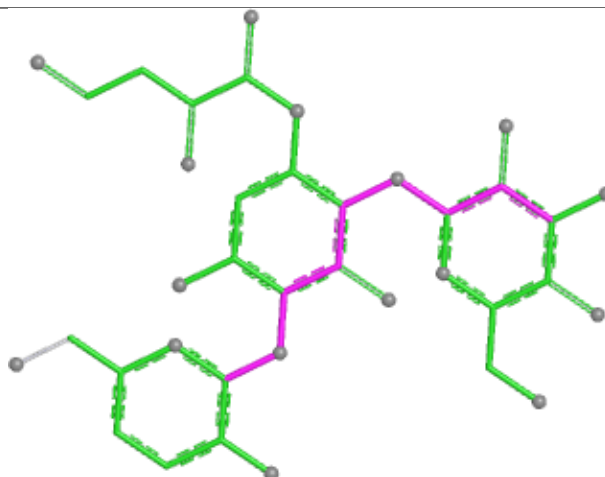


Rings

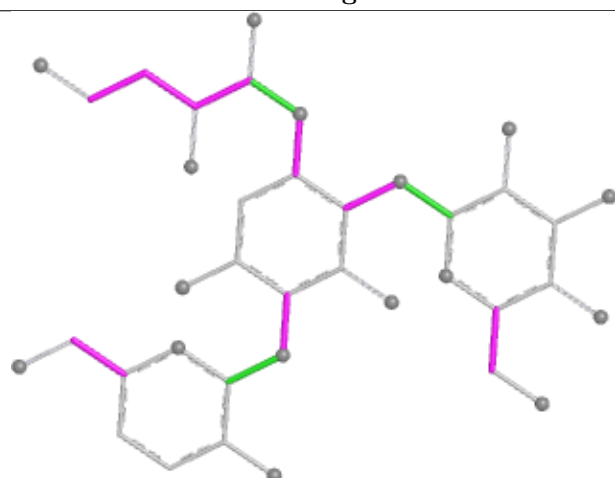
Ligand 84G 1A 5111



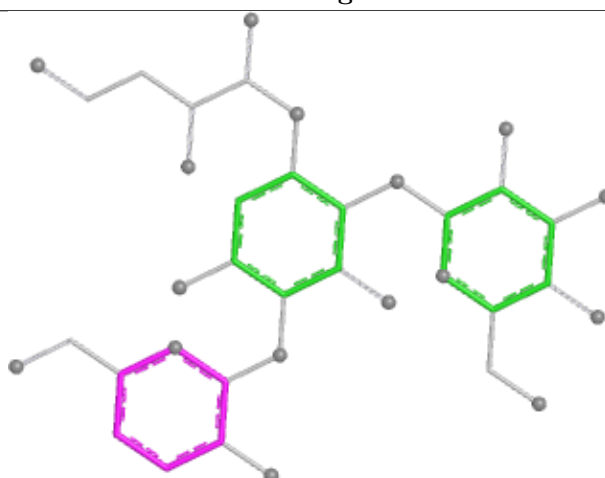
Bond lengths



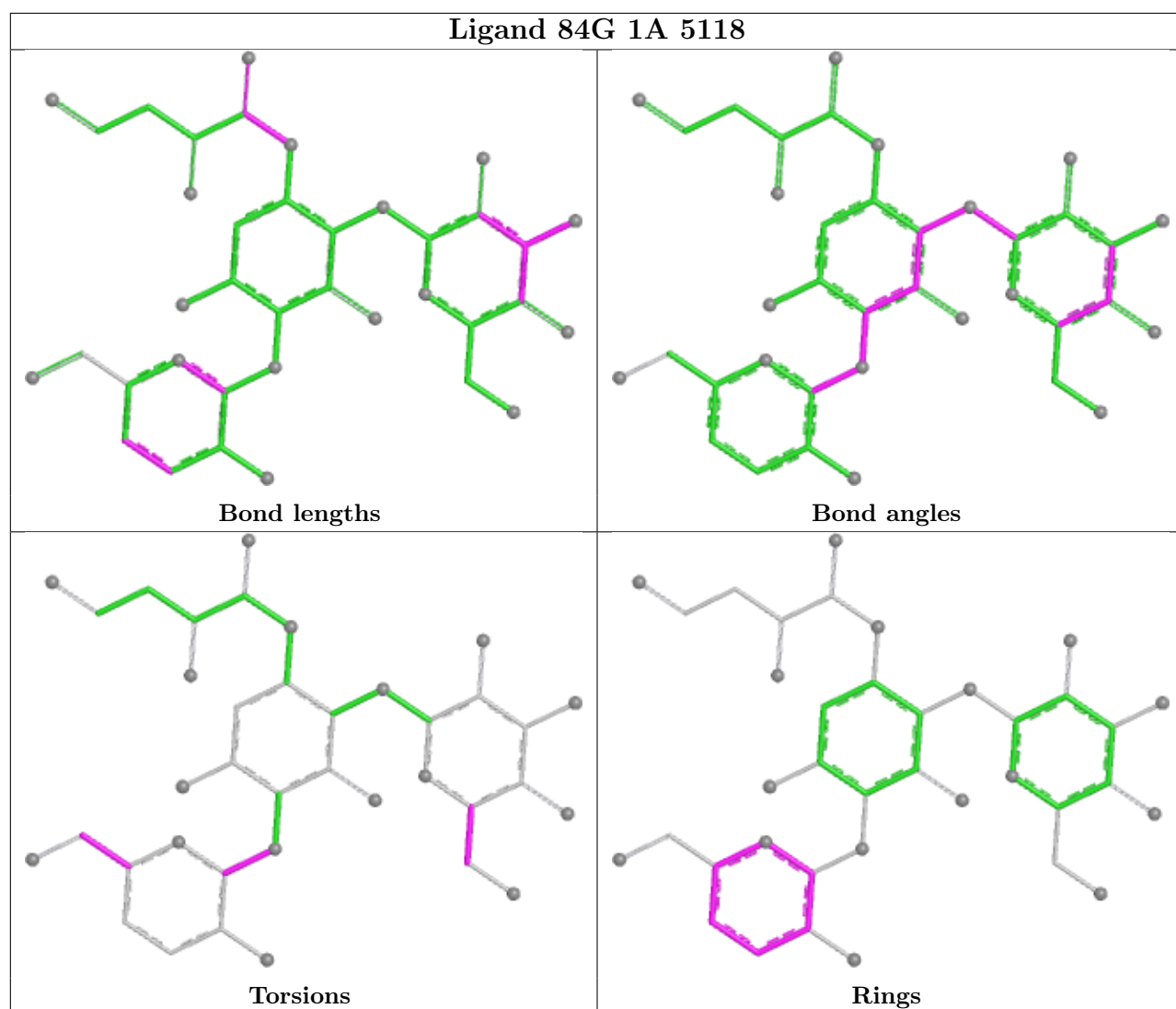
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

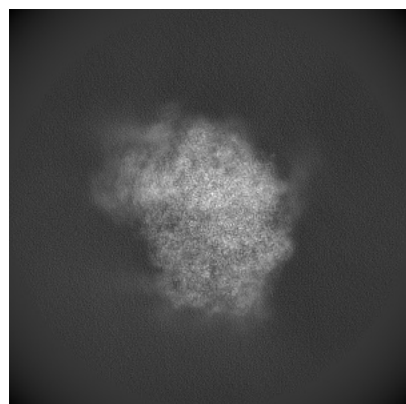
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35414. These allow visual inspection of the internal detail of the map and identification of artifacts.

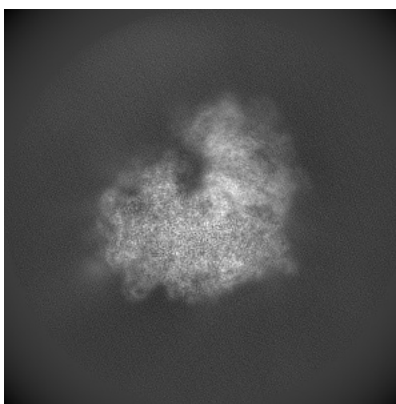
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

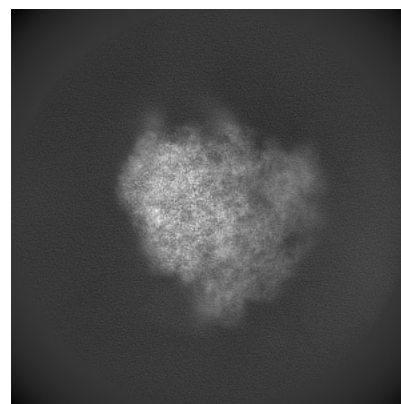
6.1.1 Primary map



X

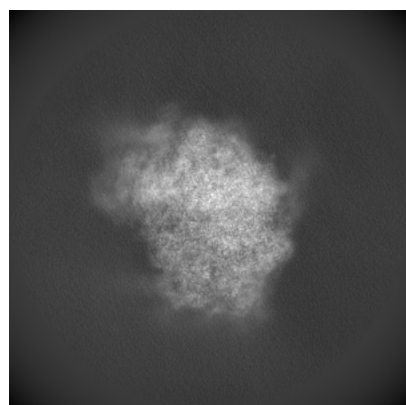


Y

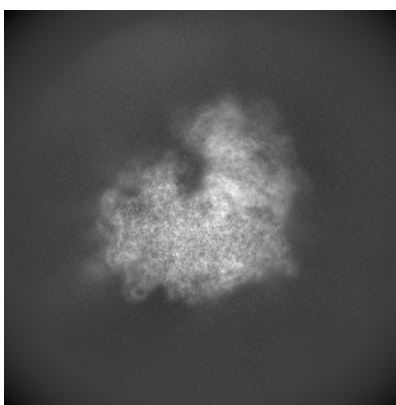


Z

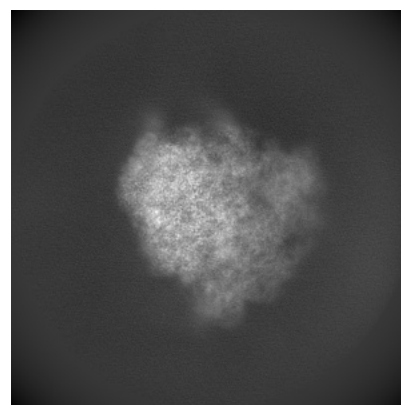
6.1.2 Raw map



X



Y

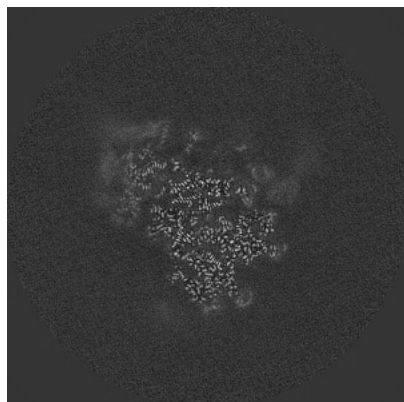


Z

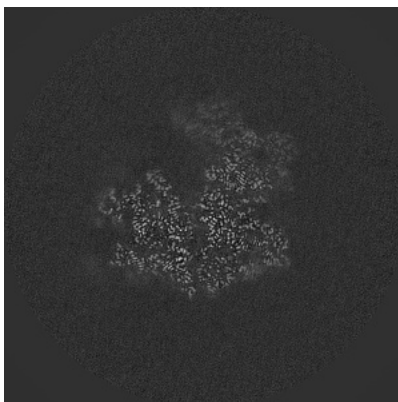
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

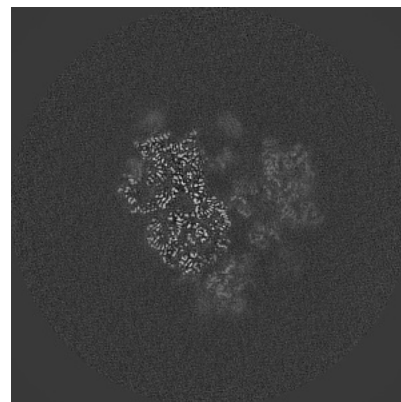
6.2.1 Primary map



X Index: 320

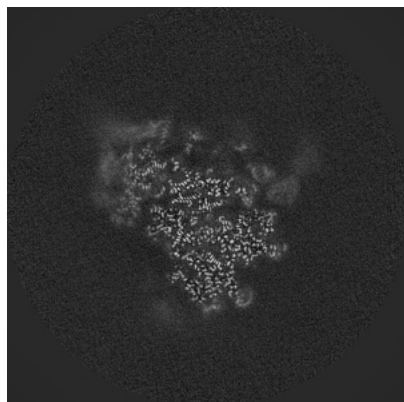


Y Index: 320

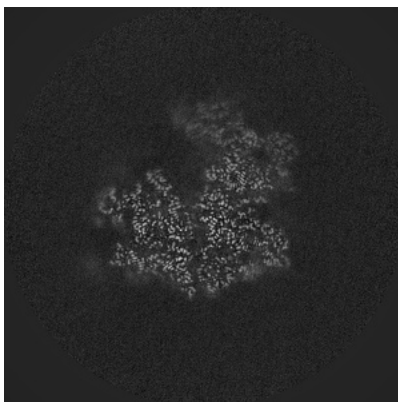


Z Index: 320

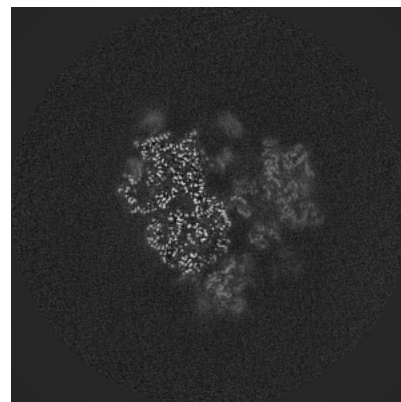
6.2.2 Raw map



X Index: 320



Y Index: 320

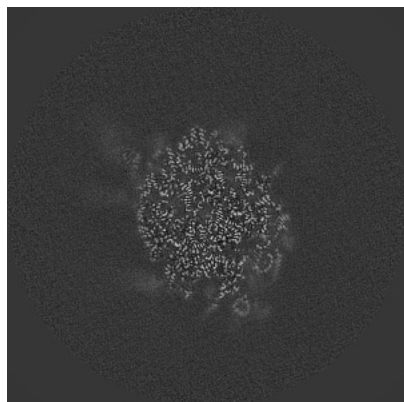


Z Index: 320

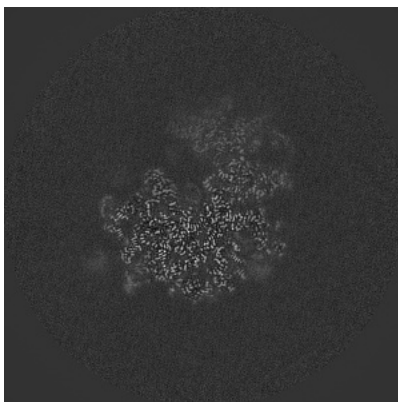
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

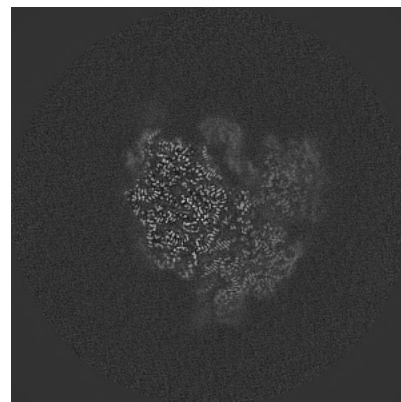
6.3.1 Primary map



X Index: 290

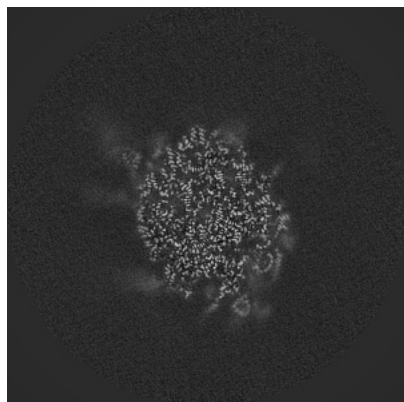


Y Index: 336

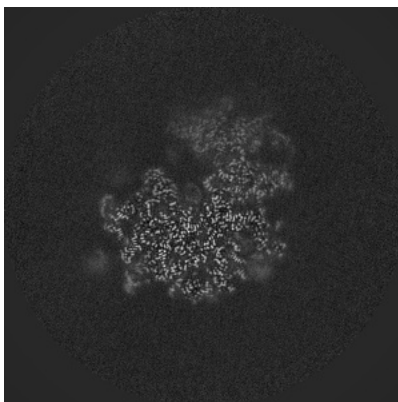


Z Index: 348

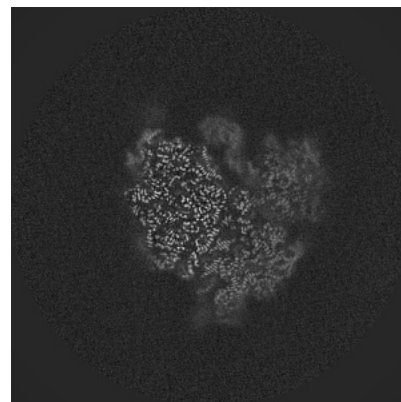
6.3.2 Raw map



X Index: 290



Y Index: 336

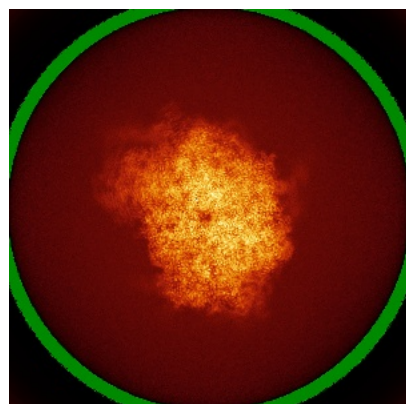


Z Index: 349

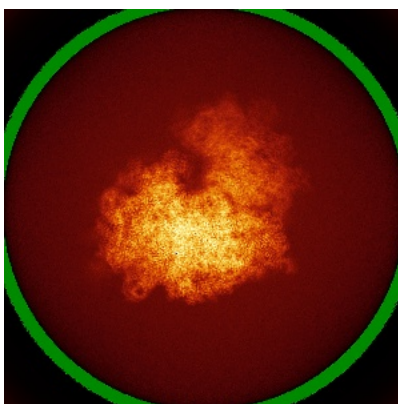
The images above show the largest variance slices of the map in three orthogonal directions.

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

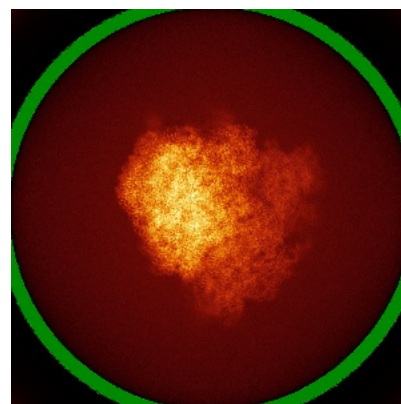
6.4.1 Primary map



X

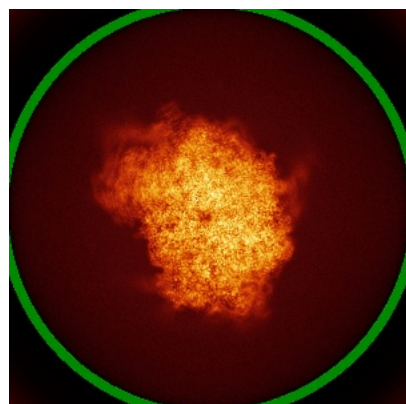


Y

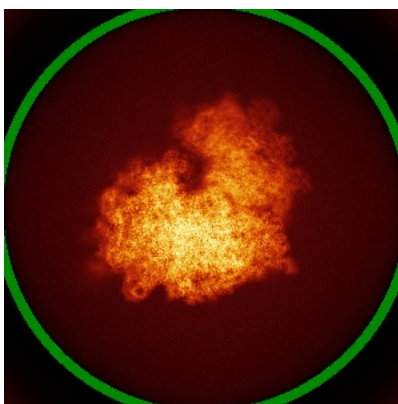


Z

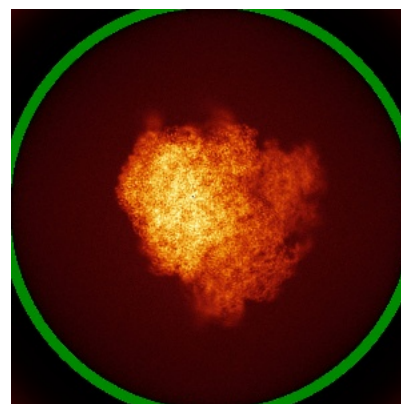
6.4.2 Raw map



X



Y



Z

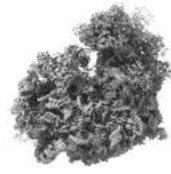
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



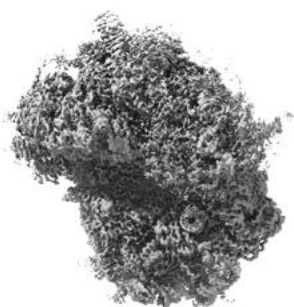
Y



Z

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

6.5.2 Raw map



X



Y



Z

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

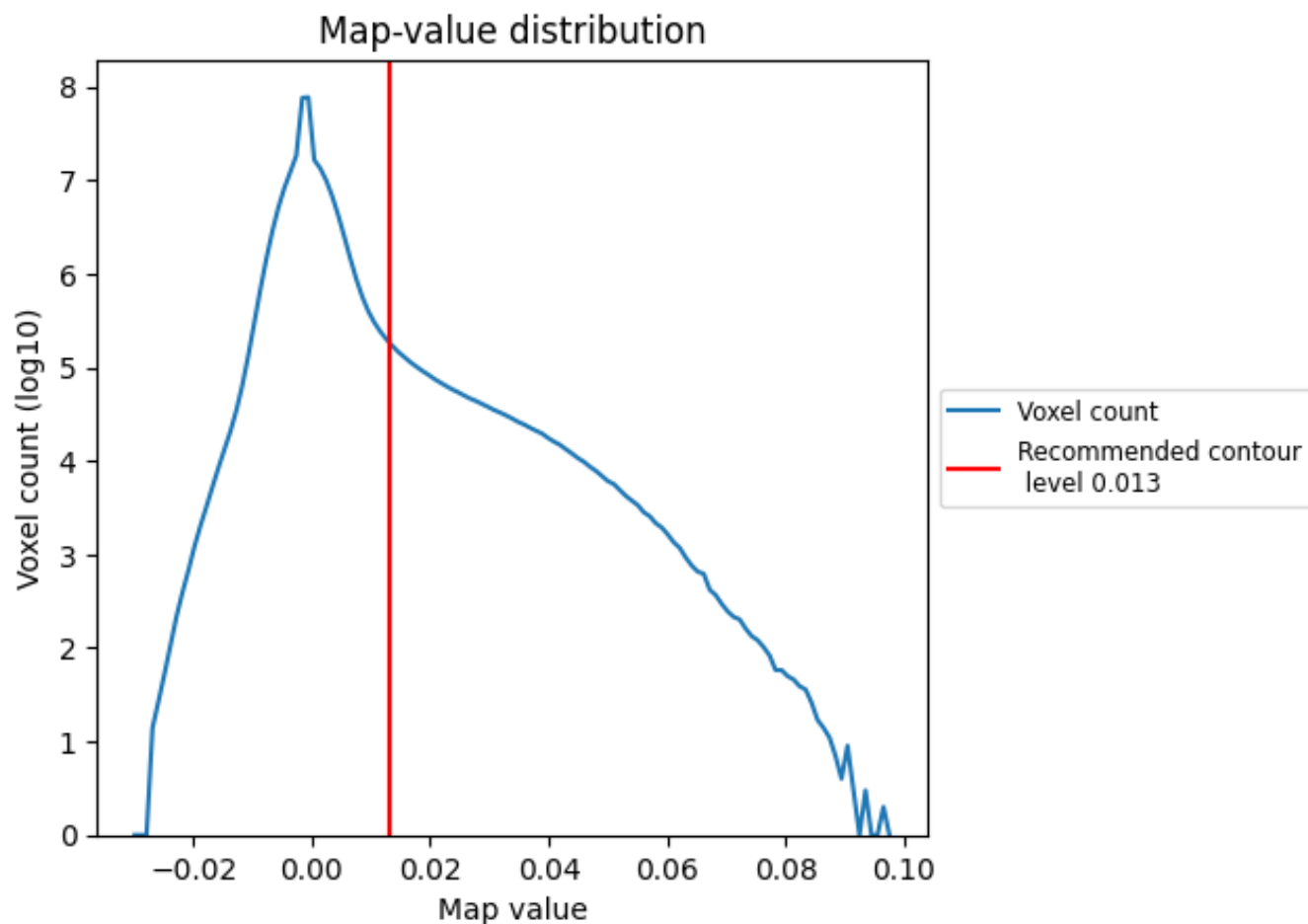
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

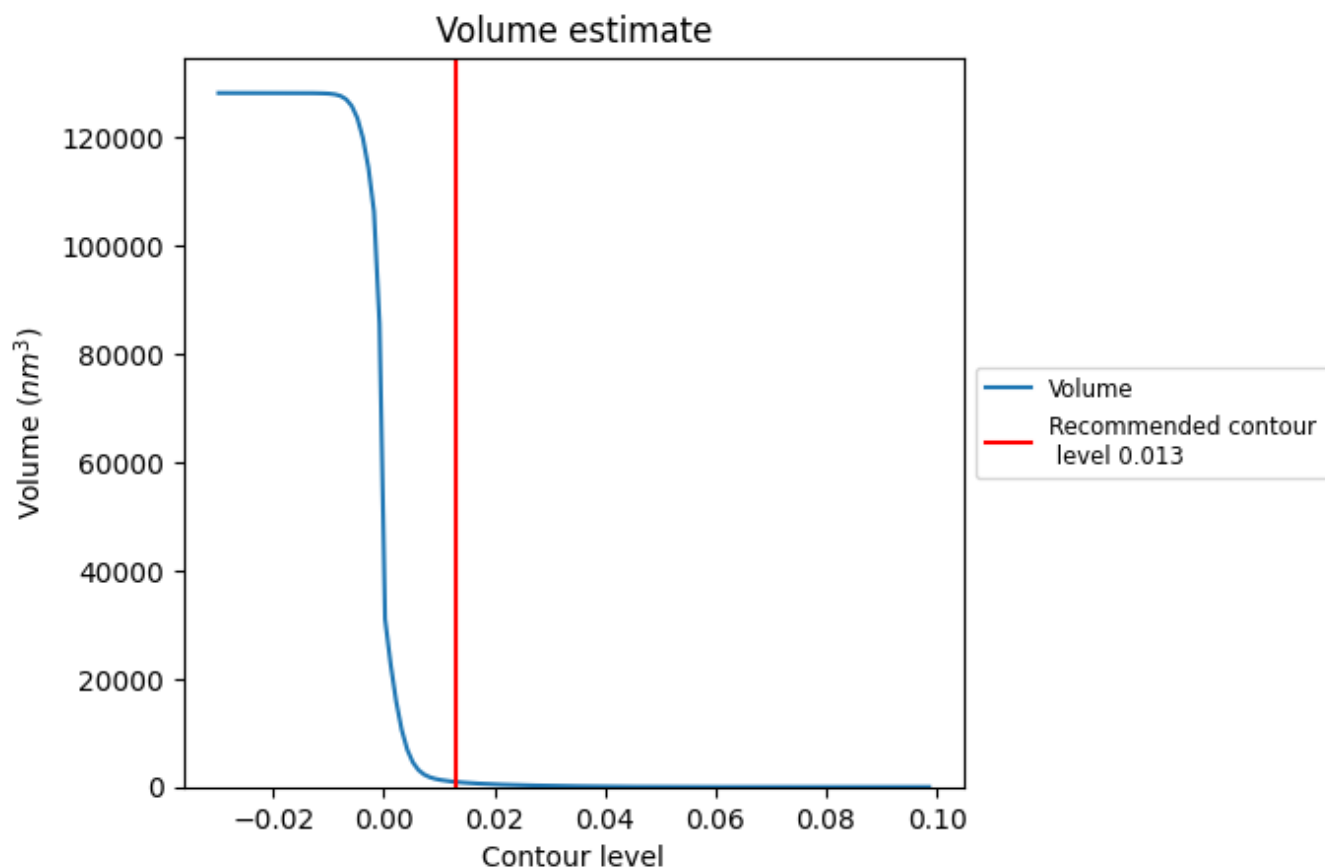
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

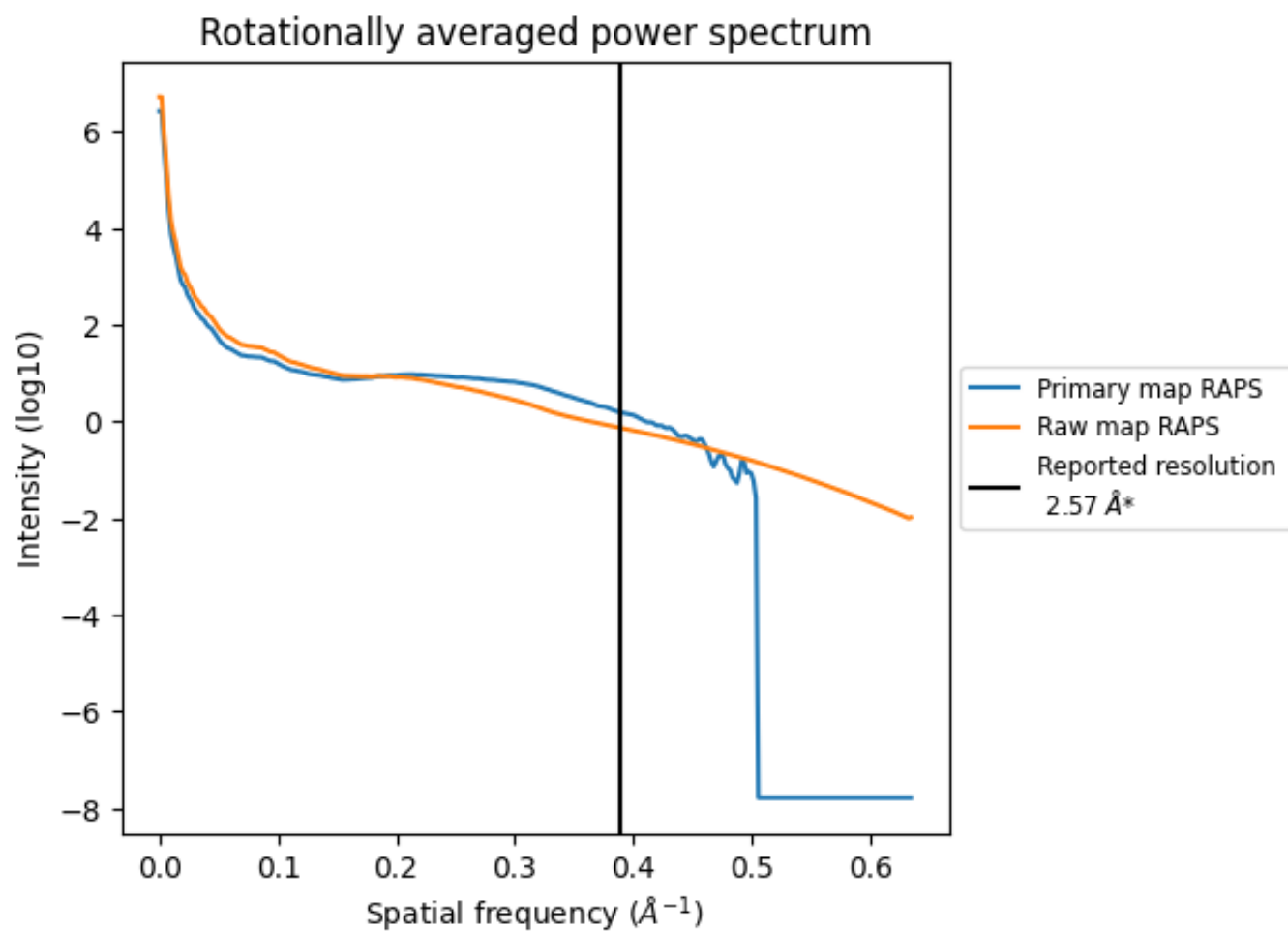
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 931 nm^3 ; this corresponds to an approximate mass of 841 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

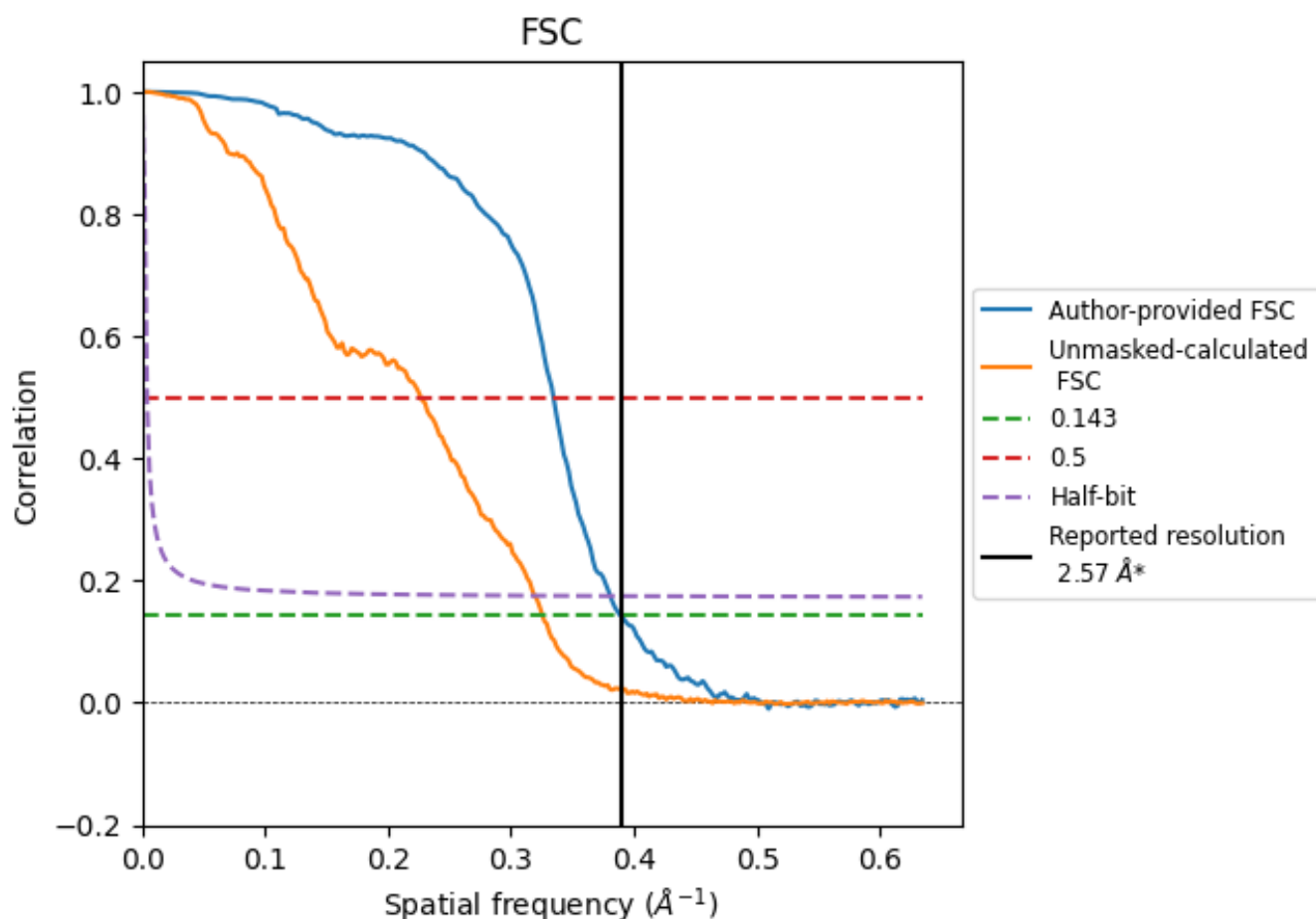


*Reported resolution corresponds to spatial frequency of $0.389 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.389 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

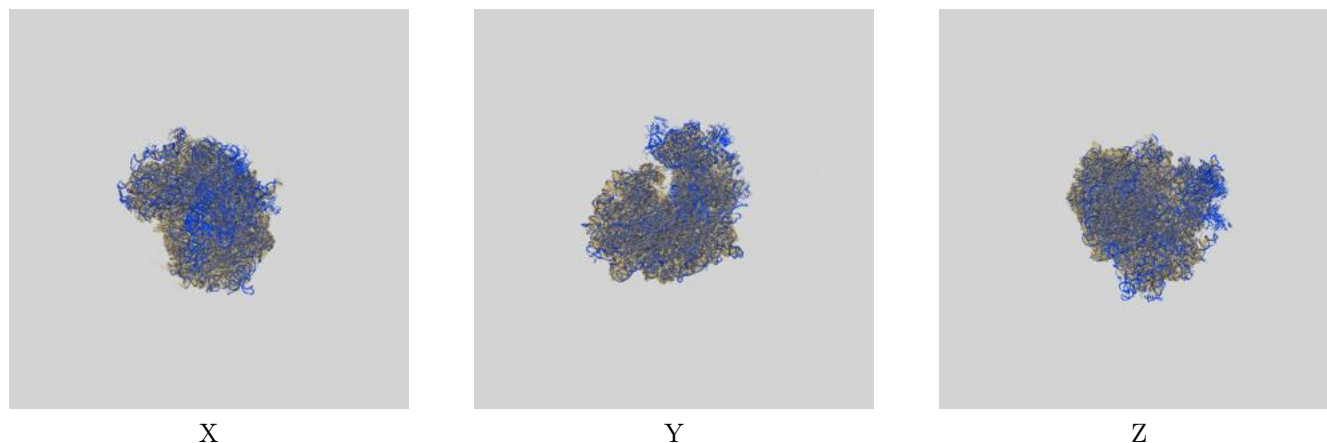
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	2.57	2.99	2.63
Unmasked-calculated*	3.07	4.41	3.13

*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 3.07 differs from the reported value 2.57 by more than 10 %

9 Map-model fit [i](#)

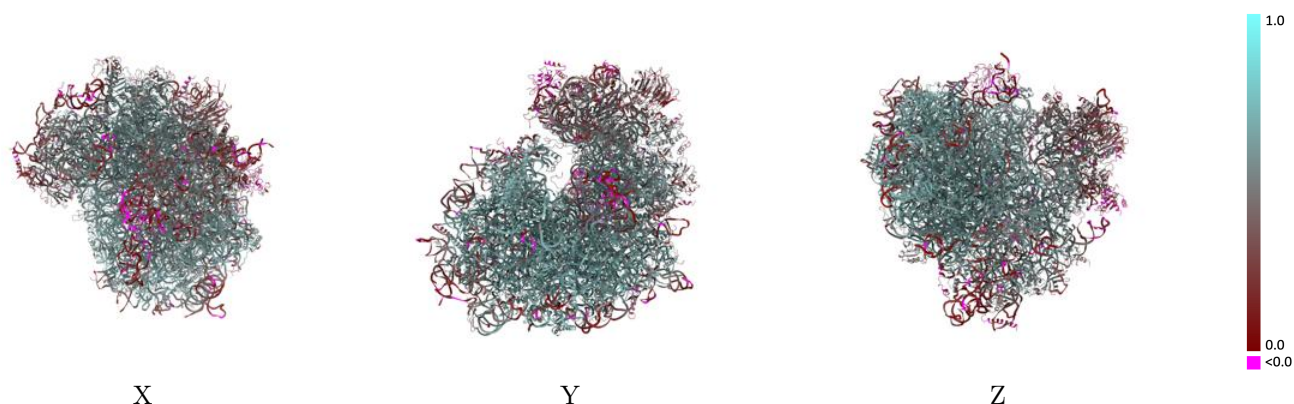
This section contains information regarding the fit between EMDB map EMD-35414 and PDB model 8IFE. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



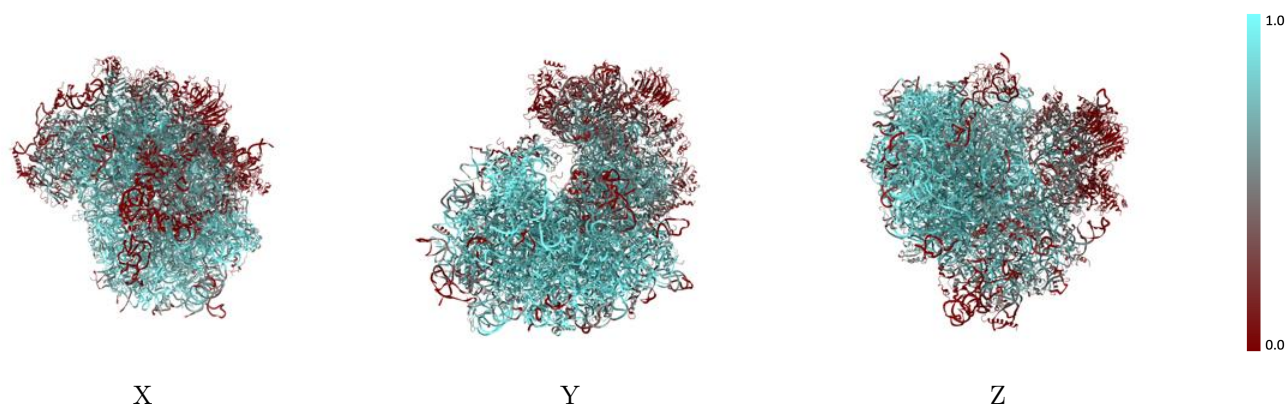
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



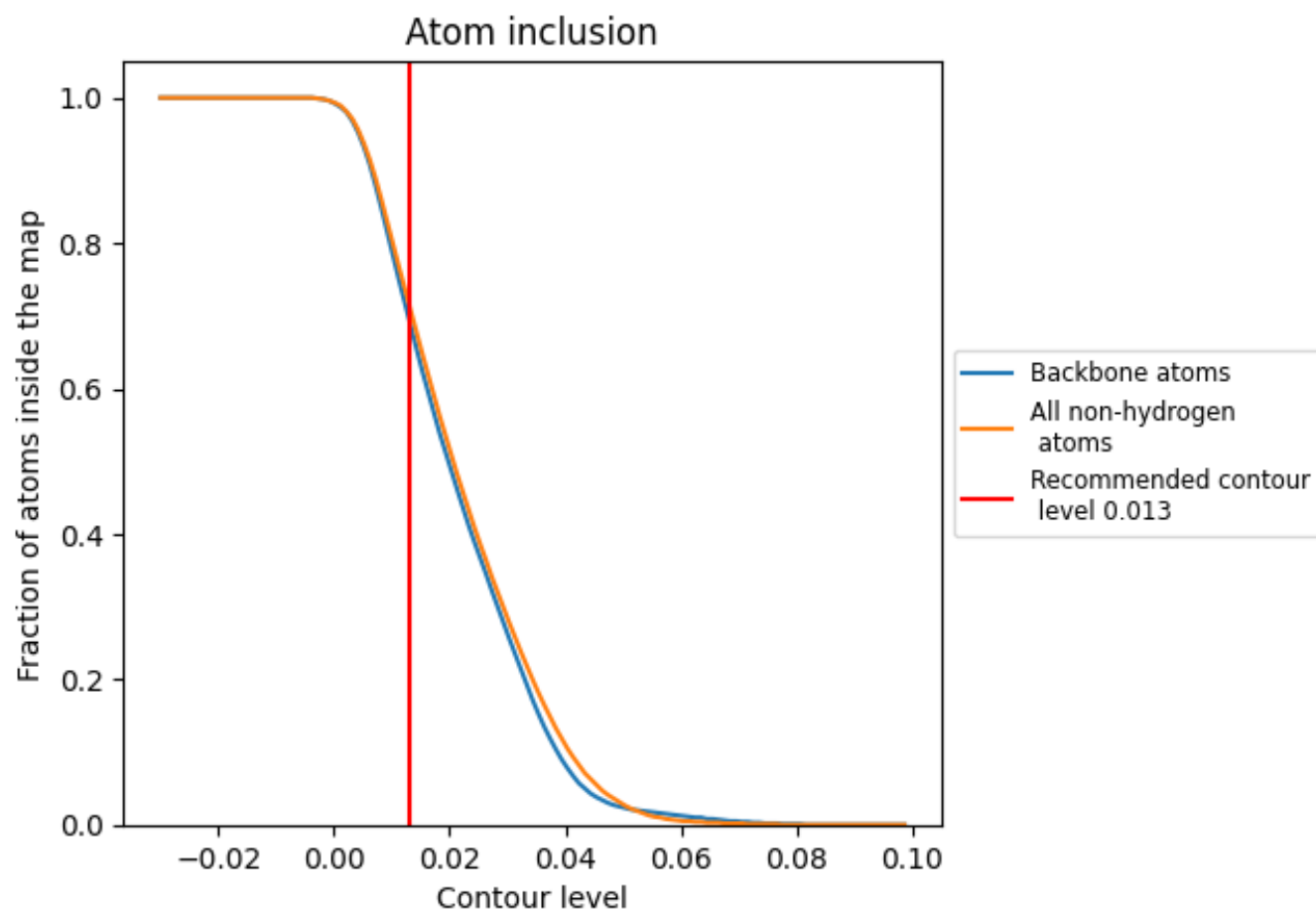
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 72% 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	 0.7160	 0.5300
1A	 0.8280	 0.5530
1B	 0.9500	 0.6200
1C	 0.9060	 0.6010
1D	 0.9320	 0.6580
1E	 0.8720	 0.6290
1F	 0.8930	 0.6350
1G	 0.8160	 0.5770
1H	 0.7630	 0.5590
20	 0.3210	 0.4190
21	 0.1650	 0.3550
2A	 0.9030	 0.6440
2B	 0.7550	 0.5620
2C	 0.8110	 0.6030
2D	 0.7030	 0.5700
2E	 0.6140	 0.5010
2F	 0.8340	 0.5990
2G	 0.8650	 0.6150
2H	 0.9540	 0.6680
2I	 0.9080	 0.6460
2J	 0.9150	 0.6550
2K	 0.9450	 0.6650
2L	 0.7650	 0.5820
2M	 0.9170	 0.6470
2N	 0.8520	 0.6210
2O	 0.5500	 0.4620
2P	 0.8770	 0.6410
2Q	 0.4250	 0.3940
2R	 0.8600	 0.6270
2S	 0.8660	 0.6270
2T	 0.8310	 0.6070
2U	 0.9320	 0.6590
2V	 0.6920	 0.5440
2W	 0.8110	 0.5930
2X	 0.8340	 0.6150



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
2Y	 0.9210	 0.6570
2Z	 0.9360	 0.6540
2a	 0.8510	 0.6190
2b	 0.8620	 0.6160
2c	 0.8350	 0.6110
2d	 0.9350	 0.6560
2e	 0.6820	 0.5600
2f	 0.8770	 0.6350
2g	 0.8420	 0.6170
2h	 0.8570	 0.6520
2i	 0.8190	 0.6130
2j	 0.8550	 0.6350
2k	 0.9150	 0.6320
2l	 0.0210	 0.1270
2m	 0.6600	 0.4670
2n	 0.3450	 0.5060
2o	 0.6210	 0.5470
2p	 0.1420	 0.3750
2q	 0.5870	 0.5320
2r	 0.3420	 0.4270
2s	 0.3190	 0.4360
2t	 0.6140	 0.5280
2u	 0.0460	 0.2860
2v	 0.6770	 0.5640
2w	 0.0910	 0.3310
2x	 0.2890	 0.4220
2y	 0.1740	 0.3940
2z	 0.2380	 0.3770
3A	 0.3680	 0.5110
3B	 0.6490	 0.5610
3C	 0.6680	 0.5500
3D	 0.2920	 0.4060
3E	 0.2600	 0.4020
3F	 0.0340	 0.2940
3G	 0.6120	 0.5400
3H	 0.3580	 0.4010
3I	 0.5520	 0.5010
3J	 0.0000	 0.0340
3K	 0.6470	 0.5820
3L	 0.6790	 0.5550
3M	 0.7190	 0.5810
3N	 0.4720	 0.4480

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Chain	Atom inclusion	Q-score
3O	 0.1820	 0.2990
3P	 0.3470	 0.4800
3Q	 0.3690	 0.4350
3R	 0.0000	 0.0470