



Full wwPDB EM Validation Report ⓘ

Jun 9, 2024 – 04:03 AM JST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

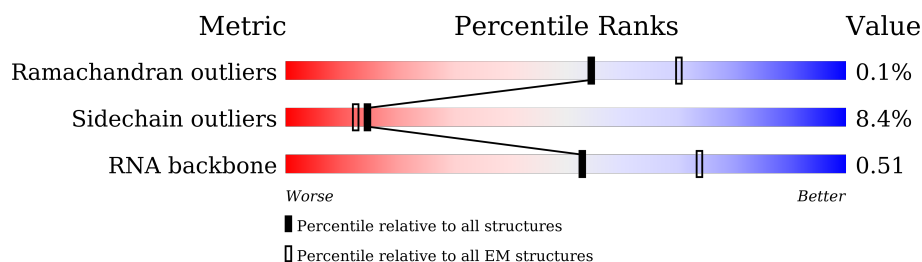
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.59 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
4	1D	257	
5	1E	403	
6	1F	427	
7	1G	297	
8	1H	288	

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Mol	Chain	Length	Quality of chain
9	2A	248	
10	2B	266	
11	2C	192	
12	2D	214	
13	2E	178	
14	2F	211	
15	2G	215	
16	2H	204	
17	2I	203	
18	2J	184	
19	2K	188	
20	2L	196	
21	2M	176	
22	2N	160	
23	2O	128	
24	2P	140	
25	2Q	157	
26	2R	156	
27	2S	145	
28	2T	136	
29	2U	148	
30	2V	159	
31	2W	115	
32	2X	125	
33	2Y	135	

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Mol	Chain	Length	Quality of chain
34	2Z	110	95% 5% .
35	2a	117	9% 93% . .
36	2b	123	. 91% 8% .
37	2c	105	. 90% 8% .
38	2d	97	84% 5% 11%
39	2e	70	7% 90% 9% .
40	2f	51	94% . .
41	2g	128	. 39% . 59%
42	2h	25	84% 12% .
43	2i	106	7% 94% 5% .
44	2j	92	. 93% 5% .
45	2k	137	. 85% 7% 9%
46	2l	217	99% 88% 12%
47	2m	1869	28% 66% 26% 7%
48	2n	295	62% 67% 8% 25%
49	2o	264	17% 75% 6% 19%
50	2p	243	92% 82% 11% 7%
51	2q	263	28% 94% 6%
52	2r	204	79% 85% 7% 7%
53	2s	194	68% 89% 7% .
54	2t	208	27% 93% 6% .
55	2u	165	59% 55% . 41%
56	2v	158	23% 87% 9% .
57	2w	145	88% 83% 5% 12%
58	2x	146	86% 89% 8% .

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Mol	Chain	Length	Quality of chain
59	2y	135	<div>95%</div> <div>89% 11%</div>
60	2z	152	<div>84%</div> <div>91% 5% 5%</div>
61	20	145	<div>85%</div> <div>90% 8%</div>
62	21	119	<div>79%</div> <div>76% 10% 13%</div>
63	3A	83	<div>65%</div> <div>86% 14%</div>
64	3B	143	<div>15%</div> <div>87% 12%</div>
65	3C	115	<div>20%</div> <div>81% 8% 11%</div>
66	3D	69	<div>70%</div> <div>88% 7%</div>
67	3E	56	<div>79%</div> <div>88% 11%</div>
68	3F	317	<div>99%</div> <div>90% 9%</div>
69	3G	293	<div>20%</div> <div>70% 6% 24%</div>
70	3H	249	<div>61%</div> <div>86% 9% 5%</div>
71	3I	194	<div>36%</div> <div>89% 7% 5%</div>
72	3J	132	<div>92%</div> <div>88% 5% 8%</div>
73	3K	151	<div>25%</div> <div>91% 8%</div>
74	3L	151	<div>19%</div> <div>82% 11% 7%</div>
75	3M	130	<div>8%</div> <div>90% 9%</div>
76	3N	133	<div>50%</div> <div>89% 10%</div>
77	3O	125	<div>57%</div> <div>50% 10% 40%</div>
78	3P	84	<div>68%</div> <div>87% 12%</div>
79	3Q	59	<div>54%</div> <div>81% 17%</div>
80	3R	156	<div>43%</div> <div>40% 57%</div>

2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 218821 atoms, of which 888 are hydrogens and 0 are deuteriums.

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 5 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

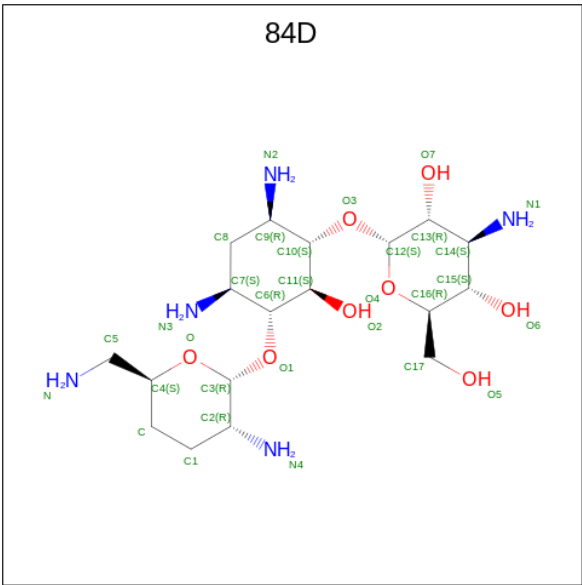
- Molecule 79 is a protein called 40S ribosomal protein S30.

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

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

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

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



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

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

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

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

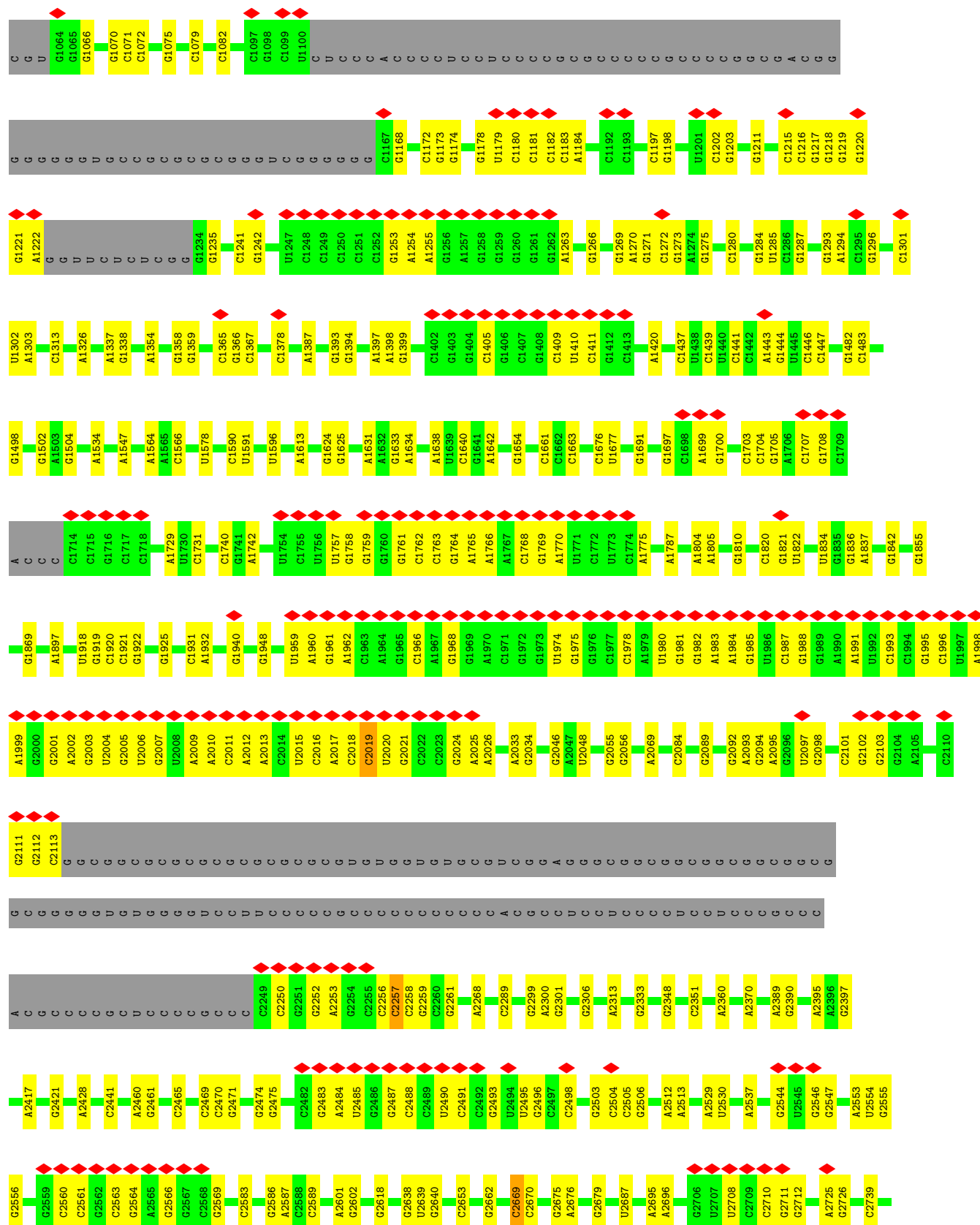
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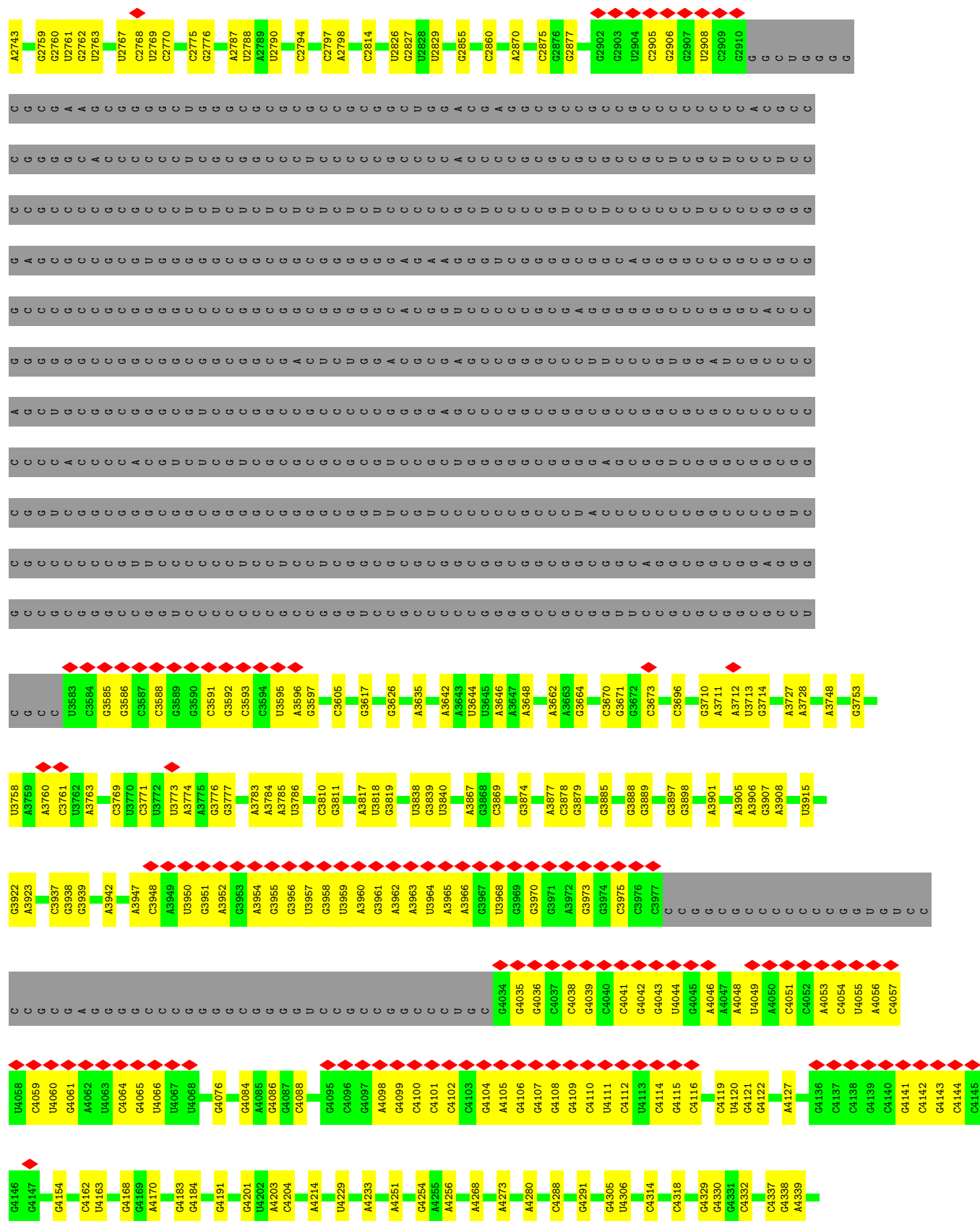
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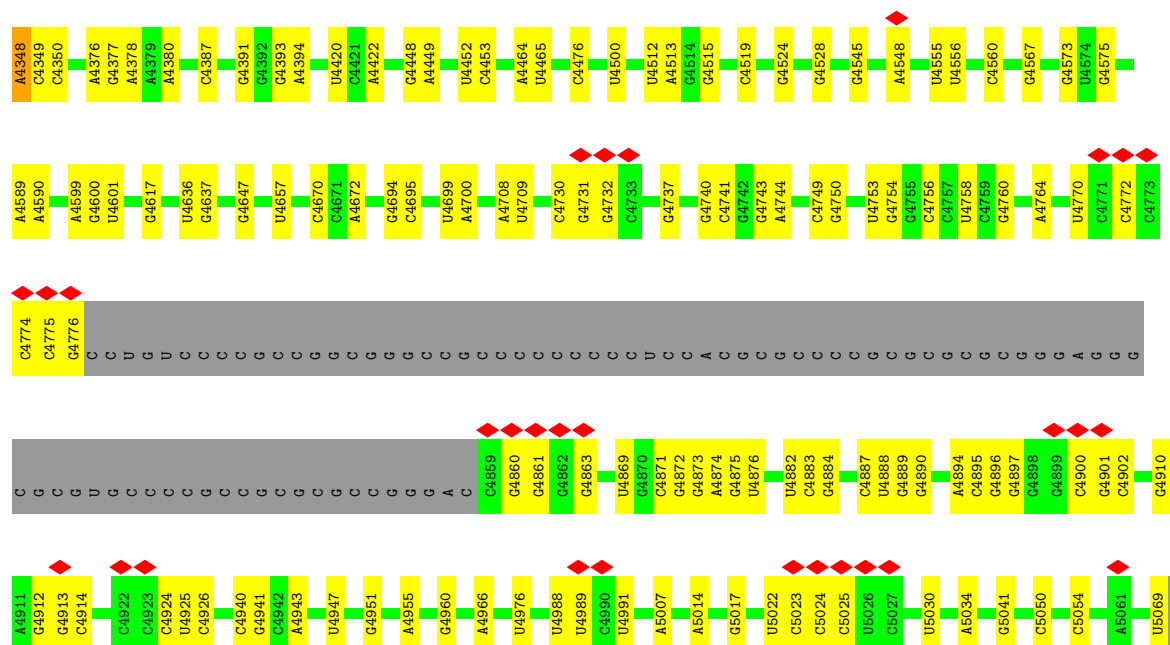
Mol	Chain	Residues	Atoms		AltConf
82	2V	1	Total 1	Mg 1	0
82	2Y	1	Total 1	Mg 1	0
82	2Z	1	Total 1	Mg 1	0
82	2a	1	Total 1	Mg 1	0
82	2d	1	Total 1	Mg 1	0
82	2m	105	Total 105	Mg 105	0
82	2o	1	Total 1	Mg 1	0
82	3H	1	Total 1	Mg 1	0
82	3K	1	Total 1	Mg 1	0
82	3L	1	Total 1	Mg 1	0

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

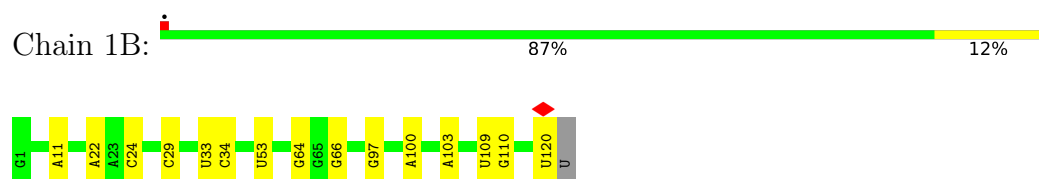
Mol	Chain	Residues	Atoms		AltConf
83	2d	1	Total 1	Zn 1	0
83	2g	1	Total 1	Zn 1	0
83	2j	1	Total 1	Zn 1	0
83	3C	1	Total 1	Zn 1	0



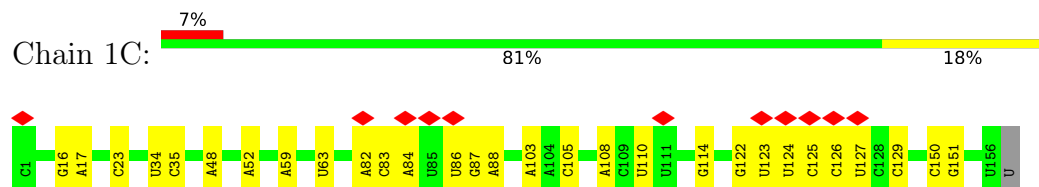




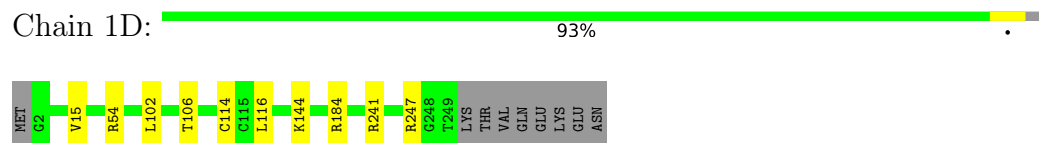
- Molecule 2: 5S ribosomal RNA



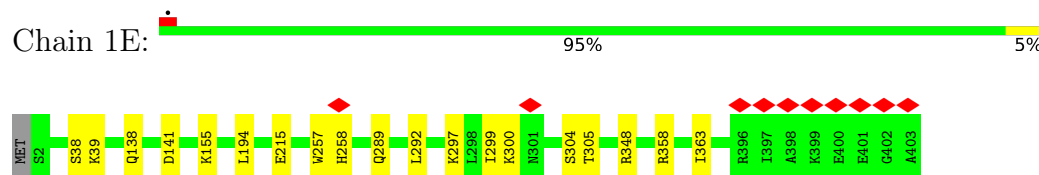
- Molecule 3: 5.8S ribosomal RNA



- Molecule 4: 60S ribosomal protein L8

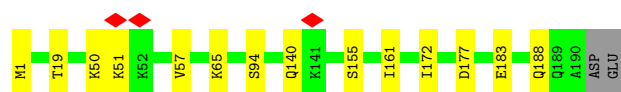


- Molecule 5: 60S ribosomal protein L3

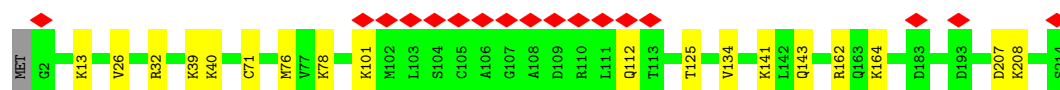


- Molecule 6: 60S ribosomal protein L4

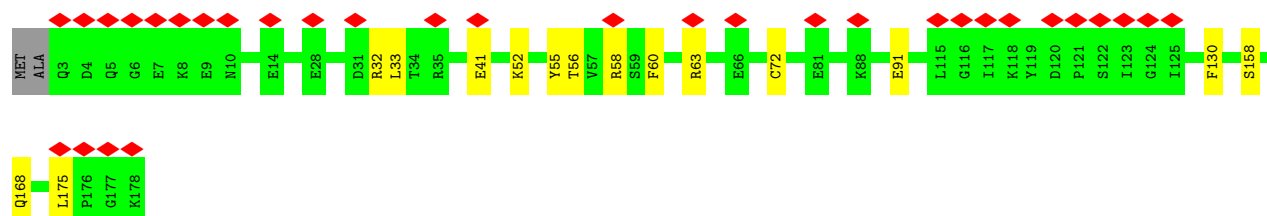




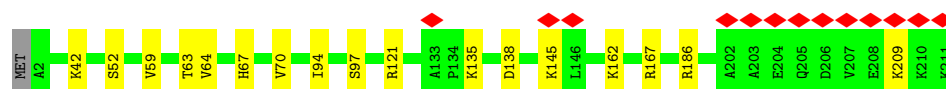
- Molecule 12: 60S ribosomal protein L10-like



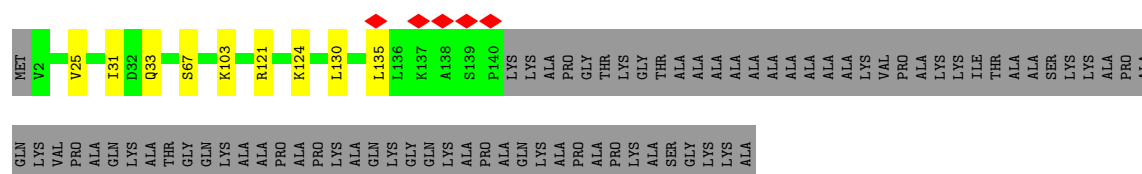
- Molecule 13: 60S ribosomal protein L11



- Molecule 14: 60S ribosomal protein L13



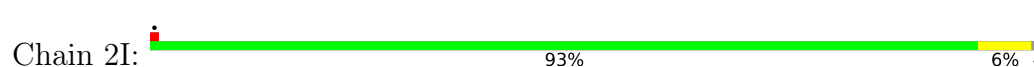
- Molecule 15: 60S ribosomal protein L14



- Molecule 16: 60S ribosomal protein L15

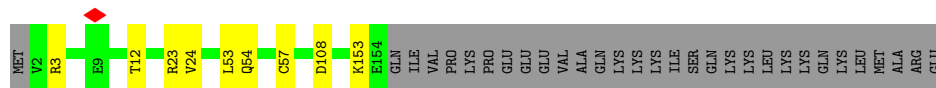
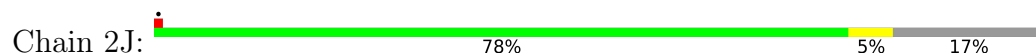


- Molecule 17: 60S ribosomal protein L13a





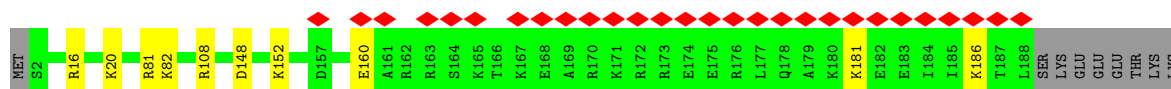
- Molecule 18: 60S ribosomal protein L17



- Molecule 19: 60S ribosomal protein L18



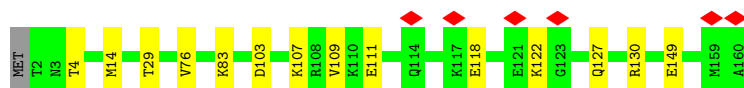
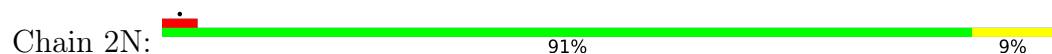
- Molecule 20: 60S ribosomal protein L19



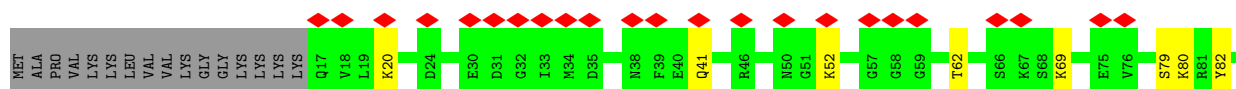
- Molecule 21: 60S ribosomal protein L18a

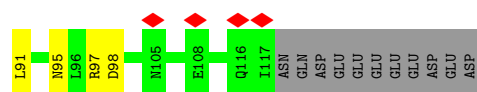


- Molecule 22: 60S ribosomal protein L21

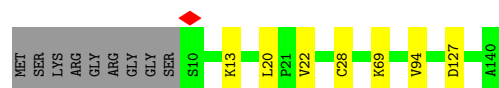
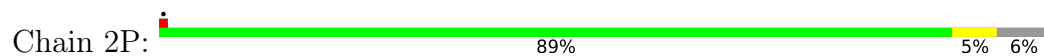


- Molecule 23: 60S ribosomal protein L22

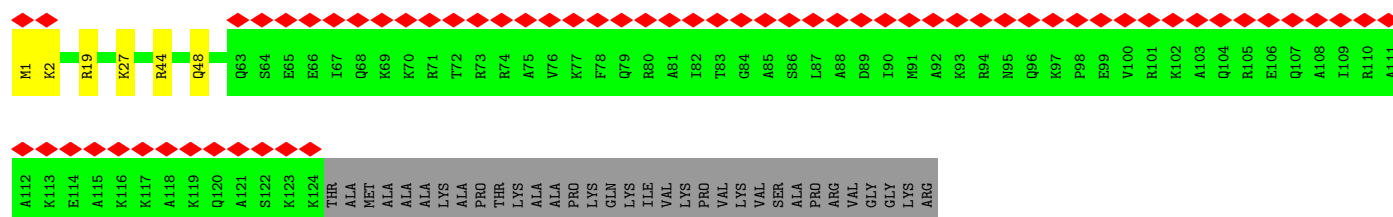
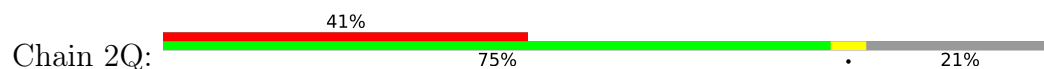




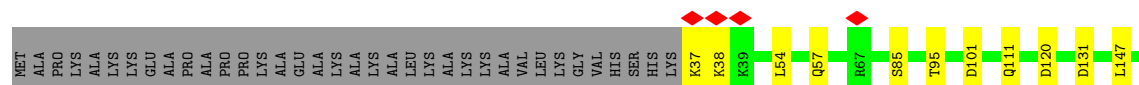
- Molecule 24: 60S ribosomal protein L23



- Molecule 25: 60S ribosomal protein L24



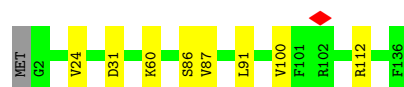
- Molecule 26: 60S ribosomal protein L23a



- Molecule 27: 60S ribosomal protein L26

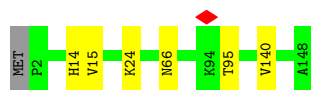


- Molecule 28: 60S ribosomal protein L27



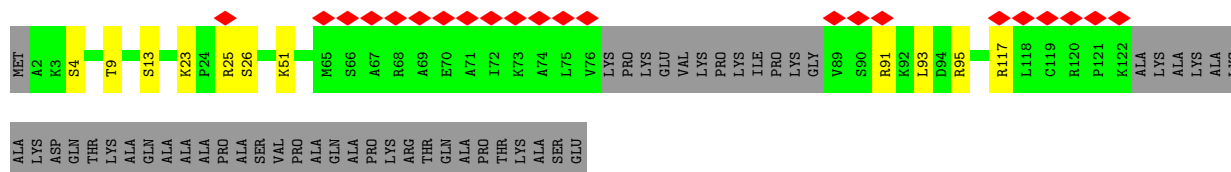
- Molecule 29: 60S ribosomal protein L27a

Chain 2U:  95% ..




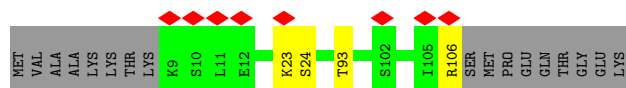
- Molecule 30: 60S ribosomal protein L29

Chain 2V:  14% 62% 7% 31%




- Molecule 31: 60S ribosomal protein L30

Chain 2W:  7% 82% . 15%



- Molecule 32: 60S ribosomal protein L31

Chain 2X:  80% 6% 14%



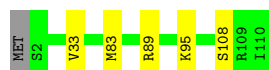
- Molecule 33: 60S ribosomal protein L32

Chain 2Y:  90% 5% 5%



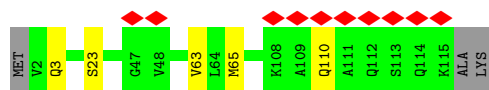
- Molecule 34: 60S ribosomal protein L35a

Chain 2Z:  95% 5% .

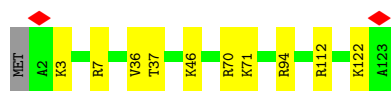


- Molecule 35: 60S ribosomal protein L34

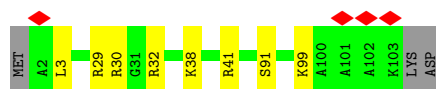
Chain 2a:  9% 93% . .



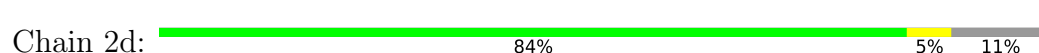
- Molecule 36: 60S ribosomal protein L35



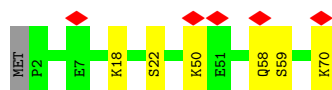
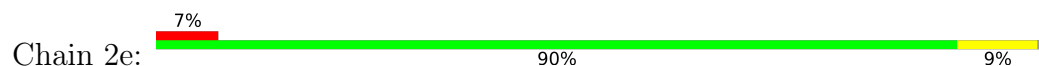
- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37



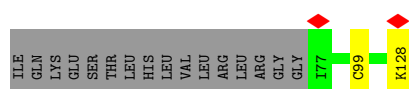
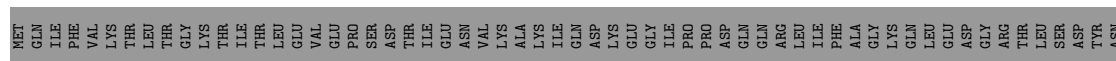
- Molecule 39: 60S ribosomal protein L38




- Molecule 40: 60S ribosomal protein L39



- Molecule 41: Large ribosomal subunit protein eL40



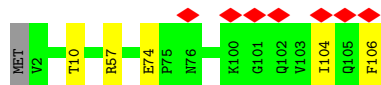
- Molecule 42: 60S ribosomal protein L41

Chain 2h:  84% 12%



- Molecule 43: 60S ribosomal protein L36a

Chain 2i:  7% 94% 5%




- Molecule 44: 60S ribosomal protein L37a

Chain 2j:  93% 5%

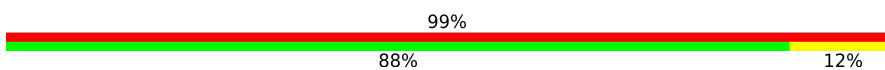


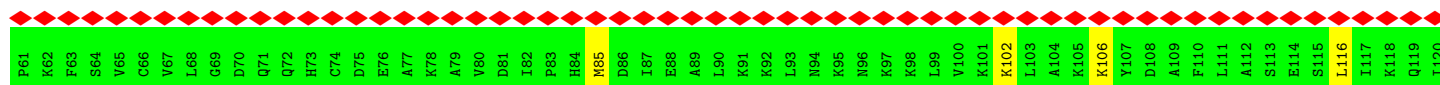
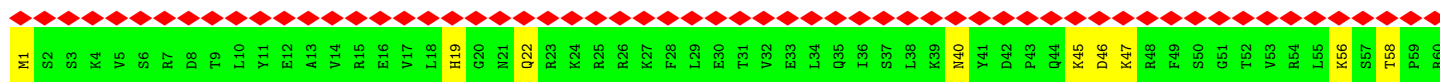
- Molecule 45: 60S ribosomal protein L28

Chain 2k:  85% 7% 9%

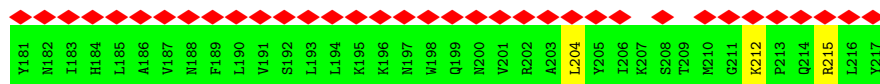


- Molecule 46: 60S ribosomal protein L10a

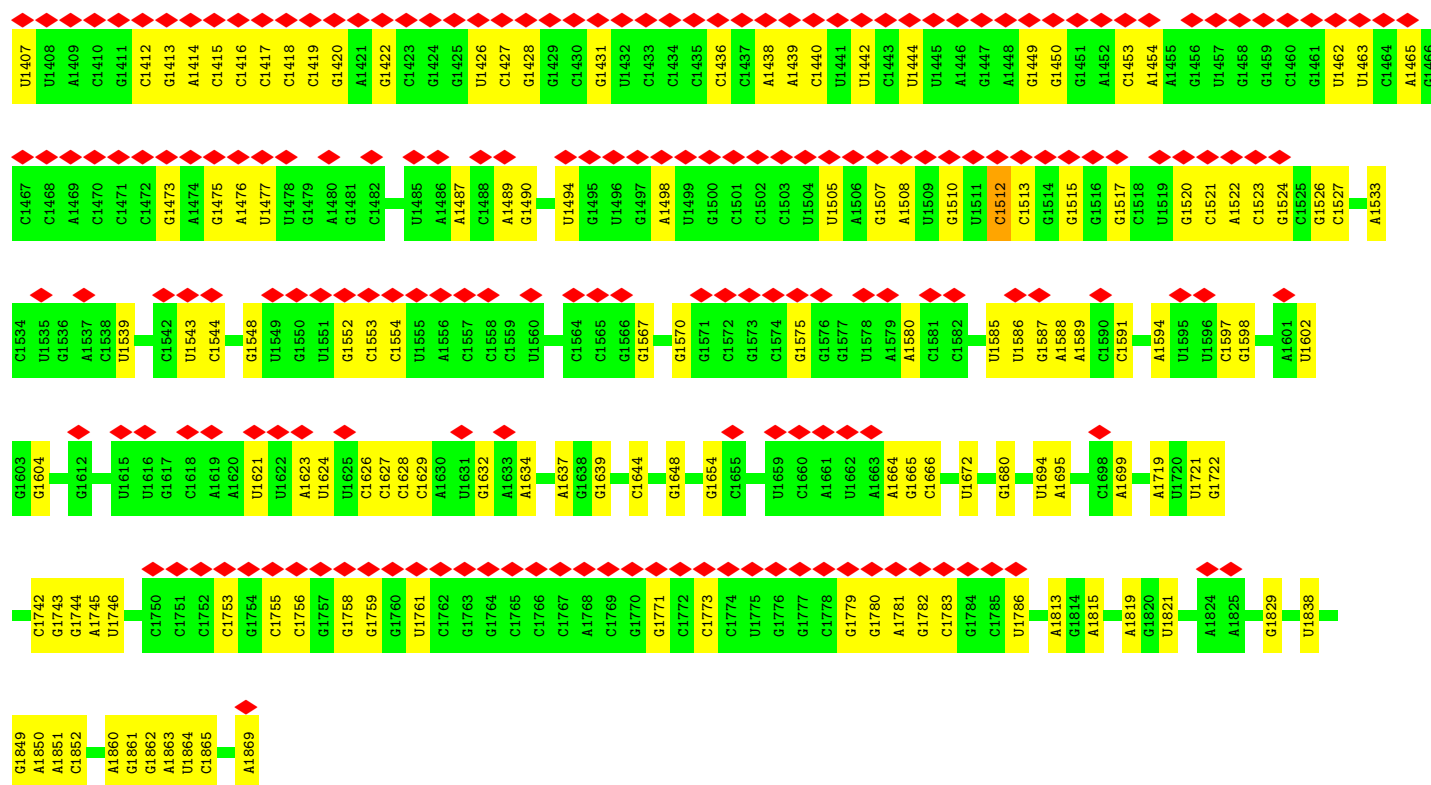
Chain 2l:  99% 88% 12%



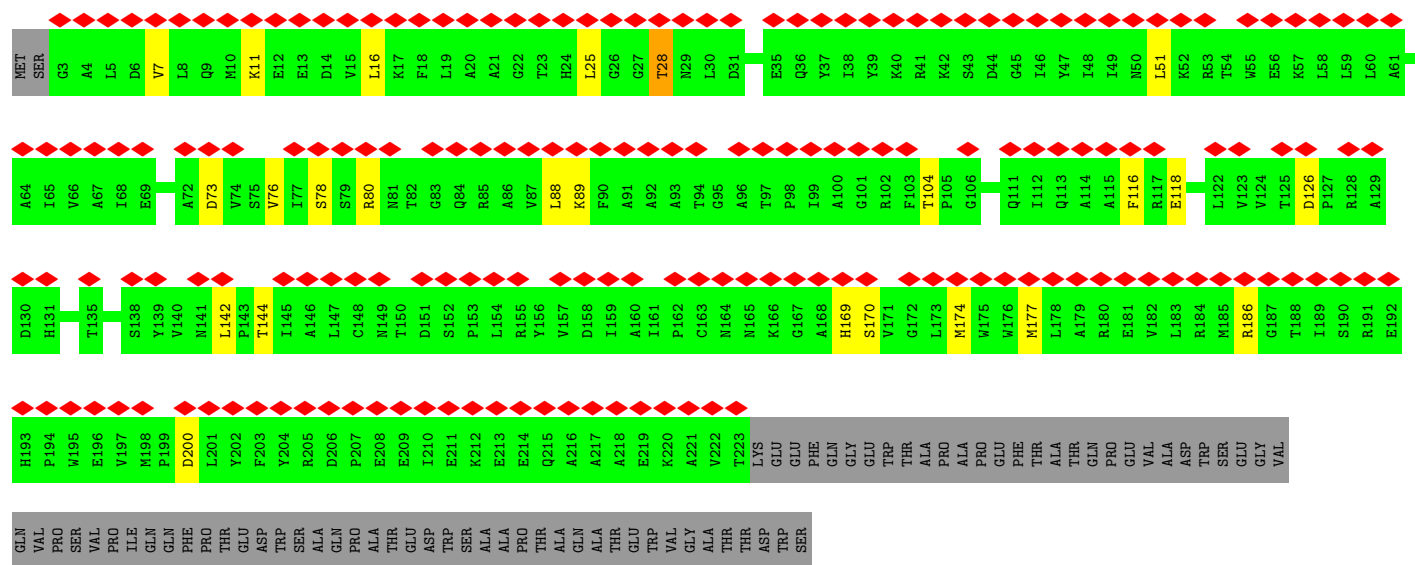
- Molecule 47: 18S ribosomal RNA



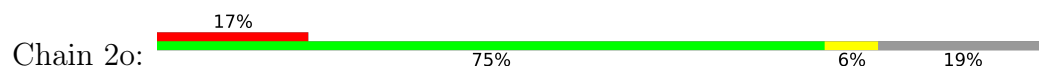


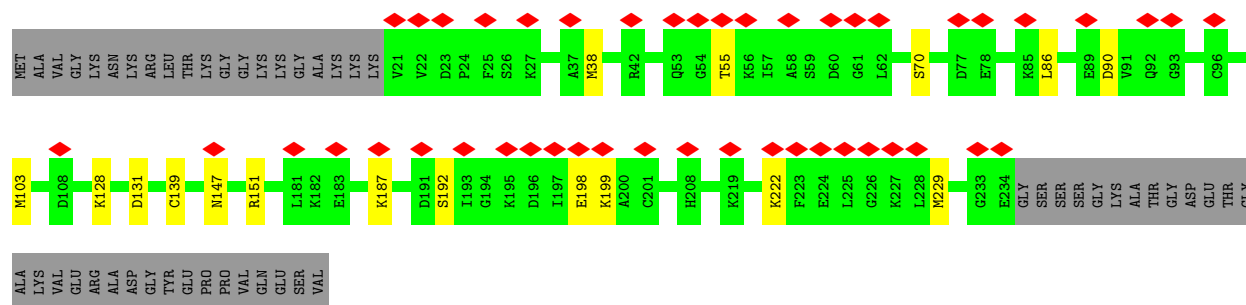


• Molecule 48: 40S ribosomal protein SA

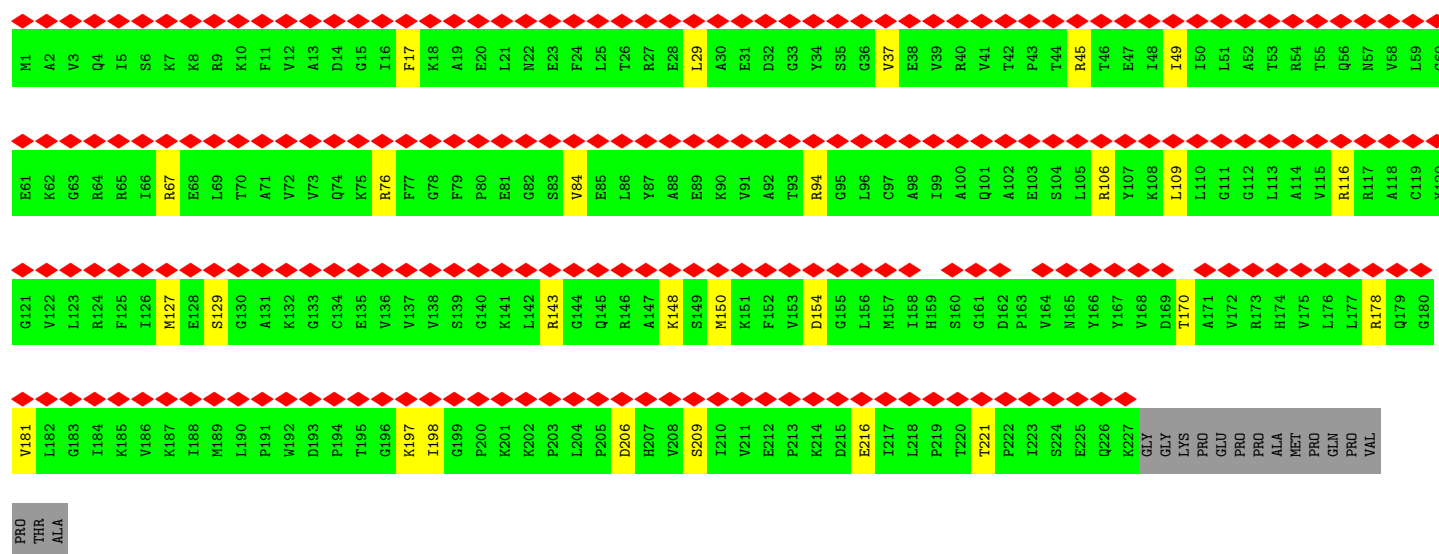
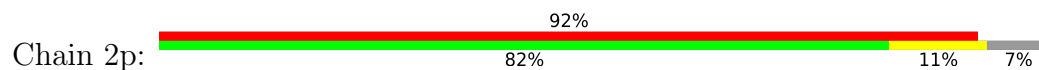


• Molecule 49: 40S ribosomal protein S3a

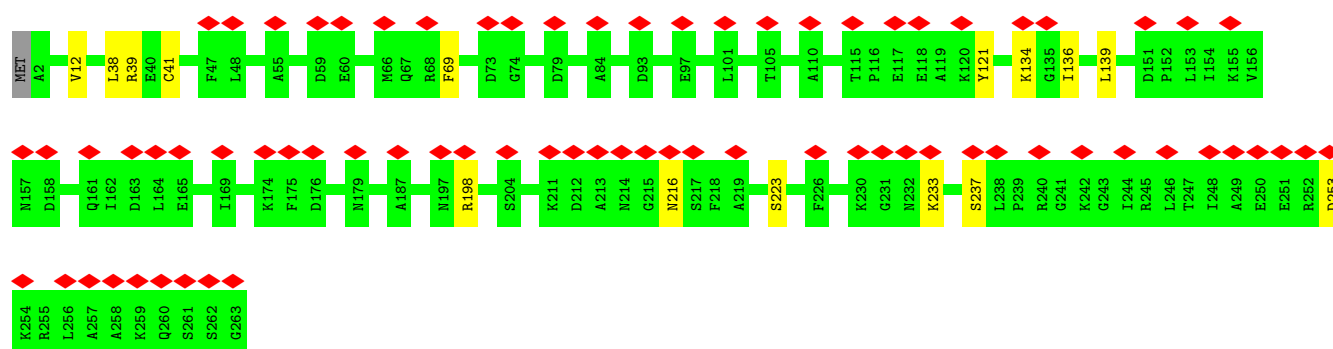




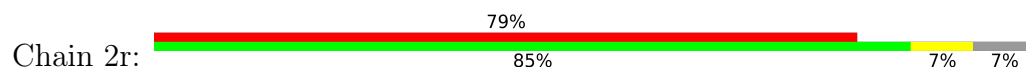
• Molecule 50: 40S ribosomal protein S3

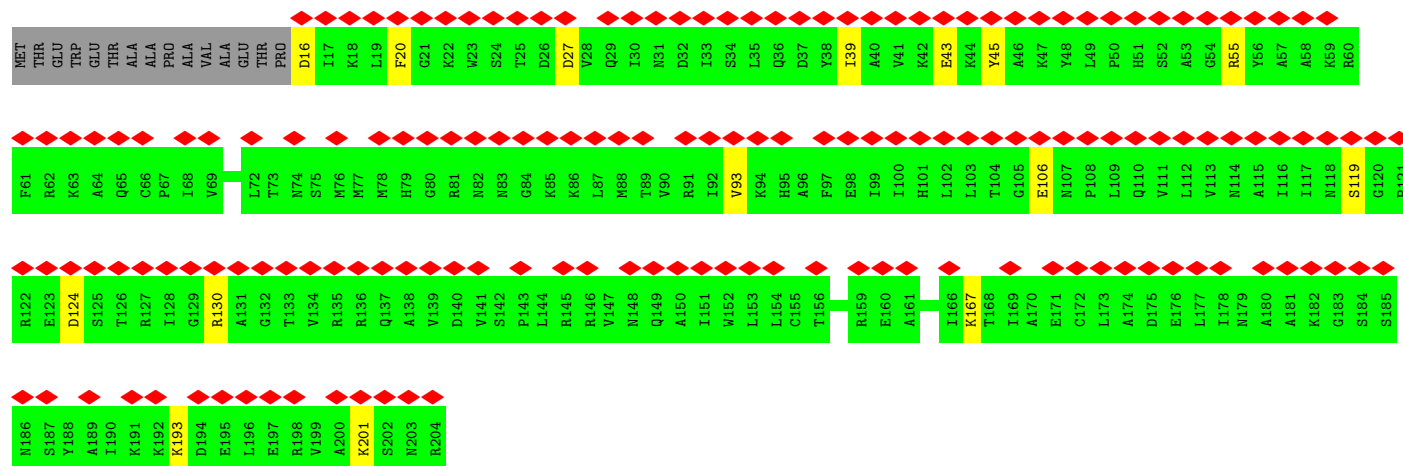


• Molecule 51: 40S ribosomal protein S4, X isoform

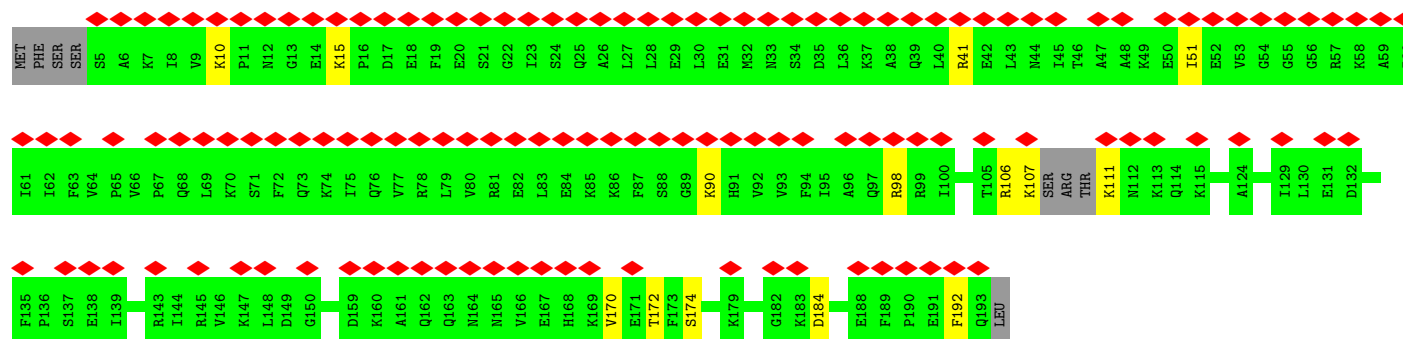
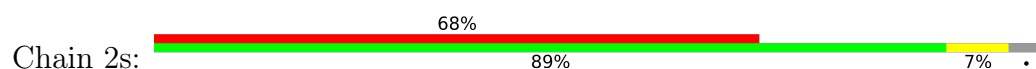


• Molecule 52: 40S ribosomal protein S5

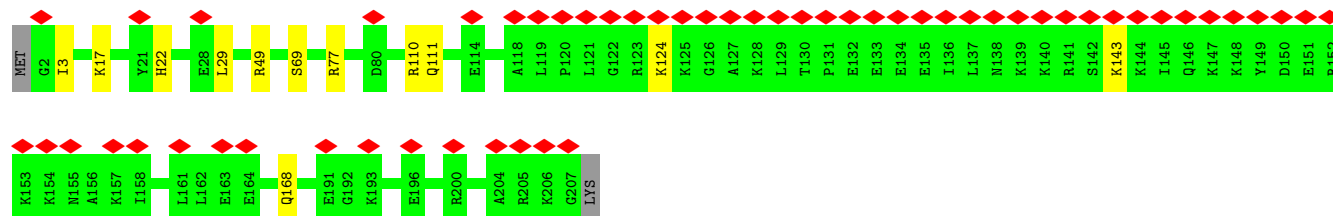




- Molecule 53: 40S ribosomal protein S7



- Molecule 54: 40S ribosomal protein S8

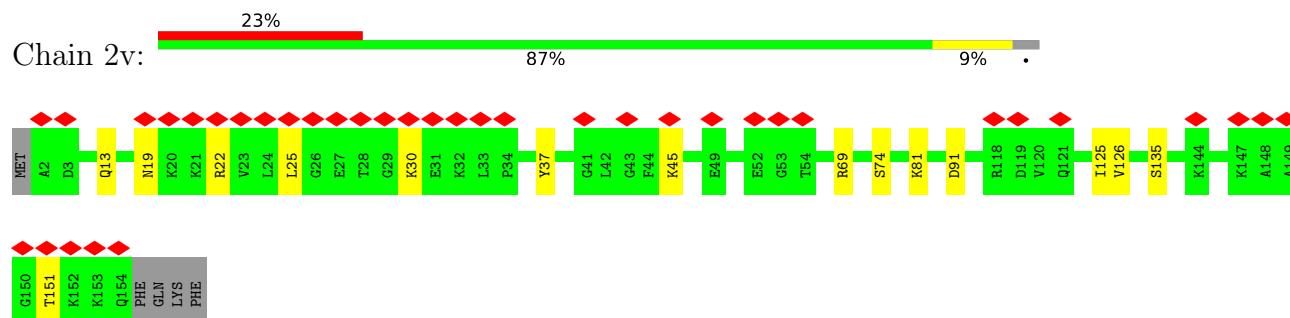


- Molecule 55: 40S ribosomal protein S10

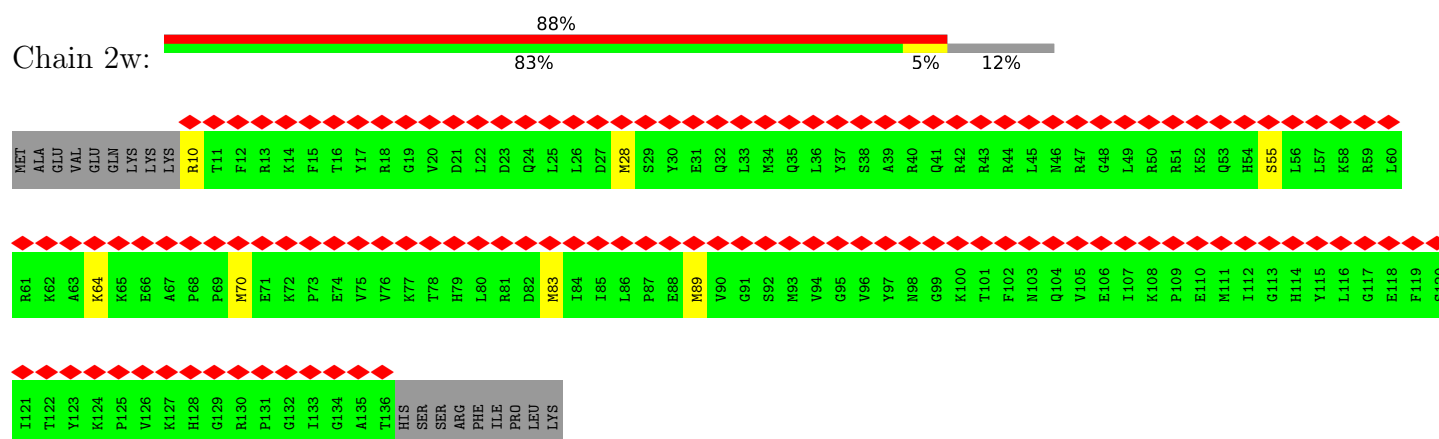


GLU
ALA
ASP
ARG
ASP
THR
TYR
ARG
ARG
SER
ALA
VAL
PRO
PRO
GLY
GLY
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LYS
ALA
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PRO
GLN

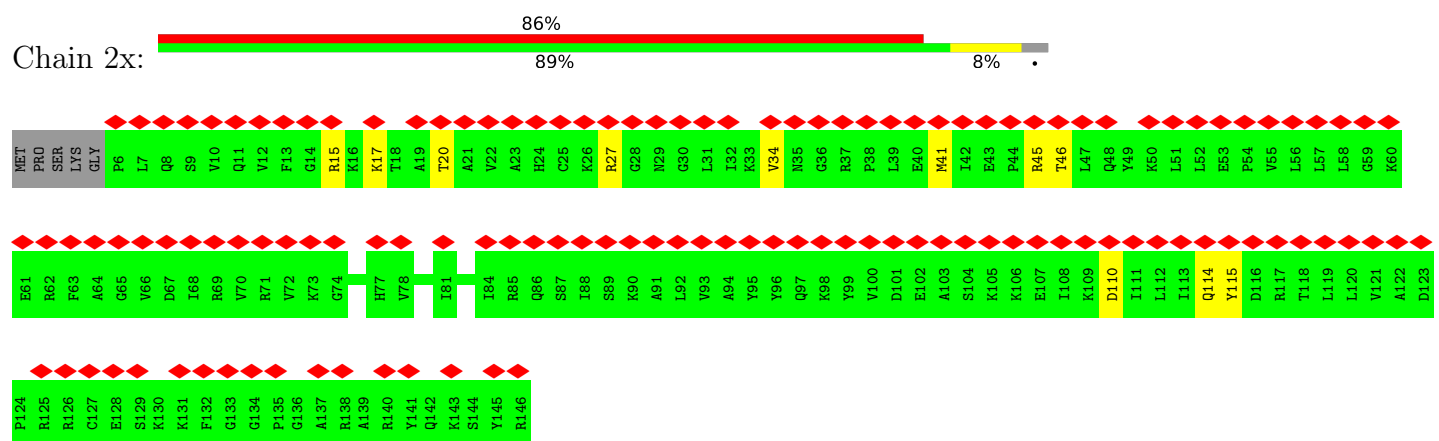
• Molecule 56: 40S ribosomal protein S11



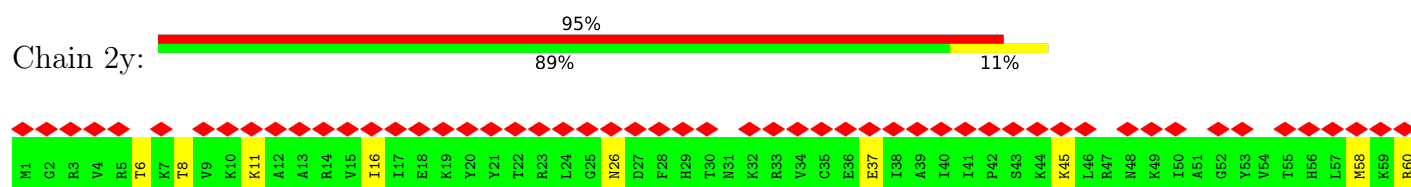
• Molecule 57: 40S ribosomal protein S15

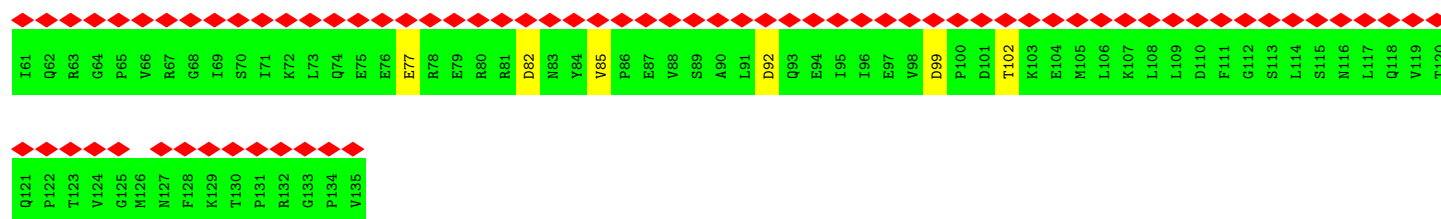


• Molecule 58: 40S ribosomal protein S16

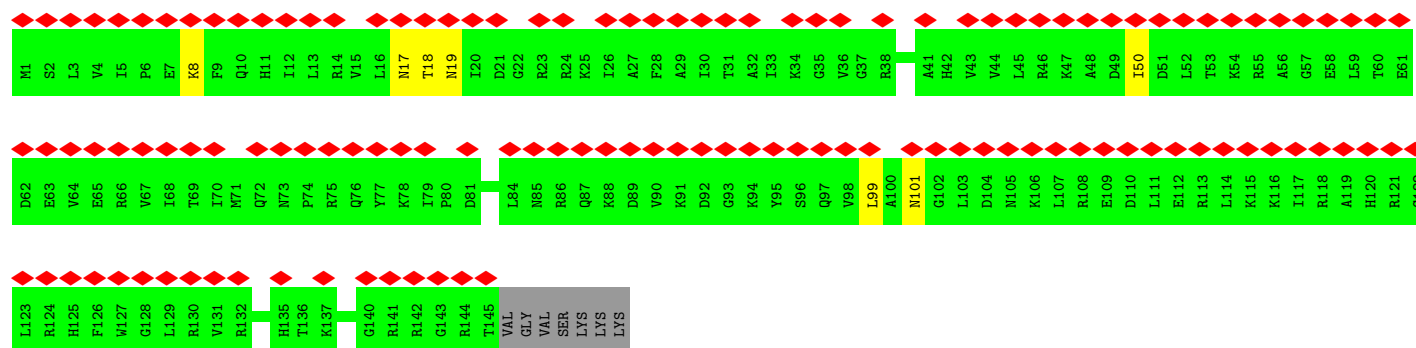
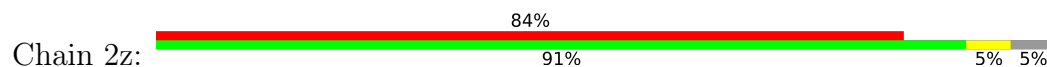


• Molecule 59: 40S ribosomal protein S17

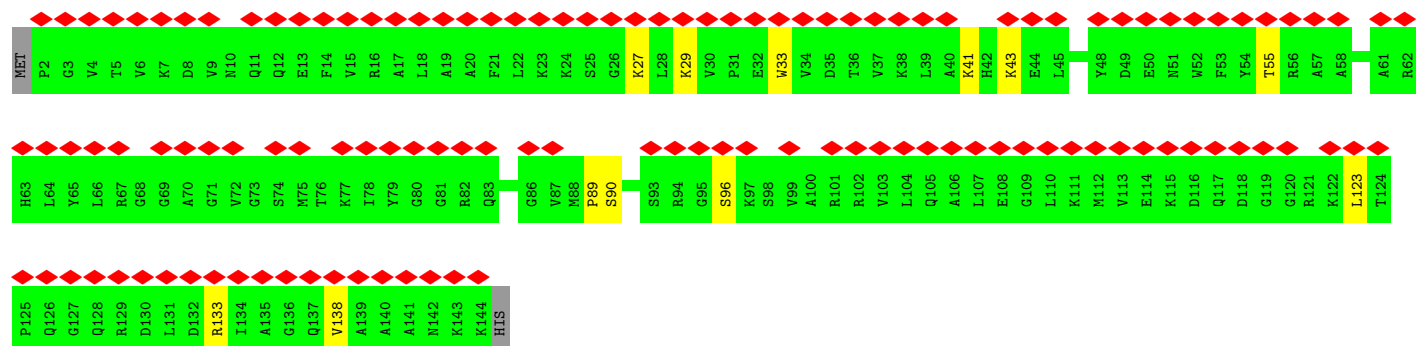
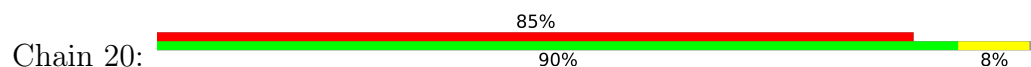




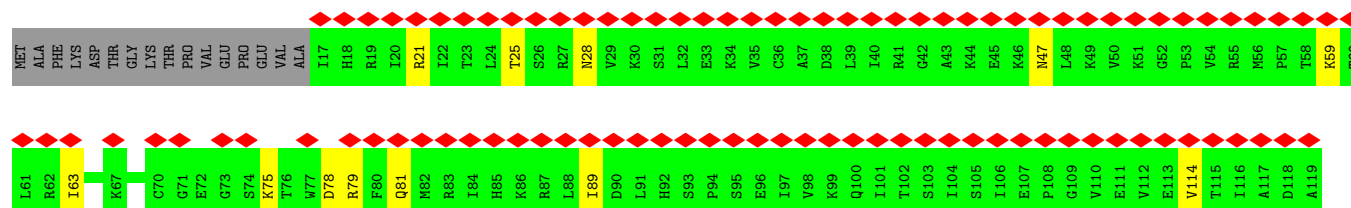
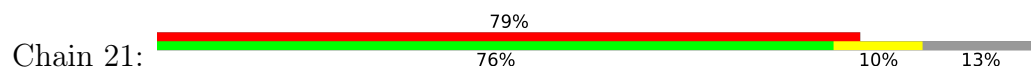
• Molecule 60: 40S ribosomal protein S18



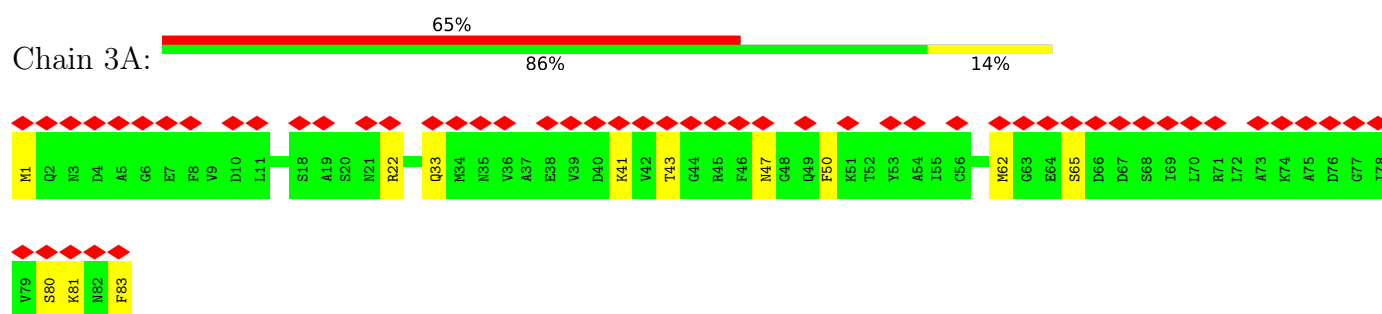
• Molecule 61: 40S ribosomal protein S19



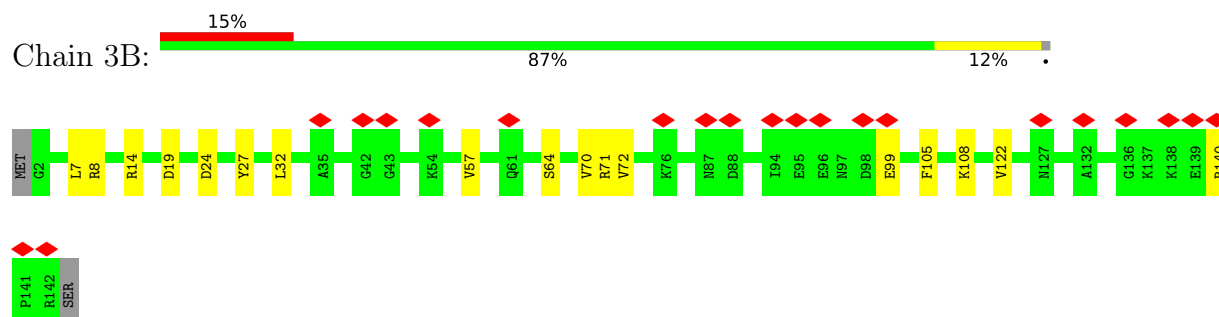
• Molecule 62: 40S ribosomal protein S20



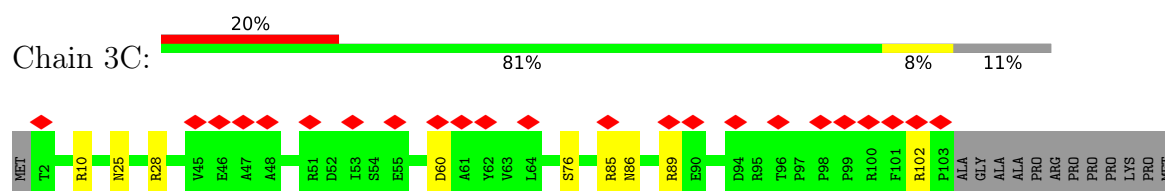
• Molecule 63: 40S ribosomal protein S21



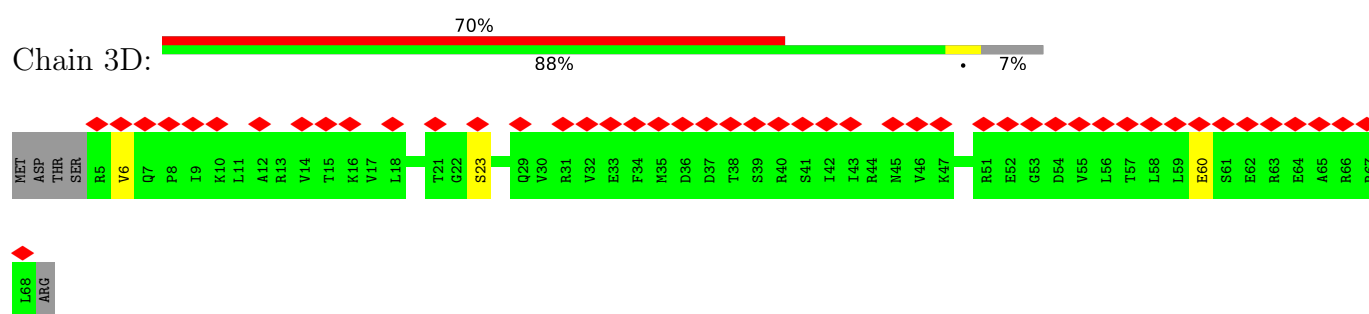
- Molecule 64: 40S ribosomal protein S23



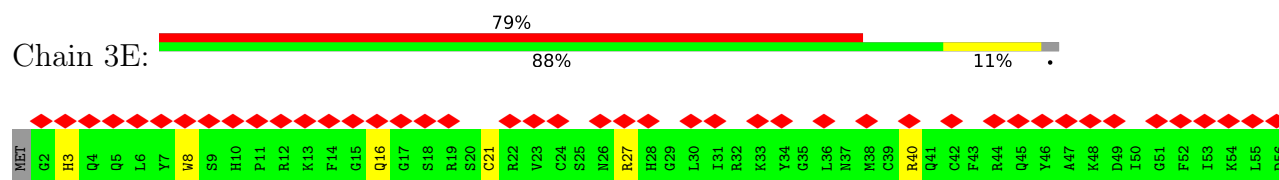
- Molecule 65: 40S ribosomal protein S26



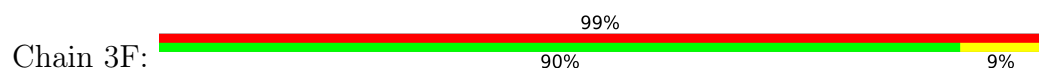
- Molecule 66: 40S ribosomal protein S28

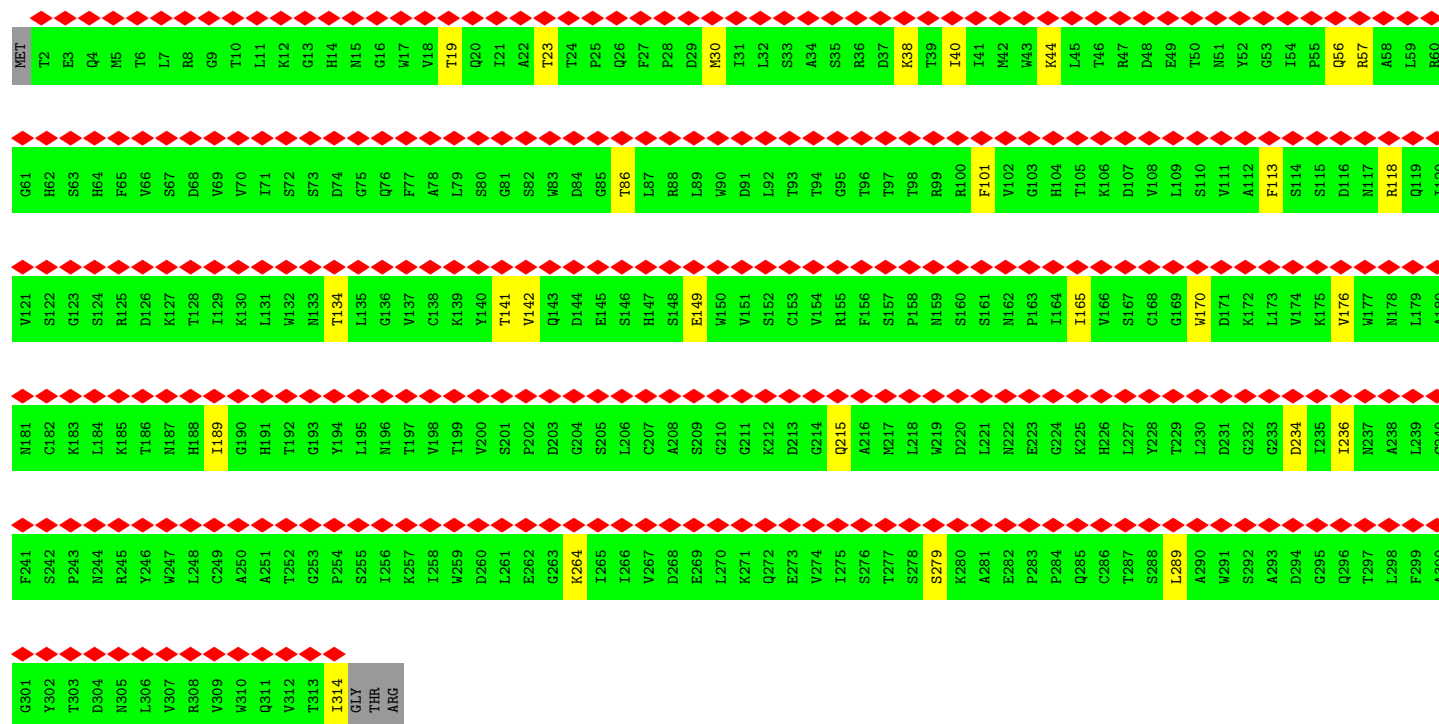


- Molecule 67: 40S ribosomal protein S29

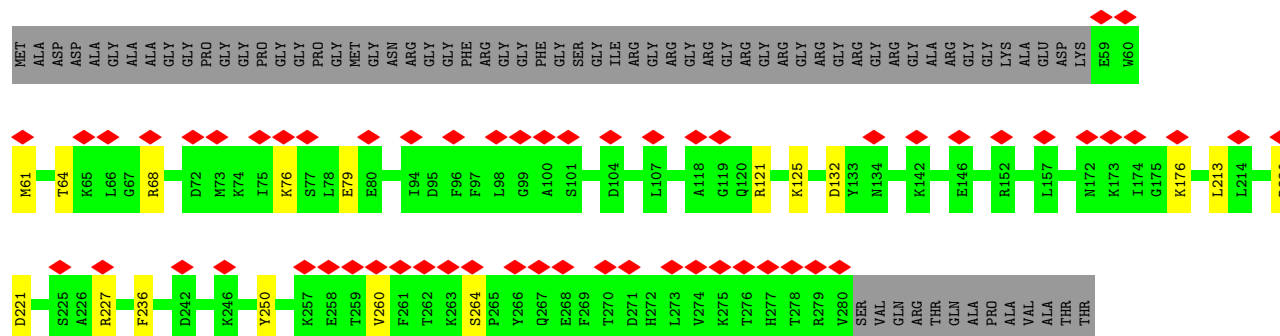
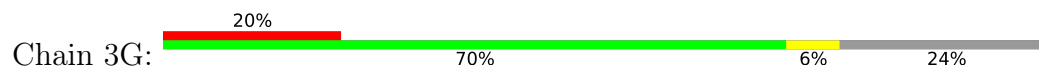


- Molecule 68: Receptor of activated protein C kinase 1

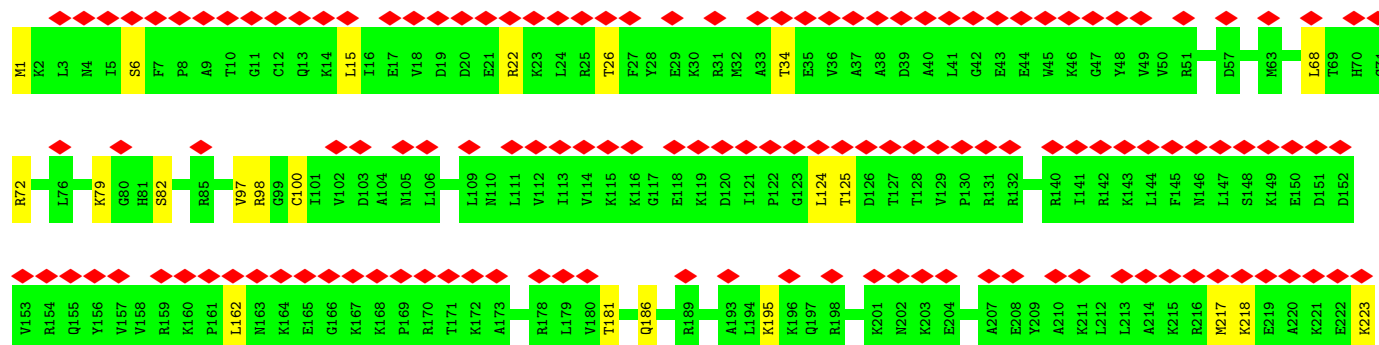
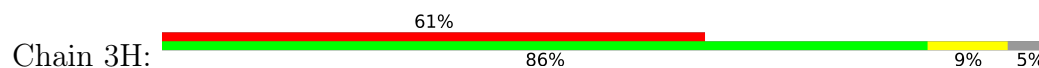


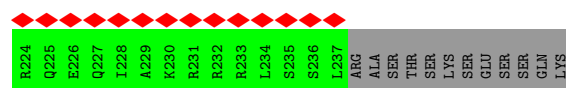


- Molecule 69: 40S ribosomal protein S2



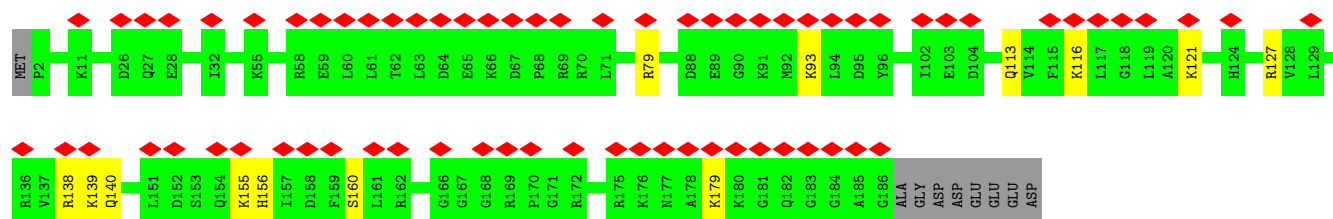
- Molecule 70: 40S ribosomal protein S6





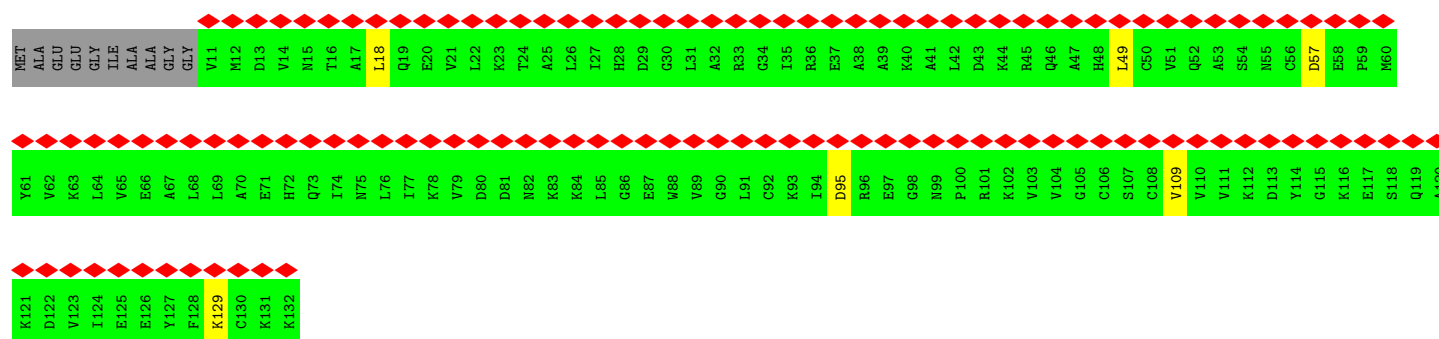
- Molecule 71: 40S ribosomal protein S9

Chain 3I:



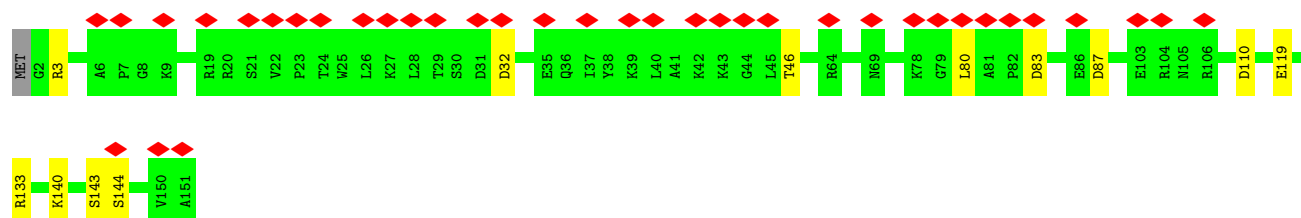
- Molecule 72: 40S ribosomal protein S12

Chain 3J:



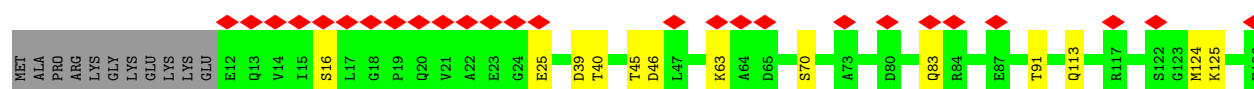
- Molecule 73: 40S ribosomal protein S13

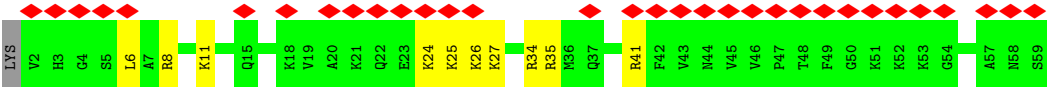
Chain 3K:



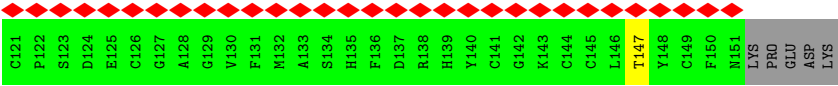
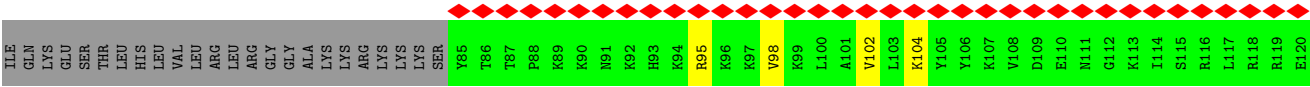
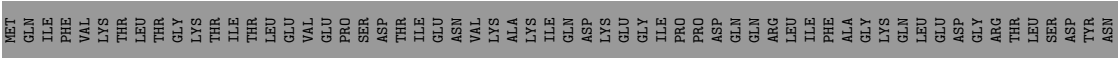
- Molecule 74: 40S ribosomal protein S14

Chain 3L:





• Molecule 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	28291	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.025	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (\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 (\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: ZN, MG, 84D, MLZ

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

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

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

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

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	4924	C	N3-C2-O2	-7.73	116.49	121.90
61	20	89	PRO	N-CD-CG	-7.51	91.94	103.20
47	2m	549	C	N1-C2-O2	7.05	123.13	118.90
61	20	89	PRO	CA-N-CD	-6.64	102.21	111.50
1	1A	456	C	O4'-C1'-N1	6.53	113.42	108.20
1	1A	129	C	N3-C2-O2	-6.50	117.35	121.90
1	1A	131	C	N3-C2-O2	-6.34	117.46	121.90
47	2m	549	C	N3-C2-O2	-6.23	117.54	121.90
47	2m	1513	C	N3-C2-O2	-6.17	117.58	121.90
1	1A	2019	C	N1-C2-O2	6.10	122.56	118.90
47	2m	322	C	N3-C2-O2	-6.05	117.66	121.90
1	1A	4924	C	N1-C2-O2	6.05	122.53	118.90
47	2m	1597	C	N3-C2-O2	-6.03	117.68	121.90
47	2m	1453	C	C2-N1-C1'	6.02	125.42	118.80
47	2m	1512	C	N1-C2-O2	5.75	122.35	118.90
1	1A	2019	C	N3-C2-O2	-5.69	117.92	121.90
1	1A	655	C	N3-C2-O2	-5.67	117.93	121.90
47	2m	1597	C	N1-C2-O2	5.64	122.28	118.90
1	1A	2669	C	O4'-C1'-N1	5.62	112.70	108.20
47	2m	1316	C	N3-C2-O2	-5.61	117.97	121.90
47	2m	958	G	C4-N9-C1'	5.50	133.65	126.50
47	2m	559	G	N3-C2-N2	-5.46	116.08	119.90
1	1A	4348	A	C3'-C2'-C1'	5.39	105.81	101.50
47	2m	321	C	N1-C2-O2	5.30	122.08	118.90
47	2m	559	G	N3-C4-N9	-5.29	122.83	126.00
47	2m	882	U	C3'-C2'-C1'	5.27	105.72	101.50
47	2m	1629	C	N3-C2-O2	-5.27	118.21	121.90
47	2m	1453	C	N1-C2-O2	5.25	122.05	118.90
47	2m	1512	C	C2-N1-C1'	5.19	124.51	118.80
1	1A	2257	C	C2-N1-C1'	5.18	124.50	118.80
47	2m	1513	C	C6-N1-C2	-5.11	118.25	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1D	246/257 (96%)	227 (92%)	19 (8%)	0	100	100
5	1E	400/403 (99%)	387 (97%)	13 (3%)	0	100	100
6	1F	366/427 (86%)	344 (94%)	22 (6%)	0	100	100
7	1G	291/297 (98%)	277 (95%)	14 (5%)	0	100	100
8	1H	232/288 (81%)	210 (90%)	22 (10%)	0	100	100
9	2A	224/248 (90%)	212 (95%)	12 (5%)	0	100	100
10	2B	240/266 (90%)	227 (95%)	13 (5%)	0	100	100
11	2C	188/192 (98%)	176 (94%)	12 (6%)	0	100	100
12	2D	211/214 (99%)	198 (94%)	13 (6%)	0	100	100
13	2E	174/178 (98%)	166 (95%)	7 (4%)	1 (1%)	25	47
14	2F	208/211 (99%)	192 (92%)	16 (8%)	0	100	100
15	2G	137/215 (64%)	129 (94%)	8 (6%)	0	100	100
16	2H	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
17	2I	199/203 (98%)	193 (97%)	6 (3%)	0	100	100
18	2J	151/184 (82%)	144 (95%)	7 (5%)	0	100	100
19	2K	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
20	2L	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
21	2M	173/176 (98%)	159 (92%)	14 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	2N	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
23	2O	99/128 (77%)	85 (86%)	14 (14%)	0	100	100
24	2P	129/140 (92%)	124 (96%)	5 (4%)	0	100	100
25	2Q	122/157 (78%)	109 (89%)	13 (11%)	0	100	100
26	2R	118/156 (76%)	113 (96%)	4 (3%)	1 (1%)	19	39
27	2S	132/145 (91%)	127 (96%)	5 (4%)	0	100	100
28	2T	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
29	2U	145/148 (98%)	141 (97%)	4 (3%)	0	100	100
30	2V	105/159 (66%)	100 (95%)	5 (5%)	0	100	100
31	2W	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
32	2X	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
33	2Y	126/135 (93%)	119 (94%)	6 (5%)	1 (1%)	19	39
34	2Z	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
35	2a	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
36	2b	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
37	2c	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
38	2d	85/97 (88%)	82 (96%)	3 (4%)	0	100	100
39	2e	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
40	2f	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
41	2g	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
42	2h	22/25 (88%)	22 (100%)	0	0	100	100
43	2i	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
44	2j	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	2k	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
46	2l	215/217 (99%)	173 (80%)	42 (20%)	0	100	100
48	2n	219/295 (74%)	199 (91%)	19 (9%)	1 (0%)	29	52
49	2o	212/264 (80%)	204 (96%)	8 (4%)	0	100	100
50	2p	225/243 (93%)	204 (91%)	21 (9%)	0	100	100
51	2q	260/263 (99%)	247 (95%)	13 (5%)	0	100	100
52	2r	187/204 (92%)	169 (90%)	18 (10%)	0	100	100
53	2s	182/194 (94%)	159 (87%)	22 (12%)	1 (0%)	29	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	2t	204/208 (98%)	193 (95%)	11 (5%)	0	100	100
55	2u	96/165 (58%)	85 (88%)	11 (12%)	0	100	100
56	2v	151/158 (96%)	138 (91%)	12 (8%)	1 (1%)	22	43
57	2w	125/145 (86%)	116 (93%)	9 (7%)	0	100	100
58	2x	139/146 (95%)	127 (91%)	12 (9%)	0	100	100
59	2y	133/135 (98%)	118 (89%)	15 (11%)	0	100	100
60	2z	143/152 (94%)	131 (92%)	12 (8%)	0	100	100
61	20	141/145 (97%)	129 (92%)	12 (8%)	0	100	100
62	21	101/119 (85%)	95 (94%)	6 (6%)	0	100	100
63	3A	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
64	3B	139/143 (97%)	130 (94%)	9 (6%)	0	100	100
65	3C	101/115 (88%)	95 (94%)	6 (6%)	0	100	100
66	3D	62/69 (90%)	51 (82%)	11 (18%)	0	100	100
67	3E	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
68	3F	311/317 (98%)	283 (91%)	28 (9%)	0	100	100
69	3G	221/293 (75%)	204 (92%)	17 (8%)	0	100	100
70	3H	235/249 (94%)	228 (97%)	7 (3%)	0	100	100
71	3I	184/194 (95%)	167 (91%)	17 (9%)	0	100	100
72	3J	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
73	3K	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
74	3L	138/151 (91%)	125 (91%)	13 (9%)	0	100	100
75	3M	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
76	3N	130/133 (98%)	127 (98%)	3 (2%)	0	100	100
77	3O	73/125 (58%)	61 (84%)	12 (16%)	0	100	100
78	3P	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
79	3Q	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
80	3R	65/156 (42%)	61 (94%)	4 (6%)	0	100	100
All	All	11562/12905 (90%)	10818 (94%)	738 (6%)	6 (0%)	54	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	2R	38	LYS

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Mol	Chain	Res	Type
33	2Y	92	ASN
53	2s	15	LYS
48	2n	28	THR
13	2E	175	LEU
56	2v	151	THR

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%)	180 (95%)	10 (5%)	22	45
5	1E	348/349 (100%)	329 (94%)	19 (6%)	21	43
6	1F	306/348 (88%)	289 (94%)	17 (6%)	21	42
7	1G	246/250 (98%)	228 (93%)	18 (7%)	14	28
8	1H	209/252 (83%)	190 (91%)	19 (9%)	9	18
9	2A	195/215 (91%)	184 (94%)	11 (6%)	21	42
10	2B	204/223 (92%)	187 (92%)	17 (8%)	11	22
11	2C	169/171 (99%)	155 (92%)	14 (8%)	11	22
12	2D	180/181 (99%)	162 (90%)	18 (10%)	7	14
13	2E	148/149 (99%)	134 (90%)	14 (10%)	8	16
14	2F	176/177 (99%)	159 (90%)	17 (10%)	8	15
15	2G	118/161 (73%)	109 (92%)	9 (8%)	13	26
16	2H	171/172 (99%)	166 (97%)	5 (3%)	42	68
17	2I	173/174 (99%)	160 (92%)	13 (8%)	13	27
18	2J	134/163 (82%)	125 (93%)	9 (7%)	16	33
19	2K	164/165 (99%)	160 (98%)	4 (2%)	49	74
20	2L	166/175 (95%)	156 (94%)	10 (6%)	19	39
21	2M	156/157 (99%)	148 (95%)	8 (5%)	24	46
22	2N	139/140 (99%)	125 (90%)	14 (10%)	7	14
23	2O	91/115 (79%)	79 (87%)	12 (13%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	2P	101/107 (94%)	94 (93%)	7 (7%)	15	31
25	2Q	103/126 (82%)	97 (94%)	6 (6%)	20	40
26	2R	108/133 (81%)	98 (91%)	10 (9%)	9	17
27	2S	124/135 (92%)	118 (95%)	6 (5%)	25	49
28	2T	117/118 (99%)	109 (93%)	8 (7%)	16	32
29	2U	120/121 (99%)	114 (95%)	6 (5%)	24	47
30	2V	89/126 (71%)	78 (88%)	11 (12%)	4	8
31	2W	83/97 (86%)	79 (95%)	4 (5%)	25	49
32	2X	98/110 (89%)	91 (93%)	7 (7%)	14	29
33	2Y	114/121 (94%)	108 (95%)	6 (5%)	22	45
34	2Z	88/89 (99%)	83 (94%)	5 (6%)	20	41
35	2a	98/100 (98%)	93 (95%)	5 (5%)	24	46
36	2b	109/110 (99%)	99 (91%)	10 (9%)	9	17
37	2c	86/89 (97%)	78 (91%)	8 (9%)	9	17
38	2d	74/80 (92%)	69 (93%)	5 (7%)	16	32
39	2e	64/65 (98%)	58 (91%)	6 (9%)	8	17
40	2f	47/48 (98%)	45 (96%)	2 (4%)	29	54
41	2g	47/115 (41%)	45 (96%)	2 (4%)	29	54
42	2h	23/24 (96%)	20 (87%)	3 (13%)	4	7
43	2i	94/94 (100%)	89 (95%)	5 (5%)	22	45
44	2j	74/75 (99%)	69 (93%)	5 (7%)	16	32
45	2k	109/121 (90%)	100 (92%)	9 (8%)	11	22
46	2l	195/196 (100%)	169 (87%)	26 (13%)	4	7
48	2n	183/243 (75%)	159 (87%)	24 (13%)	4	7
49	2o	195/231 (84%)	178 (91%)	17 (9%)	10	20
50	2p	190/202 (94%)	163 (86%)	27 (14%)	3	5
51	2q	224/225 (100%)	209 (93%)	15 (7%)	16	33
52	2r	159/170 (94%)	144 (91%)	15 (9%)	8	17
53	2s	166/174 (95%)	153 (92%)	13 (8%)	12	25
54	2t	178/180 (99%)	166 (93%)	12 (7%)	16	33
55	2u	89/136 (65%)	82 (92%)	7 (8%)	12	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	2v	137/142 (96%)	123 (90%)	14 (10%)	7	14
57	2w	113/130 (87%)	106 (94%)	7 (6%)	18	37
58	2x	117/121 (97%)	106 (91%)	11 (9%)	8	17
59	2y	122/122 (100%)	107 (88%)	15 (12%)	4	9
60	2z	126/132 (96%)	119 (94%)	7 (6%)	21	42
61	20	113/115 (98%)	102 (90%)	11 (10%)	8	15
62	21	94/107 (88%)	82 (87%)	12 (13%)	4	8
63	3A	67/67 (100%)	55 (82%)	12 (18%)	2	2
64	3B	113/115 (98%)	96 (85%)	17 (15%)	3	5
65	3C	90/98 (92%)	80 (89%)	10 (11%)	6	11
66	3D	57/62 (92%)	54 (95%)	3 (5%)	22	45
67	3E	48/49 (98%)	42 (88%)	6 (12%)	4	8
68	3F	272/275 (99%)	245 (90%)	27 (10%)	8	15
69	3G	189/225 (84%)	172 (91%)	17 (9%)	9	18
70	3H	207/218 (95%)	185 (89%)	22 (11%)	6	12
71	3I	162/168 (96%)	148 (91%)	14 (9%)	10	20
72	3J	102/108 (94%)	96 (94%)	6 (6%)	19	39
73	3K	130/131 (99%)	118 (91%)	12 (9%)	9	17
74	3L	110/119 (92%)	94 (86%)	16 (14%)	3	5
75	3M	112/113 (99%)	100 (89%)	12 (11%)	6	12
76	3N	114/115 (99%)	101 (89%)	13 (11%)	5	10
77	3O	66/103 (64%)	54 (82%)	12 (18%)	1	2
78	3P	75/76 (99%)	65 (87%)	10 (13%)	4	7
79	3Q	47/48 (98%)	37 (79%)	10 (21%)	1	1
80	3R	60/140 (43%)	55 (92%)	5 (8%)	11	22
All	All	10075/10996 (92%)	9224 (92%)	851 (8%)	14	21

All (851) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	1D	15	VAL
4	1D	54	ARG
4	1D	102	LEU

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Mol	Chain	Res	Type
4	1D	106	THR
4	1D	114	CYS
4	1D	116	LEU
4	1D	144	LYS
4	1D	184	ARG
4	1D	241	ARG
4	1D	247	ARG
5	1E	38	SER
5	1E	39	LYS
5	1E	138	GLN
5	1E	141	ASP
5	1E	155	LYS
5	1E	194	LEU
5	1E	215	GLU
5	1E	257	TRP
5	1E	258	HIS
5	1E	289	GLN
5	1E	292	LEU
5	1E	297	LYS
5	1E	299	ILE
5	1E	300	LYS
5	1E	304	SER
5	1E	305	THR
5	1E	348	ARG
5	1E	358	ARG
5	1E	363	ILE
6	1F	1	MET
6	1F	8	ILE
6	1F	14	LYS
6	1F	61	GLN
6	1F	63	SER
6	1F	122	TYR
6	1F	157	LYS
6	1F	179	ASP
6	1F	188	ARG
6	1F	204	ARG
6	1F	208	CYS
6	1F	230	LEU
6	1F	267	TRP
6	1F	291	ARG
6	1F	312	ARG
6	1F	334	THR

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Mol	Chain	Res	Type
6	1F	345	ARG
7	1G	34	LYS
7	1G	51	MET
7	1G	85	LYS
7	1G	88	VAL
7	1G	89	LYS
7	1G	93	THR
7	1G	115	MET
7	1G	154	THR
7	1G	187	SER
7	1G	213	GLU
7	1G	220	LYS
7	1G	224	SER
7	1G	238	GLU
7	1G	254	GLU
7	1G	260	GLU
7	1G	272	SER
7	1G	286	SER
7	1G	289	ARG
8	1H	49	VAL
8	1H	56	ARG
8	1H	89	LEU
8	1H	96	VAL
8	1H	100	LYS
8	1H	106	VAL
8	1H	124	LYS
8	1H	128	HIS
8	1H	130	LYS
8	1H	145	THR
8	1H	183	ARG
8	1H	191	GLN
8	1H	198	SER
8	1H	210	LYS
8	1H	221	LYS
8	1H	235	THR
8	1H	239	LYS
8	1H	255	SER
8	1H	262	LYS
9	2A	28	LEU
9	2A	36	LYS
9	2A	62	ARG
9	2A	74	MET

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Mol	Chain	Res	Type
9	2A	102	SER
9	2A	200	ARG
9	2A	215	SER
9	2A	221	LYS
9	2A	242	ARG
9	2A	247	MET
9	2A	248	ASN
10	2B	43	GLN
10	2B	88	ASP
10	2B	94	GLN
10	2B	97	LYS
10	2B	105	GLU
10	2B	111	LYS
10	2B	137[A]	ARG
10	2B	137[B]	ARG
10	2B	176	LYS
10	2B	185	LYS
10	2B	192	ARG
10	2B	207	VAL
10	2B	209	SER
10	2B	211	ASP
10	2B	223	ARG
10	2B	253	LEU
10	2B	265	LEU
11	2C	1	MET
11	2C	19	THR
11	2C	50	LYS
11	2C	51	LYS
11	2C	57	VAL
11	2C	65	LYS
11	2C	94	SER
11	2C	140	GLN
11	2C	155	SER
11	2C	161	ILE
11	2C	172	ILE
11	2C	177	ASP
11	2C	183	GLU
11	2C	188	GLN
12	2D	13	LYS
12	2D	26	VAL
12	2D	32	ARG
12	2D	39	LYS

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Mol	Chain	Res	Type
12	2D	40	LYS
12	2D	71	CYS
12	2D	76	MET
12	2D	78	LYS
12	2D	101	LYS
12	2D	112	GLN
12	2D	125	THR
12	2D	134	VAL
12	2D	141	LYS
12	2D	143	GLN
12	2D	162	ARG
12	2D	164	LYS
12	2D	207	ASP
12	2D	208	LYS
13	2E	32	ARG
13	2E	33	LEU
13	2E	41	GLU
13	2E	52	LYS
13	2E	55	TYR
13	2E	56	THR
13	2E	58	ARG
13	2E	60	PHE
13	2E	63	ARG
13	2E	72	CYS
13	2E	91	GLU
13	2E	130	PHE
13	2E	158	SER
13	2E	168	GLN
14	2F	42	LYS
14	2F	52	SER
14	2F	59	VAL
14	2F	63	THR
14	2F	64	VAL
14	2F	67	HIS
14	2F	70	VAL
14	2F	94	ILE
14	2F	97	SER
14	2F	121	ARG
14	2F	135	LYS
14	2F	138	ASP
14	2F	145	LYS
14	2F	162	LYS

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Mol	Chain	Res	Type
14	2F	167	ARG
14	2F	186	ARG
14	2F	209	LYS
15	2G	25	VAL
15	2G	31	ILE
15	2G	33	GLN
15	2G	67	SER
15	2G	103	LYS
15	2G	121	ARG
15	2G	124	LYS
15	2G	130	LEU
15	2G	135	LEU
16	2H	25	VAL
16	2H	37	HIS
16	2H	50	ARG
16	2H	169	ARG
16	2H	182	HIS
17	2I	5	GLN
17	2I	25	LYS
17	2I	27	VAL
17	2I	31	ARG
17	2I	100	ASP
17	2I	117	ARG
17	2I	141	LEU
17	2I	145	VAL
17	2I	152	VAL
17	2I	173	GLN
17	2I	186	GLU
17	2I	191	LYS
17	2I	194	GLU
18	2J	3	ARG
18	2J	12	THR
18	2J	23	ARG
18	2J	24	VAL
18	2J	53	LEU
18	2J	54	GLN
18	2J	57	CYS
18	2J	108	ASP
18	2J	153	LYS
19	2K	33	ARG
19	2K	45	GLN
19	2K	66	MET

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Mol	Chain	Res	Type
19	2K	161	SER
20	2L	16	ARG
20	2L	20	LYS
20	2L	81	ARG
20	2L	82	LYS
20	2L	108	ARG
20	2L	148	ASP
20	2L	152	LYS
20	2L	160	GLU
20	2L	181	LYS
20	2L	186	LYS
21	2M	19	THR
21	2M	31	ARG
21	2M	48	VAL
21	2M	90	THR
21	2M	135	SER
21	2M	161	ARG
21	2M	164	LYS
21	2M	169	THR
22	2N	4	THR
22	2N	14	MET
22	2N	29	THR
22	2N	76	VAL
22	2N	83	LYS
22	2N	103	ASP
22	2N	107	LYS
22	2N	109	VAL
22	2N	111	GLU
22	2N	118	GLU
22	2N	122	LYS
22	2N	127	GLN
22	2N	130	ARG
22	2N	149	GLU
23	2O	20	LYS
23	2O	41	GLN
23	2O	52	LYS
23	2O	62	THR
23	2O	69	LYS
23	2O	79	SER
23	2O	80	LYS
23	2O	82	TYR
23	2O	91	LEU

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Mol	Chain	Res	Type
23	2O	95	ASN
23	2O	97	ARG
23	2O	98	ASP
24	2P	13	LYS
24	2P	20	LEU
24	2P	22	VAL
24	2P	28	CYS
24	2P	69	LYS
24	2P	94	VAL
24	2P	127	ASP
25	2Q	1	MET
25	2Q	2	LYS
25	2Q	19	ARG
25	2Q	27	LYS
25	2Q	44	ARG
25	2Q	48	GLN
26	2R	37	LYS
26	2R	54	LEU
26	2R	57	GLN
26	2R	85	SER
26	2R	95	THR
26	2R	101	ASP
26	2R	111	GLN
26	2R	120	ASP
26	2R	131	ASP
26	2R	147	LEU
27	2S	46	SER
27	2S	74	TYR
27	2S	84	ARG
27	2S	105	VAL
27	2S	112	ASP
27	2S	127	GLN
28	2T	24	VAL
28	2T	31	ASP
28	2T	60	LYS
28	2T	86	SER
28	2T	87	VAL
28	2T	91	LEU
28	2T	100	VAL
28	2T	112	ARG
29	2U	14	HIS
29	2U	15	VAL

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Mol	Chain	Res	Type
29	2U	24	LYS
29	2U	66	ASN
29	2U	95	THR
29	2U	140	VAL
30	2V	4	SER
30	2V	9	THR
30	2V	13	SER
30	2V	23	LYS
30	2V	25	ARG
30	2V	26	SER
30	2V	51	LYS
30	2V	91	ARG
30	2V	93	LEU
30	2V	95	ARG
30	2V	117	ARG
31	2W	23	LYS
31	2W	24	SER
31	2W	93	THR
31	2W	106	ARG
32	2X	33	ILE
32	2X	50	ARG
32	2X	89	SER
32	2X	98	SER
32	2X	100	ASN
32	2X	101	LYS
32	2X	123	ASP
33	2Y	5	ARG
33	2Y	11	LYS
33	2Y	83	LYS
33	2Y	87	VAL
33	2Y	109	LYS
33	2Y	117	GLN
34	2Z	33	VAL
34	2Z	83	MET
34	2Z	89	ARG
34	2Z	95	LYS
34	2Z	108	SER
35	2a	3	GLN
35	2a	23	SER
35	2a	63	VAL
35	2a	65	MET
35	2a	110	GLN

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Mol	Chain	Res	Type
36	2b	3	LYS
36	2b	7	ARG
36	2b	36	VAL
36	2b	37	THR
36	2b	46	LYS
36	2b	70	ARG
36	2b	71	LYS
36	2b	94	ARG
36	2b	112	ARG
36	2b	122	LYS
37	2c	3	LEU
37	2c	29	ARG
37	2c	30	ARG
37	2c	32	ARG
37	2c	38	LYS
37	2c	41	ARG
37	2c	91	SER
37	2c	99	LYS
38	2d	6	SER
38	2d	22	CYS
38	2d	24	SER
38	2d	25	LYS
38	2d	32	SER
39	2e	18	LYS
39	2e	22	SER
39	2e	50	LYS
39	2e	58	GLN
39	2e	59	SER
39	2e	70	LYS
40	2f	8	ARG
40	2f	36	ARG
41	2g	99	CYS
41	2g	128	LYS
42	2h	6	ARG
42	2h	13	LEU
42	2h	24	SER
43	2i	10	THR
43	2i	57	ARG
43	2i	74	GLU
43	2i	104	ILE
43	2i	106	PHE
44	2j	36	LYS

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Mol	Chain	Res	Type
44	2j	62	LYS
44	2j	72	ASN
44	2j	81	SER
44	2j	90	LYS
45	2k	21	ASN
45	2k	24	THR
45	2k	26	SER
45	2k	32	LEU
45	2k	49	VAL
45	2k	58	LYS
45	2k	67	ARG
45	2k	78	VAL
45	2k	122	LYS
46	2l	1	MET
46	2l	19	HIS
46	2l	22	GLN
46	2l	40	ASN
46	2l	45	LYS
46	2l	46	ASP
46	2l	47	LYS
46	2l	56	LYS
46	2l	58	THR
46	2l	85	MET
46	2l	102	LYS
46	2l	106	LYS
46	2l	116	LEU
46	2l	122	ARG
46	2l	141	ASN
46	2l	144	MET
46	2l	148	VAL
46	2l	156	LYS
46	2l	159	MET
46	2l	161	LYS
46	2l	167	VAL
46	2l	174	MET
46	2l	175	THR
46	2l	204	LEU
46	2l	212	LYS
46	2l	215	ARG
48	2n	7	VAL
48	2n	11	LYS
48	2n	16	LEU

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Mol	Chain	Res	Type
48	2n	25	LEU
48	2n	28	THR
48	2n	51	LEU
48	2n	73	ASP
48	2n	76	VAL
48	2n	78	SER
48	2n	80	ARG
48	2n	88	LEU
48	2n	89	LYS
48	2n	104	THR
48	2n	116	PHE
48	2n	118	GLU
48	2n	126	ASP
48	2n	142	LEU
48	2n	144	THR
48	2n	169	HIS
48	2n	170	SER
48	2n	174	MET
48	2n	177	MET
48	2n	186	ARG
48	2n	200	ASP
49	2o	38	MET
49	2o	55	THR
49	2o	70	SER
49	2o	86	LEU
49	2o	90	ASP
49	2o	103	MET
49	2o	128	LYS
49	2o	131	ASP
49	2o	139	CYS
49	2o	147	ASN
49	2o	151	ARG
49	2o	187	LYS
49	2o	192	SER
49	2o	198	GLU
49	2o	199	LYS
49	2o	222	LYS
49	2o	229	MET
50	2p	17	PHE
50	2p	29	LEU
50	2p	37	VAL
50	2p	45	ARG

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Mol	Chain	Res	Type
50	2p	49	ILE
50	2p	67	ARG
50	2p	76	ARG
50	2p	84	VAL
50	2p	94	ARG
50	2p	106	ARG
50	2p	109	LEU
50	2p	116	ARG
50	2p	127	MET
50	2p	129	SER
50	2p	143	ARG
50	2p	148	LYS
50	2p	150	MET
50	2p	154	ASP
50	2p	170	THR
50	2p	178	ARG
50	2p	181	VAL
50	2p	197	LYS
50	2p	198	ILE
50	2p	206	ASP
50	2p	209	SER
50	2p	216	GLU
50	2p	221	THR
51	2q	12	VAL
51	2q	38	LEU
51	2q	39	ARG
51	2q	41	CYS
51	2q	69	PHE
51	2q	121	TYR
51	2q	134	LYS
51	2q	136	ILE
51	2q	139	LEU
51	2q	198	ARG
51	2q	216	ASN
51	2q	223	SER
51	2q	233	LYS
51	2q	237	SER
51	2q	253	ASP
52	2r	16	ASP
52	2r	20	PHE
52	2r	27	ASP
52	2r	39	ILE

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Mol	Chain	Res	Type
52	2r	43	GLU
52	2r	45	TYR
52	2r	55	ARG
52	2r	93	VAL
52	2r	106	GLU
52	2r	119	SER
52	2r	124	ASP
52	2r	130	ARG
52	2r	167	LYS
52	2r	193	LYS
52	2r	201	LYS
53	2s	10	LYS
53	2s	41	ARG
53	2s	51	ILE
53	2s	90	LYS
53	2s	98	ARG
53	2s	106	ARG
53	2s	107	LYS
53	2s	111	LYS
53	2s	170	VAL
53	2s	172	THR
53	2s	174	SER
53	2s	184	ASP
53	2s	192	PHE
54	2t	3	ILE
54	2t	17	LYS
54	2t	22	HIS
54	2t	29	LEU
54	2t	49	ARG
54	2t	69	SER
54	2t	77	ARG
54	2t	110	ARG
54	2t	111	GLN
54	2t	124	LYS
54	2t	143	LYS
54	2t	168	GLN
55	2u	45	VAL
55	2u	53	LYS
55	2u	69	TRP
55	2u	73	ASN
55	2u	95	ARG
55	2u	96	ARG

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Mol	Chain	Res	Type
55	2u	98	ARG
56	2v	13	GLN
56	2v	19	ASN
56	2v	22	ARG
56	2v	25	LEU
56	2v	30	LYS
56	2v	37	TYR
56	2v	45	LYS
56	2v	69	ARG
56	2v	74	SER
56	2v	81	LYS
56	2v	91	ASP
56	2v	125	ILE
56	2v	126	VAL
56	2v	135	SER
57	2w	10	ARG
57	2w	28	MET
57	2w	55	SER
57	2w	64	LYS
57	2w	70	MET
57	2w	83	MET
57	2w	89	MET
58	2x	15	ARG
58	2x	17	LYS
58	2x	20	THR
58	2x	27	ARG
58	2x	34	VAL
58	2x	41	MET
58	2x	45	ARG
58	2x	46	THR
58	2x	110	ASP
58	2x	114	GLN
58	2x	115	TYR
59	2y	6	THR
59	2y	8	THR
59	2y	11	LYS
59	2y	16	ILE
59	2y	26	ASN
59	2y	37	GLU
59	2y	45	LYS
59	2y	58	MET
59	2y	60	ARG

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Mol	Chain	Res	Type
59	2y	77	GLU
59	2y	82	ASP
59	2y	85	VAL
59	2y	92	ASP
59	2y	99	ASP
59	2y	102	THR
60	2z	8	LYS
60	2z	17	ASN
60	2z	18	THR
60	2z	19	ASN
60	2z	50	ILE
60	2z	99	LEU
60	2z	101	ASN
61	20	27	LYS
61	20	29	LYS
61	20	33	TRP
61	20	41	LYS
61	20	43	LYS
61	20	55	THR
61	20	90	SER
61	20	96	SER
61	20	123	LEU
61	20	133	ARG
61	20	138	VAL
62	21	21	ARG
62	21	25	THR
62	21	28	ASN
62	21	47	ASN
62	21	59	LYS
62	21	63	ILE
62	21	75	LYS
62	21	78	ASP
62	21	79	ARG
62	21	81	GLN
62	21	89	ILE
62	21	114	VAL
63	3A	1	MET
63	3A	22	ARG
63	3A	33	GLN
63	3A	41	LYS
63	3A	43	THR
63	3A	47	ASN

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Mol	Chain	Res	Type
63	3A	50	PHE
63	3A	62	MET
63	3A	65	SER
63	3A	80	SER
63	3A	81	LYS
63	3A	83	PHE
64	3B	7	LEU
64	3B	8	ARG
64	3B	14	ARG
64	3B	19	ASP
64	3B	24	ASP
64	3B	27	TYR
64	3B	32	LEU
64	3B	57	VAL
64	3B	64	SER
64	3B	70	VAL
64	3B	71	ARG
64	3B	72	VAL
64	3B	99	GLU
64	3B	105	PHE
64	3B	108	LYS
64	3B	122	VAL
64	3B	140	ARG
65	3C	10	ARG
65	3C	25	ASN
65	3C	28	ARG
65	3C	60	ASP
65	3C	76	SER
65	3C	85[A]	ARG
65	3C	85[B]	ARG
65	3C	86	ASN
65	3C	89	ARG
65	3C	102	ARG
66	3D	6	VAL
66	3D	23	SER
66	3D	60	GLU
67	3E	3	HIS
67	3E	8	TRP
67	3E	16	GLN
67	3E	21	CYS
67	3E	27	ARG
67	3E	40	ARG

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Mol	Chain	Res	Type
68	3F	19	THR
68	3F	23	THR
68	3F	30	MET
68	3F	38	LYS
68	3F	40	ILE
68	3F	44	LYS
68	3F	56	GLN
68	3F	57	ARG
68	3F	86	THR
68	3F	101	PHE
68	3F	113	PHE
68	3F	118	ARG
68	3F	134	THR
68	3F	141	THR
68	3F	142	VAL
68	3F	149	GLU
68	3F	165	ILE
68	3F	170	TRP
68	3F	176	VAL
68	3F	189	ILE
68	3F	215	GLN
68	3F	234	ASP
68	3F	236	ILE
68	3F	264	LYS
68	3F	279	SER
68	3F	289	LEU
68	3F	314	ILE
69	3G	61	MET
69	3G	64	THR
69	3G	68	ARG
69	3G	76	LYS
69	3G	79	GLU
69	3G	121	ARG
69	3G	125	LYS
69	3G	132	ASP
69	3G	176	LYS
69	3G	213	LEU
69	3G	220	ASP
69	3G	221	ASP
69	3G	227	ARG
69	3G	236	PHE
69	3G	250	TYR

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Mol	Chain	Res	Type
69	3G	260	VAL
69	3G	264	SER
70	3H	1	MET
70	3H	6	SER
70	3H	15	LEU
70	3H	22	ARG
70	3H	26	THR
70	3H	34	THR
70	3H	68	LEU
70	3H	72	ARG
70	3H	79	LYS
70	3H	82	SER
70	3H	97	VAL
70	3H	98	ARG
70	3H	100	CYS
70	3H	124	LEU
70	3H	125	THR
70	3H	162	LEU
70	3H	181	THR
70	3H	186	GLN
70	3H	195	LYS
70	3H	217	MET
70	3H	218	LYS
70	3H	223	LYS
71	3I	79	ARG
71	3I	93	LYS
71	3I	113	GLN
71	3I	116	LYS
71	3I	121	LYS
71	3I	127	ARG
71	3I	138[A]	ARG
71	3I	138[B]	ARG
71	3I	139	LYS
71	3I	140	GLN
71	3I	155	LYS
71	3I	156	HIS
71	3I	160	SER
71	3I	179	LYS
72	3J	18	LEU
72	3J	49	LEU
72	3J	57	ASP
72	3J	95	ASP

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Mol	Chain	Res	Type
72	3J	109	VAL
72	3J	129	LYS
73	3K	3	ARG
73	3K	32	ASP
73	3K	46	THR
73	3K	80	LEU
73	3K	83	ASP
73	3K	87	ASP
73	3K	110	ASP
73	3K	119	GLU
73	3K	133	ARG
73	3K	140	LYS
73	3K	143	SER
73	3K	144	SER
74	3L	16	SER
74	3L	25	GLU
74	3L	39	ASP
74	3L	40	THR
74	3L	45	THR
74	3L	46	ASP
74	3L	63	LYS
74	3L	70	SER
74	3L	83	GLN
74	3L	91	THR
74	3L	113	GLN
74	3L	124	MET
74	3L	125	LYS
74	3L	133	THR
74	3L	142	ARG
74	3L	149	ARG
75	3M	2	VAL
75	3M	6	VAL
75	3M	13	SER
75	3M	26	LEU
75	3M	57	ARG
75	3M	68	ARG
75	3M	70	ASN
75	3M	88	LYS
75	3M	97	ARG
75	3M	104	LEU
75	3M	112	ASP
75	3M	121	THR

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Mol	Chain	Res	Type
76	3N	10	ARG
76	3N	14	THR
76	3N	16	ARG
76	3N	22	GLN
76	3N	46	LYS
76	3N	50	THR
76	3N	57	VAL
76	3N	58	PHE
76	3N	94	HIS
76	3N	101	LYS
76	3N	105	LYS
76	3N	110	ARG
76	3N	114	MET
77	3O	43	LYS
77	3O	46	ASN
77	3O	48	VAL
77	3O	55	TYR
77	3O	69	THR
77	3O	77	LEU
77	3O	82	SER
77	3O	98	LYS
77	3O	102	LYS
77	3O	104	ARG
77	3O	110	THR
77	3O	112	ASN
78	3P	3	LEU
78	3P	17	ARG
78	3P	26	GLN
78	3P	36	LYS
78	3P	43	ILE
78	3P	44	THR
78	3P	61	THR
78	3P	62	VAL
78	3P	70	LYS
78	3P	80	ARG
79	3Q	6	LEU
79	3Q	8	ARG
79	3Q	11	LYS
79	3Q	24	LYS
79	3Q	25	LYS
79	3Q	26	LYS
79	3Q	27	LYS

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Mol	Chain	Res	Type
79	3Q	34	ARG
79	3Q	35	ARG
79	3Q	41	ARG
80	3R	95	ARG
80	3R	98	VAL
80	3R	102	VAL
80	3R	104	LYS
80	3R	147	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
7	1G	244	HIS
8	1H	245	GLN
9	2A	39	GLN
14	2F	149	GLN
19	2K	188	ASN
23	2O	41	GLN
25	2Q	45	ASN
26	2R	57	GLN
35	2a	3	GLN
35	2a	110	GLN
43	2i	19	GLN
45	2k	4	HIS
46	2l	19	HIS
46	2l	94	ASN
48	2n	113	GLN
48	2n	132	GLN
48	2n	165	ASN
50	2p	57	ASN
50	2p	101	GLN
51	2q	36	HIS
52	2r	203	ASN
54	2t	22	HIS
56	2v	11	GLN
57	2w	104	GLN
60	2z	17	ASN
64	3B	87	ASN
71	3I	156	HIS
73	3K	5	HIS
73	3K	13	GLN
74	3L	20	GLN

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Mol	Chain	Res	Type
76	3N	22	GLN
76	3N	85	ASN
76	3N	106	GLN
78	3P	26	GLN
78	3P	51	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	3704/5070 (73%)	810 (21%)	54 (1%)
2	1B	119/121 (98%)	14 (11%)	2 (1%)
3	1C	155/157 (98%)	28 (18%)	2 (1%)
47	2m	1716/1869 (91%)	494 (28%)	0
All	All	5694/7217 (78%)	1346 (23%)	58 (1%)

All (1346) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	6	C
1	1A	13	U
1	1A	39	A
1	1A	42	A
1	1A	48	G
1	1A	59	A
1	1A	64	A
1	1A	65	A
1	1A	66	A
1	1A	67	C
1	1A	73	A
1	1A	91	G
1	1A	98	A
1	1A	104	G
1	1A	109	G
1	1A	110	C
1	1A	119	G
1	1A	120	A
1	1A	121	A
1	1A	122	U
1	1A	128	C
1	1A	130	C
1	1A	131	C

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Mol	Chain	Res	Type
1	1A	133	C
1	1A	135	G
1	1A	136	C
1	1A	137	G
1	1A	144	G
1	1A	159	C
1	1A	171	U
1	1A	172	C
1	1A	179	G
1	1A	180	C
1	1A	183	C
1	1A	184	U
1	1A	185	C
1	1A	188	G
1	1A	189	G
1	1A	197	A
1	1A	200	U
1	1A	201	C
1	1A	209	U
1	1A	216	C
1	1A	217	C
1	1A	218	A
1	1A	219	G
1	1A	227	A
1	1A	233	U
1	1A	234	G
1	1A	265	C
1	1A	266	C
1	1A	275	C
1	1A	278	G
1	1A	280	G
1	1A	295	A
1	1A	297	U
1	1A	306	A
1	1A	315	G
1	1A	316	U
1	1A	340	C
1	1A	384	A
1	1A	386	A
1	1A	387	G
1	1A	396	A
1	1A	407	A

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Mol	Chain	Res	Type
1	1A	409	G
1	1A	410	A
1	1A	412	G
1	1A	413	G
1	1A	414	C
1	1A	415	G
1	1A	417	G
1	1A	418	A
1	1A	449	C
1	1A	450	G
1	1A	452	A
1	1A	453	G
1	1A	456	C
1	1A	457	G
1	1A	467	U
1	1A	484	U
1	1A	485	C
1	1A	486	C
1	1A	493	G
1	1A	494	U
1	1A	497	G
1	1A	498	C
1	1A	500	G
1	1A	502	C
1	1A	503	C
1	1A	504	G
1	1A	505	G
1	1A	507	G
1	1A	509	A
1	1A	510	U
1	1A	512	U
1	1A	513	U
1	1A	514	U
1	1A	517	C
1	1A	518	G
1	1A	643	C
1	1A	644	G
1	1A	645	G
1	1A	646	G
1	1A	654	C
1	1A	657	C
1	1A	665	C

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Mol	Chain	Res	Type
1	1A	666	G
1	1A	667	A
1	1A	668	C
1	1A	673	C
1	1A	685	C
1	1A	686	A
1	1A	687	U
1	1A	696	C
1	1A	703	G
1	1A	704	C
1	1A	706	C
1	1A	731	G
1	1A	738	C
1	1A	739	G
1	1A	740	G
1	1A	742	G
1	1A	744	G
1	1A	753	C
1	1A	754	U
1	1A	904	C
1	1A	905	C
1	1A	913	U
1	1A	914	U
1	1A	915	A
1	1A	916	C
1	1A	917	A
1	1A	923	C
1	1A	924	C
1	1A	925	C
1	1A	926	G
1	1A	932	A
1	1A	933	G
1	1A	936	C
1	1A	944	A
1	1A	945	U
1	1A	959	G
1	1A	960	A
1	1A	961	G
1	1A	962	C
1	1A	965	G
1	1A	966	A
1	1A	967	C

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Mol	Chain	Res	Type
1	1A	969	C
1	1A	970	G
1	1A	971	U
1	1A	977	C
1	1A	982	U
1	1A	984	C
1	1A	989	U
1	1A	990	C
1	1A	991	C
1	1A	992	C
1	1A	993	G
1	1A	995	C
1	1A	1048	G
1	1A	1049	C
1	1A	1051	G
1	1A	1066	G
1	1A	1070	G
1	1A	1071	C
1	1A	1072	C
1	1A	1075	G
1	1A	1079	C
1	1A	1082	C
1	1A	1168	G
1	1A	1172	C
1	1A	1173	G
1	1A	1174	G
1	1A	1178	G
1	1A	1179	U
1	1A	1180	C
1	1A	1181	C
1	1A	1182	C
1	1A	1183	C
1	1A	1184	A
1	1A	1198	G
1	1A	1202	C
1	1A	1203	G
1	1A	1211	G
1	1A	1215	C
1	1A	1216	C
1	1A	1217	G
1	1A	1218	G
1	1A	1219	G

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Mol	Chain	Res	Type
1	1A	1220	G
1	1A	1221	G
1	1A	1222	A
1	1A	1235	G
1	1A	1241	C
1	1A	1242	G
1	1A	1253	G
1	1A	1254	A
1	1A	1255	A
1	1A	1263	A
1	1A	1266	G
1	1A	1269	G
1	1A	1270	A
1	1A	1271	G
1	1A	1272	C
1	1A	1273	G
1	1A	1275	G
1	1A	1280	C
1	1A	1284	G
1	1A	1285	U
1	1A	1287	G
1	1A	1293	G
1	1A	1294	A
1	1A	1296	G
1	1A	1301	C
1	1A	1302	U
1	1A	1303	A
1	1A	1313	C
1	1A	1326	A
1	1A	1337	A
1	1A	1338	G
1	1A	1354	A
1	1A	1358	G
1	1A	1359	G
1	1A	1365	C
1	1A	1366	G
1	1A	1367	C
1	1A	1378	C
1	1A	1387	A
1	1A	1393	G
1	1A	1394	G
1	1A	1397	A

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Mol	Chain	Res	Type
1	1A	1398	A
1	1A	1399	G
1	1A	1405	C
1	1A	1409	C
1	1A	1410	U
1	1A	1411	C
1	1A	1420	A
1	1A	1437	C
1	1A	1439	C
1	1A	1441	C
1	1A	1443	A
1	1A	1444	G
1	1A	1446	C
1	1A	1447	C
1	1A	1482	G
1	1A	1483	C
1	1A	1498	G
1	1A	1502	G
1	1A	1504	G
1	1A	1534	A
1	1A	1547	A
1	1A	1564	A
1	1A	1566	C
1	1A	1578	U
1	1A	1591	U
1	1A	1596	U
1	1A	1613	A
1	1A	1624	G
1	1A	1625	G
1	1A	1631	A
1	1A	1633	G
1	1A	1634	A
1	1A	1638	A
1	1A	1640	C
1	1A	1642	A
1	1A	1654	G
1	1A	1661	C
1	1A	1663	C
1	1A	1676	C
1	1A	1677	U
1	1A	1691	G
1	1A	1697	G

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Mol	Chain	Res	Type
1	1A	1699	A
1	1A	1700	G
1	1A	1703	C
1	1A	1704	C
1	1A	1705	G
1	1A	1707	C
1	1A	1708	G
1	1A	1729	A
1	1A	1731	C
1	1A	1740	C
1	1A	1742	A
1	1A	1757	U
1	1A	1758	G
1	1A	1759	G
1	1A	1761	G
1	1A	1762	C
1	1A	1763	C
1	1A	1764	G
1	1A	1765	A
1	1A	1766	A
1	1A	1768	C
1	1A	1769	G
1	1A	1770	A
1	1A	1775	A
1	1A	1787	A
1	1A	1804	A
1	1A	1805	A
1	1A	1810	G
1	1A	1820	C
1	1A	1821	G
1	1A	1822	U
1	1A	1834	U
1	1A	1836	G
1	1A	1837	A
1	1A	1842	G
1	1A	1855	G
1	1A	1869	G
1	1A	1897	A
1	1A	1918	U
1	1A	1919	G
1	1A	1920	C
1	1A	1921	C

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Mol	Chain	Res	Type
1	1A	1922	G
1	1A	1925	G
1	1A	1931	C
1	1A	1932	A
1	1A	1940	G
1	1A	1948	G
1	1A	1959	U
1	1A	1960	A
1	1A	1961	G
1	1A	1962	A
1	1A	1966	C
1	1A	1968	G
1	1A	1974	U
1	1A	1975	G
1	1A	1978	C
1	1A	1980	U
1	1A	1981	G
1	1A	1982	G
1	1A	1983	A
1	1A	1984	A
1	1A	1985	G
1	1A	1987	C
1	1A	1988	G
1	1A	1991	A
1	1A	1993	C
1	1A	1995	G
1	1A	1996	C
1	1A	1998	A
1	1A	1999	A
1	1A	2001	G
1	1A	2002	A
1	1A	2003	G
1	1A	2004	U
1	1A	2005	G
1	1A	2006	U
1	1A	2007	G
1	1A	2009	A
1	1A	2010	A
1	1A	2011	C
1	1A	2012	A
1	1A	2013	A
1	1A	2015	U

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Mol	Chain	Res	Type
1	1A	2016	C
1	1A	2018	C
1	1A	2019	C
1	1A	2020	U
1	1A	2021	G
1	1A	2024	G
1	1A	2025	A
1	1A	2026	A
1	1A	2034	G
1	1A	2046	G
1	1A	2048	U
1	1A	2055	G
1	1A	2056	G
1	1A	2069	A
1	1A	2084	C
1	1A	2089	G
1	1A	2092	G
1	1A	2093	A
1	1A	2094	G
1	1A	2095	A
1	1A	2097	U
1	1A	2098	G
1	1A	2101	C
1	1A	2102	G
1	1A	2103	G
1	1A	2111	G
1	1A	2112	G
1	1A	2113	C
1	1A	2250	C
1	1A	2252	G
1	1A	2253	A
1	1A	2256	C
1	1A	2257	C
1	1A	2258	C
1	1A	2259	G
1	1A	2261	G
1	1A	2268	A
1	1A	2289	C
1	1A	2300	A
1	1A	2301	G
1	1A	2306	G
1	1A	2313	A

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Mol	Chain	Res	Type
1	1A	2333	G
1	1A	2348	G
1	1A	2351	C
1	1A	2360	A
1	1A	2370	A
1	1A	2390	G
1	1A	2395	A
1	1A	2397	G
1	1A	2417	A
1	1A	2421	G
1	1A	2428	A
1	1A	2441	C
1	1A	2460	A
1	1A	2461	G
1	1A	2465	C
1	1A	2469	C
1	1A	2470	C
1	1A	2471	G
1	1A	2474	G
1	1A	2475	G
1	1A	2483	G
1	1A	2484	A
1	1A	2485	U
1	1A	2487	G
1	1A	2488	C
1	1A	2490	U
1	1A	2491	C
1	1A	2493	G
1	1A	2495	U
1	1A	2496	G
1	1A	2498	C
1	1A	2503	G
1	1A	2504	C
1	1A	2505	C
1	1A	2506	G
1	1A	2512	A
1	1A	2513	A
1	1A	2529	A
1	1A	2530	U
1	1A	2537	A
1	1A	2544	G
1	1A	2546	G

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Mol	Chain	Res	Type
1	1A	2547	G
1	1A	2553	A
1	1A	2554	U
1	1A	2555	G
1	1A	2556	G
1	1A	2560	C
1	1A	2561	C
1	1A	2563	C
1	1A	2564	G
1	1A	2566	G
1	1A	2569	G
1	1A	2583	C
1	1A	2586	G
1	1A	2587	A
1	1A	2589	C
1	1A	2601	A
1	1A	2602	G
1	1A	2618	G
1	1A	2638	G
1	1A	2640	G
1	1A	2653	C
1	1A	2662	G
1	1A	2669	C
1	1A	2670	C
1	1A	2676	A
1	1A	2679	G
1	1A	2687	U
1	1A	2695	A
1	1A	2696	A
1	1A	2708	U
1	1A	2710	C
1	1A	2711	G
1	1A	2712	G
1	1A	2725	A
1	1A	2726	G
1	1A	2739	C
1	1A	2743	A
1	1A	2759	G
1	1A	2761	U
1	1A	2762	G
1	1A	2763	U
1	1A	2767	U

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Mol	Chain	Res	Type
1	1A	2768	C
1	1A	2769	U
1	1A	2770	C
1	1A	2776	G
1	1A	2787	A
1	1A	2788	U
1	1A	2790	U
1	1A	2794	C
1	1A	2797	C
1	1A	2798	A
1	1A	2814	C
1	1A	2826	U
1	1A	2827	G
1	1A	2829	U
1	1A	2855	G
1	1A	2860	C
1	1A	2870	A
1	1A	2875	C
1	1A	2877	G
1	1A	2905	C
1	1A	2906	G
1	1A	2908	U
1	1A	3585	G
1	1A	3586	G
1	1A	3588	C
1	1A	3591	C
1	1A	3592	G
1	1A	3593	C
1	1A	3595	U
1	1A	3596	A
1	1A	3597	G
1	1A	3605	C
1	1A	3617	G
1	1A	3626	G
1	1A	3635	A
1	1A	3642	A
1	1A	3644	U
1	1A	3646	A
1	1A	3648	A
1	1A	3662	A
1	1A	3664	G
1	1A	3670	C

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Mol	Chain	Res	Type
1	1A	3671	G
1	1A	3673	C
1	1A	3696	C
1	1A	3710	G
1	1A	3711	A
1	1A	3712	A
1	1A	3713	U
1	1A	3714	G
1	1A	3727	A
1	1A	3728	A
1	1A	3748	A
1	1A	3753	G
1	1A	3758	U
1	1A	3760	A
1	1A	3761	C
1	1A	3763	A
1	1A	3769	C
1	1A	3771	C
1	1A	3773	U
1	1A	3774	A
1	1A	3776	G
1	1A	3777	G
1	1A	3783	A
1	1A	3784	A
1	1A	3785	A
1	1A	3786	U
1	1A	3811	G
1	1A	3817	A
1	1A	3818	U
1	1A	3819	G
1	1A	3838	U
1	1A	3839	G
1	1A	3840	U
1	1A	3867	A
1	1A	3869	C
1	1A	3874	G
1	1A	3877	A
1	1A	3878	C
1	1A	3879	G
1	1A	3885	G
1	1A	3889	G
1	1A	3897	G

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Mol	Chain	Res	Type
1	1A	3898	G
1	1A	3901	A
1	1A	3905	A
1	1A	3906	A
1	1A	3907	G
1	1A	3908	A
1	1A	3915	U
1	1A	3922	G
1	1A	3923	A
1	1A	3937	C
1	1A	3938	G
1	1A	3939	G
1	1A	3942	A
1	1A	3947	A
1	1A	3948	C
1	1A	3950	U
1	1A	3951	G
1	1A	3952	A
1	1A	3954	A
1	1A	3955	G
1	1A	3956	G
1	1A	3957	U
1	1A	3958	G
1	1A	3959	U
1	1A	3960	A
1	1A	3961	G
1	1A	3962	A
1	1A	3963	A
1	1A	3964	U
1	1A	3965	A
1	1A	3966	A
1	1A	3968	U
1	1A	3970	G
1	1A	3973	G
1	1A	3975	C
1	1A	4035	G
1	1A	4036	G
1	1A	4038	C
1	1A	4039	G
1	1A	4041	C
1	1A	4042	G
1	1A	4043	G

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Mol	Chain	Res	Type
1	1A	4044	U
1	1A	4046	A
1	1A	4048	A
1	1A	4049	U
1	1A	4051	C
1	1A	4053	A
1	1A	4054	C
1	1A	4055	U
1	1A	4056	A
1	1A	4057	C
1	1A	4059	C
1	1A	4061	G
1	1A	4064	C
1	1A	4065	G
1	1A	4066	U
1	1A	4076	G
1	1A	4084	G
1	1A	4086	G
1	1A	4088	C
1	1A	4099	G
1	1A	4100	C
1	1A	4101	C
1	1A	4102	C
1	1A	4104	G
1	1A	4105	A
1	1A	4106	G
1	1A	4107	G
1	1A	4108	G
1	1A	4109	G
1	1A	4110	C
1	1A	4111	U
1	1A	4112	C
1	1A	4114	C
1	1A	4115	G
1	1A	4116	C
1	1A	4119	C
1	1A	4120	U
1	1A	4121	G
1	1A	4122	G
1	1A	4127	A
1	1A	4141	G
1	1A	4142	C

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Mol	Chain	Res	Type
1	1A	4143	G
1	1A	4144	C
1	1A	4154	G
1	1A	4162	C
1	1A	4163	U
1	1A	4168	G
1	1A	4170	A
1	1A	4183	G
1	1A	4184	G
1	1A	4191	G
1	1A	4201	G
1	1A	4203	A
1	1A	4204	C
1	1A	4214	A
1	1A	4229	U
1	1A	4233	A
1	1A	4251	A
1	1A	4254	G
1	1A	4256	A
1	1A	4268	A
1	1A	4273	A
1	1A	4280	A
1	1A	4288	C
1	1A	4291	G
1	1A	4305	G
1	1A	4306	U
1	1A	4314	C
1	1A	4318	C
1	1A	4329	G
1	1A	4330	G
1	1A	4332	C
1	1A	4337	C
1	1A	4338	G
1	1A	4339	A
1	1A	4348	A
1	1A	4349	C
1	1A	4350	C
1	1A	4376	A
1	1A	4377	G
1	1A	4378	A
1	1A	4380	A
1	1A	4387	C

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Mol	Chain	Res	Type
1	1A	4391	G
1	1A	4393	G
1	1A	4394	A
1	1A	4420	U
1	1A	4422	A
1	1A	4448	G
1	1A	4449	A
1	1A	4453	C
1	1A	4464	A
1	1A	4465	U
1	1A	4476	C
1	1A	4500	U
1	1A	4512	U
1	1A	4513	A
1	1A	4515	G
1	1A	4519	C
1	1A	4524	G
1	1A	4528	G
1	1A	4545	G
1	1A	4548	A
1	1A	4555	U
1	1A	4556	U
1	1A	4560	C
1	1A	4567	G
1	1A	4573	G
1	1A	4575	G
1	1A	4589	A
1	1A	4590	A
1	1A	4600	G
1	1A	4601	U
1	1A	4617	G
1	1A	4636	U
1	1A	4637	G
1	1A	4647	G
1	1A	4657	U
1	1A	4670	C
1	1A	4672	A
1	1A	4694	G
1	1A	4695	C
1	1A	4700	A
1	1A	4708	A
1	1A	4709	U

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Mol	Chain	Res	Type
1	1A	4730	C
1	1A	4731	G
1	1A	4732	G
1	1A	4737	G
1	1A	4740	G
1	1A	4741	C
1	1A	4743	G
1	1A	4744	A
1	1A	4749	C
1	1A	4750	G
1	1A	4753	U
1	1A	4754	G
1	1A	4756	C
1	1A	4758	U
1	1A	4760	G
1	1A	4764	A
1	1A	4770	U
1	1A	4772	C
1	1A	4775	C
1	1A	4776	G
1	1A	4861	G
1	1A	4863	G
1	1A	4869	U
1	1A	4871	C
1	1A	4872	G
1	1A	4873	G
1	1A	4874	A
1	1A	4875	G
1	1A	4876	U
1	1A	4882	U
1	1A	4883	C
1	1A	4884	G
1	1A	4887	C
1	1A	4888	U
1	1A	4889	G
1	1A	4890	G
1	1A	4894	A
1	1A	4895	C
1	1A	4896	G
1	1A	4897	G
1	1A	4900	C
1	1A	4901	G

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Mol	Chain	Res	Type
1	1A	4902	C
1	1A	4910	G
1	1A	4912	G
1	1A	4914	C
1	1A	4925	U
1	1A	4926	C
1	1A	4940	C
1	1A	4941	G
1	1A	4943	A
1	1A	4947	U
1	1A	4951	G
1	1A	4955	A
1	1A	4960	G
1	1A	4966	A
1	1A	4976	U
1	1A	4988	U
1	1A	4989	U
1	1A	4991	U
1	1A	5007	A
1	1A	5014	A
1	1A	5017	G
1	1A	5022	U
1	1A	5023	C
1	1A	5024	C
1	1A	5025	C
1	1A	5030	U
1	1A	5034	A
1	1A	5041	G
1	1A	5050	C
1	1A	5054	C
1	1A	5069	U
2	1B	11	A
2	1B	22	A
2	1B	24	C
2	1B	29	C
2	1B	33	U
2	1B	34	C
2	1B	53	U
2	1B	64	G
2	1B	66	G
2	1B	97	G
2	1B	100	A

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Mol	Chain	Res	Type
2	1B	103	A
2	1B	110	G
2	1B	120	U
3	1C	17	A
3	1C	23	C
3	1C	34	U
3	1C	35	C
3	1C	48	A
3	1C	52	A
3	1C	59	A
3	1C	63	U
3	1C	82	A
3	1C	83	C
3	1C	84	A
3	1C	86	U
3	1C	87	G
3	1C	88	A
3	1C	103	A
3	1C	105	C
3	1C	108	A
3	1C	110	U
3	1C	114	G
3	1C	122	G
3	1C	123	U
3	1C	124	U
3	1C	125	C
3	1C	126	C
3	1C	127	U
3	1C	129	C
3	1C	150	C
3	1C	151	G
47	2m	2	A
47	2m	17	C
47	2m	25	A
47	2m	26	U
47	2m	33	G
47	2m	41	G
47	2m	42	A
47	2m	44	U
47	2m	46	A
47	2m	56	G
47	2m	60	A

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Mol	Chain	Res	Type
47	2m	61	A
47	2m	64	A
47	2m	66	G
47	2m	67	C
47	2m	68	A
47	2m	70	G
47	2m	72	C
47	2m	73	C
47	2m	74	G
47	2m	75	G
47	2m	76	U
47	2m	77	A
47	2m	78	C
47	2m	79	A
47	2m	80	G
47	2m	103	A
47	2m	113	G
47	2m	115	U
47	2m	124	U
47	2m	125	C
47	2m	126	G
47	2m	127	C
47	2m	139	C
47	2m	141	A
47	2m	143	U
47	2m	148	U
47	2m	155	G
47	2m	159	A
47	2m	161	U
47	2m	162	C
47	2m	167	G
47	2m	168	C
47	2m	173	A
47	2m	183	G
47	2m	184	G
47	2m	188	C
47	2m	190	G
47	2m	194	C
47	2m	198	U
47	2m	199	C
47	2m	206	G
47	2m	207	G

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Mol	Chain	Res	Type
47	2m	208	G
47	2m	214	U
47	2m	215	G
47	2m	216	C
47	2m	225	G
47	2m	290	U
47	2m	291	G
47	2m	292	A
47	2m	293	C
47	2m	295	C
47	2m	302	A
47	2m	304	C
47	2m	306	C
47	2m	307	G
47	2m	308	G
47	2m	309	G
47	2m	312	G
47	2m	313	A
47	2m	317	C
47	2m	320	G
47	2m	324	C
47	2m	325	C
47	2m	326	C
47	2m	328	U
47	2m	330	G
47	2m	331	C
47	2m	332	G
47	2m	334	C
47	2m	338	G
47	2m	339	A
47	2m	340	C
47	2m	347	G
47	2m	362	C
47	2m	364	A
47	2m	370	G
47	2m	385	G
47	2m	386	C
47	2m	399	C
47	2m	400	C
47	2m	407	G
47	2m	408	A
47	2m	409	C

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Mol	Chain	Res	Type
47	2m	413	G
47	2m	418	A
47	2m	419	G
47	2m	438	G
47	2m	448	A
47	2m	450	C
47	2m	462	C
47	2m	465	A
47	2m	466	G
47	2m	471	G
47	2m	472	C
47	2m	473	A
47	2m	474	G
47	2m	482	G
47	2m	487	U
47	2m	488	U
47	2m	489	A
47	2m	492	C
47	2m	493	A
47	2m	503	C
47	2m	516	A
47	2m	532	C
47	2m	533	A
47	2m	534	G
47	2m	537	C
47	2m	538	U
47	2m	539	C
47	2m	540	U
47	2m	541	U
47	2m	542	U
47	2m	543	C
47	2m	544	G
47	2m	545	A
47	2m	547	G
47	2m	548	C
47	2m	549	C
47	2m	550	C
47	2m	551	U
47	2m	553	U
47	2m	554	A
47	2m	555	A
47	2m	556	U

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Mol	Chain	Res	Type
47	2m	557	U
47	2m	559	G
47	2m	561	A
47	2m	562	U
47	2m	563	G
47	2m	575	A
47	2m	580	U
47	2m	581	U
47	2m	582	C
47	2m	583	C
47	2m	587	A
47	2m	589	G
47	2m	590	A
47	2m	591	U
47	2m	592	C
47	2m	595	U
47	2m	596	U
47	2m	604	A
47	2m	605	A
47	2m	606	G
47	2m	608	C
47	2m	612	U
47	2m	613	G
47	2m	614	C
47	2m	615	C
47	2m	617	G
47	2m	627	U
47	2m	631	U
47	2m	632	C
47	2m	643	A
47	2m	644	G
47	2m	656	G
47	2m	660	C
47	2m	668	A
47	2m	669	A
47	2m	672	A
47	2m	688	U
47	2m	689	U
47	2m	691	G
47	2m	692	G
47	2m	693	A
47	2m	694	G

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Mol	Chain	Res	Type
47	2m	695	C
47	2m	697	G
47	2m	698	G
47	2m	732	U
47	2m	733	C
47	2m	734	C
47	2m	735	C
47	2m	736	C
47	2m	738	C
47	2m	747	U
47	2m	748	C
47	2m	749	U
47	2m	751	G
47	2m	752	G
47	2m	753	C
47	2m	787	G
47	2m	788	G
47	2m	789	G
47	2m	793	G
47	2m	795	A
47	2m	796	G
47	2m	798	A
47	2m	799	U
47	2m	801	U
47	2m	810	A
47	2m	811	A
47	2m	812	A
47	2m	821	G
47	2m	822	U
47	2m	830	A
47	2m	834	C
47	2m	836	G
47	2m	837	A
47	2m	838	G
47	2m	839	C
47	2m	840	C
47	2m	842	C
47	2m	847	A
47	2m	848	U
47	2m	851	C
47	2m	869	A
47	2m	870	A

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Mol	Chain	Res	Type
47	2m	873	G
47	2m	874	G
47	2m	875	A
47	2m	877	C
47	2m	878	G
47	2m	879	C
47	2m	880	G
47	2m	882	U
47	2m	883	U
47	2m	885	U
47	2m	886	A
47	2m	887	U
47	2m	888	U
47	2m	889	U
47	2m	890	U
47	2m	891	G
47	2m	893	U
47	2m	894	G
47	2m	895	G
47	2m	896	U
47	2m	897	U
47	2m	898	U
47	2m	899	U
47	2m	900	C
47	2m	901	G
47	2m	903	A
47	2m	904	A
47	2m	907	G
47	2m	908	A
47	2m	912	C
47	2m	913	A
47	2m	917	U
47	2m	919	A
47	2m	920	A
47	2m	922	A
47	2m	933	G
47	2m	934	G
47	2m	944	A
47	2m	958	G
47	2m	970	G
47	2m	971	G
47	2m	990	A

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Mol	Chain	Res	Type
47	2m	992	A
47	2m	996	A
47	2m	999	G
47	2m	1001	A
47	2m	1011	A
47	2m	1012	A
47	2m	1027	A
47	2m	1028	A
47	2m	1042	A
47	2m	1043	G
47	2m	1060	A
47	2m	1061	U
47	2m	1062	A
47	2m	1083	A
47	2m	1085	C
47	2m	1088	U
47	2m	1089	G
47	2m	1110	G
47	2m	1113	A
47	2m	1114	U
47	2m	1115	U
47	2m	1116	C
47	2m	1119	A
47	2m	1131	G
47	2m	1133	A
47	2m	1139	C
47	2m	1150	A
47	2m	1153	C
47	2m	1154	U
47	2m	1157	G
47	2m	1181	A
47	2m	1183	A
47	2m	1195	A
47	2m	1207	G
47	2m	1208	A
47	2m	1215	C
47	2m	1216	C
47	2m	1217	A
47	2m	1221	G
47	2m	1224	G
47	2m	1241	A
47	2m	1242	U

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Mol	Chain	Res	Type
47	2m	1243	U
47	2m	1251	A
47	2m	1253	A
47	2m	1256	G
47	2m	1257	G
47	2m	1260	A
47	2m	1261	C
47	2m	1262	C
47	2m	1263	U
47	2m	1265	A
47	2m	1273	C
47	2m	1274	G
47	2m	1275	G
47	2m	1280	G
47	2m	1281	G
47	2m	1282	A
47	2m	1283	C
47	2m	1284	A
47	2m	1285	G
47	2m	1286	G
47	2m	1288	U
47	2m	1289	U
47	2m	1290	G
47	2m	1291	A
47	2m	1293	A
47	2m	1294	G
47	2m	1297	U
47	2m	1299	A
47	2m	1300	U
47	2m	1301	A
47	2m	1302	G
47	2m	1303	C
47	2m	1304	U
47	2m	1306	U
47	2m	1307	U
47	2m	1314	U
47	2m	1315	U
47	2m	1316	C
47	2m	1318	G
47	2m	1321	G
47	2m	1326	U
47	2m	1330	G

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Mol	Chain	Res	Type
47	2m	1331	C
47	2m	1332	A
47	2m	1342	U
47	2m	1371	U
47	2m	1372	U
47	2m	1373	C
47	2m	1375	G
47	2m	1378	A
47	2m	1396	A
47	2m	1397	U
47	2m	1401	A
47	2m	1402	A
47	2m	1403	C
47	2m	1404	U
47	2m	1405	A
47	2m	1407	U
47	2m	1412	C
47	2m	1413	G
47	2m	1414	A
47	2m	1415	C
47	2m	1416	C
47	2m	1417	C
47	2m	1418	C
47	2m	1419	C
47	2m	1420	G
47	2m	1422	G
47	2m	1426	U
47	2m	1427	C
47	2m	1428	G
47	2m	1431	G
47	2m	1436	C
47	2m	1438	A
47	2m	1439	A
47	2m	1440	C
47	2m	1442	U
47	2m	1444	U
47	2m	1449	G
47	2m	1450	G
47	2m	1454	A
47	2m	1462	U
47	2m	1463	U
47	2m	1465	A

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Mol	Chain	Res	Type
47	2m	1473	G
47	2m	1475	G
47	2m	1476	A
47	2m	1477	U
47	2m	1487	A
47	2m	1489	A
47	2m	1490	G
47	2m	1494	U
47	2m	1498	A
47	2m	1505	U
47	2m	1507	G
47	2m	1508	A
47	2m	1510	G
47	2m	1512	C
47	2m	1515	G
47	2m	1517	G
47	2m	1520	G
47	2m	1521	C
47	2m	1522	A
47	2m	1523	C
47	2m	1524	G
47	2m	1526	G
47	2m	1527	C
47	2m	1533	A
47	2m	1539	U
47	2m	1543	U
47	2m	1544	C
47	2m	1548	G
47	2m	1552	G
47	2m	1553	C
47	2m	1554	C
47	2m	1567	G
47	2m	1570	G
47	2m	1575	G
47	2m	1580	A
47	2m	1585	U
47	2m	1586	U
47	2m	1587	G
47	2m	1588	A
47	2m	1589	A
47	2m	1591	C
47	2m	1594	A

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Mol	Chain	Res	Type
47	2m	1598	G
47	2m	1602	U
47	2m	1604	G
47	2m	1621	U
47	2m	1623	A
47	2m	1624	U
47	2m	1626	C
47	2m	1627	C
47	2m	1628	C
47	2m	1632	G
47	2m	1634	A
47	2m	1637	A
47	2m	1639	G
47	2m	1644	C
47	2m	1648	G
47	2m	1654	G
47	2m	1664	A
47	2m	1665	G
47	2m	1666	C
47	2m	1672	U
47	2m	1680	G
47	2m	1694	U
47	2m	1695	A
47	2m	1699	A
47	2m	1719	A
47	2m	1721	U
47	2m	1722	G
47	2m	1742	C
47	2m	1743	G
47	2m	1744	G
47	2m	1745	A
47	2m	1746	U
47	2m	1753	C
47	2m	1755	C
47	2m	1756	C
47	2m	1758	G
47	2m	1759	G
47	2m	1761	U
47	2m	1771	G
47	2m	1773	C
47	2m	1779	G
47	2m	1780	G

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Mol	Chain	Res	Type
47	2m	1781	A
47	2m	1782	G
47	2m	1783	C
47	2m	1786	U
47	2m	1813	A
47	2m	1815	A
47	2m	1819	A
47	2m	1821	U
47	2m	1829	G
47	2m	1838	U
47	2m	1849	G
47	2m	1850	A
47	2m	1851	A
47	2m	1852	C
47	2m	1860	A
47	2m	1861	G
47	2m	1862	G
47	2m	1863	A
47	2m	1864	U
47	2m	1865	C
47	2m	1869	A

All (58) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	1	C
1	1A	66	A
1	1A	179	G
1	1A	264	C
1	1A	385	A
1	1A	406	C
1	1A	408	A
1	1A	417	G
1	1A	485	C
1	1A	499	G
1	1A	504	G
1	1A	914	U
1	1A	1048	G
1	1A	1173	G
1	1A	1180	C
1	1A	1197	C
1	1A	1220	G

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Mol	Chain	Res	Type
1	1A	1590	C
1	1A	1633	G
1	1A	2017	A
1	1A	2019	C
1	1A	2033	A
1	1A	2112	G
1	1A	2299	G
1	1A	2389	A
1	1A	2503	G
1	1A	2639	U
1	1A	2675	G
1	1A	2695	A
1	1A	2710	C
1	1A	2760	G
1	1A	2775	C
1	1A	3710	G
1	1A	3773	U
1	1A	3810	C
1	1A	3888	G
1	1A	3922	G
1	1A	4060	U
1	1A	4065	G
1	1A	4098	A
1	1A	4099	G
1	1A	4108	G
1	1A	4109	G
1	1A	4110	C
1	1A	4348	A
1	1A	4452	U
1	1A	4599	A
1	1A	4600	G
1	1A	4699	U
1	1A	4731	G
1	1A	4774	C
1	1A	4860	G
1	1A	4896	G
1	1A	4913	G
2	1B	33	U
2	1B	109	U
3	1C	16	G
3	1C	87	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
41	MLZ	2g	98	41	8,9,10	0.86	0	4,9,11	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	MLZ	2g	98	41	-	1/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 425 ligands modelled in this entry, 401 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
81	84D	1A	5106	-	32,33,33	1.56	7 (21%)	40,48,48	1.13	5 (12%)
81	84D	1A	5119	-	32,33,33	1.54	6 (18%)	40,48,48	1.08	3 (7%)
81	84D	1A	5112	-	32,33,33	1.61	7 (21%)	40,48,48	1.27	5 (12%)
81	84D	1A	5105	-	32,33,33	1.61	7 (21%)	40,48,48	1.21	5 (12%)
81	84D	1A	5104	-	32,33,33	1.61	9 (28%)	40,48,48	1.81	4 (10%)
81	84D	1A	5113	-	32,33,33	1.57	7 (21%)	40,48,48	1.23	5 (12%)
81	84D	2m	1901	-	32,33,33	1.55	7 (21%)	40,48,48	1.07	7 (17%)
81	84D	1A	5121	-	32,33,33	1.54	6 (18%)	40,48,48	1.00	3 (7%)
81	84D	1A	5116	-	32,33,33	1.53	6 (18%)	40,48,48	1.01	2 (5%)
81	84D	1A	5118	-	32,33,33	1.56	7 (21%)	40,48,48	0.98	3 (7%)
81	84D	1A	5103	-	32,33,33	1.52	6 (18%)	40,48,48	1.17	3 (7%)
81	84D	1A	5108	-	32,33,33	1.55	6 (18%)	40,48,48	1.15	3 (7%)
81	84D	2m	1902	-	32,33,33	1.55	6 (18%)	40,48,48	1.10	4 (10%)
81	84D	1A	5109	-	32,33,33	1.68	7 (21%)	40,48,48	1.80	8 (20%)
81	84D	1A	5114	-	32,33,33	1.56	7 (21%)	40,48,48	1.09	4 (10%)
81	84D	1A	5120	-	32,33,33	1.54	6 (18%)	40,48,48	1.10	3 (7%)
81	84D	1A	5107	-	32,33,33	1.59	7 (21%)	40,48,48	1.11	4 (10%)
81	84D	1A	5110	-	32,33,33	1.56	6 (18%)	40,48,48	1.14	4 (10%)
81	84D	1A	5101	-	32,33,33	1.56	7 (21%)	40,48,48	1.04	3 (7%)
81	84D	1A	5102	-	32,33,33	1.57	7 (21%)	40,48,48	1.24	4 (10%)
81	84D	1A	5117	-	32,33,33	1.57	7 (21%)	40,48,48	1.17	4 (10%)
81	84D	2m	1903	-	32,33,33	1.56	6 (18%)	40,48,48	1.07	5 (12%)
81	84D	1A	5115	-	32,33,33	1.57	7 (21%)	40,48,48	1.07	5 (12%)
81	84D	1A	5111	-	32,33,33	1.56	6 (18%)	40,48,48	0.99	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	84D	1A	5106	-	-	5/12/65/65	0/3/3/3
81	84D	1A	5119	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5112	-	-	2/12/65/65	0/3/3/3
81	84D	1A	5105	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5104	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5113	-	-	2/12/65/65	0/3/3/3
81	84D	2m	1901	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5121	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5116	-	-	5/12/65/65	0/3/3/3
81	84D	1A	5118	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5103	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5108	-	-	6/12/65/65	0/3/3/3
81	84D	2m	1902	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5109	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5114	-	-	3/12/65/65	0/3/3/3
81	84D	1A	5120	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5107	-	-	2/12/65/65	0/3/3/3
81	84D	1A	5110	-	-	3/12/65/65	1/3/3/3
81	84D	1A	5101	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5102	-	-	2/12/65/65	0/3/3/3
81	84D	1A	5117	-	-	4/12/65/65	0/3/3/3
81	84D	2m	1903	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5115	-	-	4/12/65/65	0/3/3/3
81	84D	1A	5111	-	-	4/12/65/65	0/3/3/3

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	1A	5109	84D	C15-C14	-5.13	1.47	1.53
81	1A	5112	84D	C15-C14	-4.86	1.47	1.53
81	1A	5102	84D	C15-C14	-4.70	1.47	1.53
81	1A	5104	84D	C15-C14	-4.62	1.47	1.53
81	1A	5113	84D	C15-C14	-4.58	1.47	1.53
81	1A	5106	84D	C15-C14	-4.56	1.47	1.53
81	1A	5118	84D	C15-C14	-4.54	1.47	1.53
81	1A	5107	84D	C15-C14	-4.53	1.47	1.53
81	1A	5111	84D	C15-C14	-4.50	1.47	1.53
81	1A	5115	84D	C15-C14	-4.47	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	1A	5101	84D	C15-C14	-4.45	1.48	1.53
81	1A	5110	84D	C15-C14	-4.44	1.48	1.53
81	1A	5117	84D	C15-C14	-4.42	1.48	1.53
81	1A	5120	84D	C15-C14	-4.41	1.48	1.53
81	1A	5114	84D	C15-C14	-4.34	1.48	1.53
81	2m	1902	84D	C15-C14	-4.31	1.48	1.53
81	1A	5103	84D	C15-C14	-4.30	1.48	1.53
81	2m	1903	84D	C15-C14	-4.30	1.48	1.53
81	1A	5105	84D	C15-C14	-4.30	1.48	1.53
81	1A	5121	84D	C15-C14	-4.29	1.48	1.53
81	1A	5119	84D	C15-C14	-4.29	1.48	1.53
81	1A	5108	84D	C15-C14	-4.26	1.48	1.53
81	1A	5116	84D	C15-C14	-4.25	1.48	1.53
81	2m	1901	84D	C15-C14	-4.24	1.48	1.53
81	1A	5105	84D	C13-C14	-3.91	1.48	1.53
81	1A	5109	84D	C13-C14	-3.64	1.49	1.53
81	1A	5110	84D	C13-C14	-3.56	1.49	1.53
81	1A	5115	84D	C13-C14	-3.51	1.49	1.53
81	1A	5117	84D	C13-C14	-3.50	1.49	1.53
81	1A	5107	84D	C13-C14	-3.50	1.49	1.53
81	2m	1903	84D	C13-C14	-3.47	1.49	1.53
81	1A	5101	84D	C13-C14	-3.46	1.49	1.53
81	2m	1901	84D	C13-C14	-3.44	1.49	1.53
81	1A	5114	84D	C13-C14	-3.44	1.49	1.53
81	1A	5111	84D	C13-C14	-3.39	1.49	1.53
81	1A	5104	84D	C13-C14	-3.39	1.49	1.53
81	1A	5116	84D	C13-C14	-3.37	1.49	1.53
81	1A	5118	84D	C13-C14	-3.36	1.49	1.53
81	1A	5106	84D	C13-C14	-3.36	1.49	1.53
81	1A	5108	84D	C13-C14	-3.33	1.49	1.53
81	2m	1902	84D	C13-C14	-3.32	1.49	1.53
81	1A	5121	84D	C13-C14	-3.32	1.49	1.53
81	1A	5119	84D	C13-C14	-3.26	1.49	1.53
81	1A	5112	84D	C13-C14	-3.26	1.49	1.53
81	1A	5120	84D	C13-C14	-3.22	1.49	1.53
81	1A	5103	84D	C14-N1	3.20	1.52	1.47
81	1A	5113	84D	C14-N1	3.20	1.52	1.47
81	1A	5121	84D	C14-N1	3.19	1.52	1.47
81	1A	5114	84D	C14-N1	3.17	1.52	1.47
81	2m	1902	84D	C14-N1	3.17	1.52	1.47
81	2m	1903	84D	C14-N1	3.17	1.52	1.47
81	1A	5112	84D	C14-N1	3.16	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	1A	5116	84D	C14-N1	3.16	1.52	1.47
81	1A	5106	84D	C14-N1	3.15	1.52	1.47
81	1A	5105	84D	C14-N1	3.15	1.52	1.47
81	1A	5118	84D	C14-N1	3.15	1.52	1.47
81	2m	1901	84D	C14-N1	3.15	1.52	1.47
81	1A	5102	84D	C13-C14	-3.14	1.49	1.53
81	1A	5110	84D	C14-N1	3.13	1.52	1.47
81	1A	5120	84D	C14-N1	3.13	1.52	1.47
81	1A	5113	84D	C13-C14	-3.13	1.49	1.53
81	1A	5115	84D	C14-N1	3.13	1.52	1.47
81	1A	5119	84D	C14-N1	3.12	1.52	1.47
81	1A	5102	84D	C14-N1	3.12	1.52	1.47
81	1A	5117	84D	C14-N1	3.12	1.52	1.47
81	1A	5101	84D	C14-N1	3.11	1.52	1.47
81	1A	5103	84D	C13-C14	-3.11	1.49	1.53
81	1A	5108	84D	C14-N1	3.10	1.52	1.47
81	1A	5111	84D	C14-N1	3.09	1.52	1.47
81	1A	5104	84D	C14-N1	3.09	1.52	1.47
81	1A	5109	84D	C14-N1	3.09	1.52	1.47
81	1A	5107	84D	C14-N1	3.08	1.52	1.47
81	1A	5112	84D	O-C3	2.74	1.48	1.41
81	1A	5113	84D	O-C3	2.74	1.48	1.41
81	1A	5109	84D	O-C3	2.74	1.48	1.41
81	1A	5107	84D	O-C3	2.71	1.48	1.41
81	1A	5108	84D	O-C3	2.69	1.48	1.41
81	2m	1903	84D	O-C3	2.65	1.48	1.41
81	1A	5119	84D	O-C3	2.64	1.48	1.41
81	1A	5102	84D	O-C3	2.63	1.48	1.41
81	1A	5114	84D	O-C3	2.62	1.48	1.41
81	1A	5105	84D	O-C3	2.61	1.48	1.41
81	2m	1901	84D	O-C3	2.61	1.48	1.41
81	1A	5116	84D	O-C3	2.60	1.48	1.41
81	1A	5105	84D	O4-C16	2.57	1.50	1.44
81	1A	5101	84D	O-C3	2.54	1.48	1.41
81	1A	5115	84D	O-C3	2.54	1.48	1.41
81	1A	5120	84D	O-C3	2.54	1.48	1.41
81	1A	5118	84D	O-C3	2.52	1.48	1.41
81	1A	5104	84D	O-C3	2.52	1.48	1.41
81	2m	1902	84D	O-C3	2.52	1.48	1.41
81	1A	5110	84D	O-C3	2.49	1.48	1.41
81	1A	5109	84D	O4-C12	2.49	1.48	1.41
81	1A	5103	84D	O-C3	2.48	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	1A	5111	84D	O-C3	2.48	1.48	1.41
81	1A	5117	84D	O-C3	2.44	1.48	1.41
81	1A	5121	84D	O-C3	2.44	1.48	1.41
81	1A	5106	84D	O-C3	2.43	1.48	1.41
81	1A	5112	84D	O4-C12	2.39	1.47	1.41
81	1A	5107	84D	O4-C16	2.37	1.50	1.44
81	2m	1903	84D	O4-C16	2.34	1.50	1.44
81	1A	5117	84D	O4-C16	2.32	1.50	1.44
81	1A	5111	84D	O4-C16	2.31	1.50	1.44
81	1A	5114	84D	O4-C16	2.31	1.49	1.44
81	1A	5104	84D	O4-C16	2.30	1.49	1.44
81	1A	5109	84D	C-C1	-2.27	1.47	1.52
81	2m	1902	84D	O4-C16	2.27	1.49	1.44
81	1A	5113	84D	O4-C12	2.27	1.47	1.41
81	1A	5115	84D	O4-C16	2.26	1.49	1.44
81	1A	5121	84D	O4-C16	2.26	1.49	1.44
81	2m	1901	84D	O4-C16	2.26	1.49	1.44
81	1A	5108	84D	O4-C16	2.25	1.49	1.44
81	1A	5109	84D	O4-C16	2.25	1.49	1.44
81	1A	5101	84D	O4-C16	2.24	1.49	1.44
81	1A	5102	84D	O4-C12	2.24	1.47	1.41
81	1A	5110	84D	O4-C16	2.24	1.49	1.44
81	1A	5120	84D	O4-C16	2.23	1.49	1.44
81	1A	5116	84D	O4-C16	2.22	1.49	1.44
81	1A	5112	84D	O4-C16	2.22	1.49	1.44
81	1A	5104	84D	O-C4	2.21	1.47	1.44
81	1A	5113	84D	O4-C16	2.19	1.49	1.44
81	1A	5106	84D	O4-C12	2.19	1.47	1.41
81	1A	5119	84D	O4-C16	2.18	1.49	1.44
81	1A	5118	84D	O4-C16	2.17	1.49	1.44
81	1A	5113	84D	C-C1	-2.17	1.47	1.52
81	1A	5118	84D	O4-C12	2.17	1.47	1.41
81	1A	5112	84D	C-C1	-2.17	1.47	1.52
81	1A	5105	84D	O4-C12	2.17	1.47	1.41
81	1A	5114	84D	C-C1	-2.15	1.47	1.52
81	1A	5104	84D	O4-C12	2.14	1.47	1.41
81	1A	5104	84D	C-C1	-2.14	1.47	1.52
81	1A	5107	84D	O4-C12	2.13	1.47	1.41
81	1A	5107	84D	C-C1	-2.13	1.47	1.52
81	1A	5103	84D	O4-C16	2.13	1.49	1.44
81	1A	5108	84D	C-C1	-2.12	1.47	1.52
81	1A	5102	84D	C-C1	-2.12	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	1A	5106	84D	O4-C16	2.11	1.49	1.44
81	1A	5102	84D	O4-C16	2.11	1.49	1.44
81	1A	5111	84D	O4-C12	2.10	1.47	1.41
81	1A	5101	84D	O4-C12	2.10	1.47	1.41
81	1A	5119	84D	C-C1	-2.10	1.47	1.52
81	1A	5115	84D	O4-C12	2.09	1.47	1.41
81	1A	5105	84D	C-C1	-2.09	1.47	1.52
81	2m	1903	84D	C-C1	-2.08	1.47	1.52
81	1A	5116	84D	C-C1	-2.07	1.47	1.52
81	1A	5120	84D	C-C1	-2.07	1.47	1.52
81	2m	1901	84D	C-C1	-2.06	1.47	1.52
81	1A	5117	84D	O4-C12	2.06	1.47	1.41
81	1A	5115	84D	C-C1	-2.05	1.47	1.52
81	2m	1902	84D	O4-C12	2.05	1.47	1.41
81	1A	5104	84D	C1-C2	-2.05	1.47	1.52
81	1A	5118	84D	C-C1	-2.04	1.47	1.52
81	1A	5106	84D	C-C1	-2.03	1.47	1.52
81	1A	5110	84D	O4-C12	2.03	1.47	1.41
81	1A	5121	84D	O4-C12	2.02	1.47	1.41
81	1A	5114	84D	O4-C12	2.02	1.47	1.41
81	1A	5103	84D	C-C1	-2.02	1.47	1.52
81	2m	1901	84D	O4-C12	2.01	1.47	1.41
81	1A	5101	84D	C-C1	-2.00	1.47	1.52
81	1A	5117	84D	C-C1	-2.00	1.47	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	1A	5104	84D	O-C4-C	7.95	118.40	109.86
81	1A	5109	84D	C3-O-C4	4.66	118.30	113.13
81	1A	5104	84D	C3-O-C4	4.14	117.72	113.13
81	1A	5109	84D	O4-C12-C13	3.97	118.76	110.35
81	1A	5109	84D	C12-C13-C14	3.85	115.58	110.40
81	1A	5102	84D	C12-C13-C14	3.66	115.31	110.40
81	1A	5109	84D	O-C4-C	3.65	113.78	109.86
81	1A	5112	84D	C12-C13-C14	3.53	115.14	110.40
81	1A	5109	84D	O-C3-C2	3.40	117.84	110.25
81	1A	5113	84D	C12-C13-C14	3.40	114.97	110.40
81	1A	5104	84D	C1-C-C4	3.38	116.02	110.82
81	1A	5103	84D	O-C4-C	3.33	113.44	109.86
81	1A	5119	84D	O-C4-C	3.32	113.42	109.86
81	1A	5105	84D	O4-C16-C15	3.27	115.63	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	1A	5112	84D	C3-O1-C6	-3.12	110.25	117.96
81	1A	5104	84D	C-C4-C5	-3.11	106.89	112.83
81	1A	5102	84D	C3-O1-C6	-3.10	110.30	117.96
81	1A	5110	84D	O-C4-C	3.08	113.17	109.86
81	1A	5109	84D	C12-O3-C10	-3.04	110.44	117.96
81	1A	5120	84D	O-C4-C	3.02	113.11	109.86
81	1A	5117	84D	C10-C11-C6	3.02	115.22	108.96
81	1A	5103	84D	C3-O1-C6	-3.01	110.51	117.96
81	2m	1902	84D	O-C4-C	2.98	113.06	109.86
81	1A	5106	84D	C12-O3-C10	-2.96	110.65	117.96
81	1A	5107	84D	O-C4-C	2.91	112.99	109.86
81	1A	5118	84D	C3-O1-C6	-2.90	110.79	117.96
81	1A	5110	84D	C10-C11-C6	2.89	114.96	108.96
81	1A	5114	84D	C3-O1-C6	-2.86	110.89	117.96
81	1A	5117	84D	O-C4-C	2.83	112.90	109.86
81	1A	5105	84D	C3-O1-C6	-2.82	110.98	117.96
81	1A	5108	84D	O-C4-C	2.75	112.82	109.86
81	1A	5119	84D	C3-O1-C6	-2.71	111.25	117.96
81	1A	5108	84D	C10-C11-C6	2.71	114.58	108.96
81	1A	5118	84D	O-C4-C	2.70	112.77	109.86
81	1A	5112	84D	C12-O3-C10	-2.68	111.33	117.96
81	2m	1903	84D	C3-O1-C6	-2.67	111.35	117.96
81	1A	5105	84D	C12-O3-C10	-2.66	111.37	117.96
81	1A	5115	84D	C10-C11-C6	2.61	114.38	108.96
81	1A	5117	84D	C3-O1-C6	-2.60	111.53	117.96
81	1A	5102	84D	C12-O3-C10	-2.60	111.54	117.96
81	1A	5101	84D	C3-O1-C6	-2.59	111.56	117.96
81	2m	1902	84D	C10-C11-C6	2.58	114.31	108.96
81	2m	1902	84D	C3-O1-C6	-2.57	111.60	117.96
81	1A	5109	84D	C12-O4-C16	2.55	118.69	113.69
81	2m	1903	84D	O-C4-C	2.55	112.60	109.86
81	1A	5107	84D	C3-O1-C6	-2.52	111.72	117.96
81	1A	5106	84D	C12-C13-C14	2.50	113.76	110.40
81	1A	5101	84D	O-C4-C	2.46	112.50	109.86
81	1A	5121	84D	O-C4-C	2.44	112.48	109.86
81	1A	5109	84D	C10-C11-C6	2.44	114.01	108.96
81	1A	5116	84D	C3-O1-C6	-2.42	111.97	117.96
81	1A	5120	84D	C-C4-C5	-2.41	108.23	112.83
81	1A	5113	84D	C3-O1-C6	-2.40	112.03	117.96
81	1A	5114	84D	O-C4-C	2.39	112.43	109.86
81	2m	1901	84D	C12-O3-C10	-2.37	112.10	117.96
81	1A	5116	84D	O-C4-C	2.35	112.39	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	1A	5117	84D	C-C4-C5	-2.33	108.38	112.83
81	1A	5120	84D	C3-O1-C6	-2.33	112.20	117.96
81	1A	5115	84D	C12-O3-C10	-2.33	112.21	117.96
81	1A	5112	84D	O4-C12-C13	2.31	115.24	110.35
81	1A	5113	84D	C12-O3-C10	-2.30	112.26	117.96
81	1A	5106	84D	C3-O-C4	-2.29	110.60	113.13
81	1A	5110	84D	C-C4-C5	-2.29	108.46	112.83
81	1A	5111	84D	C3-O1-C6	-2.27	112.34	117.96
81	1A	5107	84D	C12-O3-C10	-2.27	112.34	117.96
81	1A	5121	84D	C10-C11-C6	2.27	113.67	108.96
81	1A	5106	84D	C3-O1-C6	-2.25	112.39	117.96
81	1A	5107	84D	C-C4-C5	-2.22	108.59	112.83
81	1A	5119	84D	C-C4-C5	-2.19	108.64	112.83
81	1A	5108	84D	C-C4-C5	-2.19	108.65	112.83
81	2m	1903	84D	O4-C16-C15	2.17	113.63	109.69
81	1A	5115	84D	C-C4-C5	-2.16	108.71	112.83
81	2m	1903	84D	C-C4-C5	-2.15	108.71	112.83
81	1A	5114	84D	C-C4-C5	-2.15	108.72	112.83
81	1A	5113	84D	O-C3-C2	2.14	115.03	110.25
81	1A	5102	84D	O4-C12-C13	2.14	114.89	110.35
81	2m	1901	84D	O-C4-C	2.12	112.14	109.86
81	2m	1901	84D	C3-O1-C6	-2.08	112.81	117.96
81	2m	1902	84D	C-C4-C5	-2.08	108.85	112.83
81	1A	5106	84D	C10-C11-C6	2.08	113.28	108.96
81	1A	5105	84D	O-C4-C	2.08	112.09	109.86
81	1A	5114	84D	O4-C16-C15	2.07	113.46	109.69
81	1A	5101	84D	C12-O3-C10	-2.07	112.84	117.96
81	1A	5110	84D	C12-O3-C10	-2.07	112.84	117.96
81	1A	5121	84D	C3-O1-C6	-2.07	112.84	117.96
81	1A	5103	84D	C-C4-C5	-2.07	108.88	112.83
81	2m	1901	84D	C-C4-C5	-2.07	108.88	112.83
81	1A	5105	84D	C-C4-C5	-2.06	108.89	112.83
81	2m	1901	84D	C10-C11-C6	2.05	113.21	108.96
81	2m	1903	84D	C17-C16-C15	-2.05	108.21	113.00
81	1A	5112	84D	C-C4-C5	-2.04	108.92	112.83
81	1A	5118	84D	C12-O3-C10	-2.04	112.91	117.96
81	1A	5115	84D	C17-C16-C15	-2.02	108.28	113.00
81	2m	1901	84D	C17-C16-C15	-2.01	108.28	113.00
81	2m	1901	84D	O4-C16-C15	2.01	113.35	109.69
81	1A	5113	84D	C-C4-C5	-2.01	108.99	112.83
81	1A	5115	84D	O-C4-C	2.00	112.02	109.86

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	1A	5101	84D	O-C4-C5-N
81	1A	5101	84D	C-C4-C5-N
81	1A	5104	84D	O-C4-C5-N
81	1A	5105	84D	O-C4-C5-N
81	1A	5105	84D	C-C4-C5-N
81	1A	5106	84D	O-C4-C5-N
81	1A	5106	84D	C-C4-C5-N
81	1A	5107	84D	O-C4-C5-N
81	1A	5108	84D	O-C4-C5-N
81	1A	5108	84D	C-C4-C5-N
81	1A	5110	84D	C2-C3-O1-C6
81	1A	5111	84D	O-C4-C5-N
81	1A	5111	84D	C-C4-C5-N
81	1A	5113	84D	O-C4-C5-N
81	1A	5113	84D	C-C4-C5-N
81	1A	5114	84D	O-C4-C5-N
81	1A	5115	84D	O-C4-C5-N
81	1A	5116	84D	O-C4-C5-N
81	1A	5116	84D	C-C4-C5-N
81	1A	5117	84D	O-C4-C5-N
81	1A	5117	84D	C-C4-C5-N
81	1A	5118	84D	O-C4-C5-N
81	1A	5119	84D	O-C4-C5-N
81	1A	5119	84D	C-C4-C5-N
81	1A	5120	84D	C-C4-C5-N
81	1A	5121	84D	O-C4-C5-N
81	1A	5121	84D	C-C4-C5-N
81	2m	1901	84D	O-C4-C5-N
81	2m	1902	84D	O-C4-C5-N
81	2m	1903	84D	O-C4-C5-N
81	1A	5118	84D	O4-C16-C17-O5
81	1A	5102	84D	O4-C16-C17-O5
81	1A	5112	84D	O4-C16-C17-O5
81	2m	1902	84D	O4-C16-C17-O5
81	1A	5106	84D	O4-C16-C17-O5
81	1A	5120	84D	O4-C16-C17-O5
81	1A	5121	84D	O4-C16-C17-O5
81	1A	5102	84D	C15-C16-C17-O5
81	1A	5109	84D	C15-C16-C17-O5
81	1A	5114	84D	C15-C16-C17-O5
81	1A	5120	84D	C15-C16-C17-O5
81	1A	5109	84D	O4-C16-C17-O5

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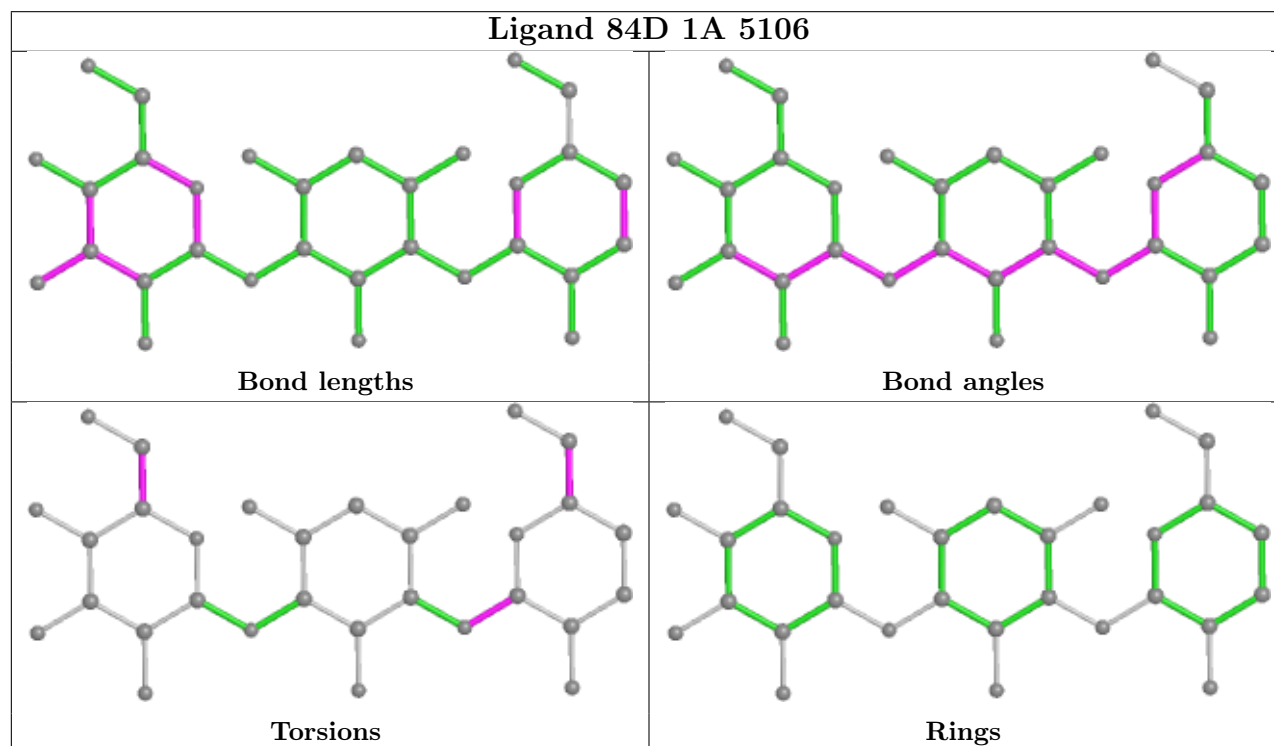
Mol	Chain	Res	Type	Atoms
81	1A	5116	84D	C15-C16-C17-O5
81	1A	5118	84D	C15-C16-C17-O5
81	1A	5114	84D	O4-C16-C17-O5
81	1A	5111	84D	C15-C16-C17-O5
81	2m	1902	84D	C15-C16-C17-O5
81	1A	5117	84D	O4-C16-C17-O5
81	1A	5112	84D	C15-C16-C17-O5
81	1A	5115	84D	O-C3-O1-C6
81	1A	5110	84D	O4-C12-O3-C10
81	1A	5110	84D	C13-C12-O3-C10
81	1A	5117	84D	C15-C16-C17-O5
81	1A	5121	84D	C15-C16-C17-O5
81	1A	5116	84D	O4-C16-C17-O5
81	2m	1903	84D	C15-C16-C17-O5
81	1A	5111	84D	O4-C16-C17-O5
81	1A	5108	84D	C15-C16-C17-O5
81	1A	5106	84D	C15-C16-C17-O5
81	1A	5118	84D	O4-C12-O3-C10
81	1A	5101	84D	O4-C16-C17-O5
81	2m	1903	84D	O4-C16-C17-O5
81	1A	5115	84D	C11-C6-O1-C3
81	1A	5103	84D	C15-C16-C17-O5
81	1A	5106	84D	O-C3-O1-C6
81	1A	5108	84D	O4-C16-C17-O5
81	1A	5108	84D	C11-C6-O1-C3
81	1A	5103	84D	O4-C16-C17-O5
81	1A	5105	84D	O4-C16-C17-O5
81	1A	5103	84D	O-C4-C5-N
81	1A	5109	84D	O-C4-C5-N
81	1A	5115	84D	C7-C6-O1-C3
81	1A	5120	84D	O-C4-C5-N
81	1A	5104	84D	C15-C16-C17-O5
81	1A	5107	84D	O4-C16-C17-O5
81	2m	1901	84D	O-C3-O1-C6
81	2m	1903	84D	O-C3-O1-C6
81	1A	5104	84D	C11-C6-O1-C3
81	1A	5108	84D	O-C3-O1-C6
81	1A	5119	84D	O4-C16-C17-O5
81	1A	5116	84D	O-C3-O1-C6
81	1A	5101	84D	C15-C16-C17-O5
81	2m	1901	84D	C11-C6-O1-C3
81	1A	5104	84D	C2-C3-O1-C6

All (1) ring outliers are listed below:

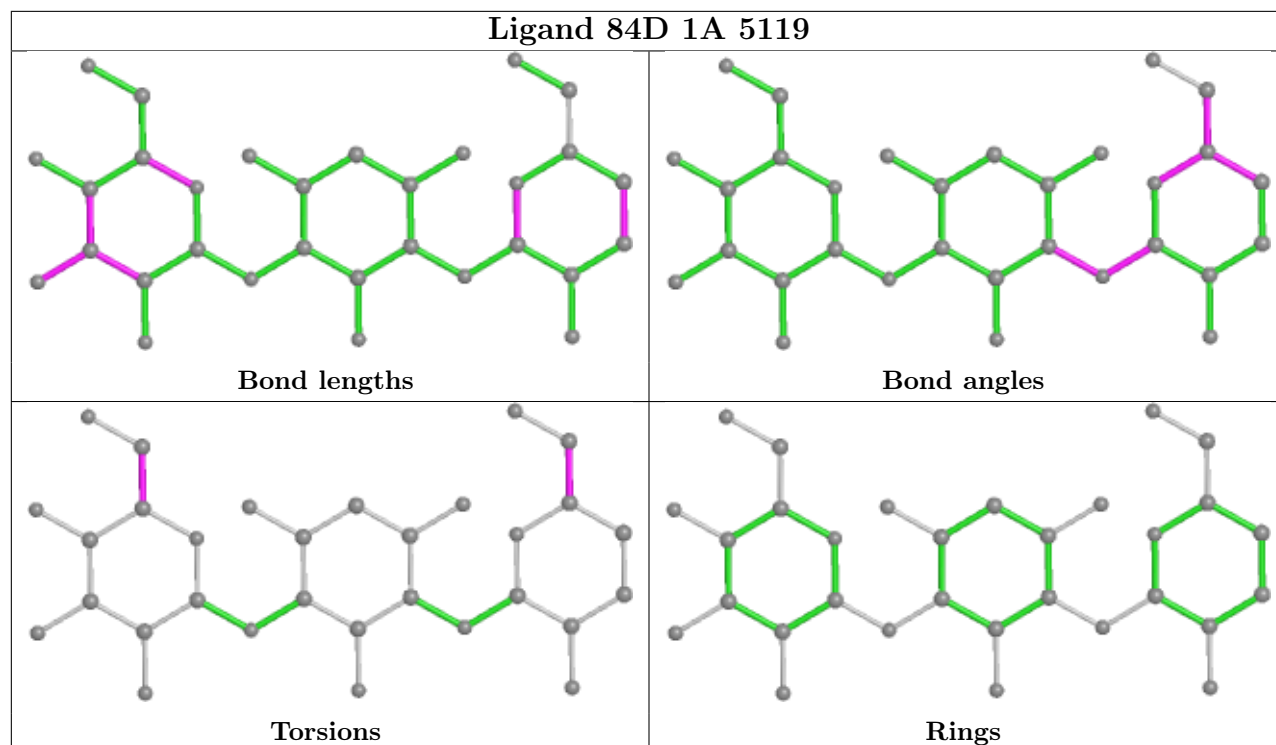
Mol	Chain	Res	Type	Atoms
81	1A	5110	84D	C-C1-C2-C3-C4-O

No monomer is involved in short contacts.

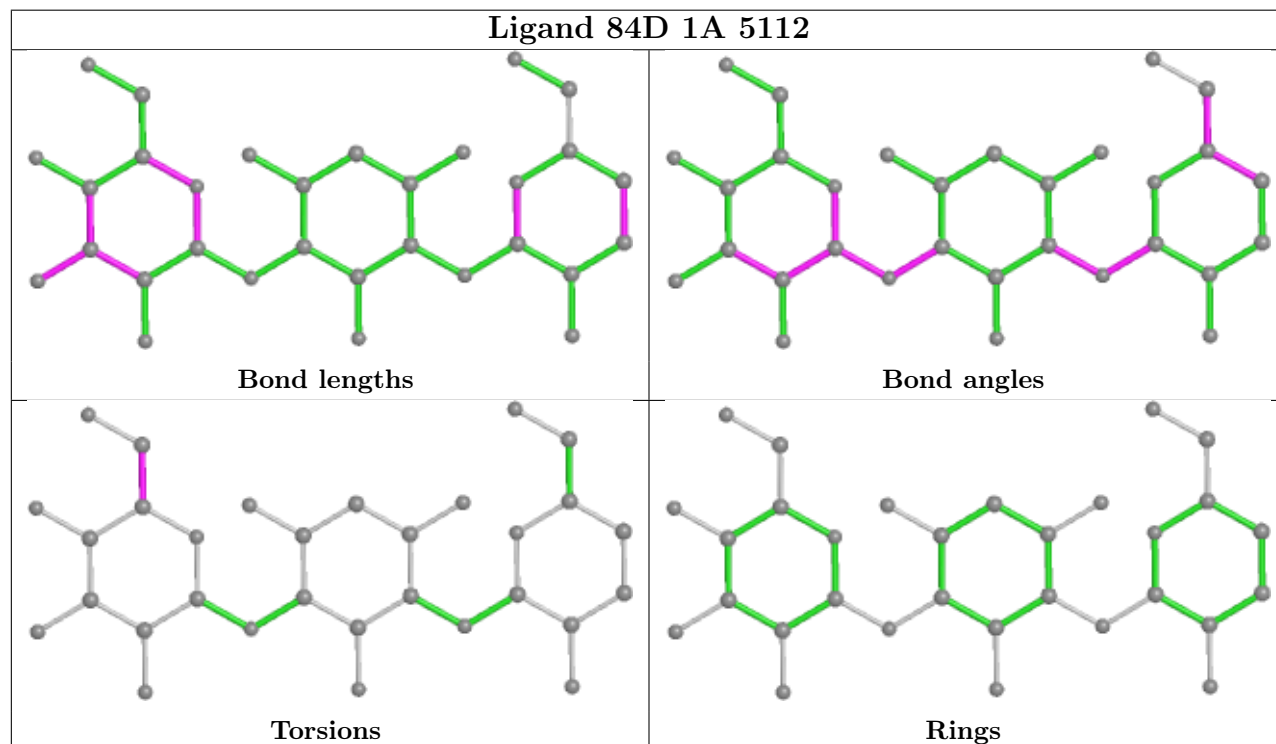
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



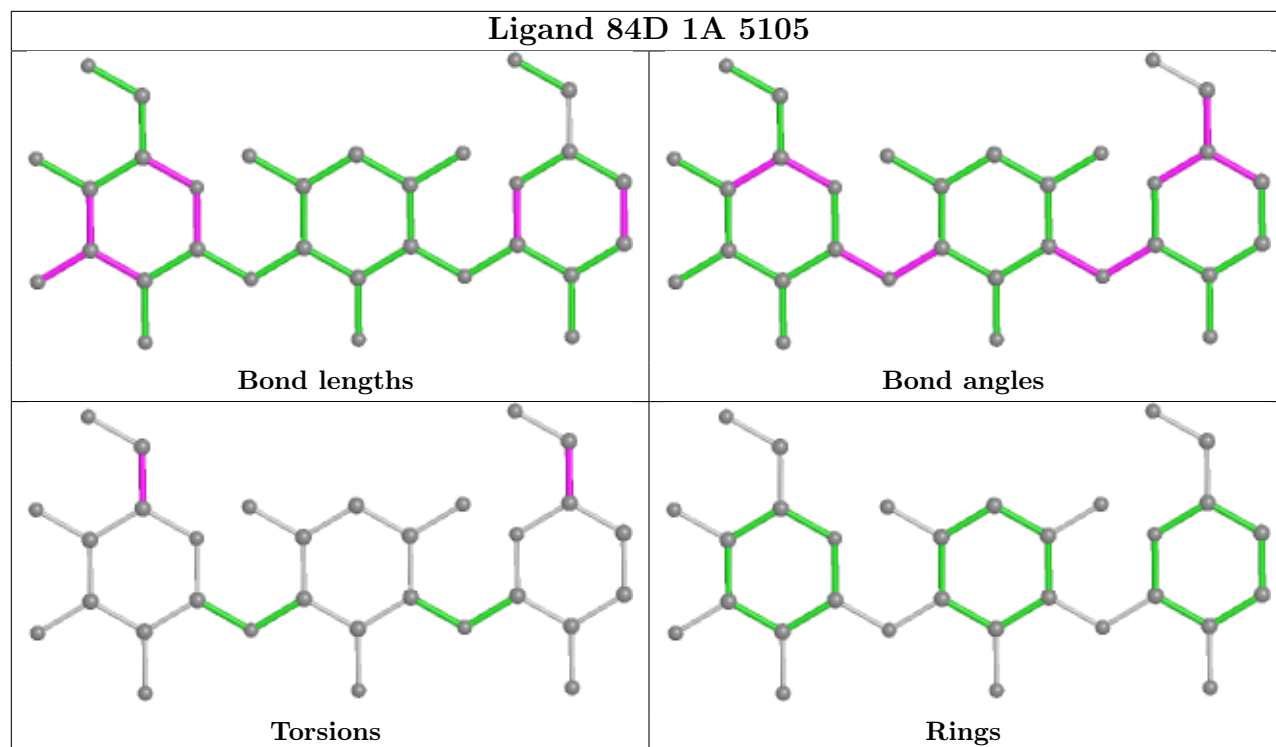
Ligand 84D 1A 5119



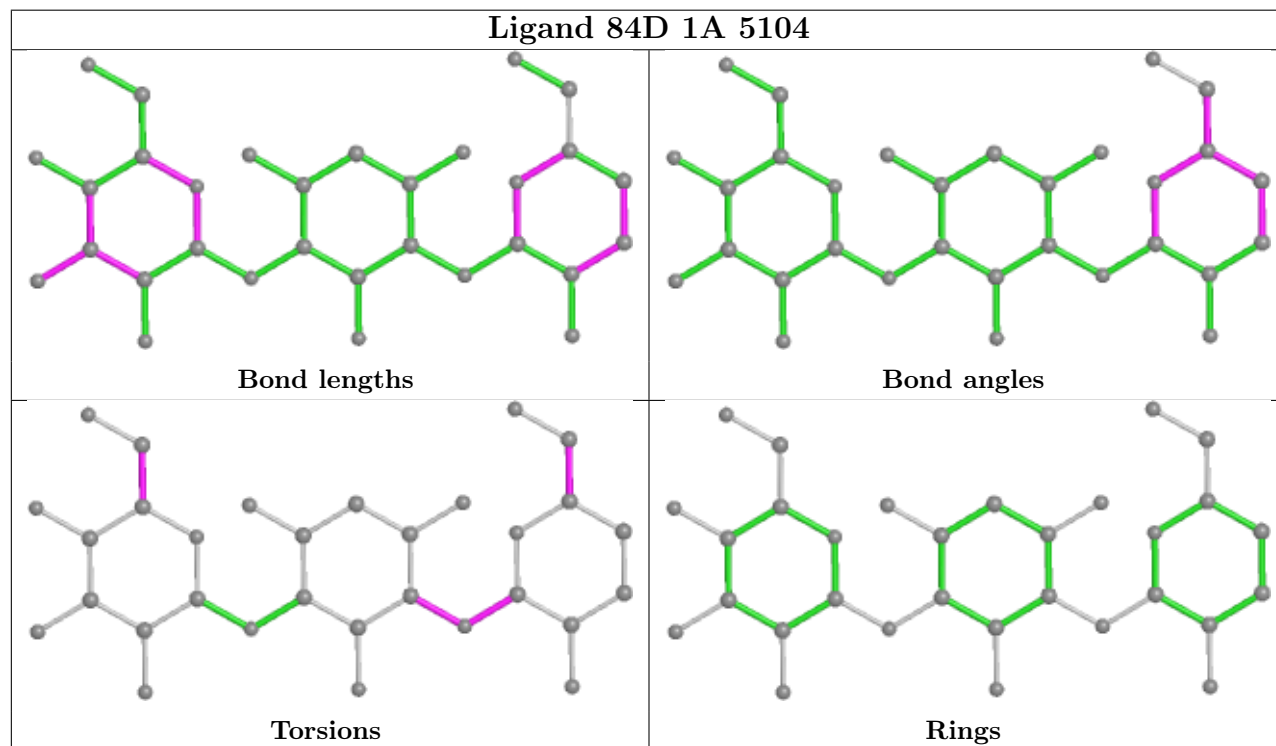
Ligand 84D 1A 5112



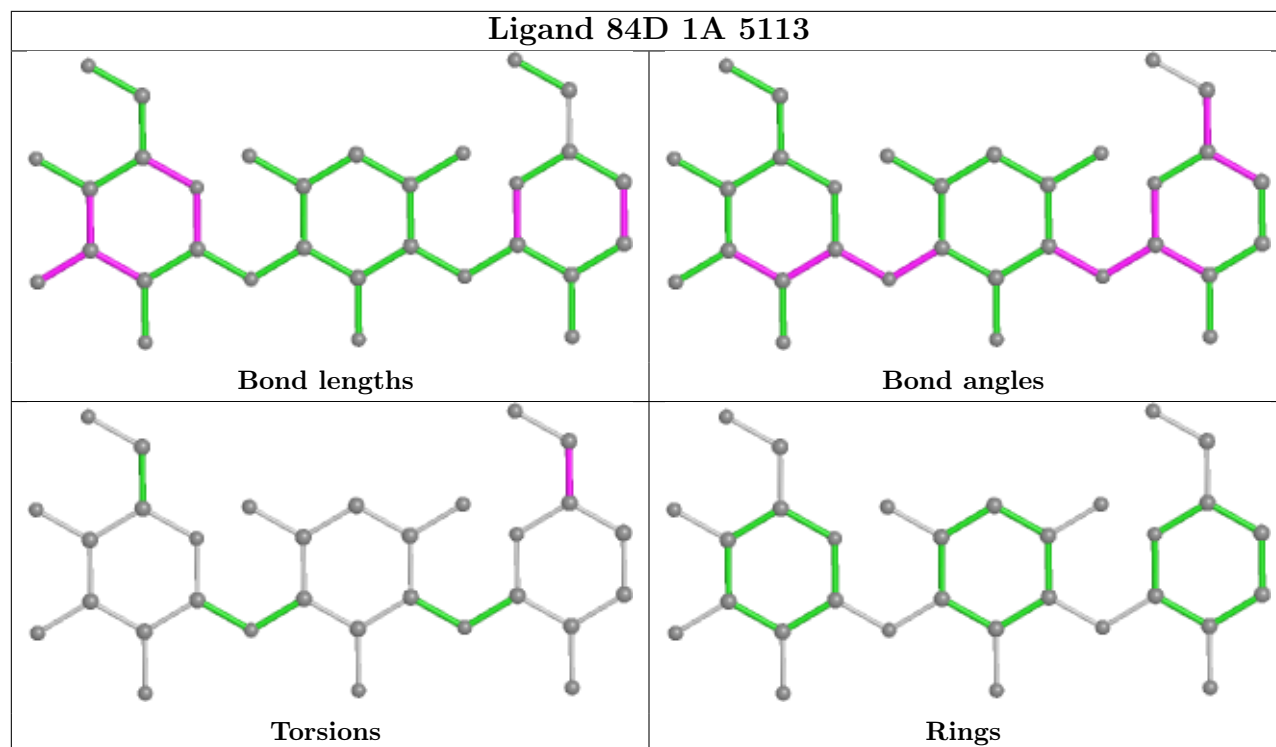
Ligand 84D 1A 5105



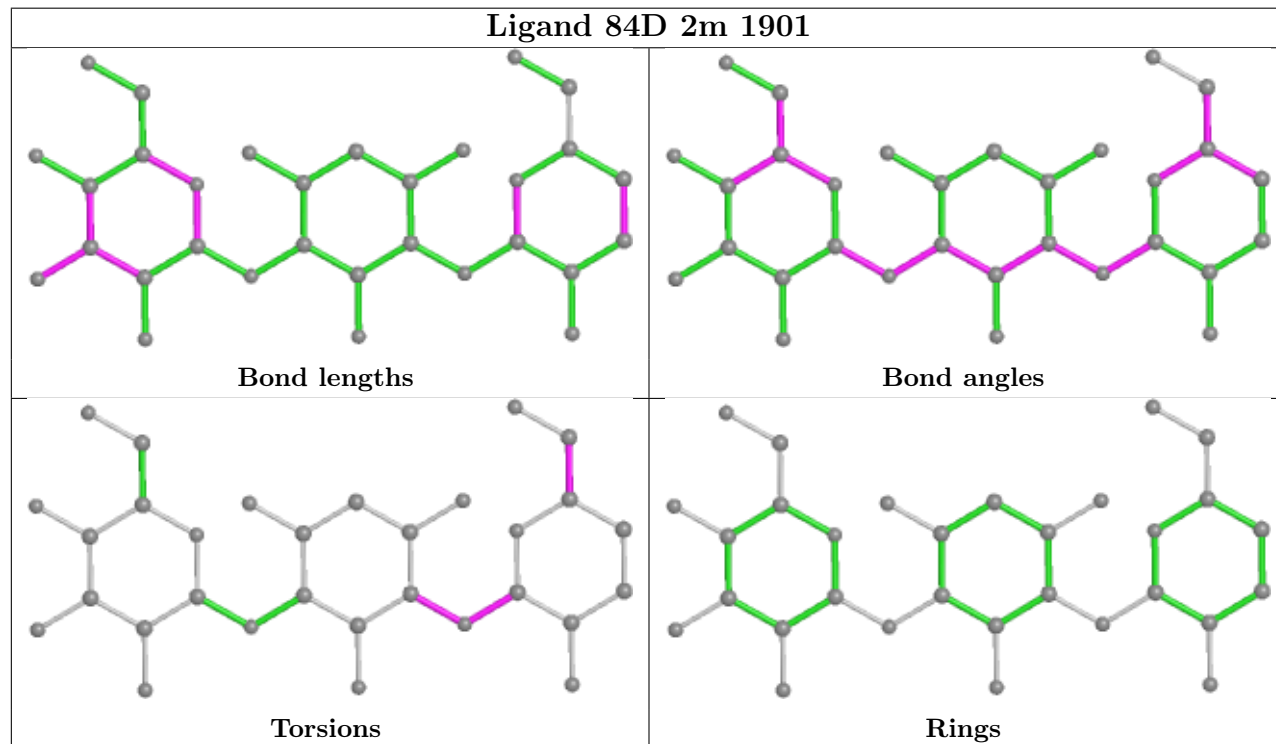
Ligand 84D 1A 5104



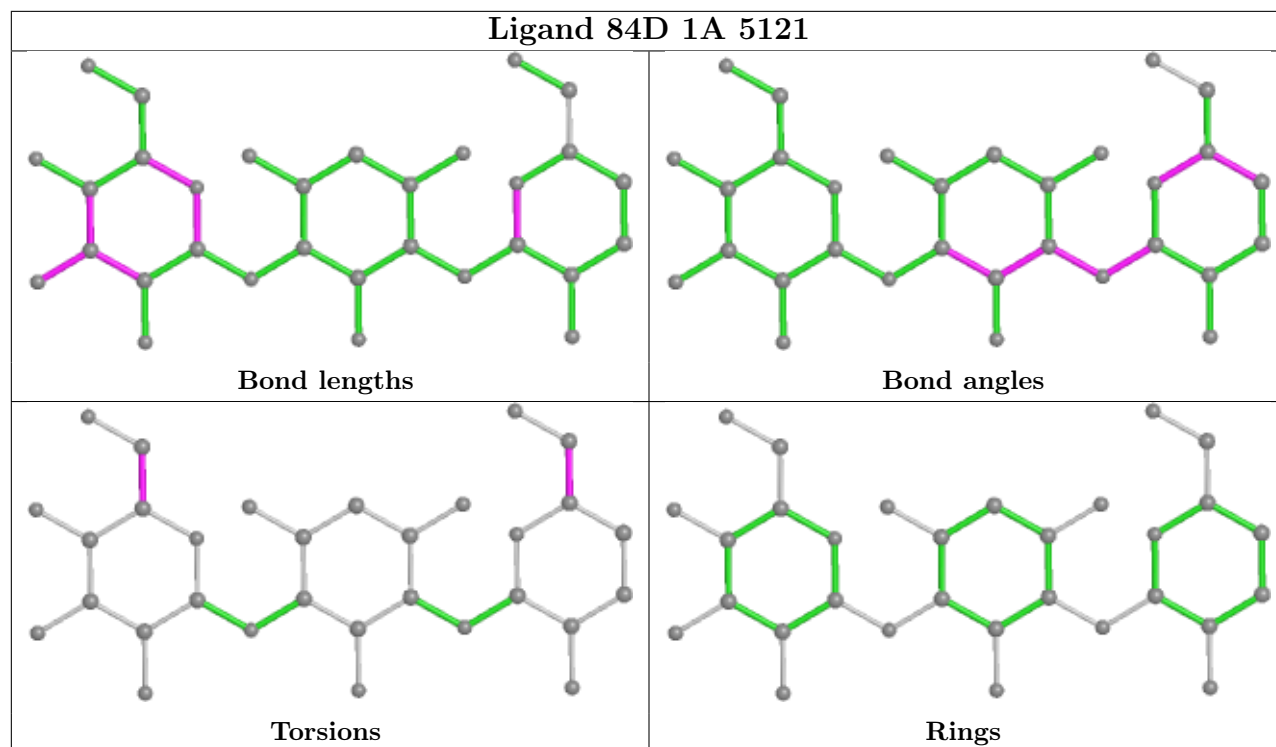
Ligand 84D 1A 5113



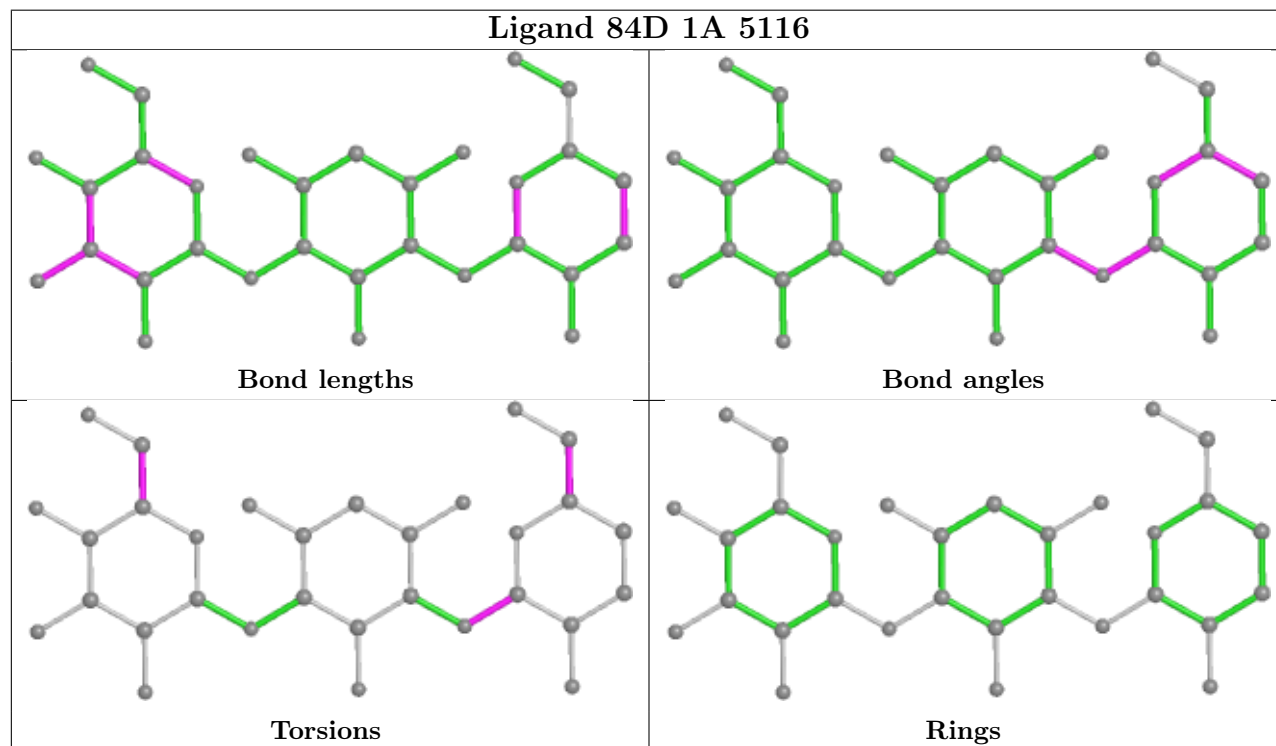
Ligand 84D 2m 1901



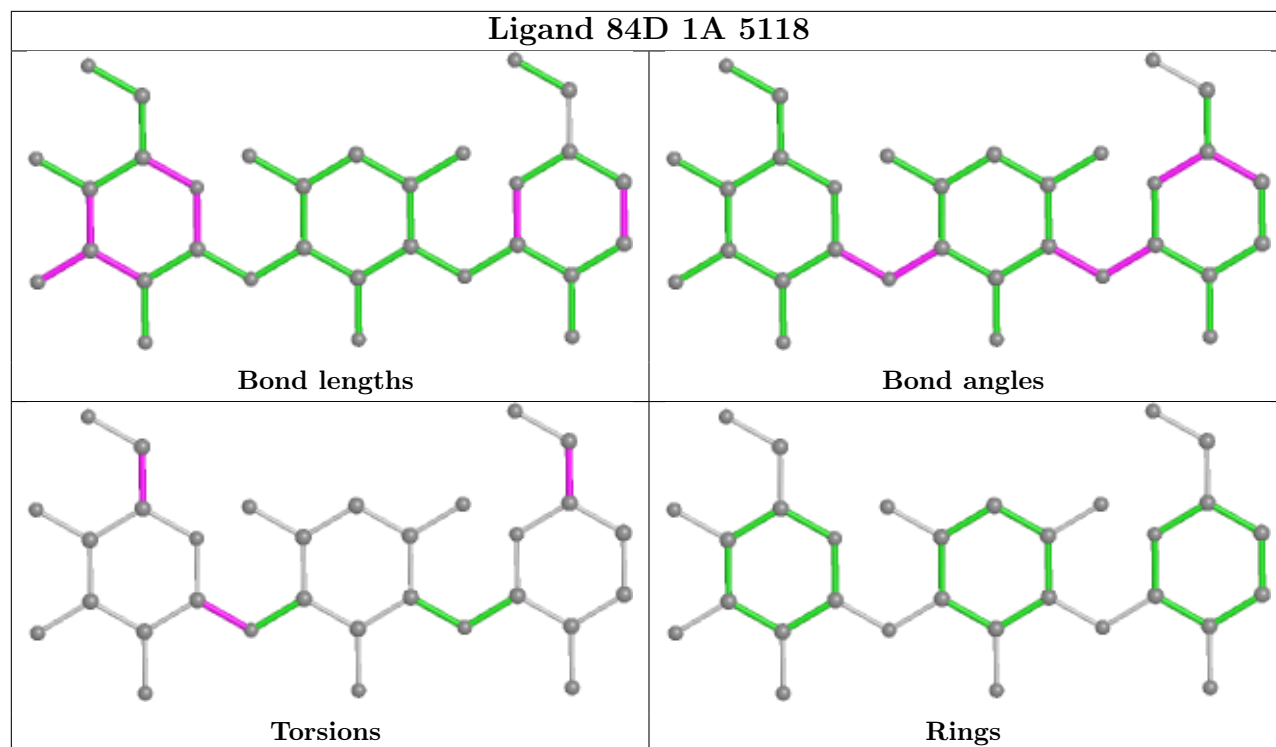
Ligand 84D 1A 5121



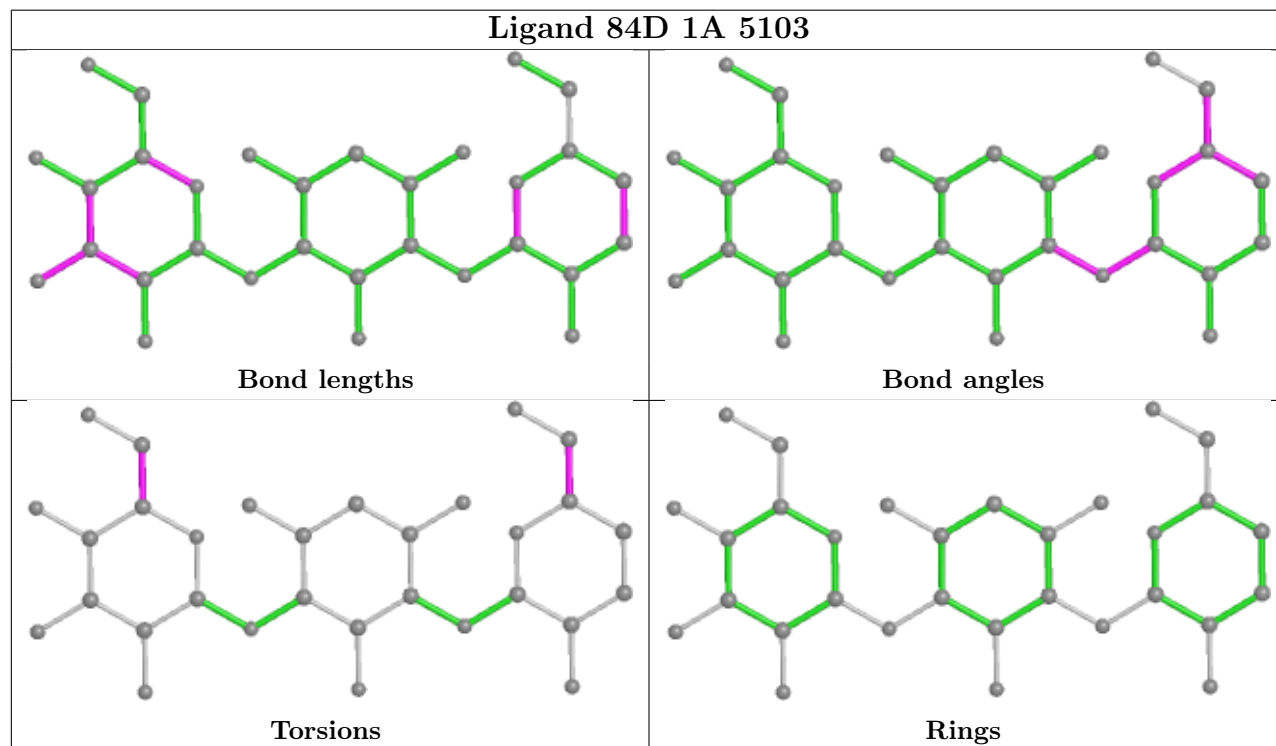
Ligand 84D 1A 5116



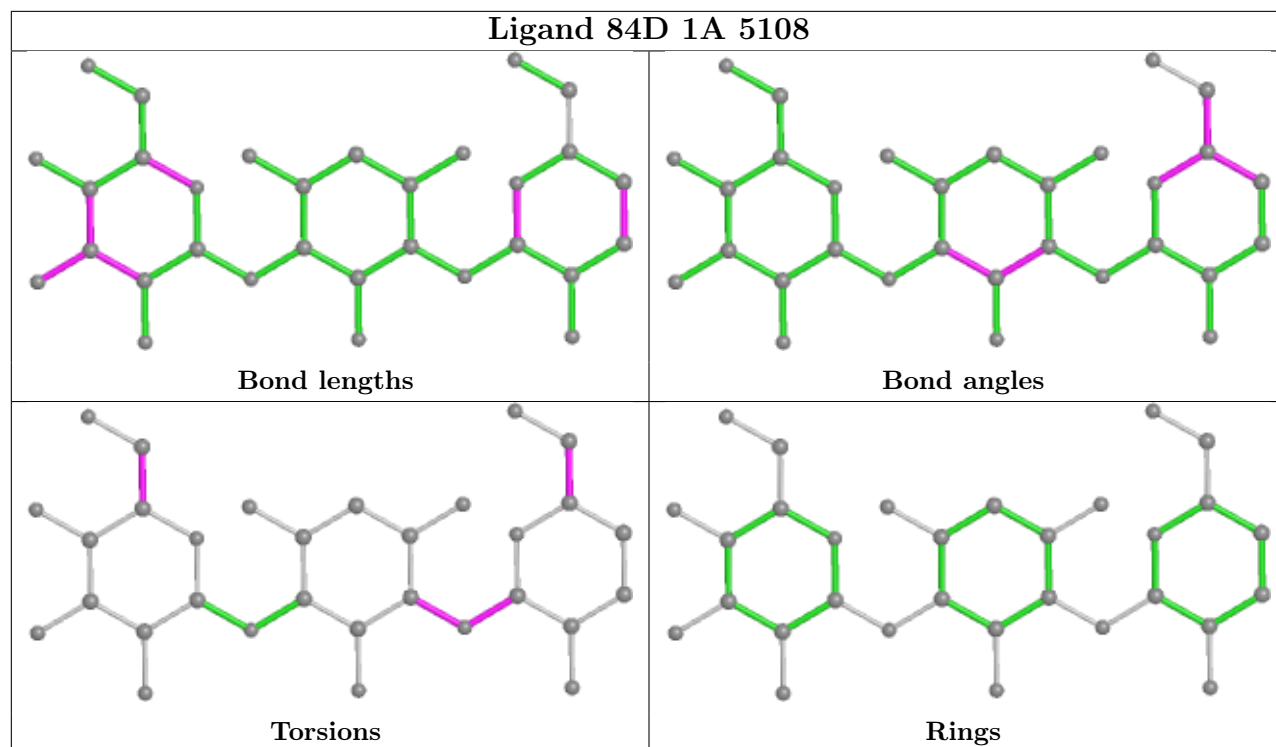
Ligand 84D 1A 5118



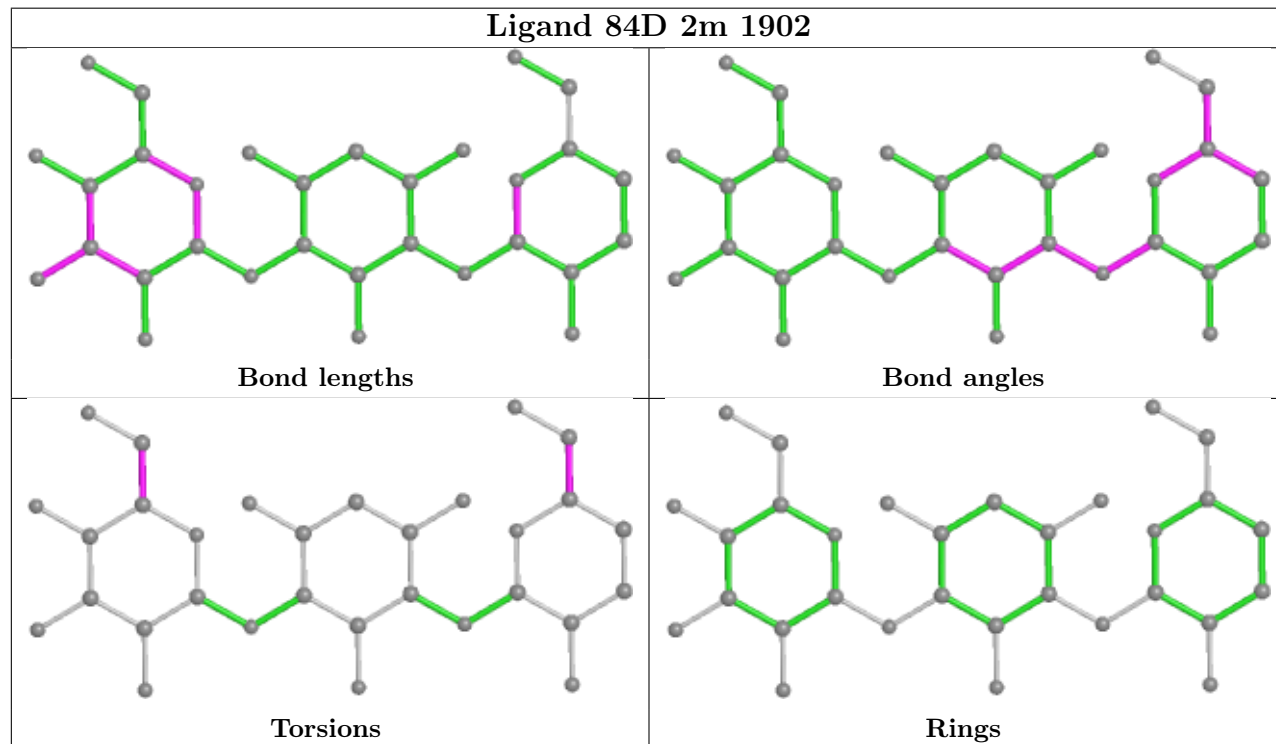
Ligand 84D 1A 5103



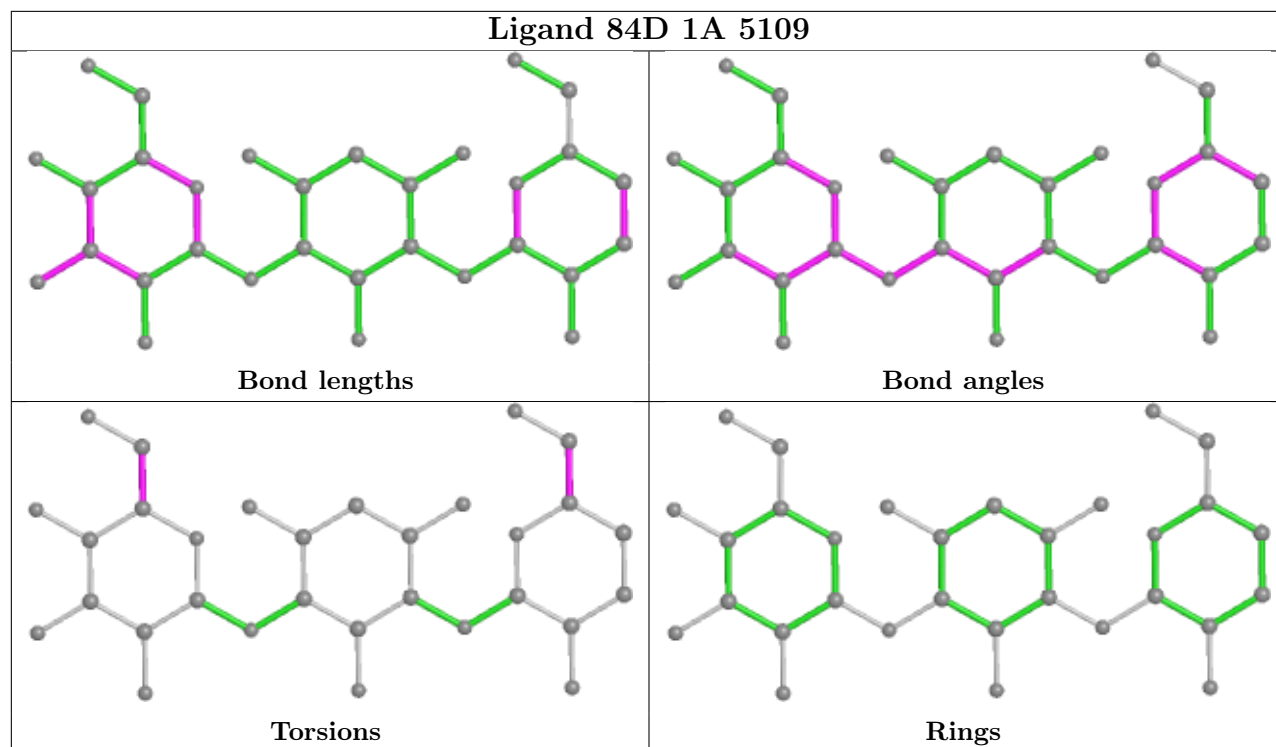
Ligand 84D 1A 5108



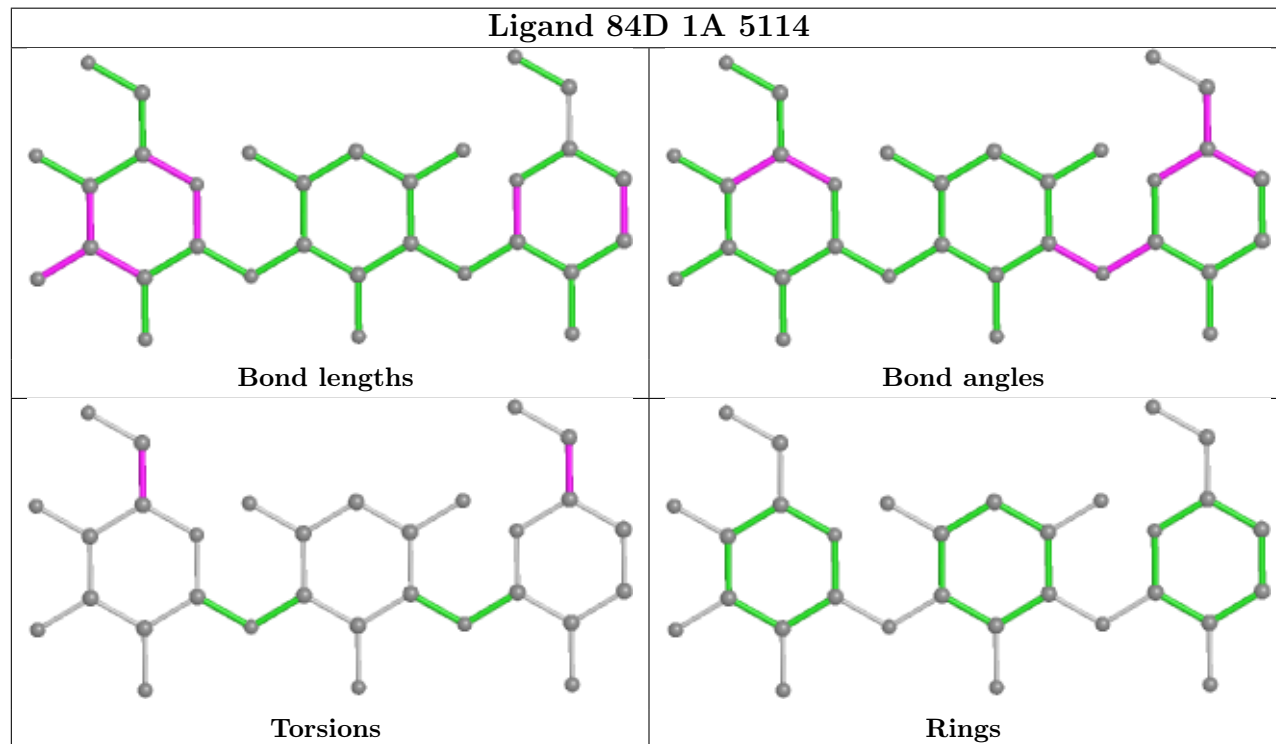
Ligand 84D 2m 1902



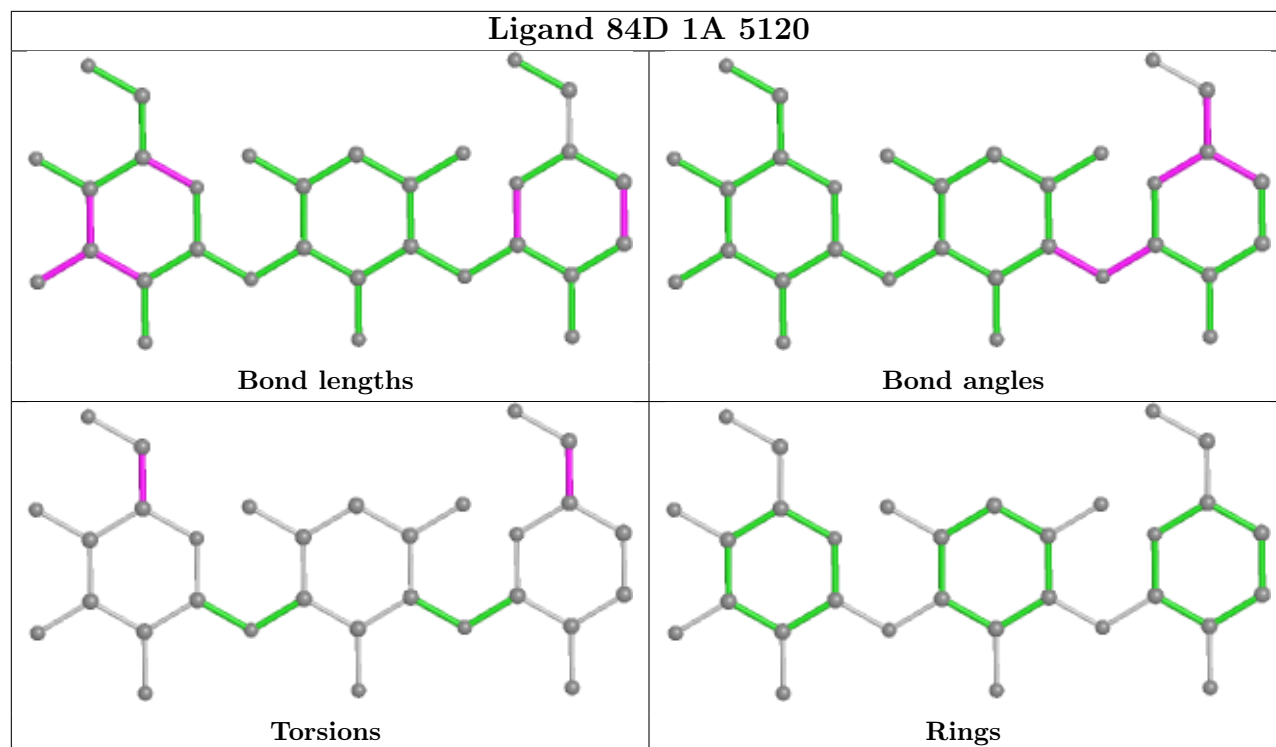
Ligand 84D 1A 5109



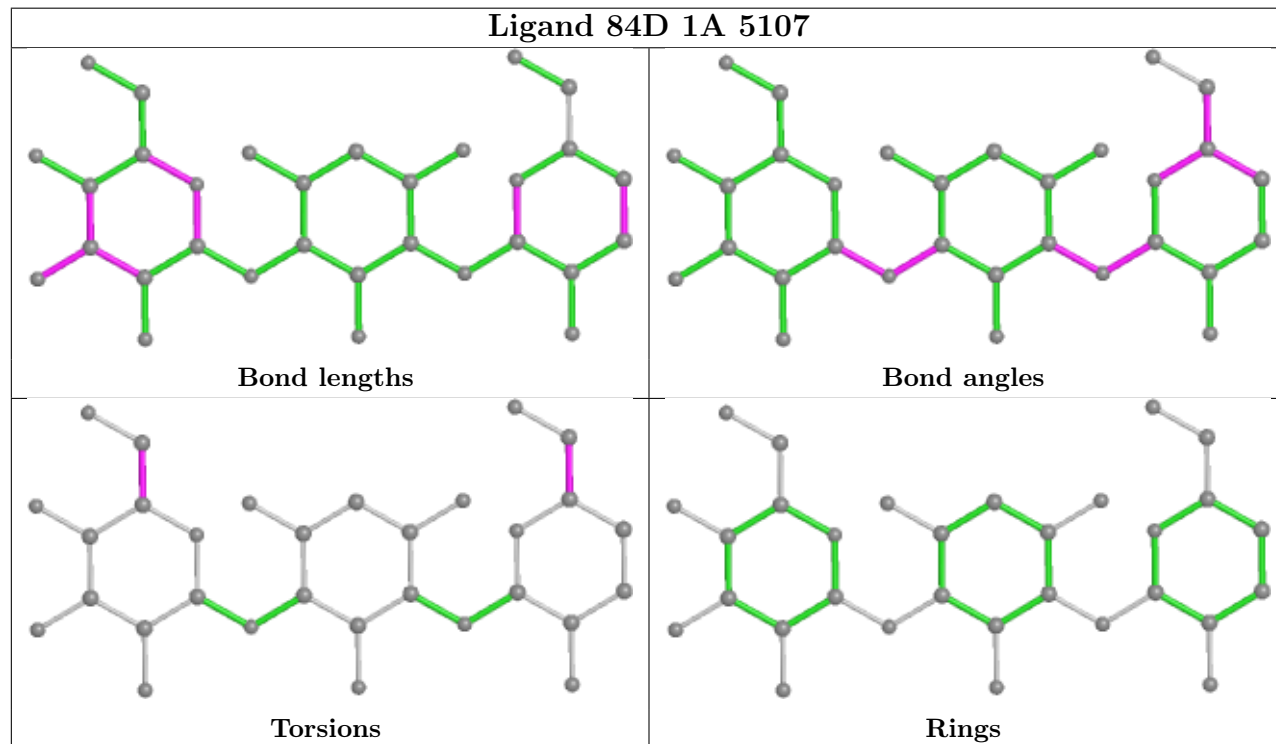
Ligand 84D 1A 5114



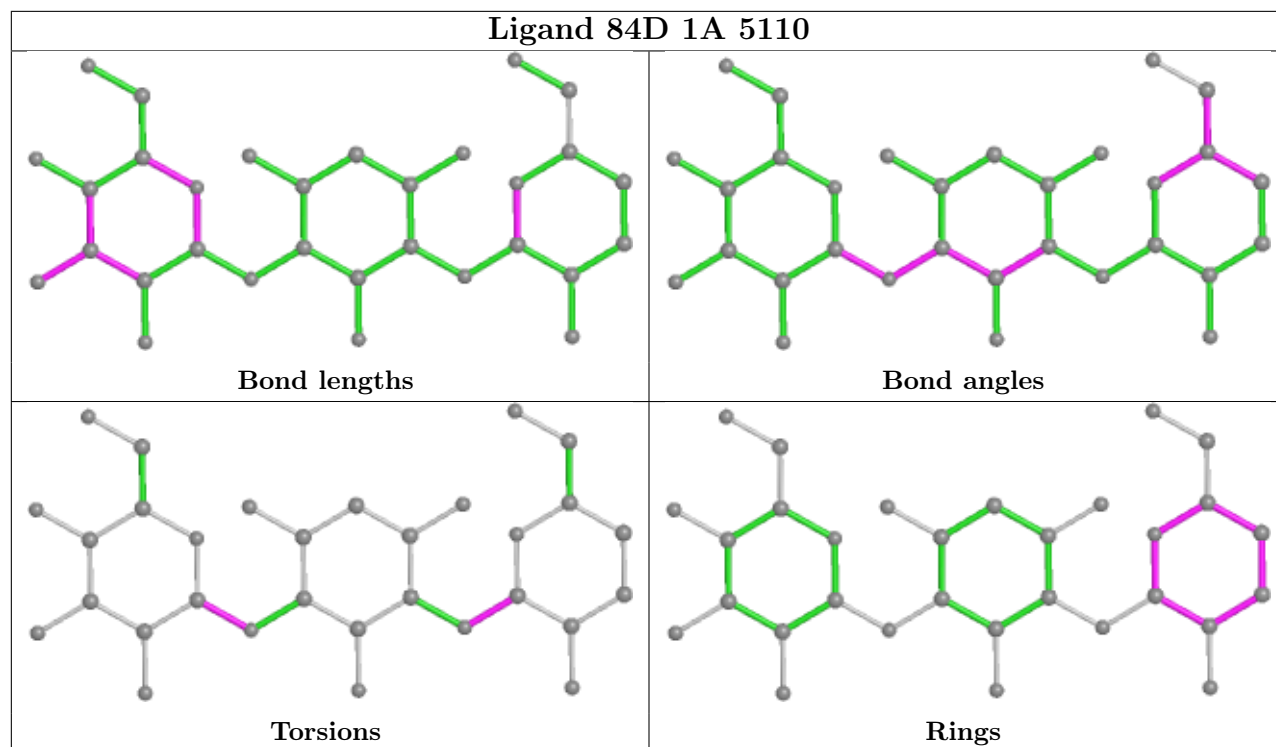
Ligand 84D 1A 5120



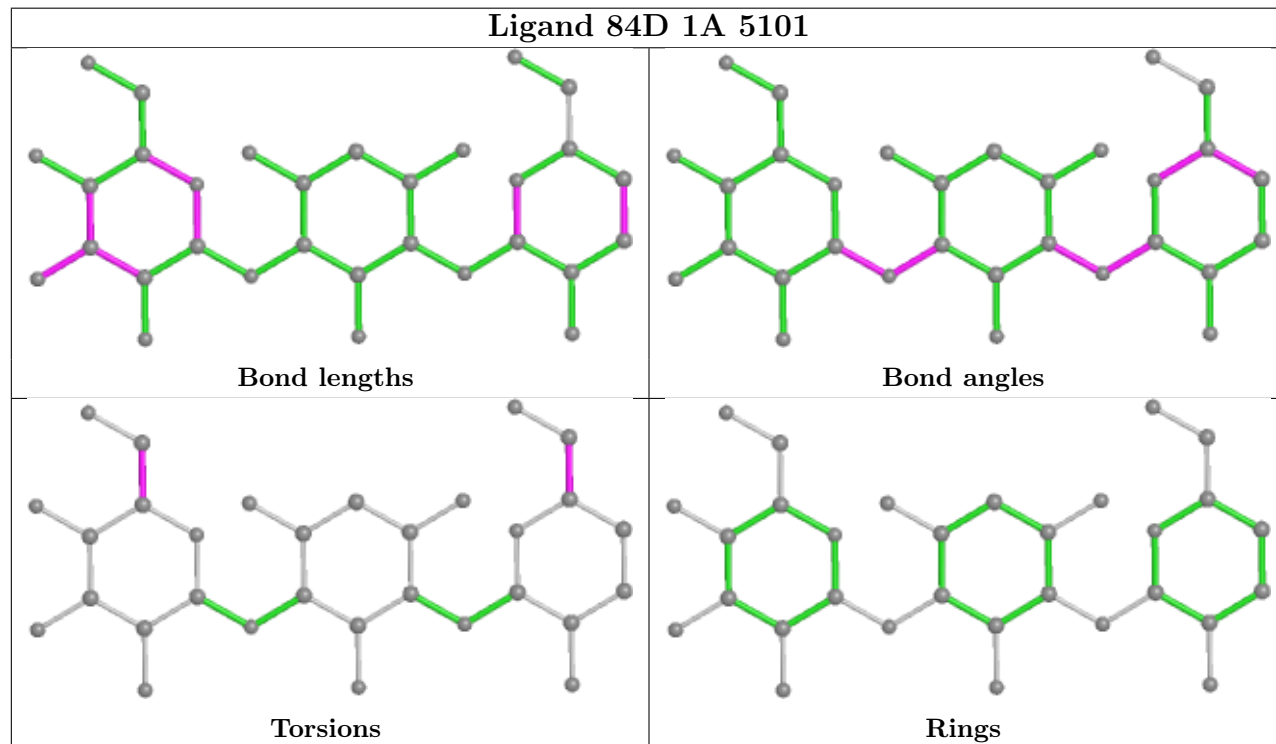
Ligand 84D 1A 5107



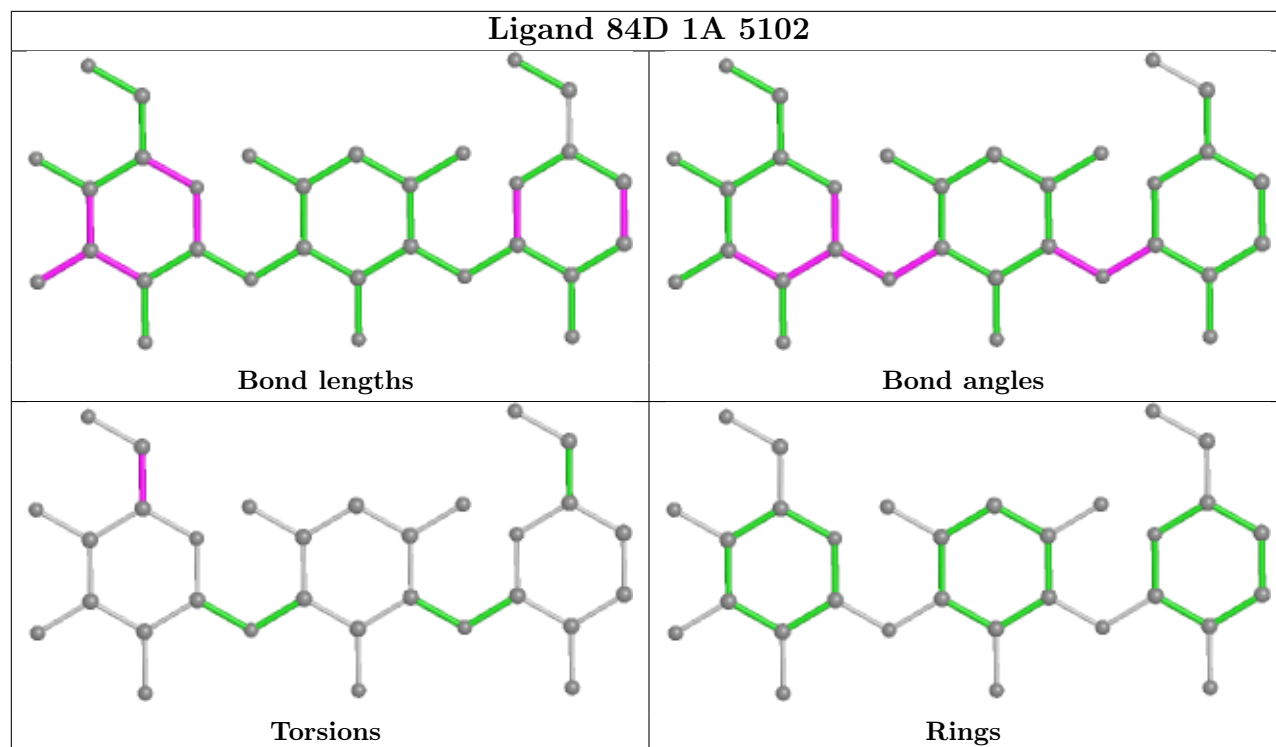
Ligand 84D 1A 5110



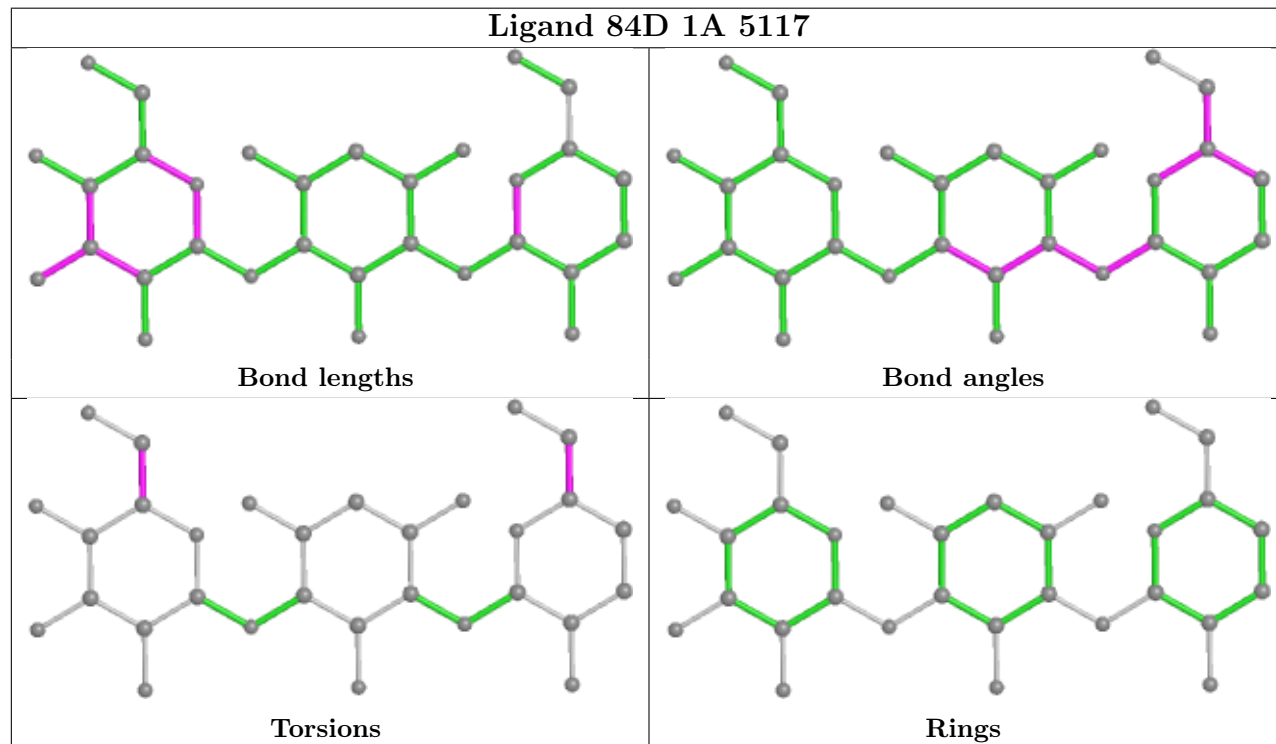
Ligand 84D 1A 5101



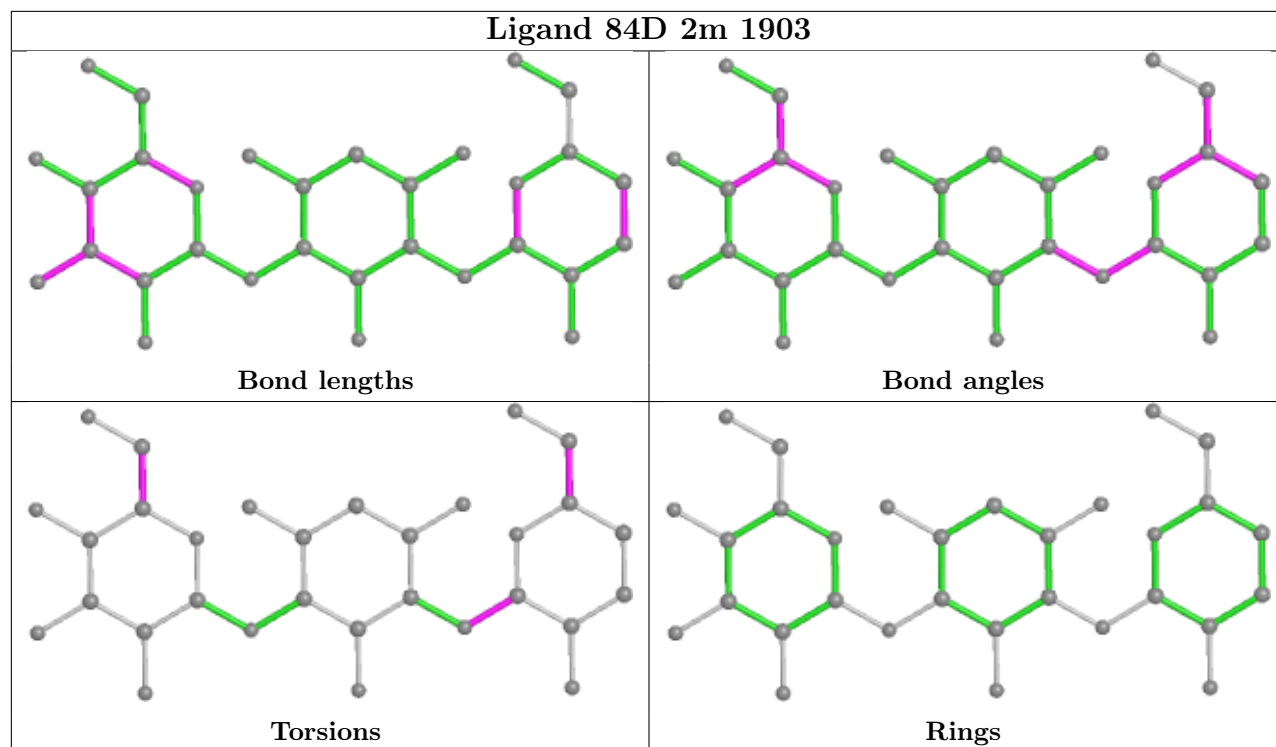
Ligand 84D 1A 5102



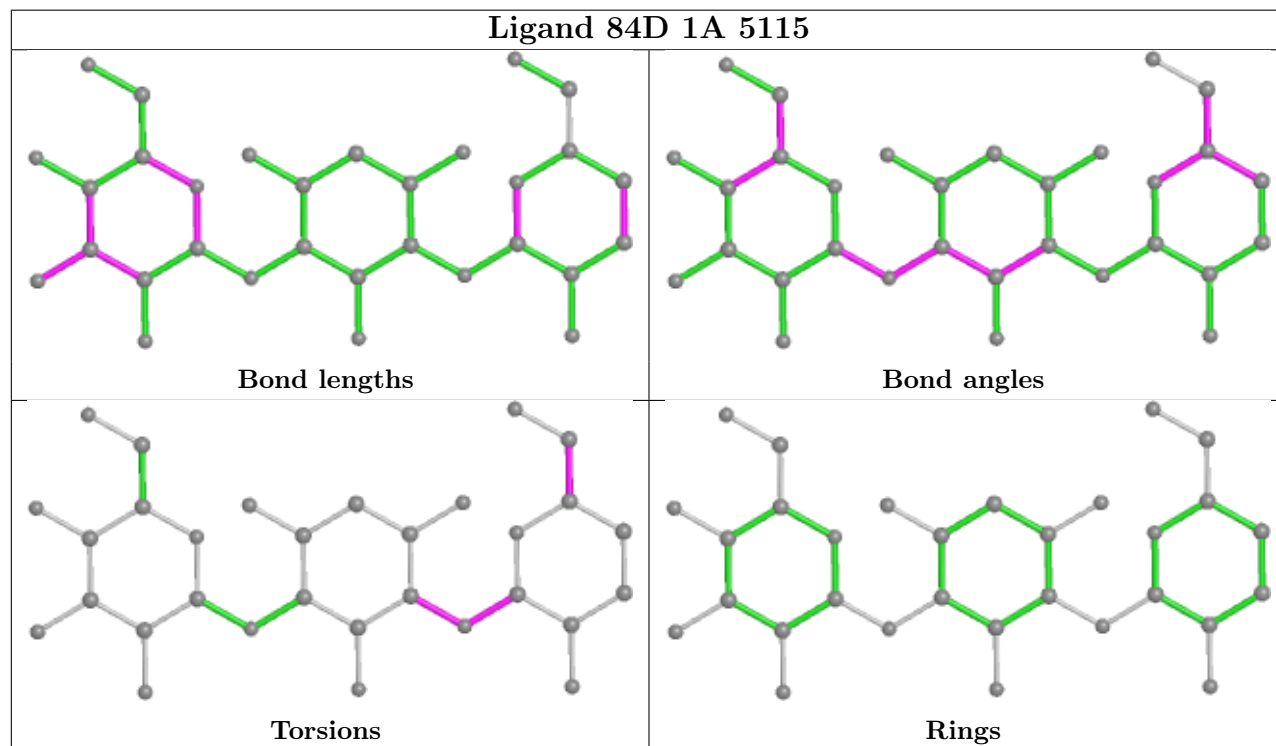
Ligand 84D 1A 5117

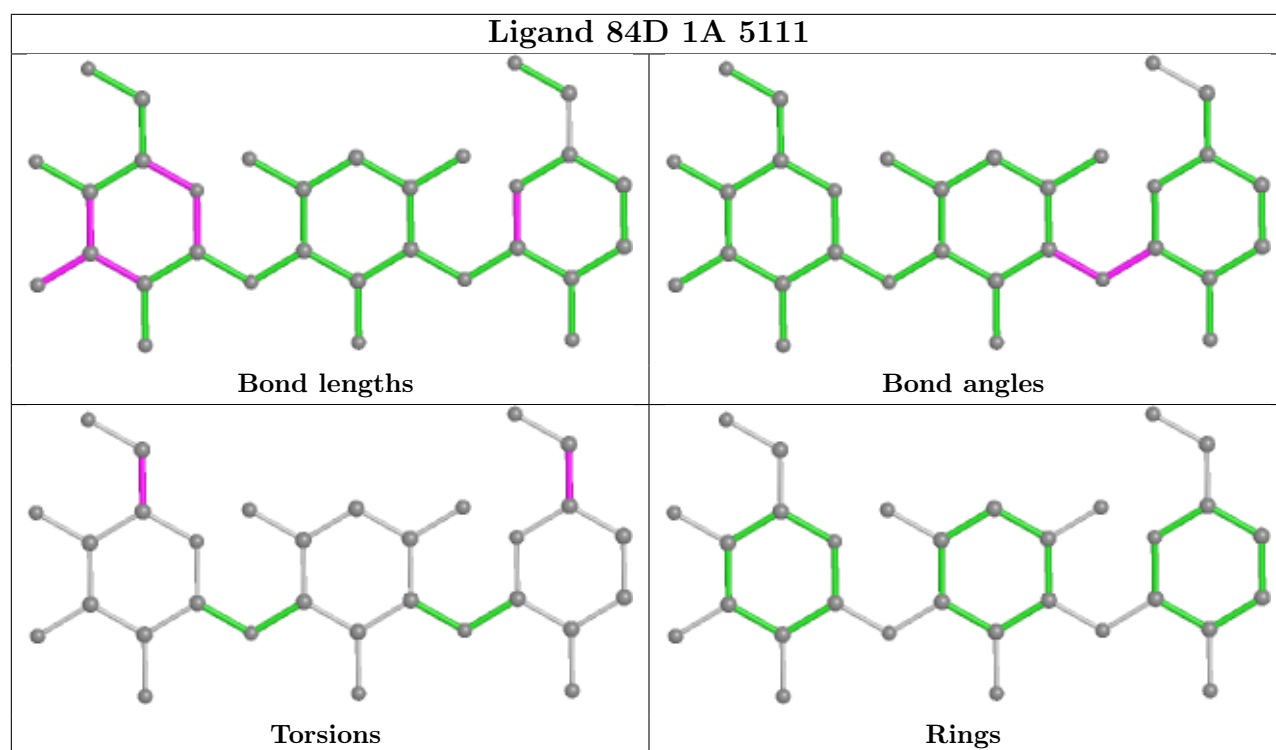


Ligand 84D 2m 1903



Ligand 84D 1A 5115





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.

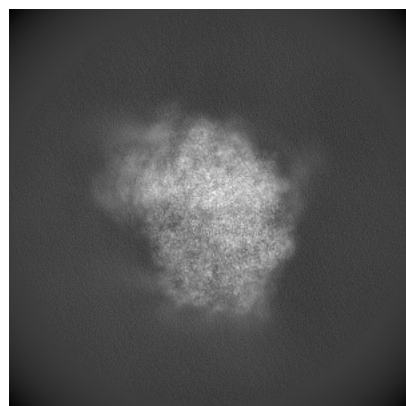
6 Map visualisation [i](#)

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

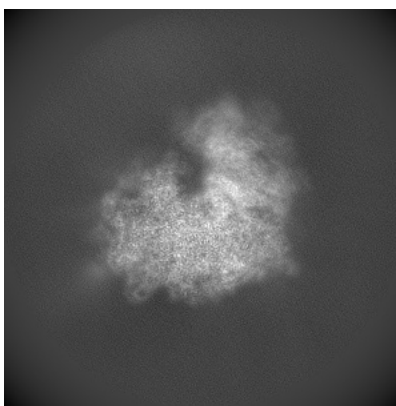
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

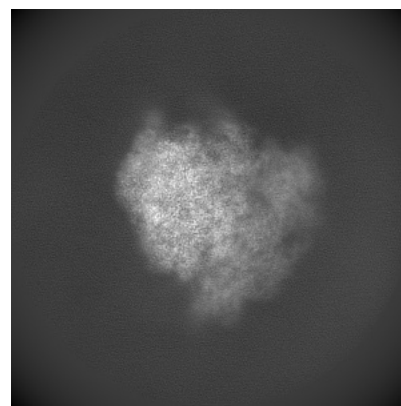
6.1.1 Primary map



X

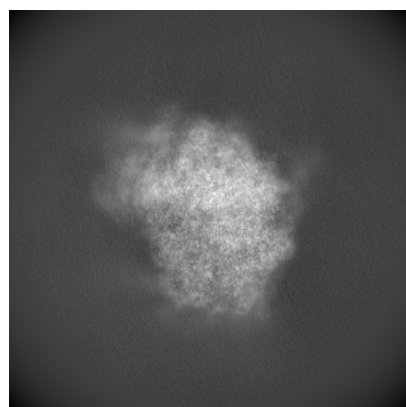


Y

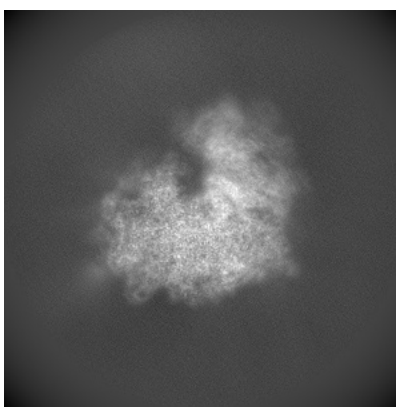


Z

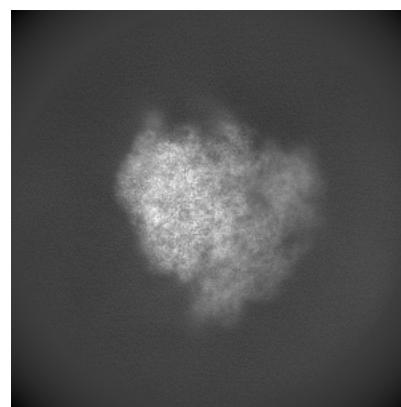
6.1.2 Raw map



X



Y

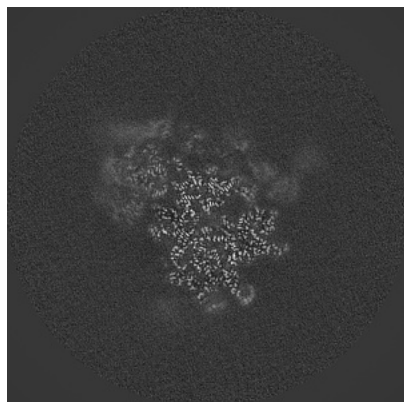


Z

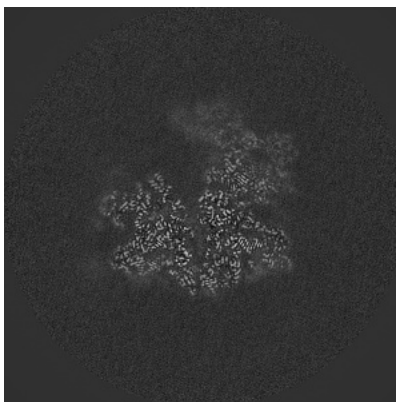
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

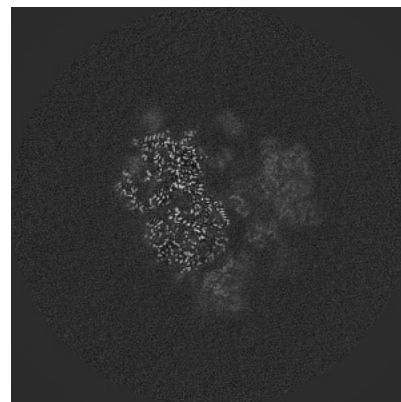
6.2.1 Primary map



X Index: 320

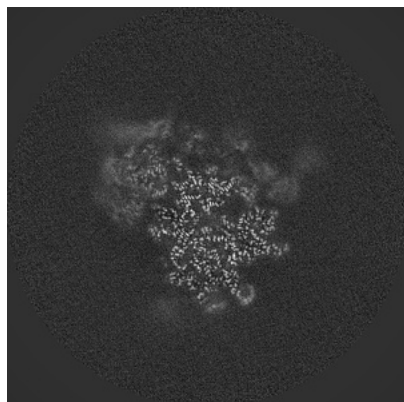


Y Index: 320

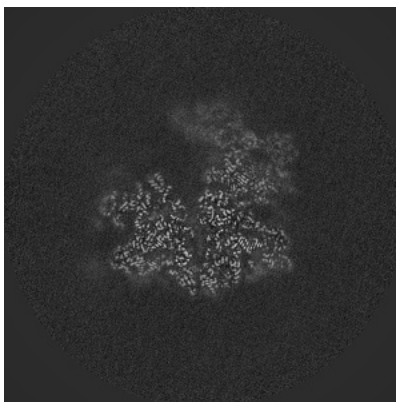


Z Index: 320

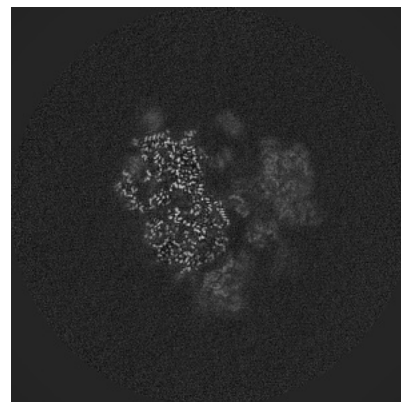
6.2.2 Raw map



X Index: 320



Y Index: 320

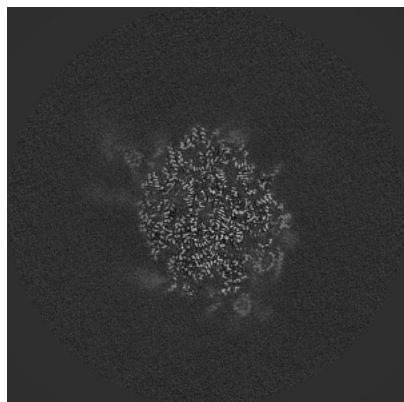


Z Index: 320

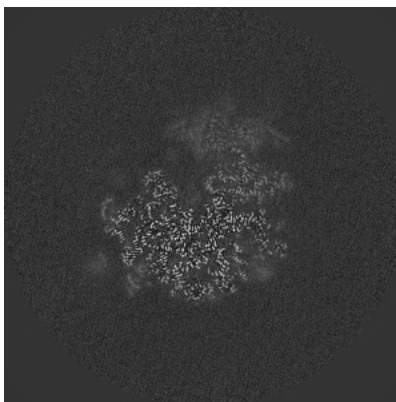
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

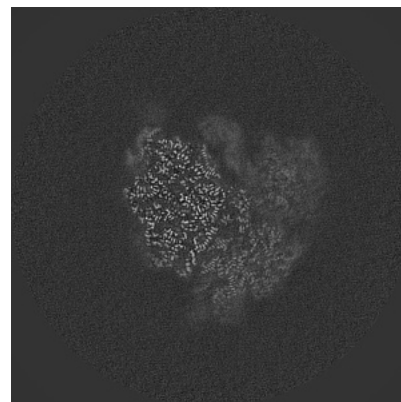
6.3.1 Primary map



X Index: 288

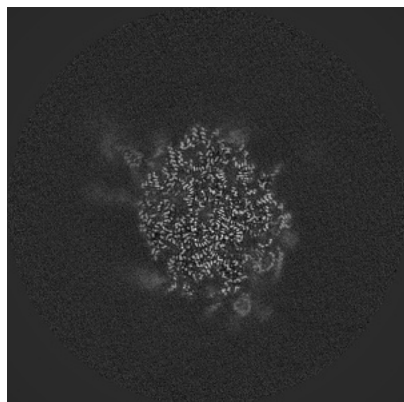


Y Index: 339

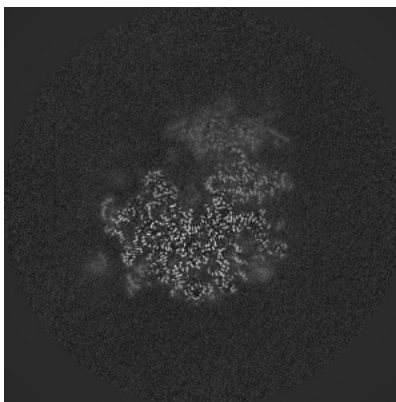


Z Index: 350

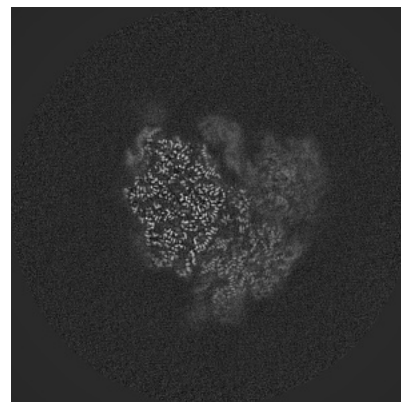
6.3.2 Raw map



X Index: 288



Y Index: 339

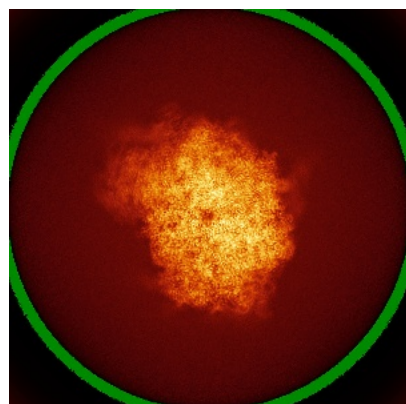


Z Index: 350

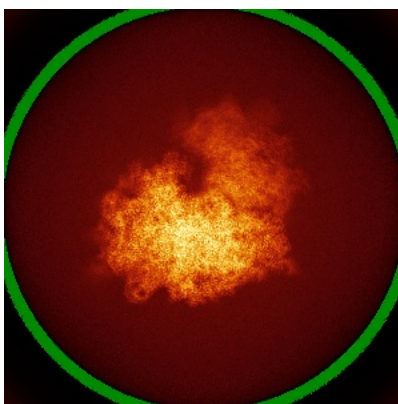
The images above show the largest variance slices of the map in three orthogonal directions.

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

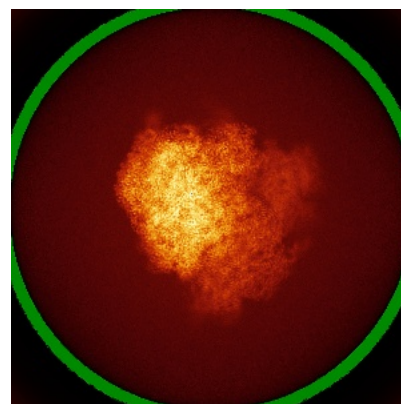
6.4.1 Primary map



X

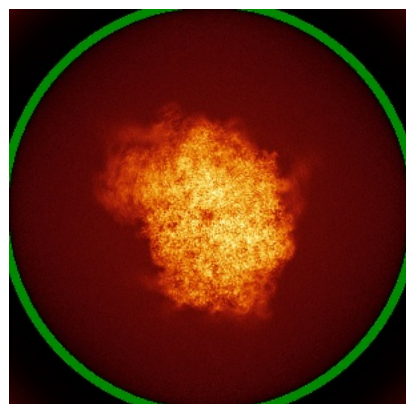


Y

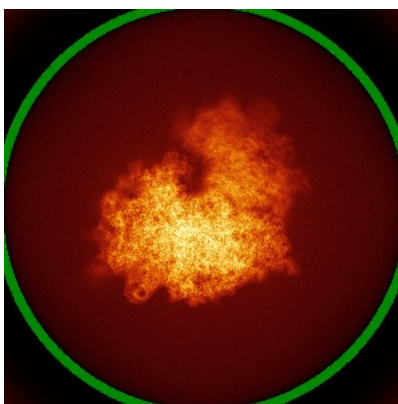


Z

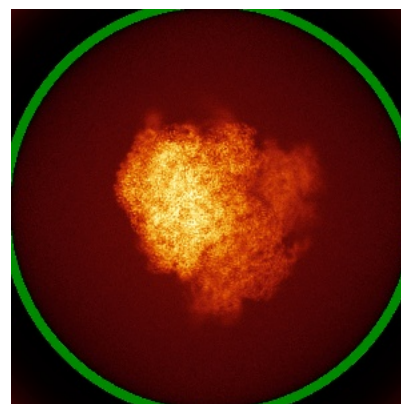
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



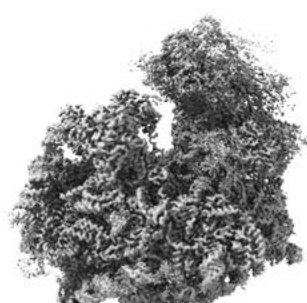
Z

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

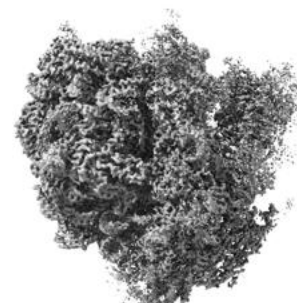
6.5.2 Raw map



X



Y



Z

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

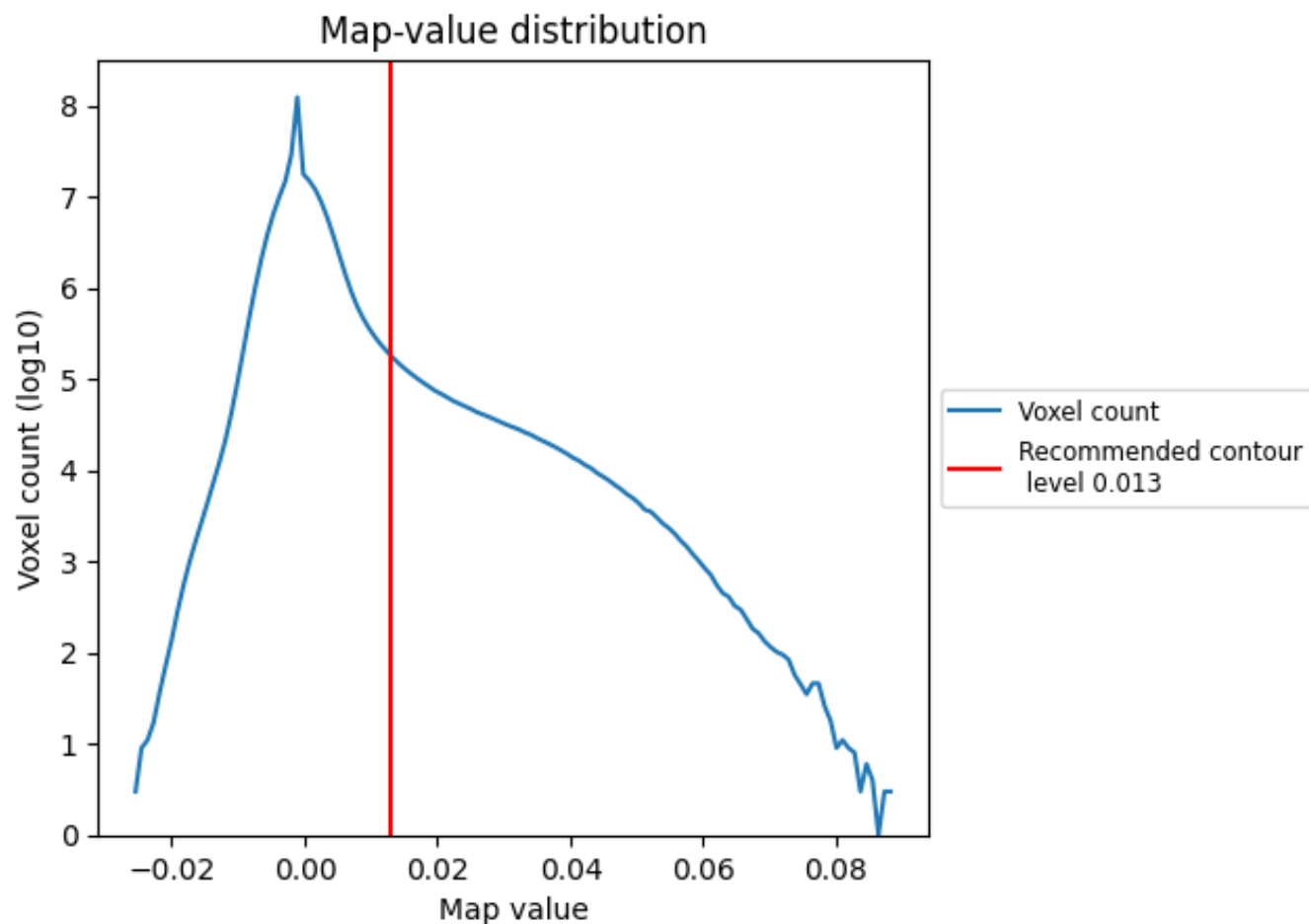
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

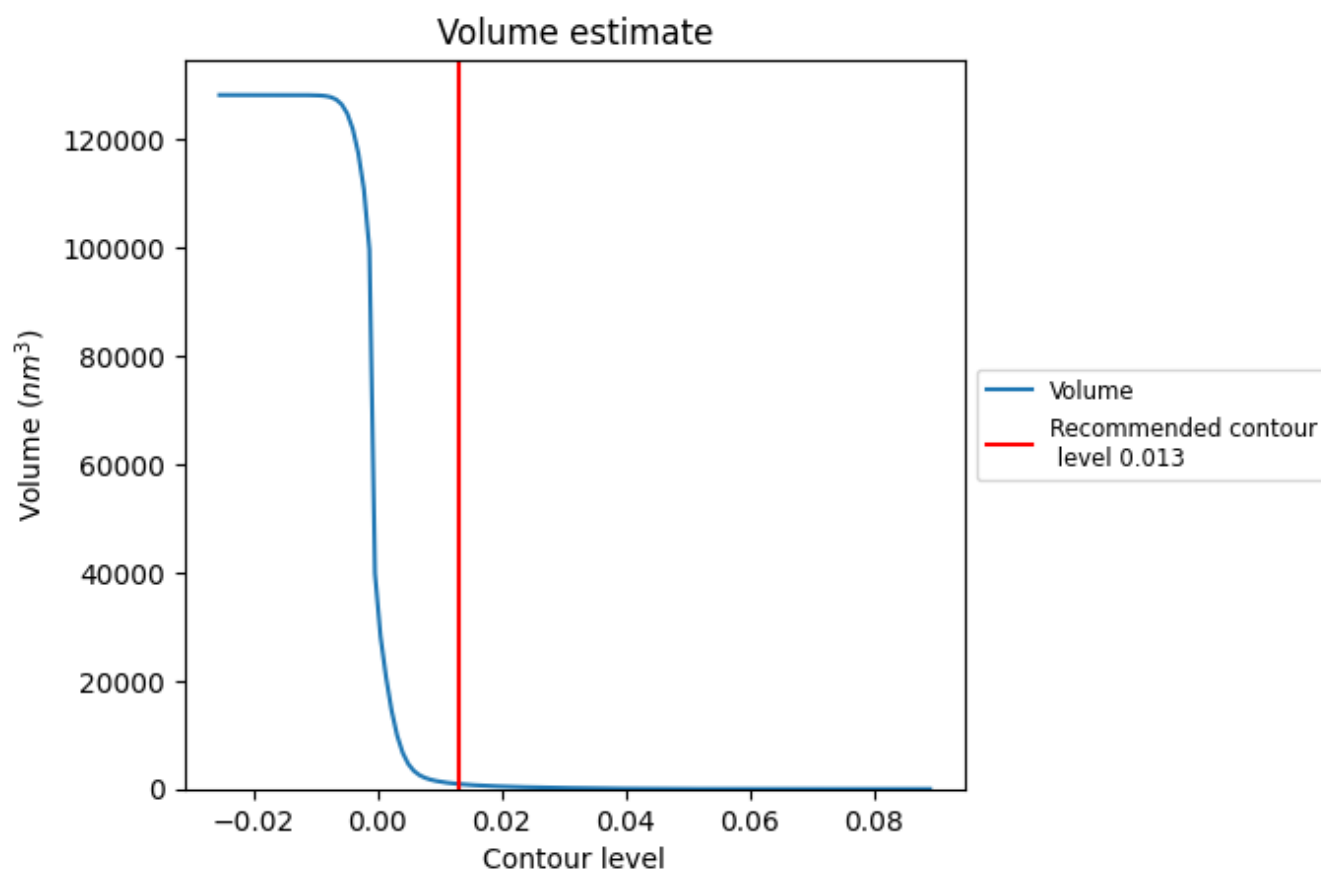
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

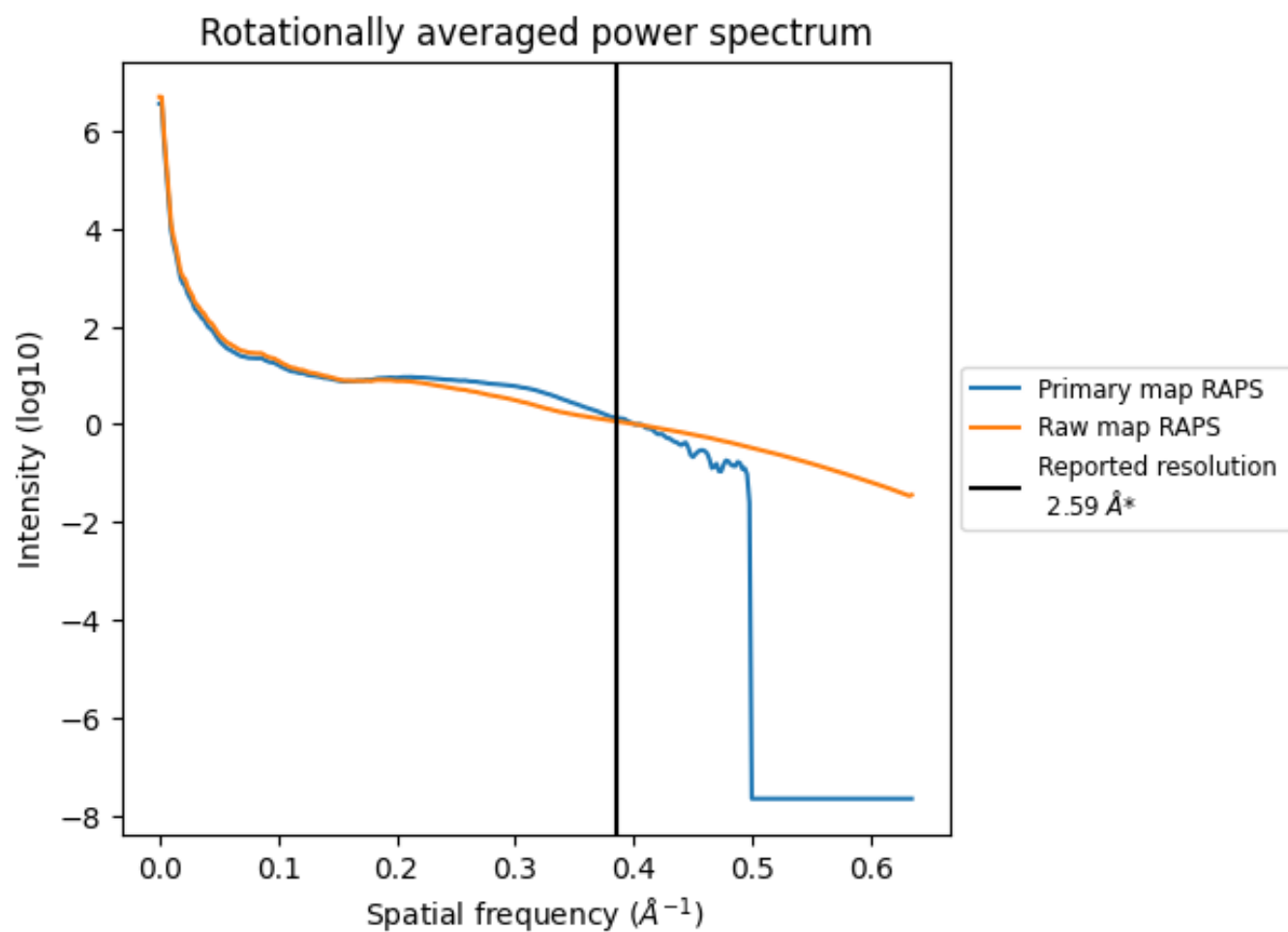
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

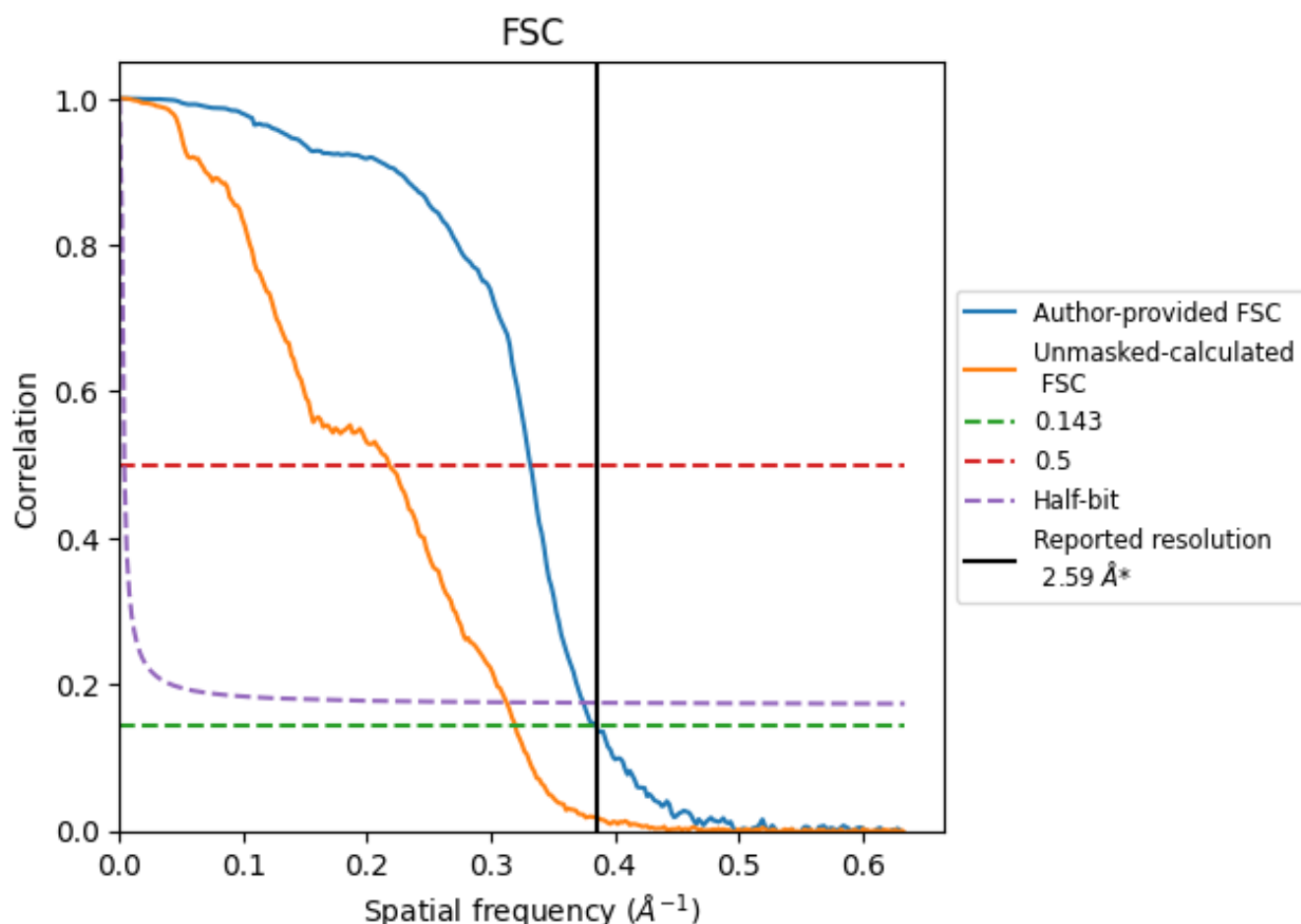


*Reported resolution corresponds to spatial frequency of 0.386 \AA^{-1}

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 0.386 Å⁻¹

8.2 Resolution estimates [i](#)

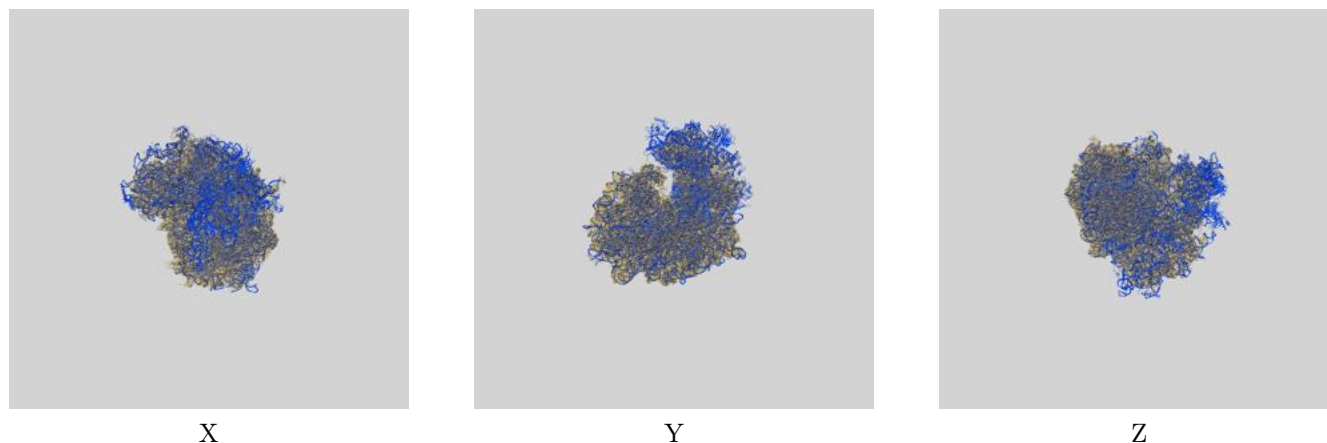
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.60	3.01	2.67
Unmasked-calculated*	3.13	4.59	3.20

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

9 Map-model fit [i](#)

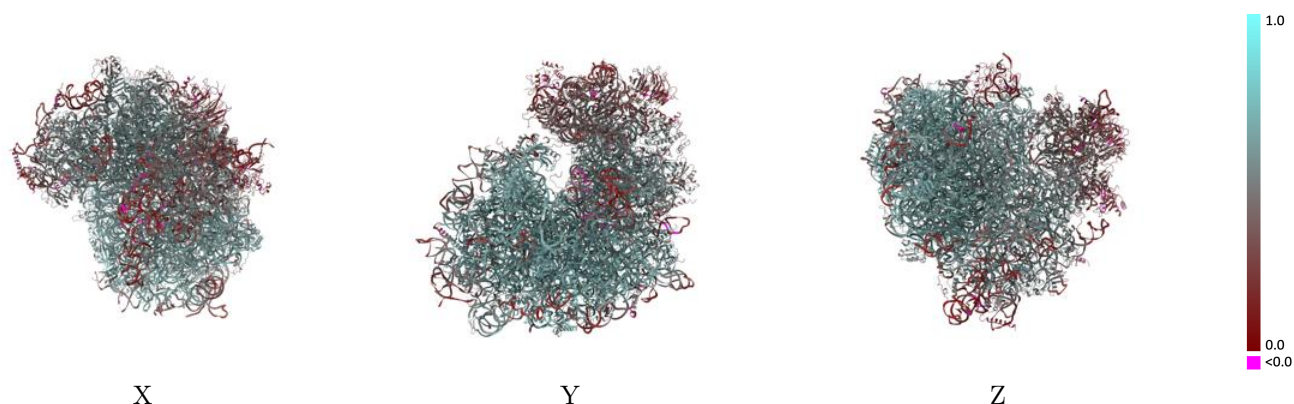
This section contains information regarding the fit between EMDB map EMD-35413 and PDB model 8IFD. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



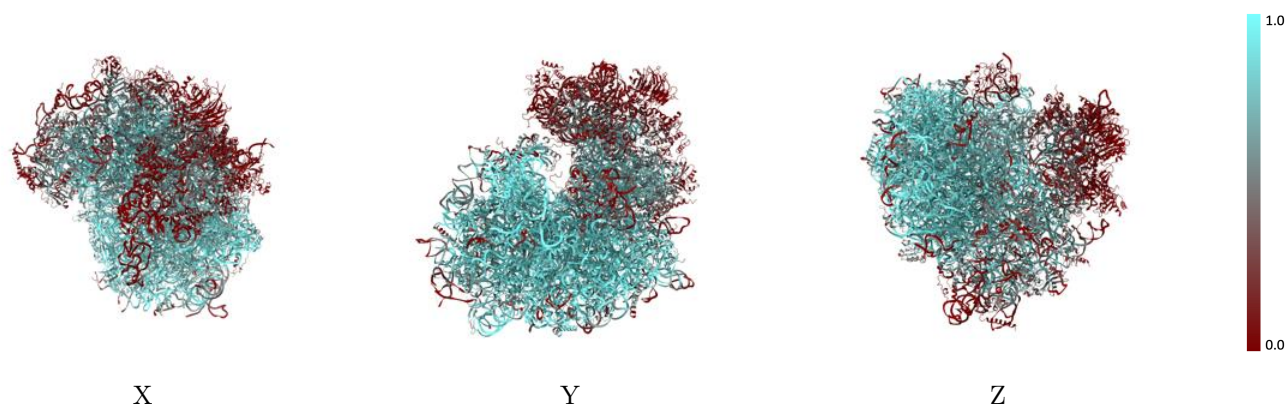
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



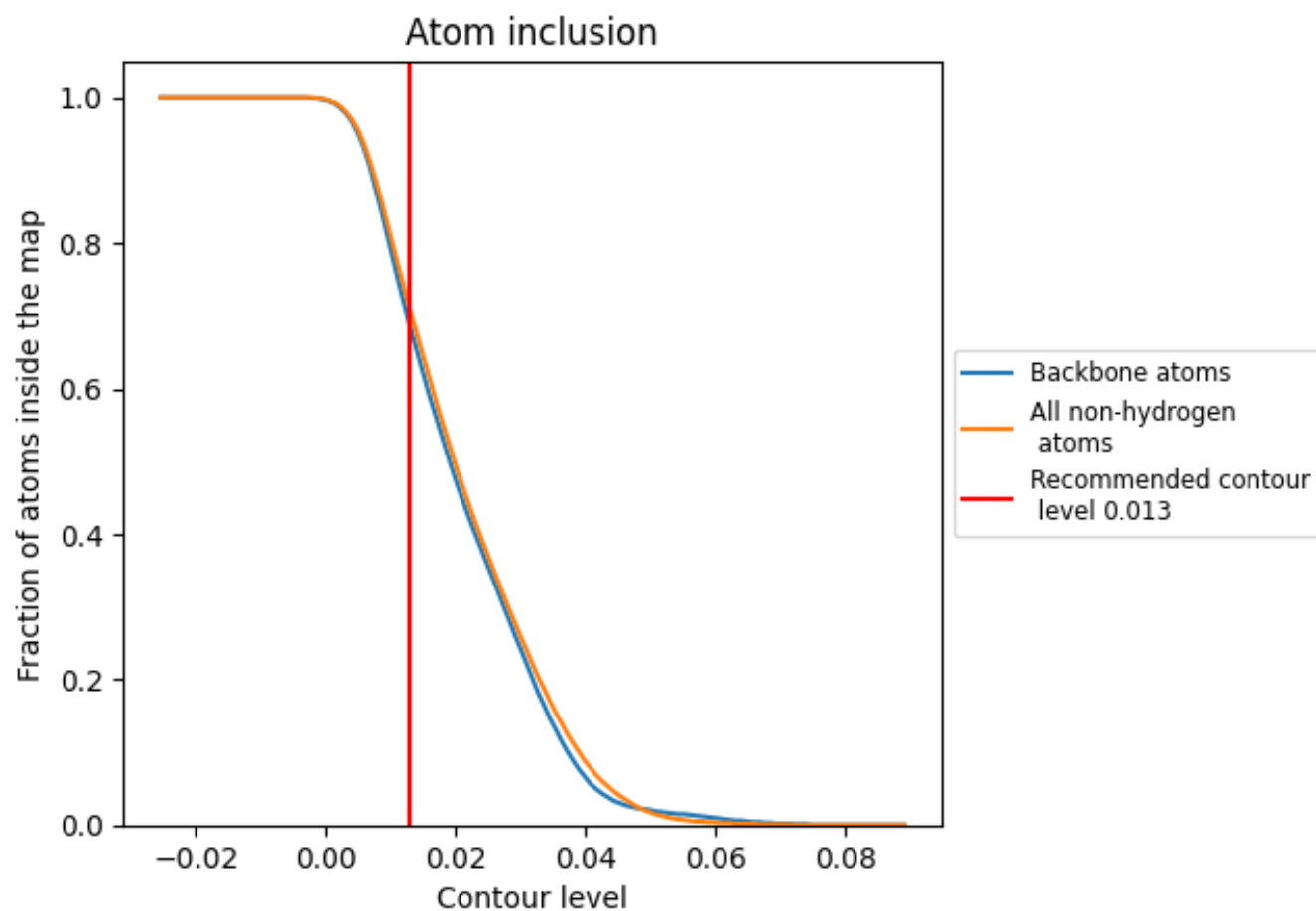
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ





















































































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

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











Continued on next page...

Continued from previous page...

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

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