wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2024 – 04:06 am BST

PDB ID	:	8OI5
Title	:	Crystal structure of the Candida albicans 80S ribosome in complex with Paromomycin (2mM)
Authors	:	Kolosova, O.; Zgadzay, Y.; Yusupov, M.
Deposited on	:	2023-03-22
Resolution	:	2.90 Å(reported)

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

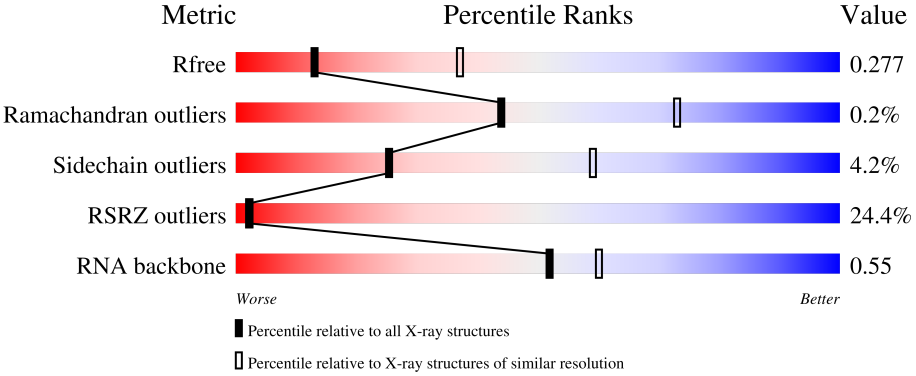
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

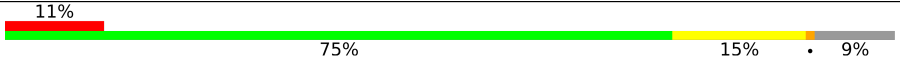
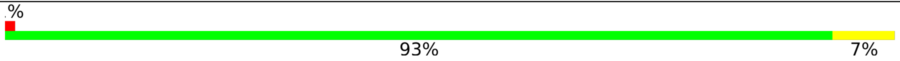
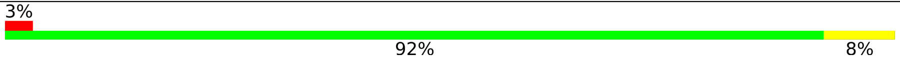
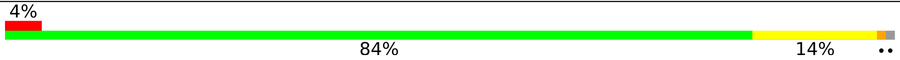
The reported resolution of this entry is 2.90 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2335 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)
RNA backbone	3690	1039 (3.10-2.70)

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

Mol	Chain	Length	Quality of chain
1	1	3359	
1	AS	3359	
2	3	121	
2	AT	121	
3	4	158	

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Mol	Chain	Length	Quality of chain
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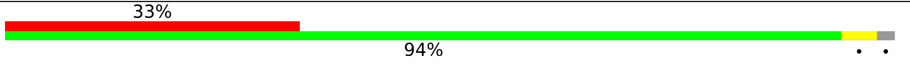
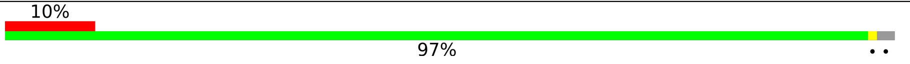
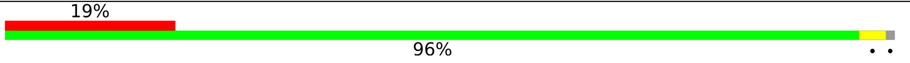
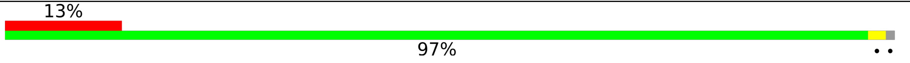
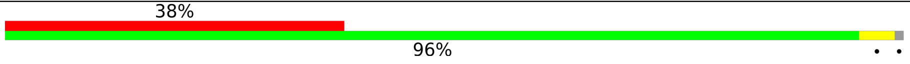
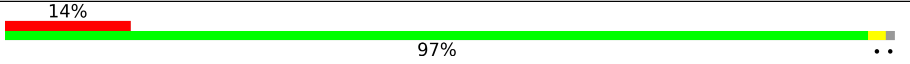
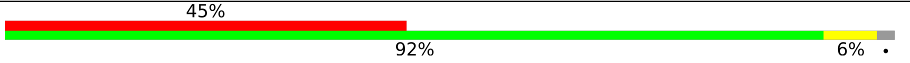
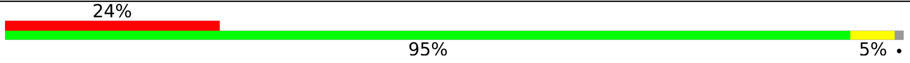
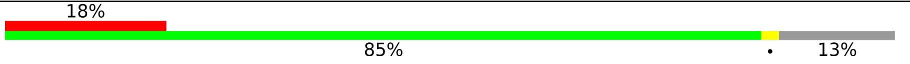
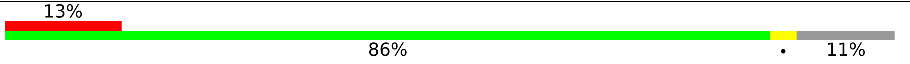
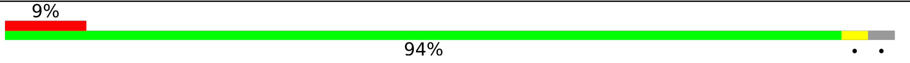
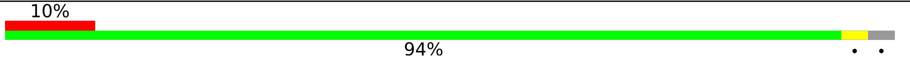
4	AW	254	
4	j	254	
5	AX	389	
5	k	389	
6	AY	363	
6	l	363	
7	AZ	298	
7	m	298	
8	BA	176	
8	n	176	
9	BB	241	
9	o	241	
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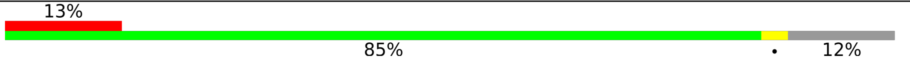
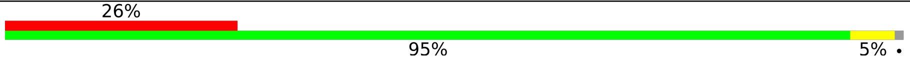
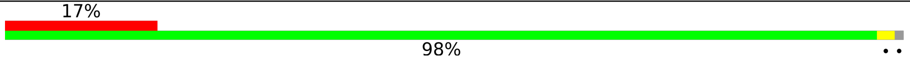
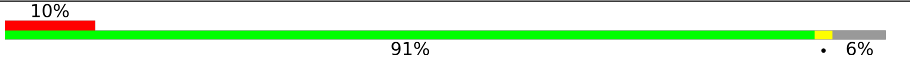
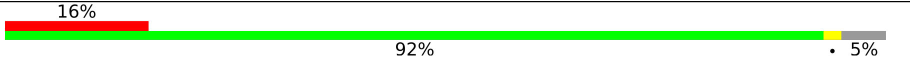
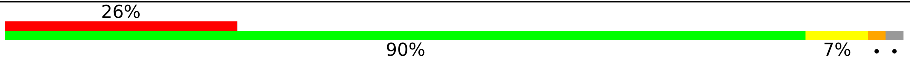
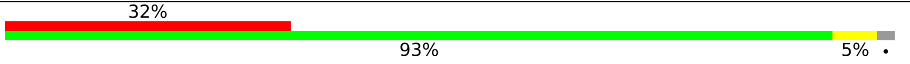
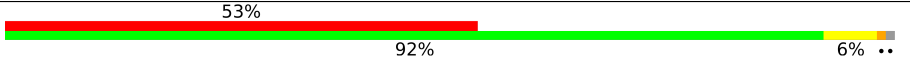
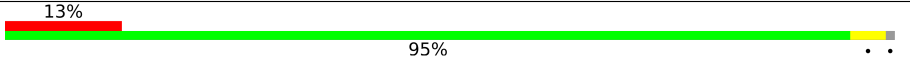
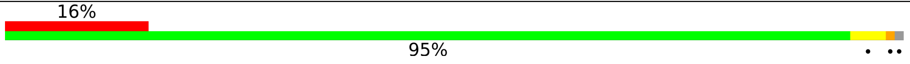
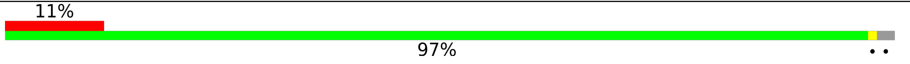
10	p	262	
11	BD	191	
11	q	191	
12	BE	220	
12	r	220	
13	BF	174	
13	s	174	
14	BG	202	
14	t	202	
15	BH	131	
15	u	131	

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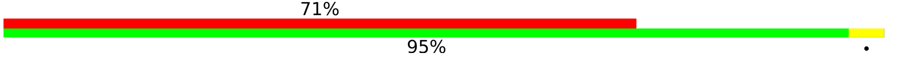
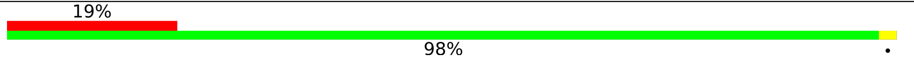
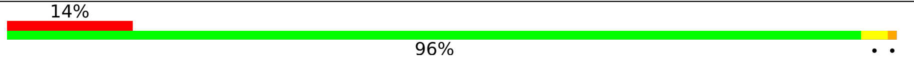
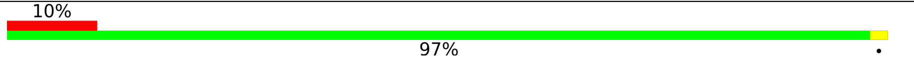
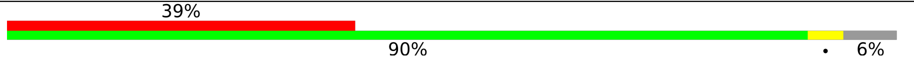
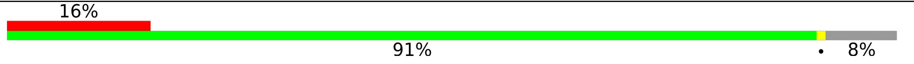
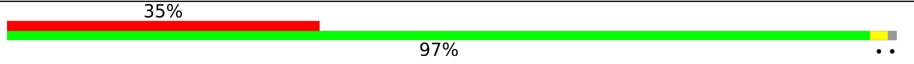
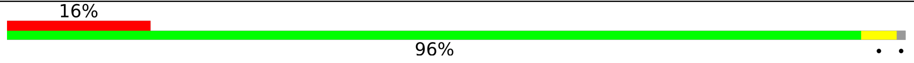
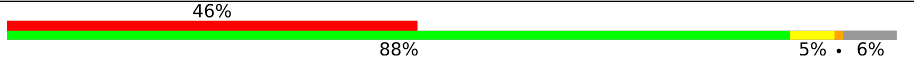
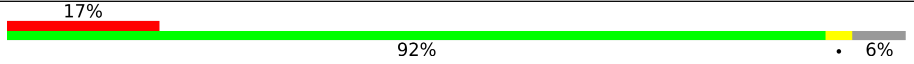
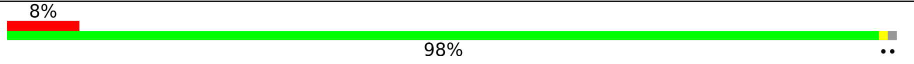
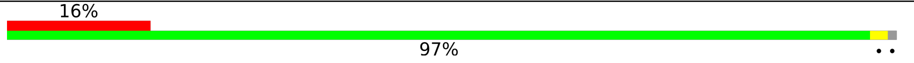
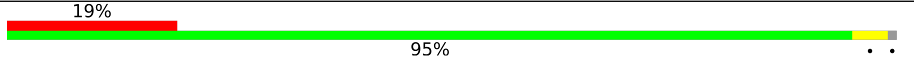
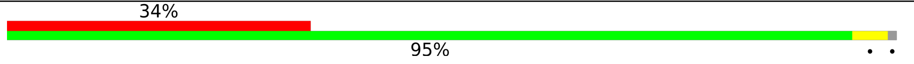
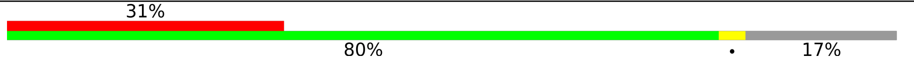
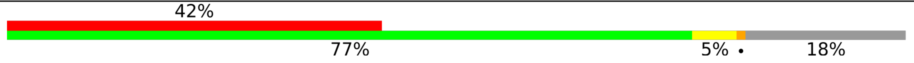
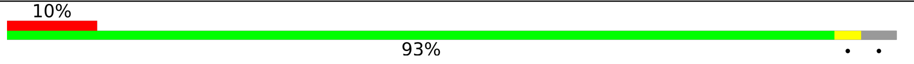
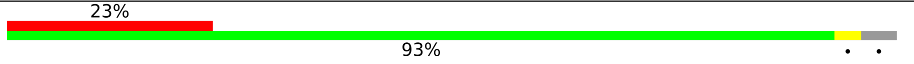
Mol	Chain	Length	Quality of chain
16	BI	204	
16	v	204	
17	BJ	200	
17	w	200	
18	BK	185	
18	x	185	
19	BL	186	
19	y	186	
20	BM	190	
20	z	190	
21	0	172	
21	BN	172	
22	2	160	
22	BO	160	
23	5	124	
23	BP	124	
24	6	137	
24	BQ	137	
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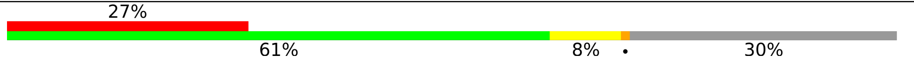
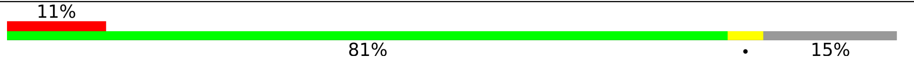
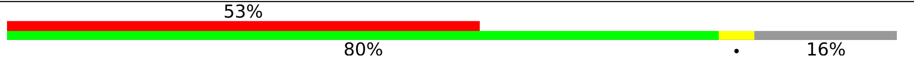
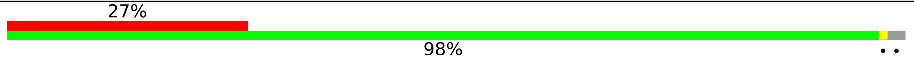
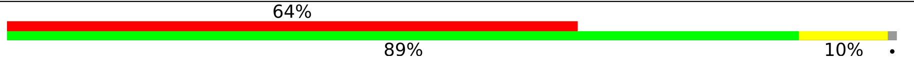
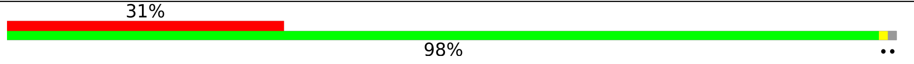
25	BR	155	
26	8	142	
26	BS	142	
27	9	127	
27	BT	127	
28	AA	136	

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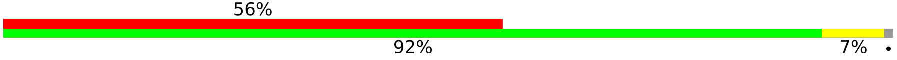
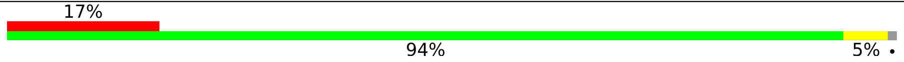
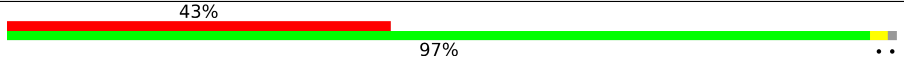
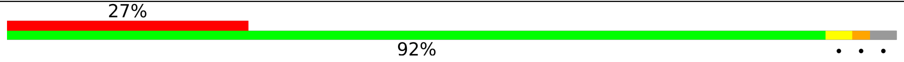
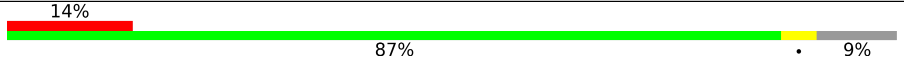
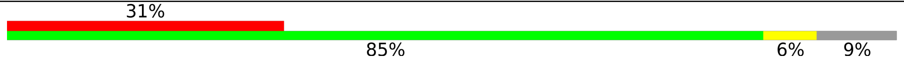
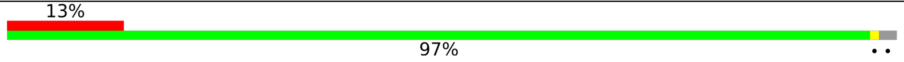
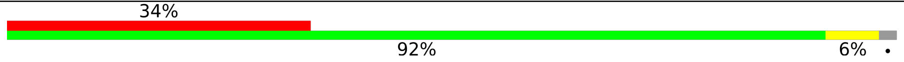
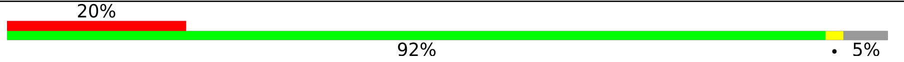
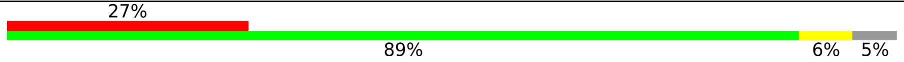
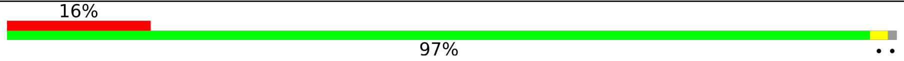
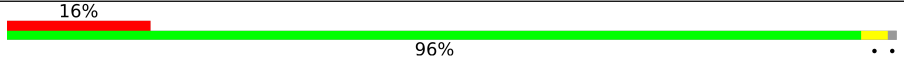
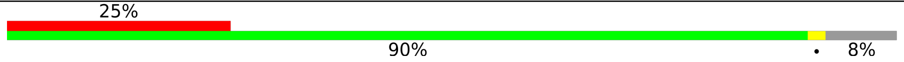
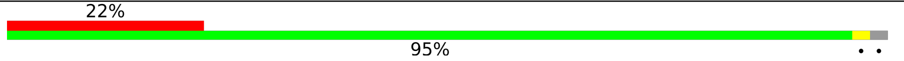
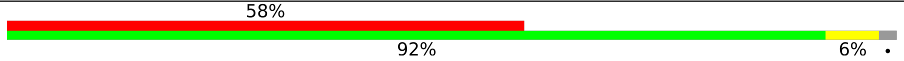
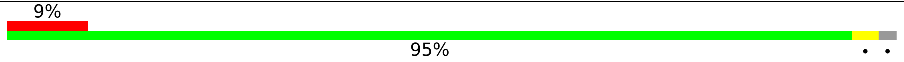
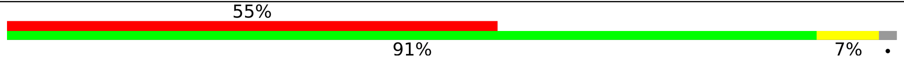
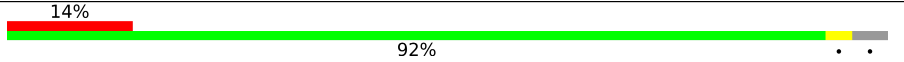
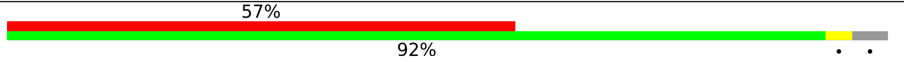
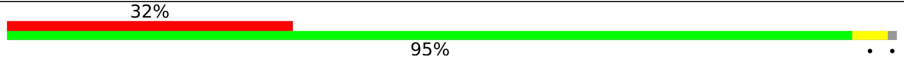
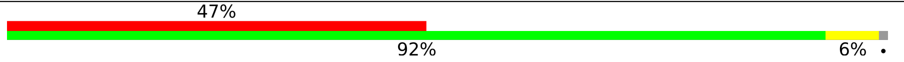
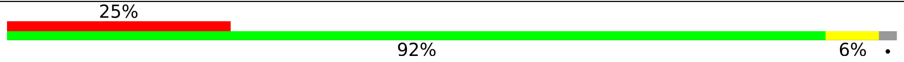
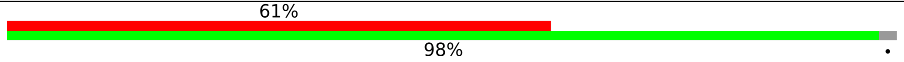
Mol	Chain	Length	Quality of chain
28	BU	136	
29	AB	149	
29	BV	149	
30	AC	63	
30	BW	63	
31	AD	106	
31	BX	106	
32	AE	112	
32	BY	112	
33	AF	131	
33	BZ	131	
34	AG	107	
34	CA	107	
35	AH	122	
35	CB	122	
36	AI	120	
36	CC	120	
37	AJ	99	
37	CD	99	
38	AK	90	
38	CE	90	
39	AL	78	
39	CF	78	
40	AM	51	
40	CG	51	

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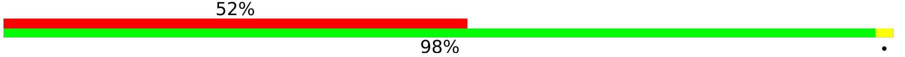
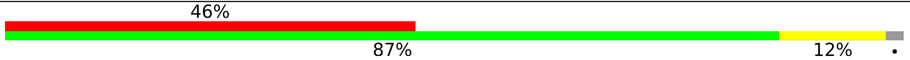
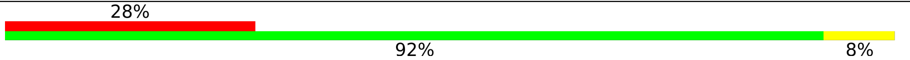
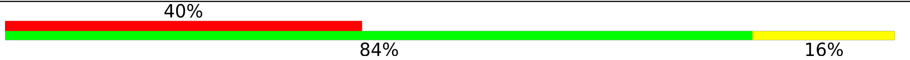
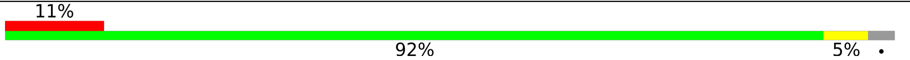
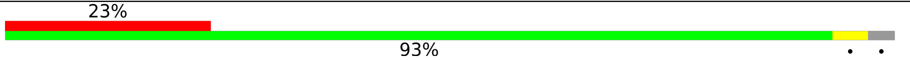
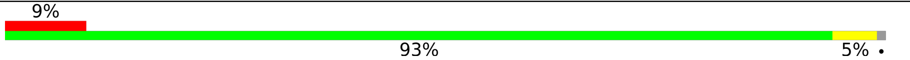
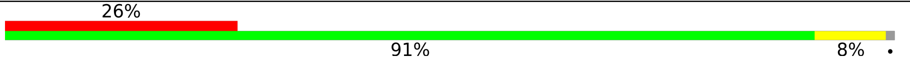
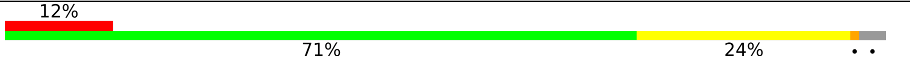
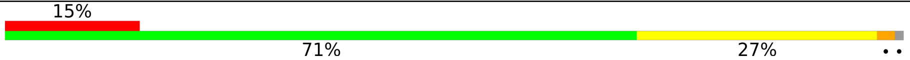
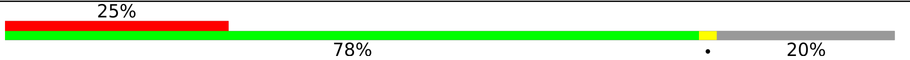
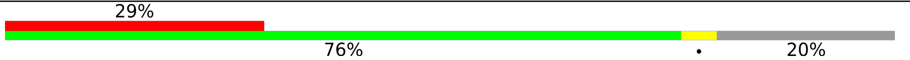
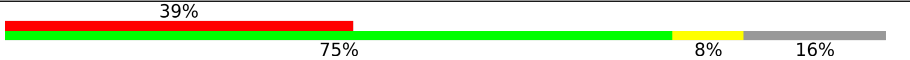
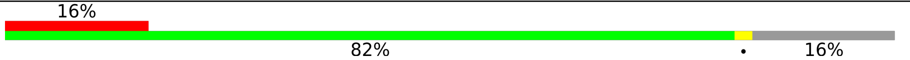
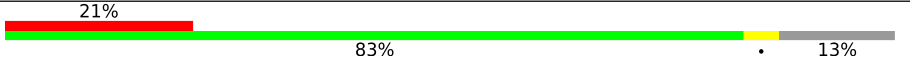
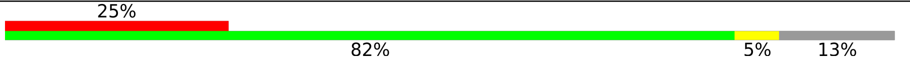
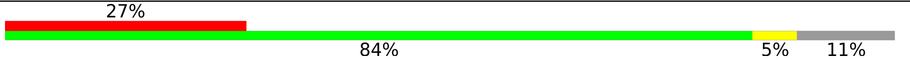
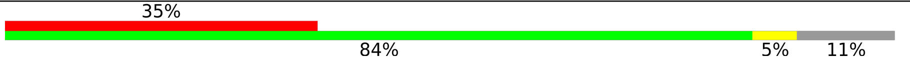
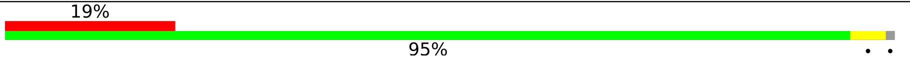
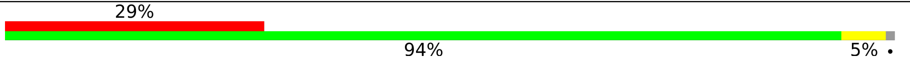
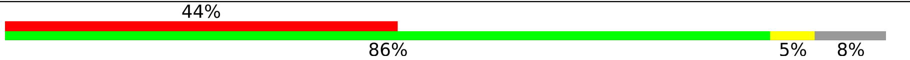
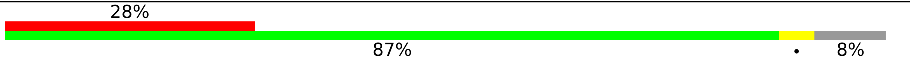
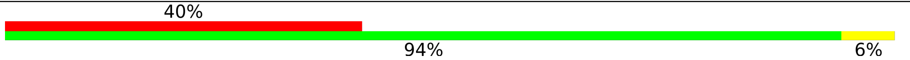
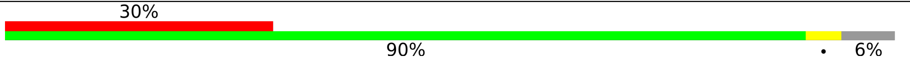
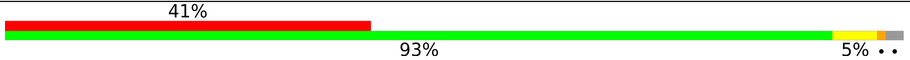
Mol	Chain	Length	Quality of chain
41	AN	52	
41	CH	52	
42	AO	25	
42	CI	25	
43	AP	106	
43	CJ	106	
44	AQ	92	
44	CK	92	
45	B	1787	
45	CM	1787	
46	C	261	
46	CN	261	
47	CO	256	
47	D	256	
48	CP	249	
48	E	249	
49	CQ	251	
49	F	251	
50	CR	262	
50	G	262	
51	CS	225	
51	H	225	
52	CT	236	
52	I	236	
53	CU	186	

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Mol	Chain	Length	Quality of chain
53	J	186	35% 91% 5% • •
54	CV	206	27% 95% • •
54	K	206	19% 96% • •
55	CW	189	34% 85% 9% 6%
55	L	189	52% 90% • 6%
56	CX	118	18% 70% 8% • 20%
56	M	118	30% 77% 6% 17%
57	CY	155	28% 87% • 9%
57	N	155	17% 89% • 9%
58	CZ	143	31% 72% 10% • 17%
58	O	143	45% 69% 12% • 19%
59	DA	151	46% 94% 5% •
59	P	151	27% 95% • •
60	DB	132	36% 94% • •
60	Q	132	20% 93% • •
61	DC	142	44% 82% • 14%
61	R	142	23% 86% 5% 9%
62	DD	142	59% 90% 5% 5%
62	S	142	39% 92% 6% •
63	DE	137	42% 85% 6% 9%
63	T	137	54% 86% • 9%
64	DF	145	41% 93% • •
64	U	145	16% 94% 6% •
65	DG	145	64% 89% 6% • •
65	V	145	33% 94% • •

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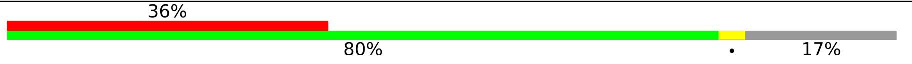
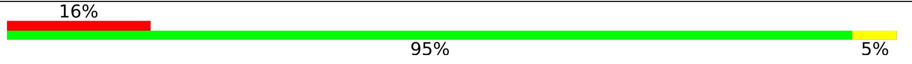
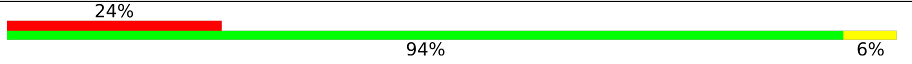
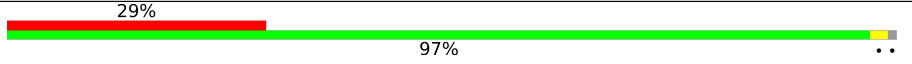
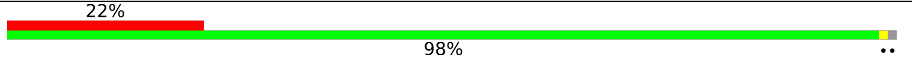
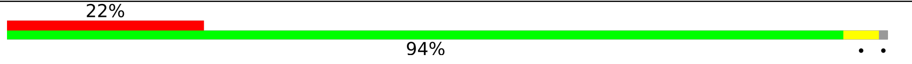
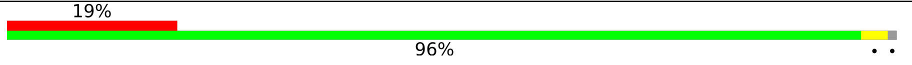
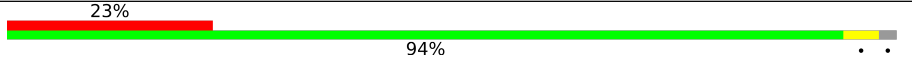
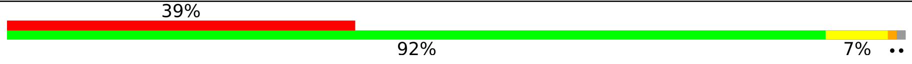
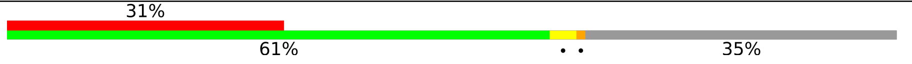
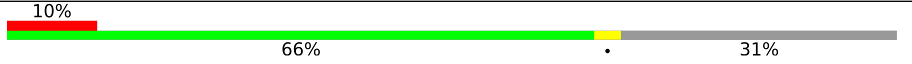
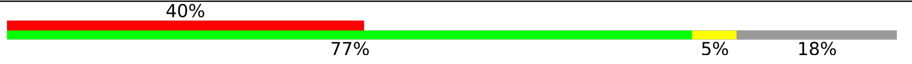
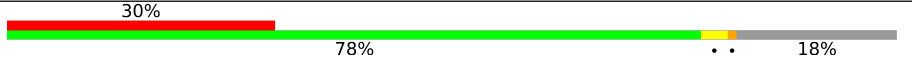
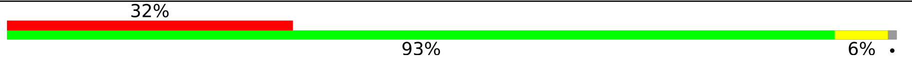
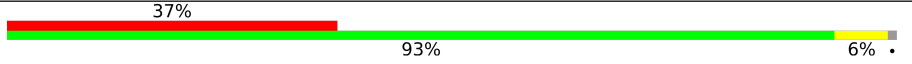
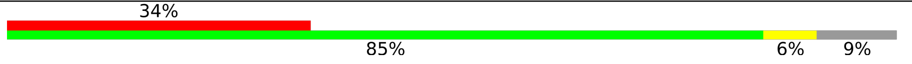
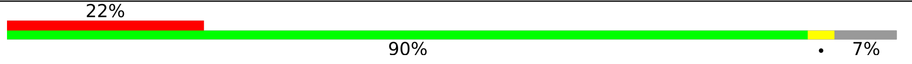
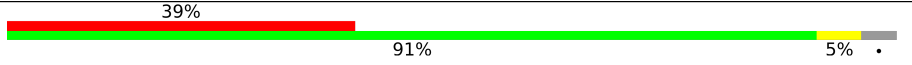
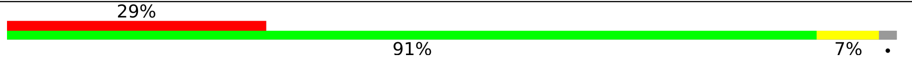
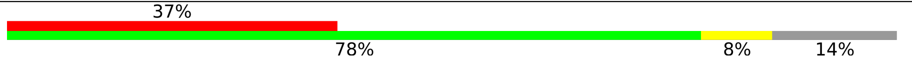
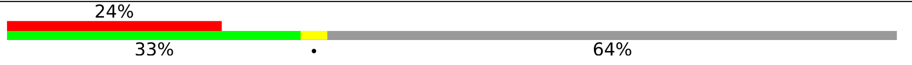
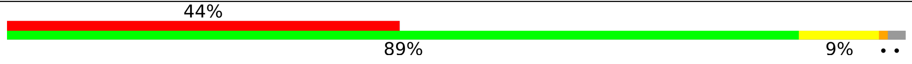
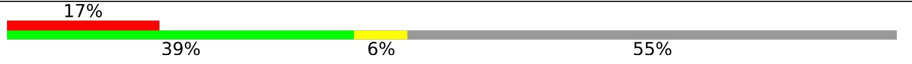
Mol	Chain	Length	Quality of chain
66	DH	119	
66	W	119	
67	DI	87	
67	X	87	
68	DJ	130	
68	Y	130	
69	DK	145	
69	Z	145	
70	DL	135	
70	a	135	
71	DM	105	
71	b	105	
72	DN	119	
72	c	119	
73	DO	82	
73	d	82	
74	DP	67	
74	e	67	
75	DQ	56	
75	f	56	
76	DR	63	
76	g	63	
77	h	193	
78	AR	317	
79	CL	267	

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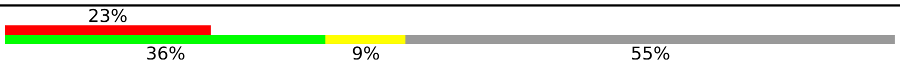
Mol	Chain	Length	Quality of chain
79	i	267	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
82	MG	1	3490	-	-	-	X
82	MG	1	3498	-	-	-	X
82	MG	AS	3469	-	-	-	X
82	MG	AS	3685	-	-	-	X
82	MG	AW	303	-	-	-	X
82	MG	B	1830	-	-	-	X
82	MG	B	1849	-	-	-	X
82	MG	B	1925	-	-	-	X

2 Entry composition (i)

There are 83 unique types of molecules in this entry. The entry contains 397530 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 25S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1	3171	67782	30282	12183	22146	3171	0	0	0
			Total	C	N	O	P			
1	AS	3065	65508	29266	11762	21415	3065	0	0	0

- Molecule 2 is a RNA chain called 5S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	3	121	2579	1153	463	842	121	0	0	0
			Total	C	N	O	P			
2	AT	121	2579	1153	463	842	121	0	0	0

- Molecule 3 is a RNA chain called 5.8S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	156	3313	1482	581	1094	156	0	0	0
			Total	C	N	O	P			
3	AU	156	3313	1482	581	1094	156	0	0	0

- Molecule 4 is a protein called 60S ribosomal protein L2-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	j	249	1894	1185	377	330	2	0	1	0
			Total	C	N	O	S			
4	AW	249	1894	1185	377	330	2	0	1	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	k	386	Total C N O S 3084 1955 584 538 7	0	1	0
5	AX	386	Total C N O S 3077 1950 582 538 7	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	l	360	Total C N O S 2745 1726 528 488 3	0	0	0
6	AY	361	Total C N O S 2751 1729 529 490 3	0	0	0

- Molecule 7 is a protein called Uncharacterized protein CaJ7.0206.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	m	296	Total C N O S 2426 1544 422 458 2	0	0	0
7	AZ	292	Total C N O S 2394 1526 416 450 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	n	157	Total C N O S 1242 796 226 219 1	0	0	0
8	BA	153	Total C N O 1210 777 221 212	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	o	234	Total C N O S 1885 1208 345 331 1	0	0	0
9	BB	234	Total C N O S 1885 1208 345 331 1	0	0	0

- Molecule 10 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	p	230	Total C N O S 1790 1147 318 322 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	BC	231	1795	1150	319	323	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	q	190	1519	958	276	281	4	0	0	0
			Total	C	N	O	S			
11	BD	190	1519	958	276	281	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	r	208	1689	1069	322	291	7	0	0	0
			Total	C	N	O	S			
12	BE	206	1671	1057	320	287	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	s	171	1371	857	260	250	4	0	0	0
			Total	C	N	O	S			
13	BF	171	1371	857	260	250	4	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	t	200	1610	1009	318	283	0	0	0
			Total	C	N	O			
14	BG	200	1610	1009	318	283	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	u	128	1015	651	190	173	1	0	0	0
			Total	C	N	O	S			
15	BH	130	1029	660	193	175	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	v	203	1713	1075	356	280	2	0	0	0
16	BI	203	1713	1075	356	280	2	0	0	0

- Molecule 17 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	w	199	1590	1025	294	269	2	0	0	0
17	BJ	199	1590	1025	294	269	2	0	0	0

- Molecule 18 is a protein called Ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	x	171	1372	846	278	248	0	0	0
18	BK	174	1396	862	282	252	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
19	y	185	1458	916	297	245	0	0	0
19	BL	185	1458	916	297	245	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	z	179	1457	901	310	243	3	0	0	0
20	BM	179	1457	901	310	243	3	0	0	0

- Molecule 21 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	0	170	1423	921	258	241	3	0	0	0
21	BN	170	1423	921	258	241	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	2	159	1262	798	241	221	2	0	0	0
22	BO	159	1262	798	241	221	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
23	5	103	831	539	138	154	0	0	0
23	BP	102	837	546	138	153	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	6	131	977	615	183	171	8	0	0	0
24	BQ	131	977	615	183	171	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	7	77	632	402	124	105	1	0	0	0
25	BR	109	877	549	178	149	1	0	0	0

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	8	121	974	622	175	176	1	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	BS	119	Total C N O S 960 613 172 174 1	0	0	0

- Molecule 27 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	9	125	Total C N O 980 613 189 178	0	0	0
27	BT	126	Total C N O 989 618 190 181	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	AA	135	Total C N O S 1087 705 197 183 2	0	0	0
28	BU	135	Total C N O S 1087 705 197 183 2	0	0	0

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	AB	148	Total C N O S 1170 741 231 197 1	0	0	0
29	BV	148	Total C N O S 1170 741 231 197 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	AC	61	Total C N O 488 304 104 80	0	0	0
30	BW	61	Total C N O 488 304 104 80	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	AD	96	Total C N O S 729 469 121 137 2	0	0	0
31	BX	96	Total C N O S 729 469 121 137 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	AE	110	894	565	168	159	2	0	0	0
32	BY	110	894	565	168	159	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	AF	124	1000	638	194	167	1	0	0	0
33	BZ	124	1004	641	195	167	1	0	0	0

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	AG	106	847	543	161	142	1	0	0	0
34	CA	106	847	543	161	142	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	AH	112	887	547	182	154	4	0	0	0
35	CB	112	887	547	182	154	4	0	0	0

- Molecule 36 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
36	AI	117	981	624	193	164	0	1	0
36	CC	118	985	626	194	165	0	1	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
37	AJ	97	Total C N O S 758 471 156 130 1	0	0	0
37	CD	97	Total C N O S 758 471 156 130 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	AK	86	Total C N O S 677 413 148 110 6	0	0	0
38	CE	86	Total C N O S 677 413 148 110 6	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
39	AL	77	Total C N O 617 393 115 109	0	0	0
39	CF	77	Total C N O 617 393 115 109	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
40	AM	50	Total C N O 438 275 97 66	0	0	0
40	CG	50	Total C N O 446 280 100 66	0	1	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	AN	52	Total C N O S 419 260 86 67 6	0	0	0
41	CH	51	Total C N O S 411 255 85 66 5	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	AO	25	Total C N O S 236 144 63 28 1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CI	25	Total 236	C 144	N 63	O 28	S 1	0	0	0

- Molecule 43 is a protein called 60S ribosomal protein L42-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AP	103	Total 828	C 521	N 165	O 137	S 5	0	0	0
43	CJ	103	Total 828	C 521	N 165	O 137	S 5	0	0	0

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AQ	91	Total 698	C 430	N 140	O 124	S 4	0	0	0
44	CK	91	Total 698	C 430	N 140	O 124	S 4	0	0	0

- Molecule 45 is a RNA chain called 18S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B	1725	Total 36771	C 16437	N 6521	O 12088	P 1725	0	0	0
45	CM	1778	Total 37902	C 16943	N 6724	O 12457	P 1778	0	0	0

- Molecule 46 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	C	208	Total 1627	C 1041	N 284	O 297	S 5	0	0	0
46	CN	208	Total 1627	C 1041	N 284	O 297	S 5	0	0	0

- Molecule 47 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	D	214	Total 1724	C 1094	N 313	O 313	S 4	0	0	0
47	CO	214	Total 1724	C 1094	N 313	O 313	S 4	0	0	0

- Molecule 48 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	E	217	Total C N O S 1629 1039 289 296 5	0	0	0
48	CP	217	Total C N O S 1629 1039 289 296 5	0	0	0

- Molecule 49 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	F	223	Total C N O S 1707 1087 311 305 4	0	0	0
49	CQ	223	Total C N O S 1707 1087 311 305 4	0	0	0

- Molecule 50 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
50	G	259	Total C N O S 2051 1304 385 357 5	0	0	0
50	CR	260	Total C N O S 2055 1306 386 358 5	0	0	0

- Molecule 51 is a protein called Ribosomal protein S7.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
51	H	206	Total C N O S 1614 1008 301 301 4	0	0	0
51	CS	206	Total C N O S 1614 1008 301 301 4	0	0	0

- Molecule 52 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	I	222	Total C N O S 1787 1113 344 324 6	0	0	0
52	CT	236	Total C N O S 1904 1184 369 345 6	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	J	181	Total 1462	C 937	N 263	O 262	0	0	0
53	CU	183	Total 1475	C 944	N 265	O 266	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	K	202	Total 1574	C 970	N 321	O 282	S 1	0	0	0
54	CV	203	Total 1579	C 973	N 322	O 283	S 1	0	0	0

- Molecule 55 is a protein called Ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	L	178	Total 1453	C 918	N 286	O 248	S 1	0	0	0
55	CW	178	Total 1453	C 918	N 286	O 248	S 1	0	0	0

- Molecule 56 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	M	98	Total 817	C 531	N 135	O 150	S 1	0	0	0
56	CX	94	Total 791	C 515	N 131	O 144	S 1	0	0	0

- Molecule 57 is a protein called 40S ribosomal protein S11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	N	141	Total 1128	C 721	N 210	O 194	S 3	0	0	0
57	CY	141	Total 1129	C 722	N 212	O 192	S 3	0	0	0

- Molecule 58 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	O	116	Total 885	C 550	N 158	O 172	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	CZ	119	Total	C	N	O	S	0	0	0
			913	566	163	179	5			

- Molecule 59 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	P	150	Total	C	N	O	S	0	0	0
			1187	757	219	210	1			
59	DA	150	Total	C	N	O	S	0	0	0
			1187	757	219	210	1			

- Molecule 60 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	Q	127	Total	C	N	O	S	0	0	0
			942	579	186	174	3			
60	DB	127	Total	C	N	O	S	0	0	0
			942	579	186	174	3			

- Molecule 61 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	R	129	Total	C	N	O	S	0	0	0
			1018	649	185	177	7			
61	DC	122	Total	C	N	O	S	0	0	0
			963	612	176	168	7			

- Molecule 62 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	S	140	Total	C	N	O	S	0	0	0
			1091	700	198	192	1			
62	DD	135	Total	C	N	O	S	0	0	0
			1053	675	192	185	1			

- Molecule 63 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	T	124	Total	C	N	O	S	0	0	0
			997	628	183	185	1			
63	DE	124	Total	C	N	O	S	0	0	0
			997	628	183	185	1			

- Molecule 64 is a protein called 40S ribosomal protein S18-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
64	U	144	1187	744	233	207	3	0	0	0
			Total	C	N	O	S			
64	DF	141	1161	727	227	204	3	0	0	0

- Molecule 65 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
65	V	141	1100	689	210	200	1	0	0	0
			Total	C	N	O	S			
65	DG	139	1089	682	208	198	1	0	0	0

- Molecule 66 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
66	W	99	782	493	145	142	2	0	0	0
			Total	C	N	O	S			
66	DH	97	763	481	140	140	2	0	0	0

- Molecule 67 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
67	X	87	676	415	126	133	2	0	0	0
			Total	C	N	O	S			
67	DI	87	676	415	126	133	2	0	0	0

- Molecule 68 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
68	Y	129	1032	655	191	183	3	0	0	0
			Total	C	N	O	S			
68	DJ	129	1032	655	191	183	3	0	0	0

- Molecule 69 is a protein called Ribosomal protein S23 (S12).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
69	Z	143	Total C N O S 1110 701 219 188 2	0	0	0
69	DK	143	Total C N O S 1110 701 219 188 2	0	0	0

- Molecule 70 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
70	a	134	Total C N O 1086 677 218 191	0	0	0
70	DL	132	Total C N O 1072 670 216 186	0	0	0

- Molecule 71 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
71	b	72	Total C N O 578 369 103 106	0	0	0
71	DM	68	Total C N O 545 351 95 99	0	0	0

- Molecule 72 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
72	c	98	Total C N O S 779 482 163 128 6	0	0	0
72	DN	98	Total C N O S 779 482 163 128 6	0	0	0

- Molecule 73 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
73	d	81	Total C N O S 614 383 110 114 7	0	0	0
73	DO	81	Total C N O S 614 383 110 114 7	0	0	0

- Molecule 74 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
74	e	62	Total C N O S 487 299 98 88 2	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
74	DP	61	Total C N O S 476 293 94 87 2	0	0	0

- Molecule 75 is a protein called 40S ribosomal protein S29A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
75	f	55	Total C N O S 454 281 94 75 4	0	0	0
75	DQ	54	Total C N O S 449 278 93 74 4	0	0	0

- Molecule 76 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
76	g	54	Total C N O S 431 271 88 70 2	0	0	0
76	DR	58	Total C N O S 461 289 93 77 2	0	0	0

- Molecule 77 is a protein called Ubiquitin-40S ribosomal protein S31 fusion protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
77	h	70	Total C N O S 574 362 113 93 6	0	0	0

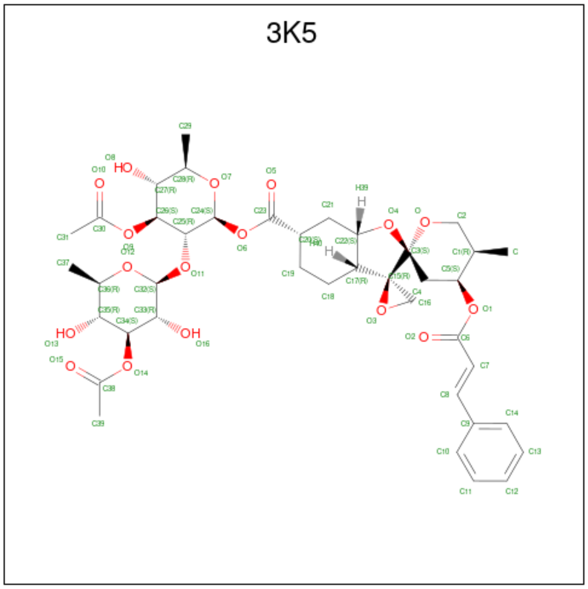
- Molecule 78 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
78	AR	311	Total C N O S 2398 1519 412 462 5	0	0	0

- Molecule 79 is a protein called 60S ribosomal protein CAALFM_C304810CA.

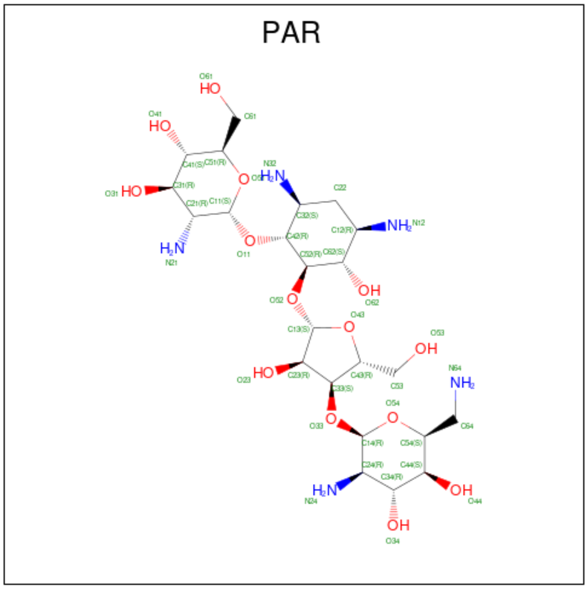
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
79	i	120	Total C N O 918 554 165 199	0	0	0
79	CL	121	Total C N O 930 563 166 201	0	0	0

- Molecule 80 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-{[(2R,2'S,3a'R,4''S,5''R,6'S,7a'S)-5''-methyl-4''-{[(2E)-3-phenylprop-2-enoyl]oxy}decahydrodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose (three-letter code: 3K5) (formula: $C_{40}H_{52}O_{17}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
80	1	1	57	40	17	0	0

- Molecule 81 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
81	1	1	42	23	5	14	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	1	1	Total C N O 42 23 5 14	0	0
81	4	1	Total C N O 42 23 5 14	0	0
81	4	1	Total C N O 42 23 5 14	0	0
81	B	1	Total C N O 42 23 5 14	0	0
81	B	1	Total C N O 42 23 5 14	0	0
81	B	1	Total C N O 42 23 5 14	0	0
81	B	1	Total C N O 42 23 5 14	0	0
81	B	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	AS	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0
81	AS	1	Total C N O 42 23 5 14	0	0
81	CM	1	Total C N O 42 23 5 14	0	0
81	CM	1	Total C N O 42 23 5 14	0	0
81	CM	1	Total C N O 42 23 5 14	0	0
81	CM	1	Total C N O 42 23 5 14	0	0
81	CM	1	Total C N O 42 23 5 14	0	0
81	CM	1	Total C N O 42 23 5 14	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	1	346	Total Mg 346 346	0	0
82	3	1	Total Mg 1 1	0	0
82	4	7	Total Mg 7 7	0	0
82	j	1	Total Mg 1 1	0	0
82	p	1	Total Mg 1 1	0	0
82	v	5	Total Mg 5 5	0	0
82	w	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	x	1	Total Mg 1 1	0	0
82	6	2	Total Mg 2 2	0	0
82	AB	1	Total Mg 1 1	0	0
82	AL	1	Total Mg 1 1	0	0
82	AP	2	Total Mg 2 2	0	0
82	B	140	Total Mg 140 140	0	0
82	C	1	Total Mg 1 1	0	0
82	E	1	Total Mg 1 1	0	0
82	F	1	Total Mg 1 1	0	0
82	G	1	Total Mg 1 1	0	0
82	K	1	Total Mg 1 1	0	0
82	f	1	Total Mg 1 1	0	0
82	AS	334	Total Mg 334 334	0	0
82	AT	1	Total Mg 1 1	0	0
82	AU	1	Total Mg 1 1	0	0
82	AW	3	Total Mg 3 3	0	0
82	AX	1	Total Mg 1 1	0	0
82	AY	1	Total Mg 1 1	0	0
82	CJ	1	Total Mg 1 1	0	0
82	CM	139	Total Mg 139 139	0	0
82	CR	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
82	DG	1	Total Mg 1 1	0	0
82	DJ	1	Total Mg 1 1	0	0
82	DK	1	Total Mg 1 1	0	0
82	CL	1	Total Mg 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	AH	1	Total Zn 1 1	0	0
83	AK	1	Total Zn 1 1	0	0
83	AN	1	Total Zn 1 1	0	0
83	AP	1	Total Zn 1 1	0	0
83	AQ	1	Total Zn 1 1	0	0
83	c	1	Total Zn 1 1	0	0
83	d	1	Total Zn 1 1	0	0
83	f	1	Total Zn 1 1	0	0
83	h	1	Total Zn 1 1	0	0
83	CB	1	Total Zn 1 1	0	0
83	CE	1	Total Zn 1 1	0	0
83	CH	1	Total Zn 1 1	0	0
83	CJ	1	Total Zn 1 1	0	0
83	CK	1	Total Zn 1 1	0	0
83	DN	1	Total Zn 1 1	0	0

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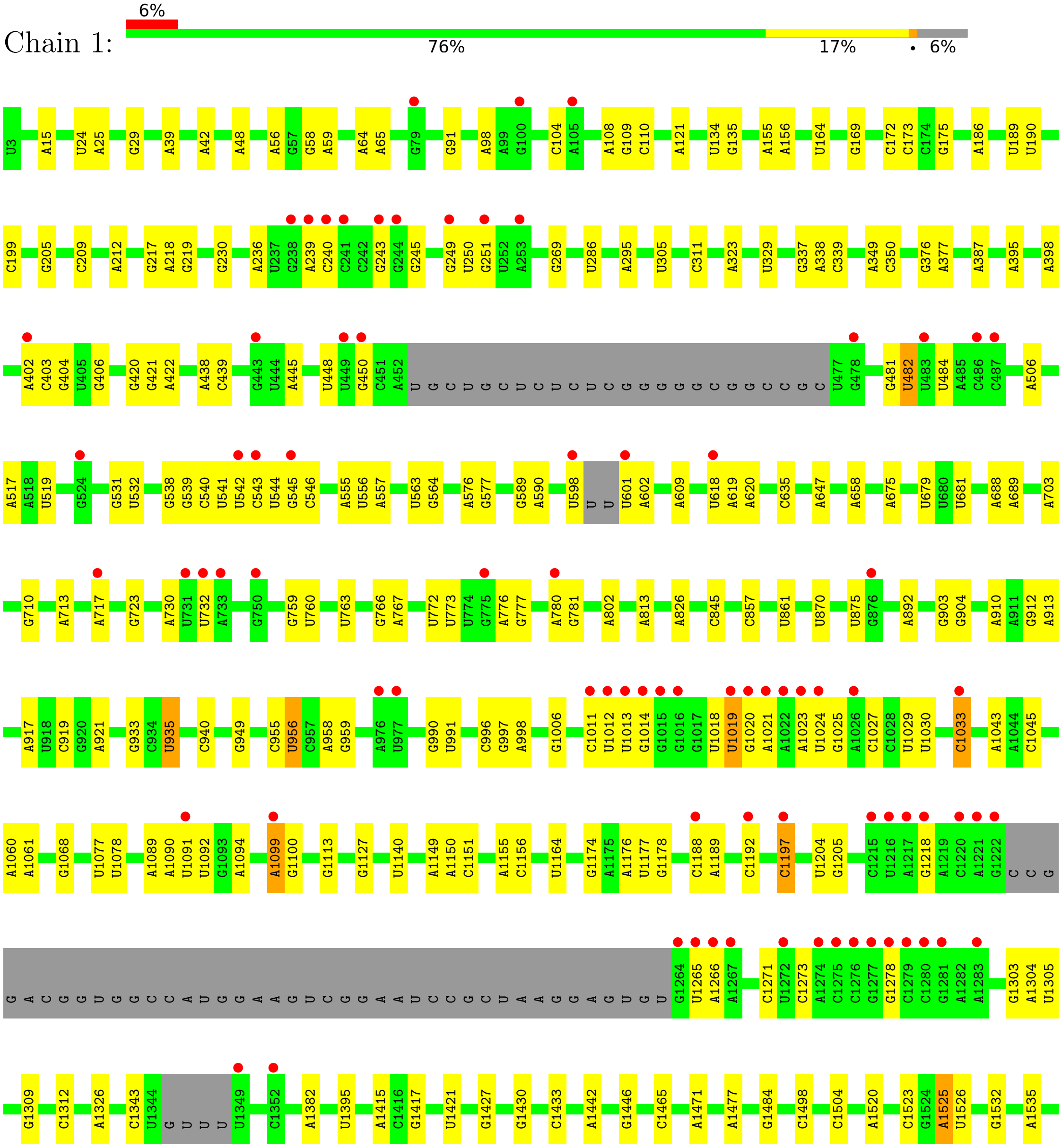
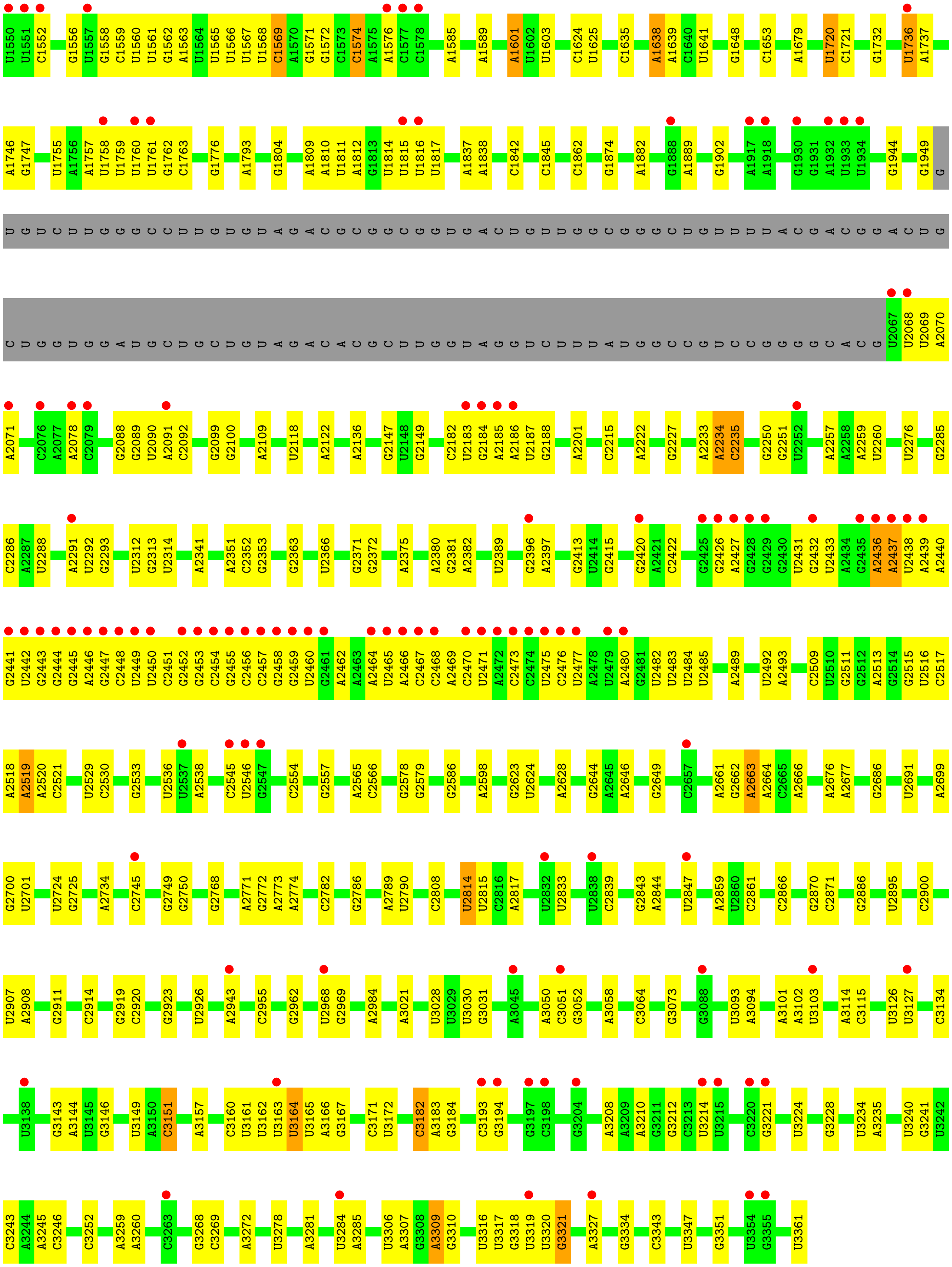
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	DO	1	Total Zn 1 1	0	0
83	DQ	1	Total Zn 1 1	0	0

3 Residue-property plots ⓘ

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

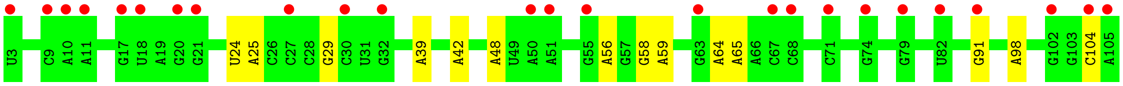
- Molecule 1: 25S

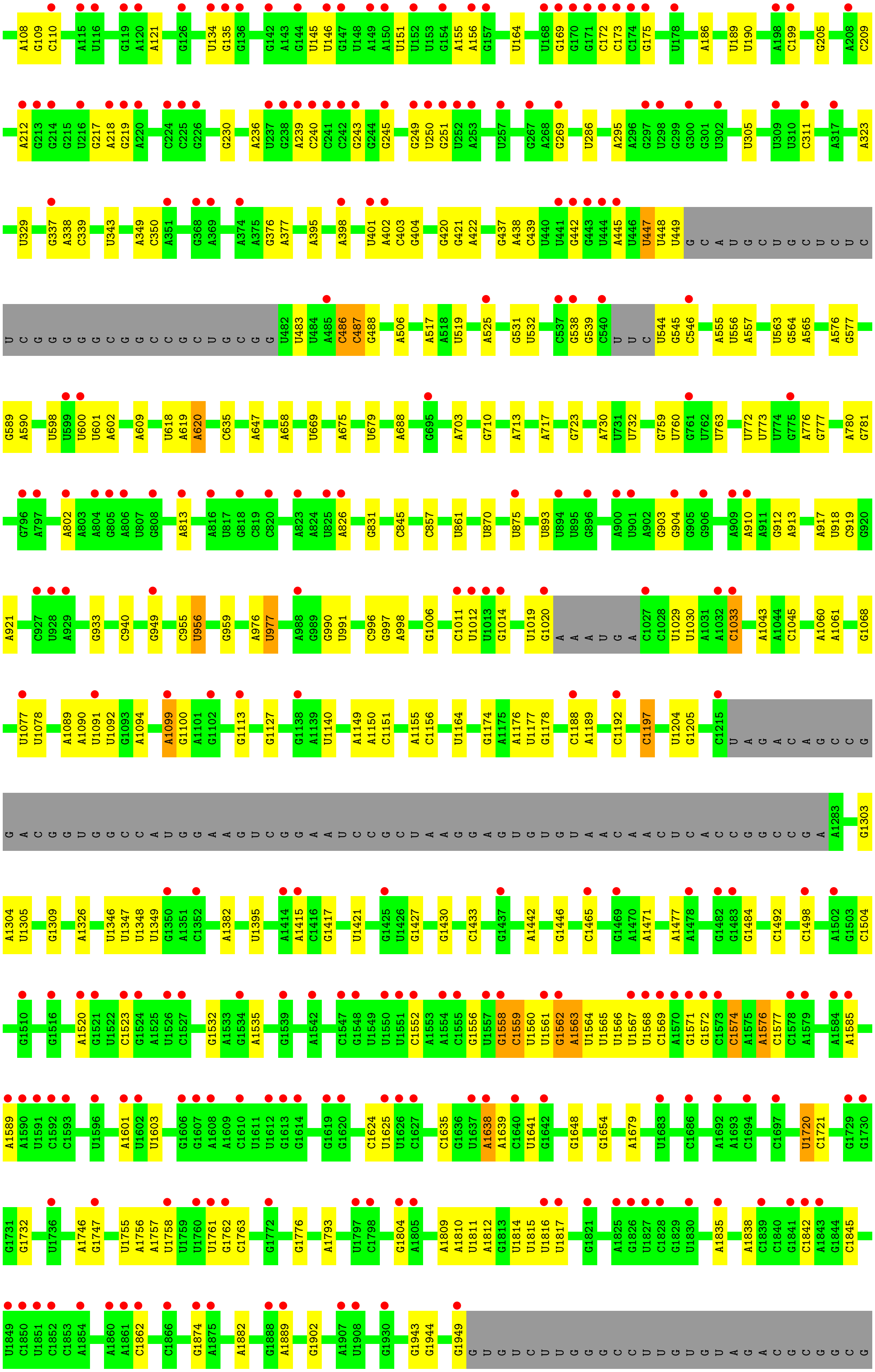


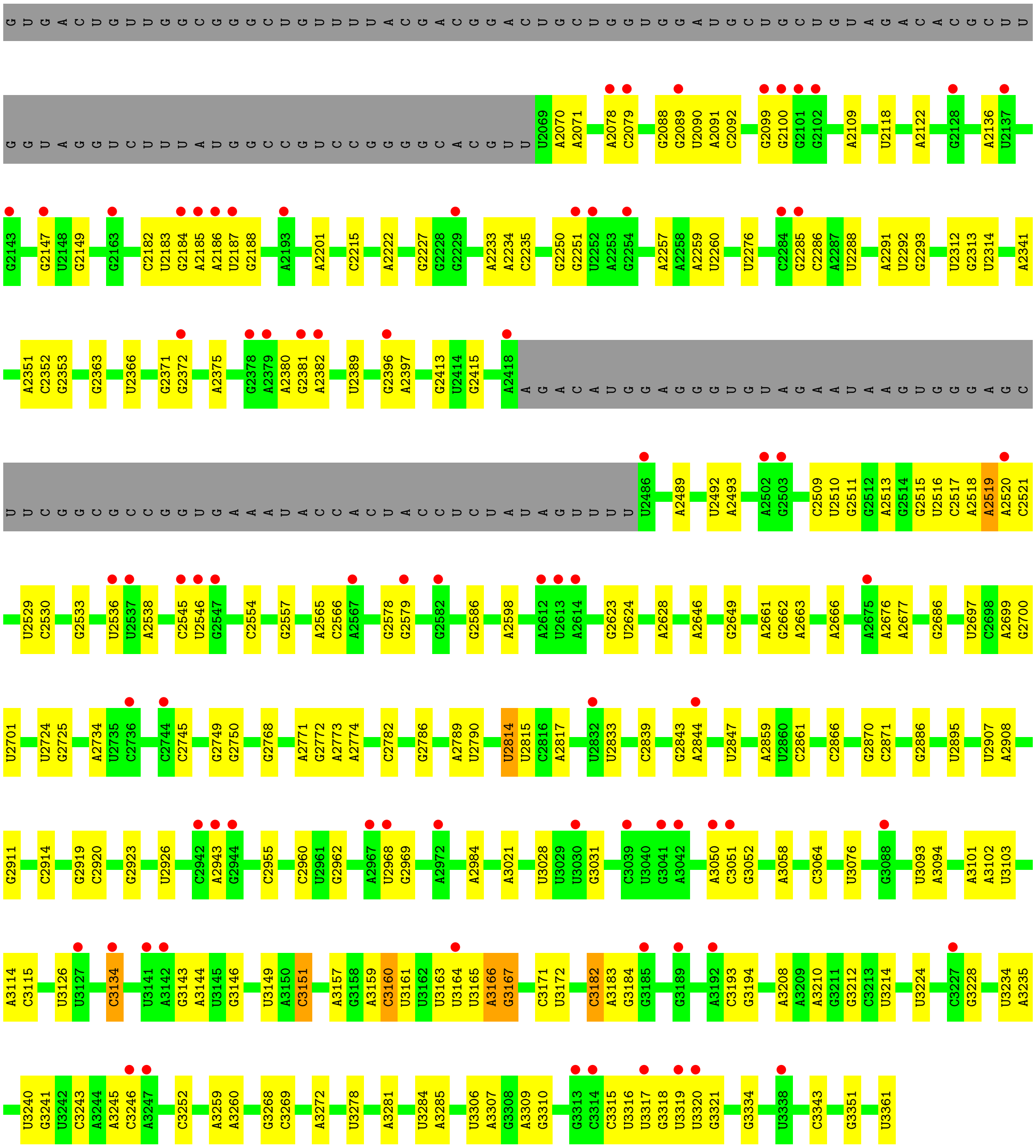


- Molecule 1: 25S

Chain AS:

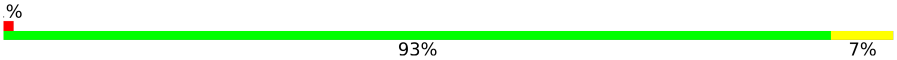


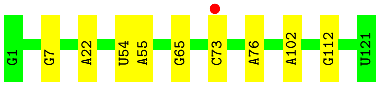

A108 G109 C110 A115 U116 G119 A120 A121 G126 U134 G135 G136 G142 A143 G144 U145 U146 G147 U148 A149 A150 U151 U152 U153 G154 A155 A156 G157 U164 U168 G169 G170 G171 C172 C173 C174 G175 U178 A186 U189 U190 A198 C199 G205 A208 C209
A212 G213 G214 G215 U216 G217 A218 G219 A220 C224 C225 G226 G230 A236 U237 G238 A239 C240 C241 C242 G243 G244 G245 G249 U250 G251 U252 A253 U257 G267 A268 G269 U286 A295 A296 G297 U298 G299 G300 G301 U302 U305 U309 U310 C311 A317 A323
U329 G337 A338 C339 U343 A349 C350 A351 G368 A369 A374 A375 G376 A377 A395 A398 U401 A402 C403 G404 G420 G421 A422 G437 A438 C439 U440 U441 G442 G443 U444 A445 U446 U447 U448 U449 G C A U G C U G C U C U C
U C G G G G G C G G C C G C U G C G G U482 U483 U484 A485 C486 C487 G488 A506 A517 A518 U519 A525 G531 U532 C537 G538 G539 C540 U U C U544 G545 C546 A555 U556 A557 U563 G564 A565 A576 G577
G589 A590 U598 U599 U600 U601 A602 A609 U618 A619 A620 C635 A647 A658 U669 A675 U679 A688 G695 A703 G710 A713 A717 G723 A730 U731 U732 G759 U760 G761 U762 U763 U772 U773 U774 G775 A776 G777 A780 G781
G796 A797 A802 A803 A804 G805 A806 U807 G808 A813 A816 U817 G818 C819 C820 A823 A824 U825 A826 G831 C845 C857 U861 U870 U875 U893 U894 U895 G896 A900 U901 A902 G903 G904 G905 G906 A909 A910 A911 G912 A913 A917 U918 C919 G920
A921 C927 U928 A929 G933 C940 G949 C955 U956 G959 A976 U977 A988 G989 G990 U991 C996 G997 A998 G1006 C1011 U1012 U1013 G1014 U1019 G1020 A A A U G A C1027 C1028 U1029 U1030 A1031 A1032 C1033 A1043 A1044 C1045 A1060 A1061 G1068
U1077 U1078 A1089 A1090 U1091 U1092 G1093 A1094 A1099 G1100 A1101 G1102 G1113 G1127 G1138 A1139 U1140 A1149 A1150 C1151 A1155 C1156 U1164 G1174 A1175 A1176 U1177 G1178 C1188 A1189 C1192 C1197 U1204 G1205 C1215 U A G A C A G C C G
G A C G G U G G C C A U G G A A G U C G G A A U C C G C U A A G G A G U G U G U A A C A A C U C A C C G G C C G A A1283 G1303
A1304 U1305 G1309 A1326 U1346 U1347 U1348 U1349 G1350 A1351 C1352 A1382 U1395 A1414 A1415 C1416 G1417 U1421 G1425 U1426 G1427 G1430 C1433 G1437 A1442 G1446 C1465 G1469 A1470 A1471 A1477 A1478 G1482 G1483 G1484 C1492 C1498 A1502 G1503 C1504
G1510 G1516 A1520 G1521 U1522 C1523 G1524 A1525 U1526 C1527 G1532 A1533 G1534 A1535 G1539 A1542 C1547 G1548 U1549 U1550 U1551 C1552 A1553 A1554 C1555 G1556 U1557 G1558 C1559 U1560 U1561 G1562 A1563 U1564 U1565 U1566 U1567 U1568 C1569 A1570 G1571 G1572 C1573 C1574 A1575 A1576 C1577 G1578 A1579 A1584 A1585
A1589 A1590 U1591 C1592 C1593 U1596 A1601 U1602 U1603 G1606 G1607 A1608 A1609 C1610 U1611 U1612 G1613 G1614 G1619 G1620 C1624 U1625 U1626 C1627 C1635 G1636 U1637 A1638 A1639 C1640 U1641 G1642 G1648 G1654 A1679 U1683 C1686 A1692 A1693 C1694 C1697 U1720 C1721 G1729 G1730
G1731 G1732 U1736 A1746 G1747 U1755 A1756 A1757 U1758 U1759 U1760 U1761 G1762 C1763 G1772 G1776 A1793 U1797 C1798 G1804 A1805 A1809 A1810 U1811 A1812 G1813 U1814 U1815 U1816 U1817 G1821 A1825 G1826 U1827 C1828 G1829 U1830 A1835 A1838 C1839 C1840 G1841 C1842 A1843 G1844 C1845
U1849 C1850 U1851 C1852 C1853 A1854 A1860 A1861 C1862 C1866 G1874 A1875 A1882 G1888 A1889 G1902 A1907 U1908 G1930 G1943 G1944 G1949 G U G U C U U G G G C C U U G U G U A G A C G C G G C G



- Molecule 2: 5S

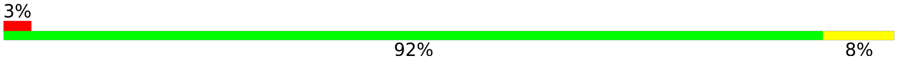
Chain 3:

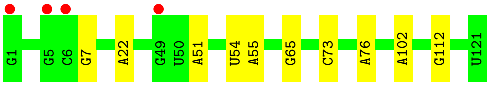




- Molecule 2: 5S

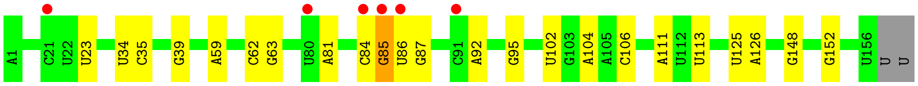
Chain AT:





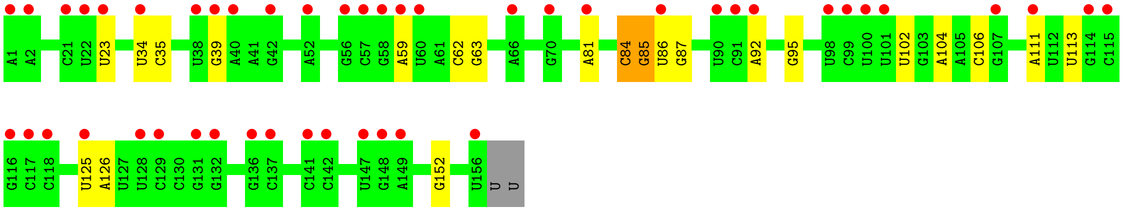
- Molecule 3: 5.8S

Chain 4:



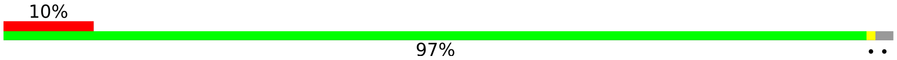
- Molecule 3: 5.8S

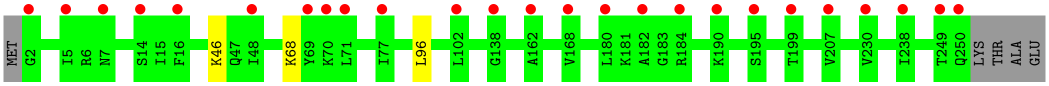
Chain AU:



- Molecule 4: 60S ribosomal protein L2-B

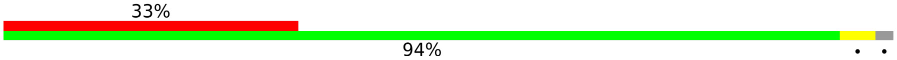
Chain j:

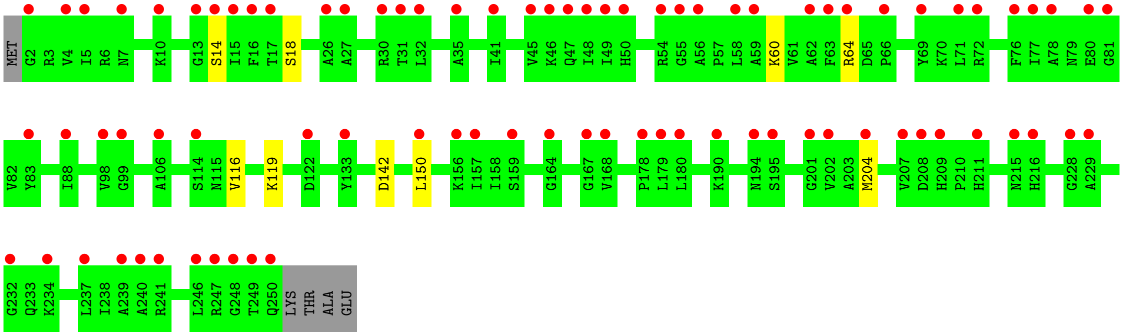




- Molecule 4: 60S ribosomal protein L2-B

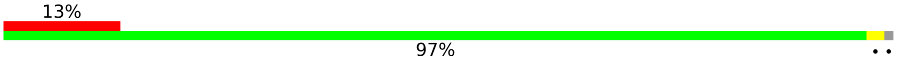
Chain AW:

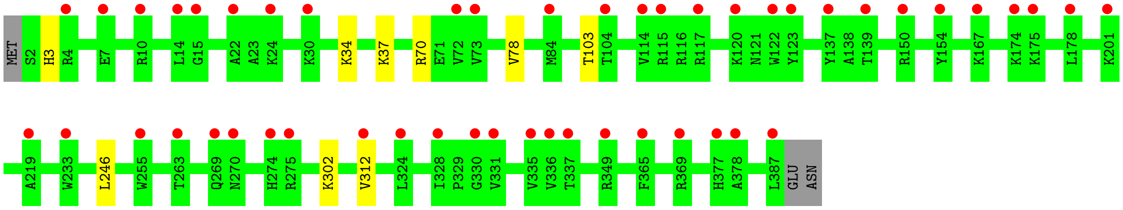




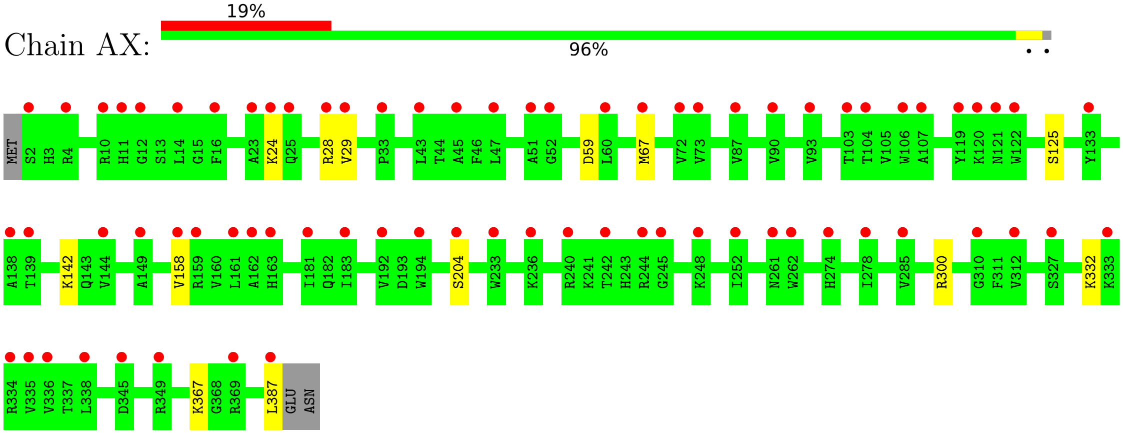
- Molecule 5: 60S ribosomal protein L3

Chain k:

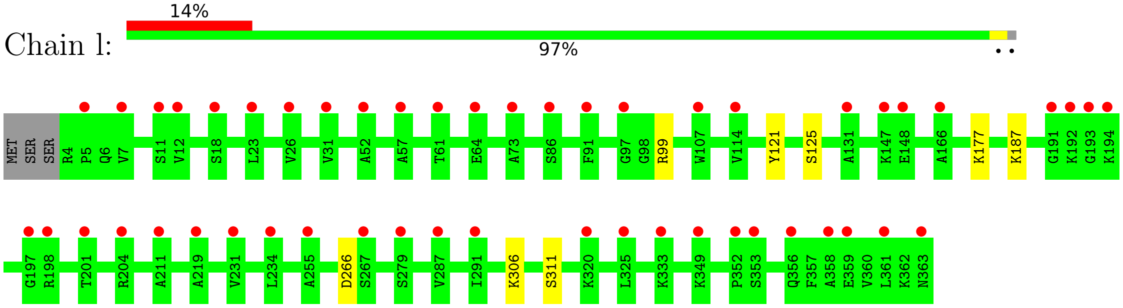




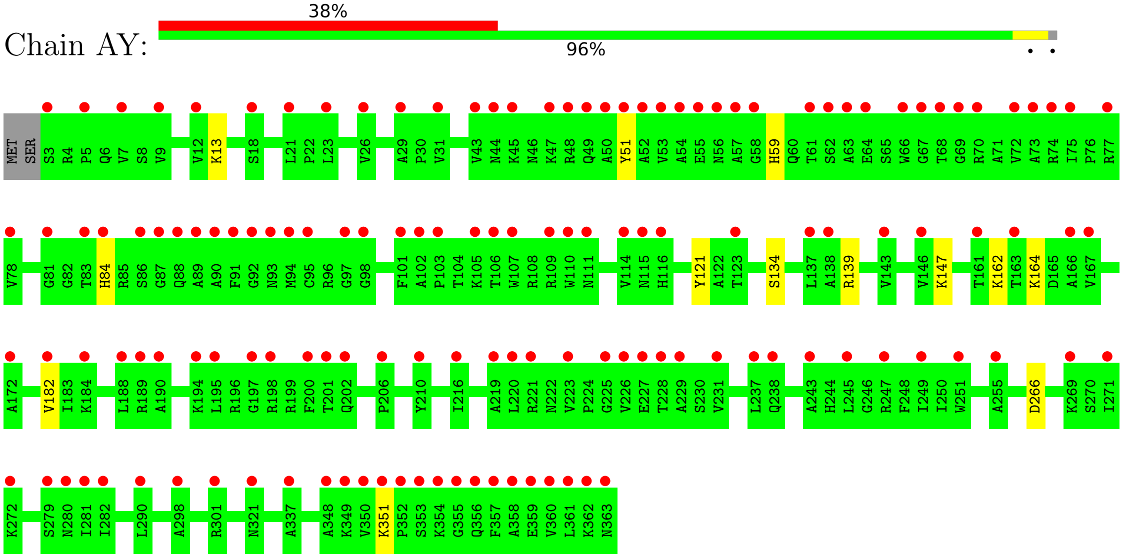
- Molecule 5: 60S ribosomal protein L3



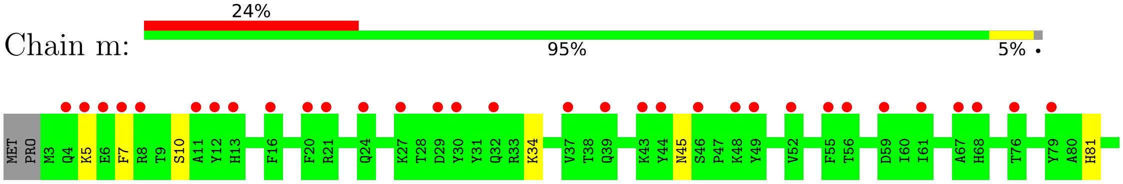
- Molecule 6: 60S ribosomal protein L4-B

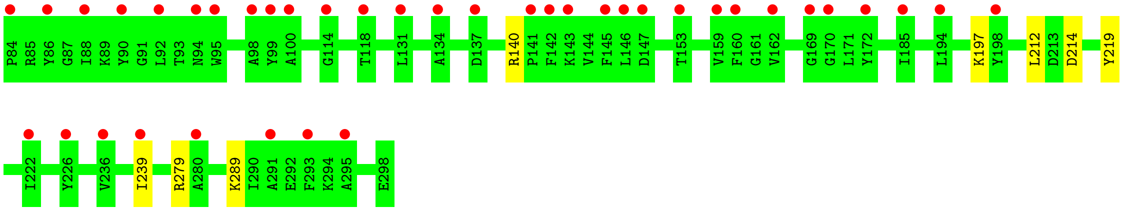


- Molecule 6: 60S ribosomal protein L4-B



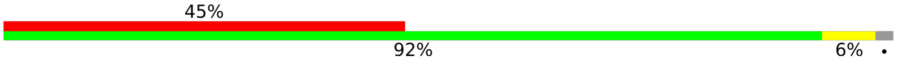
- Molecule 7: Uncharacterized protein CaJ7.0206

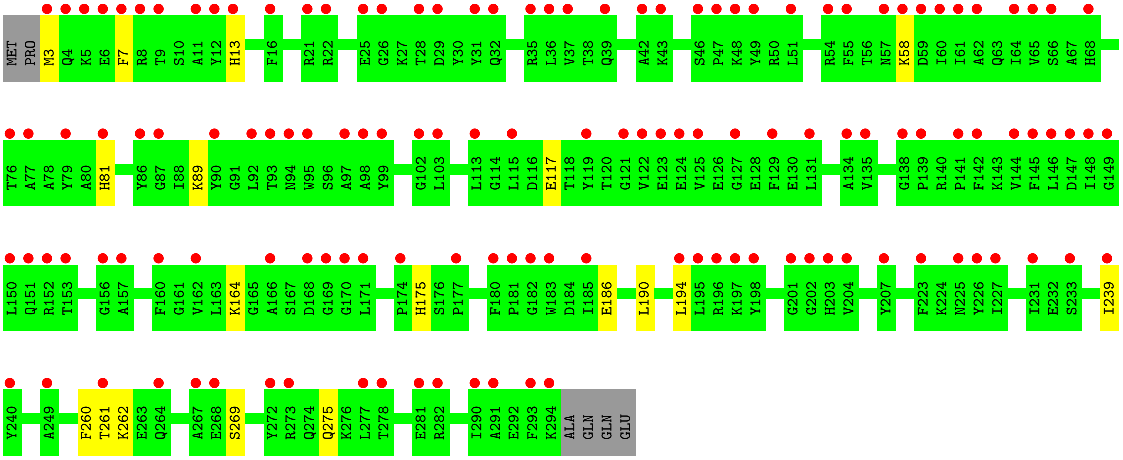




- Molecule 7: Uncharacterized protein CaJ7.0206

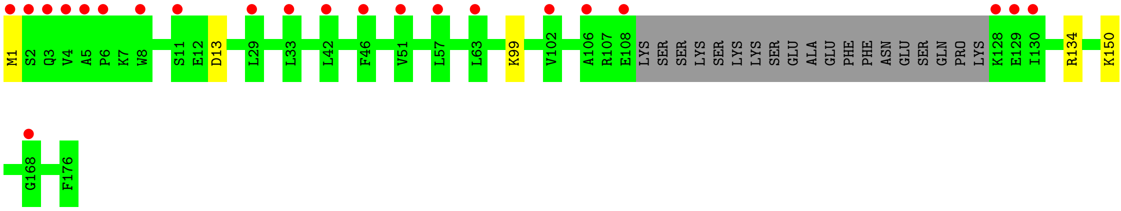
Chain AZ:





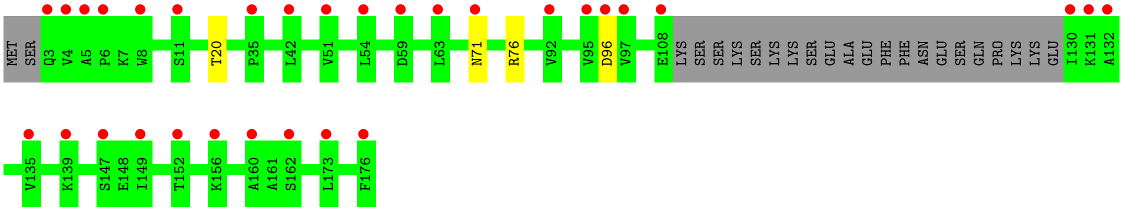
- Molecule 8: 60S ribosomal protein L6

Chain n:



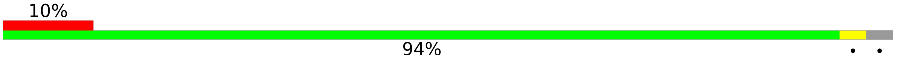
- Molecule 8: 60S ribosomal protein L6

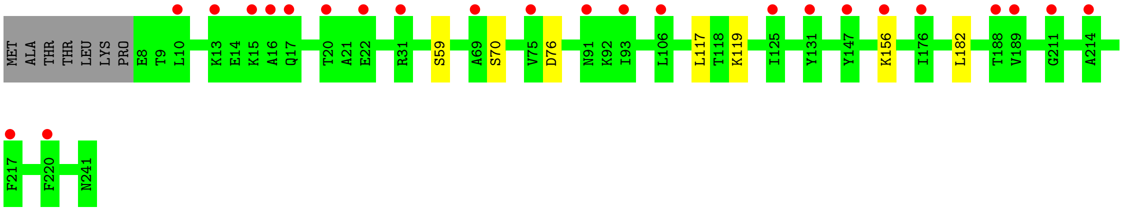
Chain BA:



- Molecule 9: 60S ribosomal protein L7-A

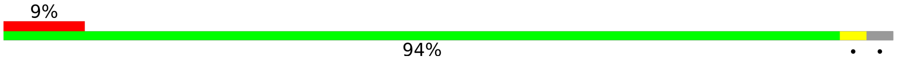
Chain o:

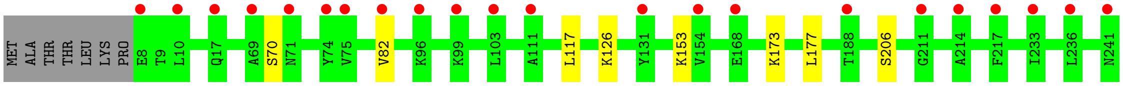




- Molecule 9: 60S ribosomal protein L7-A

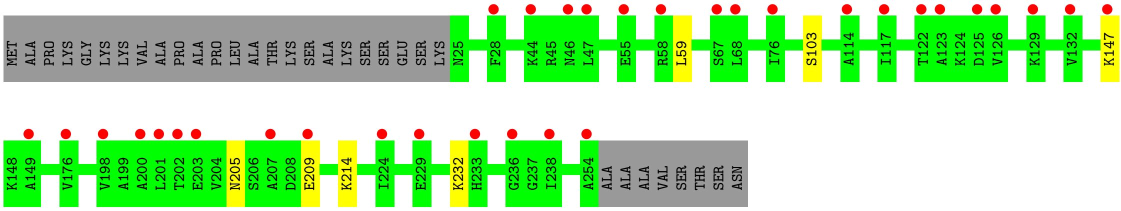
Chain BB:





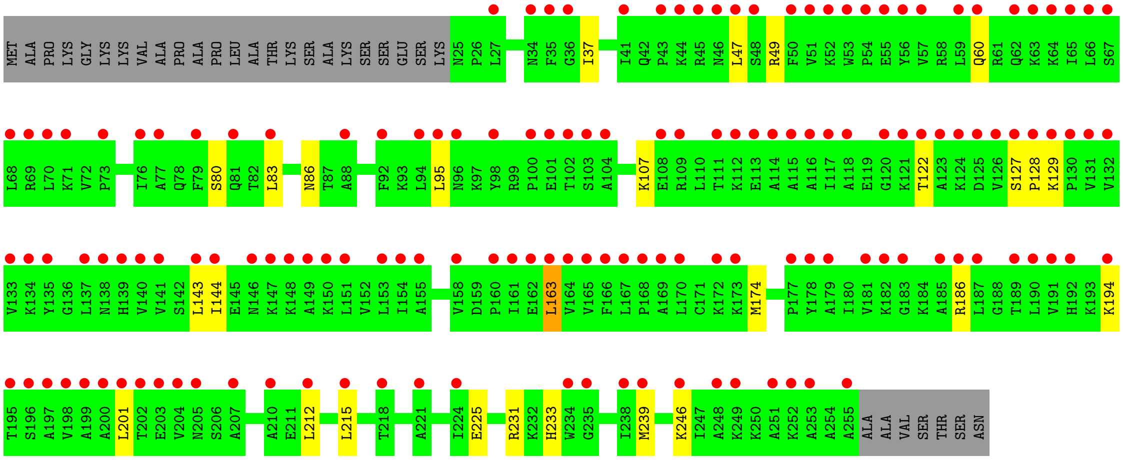
- Molecule 10: 60S ribosomal protein L8

Chain p:



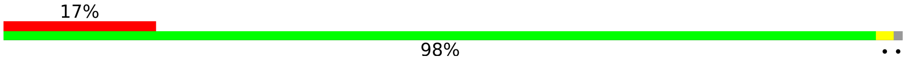
- Molecule 10: 60S ribosomal protein L8

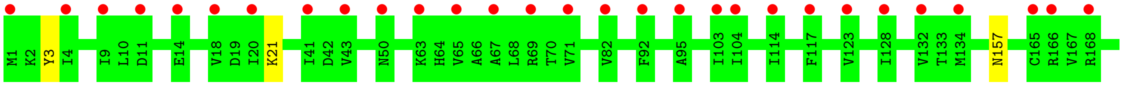
Chain BC:

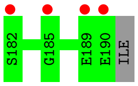


- Molecule 11: 60S ribosomal protein L9-B

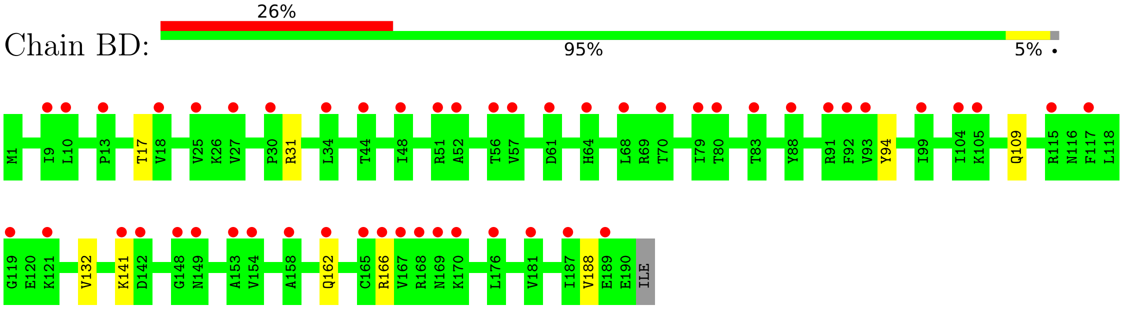
Chain q:



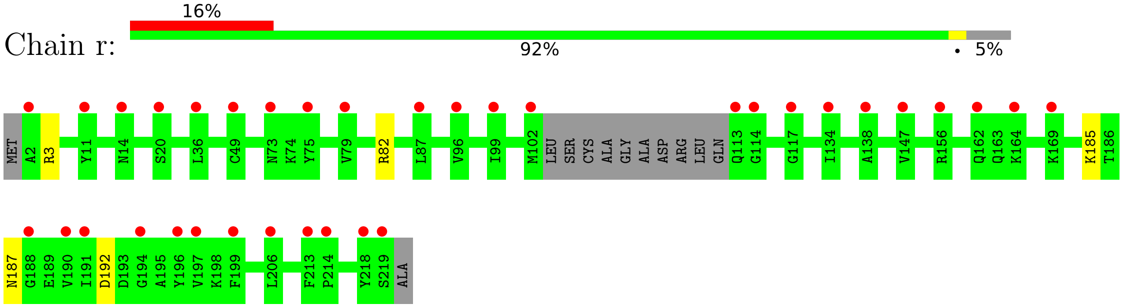




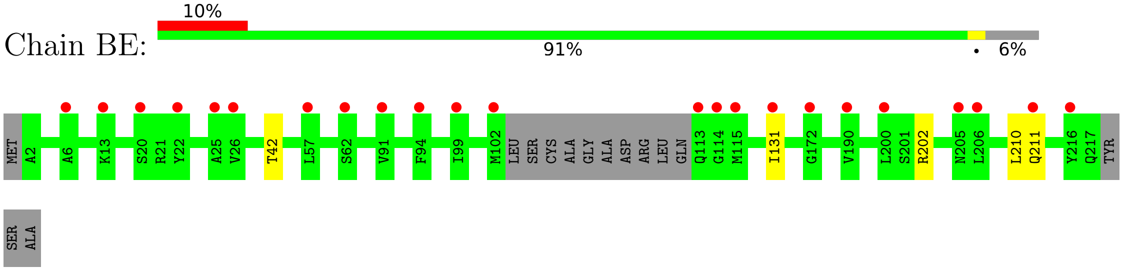
- Molecule 11: 60S ribosomal protein L9-B



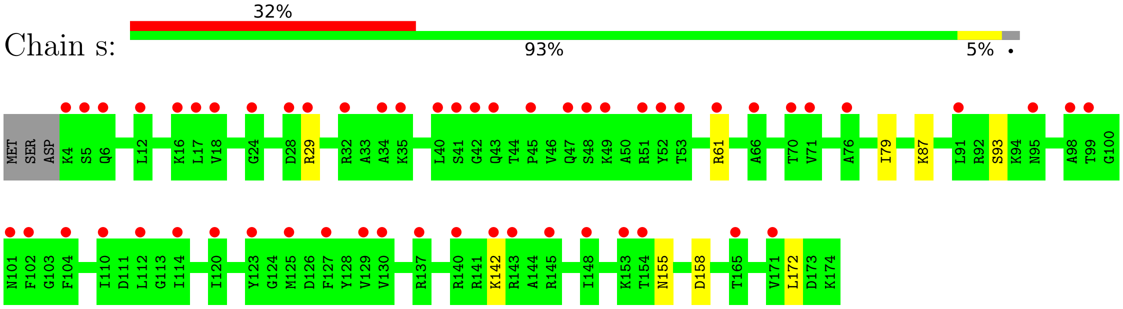
- Molecule 12: 60S ribosomal protein L10



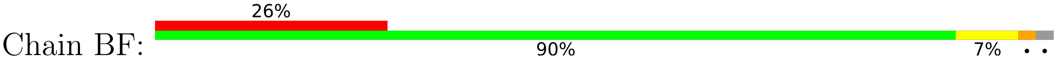
- Molecule 12: 60S ribosomal protein L10

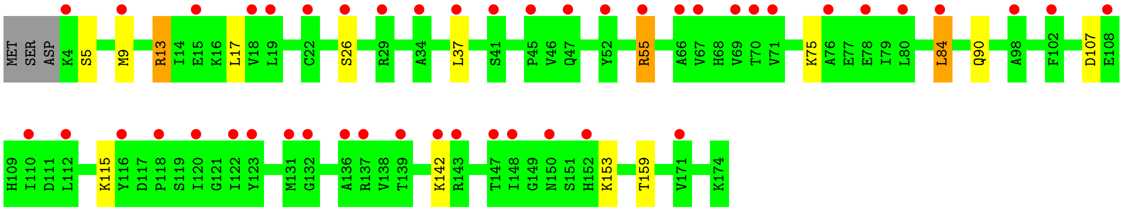


- Molecule 13: 60S ribosomal protein L11-B



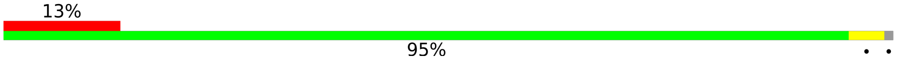
- Molecule 13: 60S ribosomal protein L11-B

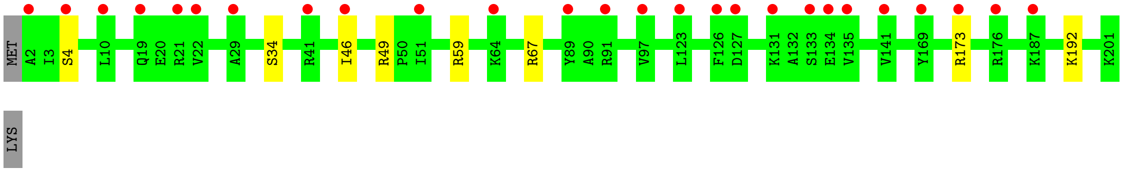




- Molecule 14: 60S ribosomal protein L13

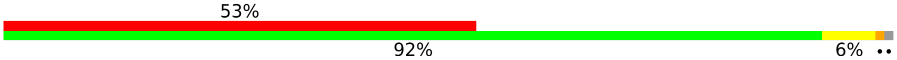
Chain t:

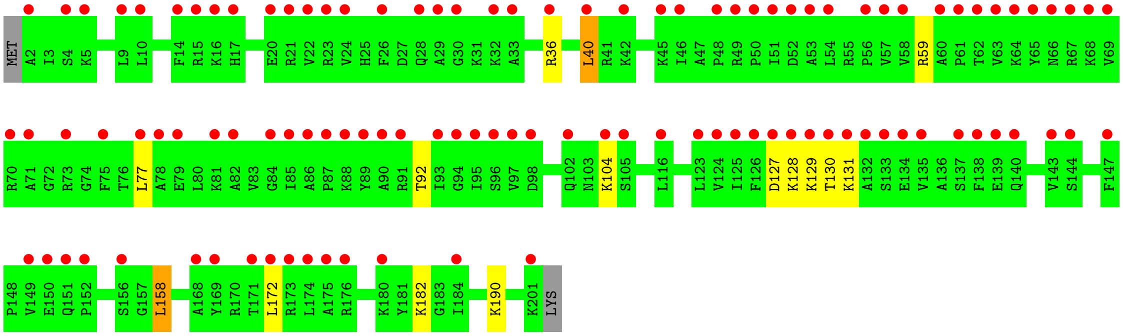




- Molecule 14: 60S ribosomal protein L13

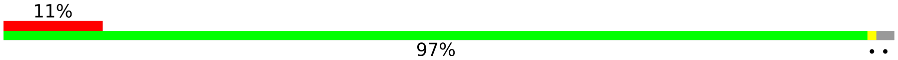
Chain BG:

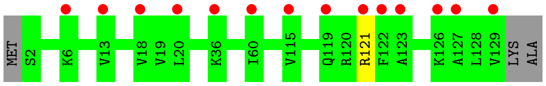




- Molecule 15: 60S ribosomal protein L14-B

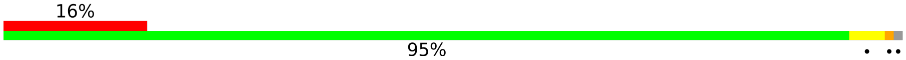
Chain u:

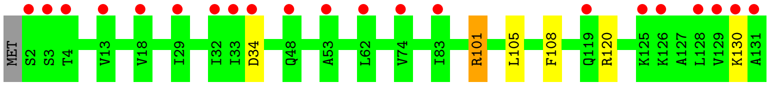




- Molecule 15: 60S ribosomal protein L14-B

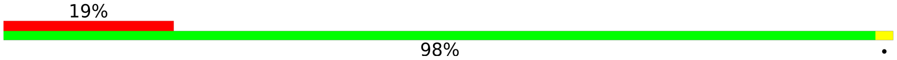
Chain BH:

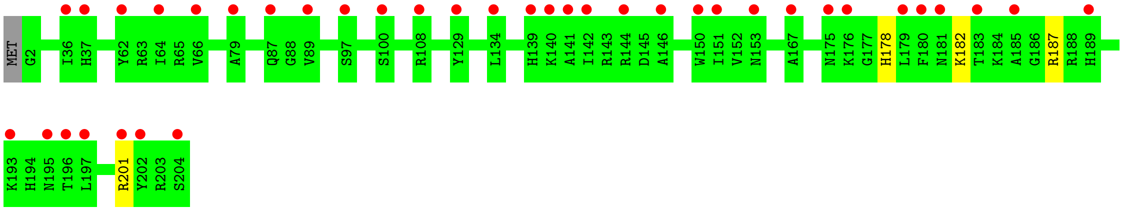




- Molecule 16: 60S ribosomal protein L15-A

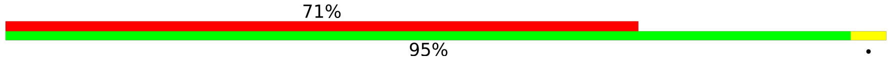
Chain v:

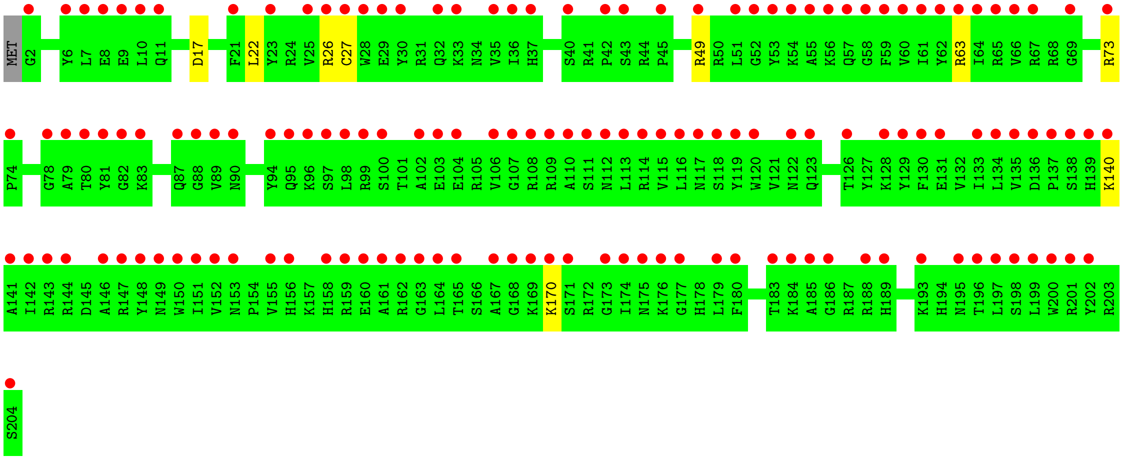




- Molecule 16: 60S ribosomal protein L15-A

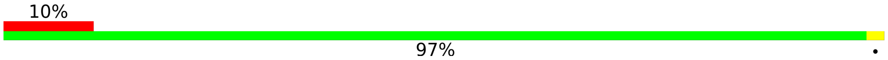
Chain BI:

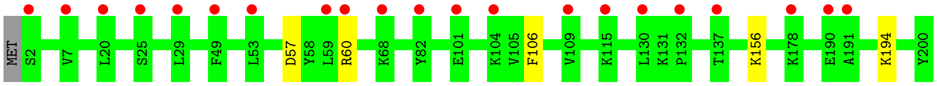




- Molecule 17: Ribosomal protein L13

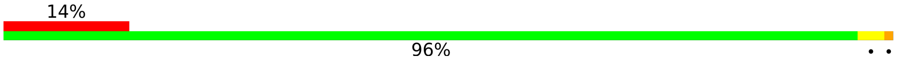
Chain w:

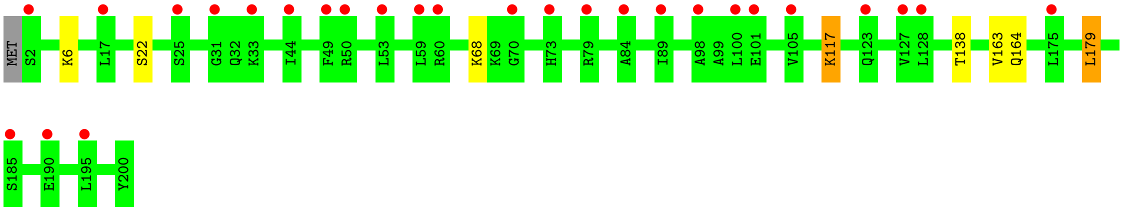




- Molecule 17: Ribosomal protein L13

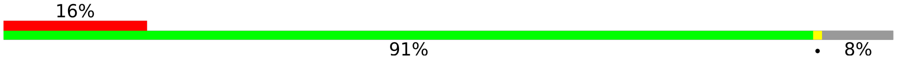
Chain BJ:

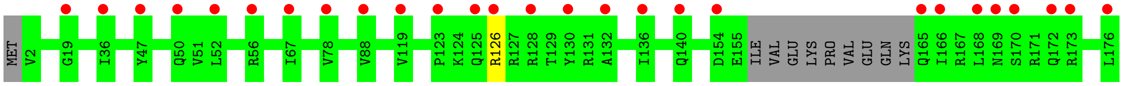


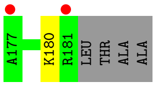


- Molecule 18: Ribosomal protein L22

Chain x:

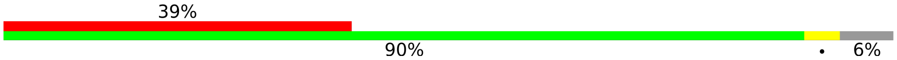


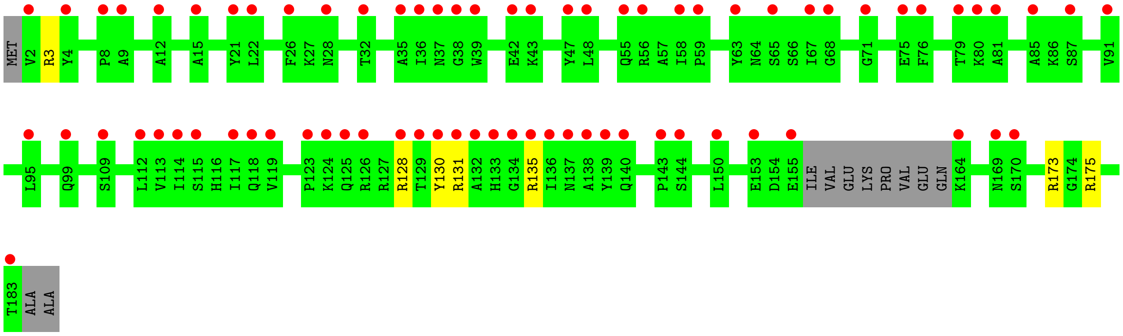




- Molecule 18: Ribosomal protein L22

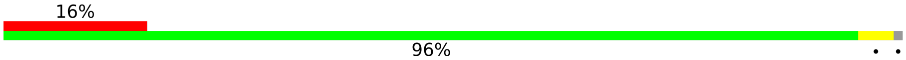
Chain BK:

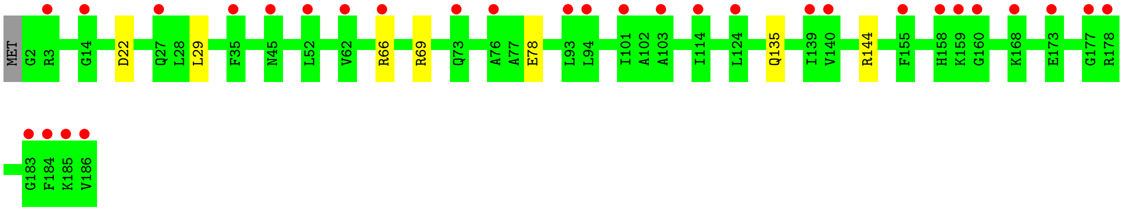




- Molecule 19: 60S ribosomal protein L18-A

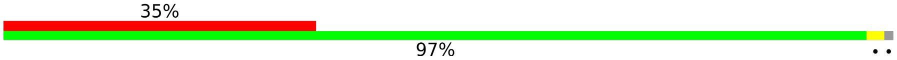
Chain y:

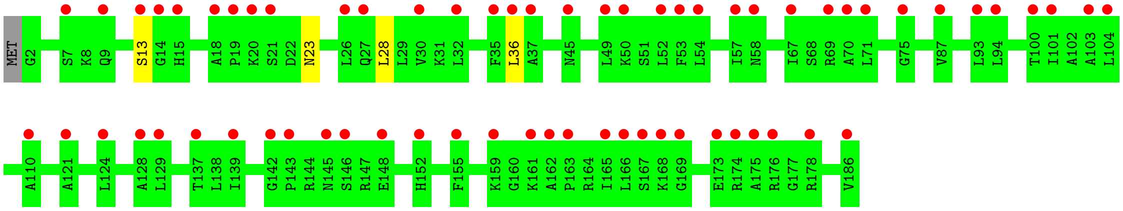




- Molecule 19: 60S ribosomal protein L18-A

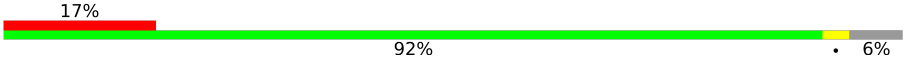
Chain BL:

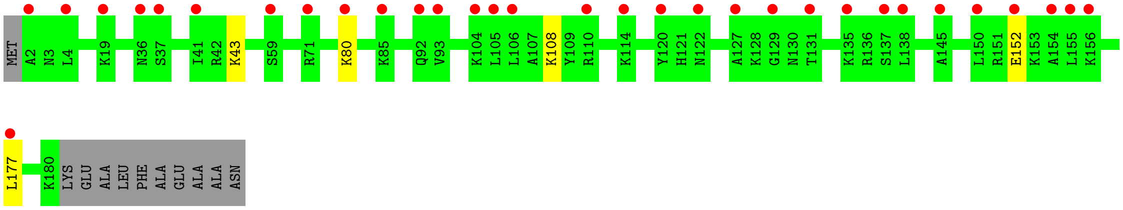




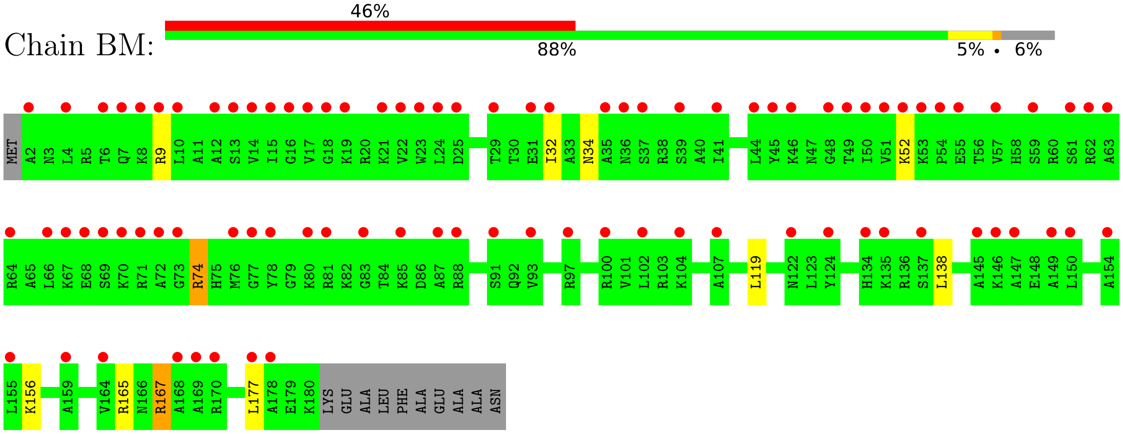
- Molecule 20: 60S ribosomal protein L19-A

Chain z:

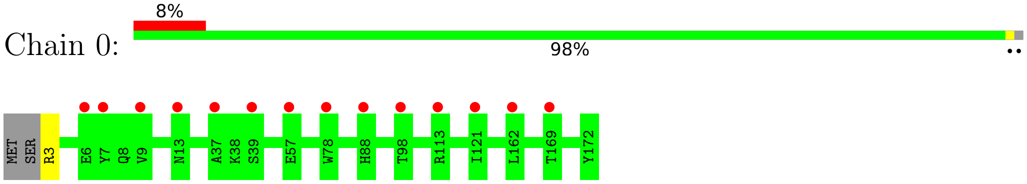




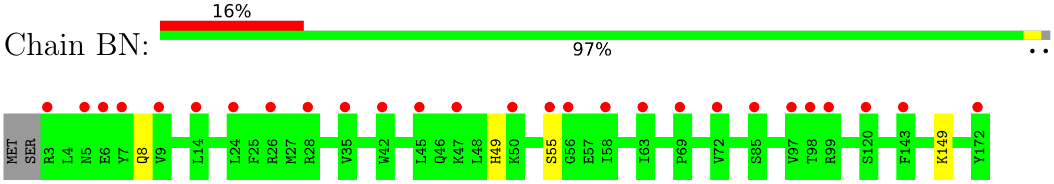
- Molecule 20: 60S ribosomal protein L19-A



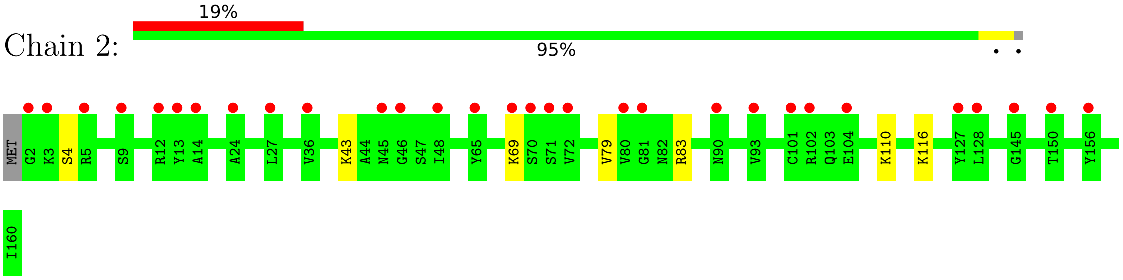
- Molecule 21: 60S ribosomal protein L20



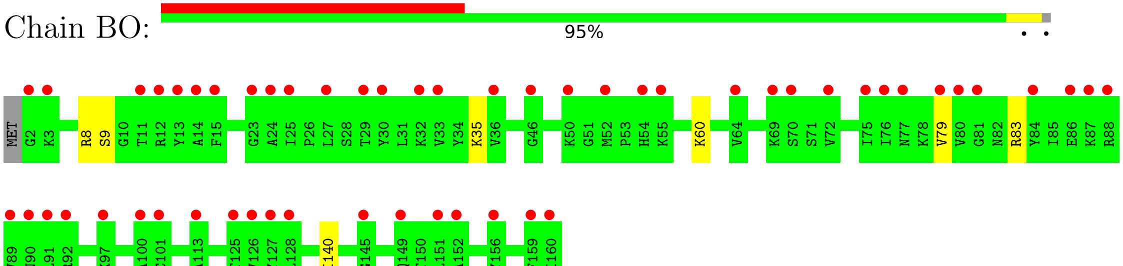
- Molecule 21: 60S ribosomal protein L20



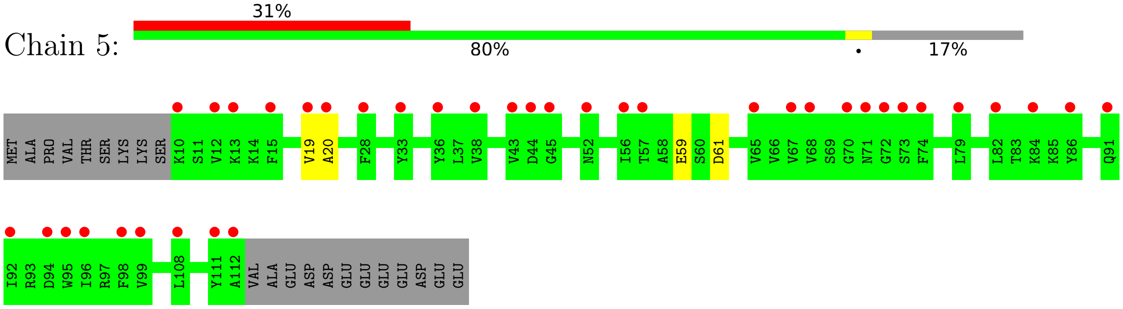
- Molecule 22: 60S ribosomal protein L21-A



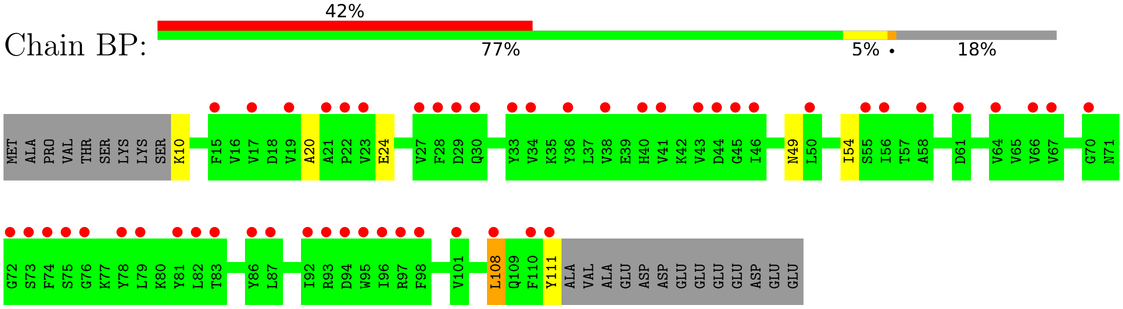
- Molecule 22: 60S ribosomal protein L21-A



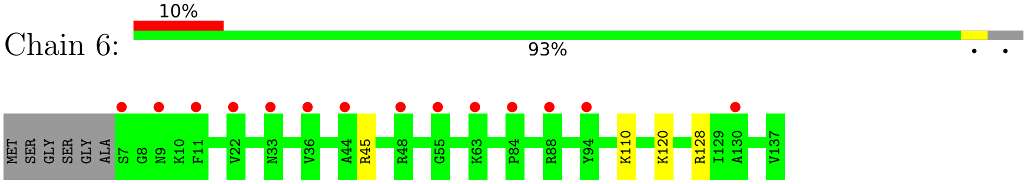
- Molecule 23: 60S ribosomal protein L22-B



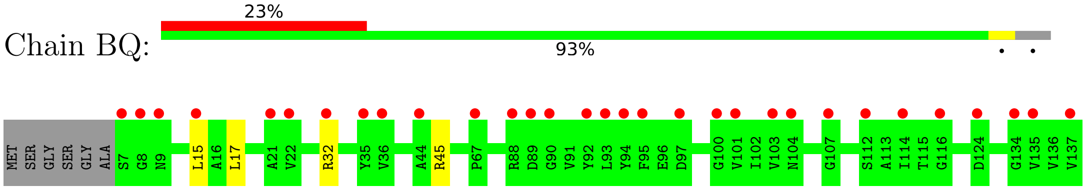
- Molecule 23: 60S ribosomal protein L22-B



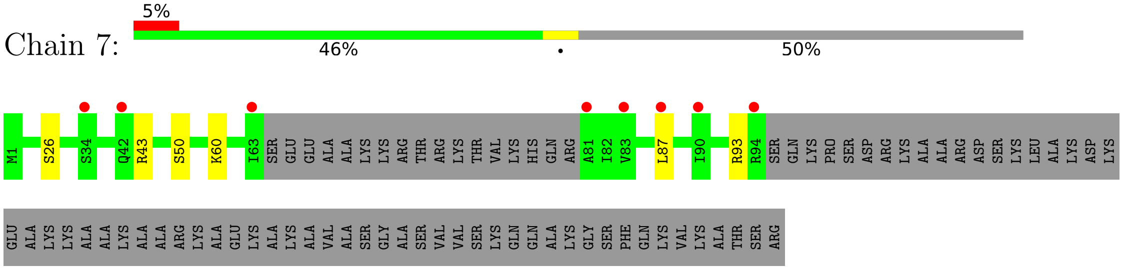
- Molecule 24: 60S ribosomal protein L23-A



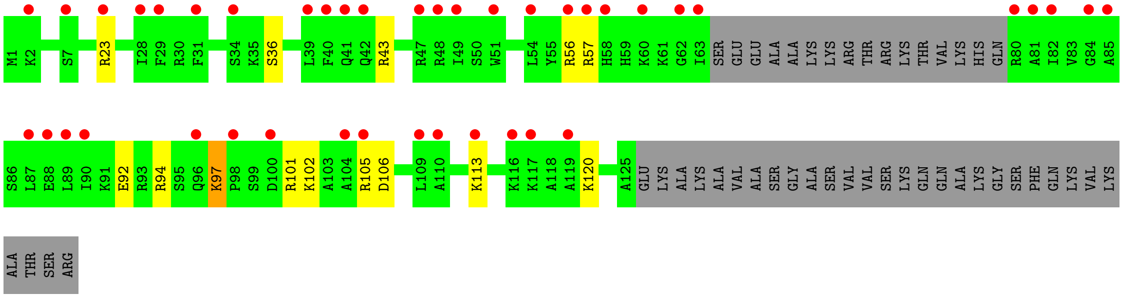
- Molecule 24: 60S ribosomal protein L23-A



- Molecule 25: 60S ribosomal protein L24-A

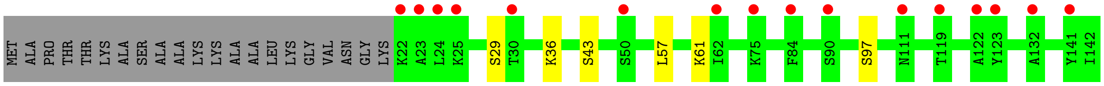


- Molecule 25: 60S ribosomal protein L24-A



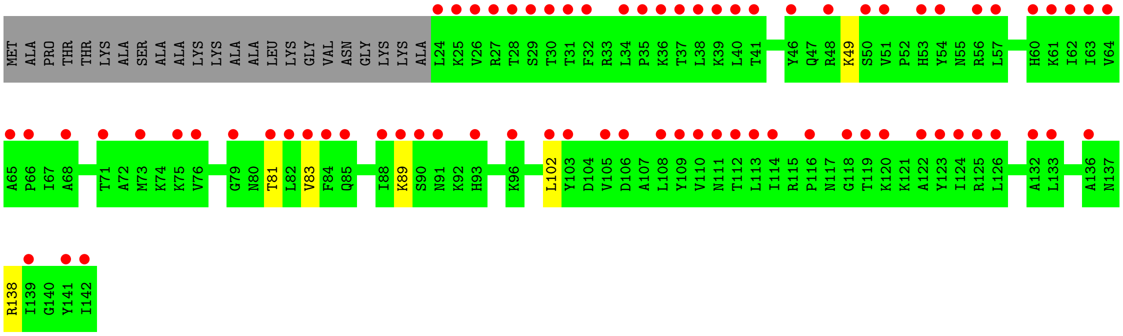
- Molecule 26: 60S ribosomal protein L25

Chain 8:



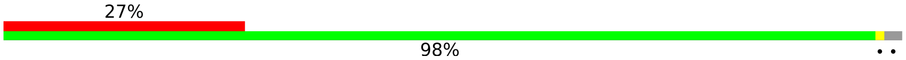
- Molecule 26: 60S ribosomal protein L25

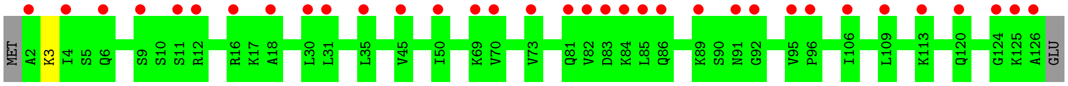
Chain BS:



- Molecule 27: Ribosomal protein L24

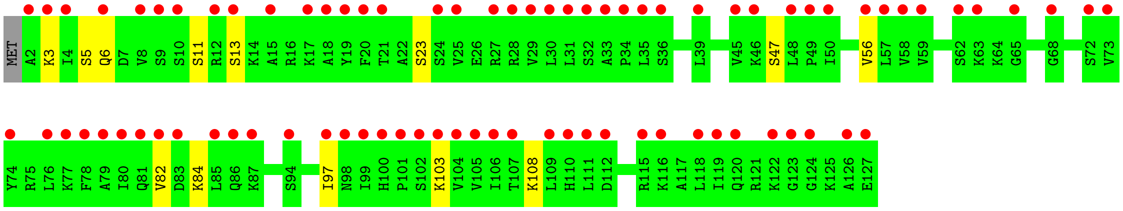
Chain 9:





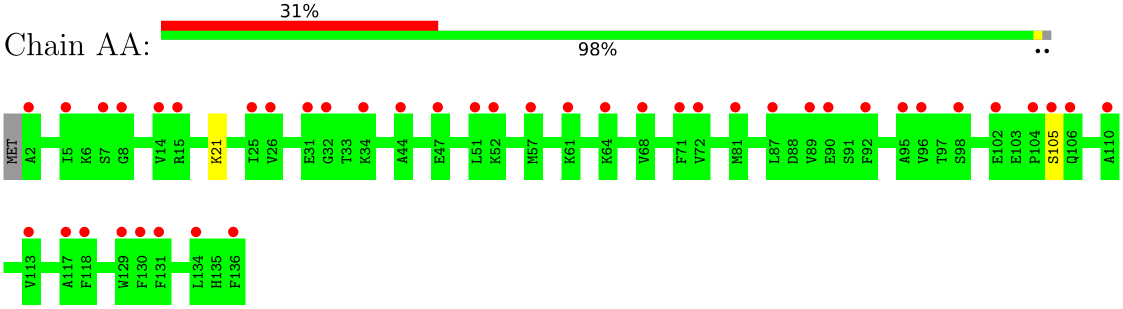
- Molecule 27: Ribosomal protein L24

Chain BT:



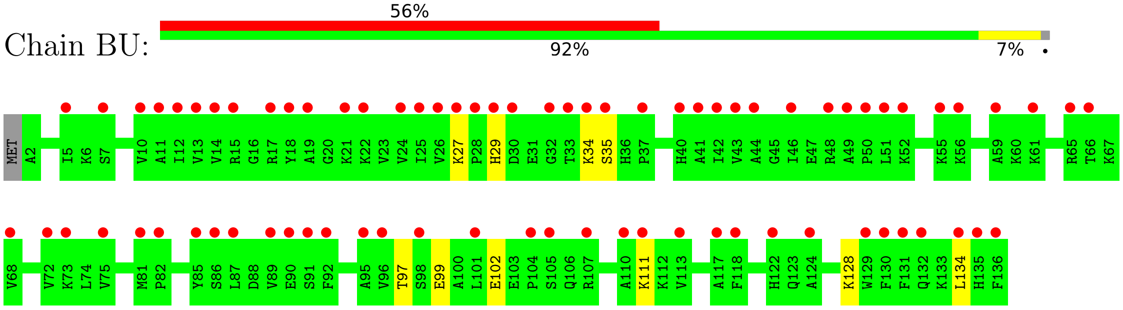
- Molecule 28: 60S ribosomal protein L27

Chain AA:



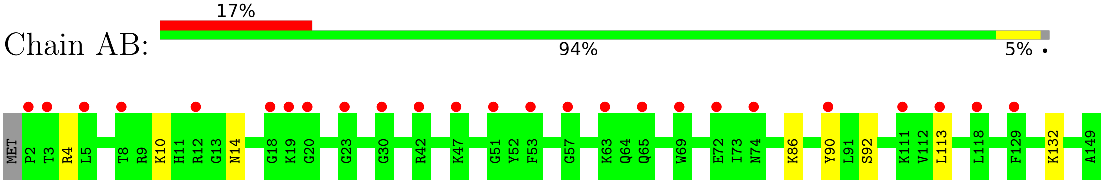
- Molecule 28: 60S ribosomal protein L27

Chain BU:



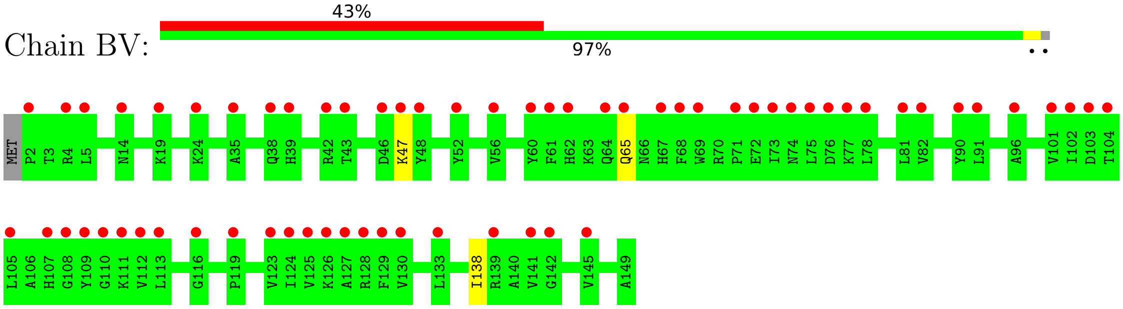
- Molecule 29: 60S ribosomal protein L28

Chain AB:



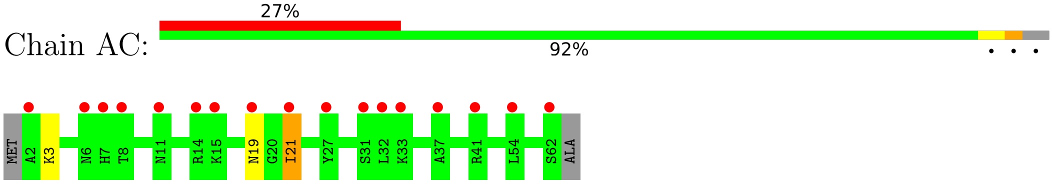
- Molecule 29: 60S ribosomal protein L28

Chain BV:

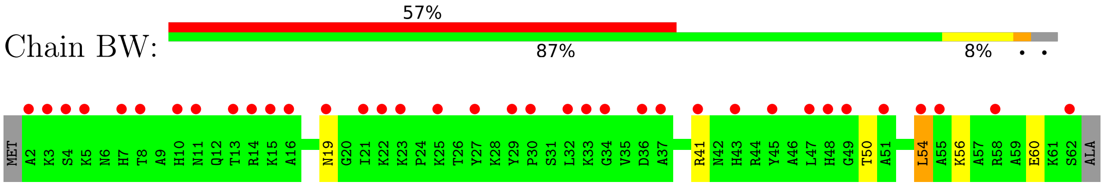


- Molecule 30: 60S ribosomal protein L29

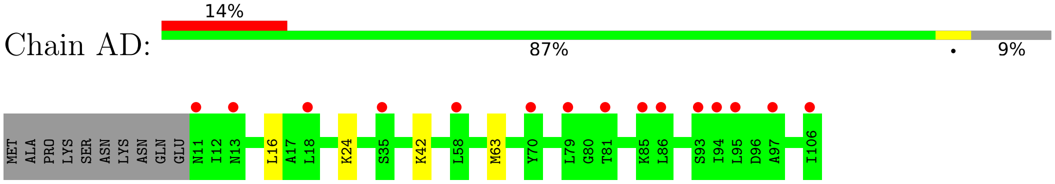
Chain AC:



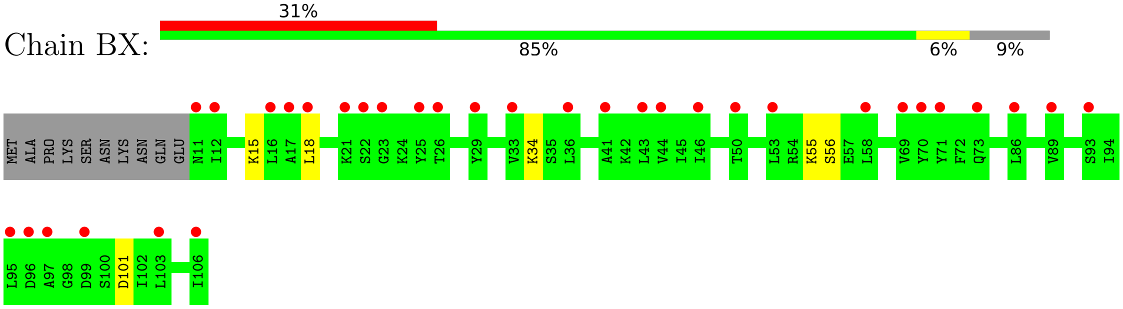
- Molecule 30: 60S ribosomal protein L29



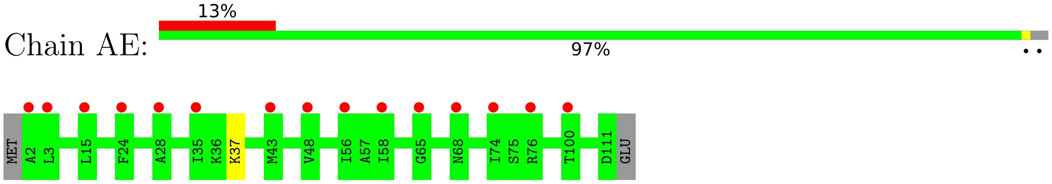
- Molecule 31: 60S ribosomal protein L30



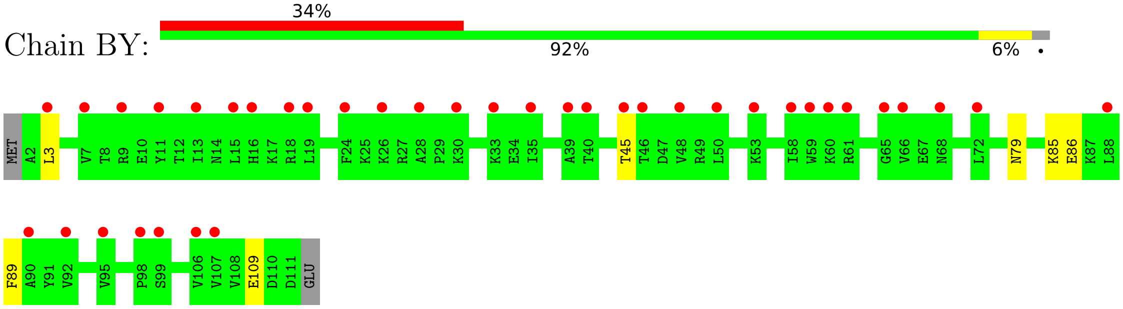
- Molecule 31: 60S ribosomal protein L30



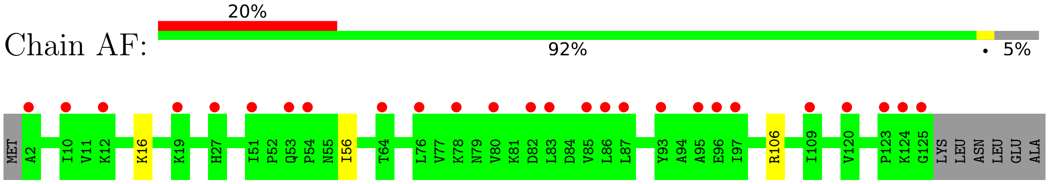
- Molecule 32: 60S ribosomal protein L31-B



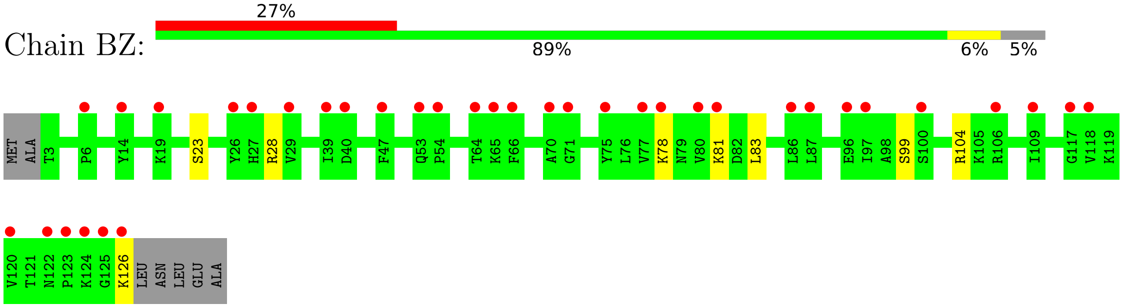
- Molecule 32: 60S ribosomal protein L31-B



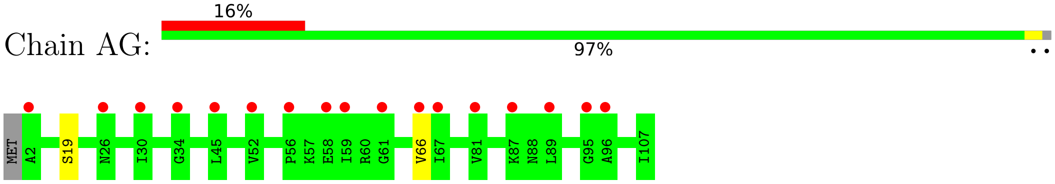
- Molecule 33: 60S ribosomal protein L32



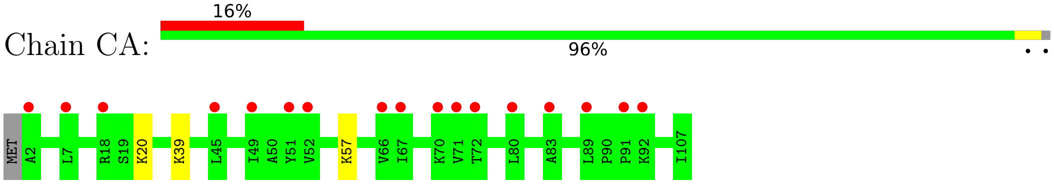
- Molecule 33: 60S ribosomal protein L32



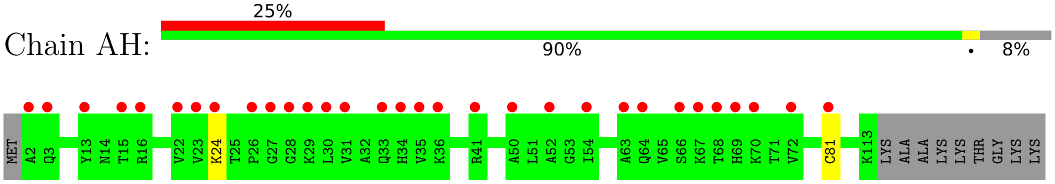
- Molecule 34: 60S ribosomal protein L33-A



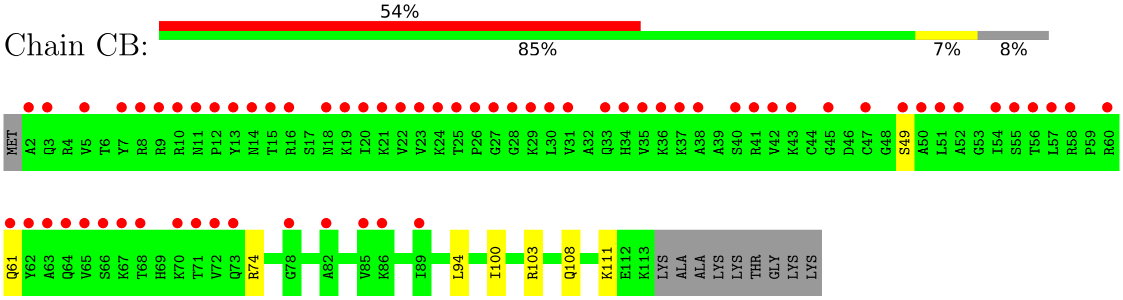
- Molecule 34: 60S ribosomal protein L33-A



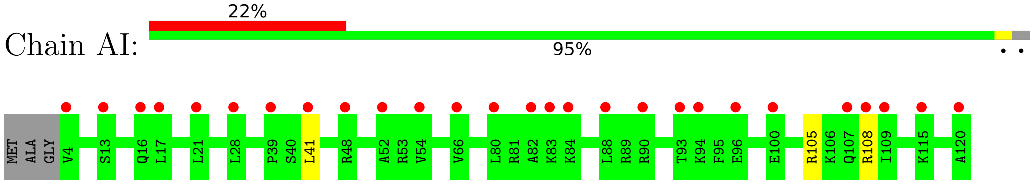
- Molecule 35: 60S ribosomal protein L34-B



- Molecule 35: 60S ribosomal protein L34-B

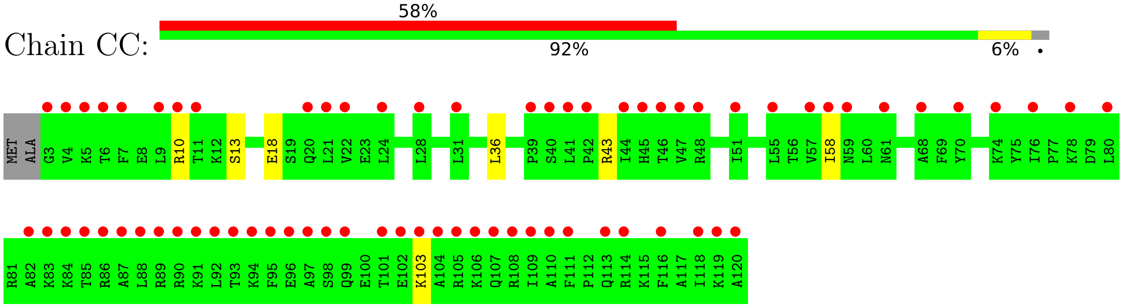


- Molecule 36: Ribosomal protein L29



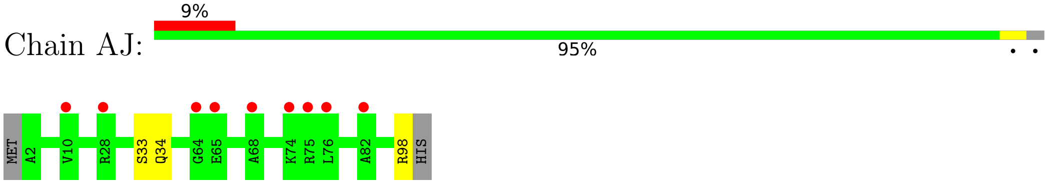
- Molecule 36: Ribosomal protein L29

Chain CC:



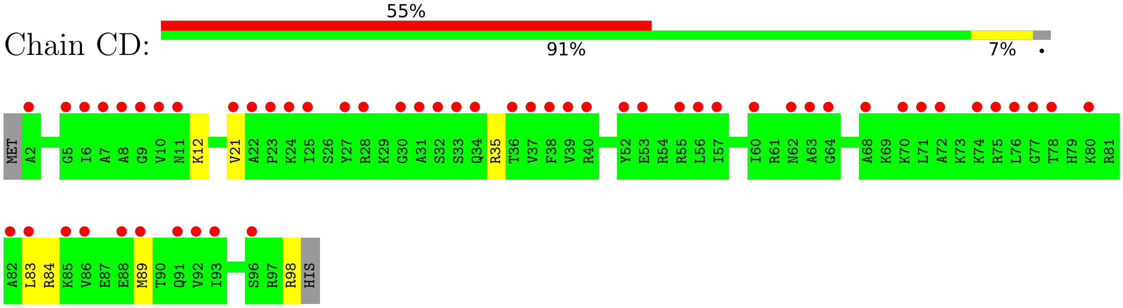
- Molecule 37: 60S ribosomal protein L36

Chain AJ:



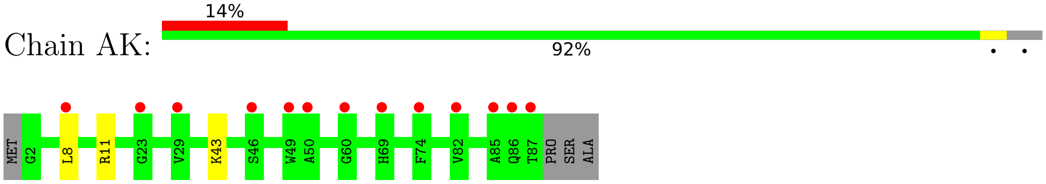
- Molecule 37: 60S ribosomal protein L36

Chain CD:



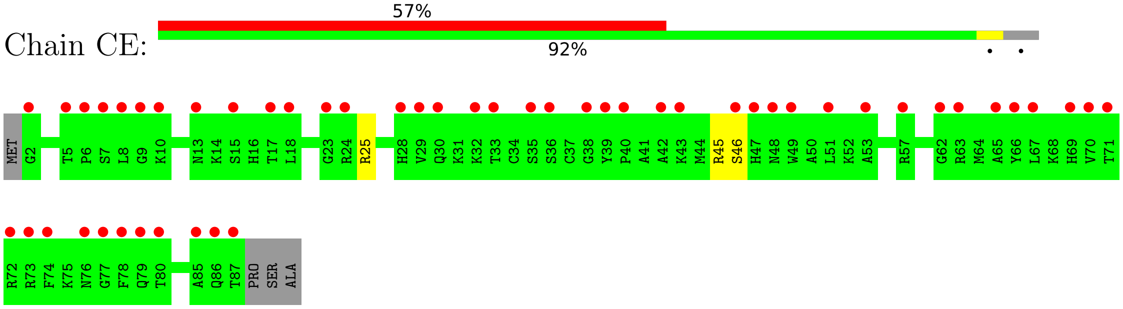
- Molecule 38: 60S ribosomal protein L37-B

Chain AK:



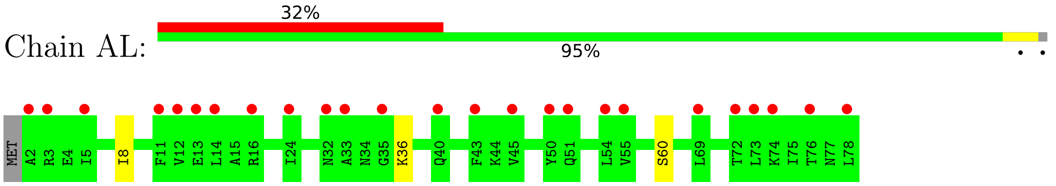
- Molecule 38: 60S ribosomal protein L37-B

Chain CE:



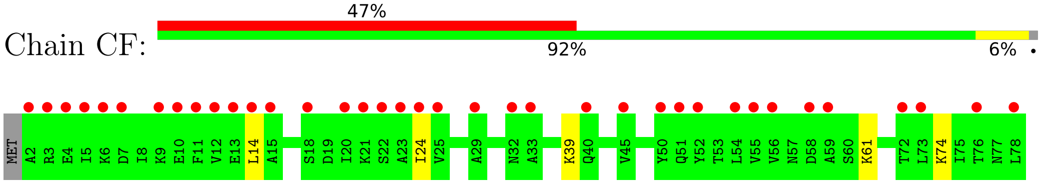
- Molecule 39: 60S ribosomal protein L38

Chain AL:



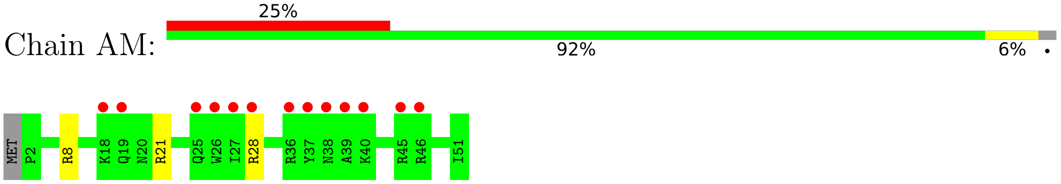
- Molecule 39: 60S ribosomal protein L38

Chain CF:



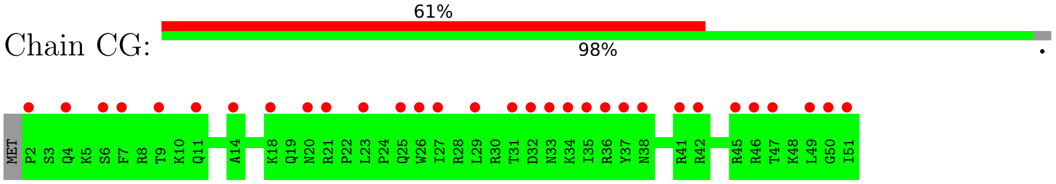
- Molecule 40: 60S ribosomal protein L39

Chain AM:



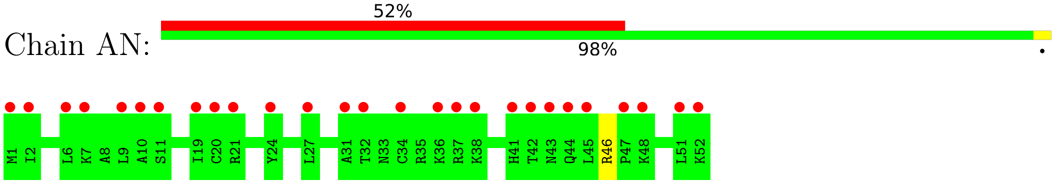
- Molecule 40: 60S ribosomal protein L39

Chain CG:



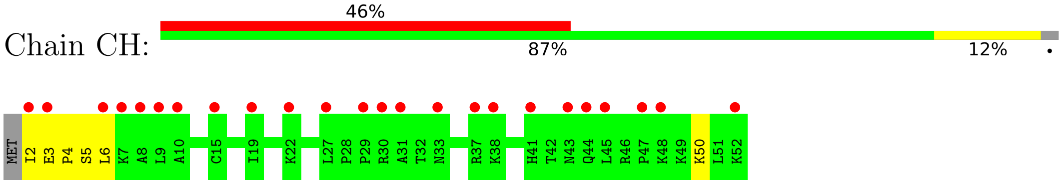
- Molecule 41: 60S ribosomal protein L40-B

Chain AN:



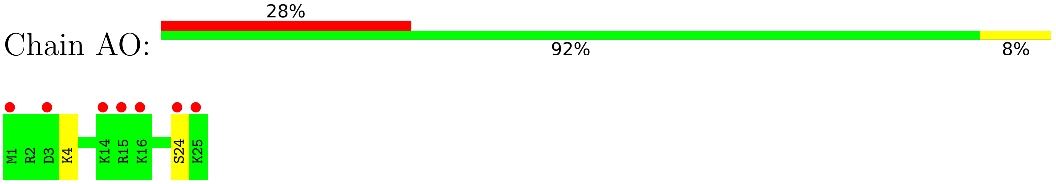
- Molecule 41: 60S ribosomal protein L40-B

Chain CH:



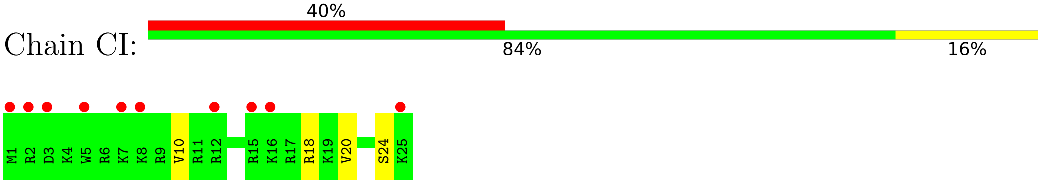
- Molecule 42: 60S ribosomal protein L41

Chain AO:



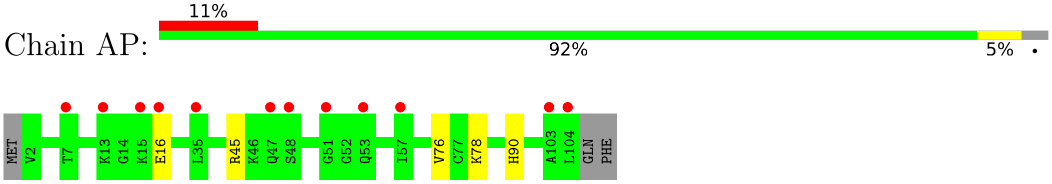
- Molecule 42: 60S ribosomal protein L41

Chain CI:



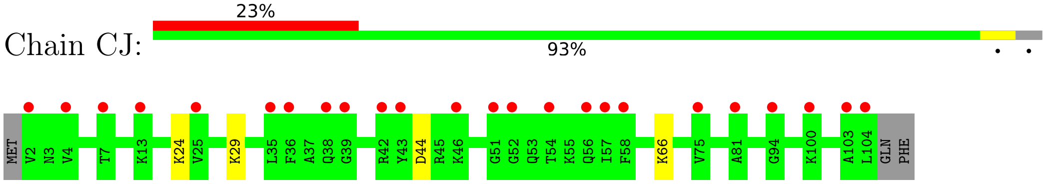
- Molecule 43: 60S ribosomal protein L42-B

Chain AP:



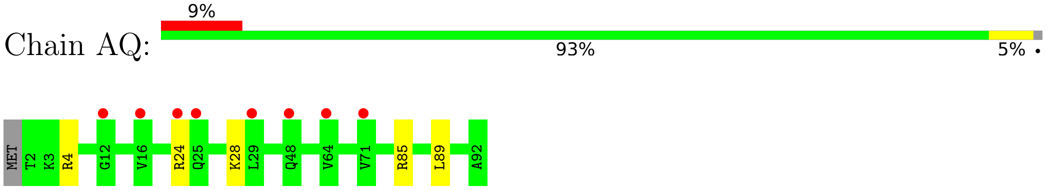
- Molecule 43: 60S ribosomal protein L42-B

Chain CJ:



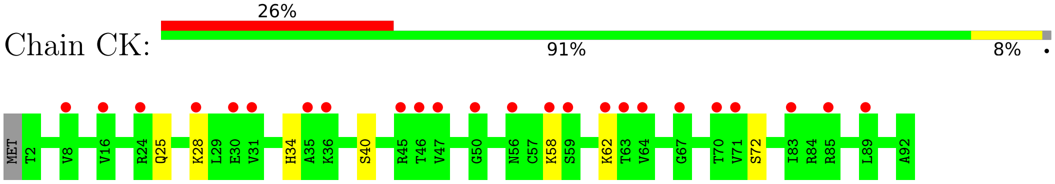
- Molecule 44: 60S ribosomal protein L43-A

Chain AQ:



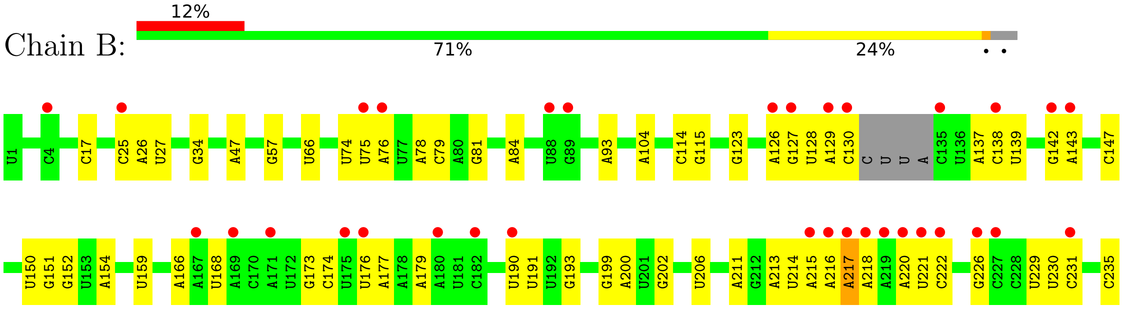
- Molecule 44: 60S ribosomal protein L43-A

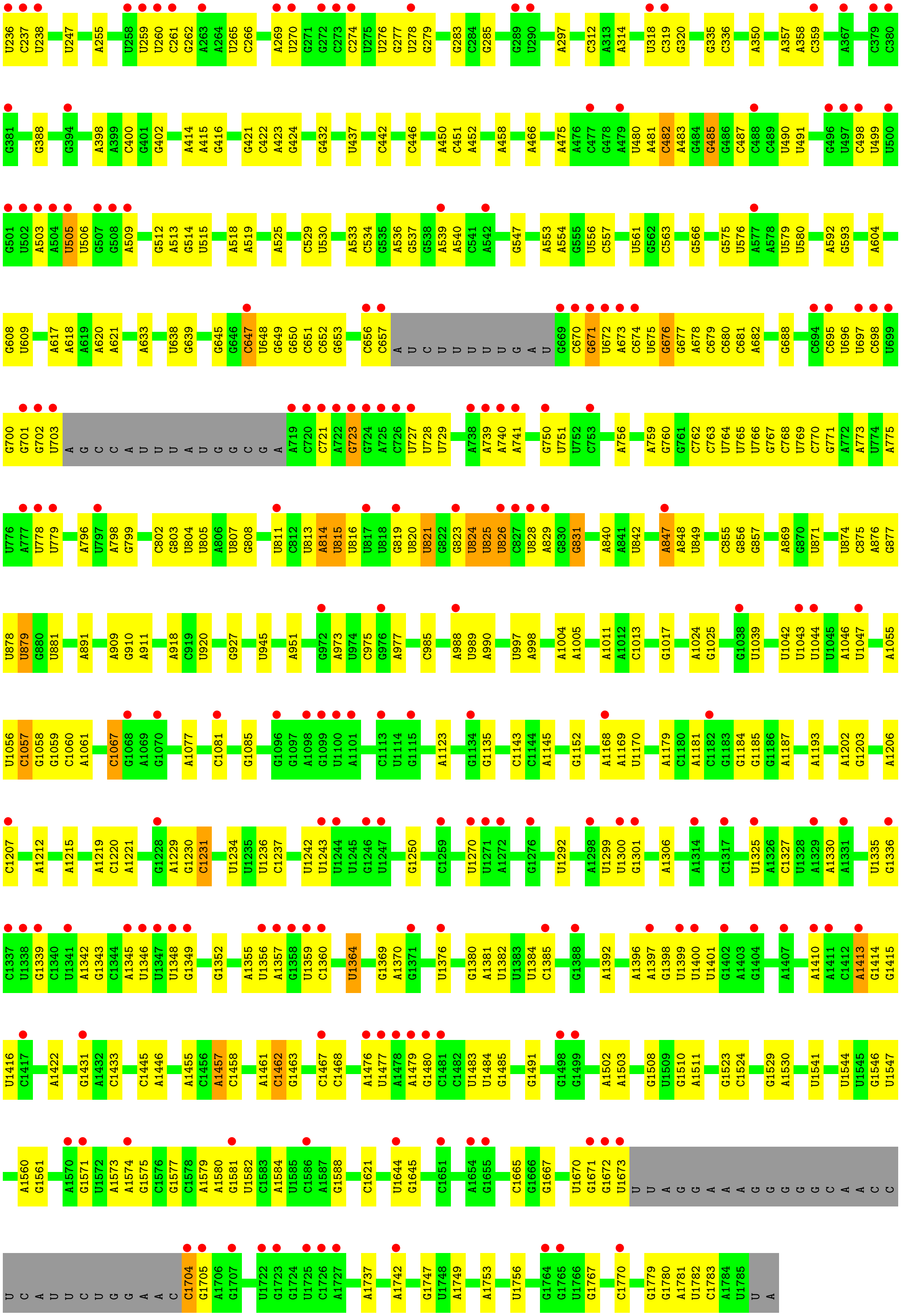
Chain CK:



- Molecule 45: 18S

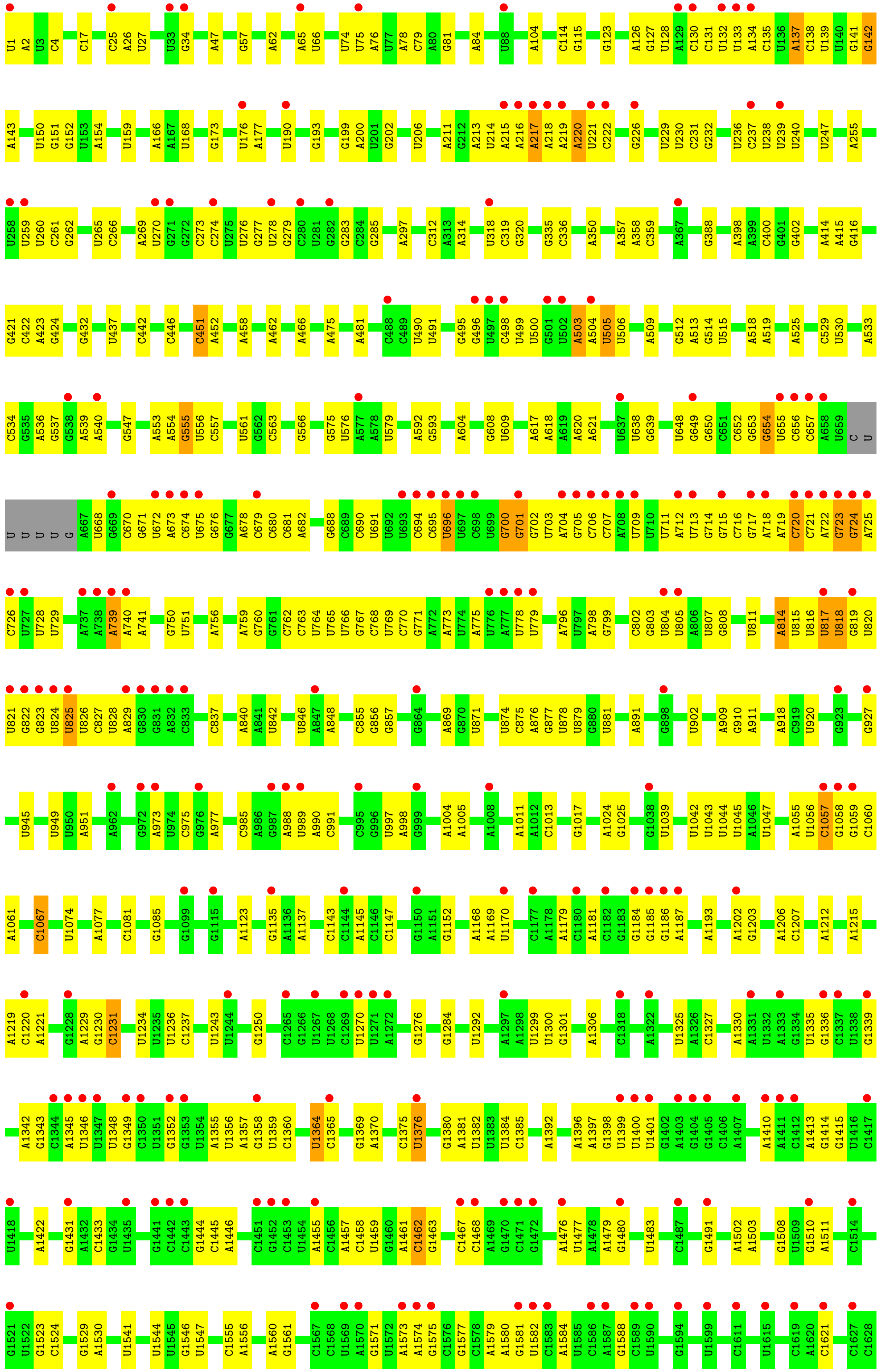
Chain B:





- Molecule 45: 18S

Chain CM: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A143 U150 G151 G152 U153 A154 U159 A166 A167 U168 G173 U176 A177 U190 G193 G199 A200 U201 G202 U206 A211 G212 A213 U214 A215 A216 A217 A218 A219 A220 U221 C222 G226 U229 U230 C231 G232 U236 C237 U238 U239 U240 U247 A255
U258 U259 U260 C261 G262 U265 C266 A269 U270 G271 G272 C273 C274 U275 U276 G277 U278 G279 C280 U281 G282 G283 C284 G285 A297 C312 A313 A314 U318 C319 G320 G335 C336 A350 A357 A358 C359 A367 G388 A398 A399 C400 G401 G402 A414 A415 G416
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C534 G535 A536 G537 G538 A539 A540 G547 A553 A554 G555 U556 C557 U561 G562 C563 G566 G575 U576 A577 A578 U579 A592 G593 A604 G608 U609 A617 A618 A619 A620 A621 U637 U638 G639 U648 G649 G650 C651 C652 G653 G654 U655 C656 C657 A658 U659 C U
U U U U G A667 U668 G669 C670 G671 U672 A673 C674 U675 G676 G677 A678 C679 C680 C681 A682 G688 C689 C690 U691 U692 U693 C694 C695 U696 U697 C698 U699 G700 G701 G702 U703 A704 G705 C706 C707 A708 U709 U710 U711 A712 U713 G714 G715 C716 G717 A718 A719 C720 C721 A722 G723 G724 A725
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U821 G822 G823 U824 U825 U826 C827 U828 A829 G830 G831 A832 C833 C837 A840 A841 U842 U846 A847 A848 C855 G856 G857 G864 A869 G870 U871 U874 C875 A876 G877 U878 U879 G880 U881 A891 G898 U902 A909 G910 A911 A918 C919 U920 G923 G927
U945 U949 U950 A951 A962 G972 A973 U974 C975 G976 A977 C985 A986 G987 A988 U989 A990 C991 C995 G996 U997 A998 G999 A1004 A1005 A1008 A1011 A1012 C1013 G1017 A1024 G1025 G1038 U1039 U1042 U1043 U1044 U1045 A1046 U1047 A1055 U1056 C1057 G1058 G1059 C1060
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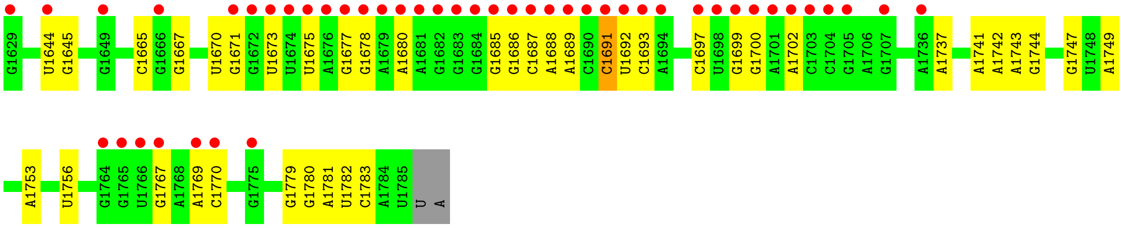
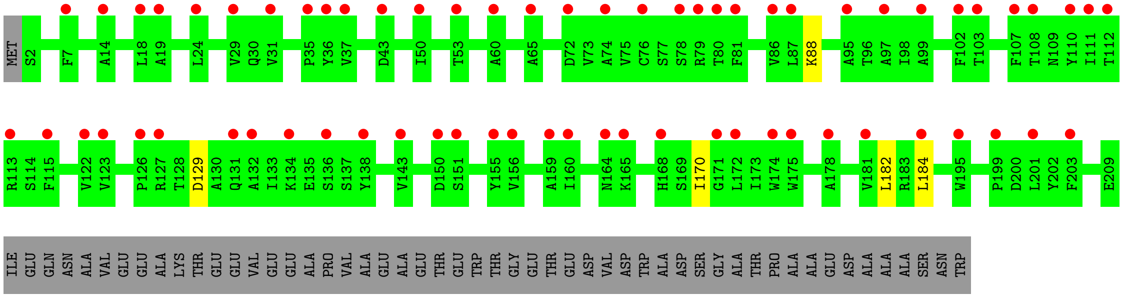


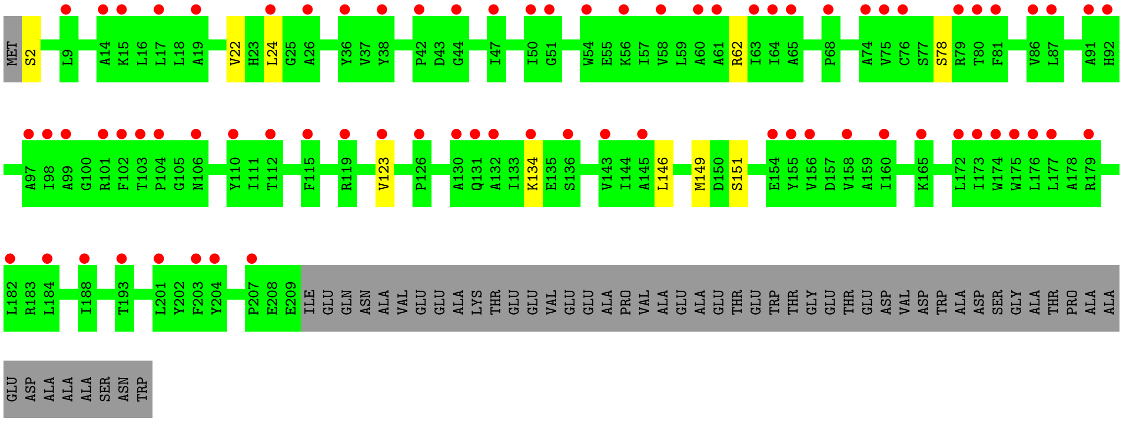
- Molecule 46: 40S ribosomal protein S0

Chain C:



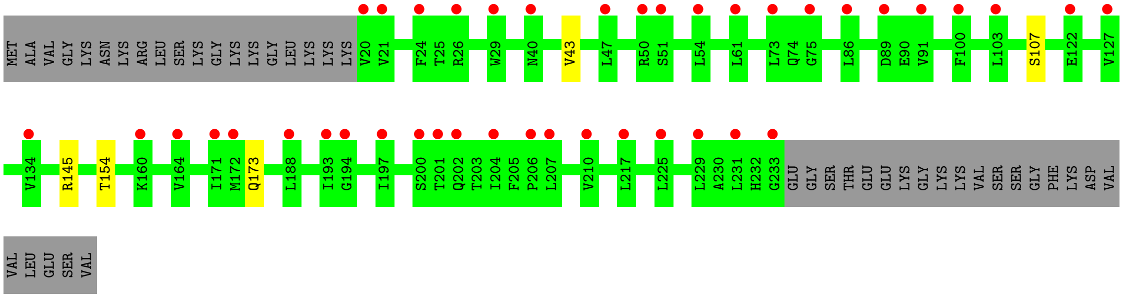
- Molecule 46: 40S ribosomal protein S0

Chain CN:



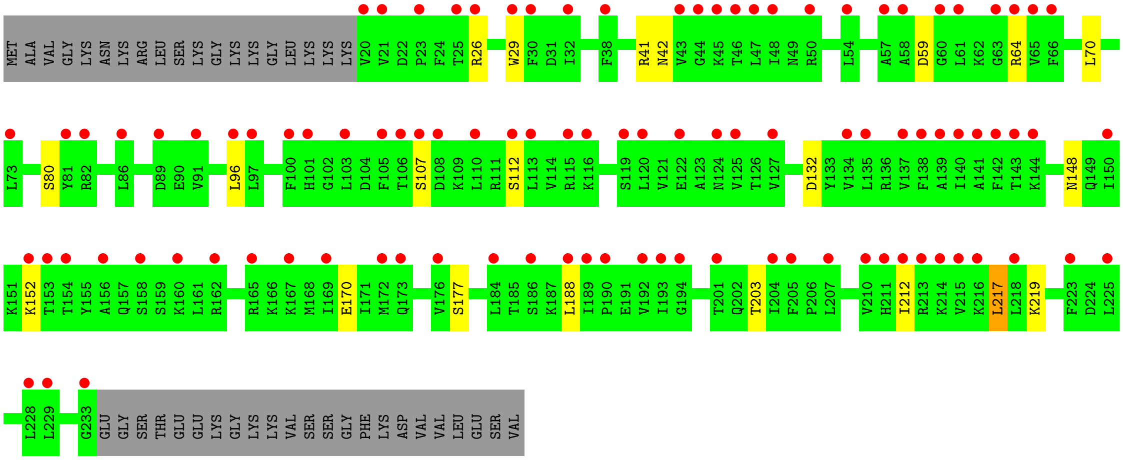
- Molecule 47: 40S ribosomal protein S1

Chain D:



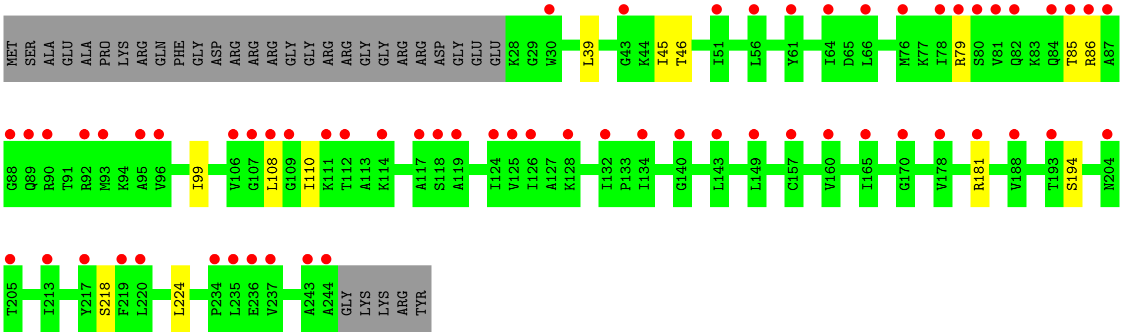
- Molecule 47: 40S ribosomal protein S1

Chain CO:



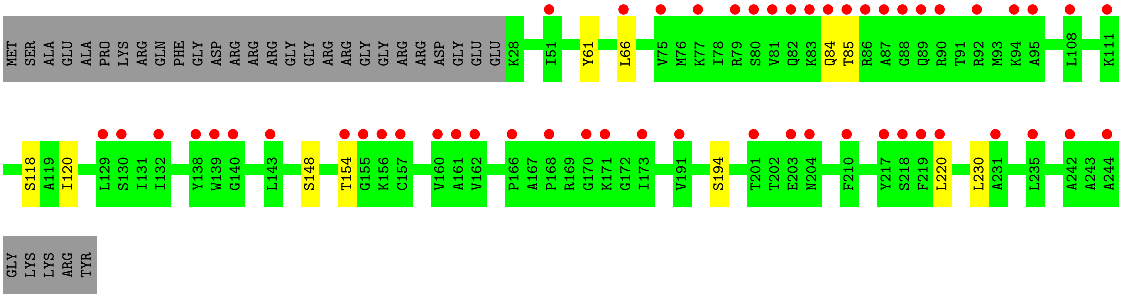
- Molecule 48: Ribosomal protein S5

Chain E:



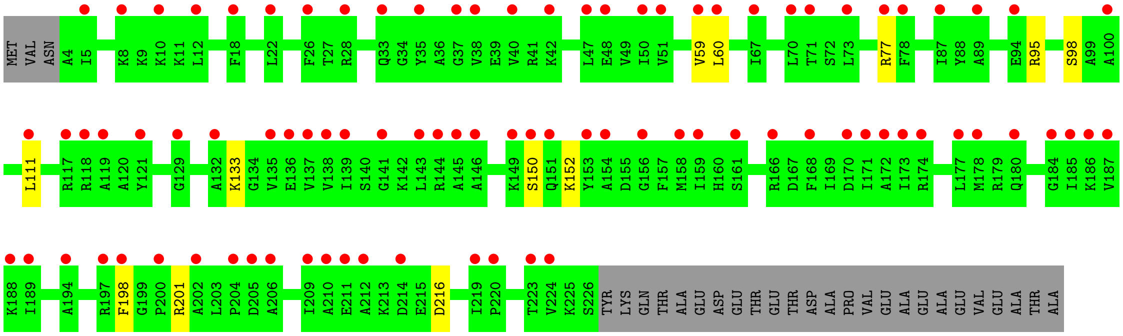
- Molecule 48: Ribosomal protein S5

Chain CP:



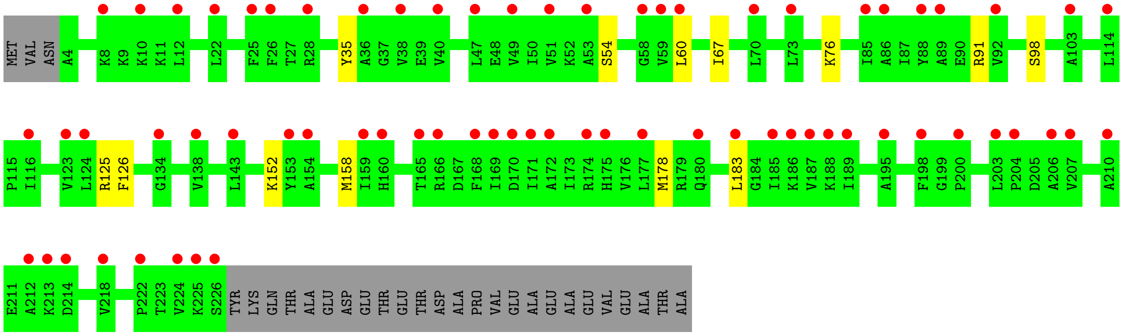
- Molecule 49: Ribosomal protein S3

Chain F:



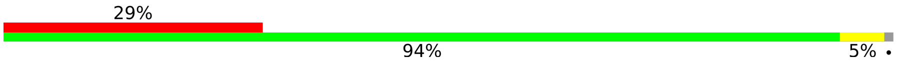
- Molecule 49: Ribosomal protein S3

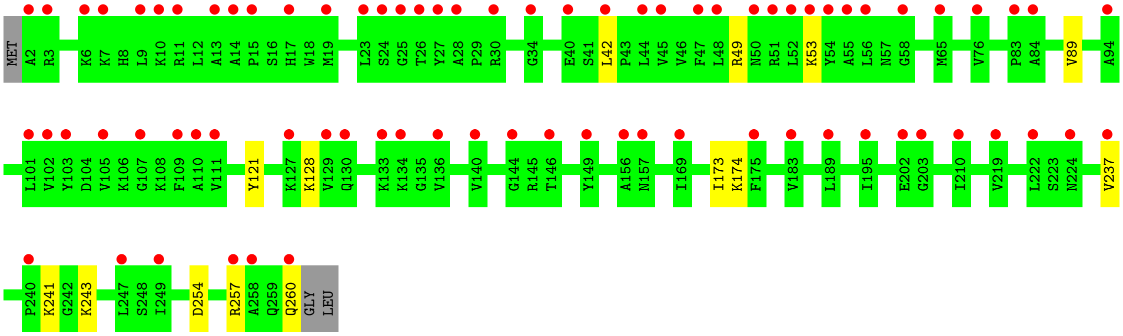
Chain CQ:



- Molecule 50: 40S ribosomal protein S4

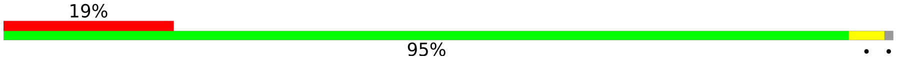
Chain G:

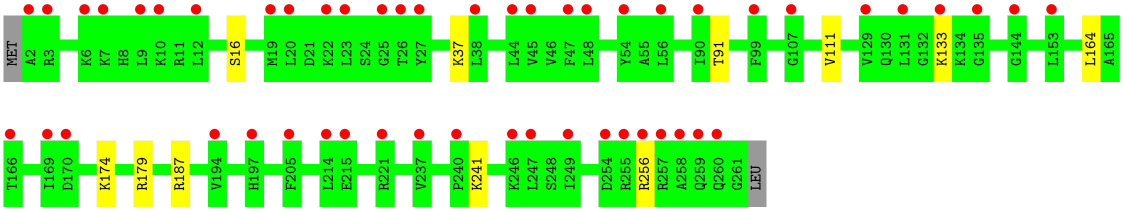




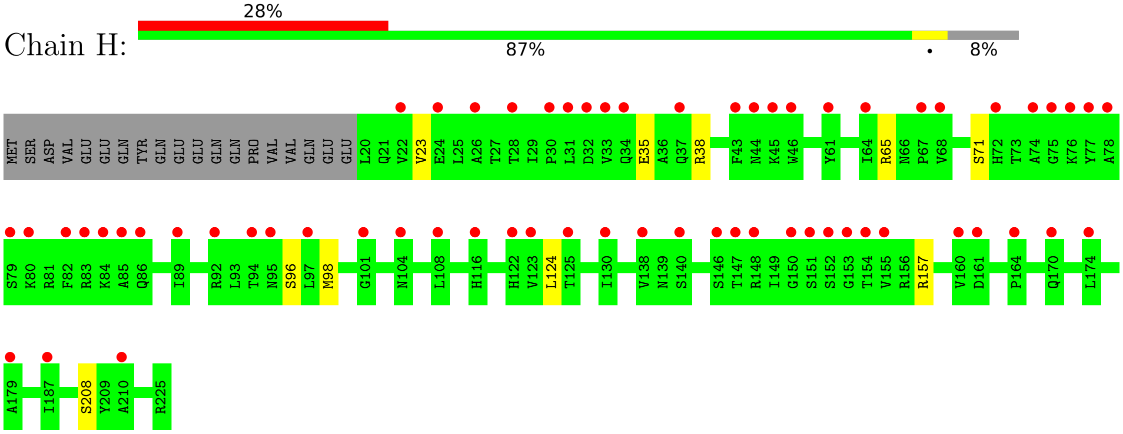
- Molecule 50: 40S ribosomal protein S4

Chain CR:

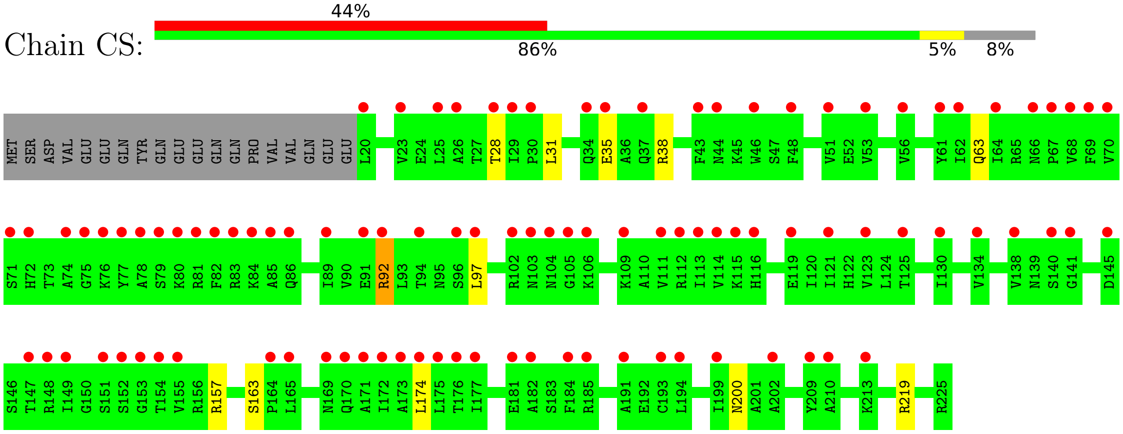




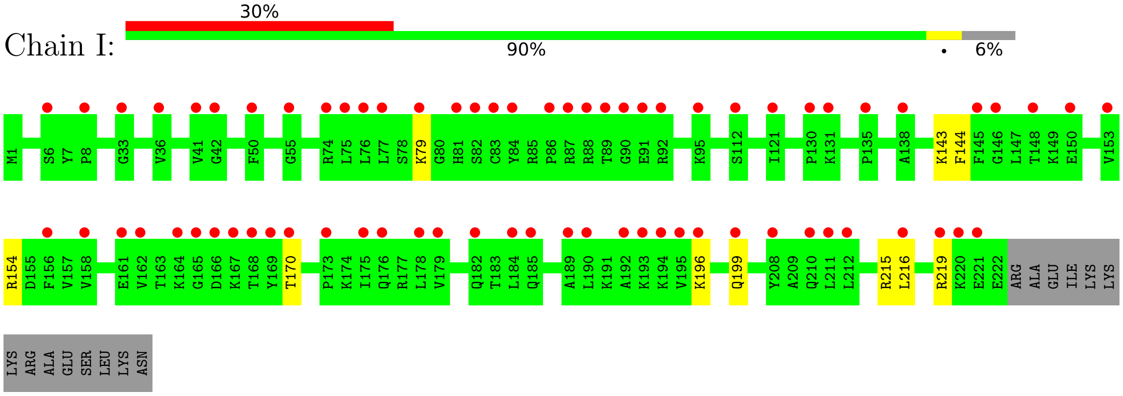
- Molecule 51: Ribosomal protein S7



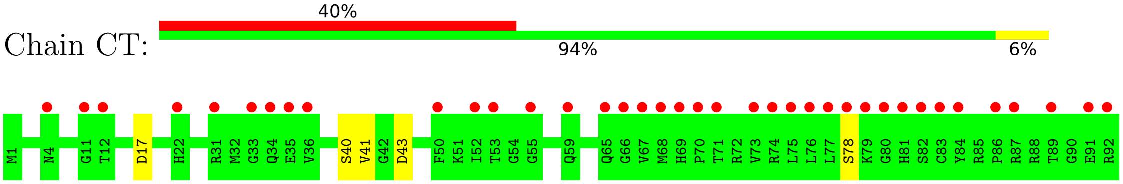
- Molecule 51: Ribosomal protein S7

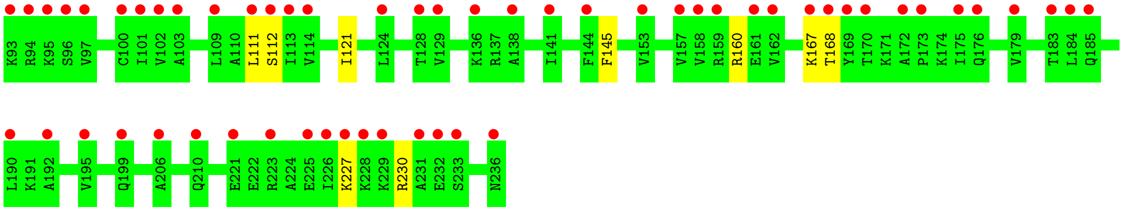


- Molecule 52: 40S ribosomal protein S6



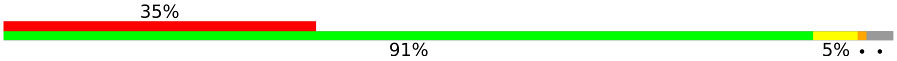
- Molecule 52: 40S ribosomal protein S6

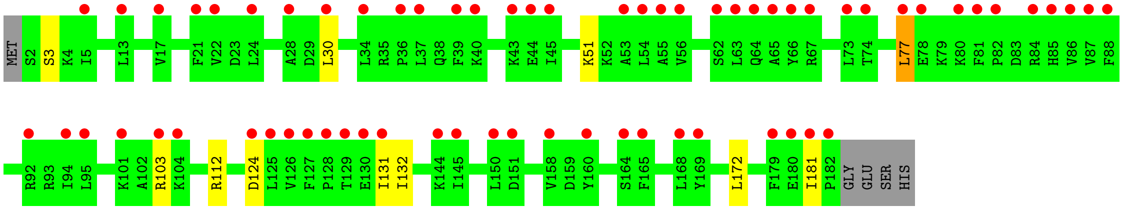




- Molecule 53: 40S ribosomal protein S7

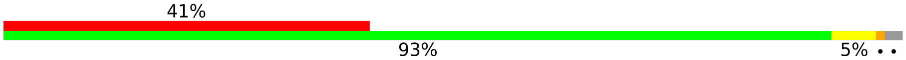
Chain J:

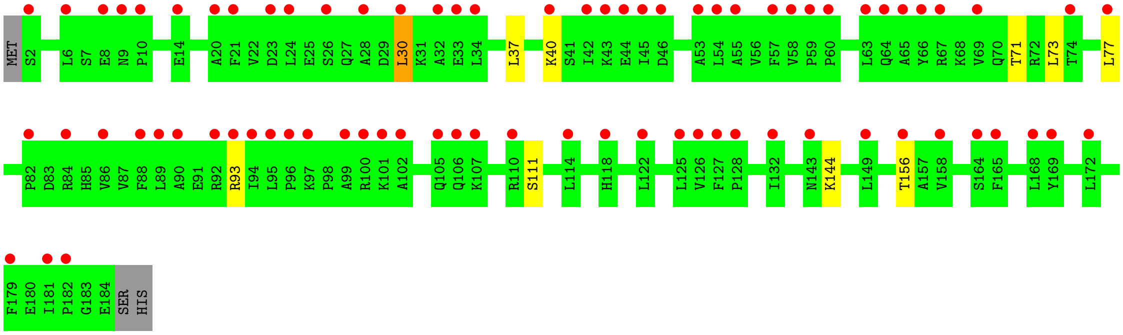




- Molecule 53: 40S ribosomal protein S7

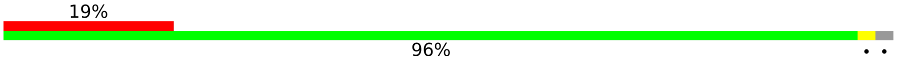
Chain CU:

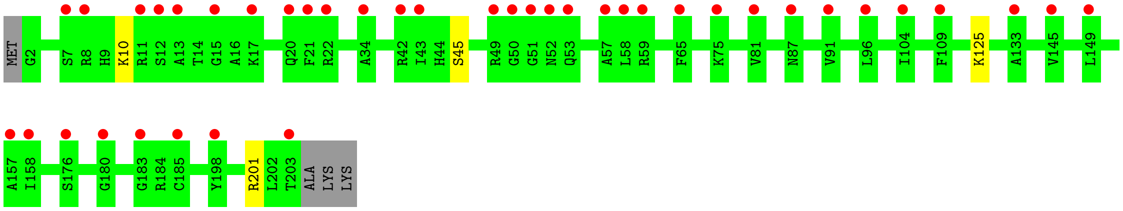




- Molecule 54: 40S ribosomal protein S8

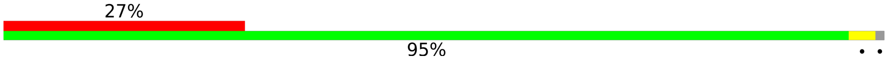
Chain K:

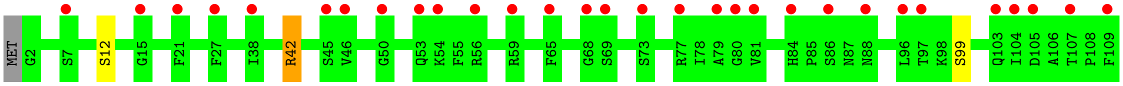


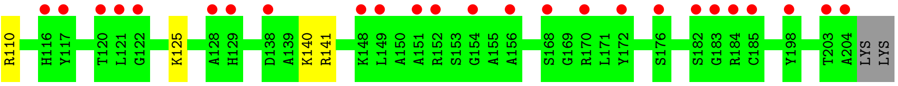


- Molecule 54: 40S ribosomal protein S8

Chain CV:

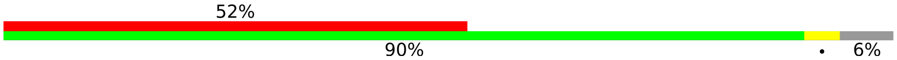


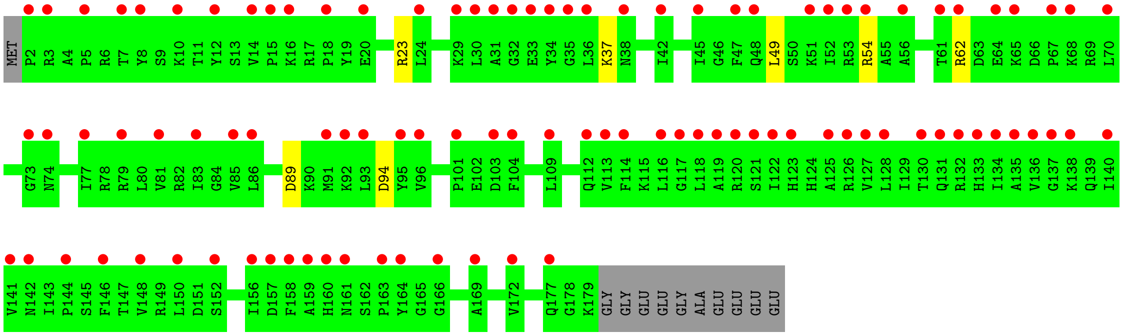




- Molecule 55: Ribosomal protein S4

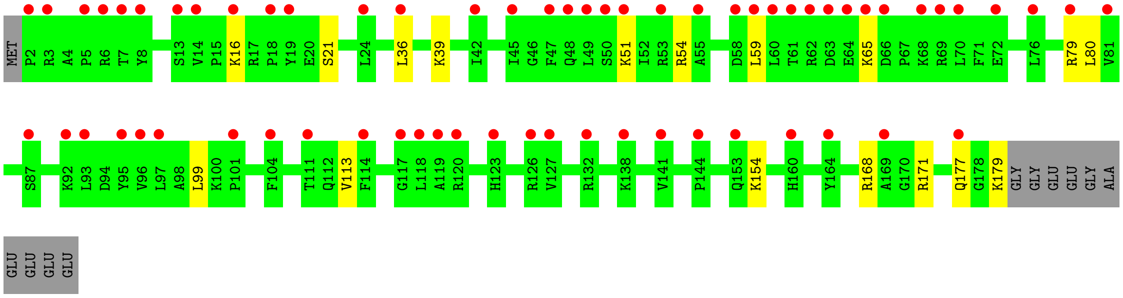
Chain L:





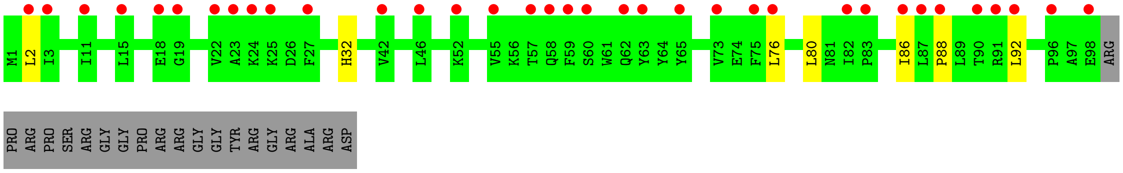
- Molecule 55: Ribosomal protein S4

Chain CW:



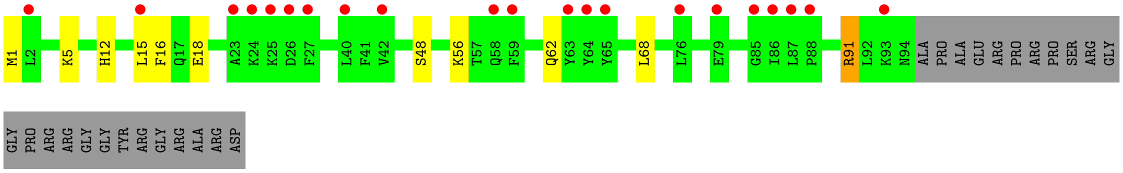
- Molecule 56: 40S ribosomal protein S10-A

Chain M:

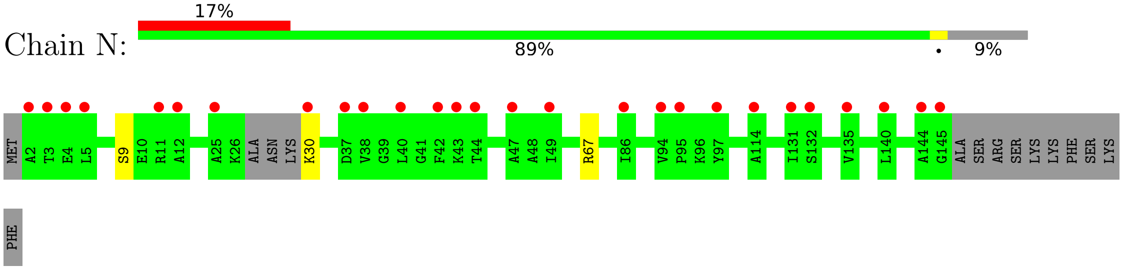


- Molecule 56: 40S ribosomal protein S10-A

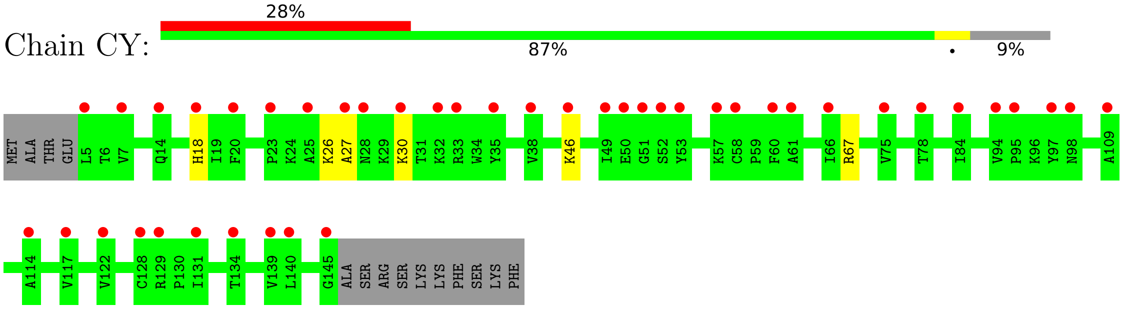
Chain CX:



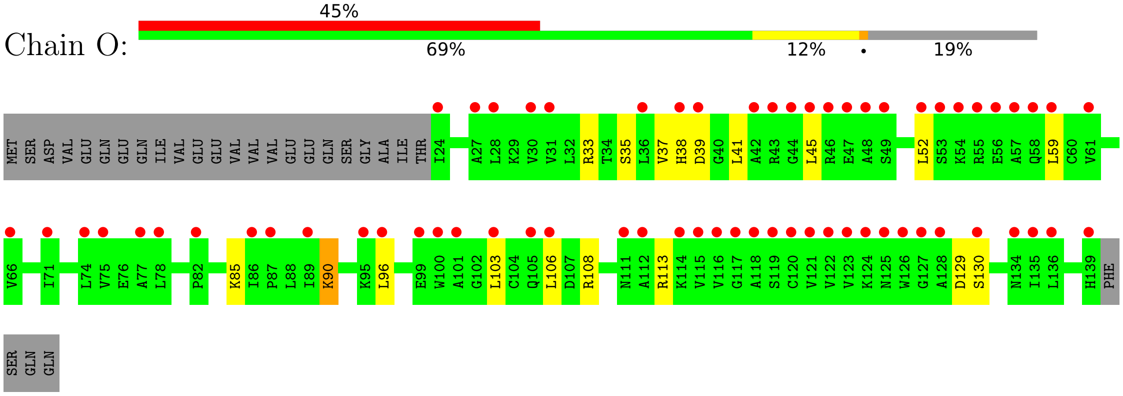
- Molecule 57: 40S ribosomal protein S11A



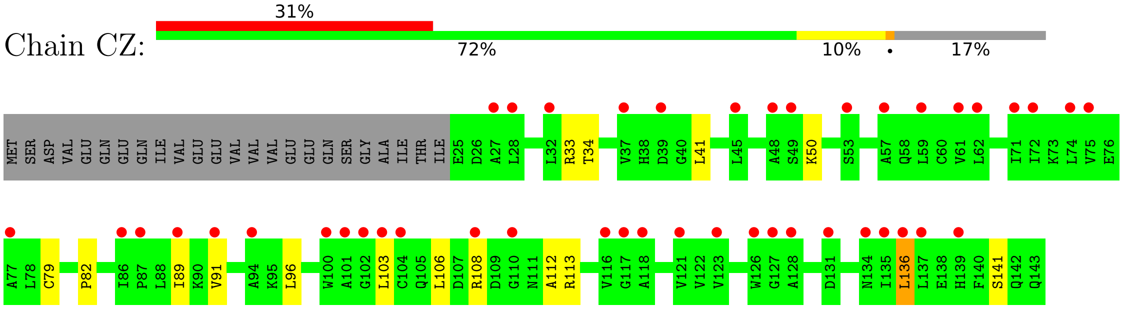
- Molecule 57: 40S ribosomal protein S11A



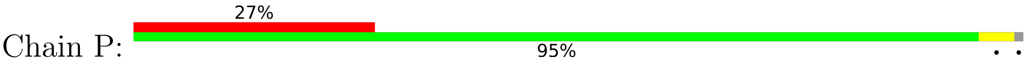
- Molecule 58: 40S ribosomal protein S12

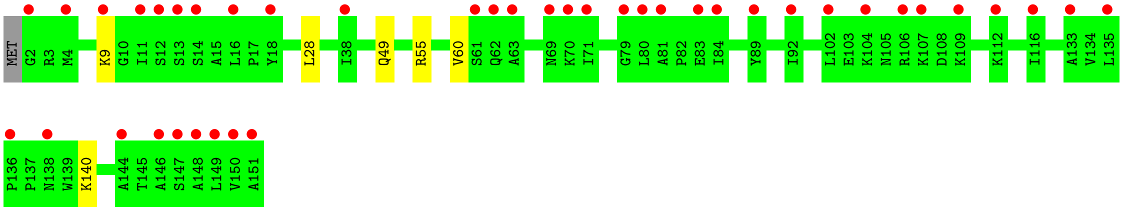


- Molecule 58: 40S ribosomal protein S12



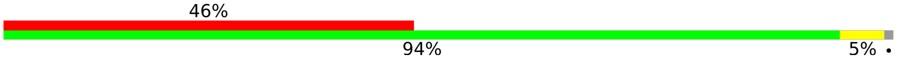
- Molecule 59: 40S ribosomal protein S13

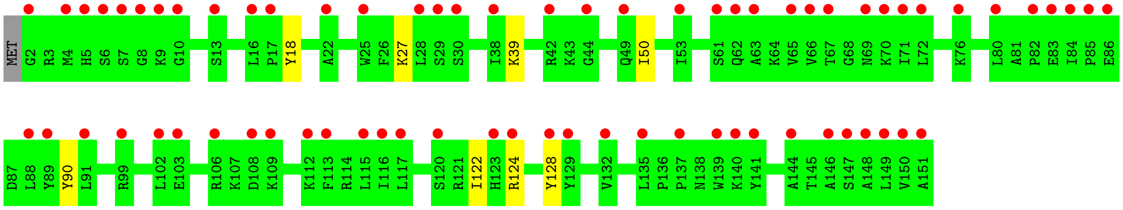




- Molecule 59: 40S ribosomal protein S13

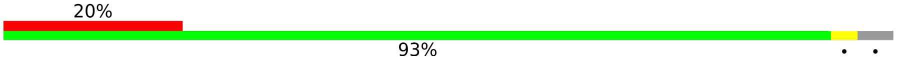
Chain DA:

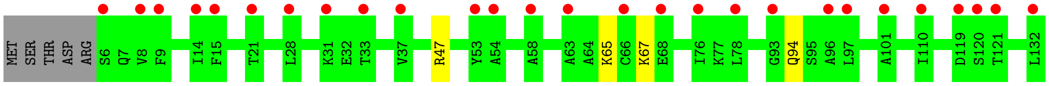




- Molecule 60: 40S ribosomal protein S14-A

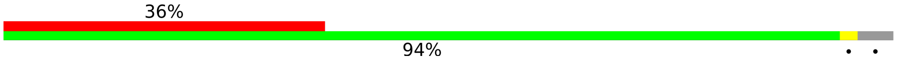
Chain Q:

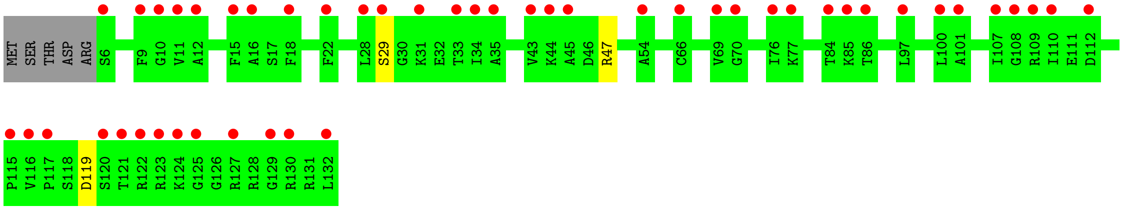




- Molecule 60: 40S ribosomal protein S14-A

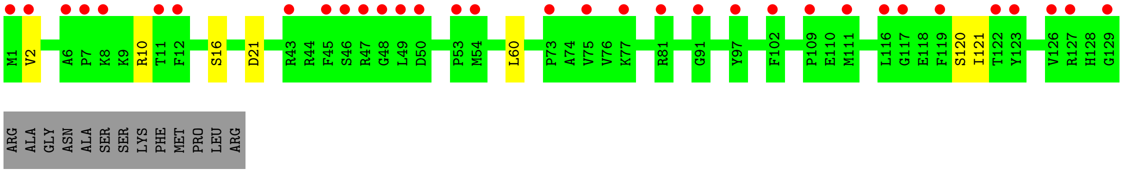
Chain DB:





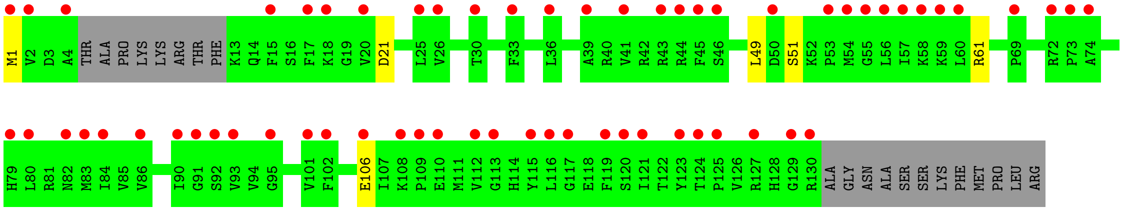
- Molecule 61: 40S ribosomal protein S15

Chain R:

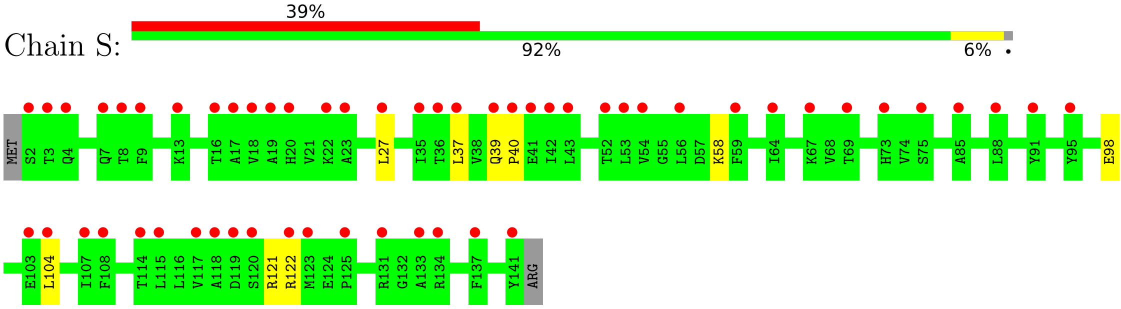


- Molecule 61: 40S ribosomal protein S15

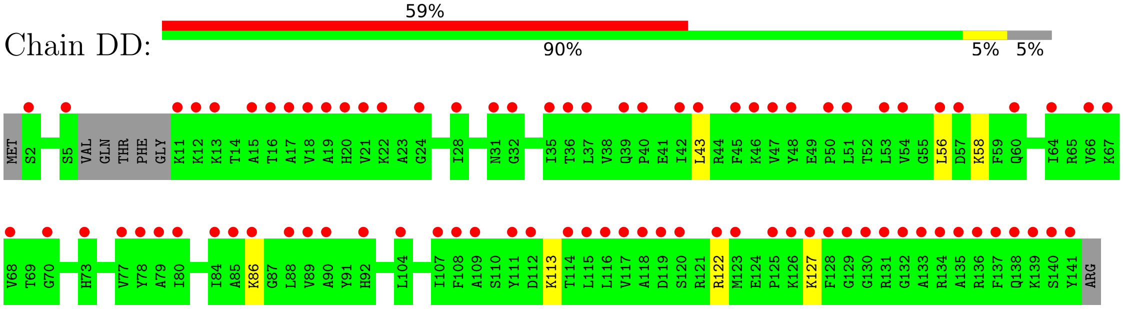
Chain DC:



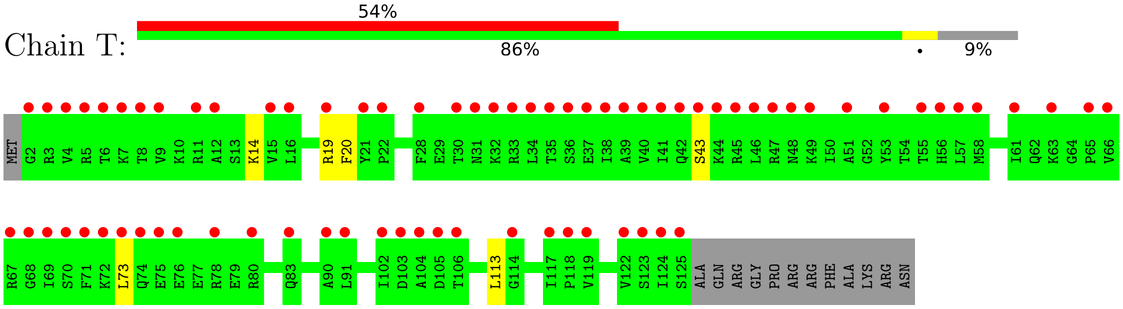
- Molecule 62: 40S ribosomal protein S16



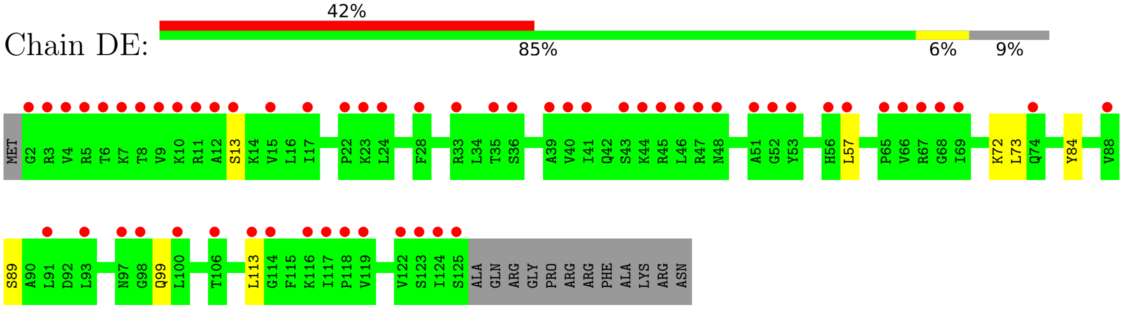
- Molecule 62: 40S ribosomal protein S16



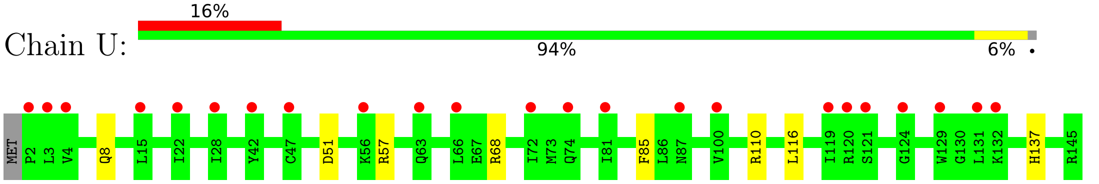
- Molecule 63: 40S ribosomal protein S17-B



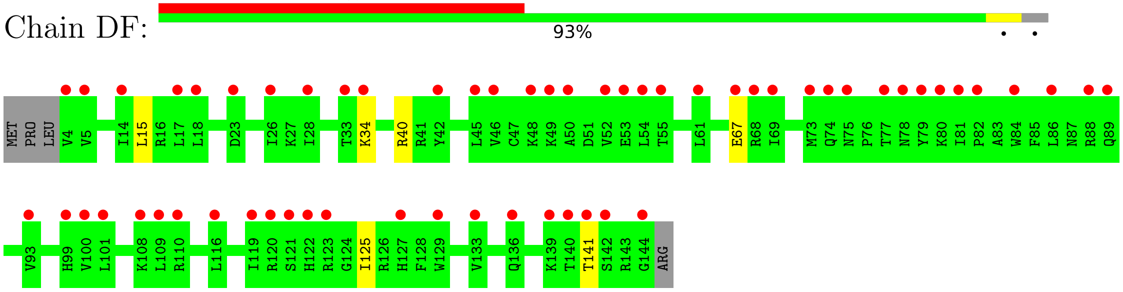
- Molecule 63: 40S ribosomal protein S17-B



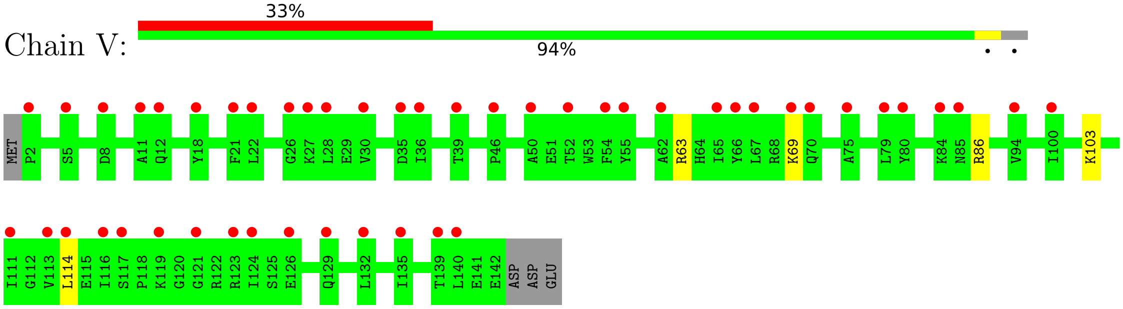
- Molecule 64: 40S ribosomal protein S18-B



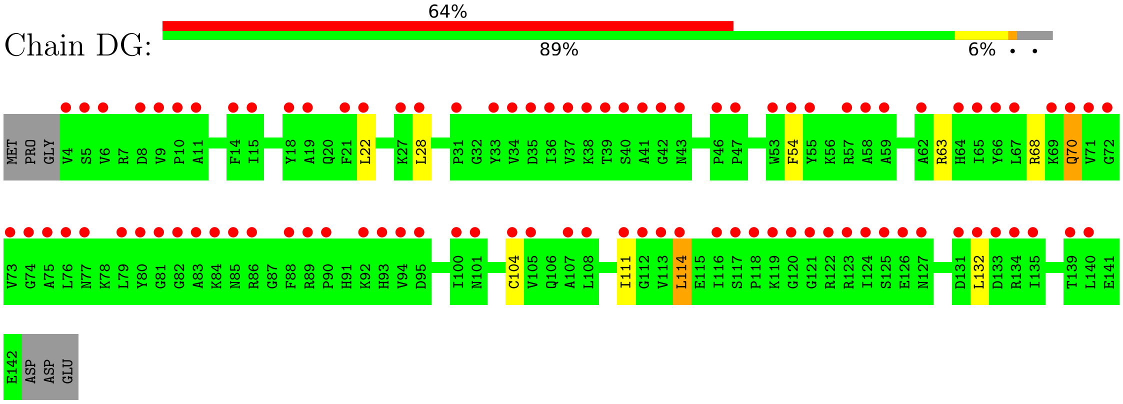
- Molecule 64: 40S ribosomal protein S18-B



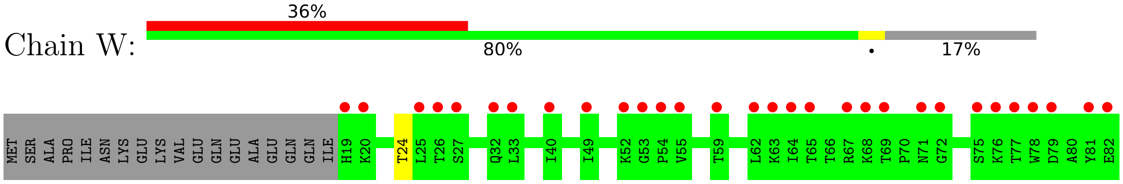
- Molecule 65: 40S ribosomal protein S19-A

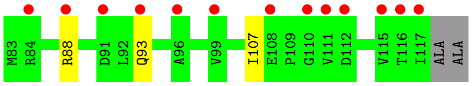


- Molecule 65: 40S ribosomal protein S19-A



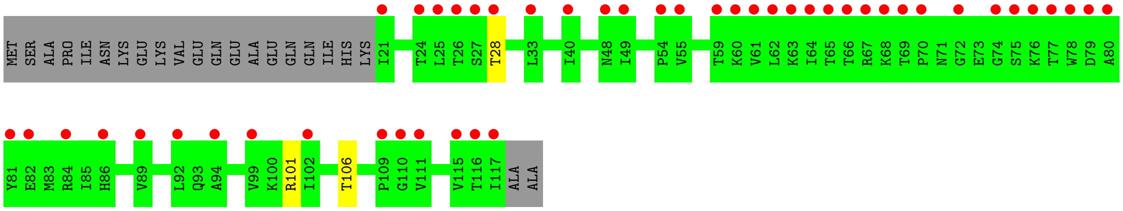
- Molecule 66: Ribosomal protein S10





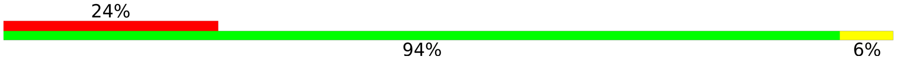
- Molecule 66: Ribosomal protein S10

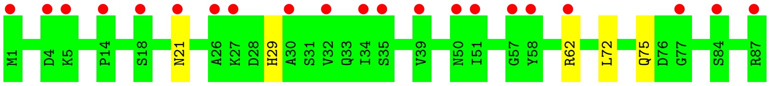
Chain DH:



- Molecule 67: 40S ribosomal protein S21

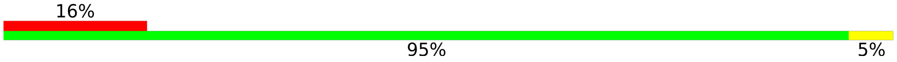
Chain X:

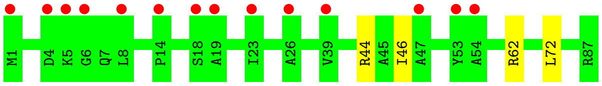




- Molecule 67: 40S ribosomal protein S21

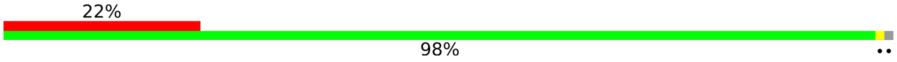
Chain DI:

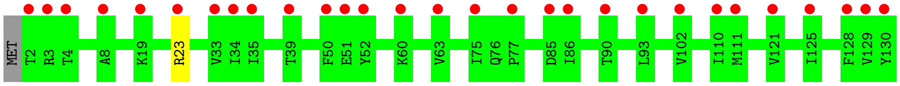




- Molecule 68: 40S ribosomal protein S22-A

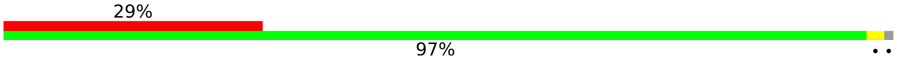
Chain Y:

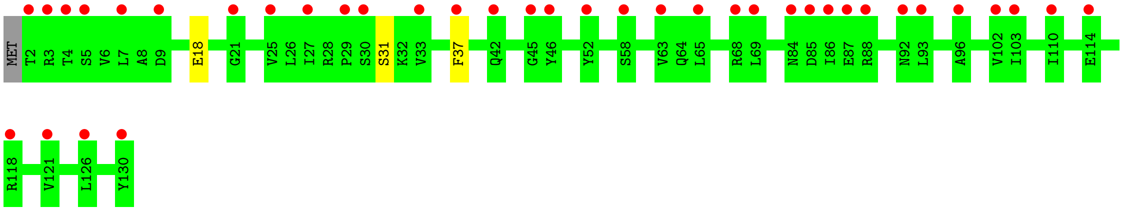




- Molecule 68: 40S ribosomal protein S22-A

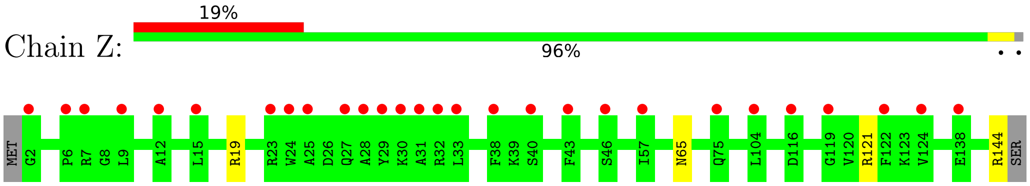
Chain DJ:





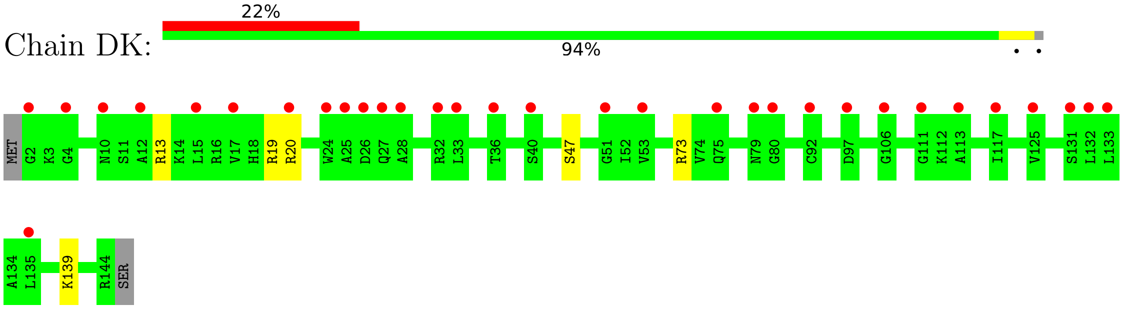
- Molecule 69: Ribosomal protein S23 (S12)

Chain Z:



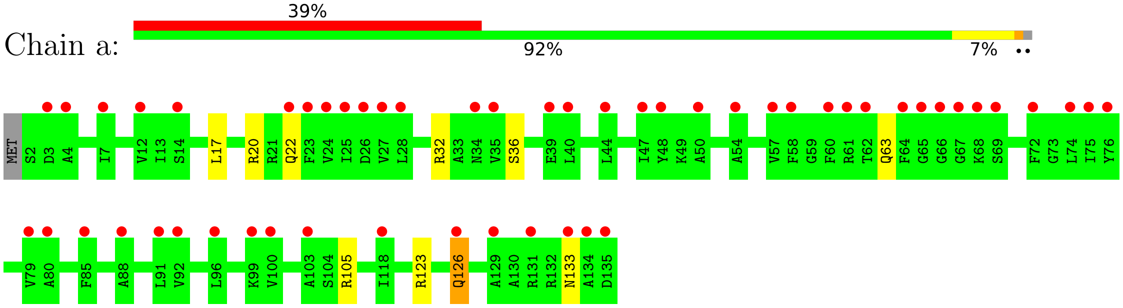
- Molecule 69: Ribosomal protein S23 (S12)

Chain DK:



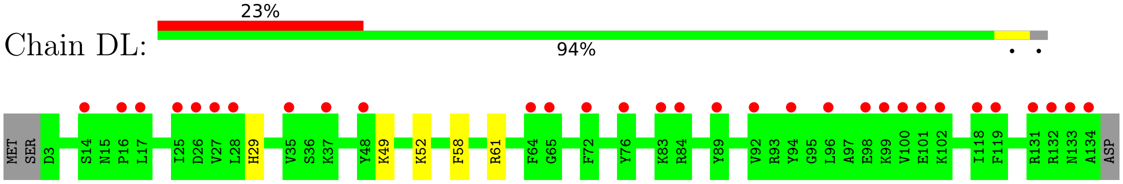
- Molecule 70: 40S ribosomal protein S24

Chain a:



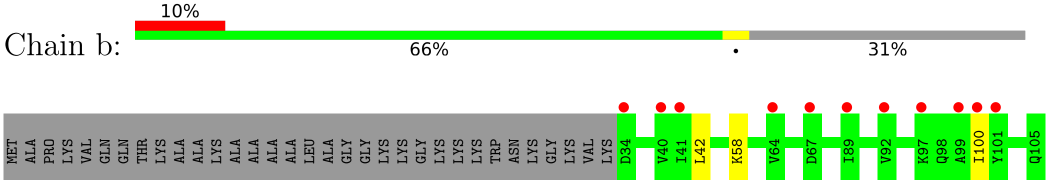
- Molecule 70: 40S ribosomal protein S24

Chain DL:



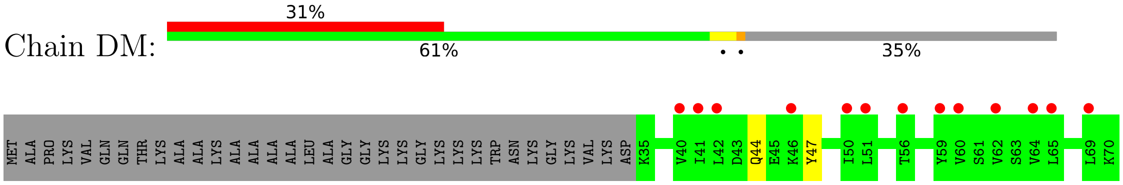
- Molecule 71: 40S ribosomal protein S25

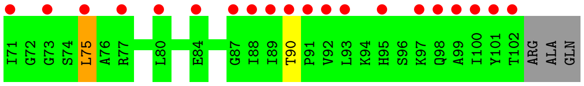
Chain b:



- Molecule 71: 40S ribosomal protein S25

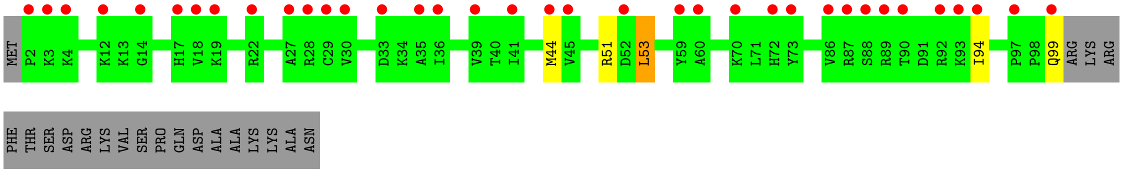
Chain DM:





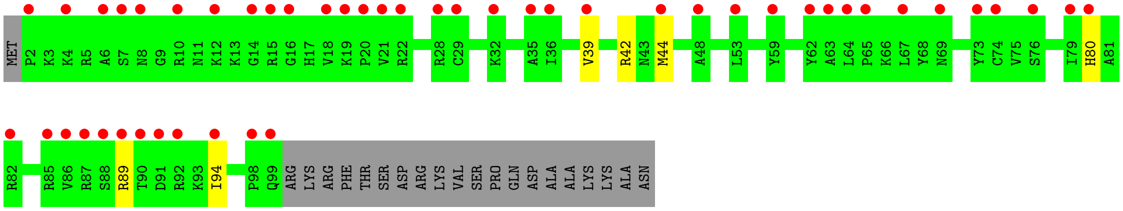
- Molecule 72: 40S ribosomal protein S26

Chain c:



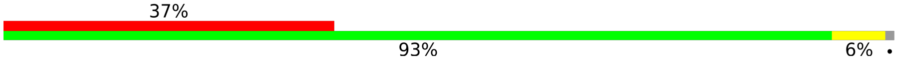
- Molecule 72: 40S ribosomal protein S26

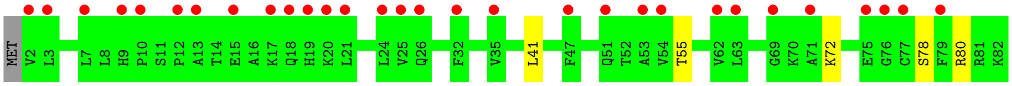
Chain DN:



- Molecule 73: 40S ribosomal protein S27

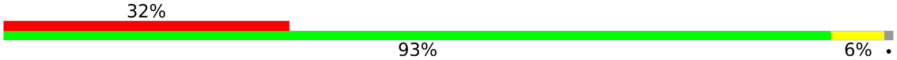
Chain d:

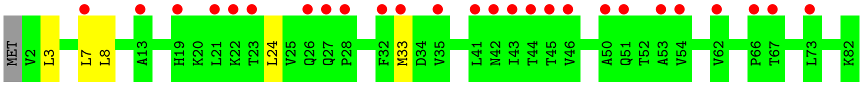




- Molecule 73: 40S ribosomal protein S27

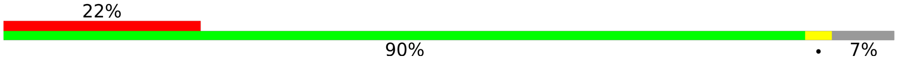
Chain DO:

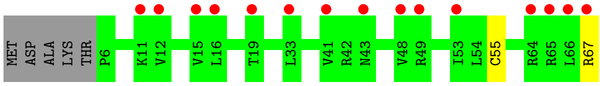




- Molecule 74: 40S ribosomal protein S28-B

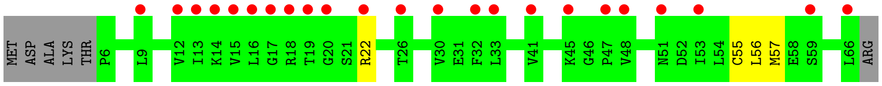
Chain e:





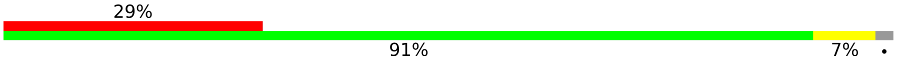
- Molecule 74: 40S ribosomal protein S28-B

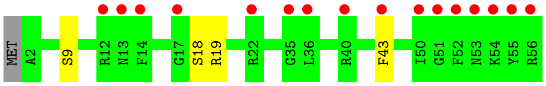
Chain DP:



- Molecule 75: 40S ribosomal protein S29A

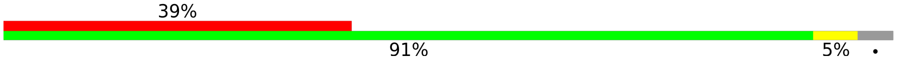
Chain f:

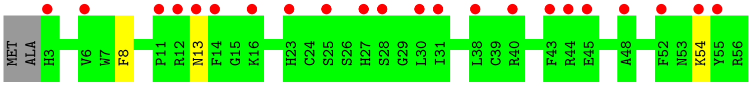




- Molecule 75: 40S ribosomal protein S29A

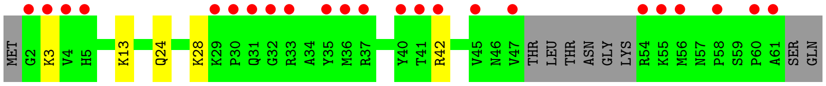
Chain DQ:





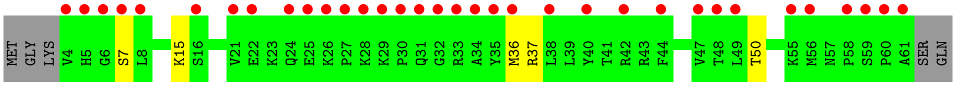
- Molecule 76: 40S ribosomal protein S30

Chain g:



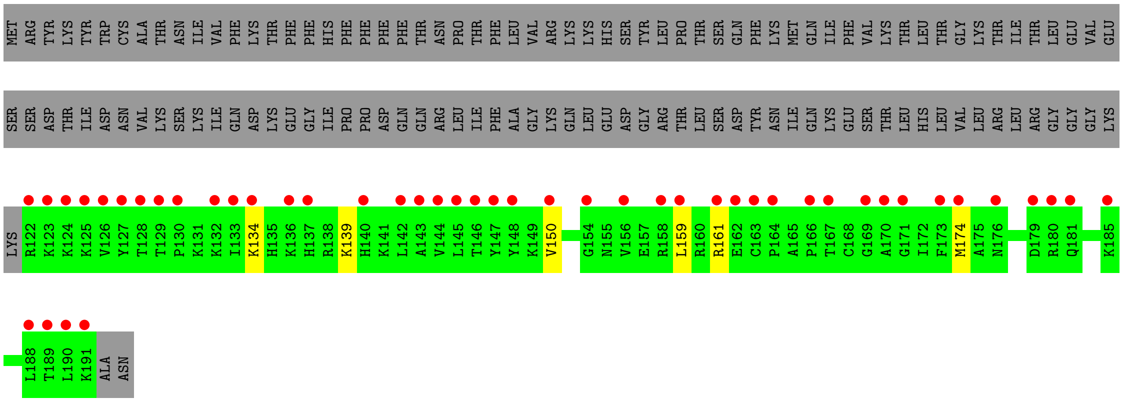
- Molecule 76: 40S ribosomal protein S30

Chain DR:

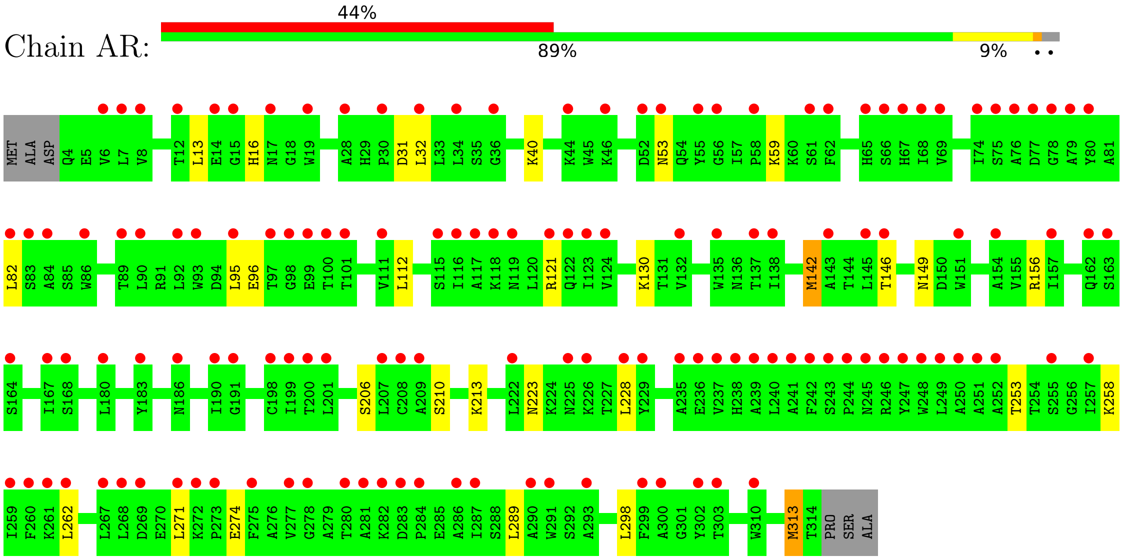


- Molecule 77: Ubiquitin-40S ribosomal protein S31 fusion protein

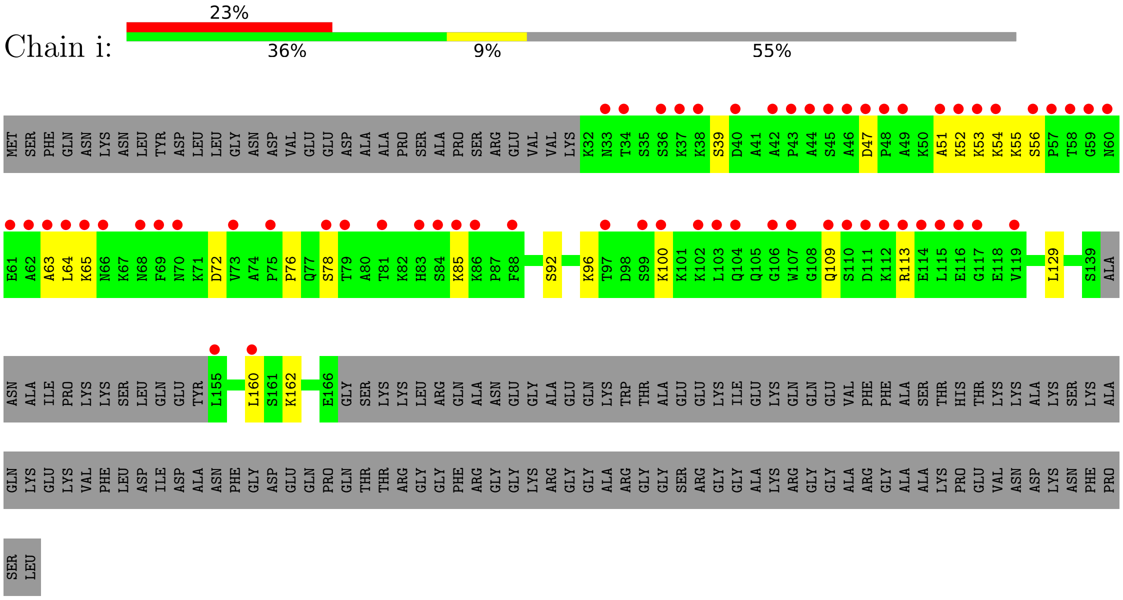
Chain h:



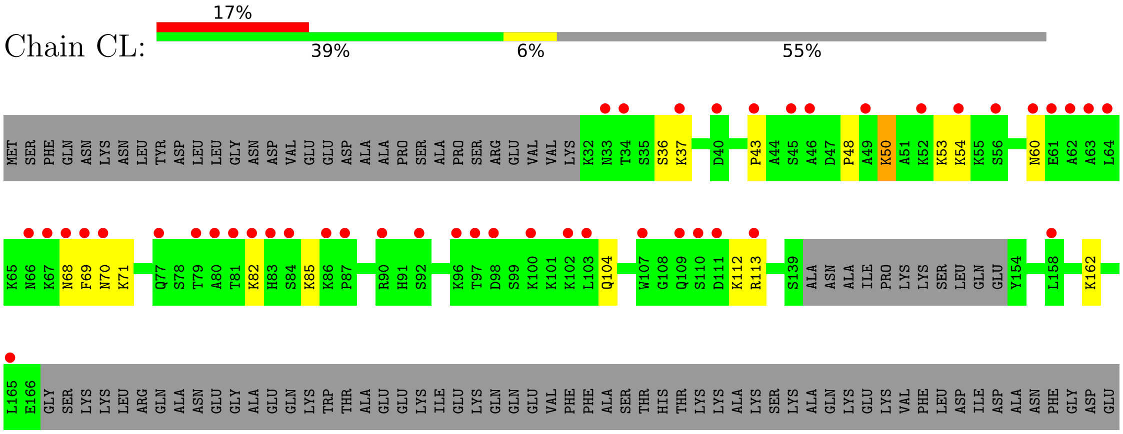
- Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 79: 60S ribosomal protein CAALFM_C304810CA



- Molecule 79: 60S ribosomal protein CAALFM_C304810CA




GLN
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LYS
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ALA
ARG
GLY
ALA
ALA
LYS
PRO
GLU
VAL
ASN
ASP
LYS
ASN
PHE
PRO
SER
LEU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	297.30Å 292.54Å 442.98Å 90.00° 99.37° 90.00°	Depositor
Resolution (Å)	163.00 – 2.90 163.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (163.00-2.90) 82.8 (163.00-2.90)	Depositor EDS
R_{merge}	0.56	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.52 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19rc4_4035	Depositor
R, R_{free}	0.257 , 0.283 0.266 , 0.277	Depositor DCC
R_{free} test set	2000 reflections (0.12%)	wwPDB-VP
Wilson B-factor (Å^2)	47.7	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	397530	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PAR, ZN, 3K5

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	1	0.34	0/75861	0.91	56/118257 (0.0%)
1	AS	0.32	0/73312	0.92	75/114279 (0.1%)
2	3	0.28	0/2884	0.81	0/4492
2	AT	0.34	0/2884	0.89	6/4492 (0.1%)
3	4	0.31	0/3702	0.87	4/5764 (0.1%)
3	AU	0.29	0/3702	0.86	3/5764 (0.1%)
4	AW	0.36	0/1931	0.81	3/2592 (0.1%)
4	j	0.34	0/1931	0.68	1/2592 (0.0%)
5	AX	0.35	0/3145	0.73	4/4231 (0.1%)
5	k	0.35	0/3156	0.72	3/4246 (0.1%)
6	AY	0.35	0/2799	0.73	1/3777 (0.0%)
6	l	0.36	0/2793	0.71	1/3769 (0.0%)
7	AZ	0.42	0/2447	0.86	4/3294 (0.1%)
7	m	0.40	0/2479	0.78	5/3337 (0.1%)
8	BA	0.38	0/1231	0.76	1/1662 (0.1%)
8	n	0.38	0/1263	0.72	1/1703 (0.1%)
9	BB	0.34	0/1918	0.65	2/2575 (0.1%)
9	o	0.39	0/1918	0.69	1/2575 (0.0%)
10	BC	0.43	0/1825	0.90	9/2458 (0.4%)
10	p	0.37	0/1820	0.71	1/2451 (0.0%)
11	BD	0.43	0/1537	0.87	1/2067 (0.0%)
11	q	0.37	0/1537	0.76	0/2067
12	BE	0.37	0/1705	0.76	2/2288 (0.1%)
12	r	0.35	0/1724	0.75	1/2314 (0.0%)
13	BF	0.39	0/1390	0.97	8/1861 (0.4%)
13	s	0.43	0/1390	0.95	2/1861 (0.1%)
14	BG	0.42	0/1637	0.89	4/2195 (0.2%)
14	t	0.38	0/1637	0.77	3/2195 (0.1%)
15	BH	0.37	0/1044	0.81	2/1407 (0.1%)
15	u	0.39	0/1030	0.77	0/1389
16	BI	0.38	0/1753	0.85	2/2347 (0.1%)
16	v	0.34	0/1753	0.73	0/2347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	BJ	0.39	0/1620	0.74	4/2167 (0.2%)
17	w	0.40	0/1620	0.73	2/2167 (0.1%)
18	BK	0.37	0/1419	0.80	1/1906 (0.1%)
18	x	0.35	0/1395	0.77	1/1874 (0.1%)
19	BL	0.38	0/1482	0.81	1/1985 (0.1%)
19	y	0.37	0/1482	0.79	1/1985 (0.1%)
20	BM	0.39	0/1475	0.93	7/1961 (0.4%)
20	z	0.35	0/1475	0.79	2/1961 (0.1%)
21	0	0.34	0/1457	0.71	0/1962
21	BN	0.37	0/1457	0.70	0/1962
22	2	0.38	0/1285	0.72	1/1723 (0.1%)
22	BO	0.39	0/1285	0.74	2/1723 (0.1%)
23	5	0.40	0/846	0.75	1/1140 (0.1%)
23	BP	0.41	0/857	0.79	1/1156 (0.1%)
24	6	0.34	0/993	0.70	0/1339
24	BQ	0.37	0/993	0.79	2/1339 (0.1%)
25	7	0.30	0/643	0.61	0/853
25	BR	0.36	0/889	0.65	0/1175
26	8	0.35	0/990	0.75	1/1337 (0.1%)
26	BS	0.42	0/976	0.84	3/1319 (0.2%)
27	9	0.38	0/990	0.72	0/1322
27	BT	0.43	0/999	0.83	3/1334 (0.2%)
28	AA	0.44	0/1112	0.74	0/1488
28	BU	0.47	0/1112	0.88	3/1488 (0.2%)
29	AB	0.35	0/1199	0.72	2/1607 (0.1%)
29	BV	0.38	0/1199	0.75	1/1607 (0.1%)
30	AC	0.35	0/498	0.87	0/661
30	BW	0.39	0/498	0.81	1/661 (0.2%)
31	AD	0.35	0/738	0.73	1/994 (0.1%)
31	BX	0.37	0/738	0.85	1/994 (0.1%)
32	AE	0.39	0/907	0.82	0/1219
32	BY	0.43	0/907	0.88	0/1219
33	AF	0.38	0/1021	0.72	0/1368
33	BZ	0.41	0/1025	0.83	4/1372 (0.3%)
34	AG	0.34	0/866	0.69	1/1165 (0.1%)
34	CA	0.38	0/866	0.75	2/1165 (0.2%)
35	AH	0.36	0/896	0.79	0/1195
35	CB	0.37	0/896	0.85	2/1195 (0.2%)
36	AI	0.34	0/995	0.87	1/1325 (0.1%)
36	CC	0.40	0/999	0.93	5/1330 (0.4%)
37	AJ	0.35	0/763	0.78	0/1012
37	CD	0.33	0/763	0.84	1/1012 (0.1%)
38	AK	0.38	0/690	0.81	2/916 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	CE	0.36	0/690	0.76	0/916
39	AL	0.37	0/623	0.75	1/831 (0.1%)
39	CF	0.38	0/623	0.77	1/831 (0.1%)
40	AM	0.34	0/447	0.83	0/594
40	CG	0.31	0/458	0.80	0/609
41	AN	0.41	0/425	0.74	0/563
41	CH	0.40	0/417	0.74	1/553 (0.2%)
42	AO	0.37	0/237	0.96	1/304 (0.3%)
42	CI	0.31	0/237	0.92	0/304
43	AP	0.36	0/840	0.72	1/1110 (0.1%)
43	CJ	0.36	0/840	0.72	1/1110 (0.1%)
44	AQ	0.42	0/705	0.77	0/940
44	CK	0.40	0/705	0.82	1/940 (0.1%)
45	B	0.33	0/41128	0.97	69/64084 (0.1%)
45	CM	0.34	0/42397	0.99	86/66069 (0.1%)
46	C	0.45	0/1666	0.88	2/2273 (0.1%)
46	CN	0.40	0/1666	0.88	6/2273 (0.3%)
47	CO	0.39	0/1750	0.92	7/2354 (0.3%)
47	D	0.38	0/1750	0.81	0/2354
48	CP	0.39	0/1657	0.77	2/2248 (0.1%)
48	E	0.40	0/1657	0.82	5/2248 (0.2%)
49	CQ	0.43	0/1731	0.95	6/2324 (0.3%)
49	F	0.38	0/1731	0.84	2/2324 (0.1%)
50	CR	0.38	0/2096	0.79	2/2822 (0.1%)
50	G	0.42	0/2092	0.85	5/2817 (0.2%)
51	CS	0.37	0/1631	0.83	3/2199 (0.1%)
51	H	0.38	0/1631	0.73	0/2199
52	CT	0.40	0/1929	0.85	2/2571 (0.1%)
52	I	0.37	0/1812	0.82	3/2420 (0.1%)
53	CU	0.40	0/1499	0.91	4/2016 (0.2%)
53	J	0.39	0/1486	0.89	6/1999 (0.3%)
54	CV	0.33	0/1606	0.78	1/2150 (0.0%)
54	K	0.36	0/1601	0.78	0/2143
55	CW	0.43	0/1478	0.96	5/1978 (0.3%)
55	L	0.37	0/1478	0.81	2/1978 (0.1%)
56	CX	0.40	0/809	0.93	3/1092 (0.3%)
56	M	0.39	0/836	0.85	3/1130 (0.3%)
57	CY	0.39	0/1154	0.75	0/1553
57	N	0.38	0/1152	0.74	0/1550
58	CZ	0.36	0/921	1.04	6/1240 (0.5%)
58	O	0.38	0/892	0.97	4/1203 (0.3%)
59	DA	0.39	0/1210	0.85	4/1631 (0.2%)
59	P	0.40	0/1210	0.81	2/1631 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	DB	0.44	0/953	0.87	1/1279 (0.1%)
60	Q	0.39	0/953	0.83	1/1279 (0.1%)
61	DC	0.35	0/980	0.77	1/1315 (0.1%)
61	R	0.41	0/1038	0.86	2/1395 (0.1%)
62	DD	0.36	0/1069	0.74	2/1430 (0.1%)
62	S	0.40	0/1109	0.86	2/1486 (0.1%)
63	DE	0.41	0/1009	0.96	3/1354 (0.2%)
63	T	0.39	0/1009	0.83	2/1354 (0.1%)
64	DF	0.36	0/1178	0.90	2/1579 (0.1%)
64	U	0.41	0/1205	0.89	3/1615 (0.2%)
65	DG	0.34	0/1108	0.77	2/1492 (0.1%)
65	V	0.44	0/1120	0.83	0/1508
66	DH	0.35	0/772	0.80	1/1045 (0.1%)
66	W	0.36	0/792	0.81	0/1071
67	DI	0.35	0/683	0.89	3/918 (0.3%)
67	X	0.43	0/683	0.82	1/918 (0.1%)
68	DJ	0.41	0/1049	0.79	0/1412
68	Y	0.39	0/1049	0.77	0/1412
69	DK	0.35	0/1128	0.82	2/1505 (0.1%)
69	Z	0.38	0/1128	0.88	1/1505 (0.1%)
70	DL	0.35	0/1086	0.80	0/1447
70	a	0.36	0/1100	0.89	2/1466 (0.1%)
71	DM	0.43	0/552	0.86	1/745 (0.1%)
71	b	0.41	0/585	0.83	2/789 (0.3%)
72	DN	0.48	0/791	0.86	2/1060 (0.2%)
72	c	0.33	0/791	0.80	2/1060 (0.2%)
73	DO	0.44	0/624	0.97	4/843 (0.5%)
73	d	0.35	0/624	0.73	1/843 (0.1%)
74	DP	0.43	0/478	1.01	4/640 (0.6%)
74	e	0.36	0/489	0.95	0/654
75	DQ	0.33	0/461	0.72	0/613
75	f	0.38	0/466	0.80	1/620 (0.2%)
76	DR	0.35	0/469	0.78	1/626 (0.2%)
76	g	0.48	0/438	0.95	2/581 (0.3%)
77	h	0.39	0/585	1.02	1/778 (0.1%)
78	AR	0.39	0/2451	0.89	12/3337 (0.4%)
79	CL	0.38	0/941	0.83	1/1257 (0.1%)
79	i	0.44	0/928	1.06	3/1239 (0.2%)
All	All	0.35	0/423231	0.89	581/621279 (0.1%)

There are no bond length outliers.

The worst 5 of 581 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	CQ	183	LEU	CB-CG-CD2	-15.59	84.49	111.00
53	CU	73	LEU	CA-CB-CG	12.79	144.72	115.30
78	AR	271	LEU	CB-CG-CD1	-11.97	90.65	111.00
13	BF	84	LEU	CB-CG-CD1	-11.31	91.78	111.00
1	AS	1576	A	O4'-C1'-N9	11.11	117.09	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	AW	248/254 (98%)	238 (96%)	10 (4%)	0	100	100
4	j	248/254 (98%)	240 (97%)	8 (3%)	0	100	100
5	AX	384/389 (99%)	371 (97%)	13 (3%)	0	100	100
5	k	385/389 (99%)	373 (97%)	12 (3%)	0	100	100
6	AY	359/363 (99%)	349 (97%)	10 (3%)	0	100	100
6	l	358/363 (99%)	347 (97%)	11 (3%)	0	100	100
7	AZ	290/298 (97%)	277 (96%)	13 (4%)	0	100	100
7	m	294/298 (99%)	283 (96%)	11 (4%)	0	100	100
8	BA	149/176 (85%)	147 (99%)	2 (1%)	0	100	100
8	n	153/176 (87%)	150 (98%)	3 (2%)	0	100	100
9	BB	232/241 (96%)	225 (97%)	7 (3%)	0	100	100
9	o	232/241 (96%)	225 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	BC	229/262 (87%)	220 (96%)	7 (3%)	2 (1%)	14	43
10	p	228/262 (87%)	220 (96%)	7 (3%)	1 (0%)	30	60
11	BD	188/191 (98%)	183 (97%)	5 (3%)	0	100	100
11	q	188/191 (98%)	184 (98%)	4 (2%)	0	100	100
12	BE	202/220 (92%)	198 (98%)	4 (2%)	0	100	100
12	r	204/220 (93%)	202 (99%)	2 (1%)	0	100	100
13	BF	169/174 (97%)	163 (96%)	6 (4%)	0	100	100
13	s	169/174 (97%)	162 (96%)	7 (4%)	0	100	100
14	BG	198/202 (98%)	194 (98%)	3 (2%)	1 (0%)	25	56
14	t	198/202 (98%)	196 (99%)	2 (1%)	0	100	100
15	BH	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
15	u	126/131 (96%)	122 (97%)	4 (3%)	0	100	100
16	BI	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
16	v	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
17	BJ	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
17	w	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
18	BK	170/185 (92%)	166 (98%)	4 (2%)	0	100	100
18	x	167/185 (90%)	163 (98%)	4 (2%)	0	100	100
19	BL	183/186 (98%)	179 (98%)	4 (2%)	0	100	100
19	y	183/186 (98%)	180 (98%)	3 (2%)	0	100	100
20	BM	177/190 (93%)	172 (97%)	5 (3%)	0	100	100
20	z	177/190 (93%)	175 (99%)	2 (1%)	0	100	100
21	0	168/172 (98%)	166 (99%)	2 (1%)	0	100	100
21	BN	168/172 (98%)	167 (99%)	1 (1%)	0	100	100
22	2	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
22	BO	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
23	5	101/124 (82%)	94 (93%)	6 (6%)	1 (1%)	13	40
23	BP	101/124 (82%)	90 (89%)	9 (9%)	2 (2%)	6	23
24	6	129/137 (94%)	127 (98%)	2 (2%)	0	100	100
24	BQ	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
25	7	73/155 (47%)	69 (94%)	3 (4%)	1 (1%)	9	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	BR	105/155 (68%)	97 (92%)	7 (7%)	1 (1%)	13	40
26	8	119/142 (84%)	118 (99%)	1 (1%)	0	100	100
26	BS	117/142 (82%)	116 (99%)	1 (1%)	0	100	100
27	9	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
27	BT	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
28	AA	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
28	BU	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
29	AB	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
29	BV	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
30	AC	59/63 (94%)	56 (95%)	1 (2%)	2 (3%)	3	13
30	BW	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
31	AD	94/106 (89%)	93 (99%)	1 (1%)	0	100	100
31	BX	94/106 (89%)	91 (97%)	3 (3%)	0	100	100
32	AE	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
32	BY	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14	43
33	AF	122/131 (93%)	122 (100%)	0	0	100	100
33	BZ	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
34	AG	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
34	CA	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
35	AH	110/122 (90%)	108 (98%)	2 (2%)	0	100	100
35	CB	110/122 (90%)	106 (96%)	4 (4%)	0	100	100
36	AI	116/120 (97%)	112 (97%)	4 (3%)	0	100	100
36	CC	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
37	AJ	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
37	CD	95/99 (96%)	93 (98%)	1 (1%)	1 (1%)	12	37
38	AK	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
38	CE	84/90 (93%)	82 (98%)	2 (2%)	0	100	100
39	AL	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
39	CF	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
40	AM	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
40	CG	49/51 (96%)	49 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	AN	50/52 (96%)	50 (100%)	0	0	100	100
41	CH	49/52 (94%)	45 (92%)	2 (4%)	2 (4%)	2	9
42	AO	23/25 (92%)	23 (100%)	0	0	100	100
42	CI	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
43	AP	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
43	CJ	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
44	AQ	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
44	CK	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
46	C	206/261 (79%)	200 (97%)	6 (3%)	0	100	100
46	CN	206/261 (79%)	198 (96%)	8 (4%)	0	100	100
47	CO	212/256 (83%)	205 (97%)	6 (3%)	1 (0%)	25	56
47	D	212/256 (83%)	207 (98%)	5 (2%)	0	100	100
48	CP	215/249 (86%)	209 (97%)	6 (3%)	0	100	100
48	E	215/249 (86%)	212 (99%)	3 (1%)	0	100	100
49	CQ	221/251 (88%)	211 (96%)	10 (4%)	0	100	100
49	F	221/251 (88%)	215 (97%)	6 (3%)	0	100	100
50	CR	258/262 (98%)	254 (98%)	4 (2%)	0	100	100
50	G	257/262 (98%)	253 (98%)	4 (2%)	0	100	100
51	CS	204/225 (91%)	195 (96%)	9 (4%)	0	100	100
51	H	204/225 (91%)	195 (96%)	8 (4%)	1 (0%)	25	56
52	CT	234/236 (99%)	229 (98%)	5 (2%)	0	100	100
52	I	220/236 (93%)	215 (98%)	5 (2%)	0	100	100
53	CU	181/186 (97%)	173 (96%)	7 (4%)	1 (1%)	22	52
53	J	179/186 (96%)	168 (94%)	11 (6%)	0	100	100
54	CV	201/206 (98%)	200 (100%)	1 (0%)	0	100	100
54	K	200/206 (97%)	199 (100%)	1 (0%)	0	100	100
55	CW	176/189 (93%)	174 (99%)	2 (1%)	0	100	100
55	L	176/189 (93%)	175 (99%)	1 (1%)	0	100	100
56	CX	92/118 (78%)	87 (95%)	5 (5%)	0	100	100
56	M	96/118 (81%)	81 (84%)	12 (12%)	3 (3%)	3	14
57	CY	139/155 (90%)	133 (96%)	4 (3%)	2 (1%)	9	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	N	137/155 (88%)	133 (97%)	4 (3%)	0	100	100
58	CZ	117/143 (82%)	91 (78%)	21 (18%)	5 (4%)	2	8
58	O	114/143 (80%)	91 (80%)	17 (15%)	6 (5%)	1	5
59	DA	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
59	P	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
60	DB	125/132 (95%)	121 (97%)	3 (2%)	1 (1%)	16	45
60	Q	125/132 (95%)	120 (96%)	5 (4%)	0	100	100
61	DC	118/142 (83%)	102 (86%)	16 (14%)	0	100	100
61	R	127/142 (89%)	115 (91%)	11 (9%)	1 (1%)	16	45
62	DD	131/142 (92%)	128 (98%)	3 (2%)	0	100	100
62	S	138/142 (97%)	134 (97%)	3 (2%)	1 (1%)	19	49
63	DE	122/137 (89%)	117 (96%)	5 (4%)	0	100	100
63	T	122/137 (89%)	117 (96%)	5 (4%)	0	100	100
64	DF	139/145 (96%)	133 (96%)	6 (4%)	0	100	100
64	U	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
65	DG	137/145 (94%)	133 (97%)	3 (2%)	1 (1%)	19	49
65	V	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
66	DH	95/119 (80%)	94 (99%)	1 (1%)	0	100	100
66	W	97/119 (82%)	94 (97%)	3 (3%)	0	100	100
67	DI	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
67	X	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
68	DJ	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
68	Y	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
69	DK	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
69	Z	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
70	DL	130/135 (96%)	130 (100%)	0	0	100	100
70	a	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
71	DM	66/105 (63%)	62 (94%)	3 (4%)	1 (2%)	8	29
71	b	70/105 (67%)	69 (99%)	1 (1%)	0	100	100
72	DN	96/119 (81%)	94 (98%)	2 (2%)	0	100	100
72	c	96/119 (81%)	94 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	DO	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
73	d	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
74	DP	59/67 (88%)	55 (93%)	4 (7%)	0	100	100
74	e	60/67 (90%)	57 (95%)	3 (5%)	0	100	100
75	DQ	52/56 (93%)	50 (96%)	2 (4%)	0	100	100
75	f	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
76	DR	56/63 (89%)	50 (89%)	5 (9%)	1 (2%)	7	25
76	g	50/63 (79%)	48 (96%)	2 (4%)	0	100	100
77	h	68/193 (35%)	56 (82%)	11 (16%)	1 (2%)	8	29
78	AR	309/317 (98%)	293 (95%)	16 (5%)	0	100	100
79	CL	117/267 (44%)	91 (78%)	22 (19%)	4 (3%)	3	13
79	i	116/267 (43%)	90 (78%)	21 (18%)	5 (4%)	2	8
All	All	21638/23766 (91%)	20895 (97%)	693 (3%)	50 (0%)	44	73

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	p	205	ASN
56	M	86	ILE
58	O	38	HIS
58	O	39	ASP
58	O	90	LYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	AW	191/194 (98%)	185 (97%)	6 (3%)	35	70
4	j	191/194 (98%)	189 (99%)	2 (1%)	73	91
5	AX	325/328 (99%)	316 (97%)	9 (3%)	38	73
5	k	326/328 (99%)	320 (98%)	6 (2%)	54	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AY	290/292 (99%)	278 (96%)	12 (4%)	26	60
6	l	289/292 (99%)	282 (98%)	7 (2%)	44	76
7	AZ	247/252 (98%)	233 (94%)	14 (6%)	17	47
7	m	250/252 (99%)	241 (96%)	9 (4%)	30	65
8	BA	132/154 (86%)	129 (98%)	3 (2%)	45	77
8	n	136/154 (88%)	132 (97%)	4 (3%)	37	72
9	BB	198/204 (97%)	192 (97%)	6 (3%)	36	71
9	o	198/204 (97%)	192 (97%)	6 (3%)	36	71
10	BC	193/216 (89%)	176 (91%)	17 (9%)	8	26
10	p	193/216 (89%)	188 (97%)	5 (3%)	41	74
11	BD	169/170 (99%)	161 (95%)	8 (5%)	22	55
11	q	169/170 (99%)	166 (98%)	3 (2%)	54	82
12	BE	176/186 (95%)	173 (98%)	3 (2%)	56	83
12	r	178/186 (96%)	174 (98%)	4 (2%)	47	78
13	BF	146/149 (98%)	135 (92%)	11 (8%)	11	33
13	s	146/149 (98%)	139 (95%)	7 (5%)	21	54
14	BG	166/168 (99%)	153 (92%)	13 (8%)	10	31
14	t	166/168 (99%)	160 (96%)	6 (4%)	30	65
15	BH	108/109 (99%)	103 (95%)	5 (5%)	23	55
15	u	107/109 (98%)	106 (99%)	1 (1%)	75	92
16	BI	177/178 (99%)	170 (96%)	7 (4%)	27	61
16	v	177/178 (99%)	173 (98%)	4 (2%)	45	77
17	BJ	166/167 (99%)	159 (96%)	7 (4%)	25	59
17	w	166/167 (99%)	163 (98%)	3 (2%)	54	82
18	BK	145/154 (94%)	139 (96%)	6 (4%)	26	60
18	x	142/154 (92%)	141 (99%)	1 (1%)	81	94
19	BL	153/154 (99%)	150 (98%)	3 (2%)	50	79
19	y	153/154 (99%)	147 (96%)	6 (4%)	27	62
20	BM	146/153 (95%)	139 (95%)	7 (5%)	21	54
20	z	146/153 (95%)	143 (98%)	3 (2%)	48	78
21	0	155/157 (99%)	154 (99%)	1 (1%)	84	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	BN	155/157 (99%)	151 (97%)	4 (3%)	41	74
22	2	133/134 (99%)	127 (96%)	6 (4%)	23	56
22	BO	133/134 (99%)	128 (96%)	5 (4%)	28	63
23	5	93/112 (83%)	91 (98%)	2 (2%)	47	78
23	BP	94/112 (84%)	89 (95%)	5 (5%)	19	49
24	6	101/104 (97%)	97 (96%)	4 (4%)	27	61
24	BQ	101/104 (97%)	99 (98%)	2 (2%)	50	79
25	7	68/127 (54%)	63 (93%)	5 (7%)	11	34
25	BR	91/127 (72%)	77 (85%)	14 (15%)	2	7
26	8	108/121 (89%)	103 (95%)	5 (5%)	23	55
26	BS	107/121 (88%)	104 (97%)	3 (3%)	38	73
27	9	110/112 (98%)	109 (99%)	1 (1%)	75	92
27	BT	111/112 (99%)	101 (91%)	10 (9%)	8	25
28	AA	117/118 (99%)	115 (98%)	2 (2%)	56	83
28	BU	117/118 (99%)	109 (93%)	8 (7%)	13	38
29	AB	120/121 (99%)	114 (95%)	6 (5%)	20	52
29	BV	120/121 (99%)	118 (98%)	2 (2%)	56	83
30	AC	48/49 (98%)	46 (96%)	2 (4%)	25	59
30	BW	48/49 (98%)	42 (88%)	6 (12%)	3	12
31	AD	81/90 (90%)	78 (96%)	3 (4%)	29	64
31	BX	81/90 (90%)	76 (94%)	5 (6%)	15	43
32	AE	98/100 (98%)	97 (99%)	1 (1%)	73	91
32	BY	98/100 (98%)	92 (94%)	6 (6%)	15	43
33	AF	109/115 (95%)	106 (97%)	3 (3%)	38	73
33	BZ	110/115 (96%)	105 (96%)	5 (4%)	23	56
34	AG	91/92 (99%)	90 (99%)	1 (1%)	70	90
34	CA	91/92 (99%)	90 (99%)	1 (1%)	70	90
35	AH	95/102 (93%)	93 (98%)	2 (2%)	48	78
35	CB	95/102 (93%)	89 (94%)	6 (6%)	15	42
36	AI	106/106 (100%)	104 (98%)	2 (2%)	52	81
36	CC	106/106 (100%)	102 (96%)	4 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	AJ	77/79 (98%)	74 (96%)	3 (4%)	27	62
37	CD	77/79 (98%)	72 (94%)	5 (6%)	14	40
38	AK	70/73 (96%)	69 (99%)	1 (1%)	62	86
38	CE	70/73 (96%)	67 (96%)	3 (4%)	25	57
39	AL	68/69 (99%)	66 (97%)	2 (3%)	37	72
39	CF	68/69 (99%)	64 (94%)	4 (6%)	16	45
40	AM	46/47 (98%)	43 (94%)	3 (6%)	14	40
40	CG	47/47 (100%)	47 (100%)	0	100	100
41	AN	47/47 (100%)	46 (98%)	1 (2%)	48	78
41	CH	46/47 (98%)	43 (94%)	3 (6%)	14	40
42	AO	24/24 (100%)	23 (96%)	1 (4%)	25	59
42	CI	24/24 (100%)	20 (83%)	4 (17%)	2	5
43	AP	88/91 (97%)	84 (96%)	4 (4%)	23	56
43	CJ	88/91 (97%)	85 (97%)	3 (3%)	32	67
44	AQ	72/73 (99%)	67 (93%)	5 (7%)	13	37
44	CK	72/73 (99%)	66 (92%)	6 (8%)	9	28
46	C	176/215 (82%)	173 (98%)	3 (2%)	56	83
46	CN	176/215 (82%)	172 (98%)	4 (2%)	45	77
47	CO	194/229 (85%)	179 (92%)	15 (8%)	10	31
47	D	194/229 (85%)	189 (97%)	5 (3%)	41	74
48	CP	175/198 (88%)	166 (95%)	9 (5%)	20	51
48	E	175/198 (88%)	167 (95%)	8 (5%)	23	55
49	CQ	174/196 (89%)	167 (96%)	7 (4%)	27	61
49	F	174/196 (89%)	164 (94%)	10 (6%)	17	47
50	CR	218/220 (99%)	209 (96%)	9 (4%)	26	60
50	G	218/220 (99%)	209 (96%)	9 (4%)	26	60
51	CS	178/197 (90%)	167 (94%)	11 (6%)	15	43
51	H	178/197 (90%)	169 (95%)	9 (5%)	20	51
52	CT	204/204 (100%)	192 (94%)	12 (6%)	16	45
52	I	192/204 (94%)	185 (96%)	7 (4%)	30	65
53	CU	164/167 (98%)	158 (96%)	6 (4%)	29	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	J	163/167 (98%)	157 (96%)	6 (4%)	29	64
54	CV	157/160 (98%)	150 (96%)	7 (4%)	23	56
54	K	157/160 (98%)	153 (98%)	4 (2%)	42	75
55	CW	153/160 (96%)	141 (92%)	12 (8%)	10	31
55	L	153/160 (96%)	148 (97%)	5 (3%)	33	68
56	CX	88/104 (85%)	79 (90%)	9 (10%)	6	19
56	M	90/104 (86%)	89 (99%)	1 (1%)	70	90
57	CY	122/134 (91%)	118 (97%)	4 (3%)	33	68
57	N	122/134 (91%)	119 (98%)	3 (2%)	42	75
58	CZ	101/123 (82%)	93 (92%)	8 (8%)	10	30
58	O	98/123 (80%)	89 (91%)	9 (9%)	7	24
59	DA	129/130 (99%)	125 (97%)	4 (3%)	35	70
59	P	129/130 (99%)	125 (97%)	4 (3%)	35	70
60	DB	97/102 (95%)	96 (99%)	1 (1%)	73	91
60	Q	97/102 (95%)	94 (97%)	3 (3%)	35	70
61	DC	105/121 (87%)	100 (95%)	5 (5%)	21	54
61	R	111/121 (92%)	107 (96%)	4 (4%)	30	65
62	DD	110/116 (95%)	105 (96%)	5 (4%)	23	56
62	S	114/116 (98%)	108 (95%)	6 (5%)	19	49
63	DE	112/122 (92%)	107 (96%)	5 (4%)	23	56
63	T	112/122 (92%)	108 (96%)	4 (4%)	30	65
64	DF	125/129 (97%)	121 (97%)	4 (3%)	34	69
64	U	128/129 (99%)	123 (96%)	5 (4%)	27	62
65	DG	112/117 (96%)	103 (92%)	9 (8%)	10	30
65	V	113/117 (97%)	108 (96%)	5 (4%)	24	57
66	DH	87/105 (83%)	85 (98%)	2 (2%)	45	77
66	W	89/105 (85%)	85 (96%)	4 (4%)	23	56
67	DI	71/71 (100%)	70 (99%)	1 (1%)	62	86
67	X	71/71 (100%)	67 (94%)	4 (6%)	17	47
68	DJ	112/113 (99%)	109 (97%)	3 (3%)	40	73
68	Y	112/113 (99%)	111 (99%)	1 (1%)	75	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	DK	116/118 (98%)	112 (97%)	4 (3%)	32	67
69	Z	116/118 (98%)	113 (97%)	3 (3%)	41	74
70	DL	109/112 (97%)	104 (95%)	5 (5%)	23	55
70	a	111/112 (99%)	102 (92%)	9 (8%)	9	29
71	DM	61/85 (72%)	58 (95%)	3 (5%)	21	53
71	b	64/85 (75%)	63 (98%)	1 (2%)	58	84
72	DN	84/102 (82%)	80 (95%)	4 (5%)	21	54
72	c	84/102 (82%)	80 (95%)	4 (5%)	21	54
73	DO	72/73 (99%)	71 (99%)	1 (1%)	62	86
73	d	72/73 (99%)	68 (94%)	4 (6%)	17	47
74	DP	53/58 (91%)	51 (96%)	2 (4%)	28	63
74	e	54/58 (93%)	52 (96%)	2 (4%)	29	64
75	DQ	47/48 (98%)	44 (94%)	3 (6%)	14	41
75	f	47/48 (98%)	44 (94%)	3 (6%)	14	41
76	DR	50/54 (93%)	47 (94%)	3 (6%)	16	44
76	g	46/54 (85%)	43 (94%)	3 (6%)	14	40
77	h	62/175 (35%)	58 (94%)	4 (6%)	14	40
78	AR	259/263 (98%)	238 (92%)	21 (8%)	9	29
79	CL	99/212 (47%)	85 (86%)	14 (14%)	3	9
79	i	98/212 (46%)	82 (84%)	16 (16%)	2	6
All	All	18570/20010 (93%)	17796 (96%)	774 (4%)	25	59

5 of 774 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	BP	49	ASN
47	CO	42	ASN
25	BR	97	LYS
23	BP	10	LYS
32	BY	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 136 such sidechains are listed below:

Mol	Chain	Res	Type
52	CT	201	GLN
56	CX	29	GLN
68	DJ	70	ASN
58	O	38	HIS
57	N	98	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3166/3359 (94%)	579 (18%)	39 (1%)
1	AS	3058/3359 (91%)	504 (16%)	38 (1%)
2	3	120/121 (99%)	9 (7%)	0
2	AT	120/121 (99%)	9 (7%)	0
3	4	155/158 (98%)	22 (14%)	2 (1%)
3	AU	155/158 (98%)	21 (13%)	2 (1%)
45	B	1721/1787 (96%)	418 (24%)	42 (2%)
45	CM	1777/1787 (99%)	461 (25%)	57 (3%)
All	All	10272/10850 (94%)	2023 (19%)	180 (1%)

5 of 2023 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	15	A
1	1	24	U
1	1	25	A
1	1	29	G
1	1	39	A

5 of 180 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AS	3234	U
45	CM	518	A
1	AS	3315	C
45	CM	176	U
45	CM	678	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1074 ligands modelled in this entry, 1018 are monoatomic - leaving 56 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	PAR	1	3418	-	45,45,45	0.71	1 (2%)	64,67,67	1.08	6 (9%)
81	PAR	CM	1804	-	45,45,45	0.45	0	64,67,67	0.90	2 (3%)
81	PAR	1	3406	-	45,45,45	0.63	1 (2%)	64,67,67	1.14	5 (7%)
81	PAR	AS	3413	-	45,45,45	0.64	1 (2%)	64,67,67	1.09	5 (7%)
81	PAR	1	3425	-	45,45,45	0.46	0	64,67,67	0.91	3 (4%)
81	PAR	AS	3410	-	45,45,45	0.53	0	64,67,67	0.95	4 (6%)
81	PAR	AS	3412	-	45,45,45	0.47	0	64,67,67	0.99	4 (6%)
81	PAR	1	3408	-	45,45,45	0.46	0	64,67,67	0.79	3 (4%)
81	PAR	B	1805	-	45,45,45	0.45	0	64,67,67	0.96	4 (6%)
81	PAR	AS	3409	-	45,45,45	0.47	0	64,67,67	0.74	2 (3%)
81	PAR	1	3422	-	45,45,45	0.66	1 (2%)	64,67,67	1.72	10 (15%)
81	PAR	1	3429	-	45,45,45	0.52	0	64,67,67	0.94	2 (3%)
81	PAR	CM	1805	-	45,45,45	0.75	1 (2%)	64,67,67	1.11	3 (4%)
81	PAR	AS	3406	-	45,45,45	0.50	0	64,67,67	1.00	5 (7%)
81	PAR	1	3423	-	45,45,45	0.46	0	64,67,67	1.07	4 (6%)
81	PAR	AS	3401	-	45,45,45	0.48	0	64,67,67	1.31	5 (7%)
81	PAR	AS	3404	-	45,45,45	0.53	0	64,67,67	0.70	2 (3%)
81	PAR	1	3402	-	45,45,45	0.48	0	64,67,67	0.67	2 (3%)
81	PAR	B	1804	-	45,45,45	0.49	0	64,67,67	0.99	4 (6%)
81	PAR	AS	3407	-	45,45,45	0.53	0	64,67,67	1.05	4 (6%)
81	PAR	CM	1802	-	45,45,45	0.46	0	64,67,67	0.80	2 (3%)
81	PAR	1	3403	-	45,45,45	0.49	0	64,67,67	0.91	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
81	PAR	AS	3403	-	45,45,45	0.51	0	64,67,67	0.61	1 (1%)
80	3K5	1	3401	-	62,63,63	2.87	28 (45%)	82,95,95	1.72	21 (25%)
81	PAR	1	3405	-	45,45,45	0.80	1 (2%)	64,67,67	1.11	5 (7%)
81	PAR	AS	3405	-	45,45,45	0.47	0	64,67,67	0.70	1 (1%)
81	PAR	CM	1801	-	45,45,45	0.61	1 (2%)	64,67,67	1.05	4 (6%)
81	PAR	1	3416	-	45,45,45	0.43	0	64,67,67	0.94	2 (3%)
81	PAR	1	3410	-	45,45,45	0.56	0	64,67,67	0.82	2 (3%)
81	PAR	4	202	-	45,45,45	0.51	0	64,67,67	1.26	3 (4%)
81	PAR	1	3409	-	45,45,45	0.47	0	64,67,67	0.94	3 (4%)
81	PAR	1	3427	-	45,45,45	0.60	0	64,67,67	0.93	3 (4%)
81	PAR	B	1802	-	45,45,45	0.46	0	64,67,67	1.21	6 (9%)
81	PAR	1	3421	-	45,45,45	0.45	0	64,67,67	0.76	2 (3%)
81	PAR	AS	3408	-	45,45,45	0.57	0	64,67,67	0.90	4 (6%)
81	PAR	1	3417	82	45,45,45	0.60	1 (2%)	64,67,67	1.23	6 (9%)
81	PAR	1	3404	-	45,45,45	0.50	0	64,67,67	0.87	3 (4%)
81	PAR	1	3415	-	45,45,45	0.49	0	64,67,67	0.83	3 (4%)
81	PAR	1	3424	-	45,45,45	0.58	1 (2%)	64,67,67	1.02	4 (6%)
81	PAR	B	1803	-	45,45,45	0.49	0	64,67,67	1.09	4 (6%)
81	PAR	1	3411	-	45,45,45	0.47	0	64,67,67	1.05	6 (9%)
81	PAR	CM	1803	-	45,45,45	0.44	0	64,67,67	0.71	2 (3%)
81	PAR	CM	1806	-	45,45,45	0.66	1 (2%)	64,67,67	0.84	1 (1%)
81	PAR	1	3430	-	45,45,45	0.61	1 (2%)	64,67,67	1.47	10 (15%)
81	PAR	AS	3411	-	45,45,45	0.45	0	64,67,67	1.12	4 (6%)
81	PAR	1	3420	-	45,45,45	0.46	0	64,67,67	0.77	2 (3%)
81	PAR	1	3428	-	45,45,45	0.50	0	64,67,67	0.85	2 (3%)
81	PAR	1	3412	-	45,45,45	0.47	0	64,67,67	0.70	1 (1%)
81	PAR	1	3426	-	45,45,45	0.55	0	64,67,67	1.03	4 (6%)
81	PAR	1	3407	-	45,45,45	0.49	0	64,67,67	0.88	2 (3%)
81	PAR	1	3414	-	45,45,45	0.50	0	64,67,67	0.91	4 (6%)
81	PAR	4	201	-	45,45,45	0.74	2 (4%)	64,67,67	0.99	5 (7%)
81	PAR	AS	3402	-	45,45,45	0.45	0	64,67,67	0.81	2 (3%)
81	PAR	B	1801	-	45,45,45	0.47	0	64,67,67	0.85	5 (7%)
81	PAR	1	3413	-	45,45,45	0.67	1 (2%)	64,67,67	1.48	8 (12%)
81	PAR	1	3419	-	45,45,45	0.45	0	64,67,67	0.66	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	PAR	1	3418	-	-	7/18/94/94	0/4/4/4
81	PAR	CM	1804	-	-	9/18/94/94	0/4/4/4
81	PAR	1	3406	-	-	8/18/94/94	0/4/4/4
81	PAR	AS	3413	-	-	9/18/94/94	0/4/4/4
81	PAR	1	3425	-	-	10/18/94/94	0/4/4/4
81	PAR	AS	3410	-	-	7/18/94/94	0/4/4/4
81	PAR	AS	3412	-	-	6/18/94/94	0/4/4/4
81	PAR	1	3408	-	-	4/18/94/94	0/4/4/4
81	PAR	B	1805	-	-	11/18/94/94	0/4/4/4
81	PAR	AS	3409	-	-	9/18/94/94	0/4/4/4
81	PAR	1	3422	-	-	5/18/94/94	0/4/4/4
81	PAR	1	3429	-	-	4/18/94/94	0/4/4/4
81	PAR	CM	1805	-	-	7/18/94/94	0/4/4/4
81	PAR	AS	3406	-	-	9/18/94/94	0/4/4/4
81	PAR	1	3423	-	-	3/18/94/94	0/4/4/4
81	PAR	AS	3401	-	-	1/18/94/94	0/4/4/4
81	PAR	AS	3404	-	-	7/18/94/94	0/4/4/4
81	PAR	1	3402	-	-	3/18/94/94	0/4/4/4
81	PAR	B	1804	-	-	7/18/94/94	0/4/4/4
81	PAR	AS	3407	-	-	5/18/94/94	1/4/4/4
81	PAR	CM	1802	-	-	6/18/94/94	0/4/4/4
81	PAR	1	3403	-	-	10/18/94/94	1/4/4/4
81	PAR	AS	3403	-	-	3/18/94/94	0/4/4/4
80	3K5	1	3401	-	-	9/29/121/121	0/7/7/7
81	PAR	1	3405	-	-	9/18/94/94	0/4/4/4
81	PAR	AS	3405	-	-	1/18/94/94	1/4/4/4
81	PAR	CM	1801	-	-	5/18/94/94	0/4/4/4
81	PAR	1	3416	-	-	3/18/94/94	0/4/4/4
81	PAR	1	3410	-	-	9/18/94/94	1/4/4/4
81	PAR	4	202	-	-	5/18/94/94	0/4/4/4
81	PAR	1	3409	-	-	7/18/94/94	0/4/4/4
81	PAR	1	3427	-	-	6/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	PAR	B	1802	-	-	5/18/94/94	0/4/4/4
81	PAR	1	3421	-	-	4/18/94/94	0/4/4/4
81	PAR	AS	3408	-	-	8/18/94/94	0/4/4/4
81	PAR	1	3417	82	-	11/18/94/94	0/4/4/4
81	PAR	1	3404	-	-	8/18/94/94	1/4/4/4
81	PAR	1	3415	-	-	3/18/94/94	0/4/4/4
81	PAR	1	3424	-	-	9/18/94/94	0/4/4/4
81	PAR	B	1803	-	-	7/18/94/94	0/4/4/4
81	PAR	1	3411	-	-	10/18/94/94	0/4/4/4
81	PAR	CM	1803	-	-	2/18/94/94	0/4/4/4
81	PAR	CM	1806	-	-	6/18/94/94	0/4/4/4
81	PAR	1	3430	-	-	9/18/94/94	0/4/4/4
81	PAR	AS	3411	-	-	9/18/94/94	1/4/4/4
81	PAR	1	3420	-	-	6/18/94/94	0/4/4/4
81	PAR	1	3428	-	-	8/18/94/94	0/4/4/4
81	PAR	1	3412	-	-	6/18/94/94	0/4/4/4
81	PAR	1	3426	-	-	2/18/94/94	0/4/4/4
81	PAR	1	3407	-	-	7/18/94/94	0/4/4/4
81	PAR	1	3414	-	-	8/18/94/94	0/4/4/4
81	PAR	4	201	-	-	5/18/94/94	0/4/4/4
81	PAR	AS	3402	-	-	8/18/94/94	0/4/4/4
81	PAR	B	1801	-	-	3/18/94/94	0/4/4/4
81	PAR	1	3413	-	-	8/18/94/94	0/4/4/4
81	PAR	1	3419	-	-	6/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	1	3401	3K5	C17-C22	-9.21	1.36	1.53
80	1	3401	3K5	O4-C22	7.32	1.59	1.43
80	1	3401	3K5	C21-C22	5.86	1.63	1.52
80	1	3401	3K5	O6-C23	4.96	1.45	1.34
80	1	3401	3K5	C20-C23	4.61	1.62	1.51

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	1	3422	PAR	O33-C14-C24	8.21	122.36	108.22
81	4	202	PAR	O11-C11-C21	7.46	121.07	108.22
81	CM	1805	PAR	O11-C11-C21	5.89	118.36	108.22
81	AS	3401	PAR	C32-C22-C12	5.59	122.67	111.18
81	1	3422	PAR	O11-C42-C52	5.56	121.61	107.48

There are no chirality outliers.

5 of 362 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	1	3401	3K5	C4-C5-O1-C6
80	1	3401	3K5	C7-C6-O1-C5
80	1	3401	3K5	O15-C38-O14-C34
80	1	3401	3K5	C39-C38-O14-C34
81	1	3403	PAR	O51-C11-O11-C42

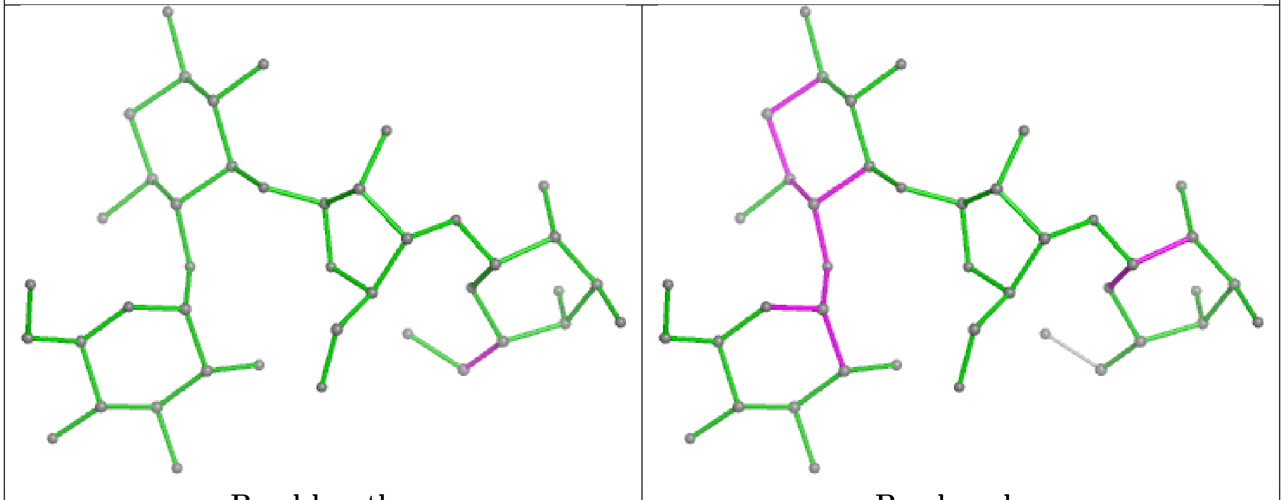
5 of 6 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
81	1	3410	PAR	C12-C22-C32-C42-C52-C62
81	AS	3407	PAR	C12-C22-C32-C42-C52-C62
81	1	3404	PAR	C12-C22-C32-C42-C52-C62
81	1	3403	PAR	C12-C22-C32-C42-C52-C62
81	AS	3405	PAR	C12-C22-C32-C42-C52-C62

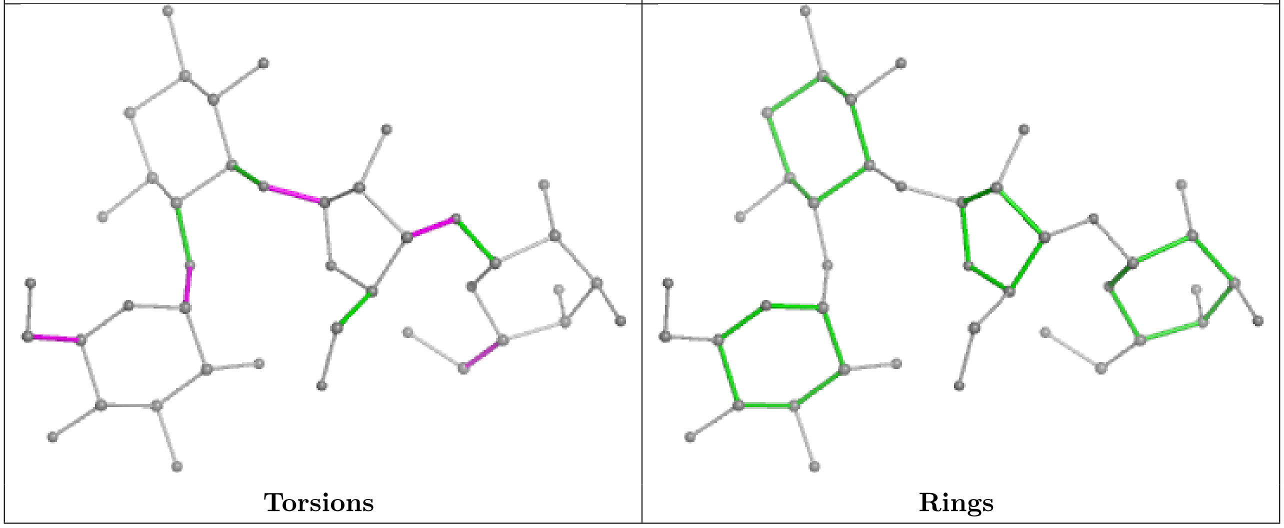
No monomer is involved in short contacts.

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

Ligand PAR 1 3418

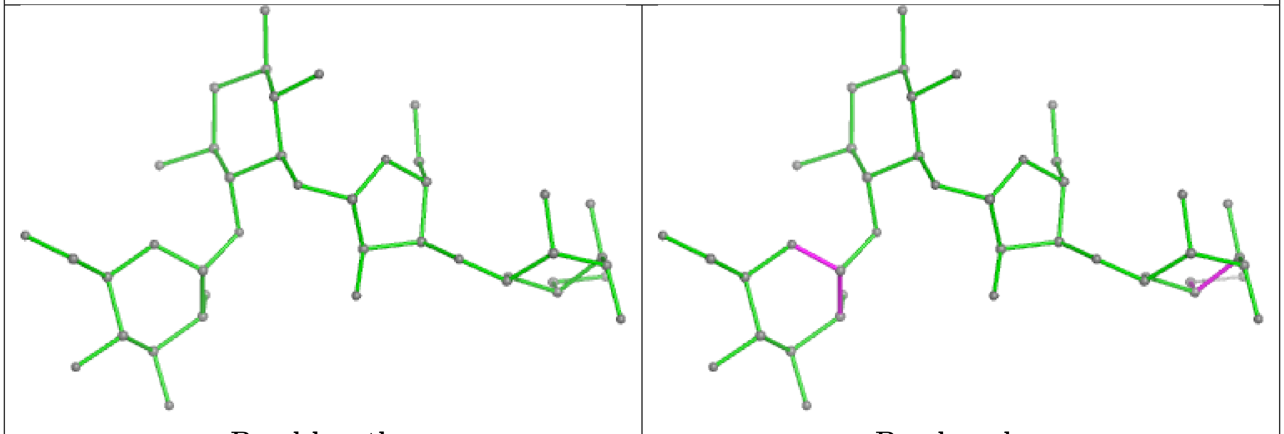


Bond lengths **Bond angles**

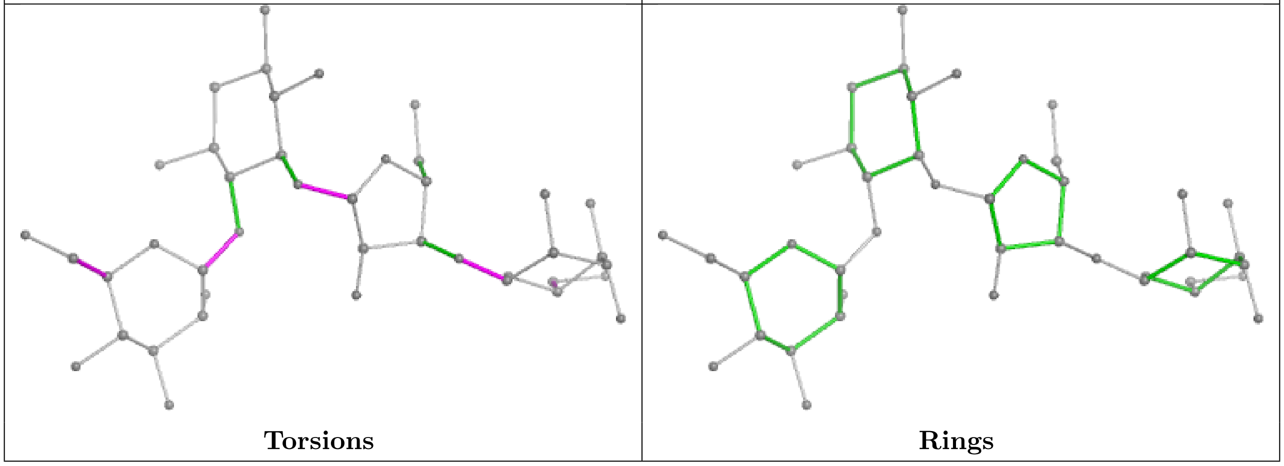


Torsions **Rings**

Ligand PAR CM 1804

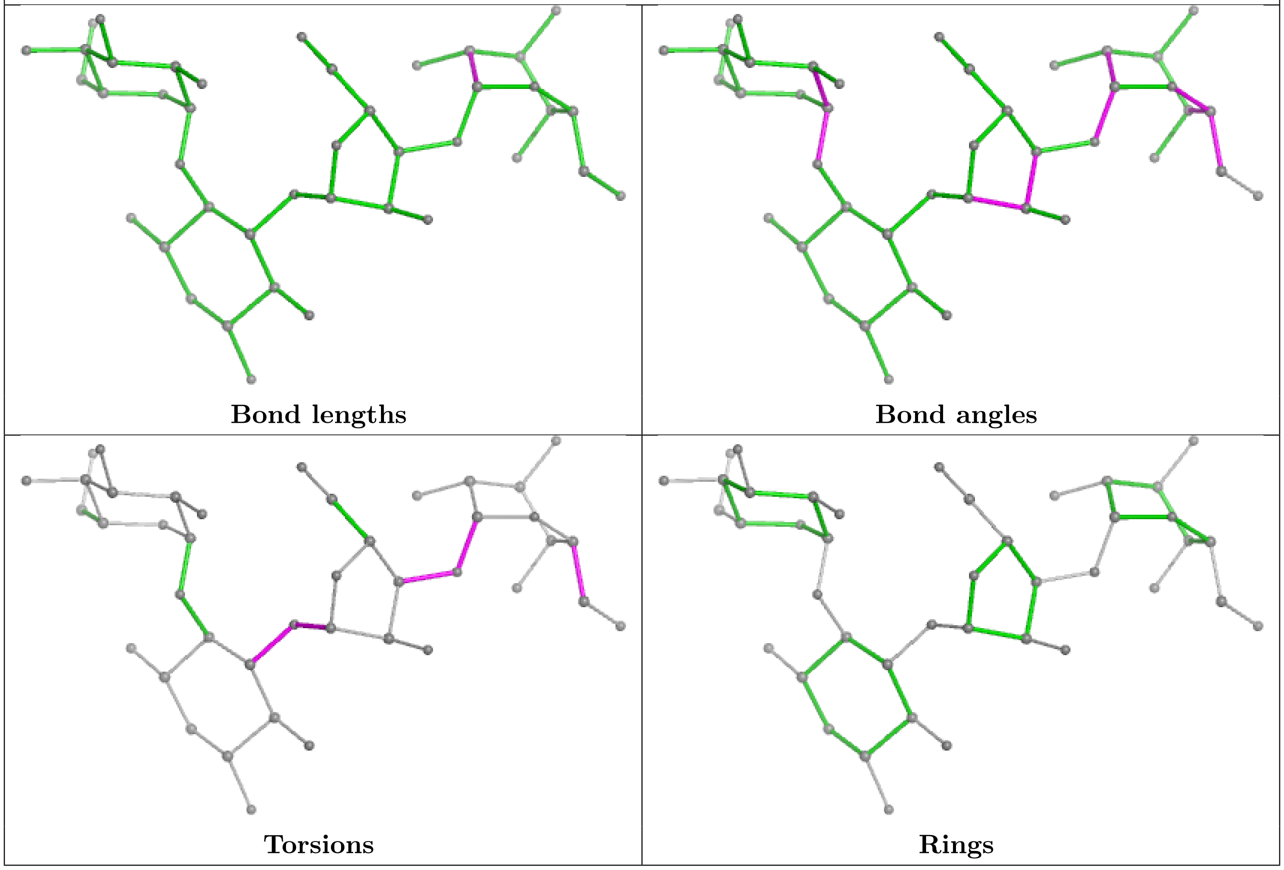


Bond lengths **Bond angles**



Torsions **Rings**

Ligand PAR 1 3406



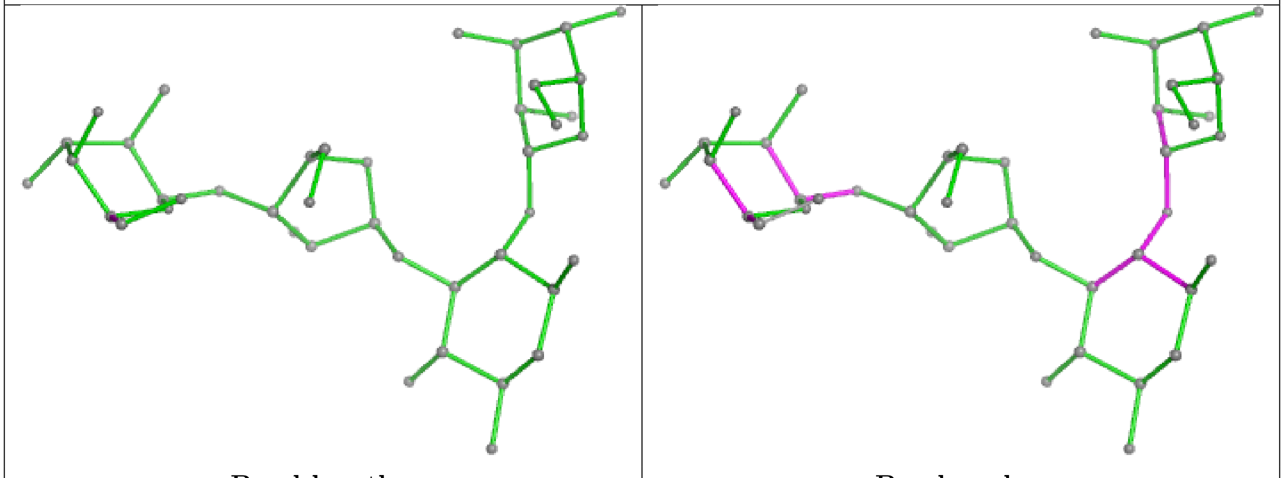
Bond lengths

Bond angles

Torsions

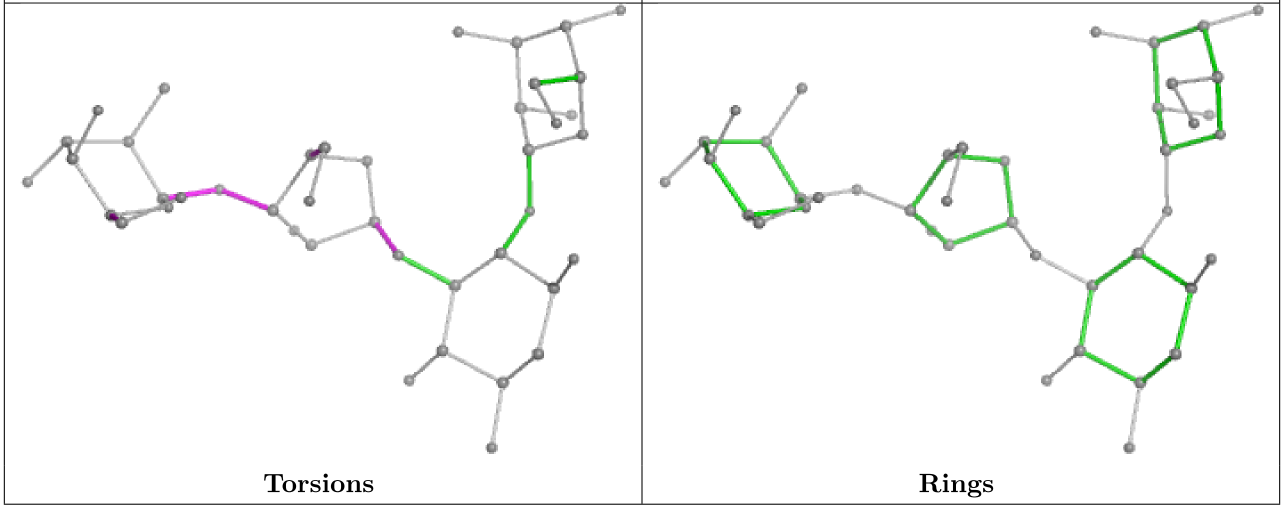
Rings

Ligand PAR AS 3413



Bond lengths

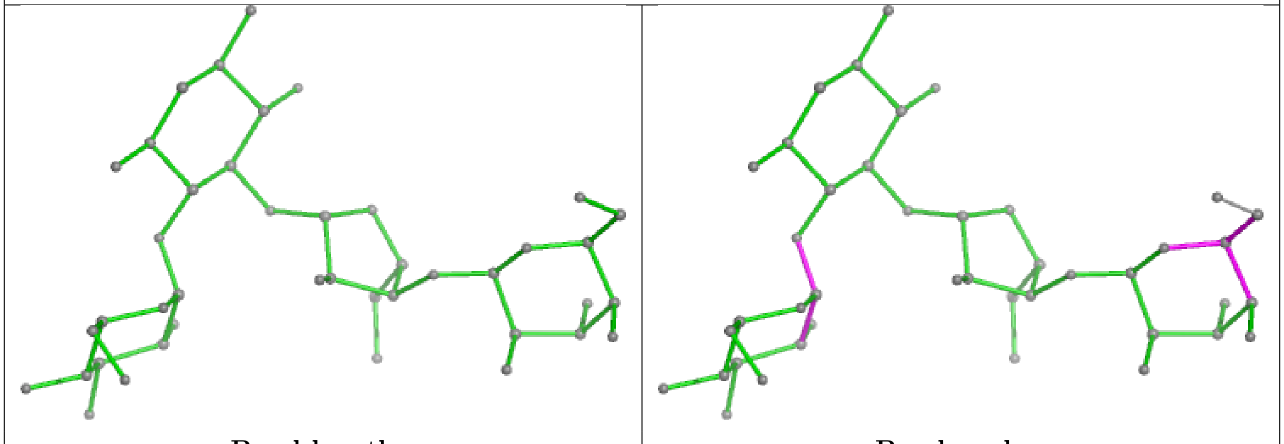
Bond angles



Torsions

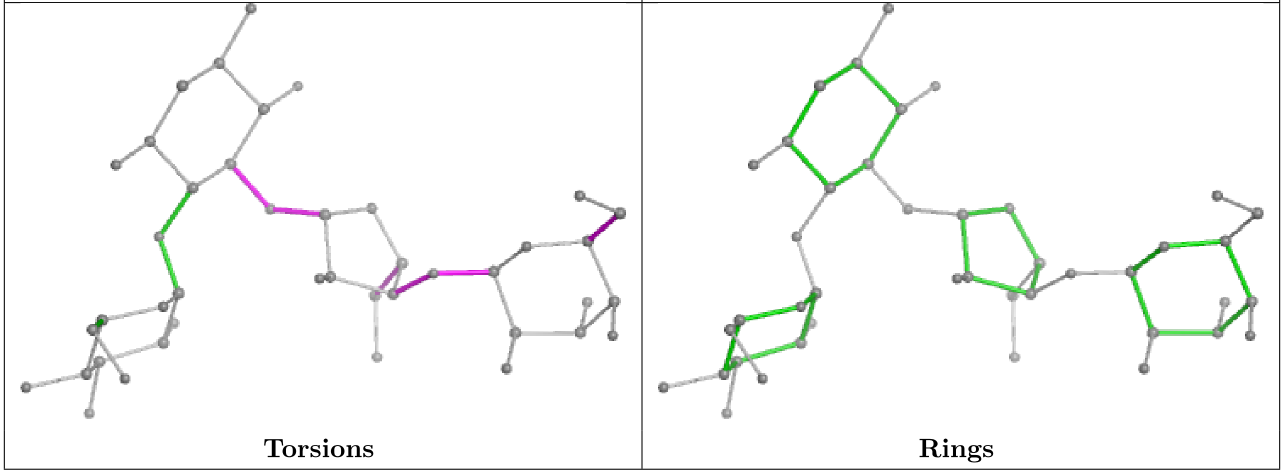
Rings

Ligand PAR 1 3425



Bond lengths

Bond angles



Torsions

Rings

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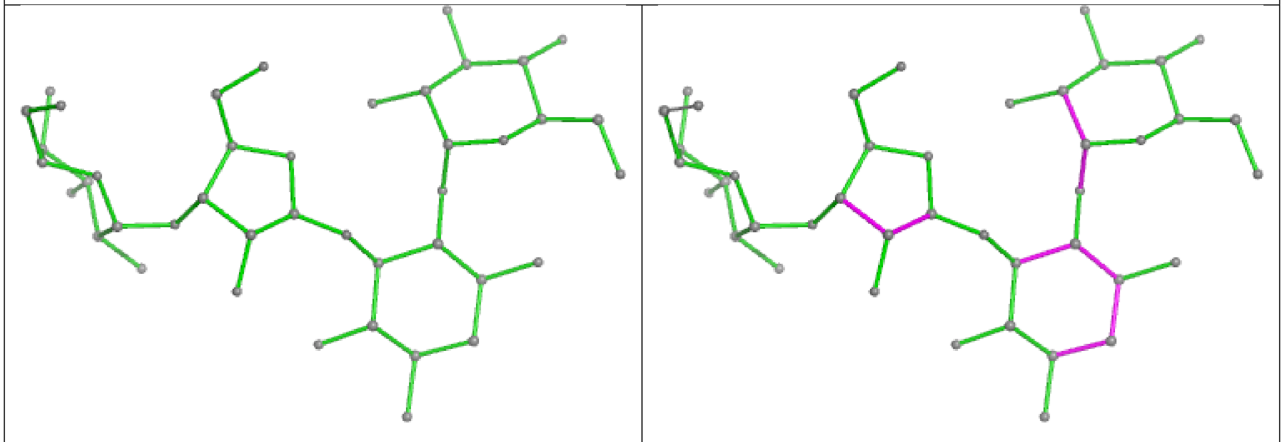
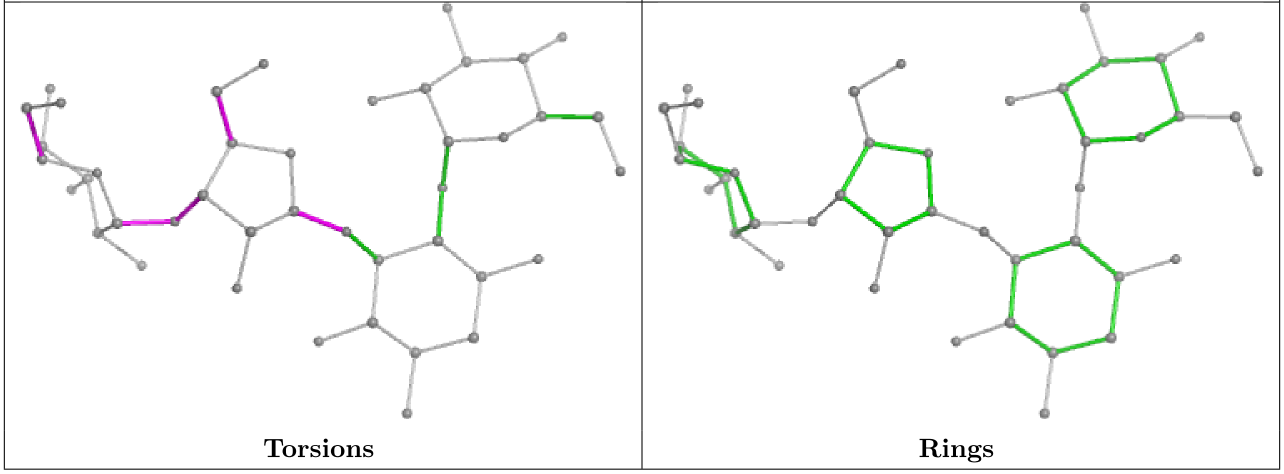


Bond lengths

Bond angles



Torsions

Rings

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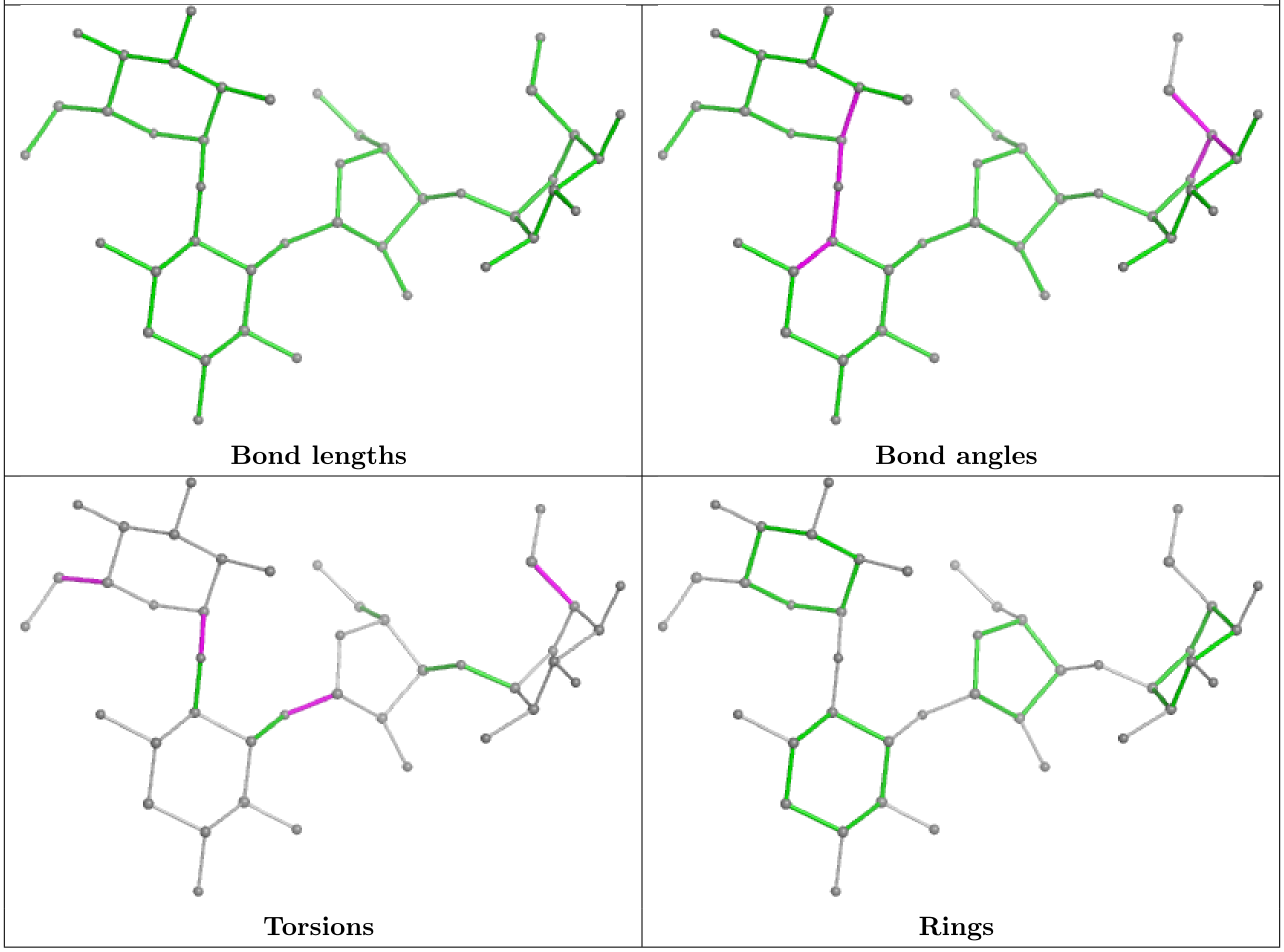


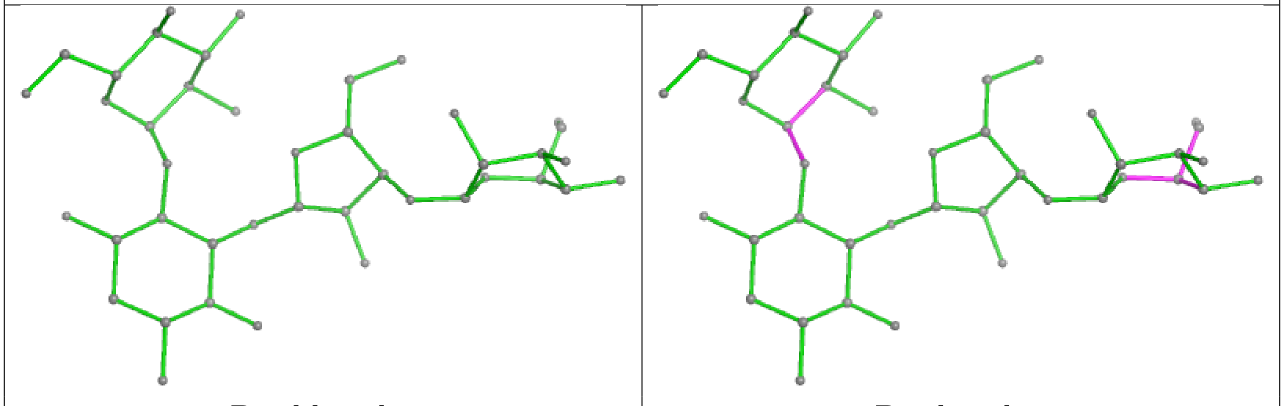
Bond lengths

Bond angles

Torsions

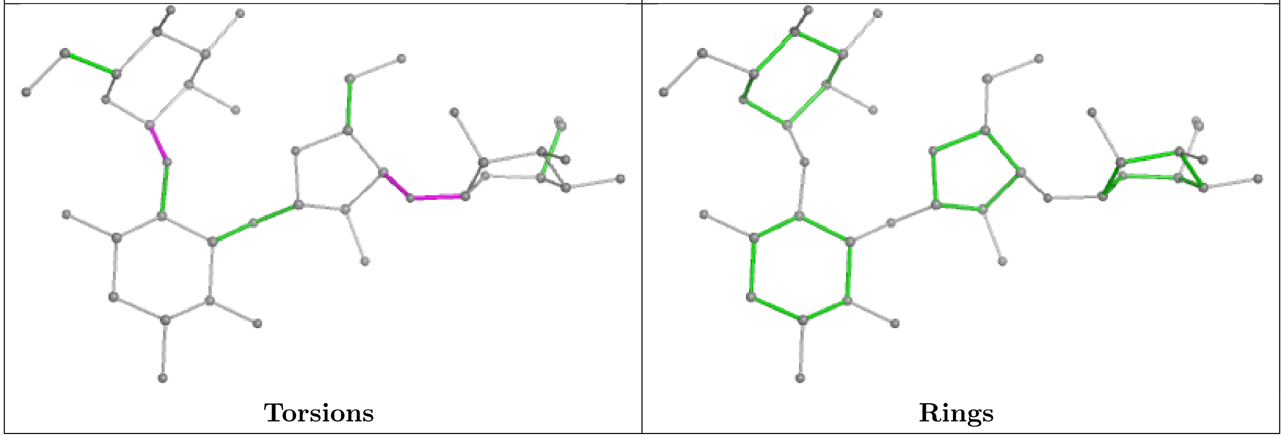
Rings

Ligand PAR 1 3408



Bond lengths

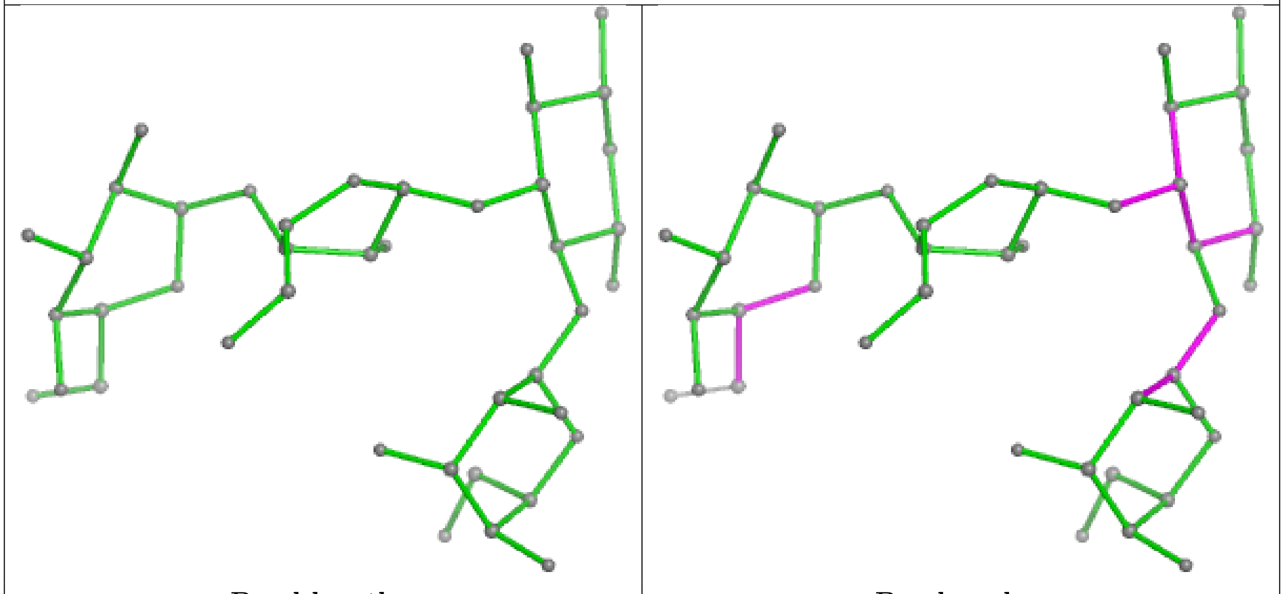
Bond angles



Torsions

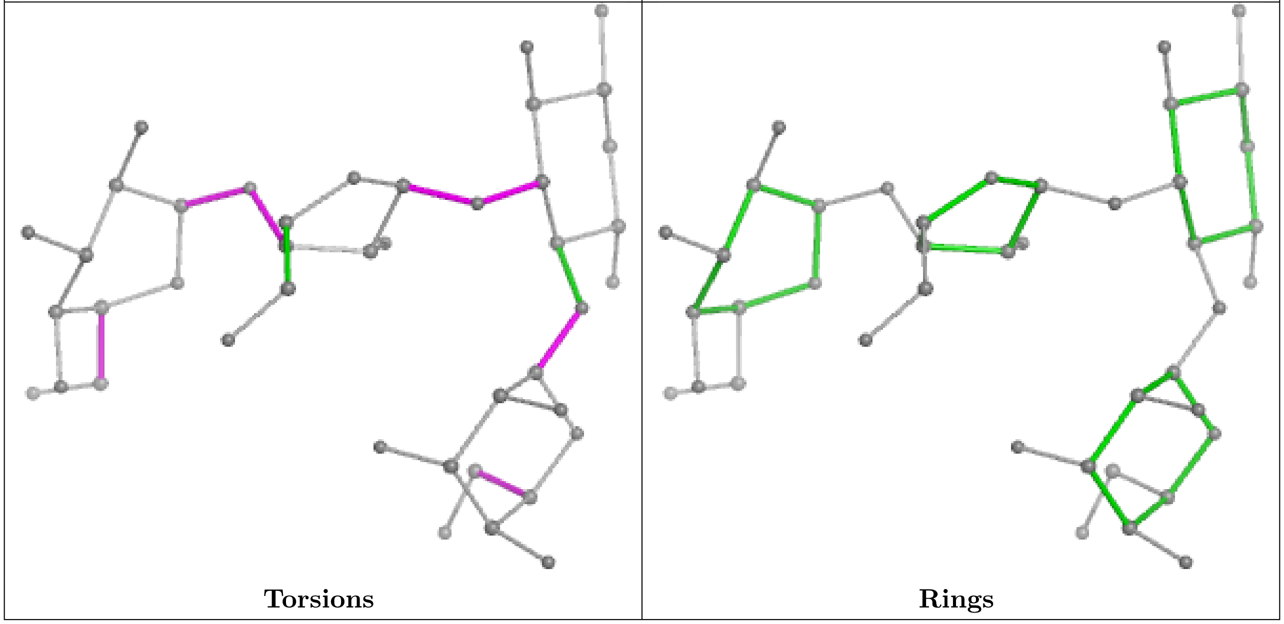
Rings

Ligand PAR B 1805



Bond lengths

Bond angles



Torsions

Rings

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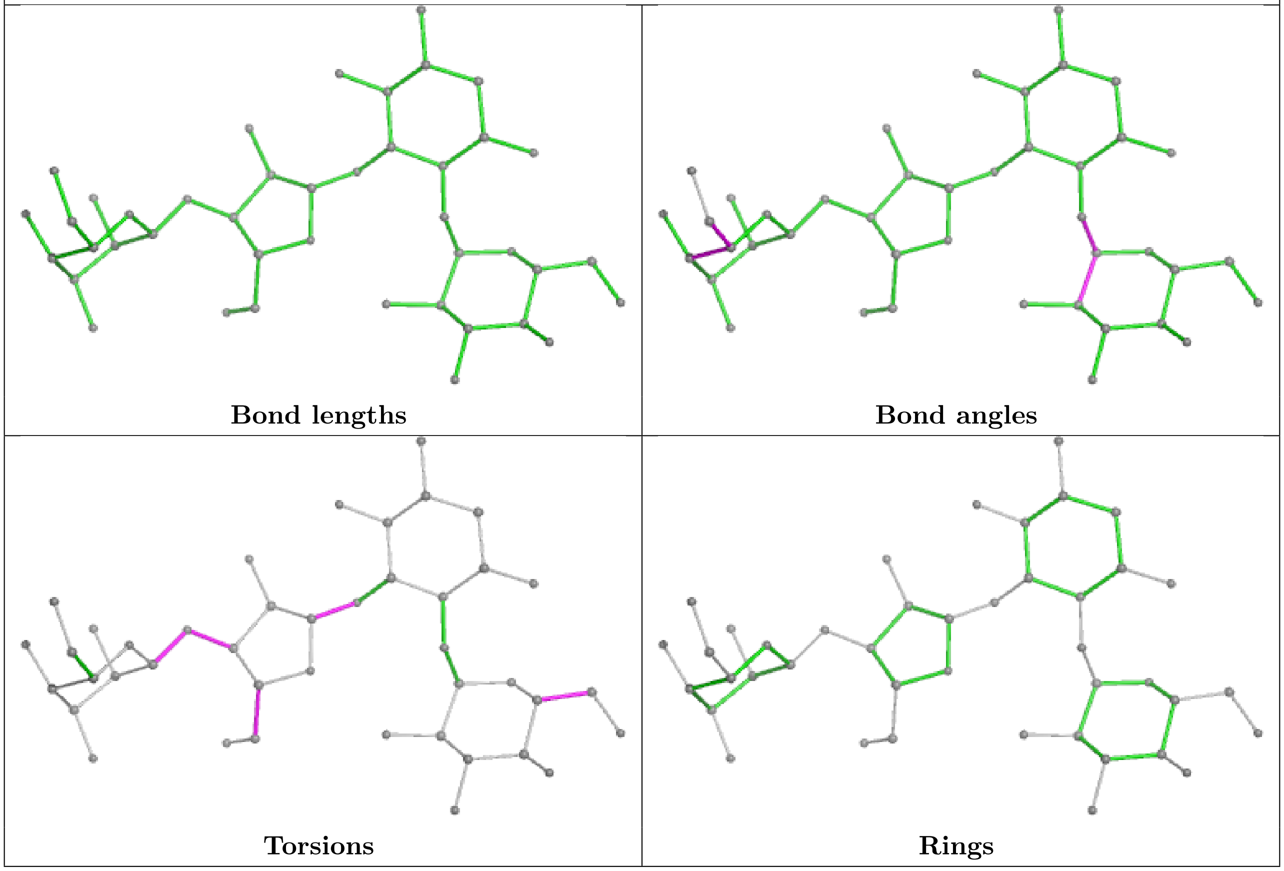


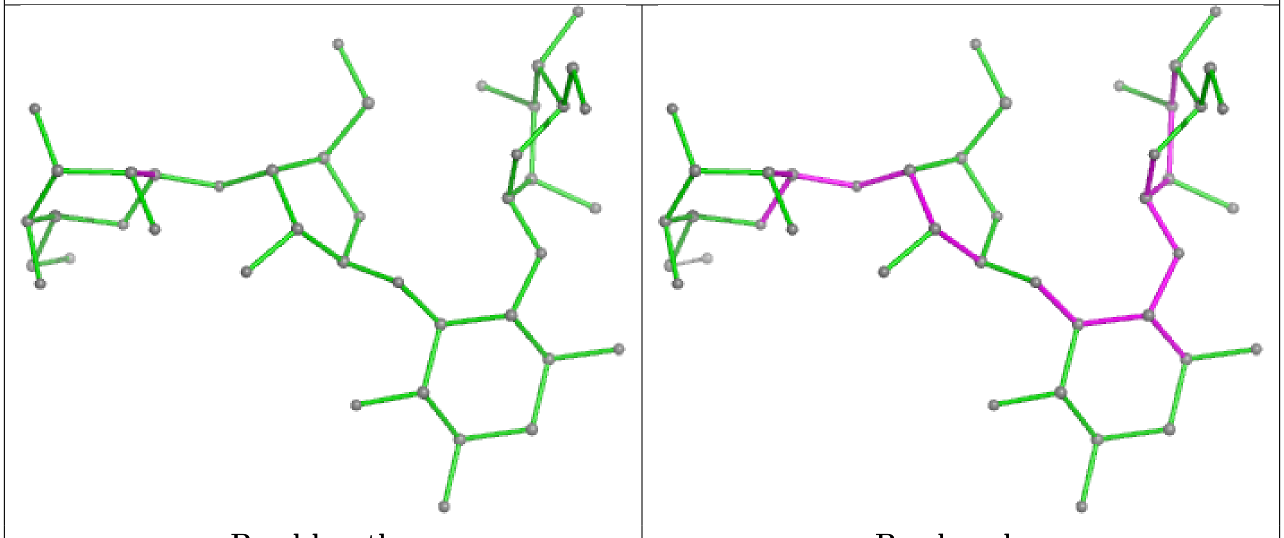
Bond lengths

Bond angles

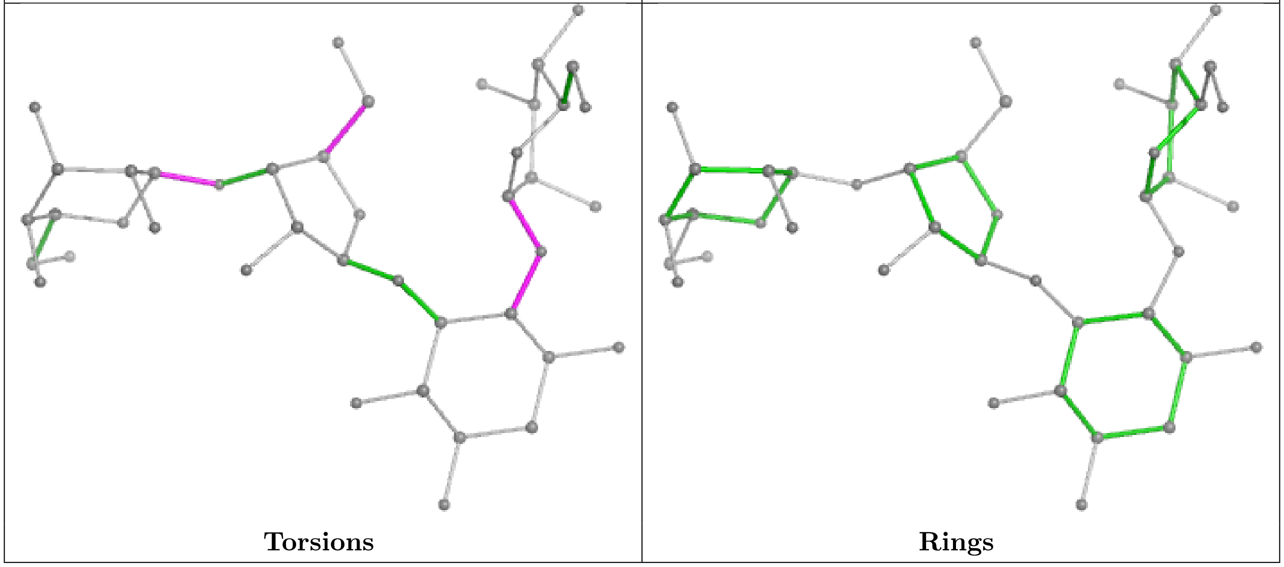
Torsions

Rings

Ligand PAR 1 3422

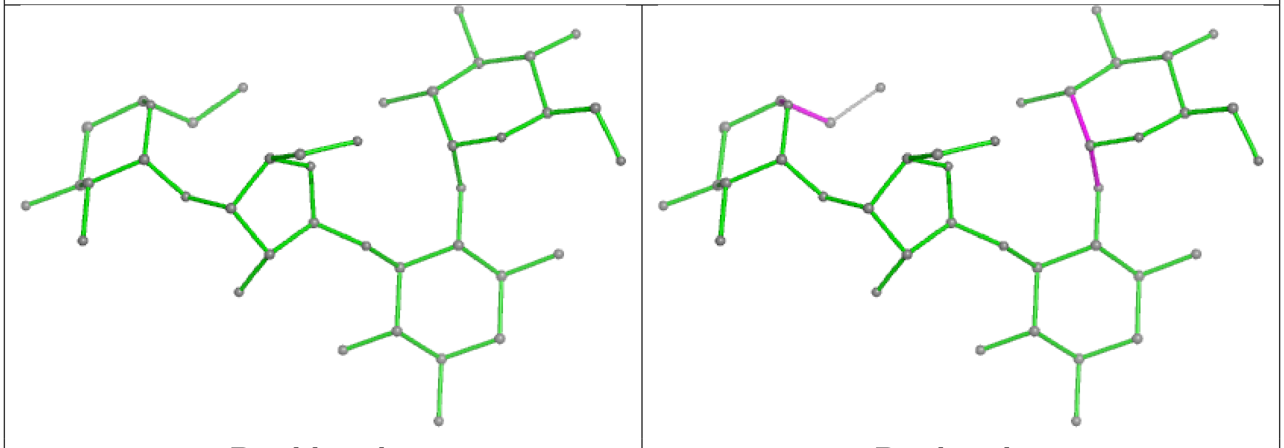


Bond lengths **Bond angles**

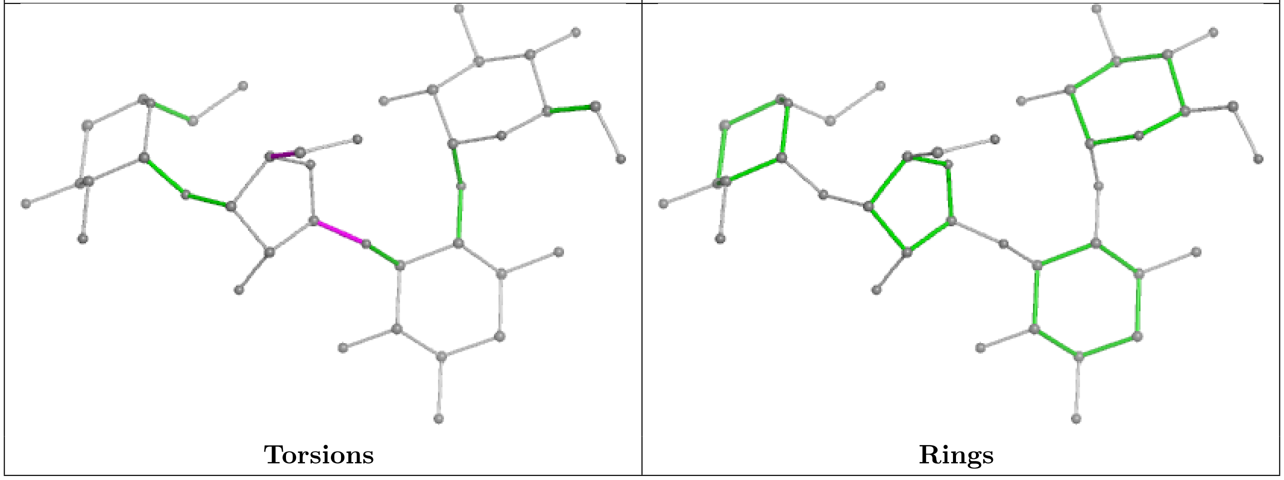


Torsions **Rings**

Ligand PAR 1 3429

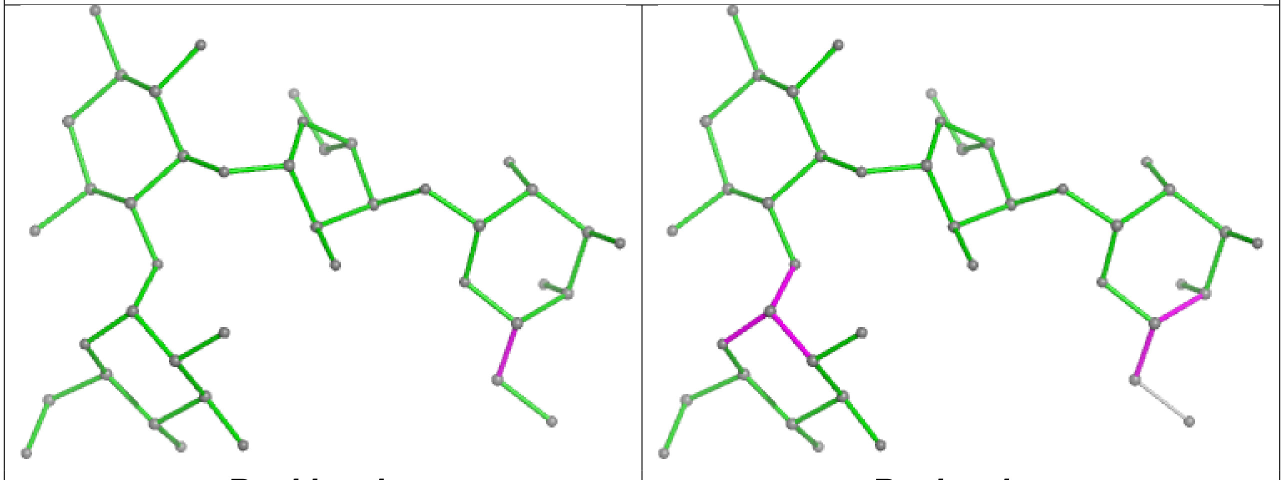


Bond lengths **Bond angles**



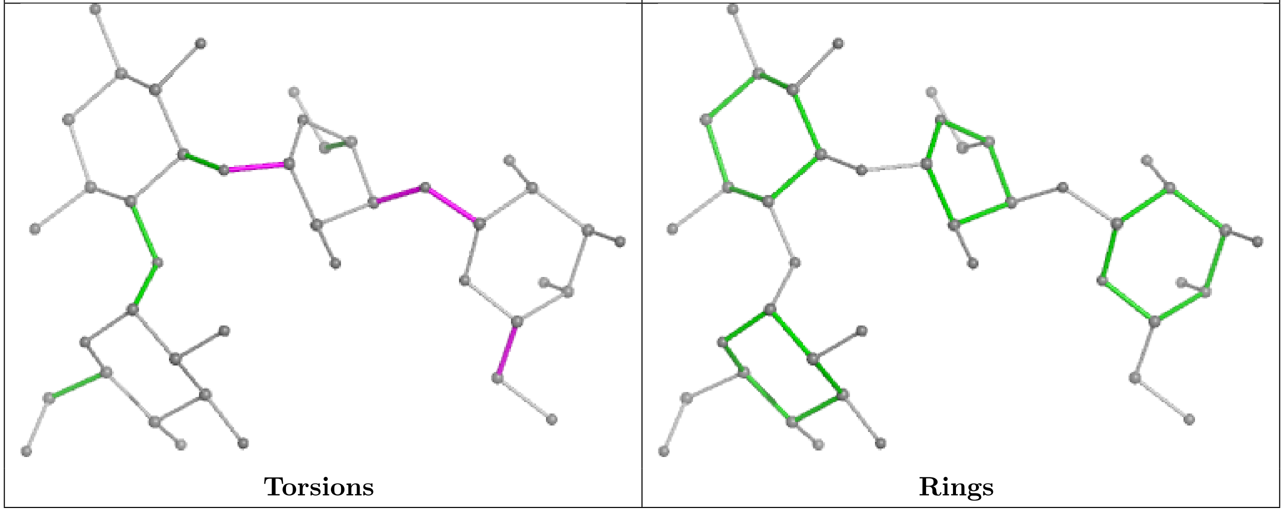
Torsions **Rings**

Ligand PAR CM 1805



Bond lengths

Bond angles



Torsions

Rings

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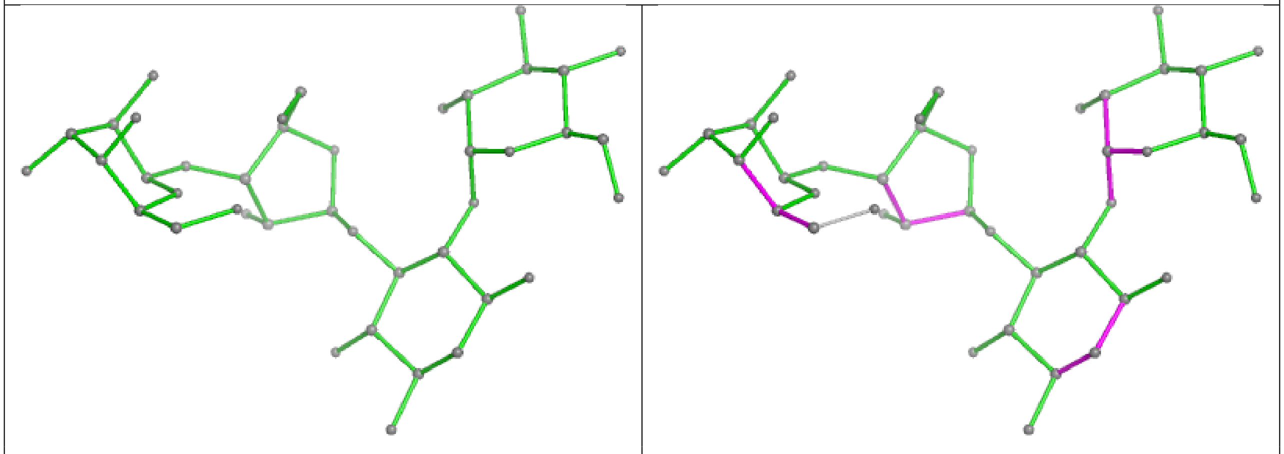

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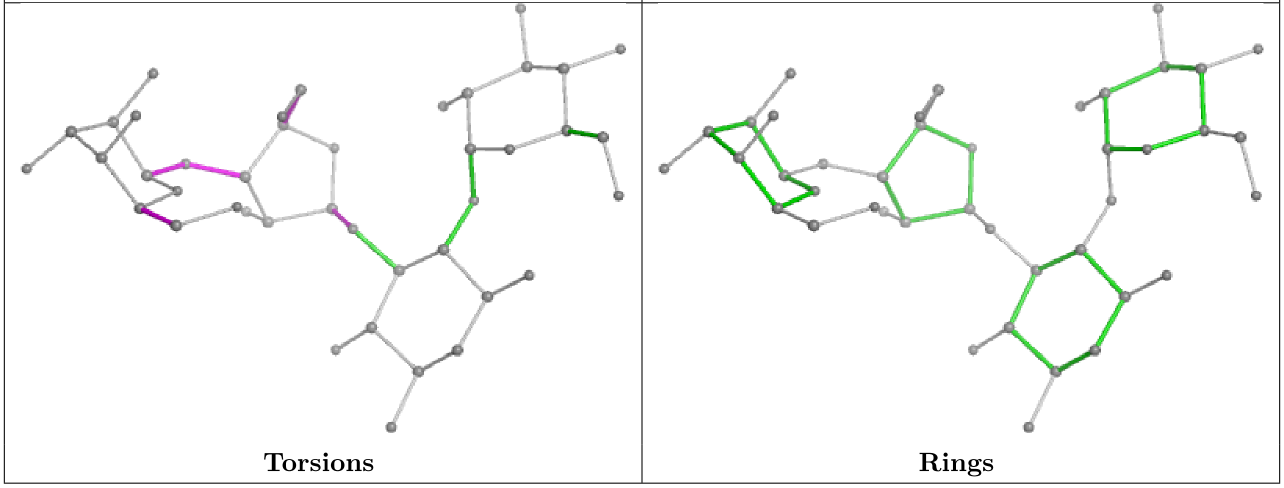

Torsions

Rings

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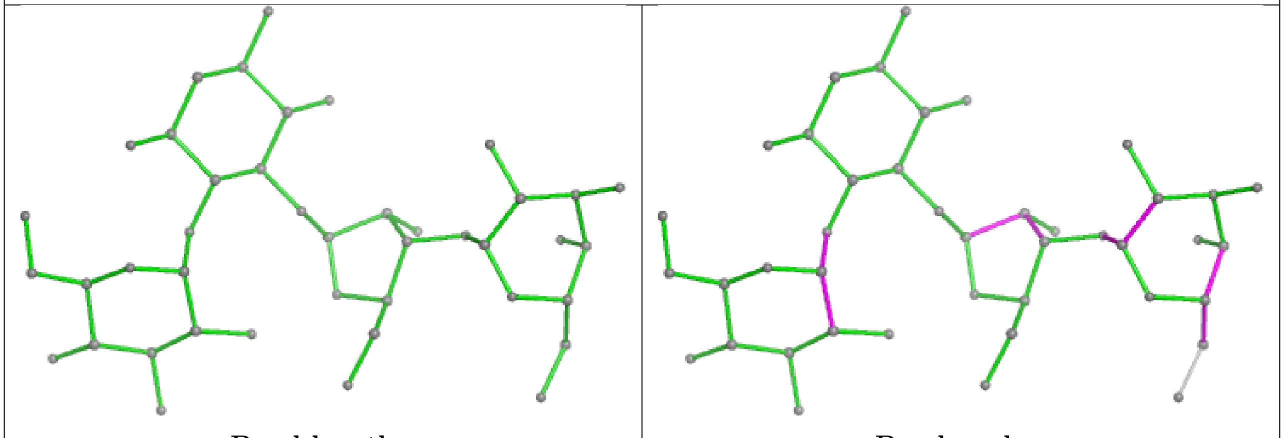
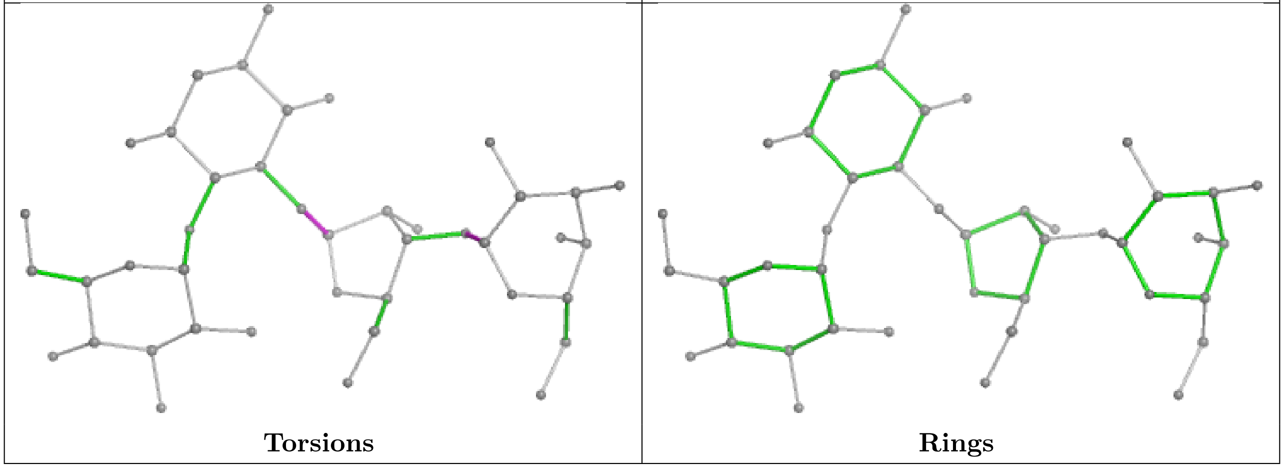


Bond lengths

Bond angles



Torsions

Rings

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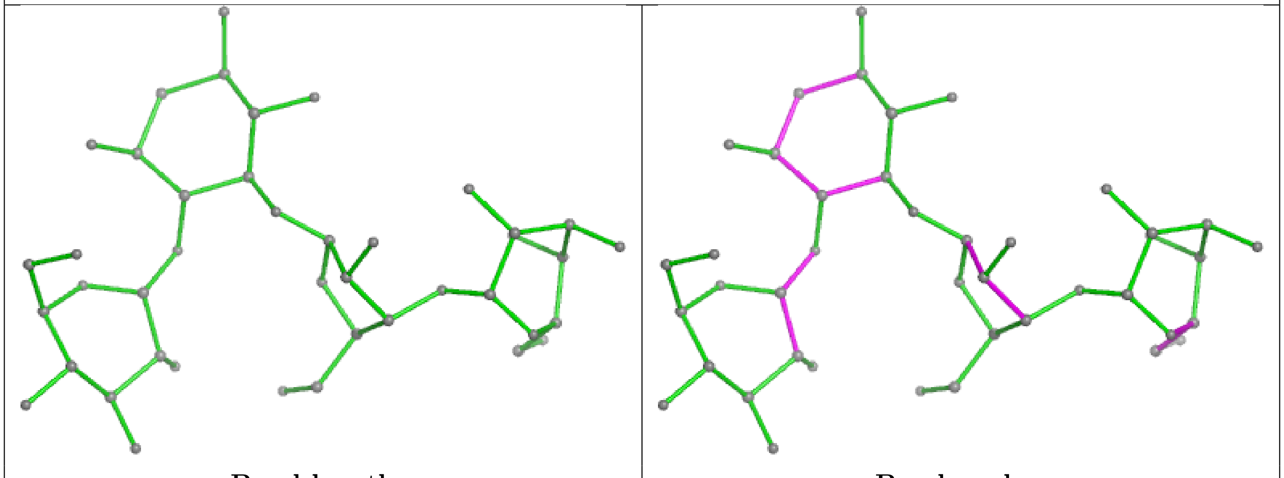

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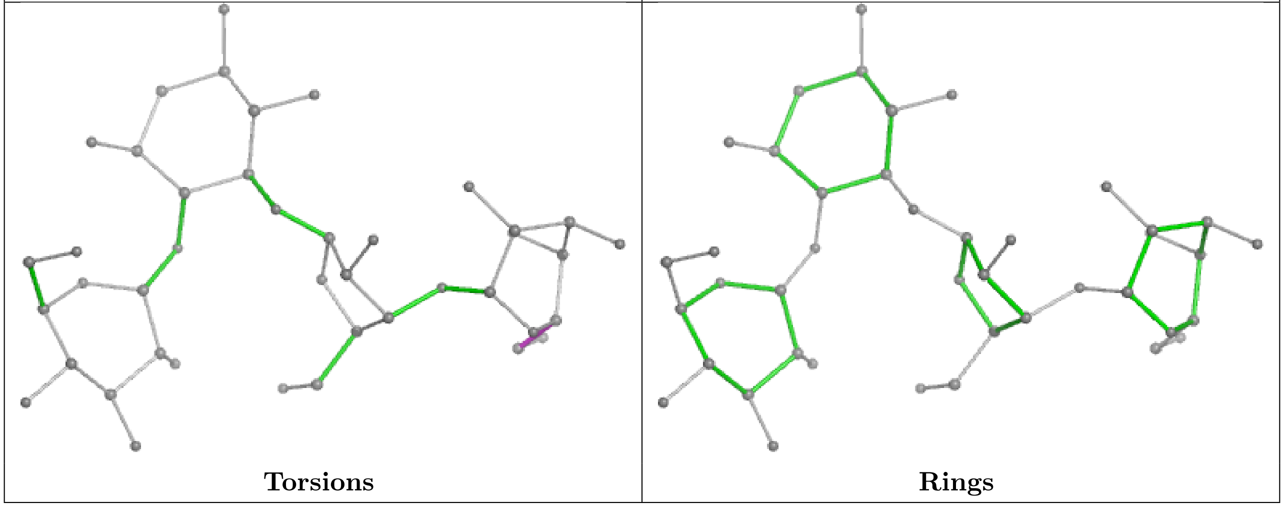

Torsions

Rings

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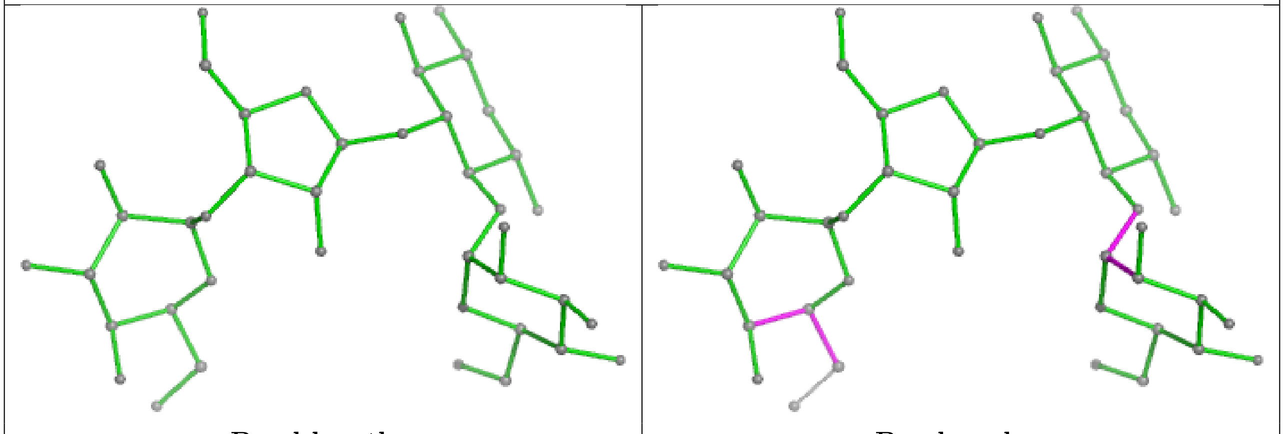

Bond lengths

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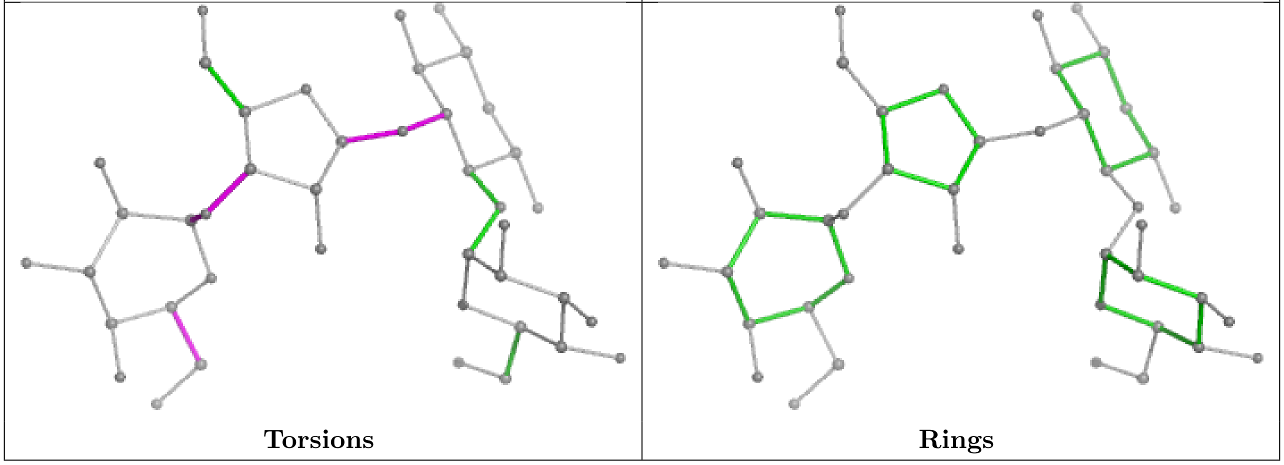

Torsions

Rings

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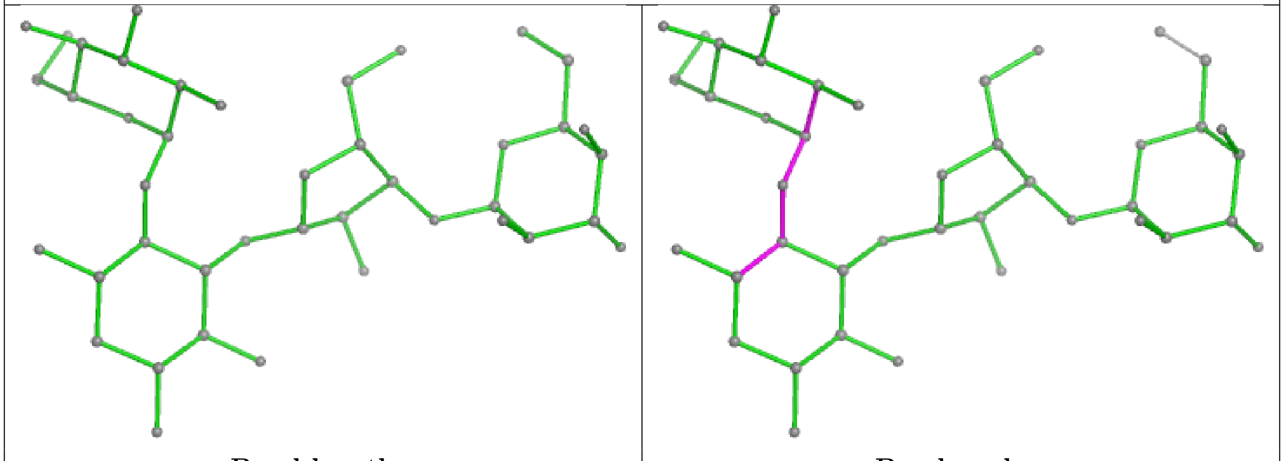
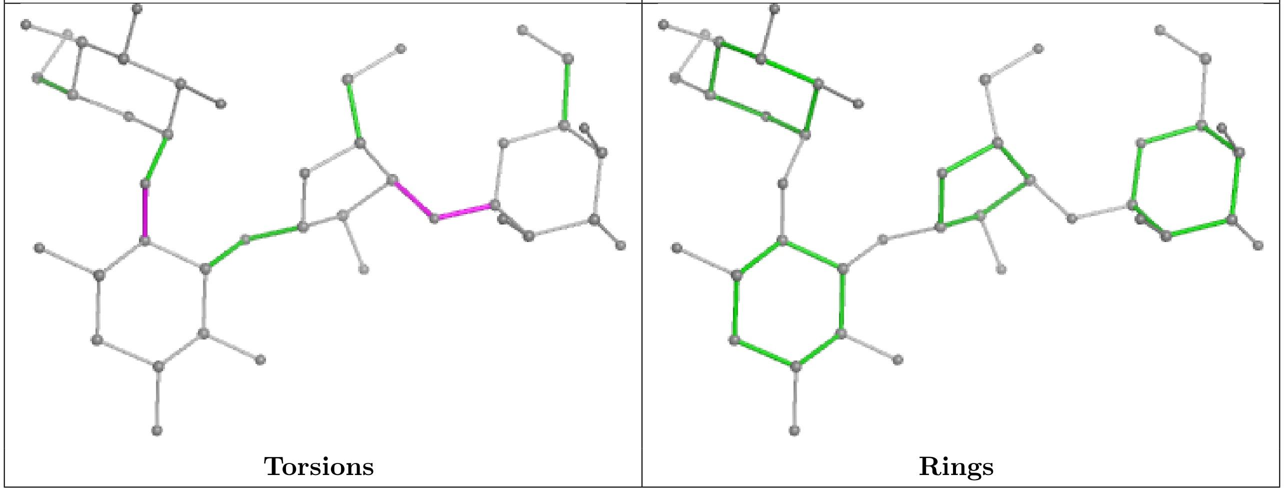
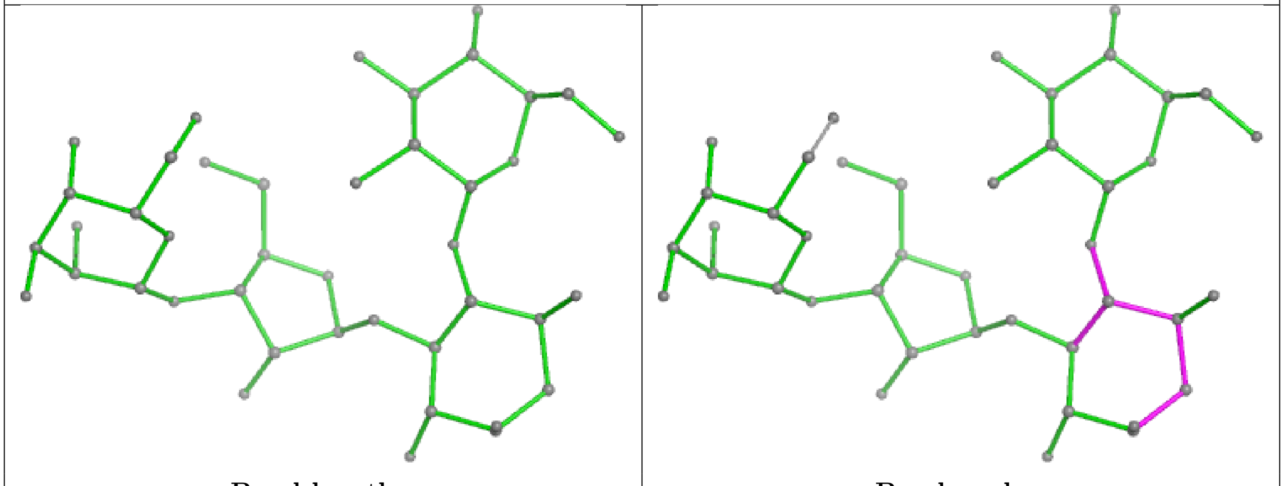


Bond lengths **Bond angles**

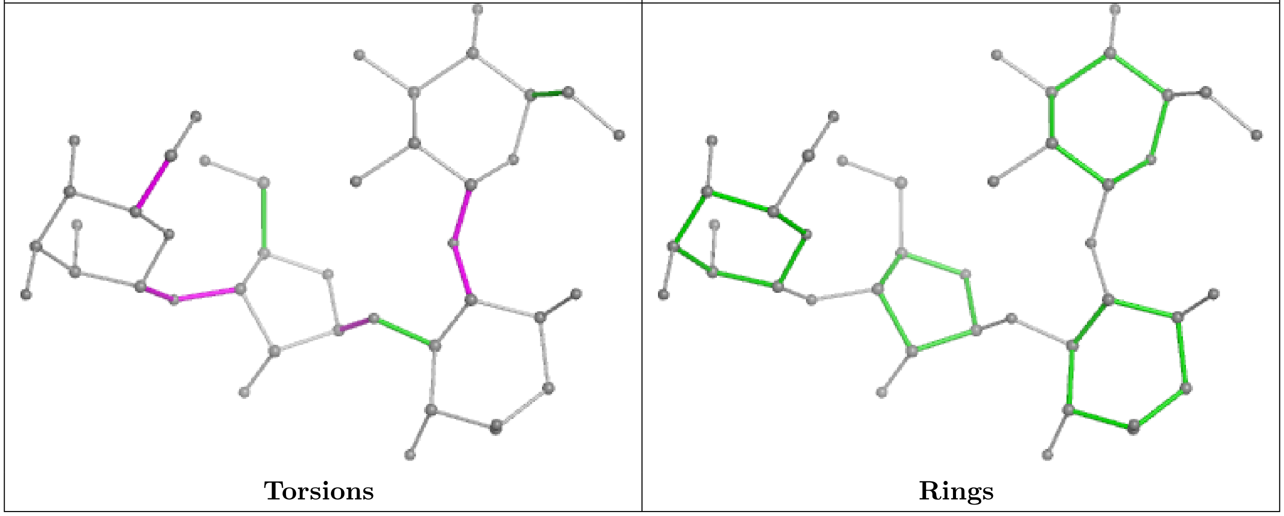


Torsions **Rings**

Ligand PAR B 1804

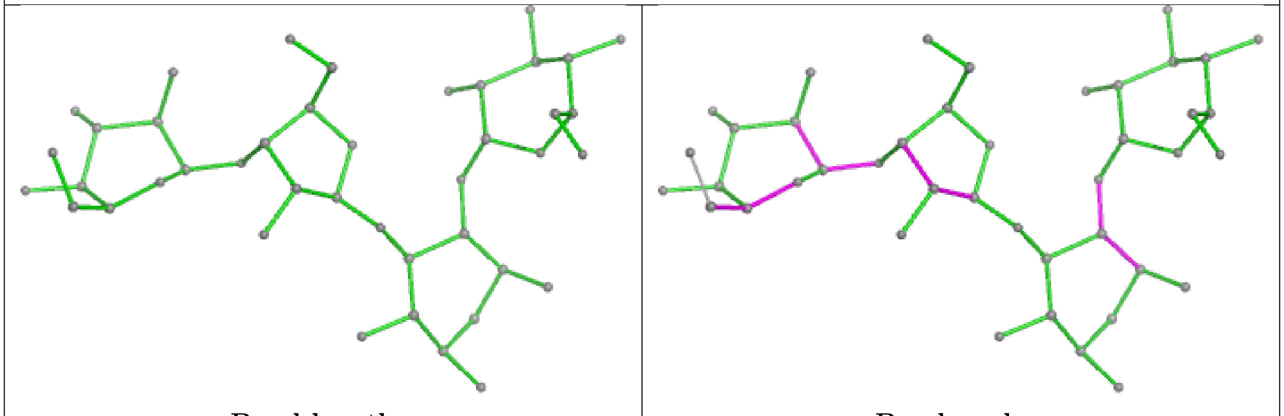


Bond lengths **Bond angles**



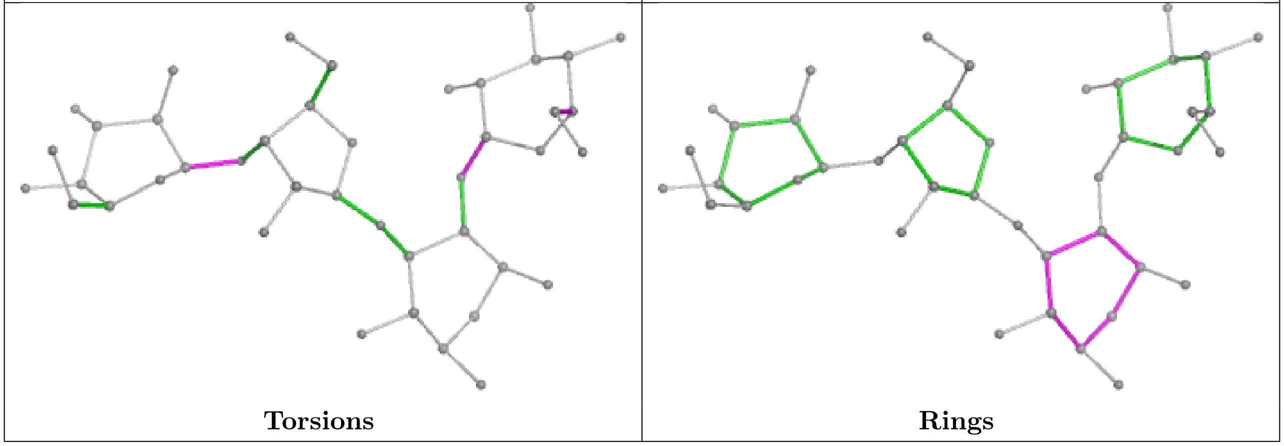
Torsions **Rings**

Ligand PAR AS 3407



Bond lengths

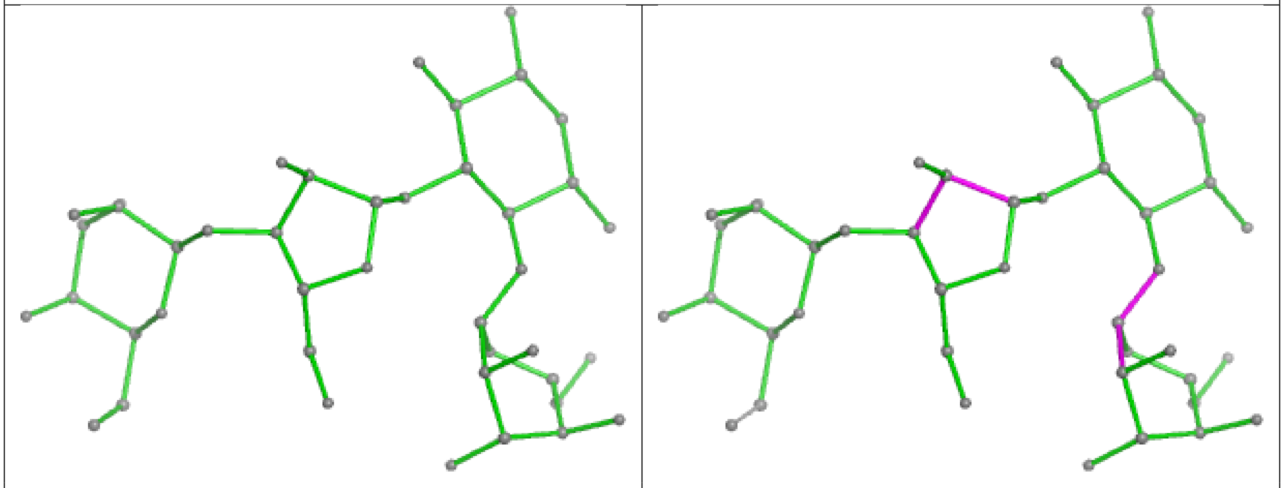
Bond angles



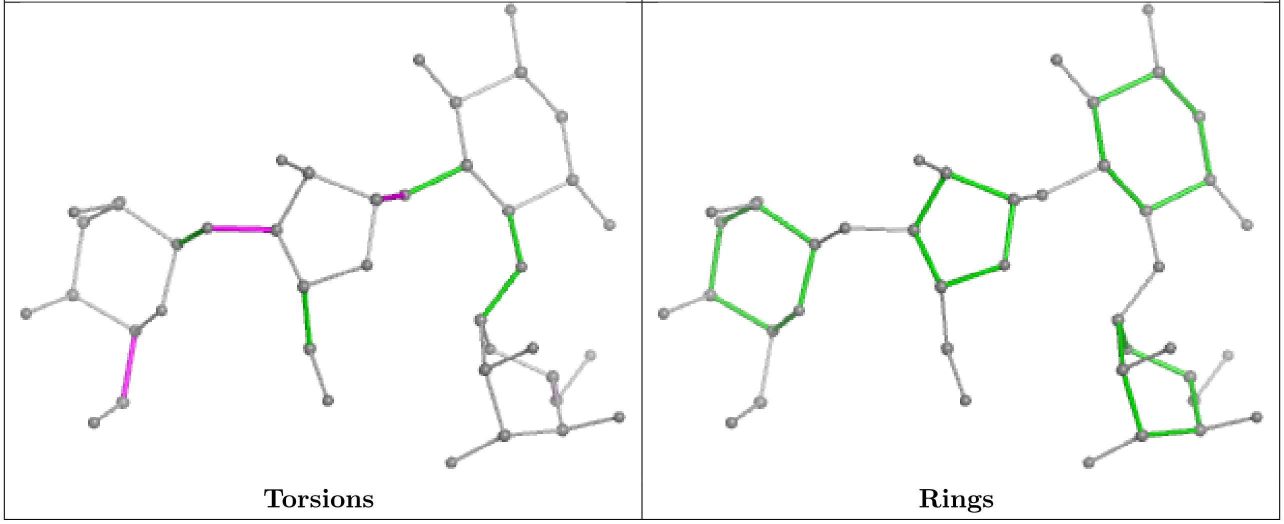
Torsions

Rings

Ligand PAR CM 1802

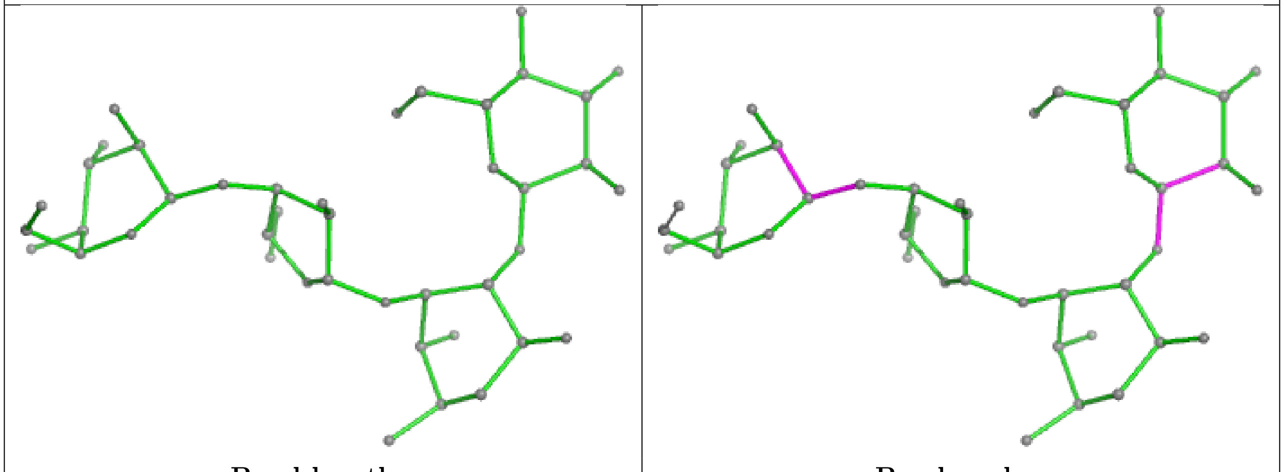


Bond lengths **Bond angles**



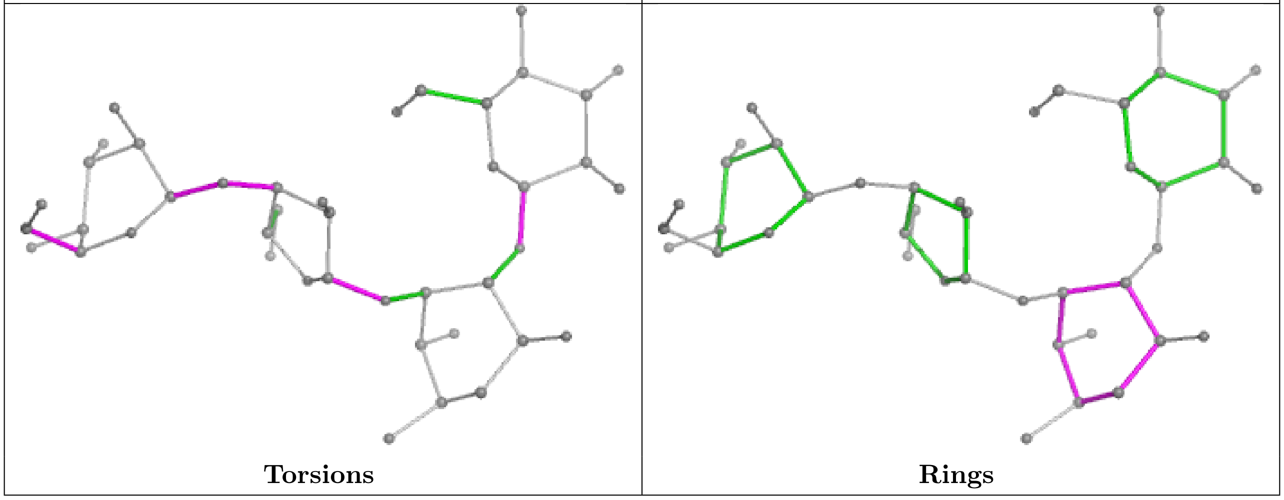
Torsions **Rings**

Ligand PAR 1 3403



Bond lengths

Bond angles



Torsions

Rings

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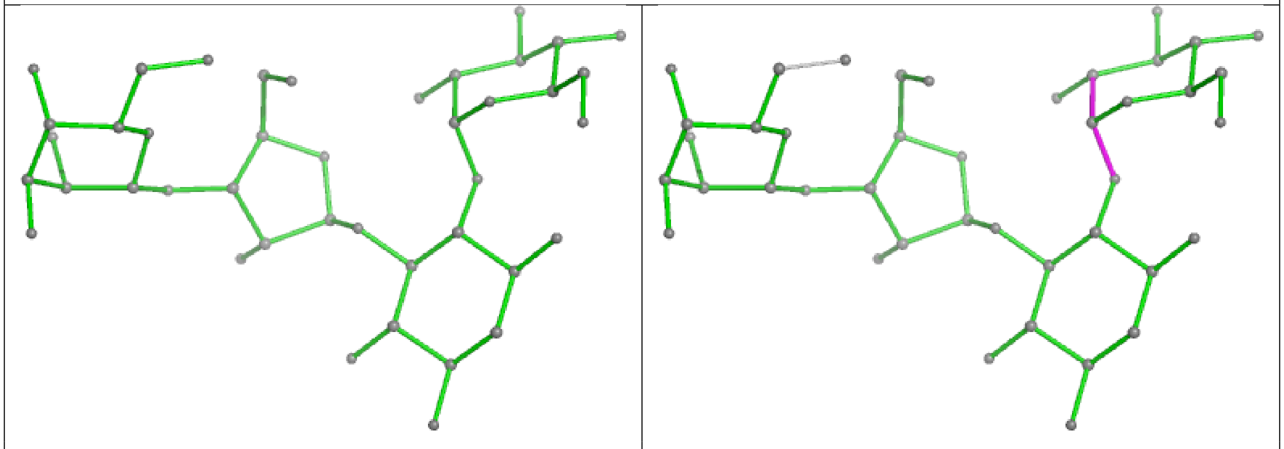

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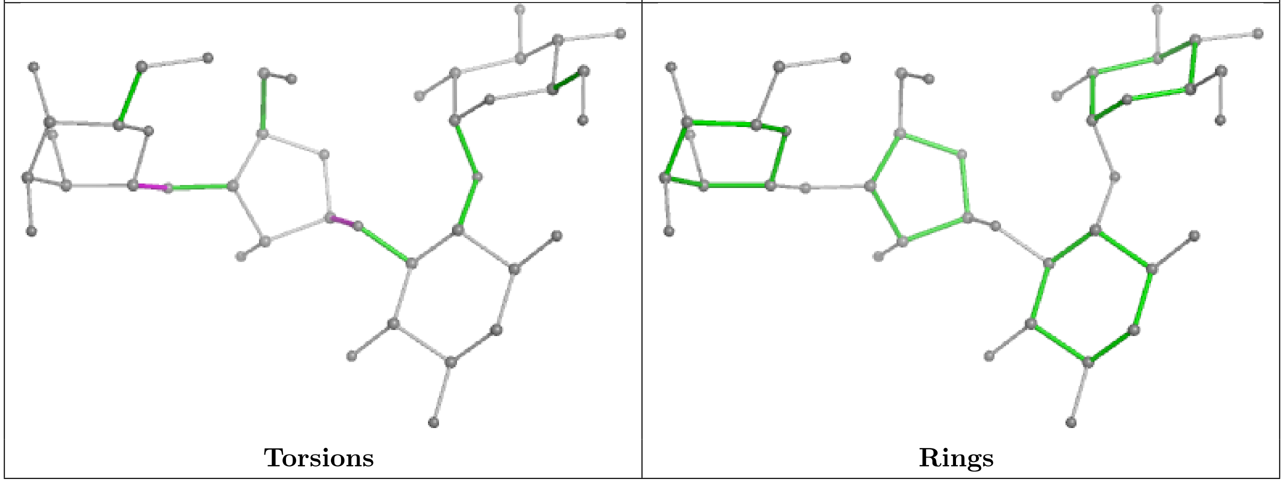
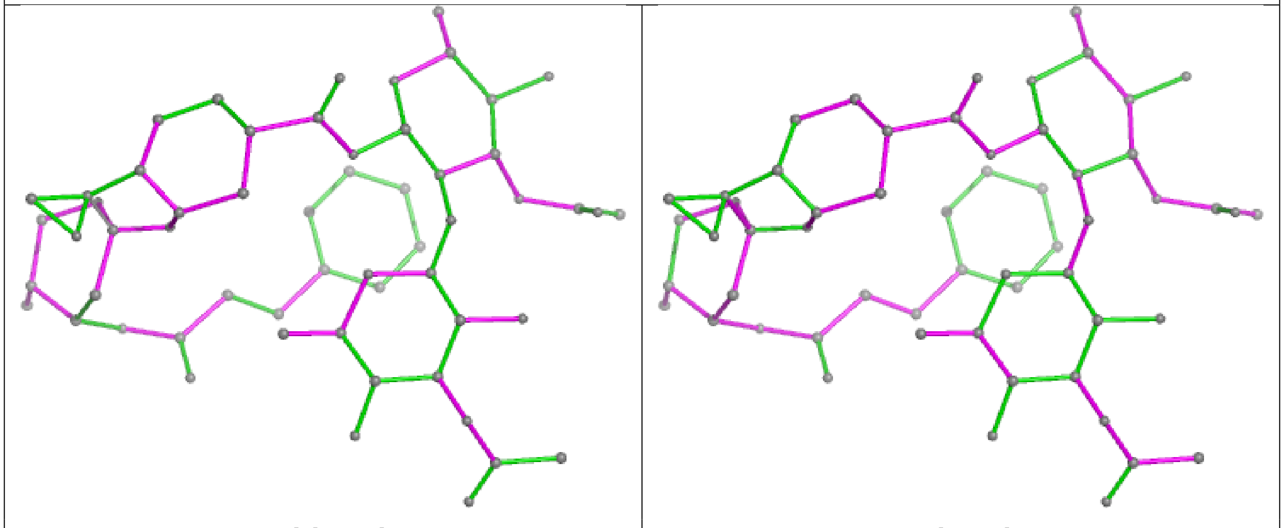


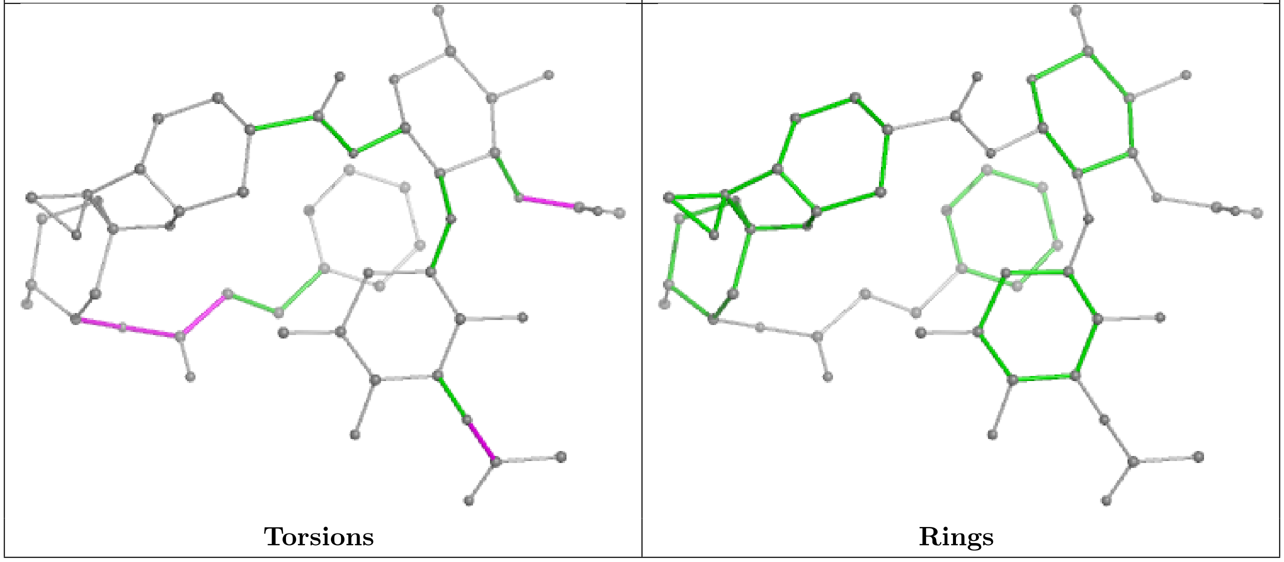
Torsions **Rings**

Ligand 3K5 1 3401



Bond lengths

Bond angles



Torsions

Rings

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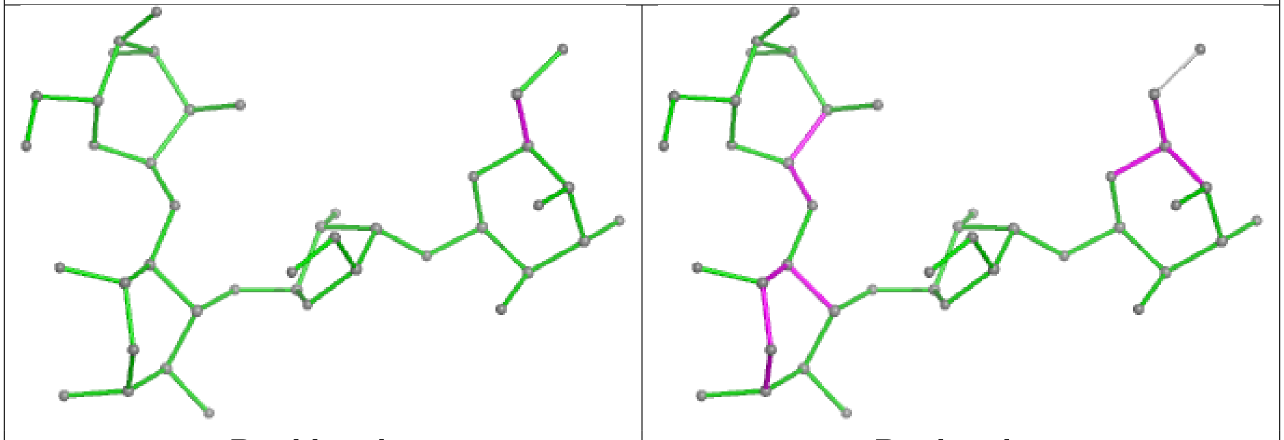
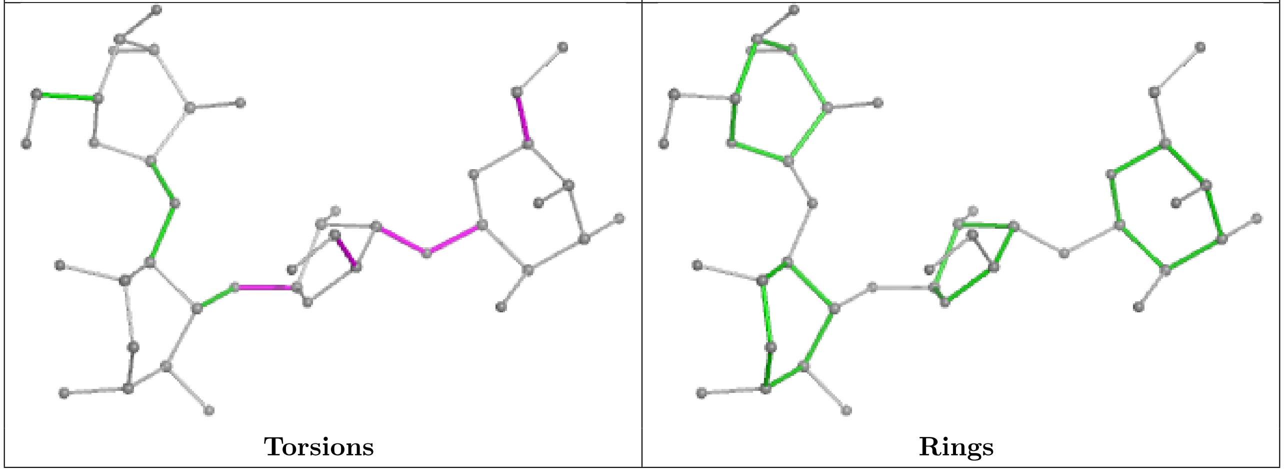


Bond lengths

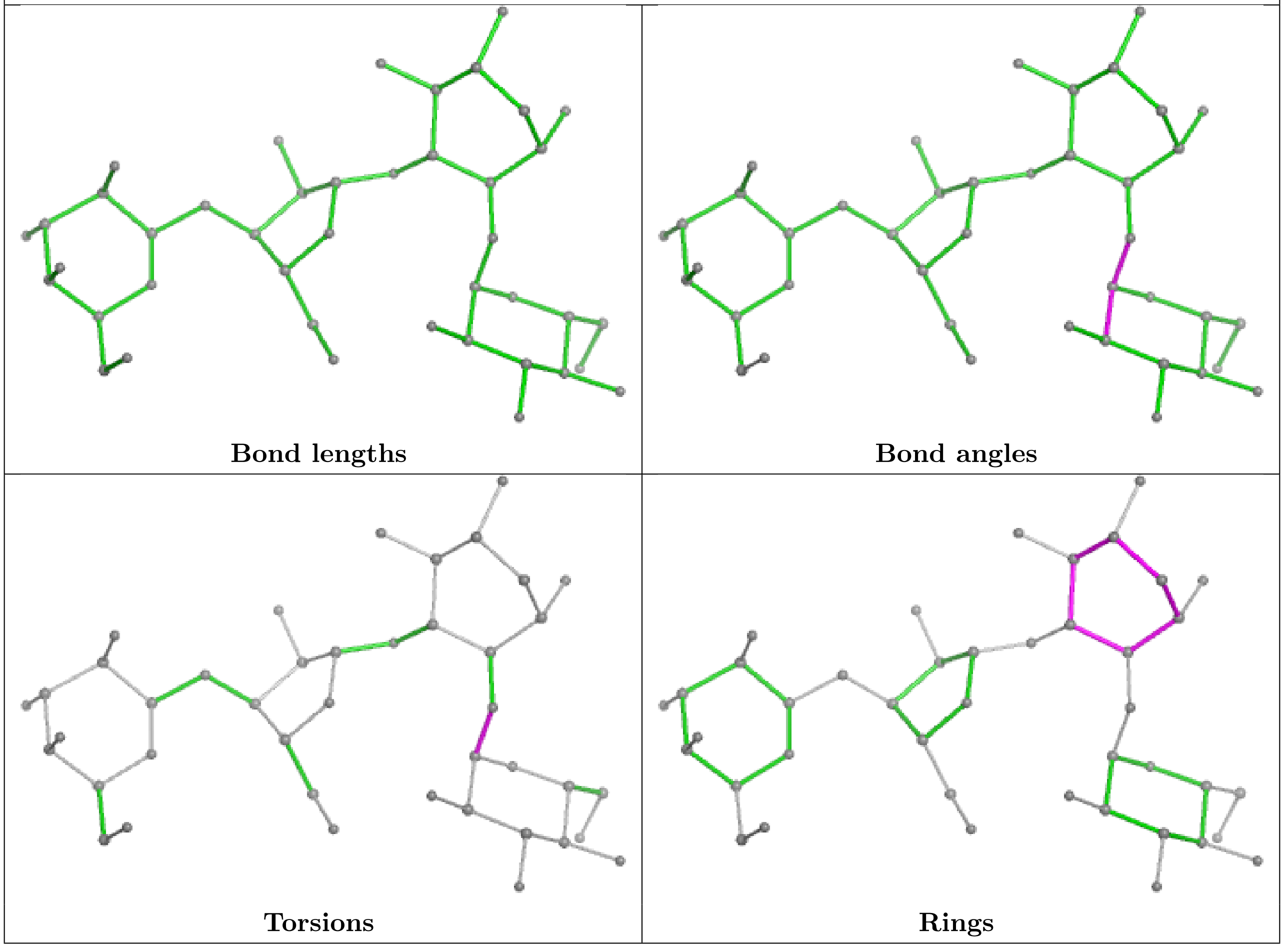
Bond angles



Torsions

Rings

Ligand PAR AS 3405



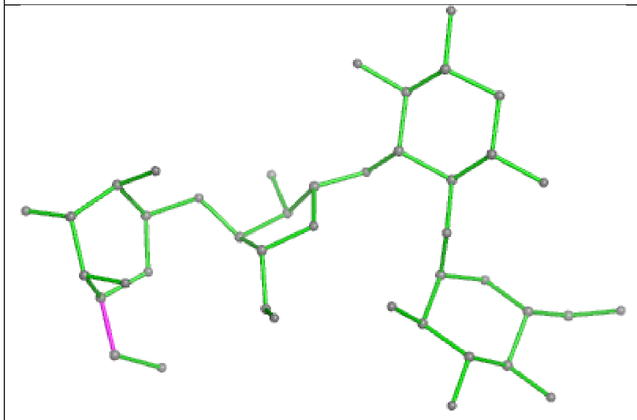
Bond lengths

Bond angles

Torsions

Rings

Ligand PAR CM 1801



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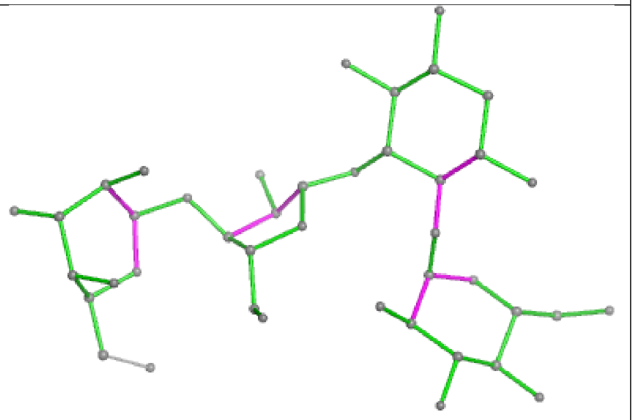

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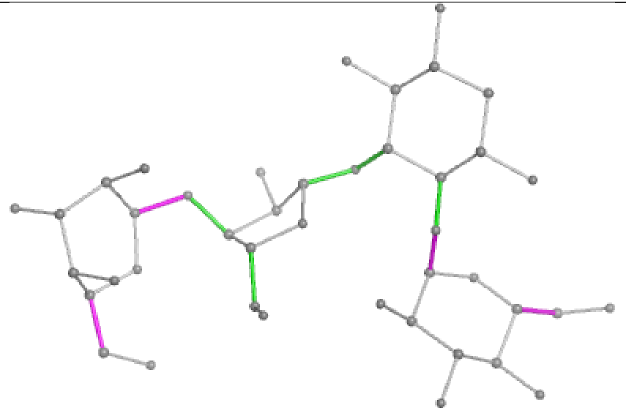
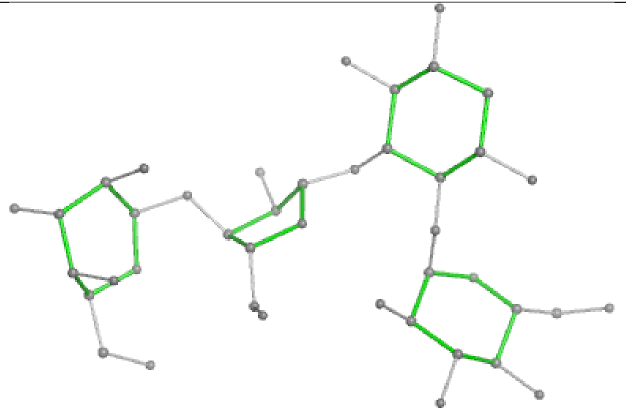
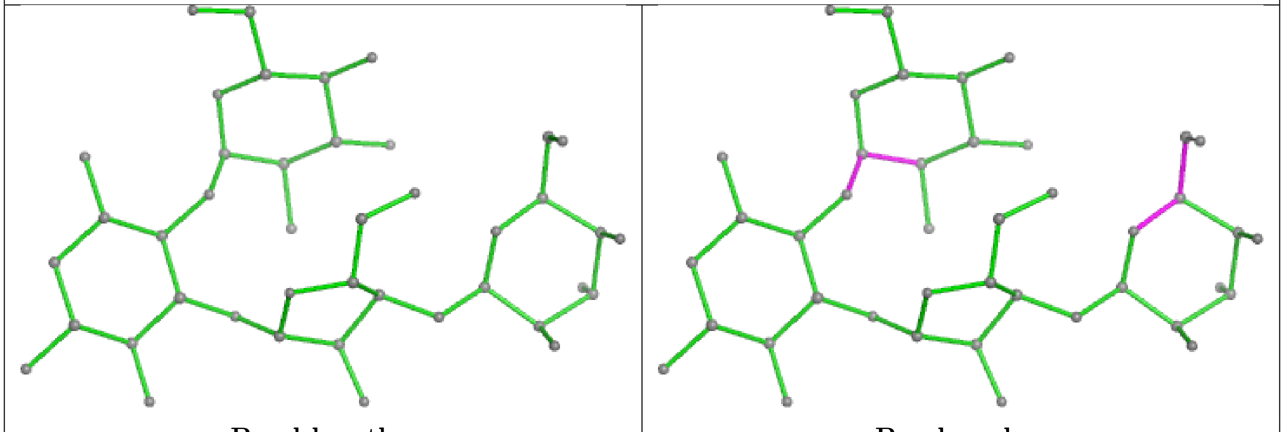


Torsions

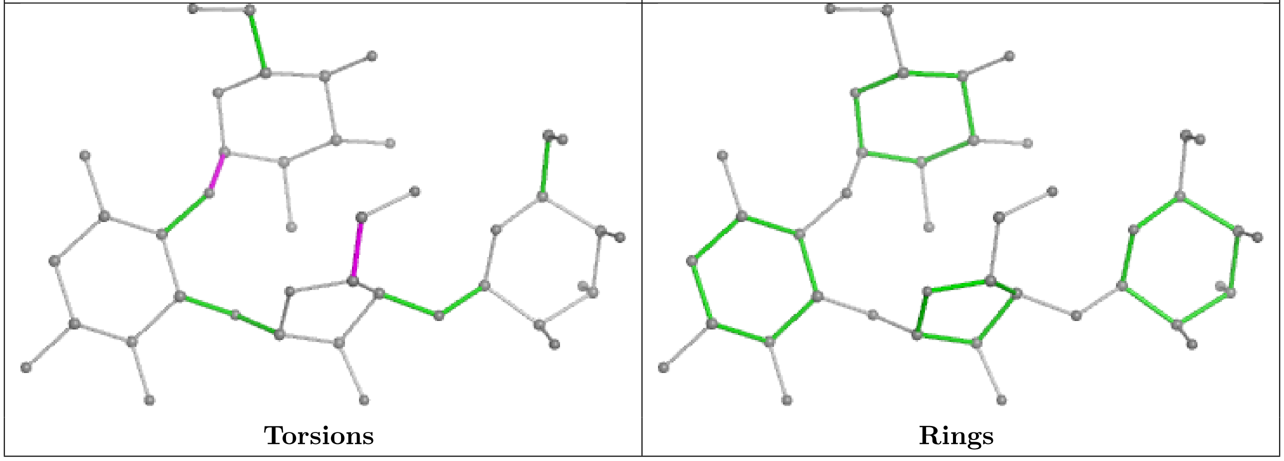


Rings

Ligand PAR 1 3416

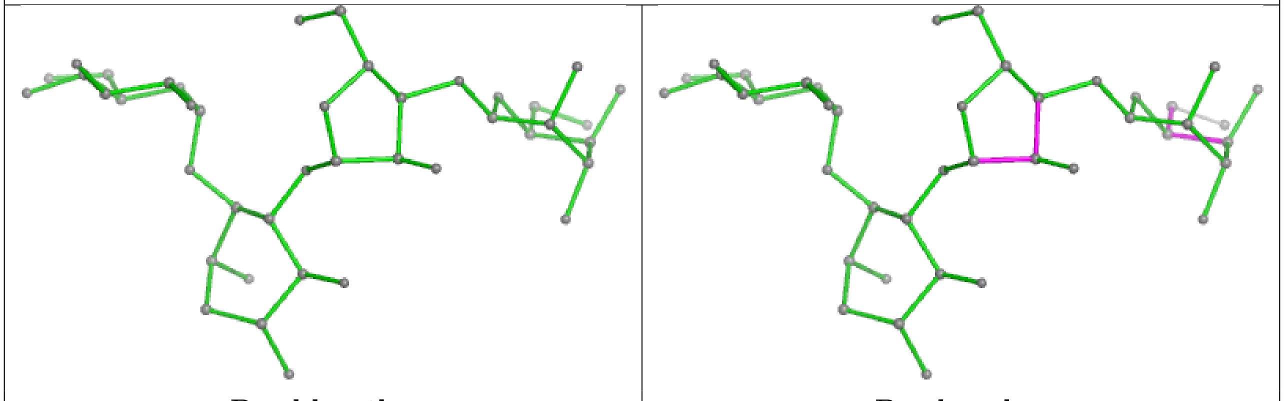


Bond lengths **Bond angles**



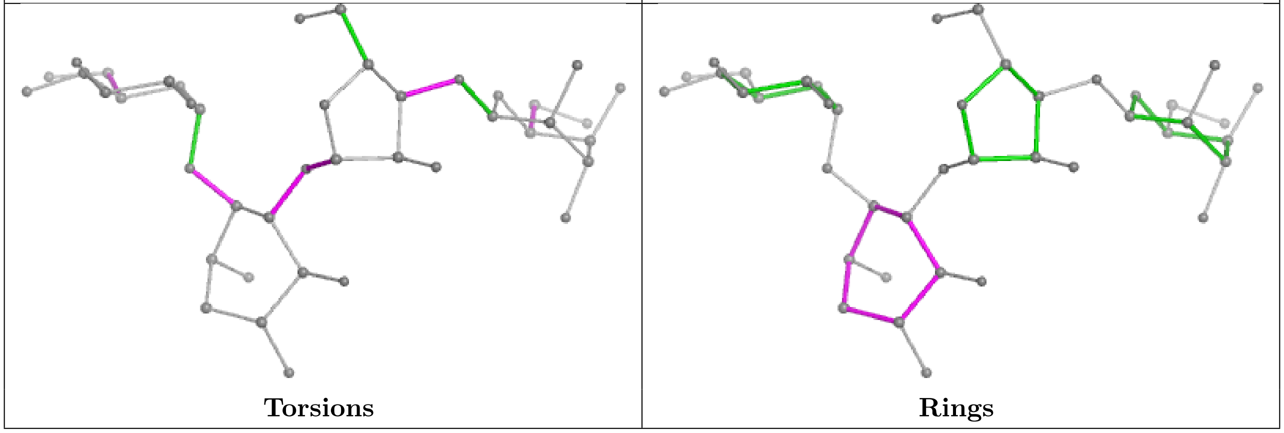
Torsions **Rings**

Ligand PAR 1 3410



Bond lengths

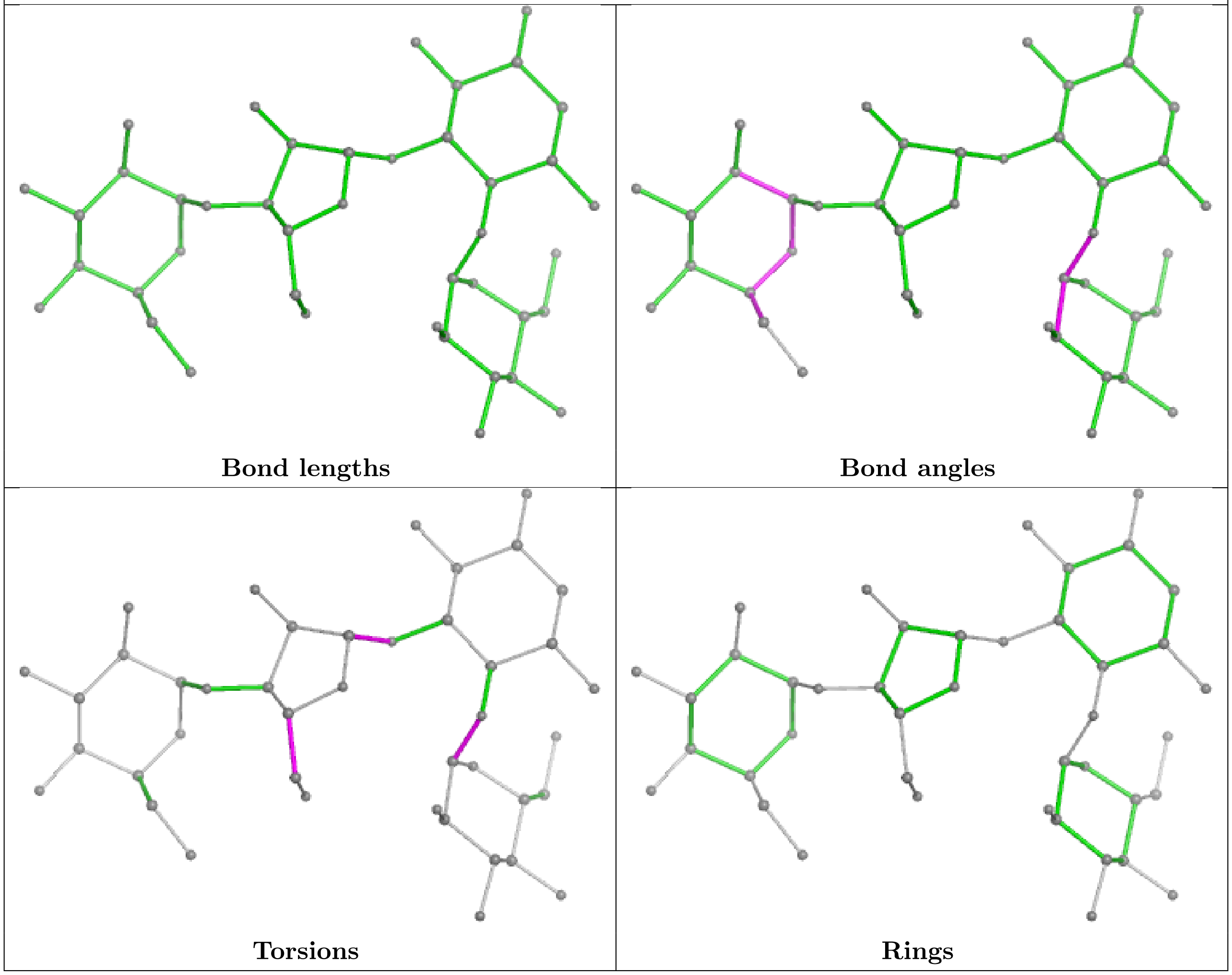
Bond angles



Torsions

Rings

Ligand PAR 4 202



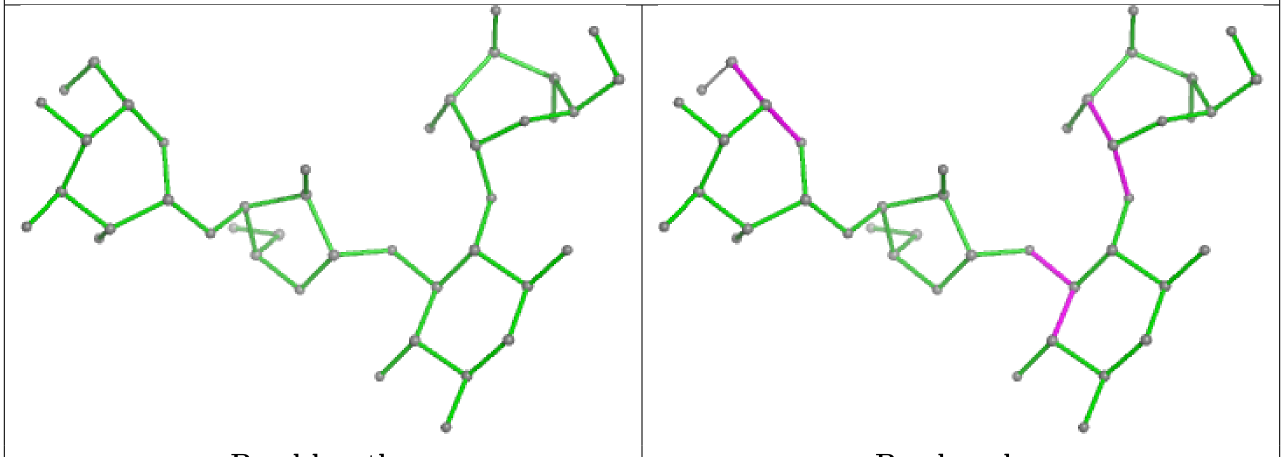
Bond lengths

Bond angles

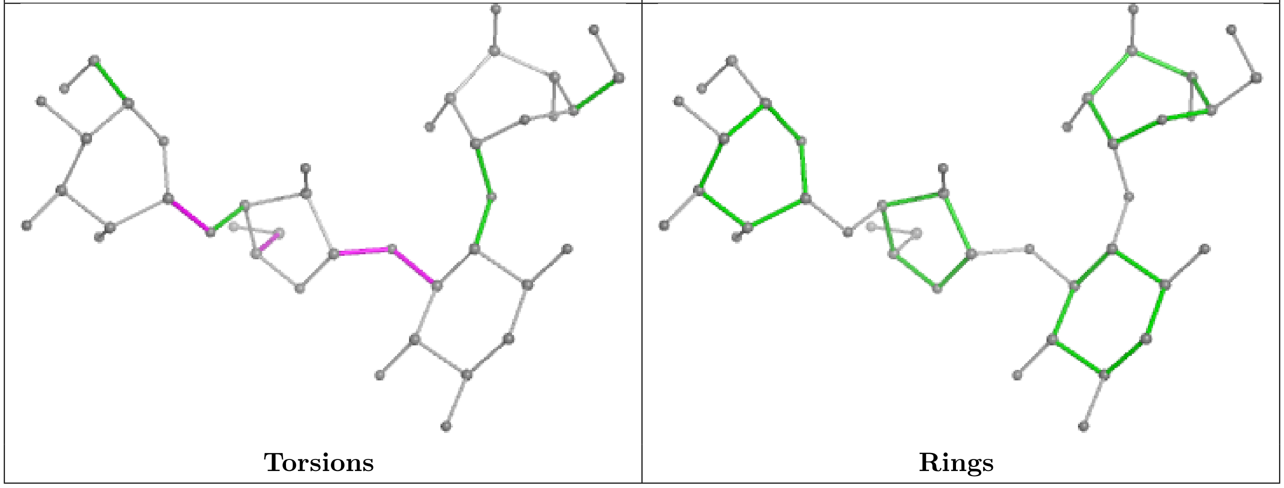
Torsions

Rings

Ligand PAR 1 3409

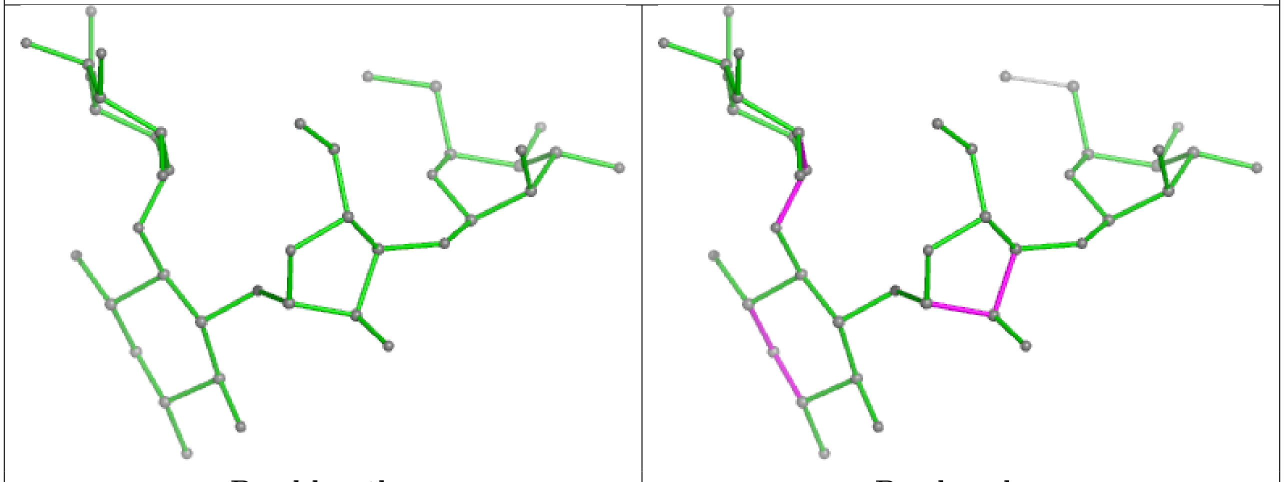


Bond lengths **Bond angles**

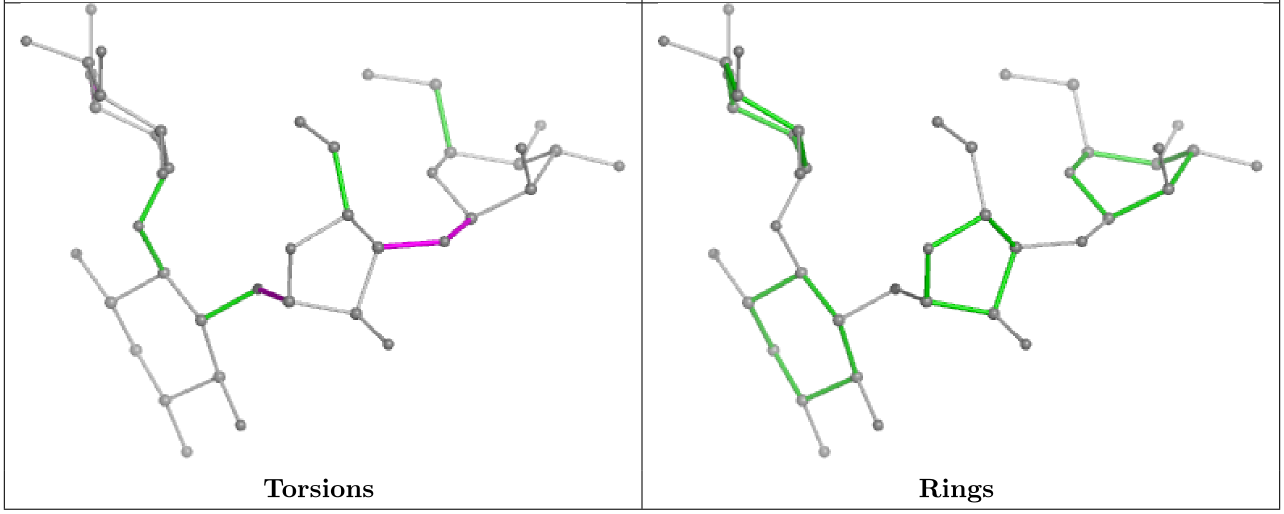


Torsions **Rings**

Ligand PAR 1 3427

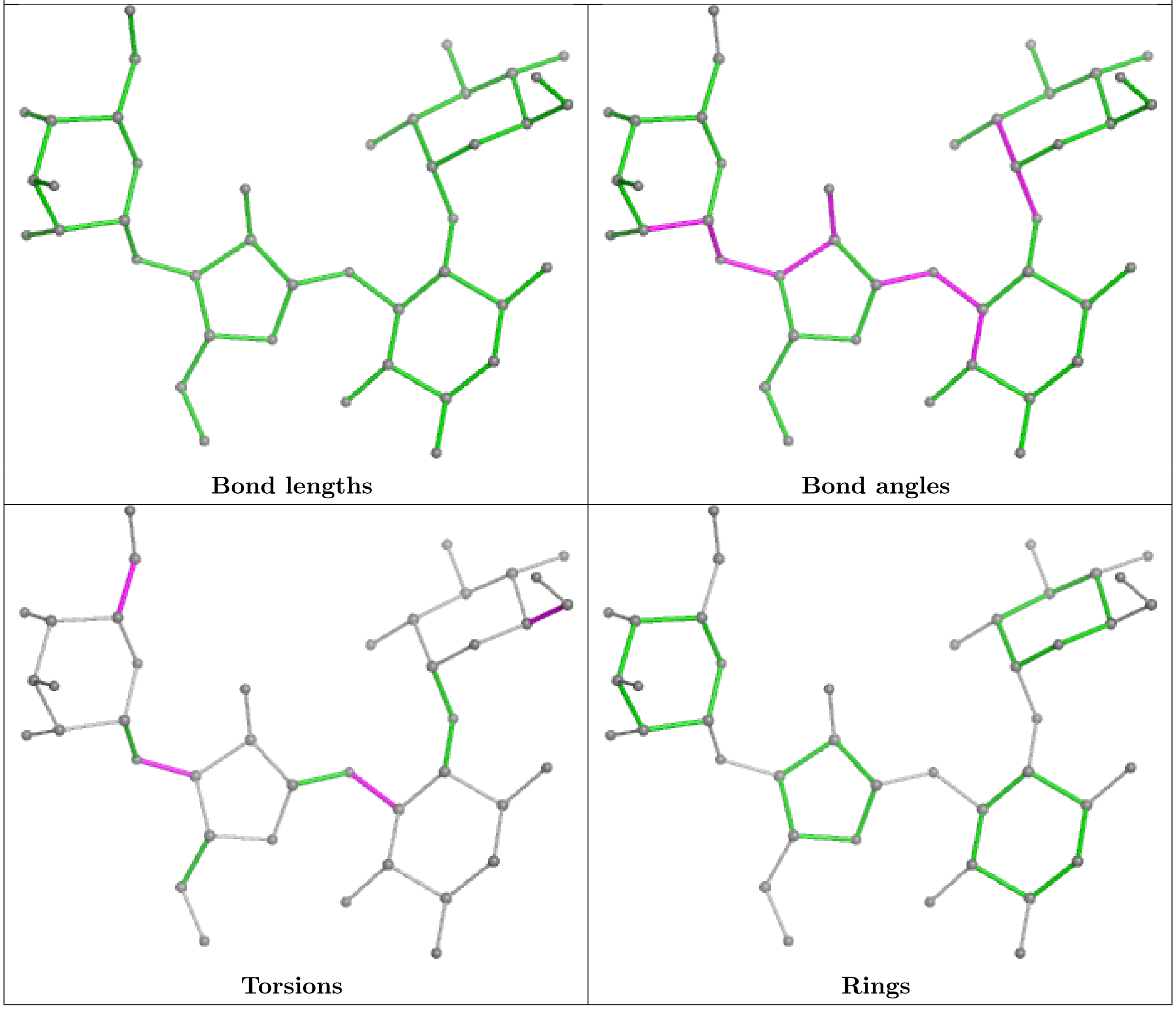


Bond lengths **Bond angles**



Torsions **Rings**

Ligand PAR B 1802



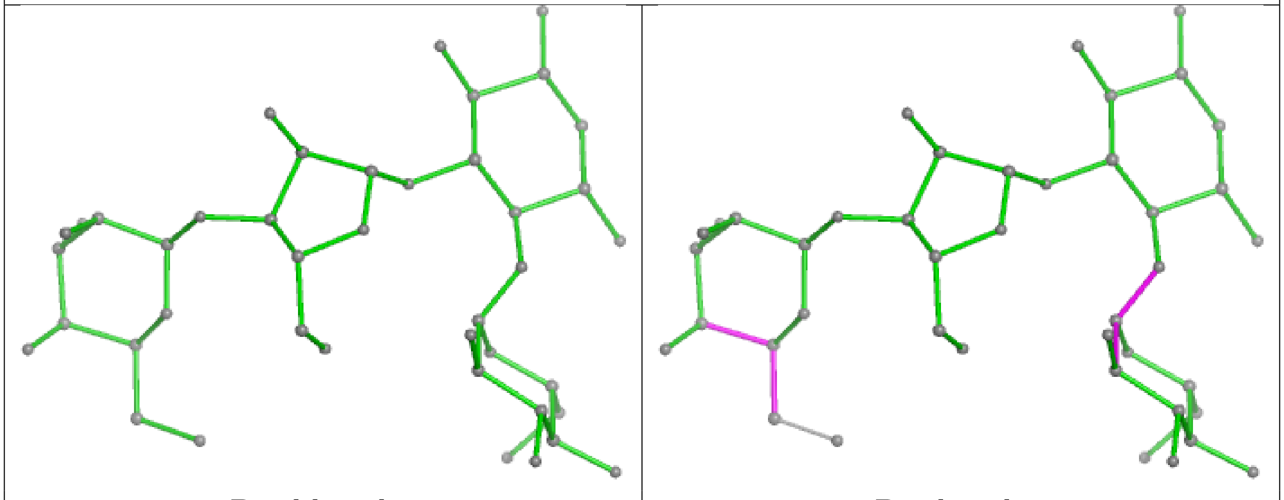
Bond lengths

Bond angles

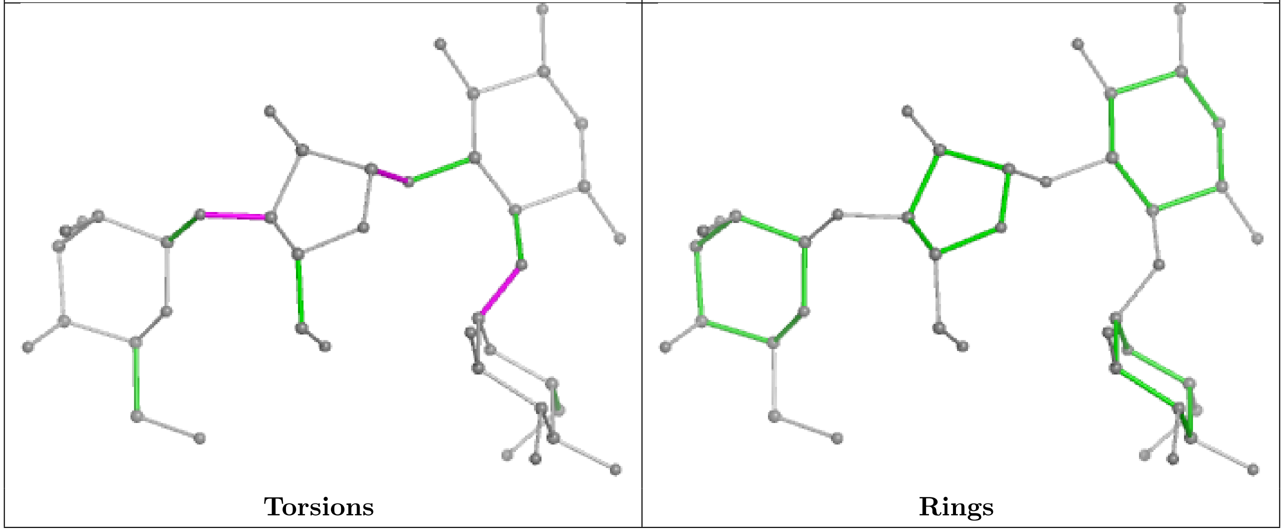
Torsions

Rings

Ligand PAR 1 3421

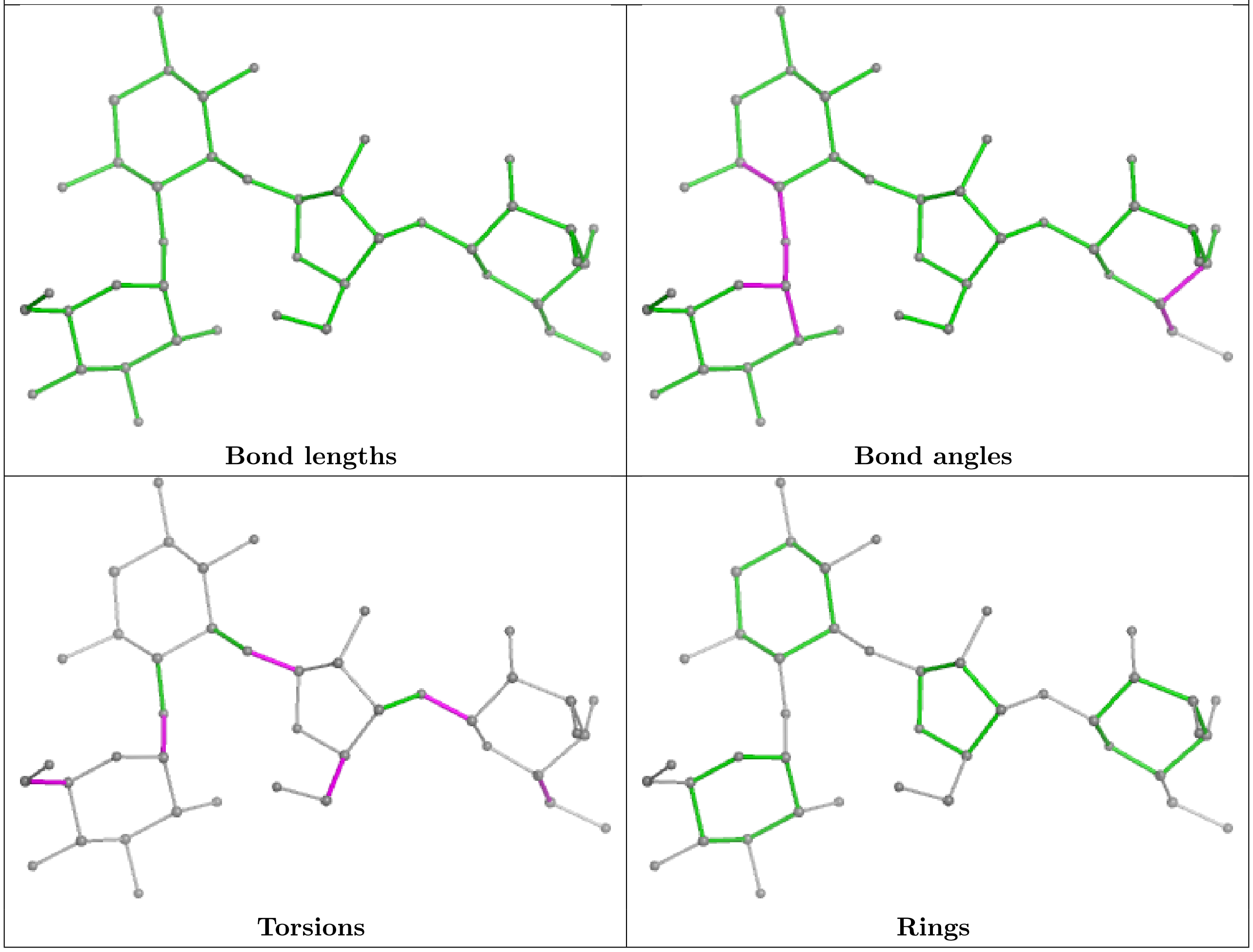


Bond lengths **Bond angles**



Torsions **Rings**

Ligand PAR AS 3408



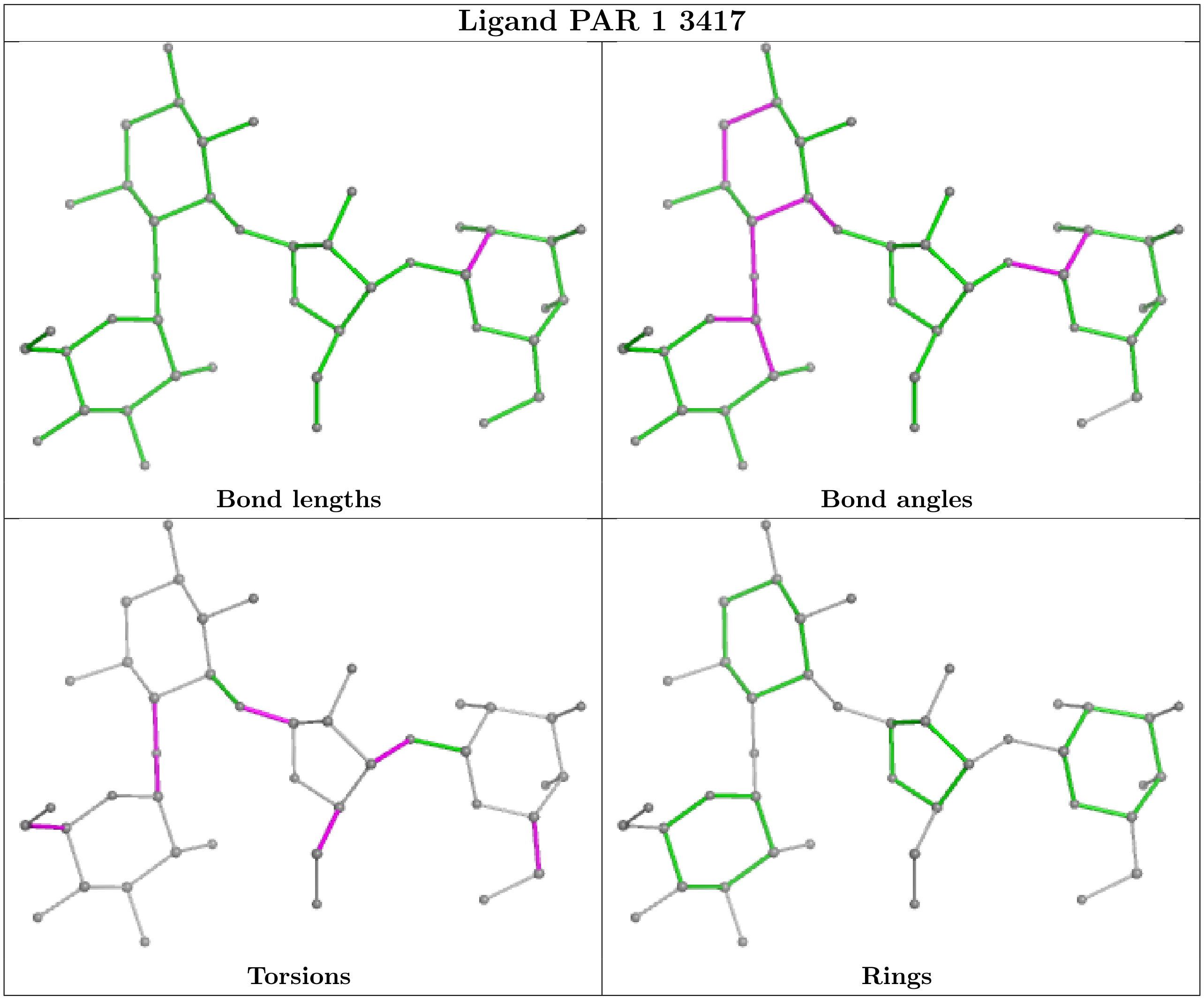
Bond lengths

Bond angles

Torsions

Rings

Ligand PAR 1 3417



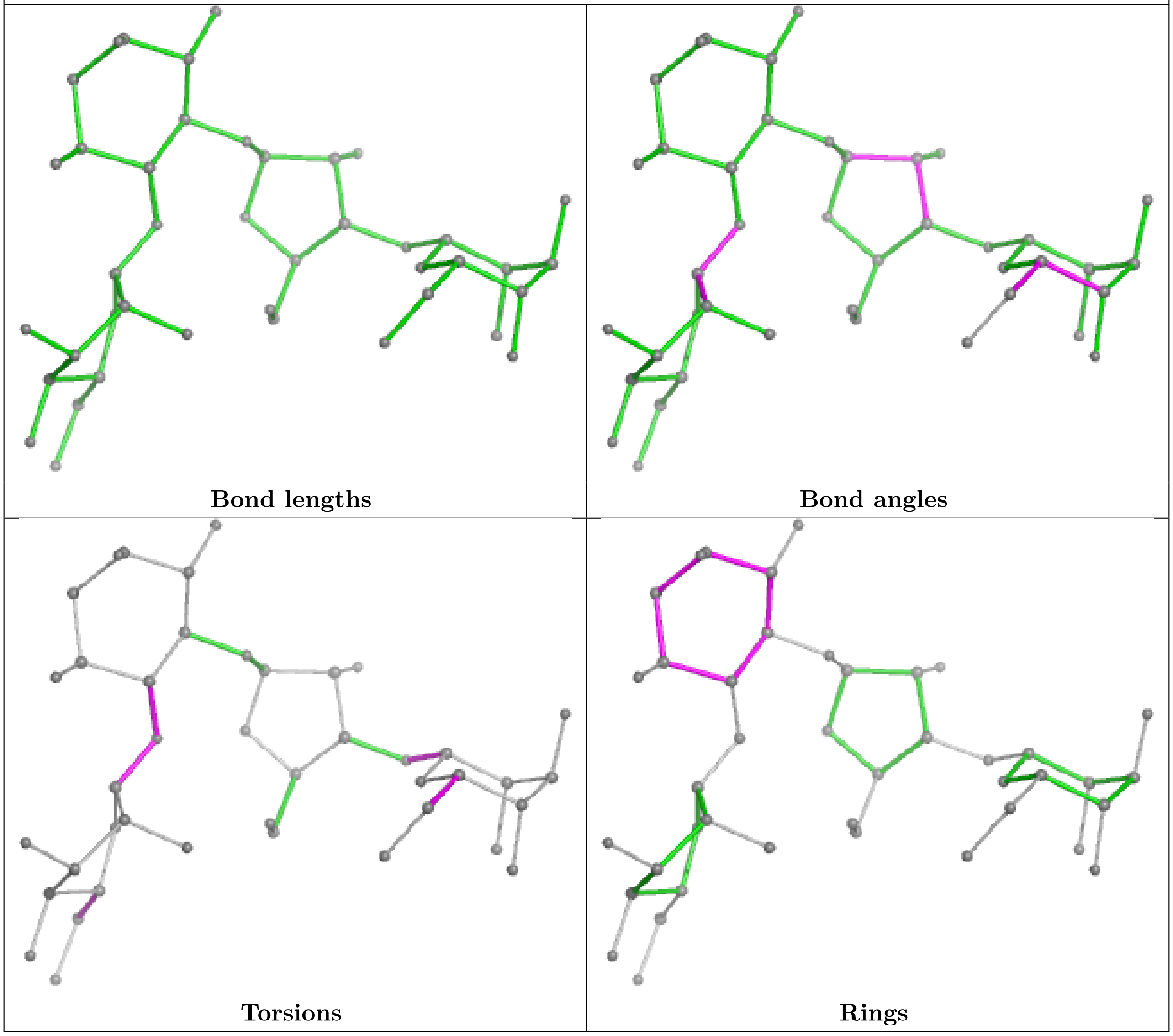
Bond lengths

Bond angles

Torsions

Rings

Ligand PAR 1 3404



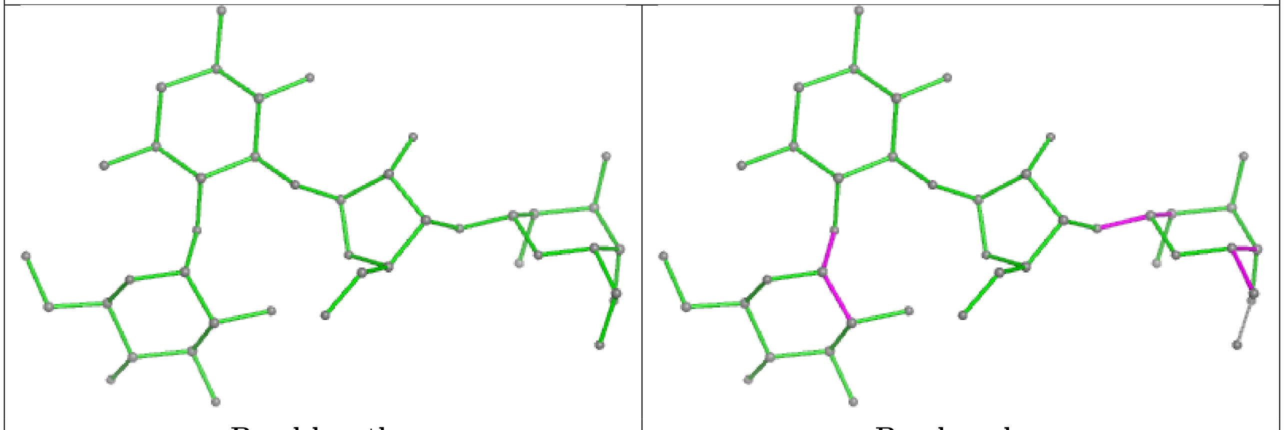
Bond lengths

Bond angles

Torsions

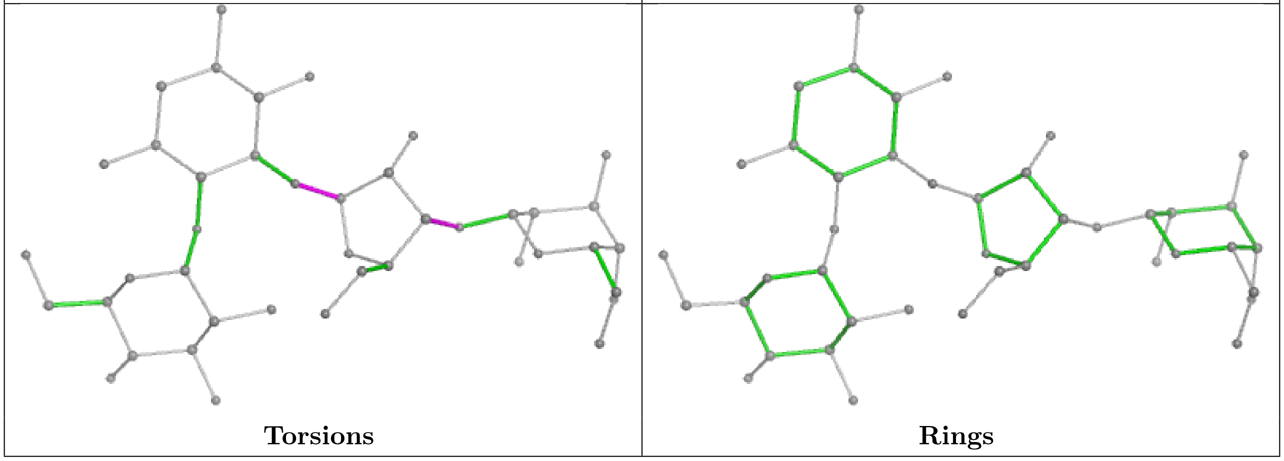
Rings

Ligand PAR 1 3415



Bond lengths

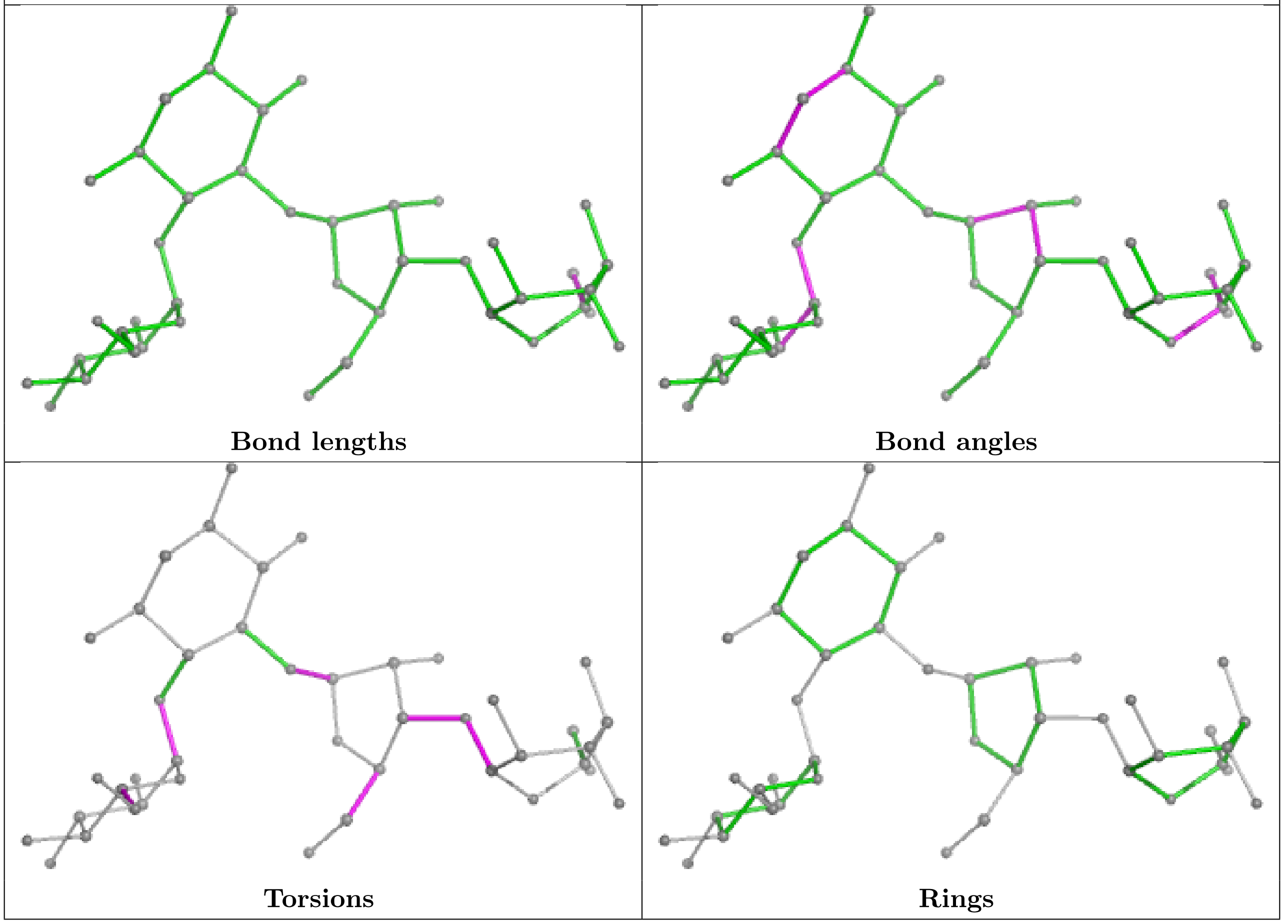
Bond angles



Torsions

Rings

Ligand PAR 1 3424



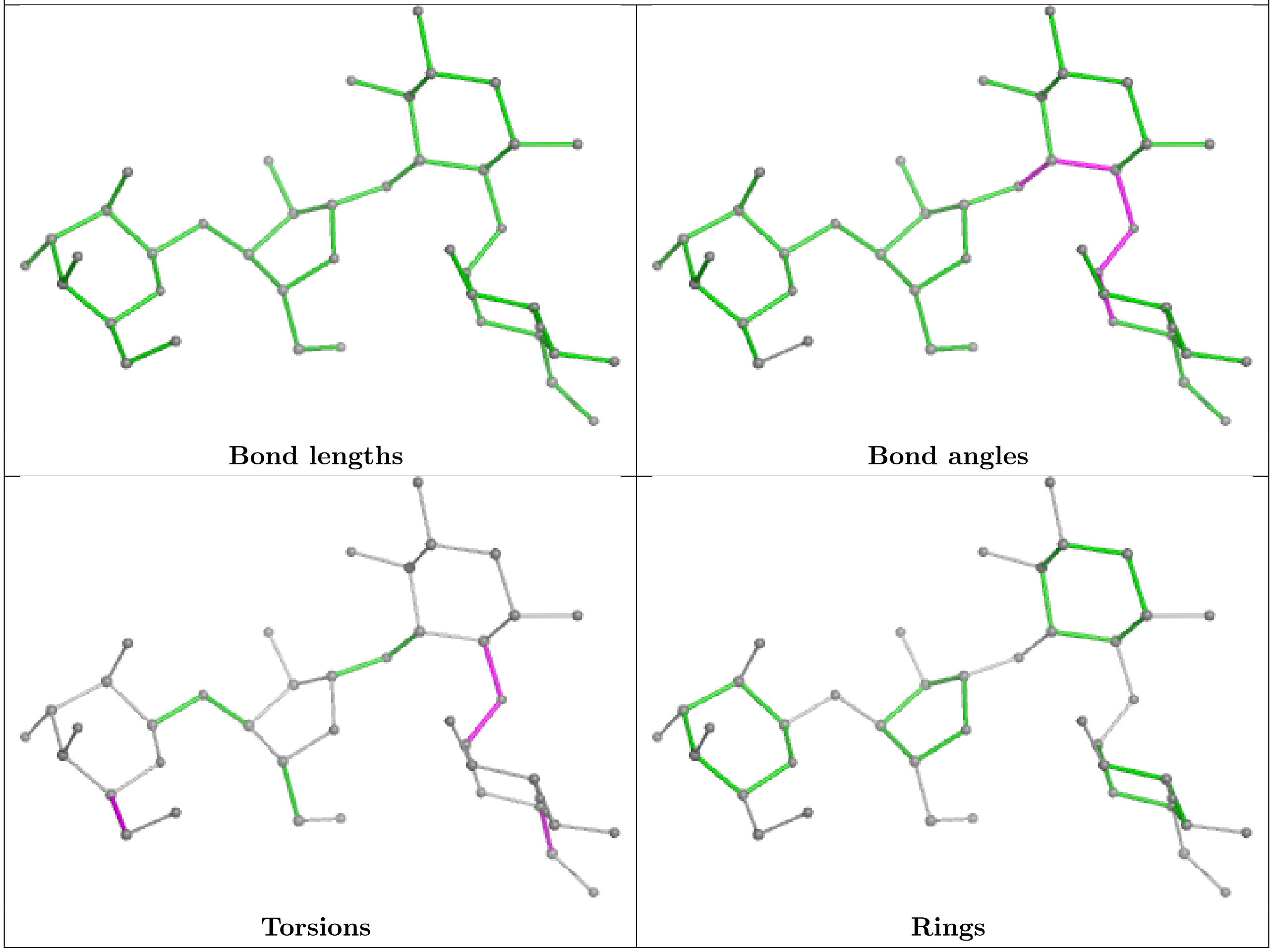
Bond lengths

Bond angles

Torsions

Rings

Ligand PAR B 1803



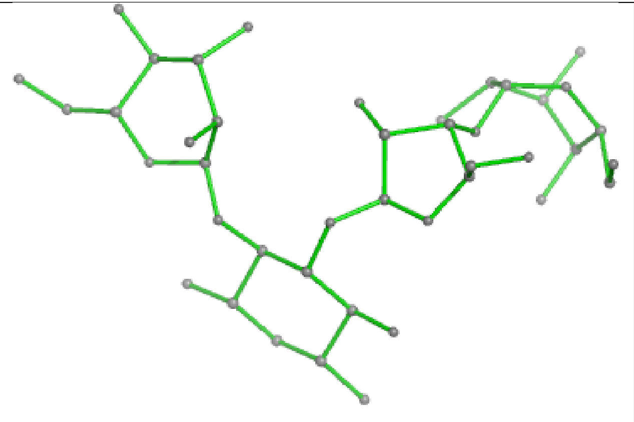
Bond lengths

Bond angles

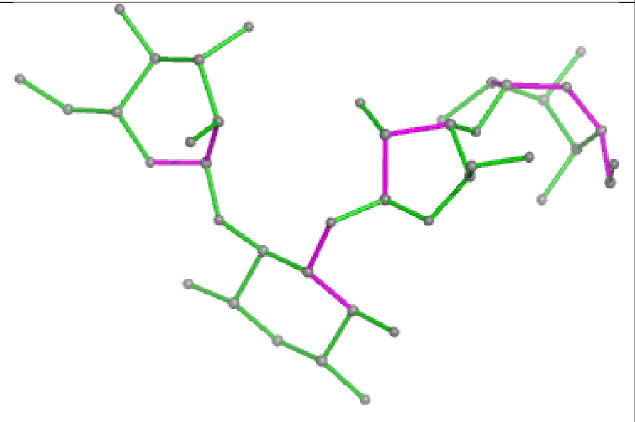
Torsions

Rings

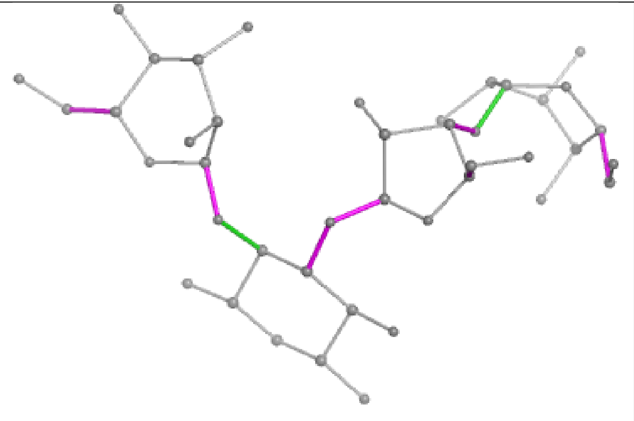
Ligand PAR 1 3411



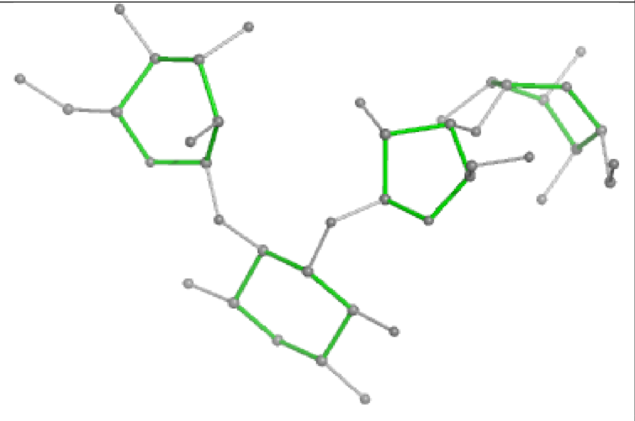
Bond lengths



Bond angles

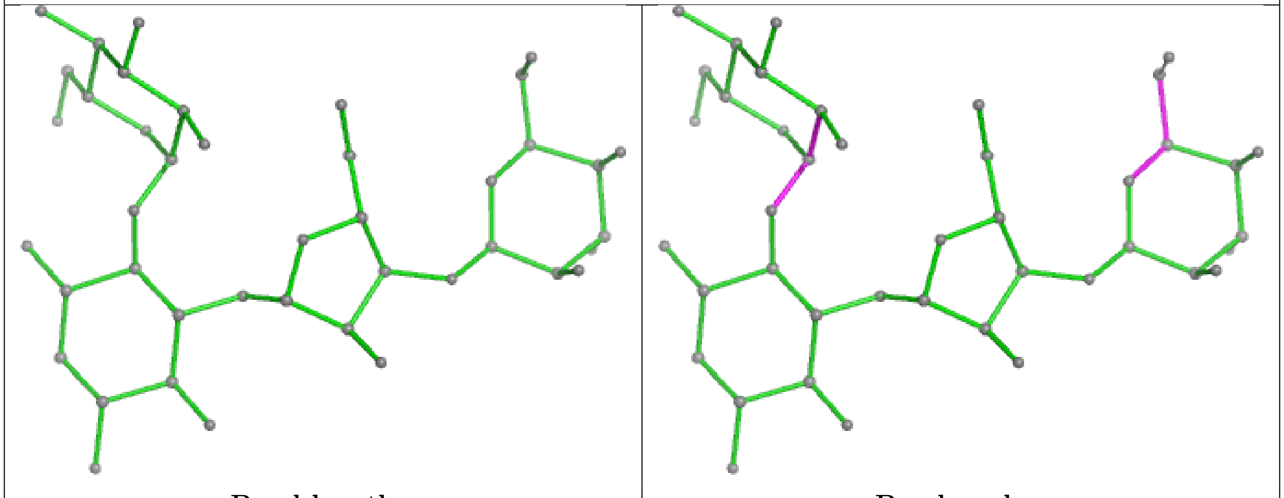


Torsions

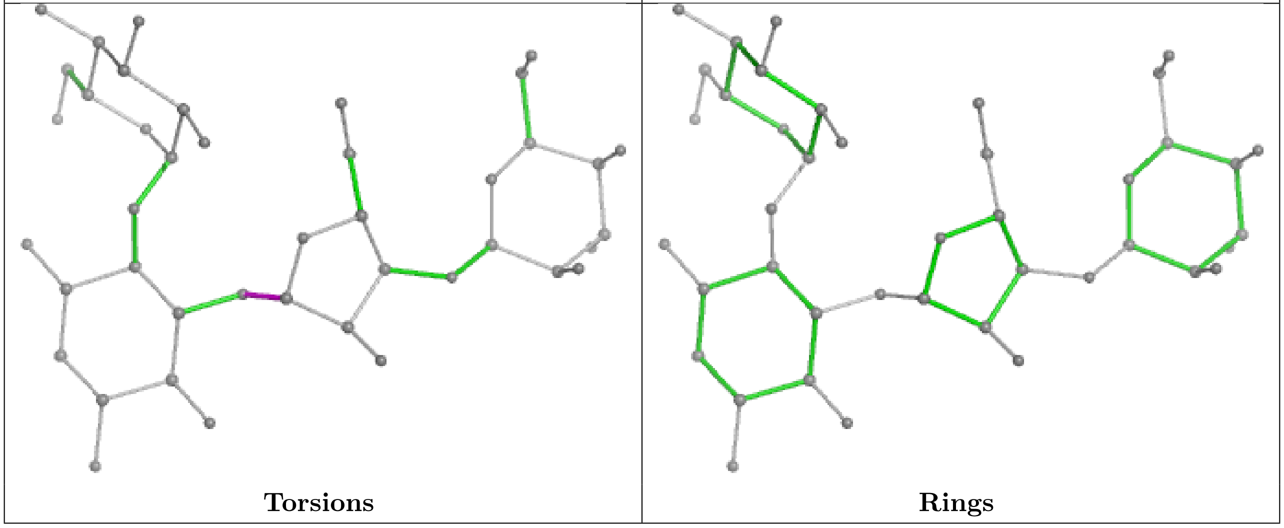


Rings

Ligand PAR CM 1803

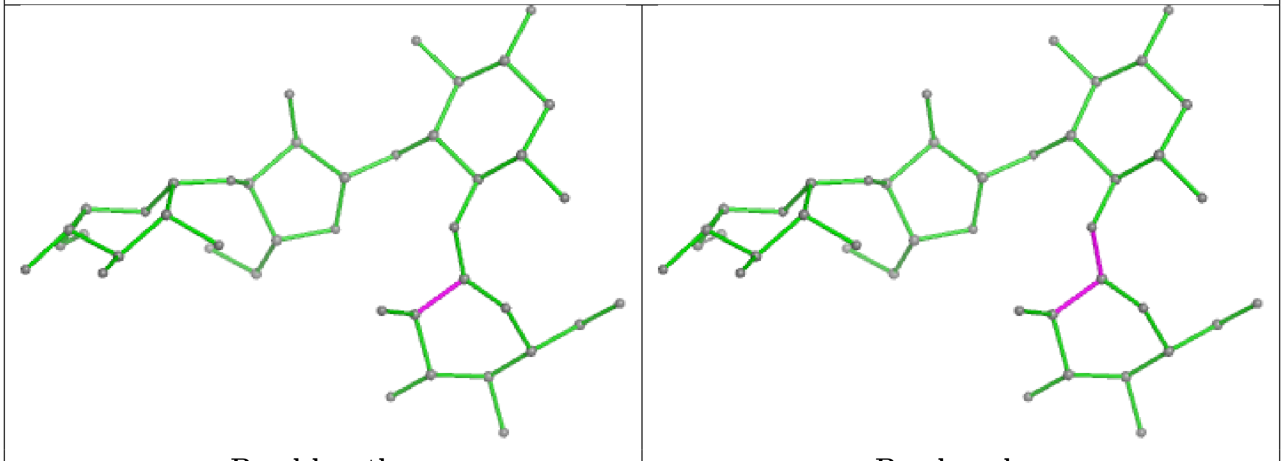


Bond lengths **Bond angles**



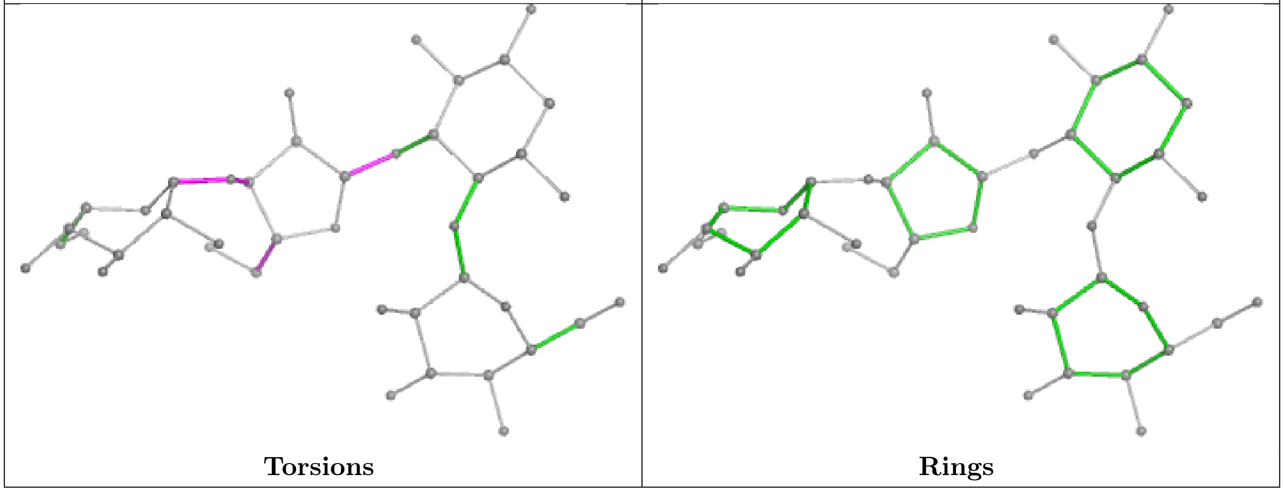
Torsions **Rings**

Ligand PAR CM 1806



Bond lengths

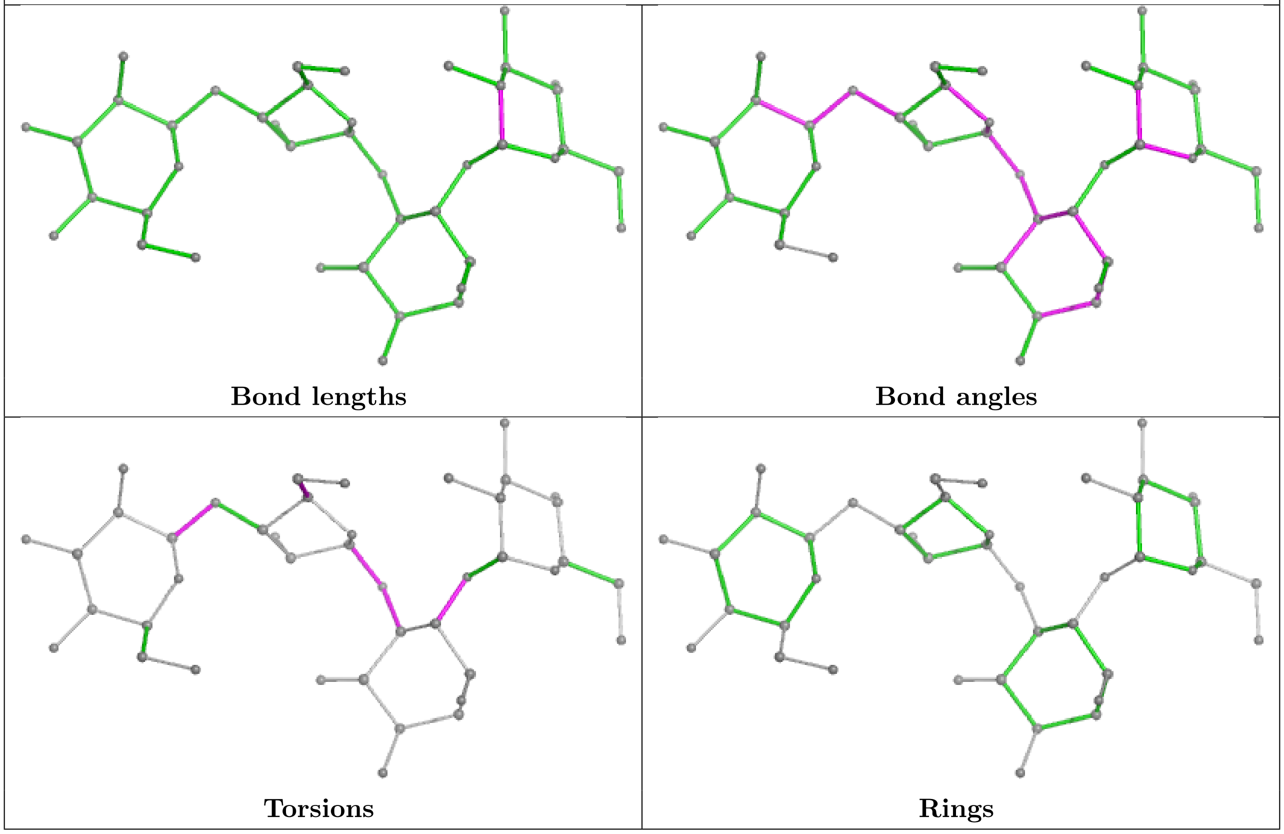
Bond angles



Torsions

Rings

Ligand PAR 1 3430



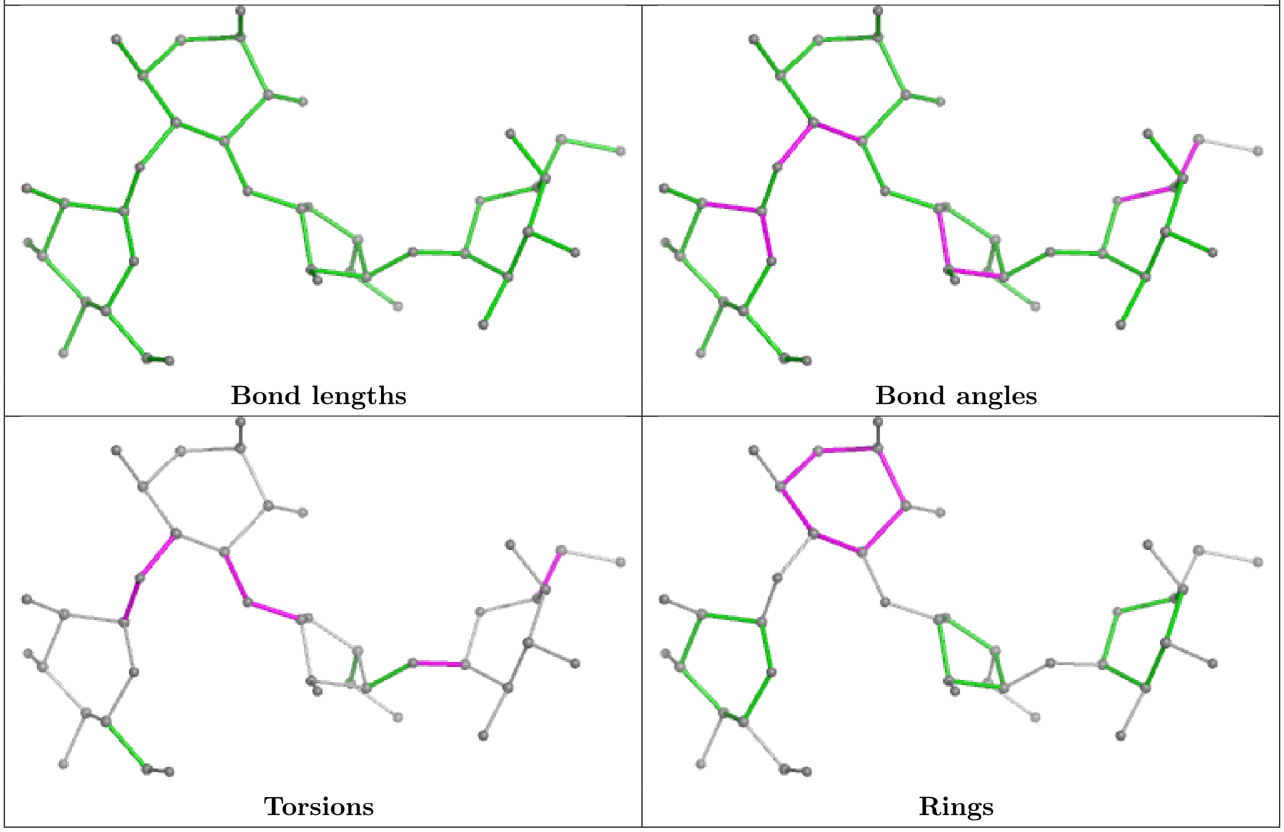
Bond lengths

Bond angles

Torsions

Rings

Ligand PAR AS 3411



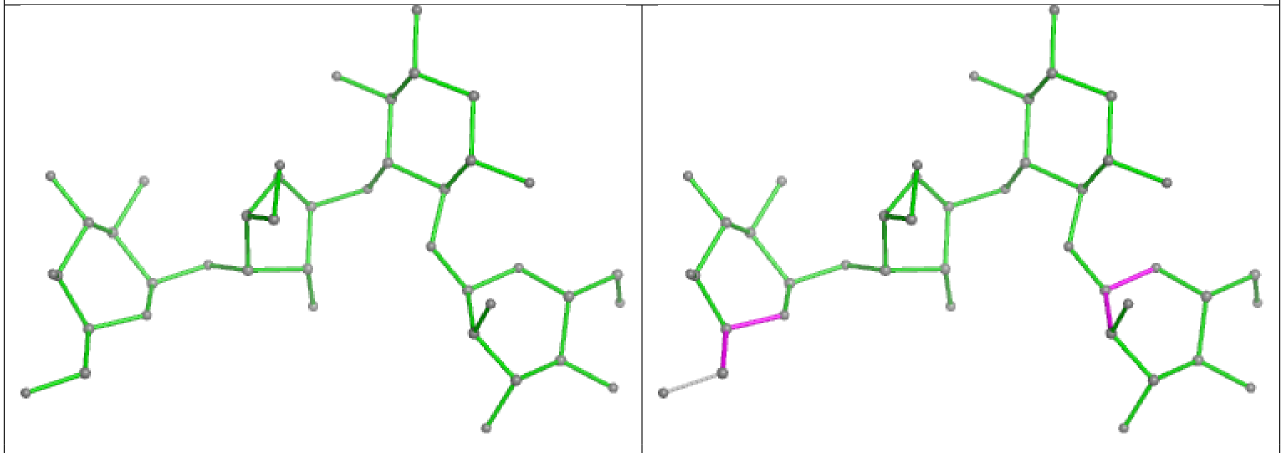
Bond lengths

Bond angles

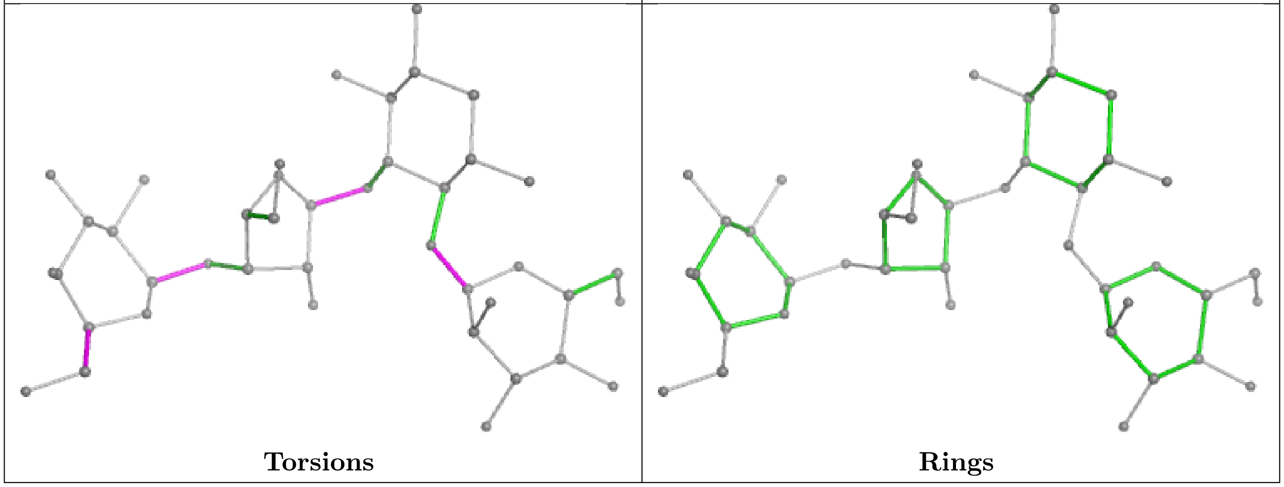
Torsions

Rings

Ligand PAR 1 3420

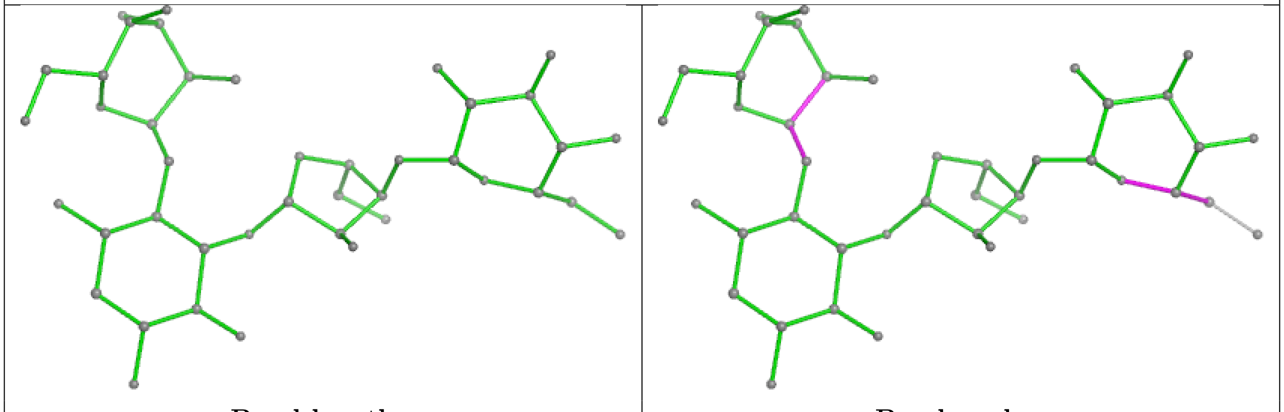


Bond lengths **Bond angles**

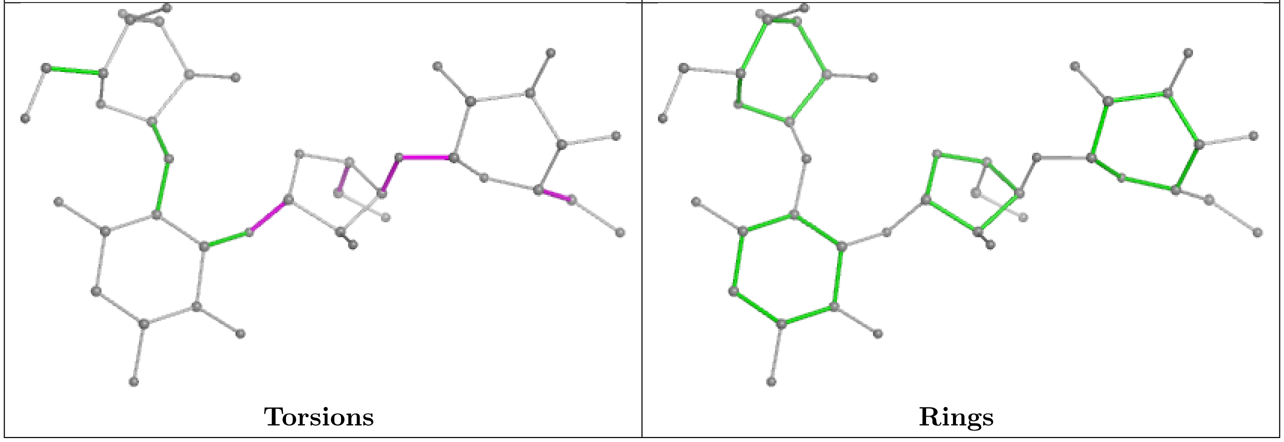


Torsions **Rings**

Ligand PAR 1 3428

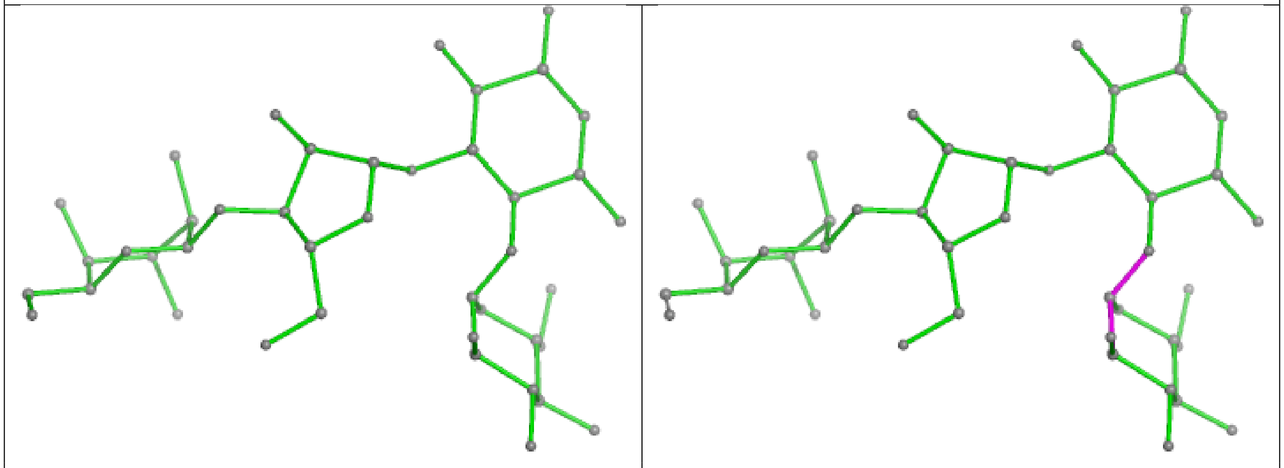


Bond lengths **Bond angles**



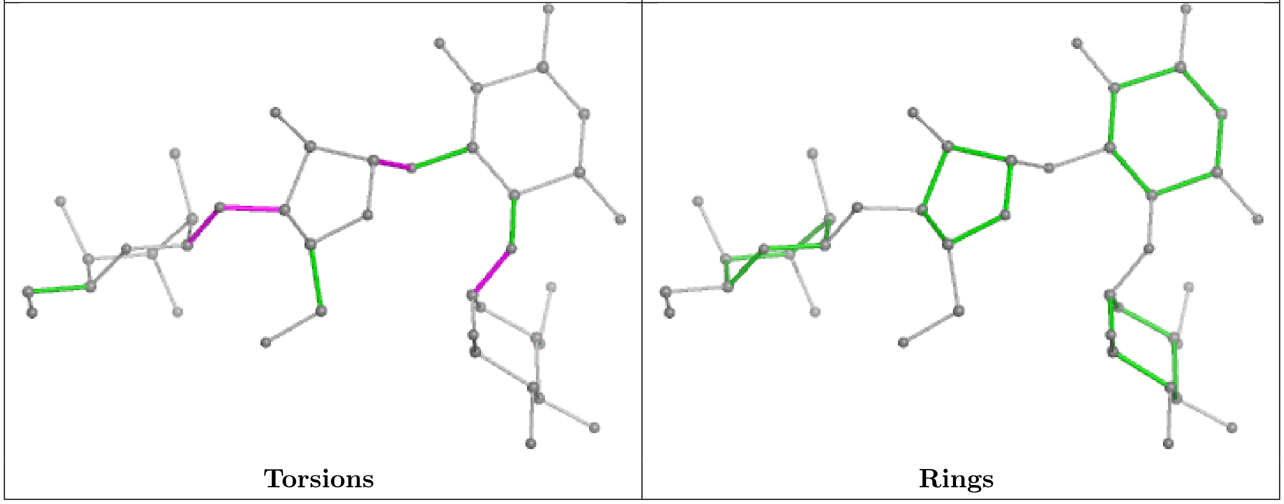
Torsions **Rings**

Ligand PAR 1 3412



Bond lengths

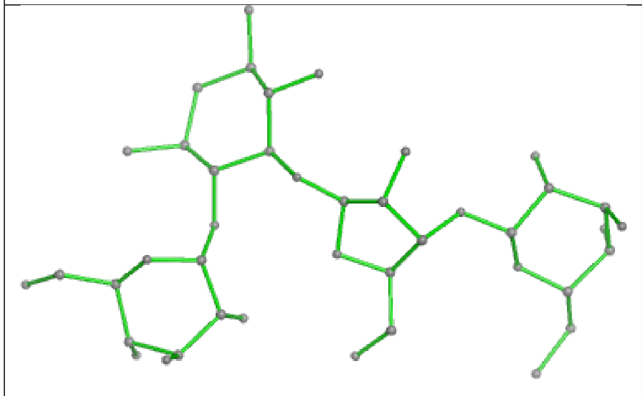
Bond angles



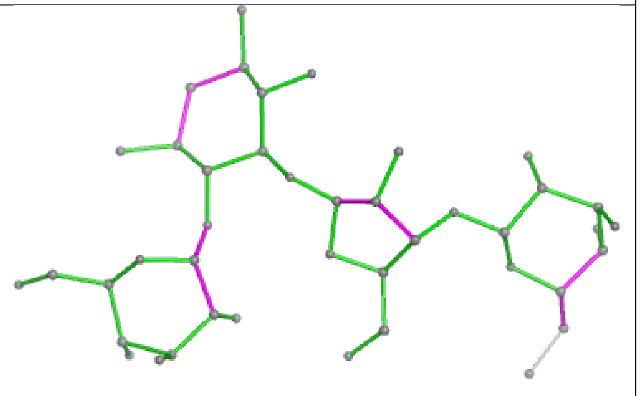
Torsions

Rings

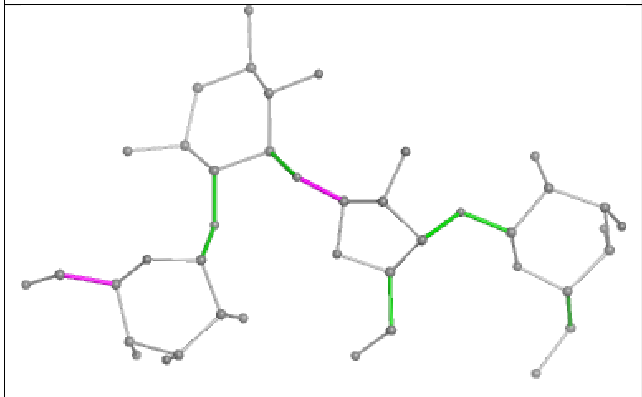
Ligand PAR 1 3426



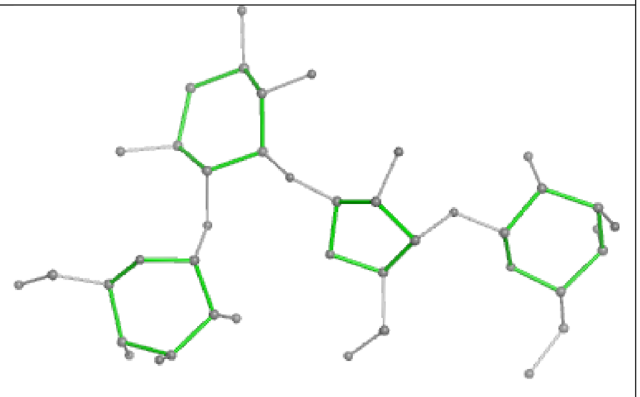
Bond lengths



Bond angles

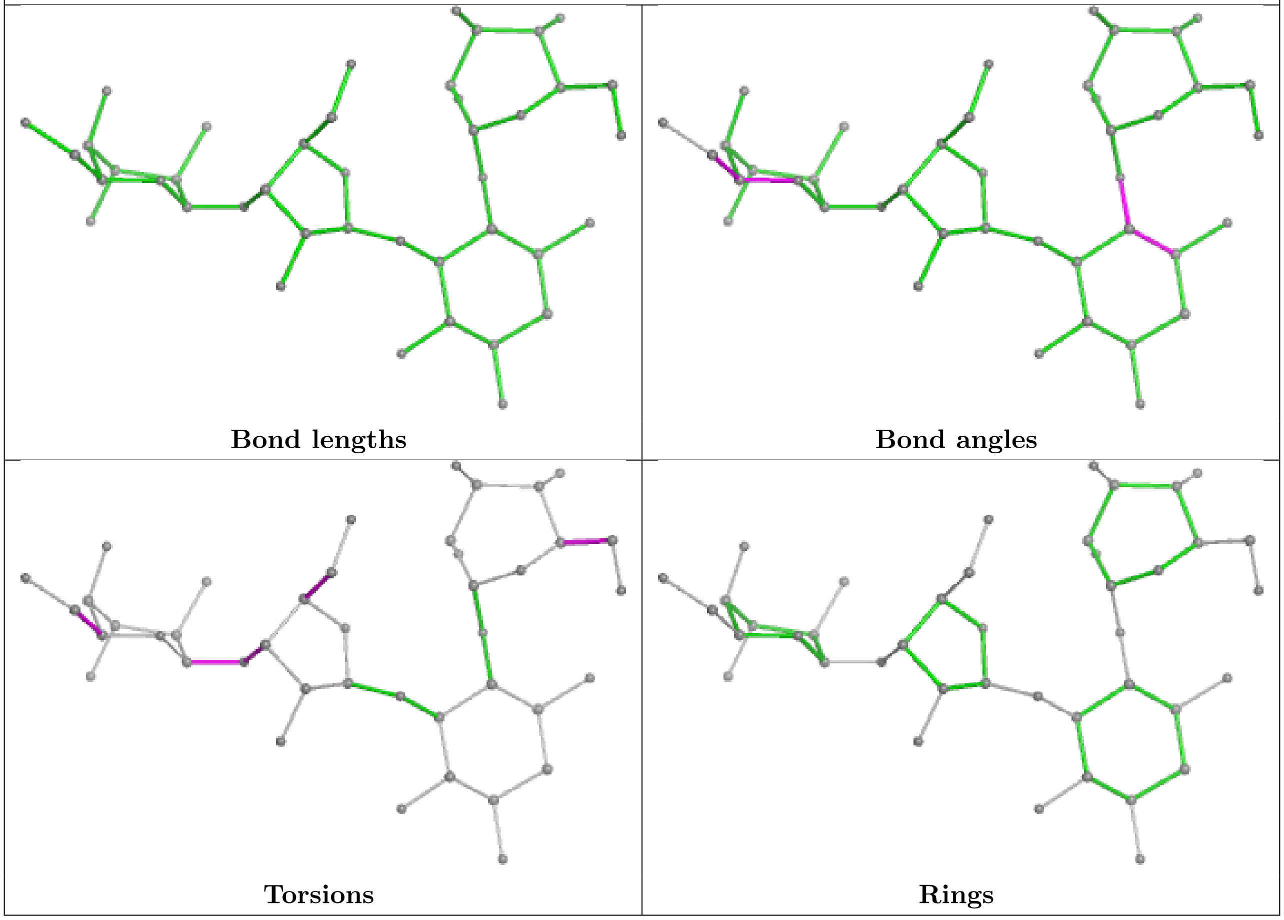


Torsions



Rings

Ligand PAR 1 3407



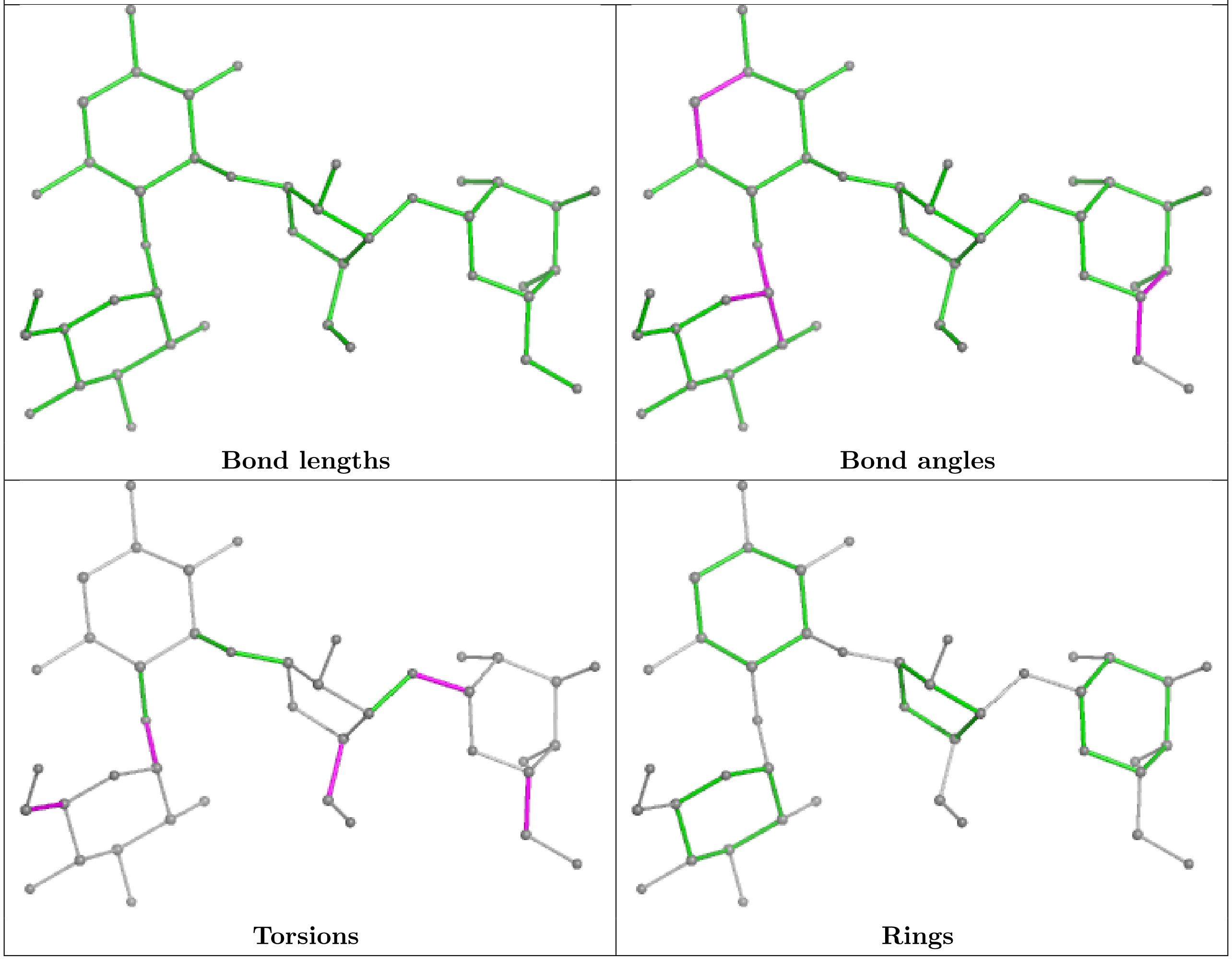
Bond lengths

Bond angles

Torsions

Rings

Ligand PAR 1 3414



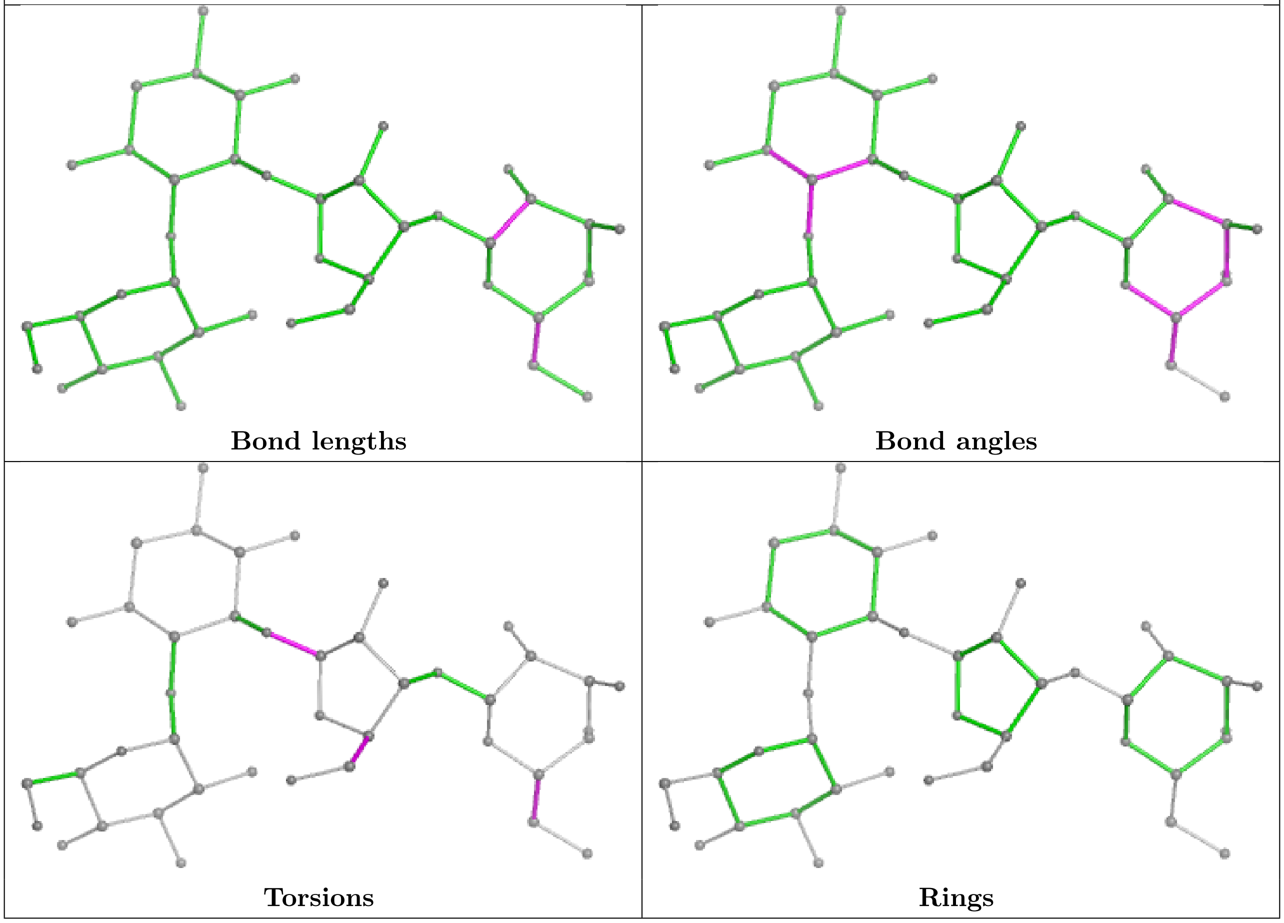
Bond lengths

Bond angles

Torsions

Rings

Ligand PAR 4 201



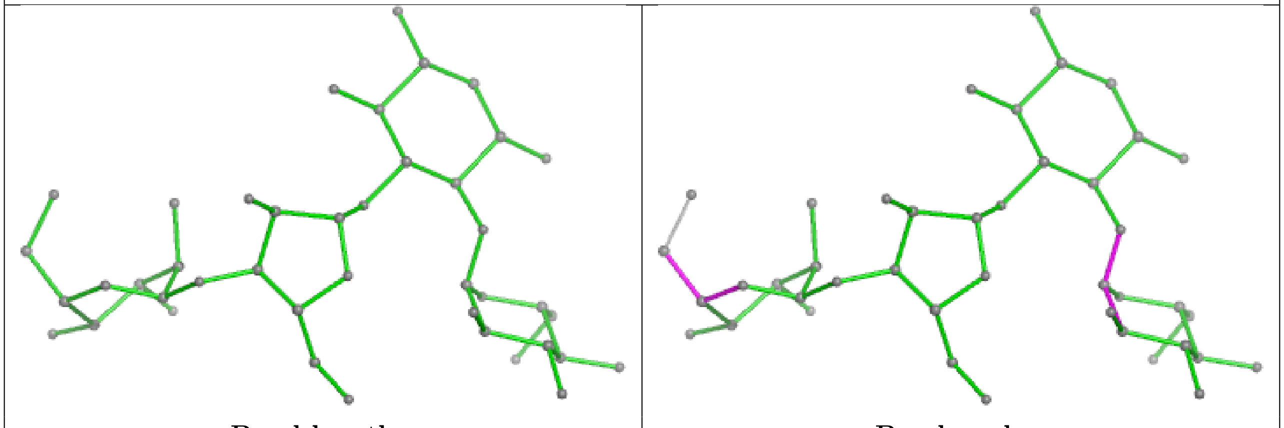
Bond lengths

Bond angles

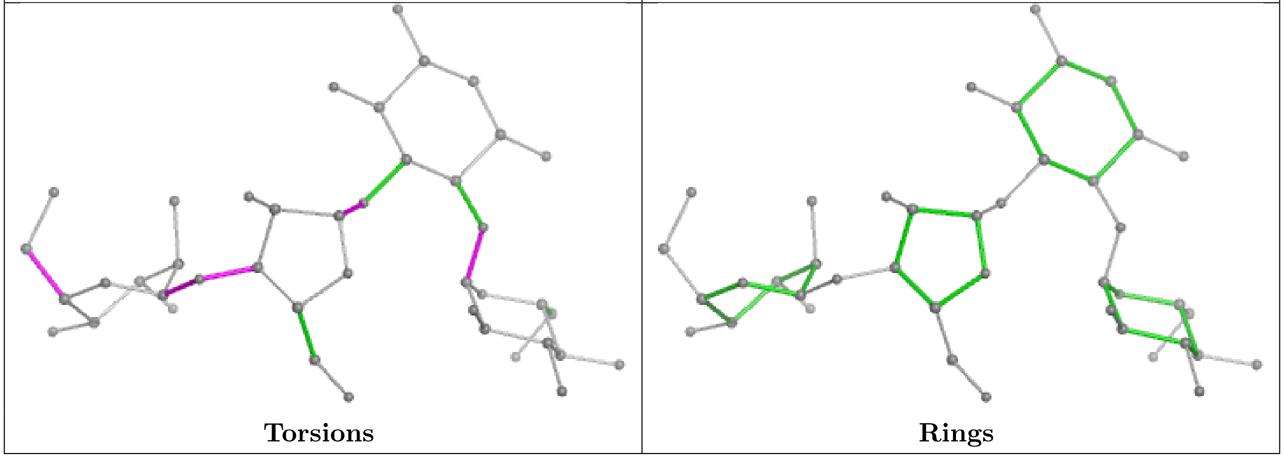
Torsions

Rings

Ligand PAR AS 3402

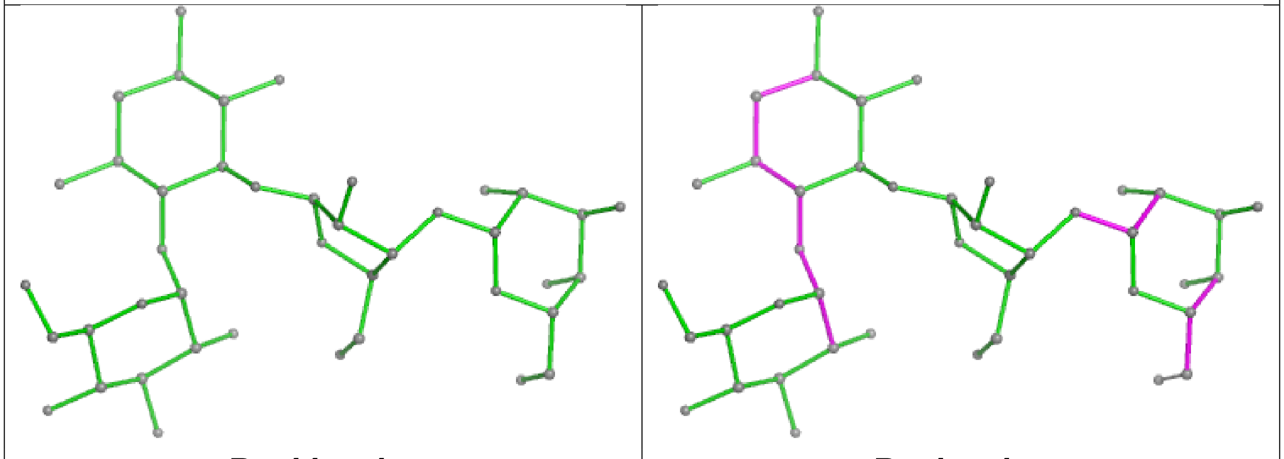


Bond lengths **Bond angles**



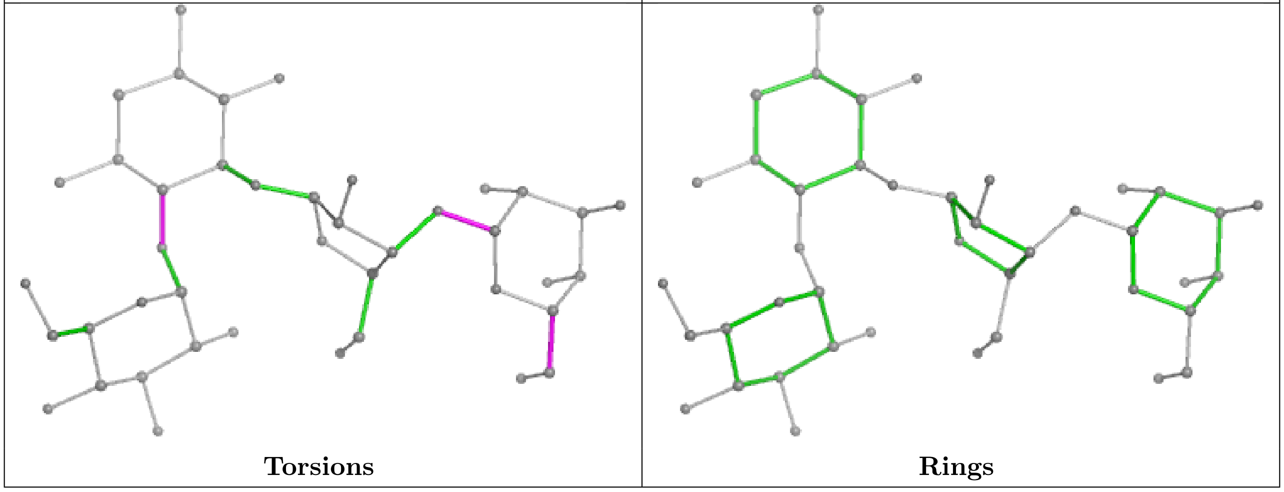
Torsions **Rings**

Ligand PAR B 1801



Bond lengths

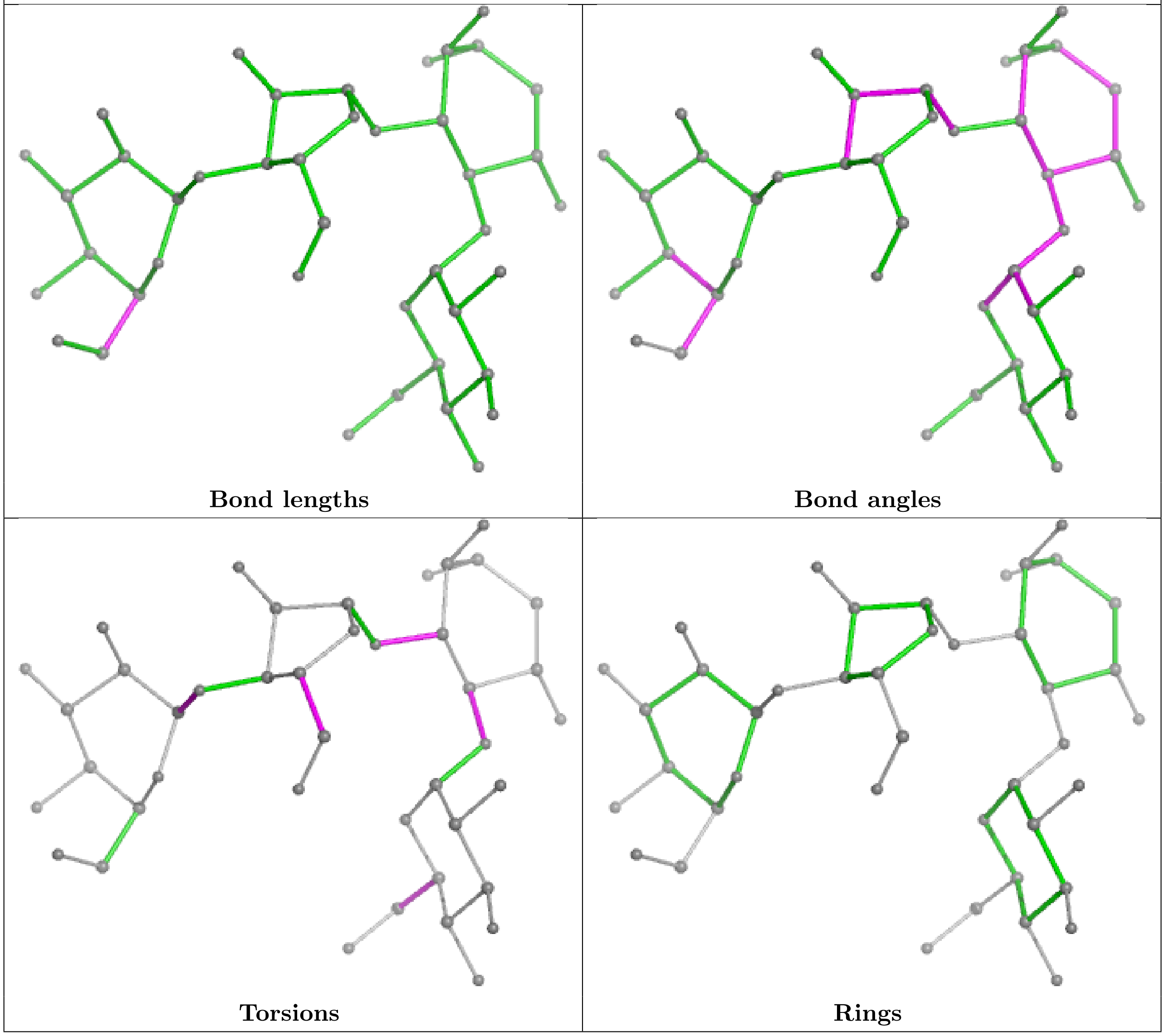
Bond angles

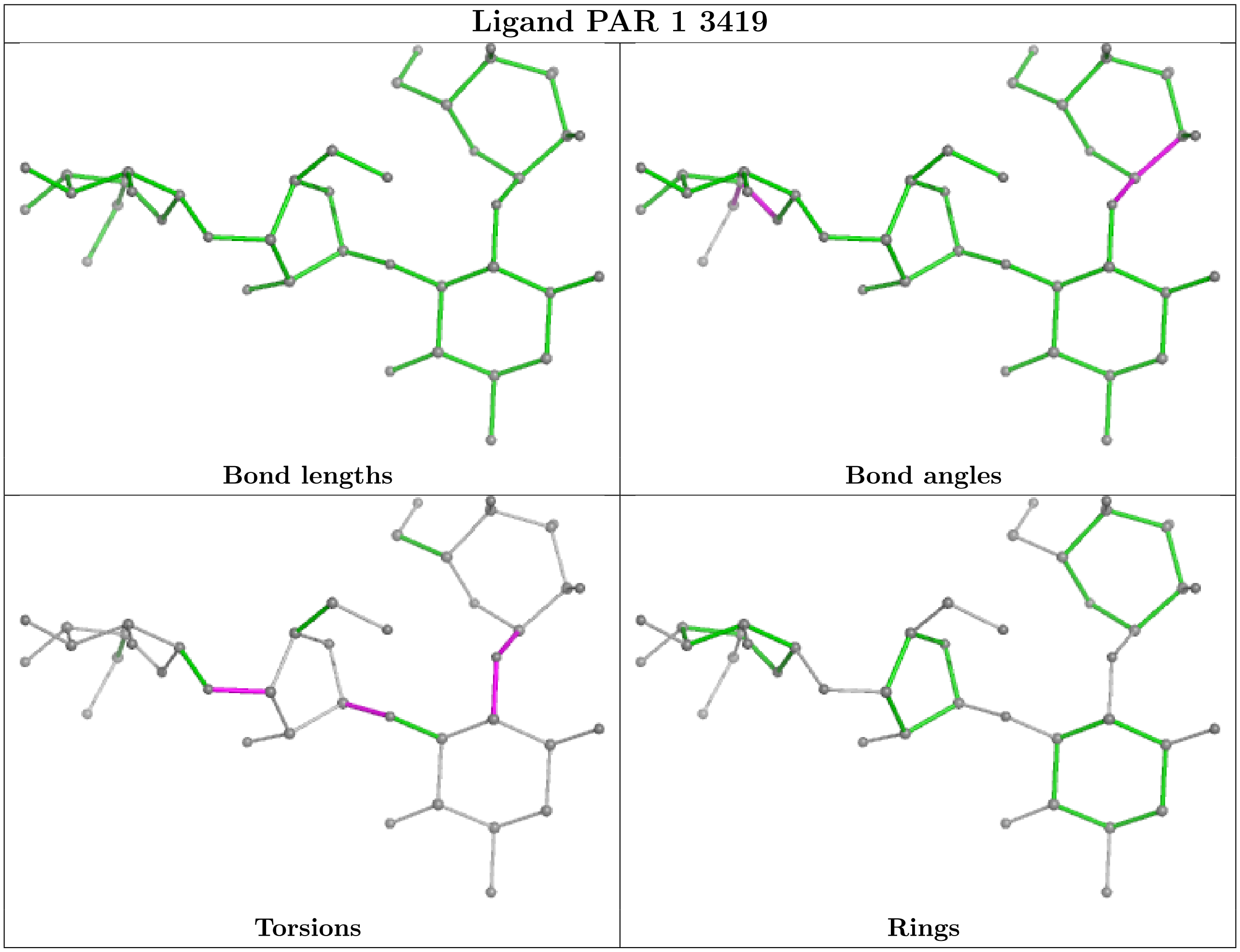


Torsions

Rings

Ligand PAR 1 3413





Ligand PAR 1 3419

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	3171/3359 (94%)	0.79	193 (6%) 28 24	29, 57, 169, 366	0
1	AS	3065/3359 (91%)	1.12	356 (11%) 11 9	38, 74, 167, 281	0
2	3	121/121 (100%)	0.64	1 (0%) 82 78	43, 75, 101, 132	0
2	AT	121/121 (100%)	0.83	4 (3%) 49 43	45, 80, 104, 137	0
3	4	156/158 (98%)	0.64	6 (3%) 44 38	39, 57, 131, 172	0
3	AU	156/158 (98%)	1.61	47 (30%) 1 1	57, 96, 147, 192	0
4	AW	249/254 (98%)	1.79	83 (33%) 1 1	44, 76, 102, 117	1 (0%)
4	j	249/254 (98%)	1.03	25 (10%) 14 12	27, 43, 67, 90	1 (0%)
5	AX	386/389 (99%)	1.31	73 (18%) 4 3	36, 67, 90, 165	0
5	k	386/389 (99%)	1.11	49 (12%) 9 8	32, 59, 82, 128	1 (0%)
6	AY	361/363 (99%)	1.83	139 (38%) 1 1	46, 75, 104, 131	0
6	l	360/363 (99%)	1.23	50 (13%) 7 6	29, 59, 94, 136	0
7	AZ	292/298 (97%)	2.07	134 (45%) 1 0	64, 99, 127, 136	0
7	m	296/298 (99%)	1.43	71 (23%) 2 2	54, 86, 114, 126	0
8	BA	153/176 (86%)	1.48	31 (20%) 3 3	50, 70, 98, 145	0
8	n	157/176 (89%)	1.17	22 (14%) 7 6	51, 70, 106, 139	0
9	BB	234/241 (97%)	1.05	22 (9%) 15 13	34, 58, 101, 154	0
9	o	234/241 (97%)	1.00	24 (10%) 13 12	41, 56, 120, 160	0
10	BC	231/262 (88%)	2.48	147 (63%) 0 0	87, 117, 150, 179	0
10	p	230/262 (87%)	1.17	33 (14%) 7 6	43, 64, 106, 129	0
11	BD	190/191 (99%)	1.42	50 (26%) 2 2	54, 75, 107, 140	0
11	q	190/191 (99%)	1.22	33 (17%) 5 4	51, 68, 89, 123	0
12	BE	206/220 (93%)	1.15	23 (11%) 11 10	44, 64, 101, 125	0
12	r	208/220 (94%)	1.24	35 (16%) 5 4	37, 63, 103, 117	0

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Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	BF	171/174 (98%)	1.54	46 (26%)	2	2	65, 87, 107, 121	0
13	s	171/174 (98%)	1.77	55 (32%)	1	1	67, 88, 110, 129	0
14	BG	200/202 (99%)	2.26	108 (54%)	0	0	50, 95, 130, 151	0
14	t	200/202 (99%)	1.12	26 (13%)	9	7	35, 66, 107, 146	0
15	BH	130/131 (99%)	1.15	21 (16%)	5	5	49, 65, 93, 117	0
15	u	128/131 (97%)	1.11	14 (10%)	12	10	45, 65, 85, 100	0
16	BI	203/204 (99%)	2.78	145 (71%)	0	0	57, 88, 107, 121	0
16	v	203/204 (99%)	1.30	38 (18%)	4	3	27, 47, 59, 82	0
17	BJ	199/200 (99%)	1.13	27 (13%)	8	7	40, 55, 89, 104	0
17	w	199/200 (99%)	1.04	21 (10%)	13	11	35, 52, 82, 102	0
18	BK	174/185 (94%)	1.81	73 (41%)	1	1	48, 74, 102, 124	0
18	x	171/185 (92%)	1.29	29 (16%)	5	4	39, 57, 122, 141	0
19	BL	185/186 (99%)	1.67	65 (35%)	1	1	47, 74, 90, 106	0
19	y	185/186 (99%)	1.24	30 (16%)	5	5	44, 58, 76, 88	0
20	BM	179/190 (94%)	2.32	88 (49%)	0	0	59, 86, 144, 167	0
20	z	179/190 (94%)	1.25	32 (17%)	4	4	44, 62, 121, 136	0
21	0	170/172 (98%)	1.05	14 (8%)	19	16	41, 56, 81, 121	0
21	BN	170/172 (98%)	1.24	27 (15%)	6	5	40, 60, 86, 107	0
22	2	159/160 (99%)	1.35	30 (18%)	4	3	41, 60, 111, 137	0
22	BO	159/160 (99%)	1.78	54 (33%)	1	1	47, 69, 116, 143	0
23	5	103/124 (83%)	1.75	38 (36%)	1	1	72, 112, 132, 156	0
23	BP	102/124 (82%)	2.03	52 (50%)	0	0	97, 129, 154, 178	1 (0%)
24	6	131/137 (95%)	1.14	14 (10%)	12	11	37, 51, 73, 102	0
24	BQ	131/137 (95%)	1.41	31 (23%)	2	2	39, 54, 71, 113	0
25	7	77/155 (49%)	0.97	8 (10%)	13	12	43, 60, 120, 137	0
25	BR	109/155 (70%)	1.74	42 (38%)	1	1	50, 82, 109, 124	0
26	8	121/142 (85%)	1.12	16 (13%)	8	7	38, 59, 83, 121	0
26	BS	119/142 (83%)	2.63	75 (63%)	0	0	64, 96, 114, 119	0
27	9	125/127 (98%)	1.64	34 (27%)	2	2	45, 72, 97, 116	0
27	BT	126/127 (99%)	2.72	81 (64%)	0	0	65, 96, 120, 140	0
28	AA	135/136 (99%)	1.49	42 (31%)	1	1	46, 72, 105, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	BU	135/136 (99%)	2.31	76 (56%) 0 0	92, 119, 177, 219	0
29	AB	148/149 (99%)	1.45	25 (16%) 5 4	33, 56, 86, 111	0
29	BV	148/149 (99%)	2.02	64 (43%) 1 1	42, 79, 103, 118	0
30	AC	61/63 (96%)	1.75	17 (27%) 2 2	42, 71, 117, 139	0
30	BW	61/63 (96%)	2.29	36 (59%) 0 0	50, 84, 123, 141	0
31	AD	96/106 (90%)	1.10	15 (15%) 6 5	47, 62, 87, 101	0
31	BX	96/106 (90%)	1.74	33 (34%) 1 1	76, 103, 127, 134	0
32	AE	110/112 (98%)	1.22	15 (13%) 8 7	50, 67, 125, 135	0
32	BY	110/112 (98%)	1.84	38 (34%) 1 1	53, 84, 122, 133	0
33	AF	124/131 (94%)	1.40	26 (20%) 3 3	36, 57, 74, 87	0
33	BZ	124/131 (94%)	1.67	36 (29%) 1 2	40, 64, 85, 109	0
34	AG	106/107 (99%)	1.10	17 (16%) 6 5	40, 54, 84, 99	0
34	CA	106/107 (99%)	1.31	17 (16%) 6 5	41, 58, 78, 87	0
35	AH	112/122 (91%)	1.61	31 (27%) 2 2	38, 60, 104, 143	0
35	CB	112/122 (91%)	2.74	66 (58%) 0 0	61, 96, 135, 161	0
36	AI	117/120 (97%)	1.51	27 (23%) 2 2	46, 67, 99, 114	1 (0%)
36	CC	118/120 (98%)	2.67	70 (59%) 0 0	71, 103, 126, 132	1 (0%)
37	AJ	97/99 (97%)	0.91	9 (9%) 16 14	45, 62, 99, 142	0
37	CD	97/99 (97%)	2.26	54 (55%) 0 0	83, 104, 137, 147	0
38	AK	86/90 (95%)	1.19	13 (15%) 6 5	32, 45, 92, 128	0
38	CE	86/90 (95%)	2.21	51 (59%) 0 0	52, 73, 107, 135	0
39	AL	77/78 (98%)	1.58	25 (32%) 1 1	63, 87, 125, 151	0
39	CF	77/78 (98%)	2.13	37 (48%) 0 0	93, 121, 152, 173	0
40	AM	50/51 (98%)	1.52	13 (26%) 2 2	41, 56, 86, 90	0
40	CG	50/51 (98%)	2.44	31 (62%) 0 0	52, 82, 97, 102	1 (2%)
41	AN	52/52 (100%)	2.02	27 (51%) 0 0	60, 83, 107, 111	0
41	CH	51/52 (98%)	2.19	24 (47%) 0 0	63, 88, 108, 120	0
42	AO	25/25 (100%)	1.61	7 (28%) 2 2	49, 60, 84, 85	0
42	CI	25/25 (100%)	2.02	10 (40%) 1 1	51, 66, 79, 83	0
43	AP	103/106 (97%)	1.05	12 (11%) 10 9	35, 57, 90, 114	0
43	CJ	103/106 (97%)	1.39	24 (23%) 2 2	57, 81, 108, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	AQ	91/92 (98%)	0.92	8 (8%) 17 15	34, 47, 80, 104	0
44	CK	91/92 (98%)	1.56	24 (26%) 2 2	52, 76, 106, 127	0
45	B	1725/1787 (96%)	1.14	222 (12%) 9 7	41, 78, 165, 331	0
45	CM	1778/1787 (99%)	1.26	264 (14%) 7 6	47, 92, 191, 459	0
46	C	208/261 (79%)	1.73	66 (31%) 1 1	72, 104, 130, 157	0
46	CN	208/261 (79%)	1.68	75 (36%) 1 1	73, 106, 137, 154	0
47	CO	214/256 (83%)	2.05	100 (46%) 0 0	88, 119, 143, 157	0
47	D	214/256 (83%)	1.28	41 (19%) 4 3	57, 84, 104, 112	0
48	CP	217/249 (87%)	1.55	53 (24%) 2 2	50, 81, 109, 128	0
48	E	217/249 (87%)	1.52	63 (29%) 1 2	44, 79, 109, 125	0
49	CQ	223/251 (88%)	1.63	69 (30%) 1 1	70, 99, 147, 166	0
49	F	223/251 (88%)	1.81	89 (39%) 1 1	62, 93, 147, 169	0
50	CR	260/262 (99%)	1.30	51 (19%) 4 3	53, 75, 102, 147	0
50	G	259/262 (98%)	1.71	77 (29%) 1 1	57, 84, 105, 144	0
51	CS	206/225 (91%)	2.04	99 (48%) 0 0	97, 120, 148, 194	0
51	H	206/225 (91%)	1.68	63 (30%) 1 1	64, 97, 131, 170	0
52	CT	236/236 (100%)	2.06	94 (39%) 1 1	59, 90, 123, 159	0
52	I	222/236 (94%)	1.72	71 (31%) 1 1	59, 97, 131, 165	0
53	CU	183/186 (98%)	1.83	77 (42%) 1 1	65, 125, 161, 174	0
53	J	181/186 (97%)	1.82	66 (36%) 1 1	60, 111, 145, 150	0
54	CV	203/206 (98%)	1.58	55 (27%) 2 2	40, 74, 132, 159	0
54	K	202/206 (98%)	1.35	40 (19%) 3 3	42, 69, 120, 137	0
55	CW	178/189 (94%)	1.77	64 (35%) 1 1	64, 88, 121, 152	0
55	L	178/189 (94%)	2.20	99 (55%) 0 0	67, 91, 119, 138	0
56	CX	94/118 (79%)	1.34	21 (22%) 3 2	78, 111, 138, 148	0
56	M	98/118 (83%)	1.73	35 (35%) 1 1	70, 105, 135, 141	0
57	CY	141/155 (90%)	1.70	43 (30%) 1 1	43, 64, 100, 155	0
57	N	141/155 (90%)	1.28	27 (19%) 4 3	43, 60, 94, 121	0
58	CZ	119/143 (83%)	1.80	44 (36%) 1 1	137, 165, 181, 188	0
58	O	116/143 (81%)	2.30	65 (56%) 0 0	141, 174, 191, 198	0
59	DA	150/151 (99%)	1.99	70 (46%) 0 0	63, 95, 117, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
59	P	150/151 (99%)	1.66	41 (27%)	2	2	43, 74, 94, 109	0
60	DB	127/132 (96%)	1.66	48 (37%)	1	1	68, 108, 129, 138	0
60	Q	127/132 (96%)	1.34	27 (21%)	3	3	36, 76, 93, 105	0
61	DC	122/142 (85%)	2.13	62 (50%)	0	0	82, 109, 129, 154	0
61	R	129/142 (90%)	1.45	33 (25%)	2	2	66, 84, 133, 148	0
62	DD	135/142 (95%)	2.47	84 (62%)	0	0	89, 119, 141, 150	0
62	S	140/142 (98%)	1.93	55 (39%)	1	1	66, 99, 134, 157	0
63	DE	124/137 (90%)	2.17	58 (46%)	0	0	88, 123, 158, 180	0
63	T	124/137 (90%)	2.42	74 (59%)	0	0	79, 115, 158, 172	0
64	DF	141/145 (97%)	1.96	59 (41%)	1	1	70, 108, 132, 153	0
64	U	144/145 (99%)	1.34	23 (15%)	6	5	63, 83, 119, 146	0
65	DG	139/145 (95%)	2.56	93 (66%)	0	0	94, 116, 133, 144	0
65	V	141/145 (97%)	1.72	48 (34%)	1	1	69, 92, 123, 148	0
66	DH	97/119 (81%)	2.13	47 (48%)	0	0	81, 113, 136, 142	0
66	W	99/119 (83%)	2.07	43 (43%)	1	1	63, 112, 137, 143	0
67	DI	87/87 (100%)	1.30	14 (16%)	5	5	72, 93, 116, 140	0
67	X	87/87 (100%)	1.56	21 (24%)	2	2	63, 91, 113, 127	0
68	DJ	129/130 (99%)	1.62	38 (29%)	1	1	56, 73, 90, 97	0
68	Y	129/130 (99%)	1.51	29 (22%)	3	2	50, 68, 84, 94	0
69	DK	143/145 (98%)	1.49	32 (22%)	3	2	49, 62, 81, 102	0
69	Z	143/145 (98%)	1.30	28 (19%)	4	3	49, 64, 80, 115	0
70	DL	132/135 (97%)	1.47	31 (23%)	2	2	66, 95, 119, 153	0
70	a	134/135 (99%)	1.87	53 (39%)	1	1	66, 104, 125, 151	0
71	DM	68/105 (64%)	1.99	33 (48%)	0	0	109, 134, 148, 159	0
71	b	72/105 (68%)	1.30	11 (15%)	6	5	82, 107, 132, 143	0
72	DN	98/119 (82%)	2.19	48 (48%)	0	0	63, 88, 131, 137	0
72	c	98/119 (82%)	1.79	36 (36%)	1	1	50, 70, 109, 150	0
73	DO	81/82 (98%)	1.79	26 (32%)	1	1	75, 107, 156, 178	0
73	d	81/82 (98%)	1.77	30 (37%)	1	1	64, 85, 145, 164	0
74	DP	61/67 (91%)	1.90	23 (37%)	1	1	105, 125, 140, 151	0
74	e	62/67 (92%)	1.55	15 (24%)	2	2	84, 105, 132, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
75	DQ	54/56 (96%)	1.80	22 (40%) 1 1	72, 91, 110, 125	0
75	f	55/56 (98%)	1.62	16 (29%) 1 2	57, 73, 101, 112	0
76	DR	58/63 (92%)	2.19	34 (58%) 0 0	65, 96, 154, 163	0
76	g	54/63 (85%)	2.14	23 (42%) 1 1	73, 97, 128, 136	0
77	h	70/193 (36%)	2.82	47 (67%) 0 0	122, 160, 179, 191	0
78	AR	311/317 (98%)	2.01	138 (44%) 1 1	101, 149, 177, 189	0
79	CL	121/267 (45%)	1.85	45 (37%) 1 1	68, 103, 129, 138	0
79	i	120/267 (44%)	2.39	62 (51%) 0 0	71, 104, 136, 146	0
All	All	32248/34616 (93%)	1.45	7858 (24%) 2 2	27, 79, 147, 459	7 (0%)

The worst 5 of 7858 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	AY	363	ASN	14.5
6	l	363	ASN	12.5
36	CC	120	ALA	11.3
52	CT	80	GLY	10.3
51	H	152	SER	10.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	AS	3630	1/1	0.26	0.38	73,73,73,73	0
82	MG	1	3654	1/1	0.32	0.35	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
82	MG	AS	3720	1/1	0.40	0.22	51,51,51,51	0
82	MG	AS	3460	1/1	0.42	0.37	75,75,75,75	0
82	MG	B	1937	1/1	0.44	0.30	72,72,72,72	0
82	MG	CM	1848	1/1	0.44	0.20	73,73,73,73	0
82	MG	B	1930	1/1	0.46	0.30	74,74,74,74	0
82	MG	B	1848	1/1	0.47	0.30	59,59,59,59	0
82	MG	B	1925	1/1	0.53	0.43	81,81,81,81	0
82	MG	CM	1839	1/1	0.54	0.17	96,96,96,96	0
82	MG	AS	3442	1/1	0.55	0.19	52,52,52,52	0
82	MG	B	1810	1/1	0.55	0.29	51,51,51,51	0
82	MG	B	1910	1/1	0.56	0.26	71,71,71,71	0
82	MG	1	3483	1/1	0.57	0.20	68,68,68,68	0
82	MG	CM	1812	1/1	0.57	0.32	73,73,73,73	0
82	MG	CM	1932	1/1	0.57	0.32	75,75,75,75	0
82	MG	AS	3716	1/1	0.58	0.28	51,51,51,51	0
82	MG	CM	1869	1/1	0.59	0.28	50,50,50,50	0
82	MG	AS	3669	1/1	0.59	0.30	80,80,80,80	0
82	MG	CM	1853	1/1	0.60	0.19	83,83,83,83	0
82	MG	AS	3738	1/1	0.60	0.25	64,64,64,64	0
82	MG	CM	1884	1/1	0.60	0.26	60,60,60,60	0
82	MG	AS	3414	1/1	0.60	0.20	57,57,57,57	0
82	MG	1	3471	1/1	0.61	0.21	50,50,50,50	0
82	MG	1	3501	1/1	0.61	0.15	65,65,65,65	0
82	MG	AS	3467	1/1	0.62	0.15	67,67,67,67	0
82	MG	CM	1851	1/1	0.62	0.29	80,80,80,80	0
82	MG	1	3762	1/1	0.62	0.17	60,60,60,60	0
82	MG	AS	3639	1/1	0.62	0.18	44,44,44,44	0
82	MG	AS	3655	1/1	0.62	0.18	41,41,41,41	0
81	PAR	CM	1806	42/42	0.62	0.16	54,78,92,94	0
82	MG	AS	3450	1/1	0.63	0.21	59,59,59,59	0
82	MG	CM	1900	1/1	0.63	0.20	63,63,63,63	0
82	MG	1	3498	1/1	0.63	0.41	64,64,64,64	0
82	MG	AS	3489	1/1	0.64	0.23	58,58,58,58	0
82	MG	AS	3620	1/1	0.64	0.25	73,73,73,73	0
82	MG	AS	3713	1/1	0.64	0.29	38,38,38,38	0
82	MG	AS	3424	1/1	0.64	0.26	65,65,65,65	0
82	MG	AS	3469	1/1	0.64	0.42	72,72,72,72	0
82	MG	B	1866	1/1	0.65	0.30	58,58,58,58	0
82	MG	AS	3728	1/1	0.65	0.15	44,44,44,44	0
82	MG	1	3584	1/1	0.65	0.18	44,44,44,44	0
81	PAR	AS	3413	42/42	0.66	0.16	20,20,20,20	0
82	MG	1	3479	1/1	0.66	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	CR	301	1/1	0.66	0.23	51,51,51,51	0
82	MG	B	1830	1/1	0.67	0.41	60,60,60,60	0
82	MG	1	3679	1/1	0.67	0.15	53,53,53,53	0
82	MG	AS	3628	1/1	0.67	0.20	52,52,52,52	0
82	MG	AS	3730	1/1	0.67	0.30	62,62,62,62	0
82	MG	AS	3420	1/1	0.67	0.25	55,55,55,55	0
82	MG	AS	3662	1/1	0.68	0.12	52,52,52,52	0
82	MG	B	1898	1/1	0.68	0.18	88,88,88,88	0
82	MG	AW	303	1/1	0.68	0.43	78,78,78,78	0
82	MG	CM	1883	1/1	0.68	0.36	67,67,67,67	0
82	MG	CM	1813	1/1	0.69	0.28	65,65,65,65	0
82	MG	AS	3493	1/1	0.69	0.17	55,55,55,55	0
82	MG	AS	3532	1/1	0.69	0.29	69,69,69,69	0
82	MG	AS	3564	1/1	0.69	0.27	60,60,60,60	0
82	MG	AS	3718	1/1	0.69	0.23	56,56,56,56	0
81	PAR	1	3407	42/42	0.69	0.24	63,82,96,104	0
82	MG	CM	1876	1/1	0.69	0.28	76,76,76,76	0
82	MG	B	1849	1/1	0.69	0.40	70,70,70,70	0
82	MG	AS	3461	1/1	0.69	0.26	55,55,55,55	0
82	MG	B	1815	1/1	0.69	0.22	49,49,49,49	0
82	MG	AS	3438	1/1	0.69	0.13	39,39,39,39	0
82	MG	1	3660	1/1	0.69	0.15	42,42,42,42	0
82	MG	1	3682	1/1	0.70	0.24	66,66,66,66	0
82	MG	1	3469	1/1	0.70	0.30	67,67,67,67	0
82	MG	AS	3732	1/1	0.70	0.33	70,70,70,70	0
81	PAR	AS	3405	42/42	0.71	0.18	67,82,94,100	42
82	MG	AS	3643	1/1	0.71	0.18	99,99,99,99	0
82	MG	1	3432	1/1	0.71	0.17	51,51,51,51	0
82	MG	1	3634	1/1	0.71	0.33	60,60,60,60	0
82	MG	1	3448	1/1	0.71	0.24	47,47,47,47	0
82	MG	AS	3670	1/1	0.71	0.19	77,77,77,77	0
82	MG	AS	3415	1/1	0.71	0.21	65,65,65,65	0
81	PAR	CM	1805	42/42	0.71	0.21	98,111,128,146	0
82	MG	CM	1831	1/1	0.71	0.26	68,68,68,68	0
82	MG	B	1822	1/1	0.71	0.29	68,68,68,68	0
83	ZN	d	101	1/1	0.71	0.14	257,257,257,257	0
83	ZN	DO	101	1/1	0.71	0.16	206,206,206,206	0
82	MG	1	3729	1/1	0.72	0.17	45,45,45,45	0
82	MG	CM	1842	1/1	0.72	0.26	56,56,56,56	0
82	MG	AS	3465	1/1	0.72	0.22	69,69,69,69	0
82	MG	B	1837	1/1	0.72	0.17	63,63,63,63	0
82	MG	1	3451	1/1	0.72	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
82	MG	CM	1862	1/1	0.72	0.21	58,58,58,58	0
82	MG	1	3649	1/1	0.72	0.26	56,56,56,56	0
81	PAR	AS	3408	42/42	0.72	0.14	83,105,119,123	0
82	MG	CM	1881	1/1	0.72	0.29	62,62,62,62	0
82	MG	AS	3526	1/1	0.72	0.18	38,38,38,38	0
82	MG	AS	3453	1/1	0.72	0.18	52,52,52,52	0
82	MG	CM	1809	1/1	0.72	0.26	60,60,60,60	0
82	MG	CM	1810	1/1	0.72	0.16	90,90,90,90	0
82	MG	1	3683	1/1	0.72	0.24	56,56,56,56	0
82	MG	AS	3685	1/1	0.72	0.41	75,75,75,75	0
82	MG	AS	3598	1/1	0.72	0.19	39,39,39,39	0
82	MG	AS	3723	1/1	0.73	0.20	46,46,46,46	0
82	MG	AS	3447	1/1	0.73	0.24	55,55,55,55	0
82	MG	AS	3645	1/1	0.73	0.38	60,60,60,60	0
82	MG	B	1943	1/1	0.73	0.21	68,68,68,68	0
81	PAR	B	1805	42/42	0.73	0.18	60,85,96,102	0
82	MG	1	3434	1/1	0.73	0.12	36,36,36,36	0
82	MG	1	3437	1/1	0.73	0.16	54,54,54,54	0
82	MG	AS	3679	1/1	0.73	0.16	68,68,68,68	0
82	MG	AS	3463	1/1	0.73	0.12	46,46,46,46	0
81	PAR	1	3413	42/42	0.73	0.39	50,82,99,113	42
82	MG	B	1823	1/1	0.73	0.27	41,41,41,41	0
82	MG	B	1940	1/1	0.73	0.40	65,65,65,65	0
82	MG	CM	1840	1/1	0.73	0.32	51,51,51,51	0
82	MG	AS	3472	1/1	0.73	0.28	55,55,55,55	0
82	MG	AL	101	1/1	0.74	0.22	94,94,94,94	0
82	MG	AS	3482	1/1	0.74	0.28	72,72,72,72	0
81	PAR	1	3403	42/42	0.74	0.21	47,63,78,89	42
82	MG	1	3663	1/1	0.74	0.27	52,52,52,52	0
82	MG	CM	1854	1/1	0.74	0.31	65,65,65,65	0
82	MG	E	301	1/1	0.74	0.23	49,49,49,49	0
82	MG	B	1895	1/1	0.74	0.23	53,53,53,53	0
82	MG	1	3724	1/1	0.74	0.40	57,57,57,57	0
82	MG	AS	3567	1/1	0.74	0.23	60,60,60,60	0
82	MG	1	3668	1/1	0.74	0.21	37,37,37,37	0
82	MG	AS	3686	1/1	0.74	0.35	47,47,47,47	0
82	MG	AS	3711	1/1	0.74	0.23	53,53,53,53	0
82	MG	1	3754	1/1	0.74	0.36	59,59,59,59	0
82	MG	CM	1832	1/1	0.74	0.22	56,56,56,56	0
82	MG	AS	3428	1/1	0.74	0.29	56,56,56,56	0
82	MG	1	3535	1/1	0.74	0.17	34,34,34,34	0
82	MG	AS	3516	1/1	0.75	0.32	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	1	3759	1/1	0.75	0.36	65,65,65,65	0
81	PAR	1	3408	42/42	0.75	0.27	64,90,104,113	42
81	PAR	AS	3401	42/42	0.75	0.21	59,75,88,93	42
82	MG	AS	3740	1/1	0.75	0.15	63,63,63,63	0
82	MG	CM	1890	1/1	0.75	0.28	62,62,62,62	0
82	MG	AS	3651	1/1	0.75	0.18	68,68,68,68	0
81	PAR	1	3414	42/42	0.75	0.20	51,85,92,99	0
82	MG	CM	1938	1/1	0.75	0.19	46,46,46,46	0
82	MG	B	1813	1/1	0.75	0.25	59,59,59,59	0
81	PAR	1	3422	42/42	0.75	0.24	56,73,85,89	42
82	MG	1	3458	1/1	0.75	0.22	56,56,56,56	0
82	MG	AS	3454	1/1	0.76	0.31	54,54,54,54	0
82	MG	AS	3519	1/1	0.76	0.18	47,47,47,47	0
82	MG	1	3541	1/1	0.76	0.18	43,43,43,43	0
82	MG	1	3746	1/1	0.76	0.16	48,48,48,48	0
82	MG	1	3750	1/1	0.76	0.18	60,60,60,60	0
81	PAR	1	3420	42/42	0.76	0.17	73,94,115,116	0
82	MG	AS	3466	1/1	0.76	0.17	62,62,62,62	0
82	MG	1	3485	1/1	0.76	0.22	64,64,64,64	0
82	MG	CM	1888	1/1	0.76	0.20	52,52,52,52	0
82	MG	AS	3627	1/1	0.76	0.40	77,77,77,77	0
82	MG	1	3439	1/1	0.76	0.16	41,41,41,41	0
82	MG	AS	3446	1/1	0.76	0.16	54,54,54,54	0
81	PAR	1	3405	42/42	0.76	0.29	41,67,84,99	42
82	MG	CM	1940	1/1	0.76	0.22	56,56,56,56	0
82	MG	CM	1942	1/1	0.76	0.15	64,64,64,64	0
82	MG	AS	3486	1/1	0.76	0.25	60,60,60,60	0
82	MG	1	3718	1/1	0.76	0.14	42,42,42,42	0
81	PAR	B	1804	42/42	0.76	0.20	76,105,123,126	0
82	MG	1	3706	1/1	0.77	0.21	46,46,46,46	0
82	MG	1	3637	1/1	0.77	0.15	50,50,50,50	0
81	PAR	1	3426	42/42	0.77	0.24	49,66,79,86	42
82	MG	1	3728	1/1	0.77	0.26	62,62,62,62	0
81	PAR	1	3409	42/42	0.77	0.18	45,81,100,109	42
82	MG	1	3521	1/1	0.77	0.17	56,56,56,56	0
82	MG	AS	3602	1/1	0.77	0.38	59,59,59,59	0
81	PAR	AS	3410	42/42	0.77	0.18	95,110,119,137	0
82	MG	B	1839	1/1	0.77	0.21	82,82,82,82	0
81	PAR	1	3416	42/42	0.77	0.21	47,71,83,85	42
82	MG	1	3755	1/1	0.77	0.21	46,46,46,46	0
82	MG	AS	3470	1/1	0.77	0.29	74,74,74,74	0
82	MG	1	3578	1/1	0.77	0.25	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	AS	3744	1/1	0.77	0.22	53,53,53,53	0
81	PAR	1	3425	42/42	0.77	0.21	52,74,87,97	42
82	MG	CM	1892	1/1	0.77	0.30	67,67,67,67	0
82	MG	CM	1897	1/1	0.77	0.15	57,57,57,57	0
82	MG	AS	3440	1/1	0.77	0.17	55,55,55,55	0
81	PAR	AS	3403	42/42	0.77	0.20	60,83,97,102	0
82	MG	AS	3492	1/1	0.77	0.17	68,68,68,68	0
82	MG	B	1808	1/1	0.77	0.12	73,73,73,73	0
82	MG	CM	1818	1/1	0.77	0.39	70,70,70,70	0
82	MG	AS	3494	1/1	0.77	0.24	55,55,55,55	0
82	MG	B	1919	1/1	0.77	0.38	65,65,65,65	0
82	MG	CM	1835	1/1	0.77	0.17	64,64,64,64	0
81	PAR	AS	3409	42/42	0.78	0.21	51,66,89,100	42
82	MG	AS	3636	1/1	0.78	0.19	92,92,92,92	0
82	MG	AS	3638	1/1	0.78	0.16	71,71,71,71	0
82	MG	1	3490	1/1	0.78	0.42	58,58,58,58	0
82	MG	CM	1825	1/1	0.78	0.22	74,74,74,74	0
82	MG	B	1873	1/1	0.78	0.20	53,53,53,53	0
82	MG	AS	3474	1/1	0.78	0.28	43,43,43,43	0
82	MG	AS	3479	1/1	0.78	0.16	39,39,39,39	0
82	MG	1	3733	1/1	0.78	0.19	56,56,56,56	0
82	MG	AS	3432	1/1	0.78	0.20	52,52,52,52	0
82	MG	1	3675	1/1	0.78	0.31	63,63,63,63	0
82	MG	B	1816	1/1	0.78	0.35	60,60,60,60	0
82	MG	AS	3674	1/1	0.78	0.13	49,49,49,49	0
82	MG	AS	3441	1/1	0.78	0.40	55,55,55,55	0
82	MG	B	1914	1/1	0.78	0.15	47,47,47,47	0
82	MG	AS	3499	1/1	0.78	0.12	48,48,48,48	0
82	MG	AS	3703	1/1	0.78	0.26	59,59,59,59	0
82	MG	AS	3501	1/1	0.78	0.38	53,53,53,53	0
82	MG	1	3431	1/1	0.78	0.38	60,60,60,60	0
82	MG	B	1920	1/1	0.78	0.28	71,71,71,71	0
82	MG	1	3477	1/1	0.78	0.19	57,57,57,57	0
82	MG	CM	1887	1/1	0.78	0.21	59,59,59,59	0
82	MG	B	1928	1/1	0.78	0.14	49,49,49,49	0
82	MG	1	3513	1/1	0.78	0.24	75,75,75,75	0
82	MG	1	3457	1/1	0.78	0.31	57,57,57,57	0
82	MG	CM	1894	1/1	0.78	0.21	91,91,91,91	0
82	MG	AS	3586	1/1	0.78	0.25	67,67,67,67	0
82	MG	1	3532	1/1	0.78	0.12	37,37,37,37	0
82	MG	CM	1916	1/1	0.78	0.17	44,44,44,44	0
82	MG	CM	1924	1/1	0.78	0.27	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	AS	3736	1/1	0.78	0.11	41,41,41,41	0
82	MG	B	1840	1/1	0.78	0.30	78,78,78,78	0
82	MG	CM	1939	1/1	0.78	0.13	57,57,57,57	0
82	MG	AS	3614	1/1	0.78	0.16	54,54,54,54	0
82	MG	AS	3743	1/1	0.78	0.15	44,44,44,44	0
82	MG	B	1845	1/1	0.78	0.19	61,61,61,61	0
82	MG	G	301	1/1	0.78	0.15	56,56,56,56	0
81	PAR	AS	3404	42/42	0.78	0.23	59,90,101,107	42
82	MG	B	1913	1/1	0.79	0.20	59,59,59,59	0
82	MG	CM	1874	1/1	0.79	0.34	73,73,73,73	0
82	MG	B	1827	1/1	0.79	0.19	64,64,64,64	0
82	MG	B	1916	1/1	0.79	0.31	59,59,59,59	0
81	PAR	1	3419	42/42	0.79	0.23	34,60,71,89	42
82	MG	AS	3629	1/1	0.79	0.32	70,70,70,70	0
82	MG	CM	1885	1/1	0.79	0.40	60,60,60,60	0
82	MG	B	1836	1/1	0.79	0.30	53,53,53,53	0
82	MG	1	3657	1/1	0.79	0.20	61,61,61,61	0
82	MG	CM	1820	1/1	0.79	0.22	46,46,46,46	0
82	MG	AS	3524	1/1	0.79	0.33	67,67,67,67	0
82	MG	B	1926	1/1	0.79	0.22	54,54,54,54	0
82	MG	AS	3423	1/1	0.79	0.14	49,49,49,49	0
82	MG	AS	3724	1/1	0.79	0.28	51,51,51,51	0
82	MG	CM	1838	1/1	0.79	0.22	79,79,79,79	0
82	MG	AS	3727	1/1	0.79	0.16	67,67,67,67	0
82	MG	AS	3534	1/1	0.79	0.19	56,56,56,56	0
82	MG	1	3507	1/1	0.79	0.12	45,45,45,45	0
82	MG	AS	3426	1/1	0.79	0.30	71,71,71,71	0
82	MG	AS	3572	1/1	0.79	0.22	61,61,61,61	0
82	MG	AS	3488	1/1	0.79	0.13	69,69,69,69	0
82	MG	1	3742	1/1	0.79	0.23	56,56,56,56	0
82	MG	DG	201	1/1	0.79	0.31	74,74,74,74	0
82	MG	CM	1857	1/1	0.79	0.14	42,42,42,42	0
82	MG	1	3757	1/1	0.79	0.39	64,64,64,64	0
82	MG	AS	3505	1/1	0.80	0.22	64,64,64,64	0
82	MG	B	1901	1/1	0.80	0.19	57,57,57,57	0
82	MG	B	1906	1/1	0.80	0.17	55,55,55,55	0
82	MG	B	1831	1/1	0.80	0.15	46,46,46,46	0
82	MG	AS	3419	1/1	0.80	0.13	50,50,50,50	0
82	MG	1	3693	1/1	0.80	0.15	39,39,39,39	0
82	MG	AS	3667	1/1	0.80	0.21	39,39,39,39	0
81	PAR	CM	1802	42/42	0.80	0.19	71,86,101,105	0
82	MG	B	1812	1/1	0.80	0.38	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	1	3600	1/1	0.80	0.10	23,23,23,23	0
82	MG	AS	3427	1/1	0.80	0.24	46,46,46,46	0
82	MG	AS	3680	1/1	0.80	0.13	50,50,50,50	0
82	MG	B	1814	1/1	0.80	0.15	46,46,46,46	0
82	MG	CM	1895	1/1	0.80	0.19	76,76,76,76	0
82	MG	1	3531	1/1	0.80	0.31	53,53,53,53	0
81	PAR	1	3423	42/42	0.80	0.28	53,68,80,84	42
82	MG	B	1927	1/1	0.80	0.25	52,52,52,52	0
82	MG	AS	3619	1/1	0.80	0.20	59,59,59,59	0
82	MG	1	3447	1/1	0.80	0.16	66,66,66,66	0
82	MG	AS	3623	1/1	0.80	0.27	65,65,65,65	0
82	MG	B	1929	1/1	0.80	0.23	51,51,51,51	0
82	MG	1	3459	1/1	0.80	0.48	55,55,55,55	0
82	MG	CM	1941	1/1	0.80	0.12	52,52,52,52	0
82	MG	B	1891	1/1	0.80	0.12	47,47,47,47	0
82	MG	B	1892	1/1	0.80	0.30	79,79,79,79	0
82	MG	1	3771	1/1	0.80	0.13	49,49,49,49	0
82	MG	AS	3729	1/1	0.80	0.30	41,41,41,41	0
81	PAR	1	3427	42/42	0.80	0.17	53,67,80,88	0
82	MG	1	3749	1/1	0.81	0.23	51,51,51,51	0
82	MG	AU	201	1/1	0.81	0.24	71,71,71,71	0
82	MG	1	3701	1/1	0.81	0.14	50,50,50,50	0
82	MG	CM	1882	1/1	0.81	0.33	52,52,52,52	0
82	MG	1	3460	1/1	0.81	0.20	51,51,51,51	0
82	MG	AS	3690	1/1	0.81	0.20	19,19,19,19	0
82	MG	AS	3699	1/1	0.81	0.23	57,57,57,57	0
82	MG	AS	3702	1/1	0.81	0.14	50,50,50,50	0
82	MG	1	3454	1/1	0.81	0.16	52,52,52,52	0
82	MG	B	1853	1/1	0.81	0.29	55,55,55,55	0
81	PAR	1	3410	42/42	0.81	0.22	40,78,96,113	0
82	MG	B	1871	1/1	0.81	0.19	52,52,52,52	0
81	PAR	B	1802	42/42	0.81	0.19	55,81,98,105	0
82	MG	1	3440	1/1	0.81	0.23	50,50,50,50	0
82	MG	AS	3530	1/1	0.81	0.26	40,40,40,40	0
82	MG	CM	1905	1/1	0.81	0.23	75,75,75,75	0
82	MG	CM	1906	1/1	0.81	0.18	85,85,85,85	0
82	MG	CM	1912	1/1	0.81	0.20	98,98,98,98	0
82	MG	AS	3435	1/1	0.81	0.11	53,53,53,53	0
82	MG	CM	1919	1/1	0.81	0.28	46,46,46,46	0
82	MG	1	3765	1/1	0.81	0.16	38,38,38,38	0
82	MG	CM	1930	1/1	0.81	0.27	57,57,57,57	0
82	MG	1	3505	1/1	0.81	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	CM	1937	1/1	0.81	0.20	51,51,51,51	0
82	MG	CM	1844	1/1	0.81	0.09	83,83,83,83	0
82	MG	AS	3565	1/1	0.81	0.18	48,48,48,48	0
82	MG	4	203	1/1	0.81	0.13	77,77,77,77	0
82	MG	B	1835	1/1	0.81	0.22	59,59,59,59	0
82	MG	AS	3444	1/1	0.81	0.22	56,56,56,56	0
82	MG	CM	1943	1/1	0.81	0.14	61,61,61,61	0
82	MG	CM	1855	1/1	0.81	0.17	47,47,47,47	0
82	MG	1	3482	1/1	0.81	0.22	42,42,42,42	0
82	MG	1	3743	1/1	0.81	0.23	65,65,65,65	0
82	MG	1	3658	1/1	0.81	0.30	42,42,42,42	0
81	PAR	1	3418	42/42	0.82	0.19	67,85,93,97	42
82	MG	1	3722	1/1	0.82	0.18	41,41,41,41	0
82	MG	1	3653	1/1	0.82	0.26	51,51,51,51	0
82	MG	CM	1843	1/1	0.82	0.17	59,59,59,59	0
82	MG	1	3522	1/1	0.82	0.21	45,45,45,45	0
82	MG	CM	1845	1/1	0.82	0.31	73,73,73,73	0
82	MG	AS	3678	1/1	0.82	0.17	49,49,49,49	0
82	MG	AS	3430	1/1	0.82	0.37	63,63,63,63	0
82	MG	AS	3514	1/1	0.82	0.15	49,49,49,49	0
82	MG	AS	3681	1/1	0.82	0.14	26,26,26,26	0
82	MG	1	3656	1/1	0.82	0.18	62,62,62,62	0
82	MG	B	1902	1/1	0.82	0.19	63,63,63,63	0
81	PAR	B	1803	42/42	0.82	0.24	46,75,88,107	0
82	MG	CM	1864	1/1	0.82	0.18	79,79,79,79	0
82	MG	CM	1865	1/1	0.82	0.21	80,80,80,80	0
82	MG	AS	3693	1/1	0.82	0.12	77,77,77,77	0
82	MG	B	1908	1/1	0.82	0.14	48,48,48,48	0
82	MG	1	3735	1/1	0.82	0.18	34,34,34,34	0
82	MG	1	3495	1/1	0.82	0.10	28,28,28,28	0
81	PAR	CM	1801	42/42	0.82	0.23	72,86,93,103	42
82	MG	AS	3538	1/1	0.82	0.22	40,40,40,40	0
82	MG	1	3500	1/1	0.82	0.21	43,43,43,43	0
82	MG	1	3574	1/1	0.82	0.25	39,39,39,39	0
81	PAR	AS	3406	42/42	0.82	0.14	62,85,101,104	0
82	MG	1	3752	1/1	0.82	0.23	43,43,43,43	0
82	MG	AS	3580	1/1	0.82	0.21	42,42,42,42	0
82	MG	1	3677	1/1	0.82	0.15	43,43,43,43	0
82	MG	AS	3455	1/1	0.82	0.31	61,61,61,61	0
81	PAR	AS	3402	42/42	0.82	0.15	45,64,74,83	0
82	MG	1	3593	1/1	0.82	0.31	44,44,44,44	0
82	MG	AS	3615	1/1	0.82	0.11	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	CM	1902	1/1	0.82	0.19	57,57,57,57	0
82	MG	AS	3617	1/1	0.82	0.18	54,54,54,54	0
81	PAR	4	201	42/42	0.82	0.21	27,47,60,67	42
82	MG	1	3684	1/1	0.82	0.18	56,56,56,56	0
82	MG	B	1935	1/1	0.82	0.18	48,48,48,48	0
82	MG	AS	3626	1/1	0.82	0.21	59,59,59,59	0
82	MG	1	3510	1/1	0.82	0.23	55,55,55,55	0
82	MG	1	3767	1/1	0.82	0.25	48,48,48,48	0
82	MG	CM	1808	1/1	0.82	0.12	87,87,87,87	0
82	MG	CM	1933	1/1	0.82	0.20	84,84,84,84	0
82	MG	B	1942	1/1	0.82	0.17	56,56,56,56	0
82	MG	1	3697	1/1	0.82	0.30	49,49,49,49	0
82	MG	B	1858	1/1	0.82	0.14	64,64,64,64	0
82	MG	AS	3478	1/1	0.82	0.16	43,43,43,43	0
82	MG	1	3444	1/1	0.82	0.18	56,56,56,56	0
82	MG	B	1867	1/1	0.82	0.38	52,52,52,52	0
82	MG	j	301	1/1	0.82	0.09	24,24,24,24	0
82	MG	1	3642	1/1	0.82	0.18	57,57,57,57	0
82	MG	AS	3654	1/1	0.82	0.22	55,55,55,55	0
82	MG	B	1880	1/1	0.82	0.22	61,61,61,61	0
82	MG	B	1887	1/1	0.82	0.24	61,61,61,61	0
82	MG	1	3455	1/1	0.83	0.16	57,57,57,57	0
82	MG	AS	3621	1/1	0.83	0.21	54,54,54,54	0
82	MG	1	3770	1/1	0.83	0.17	42,42,42,42	0
82	MG	1	3630	1/1	0.83	0.30	56,56,56,56	0
81	PAR	1	3428	42/42	0.83	0.16	48,62,70,102	0
81	PAR	AS	3411	42/42	0.83	0.17	53,69,91,96	0
82	MG	AS	3742	1/1	0.83	0.29	42,42,42,42	0
82	MG	1	3539	1/1	0.83	0.18	49,49,49,49	0
82	MG	B	1874	1/1	0.83	0.26	50,50,50,50	0
82	MG	B	1876	1/1	0.83	0.28	41,41,41,41	0
82	MG	CM	1914	1/1	0.83	0.15	80,80,80,80	0
82	MG	1	3453	1/1	0.83	0.25	54,54,54,54	0
82	MG	CM	1918	1/1	0.83	0.13	70,70,70,70	0
82	MG	1	3651	1/1	0.83	0.16	28,28,28,28	0
82	MG	CM	1858	1/1	0.83	0.15	45,45,45,45	0
82	MG	CM	1929	1/1	0.83	0.21	52,52,52,52	0
82	MG	1	3516	1/1	0.83	0.10	49,49,49,49	0
82	MG	CM	1863	1/1	0.83	0.34	41,41,41,41	0
82	MG	AS	3710	1/1	0.83	0.17	57,57,57,57	0
82	MG	AS	3456	1/1	0.83	0.21	42,42,42,42	0
81	PAR	B	1801	42/42	0.83	0.17	62,87,108,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	CM	1816	1/1	0.83	0.14	46,46,46,46	0
82	MG	AS	3497	1/1	0.83	0.18	69,69,69,69	0
82	MG	1	3463	1/1	0.83	0.41	61,61,61,61	0
82	MG	AS	3656	1/1	0.83	0.12	50,50,50,50	0
82	MG	CM	1827	1/1	0.83	0.24	37,37,37,37	0
82	MG	1	3764	1/1	0.83	0.11	34,34,34,34	0
82	MG	B	1932	1/1	0.83	0.28	66,66,66,66	0
82	MG	1	3525	1/1	0.83	0.25	49,49,49,49	0
82	MG	B	1850	1/1	0.83	0.34	52,52,52,52	0
82	MG	1	3520	1/1	0.84	0.14	59,59,59,59	0
82	MG	1	3611	1/1	0.84	0.26	35,35,35,35	0
81	PAR	1	3411	42/42	0.84	0.23	43,64,77,84	0
82	MG	1	3751	1/1	0.84	0.32	54,54,54,54	0
81	PAR	1	3415	42/42	0.84	0.19	30,66,80,91	0
82	MG	AS	3481	1/1	0.84	0.12	42,42,42,42	0
81	PAR	CM	1804	42/42	0.84	0.23	40,67,81,91	0
82	MG	AS	3725	1/1	0.84	0.26	39,39,39,39	0
82	MG	1	3638	1/1	0.84	0.15	29,29,29,29	0
82	MG	AS	3487	1/1	0.84	0.38	50,50,50,50	0
82	MG	1	3499	1/1	0.84	0.14	36,36,36,36	0
82	MG	CM	1879	1/1	0.84	0.14	82,82,82,82	0
82	MG	1	3696	1/1	0.84	0.19	43,43,43,43	0
82	MG	AS	3490	1/1	0.84	0.24	73,73,73,73	0
82	MG	1	3761	1/1	0.84	0.19	54,54,54,54	0
81	PAR	1	3412	42/42	0.84	0.24	60,78,89,98	42
82	MG	B	1918	1/1	0.84	0.28	41,41,41,41	0
82	MG	1	3650	1/1	0.84	0.32	53,53,53,53	0
82	MG	1	3442	1/1	0.84	0.27	38,38,38,38	0
82	MG	1	3537	1/1	0.84	0.17	42,42,42,42	0
82	MG	AS	3504	1/1	0.84	0.11	46,46,46,46	0
82	MG	AS	3648	1/1	0.84	0.13	41,41,41,41	0
82	MG	CM	1807	1/1	0.84	0.26	49,49,49,49	0
82	MG	1	3768	1/1	0.84	0.17	59,59,59,59	0
82	MG	AS	3508	1/1	0.84	0.14	42,42,42,42	0
81	PAR	1	3417	42/42	0.84	0.16	49,70,84,91	0
81	PAR	AS	3412	42/42	0.84	0.15	37,60,77,90	0
82	MG	AS	3657	1/1	0.84	0.17	42,42,42,42	0
82	MG	CM	1815	1/1	0.84	0.15	50,50,50,50	0
82	MG	AS	3449	1/1	0.84	0.35	47,47,47,47	0
82	MG	1	3775	1/1	0.84	0.22	49,49,49,49	0
82	MG	3	201	1/1	0.84	0.18	36,36,36,36	0
82	MG	AS	3528	1/1	0.84	0.30	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
82	MG	1	3484	1/1	0.84	0.15	47,47,47,47	0
82	MG	CM	1926	1/1	0.84	0.15	52,52,52,52	0
82	MG	CM	1829	1/1	0.84	0.24	53,53,53,53	0
82	MG	B	1933	1/1	0.84	0.12	44,44,44,44	0
82	MG	4	209	1/1	0.84	0.24	56,56,56,56	0
81	PAR	1	3404	42/42	0.84	0.18	28,57,75,84	0
82	MG	AS	3553	1/1	0.84	0.12	41,41,41,41	0
82	MG	AS	3682	1/1	0.84	0.10	31,31,31,31	0
82	MG	AS	3563	1/1	0.84	0.30	55,55,55,55	0
82	MG	x	201	1/1	0.84	0.18	26,26,26,26	0
82	MG	1	3579	1/1	0.84	0.10	46,46,46,46	0
82	MG	1	3488	1/1	0.84	0.22	47,47,47,47	0
82	MG	1	3740	1/1	0.84	0.42	57,57,57,57	0
82	MG	1	3664	1/1	0.84	0.23	48,48,48,48	0
82	MG	AS	3581	1/1	0.84	0.10	32,32,32,32	0
82	MG	CM	1852	1/1	0.84	0.18	73,73,73,73	0
82	MG	1	3518	1/1	0.84	0.27	30,30,30,30	0
82	MG	AS	3557	1/1	0.85	0.26	60,60,60,60	0
82	MG	1	3747	1/1	0.85	0.27	48,48,48,48	0
82	MG	CM	1866	1/1	0.85	0.30	70,70,70,70	0
82	MG	1	3614	1/1	0.85	0.20	37,37,37,37	0
82	MG	CM	1873	1/1	0.85	0.22	71,71,71,71	0
82	MG	AS	3660	1/1	0.85	0.21	55,55,55,55	0
82	MG	AS	3483	1/1	0.85	0.20	50,50,50,50	0
82	MG	1	3465	1/1	0.85	0.20	51,51,51,51	0
82	MG	1	3698	1/1	0.85	0.18	35,35,35,35	0
82	MG	AS	3578	1/1	0.85	0.17	46,46,46,46	0
82	MG	AS	3671	1/1	0.85	0.15	56,56,56,56	0
81	PAR	1	3424	42/42	0.85	0.26	56,76,83,87	42
82	MG	1	3661	1/1	0.85	0.22	42,42,42,42	0
82	MG	1	3452	1/1	0.85	0.15	46,46,46,46	0
82	MG	1	3555	1/1	0.85	0.25	36,36,36,36	0
82	MG	1	3503	1/1	0.85	0.23	50,50,50,50	0
82	MG	B	1885	1/1	0.85	0.29	54,54,54,54	0
82	MG	1	3725	1/1	0.85	0.16	29,29,29,29	0
82	MG	1	3726	1/1	0.85	0.18	32,32,32,32	0
82	MG	AS	3689	1/1	0.85	0.31	51,51,51,51	0
82	MG	1	3763	1/1	0.85	0.10	32,32,32,32	0
82	MG	AS	3691	1/1	0.85	0.12	19,19,19,19	0
82	MG	1	3648	1/1	0.85	0.14	52,52,52,52	0
82	MG	1	3472	1/1	0.85	0.15	37,37,37,37	0
82	MG	CM	1909	1/1	0.85	0.20	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	PAR	1	3430	42/42	0.85	0.16	40,63,77,121	0
82	MG	CM	1833	1/1	0.85	0.32	48,48,48,48	0
82	MG	1	3530	1/1	0.85	0.26	50,50,50,50	0
82	MG	AS	3709	1/1	0.85	0.21	38,38,38,38	0
82	MG	AS	3464	1/1	0.85	0.23	35,35,35,35	0
82	MG	1	3736	1/1	0.85	0.14	41,41,41,41	0
82	MG	CM	1841	1/1	0.85	0.17	66,66,66,66	0
81	PAR	AS	3407	42/42	0.85	0.18	49,75,90,103	0
82	MG	1	3772	1/1	0.85	0.23	53,53,53,53	0
82	MG	AS	3717	1/1	0.85	0.33	53,53,53,53	0
82	MG	AS	3632	1/1	0.85	0.21	51,51,51,51	0
82	MG	AS	3719	1/1	0.85	0.15	48,48,48,48	0
82	MG	CM	1850	1/1	0.85	0.21	50,50,50,50	0
81	PAR	1	3406	42/42	0.85	0.20	37,53,72,86	0
82	MG	1	3692	1/1	0.85	0.19	50,50,50,50	0
82	MG	1	3745	1/1	0.85	0.14	38,38,38,38	0
82	MG	4	206	1/1	0.85	0.34	62,62,62,62	0
82	MG	AS	3536	1/1	0.85	0.11	39,39,39,39	0
82	MG	AS	3647	1/1	0.85	0.21	64,64,64,64	0
82	MG	1	3515	1/1	0.85	0.12	47,47,47,47	0
82	MG	AS	3552	1/1	0.85	0.18	53,53,53,53	0
82	MG	B	1852	1/1	0.85	0.18	54,54,54,54	0
82	MG	AS	3659	1/1	0.86	0.21	30,30,30,30	0
82	MG	AS	3475	1/1	0.86	0.15	37,37,37,37	0
82	MG	AS	3477	1/1	0.86	0.32	81,81,81,81	0
81	PAR	1	3402	42/42	0.86	0.13	46,71,82,93	0
82	MG	1	3609	1/1	0.86	0.16	42,42,42,42	0
82	MG	1	3572	1/1	0.86	0.21	35,35,35,35	0
82	MG	CM	1875	1/1	0.86	0.12	57,57,57,57	0
82	MG	1	3509	1/1	0.86	0.15	42,42,42,42	0
82	MG	AY	401	1/1	0.86	0.35	57,57,57,57	0
82	MG	AS	3434	1/1	0.86	0.25	83,83,83,83	0
82	MG	1	3756	1/1	0.86	0.17	45,45,45,45	0
82	MG	B	1861	1/1	0.86	0.27	33,33,33,33	0
82	MG	1	3776	1/1	0.86	0.23	63,63,63,63	0
82	MG	CM	1811	1/1	0.86	0.27	54,54,54,54	0
82	MG	AS	3592	1/1	0.86	0.17	50,50,50,50	0
82	MG	B	1820	1/1	0.86	0.16	53,53,53,53	0
82	MG	B	1870	1/1	0.86	0.10	30,30,30,30	0
82	MG	B	1821	1/1	0.86	0.18	55,55,55,55	0
82	MG	B	1872	1/1	0.86	0.18	50,50,50,50	0
82	MG	1	3615	1/1	0.86	0.23	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	CM	1896	1/1	0.86	0.23	59,59,59,59	0
82	MG	CM	1822	1/1	0.86	0.27	50,50,50,50	0
82	MG	1	3716	1/1	0.86	0.21	37,37,37,37	0
82	MG	AS	3692	1/1	0.86	0.16	40,40,40,40	0
82	MG	CM	1903	1/1	0.86	0.17	81,81,81,81	0
82	MG	1	3481	1/1	0.86	0.12	60,60,60,60	0
82	MG	CM	1830	1/1	0.86	0.18	55,55,55,55	0
82	MG	CM	1907	1/1	0.86	0.13	73,73,73,73	0
82	MG	AS	3452	1/1	0.86	0.12	78,78,78,78	0
82	MG	B	1828	1/1	0.86	0.26	48,48,48,48	0
82	MG	B	1884	1/1	0.86	0.31	54,54,54,54	0
82	MG	AS	3705	1/1	0.86	0.19	52,52,52,52	0
82	MG	1	3633	1/1	0.86	0.26	55,55,55,55	0
82	MG	B	1941	1/1	0.86	0.17	41,41,41,41	0
82	MG	1	3445	1/1	0.86	0.20	43,43,43,43	0
82	MG	B	1890	1/1	0.86	0.33	46,46,46,46	0
82	MG	CM	1928	1/1	0.86	0.12	60,60,60,60	0
82	MG	AS	3714	1/1	0.86	0.32	44,44,44,44	0
82	MG	AS	3521	1/1	0.86	0.15	60,60,60,60	0
82	MG	B	1834	1/1	0.86	0.12	43,43,43,43	0
82	MG	v	302	1/1	0.86	0.24	36,36,36,36	0
82	MG	v	305	1/1	0.86	0.12	39,39,39,39	0
81	PAR	4	202	42/42	0.86	0.14	44,60,80,87	0
82	MG	B	1838	1/1	0.86	0.20	59,59,59,59	0
82	MG	6	202	1/1	0.86	0.14	20,20,20,20	0
82	MG	1	3468	1/1	0.86	0.17	36,36,36,36	0
82	MG	AS	3650	1/1	0.86	0.13	49,49,49,49	0
82	MG	AS	3471	1/1	0.86	0.09	27,27,27,27	0
82	MG	AS	3540	1/1	0.86	0.25	69,69,69,69	0
82	MG	AS	3550	1/1	0.86	0.20	44,44,44,44	0
82	MG	1	3594	1/1	0.86	0.25	54,54,54,54	0
82	MG	B	1809	1/1	0.86	0.37	54,54,54,54	0
82	MG	AS	3568	1/1	0.87	0.17	41,41,41,41	0
82	MG	B	1912	1/1	0.87	0.20	42,42,42,42	0
82	MG	AS	3574	1/1	0.87	0.27	30,30,30,30	0
82	MG	AS	3577	1/1	0.87	0.33	45,45,45,45	0
82	MG	1	3461	1/1	0.87	0.21	37,37,37,37	0
82	MG	1	3491	1/1	0.87	0.20	48,48,48,48	0
82	MG	B	1842	1/1	0.87	0.22	45,45,45,45	0
82	MG	AS	3585	1/1	0.87	0.16	44,44,44,44	0
82	MG	F	301	1/1	0.87	0.17	39,39,39,39	0
82	MG	AS	3721	1/1	0.87	0.31	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
82	MG	AS	3589	1/1	0.87	0.23	59,59,59,59	0
82	MG	B	1917	1/1	0.87	0.28	57,57,57,57	0
82	MG	1	3727	1/1	0.87	0.22	57,57,57,57	0
82	MG	B	1847	1/1	0.87	0.16	33,33,33,33	0
82	MG	AS	3603	1/1	0.87	0.20	43,43,43,43	0
82	MG	AS	3604	1/1	0.87	0.23	46,46,46,46	0
82	MG	AS	3480	1/1	0.87	0.14	28,28,28,28	0
82	MG	p	301	1/1	0.87	0.26	47,47,47,47	0
82	MG	CM	1847	1/1	0.87	0.13	38,38,38,38	0
82	MG	AS	3529	1/1	0.87	0.08	34,34,34,34	0
82	MG	1	3641	1/1	0.87	0.16	50,50,50,50	0
82	MG	1	3436	1/1	0.87	0.11	38,38,38,38	0
82	MG	CM	1917	1/1	0.87	0.21	58,58,58,58	0
82	MG	AS	3485	1/1	0.87	0.29	65,65,65,65	0
81	PAR	1	3421	42/42	0.87	0.14	53,69,76,90	42
82	MG	CM	1920	1/1	0.87	0.23	60,60,60,60	0
82	MG	1	3734	1/1	0.87	0.31	42,42,42,42	0
82	MG	AS	3745	1/1	0.87	0.31	49,49,49,49	0
82	MG	CM	1856	1/1	0.87	0.30	72,72,72,72	0
82	MG	AS	3687	1/1	0.87	0.13	38,38,38,38	0
82	MG	AW	301	1/1	0.87	0.13	50,50,50,50	0
82	MG	AS	3459	1/1	0.87	0.27	62,62,62,62	0
82	MG	AS	3542	1/1	0.87	0.22	26,26,26,26	0
82	MG	1	3719	1/1	0.87	0.28	59,59,59,59	0
82	MG	1	3753	1/1	0.87	0.35	58,58,58,58	0
82	MG	1	3721	1/1	0.87	0.24	39,39,39,39	0
82	MG	1	3737	1/1	0.87	0.31	44,44,44,44	0
82	MG	AS	3700	1/1	0.87	0.17	32,32,32,32	0
82	MG	AS	3433	1/1	0.87	0.25	49,49,49,49	0
82	MG	1	3739	1/1	0.87	0.14	46,46,46,46	0
82	MG	1	3603	1/1	0.87	0.20	23,23,23,23	0
82	MG	AS	3707	1/1	0.87	0.23	50,50,50,50	0
82	MG	CM	1880	1/1	0.87	0.25	54,54,54,54	0
83	ZN	CJ	201	1/1	0.87	0.09	187,187,187,187	0
82	MG	1	3511	1/1	0.87	0.33	52,52,52,52	0
82	MG	1	3446	1/1	0.88	0.07	31,31,31,31	0
82	MG	B	1829	1/1	0.88	0.26	36,36,36,36	0
82	MG	B	1875	1/1	0.88	0.10	53,53,53,53	0
80	3K5	1	3401	57/57	0.88	0.19	42,65,85,102	0
81	PAR	CM	1803	42/42	0.88	0.19	46,63,93,101	0
82	MG	CM	1877	1/1	0.88	0.10	53,53,53,53	0
82	MG	AX	401	1/1	0.88	0.28	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
82	MG	AS	3491	1/1	0.88	0.18	55,55,55,55	0
82	MG	CJ	202	1/1	0.88	0.25	53,53,53,53	0
82	MG	1	3686	1/1	0.88	0.14	40,40,40,40	0
82	MG	AS	3448	1/1	0.88	0.17	25,25,25,25	0
82	MG	1	3731	1/1	0.88	0.13	50,50,50,50	0
82	MG	AS	3496	1/1	0.88	0.11	36,36,36,36	0
82	MG	1	3576	1/1	0.88	0.32	28,28,28,28	0
82	MG	AS	3601	1/1	0.88	0.32	41,41,41,41	0
82	MG	w	301	1/1	0.88	0.27	52,52,52,52	0
82	MG	CM	1891	1/1	0.88	0.16	49,49,49,49	0
82	MG	1	3626	1/1	0.88	0.11	32,32,32,32	0
82	MG	1	3695	1/1	0.88	0.12	36,36,36,36	0
82	MG	AS	3605	1/1	0.88	0.30	24,24,24,24	0
82	MG	AS	3606	1/1	0.88	0.12	33,33,33,33	0
82	MG	1	3450	1/1	0.88	0.10	32,32,32,32	0
82	MG	CM	1823	1/1	0.88	0.28	60,60,60,60	0
82	MG	B	1896	1/1	0.88	0.09	48,48,48,48	0
82	MG	AS	3509	1/1	0.88	0.19	44,44,44,44	0
82	MG	AS	3511	1/1	0.88	0.13	37,37,37,37	0
82	MG	B	1807	1/1	0.88	0.32	59,59,59,59	0
82	MG	B	1900	1/1	0.88	0.34	41,41,41,41	0
82	MG	1	3462	1/1	0.88	0.23	40,40,40,40	0
82	MG	AS	3462	1/1	0.88	0.14	54,54,54,54	0
82	MG	CM	1913	1/1	0.88	0.31	46,46,46,46	0
82	MG	AS	3522	1/1	0.88	0.12	52,52,52,52	0
82	MG	1	3738	1/1	0.88	0.15	55,55,55,55	0
82	MG	B	1904	1/1	0.88	0.14	59,59,59,59	0
82	MG	AS	3417	1/1	0.88	0.16	50,50,50,50	0
82	MG	1	3536	1/1	0.88	0.12	54,54,54,54	0
82	MG	B	1811	1/1	0.88	0.29	49,49,49,49	0
82	MG	CM	1922	1/1	0.88	0.21	45,45,45,45	0
82	MG	AS	3421	1/1	0.88	0.17	60,60,60,60	0
82	MG	1	3766	1/1	0.88	0.15	31,31,31,31	0
82	MG	1	3588	1/1	0.88	0.11	28,28,28,28	0
82	MG	1	3456	1/1	0.88	0.16	31,31,31,31	0
82	MG	AS	3473	1/1	0.88	0.39	65,65,65,65	0
82	MG	1	3464	1/1	0.88	0.09	28,28,28,28	0
82	MG	1	3665	1/1	0.88	0.12	54,54,54,54	0
82	MG	1	3667	1/1	0.88	0.10	35,35,35,35	0
82	MG	1	3595	1/1	0.88	0.20	26,26,26,26	0
82	MG	1	3647	1/1	0.88	0.09	30,30,30,30	0
82	MG	AS	3731	1/1	0.88	0.24	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	PAR	1	3429	42/42	0.88	0.14	37,61,77,89	0
82	MG	AS	3735	1/1	0.88	0.10	35,35,35,35	0
82	MG	B	1923	1/1	0.88	0.29	49,49,49,49	0
82	MG	AS	3737	1/1	0.88	0.20	61,61,61,61	0
82	MG	AS	3436	1/1	0.88	0.28	48,48,48,48	0
82	MG	AS	3566	1/1	0.88	0.13	43,43,43,43	0
82	MG	AS	3437	1/1	0.88	0.20	63,63,63,63	0
82	MG	1	3542	1/1	0.88	0.33	40,40,40,40	0
82	MG	B	1826	1/1	0.89	0.18	64,64,64,64	0
82	MG	CM	1870	1/1	0.89	0.29	41,41,41,41	0
82	MG	AS	3575	1/1	0.89	0.16	47,47,47,47	0
82	MG	AS	3457	1/1	0.89	0.19	43,43,43,43	0
82	MG	v	303	1/1	0.89	0.10	39,39,39,39	0
82	MG	1	3680	1/1	0.89	0.19	25,25,25,25	0
82	MG	AS	3503	1/1	0.89	0.11	44,44,44,44	0
82	MG	B	1909	1/1	0.89	0.16	43,43,43,43	0
82	MG	B	1868	1/1	0.89	0.43	63,63,63,63	0
82	MG	1	3504	1/1	0.89	0.17	36,36,36,36	0
82	MG	1	3606	1/1	0.89	0.16	29,29,29,29	0
82	MG	AS	3595	1/1	0.89	0.23	60,60,60,60	0
82	MG	AS	3683	1/1	0.89	0.22	39,39,39,39	0
82	MG	AS	3684	1/1	0.89	0.13	85,85,85,85	0
82	MG	1	3659	1/1	0.89	0.18	45,45,45,45	0
82	MG	B	1915	1/1	0.89	0.16	43,43,43,43	0
82	MG	B	1832	1/1	0.89	0.24	41,41,41,41	0
82	MG	AS	3518	1/1	0.89	0.13	27,27,27,27	0
82	MG	1	3608	1/1	0.89	0.26	34,34,34,34	0
82	MG	AS	3520	1/1	0.89	0.17	70,70,70,70	0
82	MG	1	3467	1/1	0.89	0.33	48,48,48,48	0
82	MG	1	3662	1/1	0.89	0.10	48,48,48,48	0
82	MG	B	1879	1/1	0.89	0.26	51,51,51,51	0
82	MG	CM	1824	1/1	0.89	0.20	68,68,68,68	0
82	MG	CM	1901	1/1	0.89	0.12	39,39,39,39	0
82	MG	B	1921	1/1	0.89	0.17	38,38,38,38	0
82	MG	AS	3618	1/1	0.89	0.24	27,27,27,27	0
82	MG	1	3551	1/1	0.89	0.18	45,45,45,45	0
82	MG	B	1883	1/1	0.89	0.28	37,37,37,37	0
82	MG	1	3612	1/1	0.89	0.25	40,40,40,40	0
82	MG	1	3480	1/1	0.89	0.28	55,55,55,55	0
82	MG	B	1886	1/1	0.89	0.28	46,46,46,46	0
82	MG	1	3732	1/1	0.89	0.22	39,39,39,39	0
82	MG	CM	1837	1/1	0.89	0.21	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
82	MG	CM	1915	1/1	0.89	0.09	42,42,42,42	0
82	MG	B	1888	1/1	0.89	0.12	49,49,49,49	0
82	MG	B	1931	1/1	0.89	0.14	52,52,52,52	0
82	MG	AS	3541	1/1	0.89	0.19	49,49,49,49	0
82	MG	1	3591	1/1	0.89	0.18	31,31,31,31	0
82	MG	AS	3544	1/1	0.89	0.22	30,30,30,30	0
82	MG	AS	3546	1/1	0.89	0.28	31,31,31,31	0
82	MG	1	3557	1/1	0.89	0.24	26,26,26,26	0
82	MG	4	205	1/1	0.89	0.11	36,36,36,36	0
82	MG	AS	3644	1/1	0.89	0.11	56,56,56,56	0
82	MG	1	3496	1/1	0.89	0.24	39,39,39,39	0
82	MG	CM	1849	1/1	0.89	0.10	58,58,58,58	0
82	MG	AS	3646	1/1	0.89	0.16	66,66,66,66	0
82	MG	B	1938	1/1	0.89	0.23	39,39,39,39	0
82	MG	CM	1935	1/1	0.89	0.16	53,53,53,53	0
82	MG	CM	1936	1/1	0.89	0.16	64,64,64,64	0
82	MG	AS	3560	1/1	0.89	0.15	65,65,65,65	0
82	MG	AS	3561	1/1	0.89	0.22	32,32,32,32	0
82	MG	B	1819	1/1	0.89	0.20	66,66,66,66	0
82	MG	AS	3653	1/1	0.89	0.12	28,28,28,28	0
82	MG	1	3715	1/1	0.89	0.12	43,43,43,43	0
82	MG	1	3527	1/1	0.89	0.12	22,22,22,22	0
82	MG	1	3717	1/1	0.89	0.32	53,53,53,53	0
82	MG	CM	1944	1/1	0.89	0.27	63,63,63,63	0
82	MG	CM	1945	1/1	0.89	0.19	74,74,74,74	0
82	MG	B	1944	1/1	0.89	0.23	30,30,30,30	0
82	MG	1	3438	1/1	0.89	0.14	35,35,35,35	0
82	MG	DK	201	1/1	0.89	0.20	44,44,44,44	0
82	MG	AS	3495	1/1	0.89	0.09	28,28,28,28	0
82	MG	AS	3741	1/1	0.89	0.11	31,31,31,31	0
82	MG	AS	3661	1/1	0.89	0.29	33,33,33,33	0
82	MG	AS	3594	1/1	0.90	0.16	32,32,32,32	0
82	MG	v	301	1/1	0.90	0.06	36,36,36,36	0
82	MG	1	3548	1/1	0.90	0.13	33,33,33,33	0
82	MG	1	3700	1/1	0.90	0.09	28,28,28,28	0
82	MG	AS	3422	1/1	0.90	0.12	56,56,56,56	0
82	MG	1	3760	1/1	0.90	0.21	49,49,49,49	0
82	MG	1	3629	1/1	0.90	0.09	52,52,52,52	0
82	MG	CM	1886	1/1	0.90	0.25	44,44,44,44	0
82	MG	AS	3425	1/1	0.90	0.17	44,44,44,44	0
82	MG	AS	3527	1/1	0.90	0.31	59,59,59,59	0
82	MG	AS	3609	1/1	0.90	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
82	MG	1	3704	1/1	0.90	0.08	19,19,19,19	0
82	MG	1	3705	1/1	0.90	0.09	23,23,23,23	0
82	MG	1	3669	1/1	0.90	0.11	46,46,46,46	0
82	MG	AS	3531	1/1	0.90	0.17	72,72,72,72	0
82	MG	1	3710	1/1	0.90	0.09	37,37,37,37	0
82	MG	AS	3697	1/1	0.90	0.24	46,46,46,46	0
82	MG	CM	1898	1/1	0.90	0.18	56,56,56,56	0
82	MG	CM	1899	1/1	0.90	0.25	43,43,43,43	0
82	MG	B	1881	1/1	0.90	0.16	54,54,54,54	0
82	MG	1	3712	1/1	0.90	0.37	50,50,50,50	0
82	MG	AS	3622	1/1	0.90	0.33	38,38,38,38	0
82	MG	1	3558	1/1	0.90	0.22	52,52,52,52	0
82	MG	AS	3625	1/1	0.90	0.08	35,35,35,35	0
82	MG	1	3583	1/1	0.90	0.20	40,40,40,40	0
82	MG	AS	3708	1/1	0.90	0.25	38,38,38,38	0
82	MG	CM	1908	1/1	0.90	0.26	43,43,43,43	0
82	MG	1	3568	1/1	0.90	0.13	43,43,43,43	0
82	MG	CM	1910	1/1	0.90	0.13	67,67,67,67	0
82	MG	1	3635	1/1	0.90	0.33	70,70,70,70	0
82	MG	1	3586	1/1	0.90	0.25	30,30,30,30	0
82	MG	1	3569	1/1	0.90	0.16	35,35,35,35	0
82	MG	1	3590	1/1	0.90	0.11	35,35,35,35	0
82	MG	1	3550	1/1	0.90	0.14	21,21,21,21	0
82	MG	AS	3637	1/1	0.90	0.12	73,73,73,73	0
82	MG	B	1893	1/1	0.90	0.31	51,51,51,51	0
82	MG	AS	3554	1/1	0.90	0.27	36,36,36,36	0
82	MG	B	1851	1/1	0.90	0.10	49,49,49,49	0
82	MG	CM	1921	1/1	0.90	0.09	57,57,57,57	0
82	MG	1	3690	1/1	0.90	0.07	40,40,40,40	0
82	MG	CM	1923	1/1	0.90	0.31	58,58,58,58	0
82	MG	B	1939	1/1	0.90	0.14	41,41,41,41	0
82	MG	1	3646	1/1	0.90	0.13	38,38,38,38	0
82	MG	B	1857	1/1	0.90	0.17	39,39,39,39	0
82	MG	1	3489	1/1	0.90	0.24	34,34,34,34	0
82	MG	B	1859	1/1	0.90	0.36	38,38,38,38	0
82	MG	CM	1931	1/1	0.90	0.30	55,55,55,55	0
82	MG	B	1860	1/1	0.90	0.15	51,51,51,51	0
82	MG	AS	3652	1/1	0.90	0.13	48,48,48,48	0
82	MG	AS	3498	1/1	0.90	0.20	45,45,45,45	0
82	MG	B	1945	1/1	0.90	0.16	67,67,67,67	0
82	MG	AS	3734	1/1	0.90	0.28	49,49,49,49	0
82	MG	AS	3500	1/1	0.90	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	C	301	1/1	0.90	0.36	66,66,66,66	0
82	MG	B	1905	1/1	0.90	0.32	42,42,42,42	0
82	MG	AS	3458	1/1	0.90	0.18	40,40,40,40	0
82	MG	AS	3579	1/1	0.90	0.20	49,49,49,49	0
82	MG	4	207	1/1	0.90	0.15	35,35,35,35	0
82	MG	B	1863	1/1	0.90	0.17	74,74,74,74	0
82	MG	K	301	1/1	0.90	0.21	54,54,54,54	0
82	MG	1	3476	1/1	0.90	0.13	38,38,38,38	0
82	MG	1	3616	1/1	0.90	0.29	51,51,51,51	0
82	MG	AS	3747	1/1	0.90	0.13	41,41,41,41	0
82	MG	CL	301	1/1	0.90	0.14	87,87,87,87	0
82	MG	AS	3591	1/1	0.90	0.22	38,38,38,38	0
82	MG	AS	3673	1/1	0.90	0.19	44,44,44,44	0
82	MG	1	3666	1/1	0.90	0.24	41,41,41,41	0
82	MG	1	3493	1/1	0.91	0.22	50,50,50,50	0
82	MG	1	3441	1/1	0.91	0.26	41,41,41,41	0
82	MG	AS	3715	1/1	0.91	0.20	45,45,45,45	0
82	MG	1	3435	1/1	0.91	0.20	38,38,38,38	0
82	MG	1	3623	1/1	0.91	0.18	36,36,36,36	0
82	MG	AS	3590	1/1	0.91	0.24	26,26,26,26	0
82	MG	B	1899	1/1	0.91	0.13	42,42,42,42	0
82	MG	CM	1834	1/1	0.91	0.37	63,63,63,63	0
82	MG	B	1936	1/1	0.91	0.08	59,59,59,59	0
82	MG	1	3741	1/1	0.91	0.15	46,46,46,46	0
82	MG	1	3688	1/1	0.91	0.11	32,32,32,32	0
82	MG	AS	3596	1/1	0.91	0.17	65,65,65,65	0
82	MG	6	201	1/1	0.91	0.19	49,49,49,49	0
82	MG	1	3474	1/1	0.91	0.12	27,27,27,27	0
82	MG	AS	3664	1/1	0.91	0.17	45,45,45,45	0
82	MG	B	1833	1/1	0.91	0.22	38,38,38,38	0
82	MG	AB	201	1/1	0.91	0.15	26,26,26,26	0
82	MG	AS	3445	1/1	0.91	0.12	46,46,46,46	0
82	MG	1	3556	1/1	0.91	0.15	25,25,25,25	0
82	MG	1	3486	1/1	0.91	0.18	36,36,36,36	0
82	MG	1	3694	1/1	0.91	0.13	37,37,37,37	0
82	MG	AS	3677	1/1	0.91	0.10	59,59,59,59	0
82	MG	B	1911	1/1	0.91	0.18	58,58,58,58	0
82	MG	1	3632	1/1	0.91	0.12	15,15,15,15	0
82	MG	1	3517	1/1	0.91	0.13	36,36,36,36	0
82	MG	AS	3549	1/1	0.91	0.14	32,32,32,32	0
82	MG	1	3562	1/1	0.91	0.21	29,29,29,29	0
82	MG	AS	3551	1/1	0.91	0.16	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	1	3670	1/1	0.91	0.18	41,41,41,41	0
82	MG	f	102	1/1	0.91	0.11	55,55,55,55	0
82	MG	CM	1859	1/1	0.91	0.21	36,36,36,36	0
82	MG	AS	3746	1/1	0.91	0.07	40,40,40,40	0
82	MG	CM	1927	1/1	0.91	0.20	52,52,52,52	0
82	MG	B	1843	1/1	0.91	0.22	37,37,37,37	0
82	MG	1	3671	1/1	0.91	0.10	53,53,53,53	0
82	MG	B	1882	1/1	0.91	0.21	36,36,36,36	0
82	MG	AS	3418	1/1	0.91	0.14	35,35,35,35	0
82	MG	CM	1868	1/1	0.91	0.23	39,39,39,39	0
82	MG	B	1846	1/1	0.91	0.29	52,52,52,52	0
82	MG	4	204	1/1	0.91	0.17	51,51,51,51	0
82	MG	1	3673	1/1	0.91	0.09	22,22,22,22	0
82	MG	AS	3694	1/1	0.91	0.21	53,53,53,53	0
82	MG	B	1922	1/1	0.91	0.25	43,43,43,43	0
82	MG	1	3492	1/1	0.91	0.20	29,29,29,29	0
82	MG	1	3589	1/1	0.91	0.29	36,36,36,36	0
82	MG	CM	1878	1/1	0.91	0.25	42,42,42,42	0
82	MG	AS	3569	1/1	0.91	0.18	36,36,36,36	0
82	MG	1	3546	1/1	0.91	0.23	43,43,43,43	0
82	MG	AS	3704	1/1	0.91	0.10	61,61,61,61	0
82	MG	1	3709	1/1	0.91	0.16	29,29,29,29	0
82	MG	AS	3513	1/1	0.91	0.31	31,31,31,31	0
82	MG	AS	3468	1/1	0.91	0.18	56,56,56,56	0
82	MG	CM	1819	1/1	0.91	0.34	58,58,58,58	0
82	MG	1	3639	1/1	0.91	0.22	56,56,56,56	0
82	MG	B	1854	1/1	0.91	0.16	37,37,37,37	0
82	MG	AS	3429	1/1	0.91	0.10	38,38,38,38	0
82	MG	AS	3712	1/1	0.91	0.12	41,41,41,41	0
82	MG	1	3512	1/1	0.92	0.13	27,27,27,27	0
82	MG	AS	3635	1/1	0.92	0.08	43,43,43,43	0
82	MG	4	208	1/1	0.92	0.27	33,33,33,33	0
82	MG	1	3582	1/1	0.92	0.22	31,31,31,31	0
82	MG	CM	1821	1/1	0.92	0.12	61,61,61,61	0
82	MG	CM	1867	1/1	0.92	0.16	49,49,49,49	0
82	MG	1	3470	1/1	0.92	0.33	73,73,73,73	0
82	MG	1	3769	1/1	0.92	0.13	34,34,34,34	0
82	MG	AS	3641	1/1	0.92	0.13	29,29,29,29	0
82	MG	CM	1872	1/1	0.92	0.21	52,52,52,52	0
82	MG	AS	3642	1/1	0.92	0.18	49,49,49,49	0
82	MG	AS	3547	1/1	0.92	0.20	25,25,25,25	0
82	MG	AS	3688	1/1	0.92	0.22	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
82	MG	AS	3733	1/1	0.92	0.11	45,45,45,45	0
82	MG	AS	3510	1/1	0.92	0.17	40,40,40,40	0
82	MG	1	3676	1/1	0.92	0.20	36,36,36,36	0
82	MG	AS	3512	1/1	0.92	0.16	36,36,36,36	0
82	MG	1	3475	1/1	0.92	0.17	25,25,25,25	0
82	MG	B	1878	1/1	0.92	0.16	41,41,41,41	0
82	MG	B	1924	1/1	0.92	0.24	32,32,32,32	0
82	MG	1	3599	1/1	0.92	0.18	20,20,20,20	0
82	MG	1	3478	1/1	0.92	0.06	44,44,44,44	0
82	MG	1	3601	1/1	0.92	0.15	43,43,43,43	0
82	MG	AS	3562	1/1	0.92	0.08	37,37,37,37	0
82	MG	B	1817	1/1	0.92	0.16	48,48,48,48	0
82	MG	CM	1934	1/1	0.92	0.25	53,53,53,53	0
82	MG	B	1907	1/1	0.92	0.35	48,48,48,48	0
82	MG	CM	1889	1/1	0.92	0.09	50,50,50,50	0
82	MG	1	3640	1/1	0.92	0.10	32,32,32,32	0
82	MG	1	3748	1/1	0.92	0.16	55,55,55,55	0
82	MG	1	3554	1/1	0.92	0.23	34,34,34,34	0
82	MG	B	1862	1/1	0.92	0.16	41,41,41,41	0
82	MG	B	1934	1/1	0.92	0.21	30,30,30,30	0
82	MG	1	3577	1/1	0.92	0.08	29,29,29,29	0
82	MG	1	3563	1/1	0.92	0.21	25,25,25,25	0
82	MG	B	1844	1/1	0.92	0.24	51,51,51,51	0
82	MG	B	1806	1/1	0.92	0.17	38,38,38,38	0
82	MG	AS	3535	1/1	0.92	0.18	39,39,39,39	0
82	MG	AS	3451	1/1	0.92	0.15	59,59,59,59	0
82	MG	DJ	201	1/1	0.92	0.14	38,38,38,38	0
82	MG	AS	3502	1/1	0.92	0.14	39,39,39,39	0
82	MG	AS	3676	1/1	0.92	0.07	43,43,43,43	0
83	ZN	AH	201	1/1	0.92	0.16	134,134,134,134	0
82	MG	CM	1904	1/1	0.92	0.10	43,43,43,43	0
83	ZN	h	201	1/1	0.92	0.10	165,165,165,165	0
82	MG	AS	3539	1/1	0.92	0.15	31,31,31,31	0
82	MG	AS	3584	1/1	0.92	0.23	29,29,29,29	0
82	MG	AS	3608	1/1	0.93	0.21	38,38,38,38	0
82	MG	1	3533	1/1	0.93	0.07	22,22,22,22	0
82	MG	AS	3612	1/1	0.93	0.08	51,51,51,51	0
82	MG	1	3534	1/1	0.93	0.16	16,16,16,16	0
82	MG	1	3514	1/1	0.93	0.23	45,45,45,45	0
82	MG	1	3559	1/1	0.93	0.21	16,16,16,16	0
82	MG	AP	202	1/1	0.93	0.17	61,61,61,61	0
82	MG	CM	1814	1/1	0.93	0.25	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	1	3592	1/1	0.93	0.25	37,37,37,37	0
82	MG	1	3613	1/1	0.93	0.25	30,30,30,30	0
82	MG	CM	1817	1/1	0.93	0.20	43,43,43,43	0
82	MG	1	3773	1/1	0.93	0.11	49,49,49,49	0
82	MG	1	3560	1/1	0.93	0.18	16,16,16,16	0
82	MG	1	3561	1/1	0.93	0.24	23,23,23,23	0
82	MG	AS	3624	1/1	0.93	0.13	34,34,34,34	0
82	MG	1	3644	1/1	0.93	0.11	34,34,34,34	0
82	MG	1	3581	1/1	0.93	0.10	16,16,16,16	0
82	MG	1	3617	1/1	0.93	0.22	26,26,26,26	0
82	MG	1	3466	1/1	0.93	0.12	24,24,24,24	0
82	MG	CM	1826	1/1	0.93	0.11	28,28,28,28	0
82	MG	1	3625	1/1	0.93	0.20	24,24,24,24	0
82	MG	CM	1828	1/1	0.93	0.18	29,29,29,29	0
82	MG	1	3730	1/1	0.93	0.24	42,42,42,42	0
82	MG	AS	3582	1/1	0.93	0.17	25,25,25,25	0
82	MG	AS	3634	1/1	0.93	0.09	42,42,42,42	0
82	MG	1	3473	1/1	0.93	0.21	59,59,59,59	0
82	MG	B	1818	1/1	0.93	0.43	58,58,58,58	0
82	MG	AS	3439	1/1	0.93	0.13	50,50,50,50	0
82	MG	1	3627	1/1	0.93	0.14	34,34,34,34	0
82	MG	1	3449	1/1	0.93	0.23	32,32,32,32	0
82	MG	1	3602	1/1	0.93	0.11	16,16,16,16	0
82	MG	AS	3506	1/1	0.93	0.13	35,35,35,35	0
82	MG	AS	3593	1/1	0.93	0.24	40,40,40,40	0
82	MG	1	3655	1/1	0.93	0.13	20,20,20,20	0
82	MG	1	3707	1/1	0.93	0.23	34,34,34,34	0
82	MG	CM	1893	1/1	0.93	0.15	51,51,51,51	0
82	MG	B	1824	1/1	0.93	0.20	25,25,25,25	0
82	MG	B	1825	1/1	0.93	0.25	44,44,44,44	0
82	MG	AS	3600	1/1	0.93	0.20	38,38,38,38	0
82	MG	CM	1846	1/1	0.93	0.07	44,44,44,44	0
82	MG	1	3708	1/1	0.93	0.23	25,25,25,25	0
82	MG	AT	201	1/1	0.93	0.12	37,37,37,37	0
82	MG	1	3678	1/1	0.93	0.11	50,50,50,50	0
82	MG	1	3523	1/1	0.93	0.08	28,28,28,28	0
82	MG	AS	3515	1/1	0.93	0.09	43,43,43,43	0
82	MG	1	3605	1/1	0.93	0.19	29,29,29,29	0
82	MG	AS	3517	1/1	0.93	0.09	34,34,34,34	0
82	MG	AS	3607	1/1	0.93	0.21	32,32,32,32	0
82	MG	1	3774	1/1	0.94	0.20	57,57,57,57	0
82	MG	1	3744	1/1	0.94	0.22	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
82	MG	1	3714	1/1	0.94	0.15	28,28,28,28	0
82	MG	1	3543	1/1	0.94	0.21	20,20,20,20	0
82	MG	AS	3543	1/1	0.94	0.13	31,31,31,31	0
82	MG	1	3565	1/1	0.94	0.24	29,29,29,29	0
82	MG	AS	3599	1/1	0.94	0.38	59,59,59,59	0
82	MG	AS	3545	1/1	0.94	0.19	38,38,38,38	0
82	MG	1	3685	1/1	0.94	0.13	43,43,43,43	0
82	MG	1	3566	1/1	0.94	0.25	19,19,19,19	0
82	MG	AS	3726	1/1	0.94	0.37	53,53,53,53	0
82	MG	AS	3548	1/1	0.94	0.15	37,37,37,37	0
82	MG	1	3687	1/1	0.94	0.25	22,22,22,22	0
82	MG	AS	3663	1/1	0.94	0.21	47,47,47,47	0
82	MG	1	3544	1/1	0.94	0.12	26,26,26,26	0
82	MG	AS	3665	1/1	0.94	0.09	40,40,40,40	0
82	MG	AS	3666	1/1	0.94	0.09	73,73,73,73	0
82	MG	1	3620	1/1	0.94	0.21	25,25,25,25	0
82	MG	CM	1911	1/1	0.94	0.13	70,70,70,70	0
82	MG	B	1894	1/1	0.94	0.16	39,39,39,39	0
82	MG	1	3643	1/1	0.94	0.10	39,39,39,39	0
82	MG	1	3621	1/1	0.94	0.18	23,23,23,23	0
82	MG	AS	3555	1/1	0.94	0.09	34,34,34,34	0
82	MG	AS	3556	1/1	0.94	0.24	22,22,22,22	0
82	MG	B	1897	1/1	0.94	0.27	59,59,59,59	0
82	MG	AS	3616	1/1	0.94	0.18	71,71,71,71	0
82	MG	1	3645	1/1	0.94	0.23	22,22,22,22	0
82	MG	1	3585	1/1	0.94	0.07	33,33,33,33	0
82	MG	1	3443	1/1	0.94	0.10	36,36,36,36	0
82	MG	1	3604	1/1	0.94	0.26	24,24,24,24	0
82	MG	AS	3476	1/1	0.94	0.20	30,30,30,30	0
82	MG	CM	1861	1/1	0.94	0.08	46,46,46,46	0
82	MG	CM	1925	1/1	0.94	0.26	34,34,34,34	0
82	MG	v	304	1/1	0.94	0.22	50,50,50,50	0
82	MG	B	1864	1/1	0.94	0.22	30,30,30,30	0
82	MG	1	3570	1/1	0.94	0.08	38,38,38,38	0
82	MG	1	3547	1/1	0.94	0.17	42,42,42,42	0
82	MG	1	3607	1/1	0.94	0.21	29,29,29,29	0
82	MG	AS	3570	1/1	0.94	0.11	66,66,66,66	0
82	MG	AS	3571	1/1	0.94	0.17	23,23,23,23	0
82	MG	B	1869	1/1	0.94	0.21	38,38,38,38	0
82	MG	AS	3573	1/1	0.94	0.11	43,43,43,43	0
82	MG	1	3703	1/1	0.94	0.24	18,18,18,18	0
82	MG	AS	3633	1/1	0.94	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	AS	3523	1/1	0.94	0.24	34,34,34,34	0
82	MG	AS	3576	1/1	0.94	0.14	42,42,42,42	0
82	MG	AS	3698	1/1	0.94	0.22	42,42,42,42	0
82	MG	AS	3484	1/1	0.94	0.15	39,39,39,39	0
82	MG	1	3674	1/1	0.94	0.19	18,18,18,18	0
82	MG	AS	3701	1/1	0.94	0.20	34,34,34,34	0
82	MG	1	3652	1/1	0.94	0.14	35,35,35,35	0
82	MG	1	3631	1/1	0.94	0.07	37,37,37,37	0
82	MG	AS	3640	1/1	0.94	0.10	46,46,46,46	0
82	MG	1	3497	1/1	0.94	0.18	32,32,32,32	0
82	MG	AS	3706	1/1	0.94	0.38	49,49,49,49	0
82	MG	AP	203	1/1	0.94	0.15	33,33,33,33	0
82	MG	1	3549	1/1	0.94	0.17	39,39,39,39	0
82	MG	1	3524	1/1	0.94	0.15	32,32,32,32	0
82	MG	1	3508	1/1	0.94	0.16	27,27,27,27	0
82	MG	1	3711	1/1	0.94	0.07	40,40,40,40	0
82	MG	1	3553	1/1	0.94	0.18	25,25,25,25	0
82	MG	1	3713	1/1	0.94	0.15	21,21,21,21	0
82	MG	AS	3649	1/1	0.94	0.09	63,63,63,63	0
82	MG	AS	3696	1/1	0.95	0.21	42,42,42,42	0
82	MG	AS	3533	1/1	0.95	0.11	39,39,39,39	0
82	MG	CM	1836	1/1	0.95	0.19	56,56,56,56	0
82	MG	1	3672	1/1	0.95	0.27	27,27,27,27	0
82	MG	1	3597	1/1	0.95	0.17	26,26,26,26	0
82	MG	B	1877	1/1	0.95	0.25	42,42,42,42	0
82	MG	1	3622	1/1	0.95	0.28	25,25,25,25	0
82	MG	AS	3443	1/1	0.95	0.10	18,18,18,18	0
82	MG	AS	3675	1/1	0.95	0.06	38,38,38,38	0
82	MG	1	3487	1/1	0.95	0.04	24,24,24,24	0
82	MG	1	3723	1/1	0.95	0.22	27,27,27,27	0
82	MG	1	3691	1/1	0.95	0.10	36,36,36,36	0
82	MG	1	3610	1/1	0.95	0.21	41,41,41,41	0
82	MG	AS	3597	1/1	0.95	0.23	33,33,33,33	0
82	MG	1	3528	1/1	0.95	0.15	31,31,31,31	0
82	MG	B	1903	1/1	0.95	0.15	48,48,48,48	0
82	MG	1	3540	1/1	0.95	0.23	25,25,25,25	0
82	MG	1	3529	1/1	0.95	0.16	28,28,28,28	0
82	MG	1	3506	1/1	0.95	0.10	33,33,33,33	0
82	MG	1	3571	1/1	0.95	0.25	18,18,18,18	0
82	MG	AS	3431	1/1	0.95	0.21	25,25,25,25	0
82	MG	1	3526	1/1	0.95	0.20	22,22,22,22	0
82	MG	B	1889	1/1	0.95	0.07	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	1	3699	1/1	0.95	0.08	34,34,34,34	0
82	MG	1	3564	1/1	0.95	0.18	29,29,29,29	0
82	MG	1	3575	1/1	0.95	0.12	33,33,33,33	0
82	MG	B	1855	1/1	0.95	0.16	27,27,27,27	0
82	MG	AW	302	1/1	0.95	0.11	31,31,31,31	0
83	ZN	CB	201	1/1	0.95	0.06	159,159,159,159	0
82	MG	AS	3722	1/1	0.95	0.06	39,39,39,39	0
82	MG	AS	3416	1/1	0.95	0.13	55,55,55,55	0
82	MG	AS	3739	1/1	0.96	0.06	36,36,36,36	0
82	MG	1	3587	1/1	0.96	0.10	23,23,23,23	0
82	MG	1	3702	1/1	0.96	0.16	23,23,23,23	0
82	MG	1	3573	1/1	0.96	0.18	31,31,31,31	0
82	MG	1	3758	1/1	0.96	0.14	27,27,27,27	0
82	MG	1	3567	1/1	0.96	0.12	16,16,16,16	0
82	MG	AS	3507	1/1	0.96	0.18	48,48,48,48	0
82	MG	AS	3558	1/1	0.96	0.22	26,26,26,26	0
82	MG	AS	3559	1/1	0.96	0.17	39,39,39,39	0
82	MG	AS	3695	1/1	0.96	0.29	36,36,36,36	0
82	MG	B	1865	1/1	0.96	0.15	31,31,31,31	0
82	MG	1	3618	1/1	0.96	0.25	19,19,19,19	0
82	MG	AS	3672	1/1	0.96	0.10	34,34,34,34	0
82	MG	1	3619	1/1	0.96	0.31	22,22,22,22	0
82	MG	1	3596	1/1	0.96	0.04	11,11,11,11	0
82	MG	B	1841	1/1	0.96	0.16	40,40,40,40	0
82	MG	CM	1860	1/1	0.96	0.26	46,46,46,46	0
82	MG	1	3494	1/1	0.96	0.07	23,23,23,23	0
82	MG	B	1856	1/1	0.96	0.29	45,45,45,45	0
82	MG	1	3580	1/1	0.96	0.20	27,27,27,27	0
82	MG	AS	3587	1/1	0.96	0.09	20,20,20,20	0
82	MG	AS	3631	1/1	0.96	0.10	67,67,67,67	0
82	MG	AS	3588	1/1	0.96	0.17	20,20,20,20	0
83	ZN	AP	201	1/1	0.96	0.08	153,153,153,153	0
82	MG	1	3720	1/1	0.96	0.15	25,25,25,25	0
82	MG	AS	3611	1/1	0.96	0.12	45,45,45,45	0
82	MG	AS	3658	1/1	0.96	0.12	51,51,51,51	0
83	ZN	CE	101	1/1	0.96	0.06	68,68,68,68	0
82	MG	1	3502	1/1	0.96	0.17	36,36,36,36	0
83	ZN	CK	101	1/1	0.96	0.06	94,94,94,94	0
82	MG	AS	3613	1/1	0.96	0.10	55,55,55,55	0
82	MG	1	3538	1/1	0.97	0.11	52,52,52,52	0
82	MG	1	3552	1/1	0.97	0.05	19,19,19,19	0
82	MG	1	3628	1/1	0.97	0.10	34,34,34,34	0

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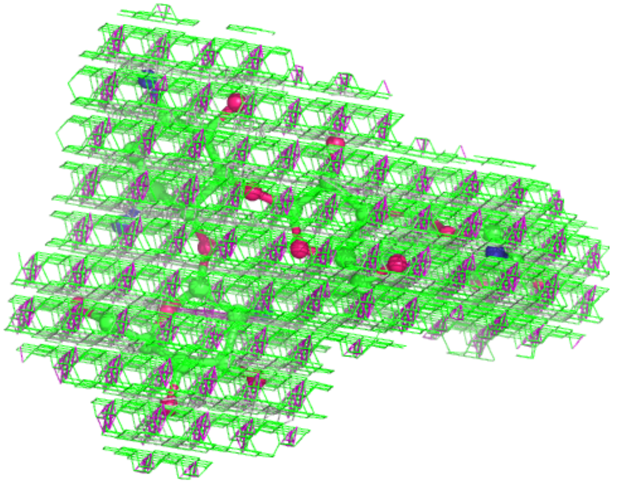
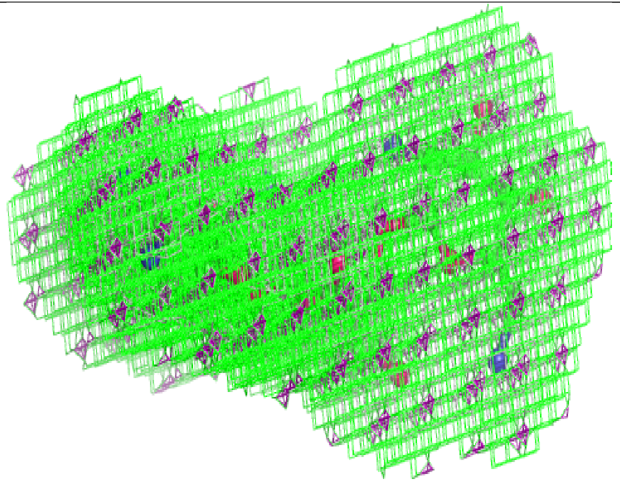
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	MG	1	3433	1/1	0.97	0.15	35,35,35,35	0
82	MG	AS	3583	1/1	0.97	0.15	17,17,17,17	0
83	ZN	AK	101	1/1	0.97	0.17	90,90,90,90	0
82	MG	1	3598	1/1	0.97	0.19	16,16,16,16	0
82	MG	AS	3525	1/1	0.97	0.11	52,52,52,52	0
82	MG	AS	3668	1/1	0.97	0.05	35,35,35,35	0
82	MG	1	3689	1/1	0.97	0.06	28,28,28,28	0
82	MG	1	3624	1/1	0.97	0.05	23,23,23,23	0
82	MG	AS	3610	1/1	0.97	0.09	33,33,33,33	0
82	MG	AS	3537	1/1	0.97	0.14	40,40,40,40	0
82	MG	1	3519	1/1	0.97	0.07	37,37,37,37	0
83	ZN	DQ	101	1/1	0.97	0.05	98,98,98,98	0
82	MG	1	3636	1/1	0.98	0.06	20,20,20,20	0
82	MG	1	3681	1/1	0.98	0.07	19,19,19,19	0
83	ZN	AQ	101	1/1	0.98	0.08	47,47,47,47	0
82	MG	1	3545	1/1	0.98	0.12	20,20,20,20	0
83	ZN	DN	201	1/1	0.98	0.05	98,98,98,98	0
83	ZN	f	101	1/1	0.98	0.05	55,55,55,55	0
82	MG	CM	1871	1/1	0.98	0.17	20,20,20,20	0
83	ZN	CH	101	1/1	0.99	0.09	68,68,68,68	0
83	ZN	c	201	1/1	0.99	0.04	73,73,73,73	0
83	ZN	AN	101	1/1	0.99	0.10	64,64,64,64	0

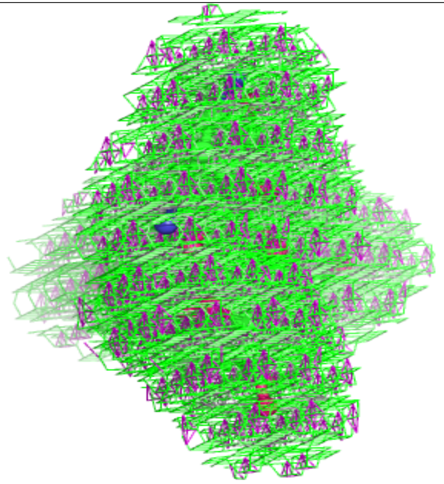
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR CM 1806:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

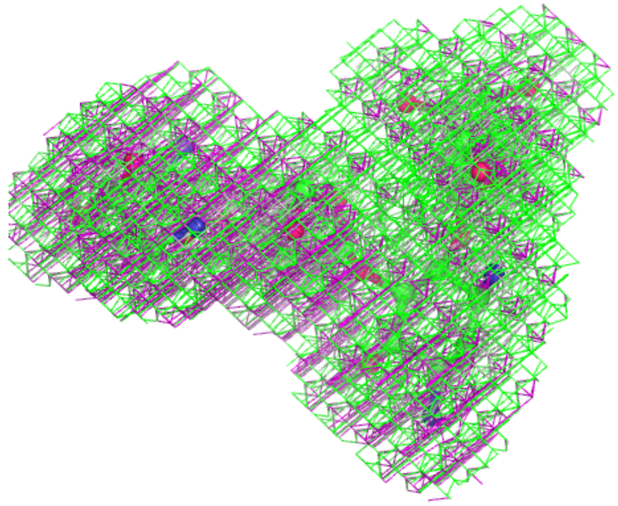


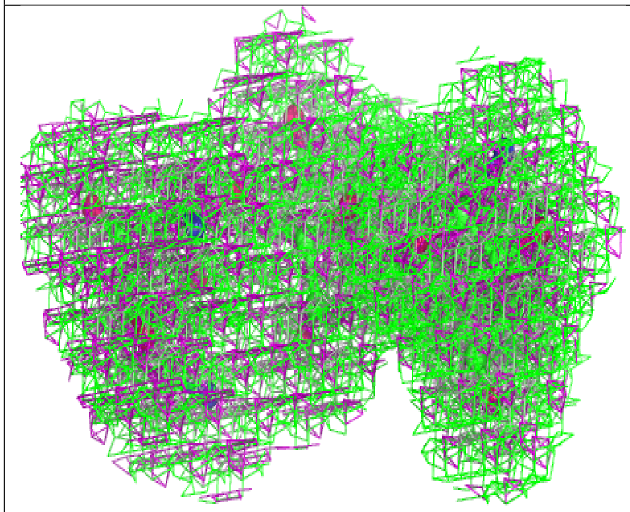


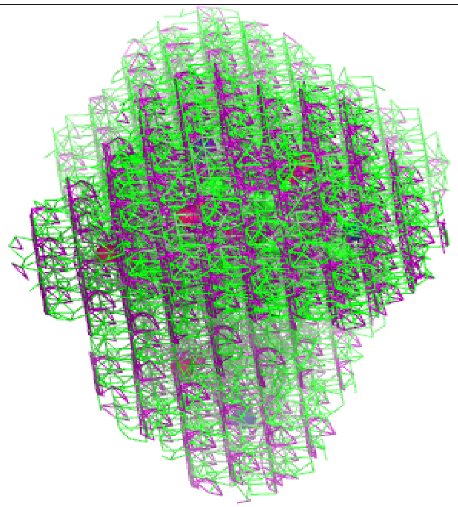


Electron density around PAR AS 3413:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

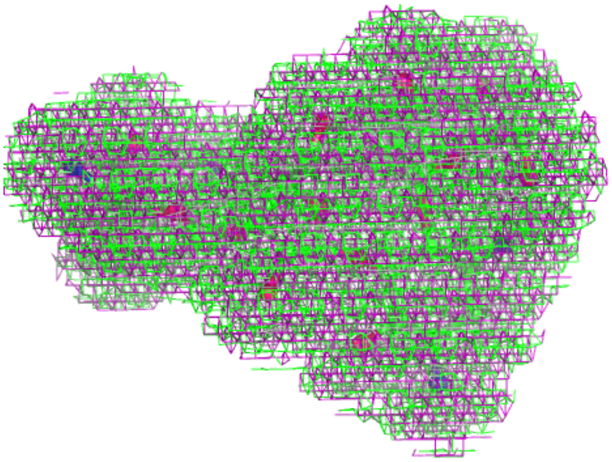


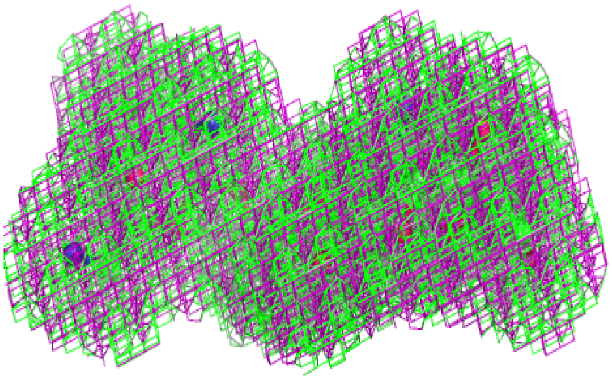


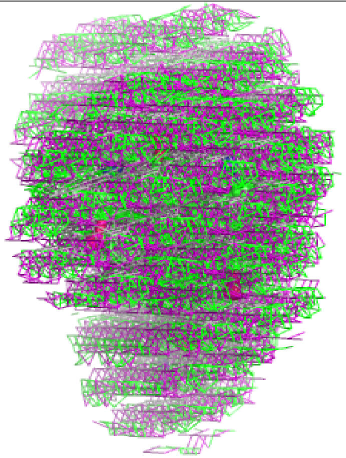


Electron density around PAR 1 3407:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

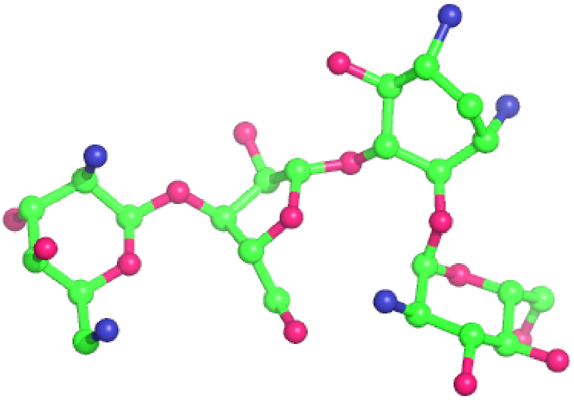


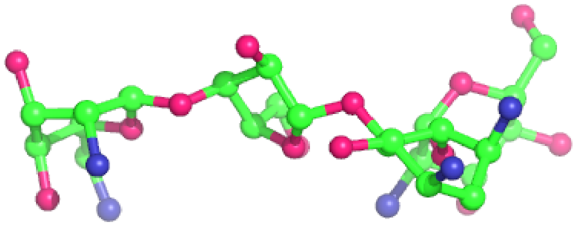


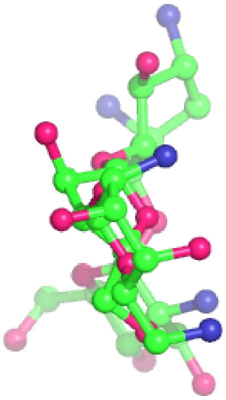


Electron density around PAR AS 3405:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

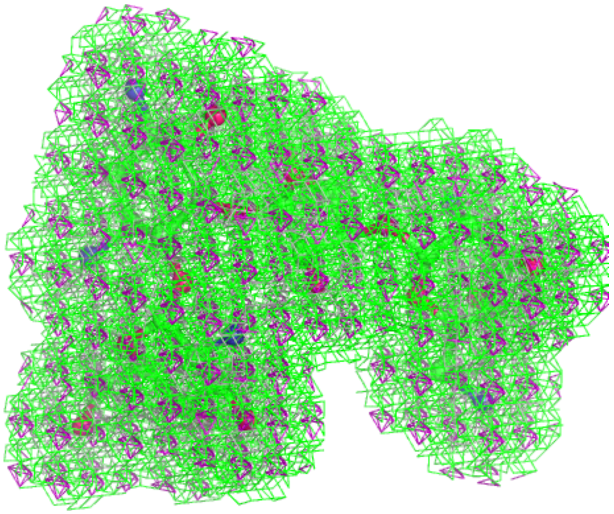


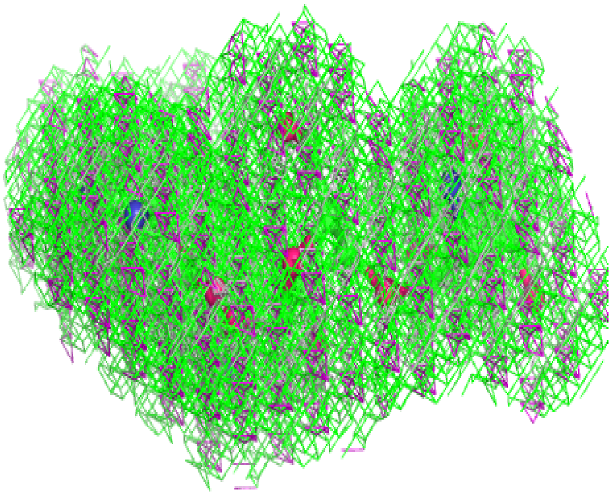


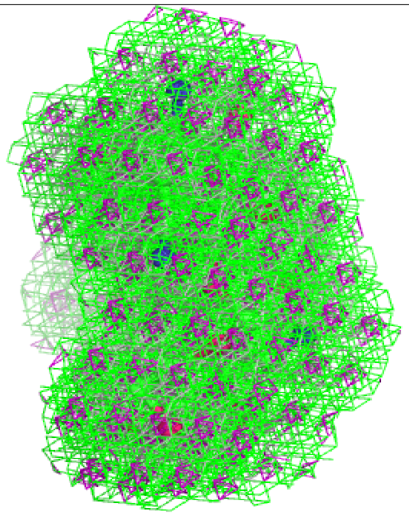


Electron density around PAR CM 1805:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

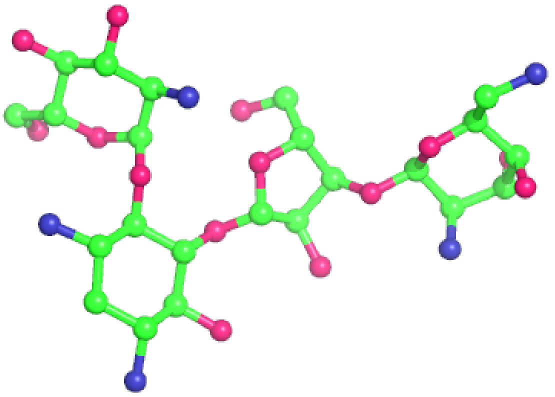


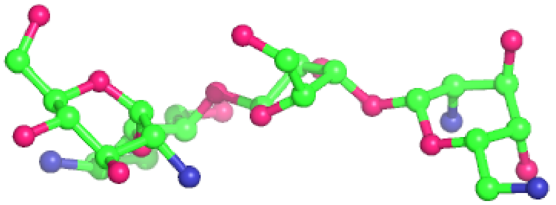


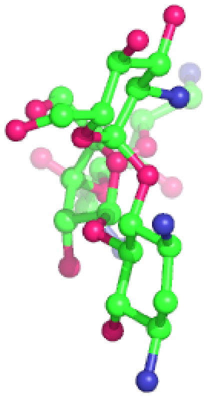


Electron density around PAR AS 3408:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

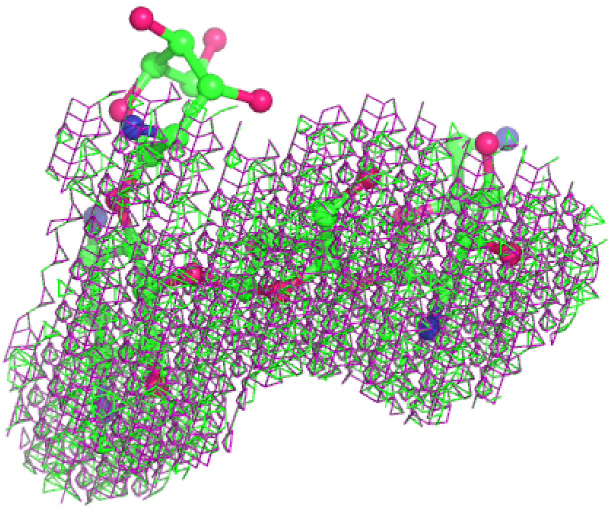


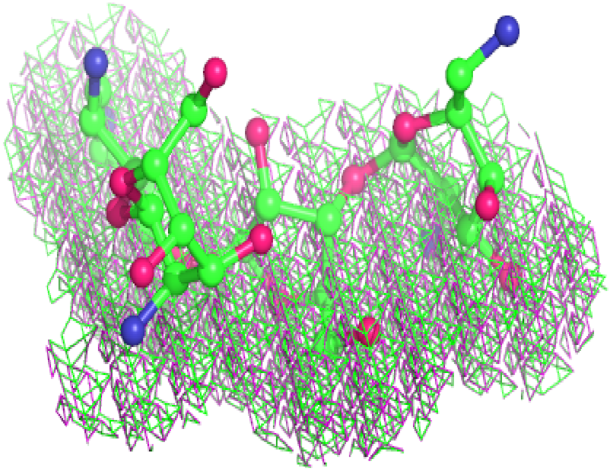


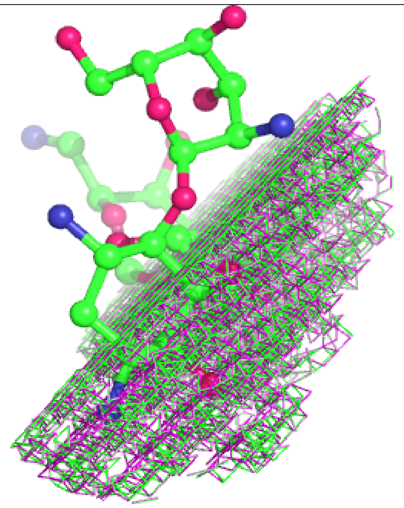


Electron density around PAR B 1805:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

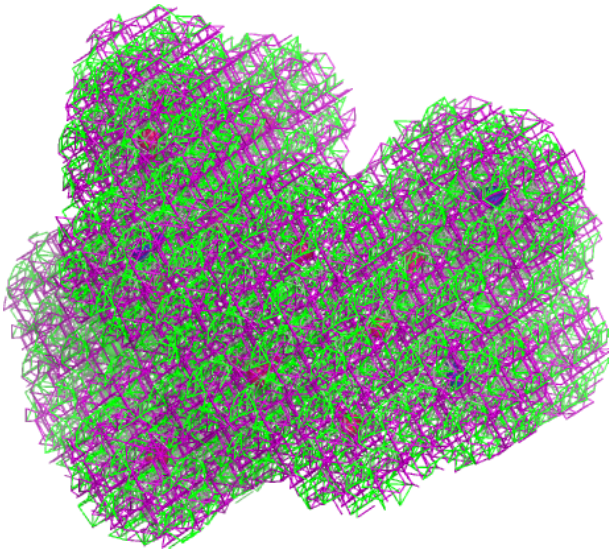


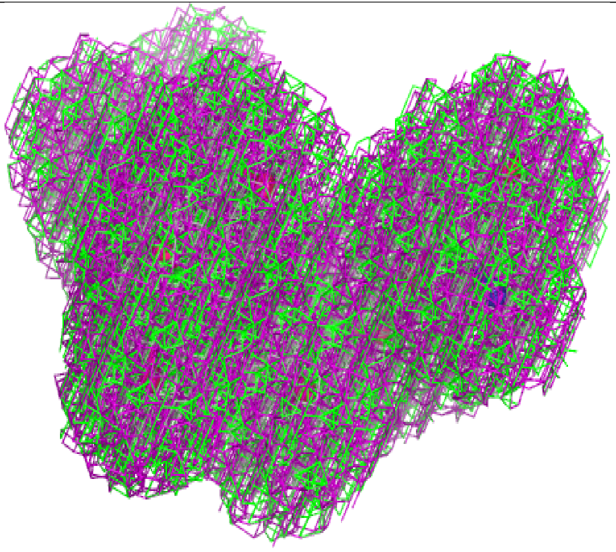


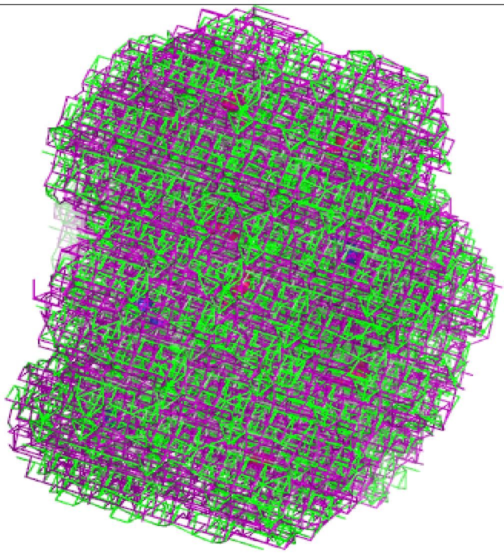


Electron density around PAR 1 3413:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

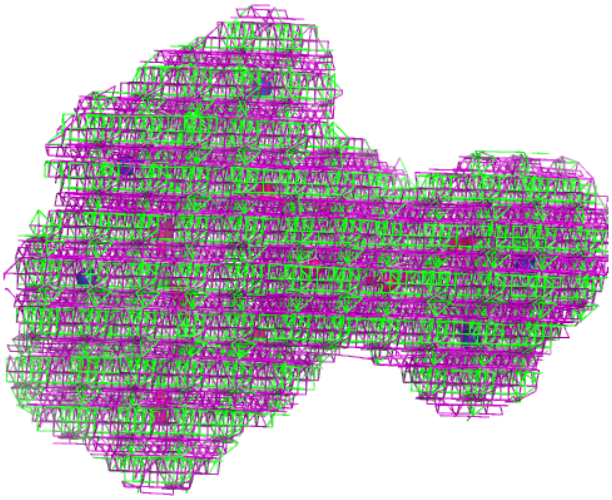


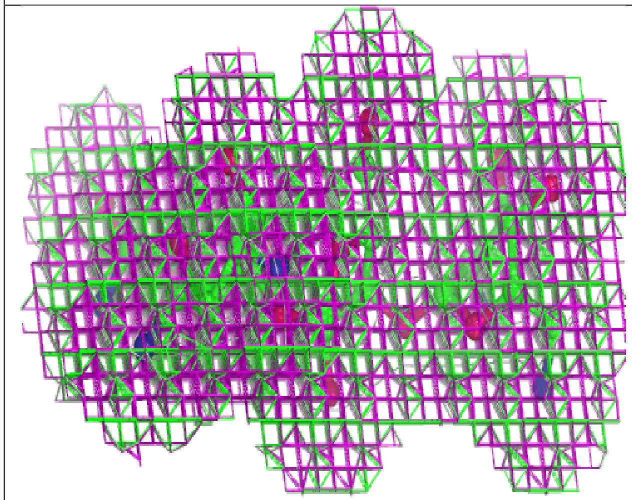


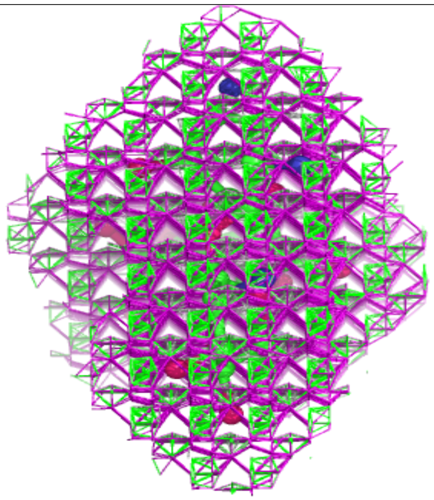


Electron density around PAR 1 3403:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

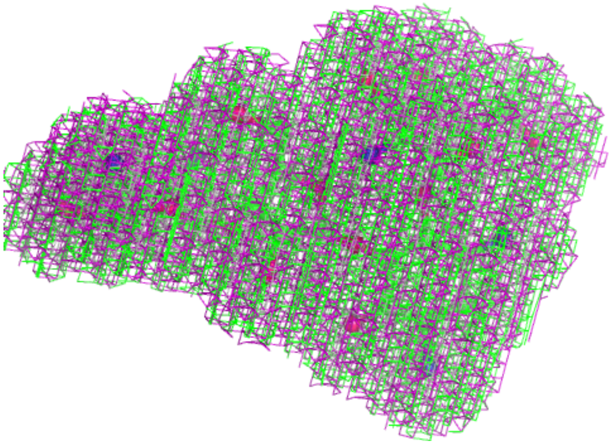


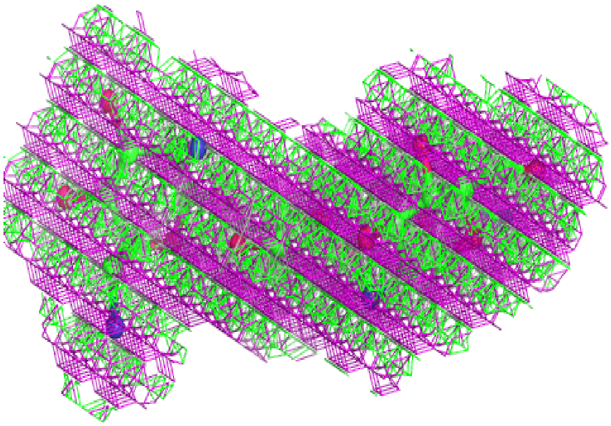


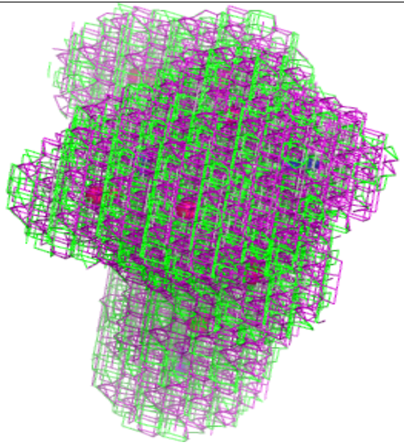


Electron density around PAR 1 3408:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

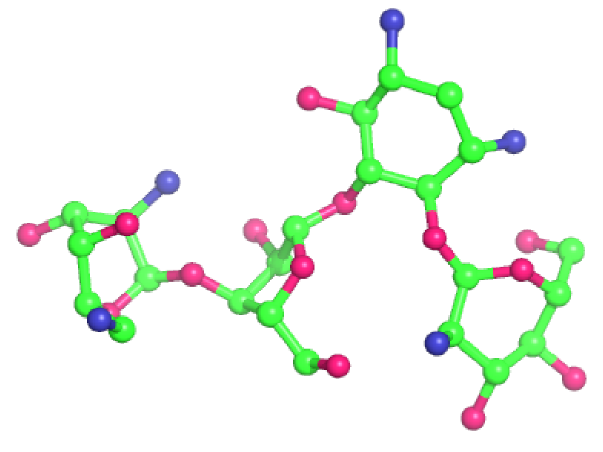


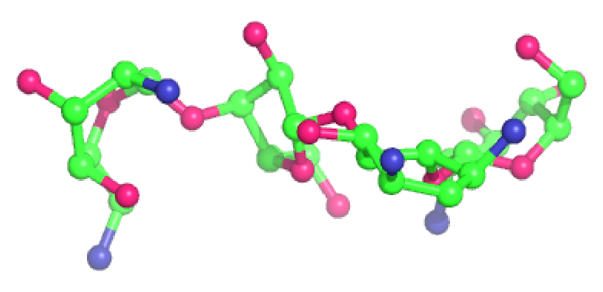


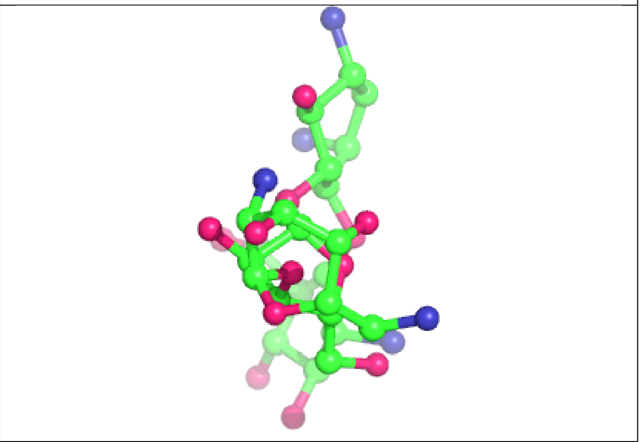


Electron density around PAR AS 3401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

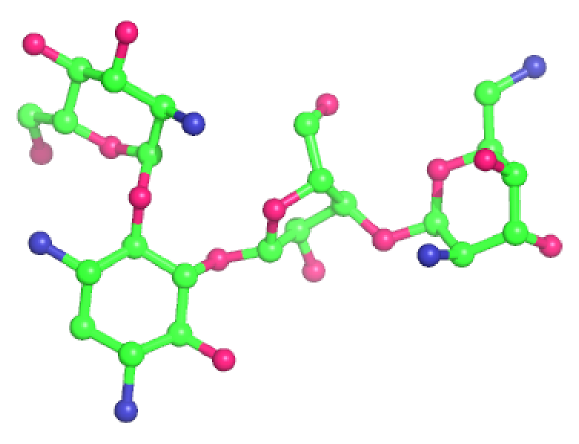


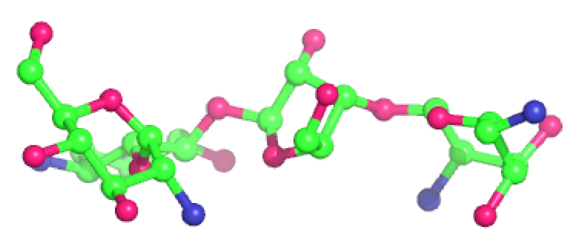


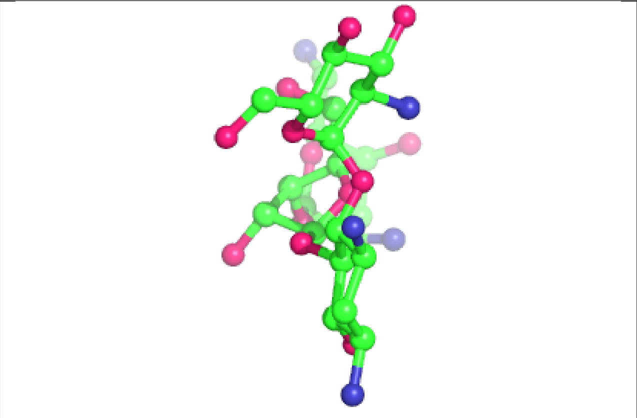


Electron density around PAR 1 3414:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

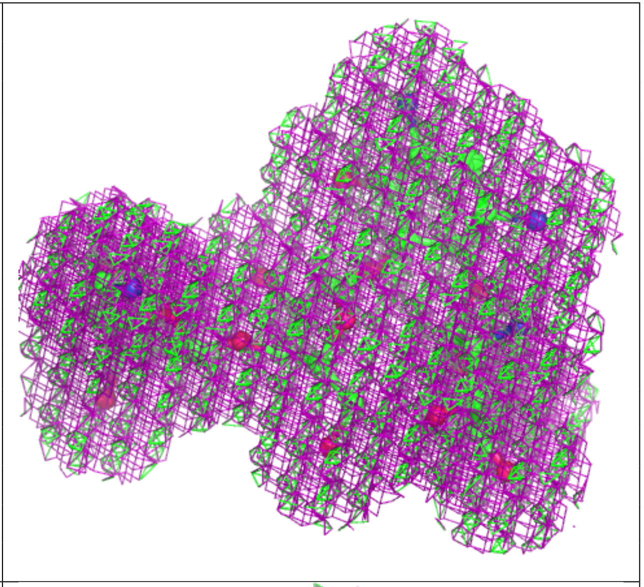


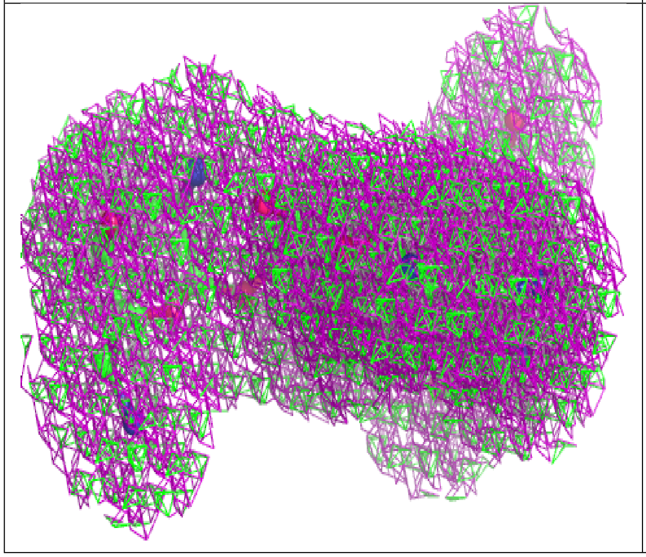


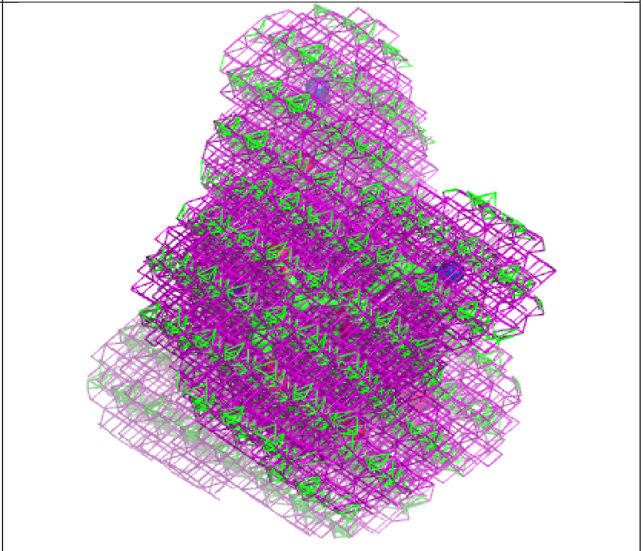


Electron density around PAR 1 3422:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

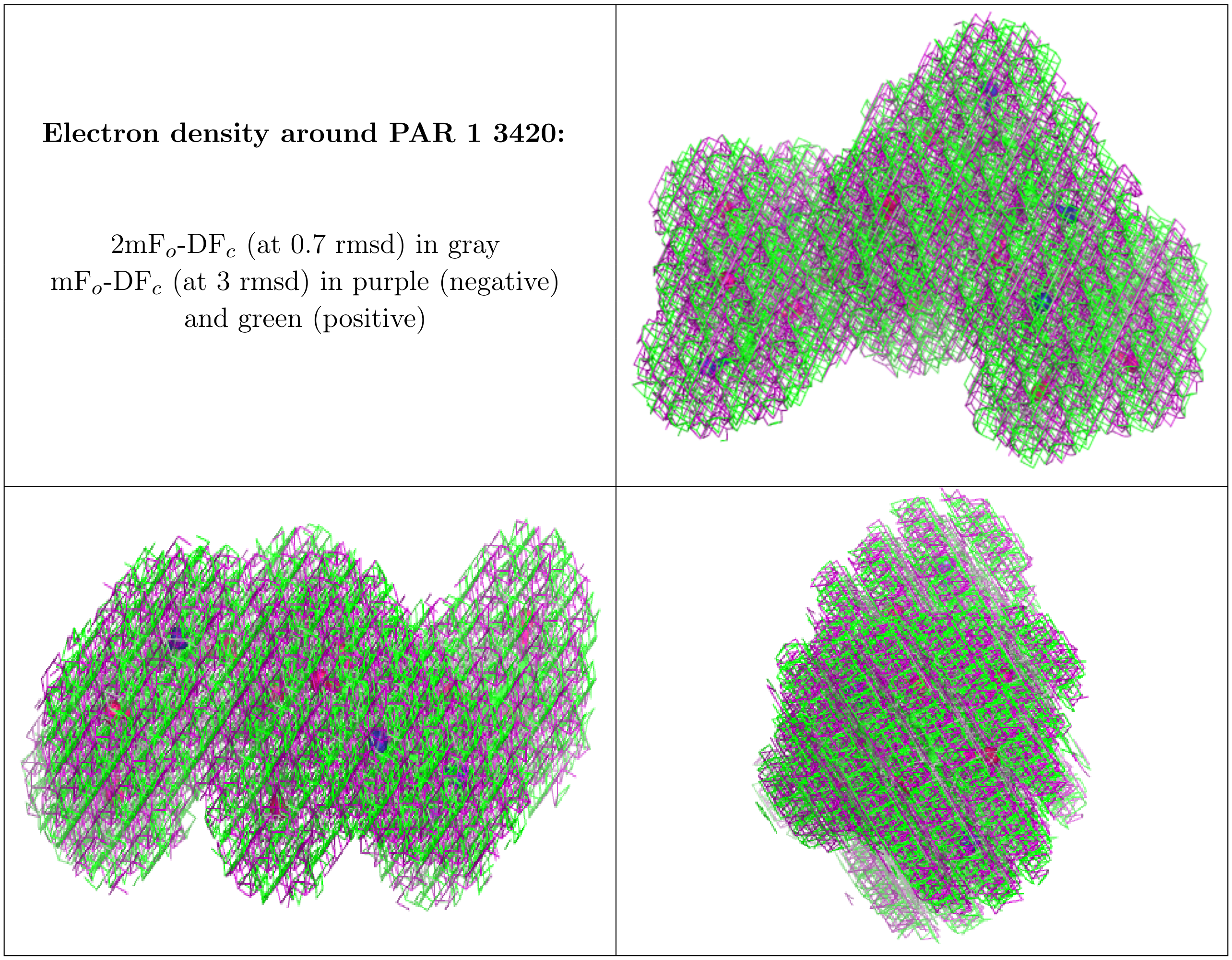






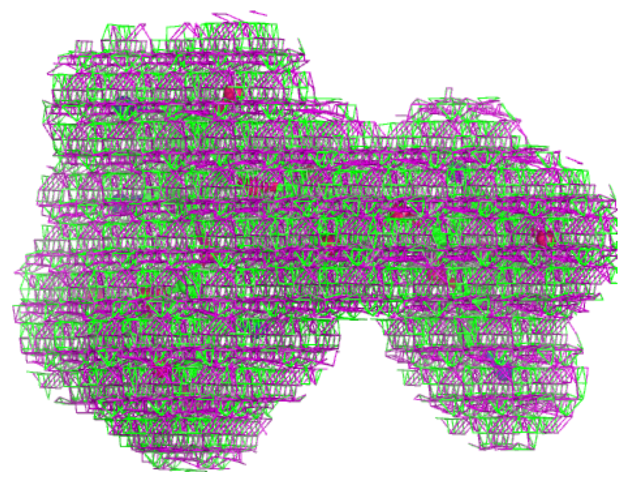
Electron density around PAR 1 3420:

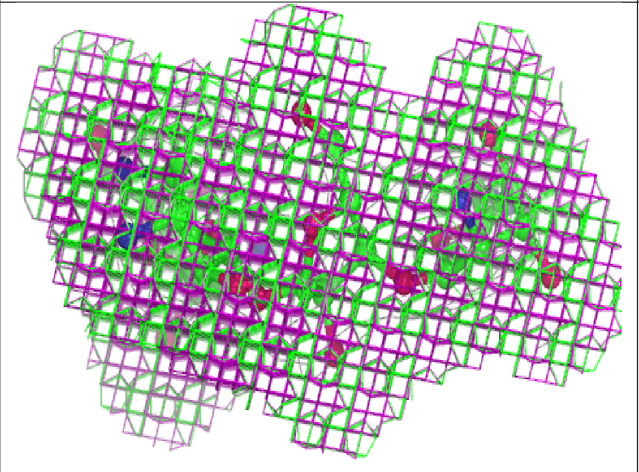
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

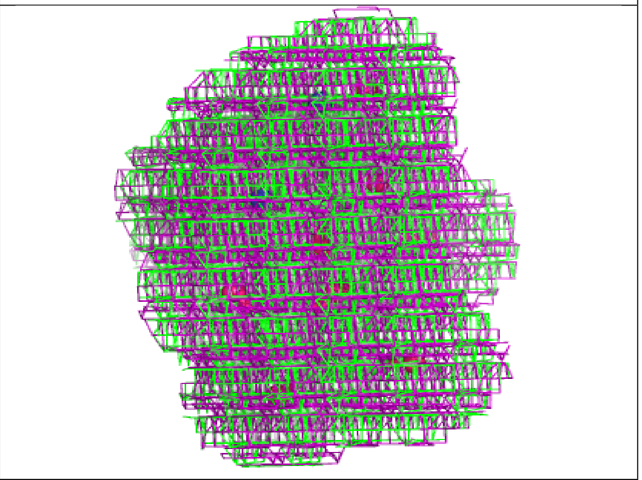


Electron density around PAR 1 3405:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

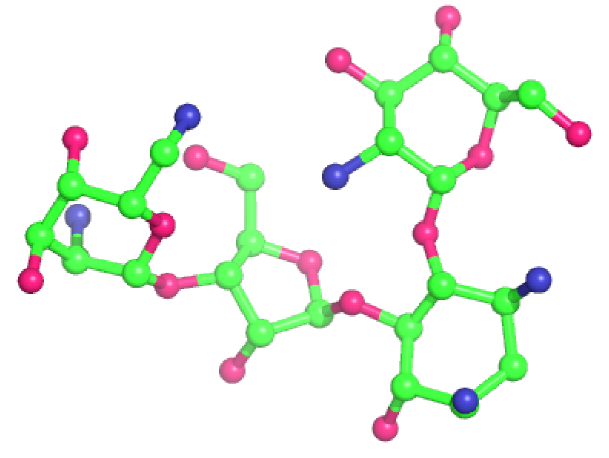


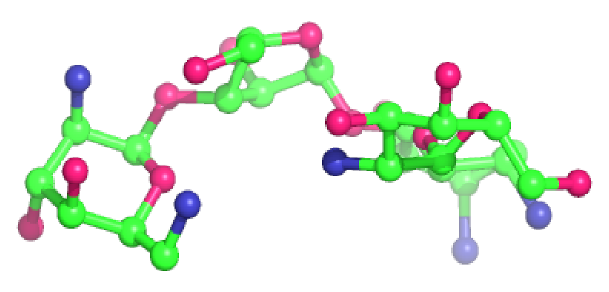


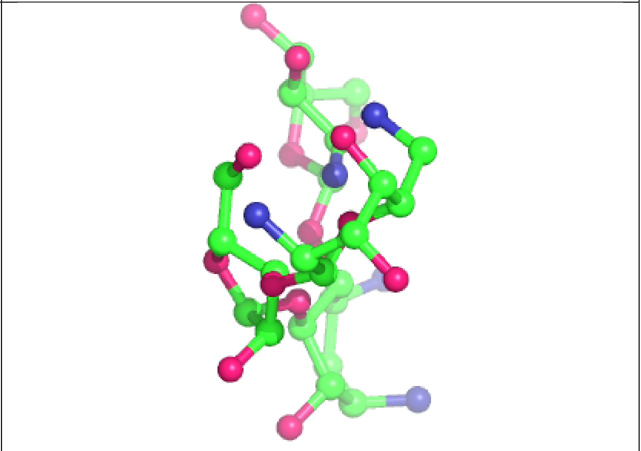


Electron density around PAR B 1804:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

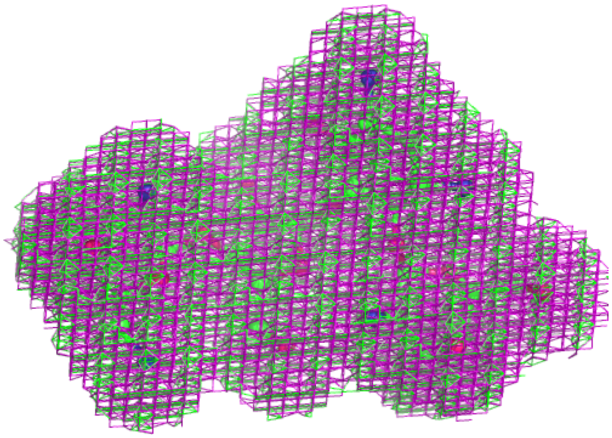


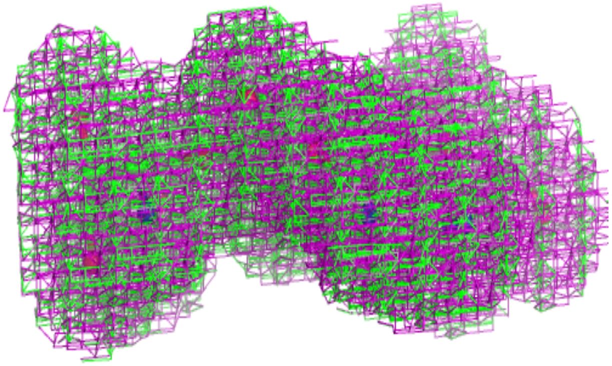


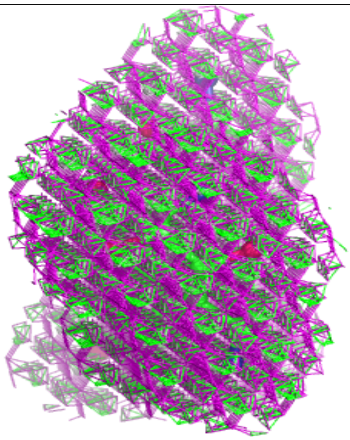


Electron density around PAR 1 3426:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

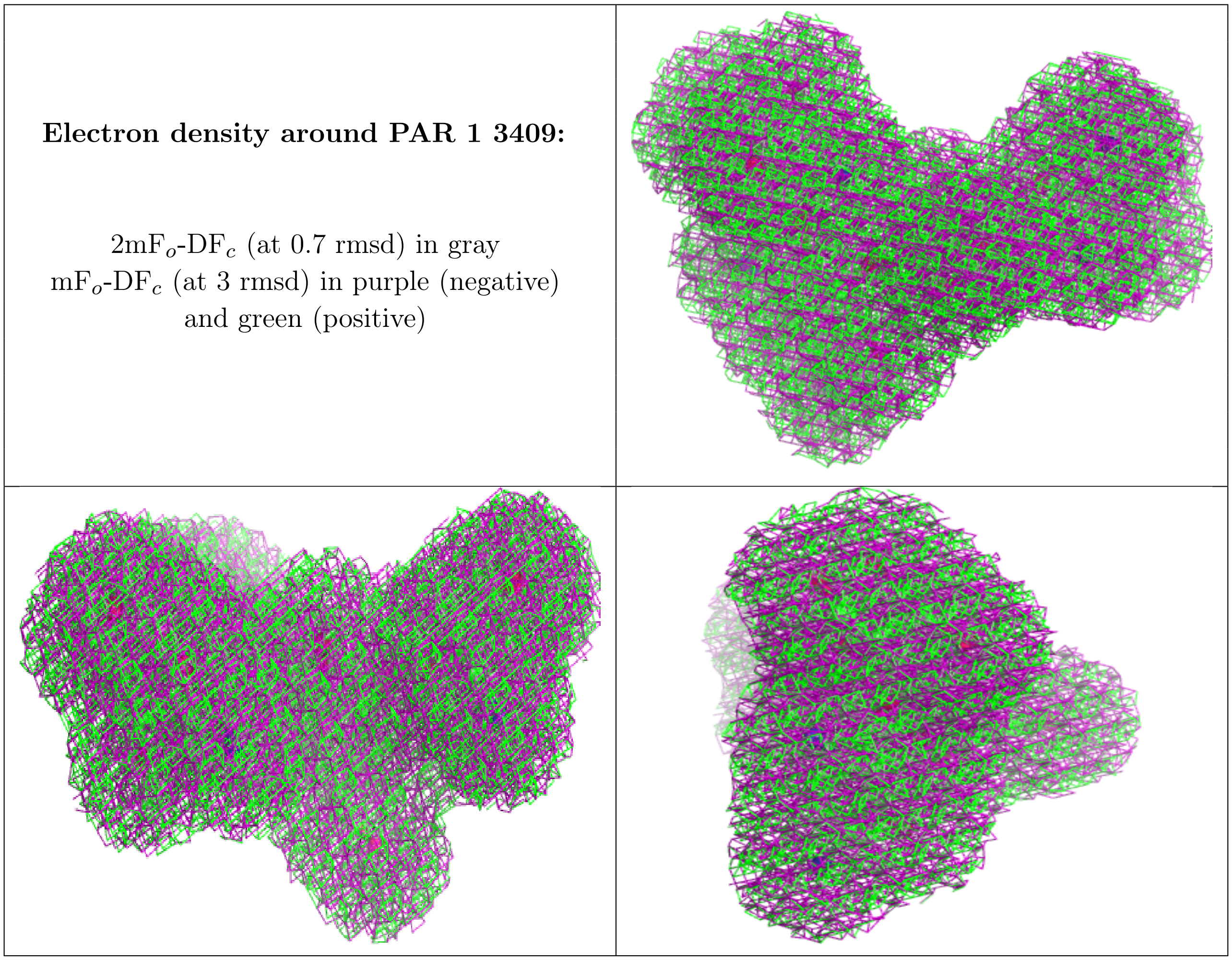






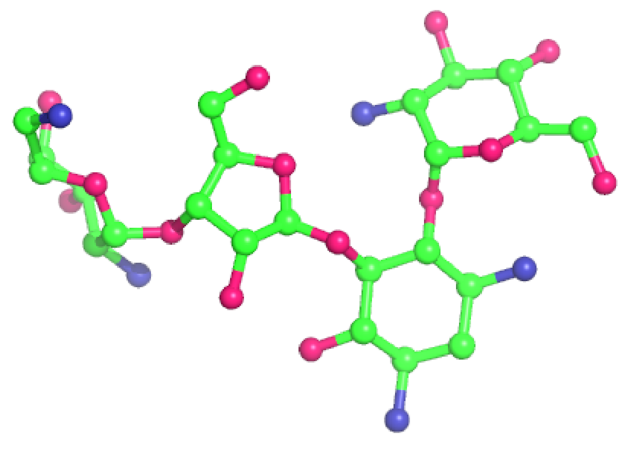
Electron density around PAR 1 3409:

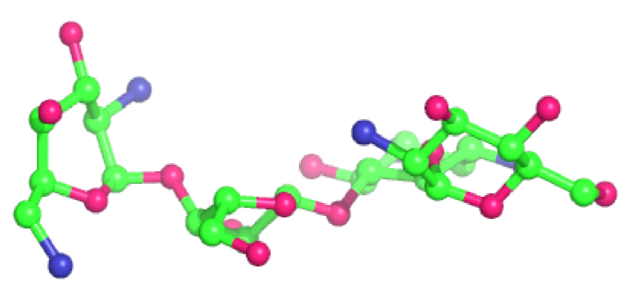
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

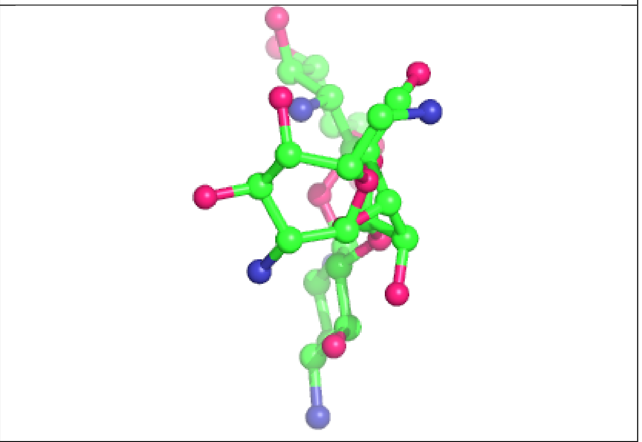


Electron density around PAR AS 3410:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

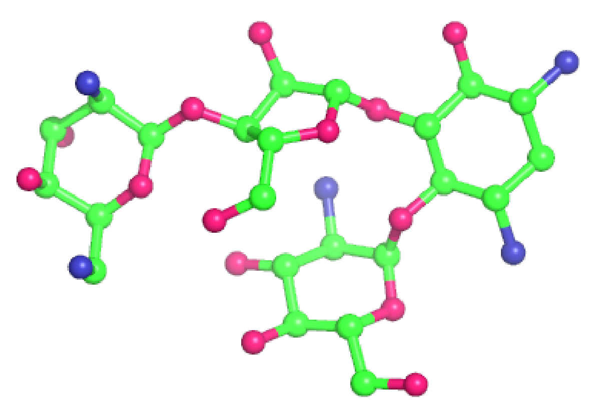


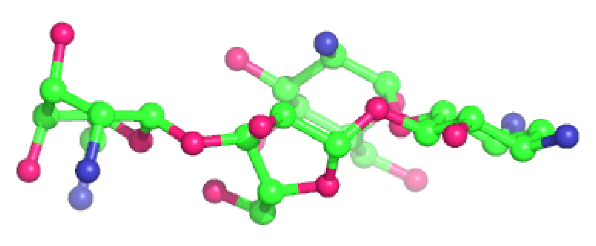


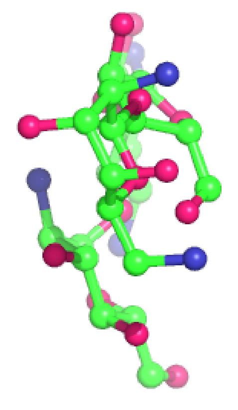


Electron density around PAR 1 3416:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

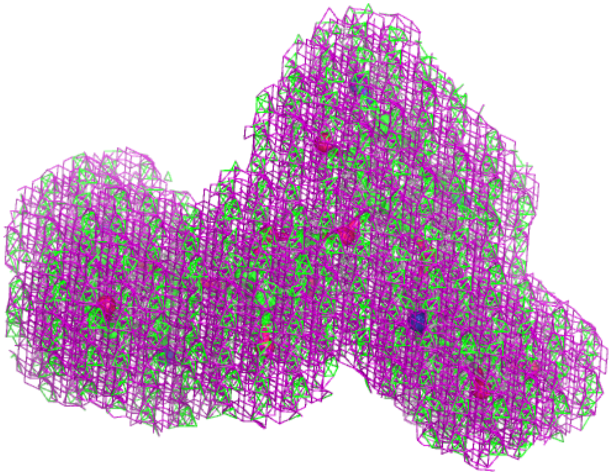


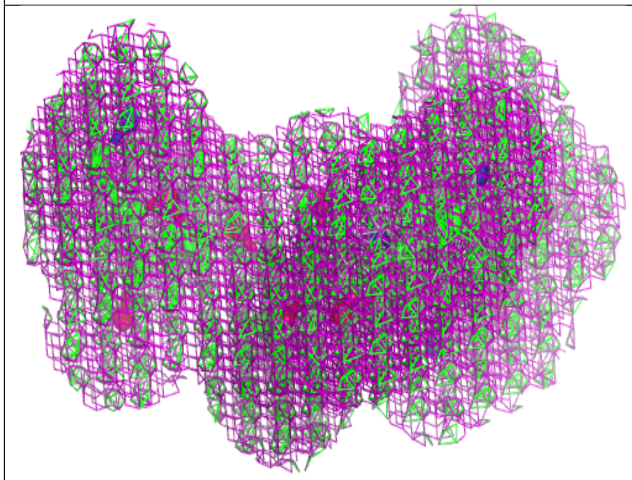


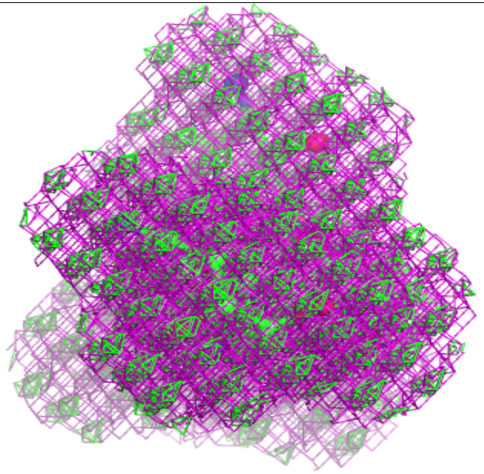


Electron density around PAR 1 3425:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

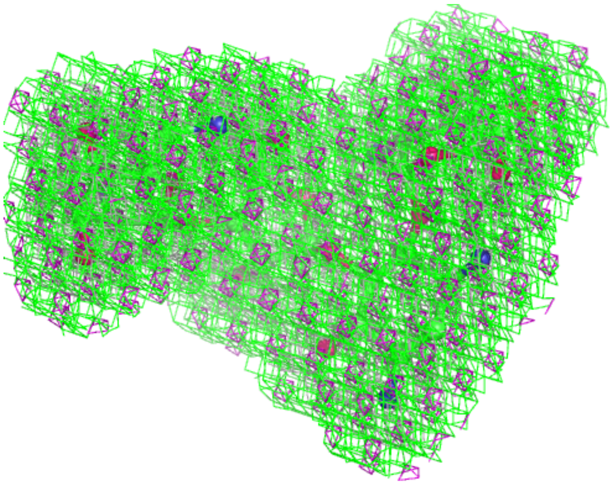


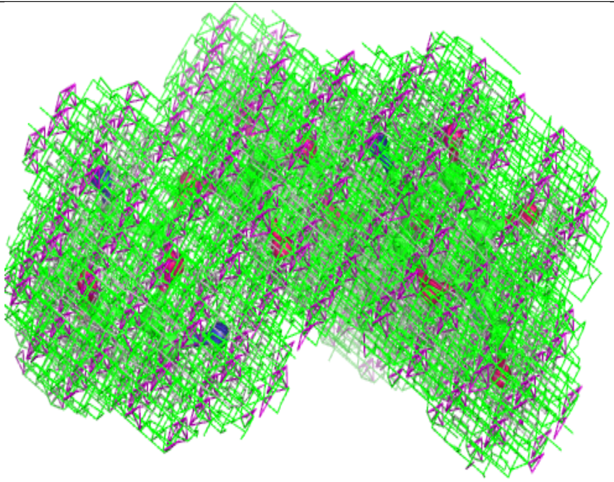


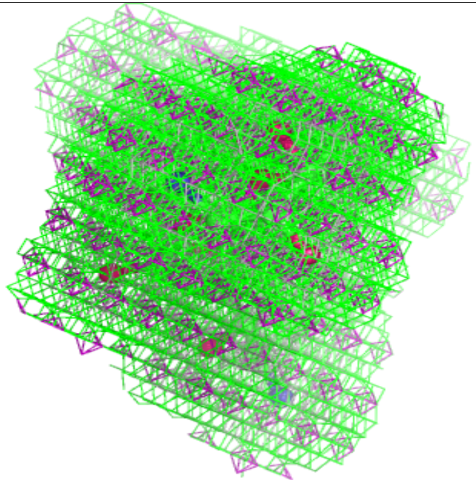


Electron density around PAR AS 3403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

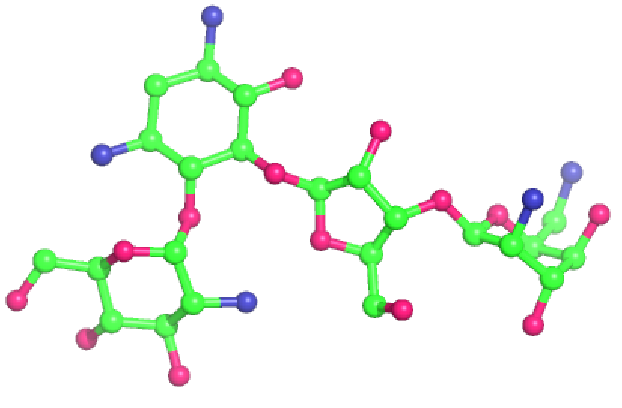


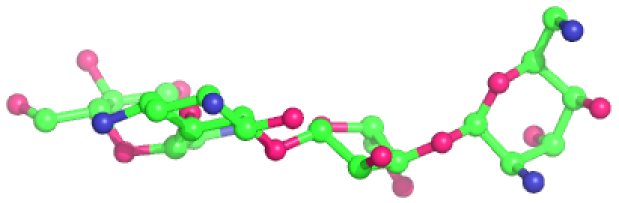


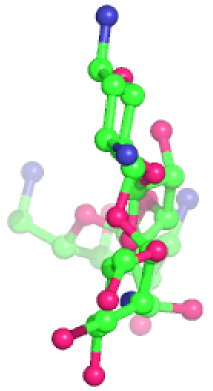


Electron density around PAR AS 3409:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

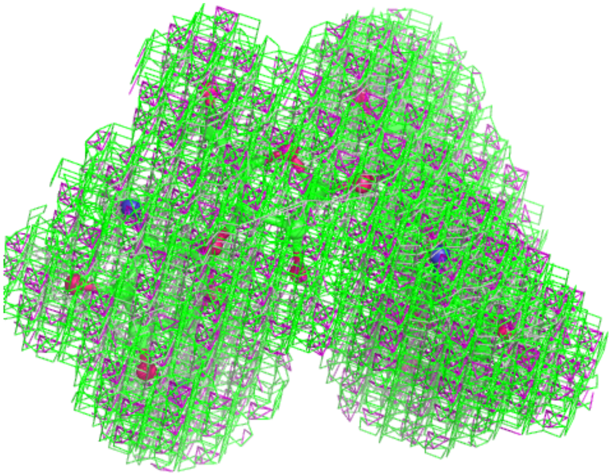


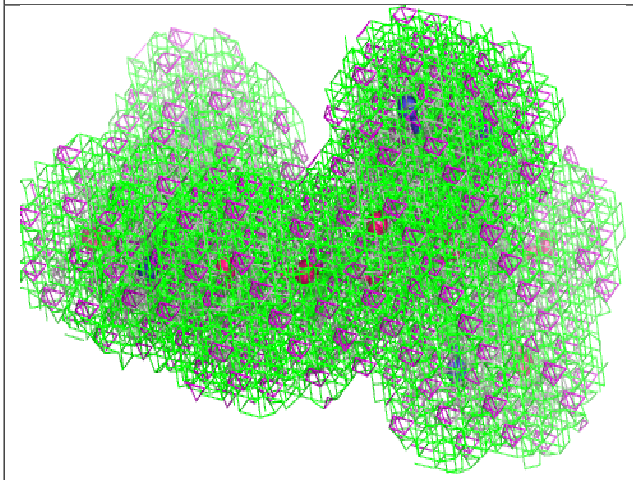


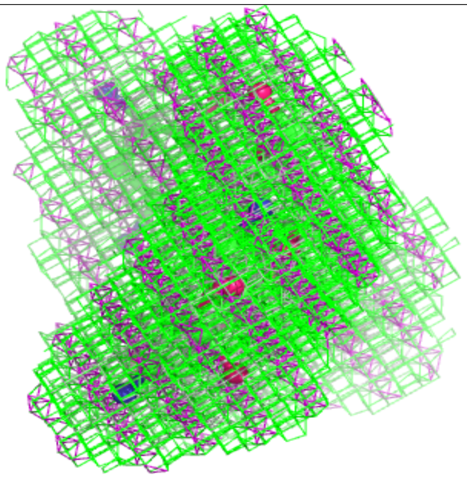


Electron density around PAR AS 3404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

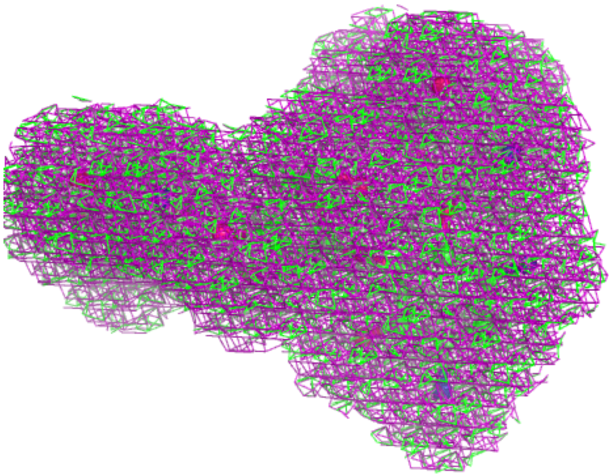


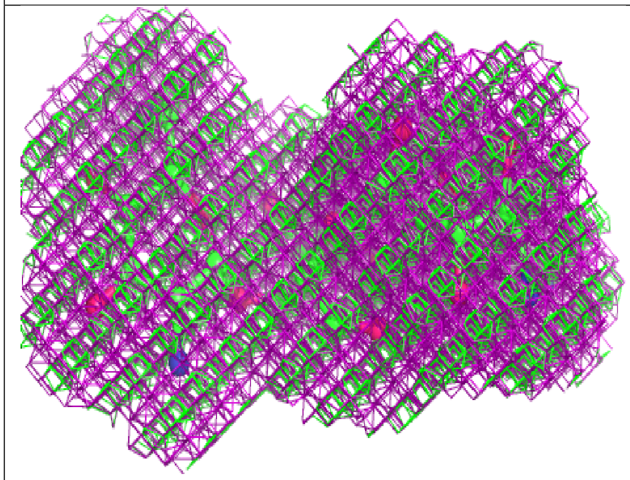


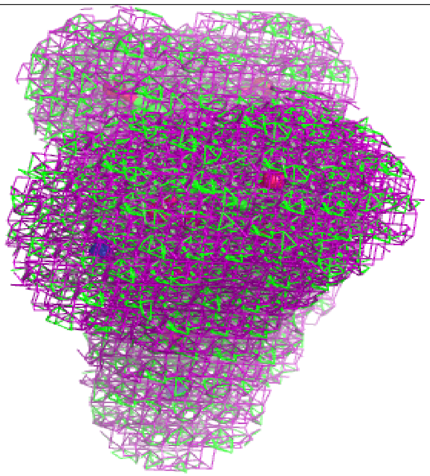


Electron density around PAR 1 3419:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

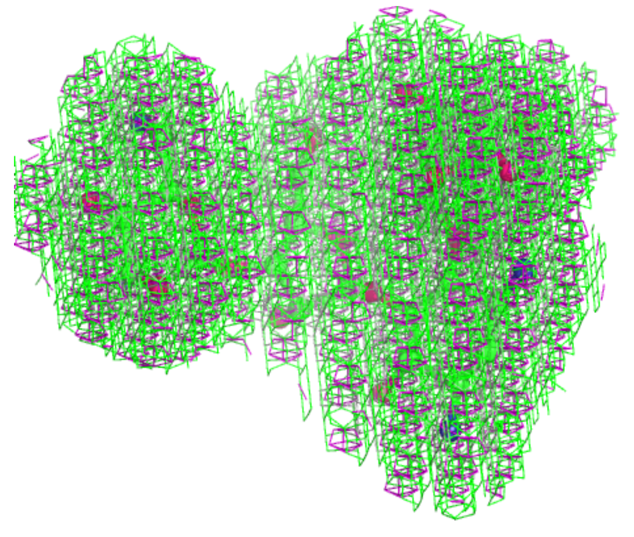


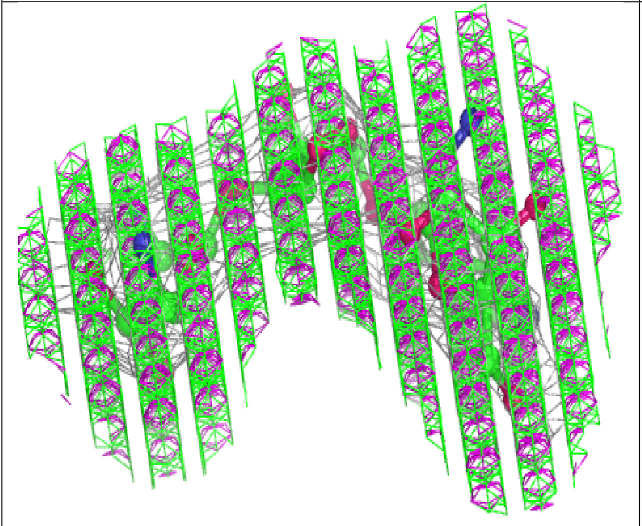


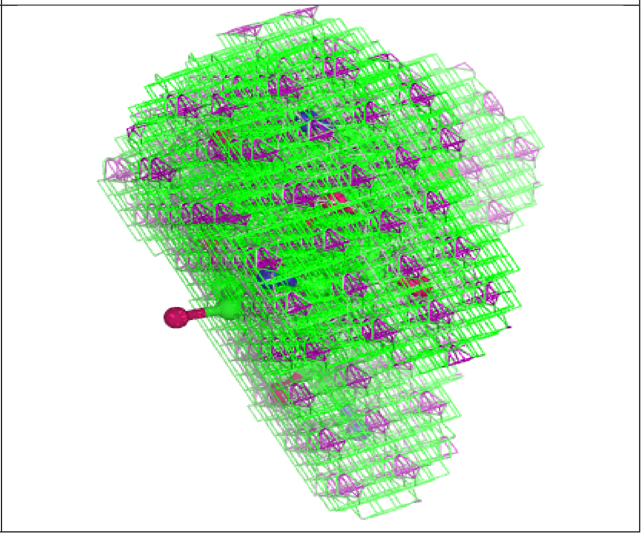


Electron density around PAR CM 1802:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

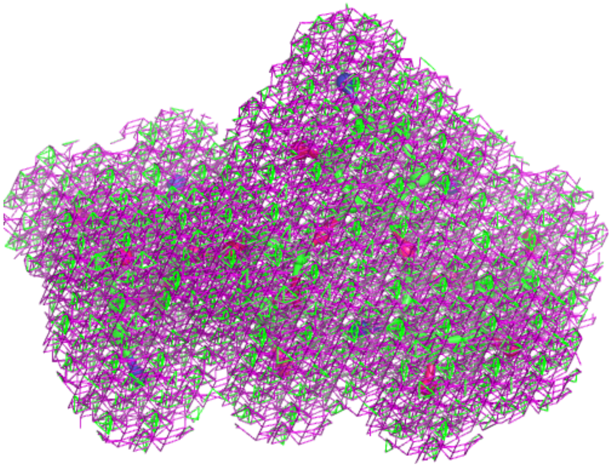


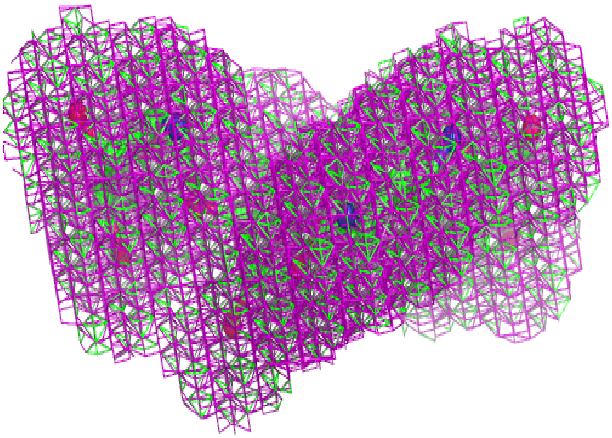


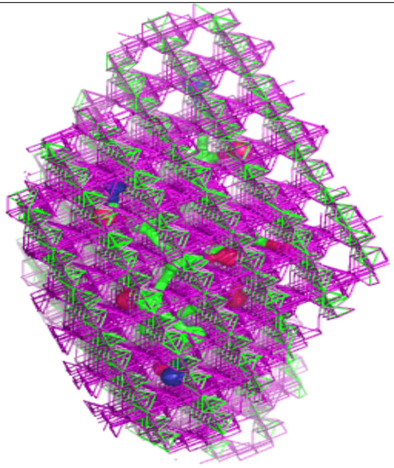


Electron density around PAR 1 3423:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

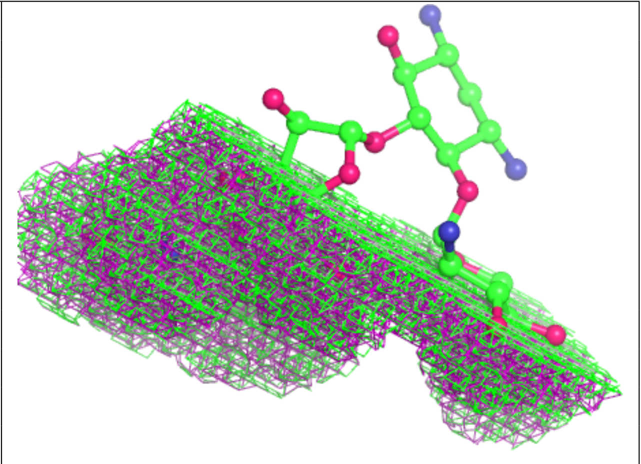


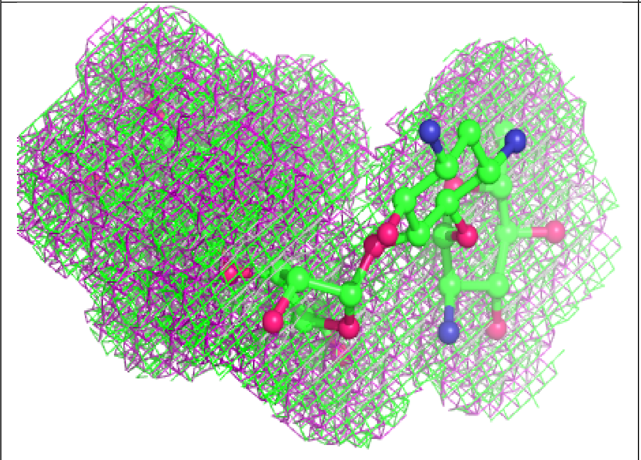


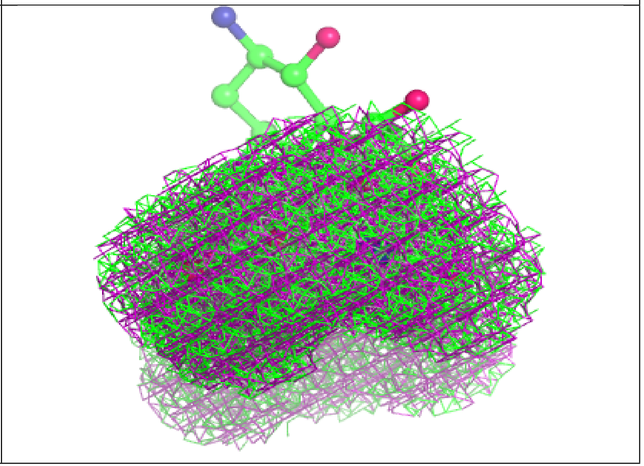


Electron density around PAR 1 3427:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

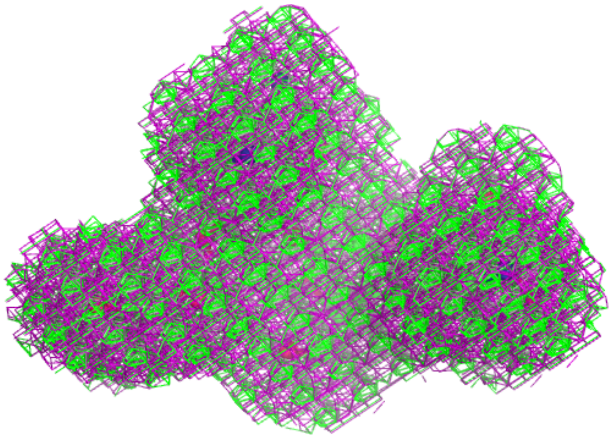


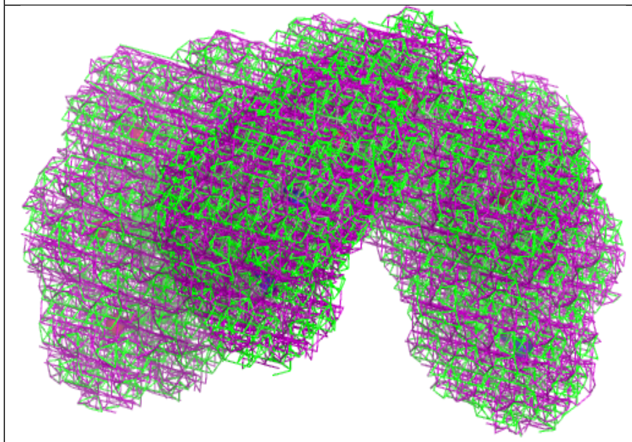


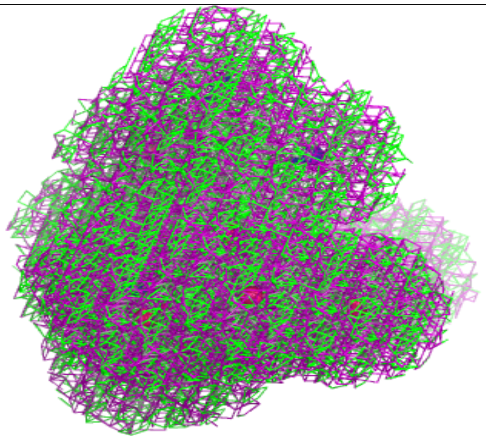


Electron density around PAR 1 3410:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

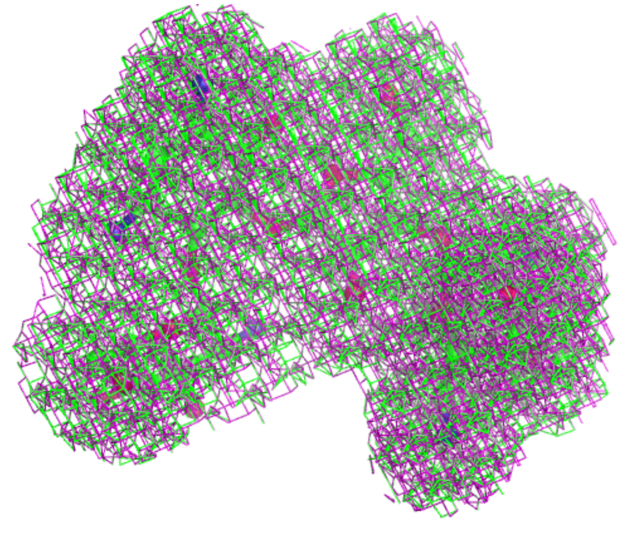


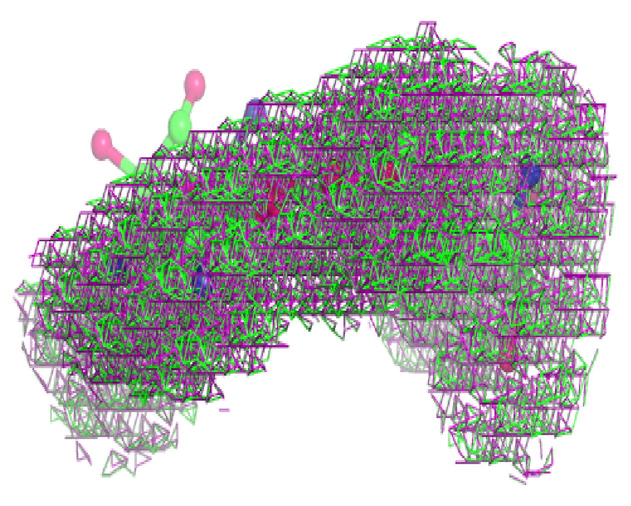


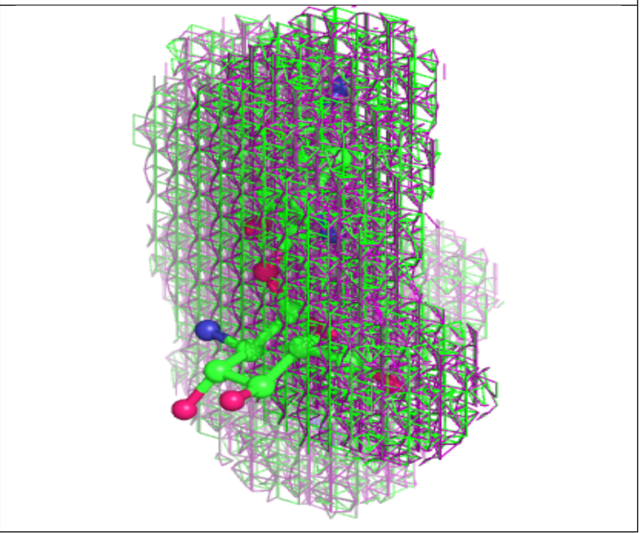


Electron density around PAR B 1802:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

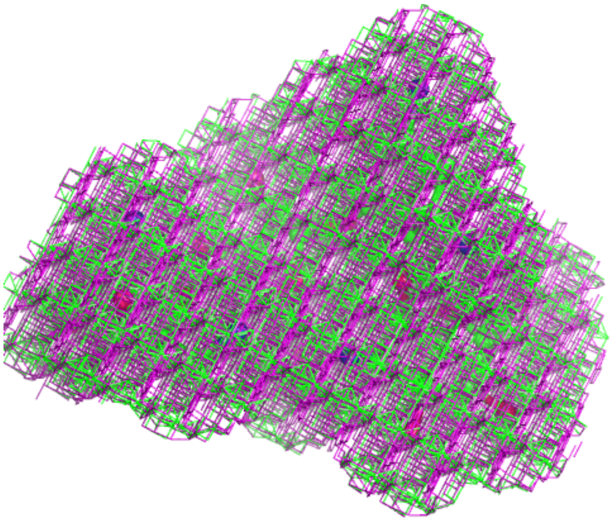


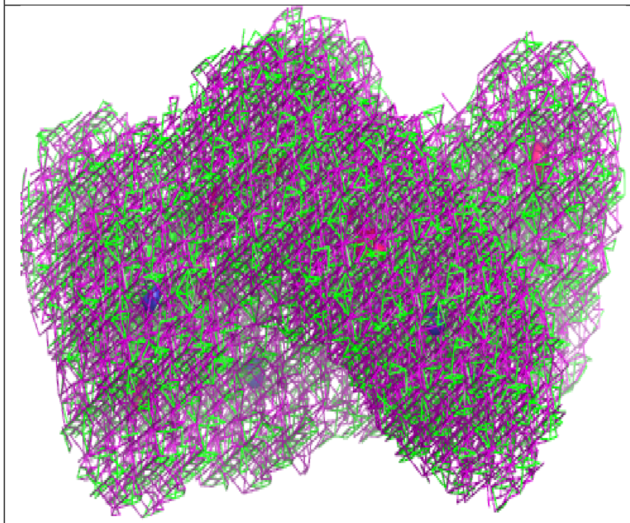


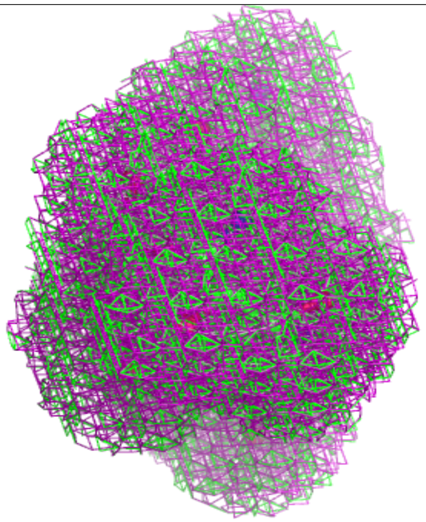


Electron density around PAR 1 3418:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

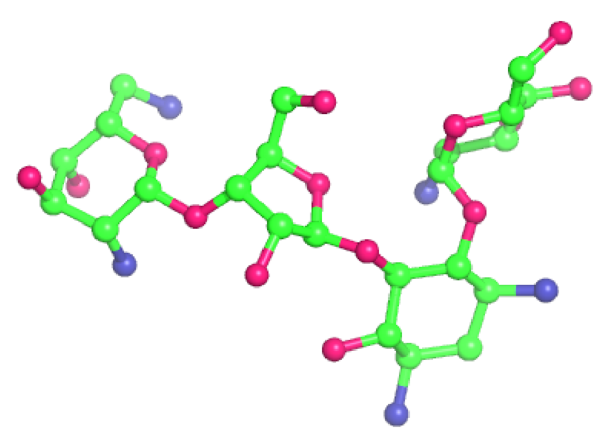


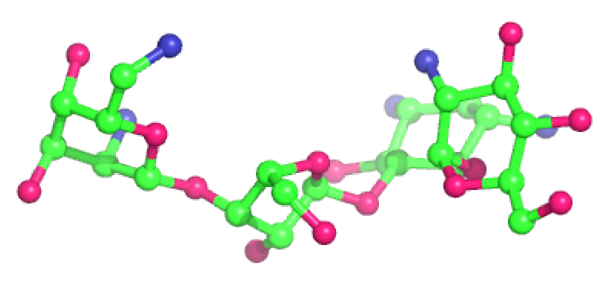


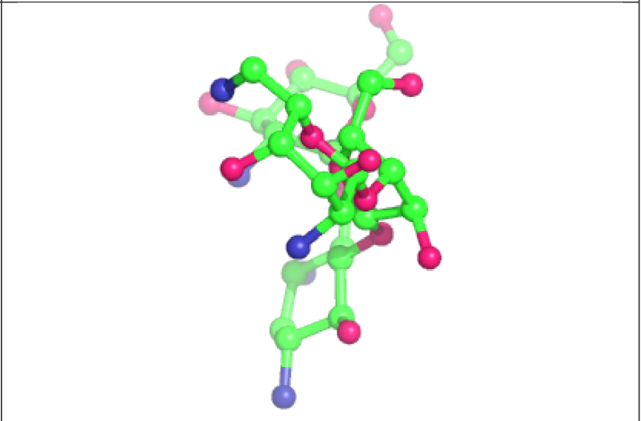


Electron density around PAR B 1803:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

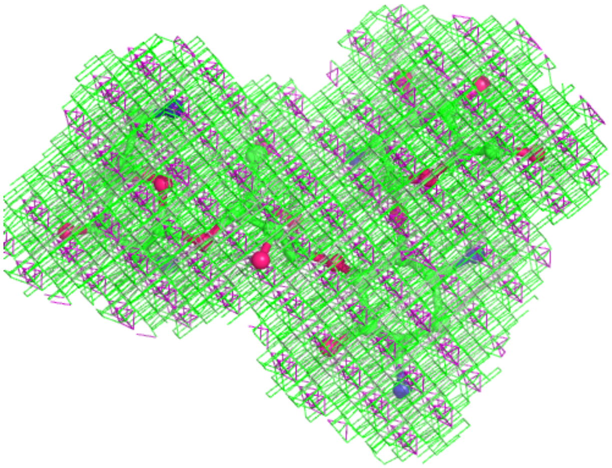


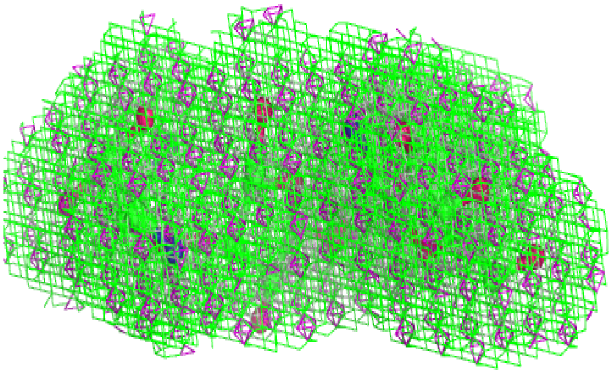


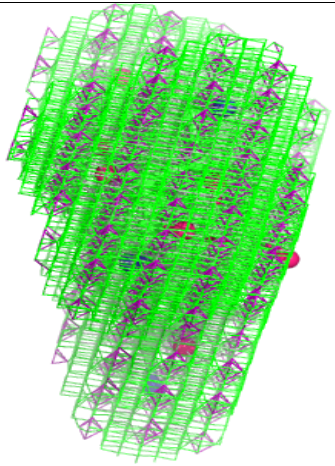


Electron density around PAR CM 1801:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

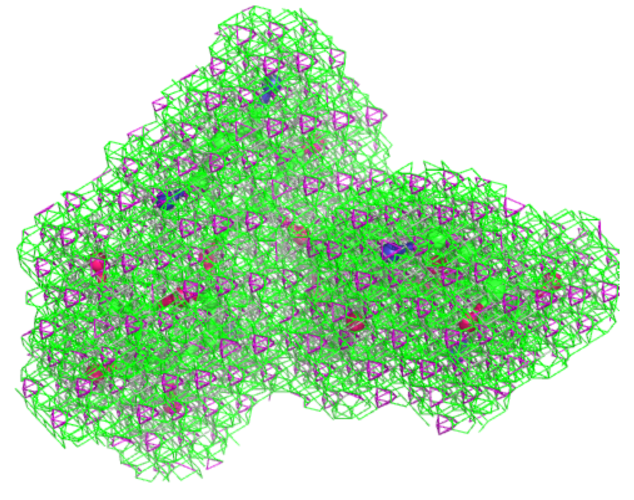


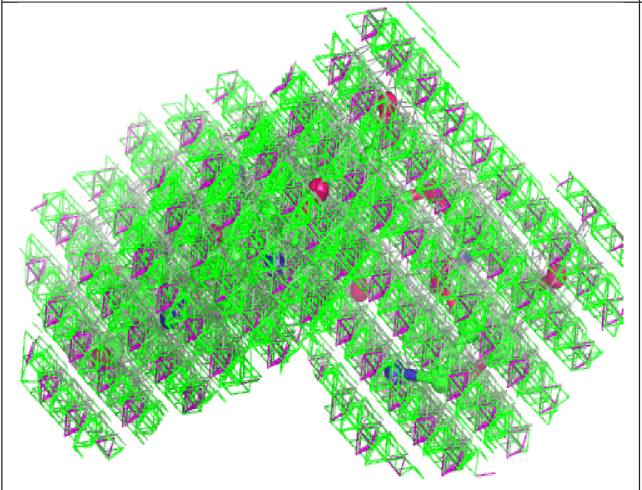


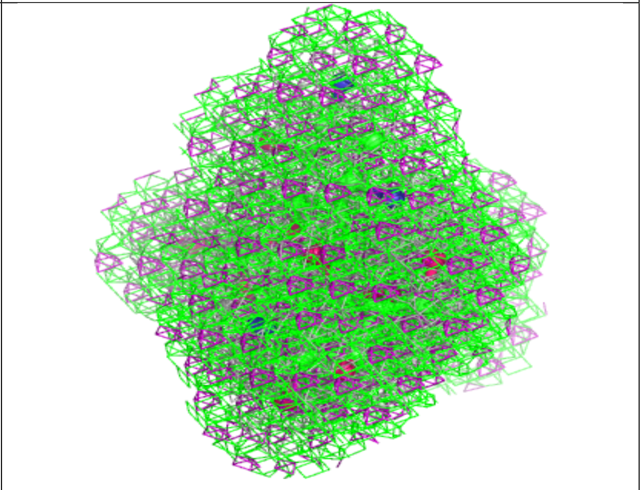


Electron density around PAR AS 3406:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

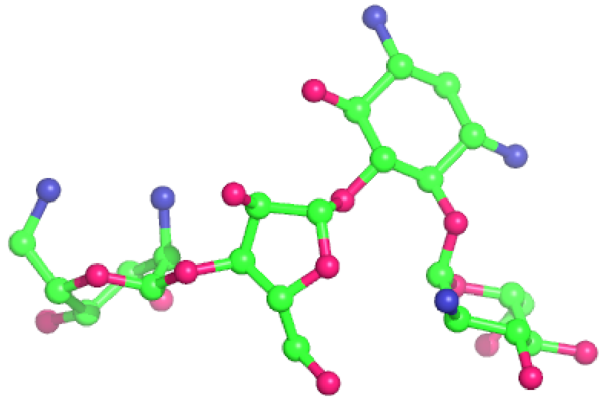


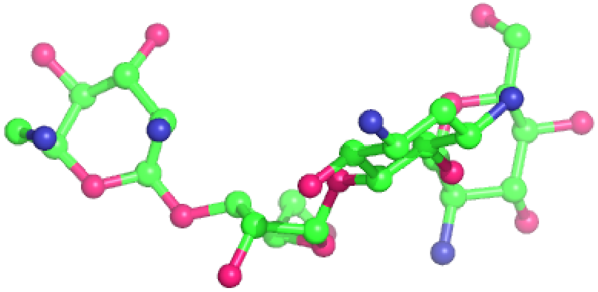


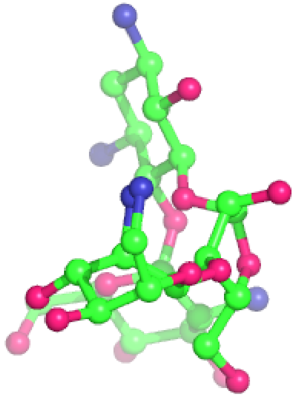


Electron density around PAR AS 3402:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

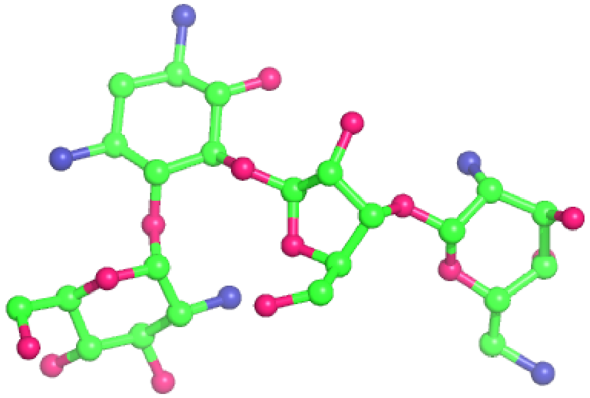


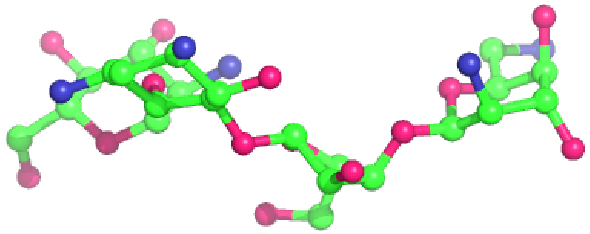


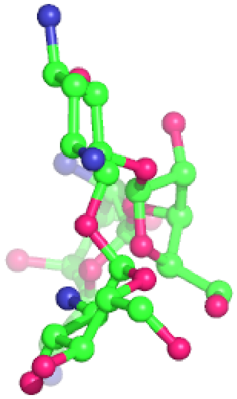


Electron density around PAR 4 201:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

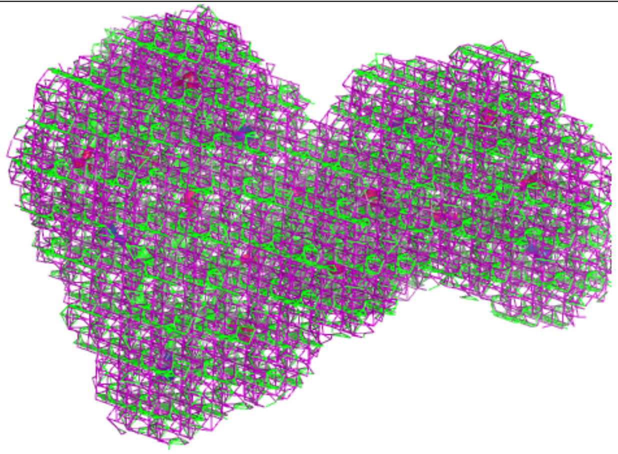


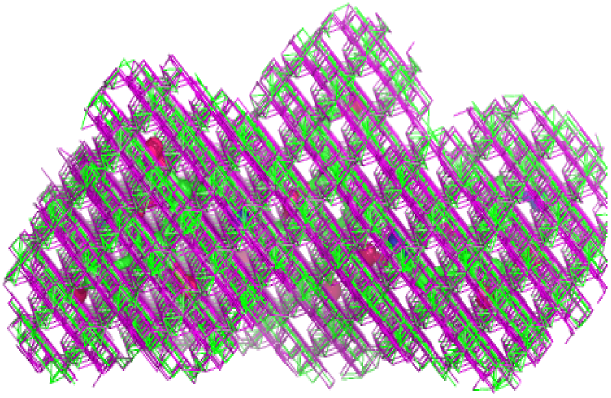


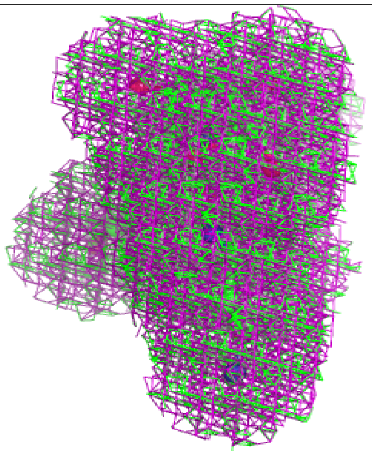


Electron density around PAR 1 3428:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

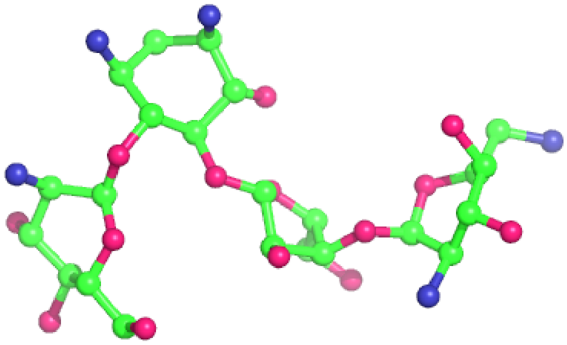


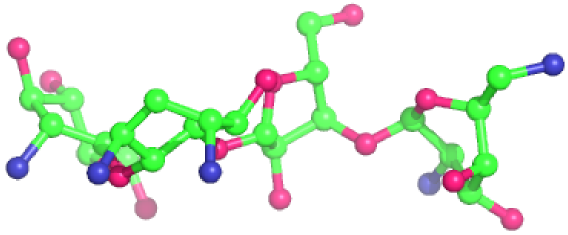


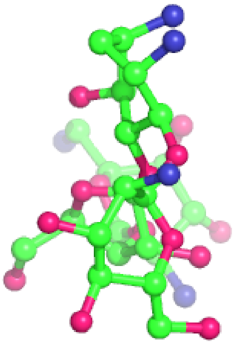


Electron density around PAR AS 3411:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

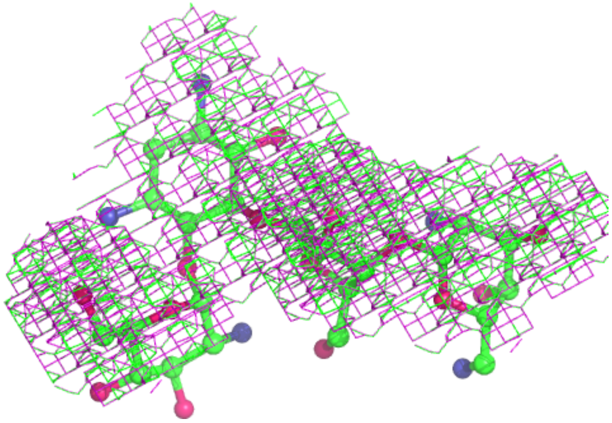


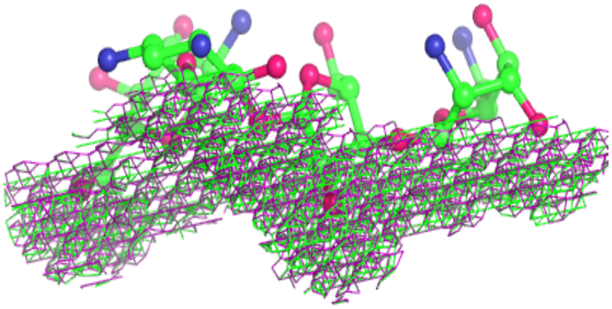


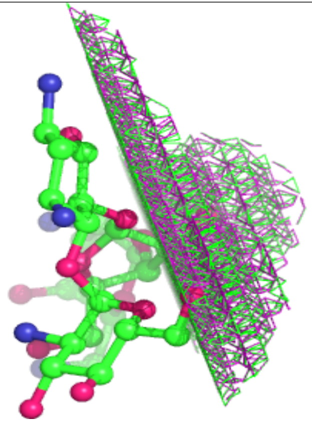


Electron density around PAR B 1801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

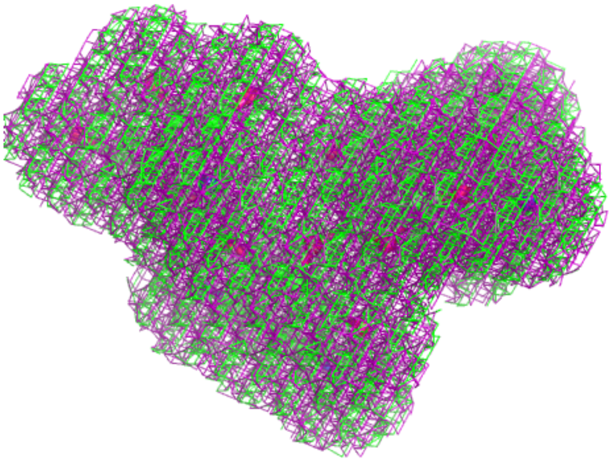


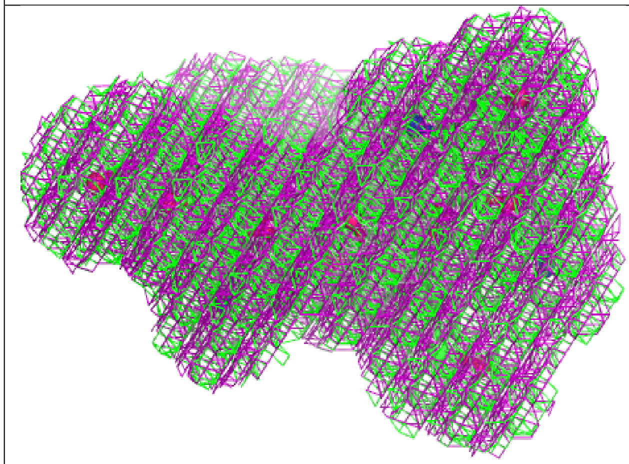


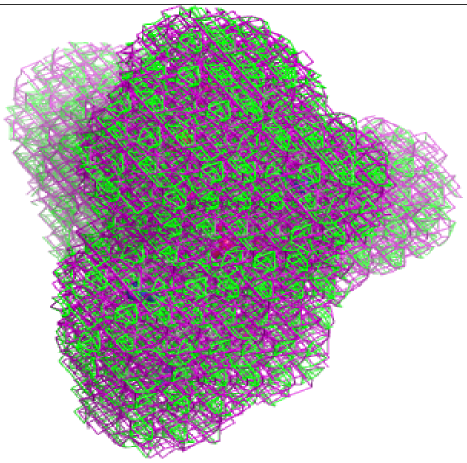


Electron density around PAR 1 3411:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

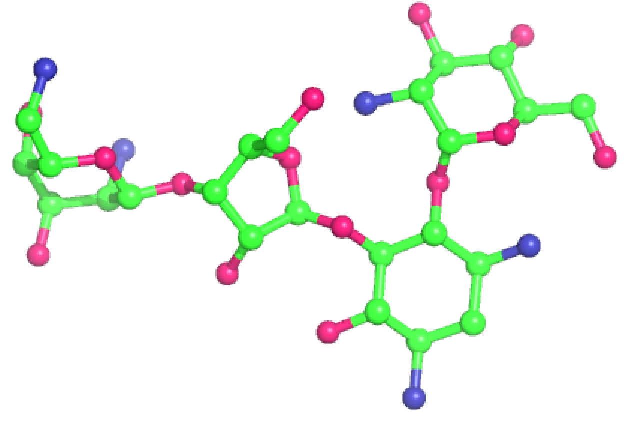


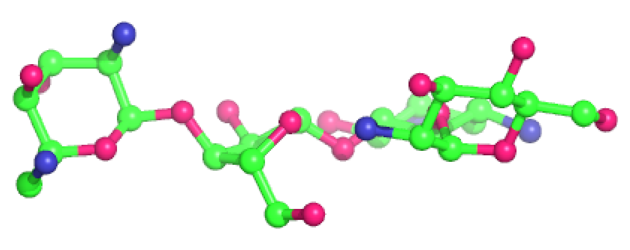


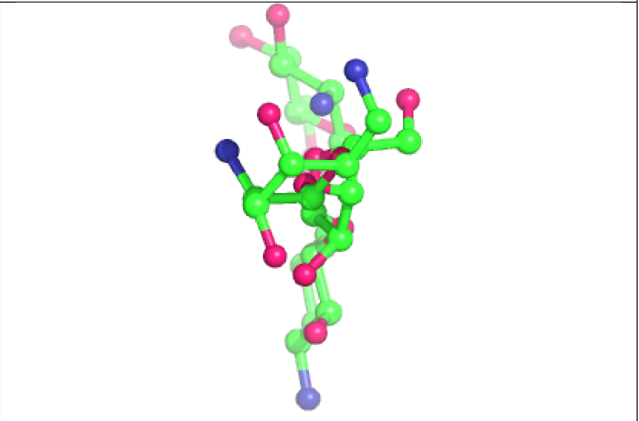


Electron density around PAR 1 3415:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

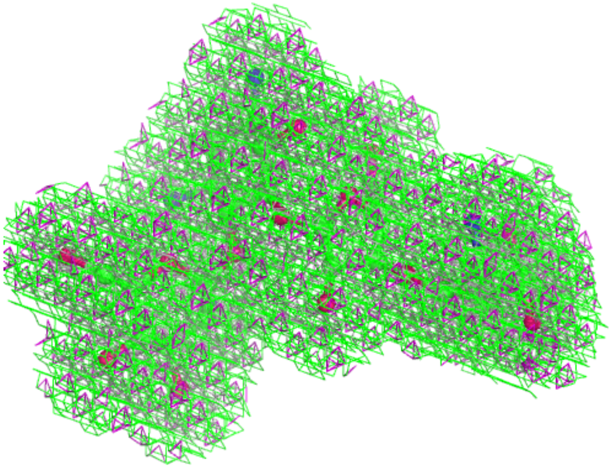


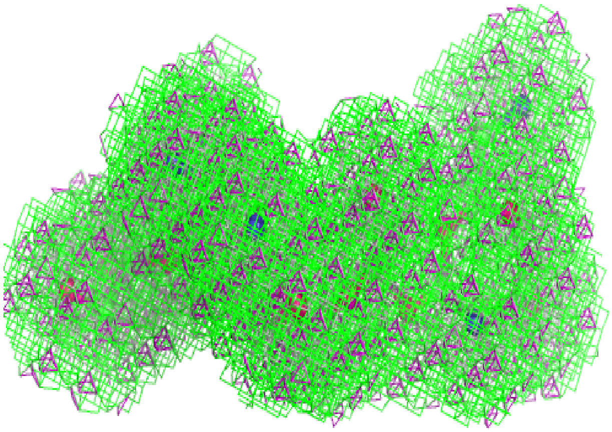


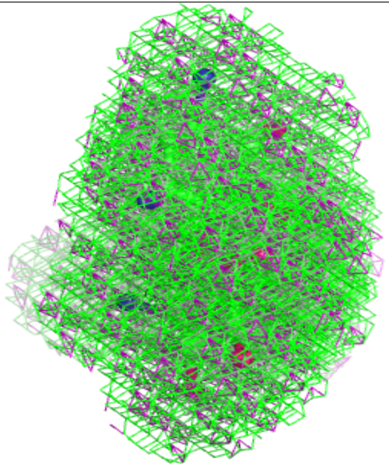


Electron density around PAR CM 1804:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

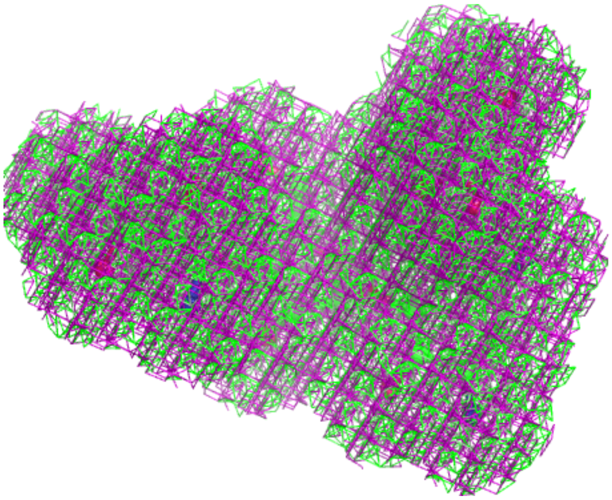


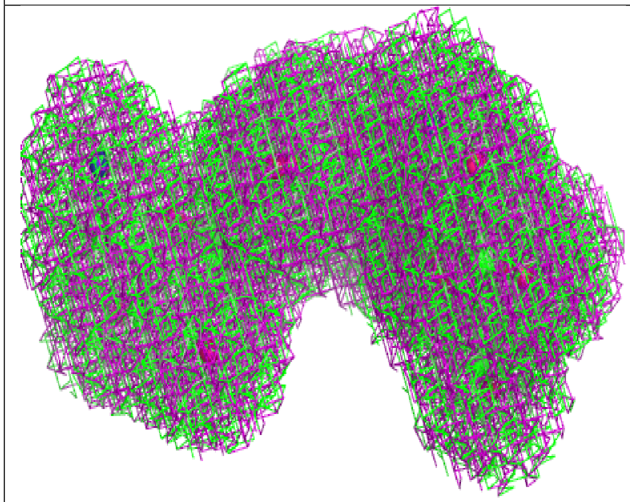


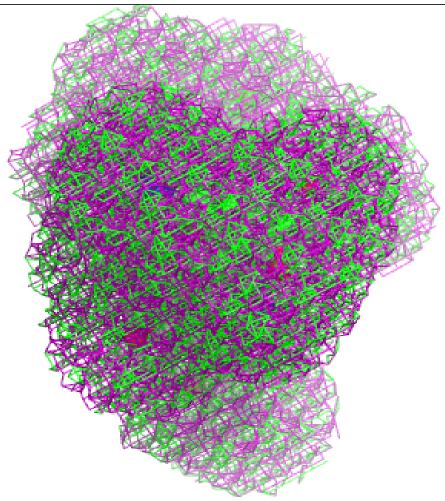


Electron density around PAR 1 3412:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

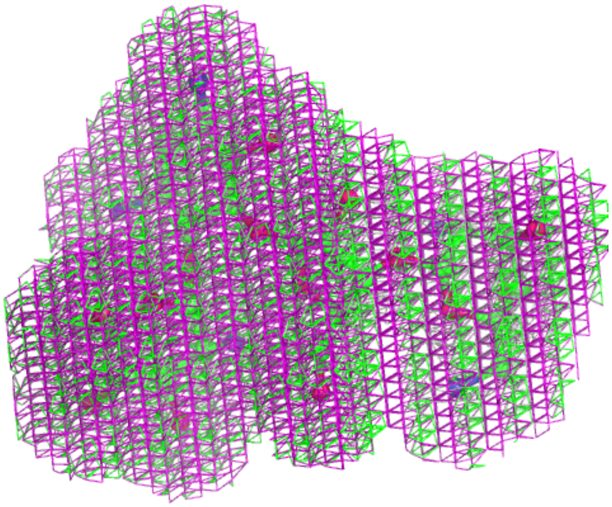


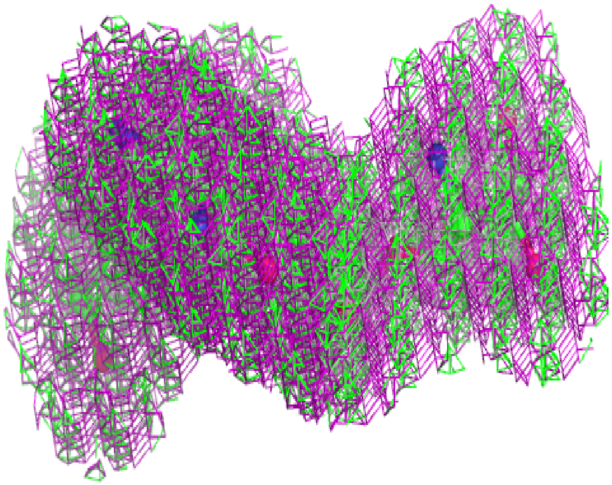


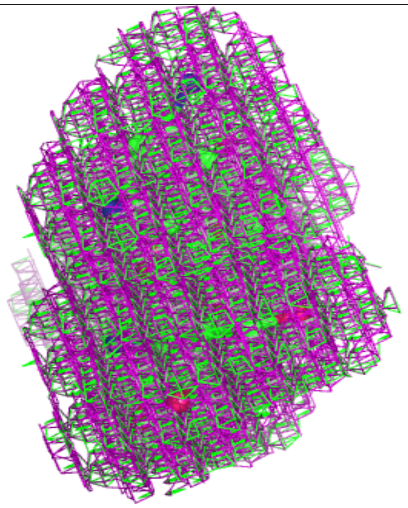


Electron density around PAR 1 3417:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

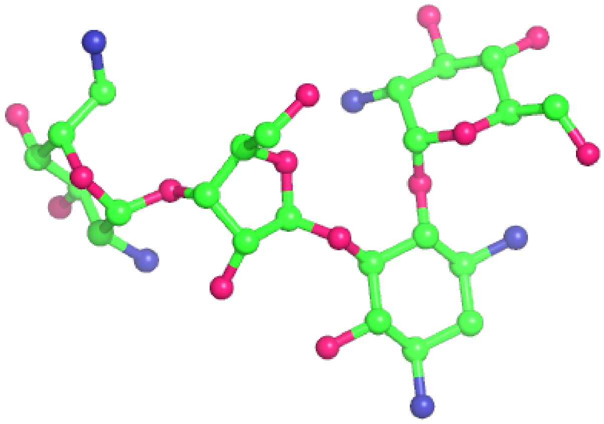


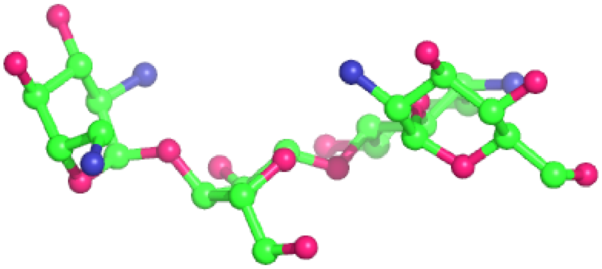


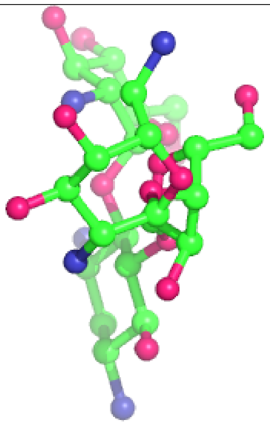


Electron density around PAR AS 3412:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

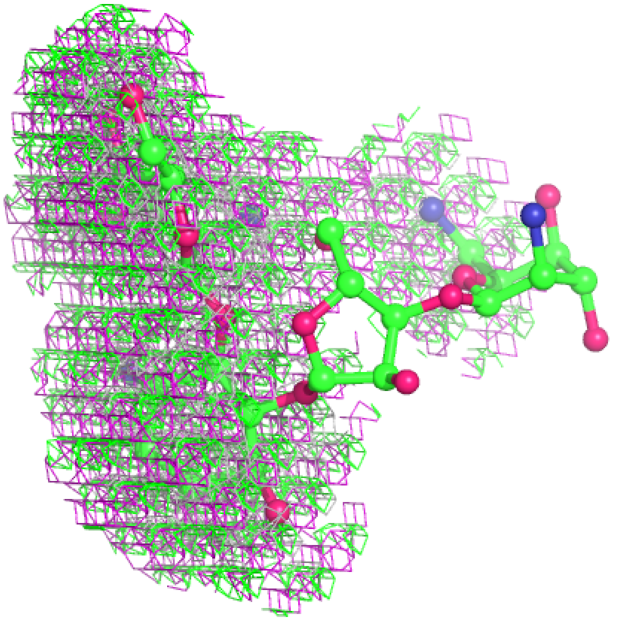


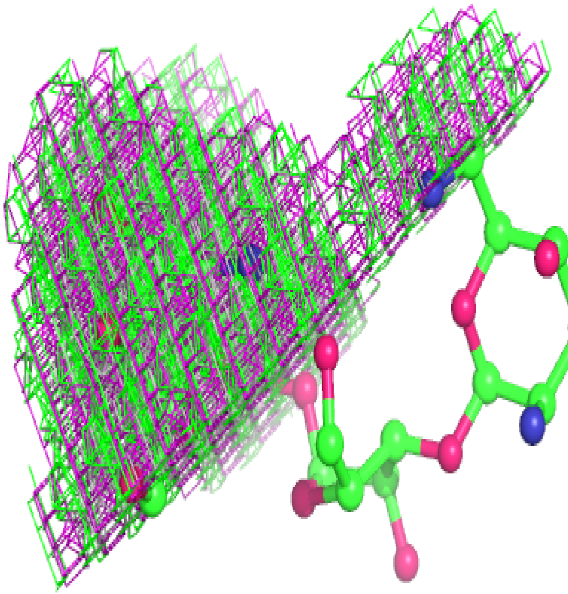


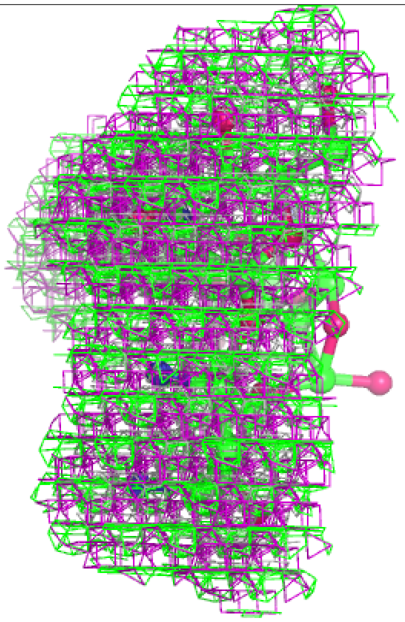


Electron density around PAR 1 3404:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

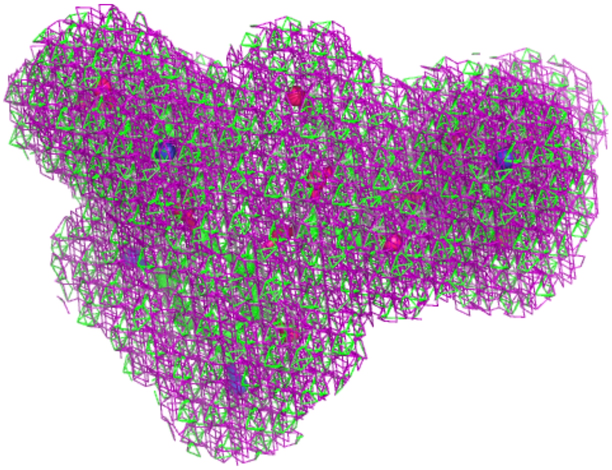


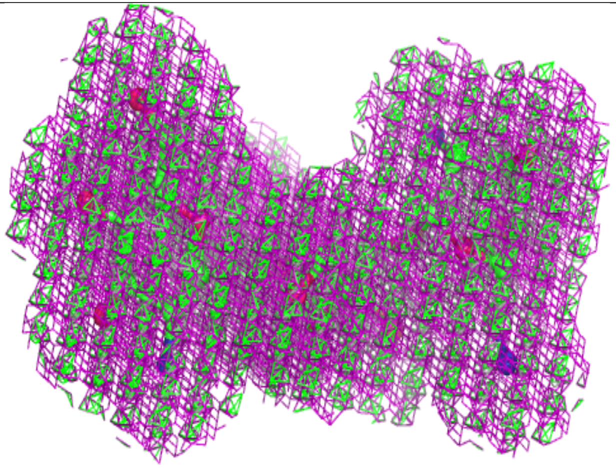


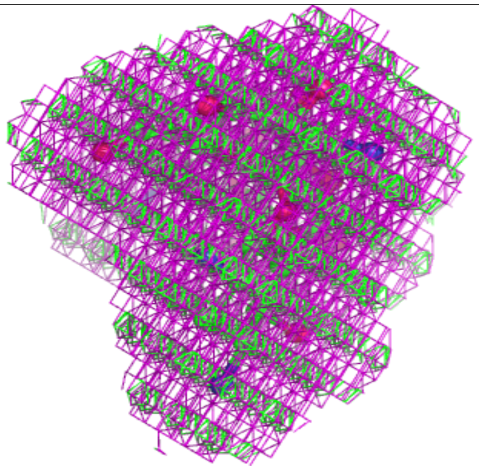


Electron density around PAR 1 3424:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

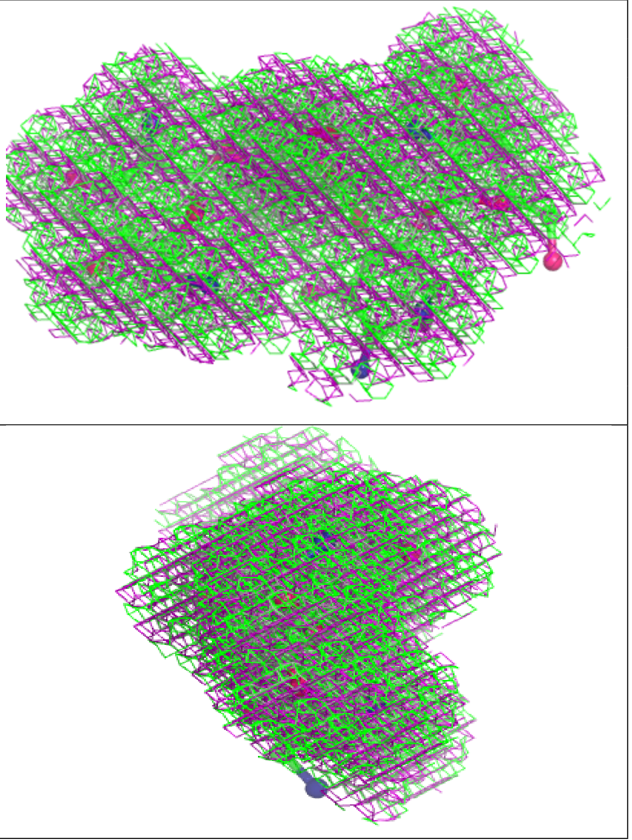






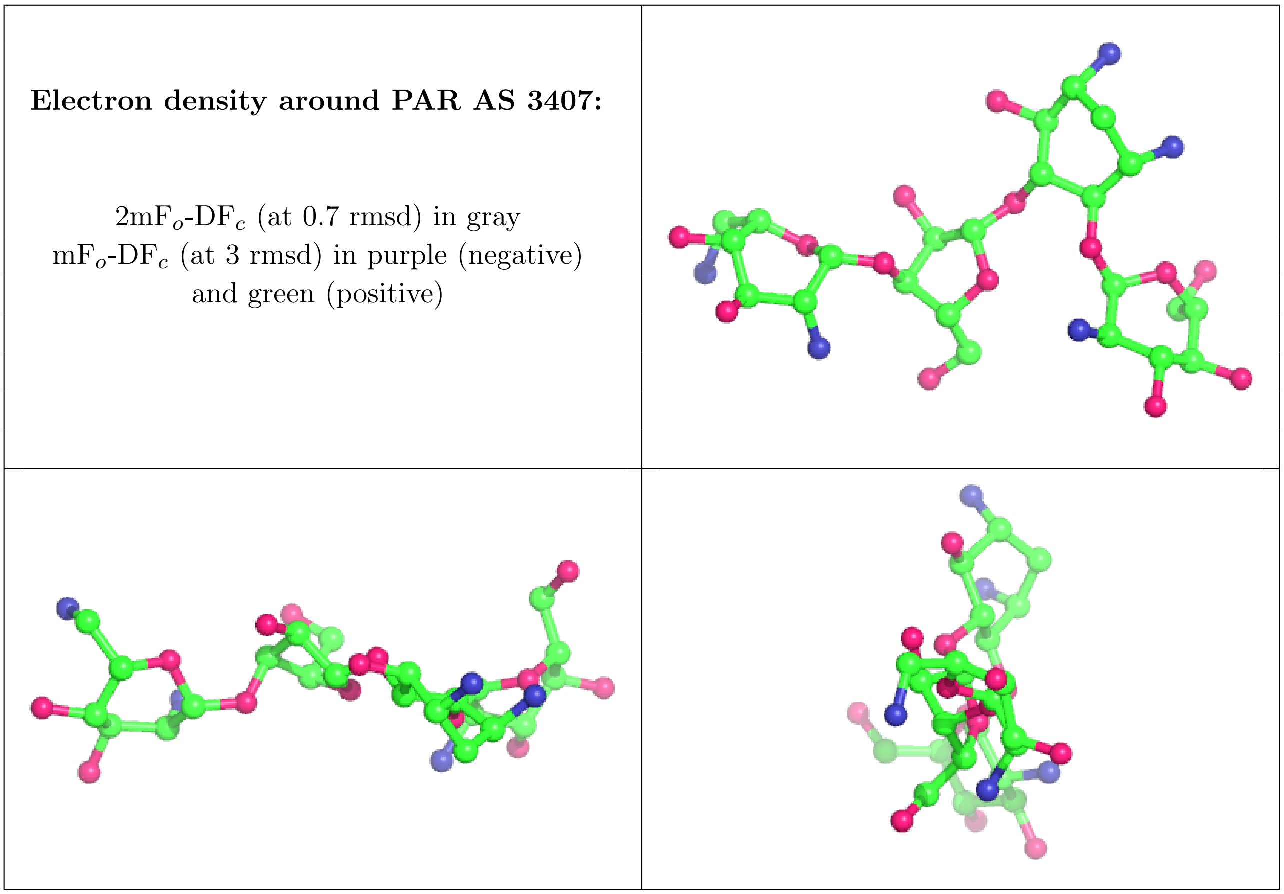
Electron density around PAR 1 3430:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



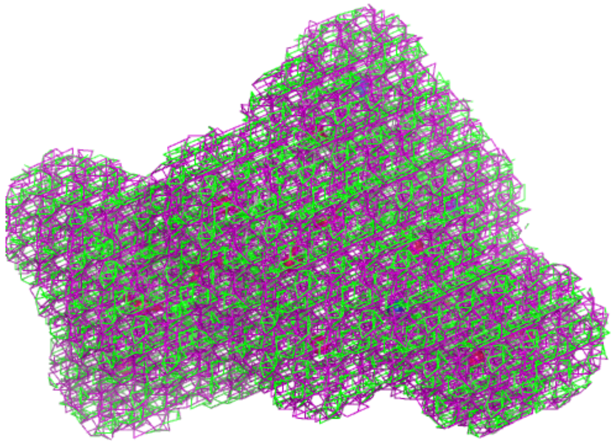
Electron density around PAR AS 3407:

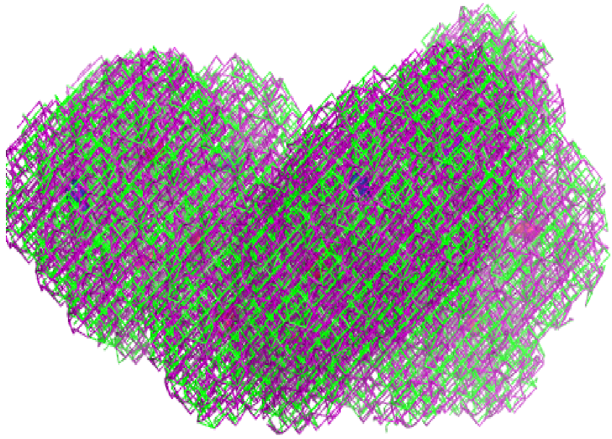
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

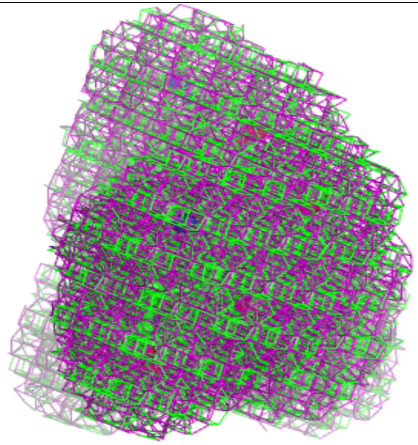


Electron density around PAR 1 3406:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

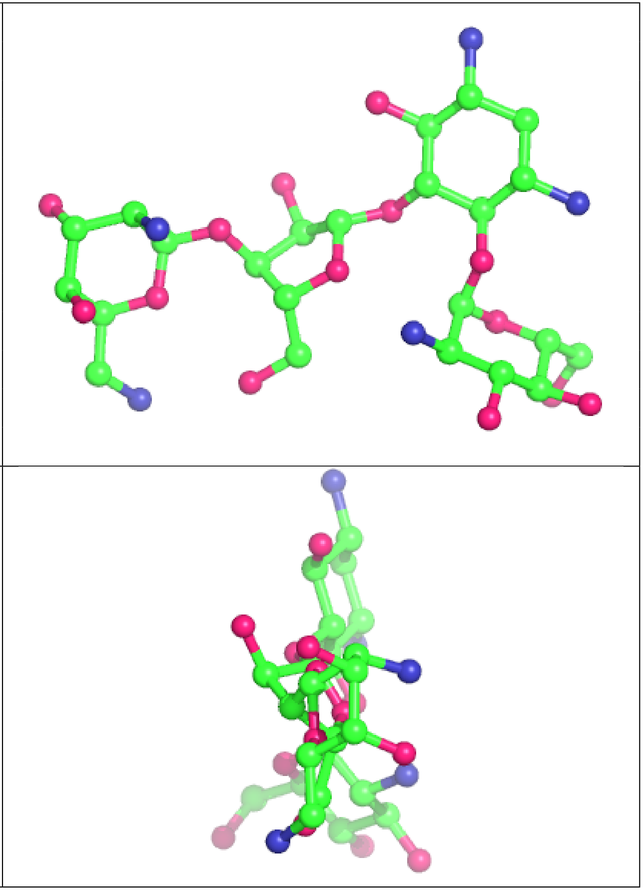






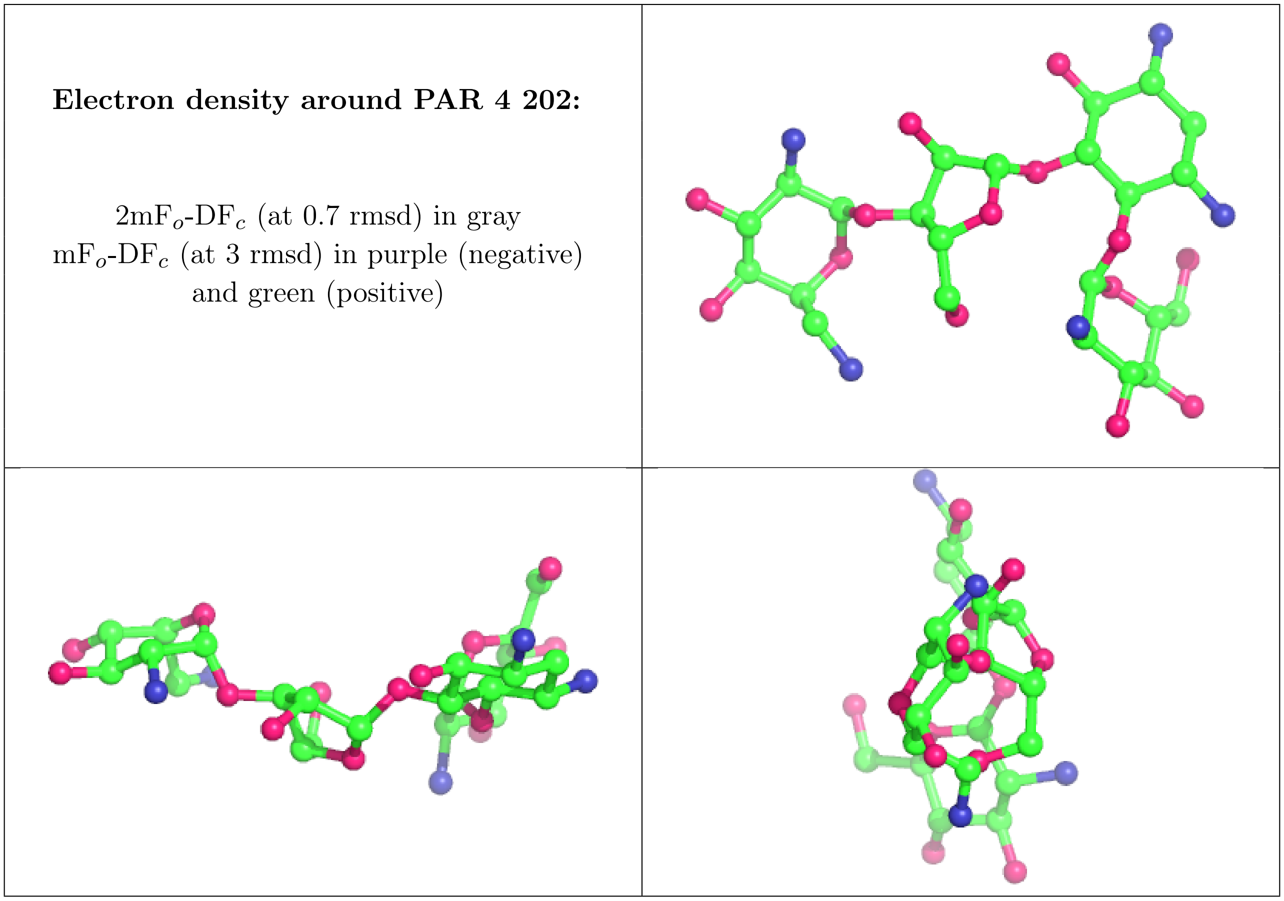
Electron density around PAR 1 3402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



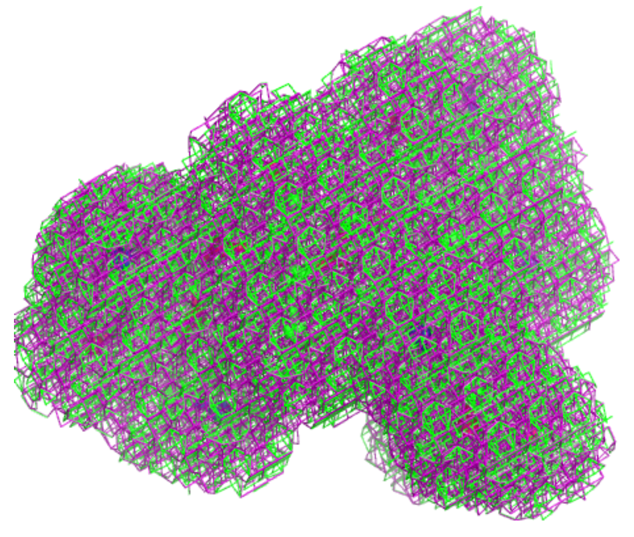
Electron density around PAR 4 202:

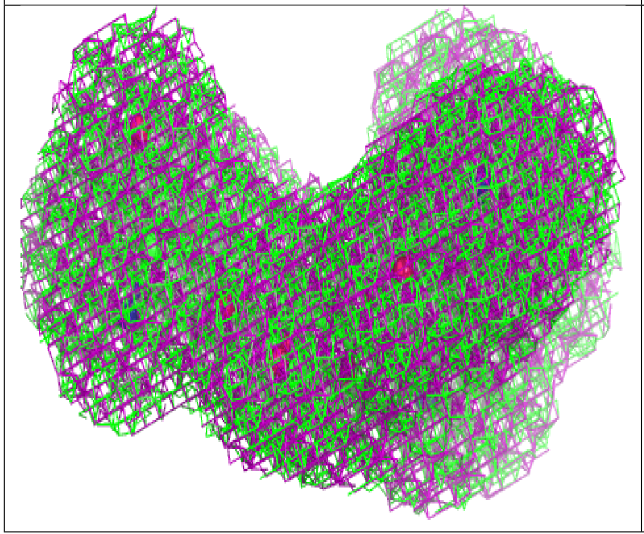
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

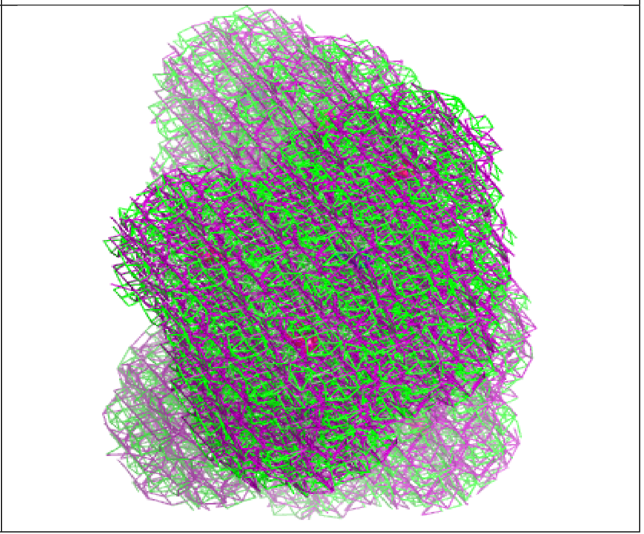


Electron density around PAR 1 3421:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

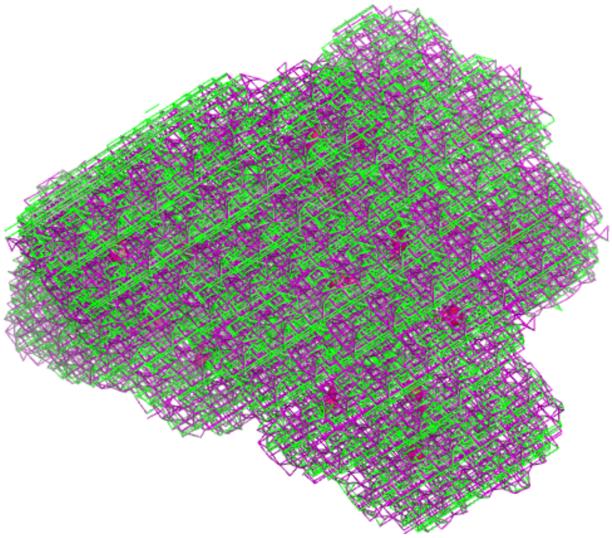


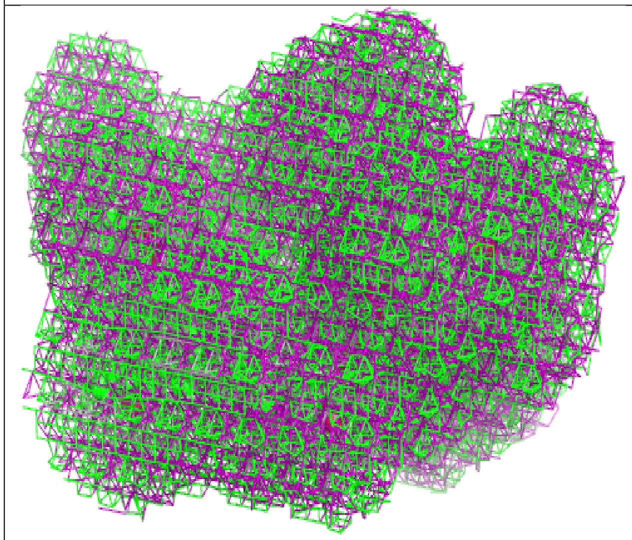


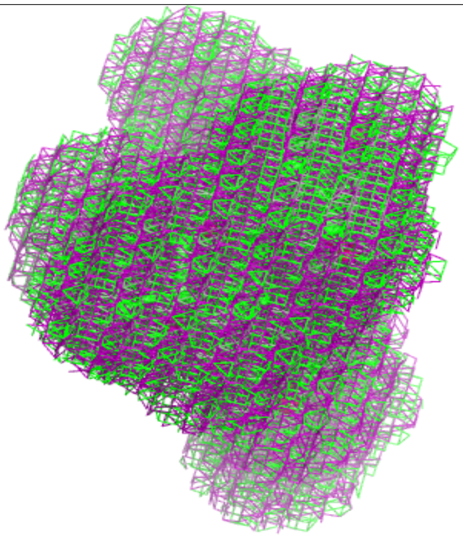


Electron density around 3K5 1 3401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

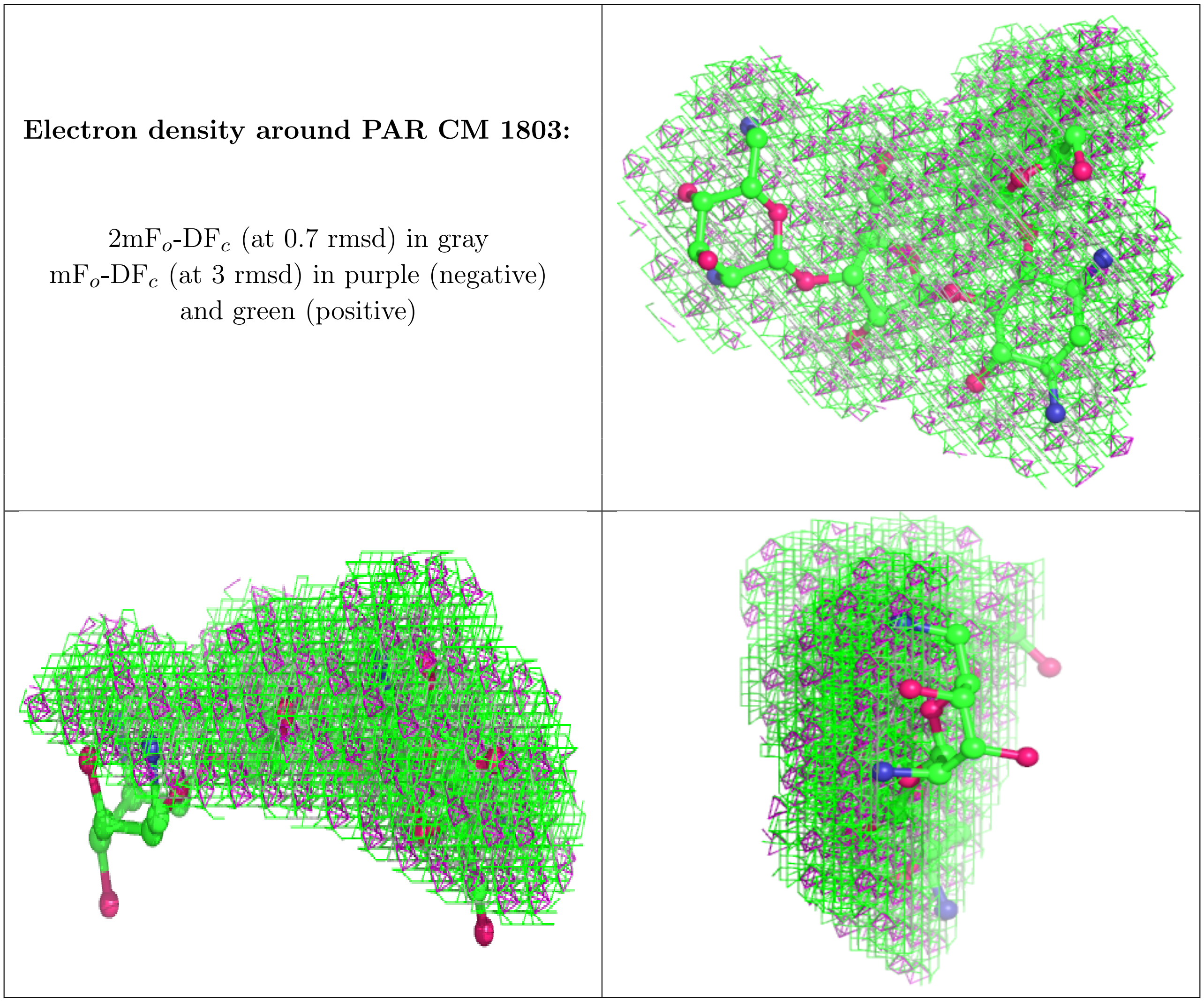






Electron density around PAR CM 1803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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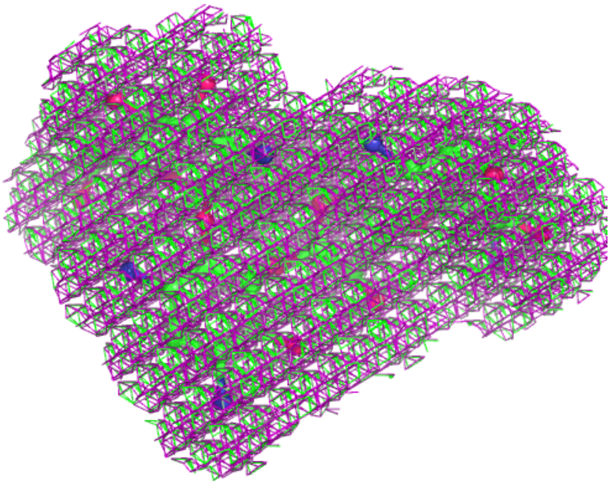
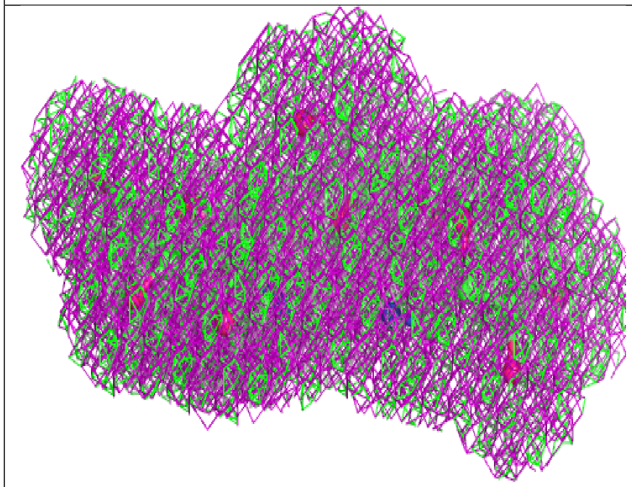
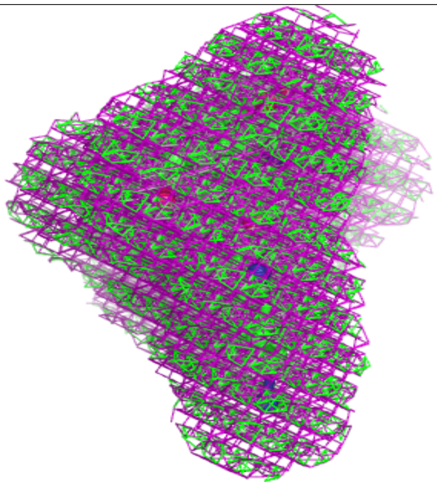
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)</td><td></td></tr>
<tr><td></td><td></td></tr>
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6.5 Other polymers

There are no such residues in this entry.