



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:59 PM UTC

PDB ID : 8OI5 / pdb_00008oi5
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)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

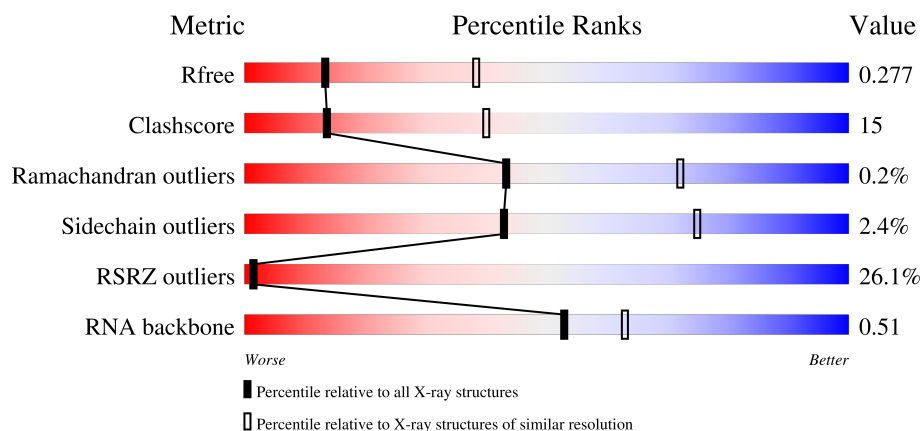
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (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 $\leq 5\%$. 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	5% 49% 37% 8% 6%
1	AS	3359	10% 46% 38% 7% 9%
2	3	121	% 60% 36% .
2	AT	121	3% 54% 43% .

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Mol	Chain	Length	Quality of chain
3	4	158	
3	AU	158	
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	
10	BC	262	
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	

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Mol	Chain	Length	Quality of chain
15	u	131	
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	
25	7	155	
25	BR	155	
26	8	142	
26	BS	142	
27	9	127	
27	BT	127	

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Mol	Chain	Length	Quality of chain
28	AA	136	
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	

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Mol	Chain	Length	Quality of chain
40	CG	51	
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	

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Mol	Chain	Length	Quality of chain
53	CU	186	
53	J	186	
54	CV	206	
54	K	206	
55	CW	189	
55	L	189	
56	CX	118	
56	M	118	
57	CY	155	
57	N	155	
58	CZ	143	
58	O	143	
59	DA	151	
59	P	151	
60	DB	132	
60	Q	132	
61	DC	142	
61	R	142	
62	DD	142	
62	S	142	
63	DE	137	
63	T	137	
64	DF	145	
64	U	145	
65	DG	145	

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Mol	Chain	Length	Quality of chain
65	V	145	
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	

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Mol	Chain	Length	Quality of chain
79	CL	267	
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	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
1	1	3171	Total	C	N	O	P	0	0	0
			67782	30282	12183	22146	3171			
1	AS	3065	Total	C	N	O	P	0	0	0
			65508	29266	11762	21415	3065			

- Molecule 2 is a RNA chain called 5S.

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

- Molecule 3 is a RNA chain called 5.8S.

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

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

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

- 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	0	1	0
			3084	1955	584	538	7			
5	AX	386	Total	C	N	O	S	0	0	0
			3077	1950	582	538	7			

- 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	0	0	0
			2745	1726	528	488	3			
6	AY	361	Total	C	N	O	S	0	0	0
			2751	1729	529	490	3			

- 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	0	0	0
			2426	1544	422	458	2			
7	AZ	292	Total	C	N	O	S	0	0	0
			2394	1526	416	450	2			

- 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	0	0	0
			1242	796	226	219	1			
8	BA	153	Total	C	N	O		0	0	0
			1210	777	221	212				

- 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	0	0	0
			1885	1208	345	331	1			
9	BB	234	Total	C	N	O	S	0	0	0
			1885	1208	345	331	1			

- 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	0	0	0
			1790	1147	318	322	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 17 is a protein called Ribosomal protein L13.

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

- Molecule 18 is a protein called Ribosomal protein L22.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

- 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	0	0	0
			1087	705	197	183	2			
28	BU	135	Total	C	N	O	S	0	0	0
			1087	705	197	183	2			

- 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	0	0	0
			1170	741	231	197	1			
29	BV	148	Total	C	N	O	S	0	0	0
			1170	741	231	197	1			

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

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

- 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	0	0	0
			729	469	121	137	2			
31	BX	96	Total	C	N	O	S	0	0	0
			729	469	121	137	2			

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

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

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

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

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

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

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

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

- Molecule 36 is a protein called Ribosomal protein L29.

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

- 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	0	0	0
			758	471	156	130	1			
37	CD	97	Total	C	N	O	S	0	0	0
			758	471	156	130	1			

- 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	0	0	0
			677	413	148	110	6			
38	CE	86	Total	C	N	O	S	0	0	0
			677	413	148	110	6			

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

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

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

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

- 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	0	0	0
			419	260	86	67	6			
41	CH	51	Total	C	N	O	S	0	0	0
			411	255	85	66	5			

- 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	0	0	0
			236	144	63	28	1			

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

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

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

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

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

- Molecule 45 is a RNA chain called 18S.

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

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

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

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

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

- Molecule 48 is a protein called Ribosomal protein S5.

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

- Molecule 49 is a protein called Ribosomal protein S3.

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

- 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	0	0	0
			2051	1304	385	357	5			
50	CR	260	Total	C	N	O	S	0	0	0
			2055	1306	386	358	5			

- Molecule 51 is a protein called Ribosomal protein S7.

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

- 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	0	0	0
			1787	1113	344	324	6			
52	CT	236	Total	C	N	O	S	0	0	0
			1904	1184	369	345	6			

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

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

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

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

- Molecule 55 is a protein called Ribosomal protein S4.

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

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

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

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

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

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

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

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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
64	U	144	Total	C	N	O	S	0	0	0
			1187	744	233	207	3			
64	DF	141	Total	C	N	O	S	0	0	0
			1161	727	227	204	3			

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

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

- Molecule 66 is a protein called Ribosomal protein S10.

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

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

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

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

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

- 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	0	0	0
			1110	701	219	188	2			
69	DK	143	Total	C	N	O	S	0	0	0
			1110	701	219	188	2			

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

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

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

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

- 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	0	0	0
			779	482	163	128	6			
72	DN	98	Total	C	N	O	S	0	0	0
			779	482	163	128	6			

- 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	0	0	0
			614	383	110	114	7			
73	DO	81	Total	C	N	O	S	0	0	0
			614	383	110	114	7			

- 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	0	0	0
			487	299	98	88	2			

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

- 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	0	0	0
			454	281	94	75	4			
75	DQ	54	Total	C	N	O	S	0	0	0
			449	278	93	74	4			

- 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	0	0	0
			431	271	88	70	2			
76	DR	58	Total	C	N	O	S	0	0	0
			461	289	93	77	2			

- 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	0	0	0
			574	362	113	93	6			

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

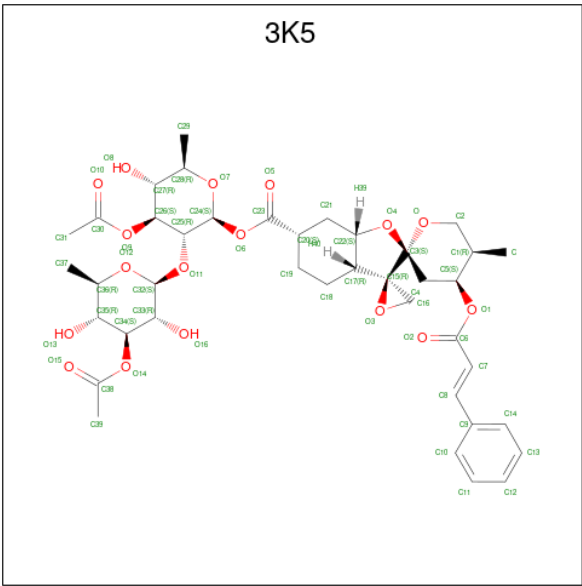
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	AR	311	Total	C	N	O	S	0	0	0
			2398	1519	412	462	5			

- 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		0	0	0
			918	554	165	199				
79	CL	121	Total	C	N	O		0	0	0
			930	563	166	201				

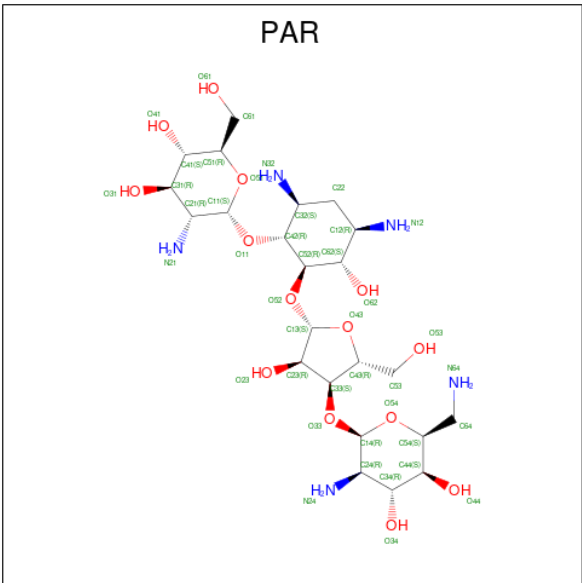
- Molecule 80 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-{{[(2R,2'S,3a'R,4''S,5''R,6'S,7a'S)-5''-methyl-4''-{[(2E)-3-phenylprop-2-enoyl]oxy}decahydrodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose (CCD ID:

3K5) (formula: C₄₀H₅₂O₁₇).



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

- Molecule 81 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄) (labeled as "Lig- and of Interest" by depositor).



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

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

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

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

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

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

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

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

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

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

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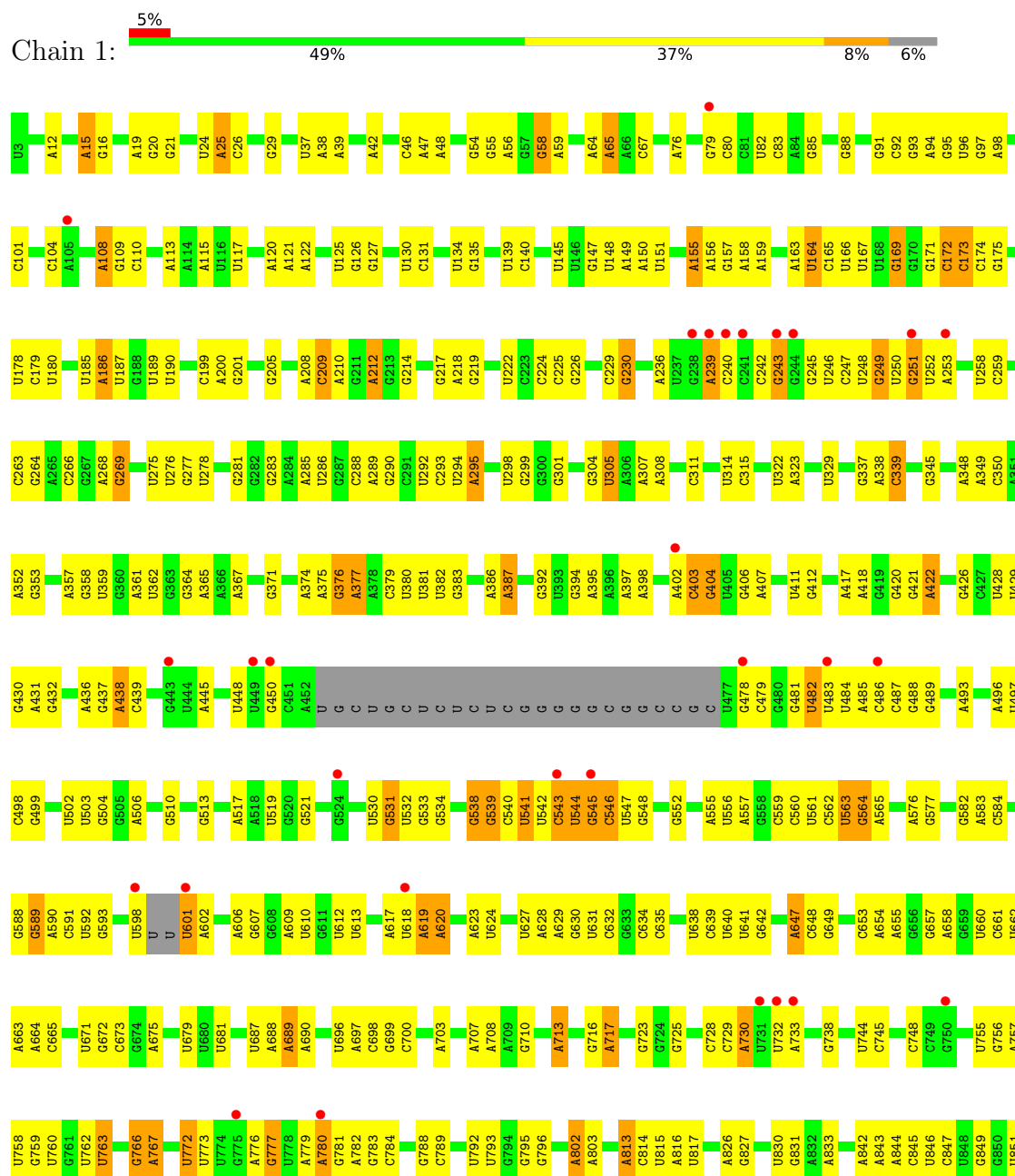
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	DO	1	Total 1	Zn 1	0	0
83	DQ	1	Total 1	Zn 1	0	0

3 Residue-property plots

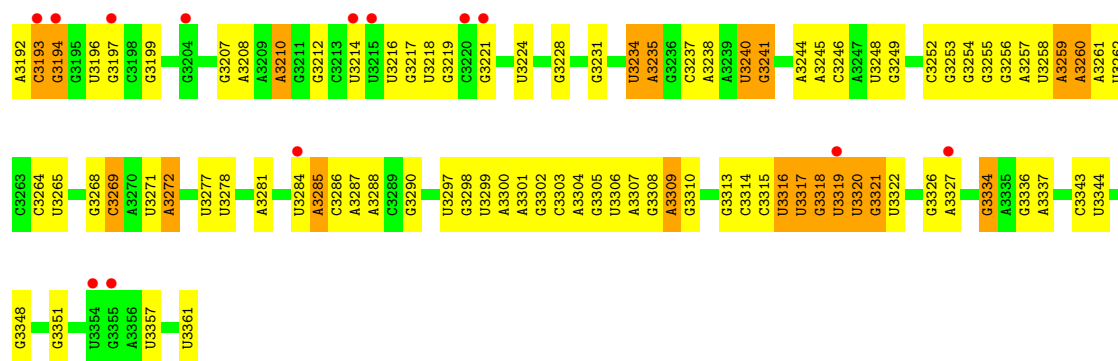
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

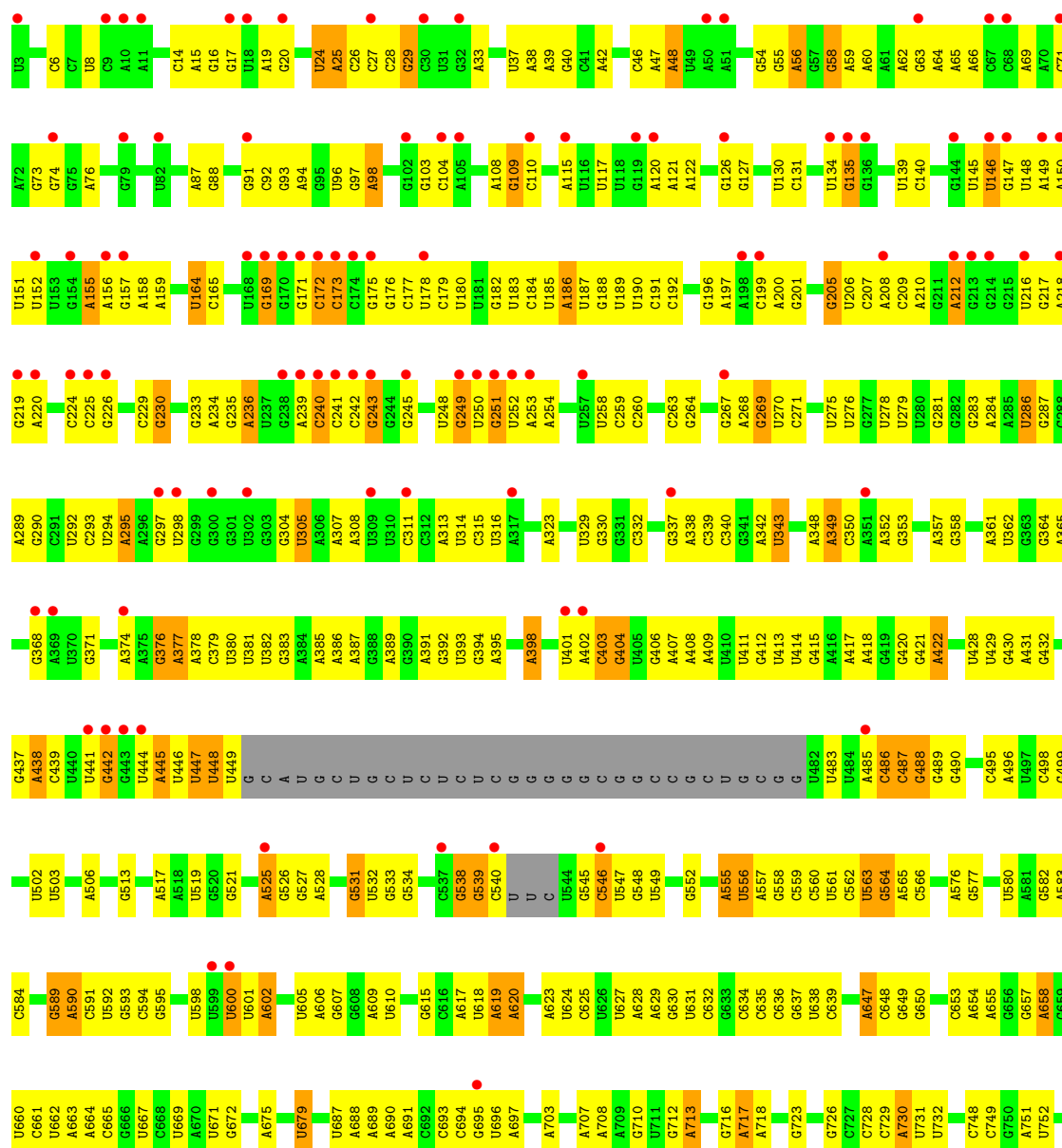


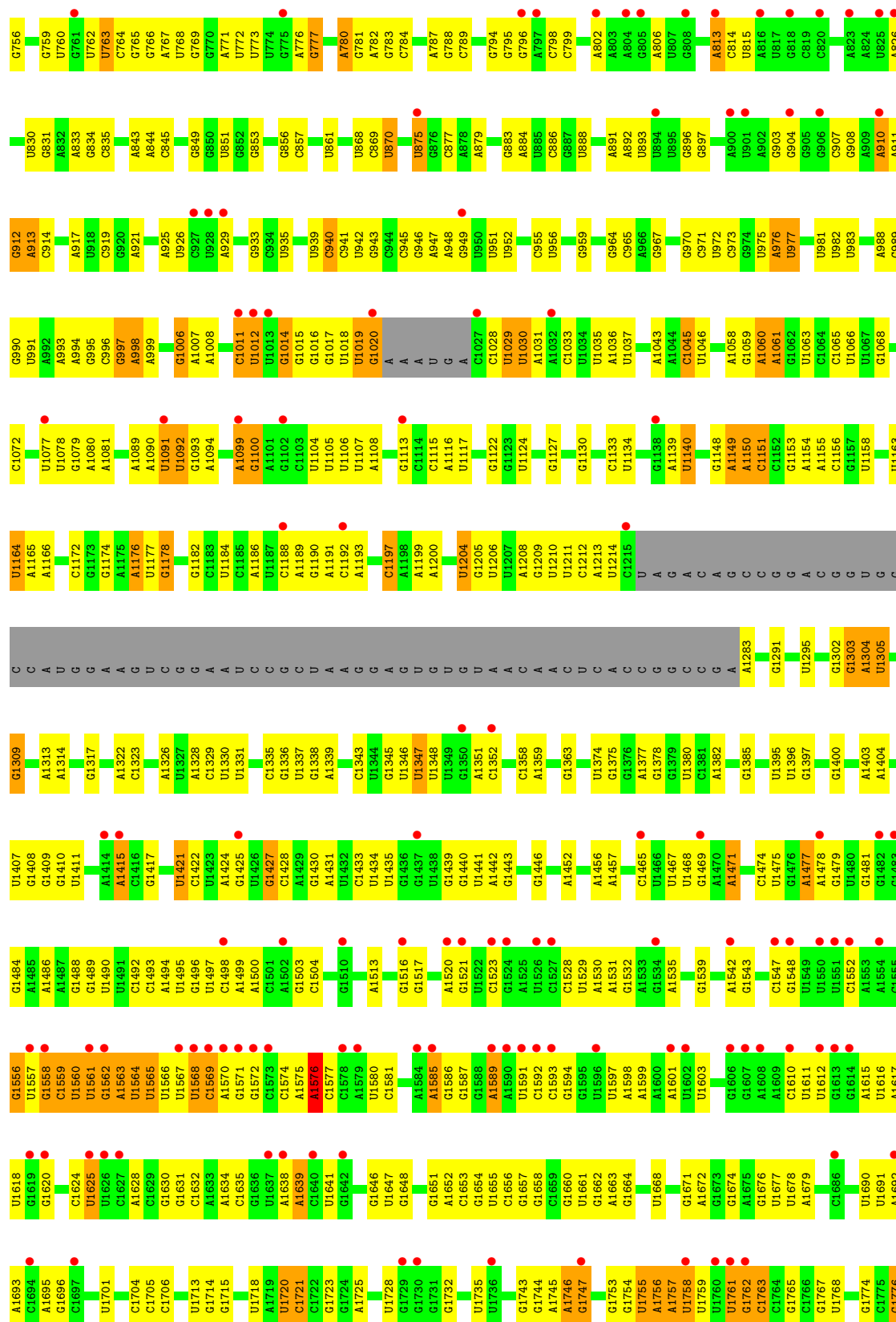


A3113	A2136	A2379	C2340	U2479	U2568	A2661	C2746	U2838	G2922	U3013	A3113
A3114	U2137	U2238	A2341	A2480	U2571	G2662	U2747	C2839	G2923	U3014	A3114
C3115	G2138	G2239	A2342	U2481	U2572	A2663	G2748	U2840	U2924	C3015	C3115
U3125	G2139	C2241	C2344	U2482	G2578	A2664	G2749	A2843	U2925	A3016	U3126
U3126	A2145	U2244	A2345	U2484	G2579	C2665	G2750	A2844	U2926	U3019	U3127
U3127	A2146	C2245	A2346	U2485	U2583	A2666	U2753	U2847	A2927	A3020	C3128
C3128	G2147	C2246	G2347	U2486	U2584	A2667	U2754	C2848	A2928	A3021	C3129
C3129	U2148	A2248	G2348	U2487	U2585	A2668	U2755	U2849	C2932	U3022	C3130
A3132	U2149	A2249	A2351	U2488	U2586	A2669	A2764	G2849	U2933	U3023	C3131
U3133	A2150	G2250	C2352	A2493	U2587	A2670	G2765	G2850	U2934	G3024	U3132
G3133	G2155	G2251	G2353	U2499	C2588	A2671	G2766	U2851	C2935	U3028	U3133
C3134	A2156	U2252	G2354	U2504	A2589	A2672	G2768	C2853	G2936	U3029	C3134
A3135	C2159	A2257	G2355	C2505	U2598	G2678	A2771	U2854	U2937	A3031	A3135
C3136	G2163	A2258	C2363	G2506	U2605	U2679	A2772	U2855	G2938	U3032	C3136
A3137	U2171	U2260	U2366	U2509	U2606	C2680	G2773	C2856	U2940	A3033	A3137
U3138	G2172	A2273	C2367	U2510	A2607	C2681	A2774	U2857	G2941	U3038	U3138
U3139	A2181	A2276	G2370	U2511	A2609	C2682	U2779	U2858	C2942	C3039	U3139
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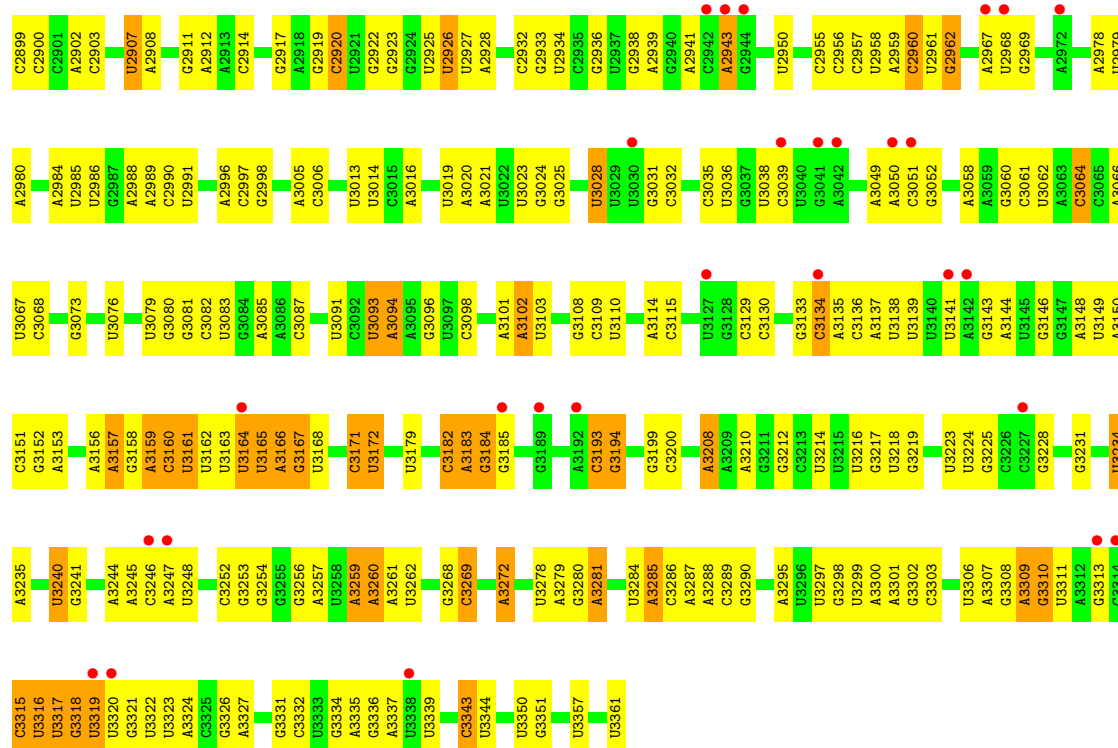


• Molecule 1: 25S





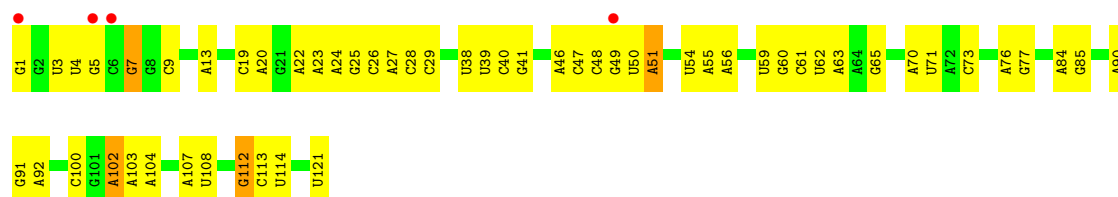
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• Molecule 2: 5S

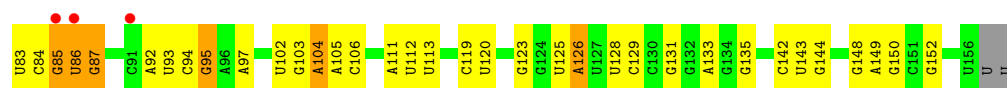


• Molecule 2: 5S

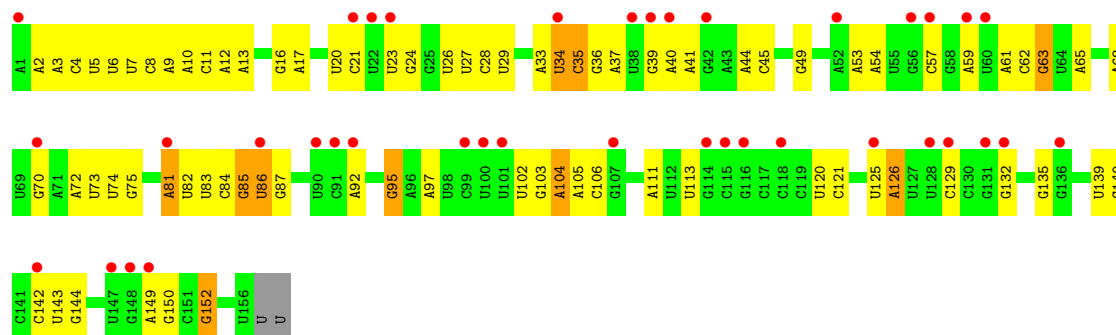


• Molecule 3: 5.8S

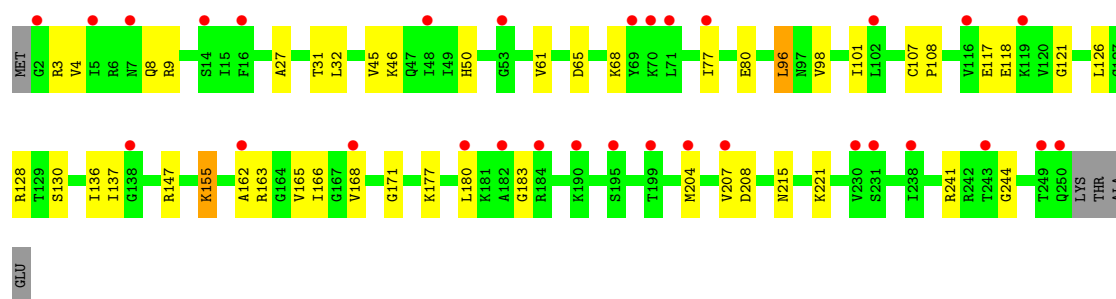
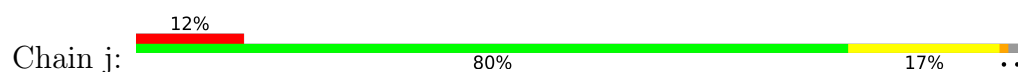




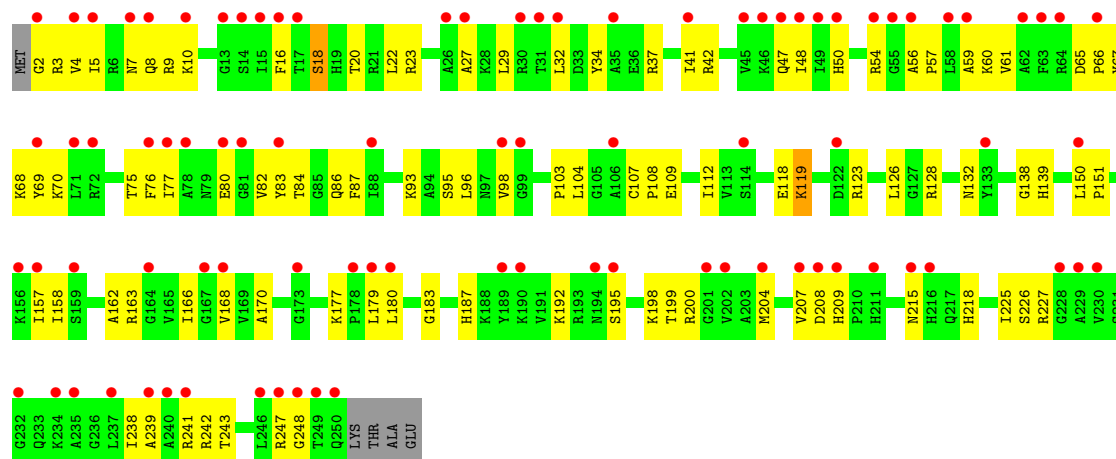
• Molecule 3: 5.8S



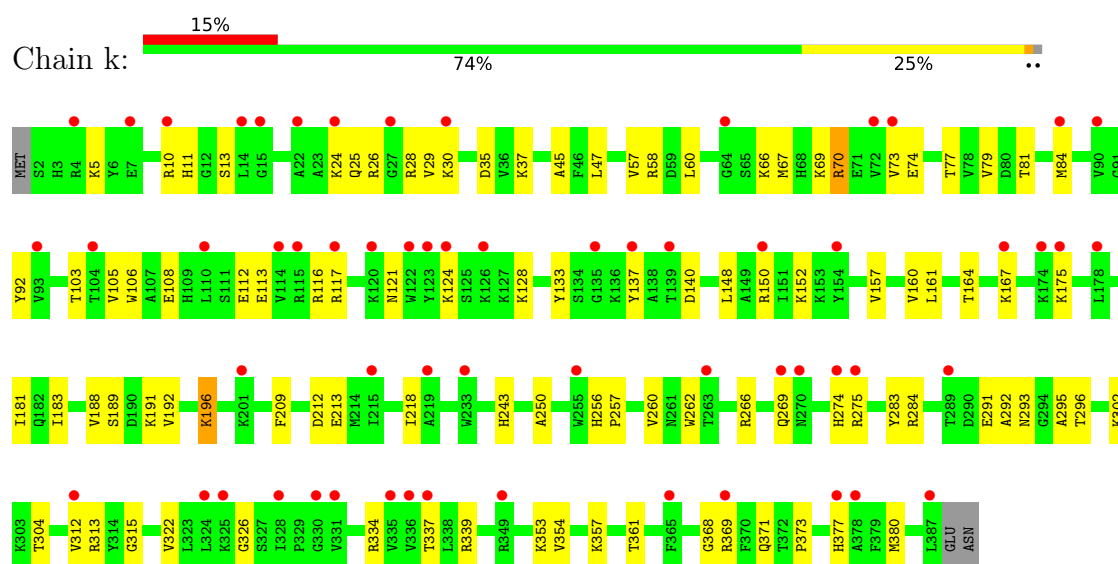
• Molecule 4: 60S ribosomal protein L2-B



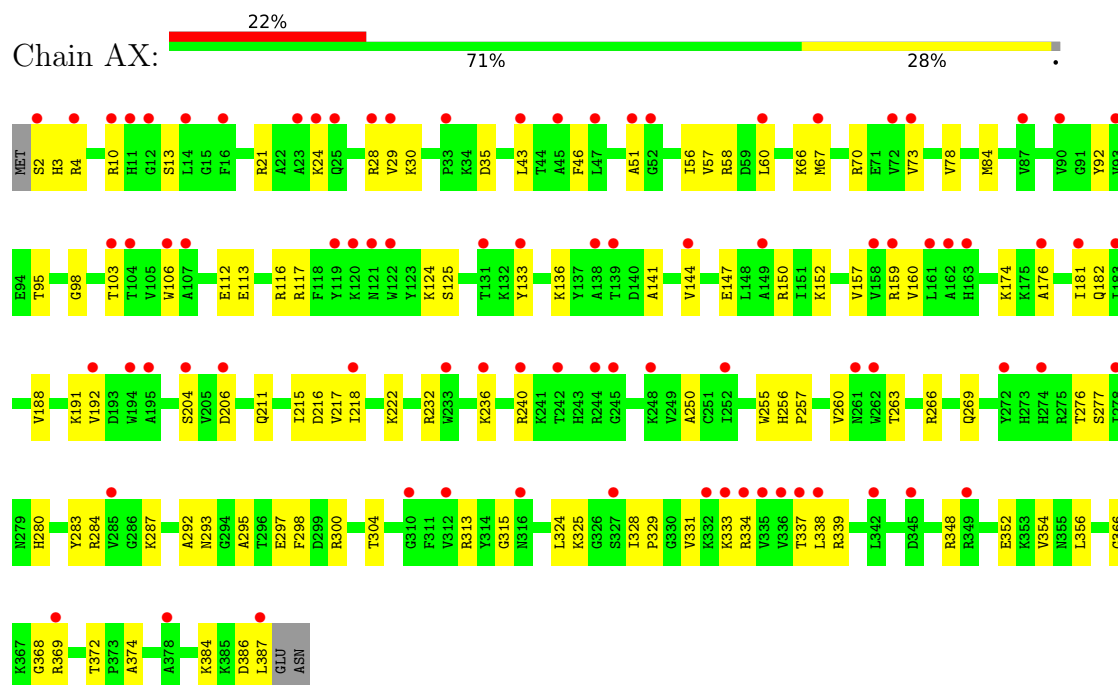
• Molecule 4: 60S ribosomal protein L2-B



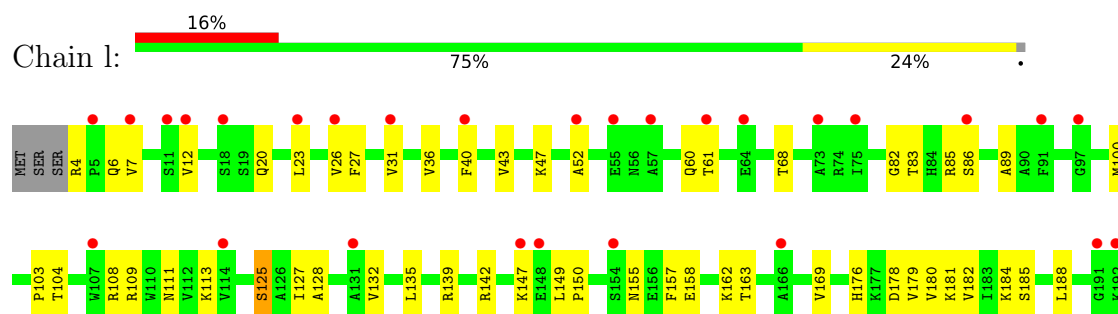
• Molecule 5: 60S ribosomal protein L3

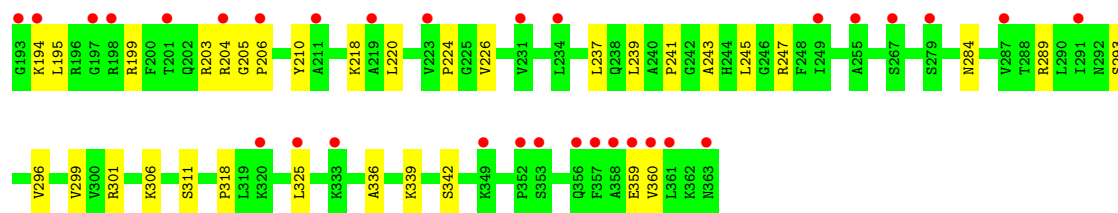


• Molecule 5: 60S ribosomal protein L3

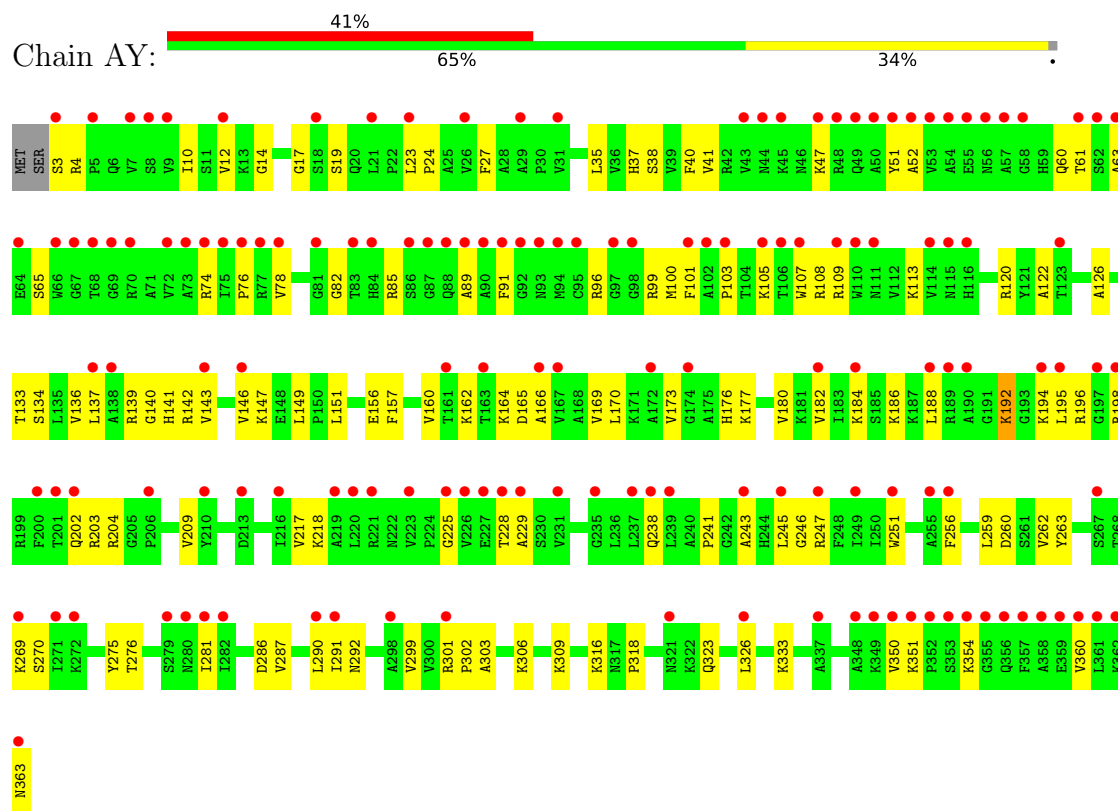


• Molecule 6: 60S ribosomal protein L4-B

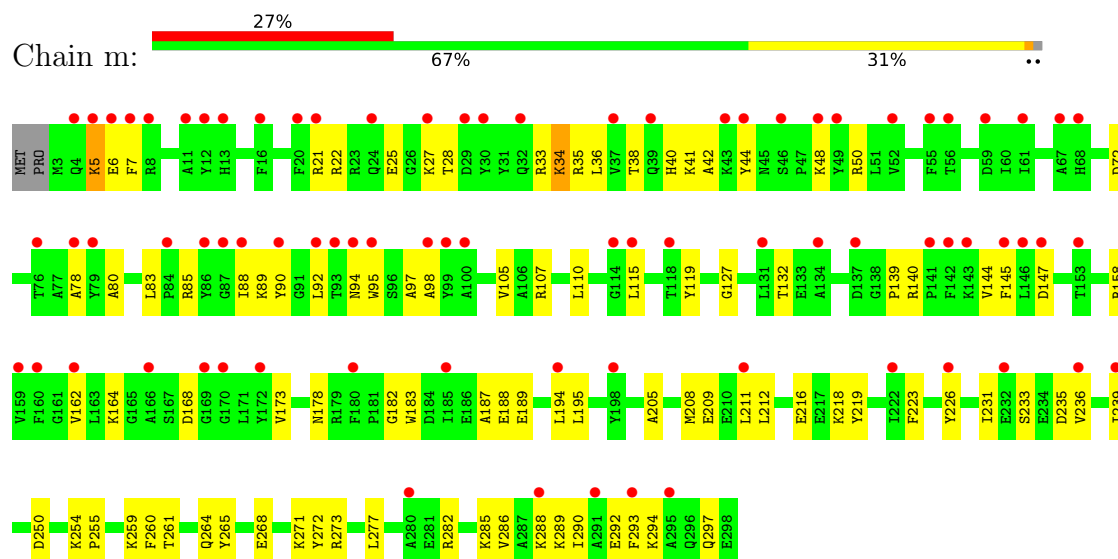




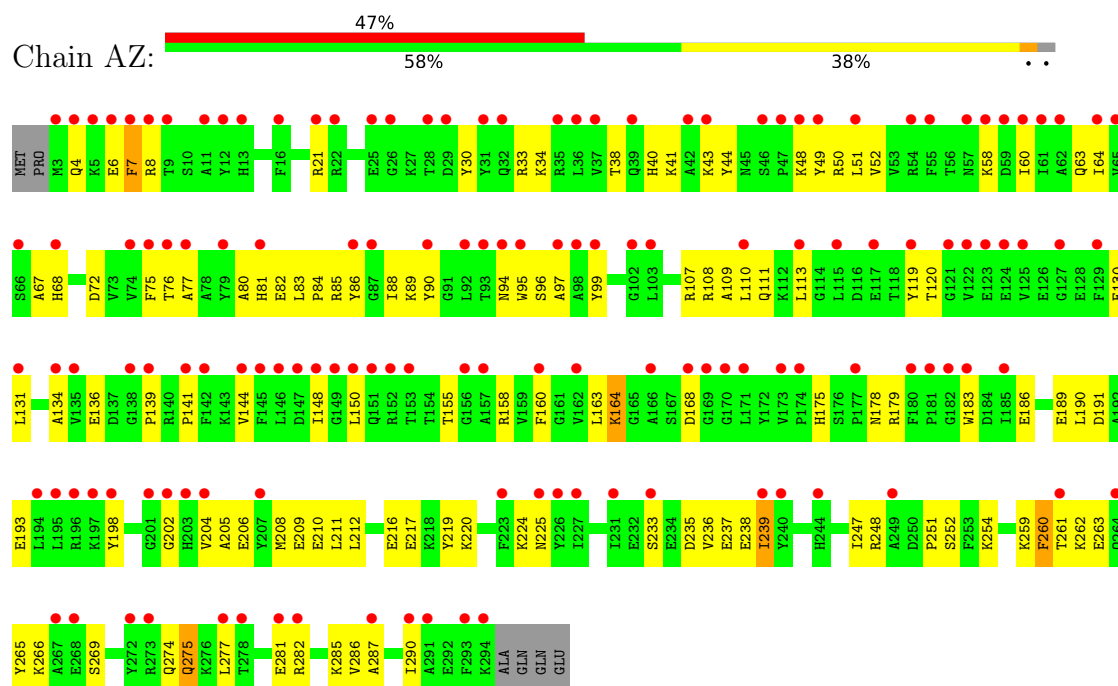
• Molecule 6: 60S ribosomal protein L4-B



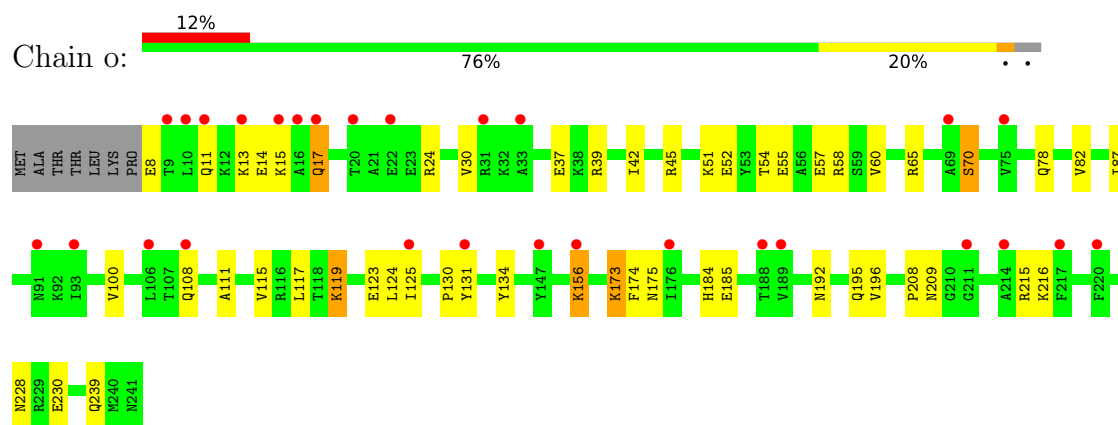
• Molecule 7: Uncharacterized protein CaJ7.0206



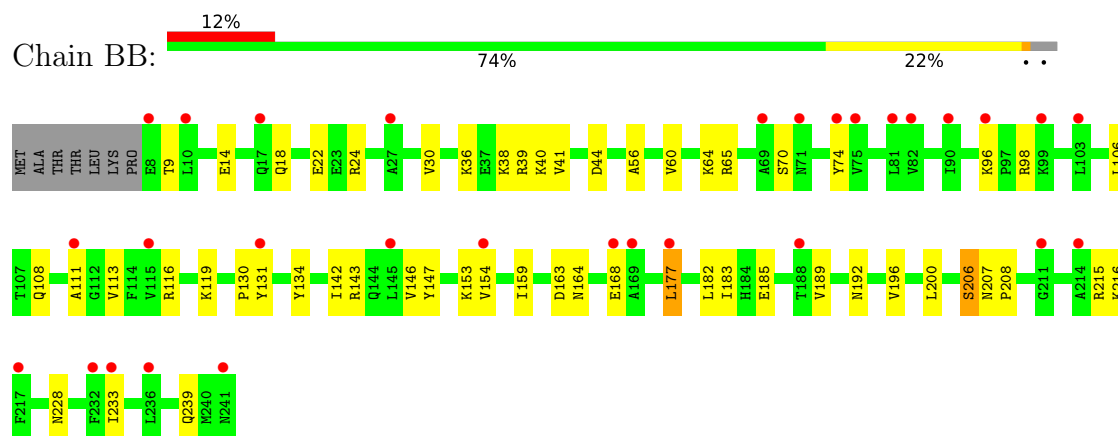
• Molecule 7: Uncharacterized protein CaJ7.0206



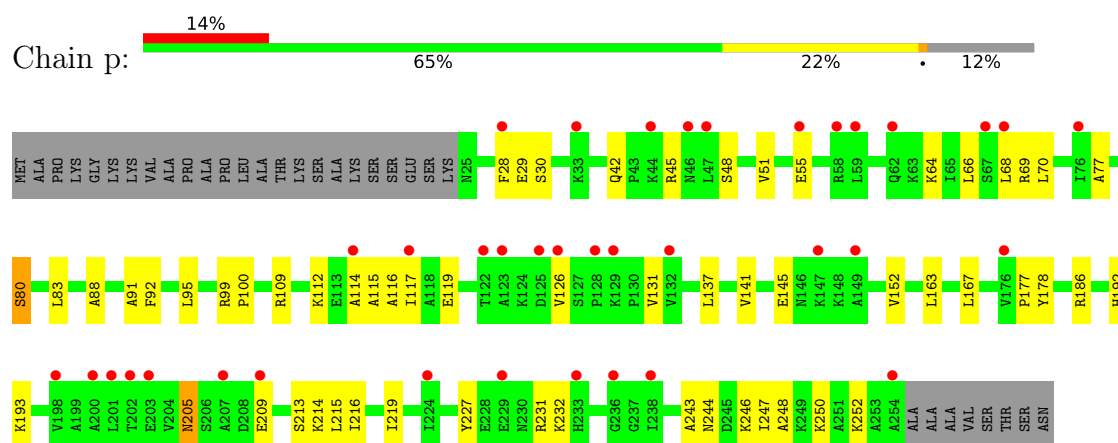
- Molecule 9: 60S ribosomal protein L7-A



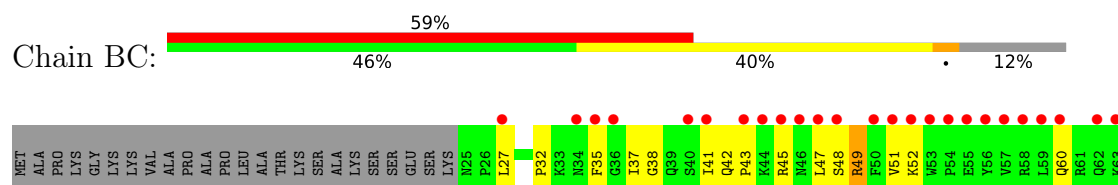
- Molecule 9: 60S ribosomal protein L7-A

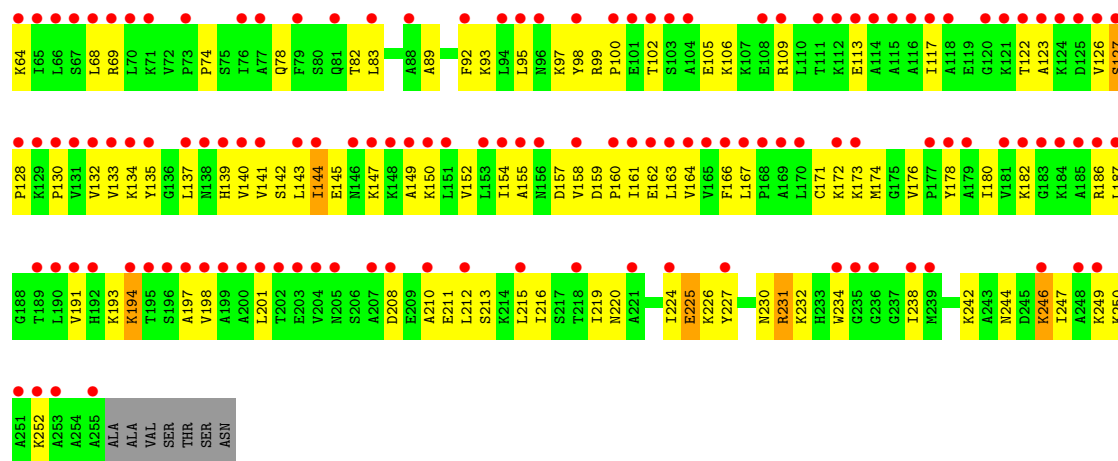


- Molecule 10: 60S ribosomal protein L8

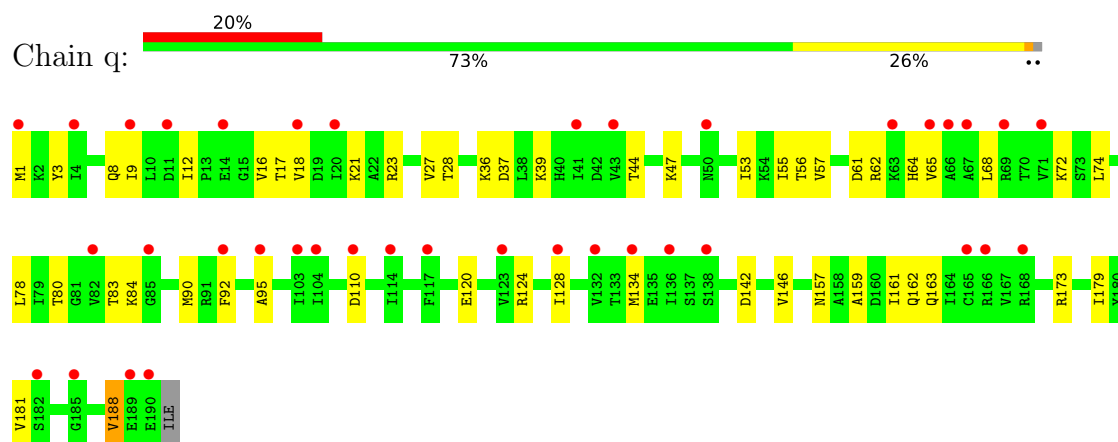


- Molecule 10: 60S ribosomal protein L8

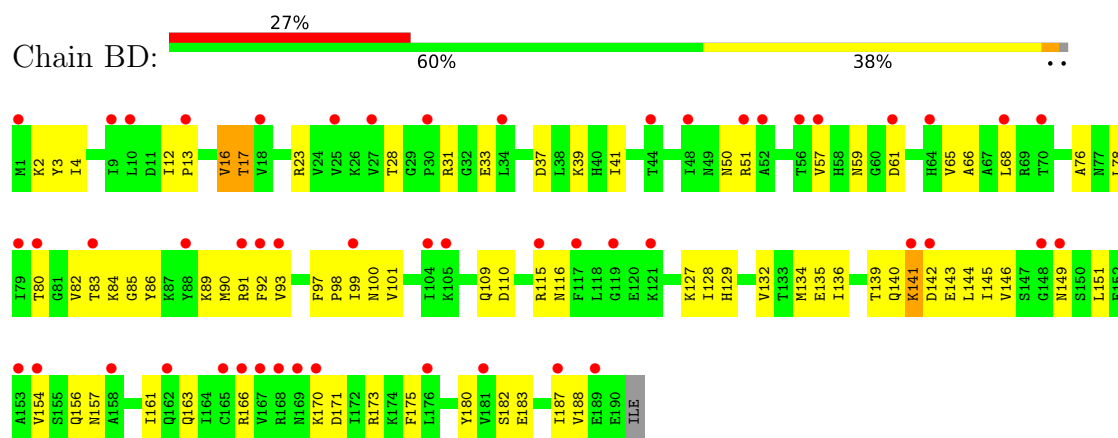




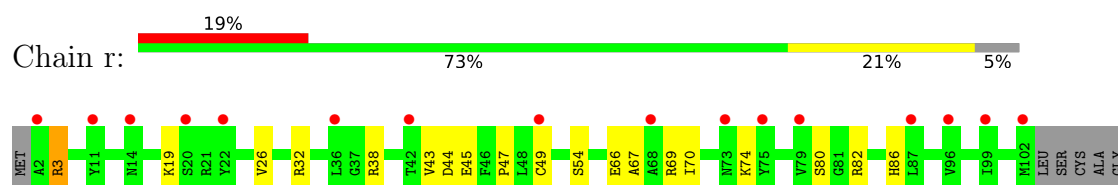
• Molecule 11: 60S ribosomal protein L9-B

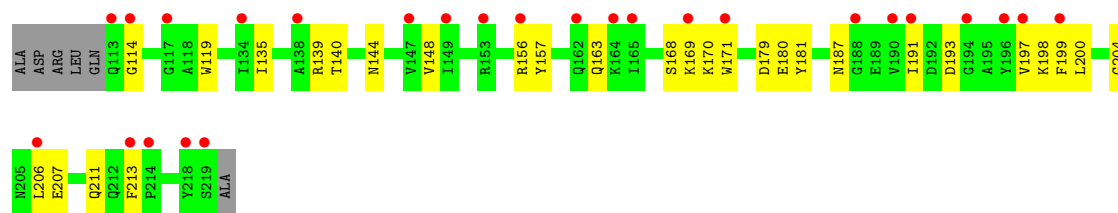


• Molecule 11: 60S ribosomal protein L9-B

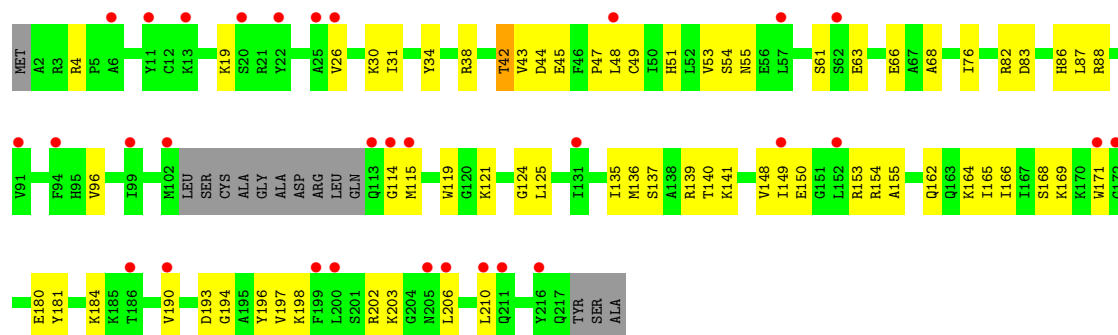


• Molecule 12: 60S ribosomal protein L10

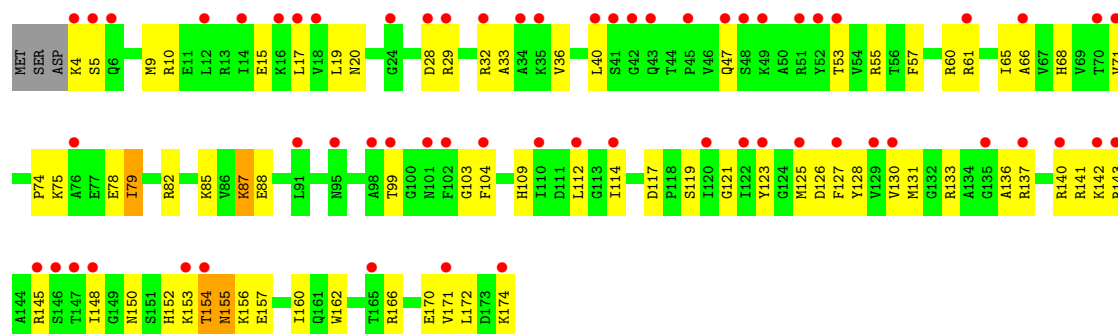




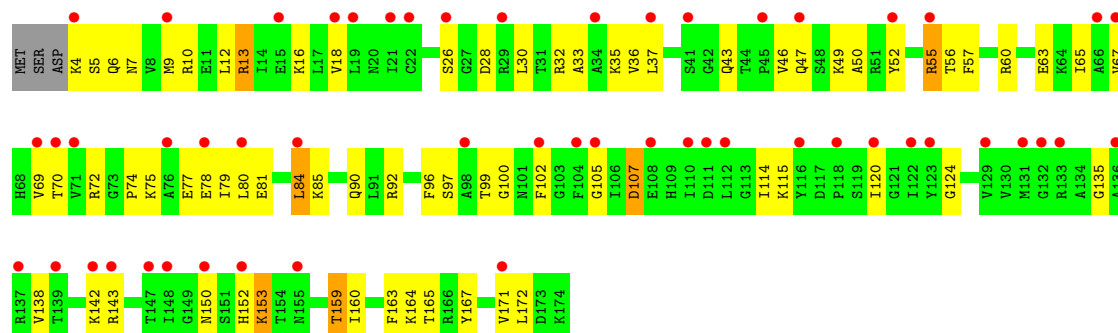
• Molecule 12: 60S ribosomal protein L10



• Molecule 13: 60S ribosomal protein L11-B



• Molecule 13: 60S ribosomal protein L11-B



Chain t:

15% 74% 23% ..

Sequence logo for Chain t showing amino acid frequencies at each position. The y-axis represents frequency from 0.00 to 0.10. The x-axis lists amino acids: MET, A2, I3, S4, L7, P8, L9, L10, H13, F14, R15, W18, Q19, E20, R21, V22, D27, Q28, A29, S34, R41, K42, I46, R49, P50, I51, D52, A53, L54, R55, P56, V57, K64, R65, N66, V69, R73, G74, K81, A82, V83, G84, I85, Y89, A90, R91, S96, V97, D98, H99, R100, Q106, L116, Y119, K122, L123, V124, I125, F126, D127, T130, K131, A132, S133, E134, V135, F138, V141, D142, V143, Q151, G157, A168, Y169, R170, R173, L174, A175, R176, K187, K192, A195, E196, A197, E198, K199, A200, K201, and LYS.

Chain BG:

55%

57%

38%

Chain u:

14% 63% 34%

Met S2 S3 T4 V5 V6 F12 V13 R17 V18 V19 L20 K24 F25 L26 L29 D34 Q35 K36 R37 V38 L39 L40 R47 L52 I55 V56 L57 T58 P59 I60 V61 L62 L65 S69 W87 W92 A93 K99 R102 S103 Q104 L105 S106 D107 F108 E109 R110 F111 Q112 V113 M114 V115 K116 K117 K118 Q119 R120 R121 F122 A123 T124 K125 K126 A127 L128 V129 LYS ALA

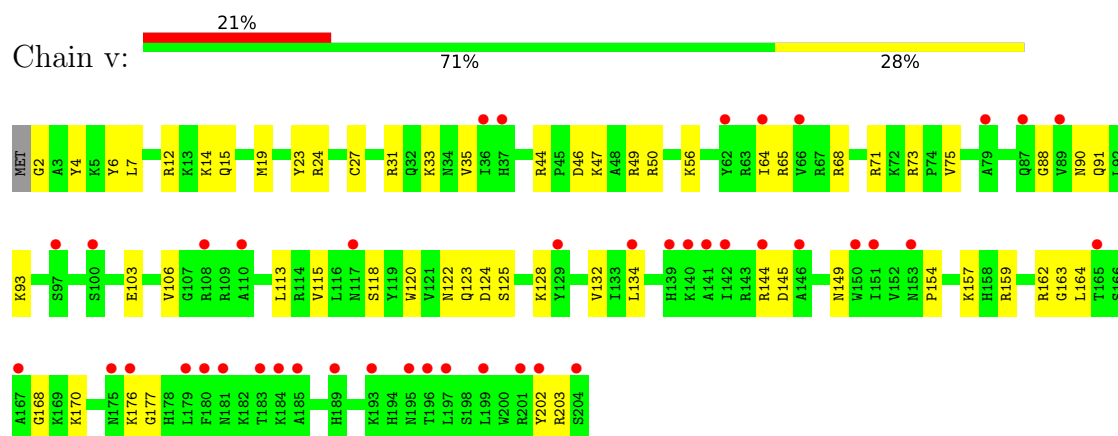
Chain BH:

Label	Color	Red Dot
MET	Grey	No
S2	Yellow	Yes
S3	Yellow	Yes
T4	Yellow	Yes
V5	Yellow	No
K6	Yellow	No
V13	Green	Yes
G16	Yellow	No
R17	Green	Yes
V18	Green	No
D22	Green	No
N23	Green	No
K24	Yellow	No
I29	Green	Yes
I32	Green	Yes
I33	Green	Yes
D34	Green	Yes
L39	Yellow	No
Q48	Yellow	Yes
A53	Green	Yes
K54	Green	No
I55	Green	Yes
L62	Yellow	Yes
A72	Yellow	No
T73	Green	No
T74	Green	Yes
T75	Green	No
K76	Yellow	No
I83	Green	Yes
W87	Yellow	No
A93	Yellow	No
K94	Green	No
K95	Green	No
R101	Brown	No
L105	Green	No
S106	Green	No
D107	Yellow	No
F108	Yellow	No
E109	Yellow	No
R110	Yellow	No
V113	Yellow	No
L116	Yellow	No

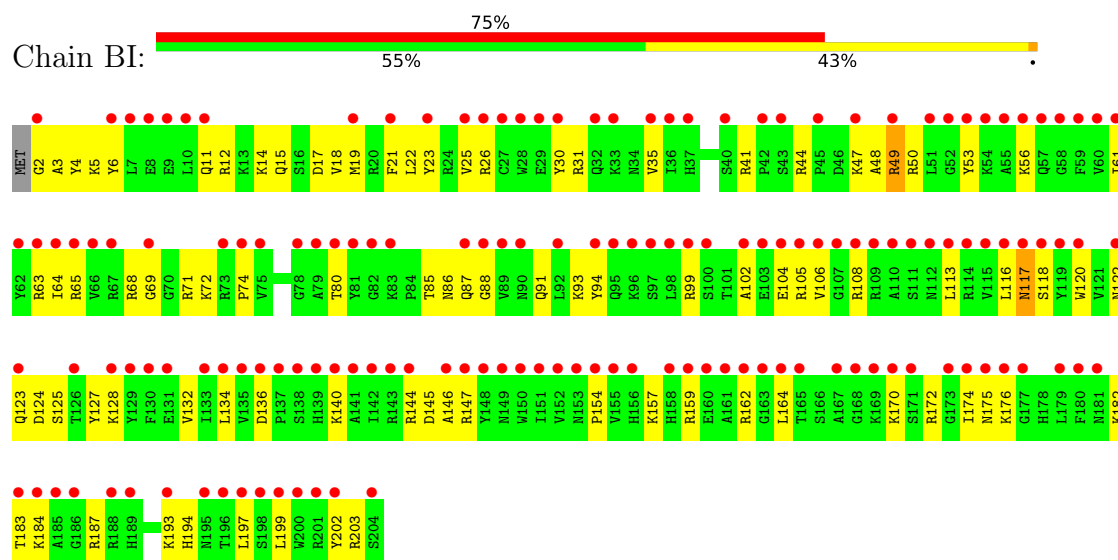
Q119, R120, K125, K126, A127, L128, V129, K130, A131

Label	Color	Red Dot
Q119	Green	Yes
R120	Green	Yes
K125	Green	Yes
K126	Green	Yes
A127	Green	Yes
L128	Green	Yes
V129	Green	Yes
K130	Green	Yes
A131	Green	Yes

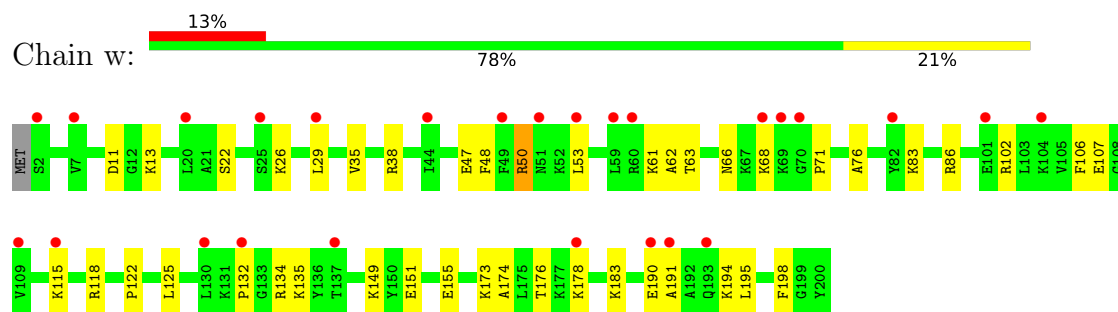
- Molecule 16: 60S ribosomal protein L15-A



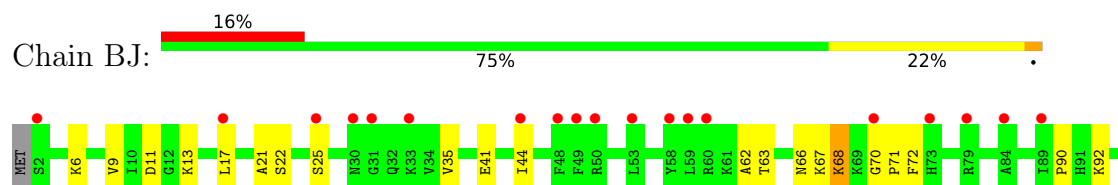
- Molecule 16: 60S ribosomal protein L15-A

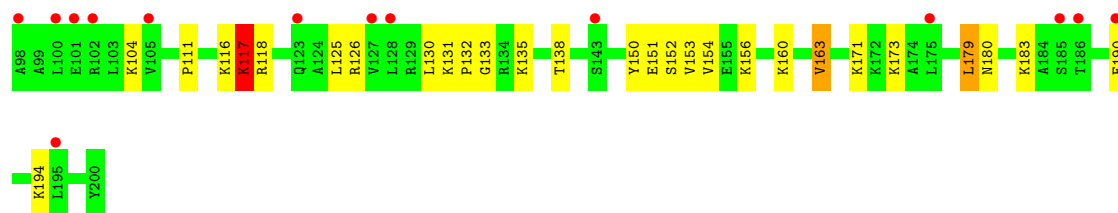


- Molecule 17: Ribosomal protein L13

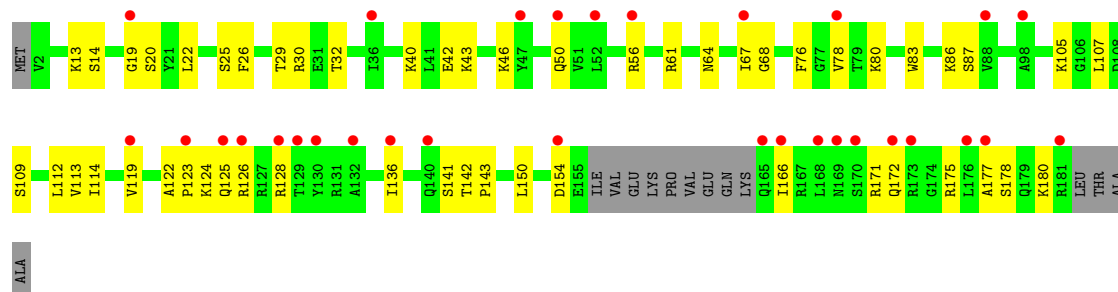


- Molecule 17: Ribosomal protein L13

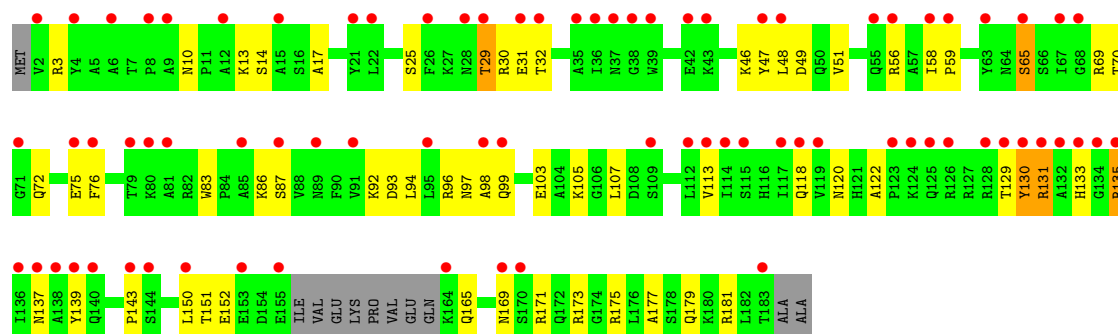
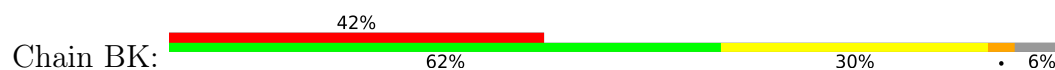




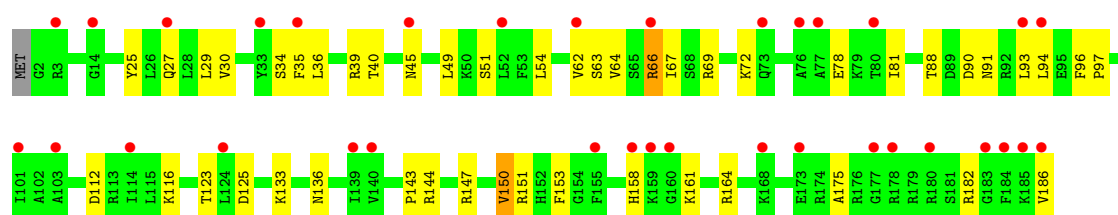
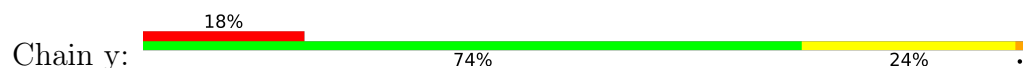
• Molecule 18: Ribosomal protein L22



• Molecule 18: Ribosomal protein L22

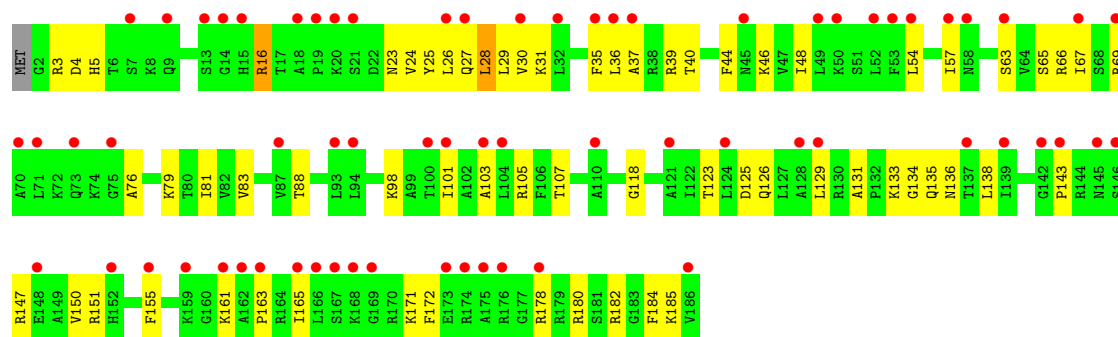


• Molecule 19: 60S ribosomal protein L18-A

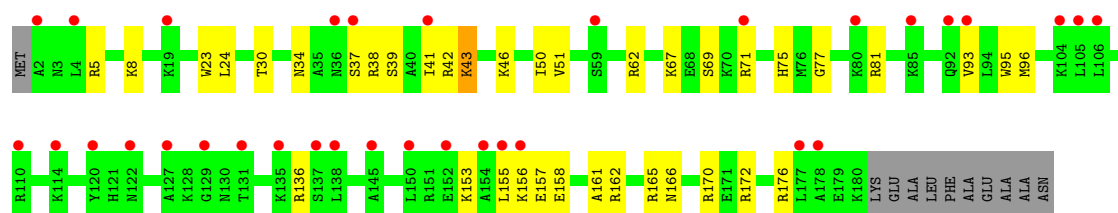


• Molecule 19: 60S ribosomal protein L18-A

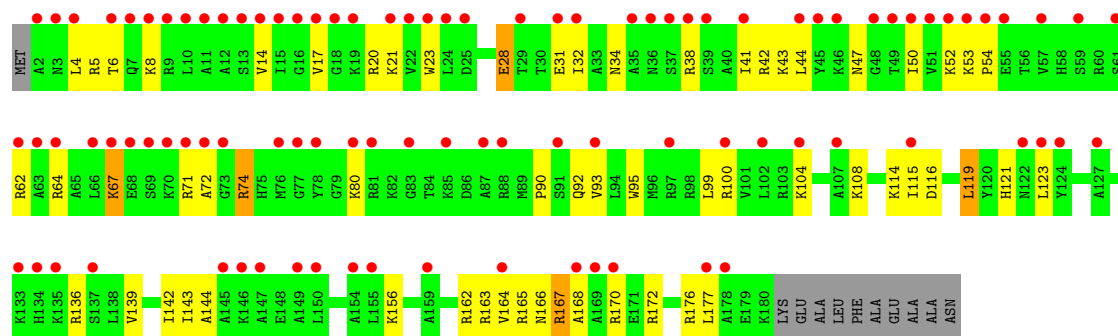




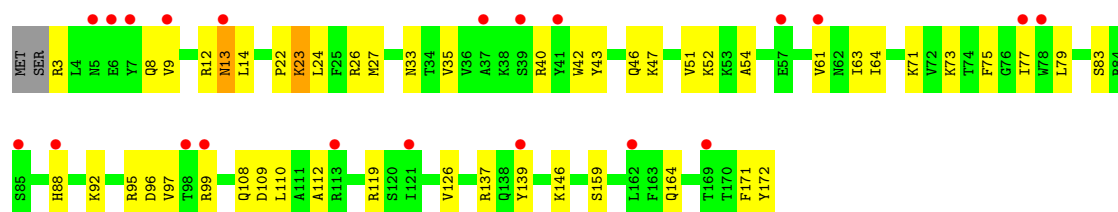
• Molecule 20: 60S ribosomal protein L19-A



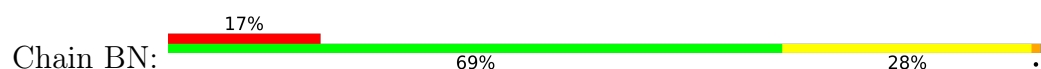
• Molecule 20: 60S ribosomal protein L19-A

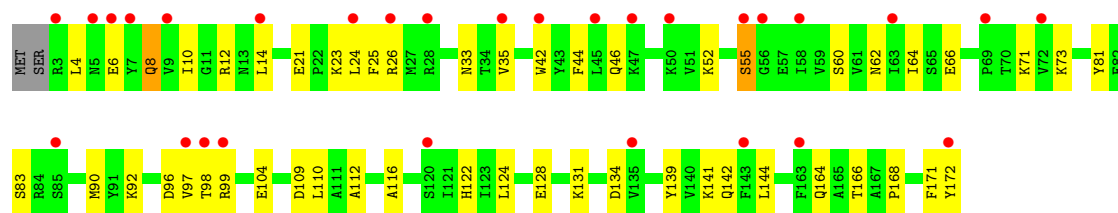


• Molecule 21: 60S ribosomal protein L20

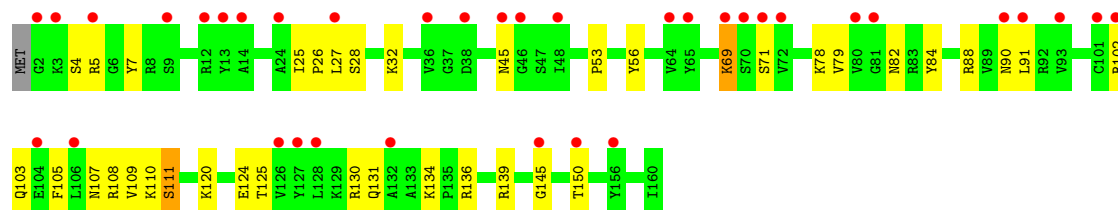
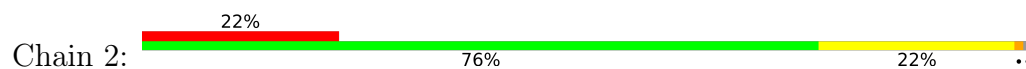


• Molecule 21: 60S ribosomal protein L20

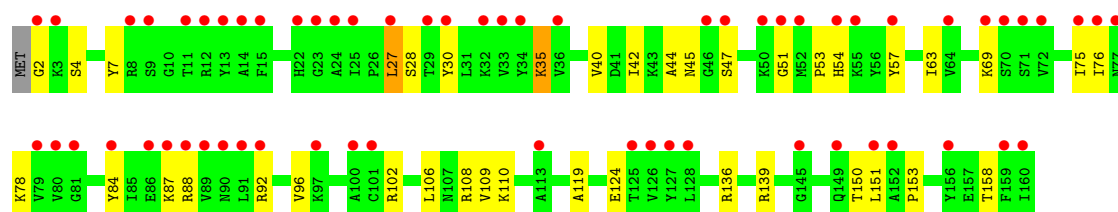
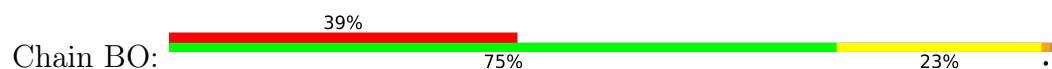




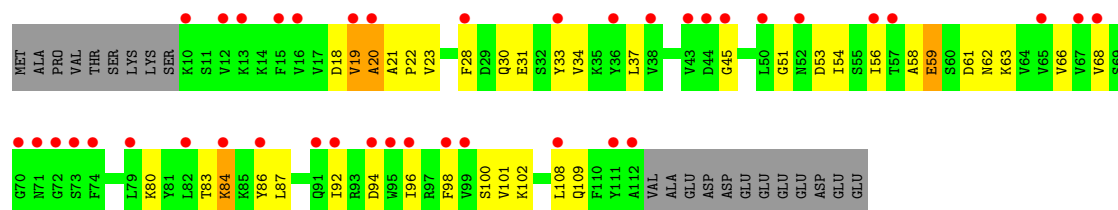
• Molecule 22: 60S ribosomal protein L21-A



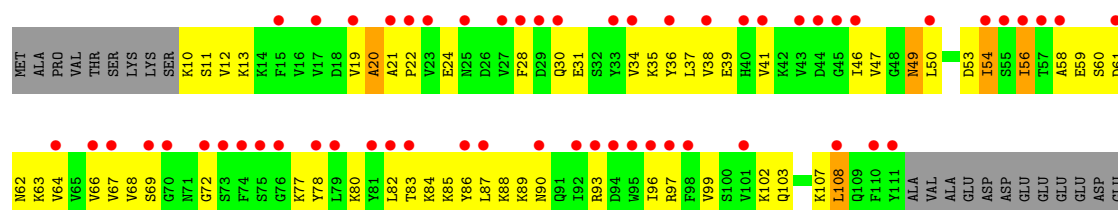
• Molecule 22: 60S ribosomal protein L21-A



• Molecule 23: 60S ribosomal protein L22-B



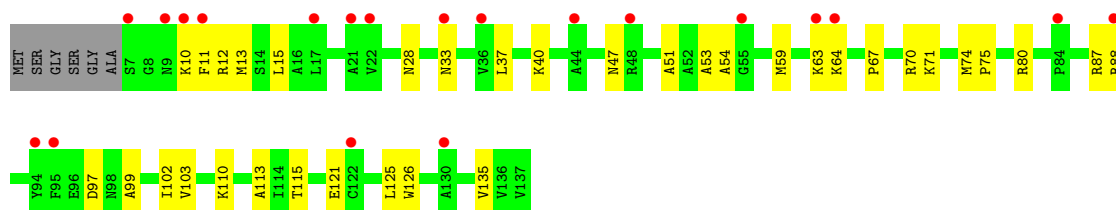
• Molecule 23: 60S ribosomal protein L22-B



GLU

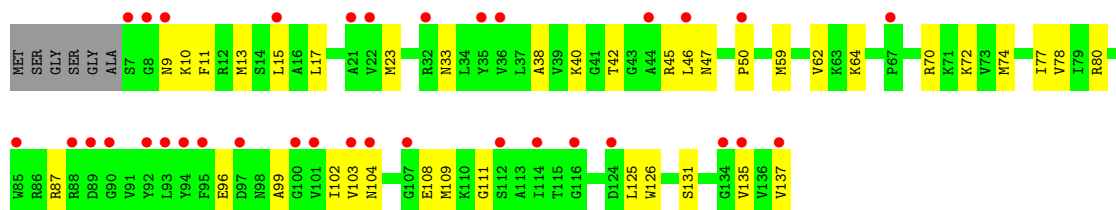
- Molecule 24: 60S ribosomal protein L23-A

Chain 6:  15% 70% 26%



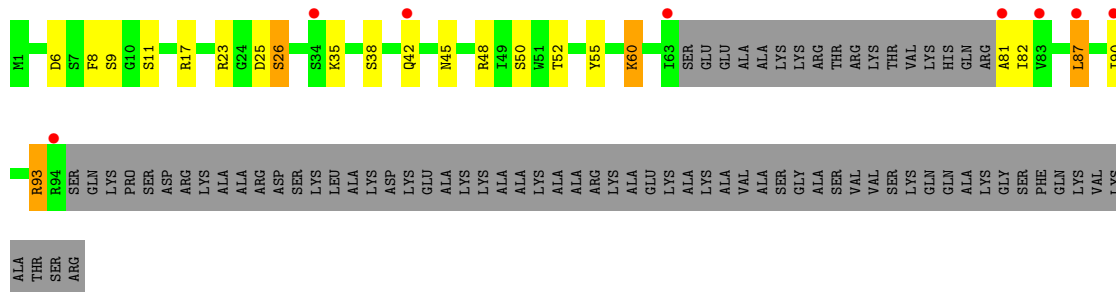
- Molecule 24: 60S ribosomal protein L23-A

Chain BQ:  25% 68% 28%



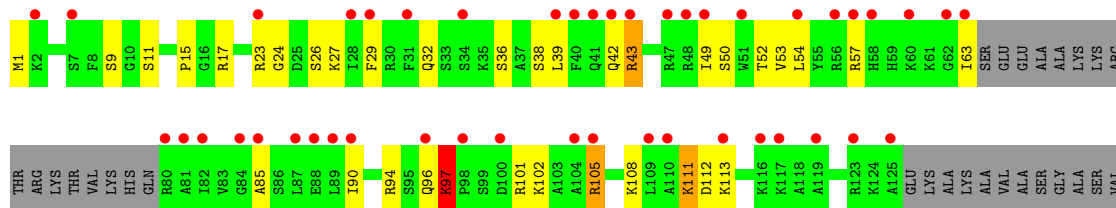
- Molecule 25: 60S ribosomal protein L24-A

Chain 7:  5% 35% 12% 50%

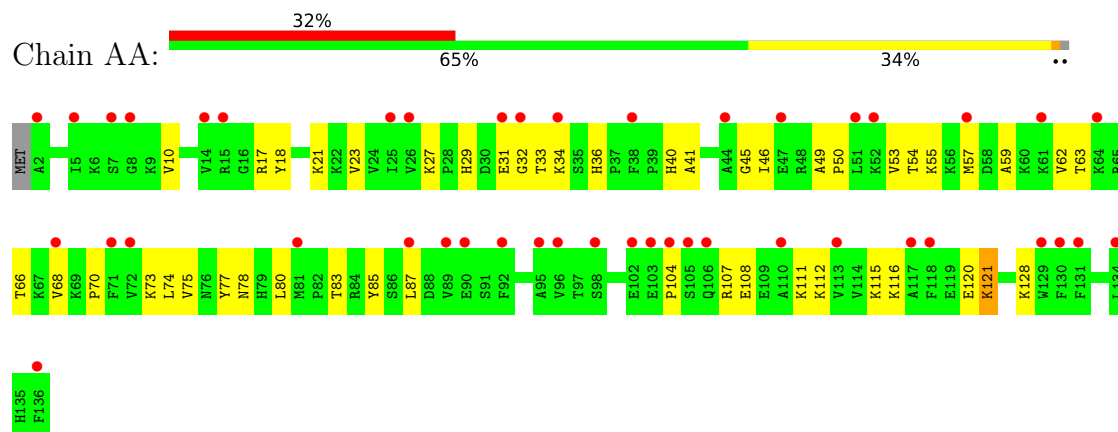


- Molecule 25: 60S ribosomal protein L24-A

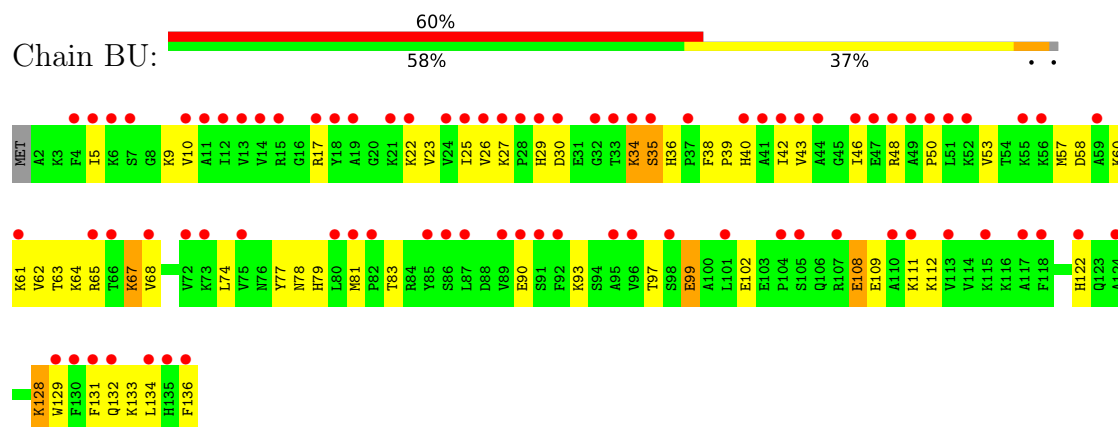
Chain BR:  29% 48% 20% 30%



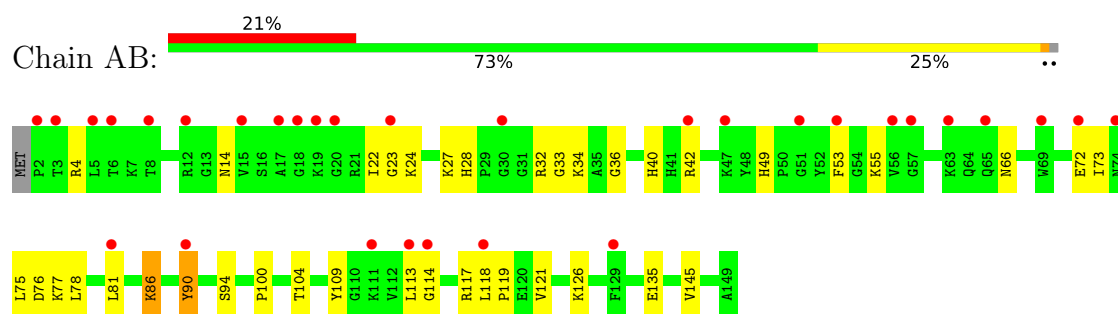
● Molecule 28: 60S ribosomal protein L27



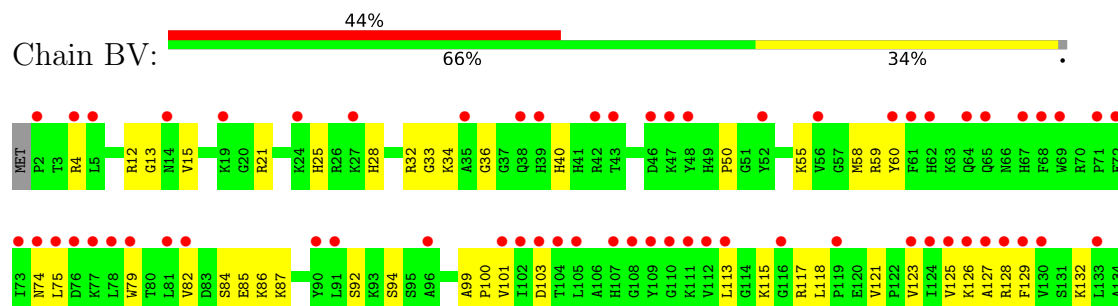
● Molecule 28: 60S ribosomal protein L27

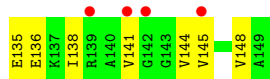


● Molecule 29: 60S ribosomal protein L28



● Molecule 29: 60S ribosomal protein L28

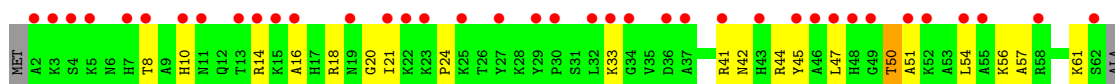




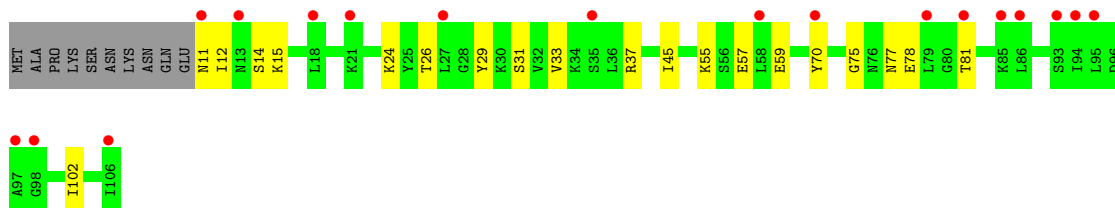
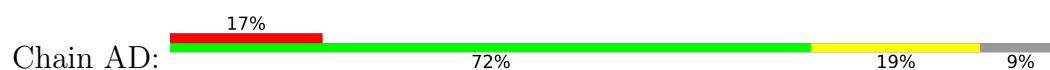
- Molecule 30: 60S ribosomal protein L29



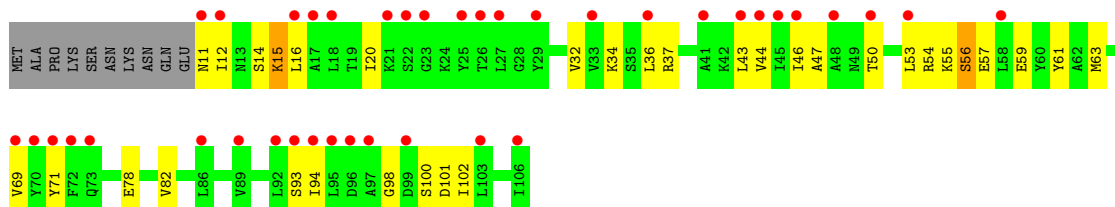
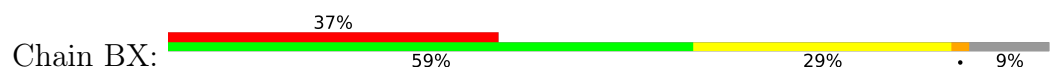
- Molecule 30: 60S ribosomal protein L29



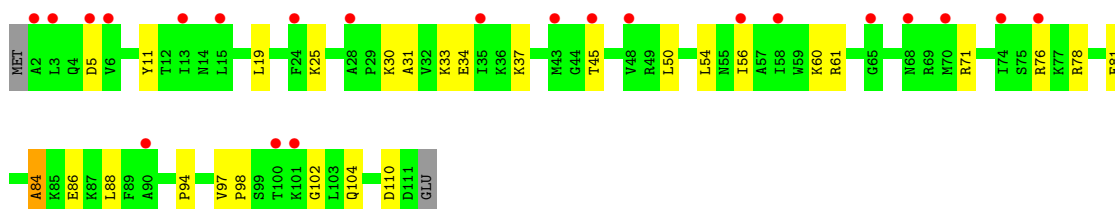
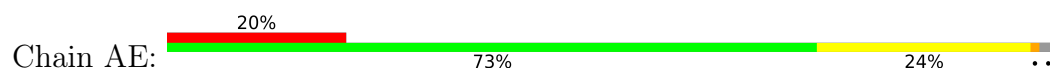
- Molecule 31: 60S ribosomal protein L30



- Molecule 31: 60S ribosomal protein L30

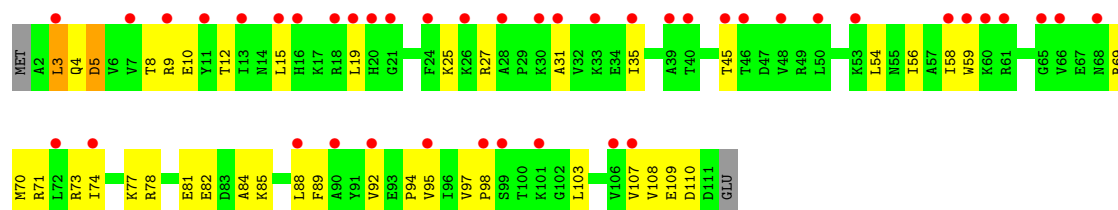


- Molecule 32: 60S ribosomal protein L31-B



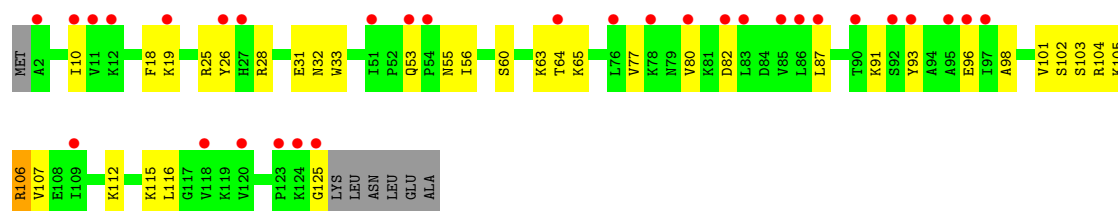
- Molecule 32: 60S ribosomal protein L31-B

Chain BY: 



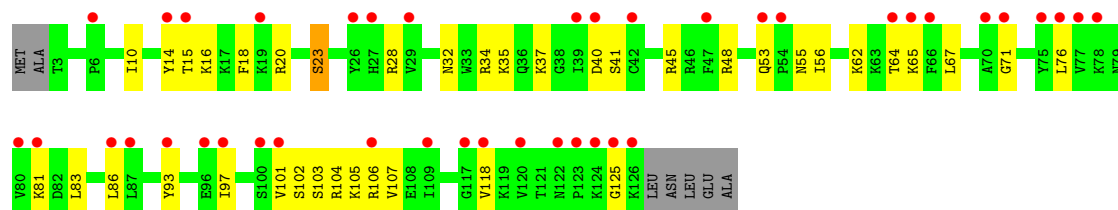
- Molecule 33: 60S ribosomal protein L32

Chain AF: 



- Molecule 33: 60S ribosomal protein L32

Chain BZ: 



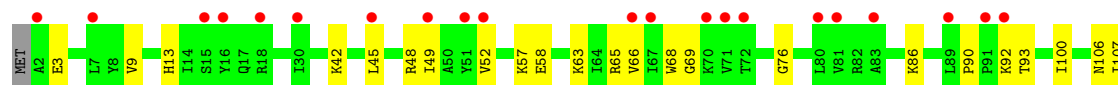
- Molecule 34: 60S ribosomal protein L33-A

Chain AG: 

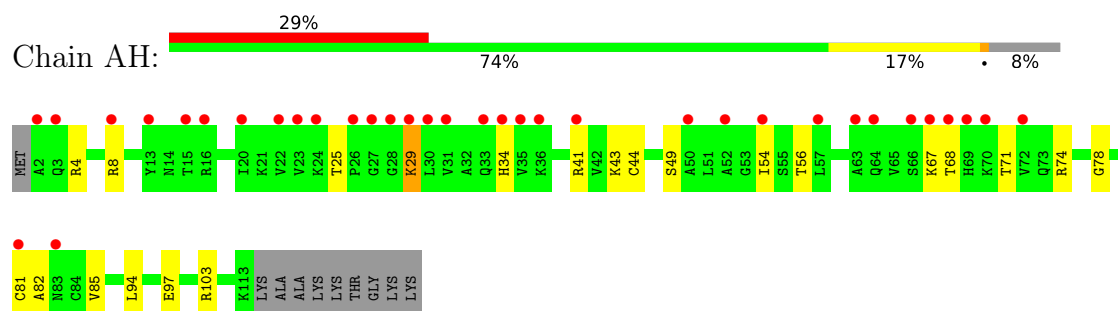


- Molecule 34: 60S ribosomal protein L33-A

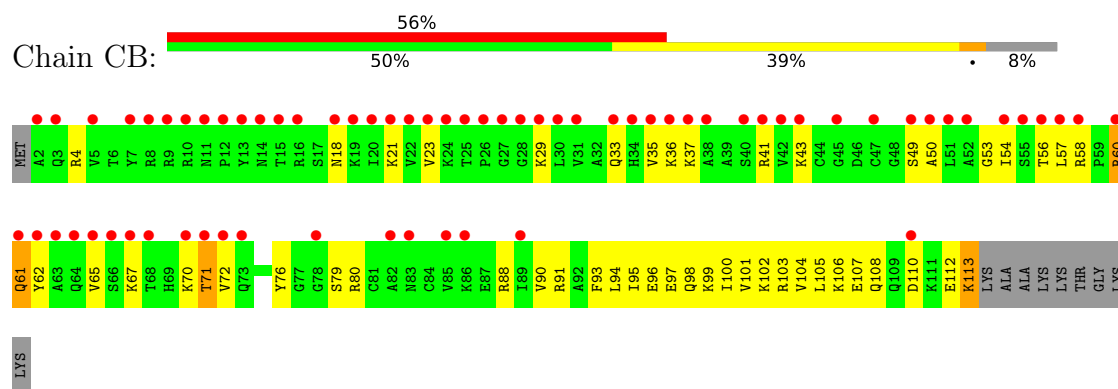
Chain CA: 



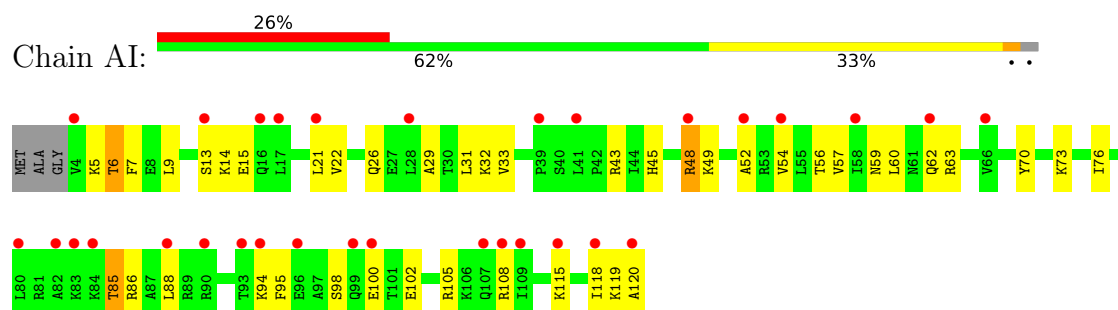
- Molecule 35: 60S ribosomal protein L34-B



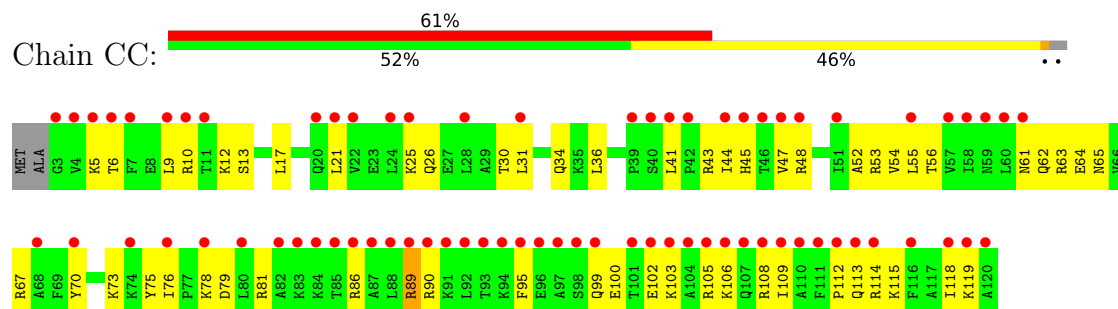
- Molecule 35: 60S ribosomal protein L34-B



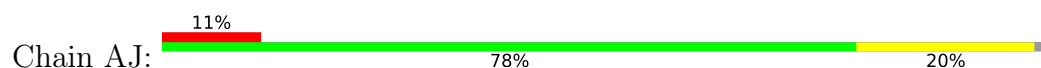
- Molecule 36: Ribosomal protein L29

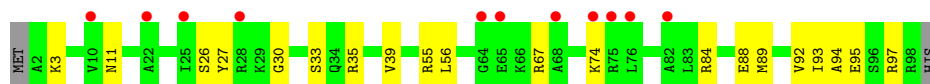


- Molecule 36: Ribosomal protein L29

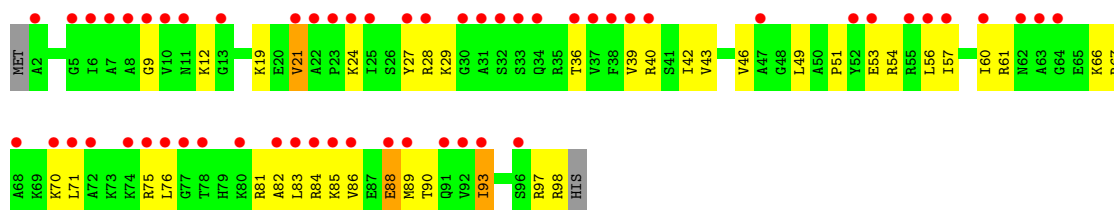


- Molecule 37: 60S ribosomal protein L36

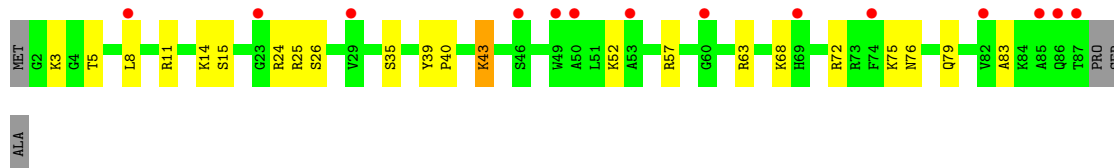
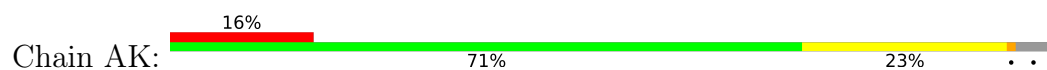




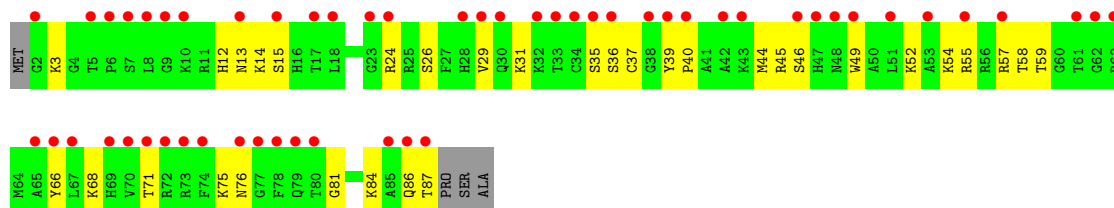
- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37-B



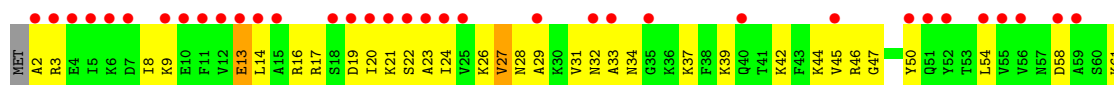
- Molecule 38: 60S ribosomal protein L37-B



- Molecule 39: 60S ribosomal protein L38

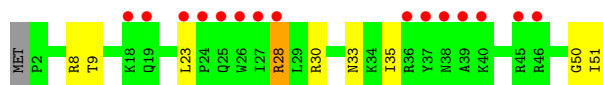
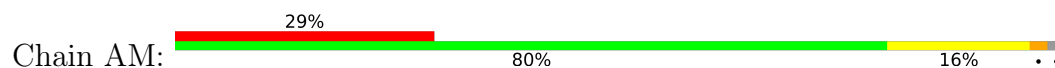


- Molecule 39: 60S ribosomal protein L38





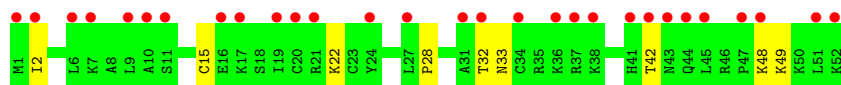
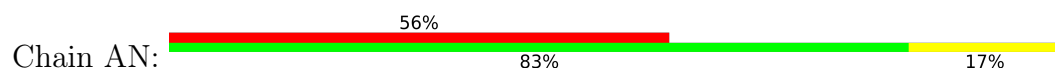
- Molecule 40: 60S ribosomal protein L39



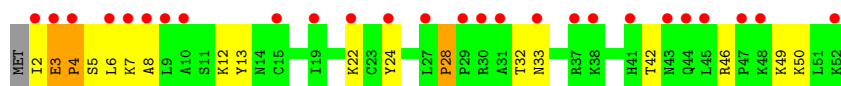
- Molecule 40: 60S ribosomal protein L39



- Molecule 41: 60S ribosomal protein L40-B



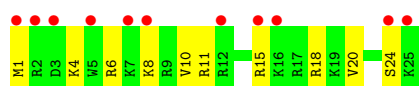
- Molecule 41: 60S ribosomal protein L40-B



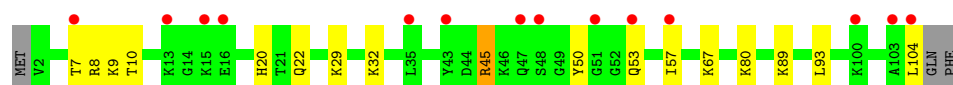
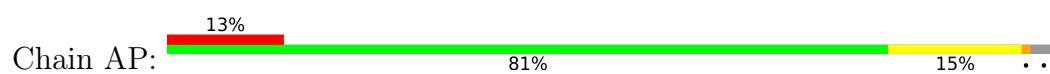
- Molecule 42: 60S ribosomal protein L41



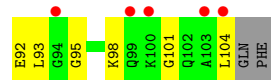
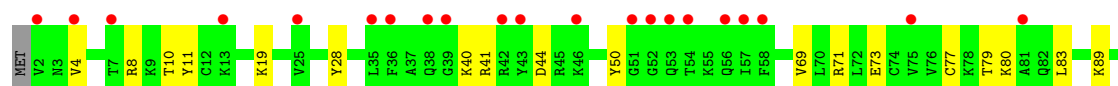
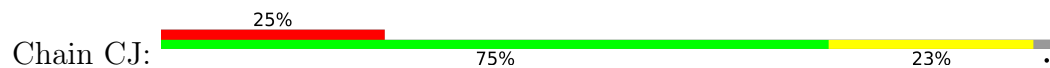
- Molecule 42: 60S ribosomal protein L41



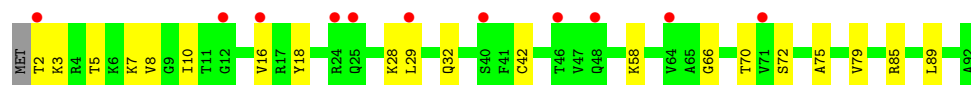
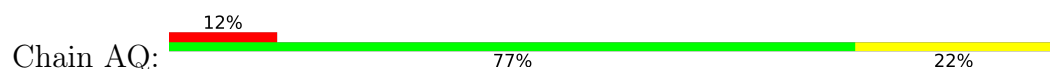
- Molecule 43: 60S ribosomal protein L42-B



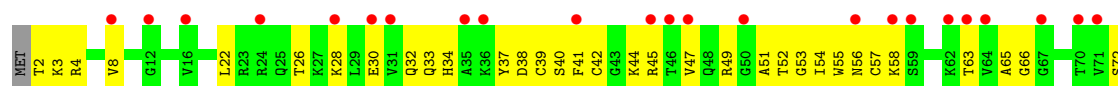
• Molecule 43: 60S ribosomal protein L42-B



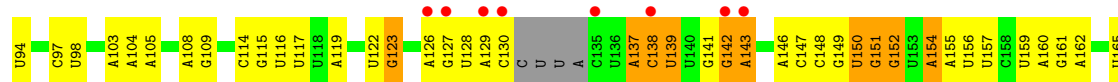
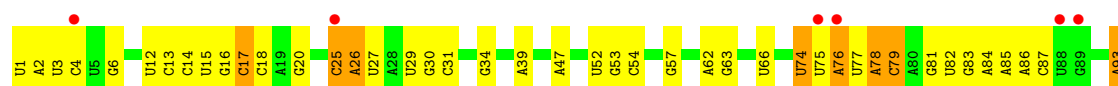
• Molecule 44: 60S ribosomal protein L43-A



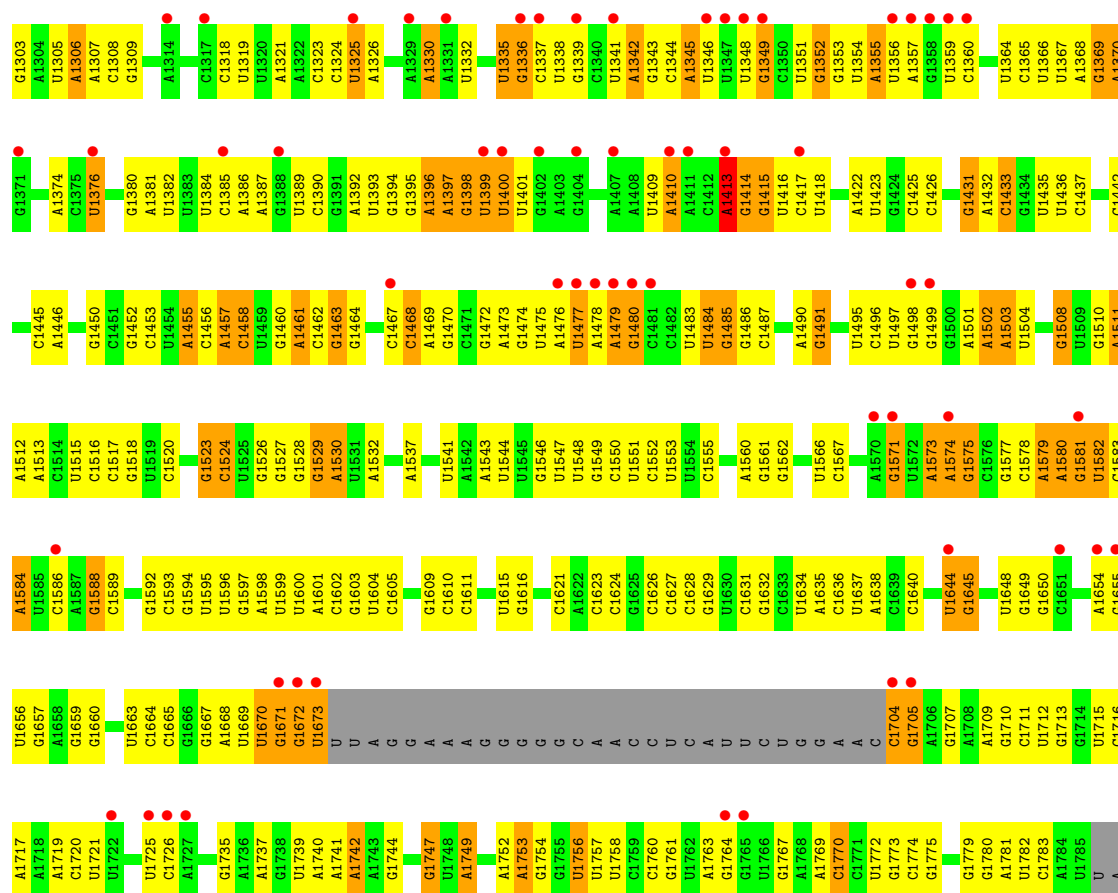
• Molecule 44: 60S ribosomal protein L43-A



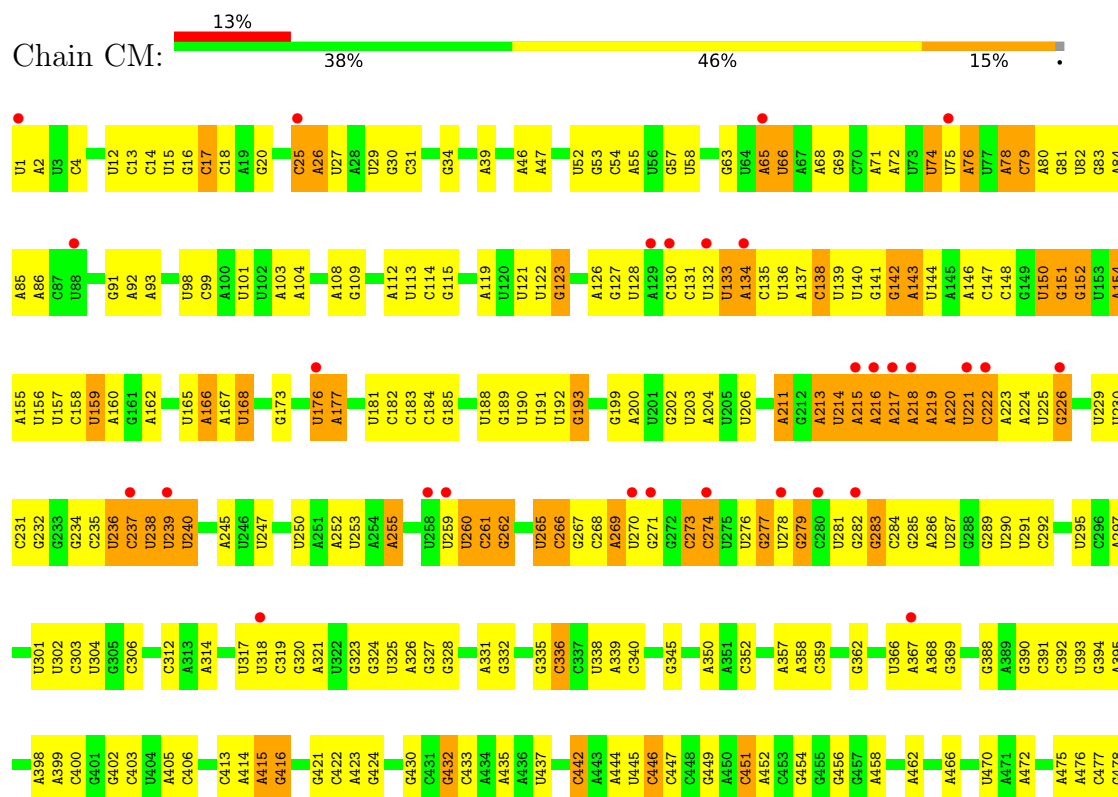
• Molecule 45: 18S

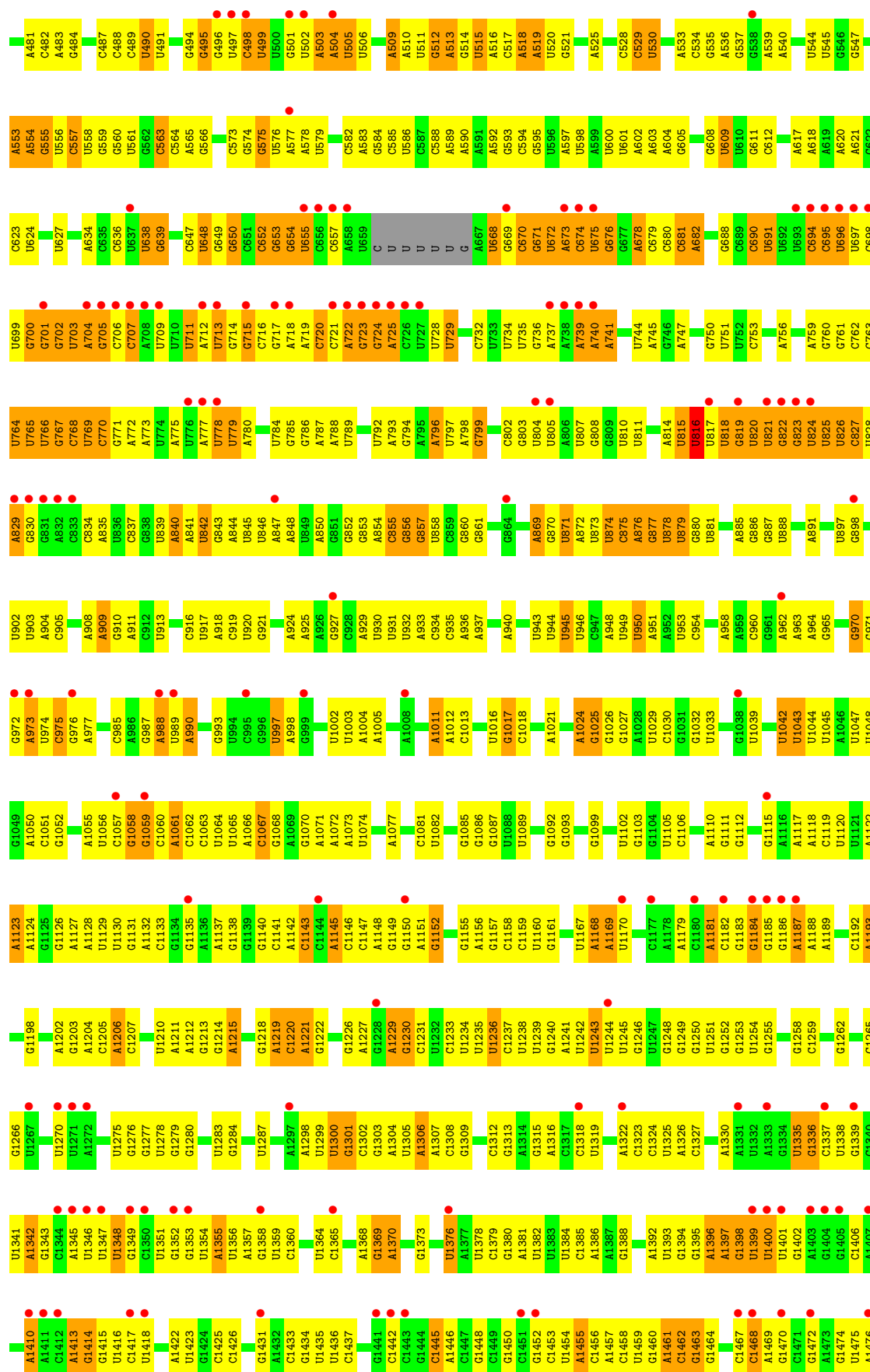


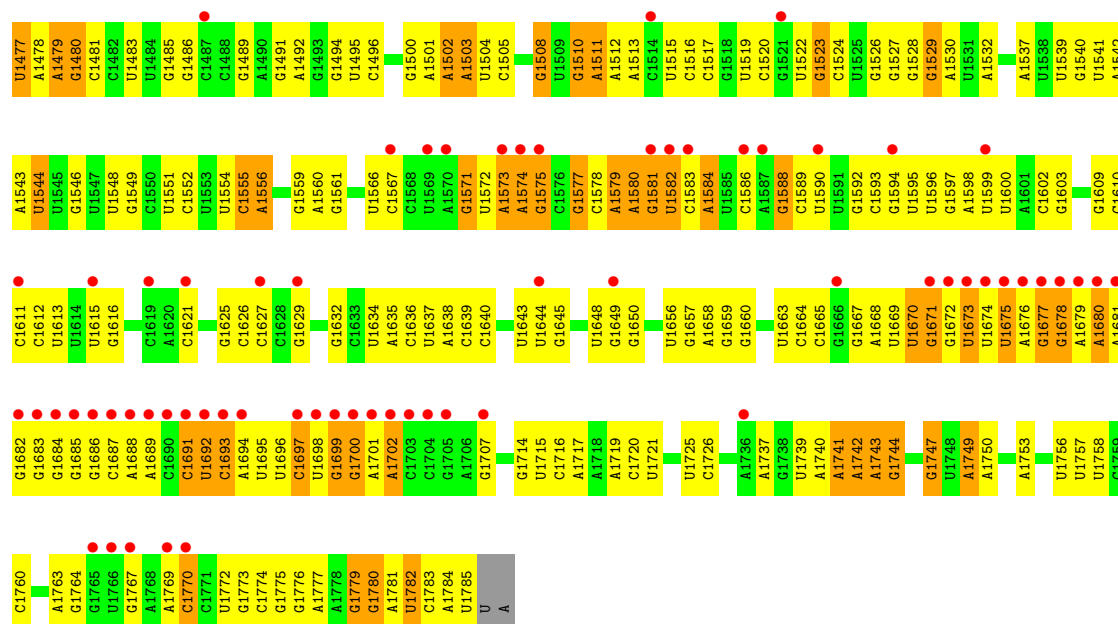




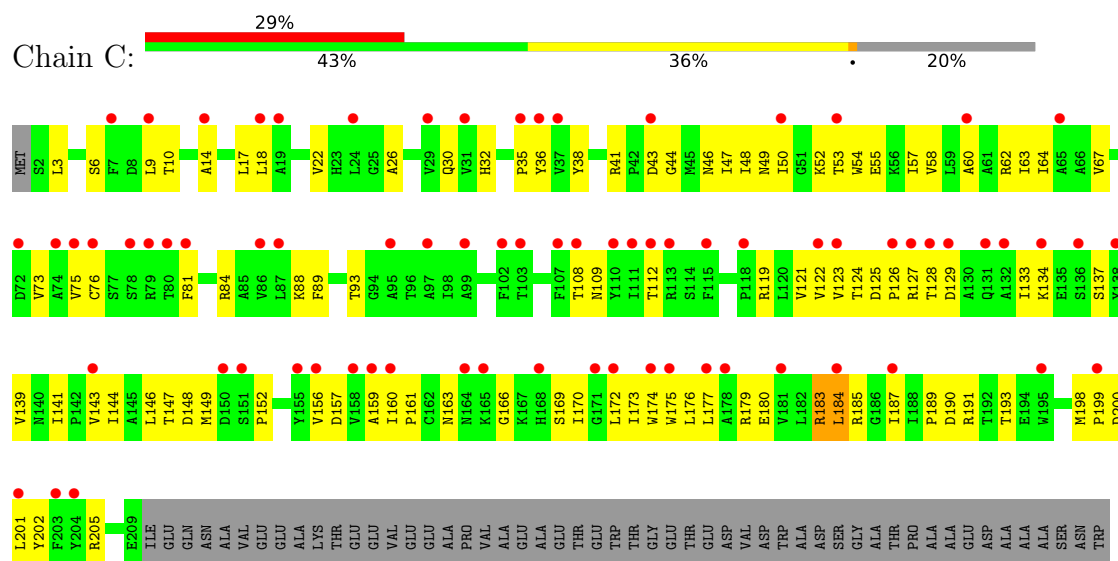
• Molecule 45: 18S



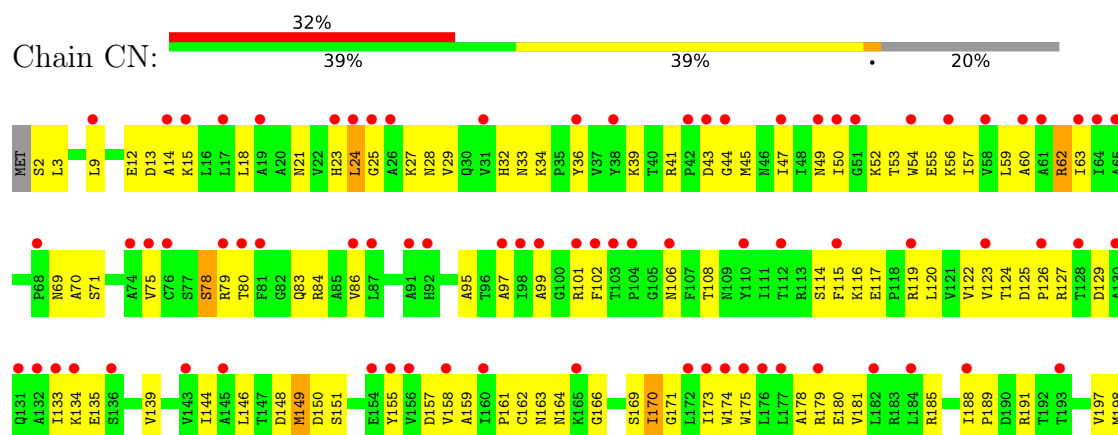


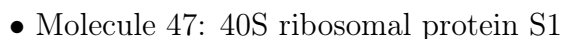
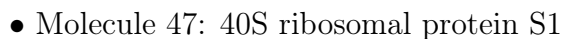


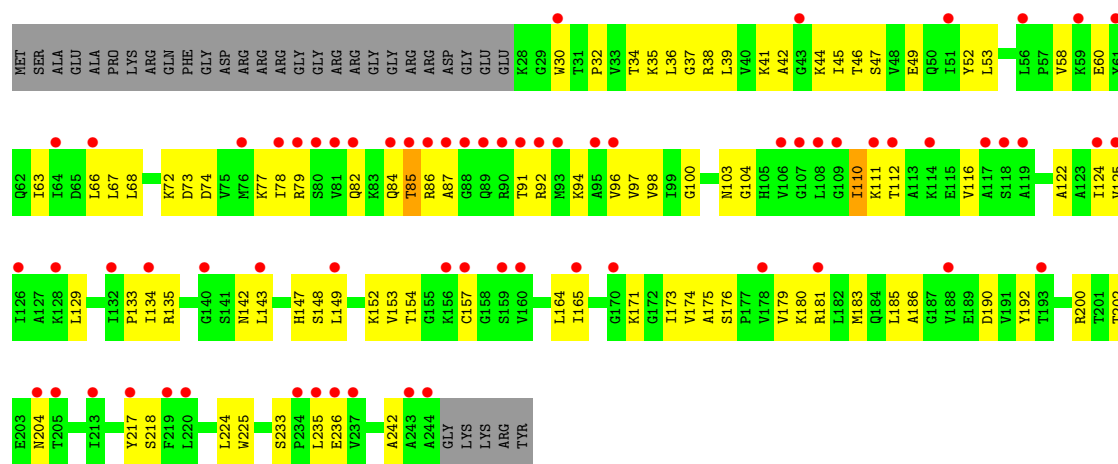
• Molecule 46: 40S ribosomal protein S0



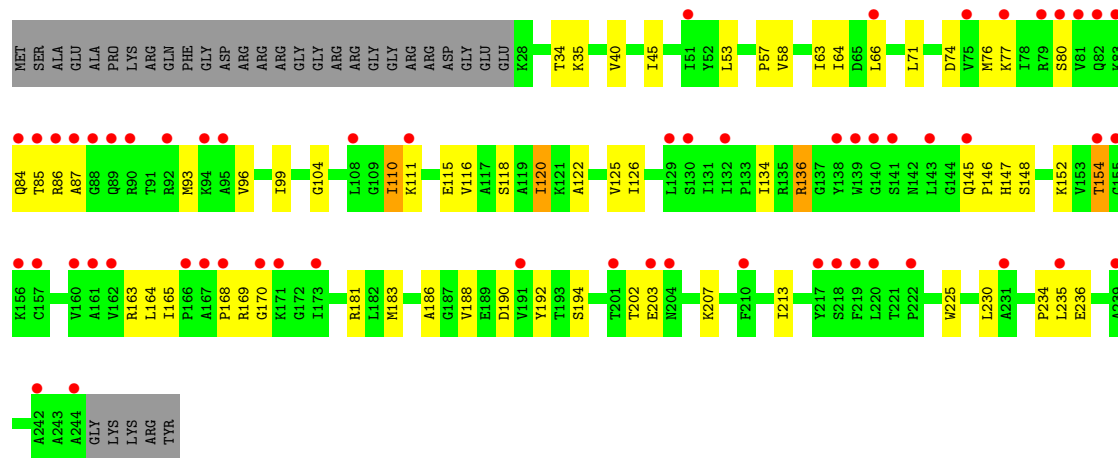
• Molecule 46: 40S ribosomal protein S0



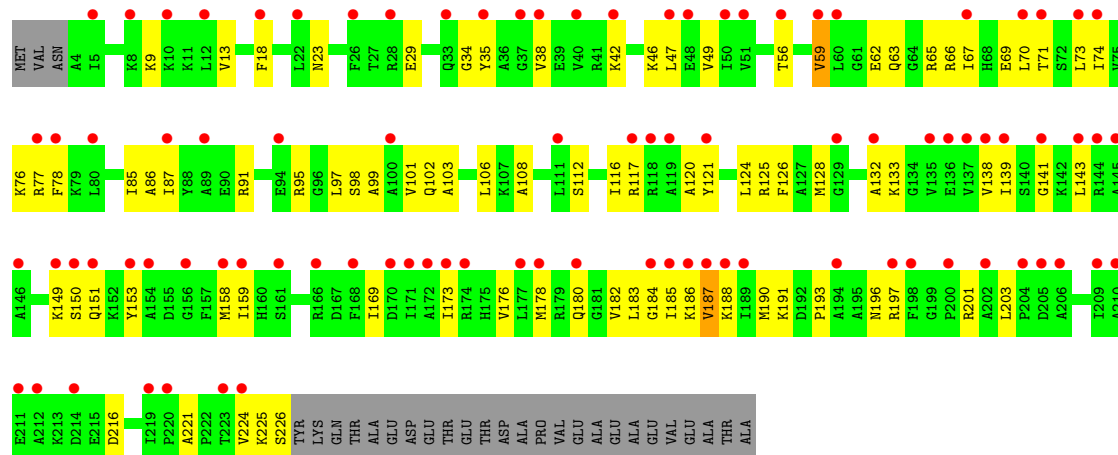




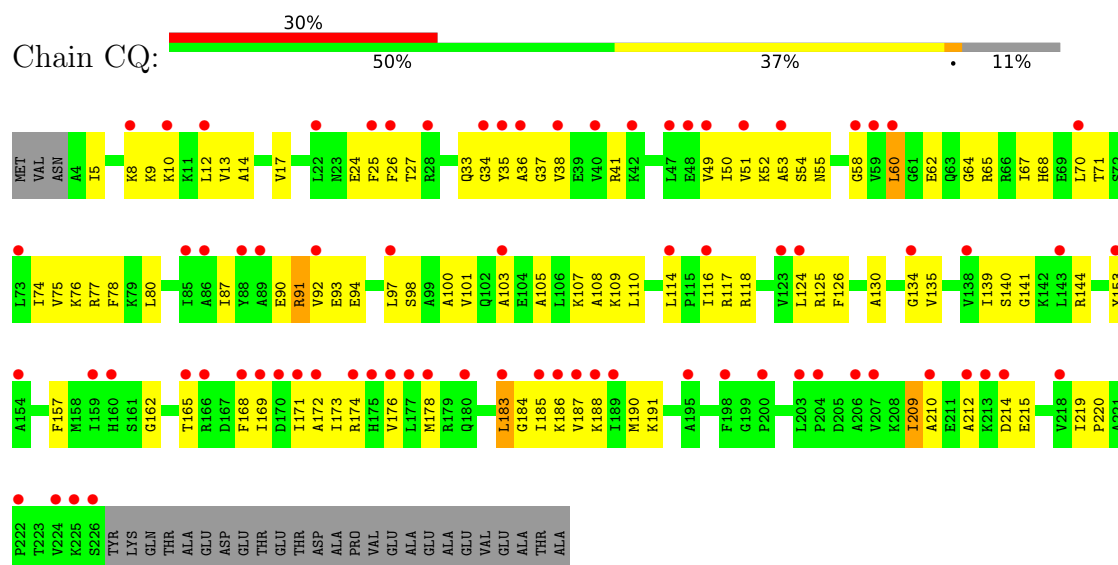
• Molecule 48: Ribosomal protein S5



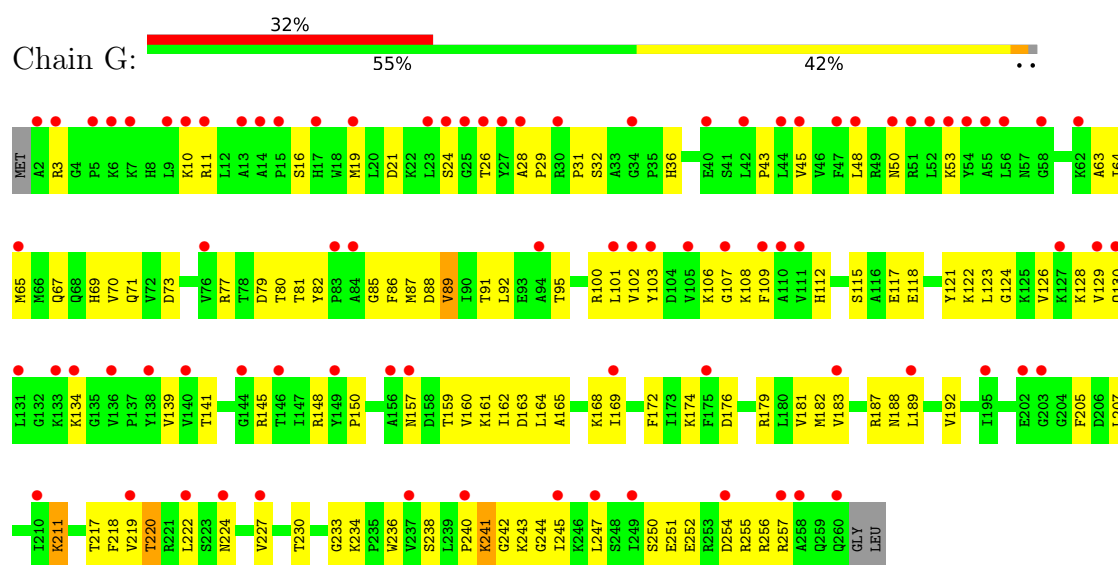
• Molecule 49: Ribosomal protein S3



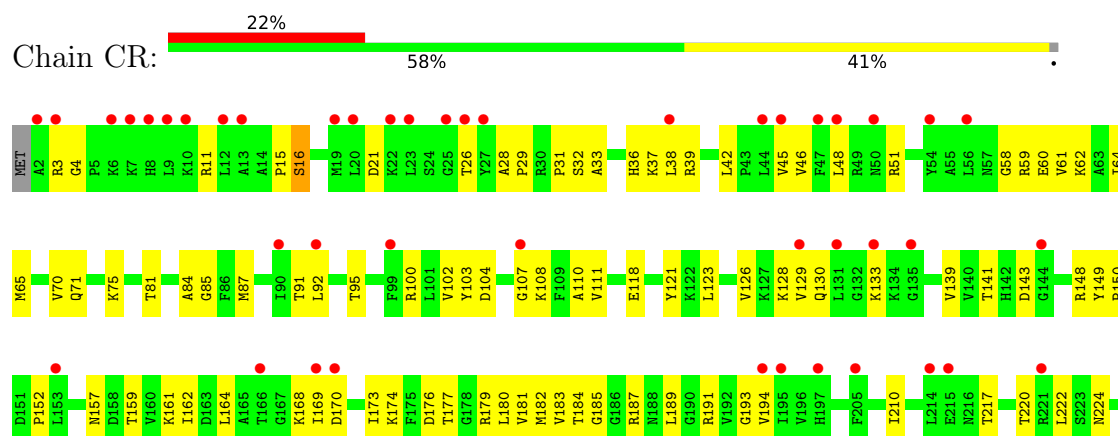
• Molecule 49: Ribosomal protein S3

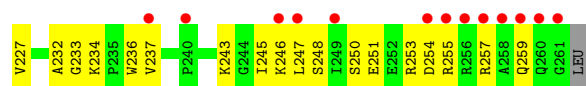


• Molecule 50: 40S ribosomal protein S4

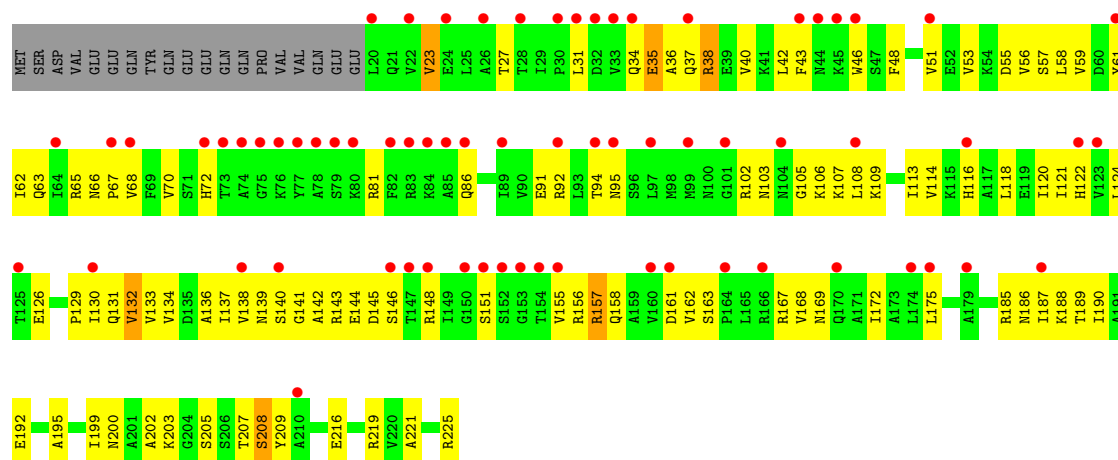


• Molecule 50: 40S ribosomal protein S4

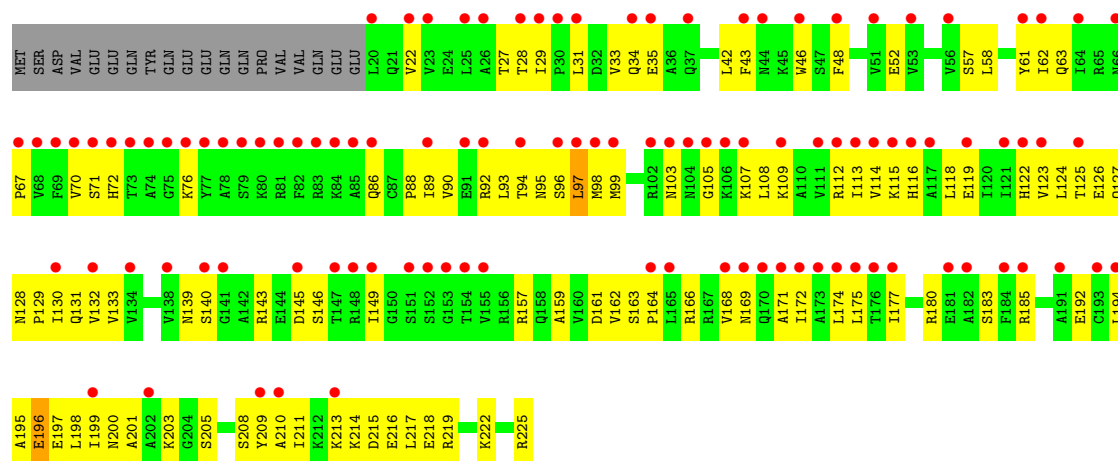




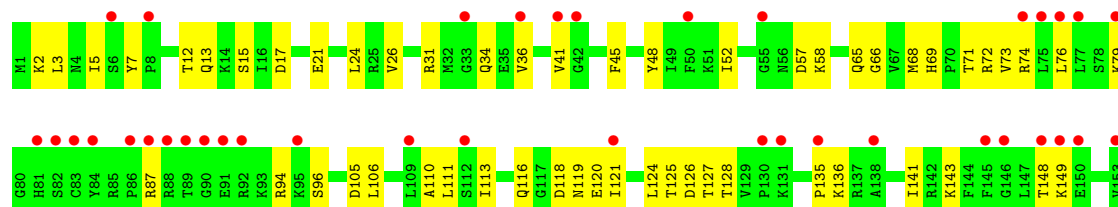
• Molecule 51: Ribosomal protein S7

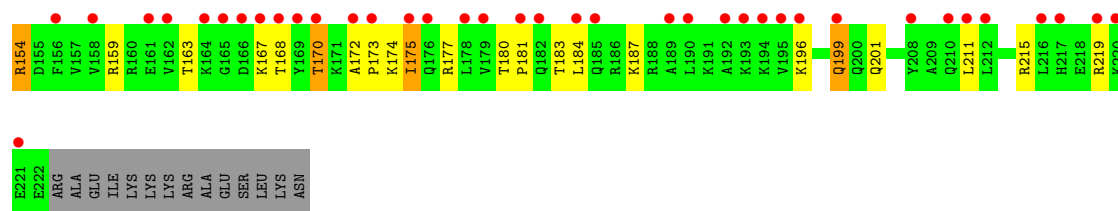


• Molecule 51: Ribosomal protein S7



• Molecule 52: 40S ribosomal protein S6

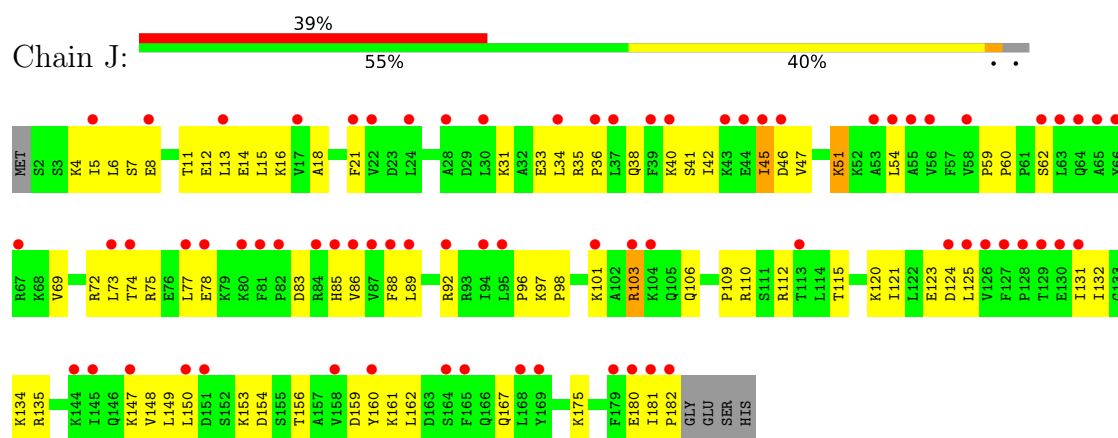




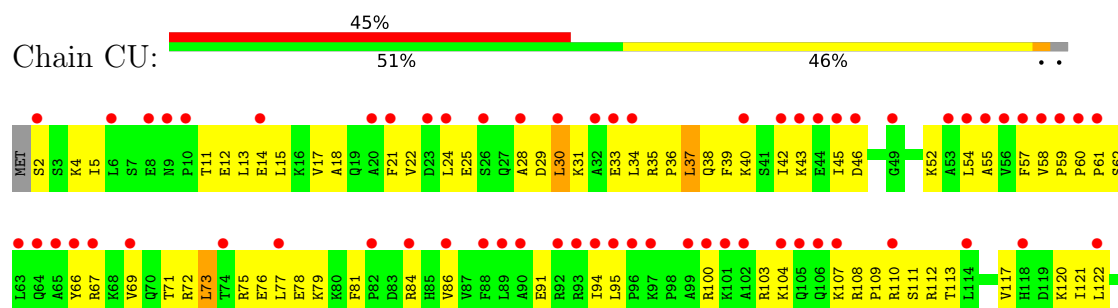
• Molecule 52: 40S ribosomal protein S6

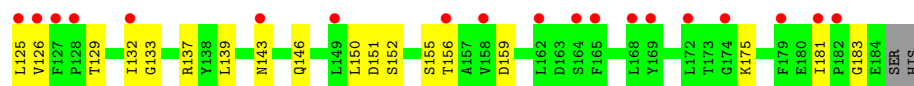


• Molecule 53: 40S ribosomal protein S7

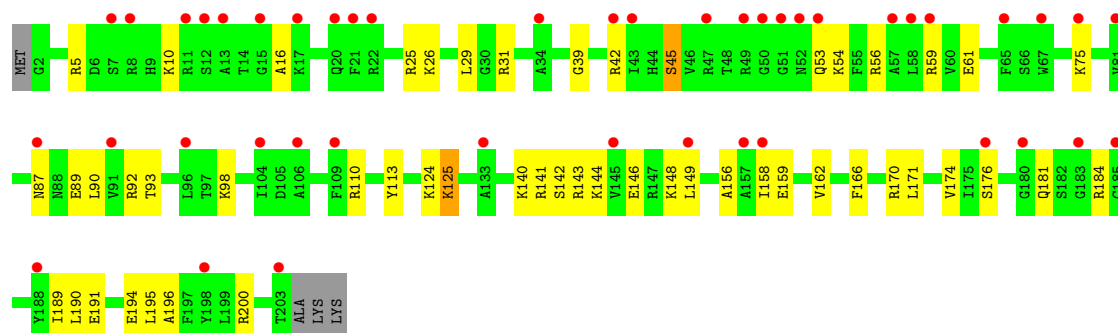
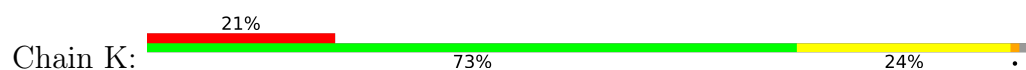


• Molecule 53: 40S ribosomal protein S7

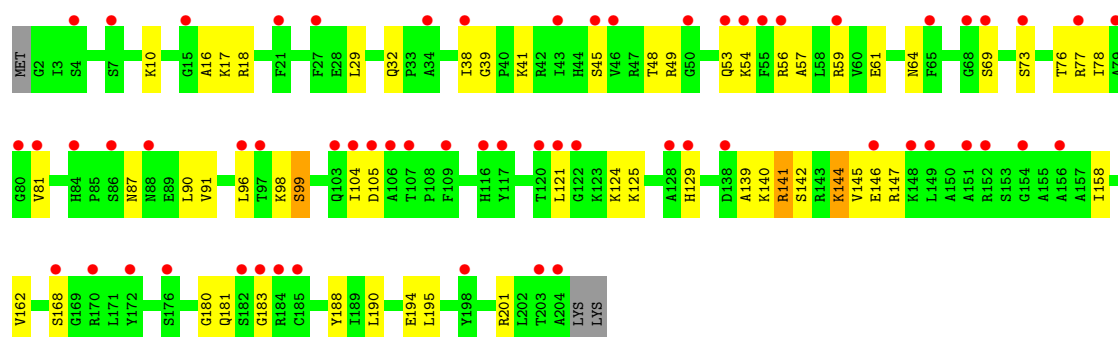
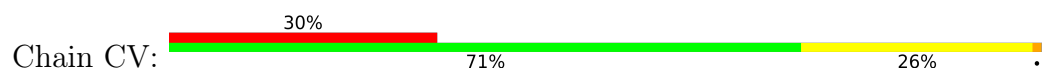




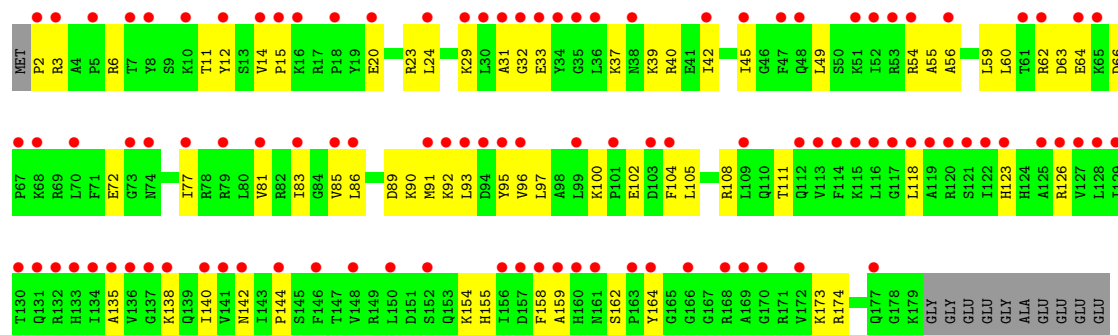
• Molecule 54: 40S ribosomal protein S8



• Molecule 54: 40S ribosomal protein S8

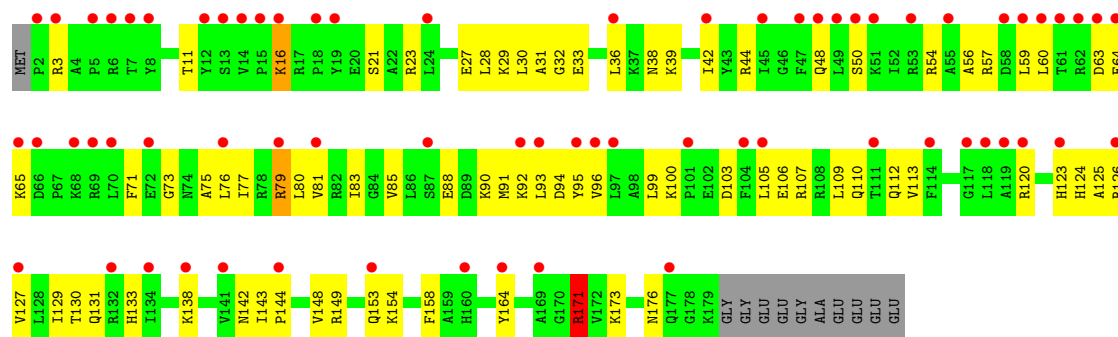


• Molecule 55: Ribosomal protein S4

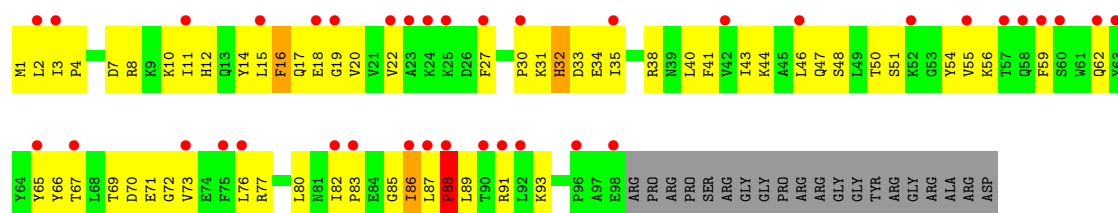


• Molecule 55: Ribosomal protein S4

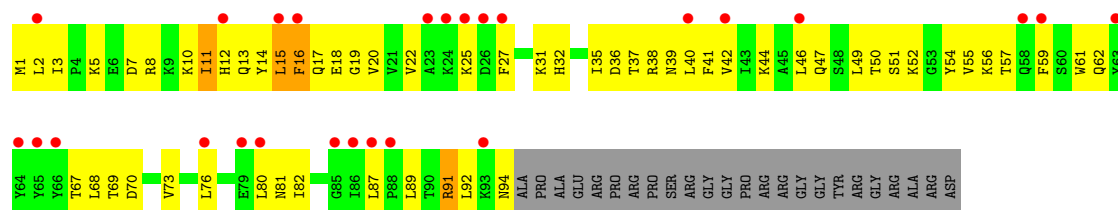




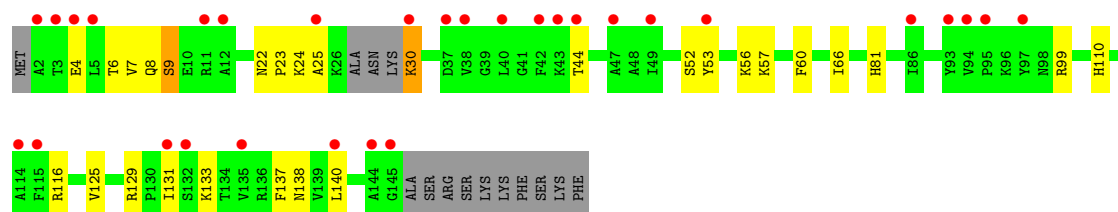
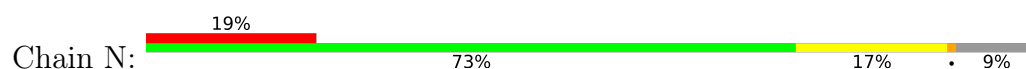
• Molecule 56: 40S ribosomal protein S10-A



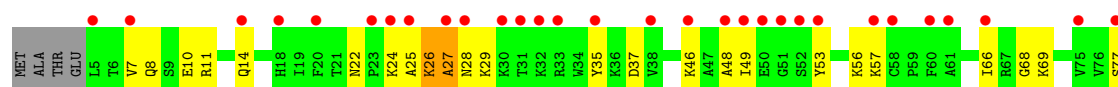
• Molecule 56: 40S ribosomal protein S10-A

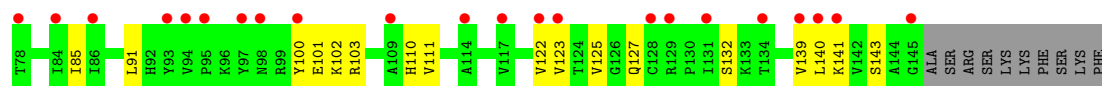


• Molecule 57: 40S ribosomal protein S11A

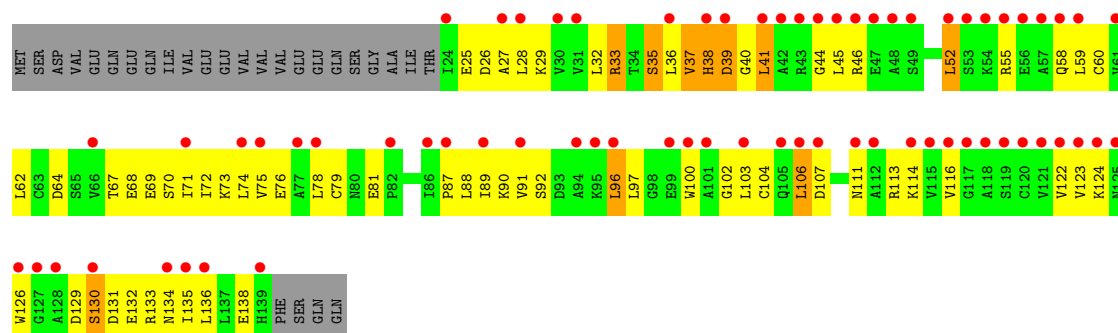


• Molecule 57: 40S ribosomal protein S11A

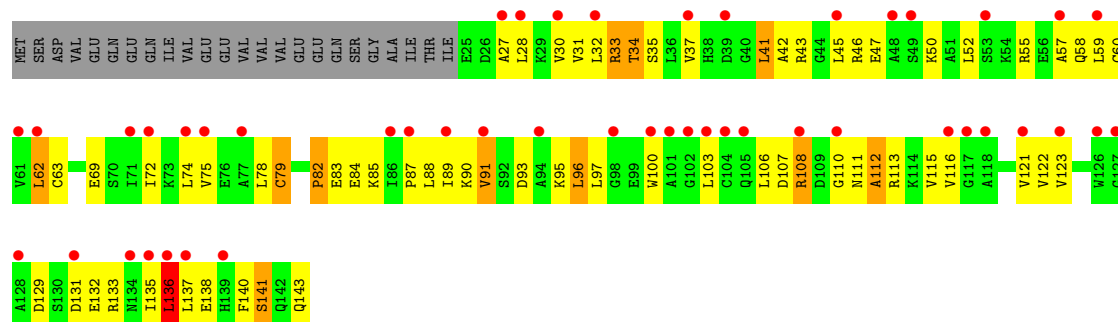




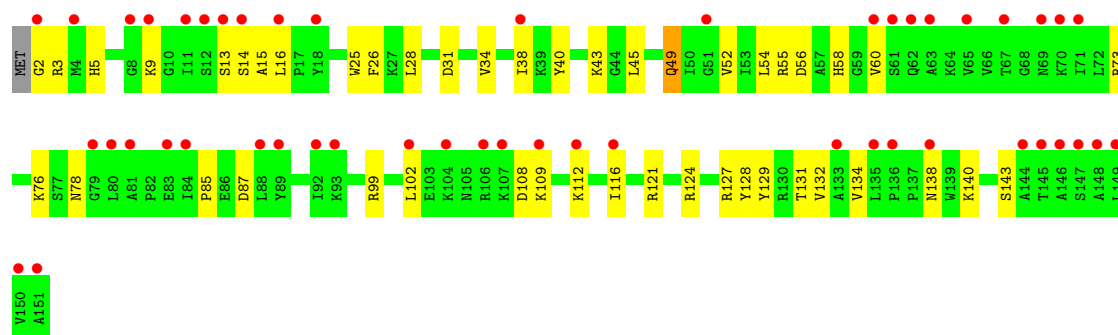
• Molecule 58: 40S ribosomal protein S12



• Molecule 58: 40S ribosomal protein S12

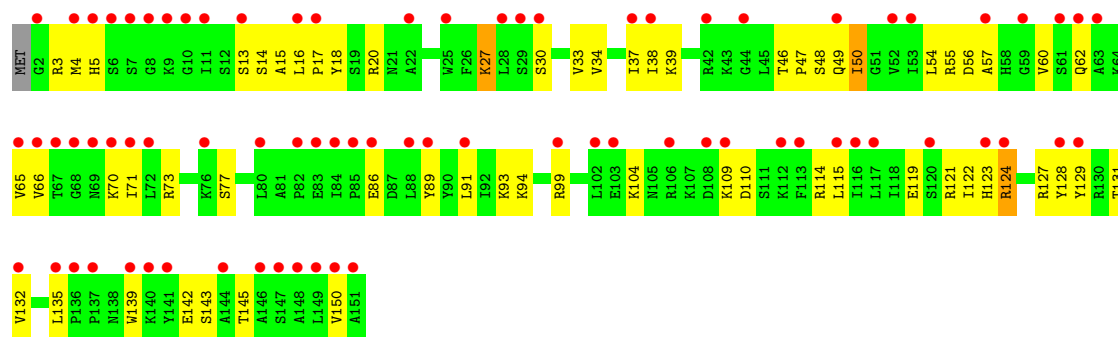


• Molecule 59: 40S ribosomal protein S13

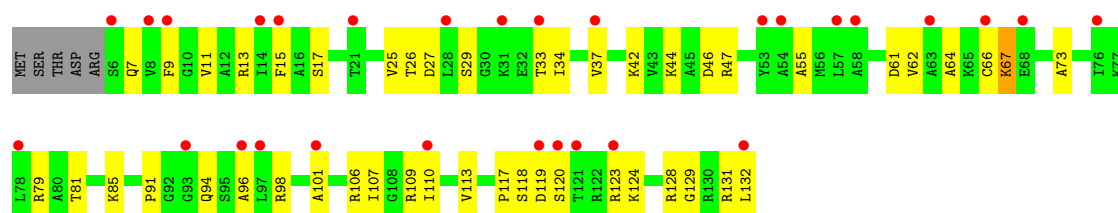


• Molecule 59: 40S ribosomal protein S13

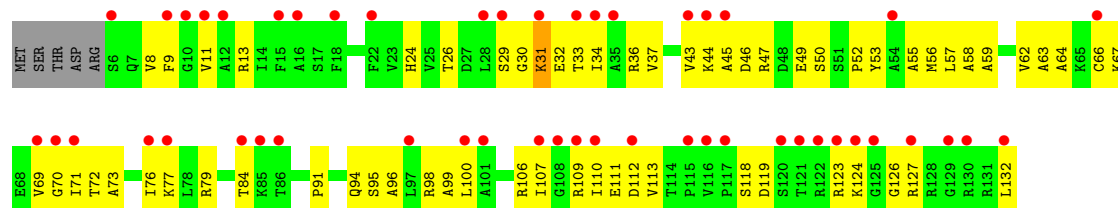
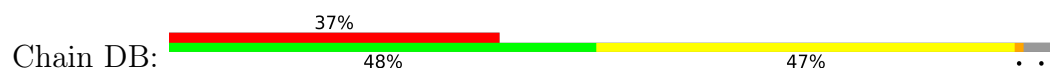




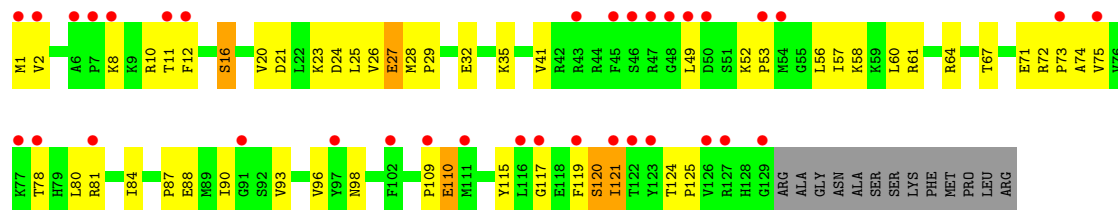
• Molecule 60: 40S ribosomal protein S14-A



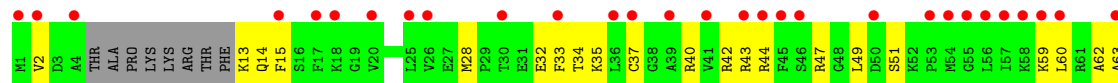
• Molecule 60: 40S ribosomal protein S14-A

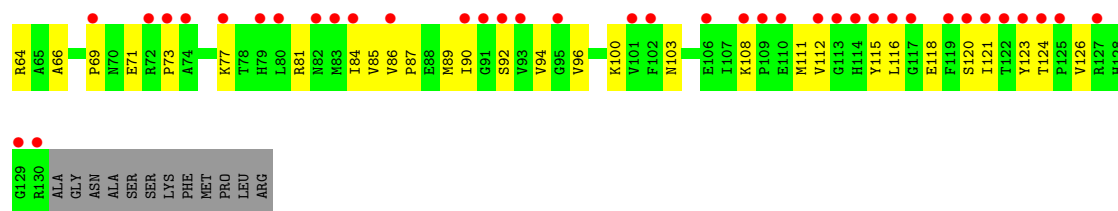


• Molecule 61: 40S ribosomal protein S15

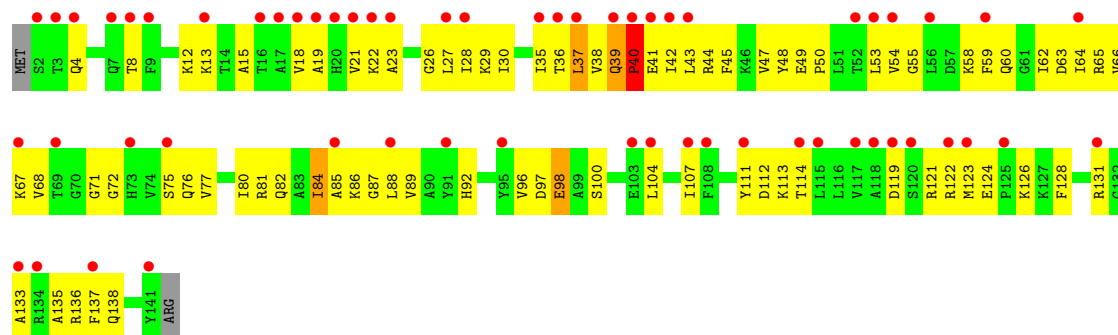
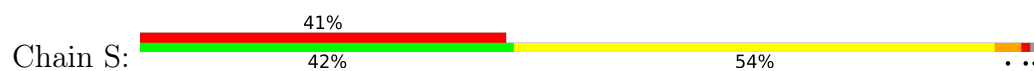


• Molecule 61: 40S ribosomal protein S15

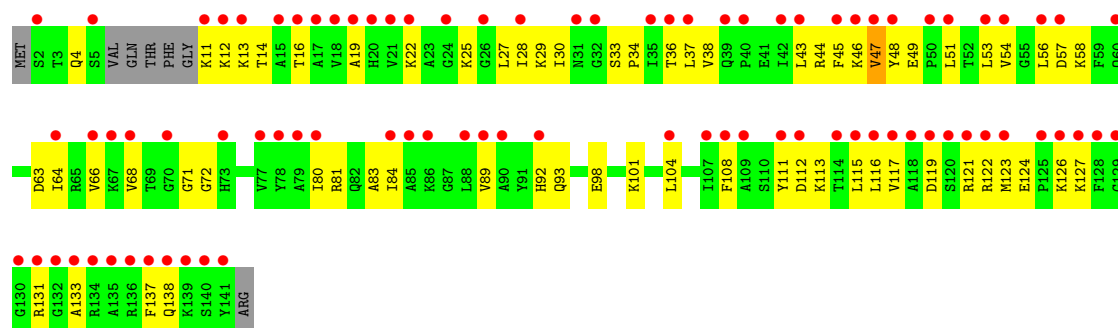




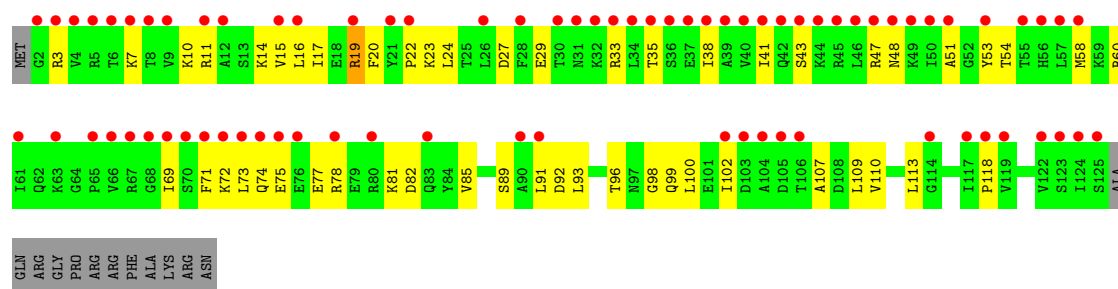
• Molecule 62: 40S ribosomal protein S16



• Molecule 62: 40S ribosomal protein S16



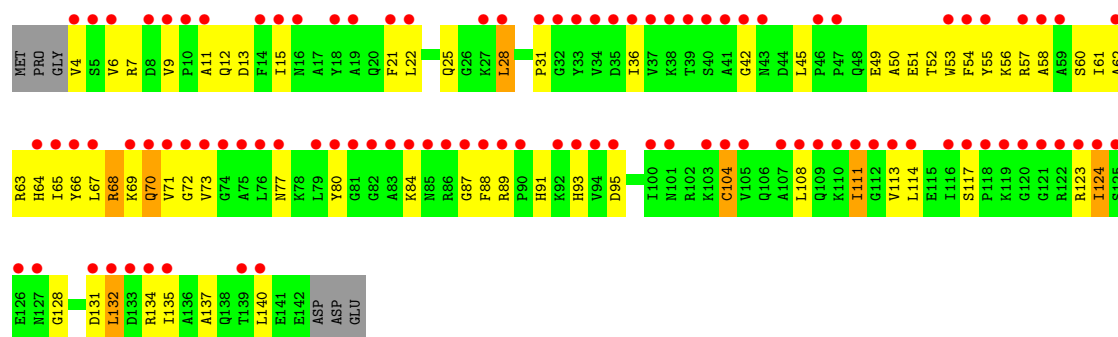
• Molecule 63: 40S ribosomal protein S17-B



• Molecule 63: 40S ribosomal protein S17-B

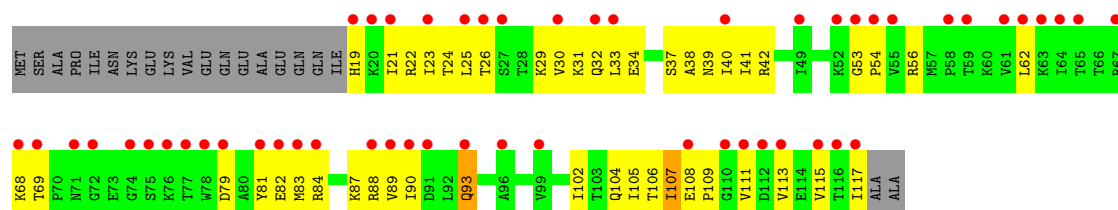


Chain DG: 



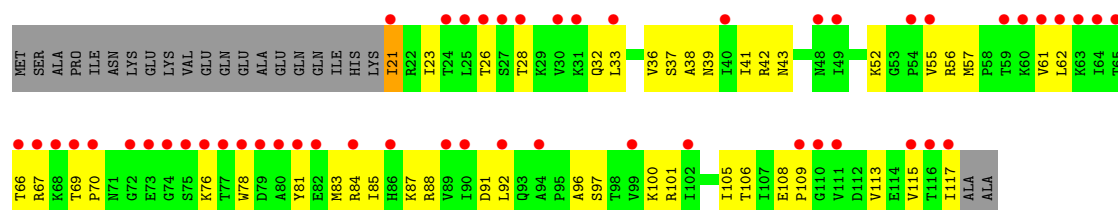
• Molecule 66: Ribosomal protein S10

Chain W: 



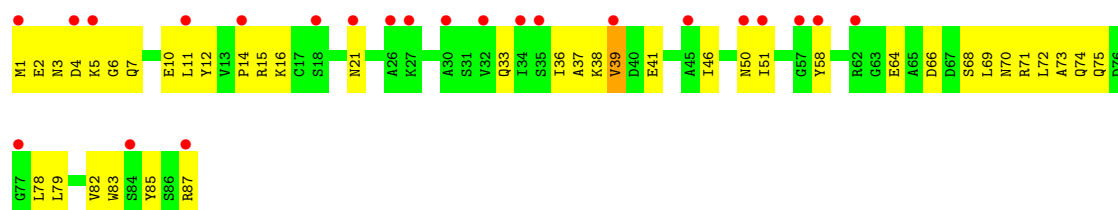
• Molecule 66: Ribosomal protein S10

Chain DH: 



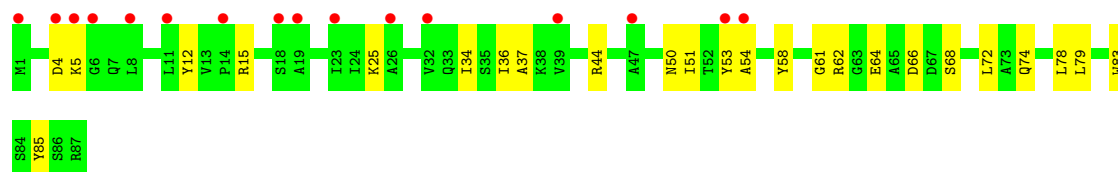
• Molecule 67: 40S ribosomal protein S21

Chain X: 

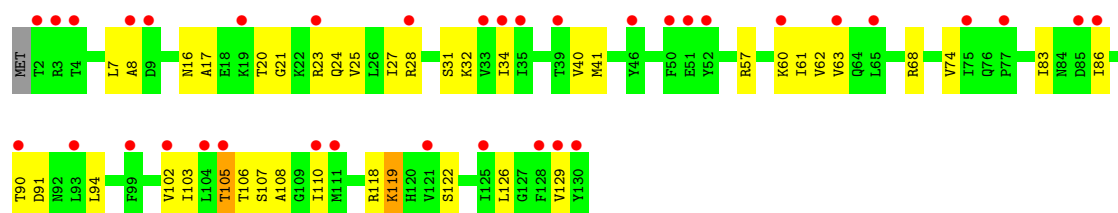


• Molecule 67: 40S ribosomal protein S21

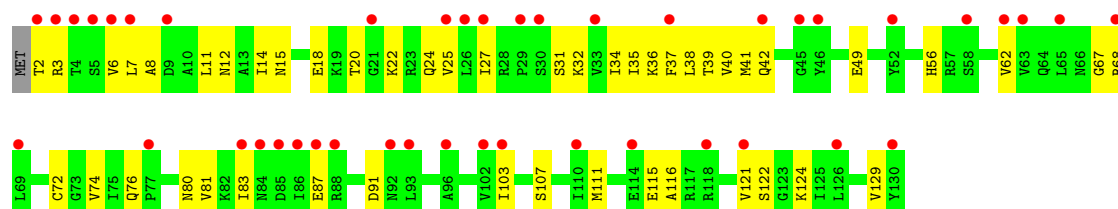
Chain DI: 



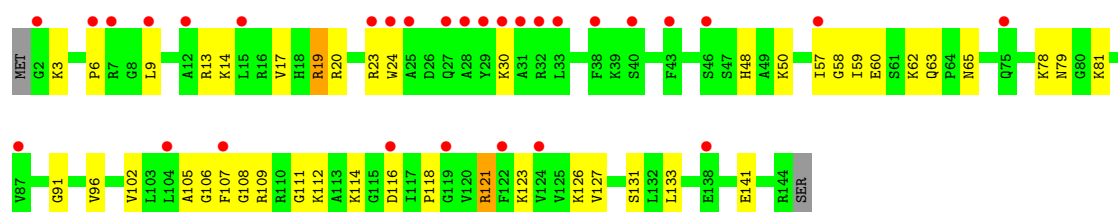
- Molecule 68: 40S ribosomal protein S22-A



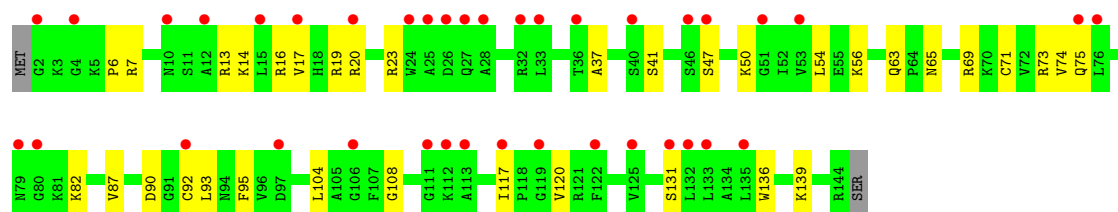
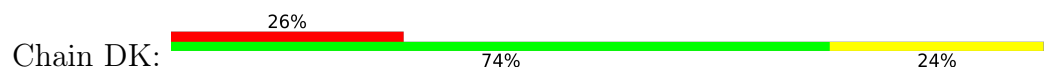
- Molecule 68: 40S ribosomal protein S22-A



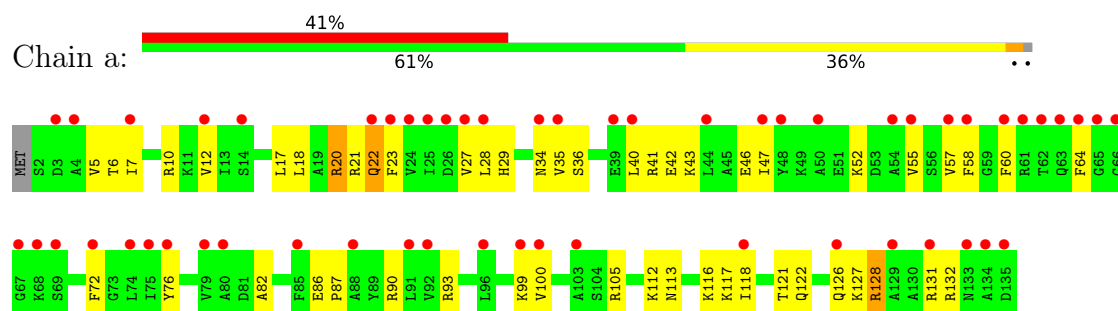
- Molecule 69: Ribosomal protein S23 (S12)



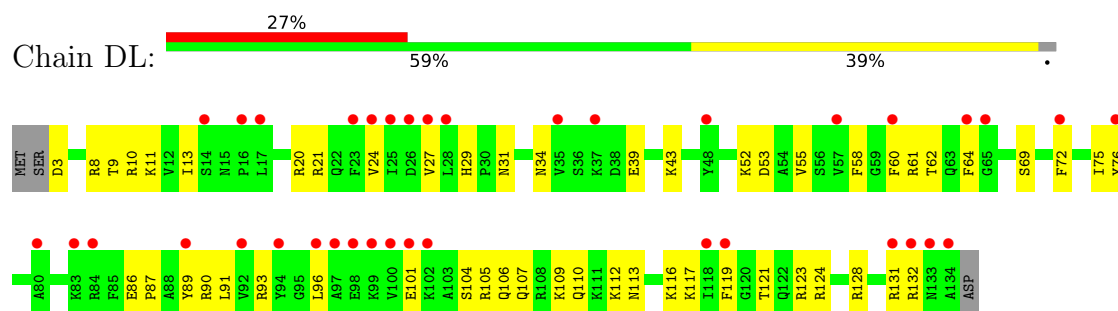
- Molecule 69: Ribosomal protein S23 (S12)



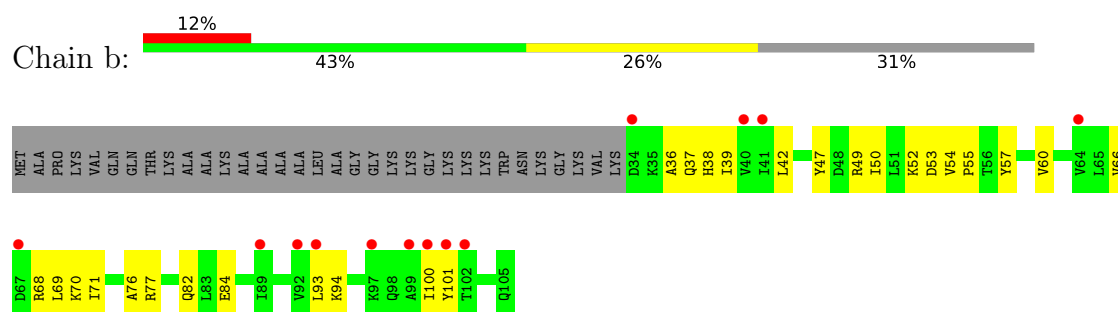
- Molecule 70: 40S ribosomal protein S24



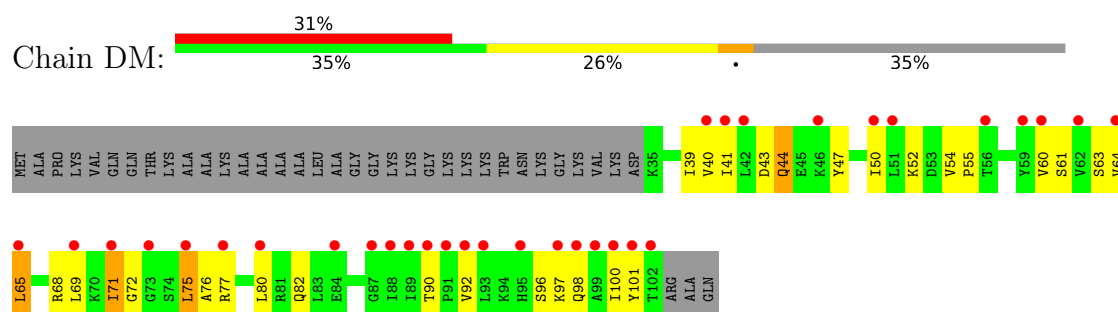
- Molecule 70: 40S ribosomal protein S24



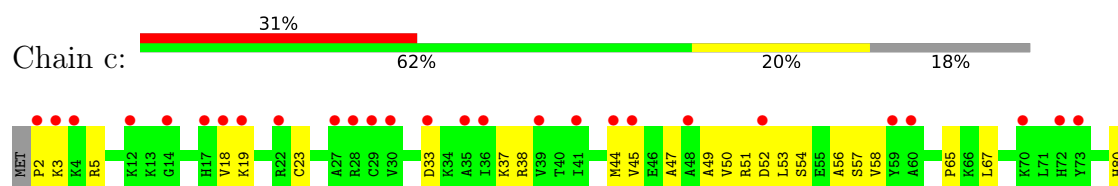
- Molecule 71: 40S ribosomal protein S25

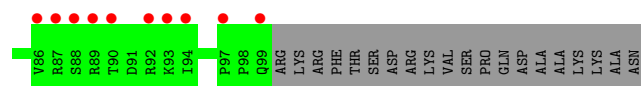


- Molecule 71: 40S ribosomal protein S25

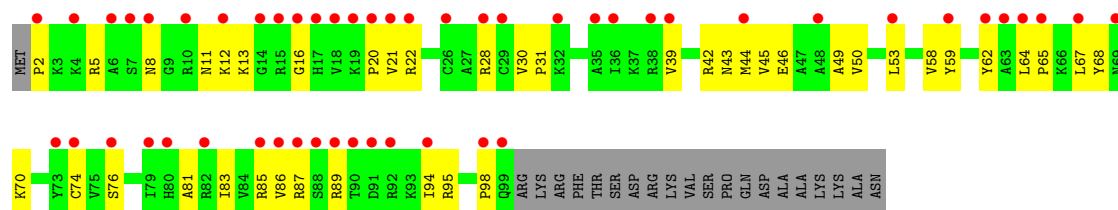
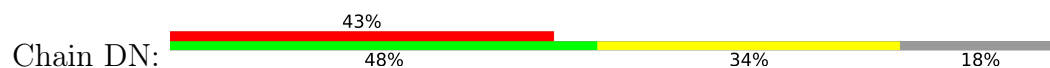


- Molecule 72: 40S ribosomal protein S26

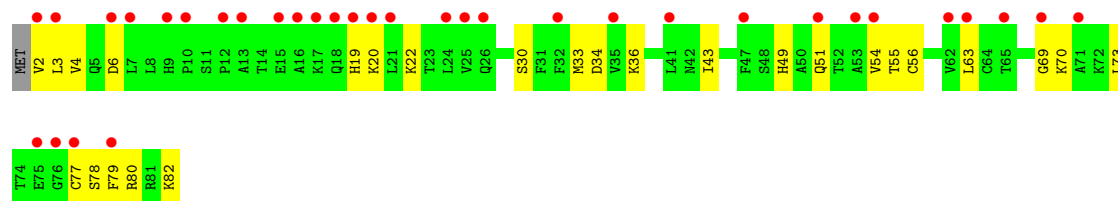
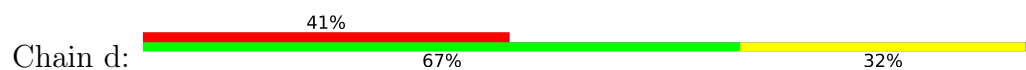




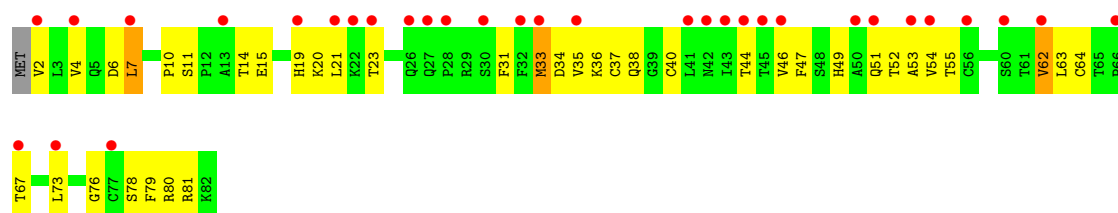
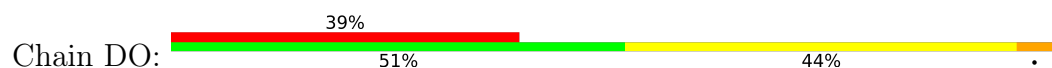
- Molecule 72: 40S ribosomal protein S26



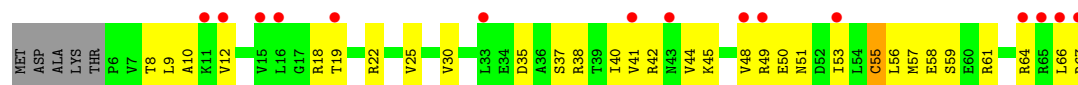
- Molecule 73: 40S ribosomal protein S27



- Molecule 73: 40S ribosomal protein S27



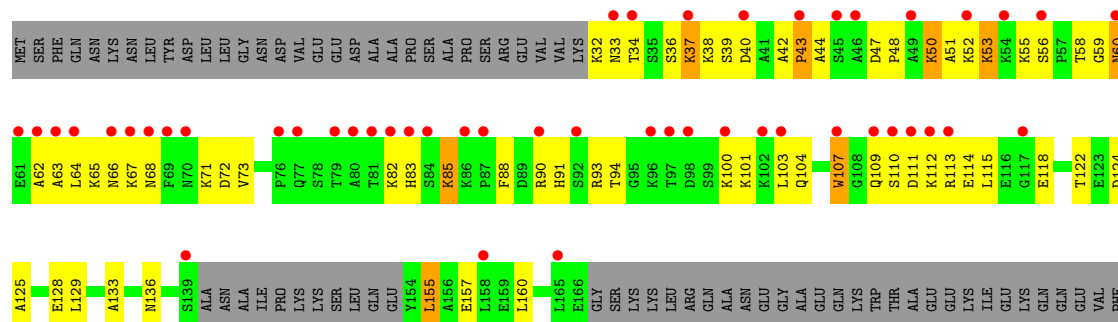
- Molecule 74: 40S ribosomal protein S28-B



- Molecule 74: 40S ribosomal protein S28-B



Chain AR: 48% 47% 46%



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
$\langle I/\sigma(I) \rangle$ 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 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 3K5, ZN, PAR, MG

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	0.20	0/75861	0.45	3/118257 (0.0%)
1	AS	0.19	0/73312	0.45	6/114279 (0.0%)
2	3	0.16	0/2884	0.34	0/4492
2	AT	0.20	0/2884	0.42	1/4492 (0.0%)
3	4	0.19	0/3702	0.43	0/5764
3	AU	0.18	0/3702	0.42	0/5764
4	AW	0.29	0/1931	0.72	1/2592 (0.0%)
4	j	0.26	0/1931	0.58	2/2592 (0.1%)
5	AX	0.27	0/3145	0.66	0/4231
5	k	0.27	0/3156	0.65	2/4246 (0.0%)
6	AY	0.28	0/2799	0.69	0/3777
6	l	0.29	0/2793	0.66	0/3769
7	AZ	0.34	0/2447	0.83	3/3294 (0.1%)
7	m	0.34	0/2479	0.75	2/3337 (0.1%)
8	BA	0.30	0/1231	0.68	1/1662 (0.1%)
8	n	0.30	0/1263	0.66	1/1703 (0.1%)
9	BB	0.27	0/1918	0.60	0/2575
9	o	0.33	0/1918	0.68	3/2575 (0.1%)
10	BC	0.39	0/1825	0.90	1/2458 (0.0%)
10	p	0.34	0/1820	0.67	0/2451
11	BD	0.37	0/1537	0.85	1/2067 (0.0%)
11	q	0.32	0/1537	0.73	0/2067
12	BE	0.31	0/1705	0.69	0/2288
12	r	0.29	0/1724	0.66	0/2314
13	BF	0.38	0/1390	0.87	4/1861 (0.2%)
13	s	0.37	0/1390	0.94	4/1861 (0.2%)
14	BG	0.37	0/1637	0.87	4/2195 (0.2%)
14	t	0.31	0/1637	0.77	5/2195 (0.2%)
15	BH	0.32	0/1044	0.78	3/1407 (0.2%)
15	u	0.37	0/1030	0.73	0/1389
16	BI	0.31	0/1753	0.79	2/2347 (0.1%)
16	v	0.25	0/1753	0.59	0/2347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	BJ	0.48	1/1620 (0.1%)	0.71	4/2167 (0.2%)
17	w	0.34	0/1620	0.69	1/2167 (0.0%)
18	BK	0.32	0/1419	0.74	1/1906 (0.1%)
18	x	0.29	0/1395	0.71	1/1874 (0.1%)
19	BL	0.33	0/1482	0.71	0/1985
19	y	0.32	0/1482	0.71	1/1985 (0.1%)
20	BM	0.36	0/1475	0.89	4/1961 (0.2%)
20	z	0.29	0/1475	0.72	0/1961
21	0	0.28	0/1457	0.63	2/1962 (0.1%)
21	BN	0.31	0/1457	0.62	0/1962
22	2	0.30	0/1285	0.68	0/1723
22	BO	0.32	0/1285	0.70	0/1723
23	5	0.32	0/846	0.77	1/1140 (0.1%)
23	BP	0.32	0/857	0.85	0/1156
24	6	0.24	0/993	0.58	0/1339
24	BQ	0.30	0/993	0.72	1/1339 (0.1%)
25	7	0.20	0/643	0.40	0/853
25	BR	0.29	0/889	0.52	0/1175
26	8	0.29	0/990	0.67	0/1337
26	BS	0.37	0/976	0.80	0/1319
27	9	0.32	0/990	0.68	0/1322
27	BT	0.38	0/999	0.84	0/1334
28	AA	0.39	0/1112	0.75	0/1488
28	BU	0.42	0/1112	0.98	5/1488 (0.3%)
29	AB	0.28	0/1199	0.64	1/1607 (0.1%)
29	BV	0.31	0/1199	0.72	0/1607
30	AC	0.36	0/498	0.97	3/661 (0.5%)
30	BW	0.34	0/498	0.76	0/661
31	AD	0.29	0/738	0.71	0/994
31	BX	0.33	0/738	0.84	0/994
32	AE	0.32	0/907	0.83	2/1219 (0.2%)
32	BY	0.37	0/907	0.85	0/1219
33	AF	0.34	0/1021	0.68	0/1368
33	BZ	0.33	0/1025	0.72	1/1372 (0.1%)
34	AG	0.27	0/866	0.59	1/1165 (0.1%)
34	CA	0.33	0/866	0.69	0/1165
35	AH	0.32	0/896	0.75	1/1195 (0.1%)
35	CB	0.34	0/896	0.82	0/1195
36	AI	0.30	0/995	0.82	1/1325 (0.1%)
36	CC	0.38	0/999	0.90	2/1330 (0.2%)
37	AJ	0.29	0/763	0.70	1/1012 (0.1%)
37	CD	0.27	0/763	0.84	2/1012 (0.2%)
38	AK	0.31	0/690	0.68	1/916 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CE	0.32	0/690	0.68	1/916 (0.1%)
39	AL	0.31	0/623	0.71	1/831 (0.1%)
39	CF	0.32	0/623	0.74	0/831
40	AM	0.28	0/447	0.64	0/594
40	CG	0.24	0/458	0.65	0/609
41	AN	0.66	1/425 (0.2%)	0.82	1/563 (0.2%)
41	CH	0.38	1/417 (0.2%)	0.74	2/553 (0.4%)
42	AO	0.32	0/237	0.84	0/304
42	CI	0.29	0/237	0.95	0/304
43	AP	0.27	0/840	0.62	0/1110
43	CJ	0.31	0/840	0.67	0/1110
44	AQ	0.34	0/705	0.70	0/940
44	CK	0.34	0/705	0.78	0/940
45	B	0.20	0/41128	0.49	4/64084 (0.0%)
45	CM	0.21	0/42397	0.50	6/66069 (0.0%)
46	C	0.44	0/1666	0.90	2/2273 (0.1%)
46	CN	0.36	0/1666	0.85	4/2273 (0.2%)
47	CO	0.39	0/1750	0.94	1/2354 (0.0%)
47	D	0.32	0/1750	0.74	0/2354
48	CP	0.33	0/1657	0.74	1/2248 (0.0%)
48	E	0.37	0/1657	0.78	2/2248 (0.1%)
49	CQ	0.37	0/1731	0.92	5/2324 (0.2%)
49	F	0.33	0/1731	0.82	0/2324
50	CR	0.36	1/2096 (0.0%)	0.74	2/2822 (0.1%)
50	G	0.36	0/2092	0.77	1/2817 (0.0%)
51	CS	0.31	0/1631	0.81	2/2199 (0.1%)
51	H	0.32	0/1631	0.70	0/2199
52	CT	0.37	0/1929	0.86	1/2571 (0.0%)
52	I	0.31	0/1812	0.78	1/2420 (0.0%)
53	CU	0.31	0/1499	0.87	2/2016 (0.1%)
53	J	0.38	0/1486	0.85	0/1999
54	CV	0.27	0/1606	0.71	0/2150
54	K	0.28	0/1601	0.70	0/2143
55	CW	0.40	0/1478	0.87	4/1978 (0.2%)
55	L	0.29	0/1478	0.69	1/1978 (0.1%)
56	CX	0.37	0/809	0.96	2/1092 (0.2%)
56	M	0.35	0/836	0.89	2/1130 (0.2%)
57	CY	0.32	0/1154	0.70	0/1553
57	N	0.30	0/1152	0.65	1/1550 (0.1%)
58	CZ	0.32	0/921	1.12	5/1240 (0.4%)
58	O	0.41	0/892	1.01	2/1203 (0.2%)
59	DA	0.35	0/1210	0.79	2/1631 (0.1%)
59	P	0.36	0/1210	0.76	0/1631

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	DB	0.39	0/953	0.86	2/1279 (0.2%)
60	Q	0.34	0/953	0.81	1/1279 (0.1%)
61	DC	0.27	0/980	0.79	0/1315
61	R	0.35	0/1038	0.83	1/1395 (0.1%)
62	DD	0.29	0/1069	0.69	0/1430
62	S	0.37	0/1109	0.86	2/1486 (0.1%)
63	DE	0.37	0/1009	0.93	2/1354 (0.1%)
63	T	0.33	0/1009	0.80	0/1354
64	DF	0.34	0/1178	0.85	3/1579 (0.2%)
64	U	0.42	0/1205	0.92	3/1615 (0.2%)
65	DG	0.26	0/1108	0.76	0/1492
65	V	0.39	0/1120	0.82	0/1508
66	DH	0.32	0/772	0.77	0/1045
66	W	0.35	0/792	0.85	0/1071
67	DI	0.31	0/683	0.80	1/918 (0.1%)
67	X	0.35	0/683	0.76	0/918
68	DJ	0.38	0/1049	0.74	0/1412
68	Y	0.34	0/1049	0.74	1/1412 (0.1%)
69	DK	0.29	0/1128	0.75	1/1505 (0.1%)
69	Z	0.31	0/1128	0.85	1/1505 (0.1%)
70	DL	0.28	0/1086	0.73	0/1447
70	a	0.31	0/1100	0.88	3/1466 (0.2%)
71	DM	0.32	0/552	0.87	1/745 (0.1%)
71	b	0.32	0/585	0.76	0/789
72	DN	0.42	0/791	0.82	1/1060 (0.1%)
72	c	0.28	0/791	0.71	0/1060
73	DO	0.37	0/624	0.91	3/843 (0.4%)
73	d	0.28	0/624	0.68	0/843
74	DP	0.37	0/478	0.96	3/640 (0.5%)
74	e	0.29	0/489	0.94	0/654
75	DQ	0.26	0/461	0.63	0/613
75	f	0.31	0/466	0.67	0/620
76	DR	0.29	0/469	0.72	0/626
76	g	0.41	0/438	1.00	3/581 (0.5%)
77	h	0.36	0/585	1.11	3/778 (0.4%)
78	AR	0.36	0/2451	0.86	3/3337 (0.1%)
79	CL	0.43	1/941 (0.1%)	0.98	2/1257 (0.2%)
79	i	0.44	0/928	1.26	4/1239 (0.3%)
All	All	0.26	5/423231 (0.0%)	0.60	188/621279 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	BJ	111	PRO	CA-C	-14.95	1.43	1.51
41	AN	28	PRO	CA-C	-11.10	1.45	1.51
79	CL	107	TRP	CA-C	7.53	1.57	1.53
50	CR	149	TYR	C-O	-6.46	1.21	1.23
41	CH	28	PRO	CA-C	5.16	1.54	1.51

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	BJ	111	PRO	O-C-N	-11.14	116.19	121.31
49	CQ	183	LEU	CB-CG-CD2	-8.74	84.49	110.70
41	AN	28	PRO	O-C-N	-8.20	117.54	121.31
53	CU	73	LEU	CA-CB-CG	8.12	144.72	116.30
46	CN	62	ARG	CG-CD-NE	7.82	129.20	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	67782	0	34070	1080	0
1	AS	65508	0	32926	1276	0
2	3	2579	0	1304	40	0
2	AT	2579	0	1304	48	0
3	4	3313	0	1674	68	0
3	AU	3313	0	1674	73	0
4	AW	1894	0	1975	97	0
4	j	1894	0	1975	36	0
5	AX	3077	0	3166	82	0
5	k	3084	0	3173	81	0
6	AY	2751	0	2879	114	0
6	l	2745	0	2874	75	0
7	AZ	2394	0	2361	111	0
7	m	2426	0	2389	93	0
8	BA	1210	0	1285	62	0
8	n	1242	0	1321	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	BB	1885	0	1977	34	0
9	o	1885	0	1977	37	0
10	BC	1795	0	1915	119	0
10	p	1790	0	1910	40	0
11	BD	1519	0	1588	73	0
11	q	1519	0	1588	39	0
12	BE	1671	0	1717	53	0
12	r	1689	0	1731	42	0
13	BF	1371	0	1410	62	0
13	s	1371	0	1410	67	0
14	BG	1610	0	1686	98	0
14	t	1610	0	1686	41	0
15	BH	1029	0	1116	25	0
15	u	1015	0	1098	47	0
16	BI	1713	0	1764	95	0
16	v	1713	0	1764	54	0
17	BJ	1590	0	1705	41	0
17	w	1590	0	1705	39	0
18	BK	1396	0	1421	52	0
18	x	1372	0	1390	45	0
19	BL	1458	0	1556	64	0
19	y	1458	0	1556	41	0
20	BM	1457	0	1564	57	0
20	z	1457	0	1564	37	0
21	0	1423	0	1480	44	0
21	BN	1423	0	1480	45	0
22	2	1262	0	1314	36	0
22	BO	1262	0	1314	36	0
23	5	831	0	848	36	0
23	BP	837	0	853	59	0
24	6	977	0	1026	28	0
24	BQ	977	0	1026	32	0
25	7	632	0	666	17	0
25	BR	877	0	939	31	0
26	8	974	0	1032	21	0
26	BS	960	0	1014	55	0
27	9	980	0	1058	32	0
27	BT	989	0	1064	63	0
28	AA	1087	0	1154	48	0
28	BU	1087	0	1154	56	0
29	AB	1170	0	1203	40	0
29	BV	1170	0	1203	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	AC	488	0	515	13	0
30	BW	488	0	515	16	0
31	AD	729	0	775	15	0
31	BX	729	0	775	30	0
32	AE	894	0	941	20	0
32	BY	894	0	941	44	0
33	AF	1000	0	1069	30	0
33	BZ	1004	0	1077	37	0
34	AG	847	0	893	19	0
34	CA	847	0	893	26	0
35	AH	887	0	947	16	0
35	CB	887	0	947	59	0
36	AI	981	0	1086	45	0
36	CC	985	0	1089	68	0
37	AJ	758	0	838	16	0
37	CD	758	0	838	39	0
38	AK	677	0	697	26	0
38	CE	677	0	697	39	0
39	AL	617	0	674	14	0
39	CF	617	0	675	36	0
40	AM	438	0	475	9	0
40	CG	446	0	488	17	0
41	AN	419	0	460	6	0
41	CH	411	0	448	13	0
42	AO	236	0	285	9	0
42	CI	236	0	285	9	0
43	AP	828	0	893	18	0
43	CJ	828	0	893	18	0
44	AQ	698	0	734	17	0
44	CK	698	0	734	40	0
45	B	36771	0	18501	822	0
45	CM	37902	0	19064	976	0
46	C	1627	0	1644	110	0
46	CN	1627	0	1644	124	0
47	CO	1724	0	1805	105	0
47	D	1724	0	1805	60	0
48	CP	1629	0	1728	59	0
48	E	1629	0	1728	89	0
49	CQ	1707	0	1807	107	0
49	F	1707	0	1807	84	0
50	CR	2055	0	2137	80	0
50	G	2051	0	2134	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	CS	1614	0	1688	114	0
51	H	1614	0	1688	112	0
52	CT	1904	0	1994	84	0
52	I	1787	0	1861	68	0
53	CU	1475	0	1567	80	0
53	J	1462	0	1558	67	0
54	CV	1579	0	1602	47	0
54	K	1574	0	1597	51	0
55	CW	1453	0	1532	86	0
55	L	1453	0	1532	59	0
56	CX	791	0	805	68	0
56	M	817	0	828	53	0
57	CY	1129	0	1183	35	0
57	N	1128	0	1176	20	0
58	CZ	913	0	934	65	0
58	O	885	0	915	63	0
59	DA	1187	0	1249	63	0
59	P	1187	0	1249	37	0
60	DB	942	0	981	72	0
60	Q	942	0	981	42	0
61	DC	963	0	1003	44	0
61	R	1018	0	1065	60	0
62	DD	1053	0	1118	72	0
62	S	1091	0	1155	86	0
63	DE	997	0	1053	77	0
63	T	997	0	1053	53	0
64	DF	1161	0	1205	67	0
64	U	1187	0	1237	46	0
65	DG	1089	0	1103	62	0
65	V	1100	0	1114	64	0
66	DH	763	0	824	42	0
66	W	782	0	844	48	0
67	DI	676	0	677	28	0
67	X	676	0	677	55	0
68	DJ	1032	0	1066	53	0
68	Y	1032	0	1066	44	0
69	DK	1110	0	1182	26	0
69	Z	1110	0	1182	39	0
70	DL	1072	0	1123	48	0
70	a	1086	0	1132	45	0
71	DM	545	0	583	35	0
71	b	578	0	613	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	DN	779	0	833	39	0
72	c	779	0	832	20	0
73	DO	614	0	630	33	0
73	d	614	0	628	25	0
74	DP	476	0	510	30	0
74	e	487	0	523	38	0
75	DQ	449	0	426	10	0
75	f	454	0	431	16	0
76	DR	461	0	499	25	0
76	g	431	0	467	28	0
77	h	574	0	606	43	0
78	AR	2398	0	2374	161	0
79	CL	930	0	905	72	0
79	i	918	0	896	63	0
80	1	57	0	52	3	0
81	1	1218	0	1305	46	0
81	4	84	0	90	2	0
81	AS	546	0	585	28	0
81	B	210	0	225	12	0
81	CM	252	0	270	9	0
82	1	346	0	0	0	0
82	3	1	0	0	0	0
82	4	7	0	0	0	0
82	6	2	0	0	0	0
82	AB	1	0	0	0	0
82	AL	1	0	0	0	0
82	AP	2	0	0	0	0
82	AS	334	0	0	0	0
82	AT	1	0	0	0	0
82	AU	1	0	0	0	0
82	AW	3	0	0	0	0
82	AX	1	0	0	0	0
82	AY	1	0	0	0	0
82	B	140	0	0	0	0
82	C	1	0	0	0	0
82	CJ	1	0	0	0	0
82	CL	1	0	0	0	0
82	CM	139	0	0	0	0
82	CR	1	0	0	0	0
82	DG	1	0	0	0	0
82	DJ	1	0	0	0	0
82	DK	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	E	1	0	0	0	0
82	F	1	0	0	0	0
82	G	1	0	0	0	0
82	K	1	0	0	0	0
82	f	1	0	0	0	0
82	j	1	0	0	0	0
82	p	1	0	0	0	0
82	v	5	0	0	0	0
82	w	1	0	0	0	0
82	x	1	0	0	0	0
83	AH	1	0	0	0	0
83	AK	1	0	0	0	0
83	AN	1	0	0	0	0
83	AP	1	0	0	0	0
83	AQ	1	0	0	0	0
83	CB	1	0	0	0	0
83	CE	1	0	0	0	0
83	CH	1	0	0	0	0
83	CJ	1	0	0	0	0
83	CK	1	0	0	0	0
83	DN	1	0	0	0	0
83	DO	1	0	0	0	0
83	DQ	1	0	0	0	0
83	c	1	0	0	0	0
83	d	1	0	0	0	0
83	f	1	0	0	0	0
83	h	1	0	0	0	0
All	All	397530	0	295439	10019	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 10019 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:CS:143:ARG:NH1	74:DP:57:MET:SD	2.24	1.10
4:AW:126:LEU:HD23	4:AW:150:LEU:HD21	1.35	1.07
63:DE:5:ARG:HD2	63:DE:49:LYS:HD2	1.23	1.07
20:BM:72:ALA:HB3	20:BM:74:ARG:HH22	1.13	1.06
51:CS:70:VAL:HB	62:DD:46:LYS:HZ2	1.20	1.05

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
10	BC	229/262 (87%)	220 (96%)	7 (3%)	2 (1%)	14	41
10	p	228/262 (87%)	220 (96%)	7 (3%)	1 (0%)	30	59
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%)	24	54
14	t	198/202 (98%)	196 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	12	39
23	BP	101/124 (82%)	90 (89%)	9 (9%)	2 (2%)	6	22
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	30
25	BR	105/155 (68%)	97 (92%)	7 (7%)	1 (1%)	12	39
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	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	41
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%)	11	36
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	CO	212/256 (83%)	205 (97%)	6 (3%)	1 (0%)	24	54
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%)	24	54
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%)	21	51
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	30
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	44
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	44
62	DD	131/142 (92%)	128 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	S	138/142 (97%)	134 (97%)	3 (2%)	1 (1%)	18	48
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%)	18	48
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	28
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
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%)	6	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	28
78	AR	309/317 (98%)	293 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	CL	117/267 (44%)	91 (78%)	22 (19%)	4 (3%)	3	12
79	i	116/267 (43%)	90 (78%)	21 (18%)	5 (4%)	2	8
All	All	21638/23766 (91%)	20895 (97%)	693 (3%)	50 (0%)	43	72

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%)	188 (98%)	3 (2%)	55	83
4	j	191/194 (98%)	189 (99%)	2 (1%)	68	89
5	AX	325/328 (99%)	322 (99%)	3 (1%)	70	90
5	k	326/328 (99%)	324 (99%)	2 (1%)	78	93
6	AY	290/292 (99%)	286 (99%)	4 (1%)	59	85
6	l	289/292 (99%)	286 (99%)	3 (1%)	68	89
7	AZ	247/252 (98%)	240 (97%)	7 (3%)	38	72
7	m	250/252 (99%)	248 (99%)	2 (1%)	73	90
8	BA	132/154 (86%)	128 (97%)	4 (3%)	36	70
8	n	136/154 (88%)	134 (98%)	2 (2%)	57	84
9	BB	198/204 (97%)	192 (97%)	6 (3%)	36	70
9	o	198/204 (97%)	192 (97%)	6 (3%)	36	70
10	BC	193/216 (89%)	185 (96%)	8 (4%)	27	61
10	p	193/216 (89%)	189 (98%)	4 (2%)	47	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	BD	169/170 (99%)	164 (97%)	5 (3%)	36	70
11	q	169/170 (99%)	166 (98%)	3 (2%)	51	80
12	BE	176/186 (95%)	174 (99%)	2 (1%)	65	88
12	r	178/186 (96%)	177 (99%)	1 (1%)	78	93
13	BF	146/149 (98%)	141 (97%)	5 (3%)	32	66
13	s	146/149 (98%)	144 (99%)	2 (1%)	59	85
14	BG	166/168 (99%)	158 (95%)	8 (5%)	23	55
14	t	166/168 (99%)	165 (99%)	1 (1%)	78	93
15	BH	108/109 (99%)	106 (98%)	2 (2%)	50	79
15	u	107/109 (98%)	106 (99%)	1 (1%)	70	90
16	BI	177/178 (99%)	173 (98%)	4 (2%)	44	76
16	v	177/178 (99%)	176 (99%)	1 (1%)	78	93
17	BJ	166/167 (99%)	161 (97%)	5 (3%)	36	70
17	w	166/167 (99%)	166 (100%)	0	100	100
18	BK	145/154 (94%)	141 (97%)	4 (3%)	38	72
18	x	142/154 (92%)	141 (99%)	1 (1%)	76	92
19	BL	153/154 (99%)	151 (99%)	2 (1%)	61	86
19	y	153/154 (99%)	149 (97%)	4 (3%)	40	73
20	BM	146/153 (95%)	141 (97%)	5 (3%)	32	66
20	z	146/153 (95%)	145 (99%)	1 (1%)	76	92
21	0	155/157 (99%)	155 (100%)	0	100	100
21	BN	155/157 (99%)	153 (99%)	2 (1%)	61	86
22	2	133/134 (99%)	131 (98%)	2 (2%)	57	84
22	BO	133/134 (99%)	130 (98%)	3 (2%)	44	76
23	5	93/112 (83%)	90 (97%)	3 (3%)	34	68
23	BP	94/112 (84%)	89 (95%)	5 (5%)	20	52
24	6	101/104 (97%)	100 (99%)	1 (1%)	68	89
24	BQ	101/104 (97%)	100 (99%)	1 (1%)	68	89
25	7	68/127 (54%)	65 (96%)	3 (4%)	25	59
25	BR	91/127 (72%)	83 (91%)	8 (9%)	9	29
26	8	108/121 (89%)	106 (98%)	2 (2%)	50	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BS	107/121 (88%)	103 (96%)	4 (4%)	30	64
27	9	110/112 (98%)	109 (99%)	1 (1%)	70	90
27	BT	111/112 (99%)	103 (93%)	8 (7%)	13	39
28	AA	117/118 (99%)	116 (99%)	1 (1%)	70	90
28	BU	117/118 (99%)	110 (94%)	7 (6%)	17	47
29	AB	120/121 (99%)	119 (99%)	1 (1%)	73	90
29	BV	120/121 (99%)	119 (99%)	1 (1%)	73	90
30	AC	48/49 (98%)	46 (96%)	2 (4%)	26	60
30	BW	48/49 (98%)	47 (98%)	1 (2%)	47	77
31	AD	81/90 (90%)	80 (99%)	1 (1%)	63	86
31	BX	81/90 (90%)	77 (95%)	4 (5%)	22	54
32	AE	98/100 (98%)	98 (100%)	0	100	100
32	BY	98/100 (98%)	96 (98%)	2 (2%)	48	78
33	AF	109/115 (95%)	107 (98%)	2 (2%)	51	80
33	BZ	110/115 (96%)	108 (98%)	2 (2%)	51	80
34	AG	91/92 (99%)	90 (99%)	1 (1%)	65	88
34	CA	91/92 (99%)	91 (100%)	0	100	100
35	AH	95/102 (93%)	94 (99%)	1 (1%)	65	88
35	CB	95/102 (93%)	90 (95%)	5 (5%)	20	52
36	AI	106/106 (100%)	104 (98%)	2 (2%)	50	79
36	CC	106/106 (100%)	102 (96%)	4 (4%)	29	64
37	AJ	77/79 (98%)	76 (99%)	1 (1%)	61	86
37	CD	77/79 (98%)	75 (97%)	2 (3%)	40	73
38	AK	70/73 (96%)	70 (100%)	0	100	100
38	CE	70/73 (96%)	69 (99%)	1 (1%)	59	85
39	AL	68/69 (99%)	66 (97%)	2 (3%)	37	71
39	CF	68/69 (99%)	65 (96%)	3 (4%)	25	59
40	AM	46/47 (98%)	45 (98%)	1 (2%)	45	77
40	CG	47/47 (100%)	47 (100%)	0	100	100
41	AN	47/47 (100%)	47 (100%)	0	100	100
41	CH	46/47 (98%)	44 (96%)	2 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	AO	24/24 (100%)	23 (96%)	1 (4%)	26	60
42	CI	24/24 (100%)	21 (88%)	3 (12%)	4	15
43	AP	88/91 (97%)	87 (99%)	1 (1%)	65	88
43	CJ	88/91 (97%)	87 (99%)	1 (1%)	65	88
44	AQ	72/73 (99%)	72 (100%)	0	100	100
44	CK	72/73 (99%)	70 (97%)	2 (3%)	38	72
46	C	176/215 (82%)	175 (99%)	1 (1%)	78	93
46	CN	176/215 (82%)	172 (98%)	4 (2%)	44	76
47	CO	194/229 (85%)	187 (96%)	7 (4%)	31	65
47	D	194/229 (85%)	191 (98%)	3 (2%)	57	84
48	CP	175/198 (88%)	167 (95%)	8 (5%)	24	57
48	E	175/198 (88%)	172 (98%)	3 (2%)	53	82
49	CQ	174/196 (89%)	171 (98%)	3 (2%)	53	82
49	F	174/196 (89%)	169 (97%)	5 (3%)	37	71
50	CR	218/220 (99%)	210 (96%)	8 (4%)	30	64
50	G	218/220 (99%)	215 (99%)	3 (1%)	59	85
51	CS	178/197 (90%)	169 (95%)	9 (5%)	21	53
51	H	178/197 (90%)	173 (97%)	5 (3%)	38	72
52	CT	204/204 (100%)	191 (94%)	13 (6%)	16	44
52	I	192/204 (94%)	188 (98%)	4 (2%)	47	77
53	CU	164/167 (98%)	160 (98%)	4 (2%)	43	75
53	J	163/167 (98%)	159 (98%)	4 (2%)	42	74
54	CV	157/160 (98%)	153 (98%)	4 (2%)	42	74
54	K	157/160 (98%)	155 (99%)	2 (1%)	61	86
55	CW	153/160 (96%)	148 (97%)	5 (3%)	33	67
55	L	153/160 (96%)	153 (100%)	0	100	100
56	CX	88/104 (85%)	86 (98%)	2 (2%)	44	76
56	M	90/104 (86%)	88 (98%)	2 (2%)	45	77
57	CY	122/134 (91%)	122 (100%)	0	100	100
57	N	122/134 (91%)	119 (98%)	3 (2%)	42	74
58	CZ	101/123 (82%)	93 (92%)	8 (8%)	11	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	O	98/123 (80%)	94 (96%)	4 (4%)	27	61
59	DA	129/130 (99%)	127 (98%)	2 (2%)	55	83
59	P	129/130 (99%)	127 (98%)	2 (2%)	55	83
60	DB	97/102 (95%)	95 (98%)	2 (2%)	47	77
60	Q	97/102 (95%)	95 (98%)	2 (2%)	47	77
61	DC	105/121 (87%)	103 (98%)	2 (2%)	50	79
61	R	111/121 (92%)	107 (96%)	4 (4%)	31	65
62	DD	110/116 (95%)	108 (98%)	2 (2%)	51	80
62	S	114/116 (98%)	110 (96%)	4 (4%)	32	66
63	DE	112/122 (92%)	108 (96%)	4 (4%)	31	65
63	T	112/122 (92%)	108 (96%)	4 (4%)	31	65
64	DF	125/129 (97%)	122 (98%)	3 (2%)	43	75
64	U	128/129 (99%)	127 (99%)	1 (1%)	73	90
65	DG	112/117 (96%)	104 (93%)	8 (7%)	13	40
65	V	113/117 (97%)	111 (98%)	2 (2%)	51	80
66	DH	87/105 (83%)	84 (97%)	3 (3%)	32	66
66	W	89/105 (85%)	86 (97%)	3 (3%)	32	66
67	DI	71/71 (100%)	71 (100%)	0	100	100
67	X	71/71 (100%)	70 (99%)	1 (1%)	59	85
68	DJ	112/113 (99%)	112 (100%)	0	100	100
68	Y	112/113 (99%)	110 (98%)	2 (2%)	51	80
69	DK	116/118 (98%)	113 (97%)	3 (3%)	40	73
69	Z	116/118 (98%)	115 (99%)	1 (1%)	70	90
70	DL	109/112 (97%)	108 (99%)	1 (1%)	70	90
70	a	111/112 (99%)	108 (97%)	3 (3%)	39	73
71	DM	61/85 (72%)	57 (93%)	4 (7%)	15	43
71	b	64/85 (75%)	63 (98%)	1 (2%)	55	83
72	DN	84/102 (82%)	82 (98%)	2 (2%)	43	75
72	c	84/102 (82%)	84 (100%)	0	100	100
73	DO	72/73 (99%)	69 (96%)	3 (4%)	26	60
73	d	72/73 (99%)	70 (97%)	2 (3%)	38	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	DP	53/58 (91%)	52 (98%)	1 (2%)	50	79
74	e	54/58 (93%)	53 (98%)	1 (2%)	50	79
75	DQ	47/48 (98%)	46 (98%)	1 (2%)	47	77
75	f	47/48 (98%)	47 (100%)	0	100	100
76	DR	50/54 (93%)	48 (96%)	2 (4%)	28	62
76	g	46/54 (85%)	46 (100%)	0	100	100
77	h	62/175 (35%)	60 (97%)	2 (3%)	34	68
78	AR	259/263 (98%)	245 (95%)	14 (5%)	20	51
79	CL	99/212 (47%)	93 (94%)	6 (6%)	17	46
79	i	98/212 (46%)	84 (86%)	14 (14%)	3	11
All	All	18570/20010 (93%)	18131 (98%)	439 (2%)	43	75

5 of 439 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	BN	55	SER
36	CC	103	LYS
79	CL	155	LEU
66	DH	21	ILE
23	BP	56	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 254 such sidechains are listed below:

Mol	Chain	Res	Type
68	Y	70	ASN
58	CZ	38	HIS
10	BC	192	HIS
57	CY	92	HIS
67	DI	70	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

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	1801	-	44,45,45	0.47	0	63,67,67	0.86	4 (6%)
81	PAR	1	3424	-	44,45,45	0.48	0	63,67,67	1.05	4 (6%)
81	PAR	AS	3410	-	44,45,45	0.50	0	63,67,67	0.97	5 (7%)
81	PAR	AS	3413	-	44,45,45	0.58	0	63,67,67	1.09	5 (7%)
81	PAR	1	3410	-	44,45,45	0.56	0	63,67,67	0.80	1 (1%)
81	PAR	AS	3411	-	44,45,45	0.45	0	63,67,67	1.11	4 (6%)
81	PAR	CM	1805	-	44,45,45	0.50	0	63,67,67	1.13	4 (6%)
81	PAR	B	1805	-	44,45,45	0.45	0	63,67,67	0.98	4 (6%)
81	PAR	AS	3407	-	44,45,45	0.49	0	63,67,67	1.06	4 (6%)
81	PAR	1	3420	-	44,45,45	0.46	0	63,67,67	0.76	2 (3%)
81	PAR	1	3402	-	44,45,45	0.48	0	63,67,67	0.68	2 (3%)
81	PAR	1	3405	-	44,45,45	0.48	0	63,67,67	1.13	5 (7%)
81	PAR	AS	3406	-	44,45,45	0.49	0	63,67,67	1.03	4 (6%)
81	PAR	1	3416	-	44,45,45	0.43	0	63,67,67	0.97	1 (1%)
81	PAR	1	3423	-	44,45,45	0.46	0	63,67,67	1.07	4 (6%)
81	PAR	4	201	-	44,45,45	0.62	1 (2%)	63,67,67	0.99	5 (7%)
81	PAR	1	3427	-	44,45,45	0.59	0	63,67,67	0.97	3 (4%)
81	PAR	4	202	-	44,45,45	0.50	0	63,67,67	1.30	3 (4%)
81	PAR	1	3428	-	44,45,45	0.51	0	63,67,67	0.88	2 (3%)
81	PAR	CM	1804	-	44,45,45	0.44	0	63,67,67	0.90	1 (1%)
81	PAR	1	3411	-	44,45,45	0.45	0	63,67,67	1.06	6 (9%)
81	PAR	1	3407	-	44,45,45	0.47	0	63,67,67	0.88	2 (3%)
81	PAR	1	3430	-	44,45,45	0.58	1 (2%)	63,67,67	1.54	11 (17%)
81	PAR	1	3422	-	44,45,45	0.64	1 (2%)	63,67,67	1.80	12 (19%)
81	PAR	AS	3404	-	44,45,45	0.53	0	63,67,67	0.70	1 (1%)
81	PAR	B	1803	-	44,45,45	0.49	0	63,67,67	1.12	4 (6%)
81	PAR	1	3418	-	44,45,45	0.52	0	63,67,67	1.14	7 (11%)
81	PAR	B	1804	-	44,45,45	0.48	0	63,67,67	1.02	4 (6%)
81	PAR	AS	3405	-	44,45,45	0.44	0	63,67,67	0.72	1 (1%)
80	3K5	1	3401	-	63,63,63	2.84	28 (44%)	84,95,95	1.74	21 (25%)
81	PAR	1	3426	-	44,45,45	0.49	0	63,67,67	1.07	4 (6%)
81	PAR	AS	3402	-	44,45,45	0.45	0	63,67,67	0.83	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
81	PAR	CM	1806	-	44,45,45	0.64	1 (2%)	63,67,67	0.83	1 (1%)
81	PAR	1	3429	-	44,45,45	0.51	0	63,67,67	0.95	3 (4%)
81	PAR	1	3403	-	44,45,45	0.44	0	63,67,67	0.94	2 (3%)
81	PAR	AS	3401	-	44,45,45	0.48	0	63,67,67	1.42	5 (7%)
81	PAR	1	3413	-	44,45,45	0.55	0	63,67,67	1.49	7 (11%)
81	PAR	AS	3408	-	44,45,45	0.52	0	63,67,67	0.92	4 (6%)
81	PAR	1	3417	82	44,45,45	0.56	1 (2%)	63,67,67	1.29	6 (9%)
81	PAR	1	3412	-	44,45,45	0.46	0	63,67,67	0.73	1 (1%)
81	PAR	CM	1803	-	44,45,45	0.44	0	63,67,67	0.73	2 (3%)
81	PAR	AS	3403	-	44,45,45	0.49	0	63,67,67	0.64	1 (1%)
81	PAR	1	3414	-	44,45,45	0.47	0	63,67,67	0.93	3 (4%)
81	PAR	1	3409	-	44,45,45	0.47	0	63,67,67	0.97	3 (4%)
81	PAR	1	3408	-	44,45,45	0.47	0	63,67,67	0.77	2 (3%)
81	PAR	1	3406	-	44,45,45	0.59	1 (2%)	63,67,67	1.15	5 (7%)
81	PAR	AS	3409	-	44,45,45	0.44	0	63,67,67	0.76	1 (1%)
81	PAR	1	3421	-	44,45,45	0.45	0	63,67,67	0.77	1 (1%)
81	PAR	AS	3412	-	44,45,45	0.45	0	63,67,67	0.99	3 (4%)
81	PAR	1	3419	-	44,45,45	0.46	0	63,67,67	0.68	2 (3%)
81	PAR	CM	1801	-	44,45,45	0.52	0	63,67,67	1.06	5 (7%)
81	PAR	B	1802	-	44,45,45	0.46	0	63,67,67	1.25	6 (9%)
81	PAR	CM	1802	-	44,45,45	0.46	0	63,67,67	0.82	2 (3%)
81	PAR	1	3404	-	44,45,45	0.49	0	63,67,67	0.90	3 (4%)
81	PAR	1	3425	-	44,45,45	0.46	0	63,67,67	0.94	2 (3%)
81	PAR	1	3415	-	44,45,45	0.47	0	63,67,67	0.84	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	B	1801	-	-	2/18/94/94	0/4/4/4
81	PAR	1	3424	-	-	9/18/94/94	0/4/4/4
81	PAR	AS	3410	-	-	7/18/94/94	0/4/4/4
81	PAR	AS	3413	-	-	9/18/94/94	0/4/4/4
81	PAR	1	3410	-	-	9/18/94/94	1/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	PAR	AS	3411	-	-	9/18/94/94	1/4/4/4
81	PAR	CM	1805	-	-	7/18/94/94	0/4/4/4
81	PAR	B	1805	-	-	12/18/94/94	0/4/4/4
81	PAR	AS	3407	-	-	5/18/94/94	1/4/4/4
81	PAR	1	3420	-	-	6/18/94/94	0/4/4/4
81	PAR	1	3402	-	-	3/18/94/94	0/4/4/4
81	PAR	1	3405	-	-	9/18/94/94	0/4/4/4
81	PAR	AS	3406	-	-	9/18/94/94	0/4/4/4
81	PAR	1	3416	-	-	3/18/94/94	0/4/4/4
81	PAR	1	3423	-	-	3/18/94/94	0/4/4/4
81	PAR	4	201	-	-	4/18/94/94	0/4/4/4
81	PAR	1	3427	-	-	6/18/94/94	0/4/4/4
81	PAR	4	202	-	-	4/18/94/94	0/4/4/4
81	PAR	1	3428	-	-	7/18/94/94	0/4/4/4
81	PAR	CM	1804	-	-	9/18/94/94	0/4/4/4
81	PAR	1	3411	-	-	9/18/94/94	0/4/4/4
81	PAR	1	3407	-	-	8/18/94/94	0/4/4/4
81	PAR	1	3430	-	-	9/18/94/94	0/4/4/4
81	PAR	1	3422	-	-	5/18/94/94	0/4/4/4
81	PAR	AS	3404	-	-	6/18/94/94	0/4/4/4
81	PAR	B	1803	-	-	7/18/94/94	0/4/4/4
81	PAR	1	3418	-	-	6/18/94/94	0/4/4/4
81	PAR	B	1804	-	-	6/18/94/94	0/4/4/4
81	PAR	AS	3405	-	-	2/18/94/94	1/4/4/4
80	3K5	1	3401	-	-	9/29/121/121	0/7/7/7
81	PAR	1	3426	-	-	1/18/94/94	0/4/4/4
81	PAR	AS	3402	-	-	8/18/94/94	0/4/4/4
81	PAR	CM	1806	-	-	6/18/94/94	0/4/4/4
81	PAR	1	3429	-	-	4/18/94/94	0/4/4/4
81	PAR	1	3403	-	-	10/18/94/94	1/4/4/4
81	PAR	AS	3401	-	-	1/18/94/94	0/4/4/4
81	PAR	1	3413	-	-	8/18/94/94	0/4/4/4
81	PAR	AS	3408	-	-	7/18/94/94	0/4/4/4
81	PAR	1	3417	82	-	11/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	PAR	1	3412	-	-	5/18/94/94	0/4/4/4
81	PAR	CM	1803	-	-	2/18/94/94	0/4/4/4
81	PAR	AS	3403	-	-	3/18/94/94	0/4/4/4
81	PAR	1	3414	-	-	8/18/94/94	0/4/4/4
81	PAR	1	3409	-	-	6/18/94/94	0/4/4/4
81	PAR	1	3408	-	-	4/18/94/94	0/4/4/4
81	PAR	1	3406	-	-	8/18/94/94	0/4/4/4
81	PAR	AS	3409	-	-	9/18/94/94	0/4/4/4
81	PAR	1	3421	-	-	4/18/94/94	0/4/4/4
81	PAR	AS	3412	-	-	6/18/94/94	0/4/4/4
81	PAR	1	3419	-	-	6/18/94/94	0/4/4/4
81	PAR	CM	1801	-	-	5/18/94/94	0/4/4/4
81	PAR	B	1802	-	-	5/18/94/94	0/4/4/4
81	PAR	CM	1802	-	-	5/18/94/94	0/4/4/4
81	PAR	1	3404	-	-	8/18/94/94	1/4/4/4
81	PAR	1	3425	-	-	10/18/94/94	0/4/4/4
81	PAR	1	3415	-	-	3/18/94/94	0/4/4/4

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	1	3401	3K5	C17-C22	-8.43	1.36	1.53
80	1	3401	3K5	O4-C22	7.27	1.59	1.43
80	1	3401	3K5	C21-C22	5.81	1.63	1.52
80	1	3401	3K5	O6-C23	5.07	1.45	1.34
80	1	3401	3K5	C20-C23	4.65	1.62	1.51

The worst 5 of 215 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	1	3422	PAR	O33-C14-C24	8.72	122.36	108.08
81	4	202	PAR	O11-C11-C21	7.94	121.07	108.08
81	AS	3401	PAR	C32-C22-C12	6.80	122.67	111.02
81	CM	1805	PAR	O11-C11-C21	6.29	118.36	108.08
81	1	3416	PAR	O11-C11-C21	5.72	117.44	108.08

There are no chirality outliers.

5 of 352 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	C39-C38-O14-C34
81	1	3403	PAR	O51-C11-O11-C42
81	1	3403	PAR	C23-C13-O52-C52

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

45 monomers are involved in 100 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	B	1801	PAR	2	0
81	1	3424	PAR	1	0
81	AS	3413	PAR	1	0
81	1	3410	PAR	2	0
81	AS	3411	PAR	2	0
81	B	1805	PAR	3	0
81	AS	3407	PAR	2	0
81	1	3420	PAR	1	0
81	1	3402	PAR	2	0
81	1	3405	PAR	1	0
81	AS	3406	PAR	1	0
81	1	3416	PAR	3	0
81	1	3423	PAR	3	0
81	1	3427	PAR	1	0
81	4	202	PAR	2	0
81	CM	1804	PAR	1	0
81	1	3430	PAR	1	0
81	1	3422	PAR	7	0
81	AS	3404	PAR	3	0
81	B	1803	PAR	4	0
81	B	1804	PAR	2	0
81	AS	3405	PAR	4	0
80	1	3401	3K5	3	0
81	1	3426	PAR	1	0
81	AS	3402	PAR	1	0

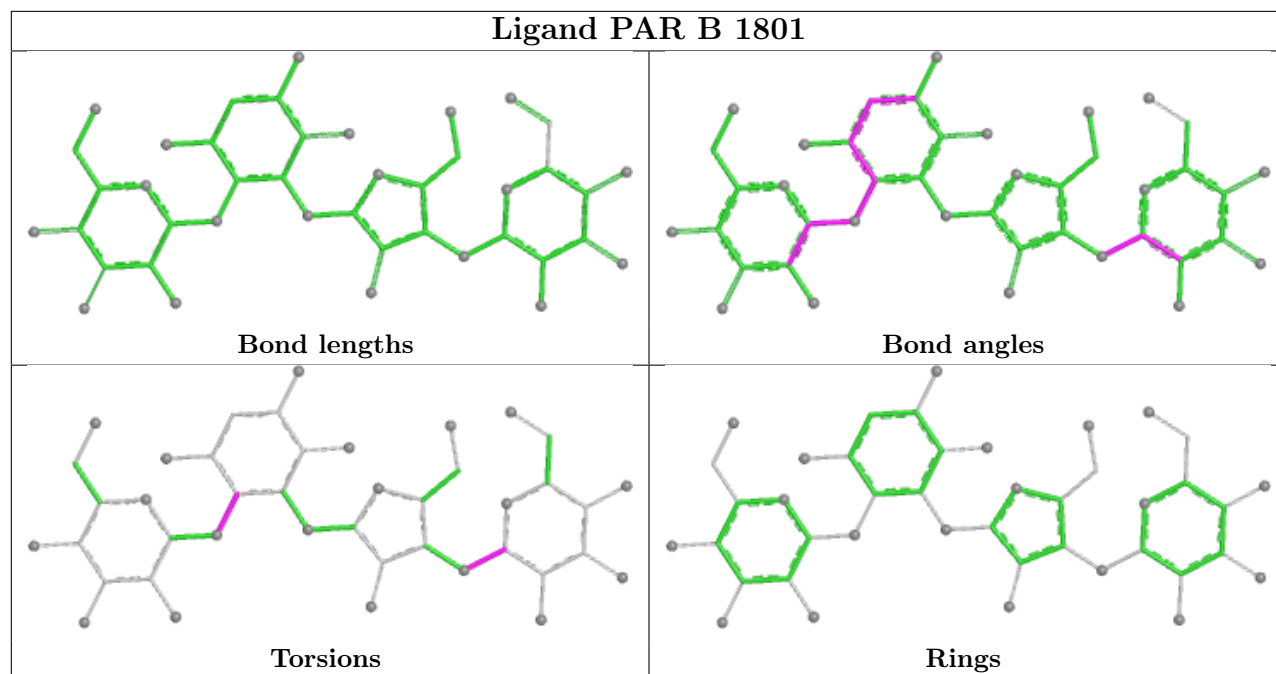
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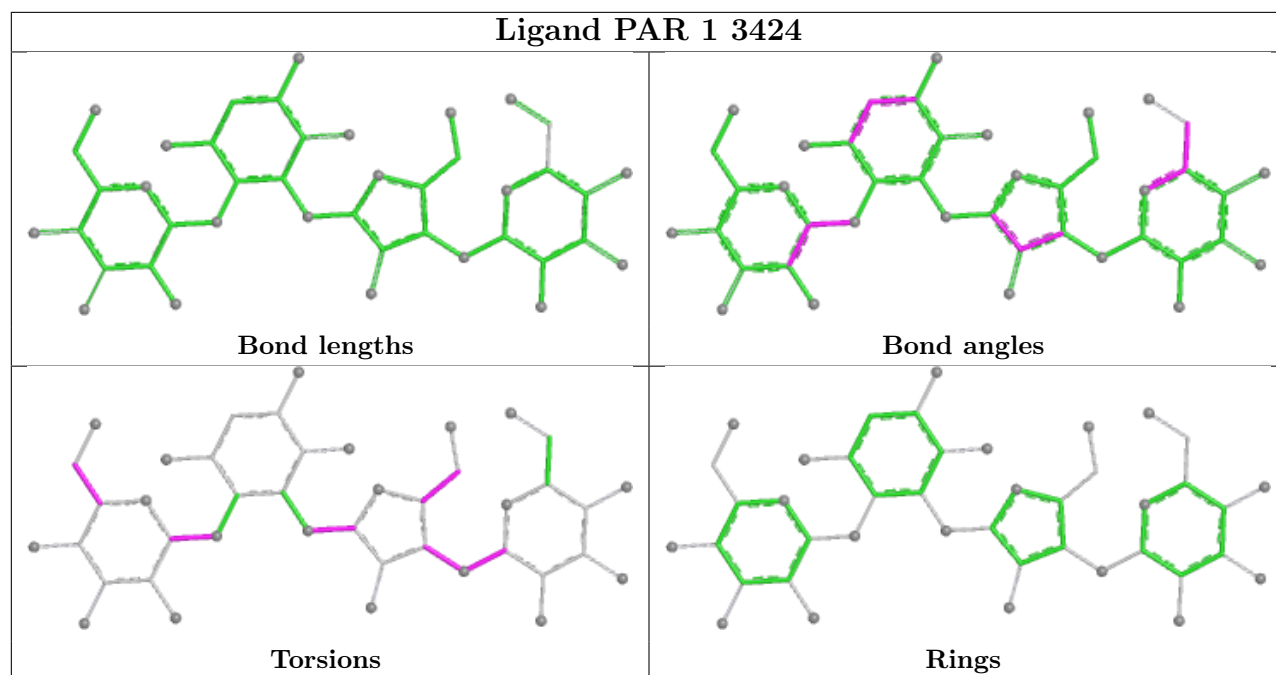
Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	CM	1806	PAR	1	0
81	1	3403	PAR	2	0
81	AS	3401	PAR	4	0
81	1	3413	PAR	2	0
81	1	3417	PAR	1	0
81	1	3412	PAR	3	0
81	CM	1803	PAR	1	0
81	AS	3403	PAR	5	0
81	1	3408	PAR	1	0
81	1	3406	PAR	5	0
81	AS	3409	PAR	4	0
81	1	3421	PAR	1	0
81	AS	3412	PAR	1	0
81	1	3419	PAR	5	0
81	CM	1801	PAR	3	0
81	B	1802	PAR	1	0
81	CM	1802	PAR	3	0
81	1	3404	PAR	1	0
81	1	3425	PAR	2	0
81	1	3415	PAR	4	0

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

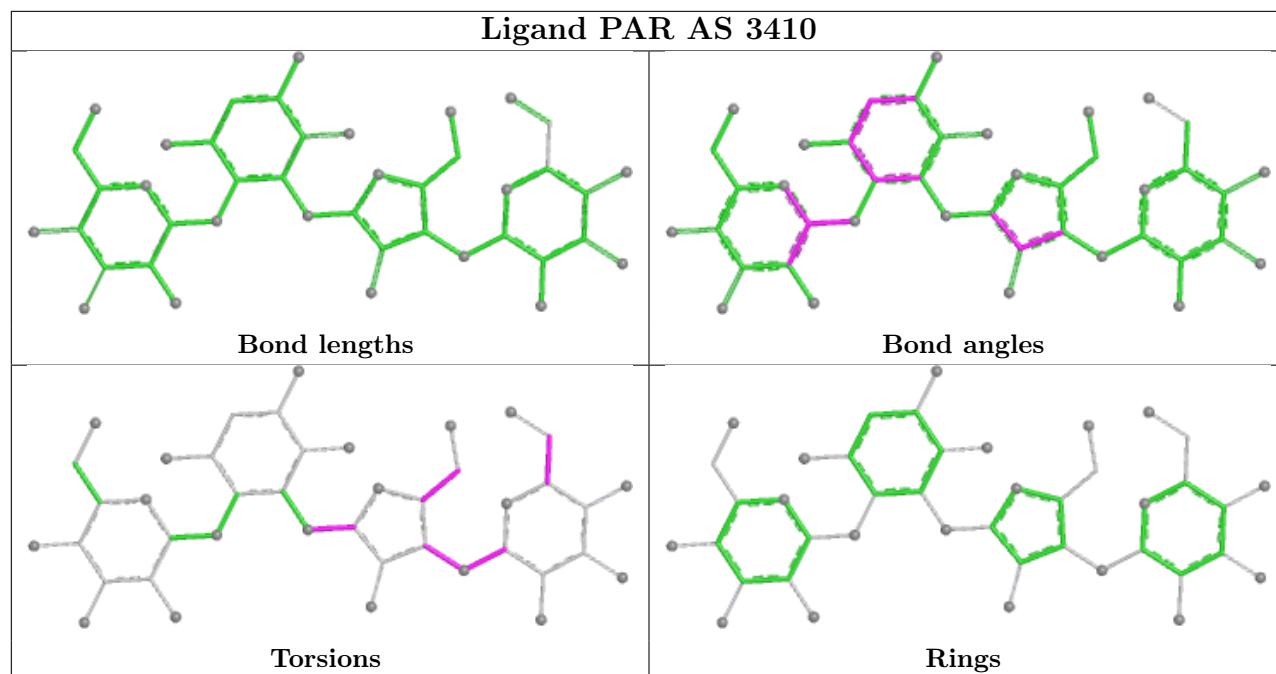
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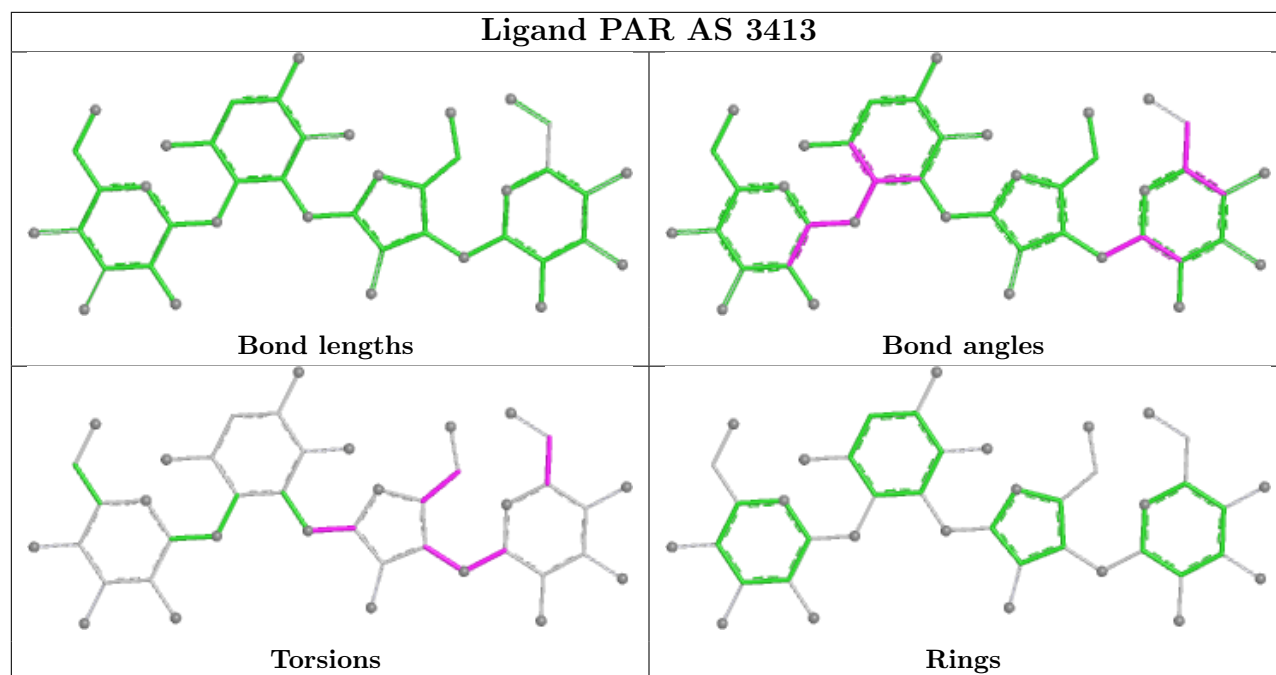
Ligand PAR 1 3424

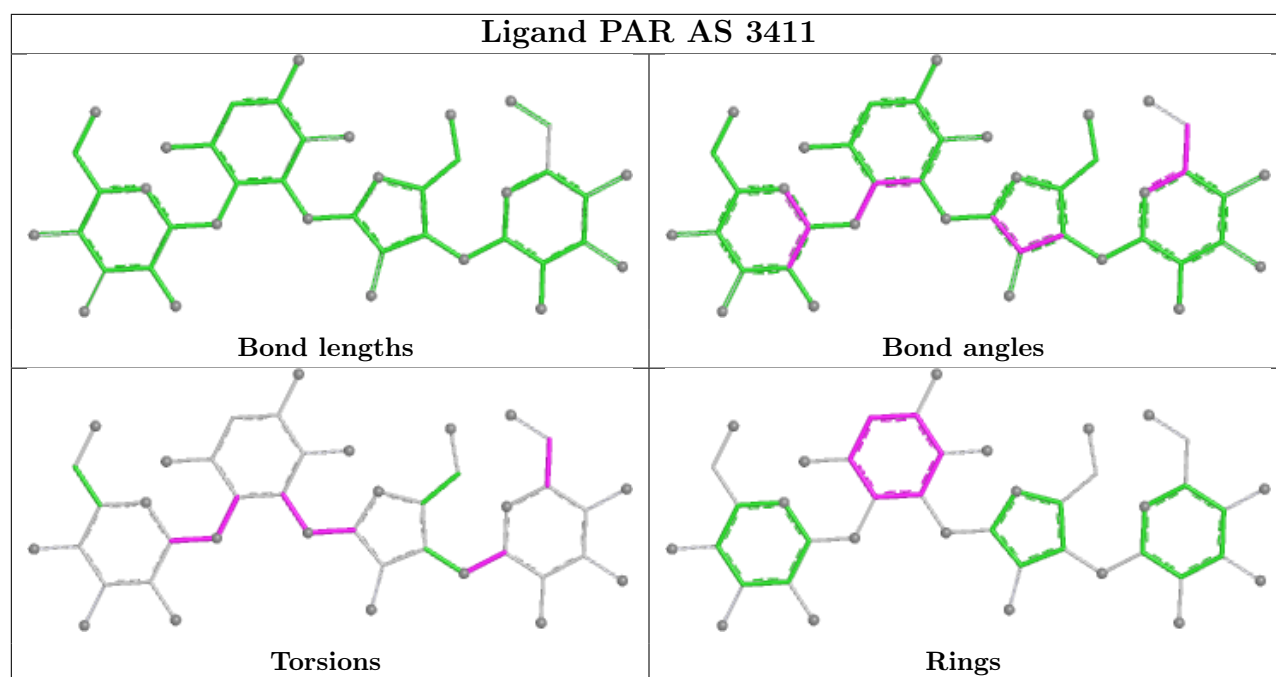
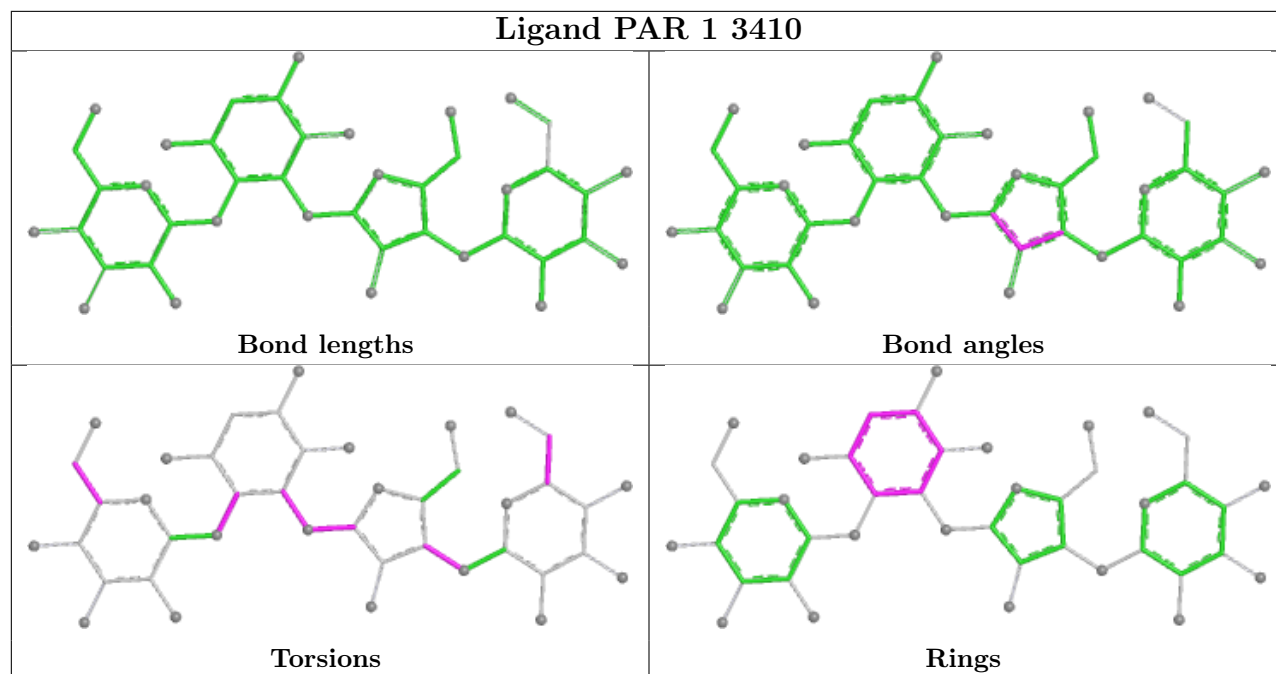


Ligand PAR AS 3410

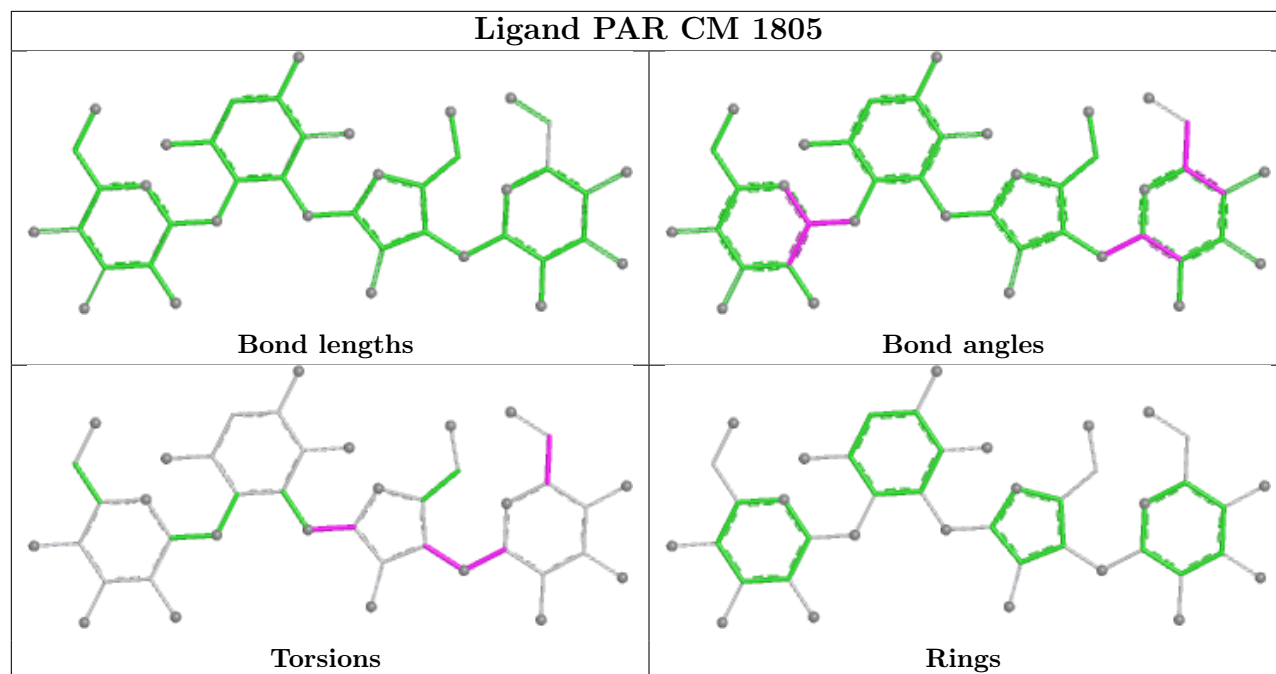


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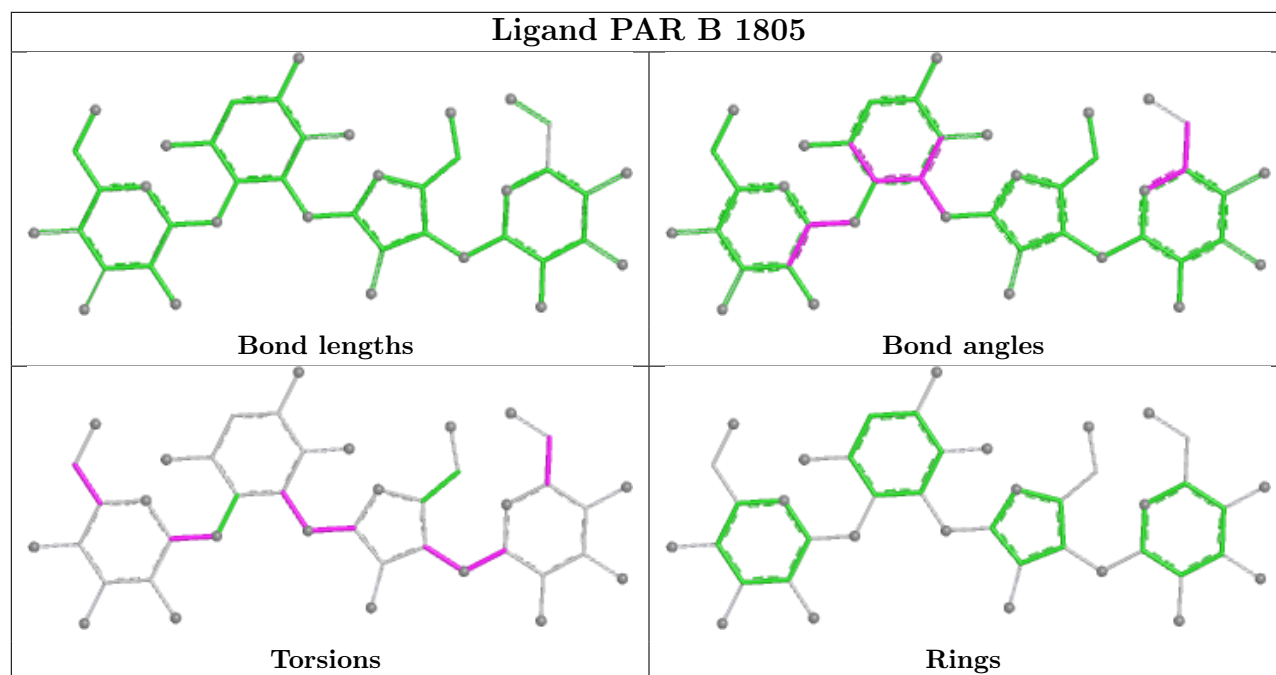




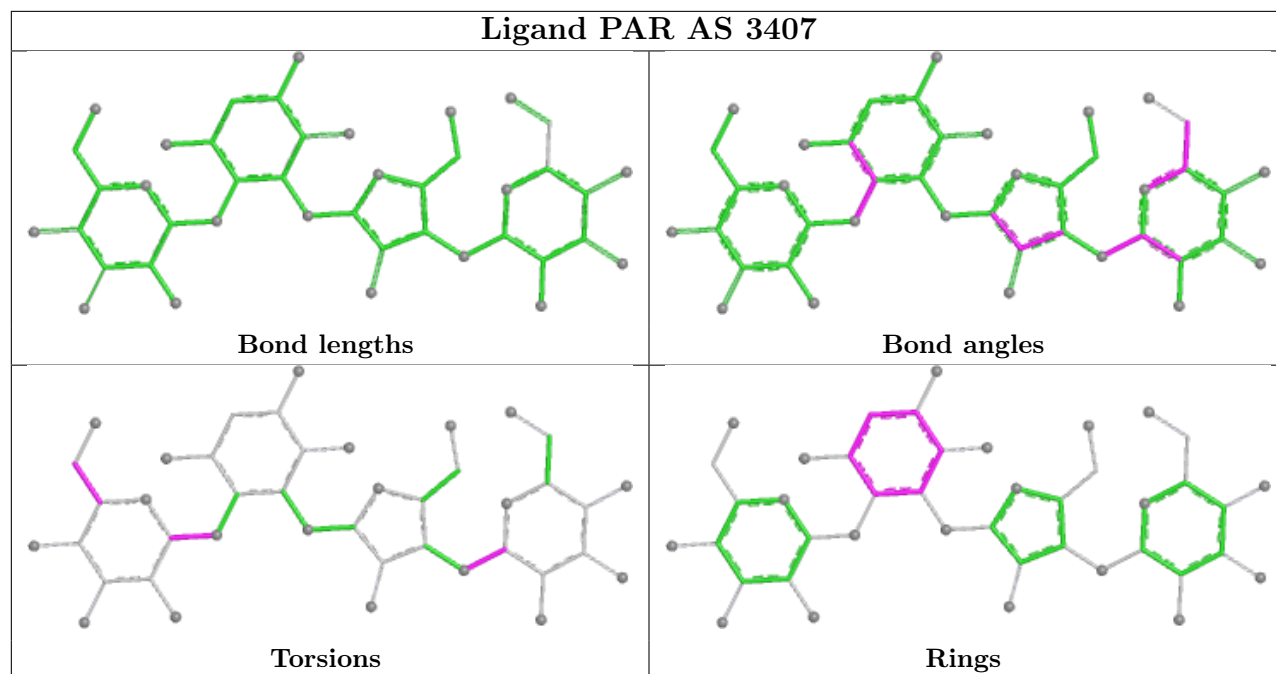
Ligand PAR CM 1805



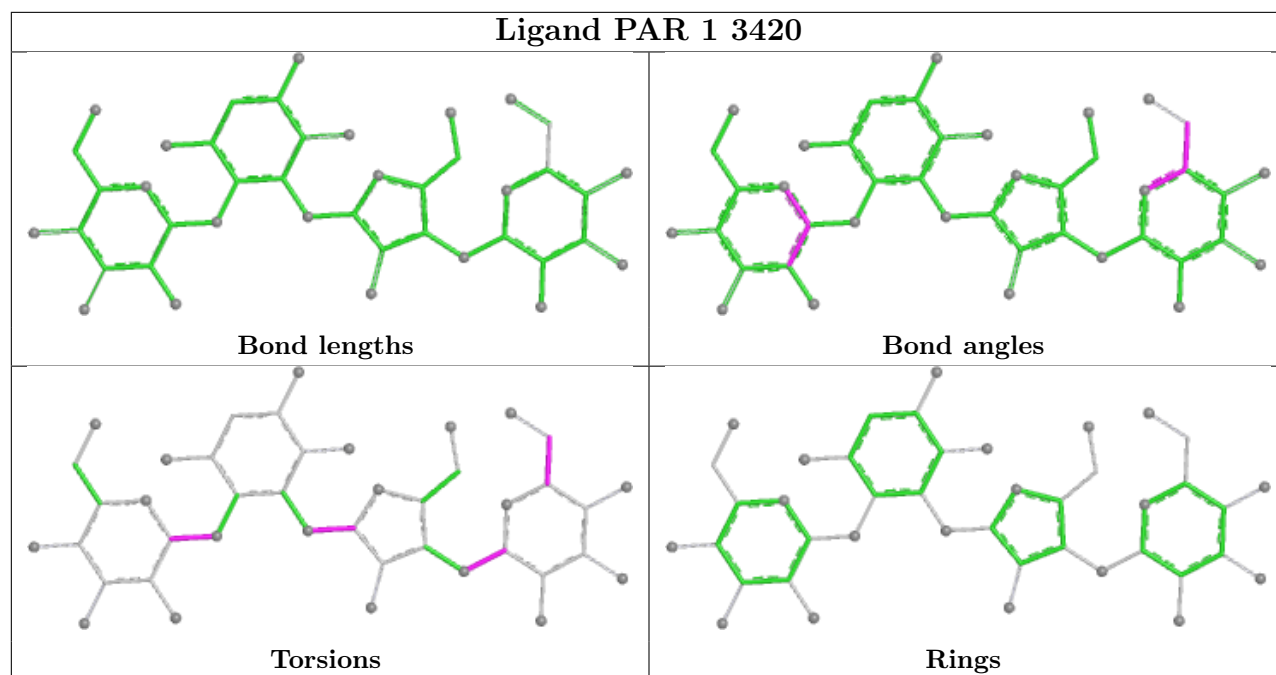
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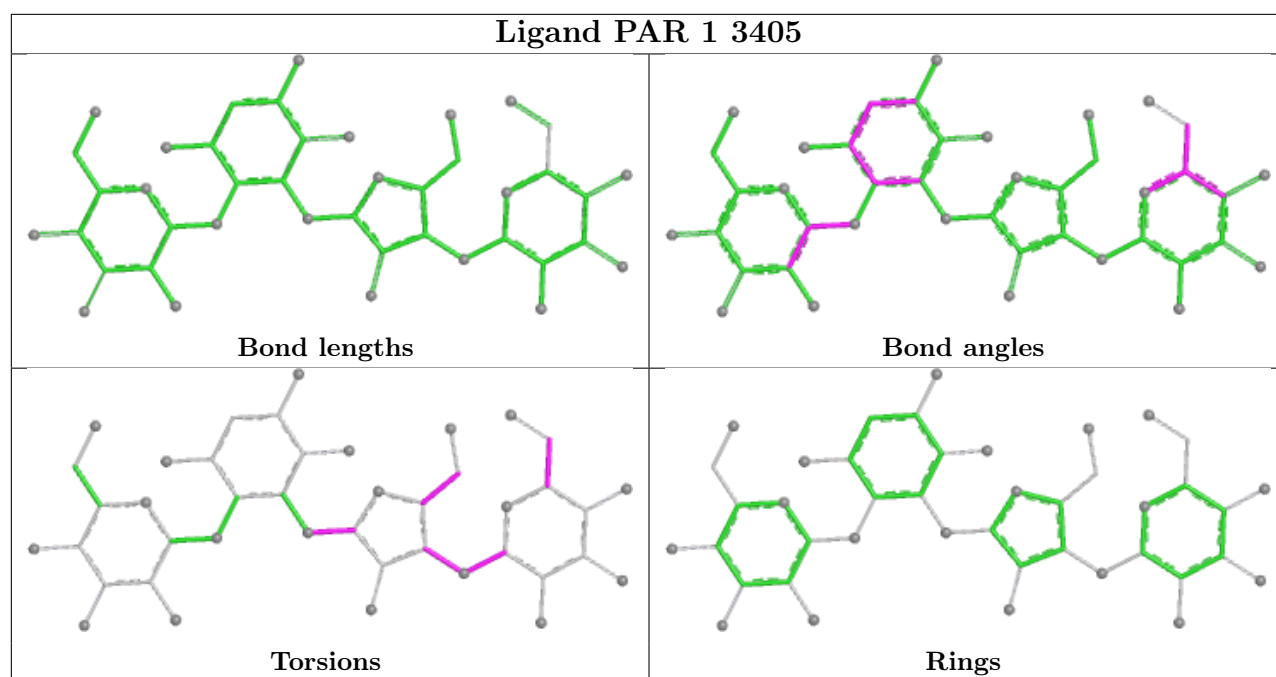
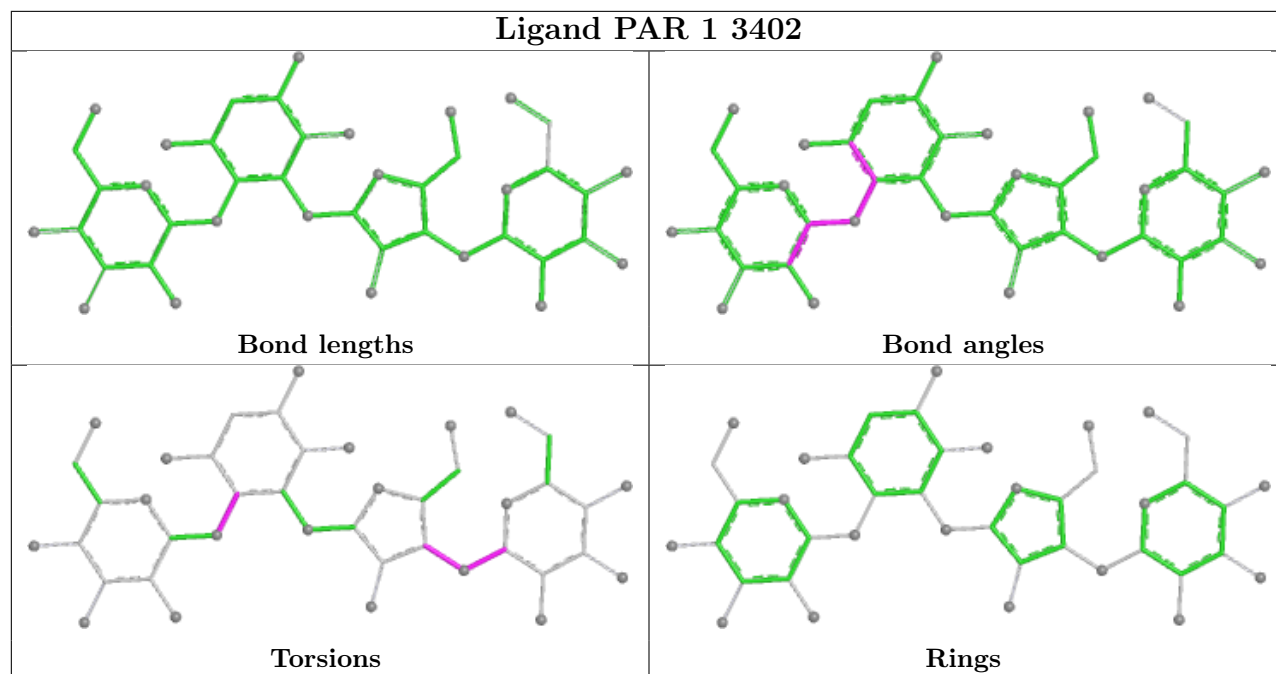


Ligand PAR AS 3407

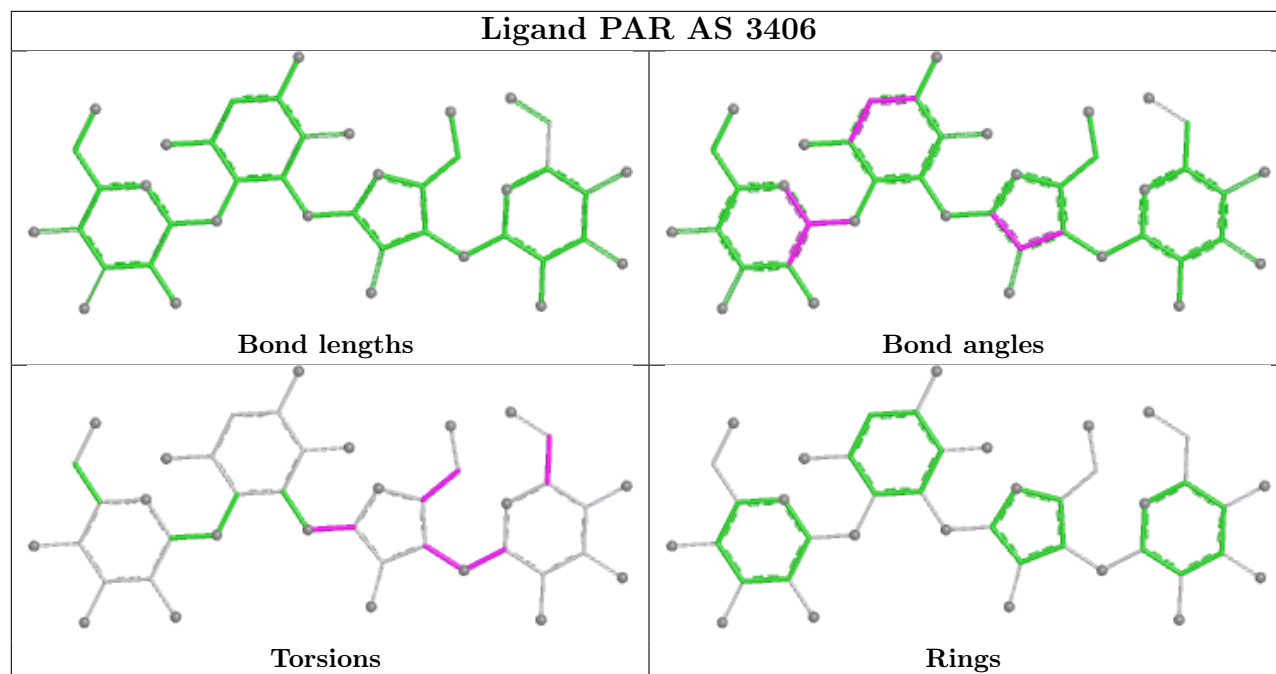


Ligand PAR 1 3420

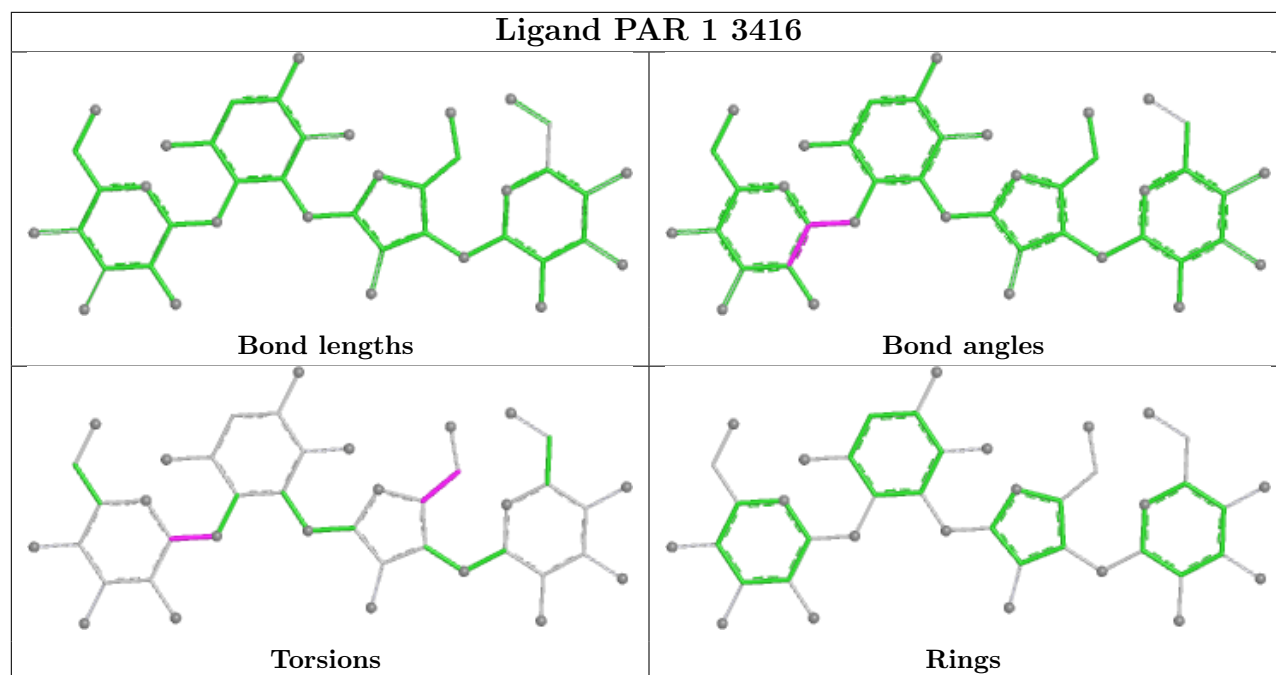


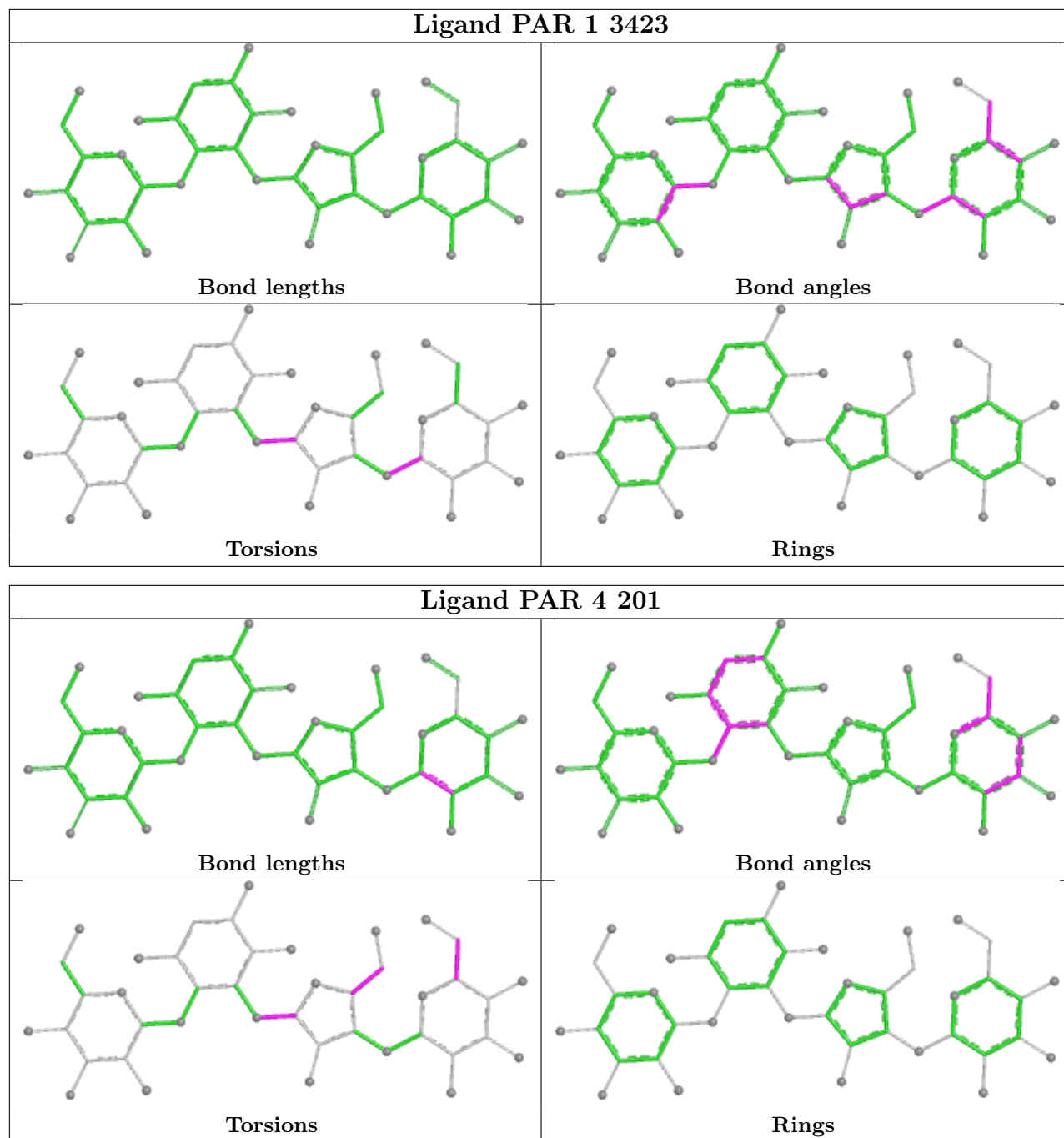


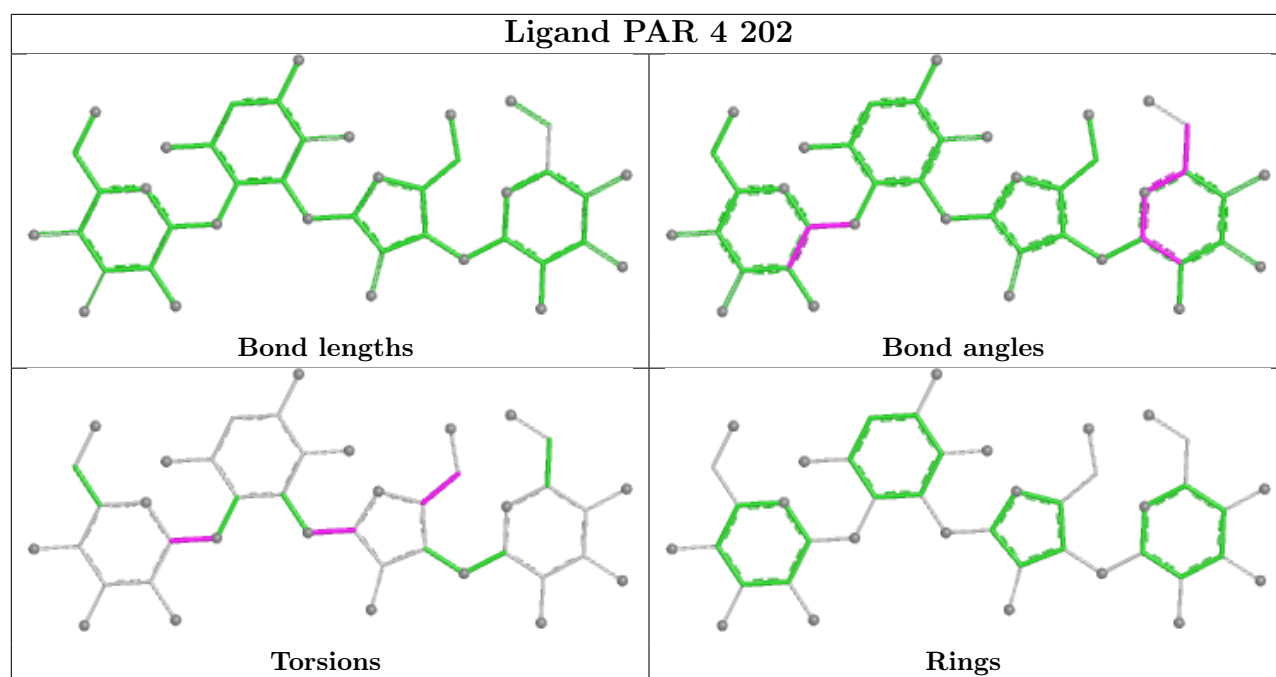
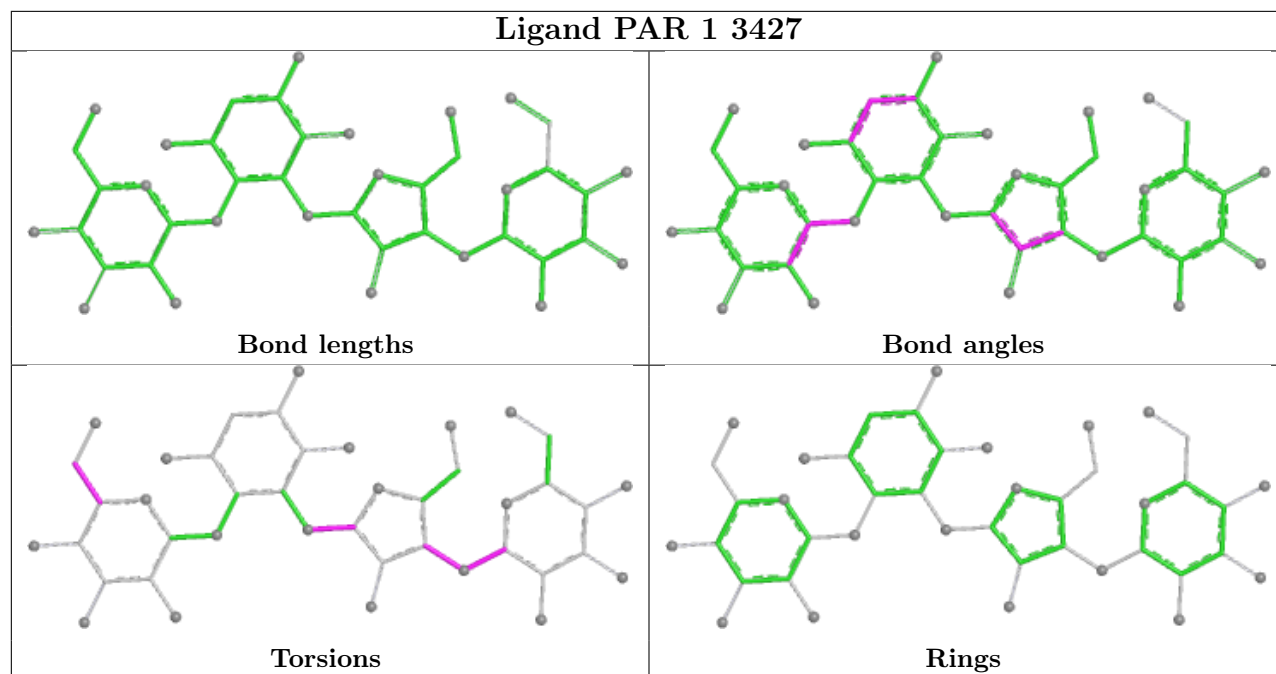
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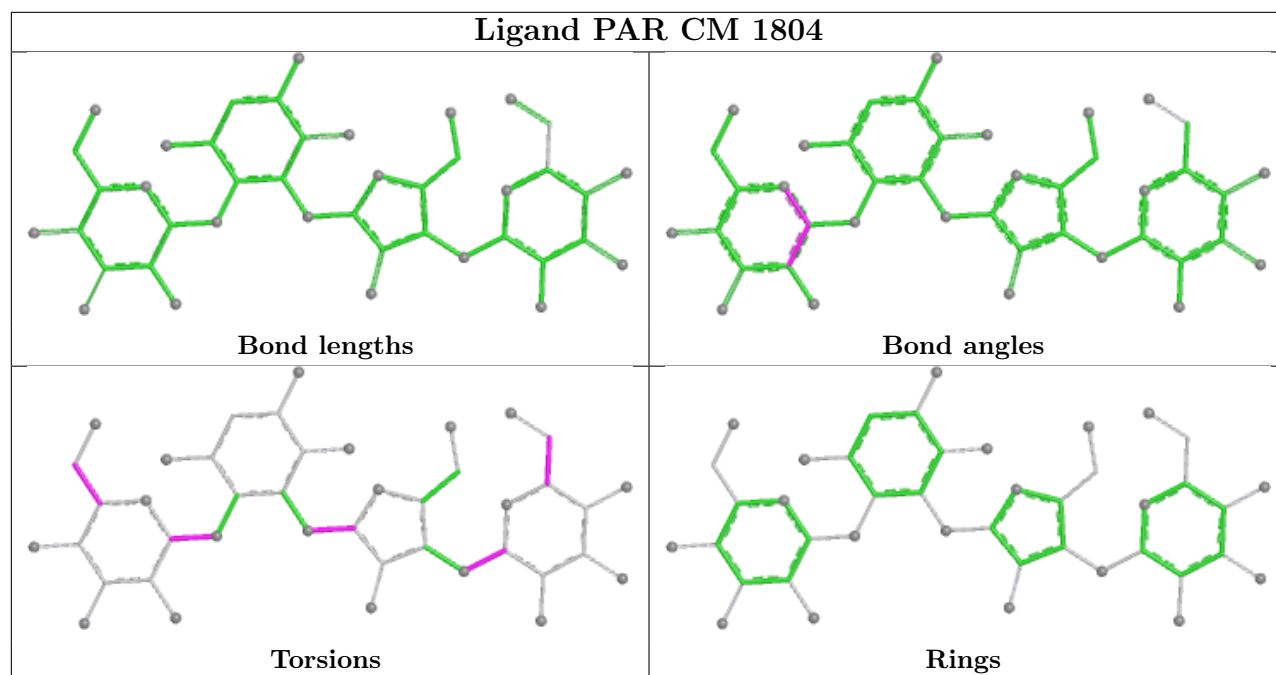
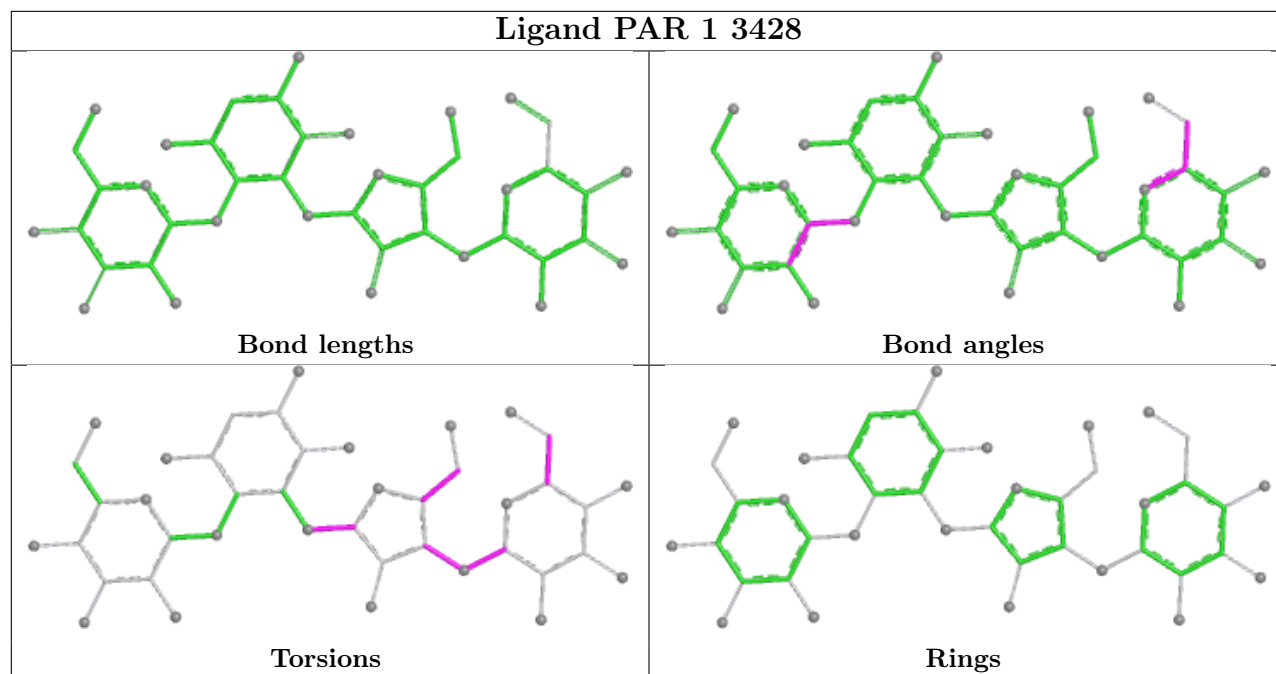


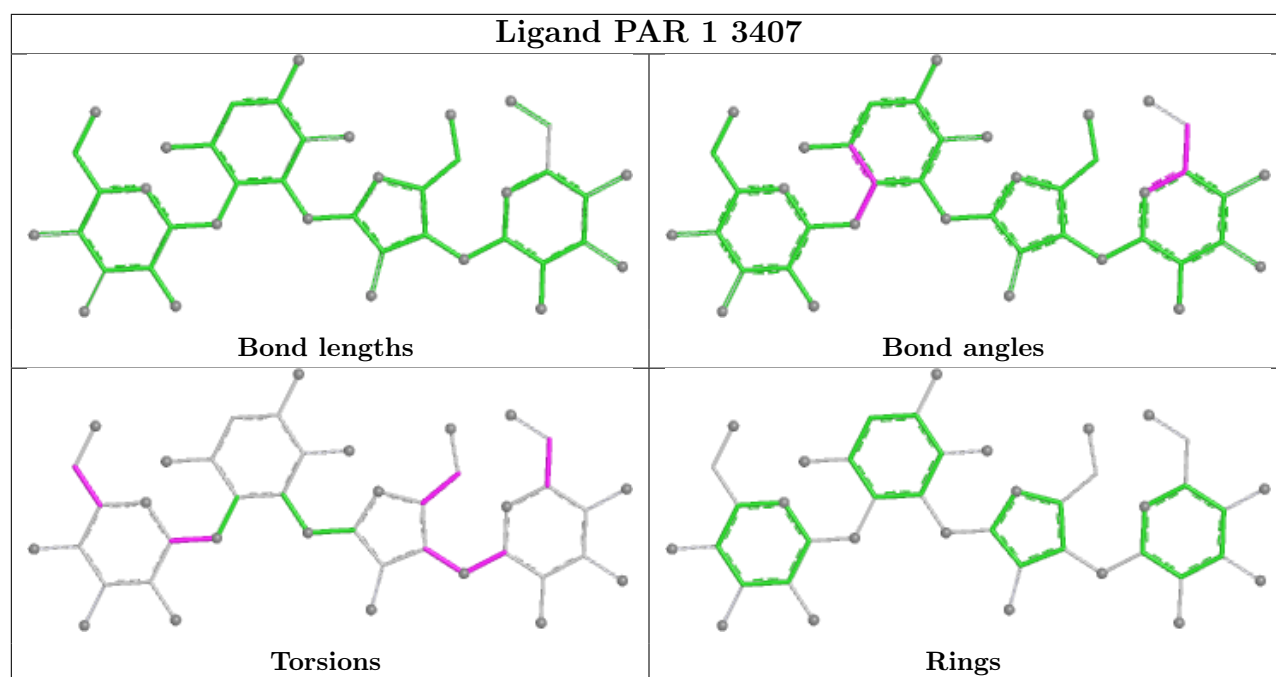
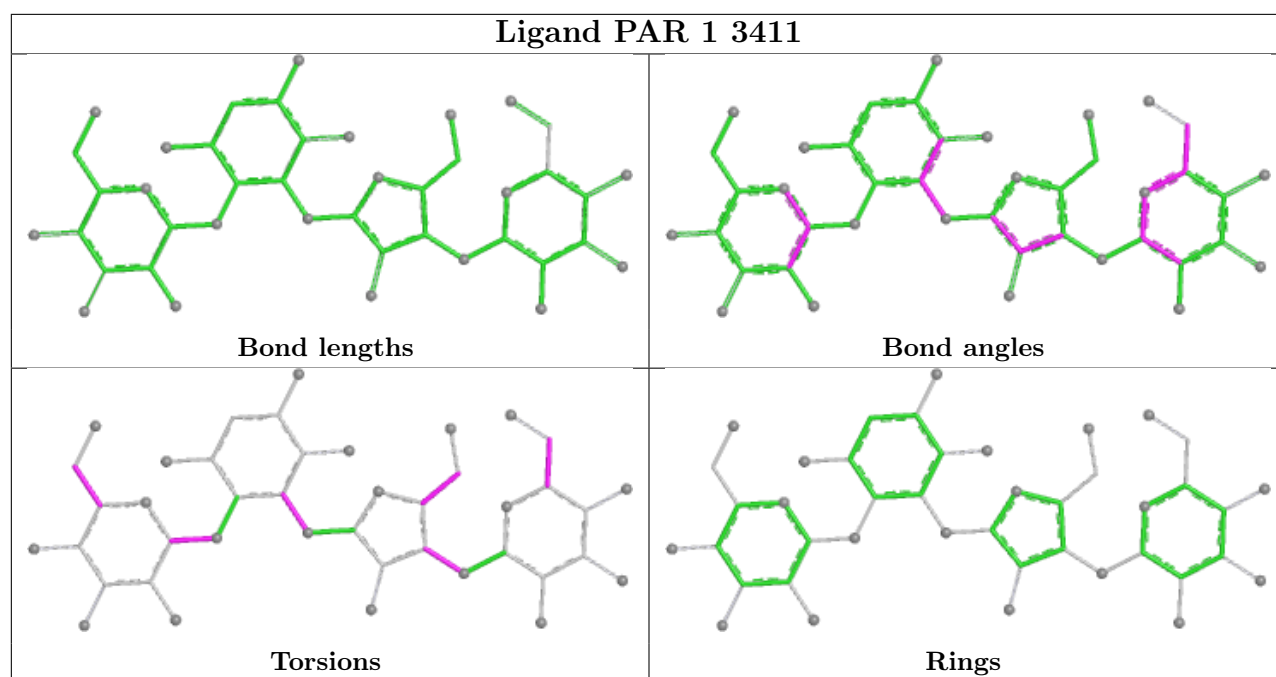
Ligand PAR 1 3416

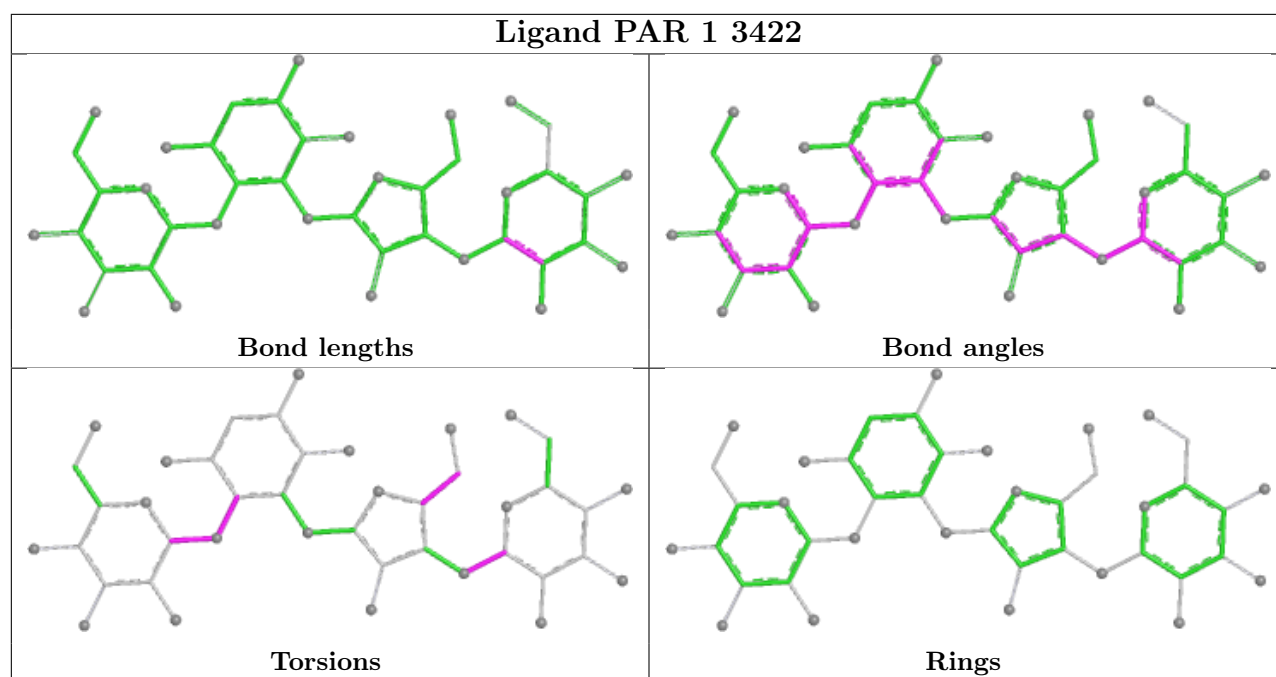
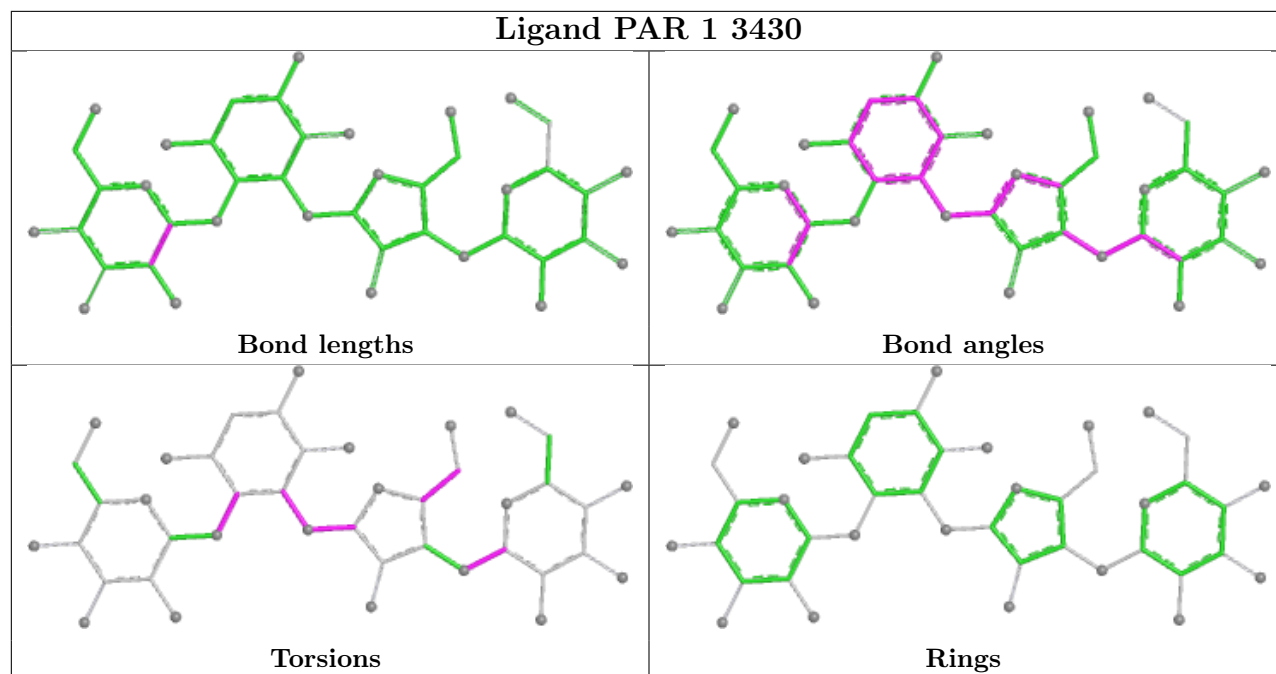




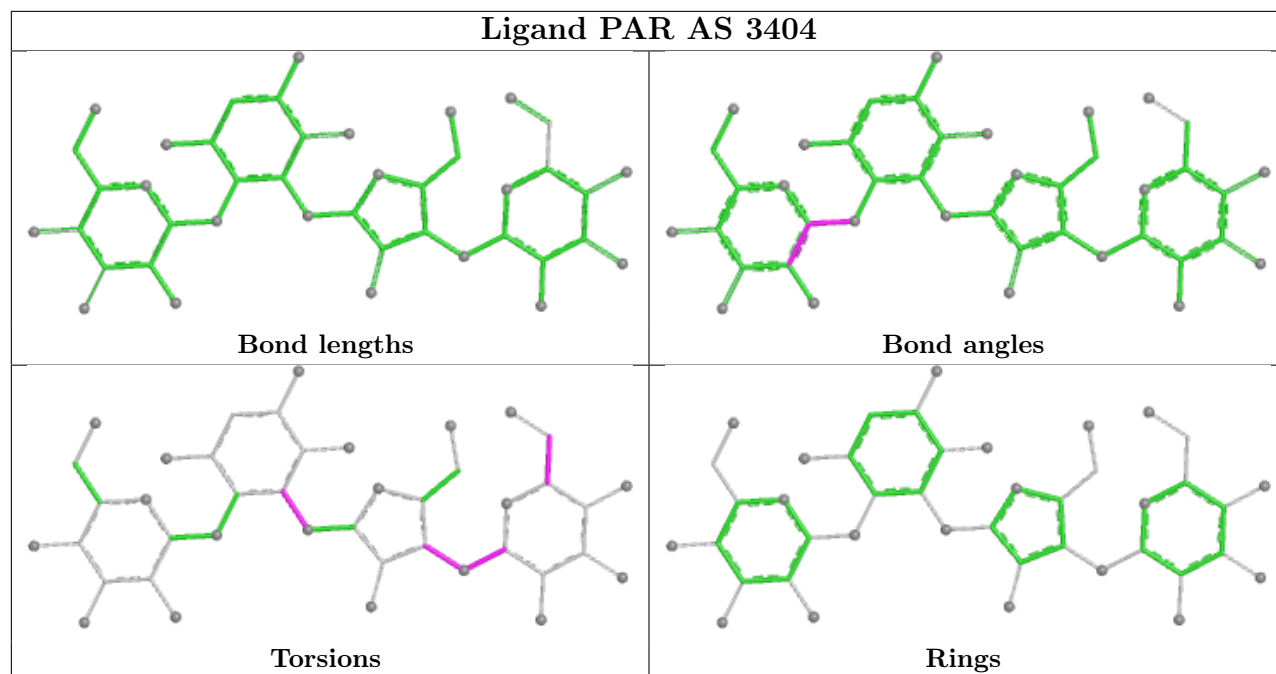




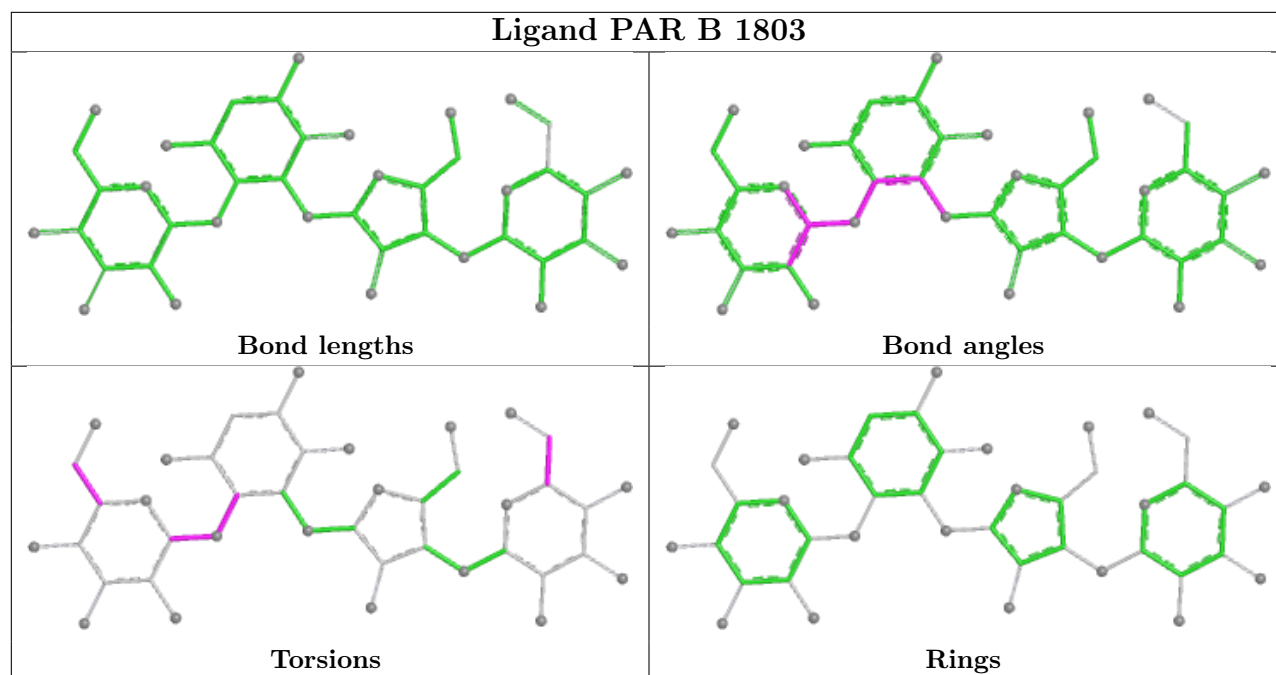


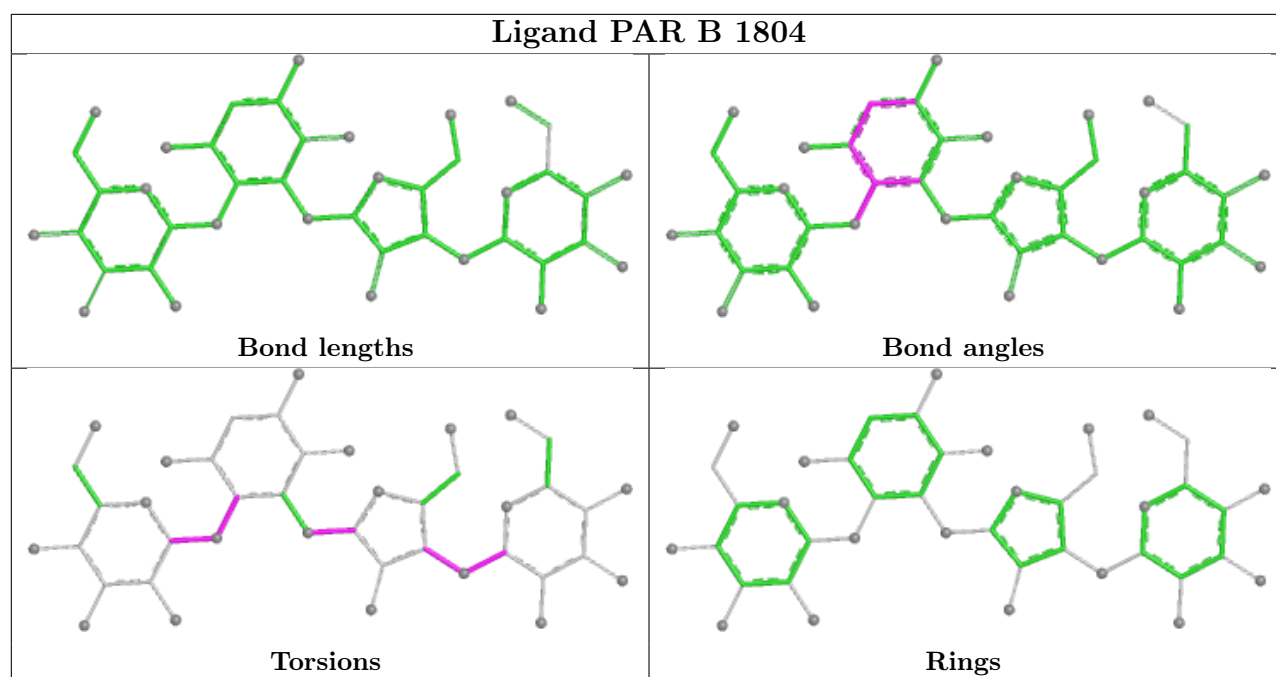
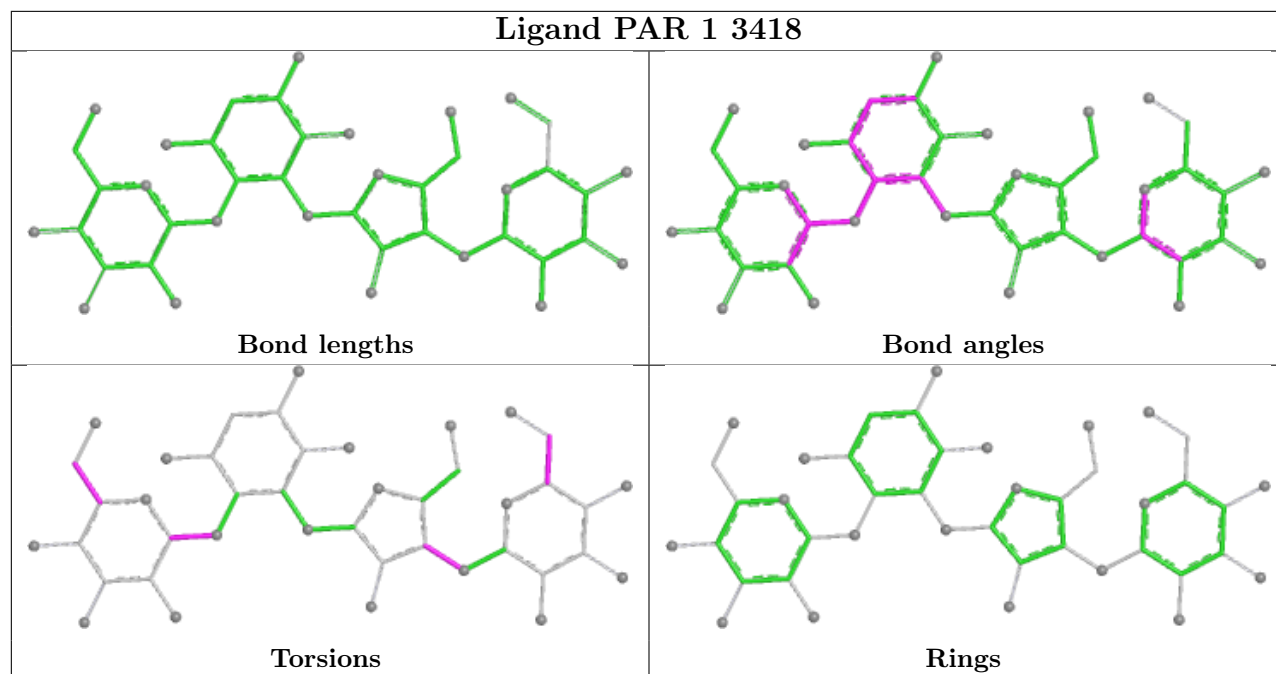


Ligand PAR AS 3404

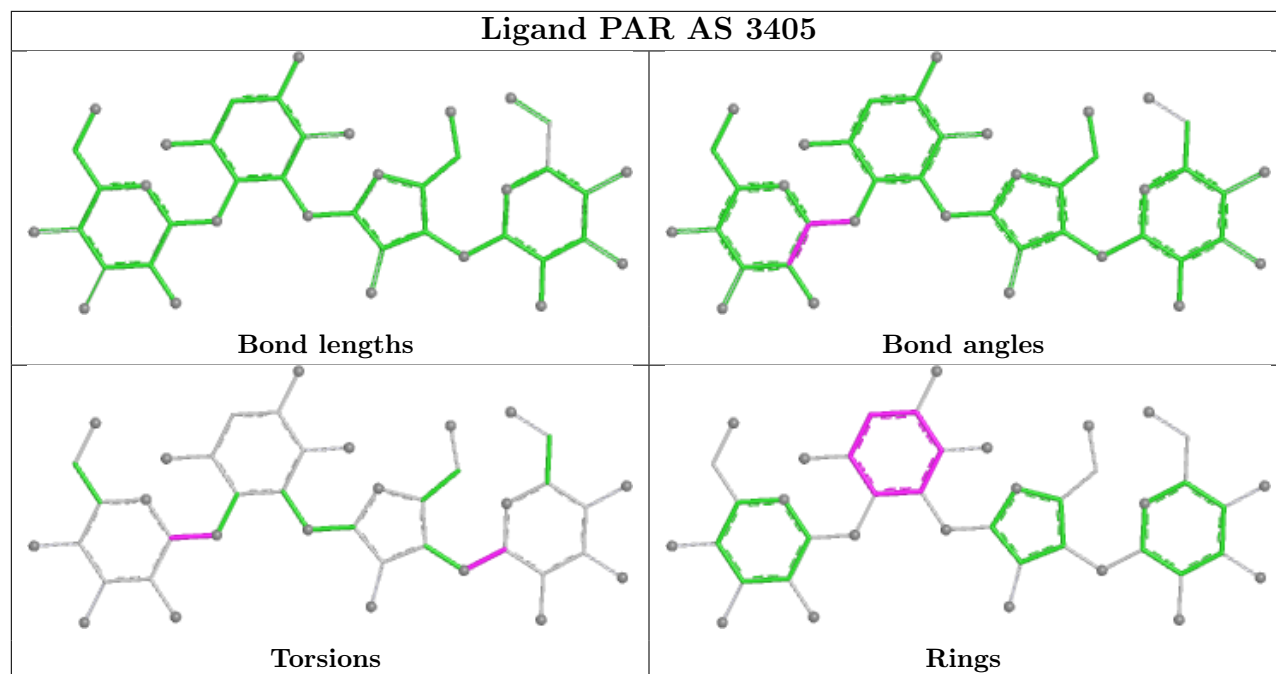


Ligand PAR B 1803

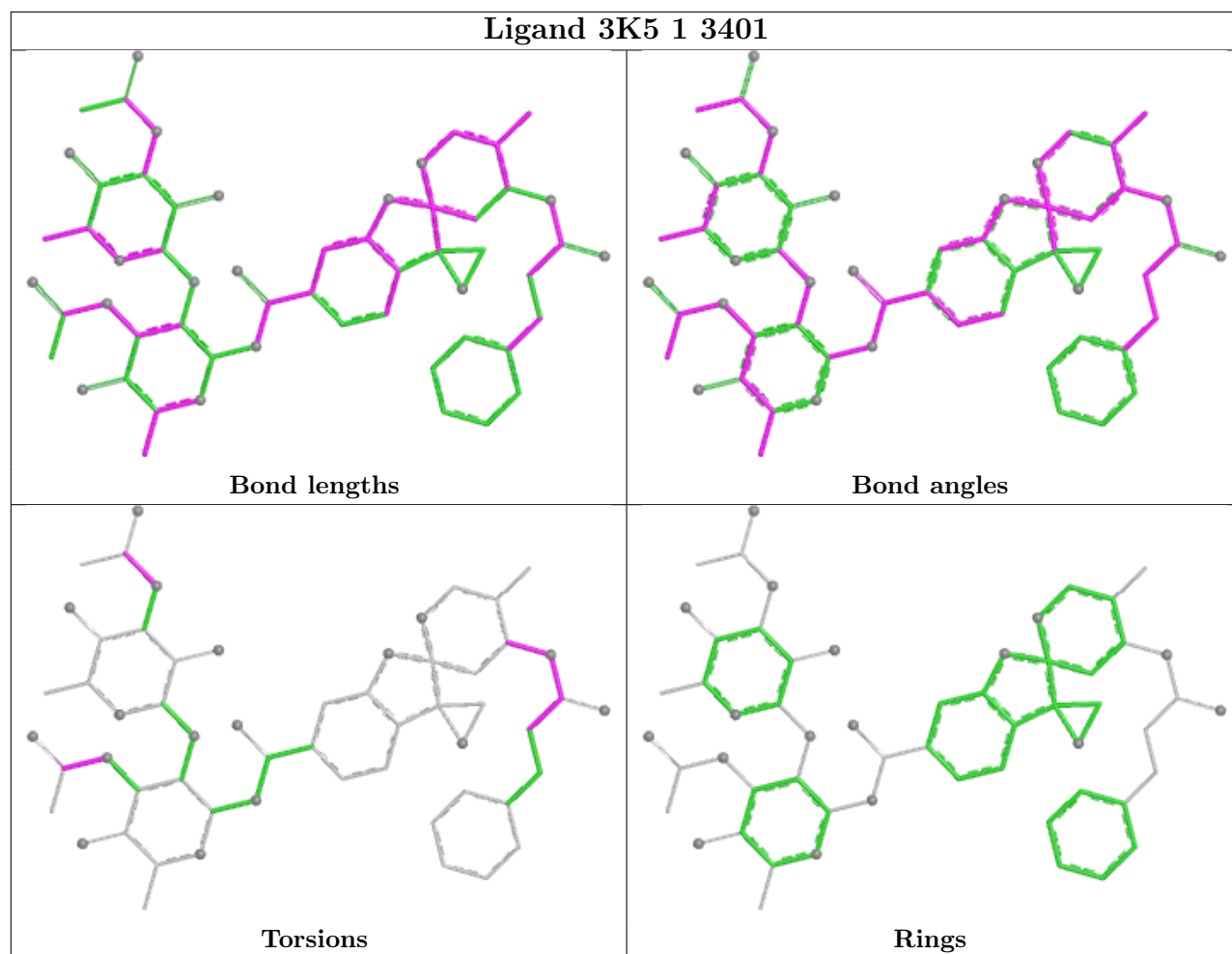


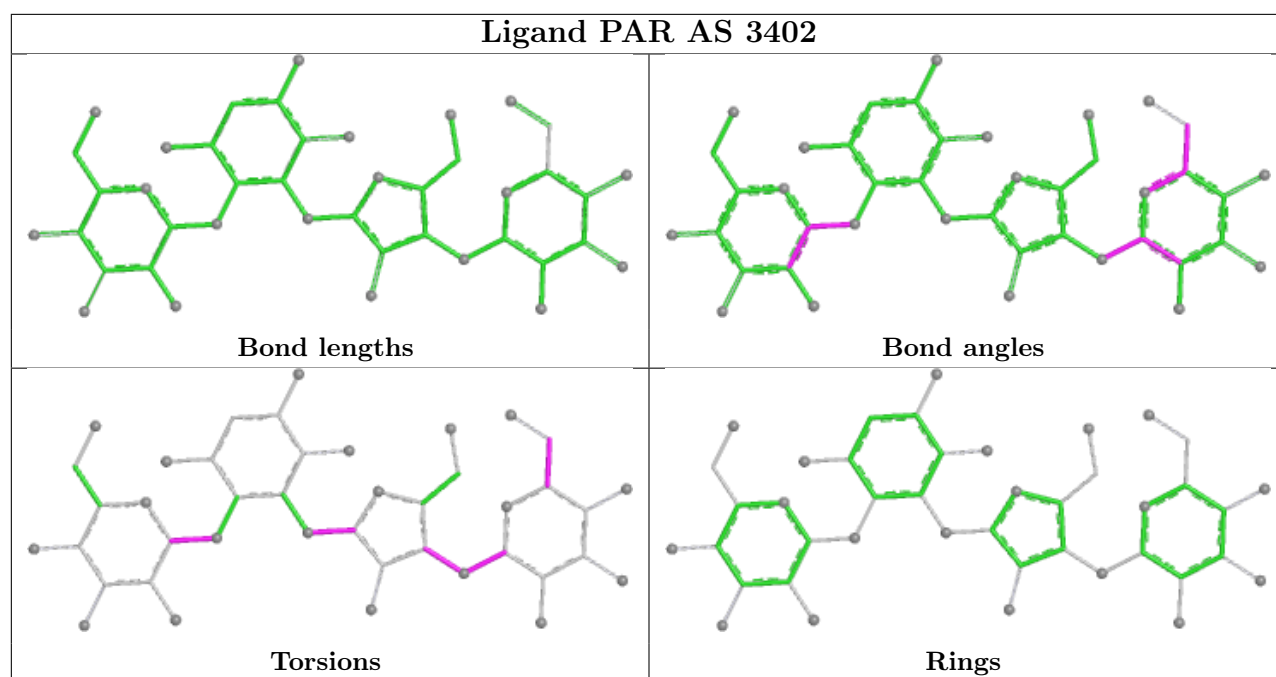
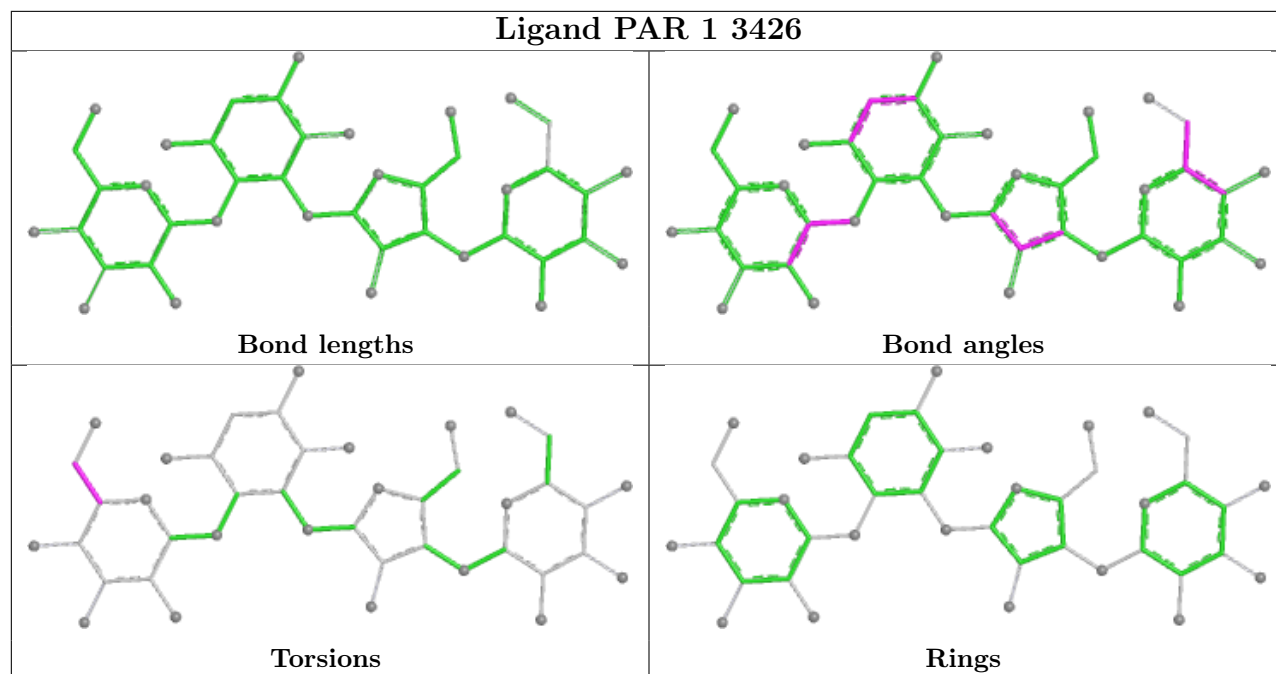


Ligand PAR AS 3405

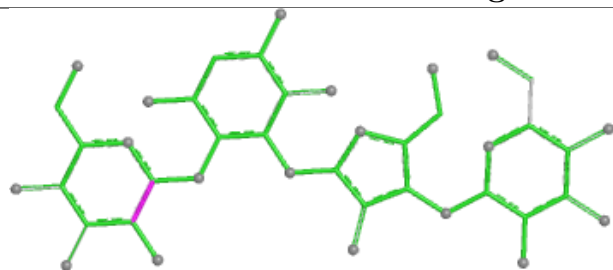


Ligand 3K5 1 3401

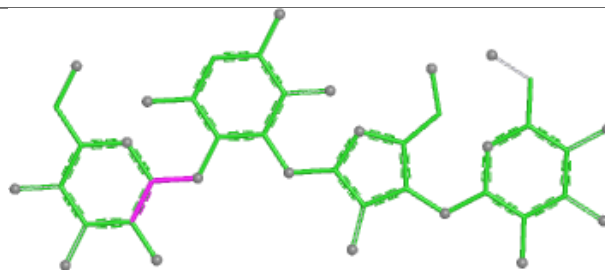




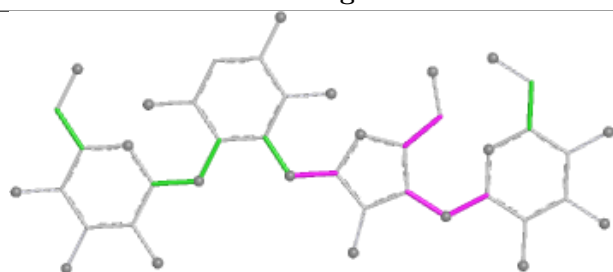
Ligand PAR CM 1806



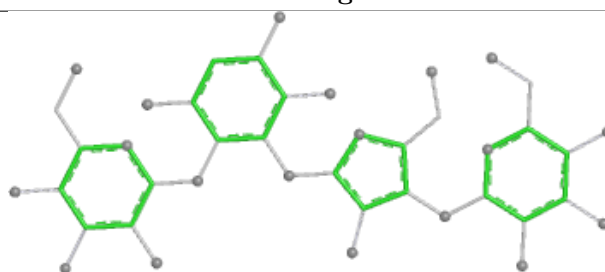
Bond lengths



Bond angles

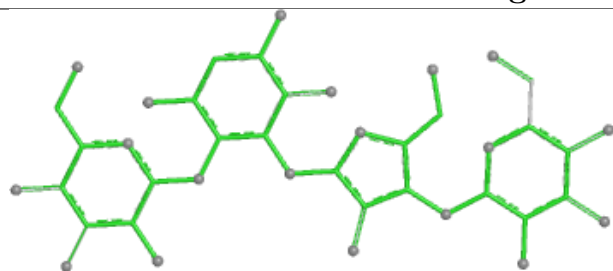


Torsions

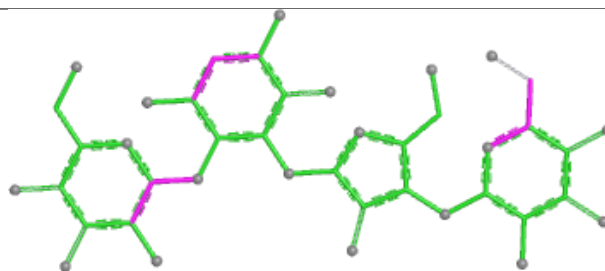


Rings

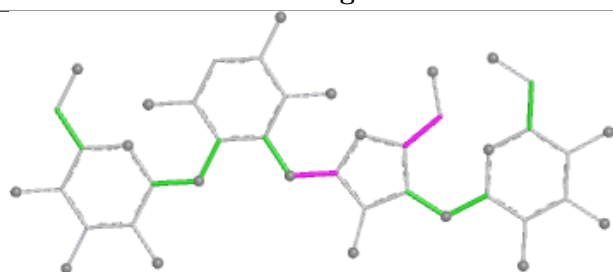
Ligand PAR 1 3429



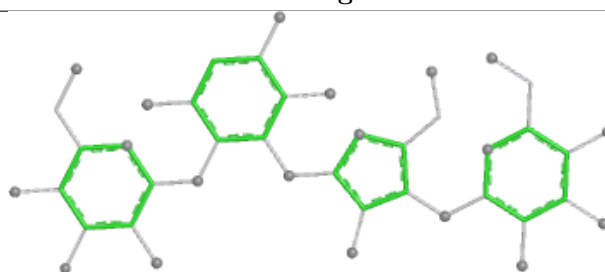
Bond lengths



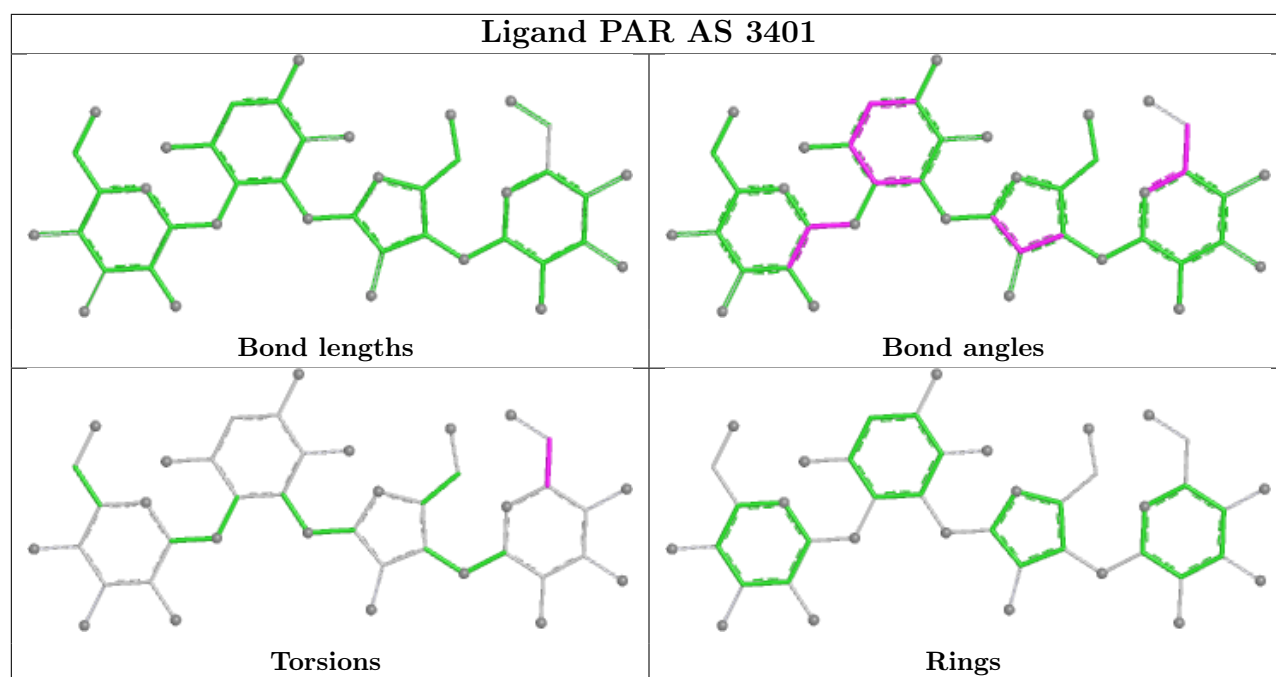
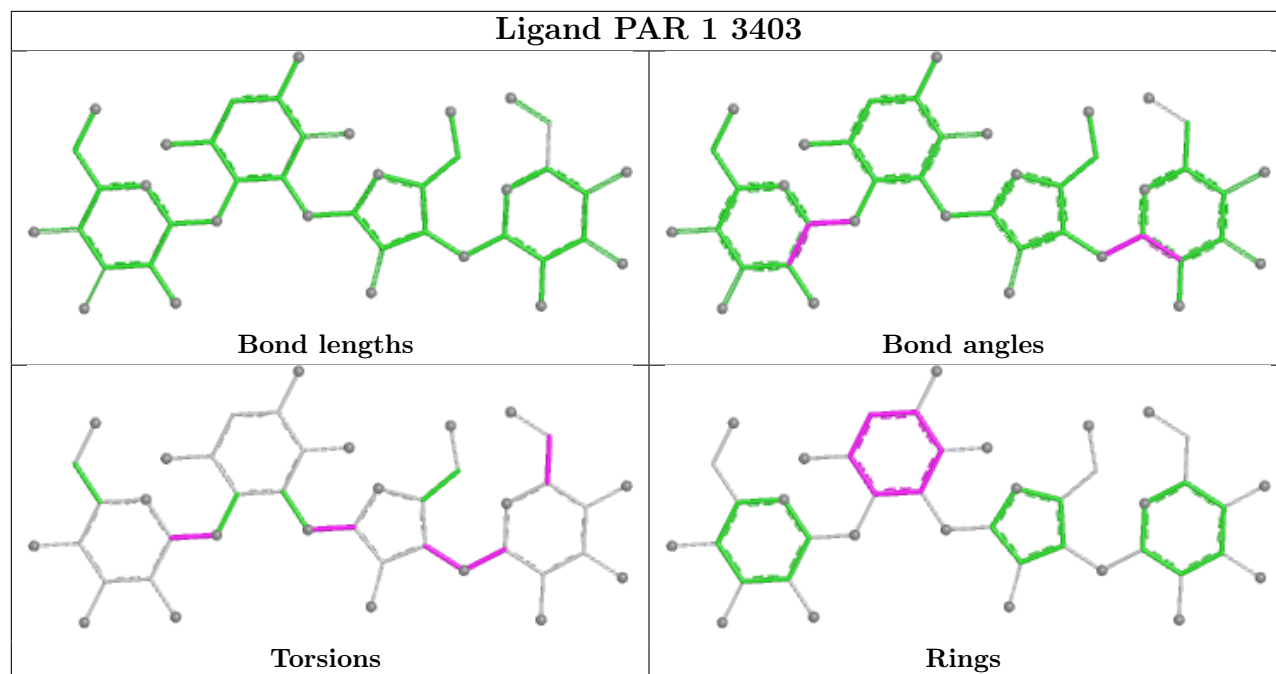
Bond angles

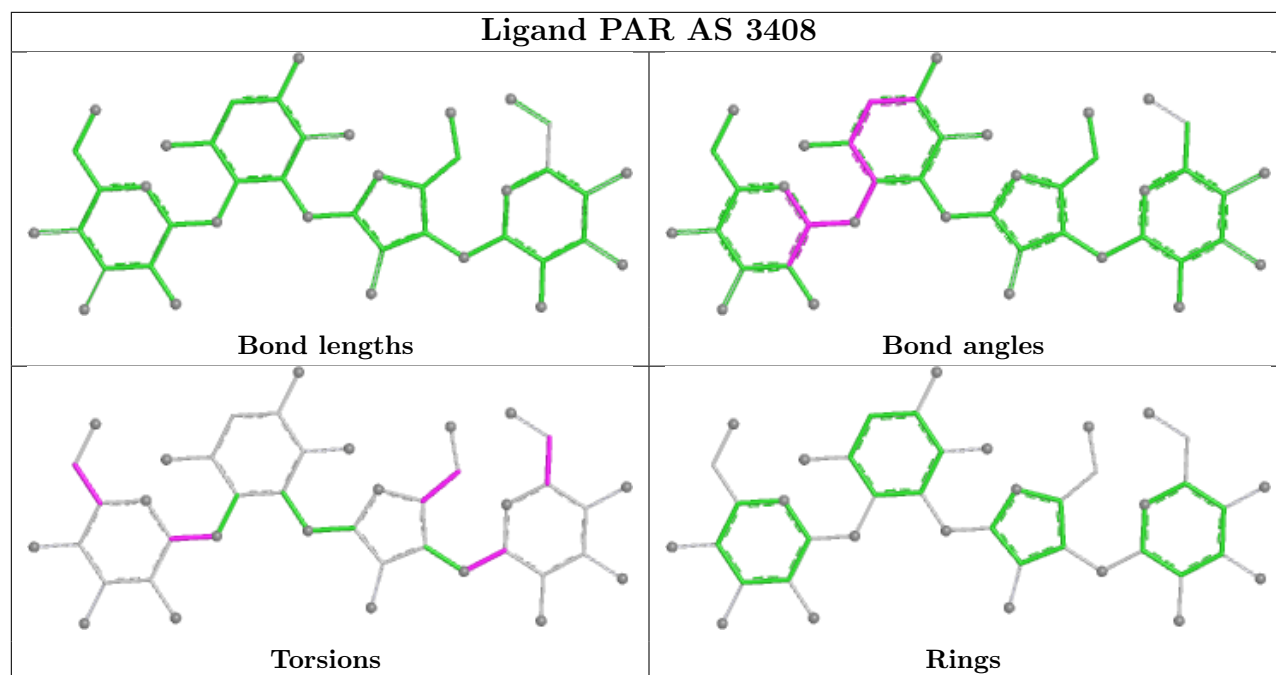
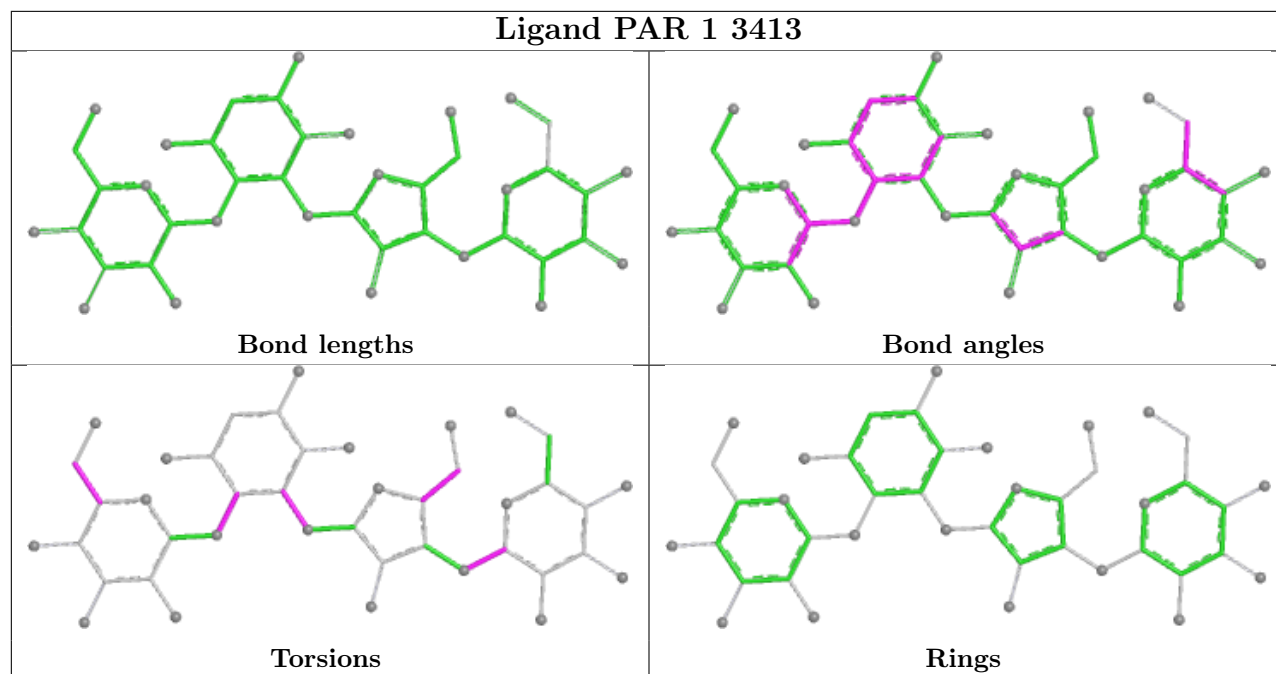


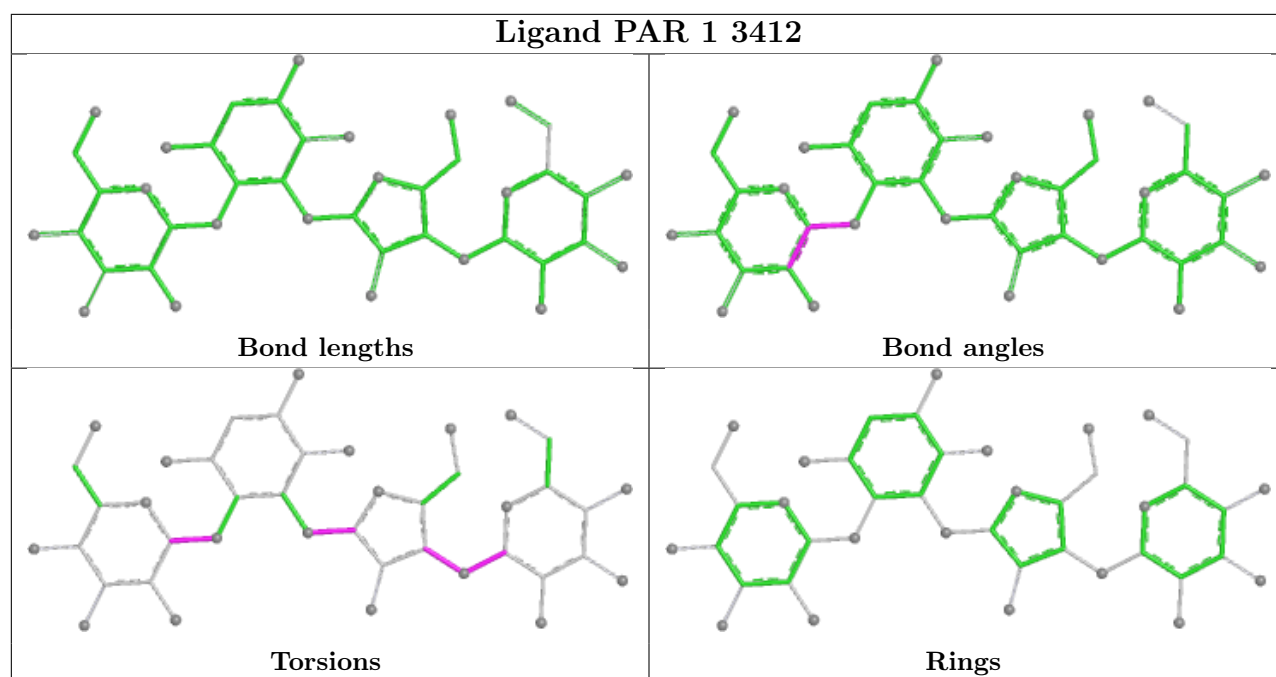
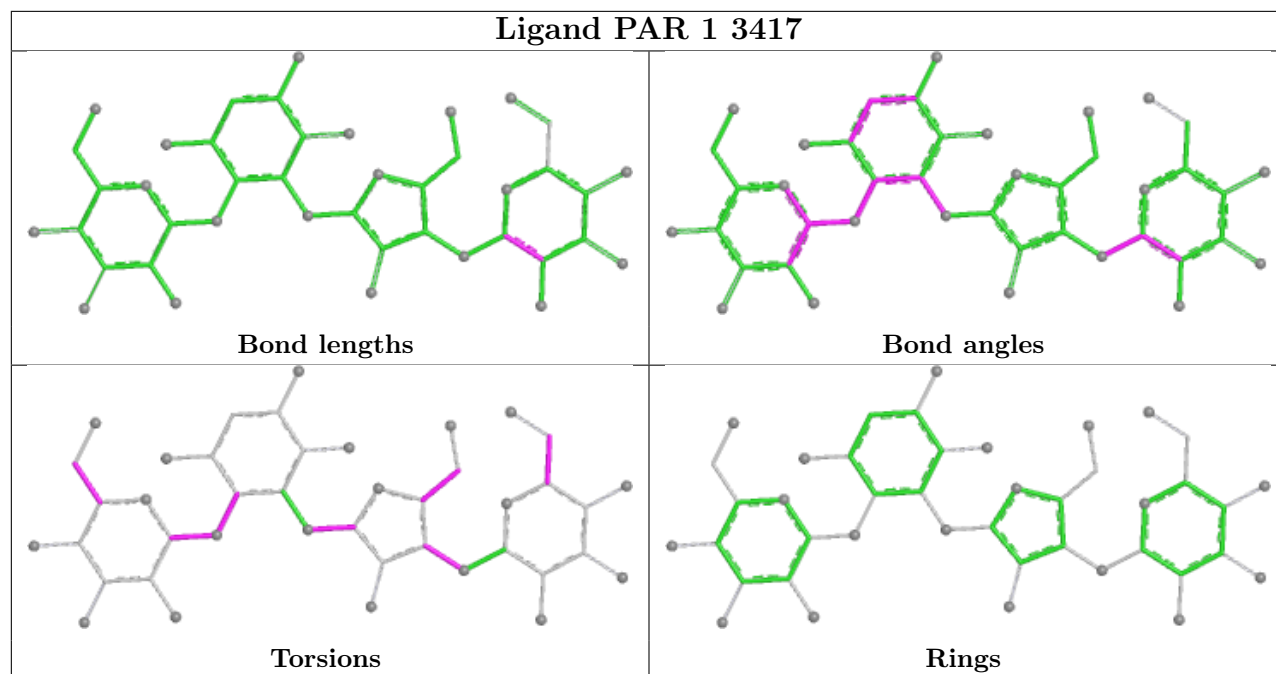
Torsions



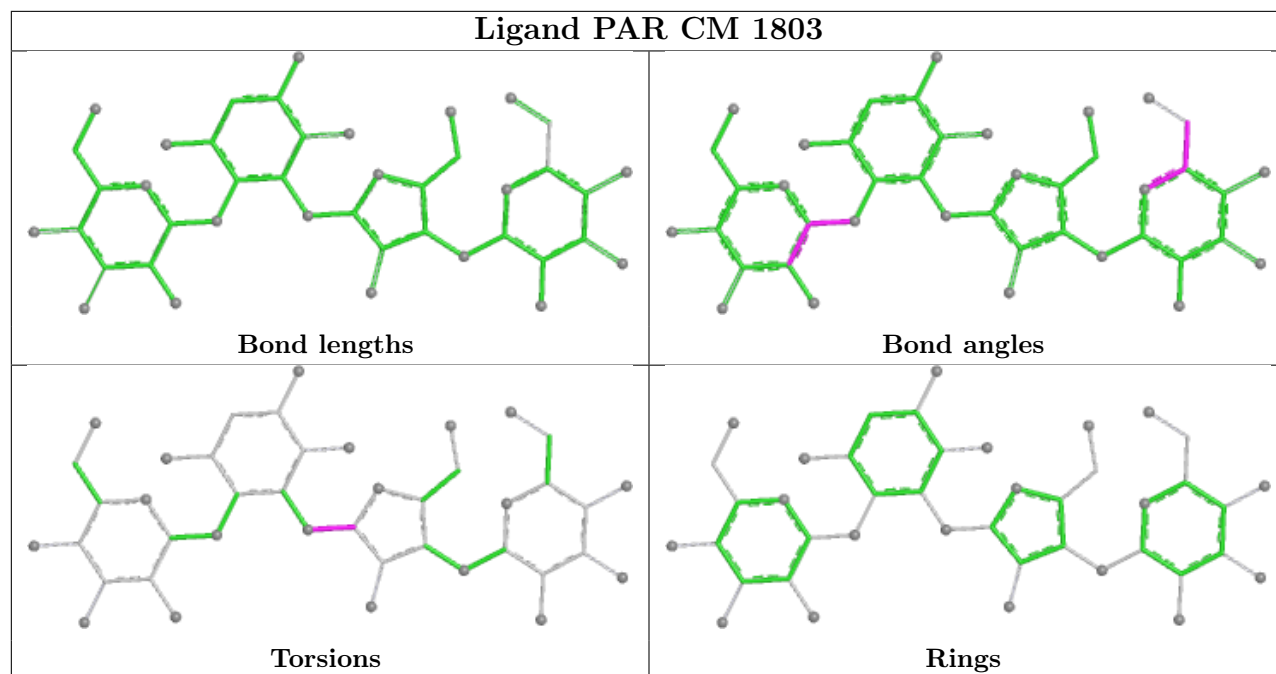
Rings



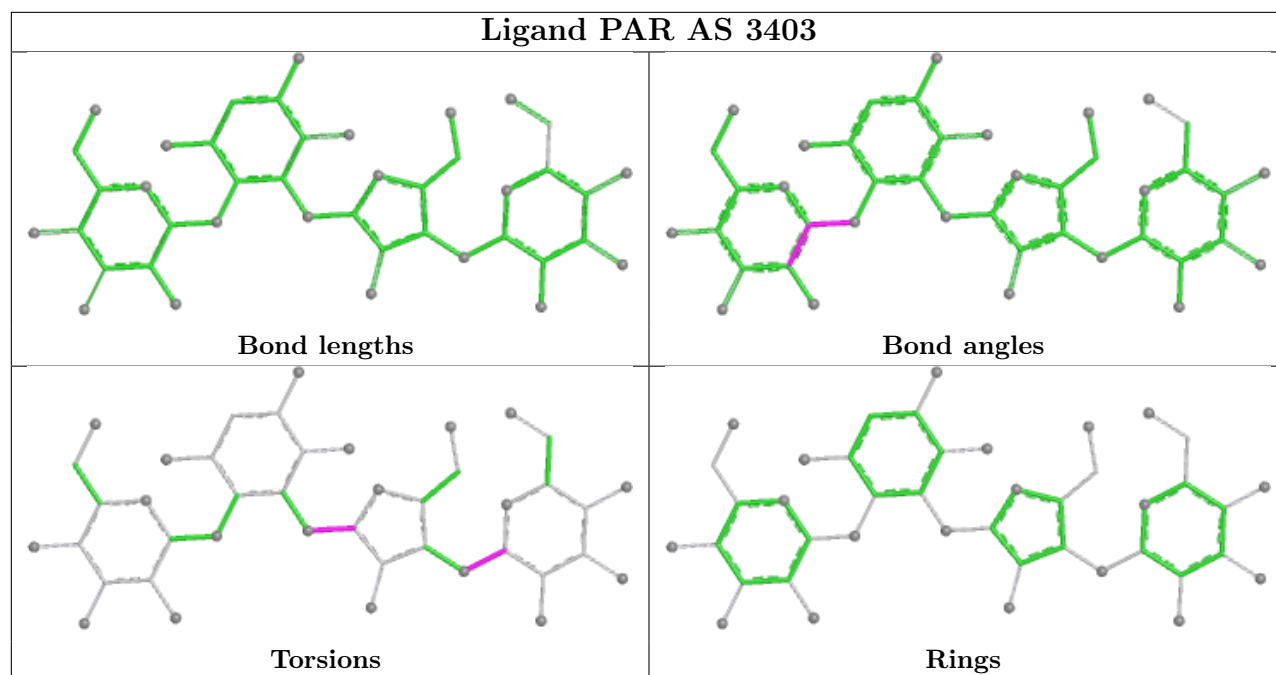


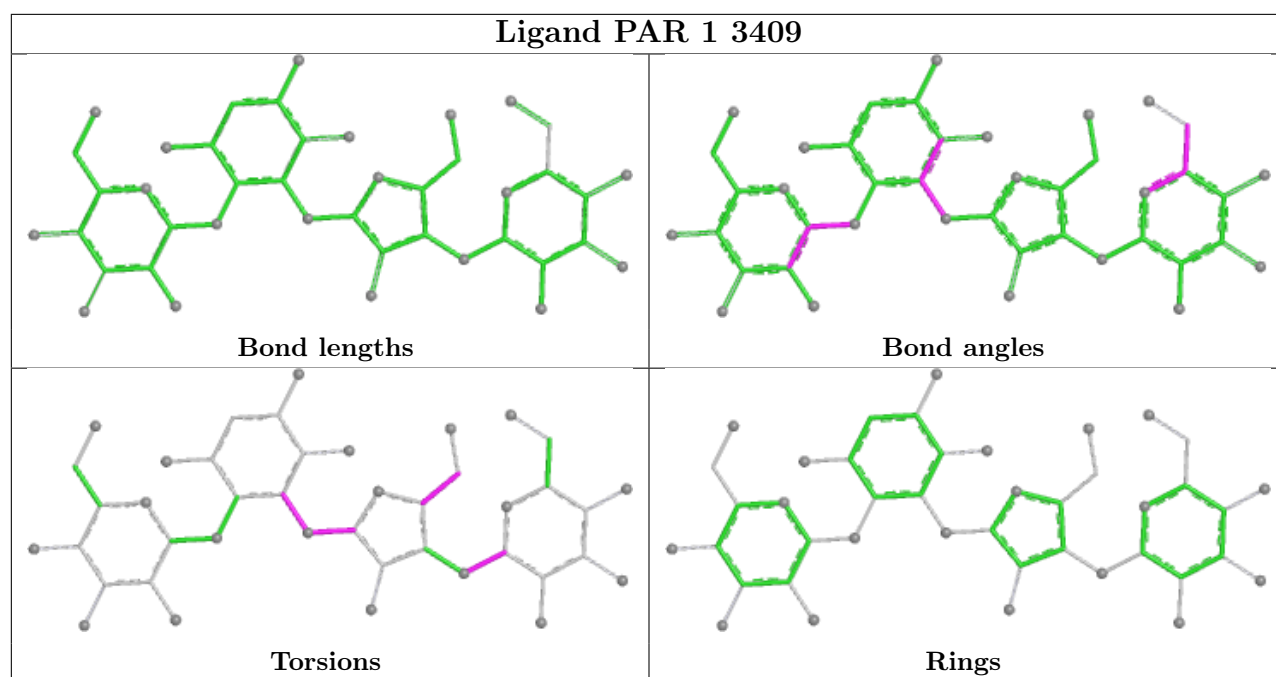
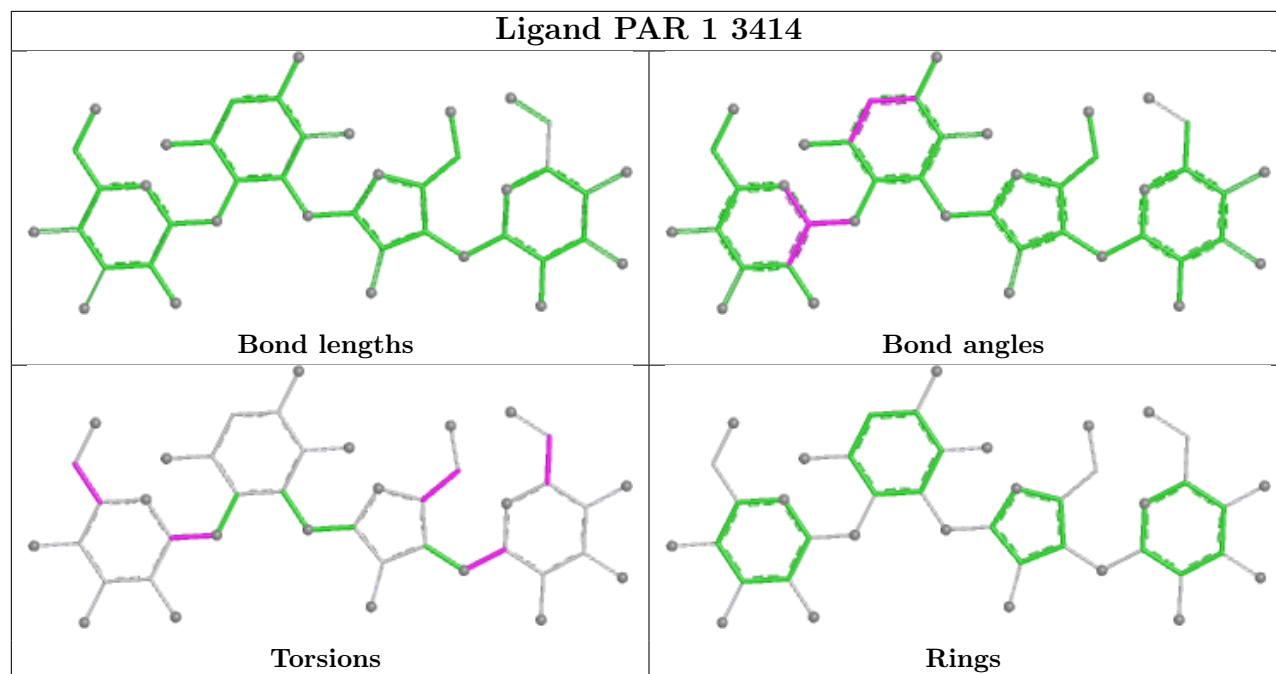


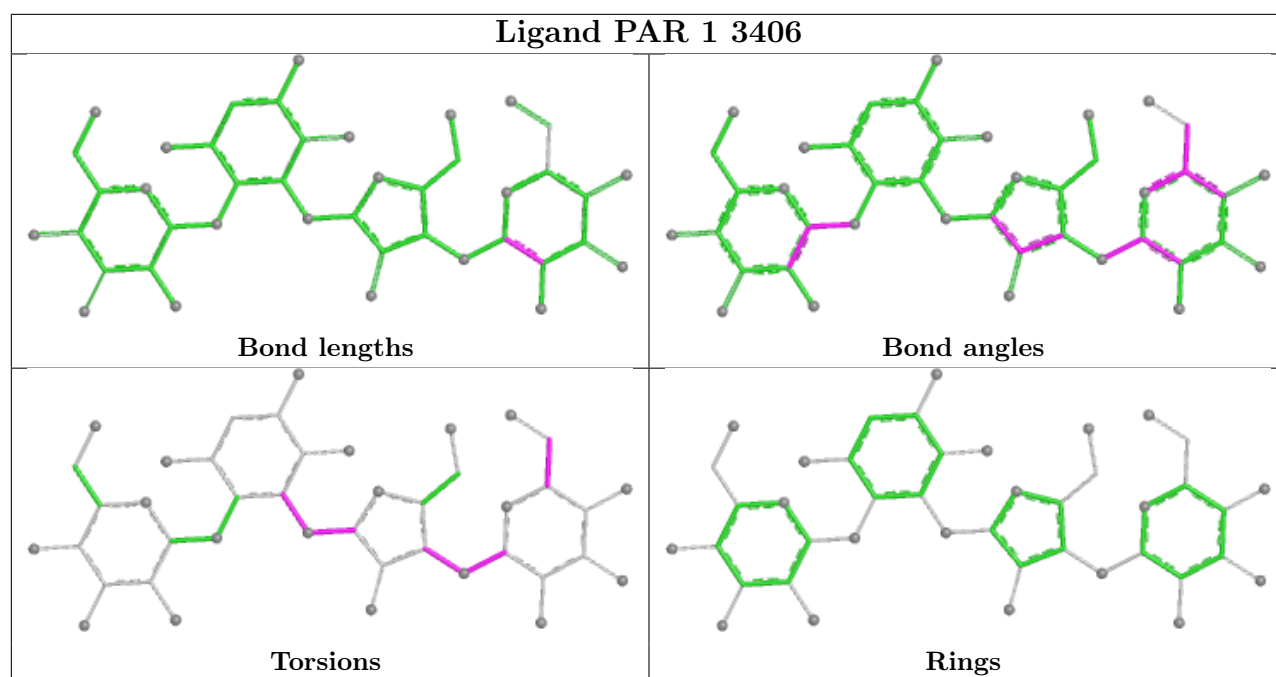
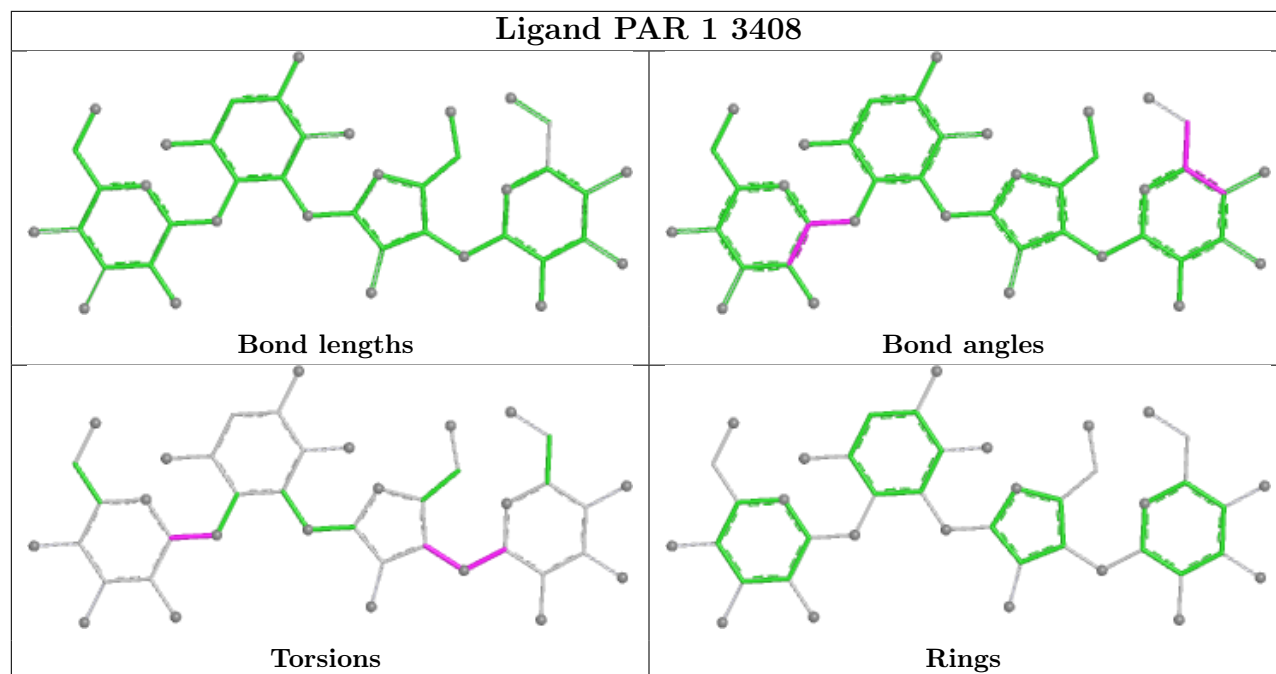
Ligand PAR CM 1803



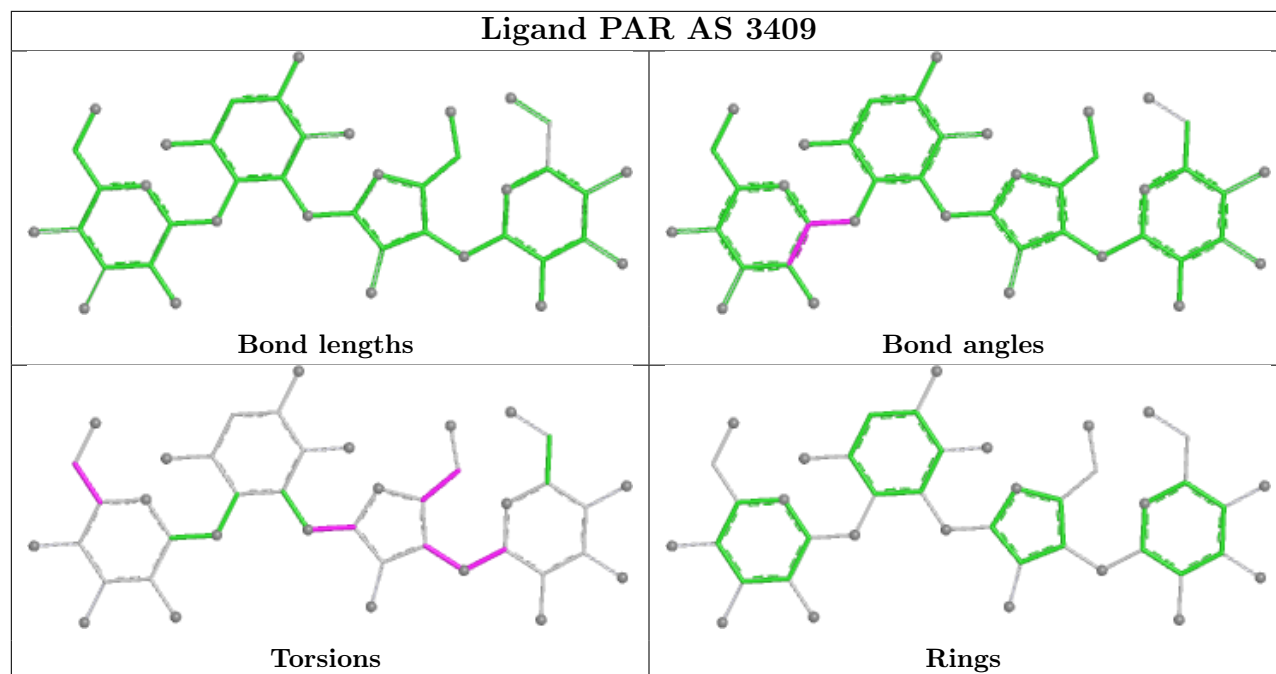
Ligand PAR AS 3403



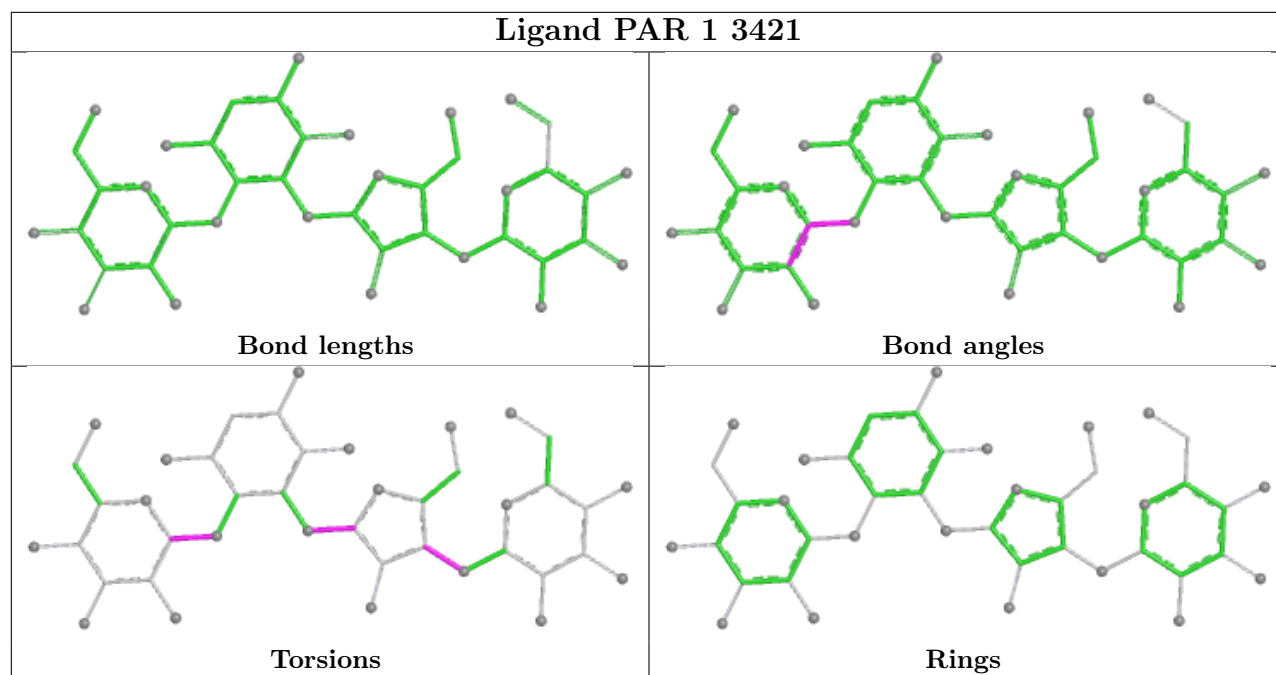




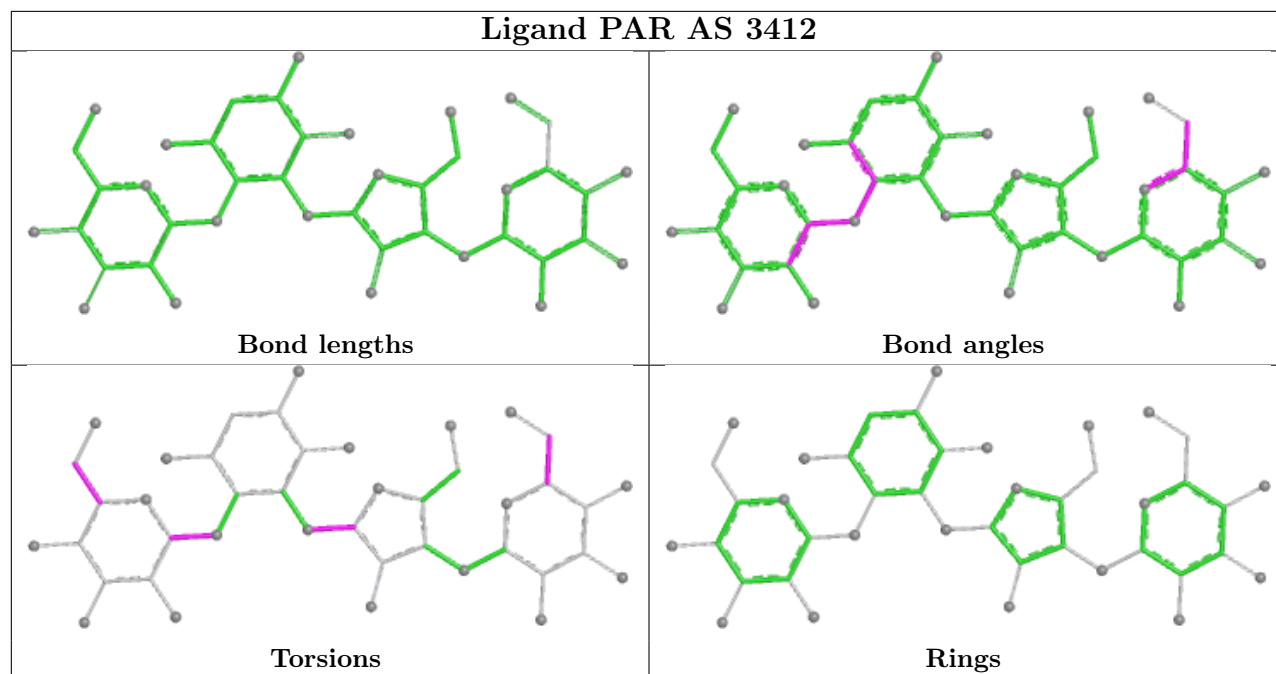
Ligand PAR AS 3409



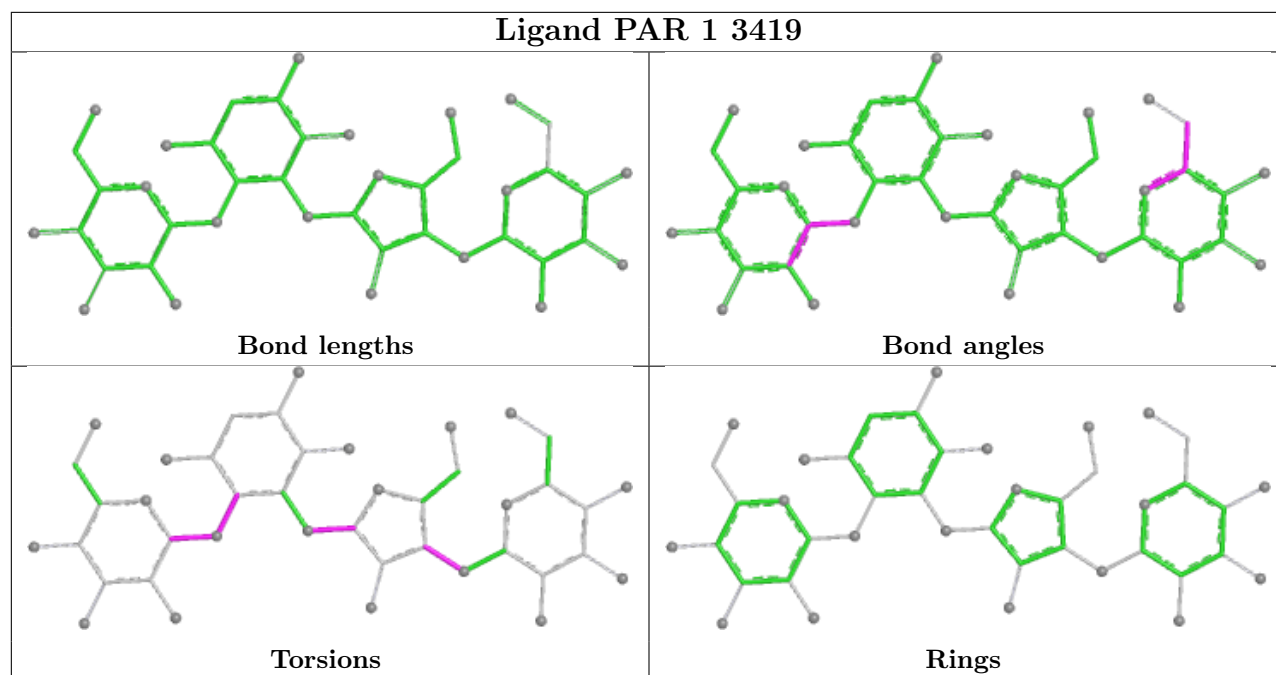
Ligand PAR 1 3421



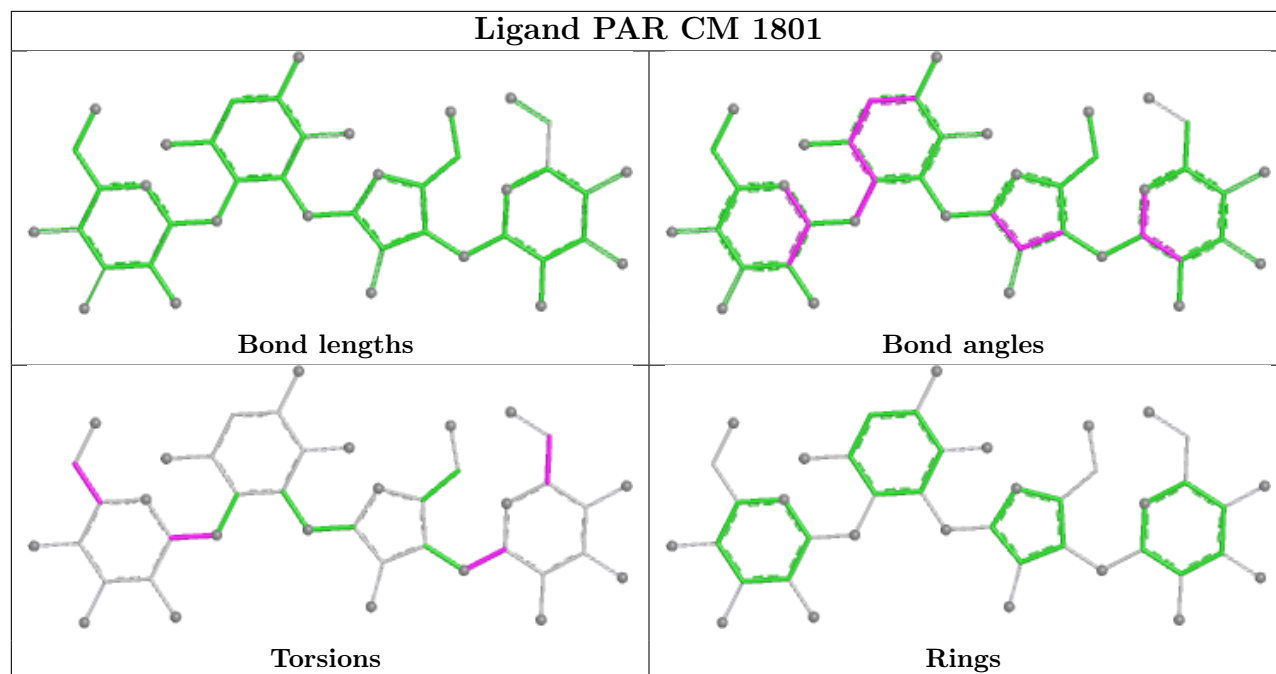
Ligand PAR AS 3412



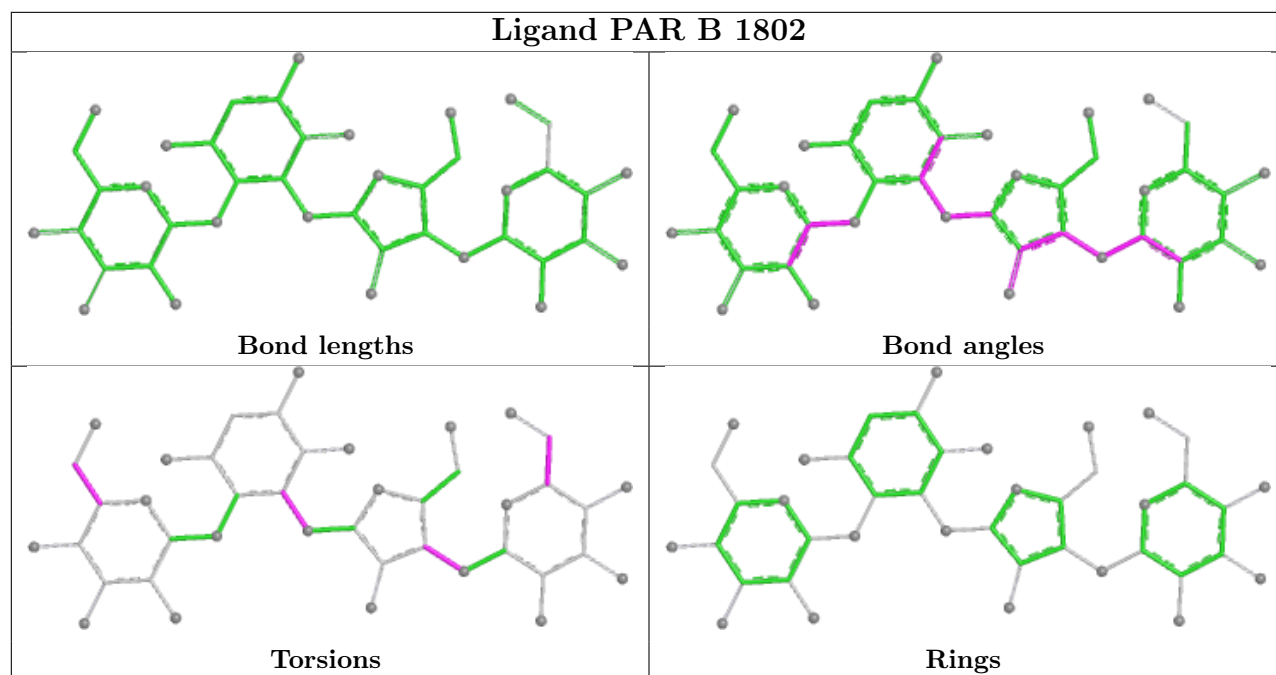
Ligand PAR 1 3419



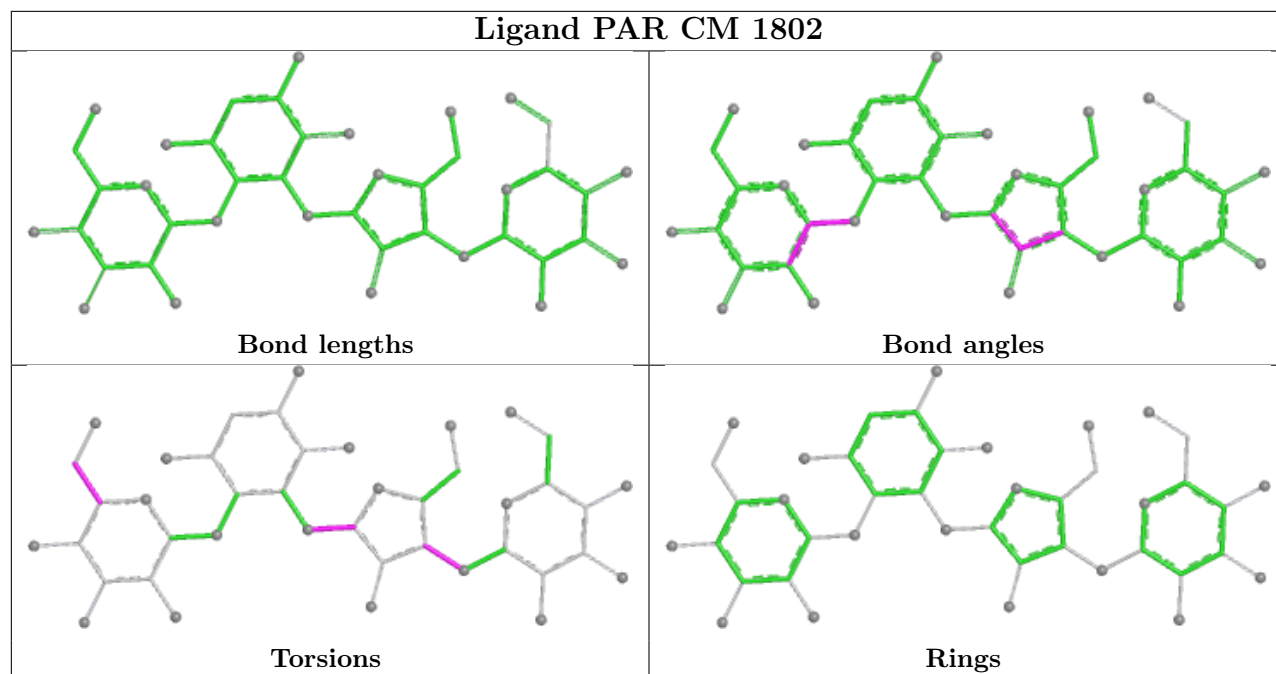
Ligand PAR CM 1801



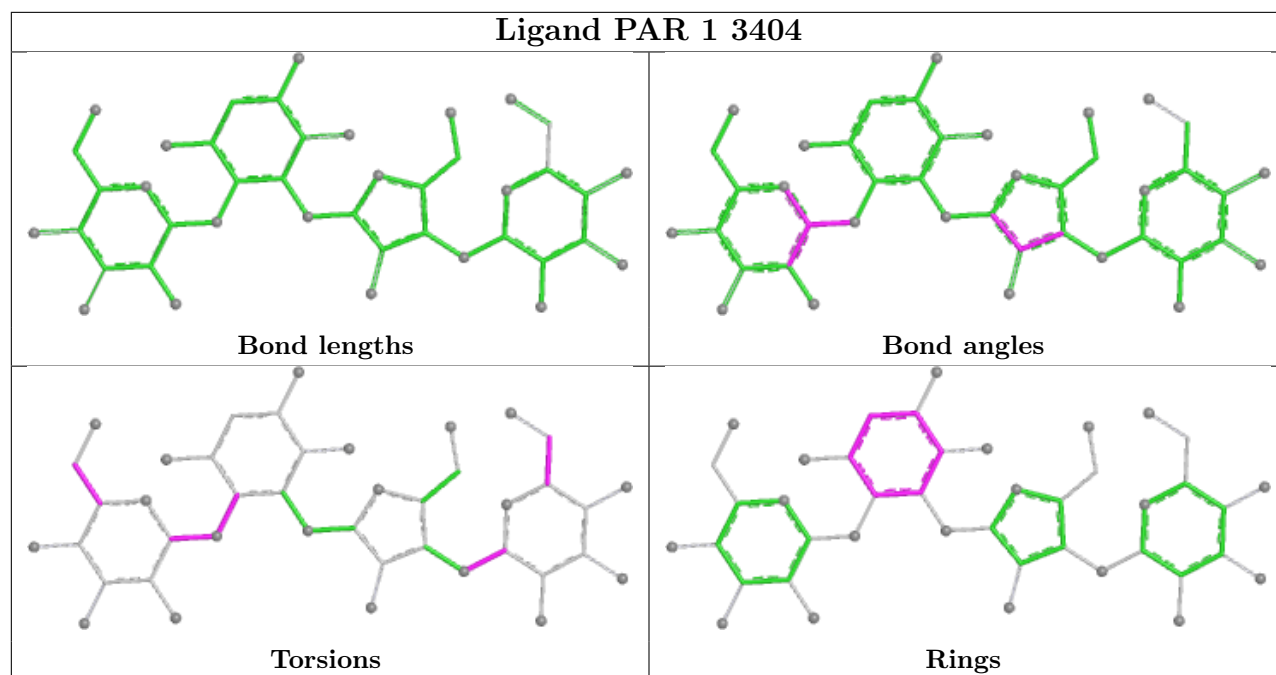
Ligand PAR B 1802

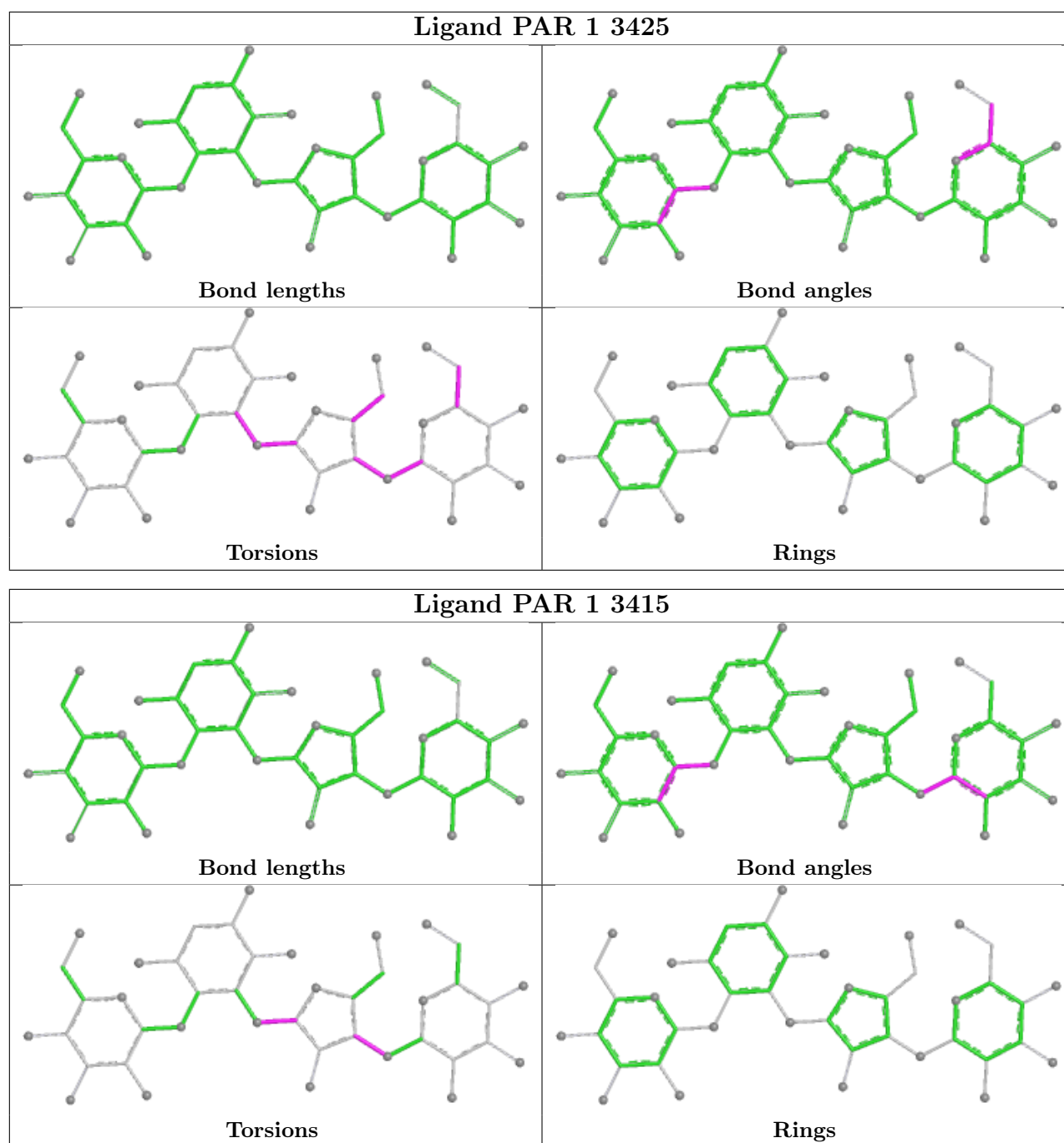


Ligand PAR CM 1802



Ligand PAR 1 3404





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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%)	0.72	179 (5%) 30 23	29, 57, 169, 366	0
1	AS	3065/3359 (91%)	1.04	323 (10%) 11 10	38, 74, 167, 281	0
2	3	121/121 (100%)	0.57	1 (0%) 82 77	43, 75, 101, 132	0
2	AT	121/121 (100%)	0.76	4 (3%) 49 40	45, 80, 104, 137	0
3	4	156/158 (98%)	0.57	5 (3%) 50 41	39, 57, 131, 172	0
3	AU	156/158 (98%)	1.53	38 (24%) 2 1	57, 96, 147, 192	0
4	AW	249/254 (98%)	1.89	88 (35%) 1 1	44, 76, 102, 117	1 (0%)
4	j	249/254 (98%)	1.15	31 (12%) 8 7	27, 43, 67, 90	1 (0%)
5	AX	386/389 (99%)	1.42	84 (21%) 2 2	36, 67, 90, 165	0
5	k	386/389 (99%)	1.22	60 (15%) 5 4	32, 59, 82, 128	1 (0%)
6	AY	361/363 (99%)	1.93	149 (41%) 0 0	46, 75, 104, 131	0
6	l	360/363 (99%)	1.34	59 (16%) 4 3	29, 59, 94, 136	0
7	AZ	292/298 (97%)	2.17	141 (48%) 0 0	64, 99, 127, 136	0
7	m	296/298 (99%)	1.54	80 (27%) 1 1	54, 86, 114, 126	0
8	BA	153/176 (86%)	1.58	36 (23%) 2 2	50, 70, 98, 145	0
8	n	157/176 (89%)	1.28	25 (15%) 5 4	51, 70, 106, 139	0
9	BB	234/241 (97%)	1.17	30 (12%) 7 6	34, 58, 101, 154	0
9	o	234/241 (97%)	1.11	28 (11%) 9 7	41, 56, 120, 160	0
10	BC	231/262 (88%)	2.57	154 (66%) 0 0	87, 117, 150, 179	0
10	p	230/262 (87%)	1.27	37 (16%) 4 4	43, 64, 106, 129	0
11	BD	190/191 (99%)	1.53	51 (26%) 1 1	54, 75, 107, 140	0
11	q	190/191 (99%)	1.34	38 (20%) 3 2	51, 68, 89, 123	0
12	BE	206/220 (93%)	1.26	31 (15%) 5 4	44, 64, 101, 125	0
12	r	208/220 (94%)	1.35	42 (20%) 3 2	37, 63, 103, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	BF	171/174 (98%)	1.64	53 (30%)	1	1	65, 87, 107, 121	0
13	s	171/174 (98%)	1.86	61 (35%)	1	0	67, 88, 110, 129	0
14	BG	200/202 (99%)	2.35	112 (56%)	0	0	50, 95, 130, 151	0
14	t	200/202 (99%)	1.23	31 (15%)	5	4	35, 66, 107, 146	0
15	BH	130/131 (99%)	1.26	23 (17%)	4	3	49, 65, 93, 117	0
15	u	128/131 (97%)	1.22	18 (14%)	6	5	45, 65, 85, 100	0
16	BI	203/204 (99%)	2.86	152 (74%)	0	0	57, 88, 107, 121	0
16	v	203/204 (99%)	1.42	43 (21%)	2	2	27, 47, 59, 82	0
17	BJ	199/200 (99%)	1.24	33 (16%)	4	3	40, 55, 89, 104	0
17	w	199/200 (99%)	1.16	26 (13%)	7	6	35, 52, 82, 102	0
18	BK	174/185 (94%)	1.91	78 (44%)	0	0	48, 74, 102, 124	0
18	x	171/185 (92%)	1.40	31 (18%)	3	3	39, 57, 122, 141	0
19	BL	185/186 (99%)	1.77	67 (36%)	1	0	47, 74, 90, 106	0
19	y	185/186 (99%)	1.35	34 (18%)	3	3	44, 58, 76, 88	0
20	BM	179/190 (94%)	2.40	95 (53%)	0	0	59, 86, 144, 167	0
20	z	179/190 (94%)	1.36	33 (18%)	3	3	44, 62, 121, 136	0
21	0	170/172 (98%)	1.17	21 (12%)	8	7	41, 56, 81, 121	0
21	BN	170/172 (98%)	1.35	29 (17%)	4	3	40, 60, 86, 107	0
22	2	159/160 (99%)	1.46	36 (22%)	2	2	41, 60, 111, 137	0
22	BO	159/160 (99%)	1.87	62 (38%)	1	0	47, 69, 116, 143	0
23	5	103/124 (83%)	1.84	40 (38%)	1	0	72, 112, 132, 156	0
23	BP	102/124 (82%)	2.12	57 (55%)	0	0	97, 129, 154, 178	1 (0%)
24	6	131/137 (95%)	1.26	20 (15%)	5	4	37, 51, 73, 102	0
24	BQ	131/137 (95%)	1.53	34 (25%)	1	1	39, 54, 71, 113	0
25	7	77/155 (49%)	1.08	8 (10%)	11	10	43, 60, 120, 137	0
25	BR	109/155 (70%)	1.84	45 (41%)	0	0	50, 82, 109, 124	0
26	8	121/142 (85%)	1.24	17 (14%)	6	5	38, 59, 83, 121	0
26	BS	119/142 (83%)	2.72	82 (68%)	0	0	64, 96, 114, 119	0
27	9	125/127 (98%)	1.74	41 (32%)	1	1	45, 72, 97, 116	0
27	BT	126/127 (99%)	2.80	83 (65%)	0	0	65, 96, 120, 140	0
28	AA	135/136 (99%)	1.60	44 (32%)	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%)	2.39	81 (60%)	0	0	92, 119, 177, 219	0
29	AB	148/149 (99%)	1.56	31 (20%)	2	2	33, 56, 86, 111	0
29	BV	148/149 (99%)	2.13	66 (44%)	0	0	42, 79, 103, 118	0
30	AC	61/63 (96%)	1.84	19 (31%)	1	1	42, 71, 117, 139	0
30	BW	61/63 (96%)	2.39	38 (62%)	0	0	50, 84, 123, 141	0
31	AD	96/106 (90%)	1.23	18 (18%)	3	3	47, 62, 87, 101	0
31	BX	96/106 (90%)	1.84	39 (40%)	0	0	76, 103, 127, 134	0
32	AE	110/112 (98%)	1.33	22 (20%)	3	2	50, 67, 125, 135	0
32	BY	110/112 (98%)	1.93	43 (39%)	1	0	53, 84, 122, 133	0
33	AF	124/131 (94%)	1.51	31 (25%)	2	1	36, 57, 74, 87	0
33	BZ	124/131 (94%)	1.78	41 (33%)	1	1	40, 64, 85, 109	0
34	AG	106/107 (99%)	1.22	20 (18%)	3	3	40, 54, 84, 99	0
34	CA	106/107 (99%)	1.42	21 (19%)	3	2	41, 58, 78, 87	0
35	AH	112/122 (91%)	1.73	35 (31%)	1	1	38, 60, 104, 143	0
35	CB	112/122 (91%)	2.82	68 (60%)	0	0	61, 96, 135, 161	0
36	AI	117/120 (97%)	1.62	31 (26%)	1	1	46, 67, 99, 114	1 (0%)
36	CC	118/120 (98%)	2.76	73 (61%)	0	0	71, 103, 126, 132	1 (0%)
37	AJ	97/99 (97%)	1.03	11 (11%)	10	9	45, 62, 99, 142	0
37	CD	97/99 (97%)	2.35	57 (58%)	0	0	83, 104, 137, 147	0
38	AK	86/90 (95%)	1.31	14 (16%)	4	3	32, 45, 92, 128	0
38	CE	86/90 (95%)	2.31	54 (62%)	0	0	52, 73, 107, 135	0
39	AL	77/78 (98%)	1.67	27 (35%)	1	1	63, 87, 125, 151	0
39	CF	77/78 (98%)	2.21	39 (50%)	0	0	93, 121, 152, 173	0
40	AM	50/51 (98%)	1.63	15 (30%)	1	1	41, 56, 86, 90	0
40	CG	50/51 (98%)	2.53	34 (68%)	0	0	52, 82, 97, 102	1 (2%)
41	AN	52/52 (100%)	2.12	29 (55%)	0	0	60, 83, 107, 111	0
41	CH	51/52 (98%)	2.28	26 (50%)	0	0	63, 88, 108, 120	0
42	AO	25/25 (100%)	1.73	9 (36%)	1	0	49, 60, 84, 85	0
42	CI	25/25 (100%)	2.12	11 (44%)	0	0	51, 66, 79, 83	0
43	AP	103/106 (97%)	1.16	14 (13%)	7	5	35, 57, 90, 114	0
43	CJ	103/106 (97%)	1.49	26 (25%)	1	1	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%)	1.04	11 (12%)	8	7	34, 47, 80, 104	0
44	CK	91/92 (98%)	1.66	26 (28%)	1	1	52, 76, 106, 127	0
45	B	1725/1787 (96%)	1.06	203 (11%)	9	7	41, 78, 165, 331	0
45	CM	1778/1787 (99%)	1.18	232 (13%)	7	6	47, 92, 191, 459	0
46	C	208/261 (79%)	1.83	75 (36%)	1	0	72, 104, 130, 157	0
46	CN	208/261 (79%)	1.78	83 (39%)	1	0	73, 106, 137, 154	0
47	CO	214/256 (83%)	2.14	106 (49%)	0	0	88, 119, 143, 157	0
47	D	214/256 (83%)	1.39	49 (22%)	2	2	57, 84, 104, 112	0
48	CP	217/249 (87%)	1.65	58 (26%)	1	1	50, 81, 109, 128	0
48	E	217/249 (87%)	1.62	67 (30%)	1	1	44, 79, 109, 125	0
49	CQ	223/251 (88%)	1.74	76 (34%)	1	1	70, 99, 147, 166	0
49	F	223/251 (88%)	1.91	92 (41%)	0	0	62, 93, 147, 169	0
50	CR	260/262 (99%)	1.41	57 (21%)	2	2	53, 75, 102, 147	0
50	G	259/262 (98%)	1.81	84 (32%)	1	1	57, 84, 105, 144	0
51	CS	206/225 (91%)	2.13	109 (52%)	0	0	97, 120, 148, 194	0
51	H	206/225 (91%)	1.78	69 (33%)	1	1	64, 97, 131, 170	0
52	CT	236/236 (100%)	2.14	100 (42%)	0	0	59, 90, 123, 159	0
52	I	222/236 (94%)	1.80	76 (34%)	1	1	59, 97, 131, 165	0
53	CU	183/186 (98%)	1.92	83 (45%)	0	0	65, 125, 161, 174	0
53	J	181/186 (97%)	1.92	72 (39%)	1	0	60, 111, 145, 150	0
54	CV	203/206 (98%)	1.68	61 (30%)	1	1	40, 74, 132, 159	0
54	K	202/206 (98%)	1.45	44 (21%)	2	2	42, 69, 120, 137	0
55	CW	178/189 (94%)	1.87	68 (38%)	1	0	64, 88, 121, 152	0
55	L	178/189 (94%)	2.30	105 (58%)	0	0	67, 91, 119, 138	0
56	CX	94/118 (79%)	1.45	26 (27%)	1	1	78, 111, 138, 148	0
56	M	98/118 (83%)	1.82	38 (38%)	1	0	70, 105, 135, 141	0
57	CY	141/155 (90%)	1.82	52 (36%)	1	0	43, 64, 100, 155	0
57	N	141/155 (90%)	1.39	30 (21%)	2	2	43, 60, 94, 121	0
58	CZ	119/143 (83%)	1.88	47 (39%)	1	0	137, 165, 181, 188	0
58	O	116/143 (81%)	2.38	69 (59%)	0	0	141, 174, 191, 198	0
59	DA	150/151 (99%)	2.09	77 (51%)	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%)	1.76	49 (32%)	1	1	43, 74, 94, 109	0
60	DB	127/132 (96%)	1.75	49 (38%)	1	0	68, 108, 129, 138	0
60	Q	127/132 (96%)	1.44	29 (22%)	2	2	36, 76, 93, 105	0
61	DC	122/142 (85%)	2.23	67 (54%)	0	0	82, 109, 129, 154	0
61	R	129/142 (90%)	1.56	35 (27%)	1	1	66, 84, 133, 148	0
62	DD	135/142 (95%)	2.56	86 (63%)	0	0	89, 119, 141, 150	0
62	S	140/142 (98%)	2.04	58 (41%)	0	0	66, 99, 134, 157	0
63	DE	124/137 (90%)	2.25	59 (47%)	0	0	88, 123, 158, 180	0
63	T	124/137 (90%)	2.49	76 (61%)	0	0	79, 115, 158, 172	0
64	DF	141/145 (97%)	2.05	65 (46%)	0	0	70, 108, 132, 153	0
64	U	144/145 (99%)	1.45	25 (17%)	4	3	63, 83, 119, 146	0
65	DG	139/145 (95%)	2.65	99 (71%)	0	0	94, 116, 133, 144	0
65	V	141/145 (97%)	1.82	55 (39%)	1	0	69, 92, 123, 148	0
66	DH	97/119 (81%)	2.23	51 (52%)	0	0	81, 113, 136, 142	0
66	W	99/119 (83%)	2.16	53 (53%)	0	0	63, 112, 137, 143	0
67	DI	87/87 (100%)	1.42	16 (18%)	3	3	72, 93, 116, 140	0
67	X	87/87 (100%)	1.66	23 (26%)	1	1	63, 91, 113, 127	0
68	DJ	129/130 (99%)	1.73	43 (33%)	1	1	56, 73, 90, 97	0
68	Y	129/130 (99%)	1.62	36 (27%)	1	1	50, 68, 84, 94	0
69	DK	143/145 (98%)	1.61	38 (26%)	1	1	49, 62, 81, 102	0
69	Z	143/145 (98%)	1.41	30 (20%)	2	2	49, 64, 80, 115	0
70	DL	132/135 (97%)	1.56	37 (28%)	1	1	66, 95, 119, 153	0
70	a	134/135 (99%)	1.97	55 (41%)	0	0	66, 104, 125, 151	0
71	DM	68/105 (64%)	2.07	33 (48%)	0	0	109, 134, 148, 159	0
71	b	72/105 (68%)	1.40	13 (18%)	3	3	82, 107, 132, 143	0
72	DN	98/119 (82%)	2.28	51 (52%)	0	0	63, 88, 131, 137	0
72	c	98/119 (82%)	1.89	37 (37%)	1	0	50, 70, 109, 150	0
73	DO	81/82 (98%)	1.89	32 (39%)	1	0	75, 107, 156, 178	0
73	d	81/82 (98%)	1.88	34 (41%)	0	0	64, 85, 145, 164	0
74	DP	61/67 (91%)	1.99	26 (42%)	0	0	105, 125, 140, 151	0
74	e	62/67 (92%)	1.65	15 (24%)	2	1	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%)	1.90	26 (48%)	0 0	72, 91, 110, 125
75	f	55/56 (98%)	1.73	20 (36%)	1 0	57, 73, 101, 112
76	DR	58/63 (92%)	2.28	34 (58%)	0 0	65, 96, 154, 163
76	g	54/63 (85%)	2.26	26 (48%)	0 0	73, 97, 128, 136
77	h	70/193 (36%)	2.89	47 (67%)	0 0	122, 160, 179, 191
78	AR	311/317 (98%)	2.10	152 (48%)	0 0	101, 149, 177, 189
79	CL	121/267 (45%)	1.94	49 (40%)	0 0	68, 103, 129, 138
79	i	120/267 (44%)	2.48	64 (53%)	0 0	71, 104, 136, 146
All	All	32248/34616 (93%)	1.49	8404 (26%)	1 1	27, 79, 147, 459

The worst 5 of 8404 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	AY	363	ASN	14.4
6	l	363	ASN	12.2
36	CC	120	ALA	11.4
51	H	152	SER	10.2
52	CT	80	GLY	9.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	1	3654	1/1	0.20	0.33	72,72,72,72	0
82	MG	AS	3630	1/1	0.23	0.38	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	B	1848	1/1	0.33	0.27	59,59,59,59	0
82	MG	AS	3460	1/1	0.35	0.35	75,75,75,75	0
82	MG	B	1937	1/1	0.42	0.30	72,72,72,72	0
82	MG	AS	3720	1/1	0.44	0.22	51,51,51,51	0
82	MG	CM	1848	1/1	0.45	0.20	73,73,73,73	0
82	MG	B	1930	1/1	0.48	0.29	74,74,74,74	0
82	MG	B	1810	1/1	0.49	0.29	51,51,51,51	0
82	MG	CM	1884	1/1	0.51	0.23	60,60,60,60	0
82	MG	B	1925	1/1	0.53	0.43	81,81,81,81	0
82	MG	B	1866	1/1	0.53	0.28	58,58,58,58	0
82	MG	CM	1831	1/1	0.54	0.25	68,68,68,68	0
82	MG	AS	3442	1/1	0.54	0.17	52,52,52,52	0
82	MG	CM	1812	1/1	0.54	0.31	73,73,73,73	0
82	MG	CM	1932	1/1	0.54	0.31	75,75,75,75	0
82	MG	B	1910	1/1	0.55	0.25	71,71,71,71	0
82	MG	CM	1839	1/1	0.56	0.16	96,96,96,96	0
82	MG	1	3483	1/1	0.57	0.20	68,68,68,68	0
82	MG	AS	3489	1/1	0.57	0.22	58,58,58,58	0
82	MG	AS	3738	1/1	0.57	0.25	64,64,64,64	0
82	MG	AS	3467	1/1	0.58	0.14	67,67,67,67	0
82	MG	CM	1853	1/1	0.59	0.18	83,83,83,83	0
82	MG	1	3762	1/1	0.59	0.17	60,60,60,60	0
82	MG	AS	3716	1/1	0.59	0.26	51,51,51,51	0
82	MG	AS	3669	1/1	0.60	0.29	80,80,80,80	0
82	MG	1	3498	1/1	0.60	0.37	64,64,64,64	0
82	MG	CM	1851	1/1	0.60	0.29	80,80,80,80	0
82	MG	AS	3728	1/1	0.61	0.15	44,44,44,44	0
82	MG	AS	3450	1/1	0.61	0.21	59,59,59,59	0
82	MG	AS	3620	1/1	0.62	0.24	73,73,73,73	0
82	MG	AS	3628	1/1	0.62	0.17	52,52,52,52	0
82	MG	AS	3730	1/1	0.62	0.30	62,62,62,62	0
81	PAR	CM	1806	42/42	0.62	0.16	54,78,92,94	0
82	MG	CM	1869	1/1	0.62	0.27	50,50,50,50	0
82	MG	AS	3469	1/1	0.62	0.41	72,72,72,72	0
82	MG	CM	1900	1/1	0.62	0.22	63,63,63,63	0
82	MG	1	3649	1/1	0.62	0.24	56,56,56,56	0
82	MG	AS	3713	1/1	0.63	0.26	38,38,38,38	0
82	MG	1	3679	1/1	0.63	0.15	53,53,53,53	0
82	MG	AS	3639	1/1	0.64	0.17	44,44,44,44	0
82	MG	AS	3420	1/1	0.64	0.25	55,55,55,55	0
82	MG	B	1830	1/1	0.65	0.40	60,60,60,60	0
81	PAR	AS	3413	42/42	0.65	0.16	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3424	1/1	0.65	0.26	65,65,65,65	0
82	MG	B	1815	1/1	0.66	0.21	49,49,49,49	0
82	MG	B	1822	1/1	0.66	0.28	68,68,68,68	0
82	MG	AS	3662	1/1	0.66	0.11	52,52,52,52	0
82	MG	1	3584	1/1	0.66	0.18	44,44,44,44	0
82	MG	E	301	1/1	0.66	0.24	49,49,49,49	0
82	MG	AS	3414	1/1	0.66	0.17	57,57,57,57	0
82	MG	AS	3718	1/1	0.66	0.20	56,56,56,56	0
82	MG	AS	3732	1/1	0.67	0.33	70,70,70,70	0
82	MG	CM	1813	1/1	0.68	0.28	65,65,65,65	0
82	MG	B	1823	1/1	0.68	0.26	41,41,41,41	0
82	MG	CM	1876	1/1	0.68	0.28	76,76,76,76	0
82	MG	AS	3655	1/1	0.68	0.16	41,41,41,41	0
82	MG	AW	303	1/1	0.68	0.43	78,78,78,78	0
82	MG	AS	3670	1/1	0.68	0.20	77,77,77,77	0
82	MG	CR	301	1/1	0.68	0.21	51,51,51,51	0
82	MG	AS	3711	1/1	0.69	0.21	53,53,53,53	0
82	MG	B	1849	1/1	0.69	0.40	70,70,70,70	0
82	MG	AS	3493	1/1	0.69	0.14	55,55,55,55	0
82	MG	CM	1840	1/1	0.69	0.32	51,51,51,51	0
82	MG	1	3471	1/1	0.69	0.20	50,50,50,50	0
82	MG	B	1898	1/1	0.69	0.17	88,88,88,88	0
81	PAR	1	3407	42/42	0.69	0.24	63,82,96,104	0
82	MG	1	3451	1/1	0.69	0.15	46,46,46,46	0
82	MG	1	3535	1/1	0.69	0.16	34,34,34,34	0
82	MG	AS	3461	1/1	0.69	0.26	55,55,55,55	0
82	MG	1	3729	1/1	0.69	0.18	45,45,45,45	0
82	MG	CM	1809	1/1	0.69	0.26	60,60,60,60	0
82	MG	1	3541	1/1	0.69	0.17	43,43,43,43	0
82	MG	AS	3532	1/1	0.70	0.26	69,69,69,69	0
82	MG	AS	3564	1/1	0.70	0.27	60,60,60,60	0
82	MG	AS	3598	1/1	0.70	0.18	39,39,39,39	0
82	MG	1	3501	1/1	0.70	0.12	65,65,65,65	0
82	MG	CM	1832	1/1	0.70	0.21	56,56,56,56	0
82	MG	1	3485	1/1	0.70	0.21	64,64,64,64	0
82	MG	1	3479	1/1	0.70	0.20	66,66,66,66	0
82	MG	1	3660	1/1	0.70	0.15	42,42,42,42	0
82	MG	AS	3472	1/1	0.71	0.26	55,55,55,55	0
81	PAR	CM	1805	42/42	0.71	0.21	98,111,128,146	0
81	PAR	AS	3405	42/42	0.71	0.18	67,82,94,100	42
82	MG	CM	1881	1/1	0.71	0.29	62,62,62,62	0
82	MG	1	3431	1/1	0.71	0.36	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3643	1/1	0.71	0.17	99,99,99,99	0
82	MG	1	3448	1/1	0.71	0.23	47,47,47,47	0
82	MG	B	1895	1/1	0.71	0.23	53,53,53,53	0
82	MG	AS	3567	1/1	0.72	0.20	60,60,60,60	0
82	MG	1	3432	1/1	0.72	0.16	51,51,51,51	0
82	MG	AS	3447	1/1	0.72	0.23	55,55,55,55	0
82	MG	AS	3415	1/1	0.72	0.20	65,65,65,65	0
82	MG	AS	3685	1/1	0.72	0.41	75,75,75,75	0
81	PAR	1	3413	42/42	0.72	0.39	50,82,99,113	42
81	PAR	AS	3408	42/42	0.72	0.14	83,105,119,123	0
82	MG	AS	3428	1/1	0.72	0.29	56,56,56,56	0
83	ZN	d	101	1/1	0.72	0.14	257,257,257,257	0
83	ZN	DO	101	1/1	0.72	0.16	206,206,206,206	0
82	MG	B	1873	1/1	0.73	0.19	53,53,53,53	0
82	MG	AS	3453	1/1	0.73	0.18	52,52,52,52	0
82	MG	AS	3723	1/1	0.73	0.18	46,46,46,46	0
82	MG	AS	3519	1/1	0.73	0.17	47,47,47,47	0
81	PAR	B	1805	42/42	0.73	0.18	60,85,96,102	0
82	MG	1	3437	1/1	0.73	0.15	54,54,54,54	0
82	MG	AS	3465	1/1	0.73	0.20	69,69,69,69	0
82	MG	AS	3679	1/1	0.73	0.15	68,68,68,68	0
82	MG	CM	1883	1/1	0.73	0.35	67,67,67,67	0
82	MG	B	1940	1/1	0.73	0.39	65,65,65,65	0
82	MG	CM	1810	1/1	0.73	0.16	90,90,90,90	0
82	MG	AS	3686	1/1	0.73	0.32	47,47,47,47	0
82	MG	B	1837	1/1	0.73	0.15	63,63,63,63	0
82	MG	B	1916	1/1	0.73	0.30	59,59,59,59	0
82	MG	AS	3486	1/1	0.73	0.23	60,60,60,60	0
82	MG	AS	3482	1/1	0.74	0.28	72,72,72,72	0
82	MG	B	1943	1/1	0.74	0.21	68,68,68,68	0
82	MG	CM	1842	1/1	0.74	0.26	56,56,56,56	0
82	MG	B	1831	1/1	0.74	0.14	46,46,46,46	0
82	MG	AS	3492	1/1	0.74	0.18	68,68,68,68	0
82	MG	AS	3645	1/1	0.74	0.36	60,60,60,60	0
82	MG	AS	3651	1/1	0.74	0.16	68,68,68,68	0
82	MG	AL	101	1/1	0.74	0.22	94,94,94,94	0
82	MG	AS	3516	1/1	0.74	0.31	58,58,58,58	0
82	MG	1	3469	1/1	0.74	0.29	67,67,67,67	0
82	MG	AS	3526	1/1	0.74	0.16	38,38,38,38	0
82	MG	1	3634	1/1	0.74	0.31	60,60,60,60	0
82	MG	1	3434	1/1	0.74	0.12	36,36,36,36	0
82	MG	CM	1938	1/1	0.74	0.18	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	CM	1941	1/1	0.74	0.11	52,52,52,52	0
82	MG	1	3750	1/1	0.74	0.18	60,60,60,60	0
82	MG	AS	3432	1/1	0.74	0.20	52,52,52,52	0
81	PAR	1	3403	42/42	0.74	0.21	47,63,78,89	42
82	MG	CM	1862	1/1	0.75	0.18	58,58,58,58	0
82	MG	1	3668	1/1	0.75	0.20	37,37,37,37	0
81	PAR	1	3420	42/42	0.75	0.17	73,94,115,116	0
82	MG	AS	3438	1/1	0.75	0.10	39,39,39,39	0
82	MG	1	3683	1/1	0.75	0.22	56,56,56,56	0
82	MG	1	3718	1/1	0.75	0.14	42,42,42,42	0
82	MG	CM	1890	1/1	0.75	0.28	62,62,62,62	0
82	MG	CM	1892	1/1	0.75	0.29	67,67,67,67	0
82	MG	1	3722	1/1	0.75	0.15	41,41,41,41	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
81	PAR	1	3414	42/42	0.75	0.20	51,85,92,99	0
82	MG	CM	1942	1/1	0.75	0.14	64,64,64,64	0
82	MG	AS	3703	1/1	0.75	0.26	59,59,59,59	0
82	MG	B	1839	1/1	0.75	0.20	82,82,82,82	0
82	MG	CM	1854	1/1	0.75	0.29	65,65,65,65	0
81	PAR	1	3405	42/42	0.76	0.29	41,67,84,99	42
82	MG	B	1845	1/1	0.76	0.18	61,61,61,61	0
82	MG	AS	3446	1/1	0.76	0.14	54,54,54,54	0
82	MG	1	3521	1/1	0.76	0.17	56,56,56,56	0
82	MG	AS	3501	1/1	0.76	0.38	53,53,53,53	0
82	MG	1	3458	1/1	0.76	0.20	56,56,56,56	0
82	MG	AS	3740	1/1	0.76	0.13	63,63,63,63	0
82	MG	1	3444	1/1	0.76	0.17	56,56,56,56	0
81	PAR	B	1804	42/42	0.76	0.20	76,105,123,126	0
82	MG	1	3675	1/1	0.76	0.31	63,63,63,63	0
82	MG	B	1827	1/1	0.76	0.16	64,64,64,64	0
82	MG	AS	3466	1/1	0.76	0.15	62,62,62,62	0
82	MG	CM	1818	1/1	0.76	0.39	70,70,70,70	0
82	MG	CM	1916	1/1	0.76	0.14	44,44,44,44	0
82	MG	CM	1820	1/1	0.76	0.20	46,46,46,46	0
82	MG	AS	3586	1/1	0.76	0.24	67,67,67,67	0
82	MG	1	3754	1/1	0.76	0.34	59,59,59,59	0
82	MG	CM	1835	1/1	0.76	0.16	64,64,64,64	0
82	MG	AS	3426	1/1	0.76	0.26	71,71,71,71	0
82	MG	1	3757	1/1	0.76	0.38	64,64,64,64	0
82	MG	1	3759	1/1	0.76	0.36	65,65,65,65	0
82	MG	1	3460	1/1	0.77	0.20	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	B	1808	1/1	0.77	0.12	73,73,73,73	0
82	MG	1	3682	1/1	0.77	0.23	66,66,66,66	0
82	MG	AS	3499	1/1	0.77	0.12	48,48,48,48	0
82	MG	AS	3441	1/1	0.77	0.38	55,55,55,55	0
81	PAR	1	3425	42/42	0.77	0.21	52,74,87,97	42
82	MG	1	3701	1/1	0.77	0.14	50,50,50,50	0
82	MG	B	1920	1/1	0.77	0.27	71,71,71,71	0
81	PAR	1	3426	42/42	0.77	0.24	49,66,79,86	42
81	PAR	AS	3410	42/42	0.77	0.18	95,110,119,137	0
82	MG	CM	1857	1/1	0.77	0.14	42,42,42,42	0
82	MG	1	3637	1/1	0.77	0.15	50,50,50,50	0
82	MG	1	3733	1/1	0.77	0.18	56,56,56,56	0
82	MG	AS	3463	1/1	0.77	0.10	46,46,46,46	0
82	MG	AS	3614	1/1	0.77	0.16	54,54,54,54	0
81	PAR	1	3416	42/42	0.77	0.21	47,71,83,85	42
81	PAR	1	3409	42/42	0.77	0.18	45,81,100,109	42
82	MG	CM	1887	1/1	0.77	0.21	59,59,59,59	0
82	MG	AS	3736	1/1	0.77	0.10	41,41,41,41	0
82	MG	AS	3629	1/1	0.77	0.31	70,70,70,70	0
82	MG	CM	1897	1/1	0.77	0.15	57,57,57,57	0
82	MG	1	3755	1/1	0.77	0.21	46,46,46,46	0
82	MG	AS	3744	1/1	0.77	0.23	53,53,53,53	0
82	MG	AS	3636	1/1	0.77	0.19	92,92,92,92	0
81	PAR	1	3422	42/42	0.77	0.24	56,73,85,89	42
82	MG	1	3457	1/1	0.77	0.29	57,57,57,57	0
81	PAR	AS	3403	42/42	0.77	0.20	60,83,97,102	0
82	MG	B	1867	1/1	0.77	0.38	52,52,52,52	0
82	MG	AS	3488	1/1	0.77	0.13	69,69,69,69	0
82	MG	AS	3660	1/1	0.77	0.21	55,55,55,55	0
82	MG	AS	3474	1/1	0.78	0.26	43,43,43,43	0
82	MG	AS	3534	1/1	0.78	0.18	56,56,56,56	0
82	MG	AS	3743	1/1	0.78	0.15	44,44,44,44	0
82	MG	AS	3479	1/1	0.78	0.16	39,39,39,39	0
82	MG	CM	1874	1/1	0.78	0.32	73,73,73,73	0
81	PAR	AS	3409	42/42	0.78	0.21	51,66,89,100	42
82	MG	1	3771	1/1	0.78	0.13	49,49,49,49	0
82	MG	AS	3454	1/1	0.78	0.29	54,54,54,54	0
82	MG	AS	3602	1/1	0.78	0.37	59,59,59,59	0
82	MG	1	3477	1/1	0.78	0.19	57,57,57,57	0
82	MG	CM	1888	1/1	0.78	0.19	52,52,52,52	0
81	PAR	AS	3404	42/42	0.78	0.23	59,90,101,107	42
82	MG	AS	3627	1/1	0.78	0.37	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	CM	1825	1/1	0.78	0.23	74,74,74,74	0
82	MG	B	1892	1/1	0.78	0.28	79,79,79,79	0
82	MG	AS	3494	1/1	0.78	0.23	55,55,55,55	0
82	MG	1	3482	1/1	0.78	0.21	42,42,42,42	0
82	MG	B	1812	1/1	0.78	0.38	65,65,65,65	0
82	MG	AS	3638	1/1	0.78	0.15	71,71,71,71	0
82	MG	AS	3504	1/1	0.78	0.10	46,46,46,46	0
82	MG	G	301	1/1	0.78	0.15	56,56,56,56	0
82	MG	1	3728	1/1	0.78	0.26	62,62,62,62	0
82	MG	1	3657	1/1	0.78	0.20	61,61,61,61	0
82	MG	B	1914	1/1	0.79	0.13	47,47,47,47	0
82	MG	AS	3617	1/1	0.79	0.18	54,54,54,54	0
82	MG	B	1814	1/1	0.79	0.14	46,46,46,46	0
82	MG	AS	3440	1/1	0.79	0.17	55,55,55,55	0
81	PAR	1	3419	42/42	0.79	0.23	34,60,71,89	42
82	MG	1	3765	1/1	0.79	0.16	38,38,38,38	0
82	MG	B	1928	1/1	0.79	0.13	49,49,49,49	0
82	MG	CM	1864	1/1	0.79	0.17	79,79,79,79	0
82	MG	CM	1865	1/1	0.79	0.21	80,80,80,80	0
82	MG	B	1929	1/1	0.79	0.23	51,51,51,51	0
82	MG	1	3706	1/1	0.79	0.17	46,46,46,46	0
82	MG	4	203	1/1	0.79	0.12	77,77,77,77	0
82	MG	B	1871	1/1	0.79	0.18	52,52,52,52	0
82	MG	AS	3508	1/1	0.79	0.12	42,42,42,42	0
82	MG	1	3677	1/1	0.79	0.14	43,43,43,43	0
82	MG	B	1876	1/1	0.79	0.27	41,41,41,41	0
82	MG	B	1887	1/1	0.79	0.24	61,61,61,61	0
82	MG	1	3532	1/1	0.79	0.12	37,37,37,37	0
81	PAR	1	3423	42/42	0.79	0.28	53,68,80,84	42
82	MG	CM	1894	1/1	0.79	0.20	91,91,91,91	0
82	MG	CM	1895	1/1	0.79	0.19	76,76,76,76	0
82	MG	AS	3419	1/1	0.79	0.13	50,50,50,50	0
82	MG	AS	3674	1/1	0.79	0.12	49,49,49,49	0
82	MG	1	3440	1/1	0.79	0.22	50,50,50,50	0
82	MG	AS	3680	1/1	0.79	0.13	50,50,50,50	0
82	MG	CM	1827	1/1	0.79	0.23	37,37,37,37	0
82	MG	CM	1940	1/1	0.79	0.21	56,56,56,56	0
82	MG	AS	3682	1/1	0.79	0.10	31,31,31,31	0
82	MG	AS	3572	1/1	0.79	0.21	61,61,61,61	0
82	MG	B	1901	1/1	0.79	0.18	57,57,57,57	0
82	MG	B	1906	1/1	0.79	0.15	55,55,55,55	0
82	MG	B	1840	1/1	0.79	0.30	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3681	1/1	0.80	0.12	26,26,26,26	0
82	MG	1	3507	1/1	0.80	0.11	45,45,45,45	0
82	MG	1	3510	1/1	0.80	0.22	55,55,55,55	0
82	MG	1	3726	1/1	0.80	0.19	32,32,32,32	0
82	MG	B	1891	1/1	0.80	0.11	47,47,47,47	0
82	MG	AS	3470	1/1	0.80	0.27	74,74,74,74	0
82	MG	1	3513	1/1	0.80	0.23	75,75,75,75	0
82	MG	CM	1855	1/1	0.80	0.15	47,47,47,47	0
82	MG	1	3656	1/1	0.80	0.18	62,62,62,62	0
82	MG	AS	3619	1/1	0.80	0.20	59,59,59,59	0
82	MG	AS	3423	1/1	0.80	0.13	49,49,49,49	0
82	MG	AS	3621	1/1	0.80	0.21	54,54,54,54	0
82	MG	AS	3724	1/1	0.80	0.28	51,51,51,51	0
82	MG	AS	3727	1/1	0.80	0.16	67,67,67,67	0
82	MG	AS	3623	1/1	0.80	0.26	65,65,65,65	0
82	MG	AS	3729	1/1	0.80	0.28	41,41,41,41	0
82	MG	AS	3626	1/1	0.80	0.21	59,59,59,59	0
82	MG	1	3520	1/1	0.80	0.12	59,59,59,59	0
82	MG	1	3737	1/1	0.80	0.29	44,44,44,44	0
81	PAR	1	3427	42/42	0.80	0.16	53,67,80,88	0
82	MG	AS	3430	1/1	0.80	0.36	63,63,63,63	0
82	MG	1	3751	1/1	0.80	0.32	54,54,54,54	0
82	MG	B	1913	1/1	0.80	0.19	59,59,59,59	0
82	MG	1	3663	1/1	0.80	0.26	52,52,52,52	0
82	MG	1	3525	1/1	0.80	0.24	49,49,49,49	0
82	MG	B	1918	1/1	0.80	0.26	41,41,41,41	0
82	MG	CM	1906	1/1	0.80	0.17	85,85,85,85	0
82	MG	CM	1912	1/1	0.80	0.20	98,98,98,98	0
81	PAR	CM	1802	42/42	0.80	0.19	71,86,101,105	0
82	MG	CM	1918	1/1	0.80	0.12	70,70,70,70	0
82	MG	1	3488	1/1	0.80	0.21	47,47,47,47	0
82	MG	CM	1933	1/1	0.80	0.18	84,84,84,84	0
82	MG	CM	1937	1/1	0.80	0.20	51,51,51,51	0
82	MG	1	3490	1/1	0.80	0.41	58,58,58,58	0
82	MG	CM	1939	1/1	0.80	0.12	57,57,57,57	0
82	MG	1	3578	1/1	0.80	0.23	25,25,25,25	0
82	MG	1	3770	1/1	0.80	0.17	42,42,42,42	0
81	PAR	1	3410	42/42	0.80	0.22	40,78,96,113	0
82	MG	1	3593	1/1	0.80	0.29	44,44,44,44	0
82	MG	1	3455	1/1	0.80	0.15	57,57,57,57	0
82	MG	AS	3565	1/1	0.80	0.18	48,48,48,48	0
82	MG	AS	3435	1/1	0.81	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	B	1835	1/1	0.81	0.22	59,59,59,59	0
82	MG	B	1836	1/1	0.81	0.28	53,53,53,53	0
82	MG	AU	201	1/1	0.81	0.24	71,71,71,71	0
82	MG	1	3749	1/1	0.81	0.22	51,51,51,51	0
82	MG	1	3693	1/1	0.81	0.15	39,39,39,39	0
82	MG	B	1942	1/1	0.81	0.18	56,56,56,56	0
82	MG	AS	3615	1/1	0.81	0.10	86,86,86,86	0
82	MG	1	3600	1/1	0.81	0.09	23,23,23,23	0
82	MG	CM	1816	1/1	0.81	0.13	46,46,46,46	0
82	MG	B	1902	1/1	0.81	0.19	63,63,63,63	0
82	MG	1	3752	1/1	0.81	0.22	43,43,43,43	0
82	MG	AS	3702	1/1	0.81	0.13	50,50,50,50	0
82	MG	B	1908	1/1	0.81	0.12	48,48,48,48	0
82	MG	1	3495	1/1	0.81	0.10	28,28,28,28	0
82	MG	1	3439	1/1	0.81	0.14	41,41,41,41	0
82	MG	AS	3505	1/1	0.81	0.21	64,64,64,64	0
82	MG	CM	1838	1/1	0.81	0.21	79,79,79,79	0
82	MG	1	3642	1/1	0.81	0.18	57,57,57,57	0
82	MG	CM	1919	1/1	0.81	0.27	46,46,46,46	0
82	MG	CM	1924	1/1	0.81	0.24	57,57,57,57	0
82	MG	AS	3514	1/1	0.81	0.15	49,49,49,49	0
82	MG	AS	3464	1/1	0.81	0.22	35,35,35,35	0
82	MG	CM	1844	1/1	0.81	0.09	83,83,83,83	0
82	MG	1	3516	1/1	0.81	0.10	49,49,49,49	0
82	MG	1	3454	1/1	0.81	0.16	52,52,52,52	0
82	MG	AS	3530	1/1	0.81	0.25	40,40,40,40	0
82	MG	1	3505	1/1	0.81	0.10	44,44,44,44	0
81	PAR	B	1802	42/42	0.81	0.19	55,81,98,105	0
82	MG	AS	3538	1/1	0.81	0.20	40,40,40,40	0
82	MG	B	1926	1/1	0.81	0.22	54,54,54,54	0
82	MG	1	3684	1/1	0.81	0.14	56,56,56,56	0
82	MG	1	3539	1/1	0.82	0.17	49,49,49,49	0
81	PAR	AS	3402	42/42	0.82	0.15	45,64,74,83	0
82	MG	1	3772	1/1	0.82	0.23	53,53,53,53	0
82	MG	B	1919	1/1	0.82	0.36	65,65,65,65	0
81	PAR	4	201	42/42	0.82	0.21	27,47,60,67	42
82	MG	B	1852	1/1	0.82	0.17	54,54,54,54	0
82	MG	x	201	1/1	0.82	0.18	26,26,26,26	0
82	MG	B	1927	1/1	0.82	0.24	52,52,52,52	0
81	PAR	1	3418	42/42	0.82	0.19	67,85,93,97	42
82	MG	1	3459	1/1	0.82	0.46	55,55,55,55	0
82	MG	1	3445	1/1	0.82	0.20	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	CM	1885	1/1	0.82	0.37	60,60,60,60	0
82	MG	B	1932	1/1	0.82	0.26	66,66,66,66	0
82	MG	B	1935	1/1	0.82	0.18	48,48,48,48	0
82	MG	AS	3654	1/1	0.82	0.22	55,55,55,55	0
82	MG	AS	3455	1/1	0.82	0.31	61,61,61,61	0
82	MG	AS	3456	1/1	0.82	0.20	42,42,42,42	0
82	MG	1	3463	1/1	0.82	0.38	61,61,61,61	0
81	PAR	B	1803	42/42	0.82	0.24	46,75,88,107	0
82	MG	B	1890	1/1	0.82	0.32	46,46,46,46	0
82	MG	AS	3552	1/1	0.82	0.18	53,53,53,53	0
82	MG	AS	3678	1/1	0.82	0.18	49,49,49,49	0
82	MG	1	3522	1/1	0.82	0.21	45,45,45,45	0
82	MG	1	3648	1/1	0.82	0.13	52,52,52,52	0
81	PAR	CM	1801	42/42	0.82	0.23	72,86,93,103	42
82	MG	1	3696	1/1	0.82	0.18	43,43,43,43	0
82	MG	AS	3580	1/1	0.82	0.22	42,42,42,42	0
82	MG	1	3697	1/1	0.82	0.29	49,49,49,49	0
82	MG	AS	3690	1/1	0.82	0.18	19,19,19,19	0
82	MG	1	3653	1/1	0.82	0.26	51,51,51,51	0
82	MG	1	3499	1/1	0.82	0.14	36,36,36,36	0
82	MG	CM	1843	1/1	0.82	0.17	59,59,59,59	0
82	MG	1	3764	1/1	0.82	0.10	34,34,34,34	0
82	MG	AS	3477	1/1	0.82	0.31	81,81,81,81	0
82	MG	CM	1943	1/1	0.82	0.13	61,61,61,61	0
81	PAR	AS	3406	42/42	0.82	0.14	62,85,101,104	0
82	MG	DG	201	1/1	0.82	0.30	74,74,74,74	0
82	MG	1	3767	1/1	0.82	0.24	48,48,48,48	0
82	MG	AS	3427	1/1	0.82	0.21	46,46,46,46	0
82	MG	AS	3497	1/1	0.83	0.18	69,69,69,69	0
82	MG	1	3734	1/1	0.83	0.29	42,42,42,42	0
82	MG	1	3736	1/1	0.83	0.13	41,41,41,41	0
82	MG	1	3633	1/1	0.83	0.26	55,55,55,55	0
82	MG	1	3742	1/1	0.83	0.21	56,56,56,56	0
82	MG	AS	3725	1/1	0.83	0.26	39,39,39,39	0
82	MG	1	3746	1/1	0.83	0.12	48,48,48,48	0
82	MG	4	209	1/1	0.83	0.24	56,56,56,56	0
82	MG	j	301	1/1	0.83	0.09	24,24,24,24	0
82	MG	1	3658	1/1	0.83	0.27	42,42,42,42	0
81	PAR	1	3411	42/42	0.83	0.23	43,64,77,84	0
82	MG	AS	3528	1/1	0.83	0.28	47,47,47,47	0
82	MG	B	1850	1/1	0.83	0.32	52,52,52,52	0
82	MG	1	3447	1/1	0.83	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3742	1/1	0.83	0.28	42,42,42,42	0
81	PAR	B	1801	42/42	0.83	0.17	62,87,108,112	0
81	PAR	1	3428	42/42	0.83	0.16	48,62,70,102	0
82	MG	AS	3540	1/1	0.83	0.24	69,69,69,69	0
82	MG	AS	3659	1/1	0.83	0.18	30,30,30,30	0
82	MG	CM	1808	1/1	0.83	0.11	87,87,87,87	0
82	MG	B	1870	1/1	0.83	0.09	30,30,30,30	0
82	MG	AS	3563	1/1	0.83	0.29	55,55,55,55	0
82	MG	B	1813	1/1	0.83	0.23	59,59,59,59	0
82	MG	1	3453	1/1	0.83	0.24	54,54,54,54	0
82	MG	CM	1914	1/1	0.83	0.15	80,80,80,80	0
82	MG	1	3724	1/1	0.83	0.38	57,57,57,57	0
82	MG	AS	3481	1/1	0.83	0.12	42,42,42,42	0
82	MG	AS	3578	1/1	0.83	0.16	46,46,46,46	0
82	MG	B	1816	1/1	0.83	0.34	60,60,60,60	0
82	MG	CM	1926	1/1	0.83	0.14	52,52,52,52	0
82	MG	CM	1930	1/1	0.83	0.25	57,57,57,57	0
82	MG	AS	3581	1/1	0.83	0.10	32,32,32,32	0
82	MG	1	3651	1/1	0.83	0.16	28,28,28,28	0
82	MG	AS	3487	1/1	0.83	0.37	50,50,50,50	0
82	MG	B	1933	1/1	0.83	0.11	44,44,44,44	0
82	MG	1	3500	1/1	0.83	0.20	43,43,43,43	0
82	MG	AS	3693	1/1	0.83	0.12	77,77,77,77	0
82	MG	AS	3699	1/1	0.83	0.22	57,57,57,57	0
81	PAR	AS	3411	42/42	0.83	0.17	53,69,91,96	0
82	MG	1	3468	1/1	0.83	0.17	36,36,36,36	0
82	MG	AS	3710	1/1	0.83	0.16	57,57,57,57	0
82	MG	CM	1845	1/1	0.83	0.29	73,73,73,73	0
82	MG	AS	3618	1/1	0.83	0.22	27,27,27,27	0
82	MG	AS	3452	1/1	0.83	0.11	78,78,78,78	0
82	MG	AS	3709	1/1	0.84	0.20	38,38,38,38	0
82	MG	CM	1882	1/1	0.84	0.31	52,52,52,52	0
82	MG	CM	1815	1/1	0.84	0.14	50,50,50,50	0
82	MG	1	3615	1/1	0.84	0.22	34,34,34,34	0
82	MG	1	3761	1/1	0.84	0.18	54,54,54,54	0
82	MG	1	3712	1/1	0.84	0.33	50,50,50,50	0
82	MG	AS	3585	1/1	0.84	0.15	44,44,44,44	0
82	MG	1	3740	1/1	0.84	0.40	57,57,57,57	0
82	MG	CM	1830	1/1	0.84	0.17	55,55,55,55	0
82	MG	AS	3719	1/1	0.84	0.14	48,48,48,48	0
82	MG	AS	3657	1/1	0.84	0.17	42,42,42,42	0
82	MG	CM	1833	1/1	0.84	0.31	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3630	1/1	0.84	0.29	56,56,56,56	0
82	MG	CM	1905	1/1	0.84	0.22	75,75,75,75	0
82	MG	1	3745	1/1	0.84	0.14	38,38,38,38	0
82	MG	B	1858	1/1	0.84	0.12	64,64,64,64	0
82	MG	AS	3667	1/1	0.84	0.18	39,39,39,39	0
82	MG	AS	3478	1/1	0.84	0.15	43,43,43,43	0
82	MG	1	3721	1/1	0.84	0.22	39,39,39,39	0
82	MG	1	3515	1/1	0.84	0.12	47,47,47,47	0
81	PAR	CM	1804	42/42	0.84	0.23	40,67,81,91	0
82	MG	3	201	1/1	0.84	0.17	36,36,36,36	0
82	MG	CM	1929	1/1	0.84	0.20	52,52,52,52	0
81	PAR	1	3417	42/42	0.84	0.16	49,70,84,91	0
82	MG	B	1874	1/1	0.84	0.26	50,50,50,50	0
82	MG	4	206	1/1	0.84	0.34	62,62,62,62	0
82	MG	AS	3557	1/1	0.84	0.25	60,60,60,60	0
82	MG	B	1880	1/1	0.84	0.21	61,61,61,61	0
82	MG	1	3464	1/1	0.84	0.09	28,28,28,28	0
82	MG	AS	3691	1/1	0.84	0.12	19,19,19,19	0
81	PAR	1	3415	42/42	0.84	0.19	30,66,80,91	0
82	MG	CM	1866	1/1	0.84	0.29	70,70,70,70	0
81	PAR	AS	3412	42/42	0.84	0.15	37,60,77,90	0
82	MG	CM	1873	1/1	0.84	0.21	71,71,71,71	0
82	MG	1	3484	1/1	0.84	0.14	47,47,47,47	0
82	MG	AS	3577	1/1	0.84	0.32	45,45,45,45	0
82	MG	CM	1879	1/1	0.84	0.13	82,82,82,82	0
82	MG	1	3739	1/1	0.85	0.12	46,46,46,46	0
82	MG	AS	3524	1/1	0.85	0.30	67,67,67,67	0
82	MG	1	3472	1/1	0.85	0.15	37,37,37,37	0
82	MG	1	3555	1/1	0.85	0.24	36,36,36,36	0
82	MG	v	305	1/1	0.85	0.11	39,39,39,39	0
82	MG	1	3743	1/1	0.85	0.22	65,65,65,65	0
82	MG	1	3574	1/1	0.85	0.22	39,39,39,39	0
82	MG	B	1941	1/1	0.85	0.15	41,41,41,41	0
81	PAR	1	3430	42/42	0.85	0.16	40,63,77,121	0
82	MG	B	1809	1/1	0.85	0.36	54,54,54,54	0
82	MG	AS	3553	1/1	0.85	0.12	41,41,41,41	0
82	MG	1	3698	1/1	0.85	0.18	35,35,35,35	0
82	MG	B	1884	1/1	0.85	0.29	54,54,54,54	0
81	PAR	1	3404	42/42	0.85	0.18	28,57,75,84	0
81	PAR	1	3412	42/42	0.85	0.24	60,78,89,98	42
82	MG	1	3442	1/1	0.85	0.24	38,38,38,38	0
82	MG	AS	3568	1/1	0.85	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	CM	1891	1/1	0.85	0.15	49,49,49,49	0
82	MG	1	3753	1/1	0.85	0.34	58,58,58,58	0
82	MG	1	3611	1/1	0.85	0.25	35,35,35,35	0
82	MG	1	3465	1/1	0.85	0.20	51,51,51,51	0
82	MG	1	3661	1/1	0.85	0.21	42,42,42,42	0
82	MG	AS	3483	1/1	0.85	0.18	50,50,50,50	0
82	MG	CM	1902	1/1	0.85	0.17	57,57,57,57	0
82	MG	CM	1903	1/1	0.85	0.17	81,81,81,81	0
82	MG	1	3626	1/1	0.85	0.09	32,32,32,32	0
82	MG	1	3725	1/1	0.85	0.15	29,29,29,29	0
82	MG	CM	1909	1/1	0.85	0.20	79,79,79,79	0
82	MG	AS	3689	1/1	0.85	0.32	51,51,51,51	0
82	MG	CM	1829	1/1	0.85	0.24	53,53,53,53	0
82	MG	AS	3589	1/1	0.85	0.23	59,59,59,59	0
82	MG	AS	3592	1/1	0.85	0.17	50,50,50,50	0
82	MG	AS	3692	1/1	0.85	0.15	40,40,40,40	0
82	MG	1	3664	1/1	0.85	0.21	48,48,48,48	0
82	MG	1	3727	1/1	0.85	0.21	57,57,57,57	0
82	MG	AS	3490	1/1	0.85	0.24	73,73,73,73	0
82	MG	1	3530	1/1	0.85	0.25	50,50,50,50	0
82	MG	1	3531	1/1	0.85	0.27	53,53,53,53	0
82	MG	B	1838	1/1	0.85	0.19	59,59,59,59	0
82	MG	1	3768	1/1	0.85	0.16	59,59,59,59	0
82	MG	1	3731	1/1	0.85	0.12	50,50,50,50	0
81	PAR	AS	3407	42/42	0.85	0.18	49,75,90,103	0
82	MG	AS	3717	1/1	0.85	0.30	53,53,53,53	0
82	MG	CM	1850	1/1	0.85	0.20	50,50,50,50	0
81	PAR	1	3406	42/42	0.85	0.20	37,53,72,86	0
82	MG	CM	1852	1/1	0.85	0.17	73,73,73,73	0
82	MG	1	3775	1/1	0.85	0.21	49,49,49,49	0
82	MG	1	3638	1/1	0.85	0.14	29,29,29,29	0
81	PAR	1	3424	42/42	0.85	0.26	56,76,83,87	42
82	MG	B	1853	1/1	0.85	0.26	55,55,55,55	0
82	MG	CM	1875	1/1	0.86	0.12	57,57,57,57	0
82	MG	AS	3687	1/1	0.86	0.12	38,38,38,38	0
82	MG	AS	3536	1/1	0.86	0.10	39,39,39,39	0
82	MG	1	3572	1/1	0.86	0.18	35,35,35,35	0
82	MG	AS	3444	1/1	0.86	0.20	56,56,56,56	0
82	MG	1	3747	1/1	0.86	0.25	48,48,48,48	0
82	MG	B	1904	1/1	0.86	0.12	59,59,59,59	0
82	MG	AS	3449	1/1	0.86	0.35	47,47,47,47	0
82	MG	AS	3560	1/1	0.86	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	CM	1822	1/1	0.86	0.27	50,50,50,50	0
82	MG	AS	3632	1/1	0.86	0.20	51,51,51,51	0
82	MG	1	3692	1/1	0.86	0.18	50,50,50,50	0
81	PAR	1	3402	42/42	0.86	0.13	46,71,82,93	0
82	MG	1	3481	1/1	0.86	0.12	60,60,60,60	0
82	MG	1	3635	1/1	0.86	0.32	70,70,70,70	0
82	MG	CM	1896	1/1	0.86	0.23	59,59,59,59	0
82	MG	AS	3714	1/1	0.86	0.31	44,44,44,44	0
82	MG	1	3579	1/1	0.86	0.09	46,46,46,46	0
82	MG	AS	3647	1/1	0.86	0.21	64,64,64,64	0
82	MG	CM	1837	1/1	0.86	0.20	62,62,62,62	0
82	MG	AS	3650	1/1	0.86	0.13	49,49,49,49	0
81	PAR	4	202	42/42	0.86	0.14	44,60,80,87	0
82	MG	CM	1907	1/1	0.86	0.12	73,73,73,73	0
82	MG	B	1917	1/1	0.86	0.28	57,57,57,57	0
82	MG	CM	1841	1/1	0.86	0.15	66,66,66,66	0
82	MG	1	3503	1/1	0.86	0.23	50,50,50,50	0
82	MG	1	3756	1/1	0.86	0.16	45,45,45,45	0
82	MG	1	3518	1/1	0.86	0.27	30,30,30,30	0
82	MG	p	301	1/1	0.86	0.25	47,47,47,47	0
82	MG	v	302	1/1	0.86	0.25	36,36,36,36	0
82	MG	1	3461	1/1	0.86	0.20	37,37,37,37	0
82	MG	CM	1928	1/1	0.86	0.11	60,60,60,60	0
82	MG	1	3650	1/1	0.86	0.31	53,53,53,53	0
82	MG	1	3614	1/1	0.86	0.19	37,37,37,37	0
82	MG	AS	3671	1/1	0.86	0.13	56,56,56,56	0
82	MG	1	3763	1/1	0.86	0.10	32,32,32,32	0
82	MG	AS	3605	1/1	0.86	0.28	24,24,24,24	0
82	MG	CM	1856	1/1	0.86	0.28	72,72,72,72	0
82	MG	AS	3436	1/1	0.86	0.27	48,48,48,48	0
82	MG	AS	3475	1/1	0.86	0.15	37,37,37,37	0
82	MG	CM	1863	1/1	0.86	0.33	41,41,41,41	0
82	MG	AS	3529	1/1	0.86	0.07	34,34,34,34	0
82	MG	1	3462	1/1	0.86	0.22	40,40,40,40	0
82	MG	B	1896	1/1	0.86	0.09	48,48,48,48	0
82	MG	AY	401	1/1	0.86	0.34	57,57,57,57	0
82	MG	CJ	202	1/1	0.86	0.24	53,53,53,53	0
82	MG	1	3509	1/1	0.86	0.14	42,42,42,42	0
82	MG	B	1861	1/1	0.87	0.26	33,33,33,33	0
82	MG	1	3446	1/1	0.87	0.07	31,31,31,31	0
82	MG	CM	1811	1/1	0.87	0.26	54,54,54,54	0
82	MG	B	1912	1/1	0.87	0.20	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3603	1/1	0.87	0.20	23,23,23,23	0
82	MG	B	1868	1/1	0.87	0.43	63,63,63,63	0
82	MG	1	3609	1/1	0.87	0.14	42,42,42,42	0
82	MG	1	3716	1/1	0.87	0.19	37,37,37,37	0
82	MG	B	1872	1/1	0.87	0.18	50,50,50,50	0
82	MG	1	3766	1/1	0.87	0.15	31,31,31,31	0
82	MG	CM	1823	1/1	0.87	0.27	60,60,60,60	0
82	MG	AS	3705	1/1	0.87	0.18	52,52,52,52	0
82	MG	B	1832	1/1	0.87	0.24	41,41,41,41	0
82	MG	AS	3550	1/1	0.87	0.18	44,44,44,44	0
82	MG	AS	3433	1/1	0.87	0.24	49,49,49,49	0
82	MG	B	1875	1/1	0.87	0.10	53,53,53,53	0
82	MG	1	3456	1/1	0.87	0.16	31,31,31,31	0
82	MG	6	202	1/1	0.87	0.14	20,20,20,20	0
82	MG	1	3735	1/1	0.87	0.16	34,34,34,34	0
82	MG	B	1885	1/1	0.87	0.27	54,54,54,54	0
82	MG	AS	3648	1/1	0.87	0.12	41,41,41,41	0
82	MG	B	1807	1/1	0.87	0.31	59,59,59,59	0
82	MG	1	3719	1/1	0.87	0.25	59,59,59,59	0
82	MG	1	3612	1/1	0.87	0.24	40,40,40,40	0
82	MG	1	3576	1/1	0.87	0.30	28,28,28,28	0
82	MG	AS	3574	1/1	0.87	0.23	30,30,30,30	0
82	MG	AS	3448	1/1	0.87	0.14	25,25,25,25	0
82	MG	B	1847	1/1	0.87	0.17	33,33,33,33	0
82	MG	CM	1847	1/1	0.87	0.11	38,38,38,38	0
82	MG	B	1938	1/1	0.87	0.22	39,39,39,39	0
82	MG	AS	3731	1/1	0.87	0.24	53,53,53,53	0
82	MG	1	3537	1/1	0.87	0.16	42,42,42,42	0
82	MG	AS	3735	1/1	0.87	0.09	35,35,35,35	0
82	MG	1	3776	1/1	0.87	0.21	63,63,63,63	0
82	MG	B	1900	1/1	0.87	0.33	41,41,41,41	0
81	PAR	1	3421	42/42	0.87	0.14	53,69,76,90	42
82	MG	1	3436	1/1	0.87	0.11	38,38,38,38	0
82	MG	AS	3459	1/1	0.87	0.27	62,62,62,62	0
82	MG	F	301	1/1	0.87	0.14	39,39,39,39	0
82	MG	AS	3604	1/1	0.87	0.24	46,46,46,46	0
82	MG	AW	301	1/1	0.87	0.11	50,50,50,50	0
82	MG	1	3491	1/1	0.87	0.20	48,48,48,48	0
82	MG	B	1820	1/1	0.87	0.15	53,53,53,53	0
82	MG	AS	3520	1/1	0.87	0.16	70,70,70,70	0
82	MG	CM	1870	1/1	0.87	0.27	41,41,41,41	0
82	MG	CM	1807	1/1	0.87	0.23	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	ZN	CJ	201	1/1	0.87	0.09	187,187,187,187	0
82	MG	AS	3521	1/1	0.87	0.13	60,60,60,60	0
82	MG	B	1923	1/1	0.88	0.29	49,49,49,49	0
81	PAR	CM	1803	42/42	0.88	0.19	46,63,93,101	0
82	MG	CM	1880	1/1	0.88	0.25	54,54,54,54	0
82	MG	1	3738	1/1	0.88	0.15	55,55,55,55	0
82	MG	B	1886	1/1	0.88	0.27	46,46,46,46	0
82	MG	AS	3700	1/1	0.88	0.16	32,32,32,32	0
82	MG	AS	3434	1/1	0.88	0.24	83,83,83,83	0
82	MG	1	3558	1/1	0.88	0.19	52,52,52,52	0
82	MG	B	1842	1/1	0.88	0.19	45,45,45,45	0
82	MG	1	3641	1/1	0.88	0.16	50,50,50,50	0
82	MG	AS	3542	1/1	0.88	0.22	26,26,26,26	0
81	PAR	1	3429	42/42	0.88	0.14	37,61,77,89	0
82	MG	1	3665	1/1	0.88	0.12	54,54,54,54	0
82	MG	AS	3485	1/1	0.88	0.28	65,65,65,65	0
82	MG	1	3667	1/1	0.88	0.10	35,35,35,35	0
82	MG	1	3646	1/1	0.88	0.13	38,38,38,38	0
82	MG	1	3647	1/1	0.88	0.09	30,30,30,30	0
82	MG	AS	3646	1/1	0.88	0.15	66,66,66,66	0
82	MG	CM	1901	1/1	0.88	0.11	39,39,39,39	0
82	MG	1	3511	1/1	0.88	0.34	52,52,52,52	0
82	MG	AS	3721	1/1	0.88	0.31	71,71,71,71	0
82	MG	1	3536	1/1	0.88	0.12	54,54,54,54	0
82	MG	AS	3566	1/1	0.88	0.13	43,43,43,43	0
82	MG	1	3680	1/1	0.88	0.19	25,25,25,25	0
82	MG	1	3450	1/1	0.88	0.09	32,32,32,32	0
80	3K5	1	3401	57/57	0.88	0.19	42,65,85,102	0
82	MG	1	3452	1/1	0.88	0.12	46,46,46,46	0
82	MG	AS	3575	1/1	0.88	0.16	47,47,47,47	0
82	MG	CM	1917	1/1	0.88	0.21	58,58,58,58	0
82	MG	1	3588	1/1	0.88	0.10	28,28,28,28	0
82	MG	B	1829	1/1	0.88	0.25	36,36,36,36	0
82	MG	CM	1920	1/1	0.88	0.22	60,60,60,60	0
82	MG	CM	1922	1/1	0.88	0.20	45,45,45,45	0
82	MG	CM	1849	1/1	0.88	0.09	58,58,58,58	0
82	MG	1	3591	1/1	0.88	0.17	31,31,31,31	0
82	MG	AS	3417	1/1	0.88	0.15	50,50,50,50	0
82	MG	AS	3737	1/1	0.88	0.20	61,61,61,61	0
82	MG	B	1915	1/1	0.88	0.14	43,43,43,43	0
82	MG	AS	3509	1/1	0.88	0.18	44,44,44,44	0
82	MG	AS	3741	1/1	0.88	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3511	1/1	0.88	0.13	37,37,37,37	0
82	MG	1	3551	1/1	0.88	0.18	45,45,45,45	0
82	MG	AS	3421	1/1	0.88	0.14	60,60,60,60	0
82	MG	AS	3518	1/1	0.88	0.11	27,27,27,27	0
82	MG	1	3594	1/1	0.88	0.24	54,54,54,54	0
82	MG	v	303	1/1	0.88	0.09	39,39,39,39	0
82	MG	AS	3683	1/1	0.88	0.22	39,39,39,39	0
82	MG	AS	3606	1/1	0.88	0.12	33,33,33,33	0
82	MG	AS	3425	1/1	0.88	0.15	44,44,44,44	0
82	MG	DK	201	1/1	0.88	0.18	44,44,44,44	0
82	MG	AS	3522	1/1	0.88	0.11	52,52,52,52	0
82	MG	1	3659	1/1	0.88	0.17	45,45,45,45	0
82	MG	w	301	1/1	0.88	0.27	52,52,52,52	0
82	MG	AS	3704	1/1	0.89	0.10	61,61,61,61	0
82	MG	1	3527	1/1	0.89	0.12	22,22,22,22	0
82	MG	AS	3707	1/1	0.89	0.21	50,50,50,50	0
82	MG	1	3542	1/1	0.89	0.32	40,40,40,40	0
82	MG	1	3662	1/1	0.89	0.09	48,48,48,48	0
82	MG	B	1939	1/1	0.89	0.13	41,41,41,41	0
82	MG	B	1879	1/1	0.89	0.26	51,51,51,51	0
82	MG	1	3489	1/1	0.89	0.23	34,34,34,34	0
82	MG	AS	3473	1/1	0.89	0.39	65,65,65,65	0
82	MG	1	3467	1/1	0.89	0.32	48,48,48,48	0
82	MG	AS	3653	1/1	0.89	0.11	28,28,28,28	0
82	MG	B	1851	1/1	0.89	0.09	49,49,49,49	0
82	MG	CM	1834	1/1	0.89	0.36	63,63,63,63	0
82	MG	B	1945	1/1	0.89	0.16	67,67,67,67	0
82	MG	CM	1899	1/1	0.89	0.24	43,43,43,43	0
82	MG	AS	3656	1/1	0.89	0.10	50,50,50,50	0
82	MG	C	301	1/1	0.89	0.35	66,66,66,66	0
82	MG	6	201	1/1	0.89	0.19	49,49,49,49	0
82	MG	AS	3595	1/1	0.89	0.21	60,60,60,60	0
82	MG	1	3688	1/1	0.89	0.10	32,32,32,32	0
82	MG	AS	3664	1/1	0.89	0.16	45,45,45,45	0
82	MG	AS	3601	1/1	0.89	0.30	41,41,41,41	0
82	MG	CM	1908	1/1	0.89	0.23	43,43,43,43	0
82	MG	B	1888	1/1	0.89	0.12	49,49,49,49	0
82	MG	AS	3603	1/1	0.89	0.19	43,43,43,43	0
82	MG	1	3557	1/1	0.89	0.22	26,26,26,26	0
82	MG	AS	3673	1/1	0.89	0.18	44,44,44,44	0
82	MG	B	1860	1/1	0.89	0.15	51,51,51,51	0
82	MG	1	3666	1/1	0.89	0.24	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3418	1/1	0.89	0.14	35,35,35,35	0
82	MG	1	3695	1/1	0.89	0.12	36,36,36,36	0
82	MG	CM	1921	1/1	0.89	0.09	57,57,57,57	0
82	MG	1	3616	1/1	0.89	0.28	51,51,51,51	0
82	MG	4	204	1/1	0.89	0.15	51,51,51,51	0
82	MG	AS	3544	1/1	0.89	0.22	30,30,30,30	0
82	MG	AS	3684	1/1	0.89	0.12	85,85,85,85	0
82	MG	AS	3747	1/1	0.89	0.12	41,41,41,41	0
82	MG	CM	1858	1/1	0.89	0.13	45,45,45,45	0
82	MG	CM	1859	1/1	0.89	0.20	36,36,36,36	0
82	MG	AS	3546	1/1	0.89	0.26	31,31,31,31	0
82	MG	CM	1935	1/1	0.89	0.15	53,53,53,53	0
82	MG	CM	1936	1/1	0.89	0.16	64,64,64,64	0
82	MG	B	1899	1/1	0.89	0.13	42,42,42,42	0
82	MG	AS	3457	1/1	0.89	0.19	43,43,43,43	0
82	MG	AS	3458	1/1	0.89	0.18	40,40,40,40	0
82	MG	1	3496	1/1	0.89	0.22	39,39,39,39	0
82	MG	AS	3498	1/1	0.89	0.20	45,45,45,45	0
82	MG	1	3606	1/1	0.89	0.16	29,29,29,29	0
82	MG	B	1931	1/1	0.89	0.13	52,52,52,52	0
82	MG	AS	3697	1/1	0.89	0.24	46,46,46,46	0
82	MG	AS	3503	1/1	0.89	0.11	44,44,44,44	0
82	MG	1	3608	1/1	0.89	0.26	34,34,34,34	0
82	MG	CM	1877	1/1	0.89	0.09	53,53,53,53	0
82	MG	AS	3637	1/1	0.89	0.11	73,73,73,73	0
82	MG	1	3705	1/1	0.89	0.09	23,23,23,23	0
82	MG	AS	3531	1/1	0.90	0.17	72,72,72,72	0
82	MG	4	205	1/1	0.90	0.10	36,36,36,36	0
82	MG	1	3760	1/1	0.90	0.21	49,49,49,49	0
82	MG	AS	3480	1/1	0.90	0.13	28,28,28,28	0
82	MG	4	207	1/1	0.90	0.14	35,35,35,35	0
82	MG	AS	3437	1/1	0.90	0.19	63,63,63,63	0
82	MG	AS	3541	1/1	0.90	0.19	49,49,49,49	0
82	MG	CM	1821	1/1	0.90	0.12	61,61,61,61	0
82	MG	4	208	1/1	0.90	0.26	33,33,33,33	0
82	MG	B	1819	1/1	0.90	0.20	66,66,66,66	0
82	MG	CM	1824	1/1	0.90	0.20	68,68,68,68	0
82	MG	1	3670	1/1	0.90	0.17	41,41,41,41	0
82	MG	B	1857	1/1	0.90	0.16	39,39,39,39	0
82	MG	1	3550	1/1	0.90	0.14	21,21,21,21	0
82	MG	1	3589	1/1	0.90	0.29	36,36,36,36	0
82	MG	CM	1898	1/1	0.90	0.19	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	v	301	1/1	0.90	0.06	36,36,36,36	0
82	MG	AS	3491	1/1	0.90	0.18	55,55,55,55	0
82	MG	AS	3640	1/1	0.90	0.08	46,46,46,46	0
82	MG	AS	3561	1/1	0.90	0.21	32,32,32,32	0
82	MG	AS	3715	1/1	0.90	0.17	45,45,45,45	0
82	MG	AS	3644	1/1	0.90	0.10	56,56,56,56	0
82	MG	B	1863	1/1	0.90	0.17	74,74,74,74	0
82	MG	B	1828	1/1	0.90	0.23	48,48,48,48	0
82	MG	B	1905	1/1	0.90	0.31	42,42,42,42	0
82	MG	AS	3495	1/1	0.90	0.08	28,28,28,28	0
82	MG	CM	1910	1/1	0.90	0.12	67,67,67,67	0
82	MG	AS	3496	1/1	0.90	0.10	36,36,36,36	0
82	MG	CM	1913	1/1	0.90	0.29	46,46,46,46	0
82	MG	1	3476	1/1	0.90	0.13	38,38,38,38	0
82	MG	AS	3652	1/1	0.90	0.14	48,48,48,48	0
82	MG	B	1907	1/1	0.90	0.34	48,48,48,48	0
82	MG	1	3632	1/1	0.90	0.11	15,15,15,15	0
82	MG	1	3700	1/1	0.90	0.09	28,28,28,28	0
82	MG	1	3577	1/1	0.90	0.07	29,29,29,29	0
82	MG	1	3568	1/1	0.90	0.13	43,43,43,43	0
82	MG	AS	3579	1/1	0.90	0.20	49,49,49,49	0
82	MG	1	3569	1/1	0.90	0.16	35,35,35,35	0
82	MG	1	3710	1/1	0.90	0.09	37,37,37,37	0
82	MG	AS	3584	1/1	0.90	0.23	29,29,29,29	0
82	MG	1	3686	1/1	0.90	0.13	40,40,40,40	0
82	MG	1	3715	1/1	0.90	0.11	43,43,43,43	0
82	MG	CM	1931	1/1	0.90	0.29	55,55,55,55	0
82	MG	1	3548	1/1	0.90	0.12	33,33,33,33	0
82	MG	AS	3422	1/1	0.90	0.11	56,56,56,56	0
82	MG	1	3717	1/1	0.90	0.30	53,53,53,53	0
82	MG	B	1881	1/1	0.90	0.15	54,54,54,54	0
82	MG	B	1922	1/1	0.90	0.24	43,43,43,43	0
82	MG	AS	3745	1/1	0.90	0.29	49,49,49,49	0
82	MG	B	1882	1/1	0.90	0.21	36,36,36,36	0
82	MG	B	1883	1/1	0.90	0.27	37,37,37,37	0
82	MG	CM	1868	1/1	0.90	0.22	39,39,39,39	0
82	MG	B	1843	1/1	0.90	0.20	37,37,37,37	0
82	MG	AS	3429	1/1	0.90	0.10	38,38,38,38	0
82	MG	CM	1945	1/1	0.90	0.17	74,74,74,74	0
82	MG	AS	3527	1/1	0.90	0.29	59,59,59,59	0
82	MG	AS	3608	1/1	0.90	0.20	38,38,38,38	0
82	MG	AS	3609	1/1	0.90	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	CL	301	1/1	0.90	0.15	87,87,87,87	0
82	MG	B	1844	1/1	0.90	0.23	51,51,51,51	0
82	MG	1	3690	1/1	0.90	0.07	40,40,40,40	0
82	MG	1	3669	1/1	0.90	0.11	46,46,46,46	0
82	MG	1	3673	1/1	0.91	0.08	22,22,22,22	0
82	MG	1	3517	1/1	0.91	0.13	36,36,36,36	0
82	MG	1	3601	1/1	0.91	0.14	43,43,43,43	0
82	MG	B	1909	1/1	0.91	0.14	43,43,43,43	0
82	MG	AS	3462	1/1	0.91	0.12	54,54,54,54	0
82	MG	AS	3734	1/1	0.91	0.28	49,49,49,49	0
82	MG	1	3629	1/1	0.91	0.08	52,52,52,52	0
82	MG	AS	3547	1/1	0.91	0.19	25,25,25,25	0
82	MG	CM	1904	1/1	0.91	0.09	43,43,43,43	0
82	MG	AS	3549	1/1	0.91	0.14	32,32,32,32	0
82	MG	1	3556	1/1	0.91	0.15	25,25,25,25	0
82	MG	AS	3551	1/1	0.91	0.15	32,32,32,32	0
82	MG	1	3492	1/1	0.91	0.19	29,29,29,29	0
82	MG	B	1859	1/1	0.91	0.38	38,38,38,38	0
82	MG	AS	3502	1/1	0.91	0.14	39,39,39,39	0
82	MG	1	3512	1/1	0.91	0.12	27,27,27,27	0
82	MG	AS	3468	1/1	0.91	0.17	56,56,56,56	0
82	MG	AS	3746	1/1	0.91	0.07	40,40,40,40	0
82	MG	AS	3625	1/1	0.91	0.07	35,35,35,35	0
82	MG	AS	3562	1/1	0.91	0.08	37,37,37,37	0
82	MG	B	1811	1/1	0.91	0.29	49,49,49,49	0
82	MG	B	1944	1/1	0.91	0.20	30,30,30,30	0
82	MG	AS	3471	1/1	0.91	0.08	27,27,27,27	0
82	MG	AS	3510	1/1	0.91	0.17	40,40,40,40	0
82	MG	1	3474	1/1	0.91	0.13	27,27,27,27	0
82	MG	CM	1923	1/1	0.91	0.29	58,58,58,58	0
82	MG	1	3709	1/1	0.91	0.16	29,29,29,29	0
82	MG	AS	3569	1/1	0.91	0.17	36,36,36,36	0
82	MG	1	3546	1/1	0.91	0.22	43,43,43,43	0
82	MG	B	1893	1/1	0.91	0.31	51,51,51,51	0
82	MG	B	1921	1/1	0.91	0.17	38,38,38,38	0
82	MG	AS	3641	1/1	0.91	0.12	29,29,29,29	0
82	MG	AS	3642	1/1	0.91	0.18	49,49,49,49	0
82	MG	K	301	1/1	0.91	0.18	54,54,54,54	0
82	MG	f	102	1/1	0.91	0.10	55,55,55,55	0
82	MG	1	3732	1/1	0.91	0.20	39,39,39,39	0
82	MG	1	3534	1/1	0.91	0.15	16,16,16,16	0
82	MG	B	1924	1/1	0.91	0.24	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3435	1/1	0.91	0.19	38,38,38,38	0
82	MG	AS	3451	1/1	0.91	0.14	59,59,59,59	0
82	MG	1	3639	1/1	0.91	0.20	56,56,56,56	0
82	MG	B	1821	1/1	0.91	0.15	55,55,55,55	0
82	MG	AS	3590	1/1	0.91	0.23	26,26,26,26	0
82	MG	CM	1944	1/1	0.91	0.26	63,63,63,63	0
82	MG	CM	1886	1/1	0.91	0.24	44,44,44,44	0
82	MG	AS	3591	1/1	0.91	0.22	38,38,38,38	0
82	MG	B	1846	1/1	0.91	0.28	52,52,52,52	0
82	MG	AS	3594	1/1	0.91	0.15	32,32,32,32	0
82	MG	1	3480	1/1	0.91	0.27	55,55,55,55	0
82	MG	AS	3596	1/1	0.91	0.17	65,65,65,65	0
82	MG	1	3694	1/1	0.91	0.13	37,37,37,37	0
82	MG	B	1826	1/1	0.91	0.17	64,64,64,64	0
82	MG	1	3599	1/1	0.92	0.18	20,20,20,20	0
82	MG	AS	3582	1/1	0.92	0.17	25,25,25,25	0
82	MG	1	3655	1/1	0.92	0.13	20,20,20,20	0
82	MG	AS	3708	1/1	0.92	0.24	38,38,38,38	0
82	MG	AS	3445	1/1	0.92	0.11	46,46,46,46	0
82	MG	v	304	1/1	0.92	0.22	50,50,50,50	0
82	MG	1	3486	1/1	0.92	0.18	36,36,36,36	0
82	MG	AS	3712	1/1	0.92	0.11	41,41,41,41	0
82	MG	1	3493	1/1	0.92	0.20	50,50,50,50	0
82	MG	1	3602	1/1	0.92	0.11	16,16,16,16	0
82	MG	1	3478	1/1	0.92	0.06	44,44,44,44	0
82	MG	1	3769	1/1	0.92	0.13	34,34,34,34	0
82	MG	AB	201	1/1	0.92	0.13	26,26,26,26	0
82	MG	AS	3539	1/1	0.92	0.14	31,31,31,31	0
82	MG	1	3582	1/1	0.92	0.22	31,31,31,31	0
82	MG	B	1878	1/1	0.92	0.16	41,41,41,41	0
82	MG	B	1806	1/1	0.92	0.16	38,38,38,38	0
82	MG	1	3562	1/1	0.92	0.19	29,29,29,29	0
82	MG	1	3586	1/1	0.92	0.25	30,30,30,30	0
82	MG	1	3773	1/1	0.92	0.11	49,49,49,49	0
82	MG	AS	3661	1/1	0.92	0.28	33,33,33,33	0
82	MG	1	3640	1/1	0.92	0.10	32,32,32,32	0
82	MG	CM	1911	1/1	0.92	0.12	70,70,70,70	0
82	MG	AS	3607	1/1	0.92	0.19	32,32,32,32	0
82	MG	1	3504	1/1	0.92	0.12	36,36,36,36	0
82	MG	1	3475	1/1	0.92	0.17	25,25,25,25	0
82	MG	AS	3612	1/1	0.92	0.07	51,51,51,51	0
82	MG	AS	3500	1/1	0.92	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3470	1/1	0.92	0.32	73,73,73,73	0
82	MG	1	3592	1/1	0.92	0.24	37,37,37,37	0
82	MG	AS	3676	1/1	0.92	0.06	43,43,43,43	0
82	MG	AS	3677	1/1	0.92	0.09	59,59,59,59	0
82	MG	1	3554	1/1	0.92	0.21	34,34,34,34	0
82	MG	1	3617	1/1	0.92	0.22	26,26,26,26	0
82	MG	B	1818	1/1	0.92	0.42	58,58,58,58	0
82	MG	CM	1925	1/1	0.92	0.24	34,34,34,34	0
82	MG	1	3623	1/1	0.92	0.17	36,36,36,36	0
82	MG	CM	1927	1/1	0.92	0.19	52,52,52,52	0
82	MG	AS	3622	1/1	0.92	0.32	38,38,38,38	0
82	MG	1	3671	1/1	0.92	0.09	53,53,53,53	0
82	MG	B	1894	1/1	0.92	0.15	39,39,39,39	0
82	MG	B	1854	1/1	0.92	0.14	37,37,37,37	0
82	MG	AT	201	1/1	0.92	0.12	37,37,37,37	0
82	MG	AS	3512	1/1	0.92	0.16	36,36,36,36	0
82	MG	CM	1867	1/1	0.92	0.16	49,49,49,49	0
82	MG	AS	3513	1/1	0.92	0.31	31,31,31,31	0
82	MG	AS	3688	1/1	0.92	0.20	45,45,45,45	0
82	MG	AX	401	1/1	0.92	0.25	43,43,43,43	0
82	MG	CM	1872	1/1	0.92	0.20	52,52,52,52	0
82	MG	1	3441	1/1	0.92	0.25	41,41,41,41	0
82	MG	1	3595	1/1	0.92	0.19	26,26,26,26	0
82	MG	B	1936	1/1	0.92	0.08	59,59,59,59	0
82	MG	AS	3634	1/1	0.92	0.09	42,42,42,42	0
82	MG	AS	3635	1/1	0.92	0.08	43,43,43,43	0
82	MG	AS	3694	1/1	0.92	0.20	53,53,53,53	0
82	MG	1	3707	1/1	0.92	0.22	34,34,34,34	0
82	MG	B	1824	1/1	0.92	0.19	25,25,25,25	0
82	MG	DJ	201	1/1	0.92	0.14	38,38,38,38	0
82	MG	B	1825	1/1	0.92	0.23	44,44,44,44	0
82	MG	AS	3701	1/1	0.92	0.19	34,34,34,34	0
83	ZN	AH	201	1/1	0.92	0.16	134,134,134,134	0
82	MG	B	1862	1/1	0.92	0.16	41,41,41,41	0
83	ZN	h	201	1/1	0.92	0.10	165,165,165,165	0
82	MG	1	3708	1/1	0.92	0.23	25,25,25,25	0
82	MG	CM	1819	1/1	0.92	0.30	58,58,58,58	0
82	MG	1	3561	1/1	0.93	0.23	23,23,23,23	0
82	MG	1	3627	1/1	0.93	0.14	34,34,34,34	0
82	MG	1	3652	1/1	0.93	0.13	35,35,35,35	0
82	MG	AS	3545	1/1	0.93	0.17	38,38,38,38	0
82	MG	AS	3649	1/1	0.93	0.08	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3674	1/1	0.93	0.18	18,18,18,18	0
82	MG	1	3583	1/1	0.93	0.20	40,40,40,40	0
82	MG	B	1864	1/1	0.93	0.21	30,30,30,30	0
82	MG	AS	3706	1/1	0.93	0.37	49,49,49,49	0
82	MG	B	1934	1/1	0.93	0.20	30,30,30,30	0
82	MG	AS	3431	1/1	0.93	0.20	25,25,25,25	0
82	MG	CM	1915	1/1	0.93	0.08	42,42,42,42	0
82	MG	1	3524	1/1	0.93	0.15	32,32,32,32	0
82	MG	1	3604	1/1	0.93	0.25	24,24,24,24	0
82	MG	AS	3554	1/1	0.93	0.27	36,36,36,36	0
82	MG	1	3605	1/1	0.93	0.18	29,29,29,29	0
82	MG	CM	1814	1/1	0.93	0.24	56,56,56,56	0
82	MG	B	1833	1/1	0.93	0.20	38,38,38,38	0
82	MG	1	3508	1/1	0.93	0.17	27,27,27,27	0
82	MG	AP	203	1/1	0.93	0.14	33,33,33,33	0
82	MG	1	3741	1/1	0.93	0.14	46,46,46,46	0
82	MG	AS	3665	1/1	0.93	0.09	40,40,40,40	0
82	MG	AS	3439	1/1	0.93	0.13	50,50,50,50	0
82	MG	AS	3515	1/1	0.93	0.09	43,43,43,43	0
82	MG	1	3713	1/1	0.93	0.14	21,21,21,21	0
82	MG	1	3466	1/1	0.93	0.11	24,24,24,24	0
82	MG	CM	1878	1/1	0.93	0.24	42,42,42,42	0
82	MG	B	1911	1/1	0.93	0.17	58,58,58,58	0
82	MG	CM	1826	1/1	0.93	0.11	28,28,28,28	0
82	MG	1	3570	1/1	0.93	0.08	38,38,38,38	0
82	MG	CM	1934	1/1	0.93	0.23	53,53,53,53	0
82	MG	1	3685	1/1	0.93	0.12	43,43,43,43	0
82	MG	1	3514	1/1	0.93	0.22	45,45,45,45	0
82	MG	AS	3523	1/1	0.93	0.24	34,34,34,34	0
82	MG	AS	3576	1/1	0.93	0.14	42,42,42,42	0
82	MG	1	3748	1/1	0.93	0.15	55,55,55,55	0
82	MG	1	3687	1/1	0.93	0.24	22,22,22,22	0
82	MG	1	3438	1/1	0.93	0.10	35,35,35,35	0
82	MG	AS	3633	1/1	0.93	0.09	28,28,28,28	0
82	MG	1	3613	1/1	0.93	0.22	30,30,30,30	0
82	MG	1	3449	1/1	0.93	0.21	32,32,32,32	0
82	MG	CM	1893	1/1	0.93	0.14	51,51,51,51	0
82	MG	B	1817	1/1	0.93	0.16	48,48,48,48	0
82	MG	1	3544	1/1	0.93	0.12	26,26,26,26	0
82	MG	1	3643	1/1	0.93	0.09	39,39,39,39	0
82	MG	1	3523	1/1	0.93	0.08	28,28,28,28	0
82	MG	1	3560	1/1	0.93	0.17	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3581	1/1	0.93	0.10	16,16,16,16	0
82	MG	CM	1846	1/1	0.93	0.06	44,44,44,44	0
82	MG	1	3730	1/1	0.93	0.22	42,42,42,42	0
82	MG	1	3625	1/1	0.93	0.20	24,24,24,24	0
82	MG	AS	3593	1/1	0.93	0.23	40,40,40,40	0
82	MG	1	3566	1/1	0.94	0.23	19,19,19,19	0
82	MG	1	3553	1/1	0.94	0.16	25,25,25,25	0
82	MG	1	3433	1/1	0.94	0.14	35,35,35,35	0
82	MG	B	1834	1/1	0.94	0.09	43,43,43,43	0
82	MG	CM	1861	1/1	0.94	0.09	46,46,46,46	0
82	MG	AS	3616	1/1	0.94	0.18	71,71,71,71	0
82	MG	B	1889	1/1	0.94	0.06	32,32,32,32	0
82	MG	AS	3570	1/1	0.94	0.11	66,66,66,66	0
82	MG	AS	3663	1/1	0.94	0.21	47,47,47,47	0
82	MG	AS	3571	1/1	0.94	0.17	23,23,23,23	0
82	MG	1	3607	1/1	0.94	0.19	29,29,29,29	0
82	MG	1	3543	1/1	0.94	0.19	20,20,20,20	0
82	MG	1	3590	1/1	0.94	0.09	35,35,35,35	0
82	MG	1	3571	1/1	0.94	0.23	18,18,18,18	0
82	MG	AS	3624	1/1	0.94	0.11	34,34,34,34	0
82	MG	AS	3535	1/1	0.94	0.17	39,39,39,39	0
82	MG	1	3529	1/1	0.94	0.15	28,28,28,28	0
82	MG	1	3473	1/1	0.94	0.20	59,59,59,59	0
82	MG	B	1869	1/1	0.94	0.19	38,38,38,38	0
82	MG	B	1897	1/1	0.94	0.26	59,59,59,59	0
82	MG	AS	3726	1/1	0.94	0.36	53,53,53,53	0
82	MG	CM	1828	1/1	0.94	0.17	29,29,29,29	0
82	MG	1	3744	1/1	0.94	0.22	47,47,47,47	0
82	MG	AS	3506	1/1	0.94	0.13	35,35,35,35	0
82	MG	AS	3543	1/1	0.94	0.13	31,31,31,31	0
82	MG	AS	3476	1/1	0.94	0.20	30,30,30,30	0
82	MG	1	3547	1/1	0.94	0.17	42,42,42,42	0
82	MG	1	3676	1/1	0.94	0.17	36,36,36,36	0
82	MG	1	3497	1/1	0.94	0.18	32,32,32,32	0
82	MG	1	3678	1/1	0.94	0.11	50,50,50,50	0
82	MG	1	3703	1/1	0.94	0.23	18,18,18,18	0
82	MG	CM	1889	1/1	0.94	0.08	50,50,50,50	0
82	MG	1	3443	1/1	0.94	0.09	36,36,36,36	0
82	MG	B	1877	1/1	0.94	0.24	42,42,42,42	0
82	MG	1	3533	1/1	0.94	0.07	22,22,22,22	0
82	MG	AS	3597	1/1	0.94	0.22	33,33,33,33	0
82	MG	AS	3517	1/1	0.94	0.08	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3599	1/1	0.94	0.36	59,59,59,59	0
82	MG	AS	3600	1/1	0.94	0.21	38,38,38,38	0
82	MG	AS	3696	1/1	0.94	0.19	42,42,42,42	0
82	MG	AS	3555	1/1	0.94	0.09	34,34,34,34	0
82	MG	AS	3698	1/1	0.94	0.21	42,42,42,42	0
82	MG	AS	3556	1/1	0.94	0.23	22,22,22,22	0
82	MG	1	3774	1/1	0.94	0.18	57,57,57,57	0
82	MG	1	3563	1/1	0.94	0.21	25,25,25,25	0
82	MG	AP	202	1/1	0.94	0.16	61,61,61,61	0
82	MG	1	3644	1/1	0.94	0.10	34,34,34,34	0
82	MG	1	3564	1/1	0.94	0.17	29,29,29,29	0
82	MG	1	3565	1/1	0.94	0.22	29,29,29,29	0
82	MG	1	3487	1/1	0.95	0.04	24,24,24,24	0
82	MG	1	3714	1/1	0.95	0.15	28,28,28,28	0
82	MG	AS	3675	1/1	0.95	0.06	38,38,38,38	0
82	MG	AS	3739	1/1	0.95	0.05	36,36,36,36	0
82	MG	AS	3587	1/1	0.95	0.08	20,20,20,20	0
82	MG	AS	3588	1/1	0.95	0.17	20,20,20,20	0
82	MG	1	3528	1/1	0.95	0.15	31,31,31,31	0
82	MG	1	3699	1/1	0.95	0.08	34,34,34,34	0
82	MG	1	3559	1/1	0.95	0.21	16,16,16,16	0
82	MG	1	3506	1/1	0.95	0.10	33,33,33,33	0
82	MG	1	3575	1/1	0.95	0.10	33,33,33,33	0
82	MG	1	3720	1/1	0.95	0.15	25,25,25,25	0
82	MG	B	1856	1/1	0.95	0.26	45,45,45,45	0
82	MG	AS	3416	1/1	0.95	0.12	55,55,55,55	0
82	MG	1	3704	1/1	0.95	0.06	19,19,19,19	0
82	MG	AW	302	1/1	0.95	0.11	31,31,31,31	0
82	MG	1	3549	1/1	0.95	0.14	39,39,39,39	0
82	MG	1	3723	1/1	0.95	0.21	27,27,27,27	0
82	MG	AS	3573	1/1	0.95	0.12	43,43,43,43	0
82	MG	AS	3658	1/1	0.95	0.12	51,51,51,51	0
82	MG	AS	3548	1/1	0.95	0.15	37,37,37,37	0
82	MG	1	3691	1/1	0.95	0.10	36,36,36,36	0
82	MG	1	3631	1/1	0.95	0.06	37,37,37,37	0
82	MG	1	3585	1/1	0.95	0.07	33,33,33,33	0
82	MG	AS	3484	1/1	0.95	0.13	39,39,39,39	0
82	MG	1	3526	1/1	0.95	0.19	22,22,22,22	0
82	MG	1	3597	1/1	0.95	0.17	26,26,26,26	0
82	MG	AS	3666	1/1	0.95	0.09	73,73,73,73	0
82	MG	1	3711	1/1	0.95	0.07	40,40,40,40	0
82	MG	1	3622	1/1	0.95	0.28	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3733	1/1	0.95	0.09	45,45,45,45	0
83	ZN	CB	201	1/1	0.95	0.06	159,159,159,159	0
82	MG	AS	3533	1/1	0.95	0.11	39,39,39,39	0
82	MG	AS	3613	1/1	0.95	0.09	55,55,55,55	0
82	MG	1	3580	1/1	0.96	0.18	27,27,27,27	0
82	MG	1	3540	1/1	0.96	0.21	25,25,25,25	0
82	MG	1	3494	1/1	0.96	0.07	23,23,23,23	0
82	MG	1	3596	1/1	0.96	0.04	11,11,11,11	0
82	MG	AS	3443	1/1	0.96	0.10	18,18,18,18	0
82	MG	1	3573	1/1	0.96	0.17	31,31,31,31	0
82	MG	B	1865	1/1	0.96	0.15	31,31,31,31	0
82	MG	1	3610	1/1	0.96	0.20	41,41,41,41	0
82	MG	CM	1860	1/1	0.96	0.26	46,46,46,46	0
82	MG	AS	3558	1/1	0.96	0.22	26,26,26,26	0
82	MG	CM	1836	1/1	0.96	0.18	56,56,56,56	0
82	MG	AS	3559	1/1	0.96	0.16	39,39,39,39	0
82	MG	1	3619	1/1	0.96	0.28	22,22,22,22	0
82	MG	1	3689	1/1	0.96	0.06	28,28,28,28	0
82	MG	1	3702	1/1	0.96	0.15	23,23,23,23	0
82	MG	AS	3583	1/1	0.96	0.14	17,17,17,17	0
82	MG	CM	1817	1/1	0.96	0.18	43,43,43,43	0
82	MG	1	3620	1/1	0.96	0.20	25,25,25,25	0
82	MG	B	1903	1/1	0.96	0.14	48,48,48,48	0
82	MG	AS	3722	1/1	0.96	0.05	39,39,39,39	0
82	MG	B	1855	1/1	0.96	0.16	27,27,27,27	0
83	ZN	AP	201	1/1	0.96	0.08	153,153,153,153	0
82	MG	B	1841	1/1	0.96	0.15	40,40,40,40	0
82	MG	1	3621	1/1	0.96	0.18	23,23,23,23	0
82	MG	AS	3610	1/1	0.96	0.08	33,33,33,33	0
83	ZN	CE	101	1/1	0.96	0.05	68,68,68,68	0
82	MG	1	3645	1/1	0.96	0.22	22,22,22,22	0
83	ZN	CK	101	1/1	0.96	0.06	94,94,94,94	0
82	MG	1	3598	1/1	0.96	0.18	16,16,16,16	0
82	MG	1	3758	1/1	0.97	0.13	27,27,27,27	0
82	MG	AS	3672	1/1	0.97	0.10	34,34,34,34	0
82	MG	1	3552	1/1	0.97	0.05	19,19,19,19	0
82	MG	1	3502	1/1	0.97	0.16	36,36,36,36	0
82	MG	1	3519	1/1	0.97	0.07	37,37,37,37	0
82	MG	1	3624	1/1	0.97	0.05	23,23,23,23	0
82	MG	1	3587	1/1	0.97	0.09	23,23,23,23	0
82	MG	AS	3631	1/1	0.97	0.09	67,67,67,67	0
82	MG	AS	3695	1/1	0.97	0.28	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
83	ZN	AK	101	1/1	0.97	0.17	90,90,90,90	0
82	MG	AS	3507	1/1	0.97	0.18	48,48,48,48	0
82	MG	1	3672	1/1	0.97	0.25	27,27,27,27	0
82	MG	1	3618	1/1	0.97	0.23	19,19,19,19	0
82	MG	1	3567	1/1	0.97	0.11	16,16,16,16	0
82	MG	1	3628	1/1	0.97	0.08	34,34,34,34	0
82	MG	AS	3537	1/1	0.97	0.13	40,40,40,40	0
82	MG	1	3538	1/1	0.97	0.10	52,52,52,52	0
82	MG	AS	3525	1/1	0.97	0.11	52,52,52,52	0
83	ZN	DQ	101	1/1	0.97	0.05	98,98,98,98	0
83	ZN	AQ	101	1/1	0.98	0.08	47,47,47,47	0
82	MG	AS	3611	1/1	0.98	0.11	45,45,45,45	0
83	ZN	f	101	1/1	0.98	0.04	55,55,55,55	0
83	ZN	DN	201	1/1	0.98	0.05	98,98,98,98	0
82	MG	CM	1871	1/1	0.98	0.16	20,20,20,20	0
82	MG	AS	3668	1/1	0.98	0.05	35,35,35,35	0
83	ZN	CH	101	1/1	0.99	0.09	68,68,68,68	0
82	MG	1	3636	1/1	0.99	0.04	20,20,20,20	0
83	ZN	AN	101	1/1	0.99	0.10	64,64,64,64	0
82	MG	1	3681	1/1	0.99	0.05	19,19,19,19	0
82	MG	1	3545	1/1	0.99	0.12	20,20,20,20	0
83	ZN	c	201	1/1	0.99	0.04	73,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.