



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:19 PM UTC

PDB ID : 8OH6 / pdb_00008oh6
Title : Crystal structure of the Candida albicans 80S ribosome in complex with Paromomycin (500umol)
Authors : Kolosova, O.; Zgadzay, Y.; Yusupov, M.
Deposited on : 2023-03-20
Resolution : 3.35 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

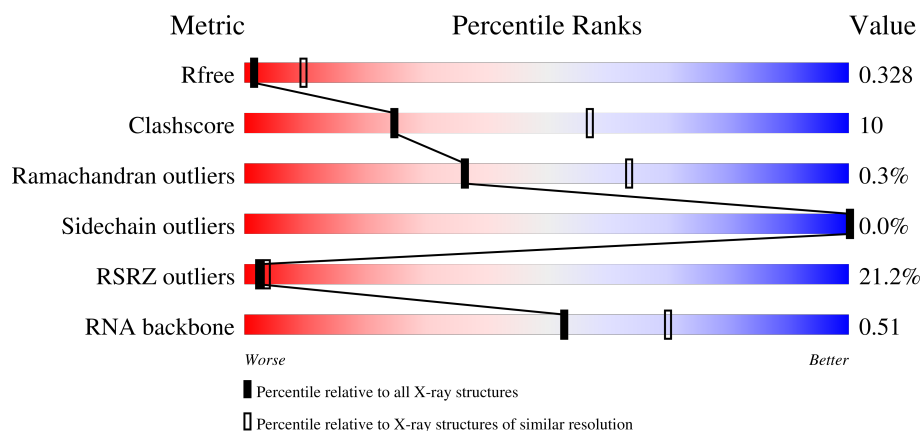
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)
RNA backbone	3983	1110 (3.72-3.00)

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	4% 50% 37% 8% .
1	AS	3359	11% 49% 36% 6% 9%
2	3	121	2% 65% 33% .
2	AT	121	6% 62% 36% .

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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	CL	267	
45	i	267	
46	B	1787	
46	CM	1787	
47	C	261	
47	CN	261	
48	CO	256	
48	D	256	
49	CP	249	
49	E	249	
50	CQ	251	
50	F	251	
51	CR	262	
51	G	262	
52	CS	225	
52	H	225	

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Mol	Chain	Length	Quality of chain
53	CT	236	
53	I	236	
54	CU	186	
54	J	186	
55	CV	206	
55	K	206	
56	CW	189	
56	L	189	
57	CX	118	
57	M	118	
58	CY	155	
58	N	155	
59	CZ	143	
59	O	143	
60	DA	151	
60	P	151	
61	DB	132	
61	Q	132	
62	DC	142	
62	R	142	
63	DD	142	
63	S	142	
64	DE	137	
64	T	137	
65	DF	145	

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

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Mol	Chain	Length	Quality of chain
78	DS	193	
78	h	193	
79	AR	317	
79	DT	317	
80	l1	217	
81	12	165	

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	3569	-	-	-	X
82	MG	1	3791	-	-	-	X
82	MG	1	3959	-	-	-	X
82	MG	1	3978	-	-	-	X
82	MG	1	4064	-	-	-	X
82	MG	1	4083	-	-	-	X
82	MG	AS	3409	-	-	-	X
82	MG	AS	3418	-	-	-	X
82	MG	AS	3580	-	-	-	X
82	MG	AS	3671	-	-	-	X
82	MG	AS	3852	-	-	-	X
82	MG	B	1866	-	-	-	X

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 401103 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 (gene name XR_002086444.1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3219	Total	C	N	O	P	0	0	0
			68814	30741	12370	22484	3219			
1	AS	3061	Total	C	N	O	P	0	0	0
			65432	29231	11756	21384	3061			

- 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	157	Total	C	N	O	P	0	0	0
			3333	1491	583	1102	157			
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	0	0
			1888	1180	376	330	2			
4	AW	248	Total	C	N	O	S	0	0	0
			1879	1175	374	328	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	361	Total	C	N	O	S	0	0	0
			2751	1729	529	490	3			
6	AY	359	Total	C	N	O	S	0	0	0
			2737	1722	526	486	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	228	Total	C	N	O	S	0	0	0
			1834	1176	336	321	1			
9	BB	227	Total	C	N	O	S	0	0	0
			1825	1171	335	318	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	p	237	Total	C	N	O	S	0	0	0
			1831	1171	325	332	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	BC	226	Total	C	N	O	S	0	0	0
			1766	1132	313	318	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	189	Total	C	N	O	S	0	0	0
			1510	953	275	278	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	130	Total	C	N	O	0	0	0
			1029	660	193	175			
15	BH	128	Total	C	N	O	0	0	0
			1015	651	190	173			

- 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	172	Total	C	N	O	0	0	0
			1380	852	279	249			
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	171	Total	C	N	O	S	0	0	0
			1386	859	293	231	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
			832	540	137	155				

- 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	118	Total	C	N	O	S	0	0	0
			945	591	192	161	1			
25	BR	111	Total	C	N	O	S	0	0	0
			896	560	183	152	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	118	Total	C	N	O	S	0	0	0
			952	607	171	173	1			

- Molecule 27 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	9	126	Total	C	N	O		0	0	0
			989	618	190	181				
27	BT	124	Total	C	N	O		0	0	0
			975	610	188	177				

- 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	62	Total	C	N	O		0	0	0
			493	307	105	81				
30	BW	60	Total	C	N	O	S	0	1	0
			489	305	105	78	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AD	99	Total	C	N	O	S	0	0	0
			755	483	126	144	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	109	Total	C	N	O	S	0	0	0
			889	562	167	158	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	1	0
			1006	643	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	3	0
			867	558	166	142	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AH	111	Total	C	N	O	S	0	0	0
			878	541	180	153	4			
35	CB	112	Total	C	N	O	S	0	4	0
			913	567	188	154	4			

- Molecule 36 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AI	120	Total	C	N	O	S	0	0	0
			992	629	195	167	1			
36	CC	117	Total	C	N	O		0	0	0
			970	615	191	164				

- 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	98	Total	C	N	O	S	0	1	0
			772	481	158	131	2			

- 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	76	Total	C	N	O		0	1	0
			618	395	115	108				

- 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	0	0
			438	275	97	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	52	Total	C	N	O	S	0	1	0
			427	265	89	67	6			

- 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	24	Total	C	N	O	S	0	0	0
			227	138	61	27	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	2	0
			841	531	168	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 protein called 60S ribosomal protein CAALFM_C304810CA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	i	121	Total	C	N	O		0	0	0
			930	563	166	201				
45	CL	107	Total	C	N	O		0	0	0
			815	490	150	175				

- Molecule 46 is a RNA chain called 18S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B	1730	Total	C	N	O	P	0	0	0
			36889	16490	6552	12117	1730			
46	CM	1704	Total	C	N	O	P	0	0	0
			36345	16246	6466	11929	1704			

- Molecule 47 is a protein called 40S ribosomal protein S0.

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

- Molecule 48 is a protein called 40S ribosomal protein S1.

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

- Molecule 49 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	E	217	Total	C	N	O	S	0	0	0
			1629	1039	289	296	5			
49	CP	216	Total	C	N	O	S	0	0	0
			1620	1033	287	295	5			

- Molecule 50 is a protein called Ribosomal protein S3.

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

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

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

- Molecule 52 is a protein called Ribosomal protein S7.

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

- Molecule 53 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	I	226	Total	C	N	O	S	0	0	0
			1820	1133	351	330	6			
53	CT	235	Total	C	N	O	S	0	0	0
			1895	1180	367	342	6			

- Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	J	185	Total	C	N	O	S	0	0	0
			1491	953	269	269				
54	CU	182	Total	C	N	O	S	0	0	0
			1466	939	264	263				

- Molecule 55 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	K	203	Total	C	N	O	S	0	0	0
			1579	973	322	283	1			
55	CV	203	Total	C	N	O	S	0	0	0
			1579	973	322	283	1			

- Molecule 56 is a protein called Ribosomal protein S4.

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

- Molecule 57 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	M	98	Total	C	N	O	S	0	0	0
			817	531	135	150	1			
57	CX	93	Total	C	N	O	S	0	0	0
			783	511	129	142	1			

- Molecule 58 is a protein called 40S ribosomal protein S11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	N	144	Total	C	N	O	S	0	0	0
			1150	734	215	198	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	CY	141	Total	C	N	O	S	0	0	0
			1129	722	212	192	3			

- Molecule 59 is a protein called 40S ribosomal protein S12.

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

- Molecule 60 is a protein called 40S ribosomal protein S13.

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

- Molecule 61 is a protein called 40S ribosomal protein S14-A.

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

- Molecule 62 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	R	129	Total	C	N	O	S	0	0	0
			1018	649	185	177	7			
62	DC	118	Total	C	N	O	S	0	0	0
			935	598	169	162	6			

- Molecule 63 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	S	139	Total	C	N	O	S	0	0	0
			1085	697	197	190	1			
63	DD	140	Total	C	N	O	S	0	0	0
			1091	700	198	192	1			

- Molecule 64 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	T	123	Total	C	N	O	S	0	0	0
			991	625	182	183	1			
64	DE	125	Total	C	N	O	S	0	0	0
			1002	631	184	186	1			

- Molecule 65 is a protein called 40S ribosomal protein S18-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	U	144	Total	C	N	O	S	0	0	0
			1187	744	233	207	3			
65	DF	142	Total	C	N	O	S	0	0	0
			1169	733	228	205	3			

- Molecule 66 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 67 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	W	102	Total	C	N	O	S	0	0	0
			808	509	150	147	2			
67	DH	100	Total	C	N	O	S	0	0	0
			790	499	146	143	2			

- Molecule 68 is a protein called 40S ribosomal protein S21.

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

- Molecule 69 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 70 is a protein called Ribosomal protein S23 (S12).

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

- Molecule 71 is a protein called 40S ribosomal protein S24.

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

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	b	71	Total	C	N	O		0	0	0
			570	365	102	103				
72	DM	72	Total	C	N	O		0	0	0
			578	369	103	106				

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	c	98	Total	C	N	O	S	0	0	0
			779	482	163	128	6			
73	DN	97	Total	C	N	O	S	0	0	0
			770	477	161	126	6			

- Molecule 74 is a protein called 40S ribosomal protein S27.

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

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

- Molecule 75 is a protein called 40S ribosomal protein S28-B.

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

- Molecule 76 is a protein called 40S ribosomal protein S29A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	f	55	Total	C	N	O	S	0	0	0
			454	281	94	75	4			
76	DQ	55	Total	C	N	O	S	0	0	0
			454	281	94	75	4			

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	g	60	Total	C	N	O	S	0	0	0
			474	297	96	79	2			
77	DR	56	Total	C	N	O	S	0	0	0
			444	278	89	75	2			

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S31 fusion protein.

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

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	AR	310	Total	C	N	O	S	0	0	0
			2389	1514	410	460	5			
79	DT	311	Total	C	N	O	S	0	0	0
			2398	1519	412	462	5			

- Molecule 80 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	11	217	Total	C	N	O	S	0	0	0
			1711	1096	294	312	9			

- Molecule 81 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
81	12	14	Total	C	N	O	0	0	0
			97	60	16	21			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	1	684	Total	Mg	0	0
			684	684		
82	3	4	Total	Mg	0	0
			4	4		
82	4	4	Total	Mg	0	0
			4	4		
82	j	1	Total	Mg	0	0
			1	1		
82	k	2	Total	Mg	0	0
			2	2		
82	o	3	Total	Mg	0	0
			3	3		
82	v	1	Total	Mg	0	0
			1	1		
82	w	1	Total	Mg	0	0
			1	1		
82	x	1	Total	Mg	0	0
			1	1		
82	y	1	Total	Mg	0	0
			1	1		
82	z	1	Total	Mg	0	0
			1	1		
82	2	1	Total	Mg	0	0
			1	1		
82	6	1	Total	Mg	0	0
			1	1		
82	9	1	Total	Mg	0	0
			1	1		
82	AA	1	Total	Mg	0	0
			1	1		

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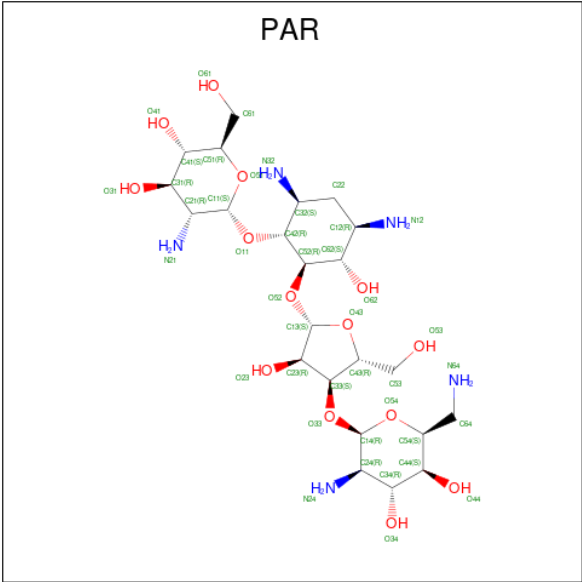
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	AB	2	Total 2	Mg 2	0	0
82	AD	1	Total 1	Mg 1	0	0
82	AF	1	Total 1	Mg 1	0	0
82	AH	1	Total 1	Mg 1	0	0
82	AI	1	Total 1	Mg 1	0	0
82	AK	2	Total 2	Mg 2	0	0
82	AN	1	Total 1	Mg 1	0	0
82	AP	2	Total 2	Mg 2	0	0
82	i	1	Total 1	Mg 1	0	0
82	B	69	Total 69	Mg 69	0	0
82	E	1	Total 1	Mg 1	0	0
82	F	1	Total 1	Mg 1	0	0
82	L	1	Total 1	Mg 1	0	0
82	Q	1	Total 1	Mg 1	0	0
82	R	1	Total 1	Mg 1	0	0
82	U	1	Total 1	Mg 1	0	0
82	Y	3	Total 3	Mg 3	0	0
82	Z	1	Total 1	Mg 1	0	0
82	c	1	Total 1	Mg 1	0	0
82	AR	1	Total 1	Mg 1	0	0
82	AS	542	Total 542	Mg 542	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
82	AT	3	Total 3	Mg 3	0	0
82	AU	2	Total 2	Mg 2	0	0
82	AW	1	Total 1	Mg 1	0	0
82	AX	1	Total 1	Mg 1	0	0
82	AZ	1	Total 1	Mg 1	0	0
82	BB	3	Total 3	Mg 3	0	0
82	BE	1	Total 1	Mg 1	0	0
82	BJ	1	Total 1	Mg 1	0	0
82	BK	1	Total 1	Mg 1	0	0
82	BO	1	Total 1	Mg 1	0	0
82	BP	1	Total 1	Mg 1	0	0
82	BQ	2	Total 2	Mg 2	0	0
82	BZ	1	Total 1	Mg 1	0	0
82	CB	1	Total 1	Mg 1	0	0
82	CE	1	Total 1	Mg 1	0	0
82	CH	1	Total 1	Mg 1	0	0
82	CM	25	Total 25	Mg 25	0	0
82	DK	1	Total 1	Mg 1	0	0

- Molecule 83 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$) (labeled as "Ligand of Interest" by depositor).



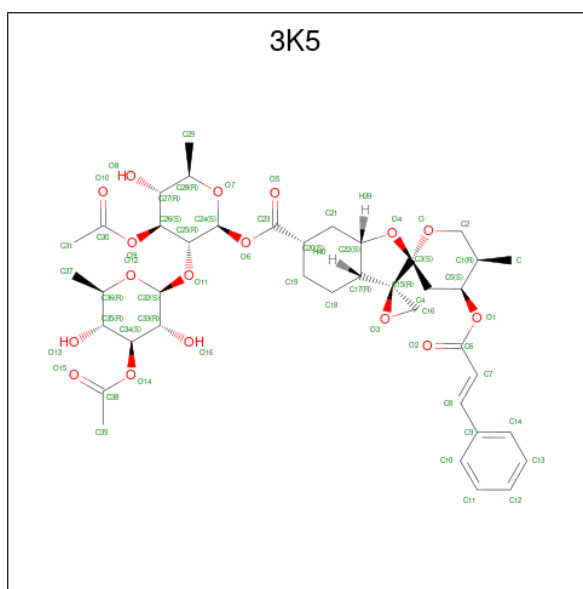
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	4	1	Total	C	N	O	0	0
			42	23	5	14		
83	B	1	Total	C	N	O	0	0
			42	23	5	14		
83	B	1	Total	C	N	O	0	0
			42	23	5	14		
83	B	1	Total	C	N	O	0	0
			42	23	5	14		

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

- Molecule 84 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
84	1	1	Total	C	O	0	0
			57	40	17		
84	AS	1	Total	C	O	0	0
			57	40	17		

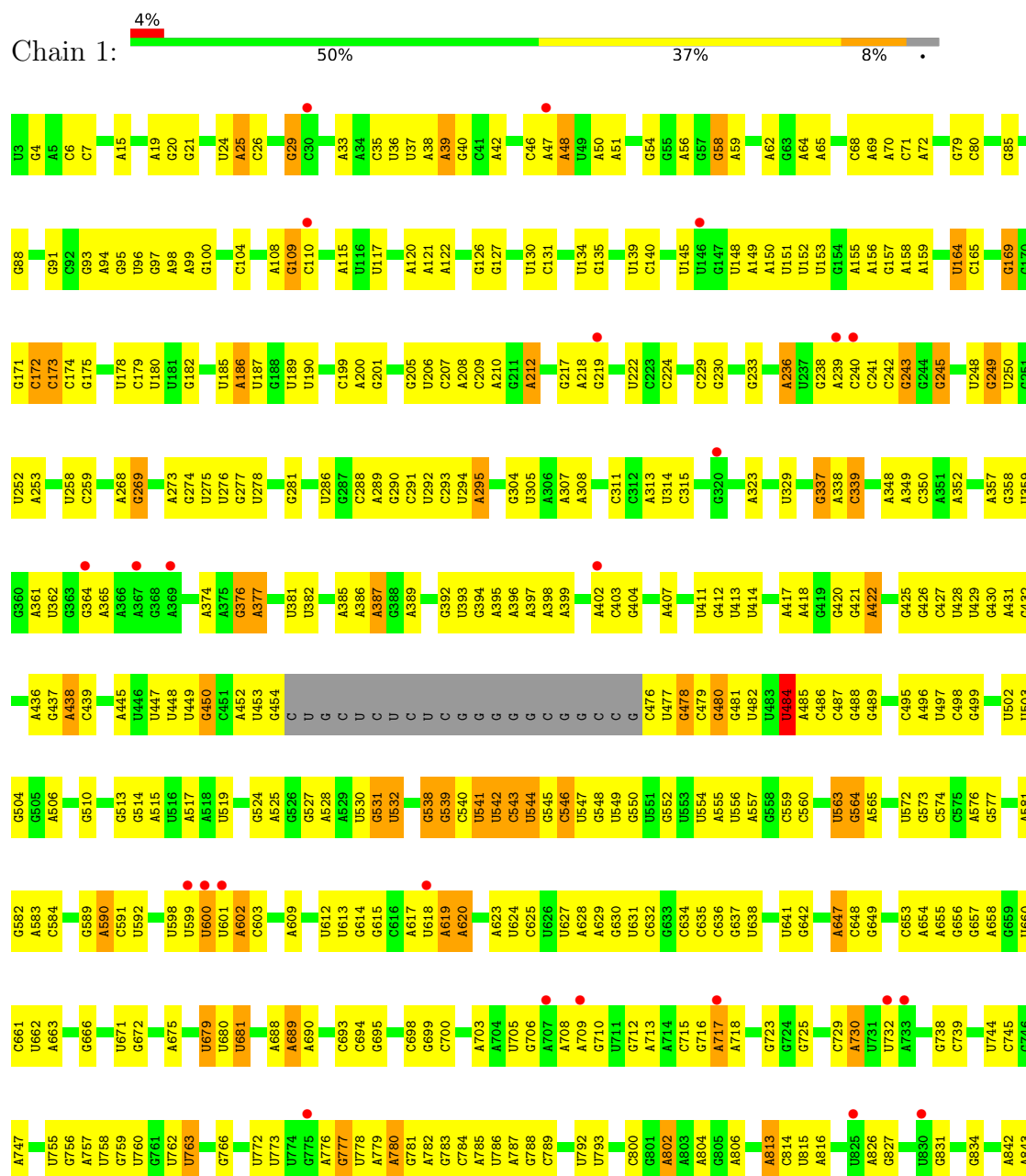
- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

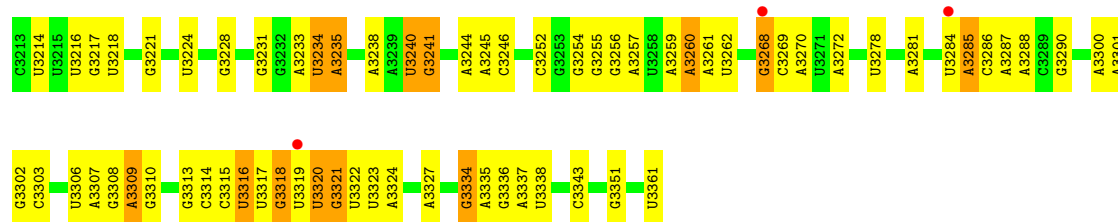
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 (gene name XR_002086444.1)

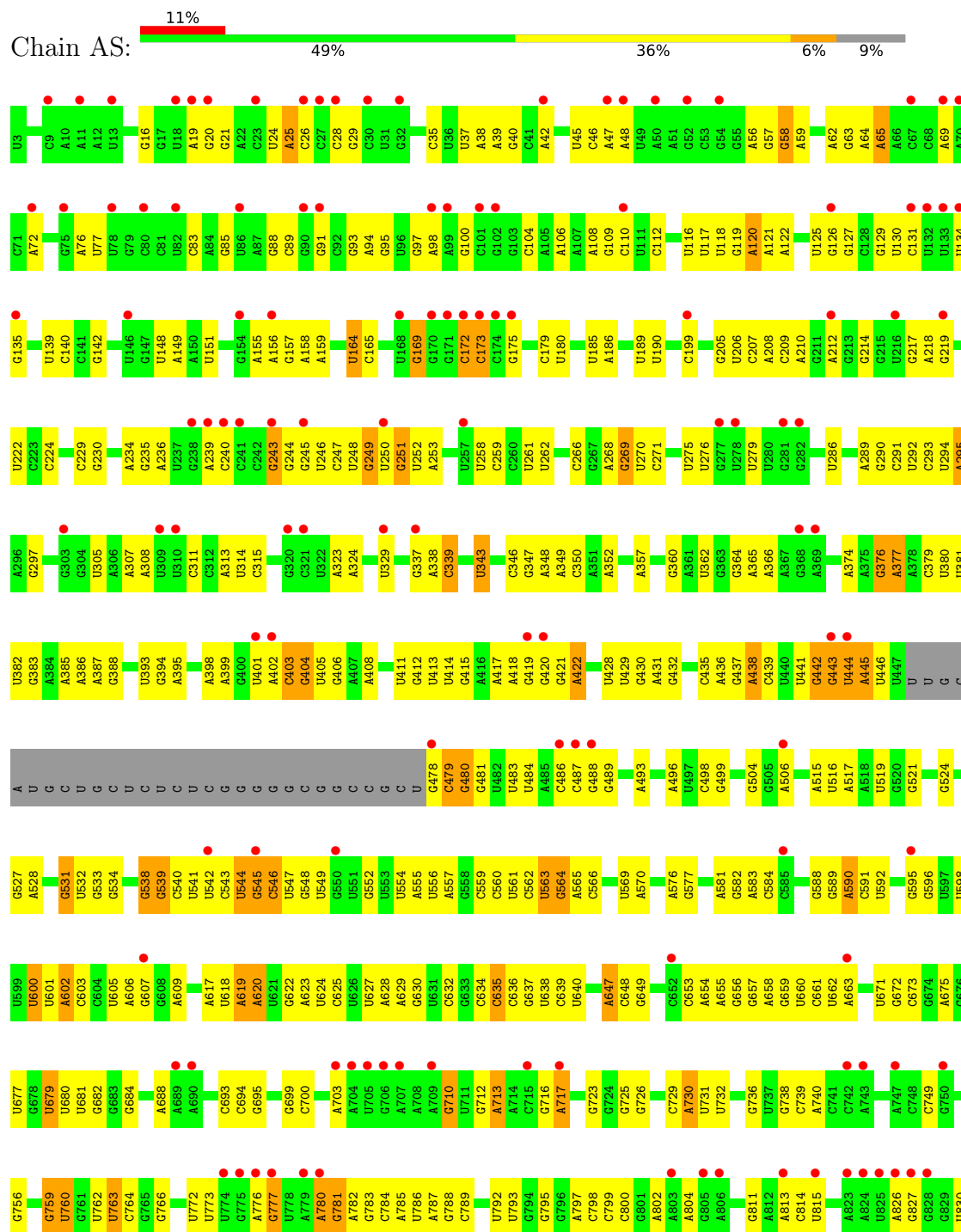


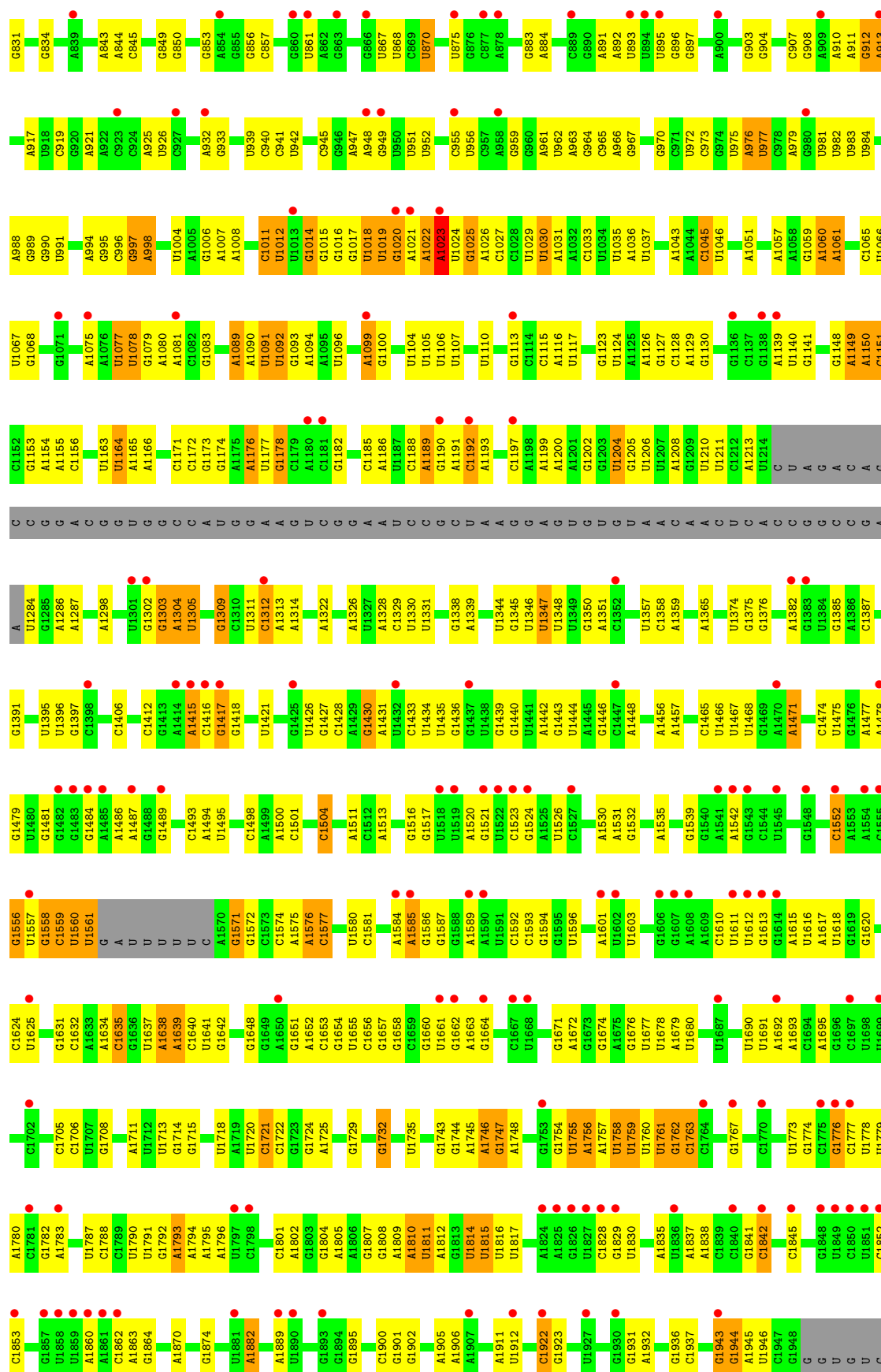


A3137	U2934	U2855	G2749	G2857	U2471	U2406	A2335	G2239	G2138	G
U3138	U2937	C2856	G2750	A2658	A2472	G2407	A2336	A2240	G2139	G
U3139	U2941	A2859	G2756	U2658	C2473	C2409	A2339	C2241	A2145	C
G3142	A2941	U2860	G2766	A2661	U2475	G2413	A2341	C2244	A2146	C
G3143	U2942	C2861	U2767	A2663	U2477	U2414	A2344	C2245	G2147	G
A3144	A2943	C2866	G2768	C2664	A2478	G2415	A2345	U2148	U2148	U2067
C3044	U2946	G2867	G2768	C2666	A2479	G2419	A2346	G2149	G2149	U2068
A3045	U2947	A2868	G2772	A2666	A2480	A2418	A2347	G2155	U2155	U2069
G3046	G2954	G2870	A2773	A2667	A2482	G2420	A2348	G2158	A2158	A2071
G3047	A2955	C2871	A2774	A2668	U2483	A2421	A2349	C2159	C2159	A2077
A3050	C2956	A2872	A2775	G2670	U2484	C2422	A2350	A2257	G2163	A2078
C3051	C2957	G2873	C2782	A2676	A2489	G2425	A2351	A2258	U2163	C2079
G3052	U2958	A2874	G2783	A2677	U2492	A2426	A2352	A2259	U2171	U2080
A3058	A2959	U2875	C2784	G2678	A2493	A2427	A2353	U2260	G2172	U2081
C3061	U2960	A2876	A2785	U2679	U2498	G2428	A2354	C2263	A2176	A2082
U3062	U2961	U2877	G2786	C2680	A2498	G2429	A2355	U2264	G2177	G2083
G2969	G2962	C2886	G2787	C2681	U2499	G2430	G2360	U2269	A2177	A2084
A2972	A2973	U2887	A2788	C2682	G2500	U2431	C2361	C2269	C2182	A2085
C2974	C2975	G2888	G2789	G2686	U2501	G2432	A2362	U2270	U2183	U2087
G2976	G2977	U2890	U2790	U2686	A2502	U2433	G2363	U2276	U2184	G2088
A2978	A2979	G2894	G2796	U2689	G2503	G2435	U2366	G2285	A2185	U2089
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G2987	A2988	C2901	C2808	A2614	G2512	A2440	G2370	G2289	A2191	G2094
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G2997	U2998	U2907	U2815	U2621	G2515	G2443	A2380	U2292	A2197	A2098
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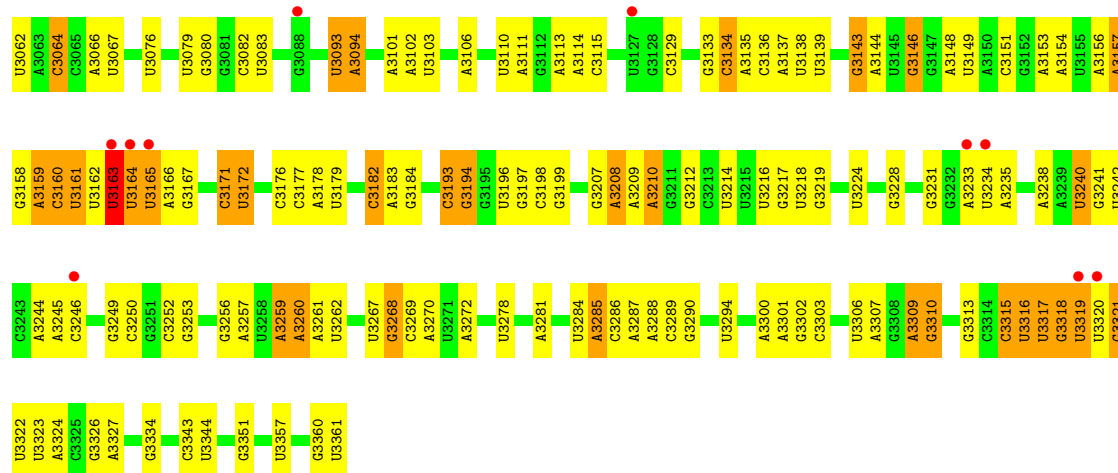


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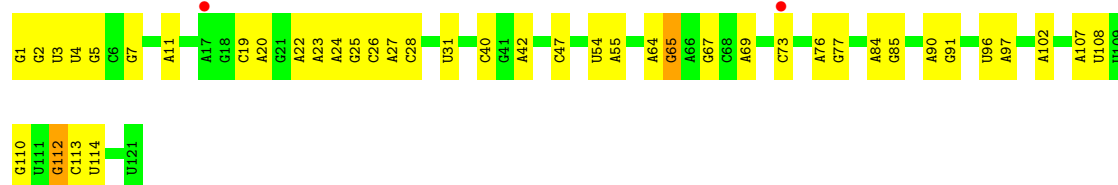




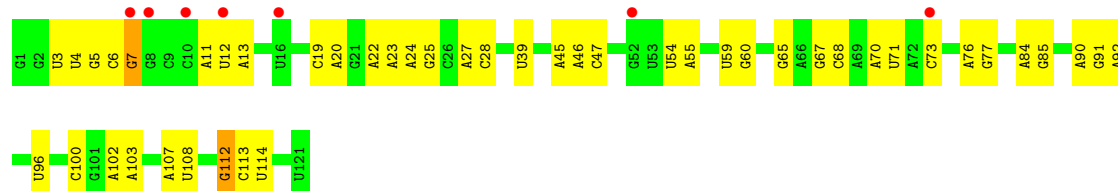




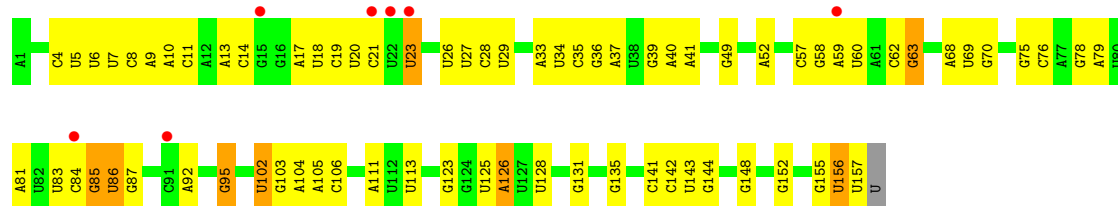
• Molecule 2: 5S



• Molecule 2: 5S

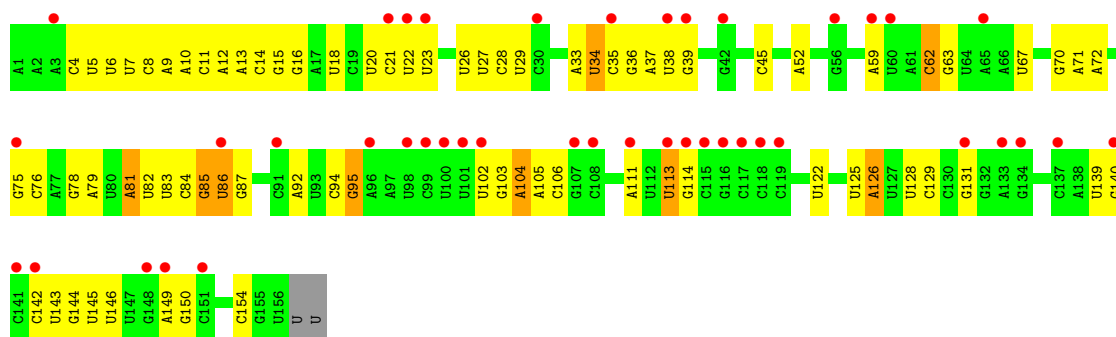


• Molecule 3: 5.8S

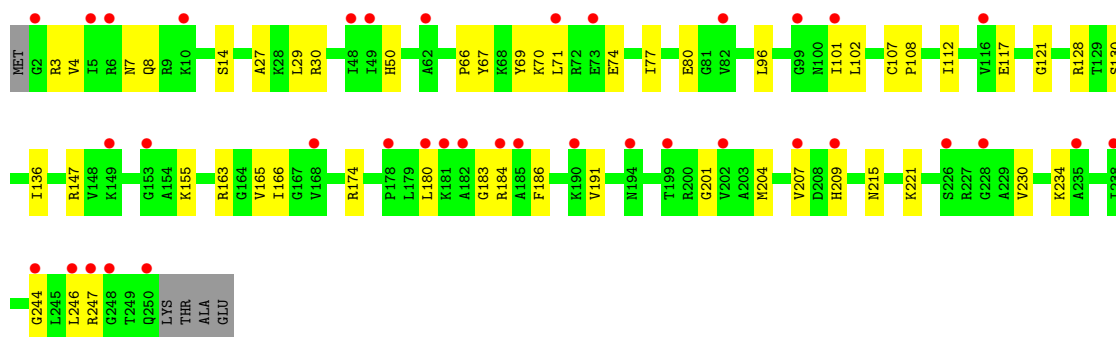
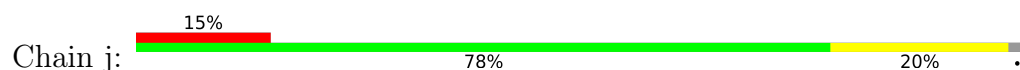


• Molecule 3: 5.8S

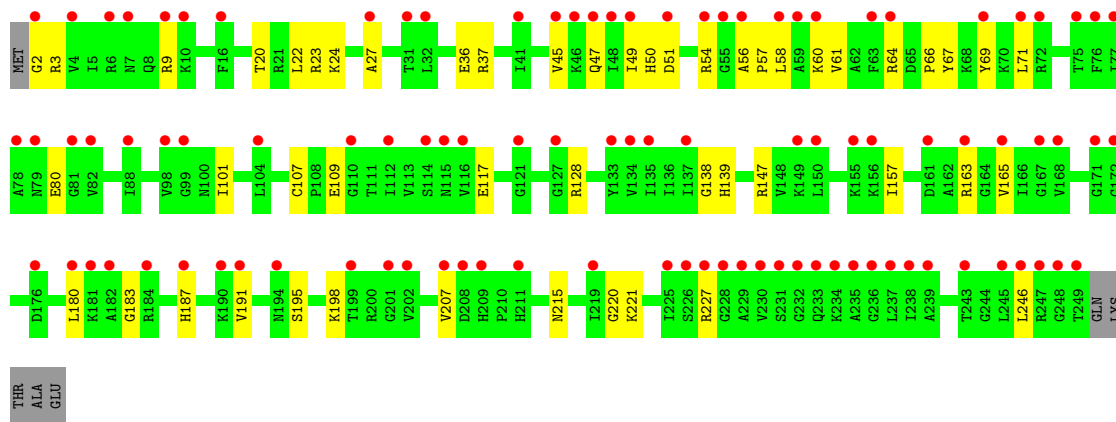
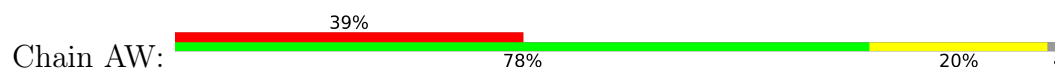




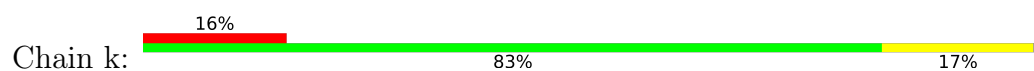
• Molecule 4: 60S ribosomal protein L2-B

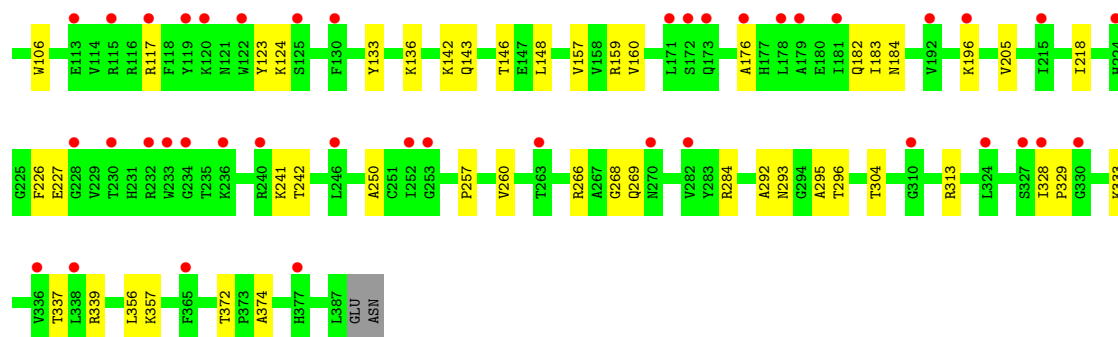


• Molecule 4: 60S ribosomal protein L2-B

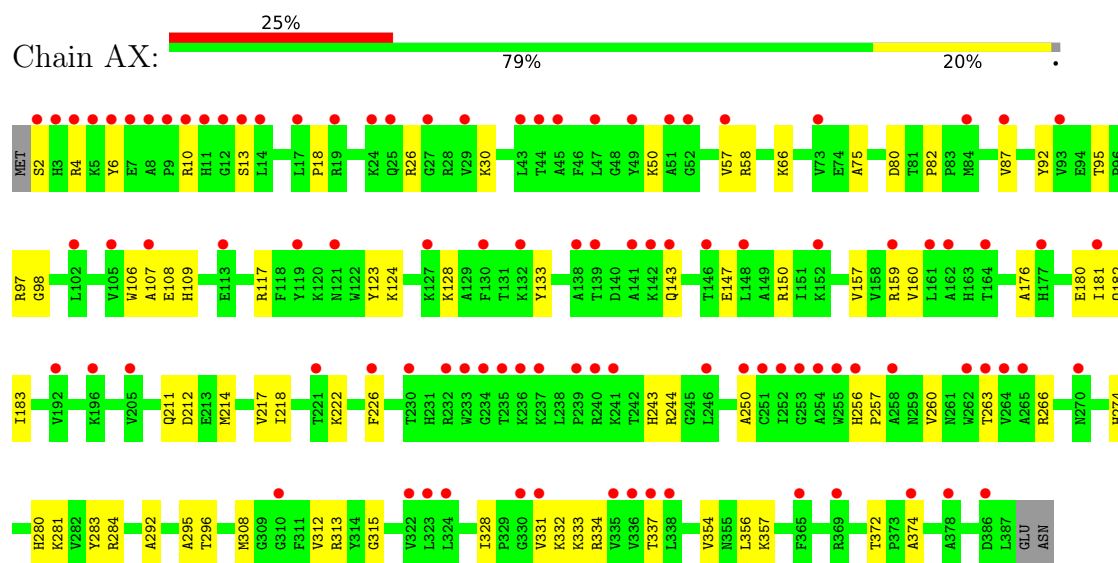


• Molecule 5: 60S ribosomal protein L3

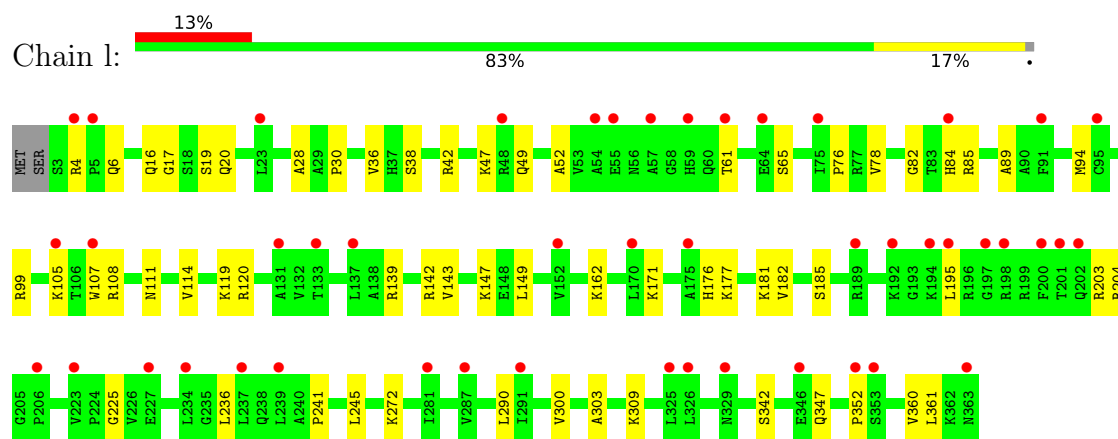




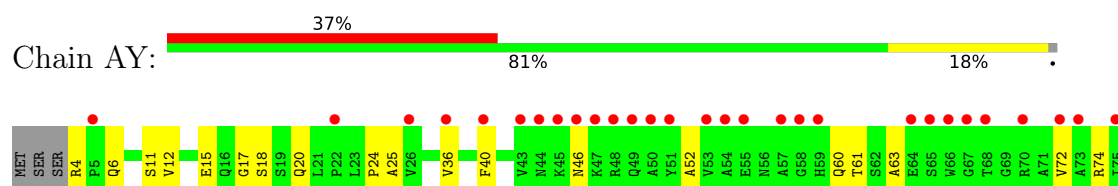
- Molecule 5: 60S ribosomal protein L3

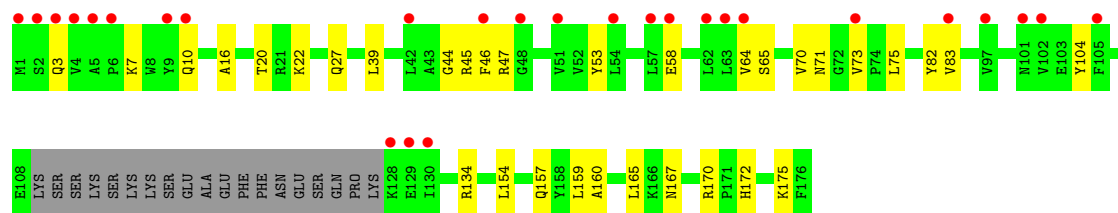


- Molecule 6: 60S ribosomal protein L4-B

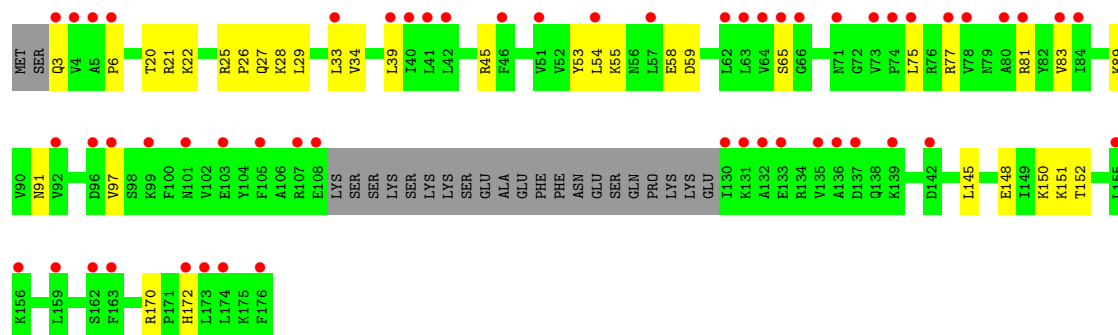


- Molecule 6: 60S ribosomal protein L4-B

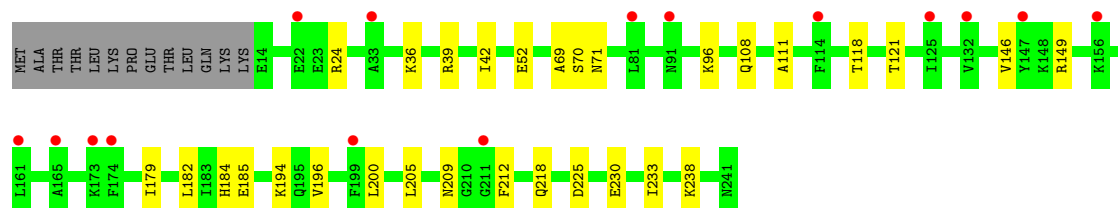
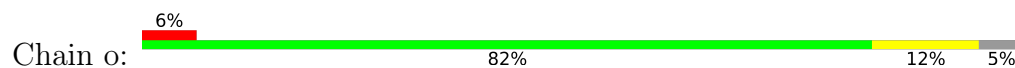




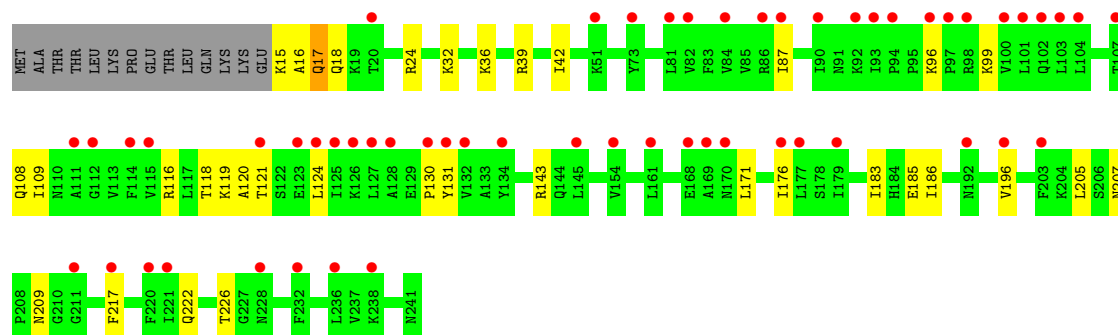
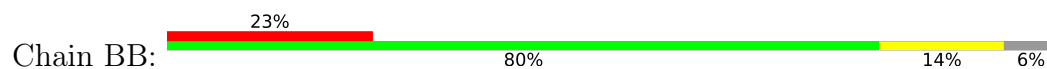
• Molecule 8: 60S ribosomal protein L6



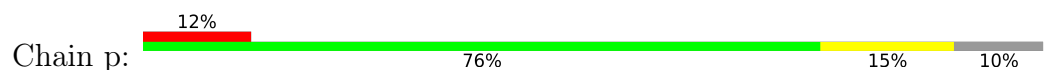
• Molecule 9: 60S ribosomal protein L7-A

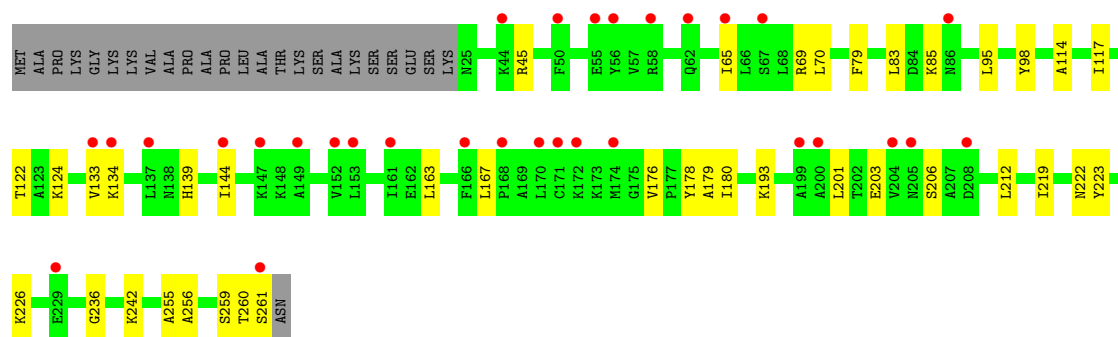


• Molecule 9: 60S ribosomal protein L7-A

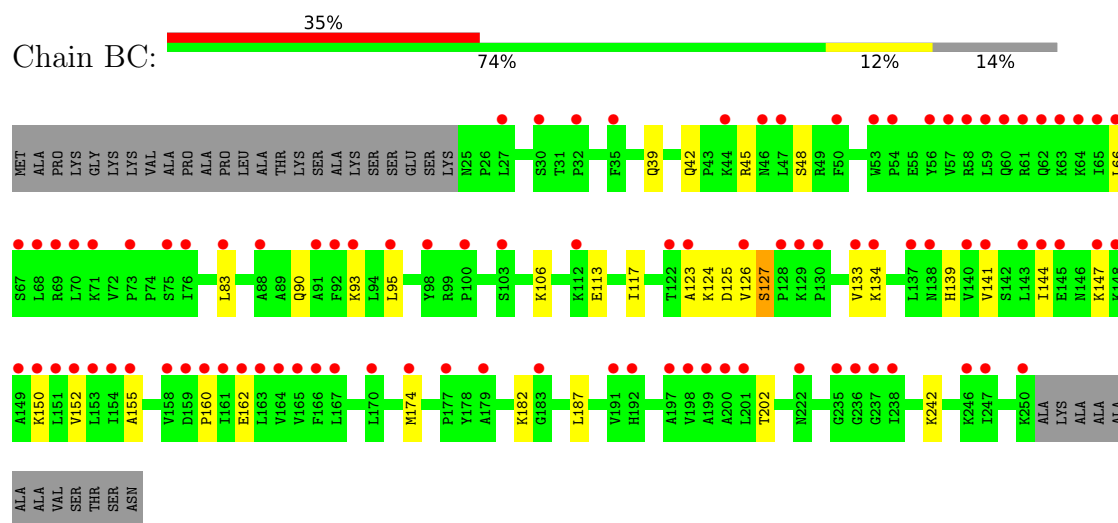


• Molecule 10: 60S ribosomal protein L8

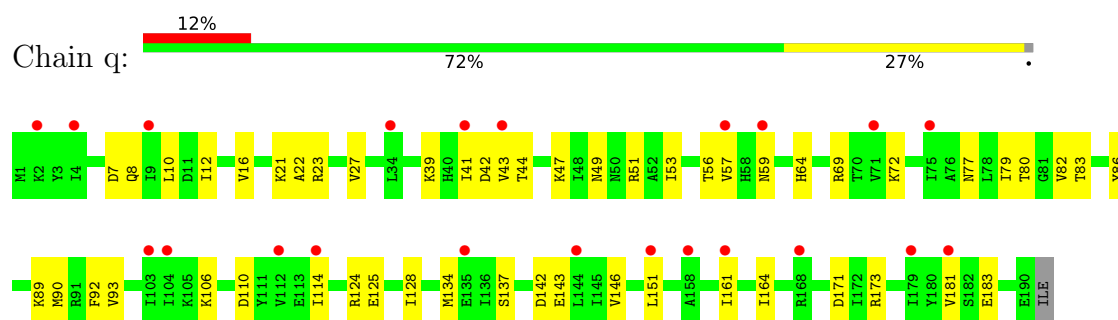




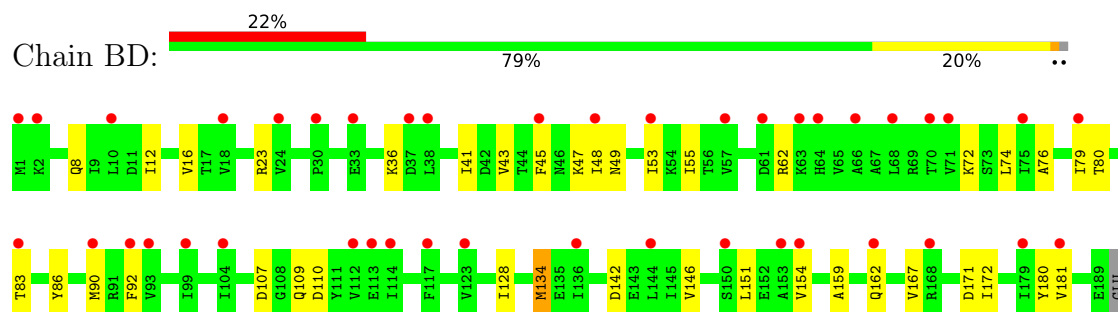
• Molecule 10: 60S ribosomal protein L8



• Molecule 11: 60S ribosomal protein L9-B



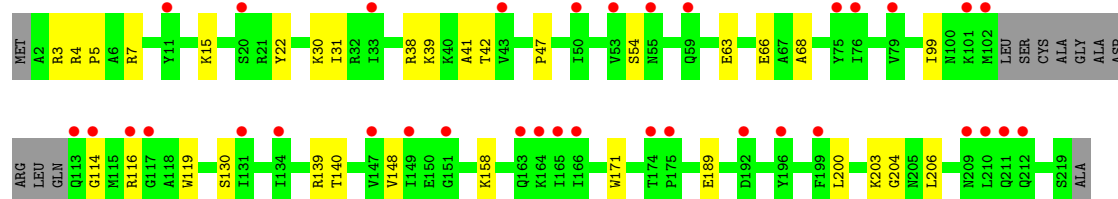
• Molecule 11: 60S ribosomal protein L9-B



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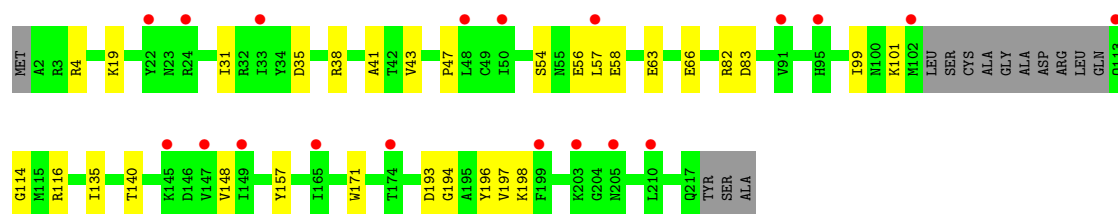
- Molecule 12: 60S ribosomal protein L10

Chain r: 



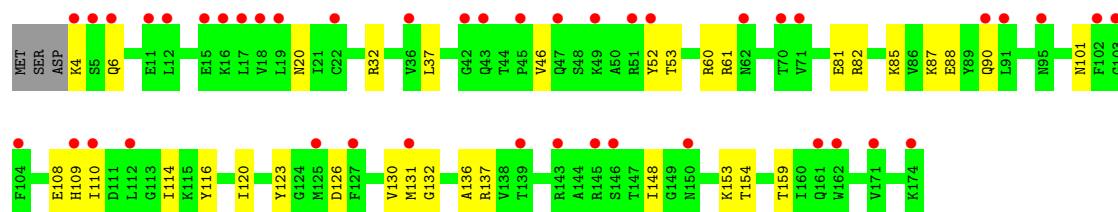
- Molecule 12: 60S ribosomal protein L10

Chain BE: 



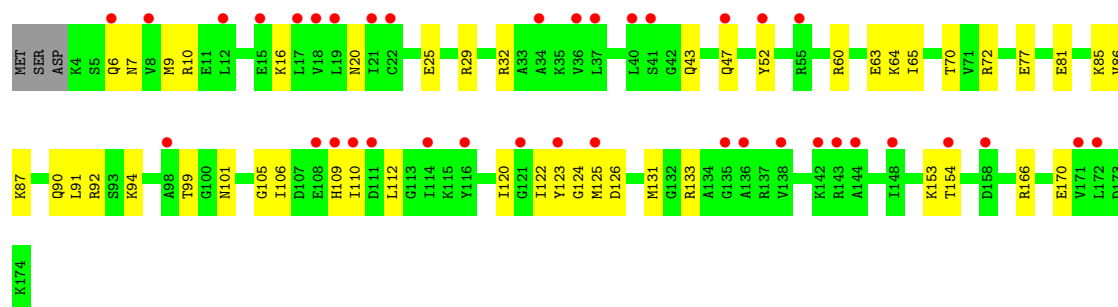
- Molecule 13: 60S ribosomal protein L11-B

Chain s: 

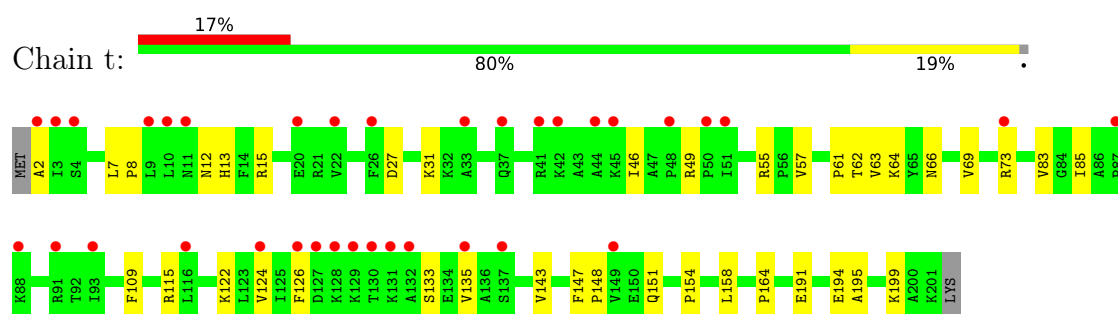


- Molecule 13: 60S ribosomal protein L11-B

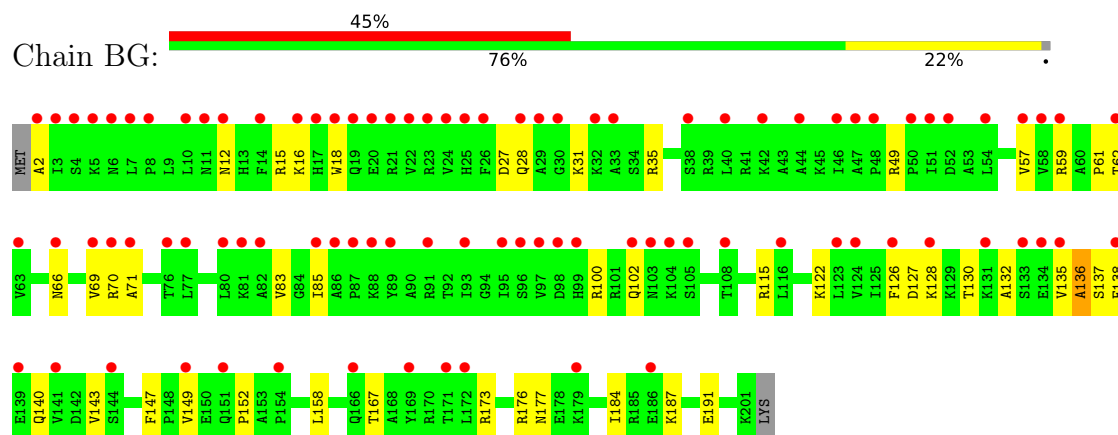
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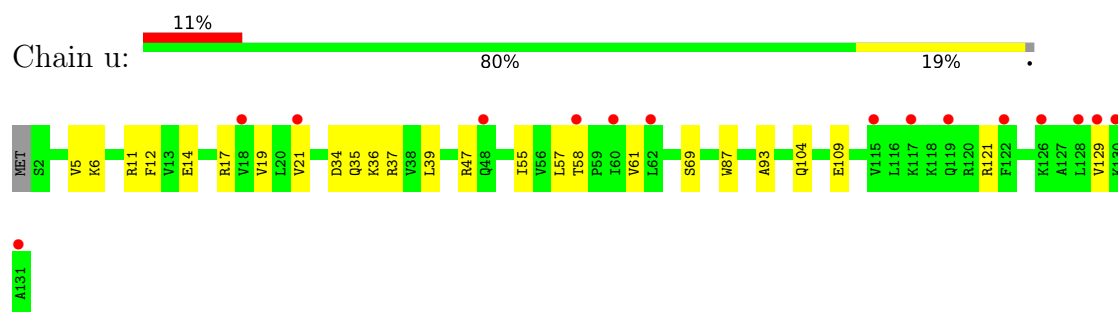
- Molecule 14: 60S ribosomal protein L13



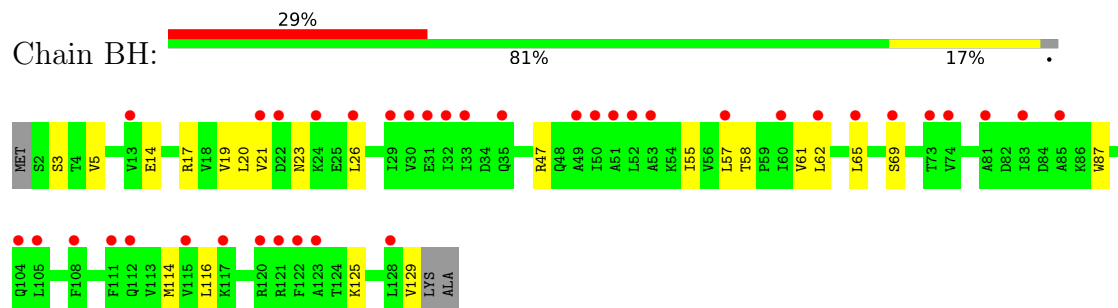
- Molecule 14: 60S ribosomal protein L13



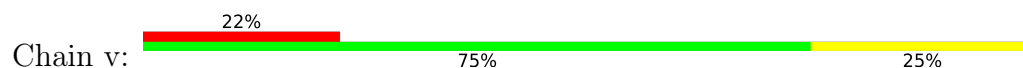
- Molecule 15: 60S ribosomal protein L14-B

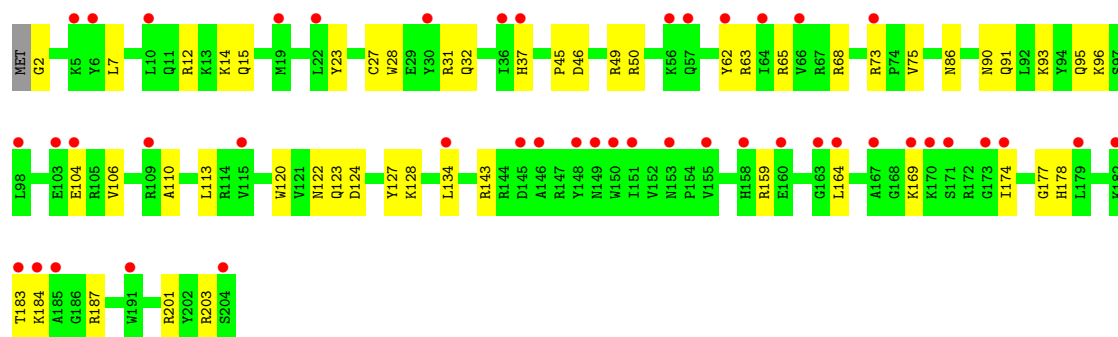


- Molecule 15: 60S ribosomal protein L14-B

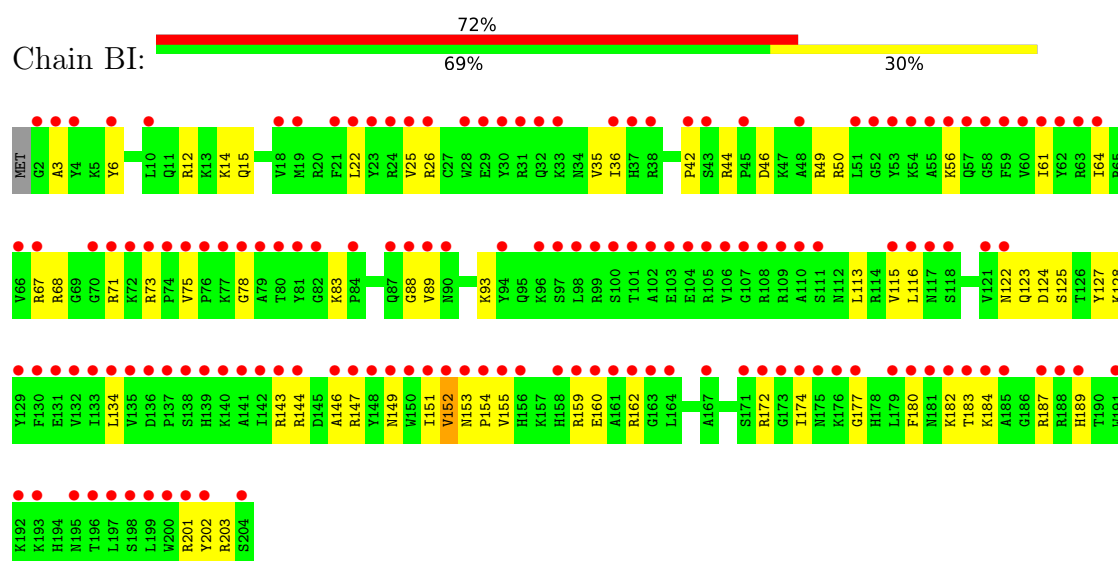


- Molecule 16: 60S ribosomal protein L15-A

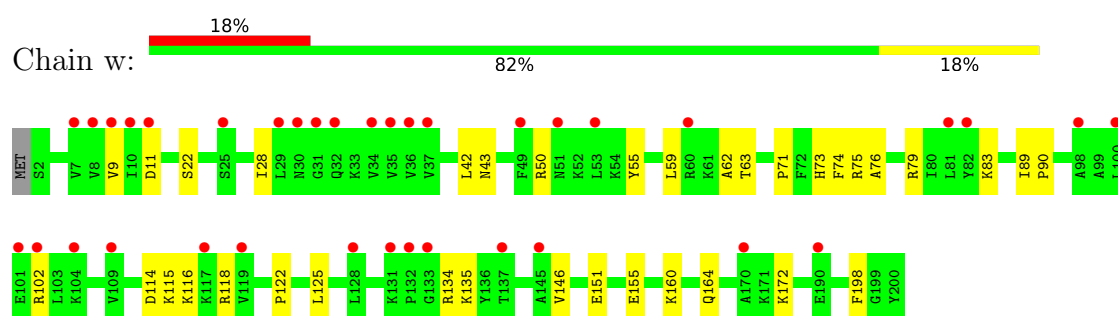




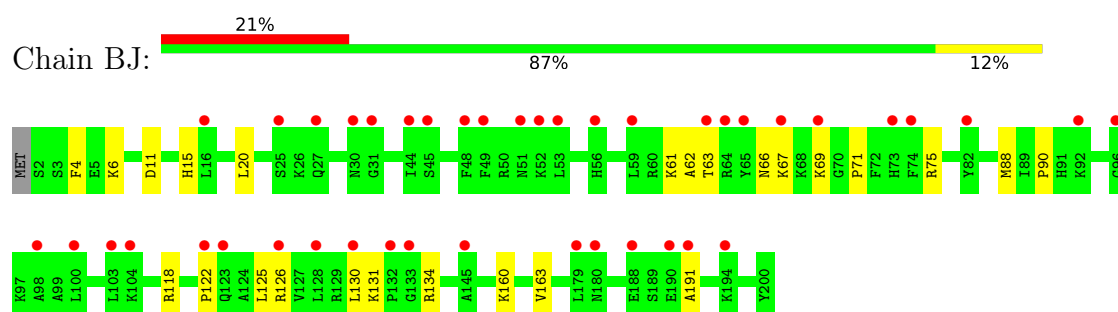
• Molecule 16: 60S ribosomal protein L15-A



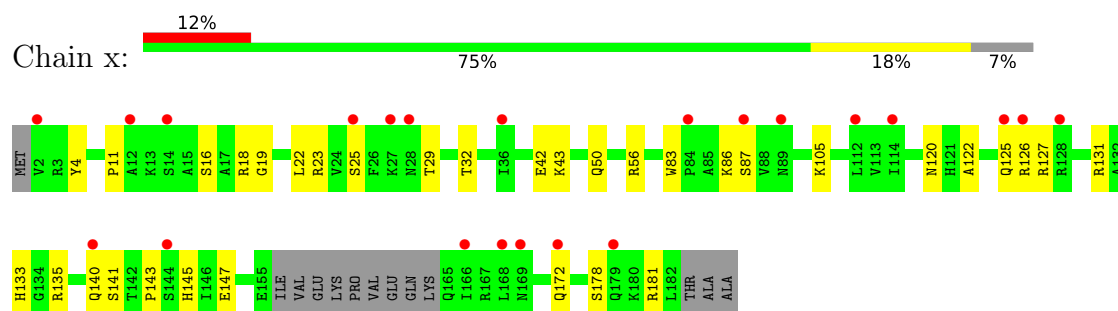
• Molecule 17: Ribosomal protein L13



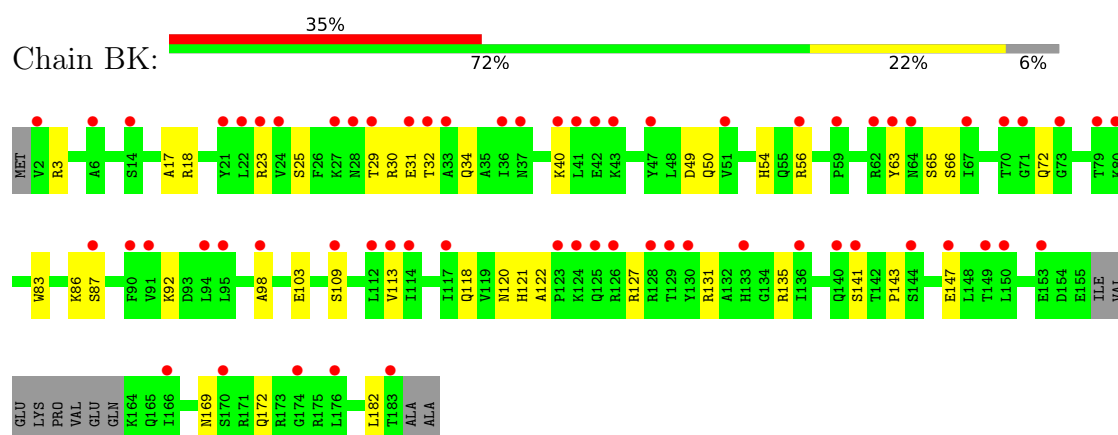
• Molecule 17: Ribosomal protein L13



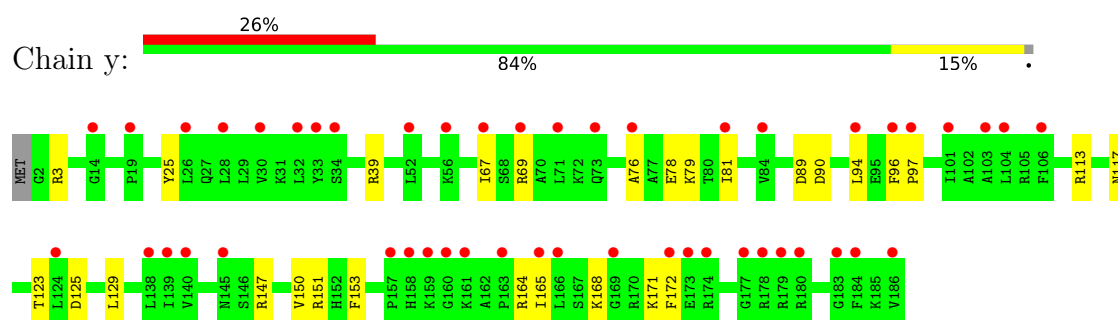
- Molecule 18: Ribosomal protein L22



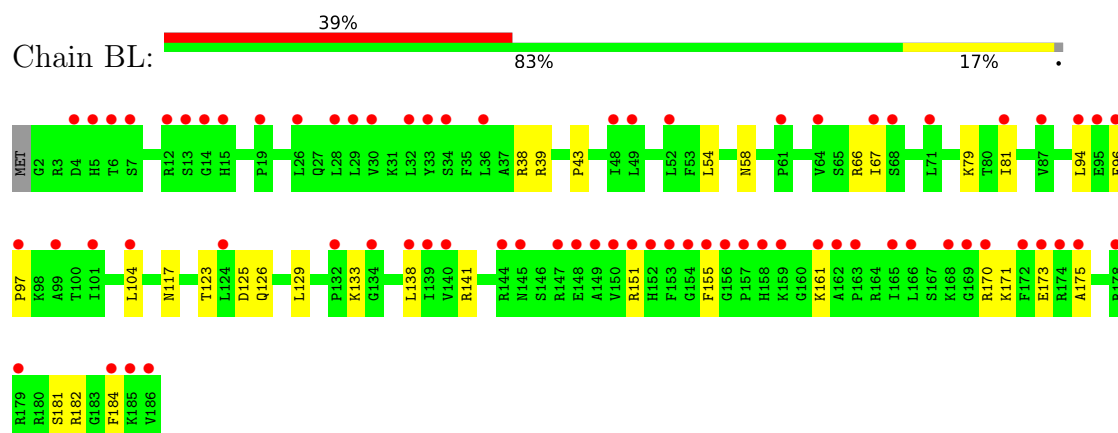
- Molecule 18: Ribosomal protein L22



- Molecule 19: 60S ribosomal protein L18-A

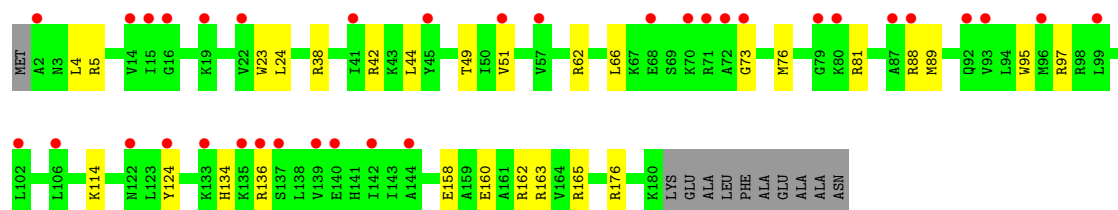


- Molecule 19: 60S ribosomal protein L18-A



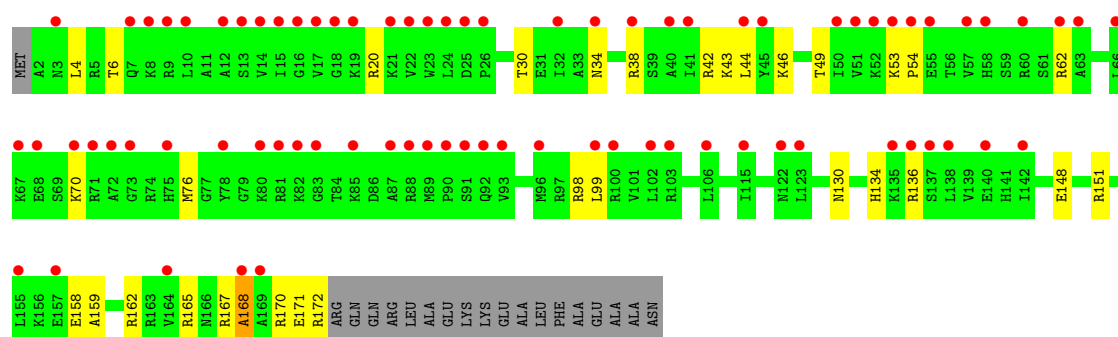
- Molecule 20: 60S ribosomal protein L19-A

Chain z: 



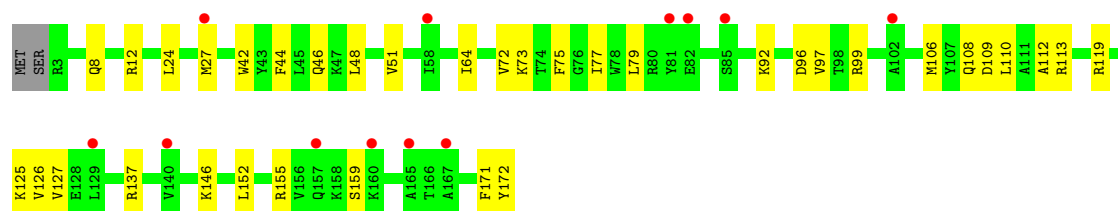
- Molecule 20: 60S ribosomal protein L19-A

Chain BM: 



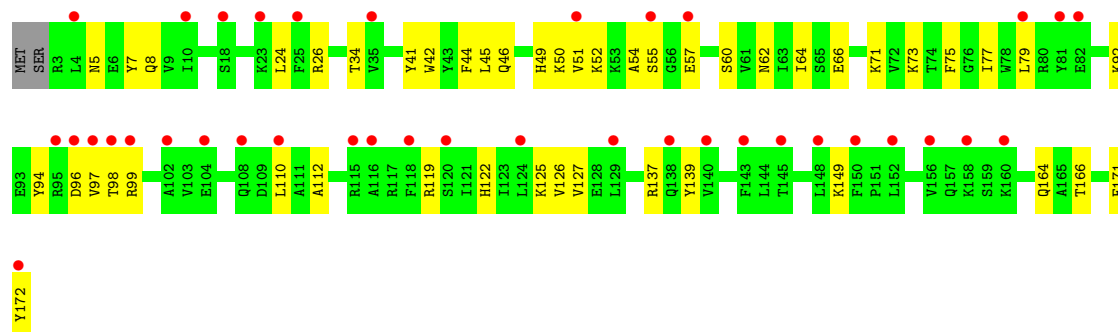
- Molecule 21: 60S ribosomal protein L20

Chain 0: 

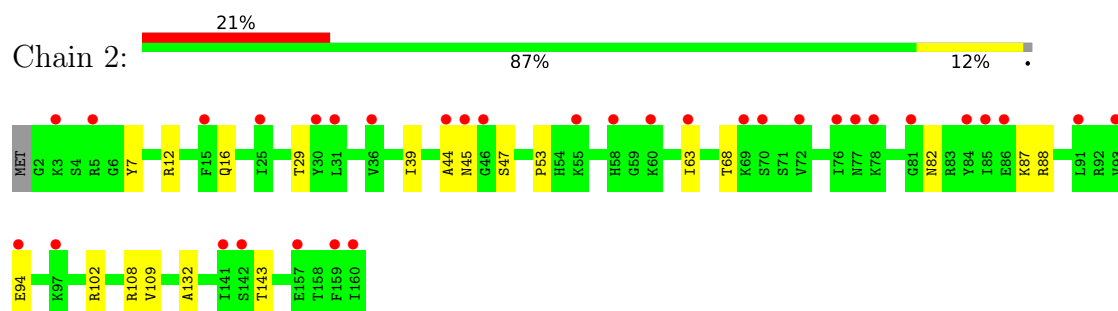


- Molecule 21: 60S ribosomal protein L20

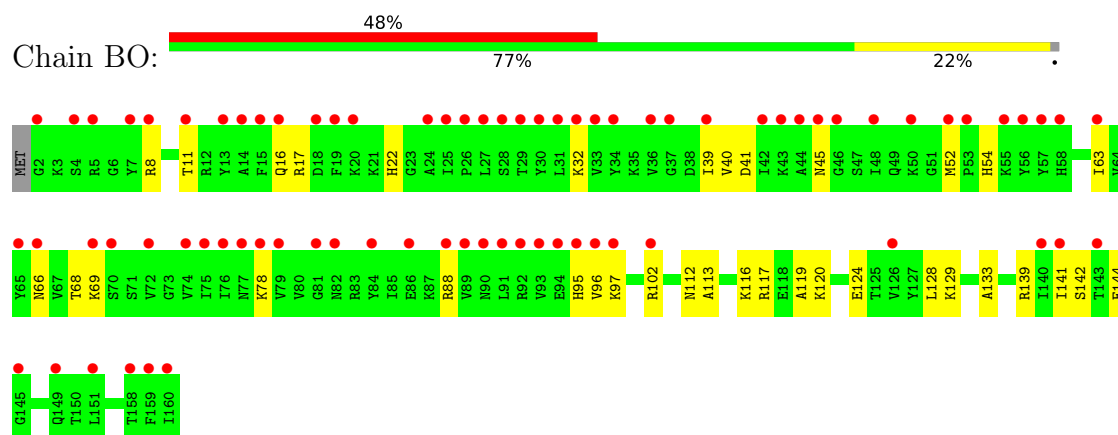
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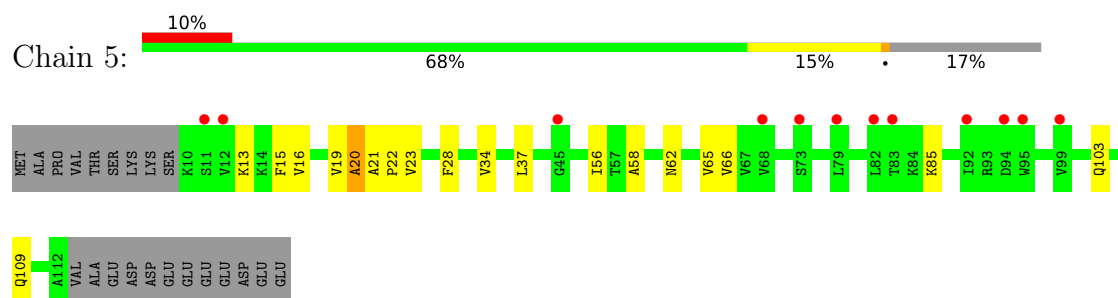
- Molecule 22: 60S ribosomal protein L21-A



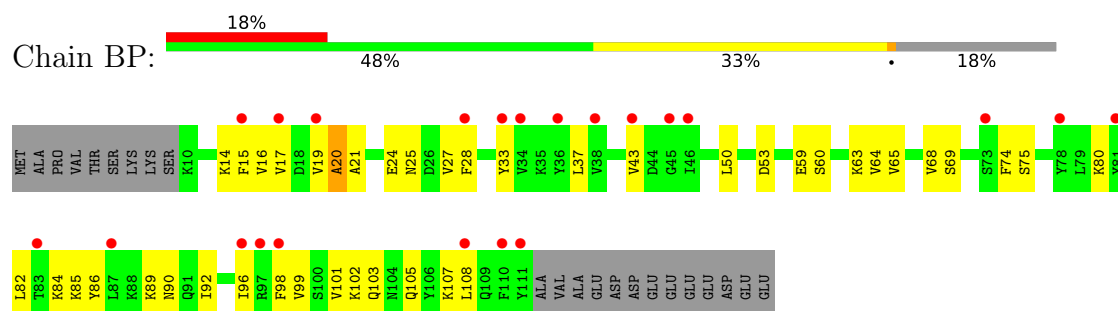
- Molecule 22: 60S ribosomal protein L21-A



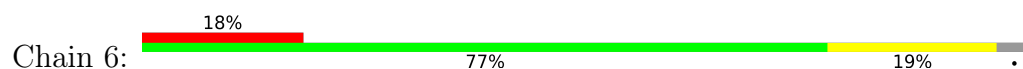
- Molecule 23: 60S ribosomal protein L22-B

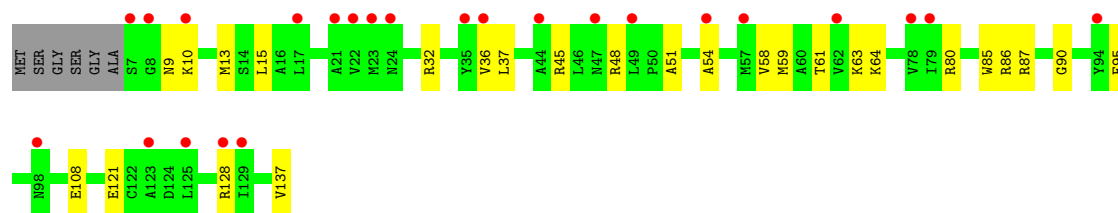


- Molecule 23: 60S ribosomal protein L22-B

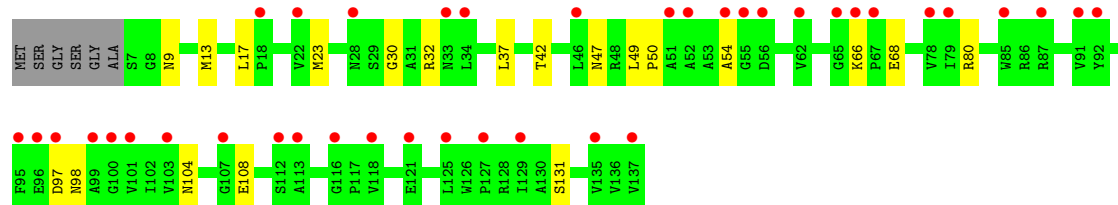
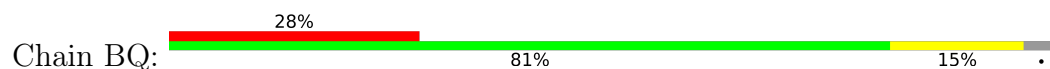


- Molecule 24: 60S ribosomal protein L23-A

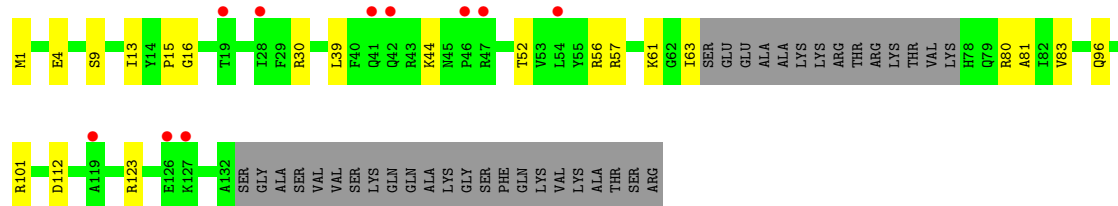




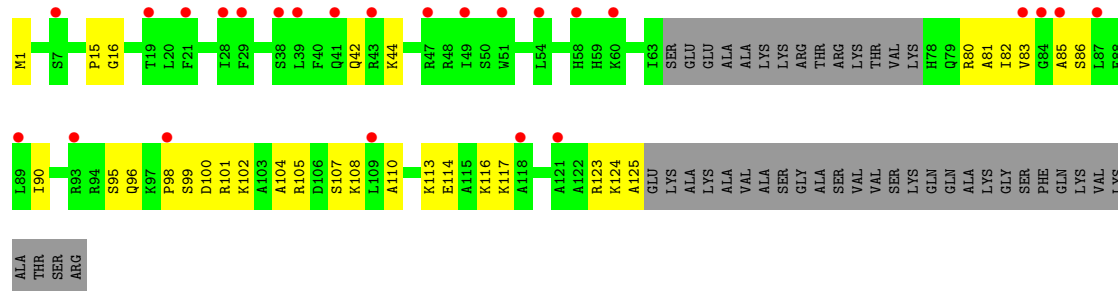
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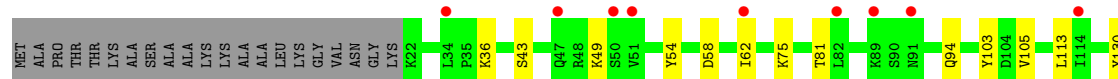
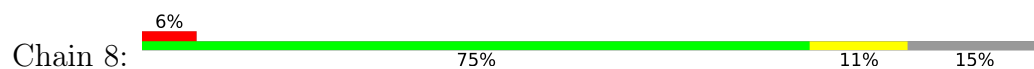
• Molecule 25: 60S ribosomal protein L24-A

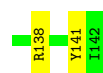


• Molecule 25: 60S ribosomal protein L24-A

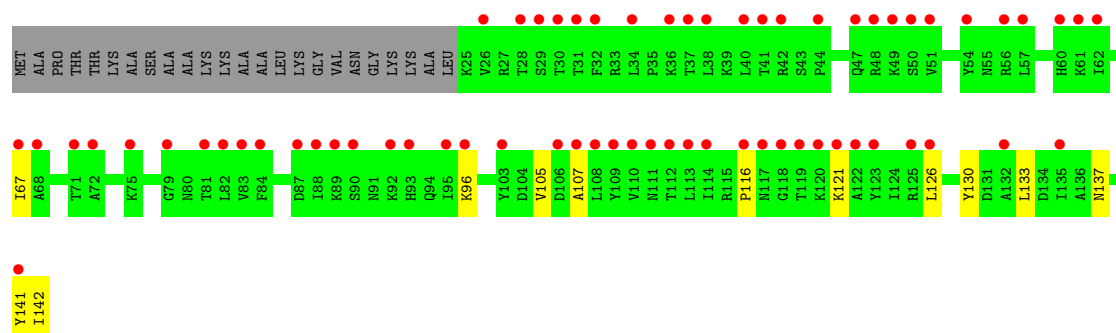
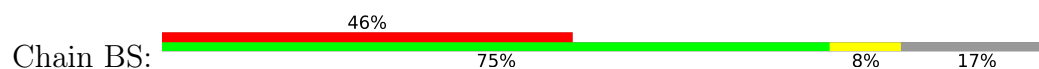


• Molecule 26: 60S ribosomal protein L25

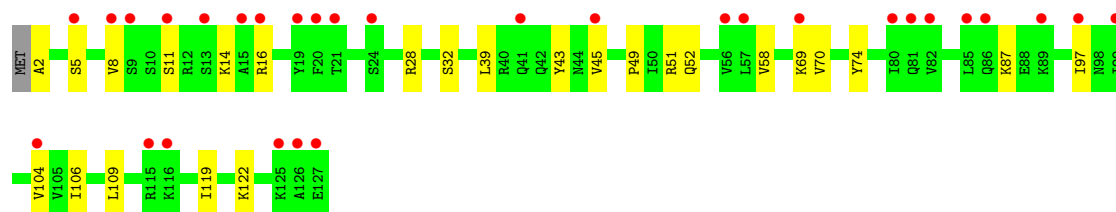
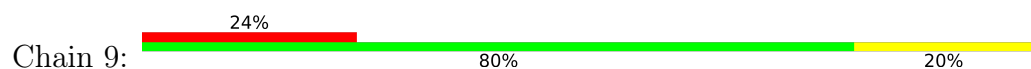




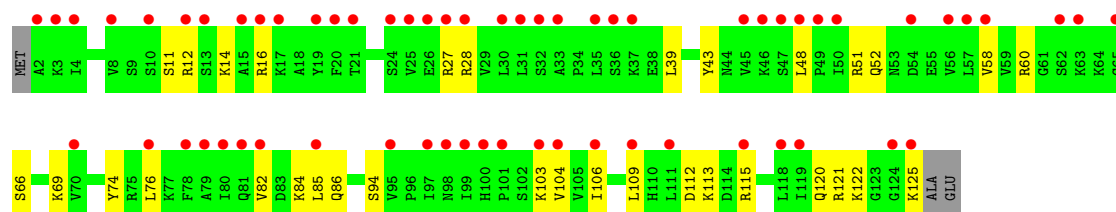
• Molecule 26: 60S ribosomal protein L25



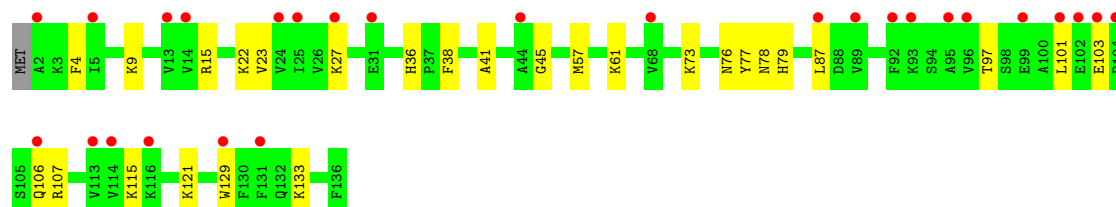
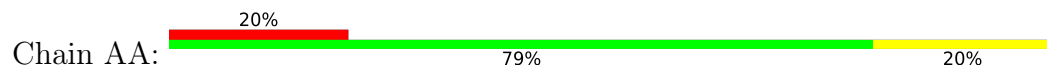
• Molecule 27: Ribosomal protein L24



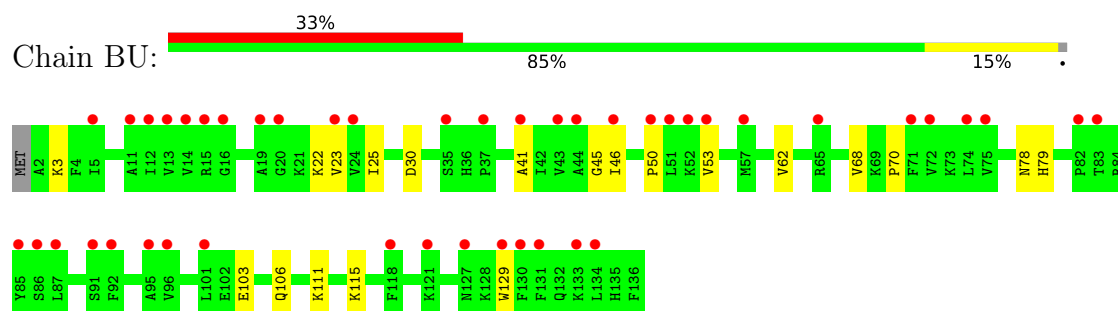
• Molecule 27: Ribosomal protein L24



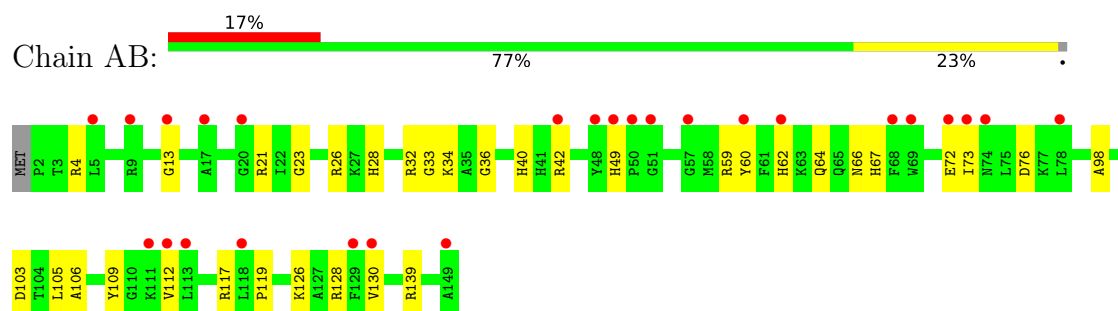
• Molecule 28: 60S ribosomal protein L27



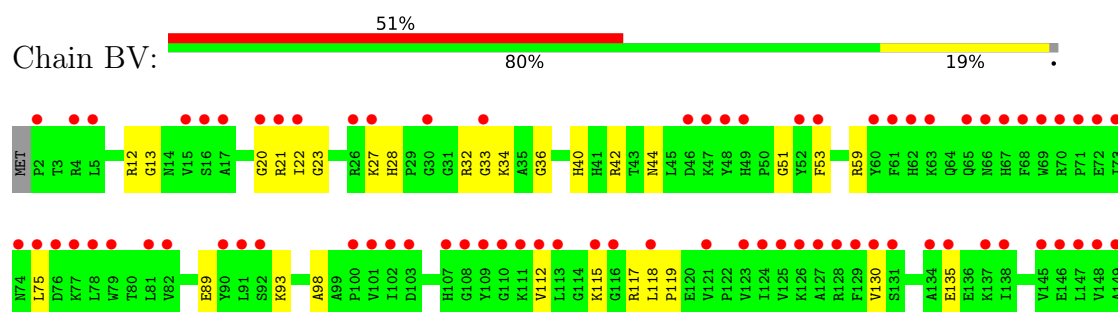
- Molecule 28: 60S ribosomal protein L27



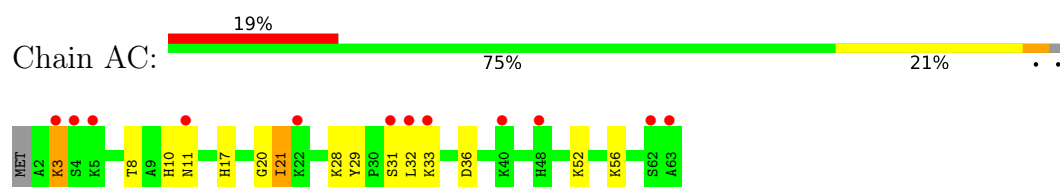
- Molecule 29: 60S ribosomal protein L28



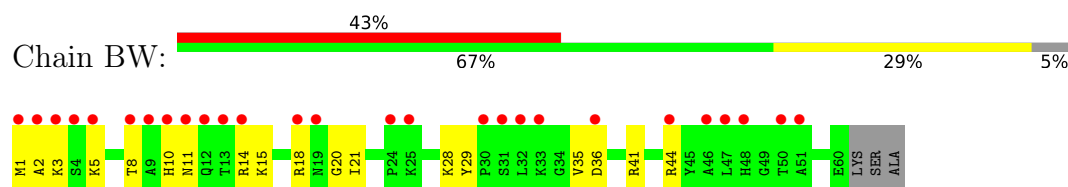
- Molecule 29: 60S ribosomal protein L28



- Molecule 30: 60S ribosomal protein L29

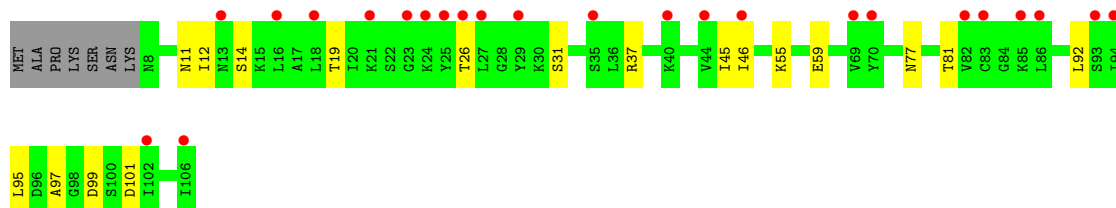


- Molecule 30: 60S ribosomal protein L29



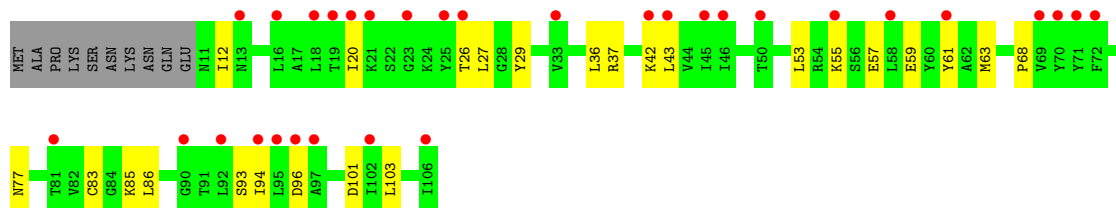
- Molecule 31: 60S ribosomal protein L30

Chain AD: 



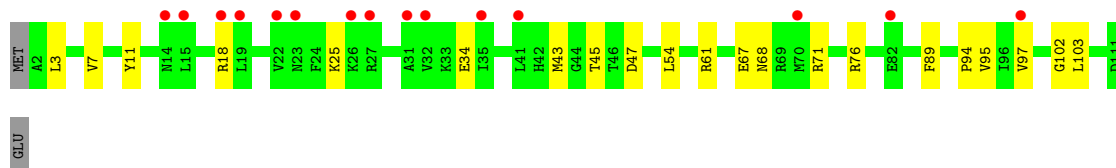
- Molecule 31: 60S ribosomal protein L30

Chain BX: 



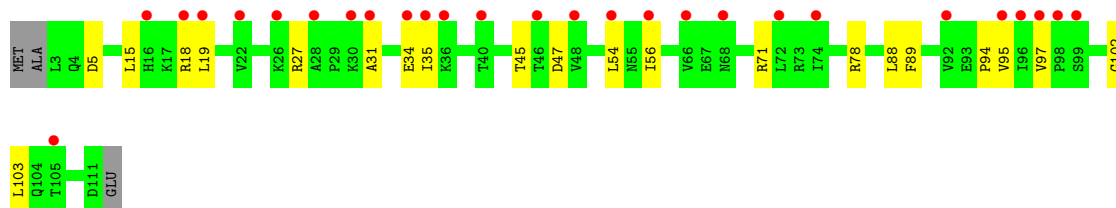
- Molecule 32: 60S ribosomal protein L31-B

Chain AE: 



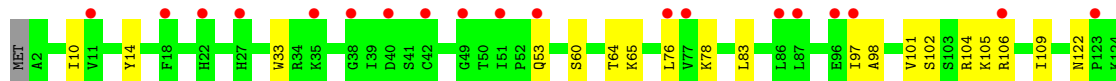
- Molecule 32: 60S ribosomal protein L31-B

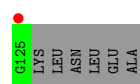
Chain BY: 



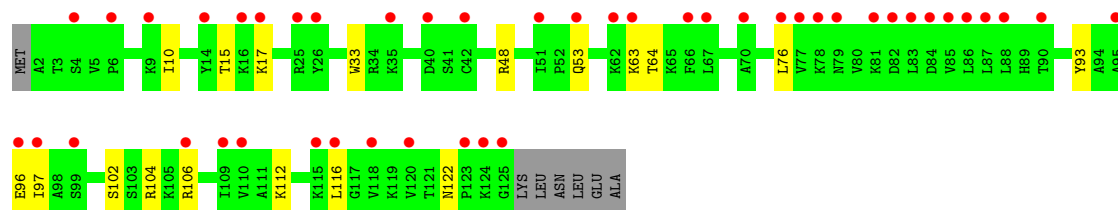
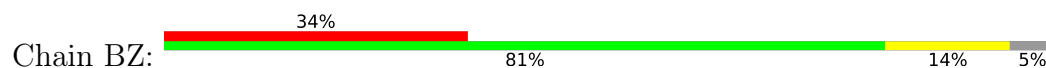
- Molecule 33: 60S ribosomal protein L32

Chain AF: 

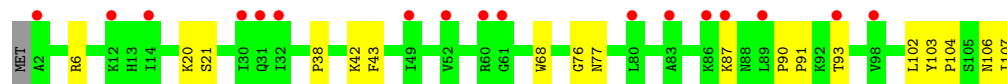
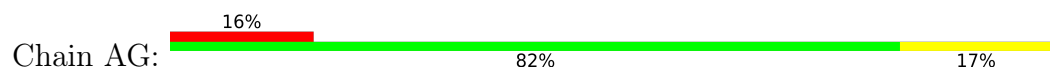




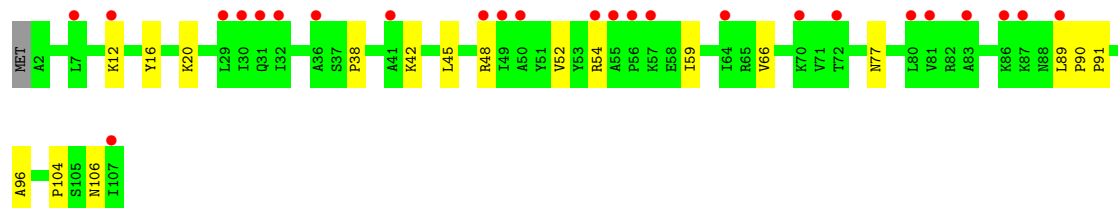
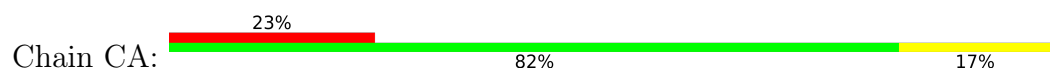
• Molecule 33: 60S ribosomal protein L32



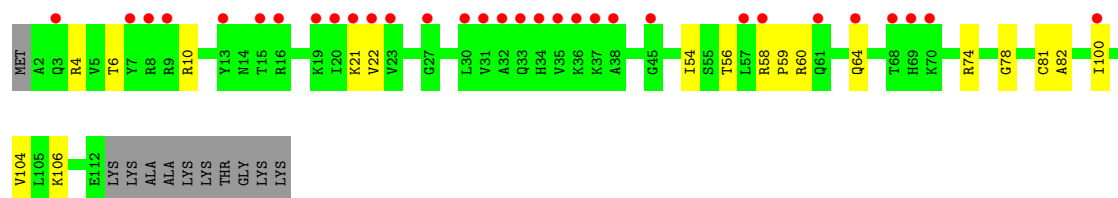
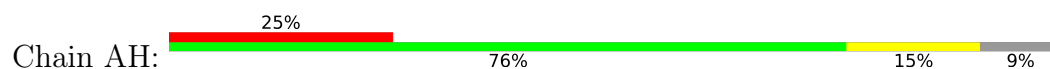
• Molecule 34: 60S ribosomal protein L33-A



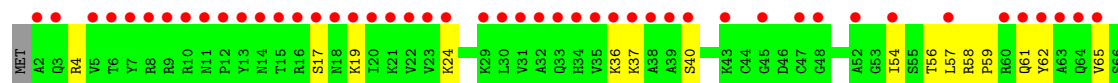
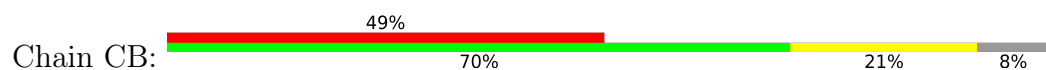
• Molecule 34: 60S ribosomal protein L33-A

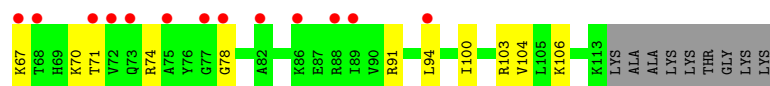


• Molecule 35: 60S ribosomal protein L34-B

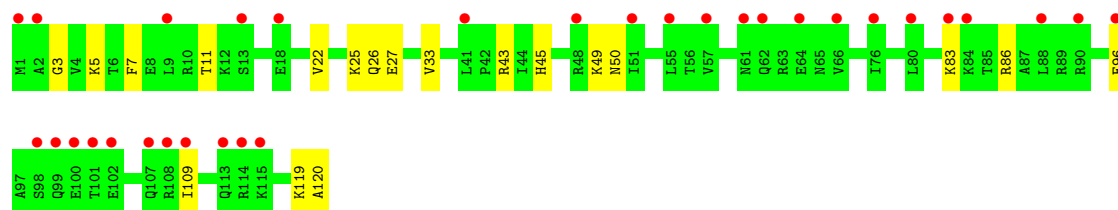
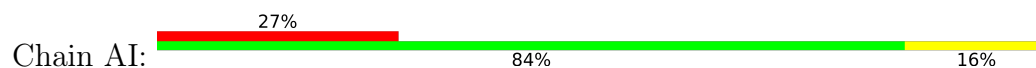


• Molecule 35: 60S ribosomal protein L34-B

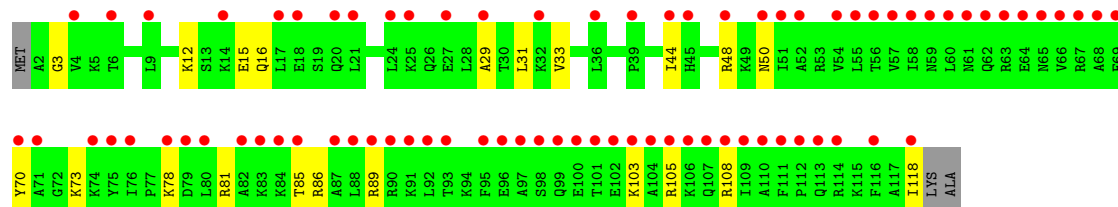
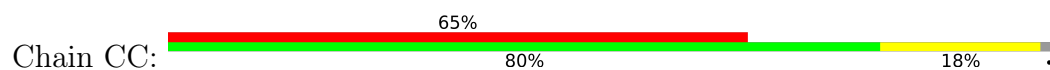




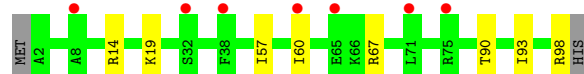
• Molecule 36: Ribosomal protein L29



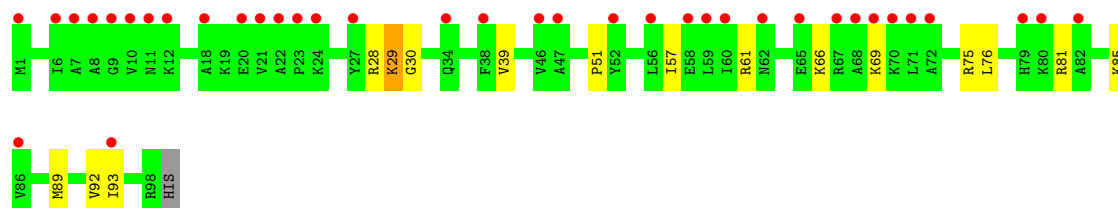
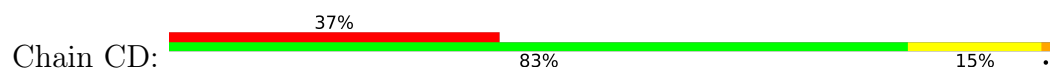
• Molecule 36: Ribosomal protein L29



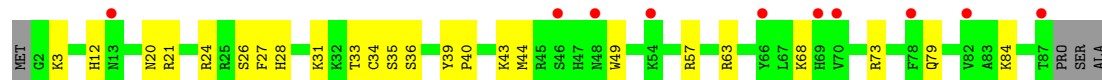
• Molecule 37: 60S ribosomal protein L36



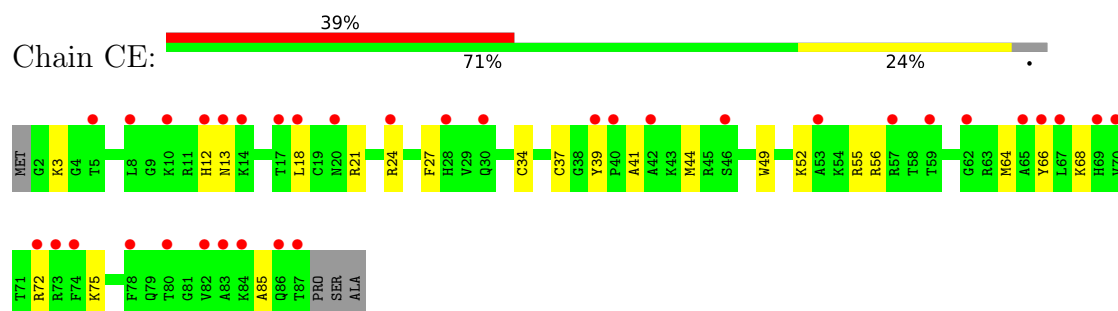
• Molecule 37: 60S ribosomal protein L36



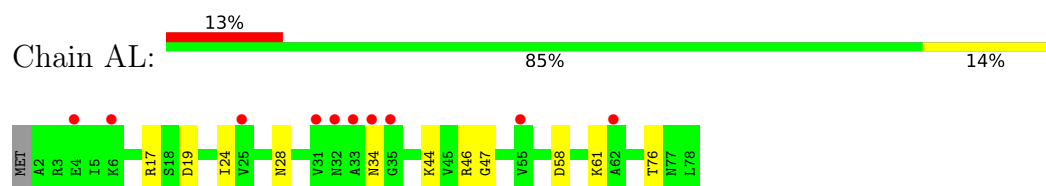
• Molecule 38: 60S ribosomal protein L37-B



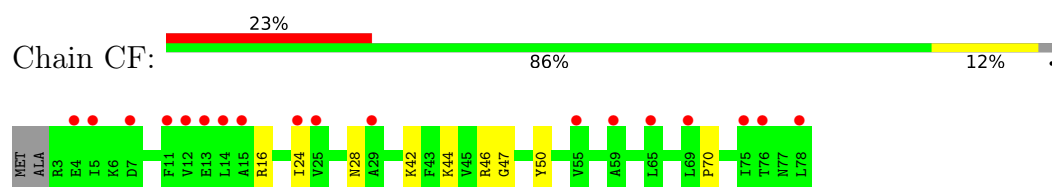
- Molecule 38: 60S ribosomal protein L37-B



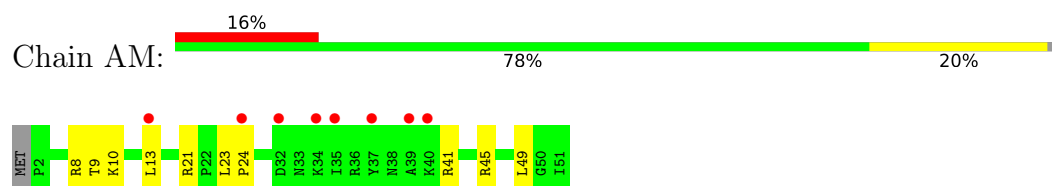
- Molecule 39: 60S ribosomal protein L38



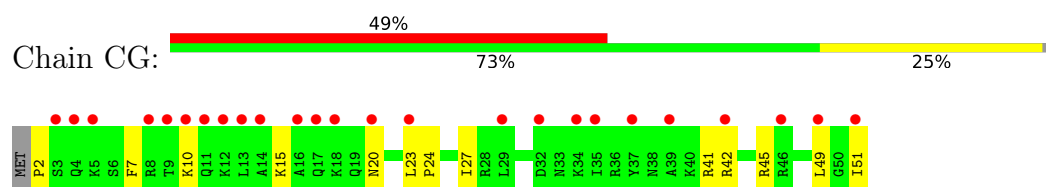
- Molecule 39: 60S ribosomal protein L38



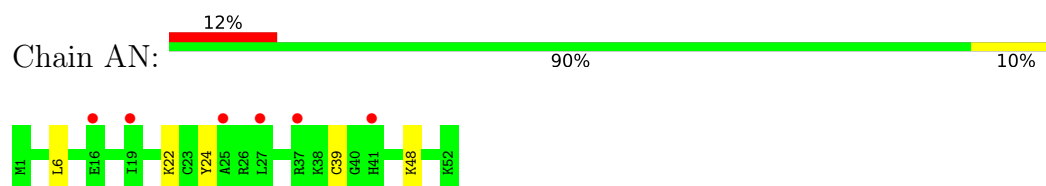
- Molecule 40: 60S ribosomal protein L39



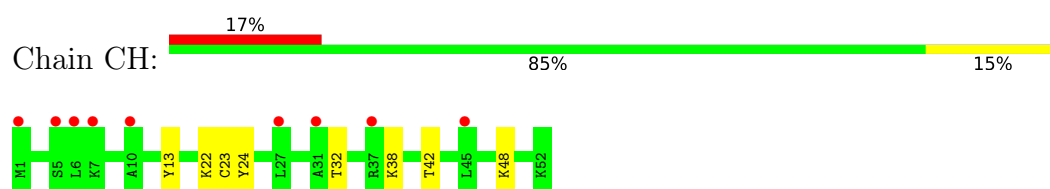
- Molecule 40: 60S ribosomal protein L39



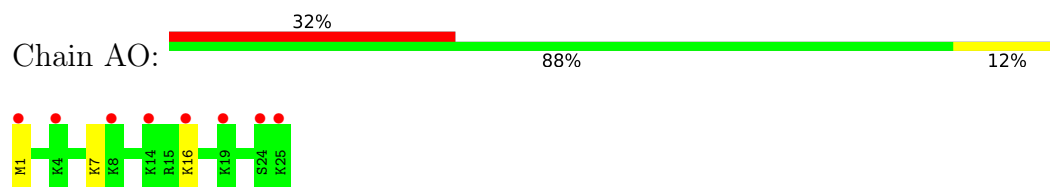
- Molecule 41: 60S ribosomal protein L40-B



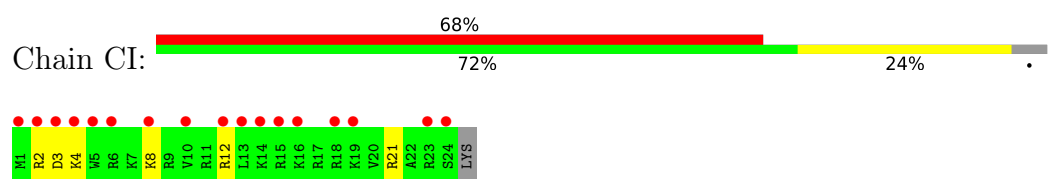
- Molecule 41: 60S ribosomal protein L40-B



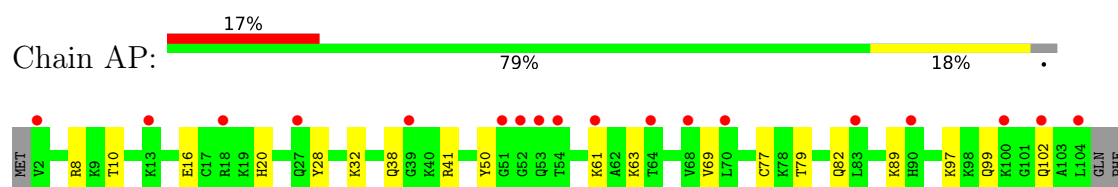
- Molecule 42: 60S ribosomal protein L41



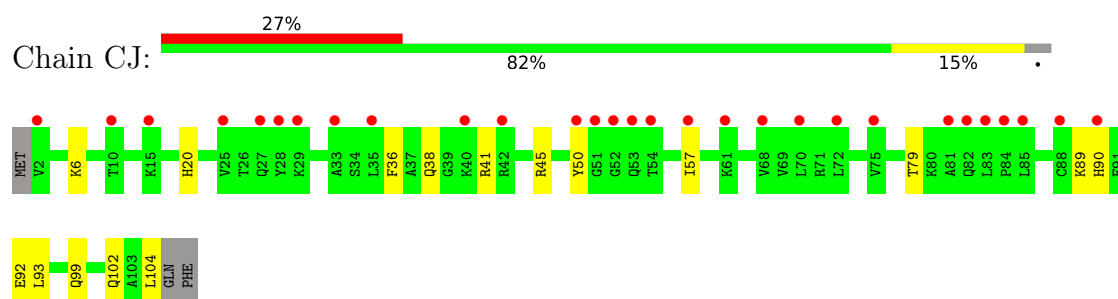
- Molecule 42: 60S ribosomal protein L41



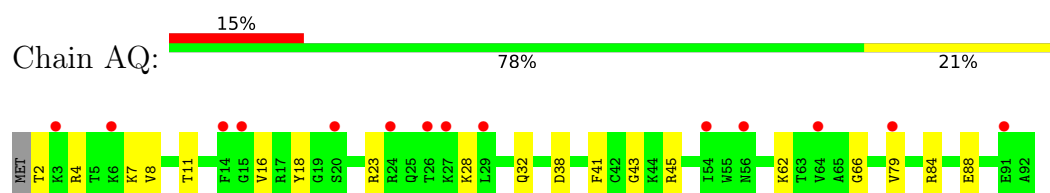
- Molecule 43: 60S ribosomal protein L42-B



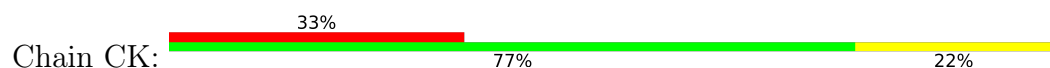
- Molecule 43: 60S ribosomal protein L42-B

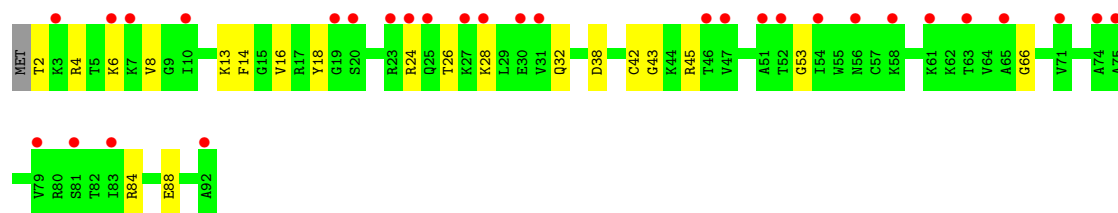


- Molecule 44: 60S ribosomal protein L43-A

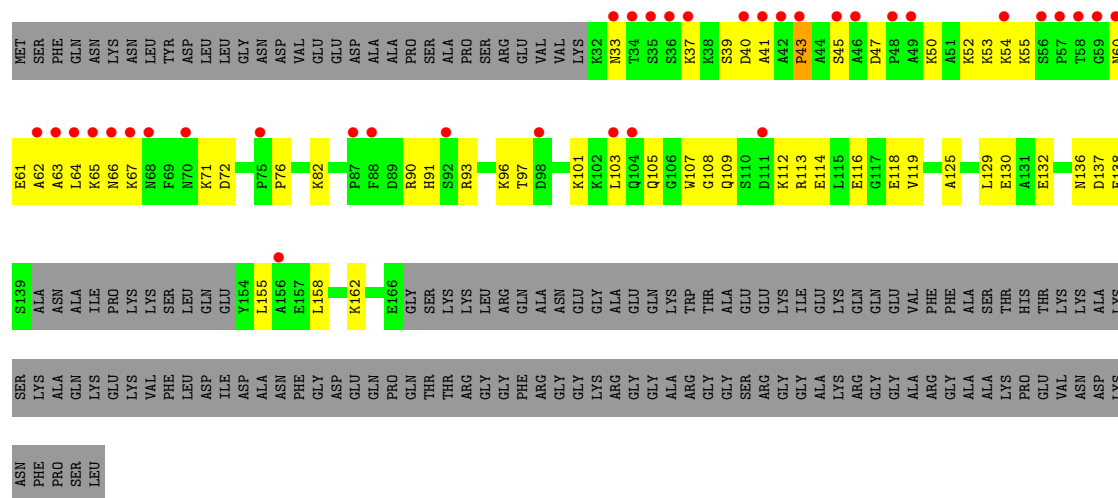


- Molecule 44: 60S ribosomal protein L43-A

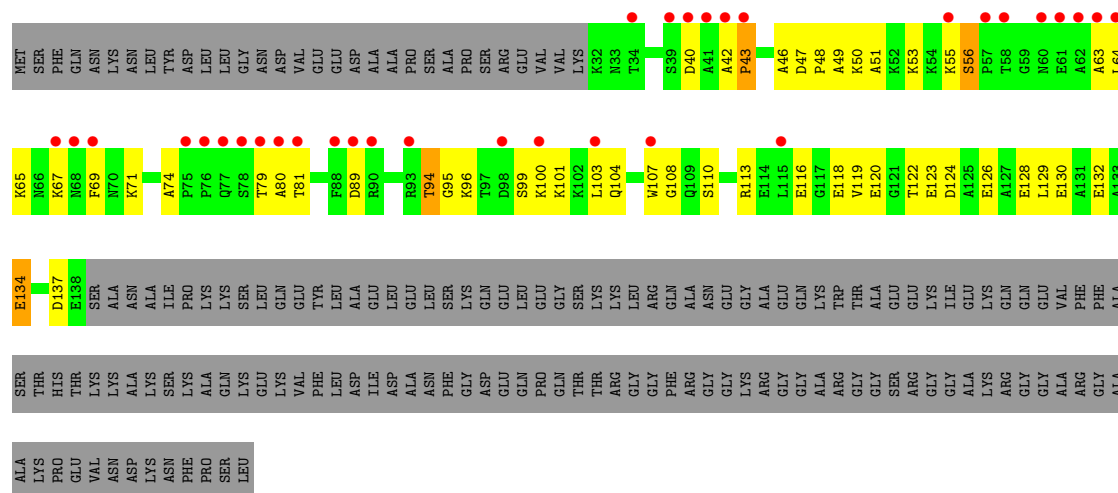




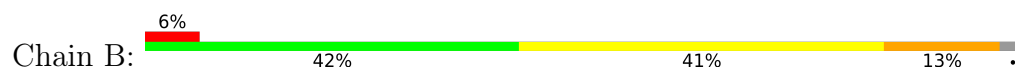
• Molecule 45: 60S ribosomal protein CAALFM_C304810CA

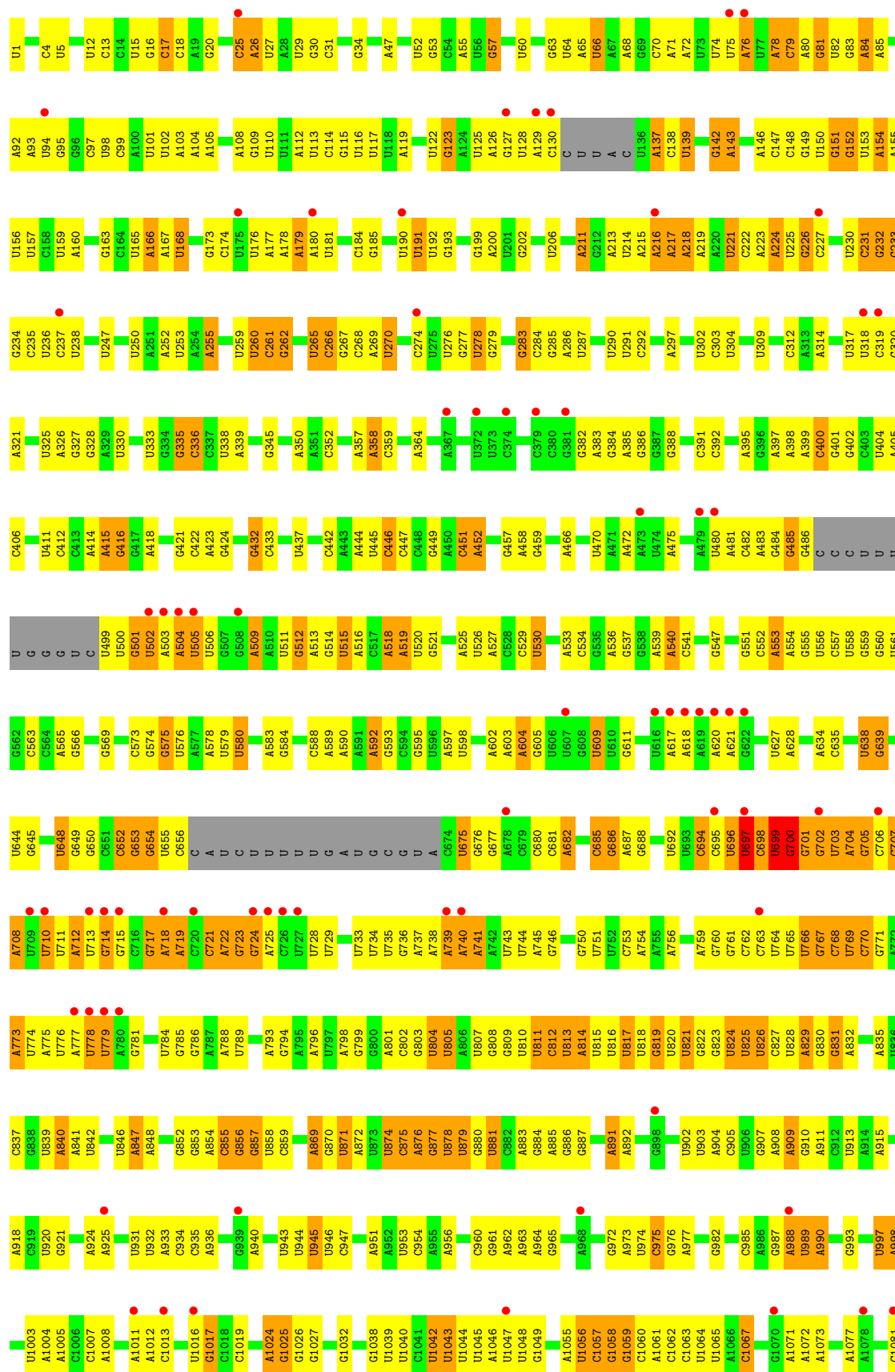


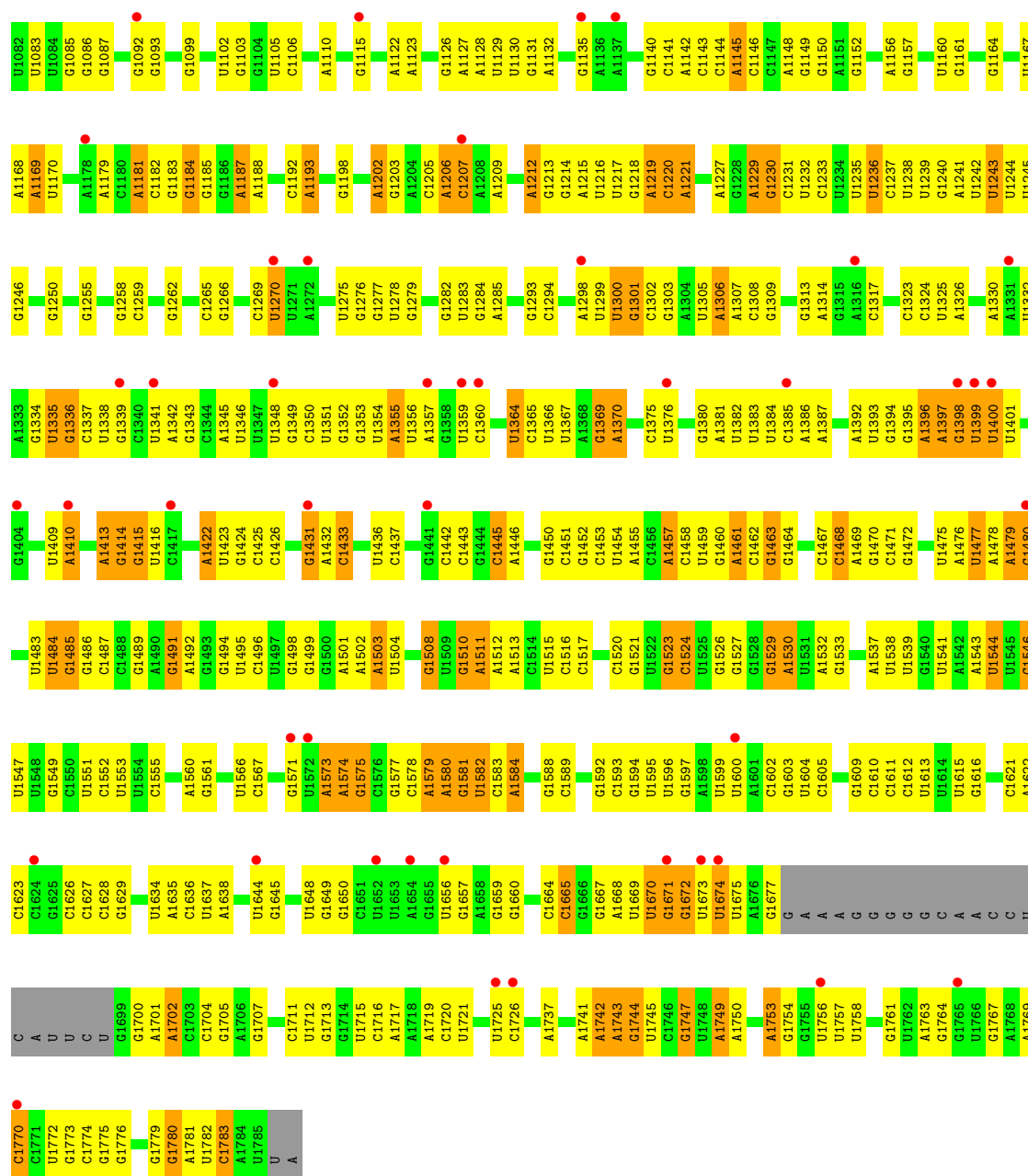
• Molecule 45: 60S ribosomal protein CAALFM_C304810CA



• Molecule 46: 18S

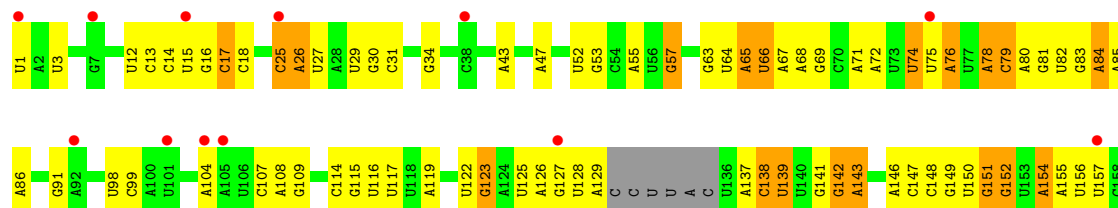




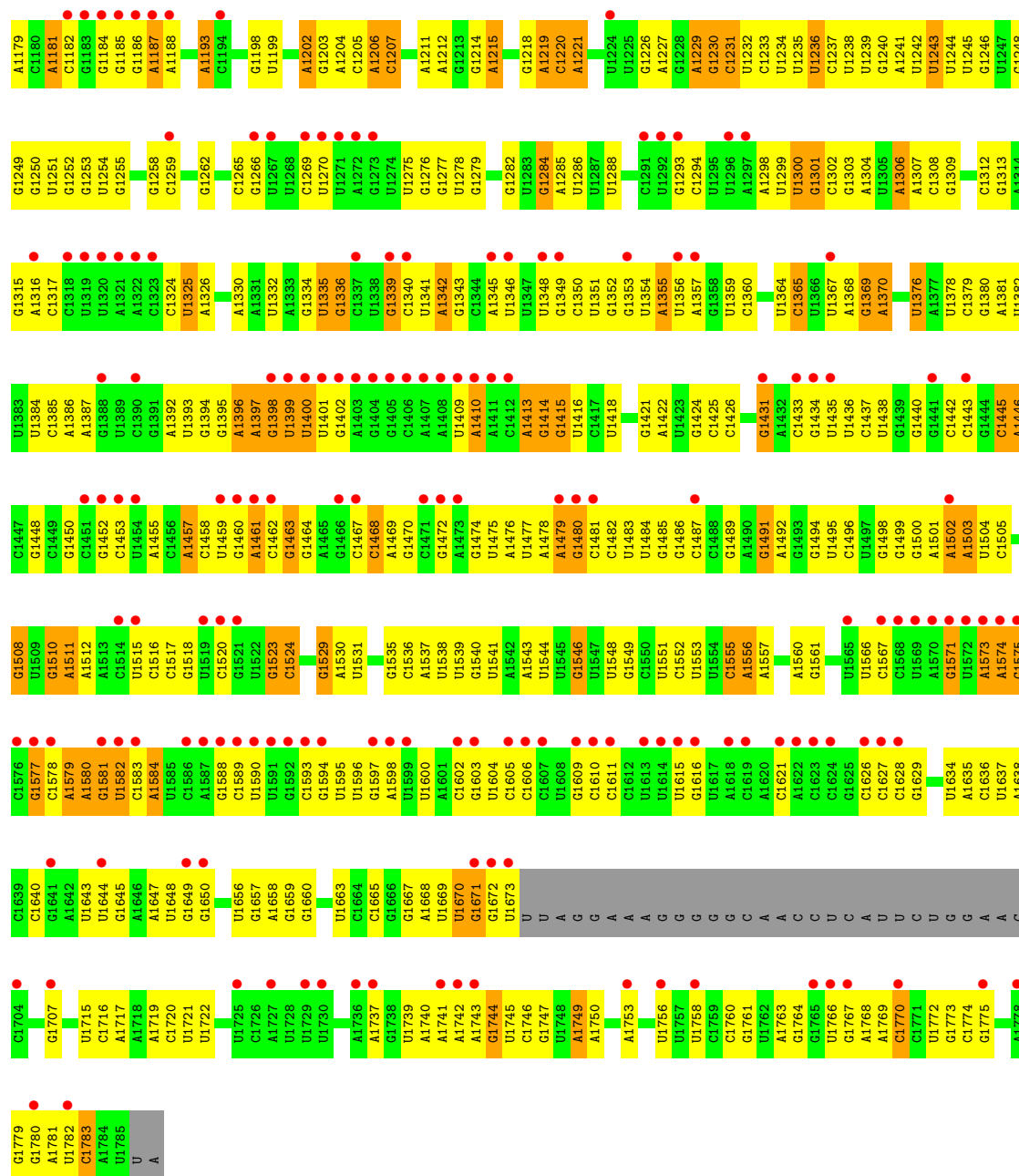


• Molecule 46: 18S

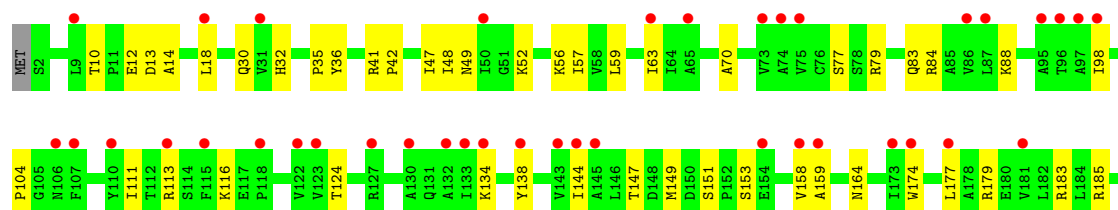
Chain CM: 19% 39% 43% 13% 5%

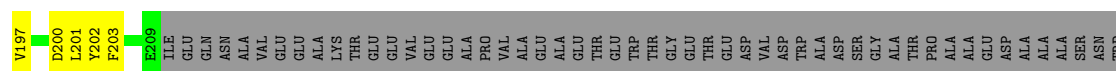




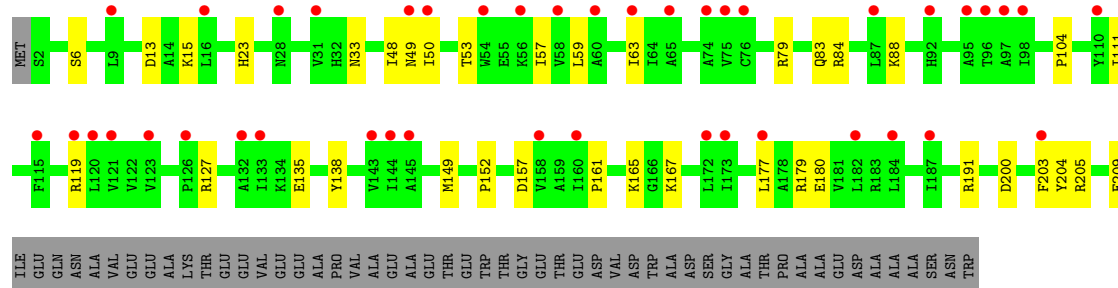


● Molecule 47: 40S ribosomal protein S0

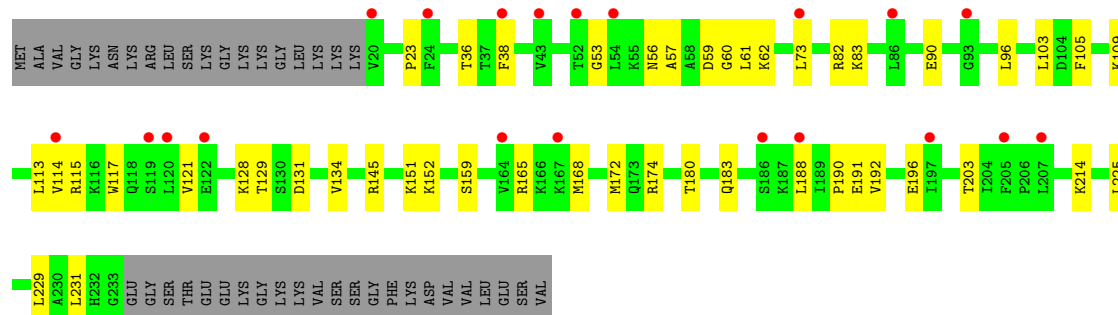




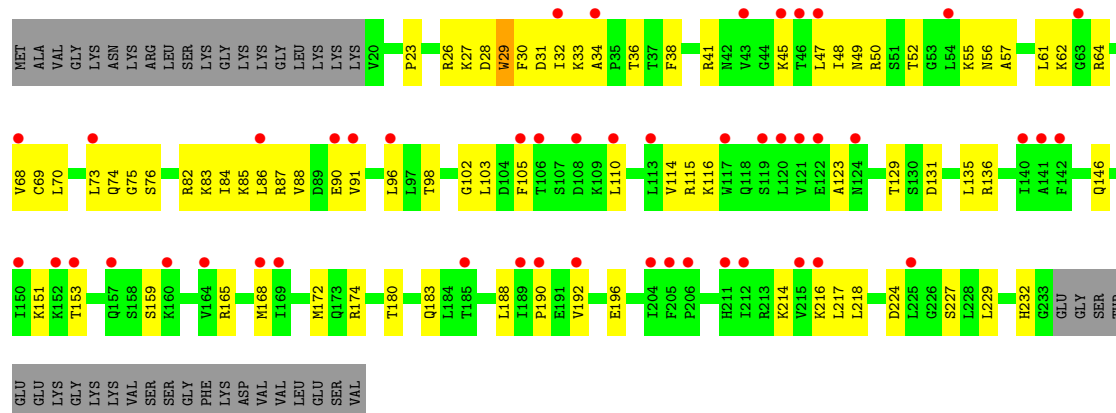
- Molecule 47: 40S ribosomal protein S0



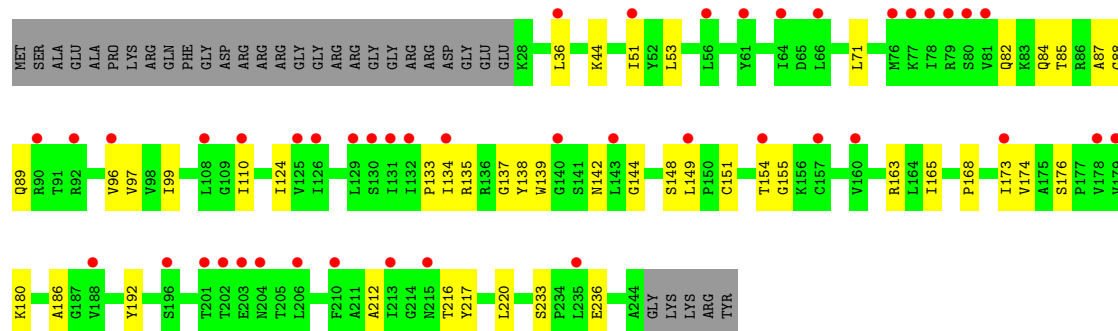
- Molecule 48: 40S ribosomal protein S1



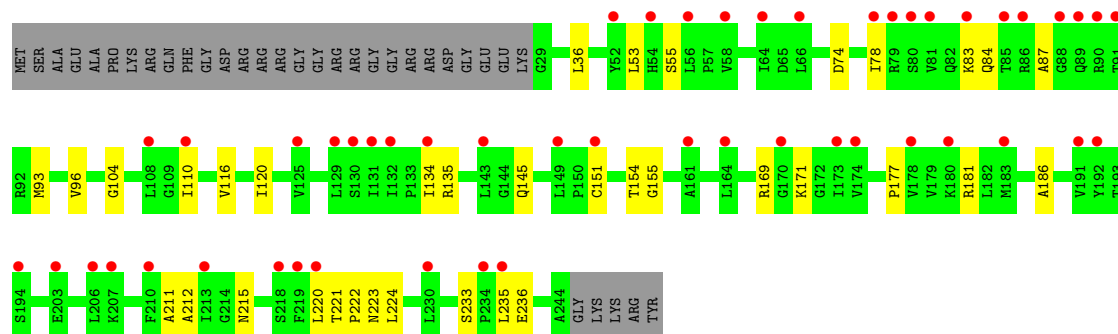
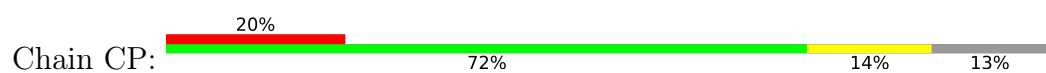
- Molecule 48: 40S ribosomal protein S1



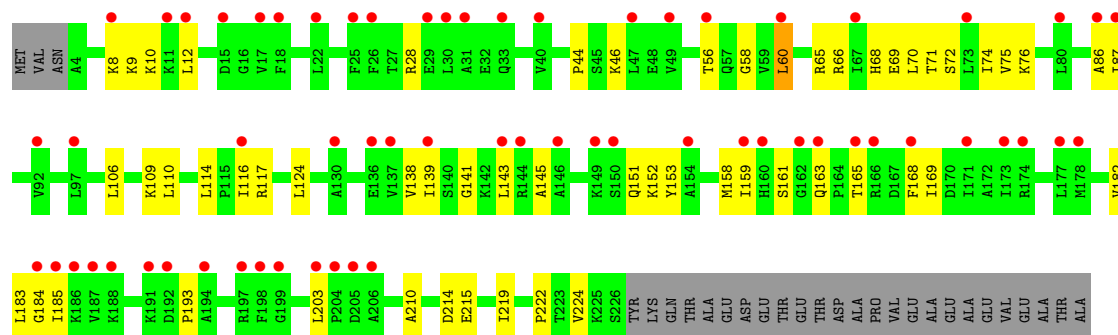
- Molecule 49: Ribosomal protein S5



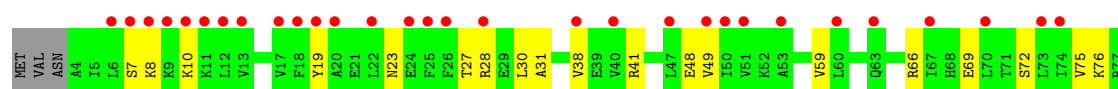
• Molecule 49: Ribosomal protein S5

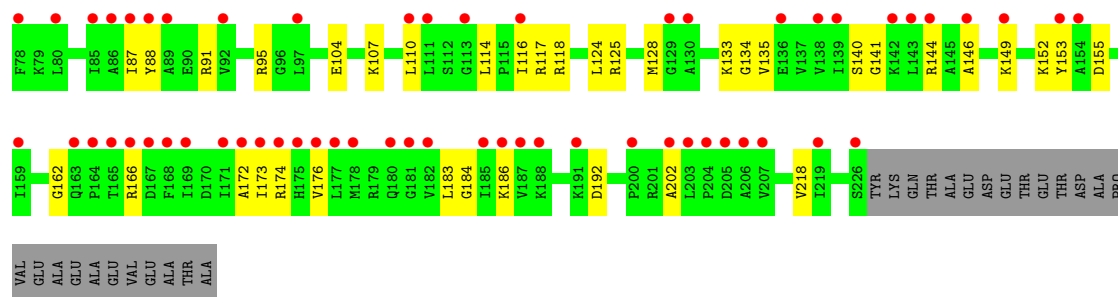


• Molecule 50: Ribosomal protein S3

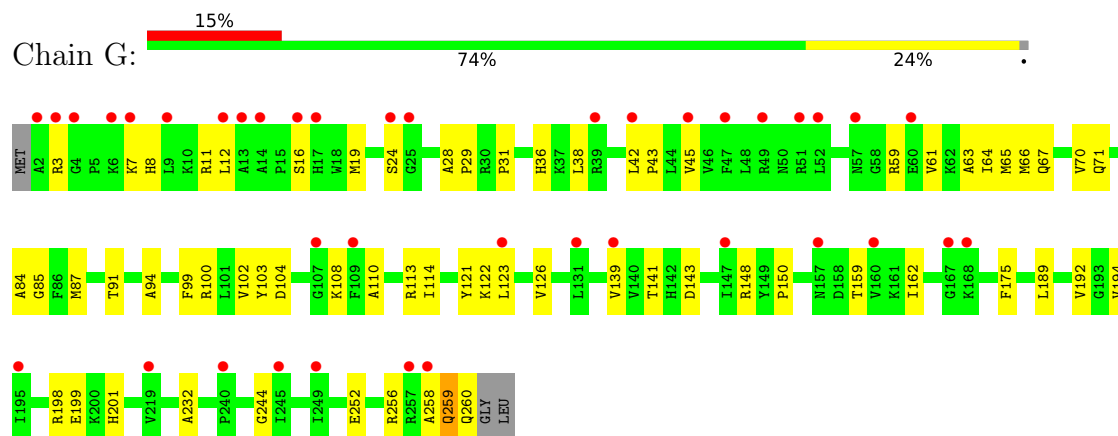


• Molecule 50: Ribosomal protein S3

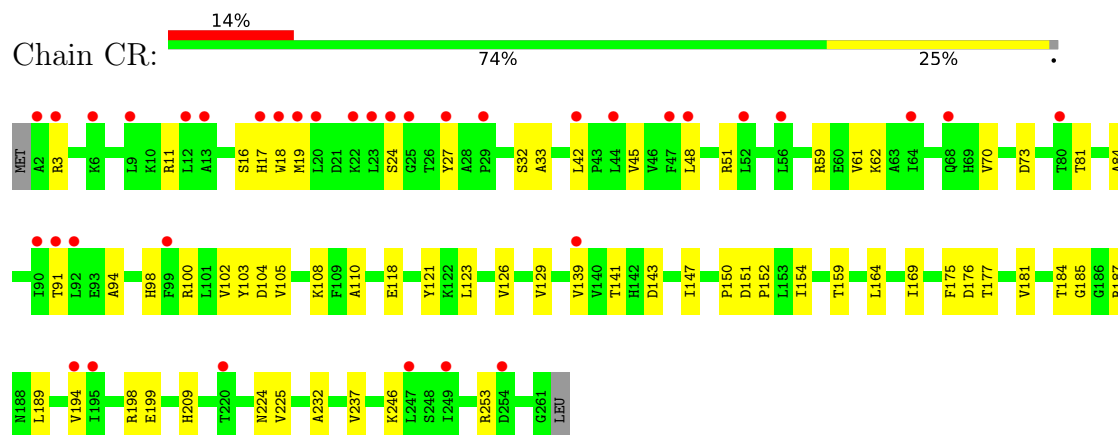




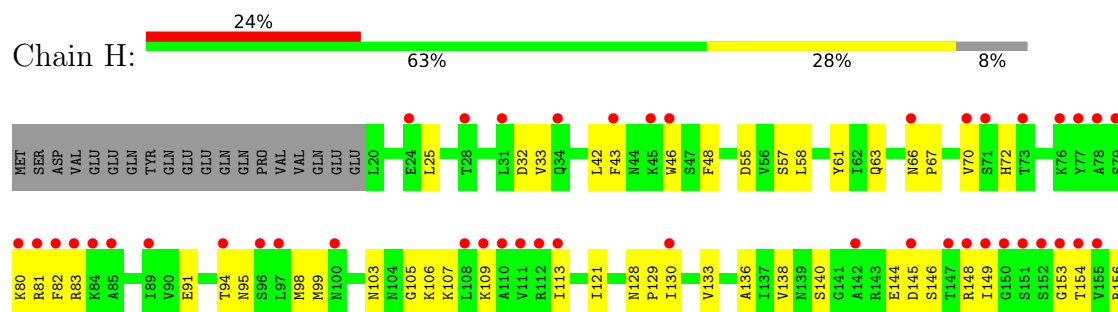
• Molecule 51: 40S ribosomal protein S4

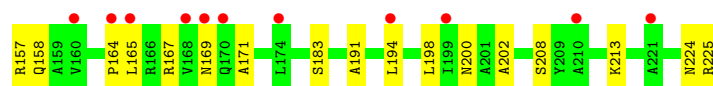


• Molecule 51: 40S ribosomal protein S4

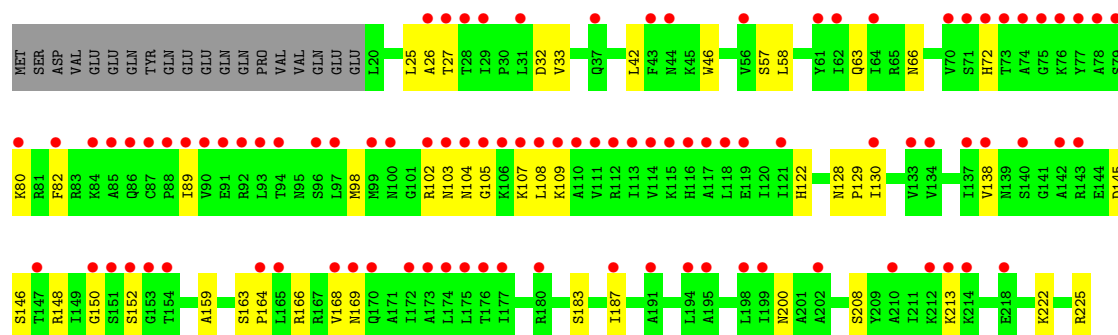
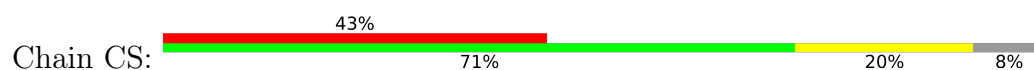


• Molecule 52: Ribosomal protein S7

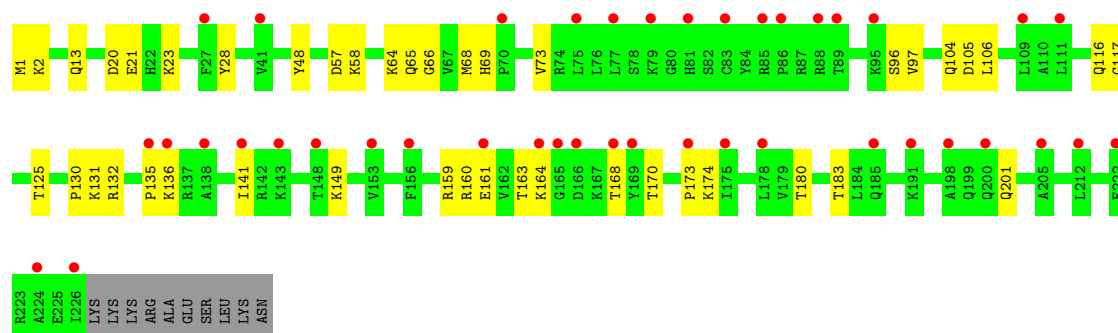
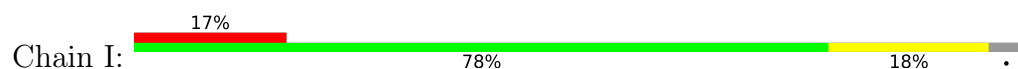




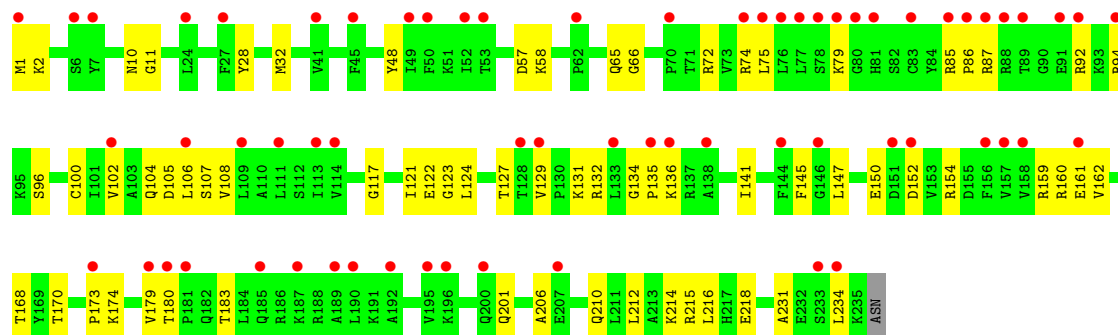
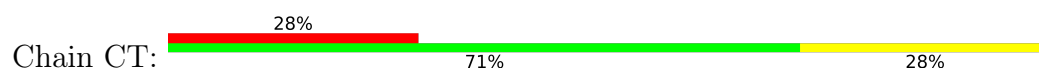
• Molecule 52: Ribosomal protein S7



• Molecule 53: 40S ribosomal protein S6

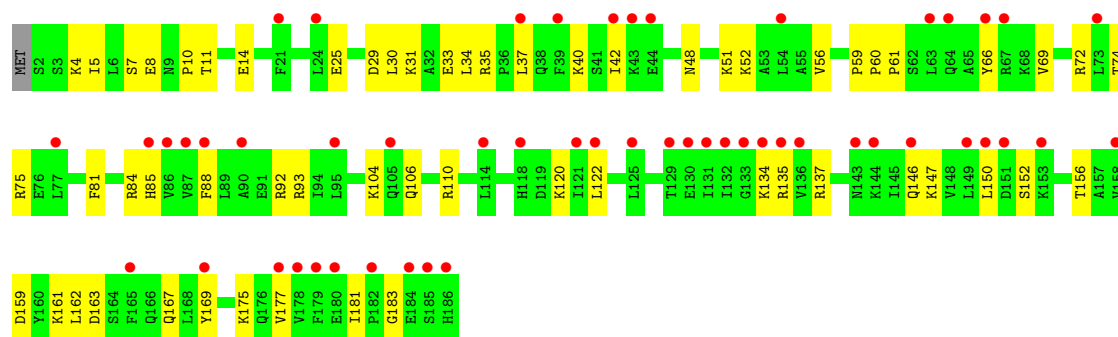


• Molecule 53: 40S ribosomal protein S6

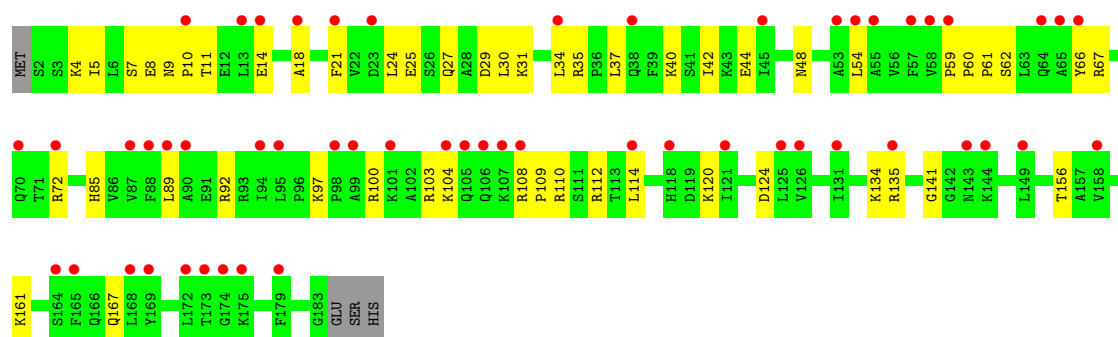
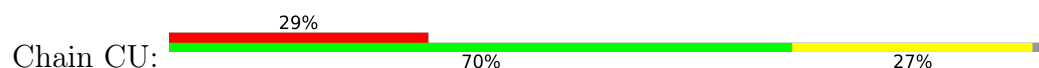


• Molecule 54: 40S ribosomal protein S7

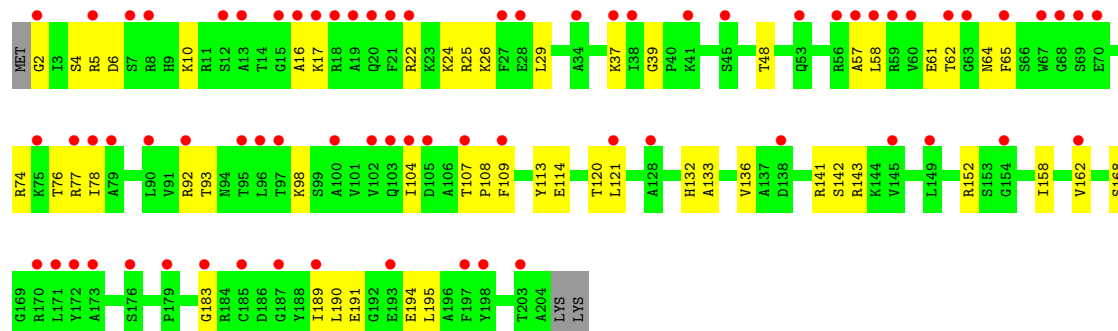
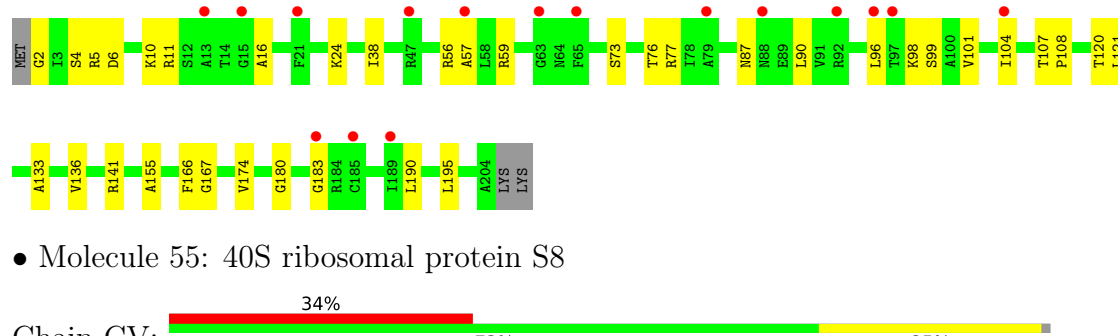
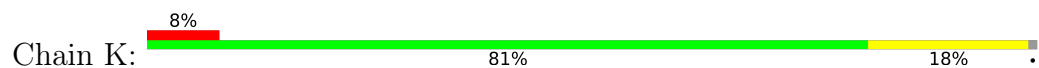




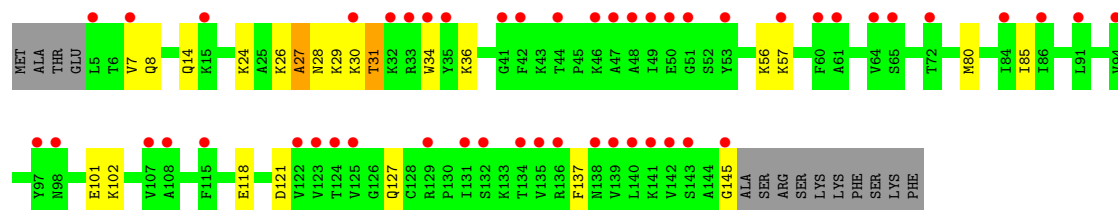
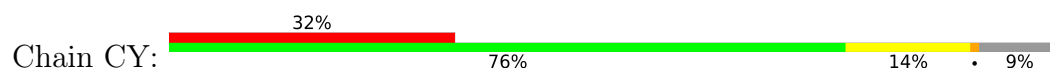
• Molecule 54: 40S ribosomal protein S7



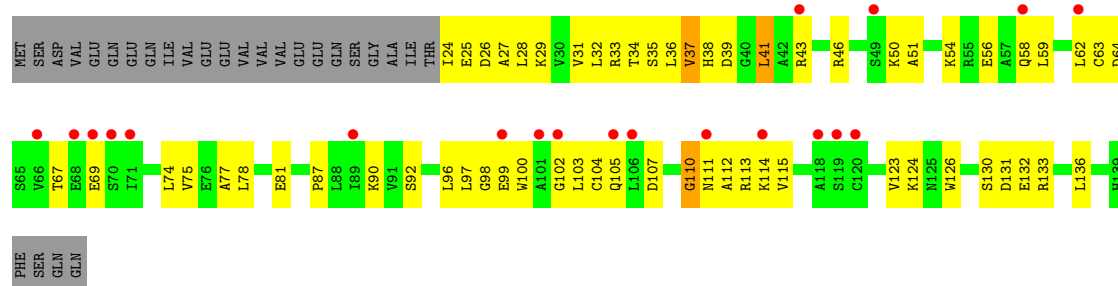
• Molecule 55: 40S ribosomal protein S8



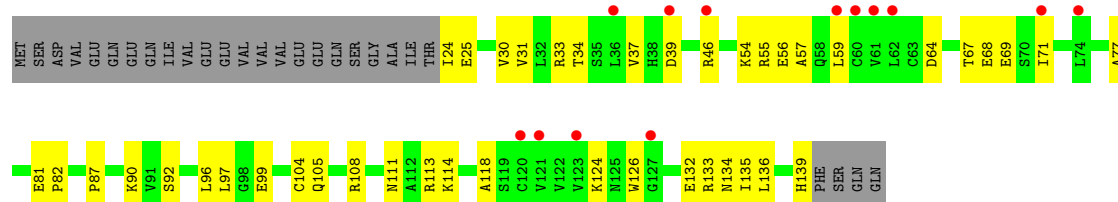
- Molecule 58: 40S ribosomal protein S11A



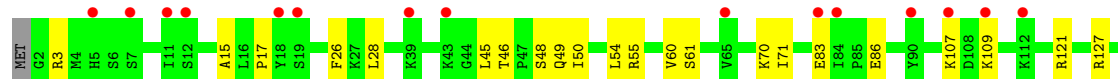
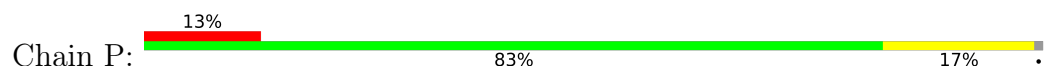
- Molecule 59: 40S ribosomal protein S12

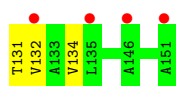


- Molecule 59: 40S ribosomal protein S12

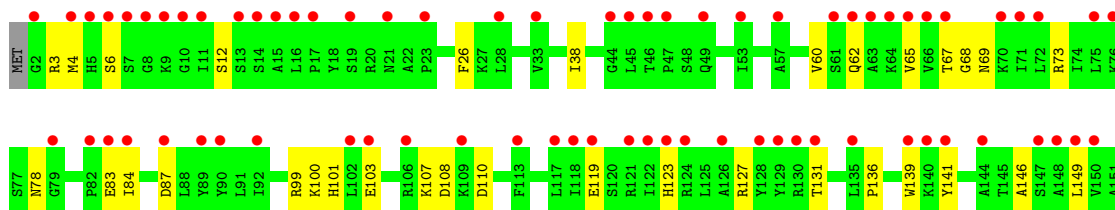
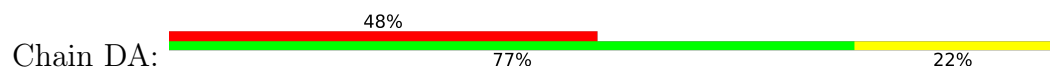


- Molecule 60: 40S ribosomal protein S13

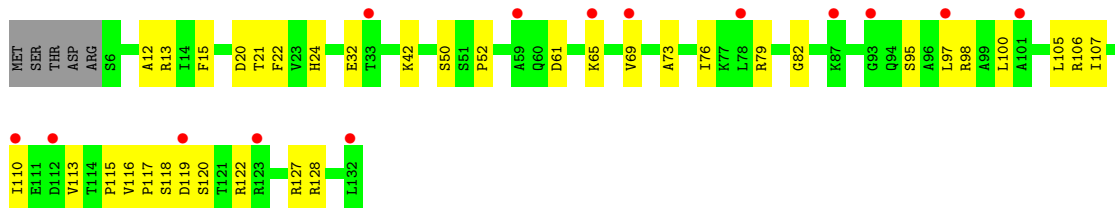




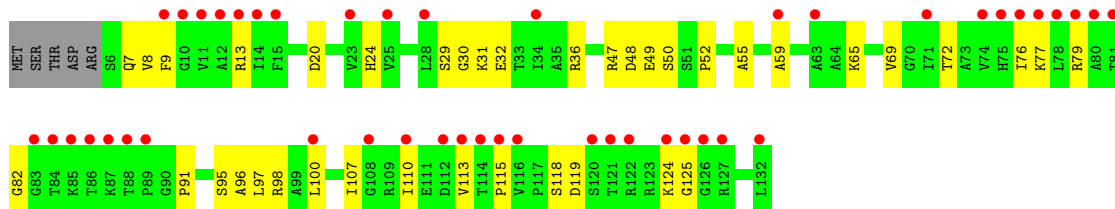
- Molecule 60: 40S ribosomal protein S13



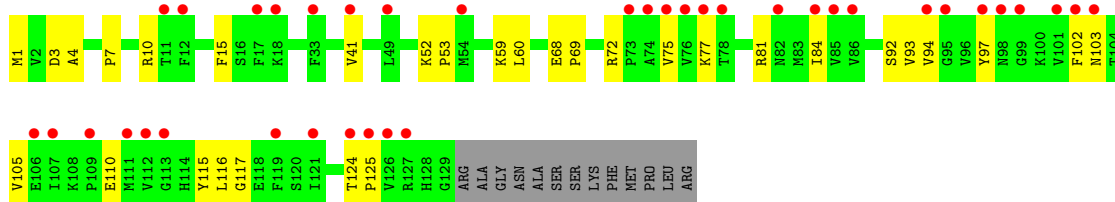
- Molecule 61: 40S ribosomal protein S14-A



- Molecule 61: 40S ribosomal protein S14-A

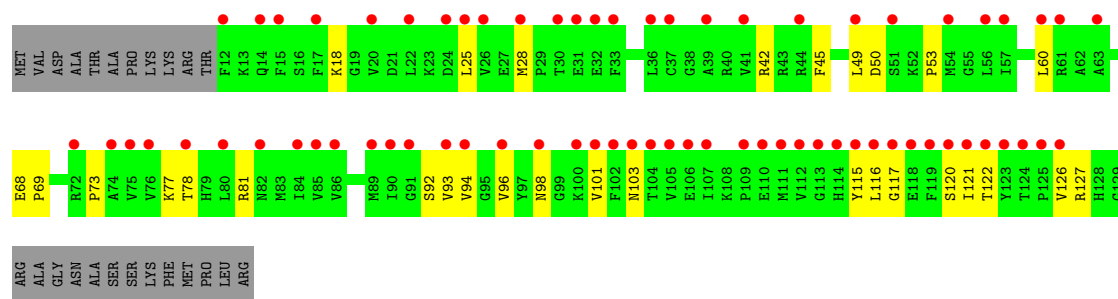


- Molecule 62: 40S ribosomal protein S15



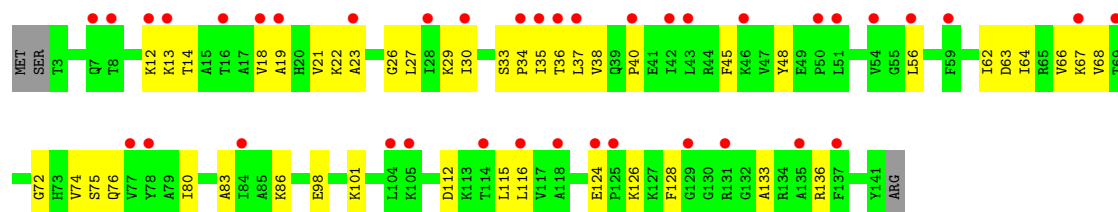
- Molecule 62: 40S ribosomal protein S15

Chain DC: 



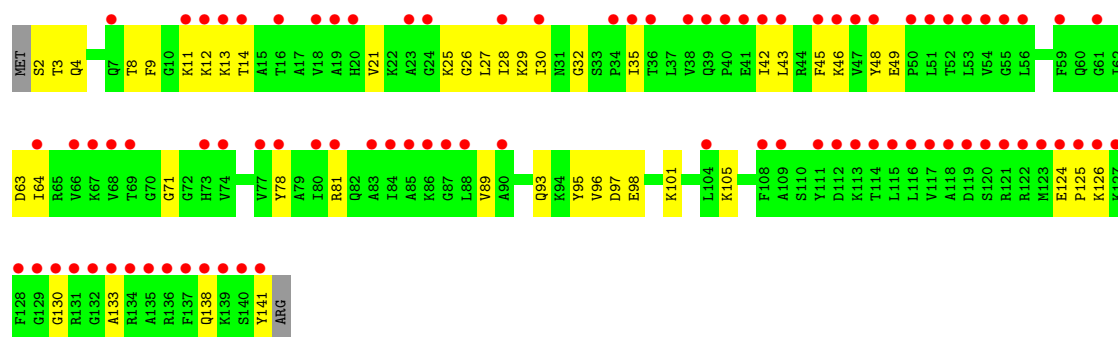
- Molecule 63: 40S ribosomal protein S16

Chain S: 



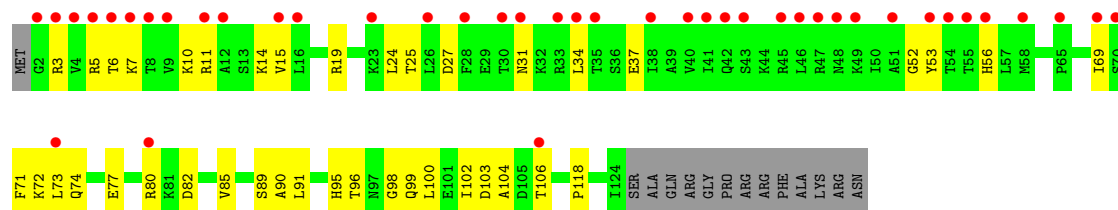
- Molecule 63: 40S ribosomal protein S16

Chain DD: 

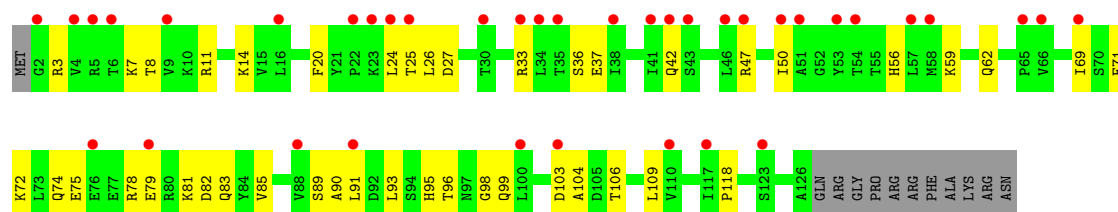


- Molecule 64: 40S ribosomal protein S17-B

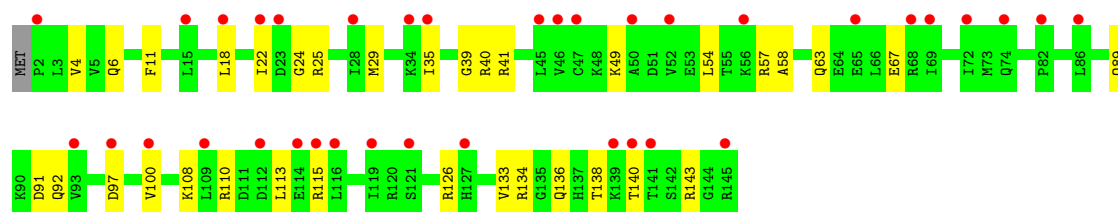
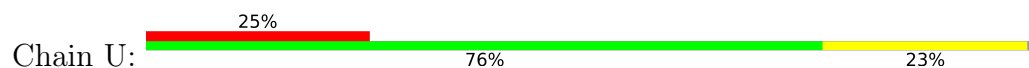
Chain T: 



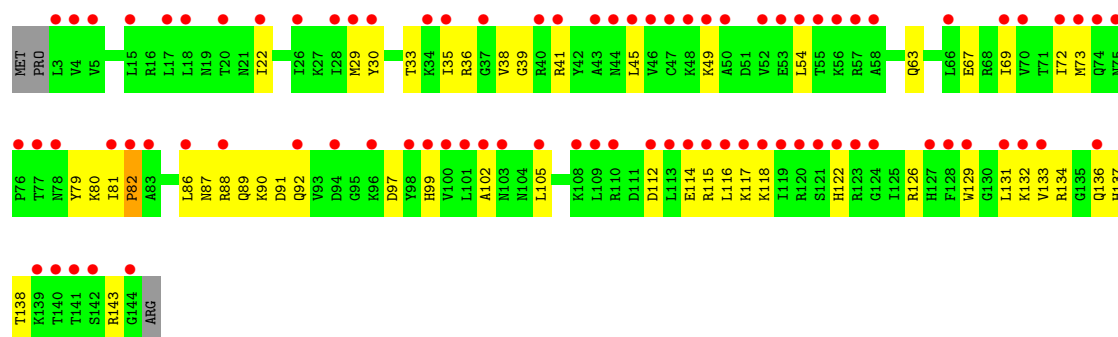
- Molecule 64: 40S ribosomal protein S17-B



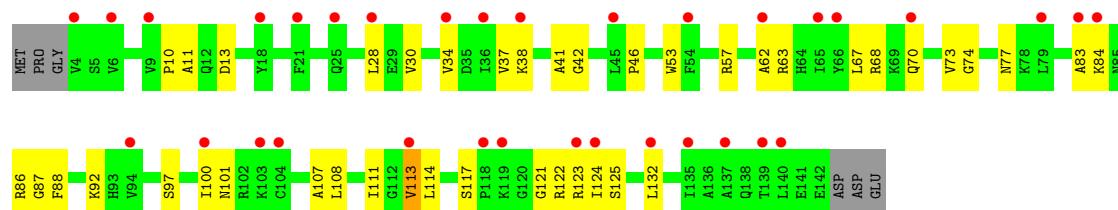
• Molecule 65: 40S ribosomal protein S18-B



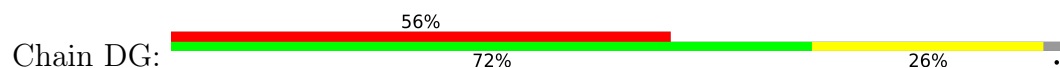
• Molecule 65: 40S ribosomal protein S18-B

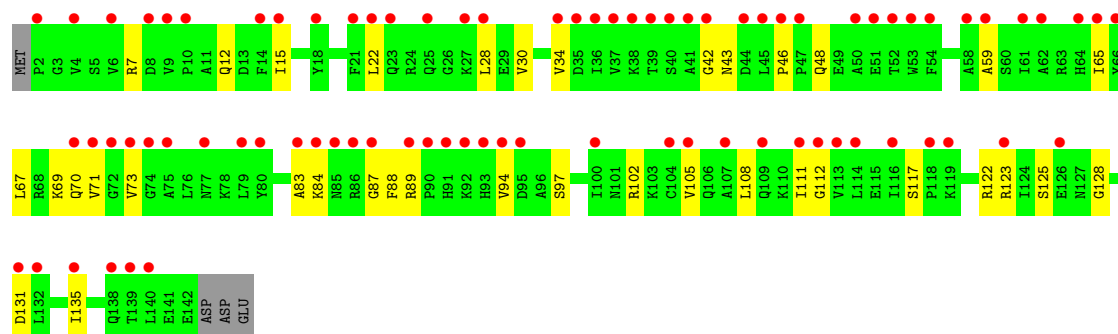


• Molecule 66: 40S ribosomal protein S19-A

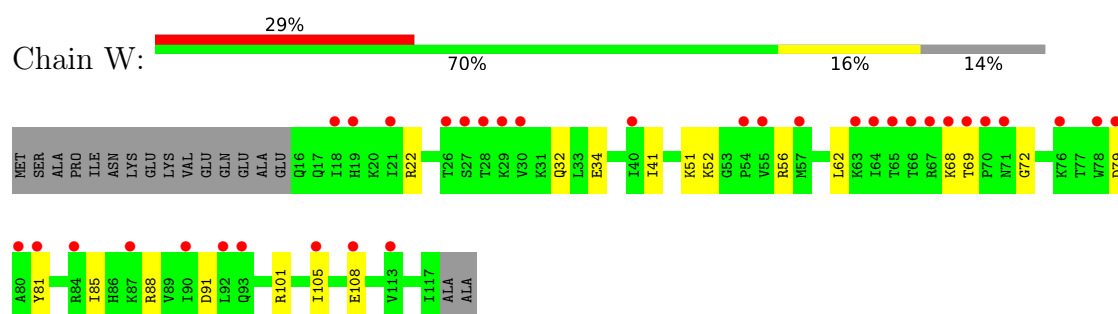


• Molecule 66: 40S ribosomal protein S19-A

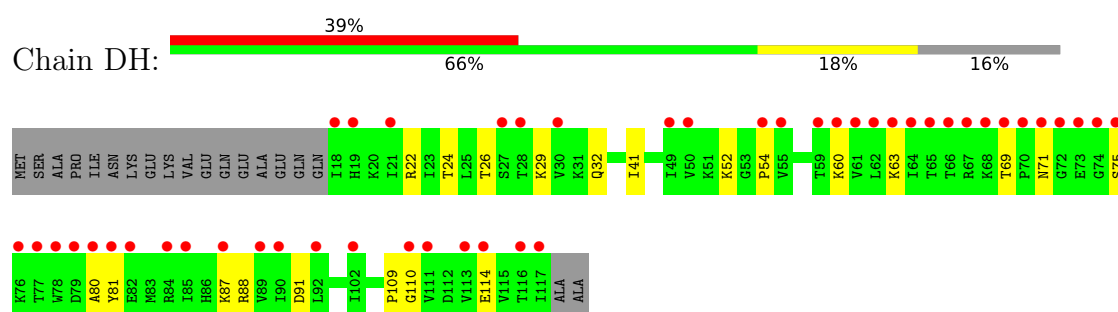




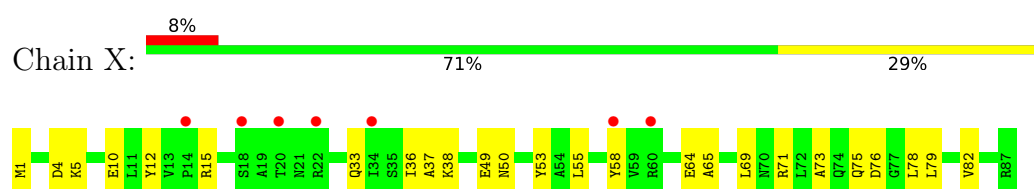
• Molecule 67: Ribosomal protein S10



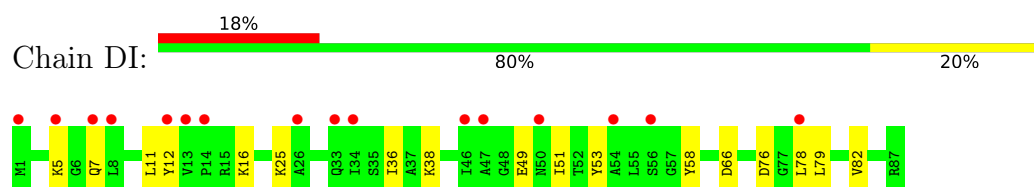
• Molecule 67: Ribosomal protein S10



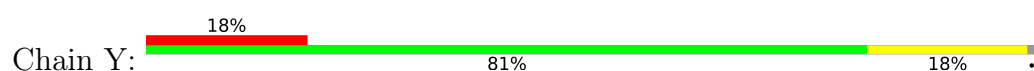
• Molecule 68: 40S ribosomal protein S21

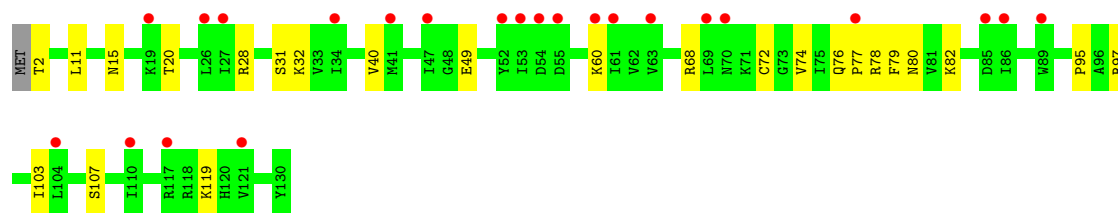


• Molecule 68: 40S ribosomal protein S21

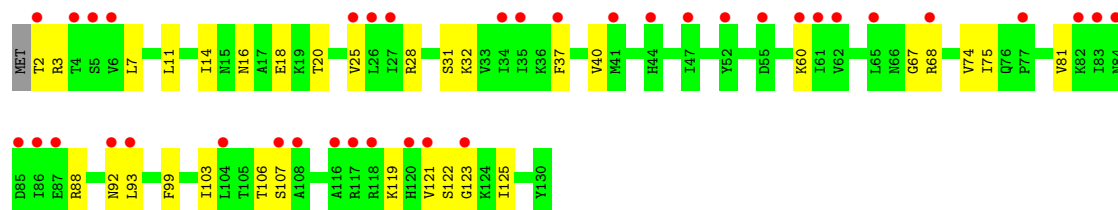
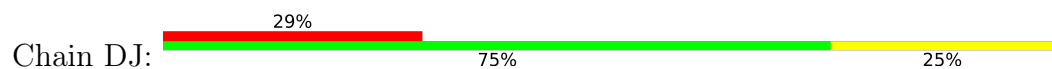


• Molecule 69: 40S ribosomal protein S22-A

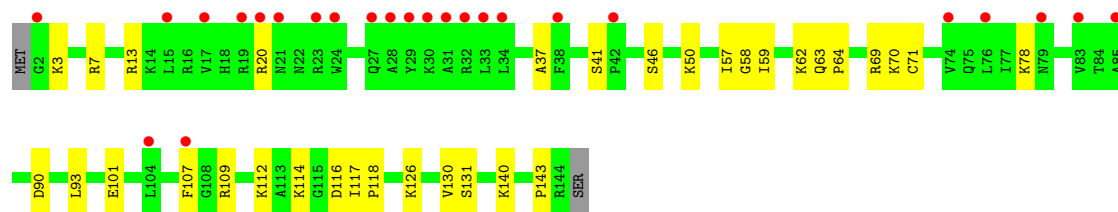
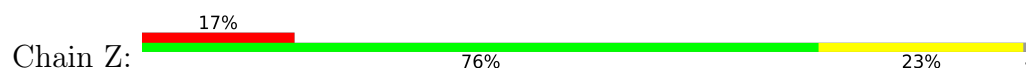




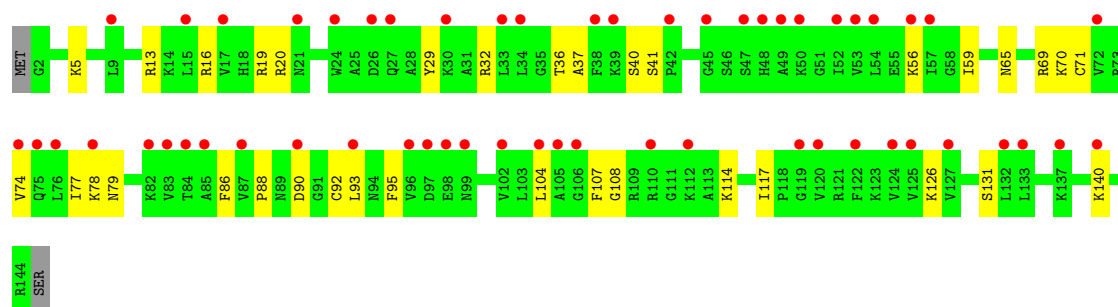
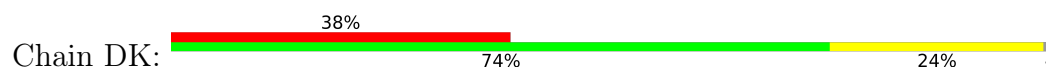
- Molecule 69: 40S ribosomal protein S22-A



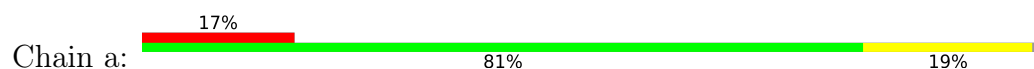
- Molecule 70: Ribosomal protein S23 (S12)

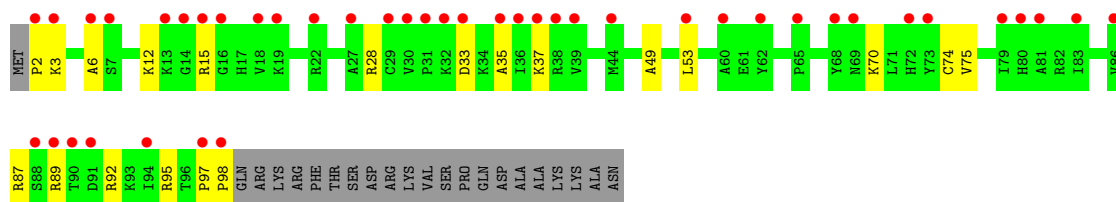


- Molecule 70: Ribosomal protein S23 (S12)

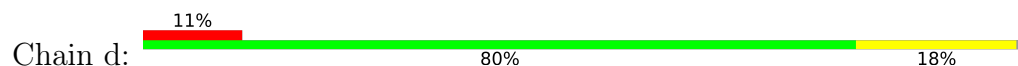


- Molecule 71: 40S ribosomal protein S24

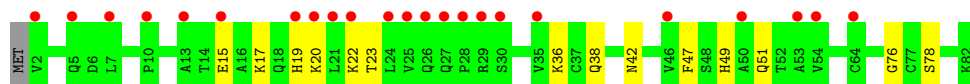
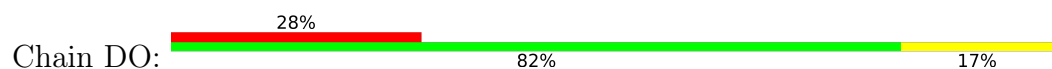




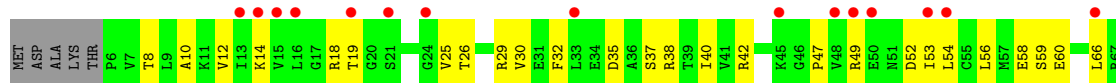
- Molecule 74: 40S ribosomal protein S27



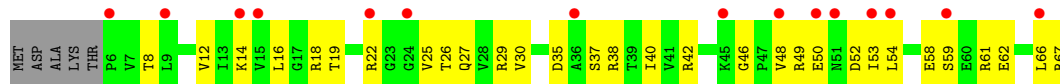
- Molecule 74: 40S ribosomal protein S27



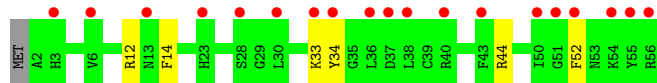
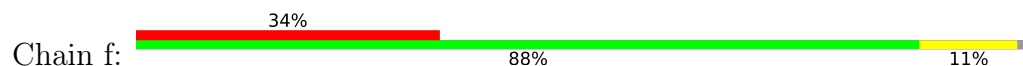
- Molecule 75: 40S ribosomal protein S28-B



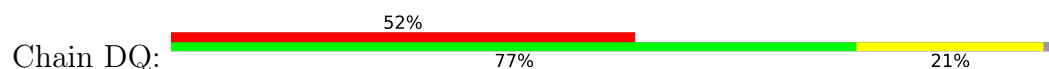
- Molecule 75: 40S ribosomal protein S28-B

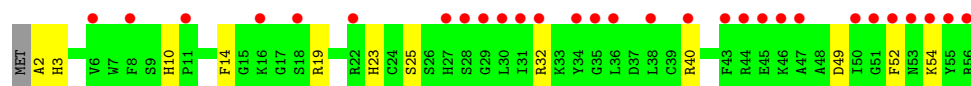


- Molecule 76: 40S ribosomal protein S29A

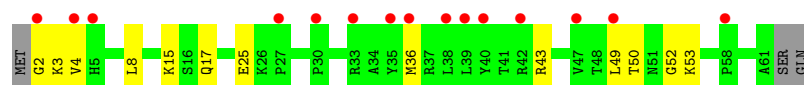
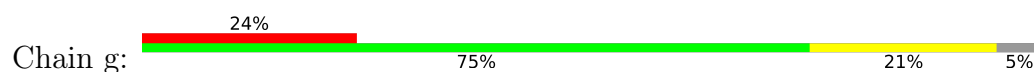


- Molecule 76: 40S ribosomal protein S29A

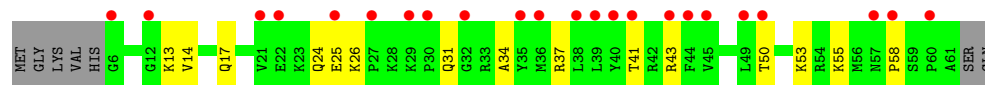
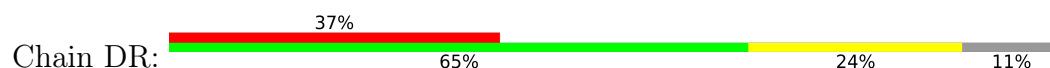




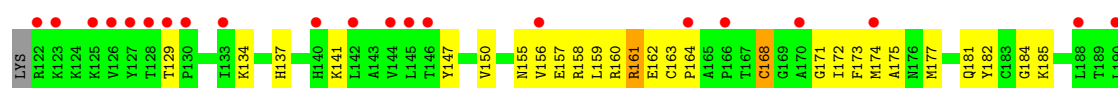
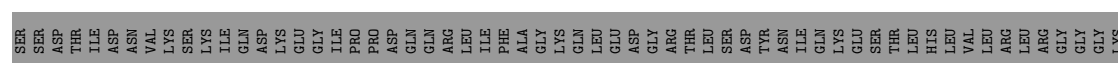
- Molecule 77: 40S ribosomal protein S30



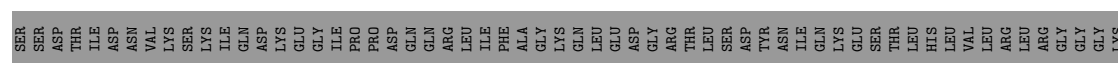
- Molecule 77: 40S ribosomal protein S30



- Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein

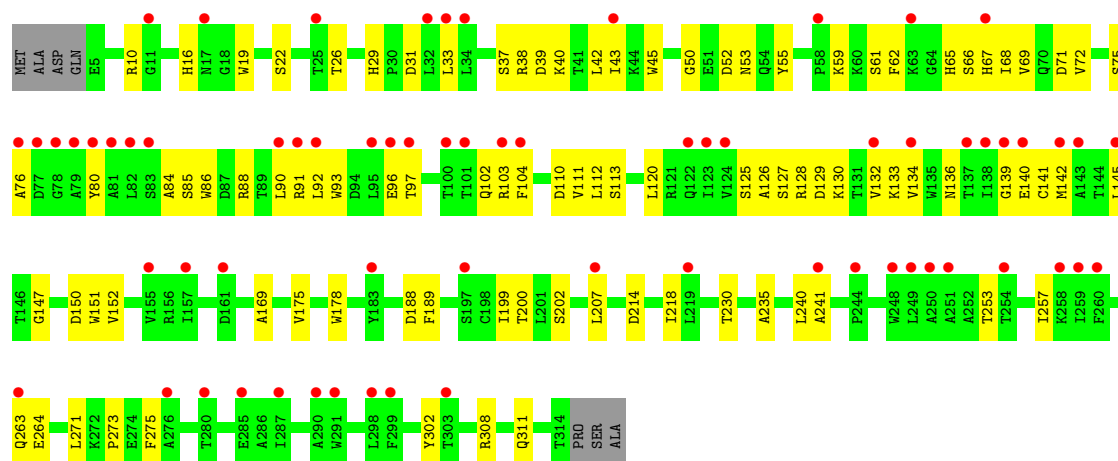


- Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein

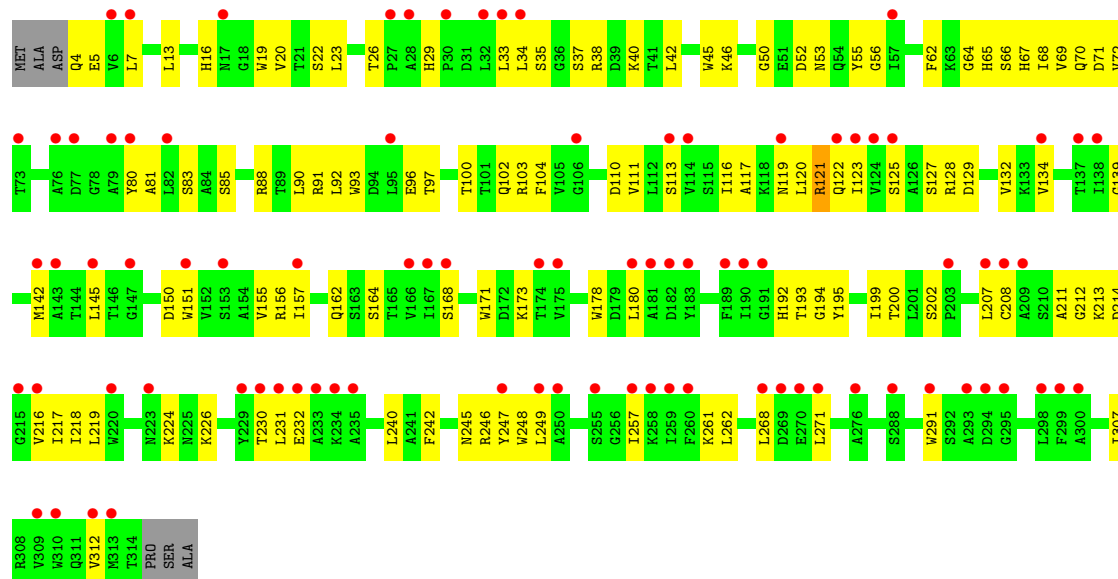


- Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

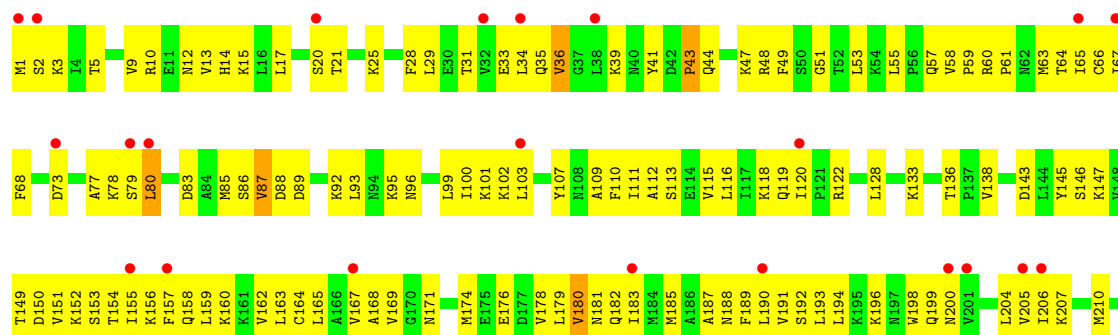




• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein



• Molecule 80: Ribosomal protein





● Molecule 81: 60S ribosomal protein L12-A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	296.89Å 293.38Å 443.00Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	175.26 – 3.35 175.26 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (175.26-3.35) 89.9 (175.26-3.35)	Depositor EDS
R_{merge}	1.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.19rc4_4035: ???)	Depositor
R, R_{free}	0.284 , 0.328 0.284 , 0.328	Depositor DCC
R_{free} test set	2000 reflections (0.15%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 12.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	401103	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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: ZN, PAR, MG, 3K5

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.17	0/77018	0.42	5/120068 (0.0%)
1	AS	0.16	0/73229	0.42	5/114152 (0.0%)
2	3	0.13	0/2884	0.30	0/4492
2	AT	0.13	0/2884	0.31	0/4492
3	4	0.14	0/3724	0.38	0/5798
3	AU	0.14	0/3702	0.37	0/5764
4	AW	0.13	0/1913	0.40	0/2569
4	j	0.15	0/1922	0.38	0/2581
5	AX	0.14	0/3145	0.41	0/4231
5	k	0.15	0/3156	0.43	0/4246
6	AY	0.13	0/2785	0.43	0/3758
6	l	0.16	0/2799	0.44	0/3777
7	AZ	0.14	0/2447	0.42	0/3294
7	m	0.15	0/2479	0.42	0/3337
8	BA	0.14	0/1231	0.41	0/1662
8	n	0.15	0/1263	0.44	0/1703
9	BB	0.13	0/1858	0.39	0/2496
9	o	0.16	0/1867	0.42	0/2508
10	BC	0.16	0/1796	0.51	0/2419
10	p	0.16	0/1861	0.46	0/2508
11	BD	0.14	0/1528	0.41	0/2055
11	q	0.18	0/1537	0.42	0/2067
12	BE	0.14	0/1705	0.41	0/2288
12	r	0.15	0/1724	0.40	0/2314
13	BF	0.15	0/1390	0.43	0/1861
13	s	0.17	0/1390	0.45	0/1861
14	BG	0.15	0/1637	0.51	0/2195
14	t	0.15	0/1637	0.42	0/2195
15	BH	0.15	0/1030	0.38	0/1389
15	u	0.17	0/1044	0.41	0/1407
16	BI	0.14	0/1753	0.41	0/2347
16	v	0.16	0/1753	0.40	0/2347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	BJ	0.13	0/1620	0.40	0/2167
17	w	0.14	0/1620	0.39	0/2167
18	BK	0.13	0/1419	0.38	0/1906
18	x	0.14	0/1403	0.41	0/1885
19	BL	0.12	0/1482	0.37	0/1985
19	y	0.14	0/1482	0.41	0/1985
20	BM	0.13	0/1404	0.43	0/1868
20	z	0.13	0/1475	0.38	0/1961
21	0	0.14	0/1457	0.38	0/1962
21	BN	0.13	0/1457	0.36	0/1962
22	2	0.13	0/1285	0.37	0/1723
22	BO	0.12	0/1285	0.36	0/1723
23	5	0.15	0/846	0.41	0/1140
23	BP	0.24	0/850	0.66	0/1145
24	6	0.13	0/993	0.38	0/1339
24	BQ	0.14	0/993	0.40	0/1339
25	7	0.12	0/958	0.29	0/1267
25	BR	0.17	0/909	0.34	0/1202
26	8	0.13	0/990	0.35	0/1337
26	BS	0.12	0/968	0.33	0/1308
27	9	0.13	0/999	0.35	0/1334
27	BT	0.15	0/985	0.41	0/1315
28	AA	0.12	0/1112	0.36	0/1488
28	BU	0.13	0/1112	0.41	0/1488
29	AB	0.14	0/1199	0.38	0/1607
29	BV	0.13	0/1199	0.43	0/1607
30	AC	0.14	0/503	0.59	0/668
30	BW	0.14	0/502	0.52	0/666
31	AD	0.13	0/764	0.35	0/1029
31	BX	0.14	0/738	0.40	0/994
32	AE	0.15	0/907	0.43	0/1219
32	BY	0.13	0/902	0.43	0/1212
33	AF	0.14	0/1021	0.42	0/1368
33	BZ	0.13	0/1030	0.43	0/1379
34	AG	0.13	0/866	0.36	0/1165
34	CA	0.22	0/895	0.39	0/1201
35	AH	0.14	0/887	0.39	0/1184
35	CB	0.15	0/934	0.42	0/1242
36	AI	0.15	0/1003	0.38	0/1336
36	CC	0.13	0/981	0.43	0/1308
37	AJ	0.12	0/763	0.37	0/1012
37	CD	0.15	0/780	0.52	0/1033
38	AK	0.15	0/690	0.42	0/916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CE	0.16	0/690	0.44	0/916
39	AL	0.14	0/623	0.42	0/831
39	CF	0.13	0/627	0.37	0/835
40	AM	0.13	0/447	0.34	0/594
40	CG	0.13	0/447	0.45	0/594
41	AN	0.16	0/425	0.44	0/563
41	CH	0.13	0/436	0.38	0/577
42	AO	0.18	0/237	0.48	0/304
42	CI	0.19	0/228	0.55	0/293
43	AP	0.15	0/840	0.41	0/1110
43	CJ	0.15	0/860	0.38	0/1136
44	AQ	0.14	0/705	0.36	0/940
44	CK	0.13	0/705	0.41	0/940
45	CL	0.28	0/826	0.94	1/1104 (0.1%)
45	i	0.24	0/941	0.89	0/1257
46	B	0.17	0/41264	0.43	6/64298 (0.0%)
46	CM	0.17	0/40656	0.44	4/63348 (0.0%)
47	C	0.13	0/1666	0.37	0/2273
47	CN	0.14	0/1666	0.43	0/2273
48	CO	0.20	0/1750	0.62	0/2354
48	D	0.13	0/1750	0.36	0/2354
49	CP	0.12	0/1648	0.37	0/2237
49	E	0.14	0/1657	0.39	0/2248
50	CQ	0.21	0/1731	0.47	0/2324
50	F	0.17	0/1731	0.51	1/2324 (0.0%)
51	CR	0.14	0/2096	0.40	0/2822
51	G	0.13	0/2092	0.37	0/2817
52	CS	0.13	0/1631	0.41	0/2199
52	H	0.18	0/1631	0.45	1/2199 (0.0%)
53	CT	0.13	0/1920	0.41	0/2560
53	I	0.14	0/1845	0.42	0/2464
54	CU	0.17	0/1490	0.44	0/2004
54	J	0.15	0/1516	0.43	0/2039
55	CV	0.14	0/1606	0.41	0/2150
55	K	0.13	0/1606	0.37	0/2150
56	CW	0.13	0/1478	0.39	0/1978
56	L	0.13	0/1478	0.35	0/1978
57	CX	0.18	0/801	0.50	0/1081
57	M	0.23	0/836	0.73	2/1130 (0.2%)
58	CY	0.18	0/1154	0.51	0/1553
58	N	0.14	0/1175	0.43	0/1582
59	CZ	0.17	0/892	0.55	0/1203
59	O	0.29	0/892	0.92	0/1203

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	DA	0.14	0/1210	0.40	0/1631
60	P	0.14	0/1210	0.40	0/1631
61	DB	0.14	0/953	0.47	0/1279
61	Q	0.13	0/953	0.40	0/1279
62	DC	0.15	0/954	0.49	0/1282
62	R	0.18	0/1038	0.55	0/1395
63	DD	0.14	0/1109	0.40	0/1486
63	S	0.16	0/1103	0.46	0/1478
64	DE	0.16	0/1014	0.47	0/1361
64	T	0.18	0/1003	0.53	0/1346
65	DF	0.16	0/1186	0.56	0/1590
65	U	0.15	0/1205	0.42	0/1615
66	DG	0.14	0/1120	0.45	0/1508
66	V	0.16	0/1108	0.55	0/1492
67	DH	0.14	0/800	0.40	0/1082
67	W	0.16	0/818	0.47	0/1106
68	DI	0.14	0/683	0.44	0/918
68	X	0.15	0/683	0.43	0/918
69	DJ	0.15	0/1049	0.42	0/1412
69	Y	0.16	0/1049	0.39	0/1412
70	DK	0.15	0/1128	0.45	0/1505
70	Z	0.15	0/1128	0.51	0/1505
71	DL	0.12	0/1086	0.37	0/1447
71	a	0.12	0/1100	0.39	0/1466
72	DM	0.14	0/585	0.39	0/789
72	b	0.14	0/577	0.37	0/778
73	DN	0.18	0/782	0.51	0/1048
73	c	0.16	0/791	0.47	0/1060
74	DO	0.13	0/624	0.43	0/843
74	d	0.14	0/624	0.43	0/843
75	DP	0.15	0/489	0.48	0/654
75	e	0.16	0/489	0.52	0/654
76	DQ	0.14	0/466	0.38	0/620
76	f	0.15	0/466	0.41	0/620
77	DR	0.16	0/451	0.50	0/601
77	g	0.15	0/482	0.49	0/642
78	DS	0.17	0/585	0.54	0/778
78	h	0.26	0/585	0.82	0/778
79	AR	0.17	0/2442	0.46	0/3325
79	DT	0.23	0/2451	0.60	1/3337 (0.0%)
80	l1	0.17	0/1737	0.46	0/2335
81	12	0.10	0/96	0.33	0/128
All	All	0.16	0/427866	0.43	26/627439 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
9	o	0	1
11	BD	0	1
52	H	0	1
57	M	0	1
61	Q	0	1
79	DT	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AS	3163	U	O5'-C5'-C4'	10.56	127.33	111.50
46	CM	1340	C	OP1-P-O3'	-9.23	80.30	108.00
46	CM	1340	C	OP2-P-O3'	-8.21	83.36	108.00
1	AS	3163	U	O5'-P-OP1	6.47	127.42	108.00
1	1	1669	G	O3'-P-O5'	6.24	113.36	104.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	2832	U	Sidechain
52	H	153	GLY	Mainchain
57	M	15	LEU	Mainchain
61	Q	119	ASP	Peptide
9	o	233	ILE	Mainchain

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	68814	0	34586	1107	0
1	AS	65432	0	32882	1064	0
2	3	2579	0	1304	32	0
2	AT	2579	0	1304	35	0
3	4	3333	0	1684	54	0
3	AU	3313	0	1674	68	0
4	AW	1879	0	1954	45	0
4	j	1888	0	1962	43	0
5	AX	3077	0	3166	62	0
5	k	3084	0	3173	51	0
6	AY	2737	0	2868	53	0
6	l	2751	0	2879	54	0
7	AZ	2394	0	2361	41	0
7	m	2426	0	2389	35	0
8	BA	1210	0	1285	27	0
8	n	1242	0	1321	29	0
9	BB	1825	0	1913	30	0
9	o	1834	0	1919	21	0
10	BC	1766	0	1882	25	0
10	p	1831	0	1951	25	0
11	BD	1510	0	1582	28	0
11	q	1519	0	1588	33	0
12	BE	1671	0	1717	20	0
12	r	1689	0	1731	24	0
13	BF	1371	0	1410	31	0
13	s	1371	0	1410	27	0
14	BG	1610	0	1686	38	0
14	t	1610	0	1686	35	0
15	BH	1015	0	1098	19	0
15	u	1029	0	1116	24	0
16	BI	1713	0	1764	56	0
16	v	1713	0	1764	42	0
17	BJ	1590	0	1705	21	0
17	w	1590	0	1705	26	0
18	BK	1396	0	1421	31	0
18	x	1380	0	1401	25	0
19	BL	1458	0	1556	28	0
19	y	1458	0	1556	27	0
20	BM	1386	0	1487	31	0
20	z	1457	0	1564	22	0
21	0	1423	0	1480	31	0
21	BN	1423	0	1480	39	0
22	2	1262	0	1314	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	BO	1262	0	1314	30	0
23	5	831	0	848	16	0
23	BP	832	0	849	35	0
24	6	977	0	1025	18	0
24	BQ	977	0	1026	15	0
25	7	945	0	1010	19	0
25	BR	896	0	954	34	0
26	8	974	0	1032	13	0
26	BS	952	0	1003	8	0
27	9	989	0	1064	18	0
27	BT	975	0	1053	34	0
28	AA	1087	0	1154	20	0
28	BU	1087	0	1154	12	0
29	AB	1170	0	1203	30	0
29	BV	1170	0	1203	26	0
30	AC	493	0	520	11	0
30	BW	489	0	522	20	0
31	AD	755	0	795	13	0
31	BX	729	0	775	20	0
32	AE	894	0	941	18	0
32	BY	889	0	936	14	0
33	AF	1000	0	1069	14	0
33	BZ	1006	0	1082	14	0
34	AG	847	0	893	19	0
34	CA	867	0	932	17	0
35	AH	878	0	934	18	0
35	CB	913	0	999	22	0
36	AI	992	0	1093	18	0
36	CC	970	0	1063	16	0
37	AJ	758	0	838	8	0
37	CD	772	0	863	13	0
38	AK	677	0	697	20	0
38	CE	677	0	697	20	0
39	AL	617	0	675	8	0
39	CF	618	0	683	9	0
40	AM	438	0	475	8	0
40	CG	438	0	475	14	0
41	AN	419	0	460	5	0
41	CH	427	0	473	7	0
42	AO	236	0	285	3	0
42	CI	227	0	272	9	0
43	AP	828	0	893	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	CJ	841	0	913	13	0
44	AQ	698	0	734	14	0
44	CK	698	0	734	19	0
45	CL	815	0	793	63	0
45	i	930	0	905	49	0
46	B	36889	0	18557	754	0
46	CM	36345	0	18285	811	0
47	C	1627	0	1644	39	0
47	CN	1627	0	1644	32	0
48	CO	1724	0	1805	62	0
48	D	1724	0	1805	34	0
49	CP	1620	0	1715	27	0
49	E	1629	0	1728	35	0
50	CQ	1707	0	1807	46	0
50	F	1707	0	1807	49	0
51	CR	2055	0	2137	45	0
51	G	2051	0	2134	46	0
52	CS	1614	0	1688	40	0
52	H	1614	0	1688	49	0
53	CT	1895	0	1988	58	0
53	I	1820	0	1896	40	0
54	CU	1466	0	1561	37	0
54	J	1491	0	1579	43	0
55	CV	1579	0	1602	43	0
55	K	1579	0	1602	27	0
56	CW	1453	0	1532	35	0
56	L	1453	0	1532	17	0
57	CX	783	0	799	41	0
57	M	817	0	828	49	0
58	CY	1129	0	1183	24	0
58	N	1150	0	1201	18	0
59	CZ	885	0	915	30	0
59	O	885	0	915	62	0
60	DA	1187	0	1249	22	0
60	P	1187	0	1249	22	0
61	DB	942	0	981	30	0
61	Q	942	0	981	23	0
62	DC	935	0	970	37	0
62	R	1018	0	1065	32	0
63	DD	1091	0	1155	38	0
63	S	1085	0	1150	42	0
64	DE	1002	0	1058	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	T	991	0	1048	39	0
65	DF	1169	0	1216	49	0
65	U	1187	0	1237	29	0
66	DG	1100	0	1114	30	0
66	V	1089	0	1103	35	0
67	DH	790	0	855	19	0
67	W	808	0	871	18	0
68	DI	676	0	677	17	0
68	X	676	0	677	19	0
69	DJ	1032	0	1066	29	0
69	Y	1032	0	1066	20	0
70	DK	1110	0	1182	35	0
70	Z	1110	0	1182	29	0
71	DL	1072	0	1123	29	0
71	a	1086	0	1132	21	0
72	DM	578	0	613	11	0
72	b	570	0	609	10	0
73	DN	770	0	825	16	0
73	c	779	0	832	12	0
74	DO	614	0	630	12	0
74	d	614	0	630	10	0
75	DP	487	0	523	24	0
75	e	487	0	523	21	0
76	DQ	454	0	432	11	0
76	f	454	0	431	10	0
77	DR	444	0	483	14	0
77	g	474	0	515	12	0
78	DS	574	0	606	19	0
78	h	574	0	606	36	0
79	AR	2389	0	2366	69	0
79	DT	2398	0	2374	87	0
80	l1	1711	0	1817	126	0
81	12	97	0	103	3	0
82	1	684	0	0	0	0
82	2	1	0	0	0	0
82	3	4	0	0	0	0
82	4	4	0	0	0	0
82	6	1	0	0	0	0
82	9	1	0	0	0	0
82	AA	1	0	0	0	0
82	AB	2	0	0	0	0
82	AD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	AF	1	0	0	0	0
82	AH	1	0	0	0	0
82	AI	1	0	0	0	0
82	AK	2	0	0	0	0
82	AN	1	0	0	0	0
82	AP	2	0	0	0	0
82	AR	1	0	0	0	0
82	AS	542	0	0	0	0
82	AT	3	0	0	0	0
82	AU	2	0	0	0	0
82	AW	1	0	0	0	0
82	AX	1	0	0	0	0
82	AZ	1	0	0	0	0
82	B	69	0	0	0	0
82	BB	3	0	0	0	0
82	BE	1	0	0	0	0
82	BJ	1	0	0	0	0
82	BK	1	0	0	0	0
82	BO	1	0	0	0	0
82	BP	1	0	0	0	0
82	BQ	2	0	0	0	0
82	BZ	1	0	0	0	0
82	CB	1	0	0	0	0
82	CE	1	0	0	0	0
82	CH	1	0	0	0	0
82	CM	25	0	0	0	0
82	DK	1	0	0	0	0
82	E	1	0	0	0	0
82	F	1	0	0	0	0
82	L	1	0	0	0	0
82	Q	1	0	0	0	0
82	R	1	0	0	0	0
82	U	1	0	0	0	0
82	Y	3	0	0	0	0
82	Z	1	0	0	0	0
82	c	1	0	0	0	0
82	i	1	0	0	0	0
82	j	1	0	0	0	0
82	k	2	0	0	0	0
82	o	3	0	0	0	0
82	v	1	0	0	0	0
82	w	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	x	1	0	0	0	0
82	y	1	0	0	0	0
82	z	1	0	0	0	0
83	1	420	0	450	32	0
83	4	42	0	45	1	0
83	AS	210	0	225	16	0
83	B	126	0	135	12	0
83	CM	84	0	90	8	0
84	1	57	0	52	3	0
84	AS	57	0	52	4	0
85	AH	1	0	0	0	0
85	AK	1	0	0	0	0
85	AN	1	0	0	0	0
85	AP	1	0	0	0	0
85	AQ	1	0	0	0	0
85	CB	1	0	0	0	0
85	CE	1	0	0	0	0
85	CH	1	0	0	0	0
85	CJ	1	0	0	0	0
85	CK	1	0	0	0	0
85	DN	1	0	0	0	0
85	DQ	1	0	0	0	0
85	DS	1	0	0	0	0
85	c	1	0	0	0	0
85	f	1	0	0	0	0
85	h	1	0	0	0	0
All	All	401103	0	298940	6780	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 10.

The worst 5 of 6780 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)
57:CX:22:VAL:CG1	57:CX:63:TYR:HE2	1.62	1.11
48:D:180:THR:HG22	48:D:183:GLN:OE1	1.53	1.07
45:CL:55:LYS:HD2	45:CL:56:SER:H	1.22	1.04
1:AS:3313:G:H1	1:AS:3322:U:H3	1.05	1.00
57:CX:22:VAL:CG1	57:CX:63:TYR:CE2	2.46	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	246/254 (97%)	239 (97%)	7 (3%)	0	100	100
4	j	247/254 (97%)	238 (96%)	9 (4%)	0	100	100
5	AX	384/389 (99%)	372 (97%)	12 (3%)	0	100	100
5	k	385/389 (99%)	373 (97%)	12 (3%)	0	100	100
6	AY	357/363 (98%)	347 (97%)	10 (3%)	0	100	100
6	l	359/363 (99%)	347 (97%)	12 (3%)	0	100	100
7	AZ	290/298 (97%)	278 (96%)	12 (4%)	0	100	100
7	m	294/298 (99%)	282 (96%)	11 (4%)	1 (0%)	36	63
8	BA	149/176 (85%)	146 (98%)	3 (2%)	0	100	100
8	n	153/176 (87%)	149 (97%)	4 (3%)	0	100	100
9	BB	225/241 (93%)	218 (97%)	6 (3%)	1 (0%)	30	58
9	o	226/241 (94%)	220 (97%)	5 (2%)	1 (0%)	30	58
10	BC	224/262 (86%)	211 (94%)	11 (5%)	2 (1%)	14	41
10	p	235/262 (90%)	228 (97%)	6 (3%)	1 (0%)	30	58
11	BD	187/191 (98%)	182 (97%)	5 (3%)	0	100	100
11	q	188/191 (98%)	183 (97%)	5 (3%)	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%)	161 (95%)	8 (5%)	0	100	100
13	s	169/174 (97%)	161 (95%)	8 (5%)	0	100	100
14	BG	198/202 (98%)	190 (96%)	6 (3%)	2 (1%)	12	38
14	t	198/202 (98%)	196 (99%)	2 (1%)	0	100	100
15	BH	126/131 (96%)	122 (97%)	4 (3%)	0	100	100
15	u	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
16	BI	201/204 (98%)	194 (96%)	6 (3%)	1 (0%)	24	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	v	201/204 (98%)	197 (98%)	4 (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	168/185 (91%)	165 (98%)	3 (2%)	0	100	100
19	BL	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
19	y	183/186 (98%)	179 (98%)	4 (2%)	0	100	100
20	BM	169/190 (89%)	164 (97%)	3 (2%)	2 (1%)	10	33
20	z	177/190 (93%)	174 (98%)	3 (2%)	0	100	100
21	0	168/172 (98%)	166 (99%)	2 (1%)	0	100	100
21	BN	168/172 (98%)	166 (99%)	2 (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	38
23	BP	101/124 (82%)	88 (87%)	11 (11%)	2 (2%)	6	24
24	6	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
24	BQ	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
25	7	114/155 (74%)	108 (95%)	6 (5%)	0	100	100
25	BR	107/155 (69%)	101 (94%)	6 (6%)	0	100	100
26	8	119/142 (84%)	119 (100%)	0	0	100	100
26	BS	116/142 (82%)	115 (99%)	1 (1%)	0	100	100
27	9	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
27	BT	122/127 (96%)	121 (99%)	1 (1%)	0	100	100
28	AA	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
28	BU	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
29	AB	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
29	BV	146/149 (98%)	138 (94%)	8 (6%)	0	100	100
30	AC	60/63 (95%)	57 (95%)	1 (2%)	2 (3%)	3	17
30	BW	59/63 (94%)	57 (97%)	1 (2%)	1 (2%)	7	27
31	AD	97/106 (92%)	95 (98%)	1 (1%)	1 (1%)	12	38
31	BX	94/106 (89%)	92 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	AE	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
32	BY	107/112 (96%)	103 (96%)	4 (4%)	0	100	100
33	AF	122/131 (93%)	122 (100%)	0	0	100	100
33	BZ	123/131 (94%)	122 (99%)	1 (1%)	0	100	100
34	AG	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
34	CA	107/107 (100%)	104 (97%)	3 (3%)	0	100	100
35	AH	109/122 (89%)	107 (98%)	2 (2%)	0	100	100
35	CB	114/122 (93%)	111 (97%)	3 (3%)	0	100	100
36	AI	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
36	CC	115/120 (96%)	113 (98%)	2 (2%)	0	100	100
37	AJ	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
37	CD	97/99 (98%)	95 (98%)	1 (1%)	1 (1%)	12	38
38	AK	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
38	CE	84/90 (93%)	80 (95%)	4 (5%)	0	100	100
39	AL	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
39	CF	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
40	AM	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	5	23
40	CG	48/51 (94%)	45 (94%)	2 (4%)	1 (2%)	5	23
41	AN	50/52 (96%)	50 (100%)	0	0	100	100
41	CH	51/52 (98%)	51 (100%)	0	0	100	100
42	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
42	CI	22/25 (88%)	22 (100%)	0	0	100	100
43	AP	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
43	CJ	103/106 (97%)	102 (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
45	CL	105/267 (39%)	76 (72%)	24 (23%)	5 (5%)	2	11
45	i	117/267 (44%)	81 (69%)	30 (26%)	6 (5%)	1	10
47	C	206/261 (79%)	201 (98%)	5 (2%)	0	100	100
47	CN	206/261 (79%)	201 (98%)	5 (2%)	0	100	100
48	CO	212/256 (83%)	199 (94%)	11 (5%)	2 (1%)	14	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	D	212/256 (83%)	207 (98%)	5 (2%)	0	100	100
49	CP	214/249 (86%)	207 (97%)	7 (3%)	0	100	100
49	E	215/249 (86%)	209 (97%)	6 (3%)	0	100	100
50	CQ	221/251 (88%)	214 (97%)	7 (3%)	0	100	100
50	F	221/251 (88%)	212 (96%)	9 (4%)	0	100	100
51	CR	258/262 (98%)	252 (98%)	6 (2%)	0	100	100
51	G	257/262 (98%)	251 (98%)	5 (2%)	1 (0%)	30	58
52	CS	204/225 (91%)	197 (97%)	7 (3%)	0	100	100
52	H	204/225 (91%)	190 (93%)	14 (7%)	0	100	100
53	CT	233/236 (99%)	226 (97%)	6 (3%)	1 (0%)	30	58
53	I	224/236 (95%)	219 (98%)	5 (2%)	0	100	100
54	CU	180/186 (97%)	169 (94%)	9 (5%)	2 (1%)	11	36
54	J	183/186 (98%)	173 (94%)	9 (5%)	1 (0%)	24	52
55	CV	201/206 (98%)	200 (100%)	1 (0%)	0	100	100
55	K	201/206 (98%)	200 (100%)	1 (0%)	0	100	100
56	CW	176/189 (93%)	175 (99%)	1 (1%)	0	100	100
56	L	176/189 (93%)	175 (99%)	1 (1%)	0	100	100
57	CX	91/118 (77%)	85 (93%)	5 (6%)	1 (1%)	11	36
57	M	96/118 (81%)	81 (84%)	13 (14%)	2 (2%)	5	23
58	CY	139/155 (90%)	131 (94%)	5 (4%)	3 (2%)	5	23
58	N	142/155 (92%)	134 (94%)	7 (5%)	1 (1%)	18	46
59	CZ	114/143 (80%)	97 (85%)	17 (15%)	0	100	100
59	O	114/143 (80%)	90 (79%)	19 (17%)	5 (4%)	2	12
60	DA	148/151 (98%)	142 (96%)	5 (3%)	1 (1%)	18	46
60	P	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
61	DB	125/132 (95%)	121 (97%)	4 (3%)	0	100	100
61	Q	125/132 (95%)	120 (96%)	5 (4%)	0	100	100
62	DC	116/142 (82%)	105 (90%)	11 (10%)	0	100	100
62	R	127/142 (89%)	112 (88%)	14 (11%)	1 (1%)	16	44
63	DD	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
63	S	137/142 (96%)	132 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	DE	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
64	T	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
65	DF	140/145 (97%)	133 (95%)	5 (4%)	2 (1%)	9	30
65	U	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
66	DG	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
66	V	137/145 (94%)	133 (97%)	3 (2%)	1 (1%)	18	46
67	DH	98/119 (82%)	95 (97%)	3 (3%)	0	100	100
67	W	100/119 (84%)	96 (96%)	4 (4%)	0	100	100
68	DI	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
68	X	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
69	DJ	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
69	Y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
70	DK	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
70	Z	141/145 (97%)	137 (97%)	4 (3%)	0	100	100
71	DL	130/135 (96%)	130 (100%)	0	0	100	100
71	a	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
72	DM	70/105 (67%)	67 (96%)	3 (4%)	0	100	100
72	b	69/105 (66%)	68 (99%)	1 (1%)	0	100	100
73	DN	95/119 (80%)	93 (98%)	2 (2%)	0	100	100
73	c	96/119 (81%)	94 (98%)	2 (2%)	0	100	100
74	DO	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
74	d	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
75	DP	60/67 (90%)	55 (92%)	5 (8%)	0	100	100
75	e	60/67 (90%)	57 (95%)	3 (5%)	0	100	100
76	DQ	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
76	f	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
77	DR	54/63 (86%)	52 (96%)	2 (4%)	0	100	100
77	g	58/63 (92%)	54 (93%)	4 (7%)	0	100	100
78	DS	68/193 (35%)	61 (90%)	7 (10%)	0	100	100
78	h	68/193 (35%)	53 (78%)	13 (19%)	2 (3%)	3	18
79	AR	308/317 (97%)	285 (92%)	22 (7%)	1 (0%)	36	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	DT	309/317 (98%)	286 (93%)	22 (7%)	1 (0%)	36	63
80	l1	215/217 (99%)	132 (61%)	74 (34%)	9 (4%)	2	13
81	12	12/165 (7%)	12 (100%)	0	0	100	100
All	All	22290/24658 (90%)	21374 (96%)	847 (4%)	69 (0%)	36	63

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	p	206	SER
45	i	54	LYS
54	J	162	LEU
59	O	37	VAL
59	O	130	SER

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	189/194 (97%)	189 (100%)	0	100	100
4	j	190/194 (98%)	190 (100%)	0	100	100
5	AX	325/328 (99%)	325 (100%)	0	100	100
5	k	326/328 (99%)	326 (100%)	0	100	100
6	AY	288/292 (99%)	288 (100%)	0	100	100
6	l	290/292 (99%)	290 (100%)	0	100	100
7	AZ	247/252 (98%)	247 (100%)	0	100	100
7	m	250/252 (99%)	250 (100%)	0	100	100
8	BA	132/154 (86%)	132 (100%)	0	100	100
8	n	136/154 (88%)	136 (100%)	0	100	100
9	BB	191/204 (94%)	191 (100%)	0	100	100
9	o	192/204 (94%)	192 (100%)	0	100	100
10	BC	192/216 (89%)	192 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	p	197/216 (91%)	197 (100%)	0	100	100
11	BD	168/170 (99%)	168 (100%)	0	100	100
11	q	169/170 (99%)	169 (100%)	0	100	100
12	BE	176/186 (95%)	176 (100%)	0	100	100
12	r	178/186 (96%)	178 (100%)	0	100	100
13	BF	146/149 (98%)	146 (100%)	0	100	100
13	s	146/149 (98%)	146 (100%)	0	100	100
14	BG	166/168 (99%)	166 (100%)	0	100	100
14	t	166/168 (99%)	166 (100%)	0	100	100
15	BH	107/109 (98%)	107 (100%)	0	100	100
15	u	108/109 (99%)	108 (100%)	0	100	100
16	BI	177/178 (99%)	177 (100%)	0	100	100
16	v	177/178 (99%)	177 (100%)	0	100	100
17	BJ	166/167 (99%)	166 (100%)	0	100	100
17	w	166/167 (99%)	166 (100%)	0	100	100
18	BK	145/154 (94%)	145 (100%)	0	100	100
18	x	143/154 (93%)	143 (100%)	0	100	100
19	BL	153/154 (99%)	153 (100%)	0	100	100
19	y	153/154 (99%)	153 (100%)	0	100	100
20	BM	139/153 (91%)	139 (100%)	0	100	100
20	z	146/153 (95%)	146 (100%)	0	100	100
21	0	155/157 (99%)	155 (100%)	0	100	100
21	BN	155/157 (99%)	155 (100%)	0	100	100
22	2	133/134 (99%)	133 (100%)	0	100	100
22	BO	133/134 (99%)	133 (100%)	0	100	100
23	5	93/112 (83%)	93 (100%)	0	100	100
23	BP	94/112 (84%)	94 (100%)	0	100	100
24	6	101/104 (97%)	101 (100%)	0	100	100
24	BQ	101/104 (97%)	101 (100%)	0	100	100
25	7	97/127 (76%)	97 (100%)	0	100	100
25	BR	93/127 (73%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	8	108/121 (89%)	108 (100%)	0	100	100
26	BS	106/121 (88%)	106 (100%)	0	100	100
27	9	111/112 (99%)	111 (100%)	0	100	100
27	BT	110/112 (98%)	110 (100%)	0	100	100
28	AA	117/118 (99%)	117 (100%)	0	100	100
28	BU	117/118 (99%)	117 (100%)	0	100	100
29	AB	120/121 (99%)	120 (100%)	0	100	100
29	BV	120/121 (99%)	120 (100%)	0	100	100
30	AC	48/49 (98%)	48 (100%)	0	100	100
30	BW	48/49 (98%)	48 (100%)	0	100	100
31	AD	84/90 (93%)	84 (100%)	0	100	100
31	BX	81/90 (90%)	81 (100%)	0	100	100
32	AE	98/100 (98%)	98 (100%)	0	100	100
32	BY	98/100 (98%)	98 (100%)	0	100	100
33	AF	109/115 (95%)	109 (100%)	0	100	100
33	BZ	110/115 (96%)	108 (98%)	2 (2%)	51	66
34	AG	91/92 (99%)	91 (100%)	0	100	100
34	CA	94/92 (102%)	94 (100%)	0	100	100
35	AH	94/102 (92%)	94 (100%)	0	100	100
35	CB	99/102 (97%)	97 (98%)	2 (2%)	48	65
36	AI	106/106 (100%)	106 (100%)	0	100	100
36	CC	104/106 (98%)	104 (100%)	0	100	100
37	AJ	77/79 (98%)	77 (100%)	0	100	100
37	CD	79/79 (100%)	79 (100%)	0	100	100
38	AK	70/73 (96%)	70 (100%)	0	100	100
38	CE	70/73 (96%)	70 (100%)	0	100	100
39	AL	68/69 (99%)	68 (100%)	0	100	100
39	CF	69/69 (100%)	69 (100%)	0	100	100
40	AM	46/47 (98%)	46 (100%)	0	100	100
40	CG	46/47 (98%)	46 (100%)	0	100	100
41	AN	47/47 (100%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	CH	48/47 (102%)	48 (100%)	0	100	100
42	AO	24/24 (100%)	24 (100%)	0	100	100
42	CI	23/24 (96%)	23 (100%)	0	100	100
43	AP	88/91 (97%)	88 (100%)	0	100	100
43	CJ	90/91 (99%)	90 (100%)	0	100	100
44	AQ	72/73 (99%)	72 (100%)	0	100	100
44	CK	72/73 (99%)	72 (100%)	0	100	100
45	CL	86/212 (41%)	86 (100%)	0	100	100
45	i	99/212 (47%)	99 (100%)	0	100	100
47	C	176/215 (82%)	176 (100%)	0	100	100
47	CN	176/215 (82%)	176 (100%)	0	100	100
48	CO	194/229 (85%)	194 (100%)	0	100	100
48	D	194/229 (85%)	194 (100%)	0	100	100
49	CP	174/198 (88%)	174 (100%)	0	100	100
49	E	175/198 (88%)	175 (100%)	0	100	100
50	CQ	174/196 (89%)	174 (100%)	0	100	100
50	F	174/196 (89%)	174 (100%)	0	100	100
51	CR	218/220 (99%)	218 (100%)	0	100	100
51	G	218/220 (99%)	218 (100%)	0	100	100
52	CS	178/197 (90%)	178 (100%)	0	100	100
52	H	178/197 (90%)	178 (100%)	0	100	100
53	CT	203/204 (100%)	203 (100%)	0	100	100
53	I	195/204 (96%)	195 (100%)	0	100	100
54	CU	163/167 (98%)	163 (100%)	0	100	100
54	J	166/167 (99%)	166 (100%)	0	100	100
55	CV	157/160 (98%)	157 (100%)	0	100	100
55	K	157/160 (98%)	157 (100%)	0	100	100
56	CW	153/160 (96%)	153 (100%)	0	100	100
56	L	153/160 (96%)	153 (100%)	0	100	100
57	CX	87/104 (84%)	87 (100%)	0	100	100
57	M	90/104 (86%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	CY	122/134 (91%)	122 (100%)	0	100	100
58	N	124/134 (92%)	124 (100%)	0	100	100
59	CZ	98/123 (80%)	98 (100%)	0	100	100
59	O	98/123 (80%)	98 (100%)	0	100	100
60	DA	129/130 (99%)	129 (100%)	0	100	100
60	P	129/130 (99%)	129 (100%)	0	100	100
61	DB	97/102 (95%)	97 (100%)	0	100	100
61	Q	97/102 (95%)	97 (100%)	0	100	100
62	DC	102/121 (84%)	102 (100%)	0	100	100
62	R	111/121 (92%)	111 (100%)	0	100	100
63	DD	114/116 (98%)	114 (100%)	0	100	100
63	S	113/116 (97%)	113 (100%)	0	100	100
64	DE	112/122 (92%)	112 (100%)	0	100	100
64	T	111/122 (91%)	111 (100%)	0	100	100
65	DF	126/129 (98%)	126 (100%)	0	100	100
65	U	128/129 (99%)	128 (100%)	0	100	100
66	DG	113/117 (97%)	113 (100%)	0	100	100
66	V	112/117 (96%)	112 (100%)	0	100	100
67	DH	90/105 (86%)	90 (100%)	0	100	100
67	W	92/105 (88%)	92 (100%)	0	100	100
68	DI	71/71 (100%)	71 (100%)	0	100	100
68	X	71/71 (100%)	71 (100%)	0	100	100
69	DJ	112/113 (99%)	112 (100%)	0	100	100
69	Y	112/113 (99%)	112 (100%)	0	100	100
70	DK	116/118 (98%)	116 (100%)	0	100	100
70	Z	116/118 (98%)	116 (100%)	0	100	100
71	DL	109/112 (97%)	109 (100%)	0	100	100
71	a	111/112 (99%)	111 (100%)	0	100	100
72	DM	64/85 (75%)	64 (100%)	0	100	100
72	b	63/85 (74%)	63 (100%)	0	100	100
73	DN	83/102 (81%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	c	84/102 (82%)	84 (100%)	0	100	100
74	DO	72/73 (99%)	72 (100%)	0	100	100
74	d	72/73 (99%)	72 (100%)	0	100	100
75	DP	54/58 (93%)	54 (100%)	0	100	100
75	e	54/58 (93%)	54 (100%)	0	100	100
76	DQ	47/48 (98%)	47 (100%)	0	100	100
76	f	47/48 (98%)	47 (100%)	0	100	100
77	DR	48/54 (89%)	48 (100%)	0	100	100
77	g	51/54 (94%)	51 (100%)	0	100	100
78	DS	62/175 (35%)	62 (100%)	0	100	100
78	h	62/175 (35%)	61 (98%)	1 (2%)	55	67
79	AR	258/263 (98%)	258 (100%)	0	100	100
79	DT	259/263 (98%)	259 (100%)	0	100	100
80	l1	196/196 (100%)	196 (100%)	0	100	100
81	l2	11/137 (8%)	11 (100%)	0	100	100
All	All	19118/20781 (92%)	19113 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
78	h	168	CYS
33	BZ	17[A]	LYS
33	BZ	17[B]	LYS
35	CB	106[A]	LYS
35	CB	106[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 188 such sidechains are listed below:

Mol	Chain	Res	Type
18	BK	120	ASN
48	CO	74	GLN
21	BN	157	GLN
29	BV	74	ASN
51	CR	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3215/3359 (95%)	617 (19%)	37 (1%)
1	AS	3054/3359 (90%)	502 (16%)	34 (1%)
2	3	120/121 (99%)	9 (7%)	0
2	AT	120/121 (99%)	9 (7%)	0
3	4	156/158 (98%)	23 (14%)	3 (1%)
3	AU	155/158 (98%)	20 (12%)	2 (1%)
46	B	1725/1787 (96%)	426 (24%)	48 (2%)
46	CM	1697/1787 (94%)	420 (24%)	45 (2%)
All	All	10242/10850 (94%)	2026 (19%)	169 (1%)

5 of 2026 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 169 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AS	3193	C
46	CM	553	A
1	AS	3309	A
46	CM	237	C
46	CM	769	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1429 ligands modelled in this entry, 1406 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
83	PAR	AS	3404	-	44,45,45	0.45	0	63,67,67	0.85	1 (1%)
83	PAR	1	3465	-	44,45,45	0.49	0	63,67,67	0.98	3 (4%)
83	PAR	4	201	-	44,45,45	0.44	0	63,67,67	1.06	2 (3%)
83	PAR	1	3459	-	44,45,45	0.47	0	63,67,67	0.83	1 (1%)
83	PAR	AS	3403	-	44,45,45	0.47	0	63,67,67	0.81	2 (3%)
83	PAR	1	3466	-	44,45,45	0.45	0	63,67,67	1.04	4 (6%)
83	PAR	1	3462	-	44,45,45	0.45	0	63,67,67	0.70	1 (1%)
84	3K5	AS	3405	-	63,63,63	0.32	0	84,95,95	0.96	4 (4%)
83	PAR	AS	3402	-	44,45,45	0.45	0	63,67,67	0.94	4 (6%)
83	PAR	AS	3406	-	44,45,45	0.48	0	63,67,67	1.27	6 (9%)
83	PAR	1	3461	-	44,45,45	0.44	0	63,67,67	0.80	1 (1%)
83	PAR	AS	3401	-	44,45,45	0.46	0	63,67,67	0.68	1 (1%)
83	PAR	B	1801	-	44,45,45	0.43	0	63,67,67	0.84	1 (1%)
83	PAR	1	3457	82	44,45,45	0.43	0	63,67,67	0.79	1 (1%)
83	PAR	B	1802	-	44,45,45	0.45	0	63,67,67	0.96	2 (3%)
83	PAR	1	3460	-	44,45,45	0.43	0	63,67,67	1.02	4 (6%)
84	3K5	1	3463	-	63,63,63	0.30	0	84,95,95	0.56	1 (1%)
83	PAR	1	3458	-	44,45,45	0.47	0	63,67,67	1.00	3 (4%)
83	PAR	B	1803	-	44,45,45	0.45	0	63,67,67	0.78	1 (1%)
83	PAR	CM	1803	-	44,45,45	0.43	0	63,67,67	0.90	2 (3%)
83	PAR	1	3464	-	44,45,45	0.44	0	63,67,67	1.00	2 (3%)
83	PAR	1	3456	-	44,45,45	0.43	0	63,67,67	0.75	2 (3%)
83	PAR	CM	1802	-	44,45,45	0.43	0	63,67,67	0.82	1 (1%)

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
83	PAR	AS	3404	-	-	4/18/94/94	0/4/4/4
83	PAR	1	3465	-	-	7/18/94/94	0/4/4/4
83	PAR	4	201	-	-	4/18/94/94	0/4/4/4
83	PAR	1	3459	-	-	6/18/94/94	0/4/4/4
83	PAR	AS	3403	-	-	5/18/94/94	0/4/4/4
83	PAR	1	3466	-	-	6/18/94/94	0/4/4/4
83	PAR	1	3462	-	-	4/18/94/94	0/4/4/4
84	3K5	AS	3405	-	-	8/29/121/121	0/7/7/7
83	PAR	AS	3402	-	-	8/18/94/94	1/4/4/4
83	PAR	AS	3406	-	-	7/18/94/94	0/4/4/4
83	PAR	1	3461	-	-	7/18/94/94	0/4/4/4
83	PAR	AS	3401	-	-	4/18/94/94	0/4/4/4
83	PAR	B	1801	-	-	3/18/94/94	0/4/4/4
83	PAR	1	3457	82	-	12/18/94/94	1/4/4/4
83	PAR	B	1802	-	-	4/18/94/94	1/4/4/4
83	PAR	1	3460	-	-	5/18/94/94	0/4/4/4
84	3K5	1	3463	-	-	2/29/121/121	0/7/7/7
83	PAR	1	3458	-	-	8/18/94/94	0/4/4/4
83	PAR	B	1803	-	-	3/18/94/94	0/4/4/4
83	PAR	CM	1803	-	-	6/18/94/94	0/4/4/4
83	PAR	1	3464	-	-	9/18/94/94	0/4/4/4
83	PAR	1	3456	-	-	3/18/94/94	0/4/4/4
83	PAR	CM	1802	-	-	4/18/94/94	0/4/4/4

There are no bond length outliers.

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	1	3466	PAR	O11-C11-C21	6.05	117.99	108.08
83	4	201	PAR	O11-C11-C21	5.69	117.39	108.08
83	AS	3406	PAR	C52-C42-C32	4.92	120.42	111.31
83	1	3464	PAR	O11-C11-C21	4.91	116.12	108.08
83	AS	3404	PAR	O11-C11-C21	4.88	116.06	108.08

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	1	3457	PAR	C43-C33-O33-C14
83	1	3458	PAR	C23-C13-O52-C52
83	1	3458	PAR	O43-C13-O52-C52
83	1	3458	PAR	C43-C33-O33-C14
83	1	3458	PAR	C24-C14-O33-C33

All (3) ring outliers are listed below:

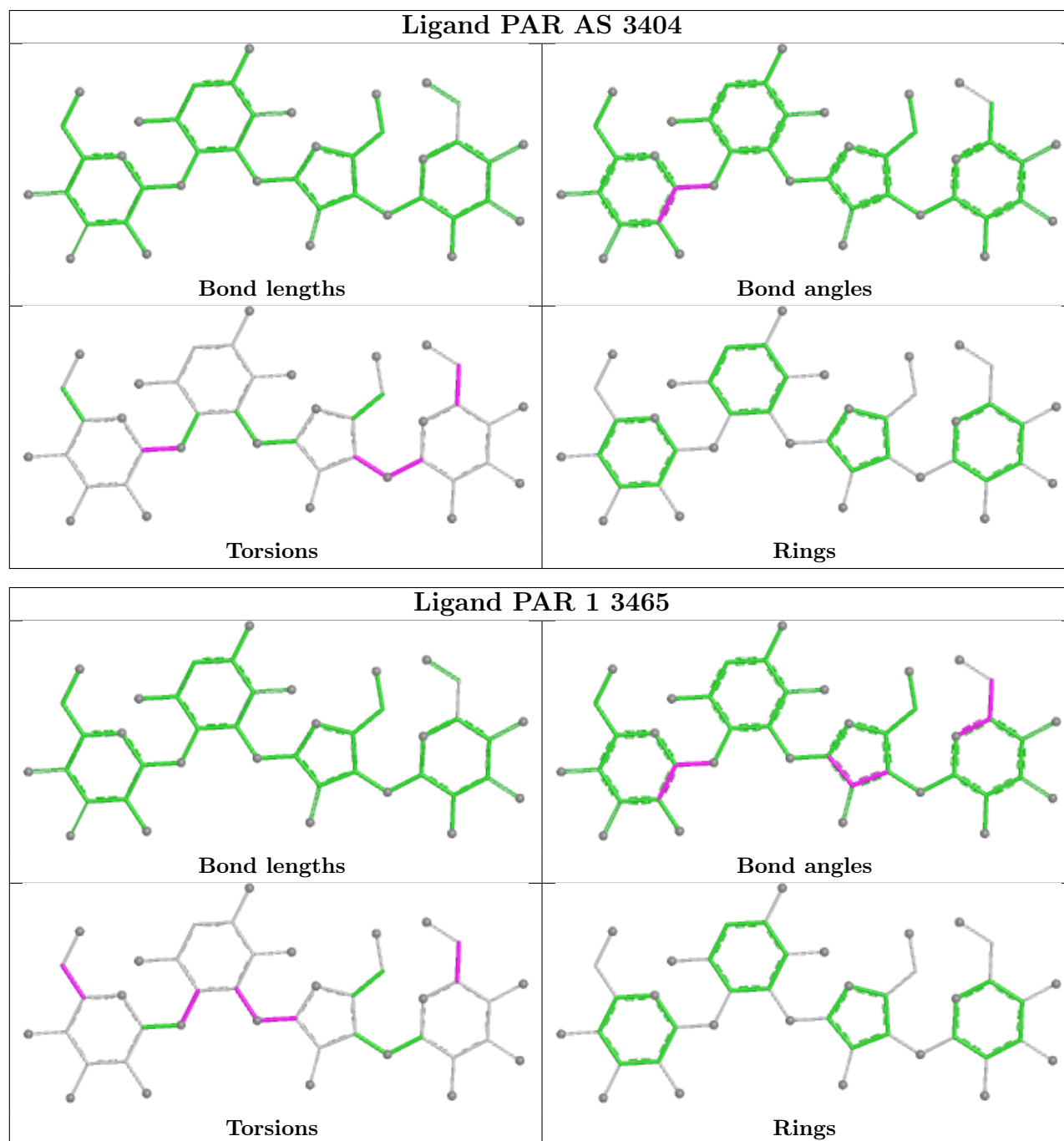
Mol	Chain	Res	Type	Atoms
83	B	1802	PAR	C12-C22-C32-C42-C52-C62
83	1	3457	PAR	C12-C22-C32-C42-C52-C62
83	AS	3402	PAR	C12-C22-C32-C42-C52-C62

23 monomers are involved in 76 short contacts:

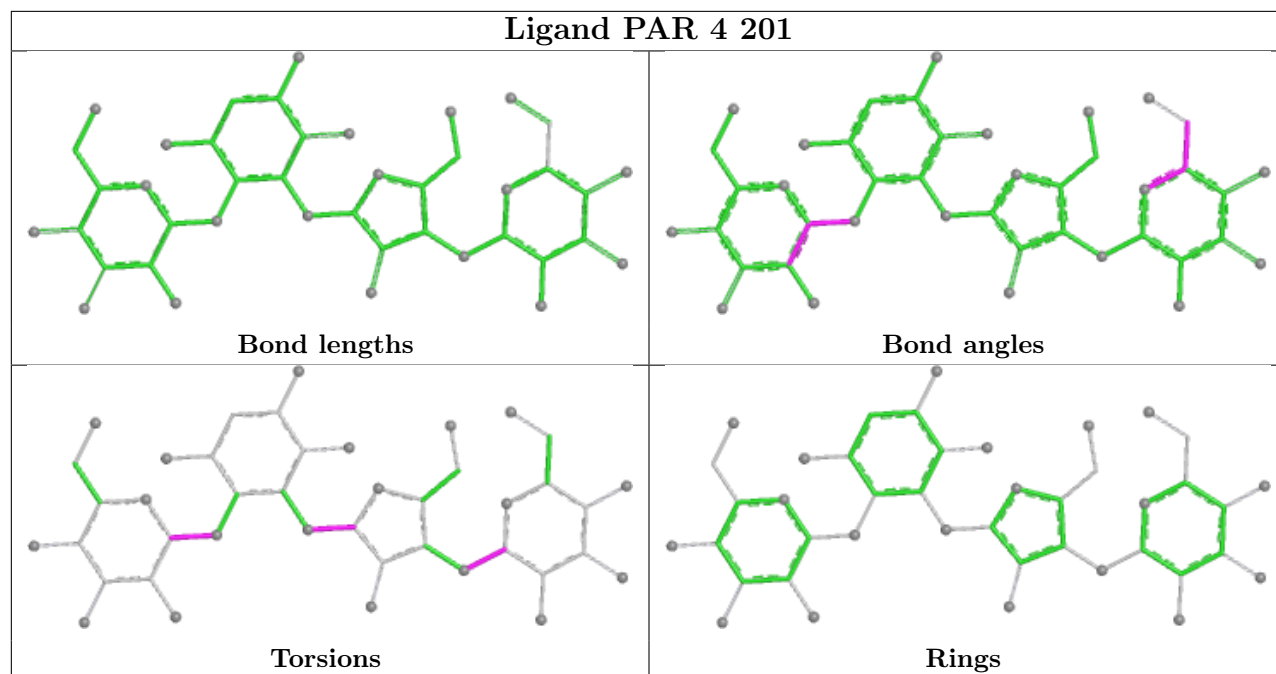
Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	AS	3404	PAR	1	0
83	1	3465	PAR	5	0
83	4	201	PAR	1	0
83	1	3459	PAR	3	0
83	AS	3403	PAR	4	0
83	1	3466	PAR	3	0
83	1	3462	PAR	6	0
84	AS	3405	3K5	4	0
83	AS	3402	PAR	5	0
83	AS	3406	PAR	5	0
83	1	3461	PAR	3	0
83	AS	3401	PAR	1	0
83	B	1801	PAR	4	0
83	1	3457	PAR	1	0
83	B	1802	PAR	2	0
83	1	3460	PAR	6	0
84	1	3463	3K5	3	0
83	1	3458	PAR	2	0
83	B	1803	PAR	6	0
83	CM	1803	PAR	5	0
83	1	3464	PAR	2	0
83	1	3456	PAR	1	0
83	CM	1802	PAR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

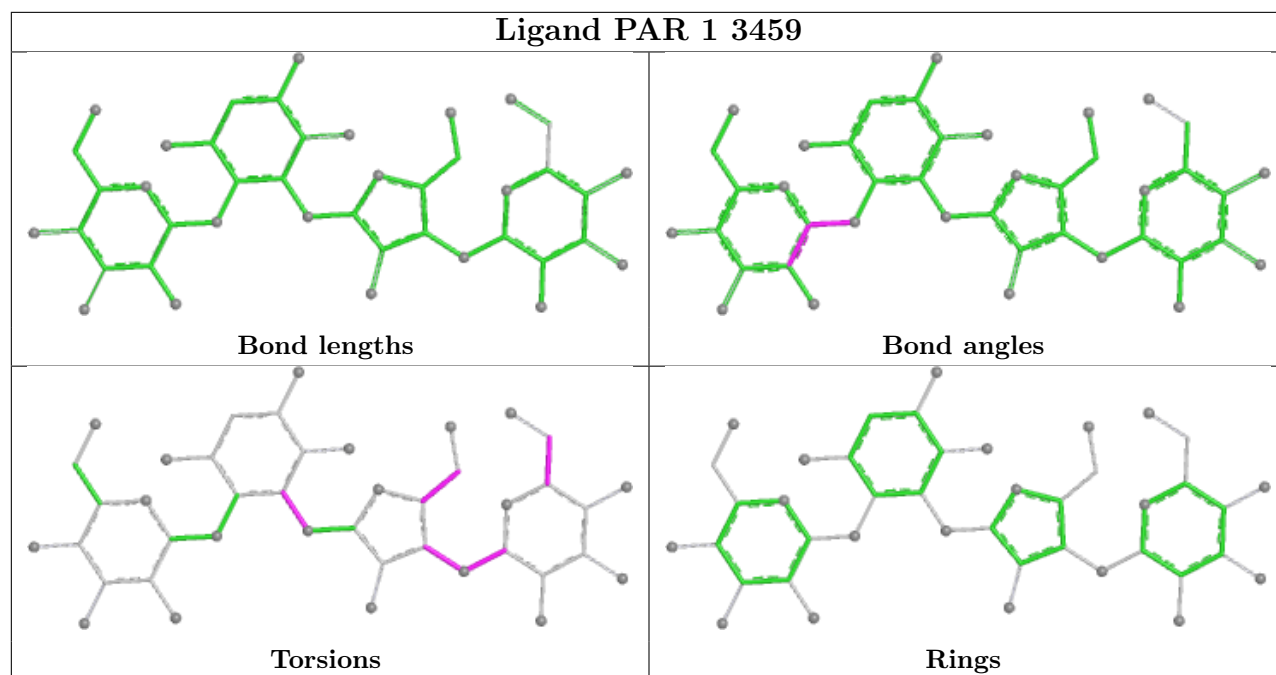
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



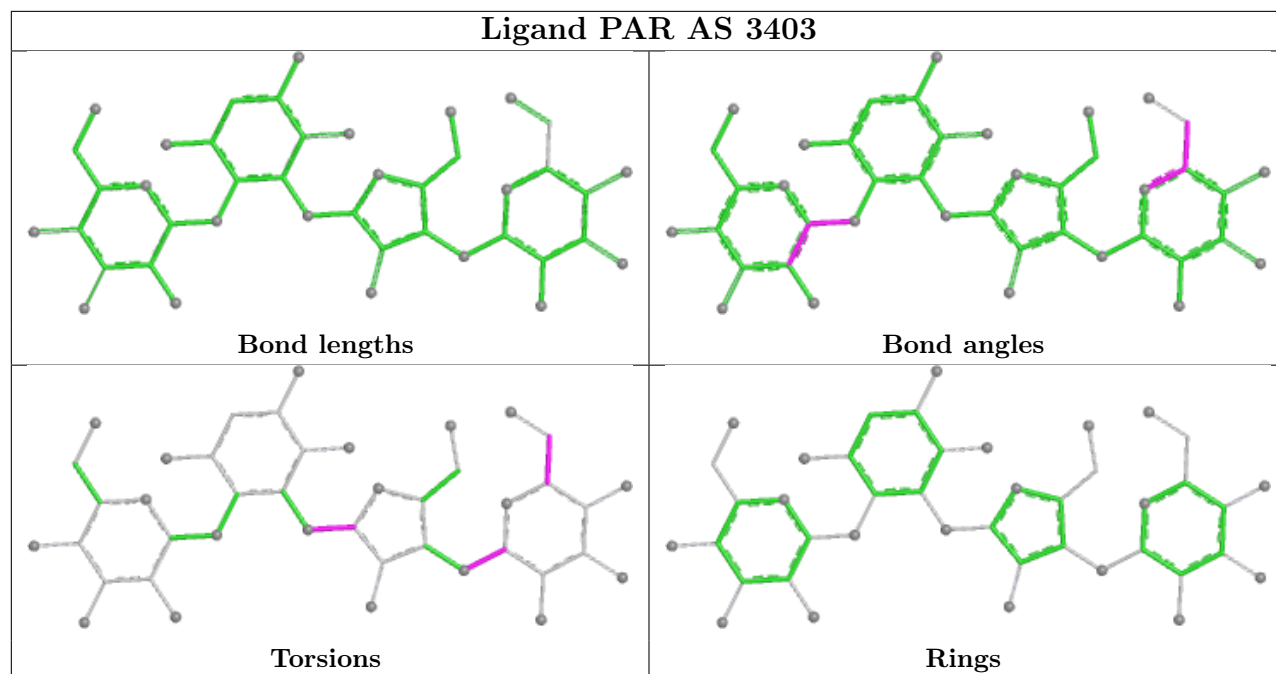
Ligand PAR 4 201



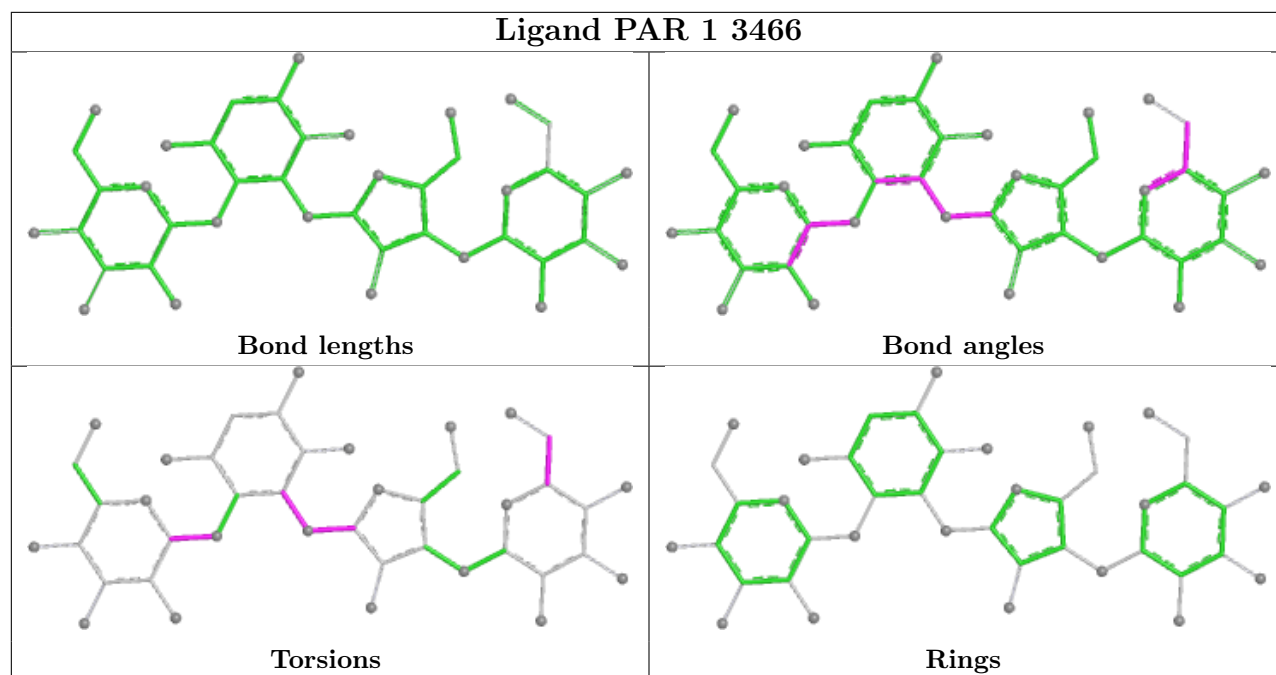
Ligand PAR 1 3459

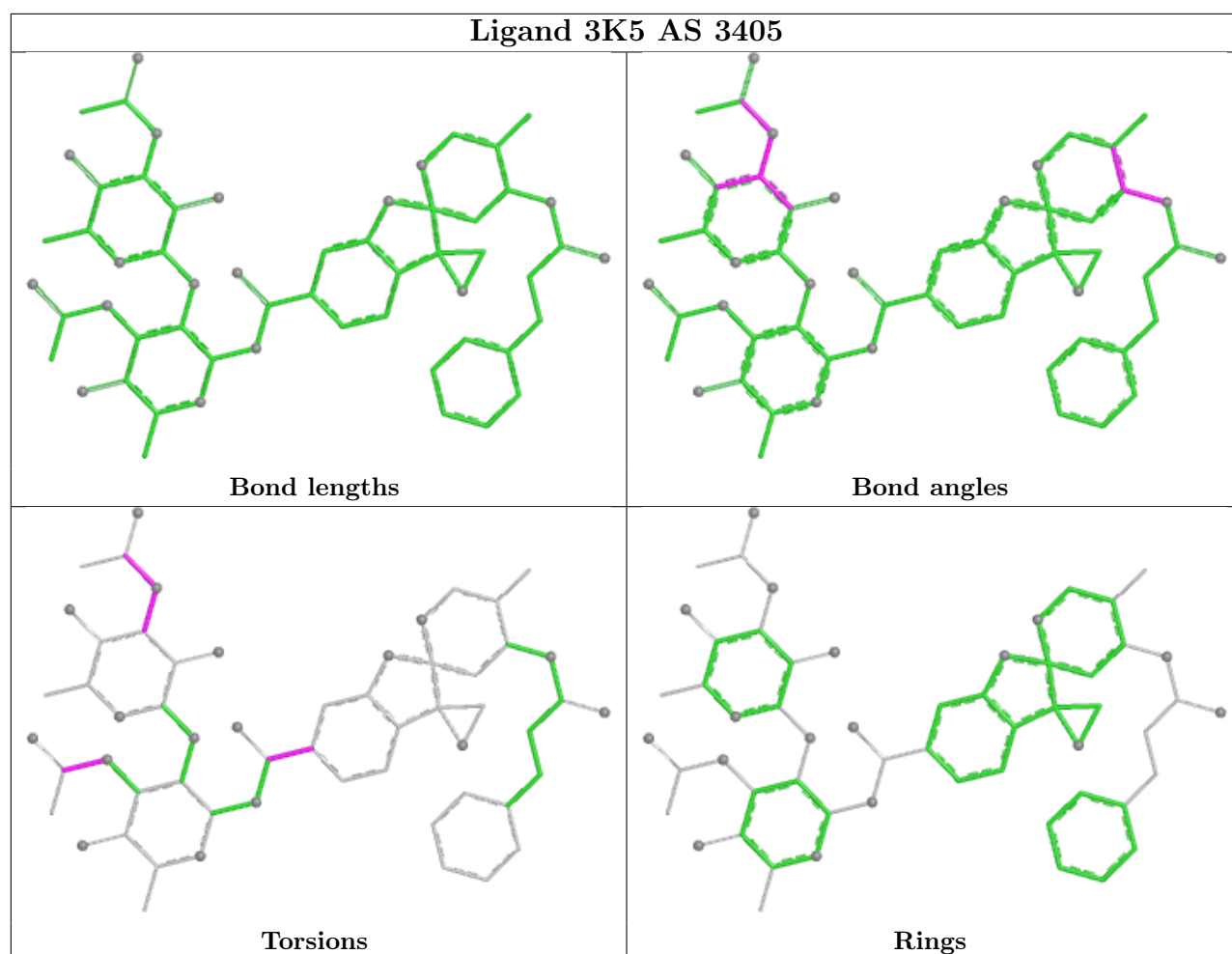
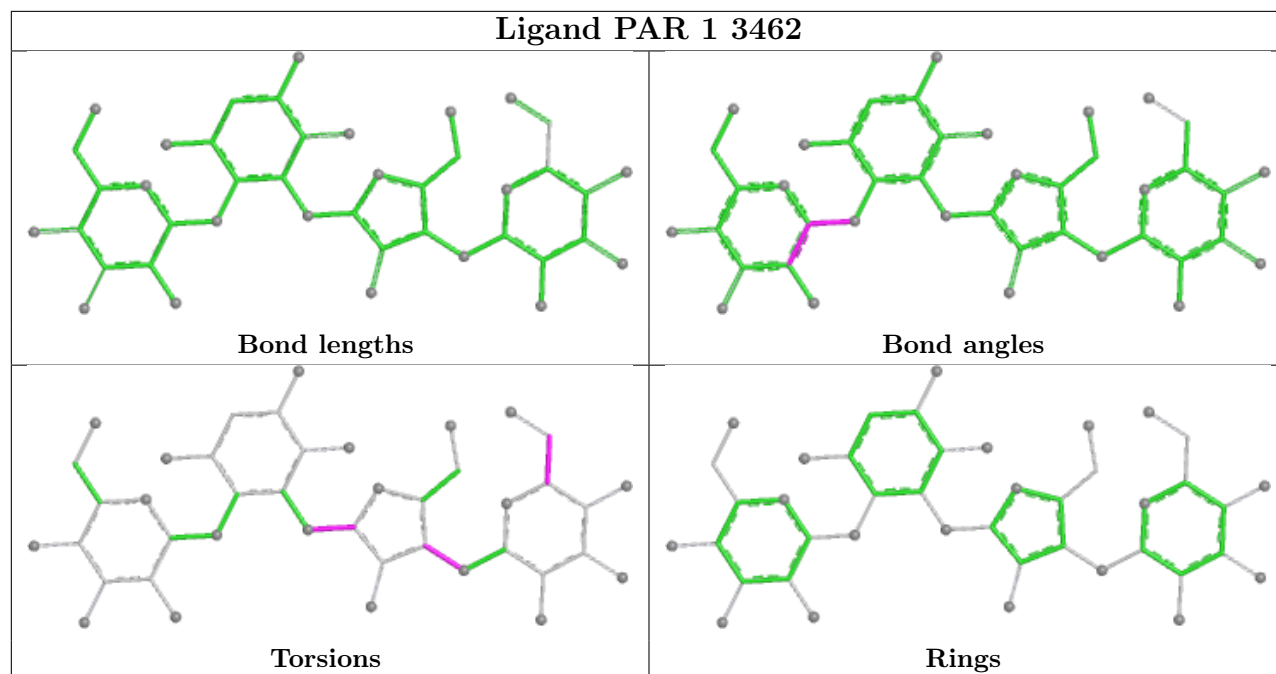


Ligand PAR AS 3403

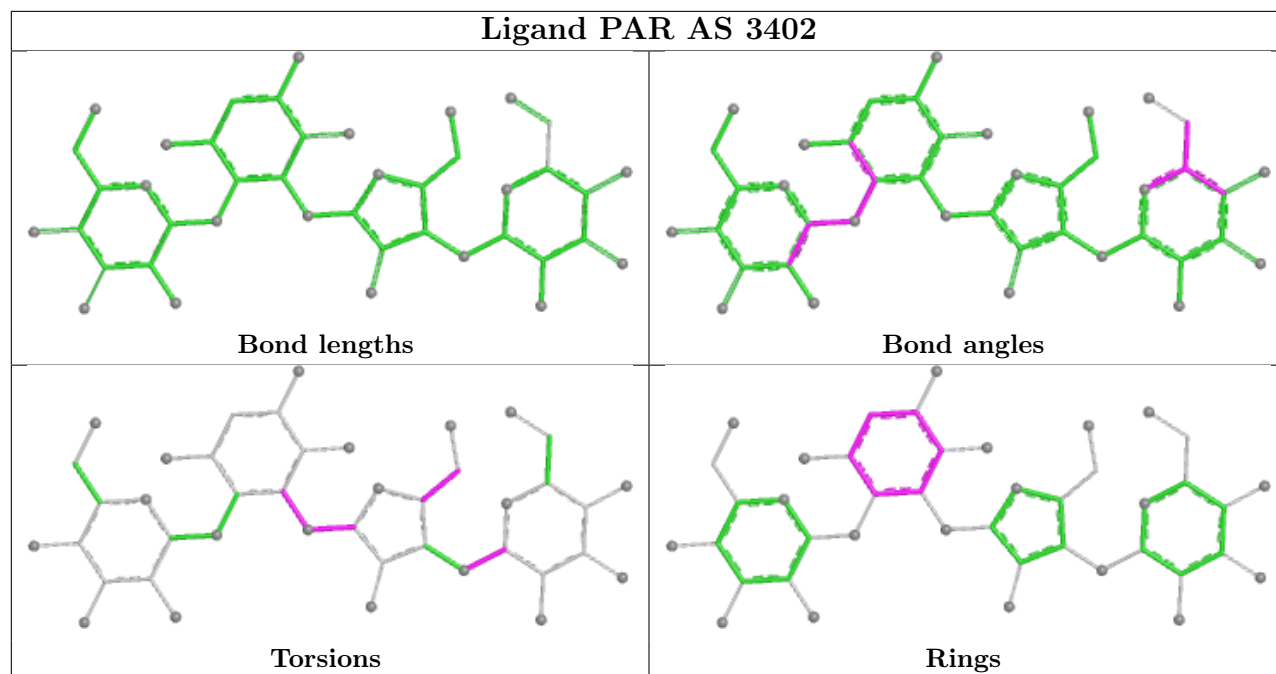


Ligand PAR 1 3466

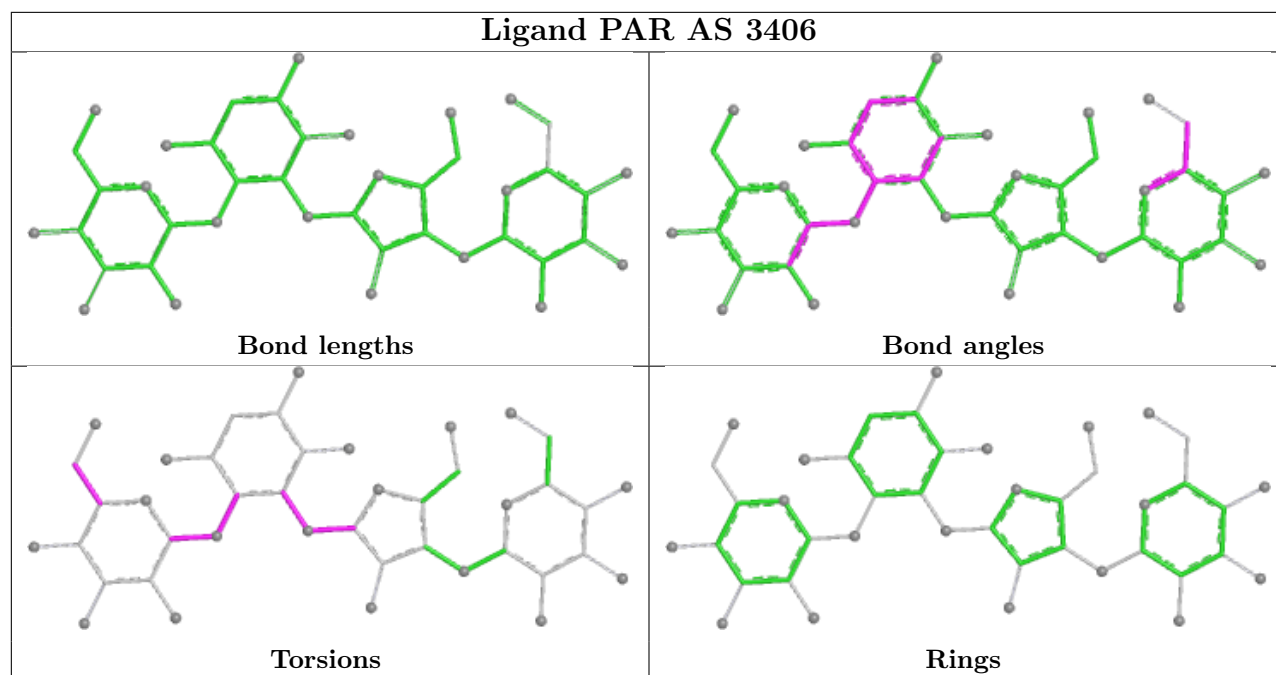


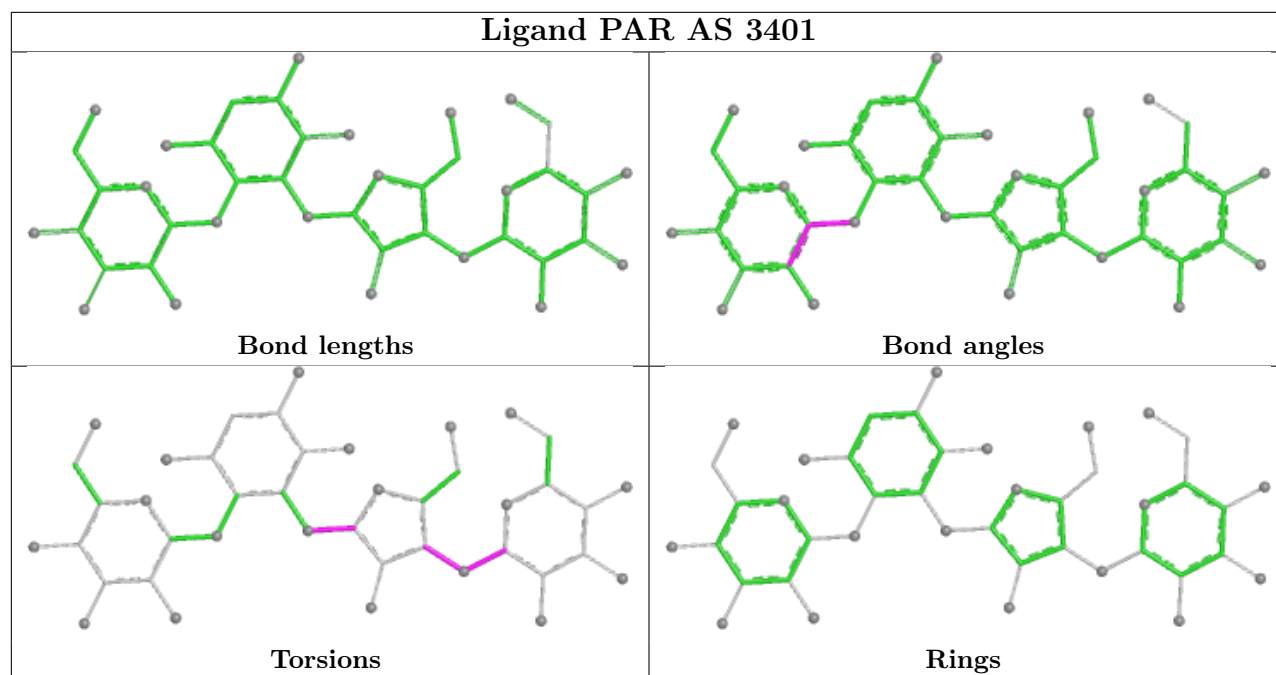
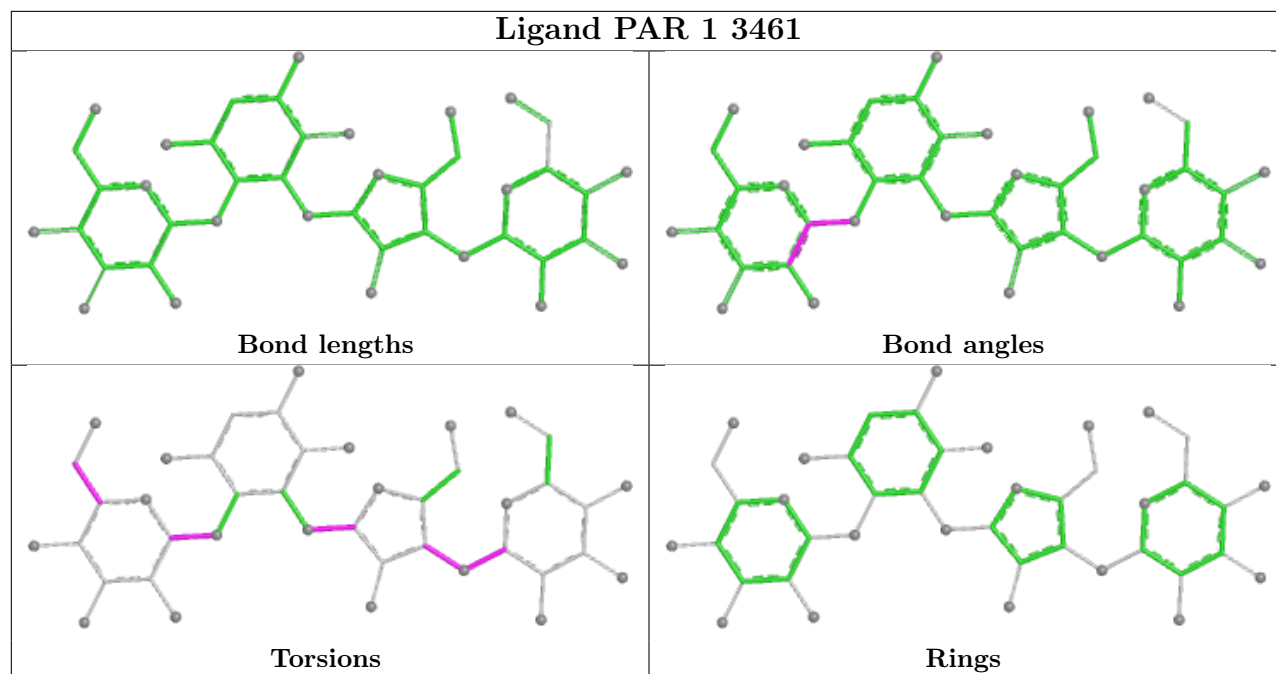


Ligand PAR AS 3402

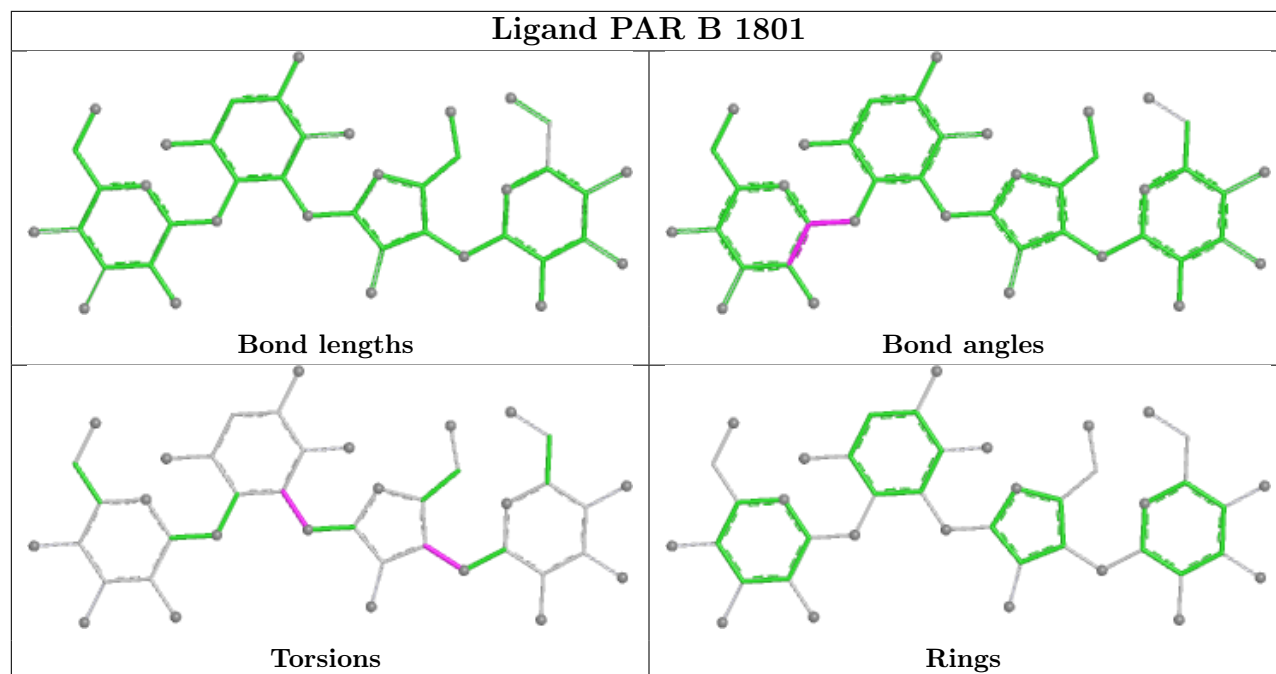


Ligand PAR AS 3406

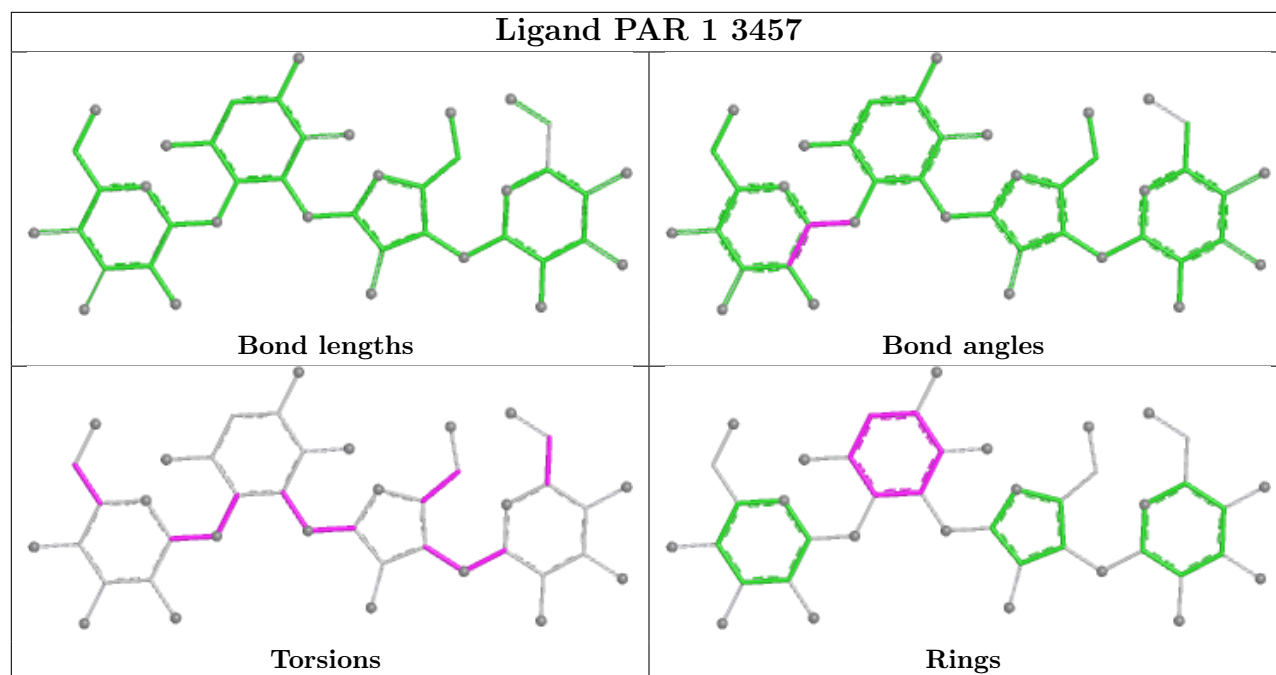


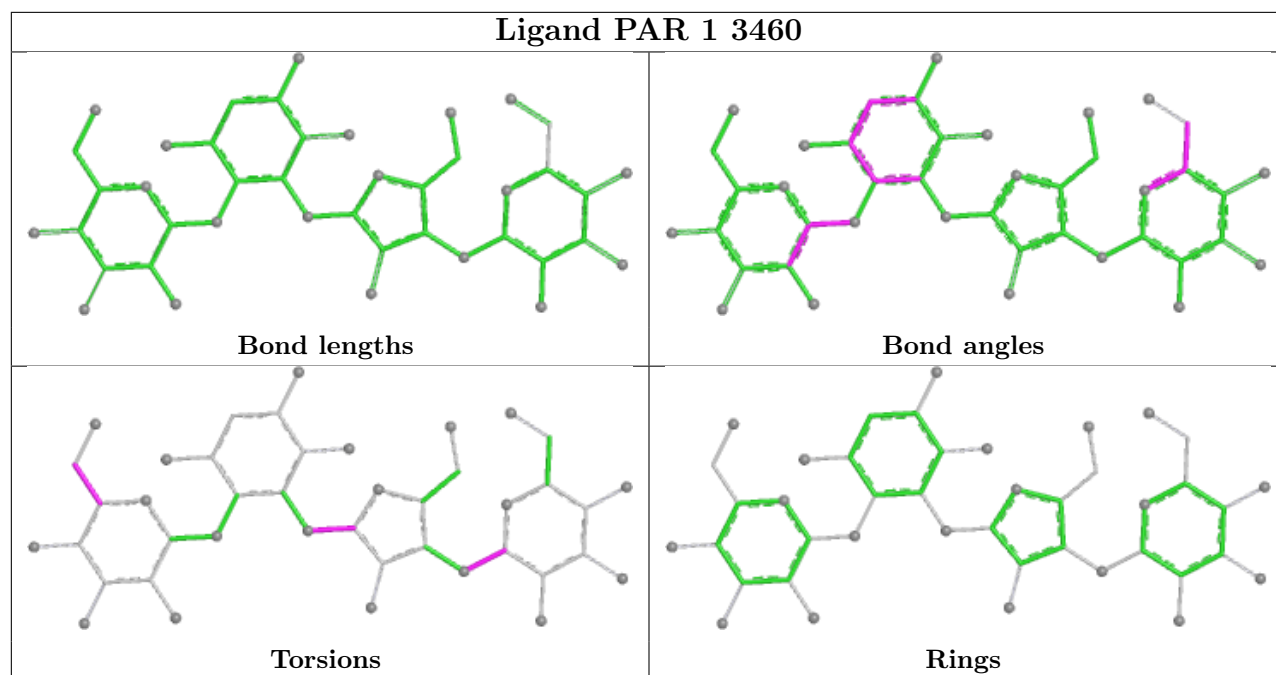
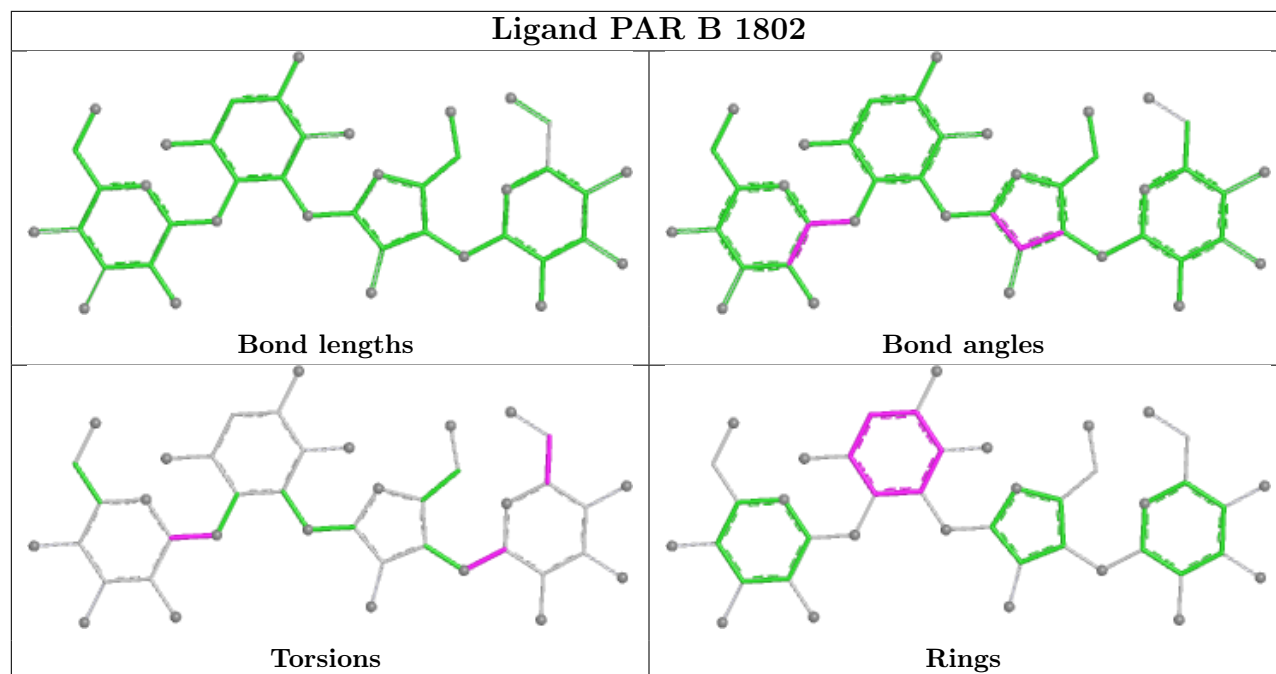


Ligand PAR B 1801

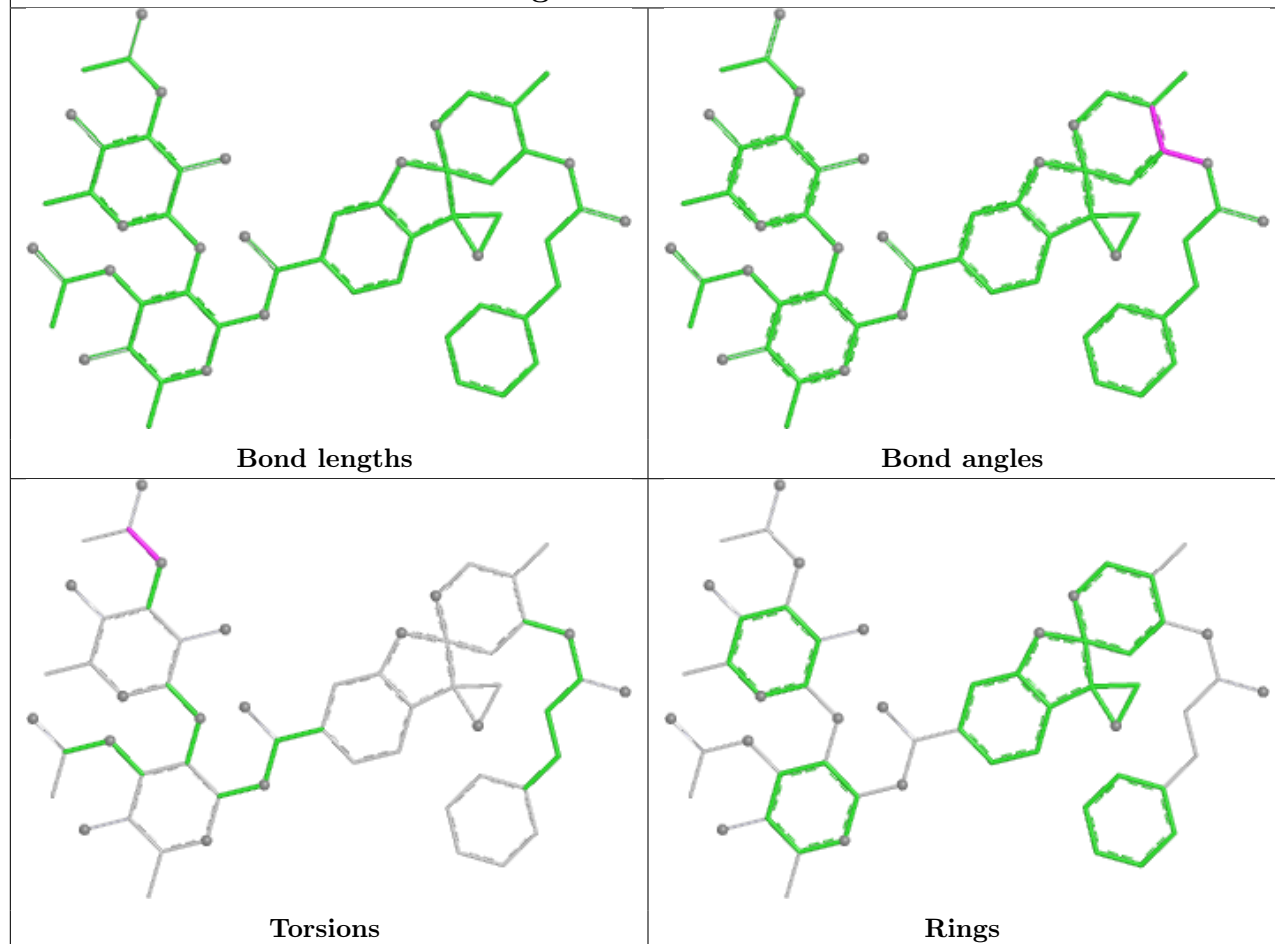


Ligand PAR 1 3457

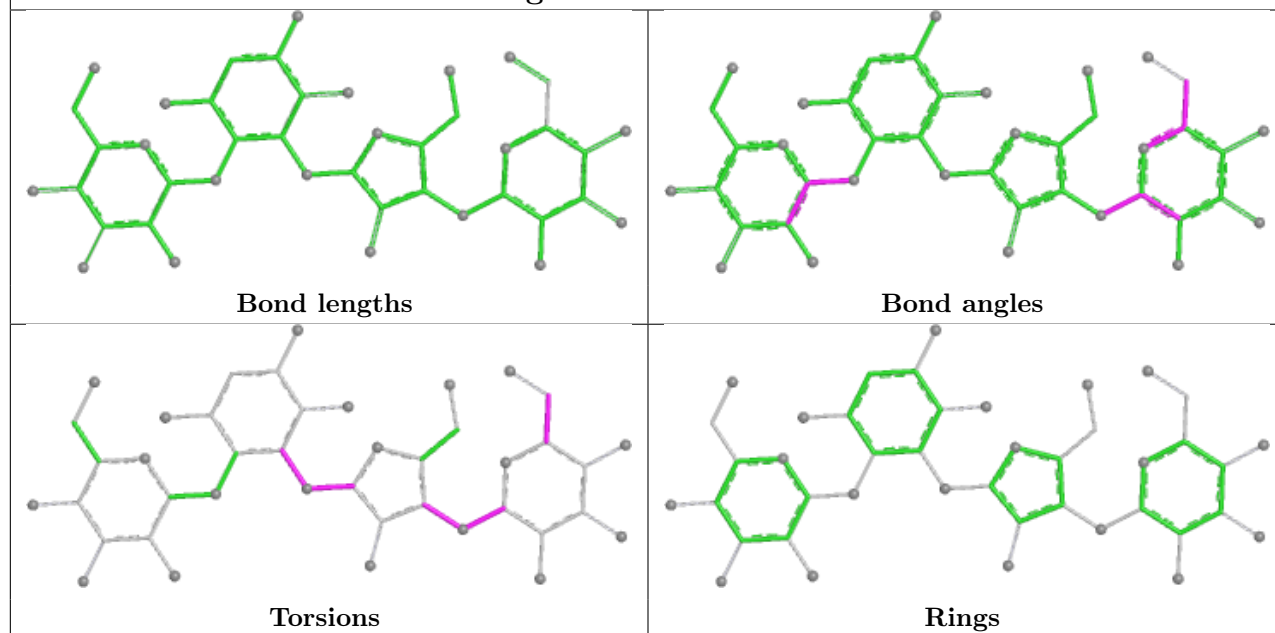




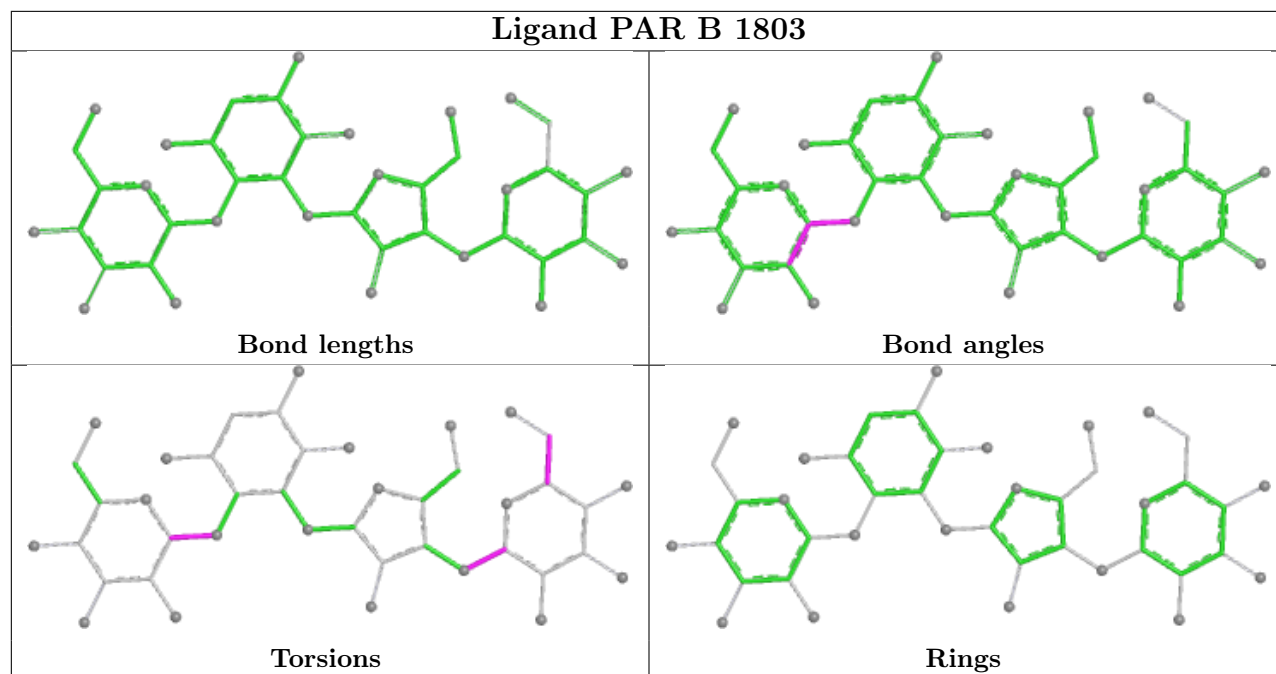
Ligand 3K5 1 3463



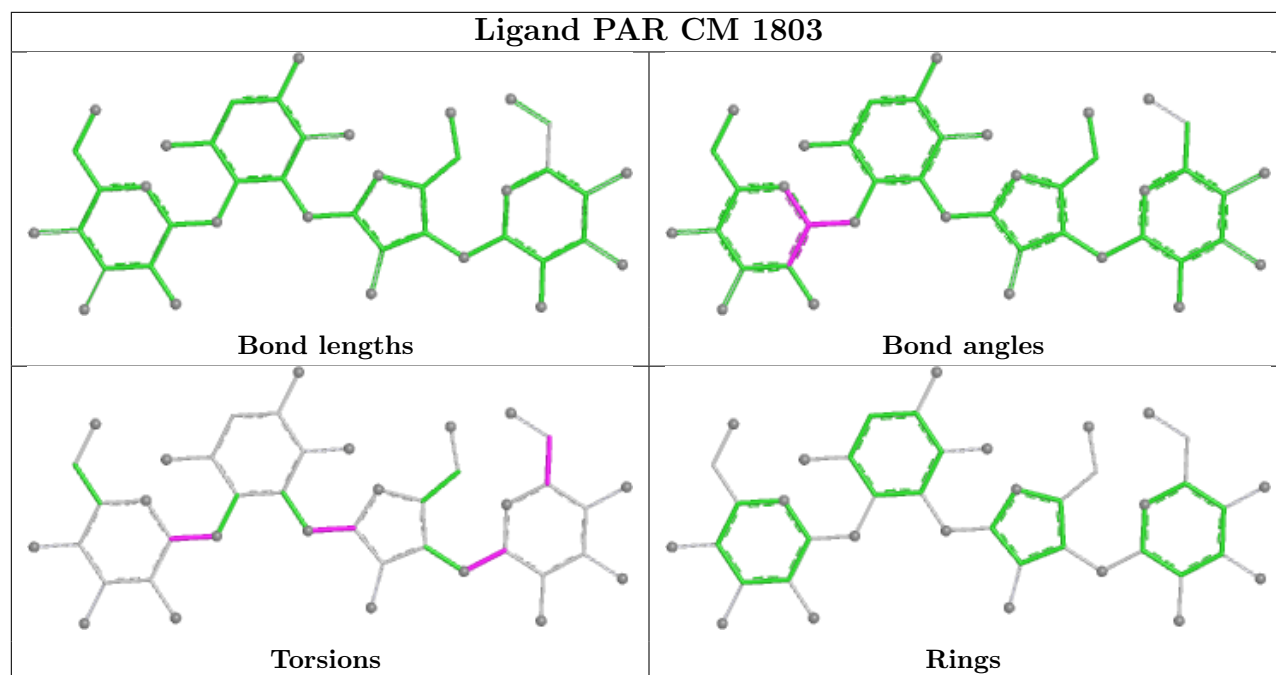
Ligand PAR 1 3458

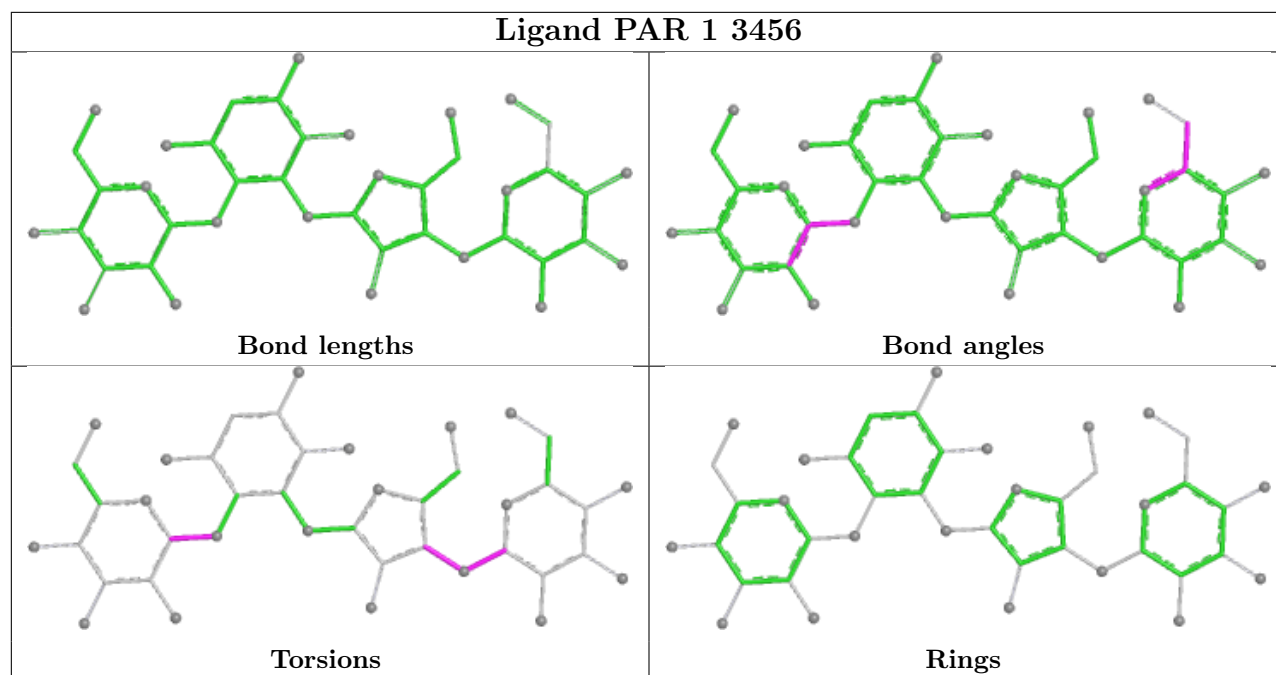
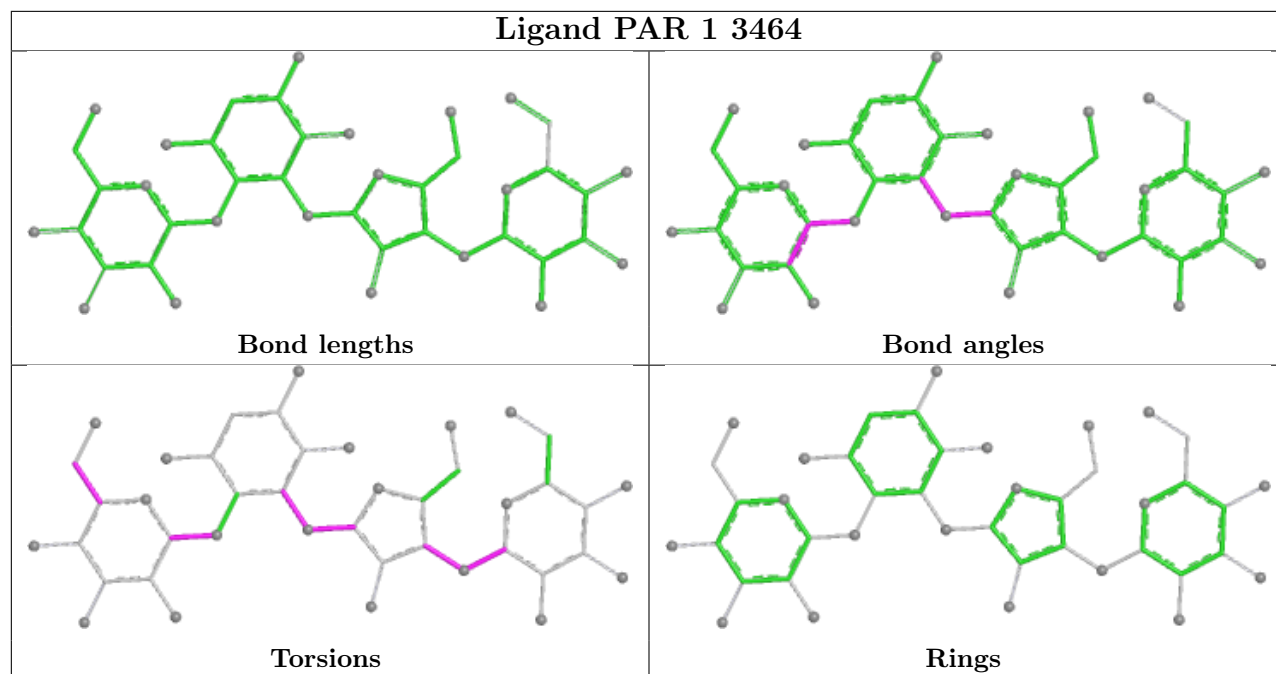


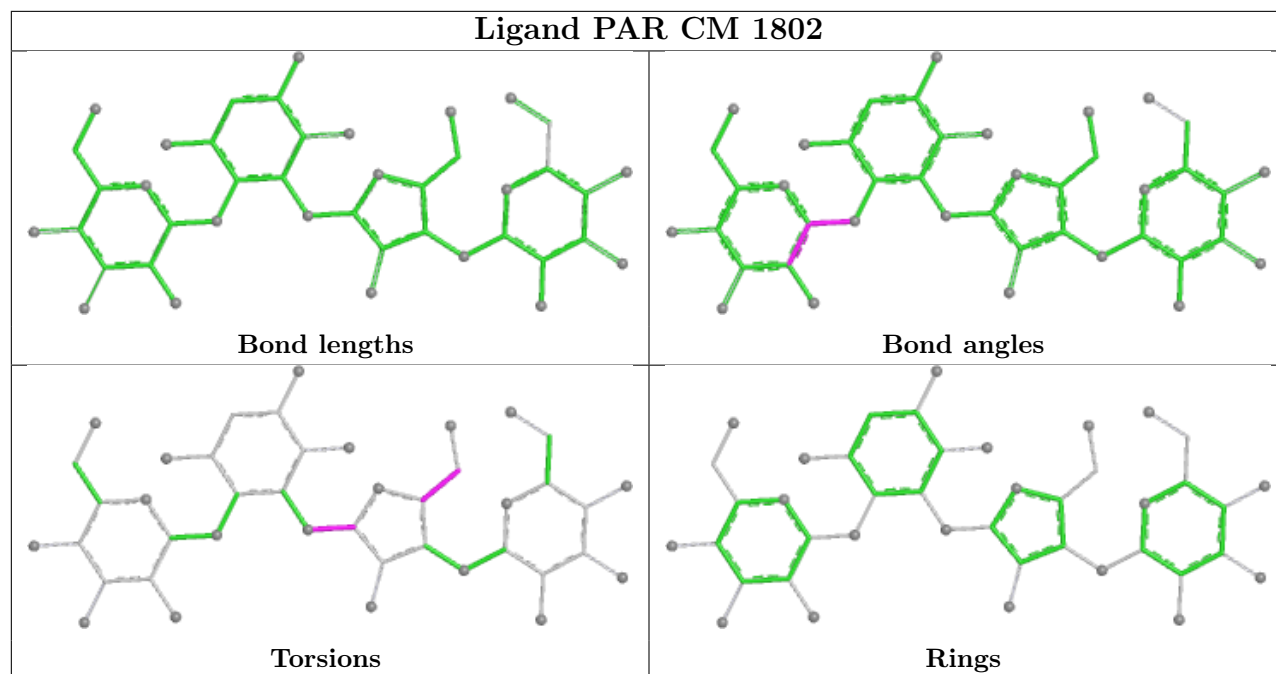
Ligand PAR B 1803



Ligand PAR CM 1803







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	3219/3359 (95%)	0.55	122 (3%) 44 31	16, 47, 179, 355	0
1	AS	3061/3359 (91%)	1.03	384 (12%) 8 8	38, 85, 181, 329	0
2	3	121/121 (100%)	0.33	2 (1%) 69 53	27, 70, 89, 129	0
2	AT	121/121 (100%)	0.67	7 (5%) 29 21	40, 98, 127, 132	0
3	4	157/158 (99%)	0.49	7 (4%) 38 27	28, 47, 130, 207	0
3	AU	156/158 (98%)	1.58	42 (26%) 1 2	63, 114, 159, 213	0
4	AW	248/254 (97%)	2.01	99 (39%) 1 0	48, 92, 123, 139	0
4	j	249/254 (98%)	1.10	37 (14%) 5 6	13, 33, 54, 89	0
5	AX	386/389 (99%)	1.53	98 (25%) 1 3	33, 72, 107, 187	0
5	k	386/389 (99%)	1.15	61 (15%) 5 6	19, 45, 69, 111	1 (0%)
6	AY	359/363 (98%)	1.87	136 (37%) 1 1	41, 84, 111, 137	0
6	l	361/363 (99%)	1.05	47 (13%) 7 8	18, 46, 81, 124	0
7	AZ	292/298 (97%)	2.08	118 (40%) 0 0	66, 116, 146, 177	0
7	m	296/298 (99%)	1.13	56 (18%) 3 4	36, 81, 114, 144	0
8	BA	153/176 (86%)	1.75	55 (35%) 1 1	54, 80, 109, 165	0
8	n	157/176 (89%)	1.10	27 (17%) 4 5	33, 61, 101, 142	0
9	BB	227/241 (94%)	1.41	56 (24%) 2 3	40, 65, 92, 112	0
9	o	228/241 (94%)	0.79	15 (6%) 24 18	21, 44, 87, 122	0
10	BC	226/262 (86%)	2.19	93 (41%) 0 0	101, 138, 165, 196	0
10	p	237/262 (90%)	1.06	31 (13%) 7 8	28, 56, 112, 156	0
11	BD	189/191 (98%)	1.37	42 (22%) 2 3	58, 88, 119, 137	0
11	q	190/191 (99%)	0.98	22 (11%) 9 9	36, 53, 81, 99	0
12	BE	206/220 (93%)	0.88	19 (9%) 14 13	39, 65, 110, 143	0
12	r	208/220 (94%)	1.21	35 (16%) 4 5	24, 51, 104, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	BF	171/174 (98%)	1.27	38 (22%)	2	3	74, 102, 126, 146	0
13	s	171/174 (98%)	1.48	43 (25%)	1	3	46, 86, 113, 146	0
14	BG	200/202 (99%)	2.24	91 (45%)	0	0	49, 111, 147, 171	0
14	t	200/202 (99%)	1.03	35 (17%)	4	5	20, 58, 113, 141	0
15	BH	128/131 (97%)	1.61	38 (29%)	1	2	57, 88, 108, 134	0
15	u	130/131 (99%)	0.95	15 (11%)	9	10	20, 54, 81, 113	0
16	BI	203/204 (99%)	3.04	147 (72%)	0	0	58, 109, 134, 149	0
16	v	203/204 (99%)	1.36	45 (22%)	2	3	19, 36, 49, 73	0
17	BJ	199/200 (99%)	1.36	42 (21%)	2	4	36, 60, 106, 125	0
17	w	199/200 (99%)	1.25	36 (18%)	3	4	16, 42, 85, 108	0
18	BK	174/185 (94%)	1.92	64 (36%)	1	1	49, 80, 112, 135	0
18	x	172/185 (92%)	1.20	22 (12%)	7	8	18, 45, 143, 168	0
19	BL	185/186 (99%)	1.83	72 (38%)	1	1	53, 83, 111, 131	0
19	y	185/186 (99%)	1.30	48 (25%)	1	2	25, 47, 64, 79	0
20	BM	171/190 (90%)	2.16	78 (45%)	0	0	66, 100, 123, 136	0
20	z	179/190 (94%)	1.18	35 (19%)	3	4	30, 53, 94, 115	0
21	0	170/172 (98%)	0.86	12 (7%)	22	17	24, 43, 71, 120	0
21	BN	170/172 (98%)	1.47	38 (22%)	2	3	43, 69, 104, 120	0
22	2	159/160 (99%)	1.35	33 (20%)	2	4	29, 49, 115, 157	0
22	BO	159/160 (99%)	2.29	77 (48%)	0	0	48, 84, 118, 170	0
23	5	103/124 (83%)	0.99	12 (11%)	9	9	55, 92, 126, 139	0
23	BP	102/124 (82%)	1.33	22 (21%)	2	4	108, 141, 177, 201	1 (0%)
24	6	131/137 (95%)	1.27	24 (18%)	3	4	17, 39, 61, 82	0
24	BQ	131/137 (95%)	1.62	39 (29%)	1	2	31, 55, 77, 85	0
25	7	118/155 (76%)	1.06	10 (8%)	16	14	25, 61, 144, 161	0
25	BR	111/155 (71%)	1.44	25 (22%)	2	3	51, 87, 138, 179	0
26	8	121/142 (85%)	0.95	9 (7%)	20	16	26, 49, 74, 124	0
26	BS	118/142 (83%)	2.39	66 (55%)	0	0	56, 104, 131, 153	0
27	9	126/127 (99%)	1.44	30 (23%)	2	3	26, 56, 93, 133	0
27	BT	124/127 (97%)	2.22	62 (50%)	0	0	54, 103, 134, 154	0
28	AA	135/136 (99%)	1.26	27 (20%)	3	4	30, 57, 91, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	BU	135/136 (99%)	1.69	45 (33%)	1	1	92, 124, 146, 157	0
29	AB	148/149 (99%)	1.23	26 (17%)	4	5	16, 47, 71, 82	0
29	BV	148/149 (99%)	2.34	76 (51%)	0	0	46, 95, 118, 131	0
30	AC	62/63 (98%)	1.48	12 (19%)	3	4	26, 59, 116, 143	0
30	BW	60/63 (95%)	2.20	27 (45%)	0	0	50, 103, 122, 131	1 (1%)
31	AD	99/106 (93%)	1.23	24 (24%)	2	3	35, 55, 88, 100	0
31	BX	96/106 (90%)	1.74	31 (32%)	1	1	79, 112, 136, 158	0
32	AE	110/112 (98%)	1.07	15 (13%)	7	7	27, 56, 135, 154	0
32	BY	109/112 (97%)	1.42	27 (24%)	2	3	43, 88, 131, 154	0
33	AF	124/131 (94%)	1.12	20 (16%)	4	5	21, 42, 57, 73	0
33	BZ	124/131 (94%)	1.91	45 (36%)	1	1	40, 62, 94, 113	1 (0%)
34	AG	106/107 (99%)	1.15	17 (16%)	5	5	21, 36, 72, 111	0
34	CA	106/107 (99%)	1.42	25 (23%)	2	3	35, 58, 99, 119	3 (2%)
35	AH	111/122 (90%)	1.74	31 (27%)	1	2	25, 51, 99, 120	0
35	CB	112/122 (91%)	2.85	60 (53%)	0	0	69, 115, 152, 186	4 (3%)
36	AI	120/120 (100%)	1.57	32 (26%)	1	2	31, 53, 86, 120	0
36	CC	117/120 (97%)	2.84	78 (66%)	0	0	78, 111, 131, 140	0
37	AJ	97/99 (97%)	0.86	7 (7%)	21	17	43, 60, 88, 110	0
37	CD	98/99 (98%)	1.86	37 (37%)	1	1	75, 126, 159, 163	1 (1%)
38	AK	86/90 (95%)	1.02	10 (11%)	9	9	19, 29, 75, 109	0
38	CE	86/90 (95%)	2.13	35 (40%)	0	0	52, 80, 129, 160	0
39	AL	77/78 (98%)	1.11	10 (12%)	7	8	44, 75, 121, 178	0
39	CF	76/78 (97%)	1.40	18 (23%)	2	3	88, 145, 194, 210	1 (1%)
40	AM	50/51 (98%)	1.44	8 (16%)	5	5	19, 47, 67, 81	0
40	CG	50/51 (98%)	2.31	25 (50%)	0	0	57, 87, 113, 125	0
41	AN	52/52 (100%)	0.82	6 (11%)	9	10	28, 46, 69, 104	0
41	CH	52/52 (100%)	1.13	9 (17%)	4	5	41, 62, 107, 122	1 (1%)
42	AO	25/25 (100%)	1.75	8 (32%)	1	1	38, 56, 72, 80	0
42	CI	24/25 (96%)	2.70	17 (70%)	0	0	56, 78, 94, 98	0
43	AP	103/106 (97%)	1.19	18 (17%)	4	5	28, 53, 85, 98	0
43	CJ	103/106 (97%)	1.45	29 (28%)	1	2	50, 97, 145, 170	2 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	AQ	91/92 (98%)	1.17	14 (15%)	5	6	24, 34, 69, 99	0
44	CK	91/92 (98%)	1.53	30 (32%)	1	1	45, 90, 107, 119	0
45	CL	107/267 (40%)	1.43	33 (30%)	1	1	71, 110, 149, 174	0
45	i	121/267 (45%)	1.65	36 (29%)	1	2	48, 87, 128, 163	0
46	B	1730/1787 (96%)	0.71	116 (6%)	24	18	17, 66, 198, 403	0
46	CM	1704/1787 (95%)	1.28	334 (19%)	3	4	37, 105, 207, 346	0
47	C	208/261 (79%)	1.20	39 (18%)	3	4	45, 84, 117, 185	0
47	CN	208/261 (79%)	1.35	42 (20%)	3	4	65, 121, 160, 180	0
48	CO	214/256 (83%)	1.48	48 (22%)	2	3	89, 136, 180, 202	0
48	D	214/256 (83%)	0.83	20 (9%)	14	13	42, 71, 101, 120	0
49	CP	216/249 (86%)	1.38	50 (23%)	2	3	52, 82, 118, 138	0
49	E	217/249 (87%)	1.21	44 (20%)	3	4	34, 57, 92, 121	0
50	CQ	223/251 (88%)	1.95	88 (39%)	1	1	92, 134, 178, 204	0
50	F	223/251 (88%)	1.66	63 (28%)	1	2	37, 80, 139, 164	0
51	CR	260/262 (99%)	1.04	36 (13%)	6	7	45, 66, 104, 145	0
51	G	259/262 (98%)	1.14	39 (15%)	5	6	35, 59, 91, 135	0
52	CS	206/225 (91%)	2.27	96 (46%)	0	0	102, 164, 185, 206	0
52	H	206/225 (91%)	1.57	55 (26%)	1	2	53, 90, 128, 172	0
53	CT	235/236 (99%)	1.50	65 (27%)	1	2	53, 94, 124, 154	0
53	I	226/236 (95%)	1.18	41 (18%)	3	4	50, 84, 136, 181	0
54	CU	182/186 (97%)	1.59	54 (29%)	1	2	66, 125, 174, 199	0
54	J	185/186 (99%)	1.47	52 (28%)	1	2	40, 90, 142, 231	0
55	CV	203/206 (98%)	1.82	71 (34%)	1	1	48, 76, 131, 154	0
55	K	203/206 (98%)	0.86	16 (7%)	18	15	35, 54, 120, 151	0
56	CW	178/189 (94%)	1.78	59 (33%)	1	1	58, 90, 119, 148	0
56	L	178/189 (94%)	1.60	50 (28%)	1	2	41, 70, 102, 120	0
57	CX	93/118 (78%)	1.37	23 (24%)	2	3	107, 157, 193, 218	0
57	M	98/118 (83%)	1.33	20 (20%)	3	4	52, 91, 129, 176	0
58	CY	141/155 (90%)	1.71	50 (35%)	1	1	27, 60, 102, 155	0
58	N	144/155 (92%)	0.93	13 (9%)	15	13	24, 47, 102, 133	0
59	CZ	116/143 (81%)	1.13	13 (11%)	10	10	156, 200, 230, 249	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
59	O	116/143 (81%)	1.27	20 (17%)	4	5	112, 154, 189, 202	0
60	DA	150/151 (99%)	2.08	72 (48%)	0	0	62, 104, 129, 143	0
60	P	150/151 (99%)	1.09	19 (12%)	8	8	26, 56, 73, 88	0
61	DB	127/132 (96%)	1.80	45 (35%)	1	1	78, 141, 165, 191	0
61	Q	127/132 (96%)	0.95	14 (11%)	10	10	23, 61, 90, 99	0
62	DC	118/142 (83%)	2.44	70 (59%)	0	0	94, 148, 166, 189	0
62	R	129/142 (90%)	1.54	38 (29%)	1	2	40, 85, 140, 173	0
63	DD	140/142 (98%)	2.93	87 (62%)	0	0	111, 156, 187, 203	0
63	S	139/142 (97%)	1.60	39 (28%)	1	2	48, 93, 127, 139	0
64	DE	125/137 (91%)	1.66	38 (30%)	1	1	94, 136, 170, 193	0
64	T	123/137 (89%)	1.65	42 (34%)	1	1	58, 99, 146, 158	0
65	DF	142/145 (97%)	2.49	85 (59%)	0	0	100, 145, 184, 200	0
65	U	144/145 (99%)	1.34	36 (25%)	2	3	41, 75, 111, 159	0
66	DG	141/145 (97%)	2.39	81 (57%)	0	0	116, 155, 177, 210	0
66	V	139/145 (95%)	1.46	33 (23%)	2	3	58, 92, 129, 143	0
67	DH	100/119 (84%)	2.62	47 (47%)	0	0	101, 140, 166, 184	0
67	W	102/119 (85%)	1.79	34 (33%)	1	1	39, 94, 139, 153	0
68	DI	87/87 (100%)	1.22	16 (18%)	3	4	60, 94, 129, 173	0
68	X	87/87 (100%)	0.86	7 (8%)	18	15	35, 71, 109, 130	0
69	DJ	129/130 (99%)	1.53	38 (29%)	1	2	49, 75, 95, 104	0
69	Y	129/130 (99%)	1.33	23 (17%)	4	4	28, 51, 69, 78	0
70	DK	143/145 (98%)	1.91	55 (38%)	1	1	40, 69, 104, 112	0
70	Z	143/145 (98%)	1.18	25 (17%)	4	5	30, 52, 73, 121	0
71	DL	132/135 (97%)	1.08	13 (9%)	13	12	63, 90, 119, 131	0
71	a	134/135 (99%)	1.14	23 (17%)	4	5	52, 79, 114, 136	0
72	DM	72/105 (68%)	1.64	23 (31%)	1	1	138, 173, 196, 208	0
72	b	71/105 (67%)	0.86	4 (5%)	30	22	73, 96, 137, 151	0
73	DN	97/119 (81%)	2.08	43 (44%)	0	0	62, 104, 154, 168	0
73	c	98/119 (82%)	1.51	28 (28%)	1	2	33, 55, 107, 119	0
74	DO	81/82 (98%)	1.68	23 (28%)	1	2	70, 113, 149, 174	0
74	d	81/82 (98%)	1.03	9 (11%)	10	10	43, 64, 130, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
75	DP	62/67 (92%)	1.43	15 (24%)	2	3	120, 160, 182, 199	0
75	e	62/67 (92%)	1.45	15 (24%)	2	3	77, 100, 125, 139	0
76	DQ	55/56 (98%)	2.40	29 (52%)	0	0	106, 131, 173, 202	0
76	f	55/56 (98%)	1.74	19 (34%)	1	1	48, 66, 94, 118	0
77	DR	56/63 (88%)	1.85	23 (41%)	0	0	76, 103, 164, 198	0
77	g	60/63 (95%)	1.30	15 (25%)	2	3	51, 81, 136, 166	0
78	DS	70/193 (36%)	1.65	20 (28%)	1	2	131, 203, 236, 256	0
78	h	70/193 (36%)	1.49	21 (30%)	1	2	94, 130, 155, 171	0
79	AR	310/317 (97%)	1.42	67 (21%)	2	4	75, 132, 174, 198	0
79	DT	311/317 (98%)	1.64	87 (27%)	1	2	136, 182, 213, 224	0
80	l1	217/217 (100%)	0.95	24 (11%)	10	10	94, 150, 201, 233	0
81	12	14/165 (8%)	1.08	3 (21%)	2	4	129, 177, 198, 221	0
All	All	32865/35508 (92%)	1.30	6952 (21%)	2	4	13, 78, 169, 403	16 (0%)

The worst 5 of 6952 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
67	DH	79	ASP	18.2
52	H	152	SER	17.8
35	CB	64	GLN	13.2
46	CM	726	C	12.1
7	AZ	49	TYR	11.9

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	AS	3842	1/1	0.03	0.16	94,94,94,94	0
82	MG	AS	3808	1/1	0.05	0.23	96,96,96,96	0
82	MG	1	3867	1/1	0.10	0.28	35,35,35,35	0
82	MG	1	3671	1/1	0.12	0.30	49,49,49,49	0
82	MG	1	3948	1/1	0.16	0.16	53,53,53,53	0
82	MG	AS	3736	1/1	0.16	0.25	73,73,73,73	0
82	MG	AS	3872	1/1	0.17	0.14	74,74,74,74	0
82	MG	AS	3521	1/1	0.18	0.21	47,47,47,47	0
82	MG	AS	3596	1/1	0.20	0.19	50,50,50,50	0
82	MG	AS	3418	1/1	0.21	0.49	84,84,84,84	0
82	MG	AS	3574	1/1	0.23	0.24	50,50,50,50	0
82	MG	1	3984	1/1	0.23	0.35	40,40,40,40	0
82	MG	AS	3899	1/1	0.23	0.13	55,55,55,55	0
82	MG	1	3919	1/1	0.24	0.14	38,38,38,38	0
82	MG	AS	3902	1/1	0.24	0.22	36,36,36,36	0
82	MG	1	4046	1/1	0.25	0.35	66,66,66,66	0
82	MG	1	3858	1/1	0.27	0.24	58,58,58,58	0
82	MG	1	3685	1/1	0.27	0.20	52,52,52,52	0
82	MG	1	3659	1/1	0.28	0.24	52,52,52,52	0
82	MG	AS	3516	1/1	0.29	0.34	73,73,73,73	0
82	MG	1	4030	1/1	0.29	0.16	34,34,34,34	0
82	MG	AS	3633	1/1	0.30	0.27	49,49,49,49	0
82	MG	1	3946	1/1	0.34	0.22	41,41,41,41	0
82	MG	1	3922	1/1	0.35	0.17	50,50,50,50	0
82	MG	AS	3858	1/1	0.36	0.24	64,64,64,64	0
82	MG	AS	3947	1/1	0.36	0.15	25,25,25,25	0
82	MG	1	4047	1/1	0.37	0.26	57,57,57,57	0
82	MG	1	3760	1/1	0.37	0.19	45,45,45,45	0
82	MG	AS	3908	1/1	0.37	0.10	55,55,55,55	0
82	MG	1	4013	1/1	0.37	0.23	55,55,55,55	0
82	MG	1	3743	1/1	0.38	0.16	16,16,16,16	0
82	MG	1	4029	1/1	0.38	0.19	98,98,98,98	0
82	MG	1	4076	1/1	0.39	0.39	52,52,52,52	0
82	MG	1	3731	1/1	0.39	0.19	10,10,10,10	0
82	MG	1	3827	1/1	0.39	0.18	53,53,53,53	0
82	MG	AS	3603	1/1	0.39	0.32	63,63,63,63	0
82	MG	AS	3921	1/1	0.39	0.18	107,107,107,107	0
82	MG	AS	3631	1/1	0.39	0.23	58,58,58,58	0
82	MG	1	3697	1/1	0.40	0.18	26,26,26,26	0
82	MG	AS	3643	1/1	0.40	0.27	35,35,35,35	0
82	MG	1	3917	1/1	0.41	0.20	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3968	1/1	0.41	0.11	67,67,67,67	0
82	MG	AS	3859	1/1	0.41	0.28	47,47,47,47	0
82	MG	AS	3617	1/1	0.43	0.14	57,57,57,57	0
82	MG	AS	3772	1/1	0.43	0.22	44,44,44,44	0
82	MG	1	3833	1/1	0.43	0.14	22,22,22,22	0
82	MG	1	3589	1/1	0.44	0.30	47,47,47,47	0
82	MG	AS	3701	1/1	0.44	0.19	50,50,50,50	0
82	MG	AS	3426	1/1	0.44	0.26	41,41,41,41	0
82	MG	AS	3752	1/1	0.44	0.12	31,31,31,31	0
82	MG	1	3530	1/1	0.44	0.17	54,54,54,54	0
82	MG	AS	3779	1/1	0.44	0.23	54,54,54,54	0
82	MG	1	4014	1/1	0.44	0.20	62,62,62,62	0
82	MG	AS	3930	1/1	0.44	0.16	57,57,57,57	0
82	MG	1	3978	1/1	0.44	0.47	85,85,85,85	0
82	MG	AS	3588	1/1	0.45	0.30	53,53,53,53	0
82	MG	AS	3681	1/1	0.45	0.30	54,54,54,54	0
82	MG	AS	3764	1/1	0.45	0.16	65,65,65,65	0
82	MG	1	4005	1/1	0.45	0.14	48,48,48,48	0
82	MG	AS	3715	1/1	0.45	0.15	8,8,8,8	0
82	MG	AS	3891	1/1	0.45	0.21	47,47,47,47	0
82	MG	AS	3642	1/1	0.46	0.18	61,61,61,61	0
82	MG	1	3730	1/1	0.46	0.16	24,24,24,24	0
82	MG	1	4064	1/1	0.47	0.41	55,55,55,55	0
82	MG	1	3620	1/1	0.47	0.13	50,50,50,50	0
82	MG	AI	201	1/1	0.47	0.16	43,43,43,43	0
82	MG	AS	3852	1/1	0.47	0.44	89,89,89,89	0
82	MG	AS	3411	1/1	0.47	0.18	27,27,27,27	0
82	MG	1	4026	1/1	0.47	0.16	53,53,53,53	0
82	MG	1	3840	1/1	0.47	0.22	37,37,37,37	1
82	MG	AS	3822	1/1	0.48	0.15	98,98,98,98	0
82	MG	1	3916	1/1	0.48	0.26	82,82,82,82	0
82	MG	1	3902	1/1	0.48	0.16	49,49,49,49	0
82	MG	1	4009	1/1	0.48	0.23	72,72,72,72	0
82	MG	AS	3918	1/1	0.48	0.15	46,46,46,46	0
82	MG	AF	201	1/1	0.48	0.22	34,34,34,34	0
82	MG	AS	3461	1/1	0.48	0.15	26,26,26,26	0
82	MG	AS	3883	1/1	0.48	0.11	24,24,24,24	0
82	MG	AS	3523	1/1	0.50	0.17	46,46,46,46	0
82	MG	AS	3806	1/1	0.50	0.10	41,41,41,41	0
82	MG	AS	3729	1/1	0.50	0.21	56,56,56,56	0
82	MG	1	3769	1/1	0.51	0.12	9,9,9,9	0
82	MG	AS	3909	1/1	0.51	0.18	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	1	3754	1/1	0.51	0.10	32,32,32,32	0
82	MG	AS	3895	1/1	0.51	0.35	72,72,72,72	0
82	MG	AS	3407	1/1	0.51	0.39	42,42,42,42	0
82	MG	1	3669	1/1	0.51	0.16	35,35,35,35	0
82	MG	1	4044	1/1	0.52	0.17	57,57,57,57	0
82	MG	1	3974	1/1	0.52	0.23	36,36,36,36	0
82	MG	1	3889	1/1	0.52	0.07	10,10,10,10	0
82	MG	AS	3584	1/1	0.52	0.17	41,41,41,41	0
82	MG	AS	3937	1/1	0.52	0.34	54,54,54,54	0
82	MG	AS	3414	1/1	0.52	0.24	64,64,64,64	0
82	MG	1	3839	1/1	0.53	0.08	16,16,16,16	0
82	MG	1	3627	1/1	0.53	0.14	10,10,10,10	0
82	MG	1	3653	1/1	0.53	0.22	45,45,45,45	0
82	MG	1	3656	1/1	0.53	0.12	36,36,36,36	0
82	MG	1	3619	1/1	0.53	0.25	39,39,39,39	0
82	MG	1	4016	1/1	0.53	0.12	75,75,75,75	0
82	MG	1	4058	1/1	0.53	0.26	56,56,56,56	0
82	MG	AS	3751	1/1	0.53	0.12	25,25,25,25	0
82	MG	1	3938	1/1	0.54	0.30	36,36,36,36	0
82	MG	1	3664	1/1	0.54	0.18	32,32,32,32	0
82	MG	B	1867	1/1	0.54	0.16	43,43,43,43	0
82	MG	1	3771	1/1	0.54	0.20	41,41,41,41	0
82	MG	AX	401	1/1	0.54	0.12	31,31,31,31	0
82	MG	1	3567	1/1	0.55	0.15	38,38,38,38	0
82	MG	AS	3857	1/1	0.55	0.19	45,45,45,45	0
82	MG	AS	3797	1/1	0.55	0.18	37,37,37,37	0
82	MG	AS	3830	1/1	0.55	0.13	69,69,69,69	0
82	MG	AS	3580	1/1	0.55	0.69	44,44,44,44	0
82	MG	AS	3843	1/1	0.55	0.12	71,71,71,71	0
85	ZN	CB	201	1/1	0.55	0.20	327,327,327,327	0
82	MG	1	3690	1/1	0.56	0.36	35,35,35,35	0
82	MG	CM	1801	1/1	0.56	0.17	42,42,42,42	0
82	MG	AS	3766	1/1	0.56	0.19	50,50,50,50	0
82	MG	1	3861	1/1	0.57	0.14	27,27,27,27	0
82	MG	AS	3735	1/1	0.57	0.12	29,29,29,29	0
82	MG	AS	3676	1/1	0.57	0.13	24,24,24,24	0
82	MG	AT	203	1/1	0.57	0.18	33,33,33,33	0
82	MG	1	4052	1/1	0.57	0.17	23,23,23,23	0
82	MG	AS	3478	1/1	0.57	0.14	15,15,15,15	0
82	MG	1	3995	1/1	0.57	0.14	32,32,32,32	0
82	MG	AS	3835	1/1	0.58	0.18	48,48,48,48	0
82	MG	AS	3809	1/1	0.58	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	4061	1/1	0.58	0.20	40,40,40,40	0
82	MG	9	201	1/1	0.58	0.25	52,52,52,52	0
82	MG	1	3991	1/1	0.59	0.09	28,28,28,28	0
82	MG	1	3911	1/1	0.59	0.23	24,24,24,24	0
82	MG	AS	3767	1/1	0.59	0.13	57,57,57,57	0
82	MG	1	4020	1/1	0.59	0.16	27,27,27,27	0
82	MG	1	3869	1/1	0.59	0.14	23,23,23,23	0
82	MG	AS	3924	1/1	0.59	0.13	98,98,98,98	0
82	MG	1	3808	1/1	0.59	0.15	12,12,12,12	0
82	MG	AS	3475	1/1	0.59	0.15	40,40,40,40	0
82	MG	1	4060	1/1	0.59	0.13	35,35,35,35	0
82	MG	1	3555	1/1	0.59	0.19	16,16,16,16	0
82	MG	AS	3811	1/1	0.59	0.11	73,73,73,73	0
82	MG	AS	3409	1/1	0.59	0.41	56,56,56,56	0
82	MG	AS	3410	1/1	0.59	0.31	35,35,35,35	0
82	MG	1	3630	1/1	0.60	0.14	40,40,40,40	0
82	MG	1	3945	1/1	0.60	0.29	33,33,33,33	0
82	MG	AS	3592	1/1	0.60	0.14	14,14,14,14	0
82	MG	AS	3763	1/1	0.60	0.09	40,40,40,40	0
82	MG	AS	3879	1/1	0.60	0.19	32,32,32,32	0
82	MG	E	301	1/1	0.60	0.20	24,24,24,24	0
82	MG	AS	3942	1/1	0.60	0.12	28,28,28,28	0
82	MG	1	3424	1/1	0.60	0.17	12,12,12,12	0
82	MG	AS	3568	1/1	0.60	0.22	42,42,42,42	0
82	MG	AS	3719	1/1	0.60	0.18	43,43,43,43	0
82	MG	1	4040	1/1	0.60	0.30	50,50,50,50	0
82	MG	1	3824	1/1	0.60	0.11	56,56,56,56	0
82	MG	AS	3915	1/1	0.61	0.15	48,48,48,48	0
82	MG	1	4015	1/1	0.61	0.13	216,216,216,216	0
82	MG	AS	3585	1/1	0.61	0.18	43,43,43,43	0
82	MG	AS	3874	1/1	0.61	0.14	29,29,29,29	0
82	MG	1	4036	1/1	0.61	0.32	50,50,50,50	0
82	MG	AS	3509	1/1	0.61	0.09	18,18,18,18	0
82	MG	1	4008	1/1	0.61	0.11	43,43,43,43	0
82	MG	AP	202	1/1	0.61	0.25	24,24,24,24	0
82	MG	1	3707	1/1	0.61	0.14	32,32,32,32	0
82	MG	AS	3422	1/1	0.61	0.34	139,139,139,139	0
82	MG	1	3683	1/1	0.61	0.19	40,40,40,40	0
83	PAR	AS	3404	42/42	0.61	0.14	94,112,135,146	0
82	MG	1	3559	1/1	0.61	0.13	17,17,17,17	0
82	MG	AS	3612	1/1	0.62	0.13	47,47,47,47	0
82	MG	1	3828	1/1	0.62	0.16	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	AS	3672	1/1	0.62	0.38	26,26,26,26	0
82	MG	AS	3824	1/1	0.62	0.17	28,28,28,28	0
82	MG	BZ	201	1/1	0.62	0.22	49,49,49,49	0
82	MG	1	3631	1/1	0.62	0.13	28,28,28,28	0
82	MG	AS	3731	1/1	0.62	0.14	32,32,32,32	0
82	MG	AS	3544	1/1	0.62	0.15	45,45,45,45	0
82	MG	1	3592	1/1	0.63	0.32	27,27,27,27	0
82	MG	AS	3632	1/1	0.63	0.15	34,34,34,34	0
82	MG	AS	3695	1/1	0.63	0.14	26,26,26,26	0
82	MG	AS	3739	1/1	0.63	0.12	22,22,22,22	0
82	MG	AS	3466	1/1	0.63	0.14	58,58,58,58	0
82	MG	1	3933	1/1	0.63	0.33	27,27,27,27	0
82	MG	1	3602	1/1	0.63	0.09	22,22,22,22	0
82	MG	AS	3844	1/1	0.63	0.12	65,65,65,65	0
82	MG	1	3511	1/1	0.63	0.19	20,20,20,20	0
82	MG	AS	3664	1/1	0.64	0.26	62,62,62,62	0
82	MG	AS	3897	1/1	0.64	0.14	42,42,42,42	0
82	MG	AS	3723	1/1	0.64	0.14	52,52,52,52	0
82	MG	1	4065	1/1	0.64	0.10	31,31,31,31	0
82	MG	1	3538	1/1	0.64	0.20	45,45,45,45	0
82	MG	1	3686	1/1	0.64	0.19	7,7,7,7	0
82	MG	AS	3688	1/1	0.64	0.18	28,28,28,28	0
82	MG	1	4011	1/1	0.64	0.17	36,36,36,36	0
82	MG	AS	3611	1/1	0.64	0.27	80,80,80,80	0
82	MG	1	4028	1/1	0.64	0.17	20,20,20,20	0
82	MG	1	3829	1/1	0.65	0.12	45,45,45,45	0
82	MG	AS	3604	1/1	0.65	0.15	37,37,37,37	0
82	MG	1	3856	1/1	0.65	0.30	41,41,41,41	0
82	MG	AS	3581	1/1	0.65	0.17	48,48,48,48	0
82	MG	1	3676	1/1	0.65	0.24	69,69,69,69	0
82	MG	AS	3893	1/1	0.65	0.11	15,15,15,15	0
82	MG	AS	3791	1/1	0.65	0.22	44,44,44,44	0
82	MG	1	3751	1/1	0.65	0.18	28,28,28,28	0
82	MG	AW	301	1/1	0.65	0.11	35,35,35,35	0
82	MG	1	3864	1/1	0.65	0.12	12,12,12,12	0
82	MG	2	201	1/1	0.65	0.14	14,14,14,14	0
82	MG	AS	3708	1/1	0.65	0.10	23,23,23,23	0
82	MG	AS	3570	1/1	0.65	0.23	66,66,66,66	0
82	MG	AS	3860	1/1	0.65	0.13	33,33,33,33	0
82	MG	1	3718	1/1	0.66	0.32	32,32,32,32	0
82	MG	1	4004	1/1	0.66	0.10	54,54,54,54	0
82	MG	i	301	1/1	0.66	0.31	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3857	1/1	0.66	0.26	33,33,33,33	0
82	MG	AS	3737	1/1	0.66	0.11	36,36,36,36	0
82	MG	1	3791	1/1	0.66	0.41	57,57,57,57	0
82	MG	AS	3639	1/1	0.66	0.14	49,49,49,49	0
82	MG	1	3989	1/1	0.66	0.10	45,45,45,45	0
82	MG	AS	3756	1/1	0.66	0.32	44,44,44,44	0
82	MG	AS	3609	1/1	0.66	0.10	41,41,41,41	0
82	MG	AS	3653	1/1	0.66	0.17	27,27,27,27	0
82	MG	1	3844	1/1	0.66	0.17	15,15,15,15	0
82	MG	1	3596	1/1	0.67	0.16	26,26,26,26	0
82	MG	AS	3558	1/1	0.67	0.37	40,40,40,40	0
82	MG	AS	3421	1/1	0.67	0.19	78,78,78,78	0
82	MG	AA	201	1/1	0.67	0.25	40,40,40,40	0
82	MG	1	3959	1/1	0.67	0.41	49,49,49,49	0
82	MG	BE	301	1/1	0.67	0.12	27,27,27,27	0
82	MG	B	1871	1/1	0.67	0.10	11,11,11,11	0
82	MG	AS	3896	1/1	0.67	0.13	42,42,42,42	0
82	MG	AS	3870	1/1	0.67	0.20	54,54,54,54	0
82	MG	1	3658	1/1	0.67	0.11	13,13,13,13	0
82	MG	AS	3817	1/1	0.68	0.10	26,26,26,26	0
82	MG	AR	401	1/1	0.68	0.09	17,17,17,17	0
82	MG	1	3533	1/1	0.68	0.14	46,46,46,46	0
82	MG	AS	3869	1/1	0.68	0.17	67,67,67,67	0
82	MG	1	3763	1/1	0.68	0.14	30,30,30,30	0
82	MG	1	3810	1/1	0.68	0.33	37,37,37,37	0
82	MG	AS	3671	1/1	0.68	0.58	41,41,41,41	0
82	MG	1	3947	1/1	0.68	0.12	58,58,58,58	0
82	MG	1	3883	1/1	0.68	0.12	12,12,12,12	0
82	MG	1	3706	1/1	0.68	0.19	25,25,25,25	0
83	PAR	1	3466	42/42	0.68	0.11	43,75,94,96	0
82	MG	1	3679	1/1	0.68	0.17	42,42,42,42	0
82	MG	AS	3926	1/1	0.68	0.13	42,42,42,42	0
82	MG	AS	3815	1/1	0.69	0.10	51,51,51,51	0
82	MG	1	3485	1/1	0.69	0.23	5,5,5,5	0
82	MG	1	3520	1/1	0.69	0.19	33,33,33,33	0
82	MG	1	3527	1/1	0.69	0.13	32,32,32,32	0
82	MG	1	3600	1/1	0.69	0.25	37,37,37,37	0
82	MG	AS	3728	1/1	0.69	0.24	37,37,37,37	0
82	MG	AS	3836	1/1	0.69	0.12	28,28,28,28	0
82	MG	1	3576	1/1	0.69	0.16	43,43,43,43	0
82	MG	AS	3586	1/1	0.69	0.11	36,36,36,36	0
82	MG	AS	3625	1/1	0.69	0.22	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3561	1/1	0.69	0.24	35,35,35,35	0
82	MG	AS	3803	1/1	0.69	0.18	58,58,58,58	0
82	MG	AS	3682	1/1	0.69	0.17	44,44,44,44	0
83	PAR	1	3457	42/42	0.69	0.19	30,63,83,97	0
82	MG	1	3640	1/1	0.69	0.05	7,7,7,7	0
82	MG	1	3944	1/1	0.69	0.26	40,40,40,40	0
82	MG	AS	3601	1/1	0.69	0.15	41,41,41,41	0
82	MG	AS	3606	1/1	0.70	0.11	40,40,40,40	0
82	MG	AS	3687	1/1	0.70	0.17	32,32,32,32	0
82	MG	1	4048	1/1	0.70	0.28	51,51,51,51	0
82	MG	AS	3734	1/1	0.70	0.17	43,43,43,43	0
82	MG	AS	3665	1/1	0.70	0.16	66,66,66,66	0
82	MG	1	3835	1/1	0.70	0.13	34,34,34,34	0
82	MG	1	4056	1/1	0.70	0.19	18,18,18,18	0
82	MG	AS	3673	1/1	0.70	0.22	16,16,16,16	0
83	PAR	1	3460	42/42	0.70	0.18	49,74,88,100	42
82	MG	1	3931	1/1	0.70	0.14	38,38,38,38	0
82	MG	AS	3868	1/1	0.70	0.23	63,63,63,63	0
82	MG	AS	3412	1/1	0.70	0.14	22,22,22,22	0
82	MG	1	3900	1/1	0.71	0.17	20,20,20,20	0
82	MG	AS	3851	1/1	0.71	0.13	25,25,25,25	0
82	MG	AS	3655	1/1	0.71	0.16	33,33,33,33	0
82	MG	AS	3663	1/1	0.71	0.30	45,45,45,45	0
82	MG	1	3777	1/1	0.71	0.09	23,23,23,23	0
82	MG	AS	3419	1/1	0.71	0.12	65,65,65,65	0
82	MG	AS	3771	1/1	0.71	0.22	54,54,54,54	0
82	MG	1	3811	1/1	0.71	0.34	22,22,22,22	0
82	MG	AS	3703	1/1	0.71	0.15	39,39,39,39	0
82	MG	AS	3913	1/1	0.71	0.09	47,47,47,47	0
82	MG	AS	3704	1/1	0.71	0.17	41,41,41,41	0
82	MG	AS	3527	1/1	0.71	0.12	53,53,53,53	0
82	MG	AS	3841	1/1	0.71	0.12	52,52,52,52	0
82	MG	1	4078	1/1	0.71	0.16	53,53,53,53	0
83	PAR	AS	3406	42/42	0.71	0.12	89,116,138,142	0
82	MG	AS	3549	1/1	0.71	0.17	51,51,51,51	0
82	MG	AS	3648	1/1	0.72	0.14	24,24,24,24	0
82	MG	B	1829	1/1	0.72	0.16	25,25,25,25	0
82	MG	B	1850	1/1	0.72	0.18	8,8,8,8	0
82	MG	AS	3823	1/1	0.72	0.12	65,65,65,65	0
82	MG	AS	3900	1/1	0.72	0.11	15,15,15,15	0
82	MG	AS	3472	1/1	0.72	0.37	16,16,16,16	0
82	MG	1	3468	1/1	0.72	0.16	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3920	1/1	0.72	0.09	30,30,30,30	0
82	MG	1	3729	1/1	0.72	0.20	27,27,27,27	0
82	MG	1	3525	1/1	0.72	0.20	21,21,21,21	0
82	MG	AS	3916	1/1	0.72	0.15	33,33,33,33	0
82	MG	1	3834	1/1	0.72	0.15	37,37,37,37	0
82	MG	AS	3753	1/1	0.72	0.08	11,11,11,11	0
82	MG	1	4071	1/1	0.72	0.09	25,25,25,25	0
82	MG	1	3934	1/1	0.72	0.24	31,31,31,31	0
82	MG	1	3548	1/1	0.72	0.14	20,20,20,20	0
82	MG	1	3885	1/1	0.72	0.21	40,40,40,40	0
82	MG	1	3554	1/1	0.72	0.15	29,29,29,29	0
82	MG	AS	3415	1/1	0.72	0.17	56,56,56,56	0
82	MG	AT	202	1/1	0.72	0.10	26,26,26,26	0
82	MG	AS	3622	1/1	0.72	0.17	48,48,48,48	0
82	MG	AS	3867	1/1	0.72	0.25	43,43,43,43	0
82	MG	AS	3773	1/1	0.72	0.31	40,40,40,40	0
82	MG	1	3415	1/1	0.72	0.19	16,16,16,16	0
82	MG	AS	3569	1/1	0.72	0.11	119,119,119,119	0
82	MG	1	3529	1/1	0.72	0.08	9,9,9,9	0
82	MG	AS	3710	1/1	0.72	0.13	44,44,44,44	0
82	MG	AS	3572	1/1	0.72	0.11	51,51,51,51	0
83	PAR	1	3461	42/42	0.72	0.13	76,95,111,114	0
82	MG	AS	3880	1/1	0.72	0.20	58,58,58,58	0
82	MG	1	3445	1/1	0.72	0.24	26,26,26,26	0
82	MG	1	3826	1/1	0.72	0.17	14,14,14,14	0
82	MG	1	3712	1/1	0.72	0.33	16,16,16,16	0
82	MG	AS	3816	1/1	0.73	0.23	14,14,14,14	0
82	MG	AS	3649	1/1	0.73	0.08	17,17,17,17	0
82	MG	AS	3435	1/1	0.73	0.12	50,50,50,50	0
82	MG	1	3886	1/1	0.73	0.20	31,31,31,31	0
82	MG	B	1820	1/1	0.73	0.17	17,17,17,17	0
82	MG	1	3414	1/1	0.73	0.09	14,14,14,14	0
82	MG	B	1836	1/1	0.73	0.11	20,20,20,20	0
82	MG	AS	3740	1/1	0.73	0.12	15,15,15,15	0
82	MG	AS	3838	1/1	0.73	0.11	18,18,18,18	0
82	MG	AS	3594	1/1	0.73	0.21	44,44,44,44	0
82	MG	1	3847	1/1	0.73	0.16	14,14,14,14	0
82	MG	1	3853	1/1	0.73	0.22	30,30,30,30	0
82	MG	1	3779	1/1	0.73	0.13	12,12,12,12	0
82	MG	AS	3518	1/1	0.73	0.16	71,71,71,71	0
82	MG	1	3955	1/1	0.73	0.15	22,22,22,22	0
82	MG	1	3783	1/1	0.73	0.19	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3962	1/1	0.73	0.13	46,46,46,46	0
82	MG	1	3598	1/1	0.73	0.15	23,23,23,23	0
82	MG	1	3807	1/1	0.73	0.13	23,23,23,23	0
82	MG	1	3863	1/1	0.73	0.14	12,12,12,12	0
82	MG	1	4079	1/1	0.73	0.12	68,68,68,68	0
82	MG	AS	3780	1/1	0.73	0.10	17,17,17,17	0
82	MG	AS	3707	1/1	0.73	0.18	47,47,47,47	0
82	MG	o	302	1/1	0.73	0.18	73,73,73,73	0
82	MG	AS	3800	1/1	0.73	0.16	29,29,29,29	0
82	MG	AS	3878	1/1	0.73	0.18	33,33,33,33	0
82	MG	1	3667	1/1	0.73	0.32	37,37,37,37	0
82	MG	1	3929	1/1	0.73	0.18	16,16,16,16	0
82	MG	1	3809	1/1	0.73	0.13	27,27,27,27	0
83	PAR	AS	3402	42/42	0.73	0.16	84,103,121,128	42
82	MG	1	3605	1/1	0.73	0.27	19,19,19,19	0
82	MG	1	3722	1/1	0.73	0.13	31,31,31,31	0
82	MG	1	3820	1/1	0.73	0.14	24,24,24,24	0
82	MG	AS	3556	1/1	0.74	0.15	41,41,41,41	0
82	MG	B	1860	1/1	0.74	0.17	24,24,24,24	0
82	MG	AS	3943	1/1	0.74	0.17	22,22,22,22	0
82	MG	1	3758	1/1	0.74	0.13	26,26,26,26	0
82	MG	AS	3416	1/1	0.74	0.20	111,111,111,111	0
82	MG	AS	3595	1/1	0.74	0.12	38,38,38,38	0
82	MG	k	401	1/1	0.74	0.15	15,15,15,15	0
82	MG	1	3952	1/1	0.74	0.15	12,12,12,12	0
82	MG	AS	3677	1/1	0.74	0.14	30,30,30,30	0
82	MG	B	1804	1/1	0.74	0.15	14,14,14,14	0
82	MG	AS	3911	1/1	0.74	0.10	31,31,31,31	0
82	MG	1	3639	1/1	0.74	0.13	28,28,28,28	0
82	MG	B	1827	1/1	0.74	0.15	4,4,4,4	0
82	MG	1	3519	1/1	0.74	0.29	24,24,24,24	0
82	MG	AS	3690	1/1	0.74	0.16	44,44,44,44	0
82	MG	1	3996	1/1	0.74	0.19	28,28,28,28	0
82	MG	AS	3699	1/1	0.74	0.30	35,35,35,35	0
82	MG	1	3999	1/1	0.74	0.17	32,32,32,32	0
82	MG	AS	3661	1/1	0.74	0.17	27,27,27,27	0
82	MG	1	4081	1/1	0.75	0.12	17,17,17,17	0
82	MG	AS	3917	1/1	0.75	0.12	28,28,28,28	0
82	MG	AS	3658	1/1	0.75	0.17	5,5,5,5	0
82	MG	AS	3575	1/1	0.75	0.10	18,18,18,18	0
82	MG	AS	3628	1/1	0.75	0.13	29,29,29,29	0
82	MG	AS	3600	1/1	0.75	0.22	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	4085	1/1	0.75	0.14	33,33,33,33	0
82	MG	AS	3666	1/1	0.75	0.29	32,32,32,32	0
82	MG	4	203	1/1	0.75	0.11	11,11,11,11	0
82	MG	AS	3884	1/1	0.75	0.08	30,30,30,30	0
82	MG	AS	3888	1/1	0.75	0.15	45,45,45,45	0
82	MG	AS	3890	1/1	0.75	0.17	59,59,59,59	0
82	MG	AS	3794	1/1	0.75	0.22	39,39,39,39	0
82	MG	1	3860	1/1	0.75	0.16	37,37,37,37	0
82	MG	AS	3743	1/1	0.75	0.32	12,12,12,12	0
82	MG	AS	3747	1/1	0.75	0.24	35,35,35,35	0
82	MG	AS	3804	1/1	0.75	0.12	39,39,39,39	0
82	MG	AS	3563	1/1	0.75	0.26	75,75,75,75	0
82	MG	AS	3856	1/1	0.75	0.07	23,23,23,23	0
82	MG	1	3784	1/1	0.75	0.19	14,14,14,14	0
82	MG	1	3546	1/1	0.75	0.13	39,39,39,39	0
83	PAR	1	3465	42/42	0.75	0.16	50,82,98,106	0
82	MG	AS	3542	1/1	0.75	0.36	51,51,51,51	0
83	PAR	B	1803	42/42	0.75	0.14	60,88,102,111	0
82	MG	AS	3812	1/1	0.75	0.09	20,20,20,20	0
82	MG	AS	3912	1/1	0.75	0.09	27,27,27,27	0
82	MG	AS	3722	1/1	0.75	0.10	17,17,17,17	0
82	MG	1	3903	1/1	0.75	0.20	35,35,35,35	0
82	MG	1	4057	1/1	0.76	0.18	15,15,15,15	0
82	MG	1	3998	1/1	0.76	0.13	17,17,17,17	0
82	MG	AS	3833	1/1	0.76	0.15	55,55,55,55	0
82	MG	AS	3610	1/1	0.76	0.15	92,92,92,92	0
82	MG	AS	3940	1/1	0.76	0.18	43,43,43,43	0
82	MG	1	3759	1/1	0.76	0.13	27,27,27,27	0
82	MG	1	3637	1/1	0.76	0.28	32,32,32,32	0
82	MG	AS	3946	1/1	0.76	0.11	15,15,15,15	0
82	MG	1	3528	1/1	0.76	0.13	30,30,30,30	0
82	MG	AS	3511	1/1	0.76	0.18	75,75,75,75	0
82	MG	AS	3513	1/1	0.76	0.10	42,42,42,42	0
82	MG	AS	3795	1/1	0.76	0.08	46,46,46,46	0
82	MG	1	4031	1/1	0.76	0.15	17,17,17,17	0
82	MG	1	3880	1/1	0.76	0.24	30,30,30,30	0
82	MG	BJ	301	1/1	0.76	0.35	51,51,51,51	0
82	MG	1	3914	1/1	0.76	0.10	52,52,52,52	0
82	MG	B	1807	1/1	0.76	0.30	13,13,13,13	0
82	MG	1	3413	1/1	0.76	0.15	5,5,5,5	0
82	MG	1	3675	1/1	0.76	0.11	41,41,41,41	0
82	MG	1	3588	1/1	0.76	0.10	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3678	1/1	0.76	0.24	21,21,21,21	0
82	MG	AS	3553	1/1	0.76	0.14	61,61,61,61	0
83	PAR	B	1801	42/42	0.76	0.18	49,65,83,104	0
82	MG	1	4086	1/1	0.76	0.16	17,17,17,17	0
82	MG	1	3921	1/1	0.76	0.15	27,27,27,27	0
82	MG	1	4053	1/1	0.76	0.16	40,40,40,40	0
82	MG	1	3894	1/1	0.76	0.15	26,26,26,26	0
82	MG	AS	3662	1/1	0.76	0.10	32,32,32,32	0
82	MG	AS	3577	1/1	0.77	0.21	68,68,68,68	1
82	MG	1	3512	1/1	0.77	0.14	24,24,24,24	0
82	MG	1	4032	1/1	0.77	0.11	8,8,8,8	0
82	MG	AS	3417	1/1	0.77	0.16	53,53,53,53	0
82	MG	1	3583	1/1	0.77	0.09	35,35,35,35	0
82	MG	1	3473	1/1	0.77	0.34	9,9,9,9	0
82	MG	AS	3738	1/1	0.77	0.12	48,48,48,48	0
82	MG	1	3850	1/1	0.77	0.08	16,16,16,16	0
82	MG	AS	3686	1/1	0.77	0.10	35,35,35,35	0
82	MG	AS	3636	1/1	0.77	0.18	45,45,45,45	0
82	MG	AS	3744	1/1	0.77	0.13	47,47,47,47	0
82	MG	B	1866	1/1	0.77	0.43	21,21,21,21	0
82	MG	AS	3818	1/1	0.77	0.31	17,17,17,17	0
82	MG	AS	3887	1/1	0.77	0.17	10,10,10,10	0
82	MG	1	3665	1/1	0.77	0.14	30,30,30,30	0
82	MG	AS	3428	1/1	0.77	0.18	17,17,17,17	0
82	MG	AS	3697	1/1	0.77	0.15	32,32,32,32	0
82	MG	1	4073	1/1	0.77	0.34	33,33,33,33	0
82	MG	AS	3760	1/1	0.77	0.13	6,6,6,6	0
82	MG	1	3699	1/1	0.77	0.17	26,26,26,26	0
82	MG	AS	3465	1/1	0.77	0.19	35,35,35,35	0
82	MG	AK	102	1/1	0.77	0.07	11,11,11,11	0
82	MG	1	3877	1/1	0.77	0.15	22,22,22,22	0
82	MG	AS	3659	1/1	0.77	0.17	46,46,46,46	0
82	MG	1	3405	1/1	0.77	0.20	14,14,14,14	0
82	MG	AS	3607	1/1	0.77	0.09	20,20,20,20	0
83	PAR	B	1802	42/42	0.77	0.15	63,92,109,117	0
82	MG	1	3882	1/1	0.77	0.33	39,39,39,39	0
82	MG	1	3469	1/1	0.77	0.16	28,28,28,28	0
82	MG	B	1811	1/1	0.77	0.17	5,5,5,5	0
82	MG	AS	3725	1/1	0.77	0.12	14,14,14,14	0
82	MG	1	3940	1/1	0.77	0.12	30,30,30,30	0
82	MG	AS	3783	1/1	0.78	0.17	63,63,63,63	0
82	MG	B	1857	1/1	0.78	0.15	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3560	1/1	0.78	0.18	8,8,8,8	0
82	MG	AS	3885	1/1	0.78	0.16	18,18,18,18	0
82	MG	1	3986	1/1	0.78	0.12	18,18,18,18	0
82	MG	AS	3840	1/1	0.78	0.13	30,30,30,30	0
82	MG	AS	3590	1/1	0.78	0.14	41,41,41,41	0
82	MG	1	3778	1/1	0.78	0.10	50,50,50,50	0
82	MG	AS	3802	1/1	0.78	0.07	15,15,15,15	0
82	MG	1	4034	1/1	0.78	0.19	14,14,14,14	0
82	MG	AS	3846	1/1	0.78	0.17	46,46,46,46	0
82	MG	AS	3492	1/1	0.78	0.15	51,51,51,51	0
82	MG	1	3503	1/1	0.78	0.32	34,34,34,34	0
82	MG	AS	3855	1/1	0.78	0.32	20,20,20,20	0
82	MG	1	4038	1/1	0.78	0.13	29,29,29,29	0
82	MG	CM	1816	1/1	0.78	0.10	45,45,45,45	0
83	PAR	1	3456	42/42	0.78	0.12	54,79,95,95	0
82	MG	1	3756	1/1	0.78	0.14	31,31,31,31	0
83	PAR	1	3459	42/42	0.78	0.20	42,69,104,117	0
82	MG	AS	3810	1/1	0.78	0.14	29,29,29,29	0
82	MG	1	3859	1/1	0.78	0.09	41,41,41,41	0
82	MG	1	4083	1/1	0.78	0.47	50,50,50,50	0
82	MG	AS	3727	1/1	0.78	0.18	12,12,12,12	0
82	MG	AS	3520	1/1	0.78	0.12	39,39,39,39	0
82	MG	1	3776	1/1	0.78	0.06	18,18,18,18	0
82	MG	AS	3445	1/1	0.78	0.12	22,22,22,22	0
82	MG	AS	3456	1/1	0.78	0.11	29,29,29,29	0
82	MG	AS	3538	1/1	0.78	0.07	20,20,20,20	0
82	MG	B	1853	1/1	0.78	0.11	26,26,26,26	0
82	MG	AS	3698	1/1	0.78	0.26	37,37,37,37	0
82	MG	AS	3540	1/1	0.79	0.15	9,9,9,9	0
82	MG	AS	3541	1/1	0.79	0.08	12,12,12,12	0
82	MG	F	301	1/1	0.79	0.10	35,35,35,35	0
82	MG	R	201	1/1	0.79	0.22	45,45,45,45	0
82	MG	AS	3548	1/1	0.79	0.22	44,44,44,44	0
82	MG	AS	3448	1/1	0.79	0.11	51,51,51,51	0
82	MG	1	3545	1/1	0.79	0.13	34,34,34,34	0
82	MG	AS	3796	1/1	0.79	0.08	10,10,10,10	0
82	MG	1	3819	1/1	0.79	0.17	20,20,20,20	0
82	MG	B	1812	1/1	0.79	0.13	8,8,8,8	0
82	MG	1	3594	1/1	0.79	0.20	31,31,31,31	0
82	MG	AS	3866	1/1	0.79	0.25	67,67,67,67	0
82	MG	B	1825	1/1	0.79	0.18	17,17,17,17	0
82	MG	1	3964	1/1	0.79	0.08	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3569	1/1	0.79	0.46	38,38,38,38	0
82	MG	AS	3487	1/1	0.79	0.10	12,12,12,12	0
82	MG	1	3674	1/1	0.79	0.12	9,9,9,9	0
82	MG	1	3942	1/1	0.79	0.06	37,37,37,37	0
82	MG	1	3983	1/1	0.79	0.33	27,27,27,27	0
82	MG	1	3862	1/1	0.79	0.16	11,11,11,11	0
82	MG	1	3650	1/1	0.79	0.17	17,17,17,17	0
82	MG	1	3635	1/1	0.79	0.09	17,17,17,17	0
82	MG	BQ	201	1/1	0.79	0.08	12,12,12,12	0
82	MG	AS	3745	1/1	0.79	0.12	17,17,17,17	0
82	MG	1	3719	1/1	0.79	0.12	7,7,7,7	0
82	MG	AS	3886	1/1	0.79	0.17	25,25,25,25	0
82	MG	AS	3692	1/1	0.79	0.14	38,38,38,38	0
82	MG	AS	3693	1/1	0.79	0.16	40,40,40,40	0
82	MG	AS	3638	1/1	0.79	0.17	36,36,36,36	0
82	MG	AS	3827	1/1	0.79	0.19	80,80,80,80	0
82	MG	AS	3829	1/1	0.79	0.08	28,28,28,28	0
82	MG	AS	3696	1/1	0.79	0.13	26,26,26,26	0
82	MG	AS	3832	1/1	0.79	0.15	33,33,33,33	0
82	MG	AS	3425	1/1	0.79	0.17	23,23,23,23	0
82	MG	AS	3641	1/1	0.79	0.23	8,8,8,8	0
82	MG	1	3927	1/1	0.79	0.13	32,32,32,32	0
83	PAR	AS	3401	42/42	0.79	0.18	74,102,111,126	42
82	MG	1	3692	1/1	0.79	0.16	7,7,7,7	0
83	PAR	AS	3403	42/42	0.79	0.16	75,109,128,132	0
82	MG	AS	3537	1/1	0.79	0.14	41,41,41,41	0
82	MG	AS	3432	1/1	0.79	0.11	23,23,23,23	0
82	MG	AS	3650	1/1	0.79	0.09	15,15,15,15	0
82	MG	1	3728	1/1	0.80	0.08	34,34,34,34	0
82	MG	AS	3732	1/1	0.80	0.17	32,32,32,32	0
82	MG	AS	3457	1/1	0.80	0.10	34,34,34,34	0
82	MG	1	3668	1/1	0.80	0.11	23,23,23,23	0
82	MG	1	3452	1/1	0.80	0.10	12,12,12,12	0
82	MG	CB	202	1/1	0.80	0.15	36,36,36,36	0
82	MG	1	3830	1/1	0.80	0.12	13,13,13,13	0
82	MG	1	3681	1/1	0.80	0.17	22,22,22,22	0
82	MG	AS	3675	1/1	0.80	0.17	31,31,31,31	0
82	MG	AS	3920	1/1	0.80	0.18	56,56,56,56	0
82	MG	1	3982	1/1	0.80	0.16	37,37,37,37	0
82	MG	1	3868	1/1	0.80	0.12	23,23,23,23	0
82	MG	AN	102	1/1	0.80	0.10	18,18,18,18	0
82	MG	1	4039	1/1	0.80	0.28	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3936	1/1	0.80	0.12	26,26,26,26	0
83	PAR	4	201	42/42	0.80	0.19	43,75,89,97	0
82	MG	B	1854	1/1	0.80	0.23	22,22,22,22	0
82	MG	AS	3894	1/1	0.80	0.06	7,7,7,7	0
82	MG	AS	3551	1/1	0.80	0.18	51,51,51,51	0
82	MG	1	4002	1/1	0.80	0.23	40,40,40,40	0
82	MG	AS	3441	1/1	0.80	0.15	21,21,21,21	0
82	MG	1	3633	1/1	0.80	0.12	13,13,13,13	0
82	MG	1	3985	1/1	0.80	0.23	4,4,4,4	0
82	MG	AS	3453	1/1	0.80	0.25	7,7,7,7	0
82	MG	AS	3807	1/1	0.80	0.08	44,44,44,44	0
82	MG	B	1810	1/1	0.81	0.13	11,11,11,11	0
82	MG	1	3557	1/1	0.81	0.15	10,10,10,10	0
82	MG	1	3705	1/1	0.81	0.10	21,21,21,21	0
82	MG	Y	203	1/1	0.81	0.17	33,33,33,33	0
82	MG	o	301	1/1	0.81	0.28	16,16,16,16	0
82	MG	AS	3440	1/1	0.81	0.16	12,12,12,12	0
82	MG	AS	3660	1/1	0.81	0.21	48,48,48,48	0
82	MG	AZ	301	1/1	0.81	0.19	60,60,60,60	0
82	MG	1	3590	1/1	0.81	0.14	19,19,19,19	0
82	MG	1	3898	1/1	0.81	0.16	39,39,39,39	0
82	MG	AS	3750	1/1	0.81	0.20	22,22,22,22	0
82	MG	1	3738	1/1	0.81	0.28	11,11,11,11	0
82	MG	1	3660	1/1	0.81	0.14	41,41,41,41	0
82	MG	AS	3578	1/1	0.81	0.10	37,37,37,37	0
82	MG	CM	1805	1/1	0.81	0.22	7,7,7,7	0
82	MG	CM	1807	1/1	0.81	0.17	20,20,20,20	0
82	MG	AS	3910	1/1	0.81	0.09	26,26,26,26	0
82	MG	AS	3529	1/1	0.81	0.14	34,34,34,34	0
82	MG	1	3873	1/1	0.81	0.25	19,19,19,19	0
82	MG	1	3440	1/1	0.81	0.10	15,15,15,15	0
82	MG	1	4025	1/1	0.81	0.16	35,35,35,35	0
82	MG	AS	3464	1/1	0.81	0.20	30,30,30,30	0
82	MG	1	3447	1/1	0.81	0.11	16,16,16,16	0
82	MG	B	1859	1/1	0.81	0.23	16,16,16,16	0
82	MG	1	3939	1/1	0.81	0.13	21,21,21,21	0
82	MG	1	3612	1/1	0.81	0.07	15,15,15,15	0
82	MG	AS	3923	1/1	0.81	0.11	16,16,16,16	0
82	MG	AS	3778	1/1	0.81	0.12	23,23,23,23	0
82	MG	AS	3683	1/1	0.81	0.08	23,23,23,23	0
82	MG	1	3696	1/1	0.81	0.21	33,33,33,33	0
82	MG	AS	3781	1/1	0.81	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3521	1/1	0.81	0.09	18,18,18,18	0
82	MG	AS	3491	1/1	0.81	0.17	7,7,7,7	0
84	3K5	AS	3405	57/57	0.81	0.21	83,102,131,138	0
82	MG	AS	3689	1/1	0.81	0.13	47,47,47,47	0
82	MG	1	3895	1/1	0.82	0.20	29,29,29,29	0
82	MG	1	3896	1/1	0.82	0.36	23,23,23,23	0
82	MG	1	3565	1/1	0.82	0.27	10,10,10,10	0
82	MG	AS	3939	1/1	0.82	0.18	35,35,35,35	0
82	MG	1	3492	1/1	0.82	0.22	8,8,8,8	0
82	MG	AS	3640	1/1	0.82	0.09	32,32,32,32	0
82	MG	AS	3535	1/1	0.82	0.14	9,9,9,9	0
82	MG	AS	3881	1/1	0.82	0.18	12,12,12,12	0
82	MG	AS	3820	1/1	0.82	0.11	75,75,75,75	0
82	MG	1	3617	1/1	0.82	0.09	33,33,33,33	0
82	MG	AS	3589	1/1	0.82	0.19	65,65,65,65	0
82	MG	AS	3646	1/1	0.82	0.09	21,21,21,21	0
82	MG	1	3638	1/1	0.82	0.20	6,6,6,6	0
82	MG	1	4092	1/1	0.82	0.18	24,24,24,24	0
82	MG	1	3848	1/1	0.82	0.16	48,48,48,48	0
82	MG	j	301	1/1	0.82	0.14	8,8,8,8	0
82	MG	1	3736	1/1	0.82	0.22	58,58,58,58	0
82	MG	1	3523	1/1	0.82	0.13	12,12,12,12	0
82	MG	AS	3468	1/1	0.82	0.17	35,35,35,35	0
82	MG	1	3401	1/1	0.82	0.14	5,5,5,5	0
82	MG	v	301	1/1	0.82	0.13	13,13,13,13	0
82	MG	AS	3898	1/1	0.82	0.06	23,23,23,23	0
82	MG	1	3647	1/1	0.82	0.09	11,11,11,11	0
82	MG	CM	1819	1/1	0.82	0.27	63,63,63,63	0
82	MG	AS	3479	1/1	0.82	0.12	37,37,37,37	0
82	MG	AS	3724	1/1	0.82	0.19	27,27,27,27	0
82	MG	AS	3608	1/1	0.82	0.12	14,14,14,14	0
82	MG	AS	3483	1/1	0.82	0.15	28,28,28,28	0
82	MG	1	3547	1/1	0.82	0.10	18,18,18,18	0
82	MG	1	3432	1/1	0.82	0.15	16,16,16,16	0
82	MG	1	3720	1/1	0.82	0.17	31,31,31,31	0
82	MG	B	1862	1/1	0.82	0.19	16,16,16,16	0
82	MG	AS	3914	1/1	0.82	0.09	23,23,23,23	0
82	MG	AS	3618	1/1	0.82	0.08	36,36,36,36	0
82	MG	1	3888	1/1	0.82	0.12	25,25,25,25	0
82	MG	AS	3624	1/1	0.82	0.10	38,38,38,38	0
82	MG	1	4035	1/1	0.82	0.19	6,6,6,6	0
82	MG	AS	3865	1/1	0.82	0.17	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3563	1/1	0.82	0.29	8,8,8,8	0
82	MG	AS	3630	1/1	0.82	0.15	33,33,33,33	0
82	MG	AS	3433	1/1	0.82	0.16	16,16,16,16	0
82	MG	1	3727	1/1	0.82	0.11	52,52,52,52	0
85	ZN	DS	201	1/1	0.82	0.11	278,278,278,278	0
82	MG	1	3450	1/1	0.83	0.09	20,20,20,20	0
82	MG	1	3615	1/1	0.83	0.10	20,20,20,20	0
82	MG	1	3951	1/1	0.83	0.12	45,45,45,45	0
82	MG	BO	201	1/1	0.83	0.09	38,38,38,38	0
82	MG	AS	3451	1/1	0.83	0.13	7,7,7,7	0
82	MG	AS	3652	1/1	0.83	0.08	32,32,32,32	0
82	MG	1	3572	1/1	0.83	0.11	13,13,13,13	0
82	MG	1	4019	1/1	0.83	0.10	46,46,46,46	0
82	MG	1	3932	1/1	0.83	0.34	60,60,60,60	0
82	MG	AS	3460	1/1	0.83	0.20	38,38,38,38	0
82	MG	CM	1812	1/1	0.83	0.20	20,20,20,20	0
82	MG	1	3575	1/1	0.83	0.10	8,8,8,8	0
82	MG	AS	3882	1/1	0.83	0.18	25,25,25,25	0
82	MG	AS	3919	1/1	0.83	0.07	67,67,67,67	0
82	MG	AS	3462	1/1	0.83	0.19	52,52,52,52	0
83	PAR	1	3458	42/42	0.83	0.17	35,50,61,65	0
82	MG	1	3422	1/1	0.83	0.11	11,11,11,11	0
82	MG	1	4051	1/1	0.83	0.13	7,7,7,7	0
82	MG	1	3818	1/1	0.83	0.16	35,35,35,35	0
83	PAR	1	3464	42/42	0.83	0.16	38,60,76,81	0
82	MG	B	1861	1/1	0.83	0.22	12,12,12,12	0
82	MG	1	3408	1/1	0.83	0.17	13,13,13,13	0
82	MG	AS	3474	1/1	0.83	0.21	10,10,10,10	0
82	MG	1	3765	1/1	0.83	0.12	28,28,28,28	0
82	MG	3	201	1/1	0.83	0.12	28,28,28,28	0
82	MG	AS	3758	1/1	0.83	0.17	44,44,44,44	0
82	MG	B	1809	1/1	0.83	0.20	15,15,15,15	0
82	MG	1	3787	1/1	0.83	0.12	10,10,10,10	0
82	MG	1	3677	1/1	0.83	0.15	32,32,32,32	0
82	MG	AS	3678	1/1	0.83	0.15	37,37,37,37	0
82	MG	1	3797	1/1	0.83	0.10	21,21,21,21	0
82	MG	B	1815	1/1	0.83	0.29	20,20,20,20	0
82	MG	1	3805	1/1	0.83	0.17	24,24,24,24	0
82	MG	AS	3906	1/1	0.83	0.11	26,26,26,26	0
82	MG	1	3794	1/1	0.84	0.07	22,22,22,22	0
82	MG	1	3825	1/1	0.84	0.14	4,4,4,4	0
82	MG	AS	3761	1/1	0.84	0.13	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3904	1/1	0.84	0.06	37,37,37,37	0
82	MG	AS	3519	1/1	0.84	0.22	72,72,72,72	0
82	MG	AS	3863	1/1	0.84	0.23	27,27,27,27	0
82	MG	B	1863	1/1	0.84	0.16	16,16,16,16	0
82	MG	1	3740	1/1	0.84	0.13	22,22,22,22	0
82	MG	1	3544	1/1	0.84	0.14	32,32,32,32	0
82	MG	AS	3769	1/1	0.84	0.15	71,71,71,71	0
82	MG	AS	3821	1/1	0.84	0.08	6,6,6,6	0
82	MG	CM	1808	1/1	0.84	0.20	11,11,11,11	0
82	MG	1	3901	1/1	0.84	0.13	30,30,30,30	0
82	MG	CM	1814	1/1	0.84	0.06	14,14,14,14	0
82	MG	AS	3871	1/1	0.84	0.28	87,87,87,87	0
82	MG	CM	1818	1/1	0.84	0.28	52,52,52,52	0
82	MG	1	3570	1/1	0.84	0.14	18,18,18,18	0
82	MG	B	1824	1/1	0.84	0.10	14,14,14,14	0
82	MG	AS	3427	1/1	0.84	0.15	18,18,18,18	0
82	MG	1	3435	1/1	0.84	0.12	13,13,13,13	0
82	MG	AS	3430	1/1	0.84	0.14	14,14,14,14	0
82	MG	1	3483	1/1	0.84	0.18	9,9,9,9	0
82	MG	AS	3627	1/1	0.84	0.28	82,82,82,82	0
83	PAR	1	3462	42/42	0.84	0.19	50,66,105,114	0
82	MG	1	3966	1/1	0.84	0.15	42,42,42,42	0
82	MG	1	3629	1/1	0.84	0.21	17,17,17,17	0
82	MG	AK	103	1/1	0.84	0.22	15,15,15,15	0
82	MG	AS	3933	1/1	0.84	0.09	49,49,49,49	0
82	MG	1	3556	1/1	0.84	0.22	14,14,14,14	0
82	MG	1	3817	1/1	0.84	0.20	14,14,14,14	0
82	MG	AS	3746	1/1	0.84	0.15	40,40,40,40	0
82	MG	1	3735	1/1	0.84	0.30	12,12,12,12	0
82	MG	AS	3499	1/1	0.84	0.12	21,21,21,21	0
82	MG	1	3614	1/1	0.84	0.11	24,24,24,24	0
82	MG	1	3420	1/1	0.84	0.16	18,18,18,18	0
82	MG	AS	3455	1/1	0.84	0.17	8,8,8,8	0
83	PAR	CM	1803	42/42	0.84	0.24	51,79,99,113	0
82	MG	AS	3854	1/1	0.84	0.09	29,29,29,29	0
82	MG	AS	3755	1/1	0.84	0.14	26,26,26,26	0
82	MG	AS	3720	1/1	0.84	0.18	13,13,13,13	0
82	MG	1	4010	1/1	0.85	0.20	55,55,55,55	0
82	MG	1	3504	1/1	0.85	0.13	14,14,14,14	0
82	MG	AS	3934	1/1	0.85	0.16	40,40,40,40	0
82	MG	AS	3935	1/1	0.85	0.10	34,34,34,34	0
82	MG	AS	3446	1/1	0.85	0.18	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3786	1/1	0.85	0.09	11,11,11,11	0
82	MG	B	1846	1/1	0.85	0.15	17,17,17,17	0
82	MG	1	3732	1/1	0.85	0.14	3,3,3,3	0
82	MG	1	3734	1/1	0.85	0.32	12,12,12,12	0
82	MG	1	3603	1/1	0.85	0.26	16,16,16,16	0
82	MG	1	4080	1/1	0.85	0.10	16,16,16,16	0
82	MG	1	3822	1/1	0.85	0.19	6,6,6,6	0
82	MG	1	3433	1/1	0.85	0.06	5,5,5,5	0
82	MG	1	3960	1/1	0.85	0.08	31,31,31,31	0
82	MG	1	3961	1/1	0.85	0.29	21,21,21,21	0
82	MG	1	3913	1/1	0.85	0.11	10,10,10,10	0
82	MG	1	3643	1/1	0.85	0.15	6,6,6,6	0
82	MG	1	3965	1/1	0.85	0.16	23,23,23,23	0
82	MG	B	1868	1/1	0.85	0.13	5,5,5,5	0
82	MG	1	3915	1/1	0.85	0.11	17,17,17,17	0
82	MG	1	3714	1/1	0.85	0.37	43,43,43,43	0
82	MG	1	3970	1/1	0.85	0.11	24,24,24,24	0
82	MG	Q	201	1/1	0.85	0.35	16,16,16,16	0
82	MG	AS	3587	1/1	0.85	0.12	32,32,32,32	0
82	MG	1	3741	1/1	0.85	0.09	12,12,12,12	0
82	MG	1	3975	1/1	0.85	0.13	29,29,29,29	0
82	MG	w	301	1/1	0.85	0.07	6,6,6,6	0
82	MG	CM	1811	1/1	0.85	0.09	10,10,10,10	0
82	MG	AS	3490	1/1	0.85	0.12	20,20,20,20	0
82	MG	1	3977	1/1	0.85	0.16	18,18,18,18	0
82	MG	1	3866	1/1	0.85	0.10	22,22,22,22	0
82	MG	1	3742	1/1	0.85	0.18	5,5,5,5	0
82	MG	1	3786	1/1	0.85	0.09	20,20,20,20	0
82	MG	CM	1822	1/1	0.85	0.10	19,19,19,19	0
82	MG	1	4041	1/1	0.85	1.37	52,52,52,52	0
82	MG	1	3666	1/1	0.85	0.12	12,12,12,12	0
82	MG	AS	3831	1/1	0.85	0.08	54,54,54,54	0
82	MG	1	3750	1/1	0.85	0.13	17,17,17,17	0
82	MG	1	3876	1/1	0.85	0.08	30,30,30,30	0
82	MG	AS	3754	1/1	0.85	0.13	117,117,117,117	0
82	MG	1	3449	1/1	0.85	0.07	7,7,7,7	0
82	MG	AS	3837	1/1	0.85	0.07	23,23,23,23	0
82	MG	1	3795	1/1	0.85	0.20	23,23,23,23	0
82	MG	1	3648	1/1	0.85	0.12	13,13,13,13	0
82	MG	AS	3522	1/1	0.85	0.10	17,17,17,17	0
82	MG	1	3526	1/1	0.85	0.24	26,26,26,26	0
82	MG	1	4054	1/1	0.85	0.15	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3841	1/1	0.85	0.12	11,11,11,11	0
82	MG	1	3843	1/1	0.85	0.13	15,15,15,15	0
82	MG	AS	3850	1/1	0.85	0.18	23,23,23,23	0
82	MG	1	3757	1/1	0.85	0.10	35,35,35,35	0
82	MG	1	3652	1/1	0.85	0.21	15,15,15,15	0
82	MG	B	1818	1/1	0.85	0.15	6,6,6,6	0
82	MG	1	3564	1/1	0.85	0.29	17,17,17,17	0
82	MG	1	4062	1/1	0.85	0.08	16,16,16,16	0
82	MG	1	3438	1/1	0.85	0.17	28,28,28,28	0
82	MG	1	3451	1/1	0.85	0.09	8,8,8,8	0
82	MG	1	4095	1/1	0.86	0.14	34,34,34,34	0
82	MG	1	3580	1/1	0.86	0.15	36,36,36,36	0
82	MG	1	3806	1/1	0.86	0.08	18,18,18,18	0
82	MG	1	3490	1/1	0.86	0.29	9,9,9,9	0
82	MG	1	3953	1/1	0.86	0.24	14,14,14,14	0
82	MG	1	3838	1/1	0.86	0.10	55,55,55,55	0
82	MG	AS	3593	1/1	0.86	0.10	53,53,53,53	0
82	MG	1	3958	1/1	0.86	0.15	18,18,18,18	0
82	MG	AS	3437	1/1	0.86	0.15	19,19,19,19	0
82	MG	1	3491	1/1	0.86	0.40	17,17,17,17	0
82	MG	1	3702	1/1	0.86	0.12	7,7,7,7	0
82	MG	1	3540	1/1	0.86	0.08	17,17,17,17	0
82	MG	B	1865	1/1	0.86	0.08	30,30,30,30	0
82	MG	AS	3670	1/1	0.86	0.15	31,31,31,31	0
82	MG	AS	3531	1/1	0.86	0.17	72,72,72,72	0
82	MG	1	3412	1/1	0.86	0.09	17,17,17,17	0
82	MG	1	3812	1/1	0.86	0.28	9,9,9,9	0
82	MG	AS	3674	1/1	0.86	0.07	21,21,21,21	0
82	MG	1	3493	1/1	0.86	0.11	11,11,11,11	0
82	MG	AS	3454	1/1	0.86	0.31	17,17,17,17	0
82	MG	1	3711	1/1	0.86	0.11	15,15,15,15	0
82	MG	CM	1806	1/1	0.86	0.16	19,19,19,19	0
82	MG	1	3928	1/1	0.86	0.12	30,30,30,30	0
82	MG	AS	3828	1/1	0.86	0.16	43,43,43,43	0
82	MG	1	4018	1/1	0.86	0.09	37,37,37,37	0
82	MG	AS	3614	1/1	0.86	0.14	45,45,45,45	0
82	MG	1	3431	1/1	0.86	0.11	13,13,13,13	0
82	MG	CM	1815	1/1	0.86	0.28	28,28,28,28	0
82	MG	AS	3684	1/1	0.86	0.07	14,14,14,14	0
82	MG	1	3972	1/1	0.86	0.13	8,8,8,8	0
82	MG	1	3478	1/1	0.86	0.31	15,15,15,15	0
82	MG	AS	3757	1/1	0.86	0.07	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	4066	1/1	0.86	0.07	19,19,19,19	0
82	MG	AS	3907	1/1	0.86	0.13	48,48,48,48	0
82	MG	1	3510	1/1	0.86	0.08	9,9,9,9	0
82	MG	AS	3839	1/1	0.86	0.08	31,31,31,31	0
82	MG	1	3823	1/1	0.86	0.13	11,11,11,11	0
82	MG	1	4075	1/1	0.86	0.07	11,11,11,11	0
82	MG	AS	3629	1/1	0.86	0.16	17,17,17,17	0
82	MG	AS	3562	1/1	0.86	0.23	52,52,52,52	0
82	MG	1	3749	1/1	0.86	0.11	4,4,4,4	0
82	MG	1	4077	1/1	0.86	0.09	16,16,16,16	0
82	MG	1	3549	1/1	0.86	0.14	17,17,17,17	0
82	MG	1	3467	1/1	0.86	0.27	8,8,8,8	0
82	MG	1	3446	1/1	0.86	0.13	12,12,12,12	0
82	MG	1	3604	1/1	0.86	0.13	17,17,17,17	0
82	MG	1	3514	1/1	0.86	0.11	10,10,10,10	0
82	MG	1	3607	1/1	0.86	0.11	22,22,22,22	0
82	MG	1	3907	1/1	0.86	0.20	20,20,20,20	0
82	MG	AS	3709	1/1	0.86	0.11	10,10,10,10	0
82	MG	1	3910	1/1	0.86	0.10	6,6,6,6	0
82	MG	AS	3496	1/1	0.86	0.23	35,35,35,35	0
84	3K5	1	3463	57/57	0.86	0.23	47,66,95,131	0
82	MG	B	1838	1/1	0.86	0.10	19,19,19,19	0
82	MG	AS	3503	1/1	0.86	0.12	22,22,22,22	0
82	MG	AS	3721	1/1	0.86	0.11	19,19,19,19	0
82	MG	1	4070	1/1	0.87	0.17	8,8,8,8	0
82	MG	1	3421	1/1	0.87	0.04	7,7,7,7	0
82	MG	AS	3517	1/1	0.87	0.16	49,49,49,49	0
82	MG	1	3621	1/1	0.87	0.16	28,28,28,28	0
82	MG	AS	3759	1/1	0.87	0.14	15,15,15,15	0
82	MG	1	3846	1/1	0.87	0.22	16,16,16,16	0
82	MG	1	3926	1/1	0.87	0.21	25,25,25,25	0
82	MG	1	4027	1/1	0.87	0.11	11,11,11,11	0
82	MG	1	3684	1/1	0.87	0.29	7,7,7,7	0
82	MG	1	3717	1/1	0.87	0.16	21,21,21,21	0
82	MG	B	1830	1/1	0.87	0.21	18,18,18,18	0
82	MG	1	3584	1/1	0.87	0.09	7,7,7,7	0
82	MG	1	3930	1/1	0.87	0.20	19,19,19,19	0
82	MG	AS	3533	1/1	0.87	0.13	14,14,14,14	0
82	MG	AS	3862	1/1	0.87	0.26	27,27,27,27	0
82	MG	AS	3691	1/1	0.87	0.08	16,16,16,16	0
82	MG	AS	3864	1/1	0.87	0.17	34,34,34,34	0
82	MG	AT	201	1/1	0.87	0.22	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3534	1/1	0.87	0.05	11,11,11,11	0
82	MG	AS	3615	1/1	0.87	0.07	35,35,35,35	0
82	MG	1	3568	1/1	0.87	0.24	11,11,11,11	0
82	MG	1	3892	1/1	0.87	0.11	23,23,23,23	0
82	MG	AS	3619	1/1	0.87	0.09	20,20,20,20	0
82	MG	BB	302	1/1	0.87	0.27	17,17,17,17	0
82	MG	1	3746	1/1	0.87	0.15	17,17,17,17	0
82	MG	1	3558	1/1	0.87	0.14	19,19,19,19	0
82	MG	B	1855	1/1	0.87	0.20	20,20,20,20	0
82	MG	1	4037	1/1	0.87	0.27	5,5,5,5	0
82	MG	1	3721	1/1	0.87	0.08	11,11,11,11	0
82	MG	AS	3705	1/1	0.87	0.24	30,30,30,30	0
82	MG	AS	3545	1/1	0.87	0.07	28,28,28,28	0
82	MG	AS	3547	1/1	0.87	0.16	58,58,58,58	0
82	MG	1	3691	1/1	0.87	0.09	13,13,13,13	0
82	MG	1	3753	1/1	0.87	0.25	7,7,7,7	0
82	MG	1	3482	1/1	0.87	0.21	8,8,8,8	0
82	MG	1	3993	1/1	0.87	0.11	35,35,35,35	0
82	MG	1	3542	1/1	0.87	0.13	7,7,7,7	0
82	MG	1	3501	1/1	0.87	0.20	11,11,11,11	0
82	MG	1	3904	1/1	0.87	0.14	62,62,62,62	0
82	MG	x	201	1/1	0.87	0.19	8,8,8,8	0
82	MG	y	201	1/1	0.87	0.14	14,14,14,14	0
82	MG	B	1872	1/1	0.87	0.18	41,41,41,41	0
82	MG	1	3905	1/1	0.87	0.11	13,13,13,13	0
82	MG	1	3906	1/1	0.87	0.12	30,30,30,30	0
82	MG	1	3803	1/1	0.87	0.15	36,36,36,36	0
82	MG	AS	3819	1/1	0.87	0.25	46,46,46,46	0
82	MG	AB	202	1/1	0.87	0.11	9,9,9,9	0
82	MG	Y	202	1/1	0.87	0.12	22,22,22,22	0
82	MG	AS	3477	1/1	0.87	0.22	10,10,10,10	0
82	MG	AS	3901	1/1	0.87	0.08	17,17,17,17	0
82	MG	1	3804	1/1	0.87	0.21	17,17,17,17	0
82	MG	AS	3656	1/1	0.87	0.11	21,21,21,21	0
82	MG	AS	3905	1/1	0.87	0.14	48,48,48,48	0
82	MG	AS	3579	1/1	0.87	0.09	23,23,23,23	0
82	MG	1	3407	1/1	0.87	0.18	12,12,12,12	0
82	MG	1	3536	1/1	0.87	0.20	13,13,13,13	0
82	MG	AS	3583	1/1	0.87	0.12	38,38,38,38	0
82	MG	1	3581	1/1	0.87	0.15	13,13,13,13	0
82	MG	1	4059	1/1	0.87	0.15	16,16,16,16	0
82	MG	1	3761	1/1	0.87	0.26	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	3875	1/1	0.87	0.14	16,16,16,16	0
82	MG	1	3661	1/1	0.87	0.12	9,9,9,9	0
82	MG	1	3918	1/1	0.87	0.19	27,27,27,27	0
82	MG	AS	3502	1/1	0.87	0.07	22,22,22,22	0
82	MG	1	3963	1/1	0.87	0.15	27,27,27,27	0
82	MG	1	3663	1/1	0.87	0.17	23,23,23,23	0
85	ZN	CJ	201	1/1	0.87	0.09	224,224,224,224	0
82	MG	1	4069	1/1	0.87	0.21	20,20,20,20	0
82	MG	AS	3452	1/1	0.88	0.13	29,29,29,29	0
82	MG	1	3780	1/1	0.88	0.08	4,4,4,4	0
82	MG	1	3628	1/1	0.88	0.14	23,23,23,23	0
82	MG	1	3402	1/1	0.88	0.27	16,16,16,16	0
82	MG	AS	3941	1/1	0.88	0.48	38,38,38,38	0
82	MG	AS	3525	1/1	0.88	0.10	12,12,12,12	0
82	MG	1	3698	1/1	0.88	0.23	18,18,18,18	0
82	MG	AS	3528	1/1	0.88	0.18	14,14,14,14	0
82	MG	1	3507	1/1	0.88	0.30	20,20,20,20	0
82	MG	AS	3458	1/1	0.88	0.23	20,20,20,20	0
82	MG	AS	3876	1/1	0.88	0.07	19,19,19,19	0
82	MG	AS	3599	1/1	0.88	0.15	23,23,23,23	0
82	MG	1	4067	1/1	0.88	0.16	15,15,15,15	0
82	MG	1	3941	1/1	0.88	0.12	69,69,69,69	0
82	MG	AS	3667	1/1	0.88	0.15	26,26,26,26	0
82	MG	1	3494	1/1	0.88	0.13	16,16,16,16	0
82	MG	1	3726	1/1	0.88	0.19	8,8,8,8	0
82	MG	1	4072	1/1	0.88	0.10	33,33,33,33	0
82	MG	AS	3539	1/1	0.88	0.07	16,16,16,16	0
82	MG	1	3499	1/1	0.88	0.13	5,5,5,5	0
82	MG	AS	3741	1/1	0.88	0.08	13,13,13,13	0
82	MG	1	3486	1/1	0.88	0.10	10,10,10,10	0
82	MG	AS	3470	1/1	0.88	0.12	26,26,26,26	0
82	MG	1	3897	1/1	0.88	0.08	5,5,5,5	0
82	MG	AS	3892	1/1	0.88	0.19	69,69,69,69	0
82	MG	1	3748	1/1	0.88	0.14	15,15,15,15	0
82	MG	1	3979	1/1	0.88	0.23	24,24,24,24	0
82	MG	1	3687	1/1	0.88	0.21	4,4,4,4	0
82	MG	1	3772	1/1	0.88	0.05	21,21,21,21	0
82	MG	1	3874	1/1	0.88	0.08	5,5,5,5	0
82	MG	AS	3482	1/1	0.88	0.12	50,50,50,50	0
82	MG	1	3651	1/1	0.88	0.09	21,21,21,21	0
82	MG	AS	3484	1/1	0.88	0.10	18,18,18,18	0
82	MG	AS	3560	1/1	0.88	0.21	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	AS	3485	1/1	0.88	0.10	20,20,20,20	0
82	MG	B	1864	1/1	0.88	0.08	8,8,8,8	0
82	MG	1	4084	1/1	0.88	0.10	195,195,195,195	0
82	MG	AS	3566	1/1	0.88	0.21	40,40,40,40	0
82	MG	AS	3431	1/1	0.88	0.30	32,32,32,32	0
82	MG	AS	3762	1/1	0.88	0.08	33,33,33,33	0
82	MG	B	1806	1/1	0.88	0.12	15,15,15,15	0
82	MG	AS	3493	1/1	0.88	0.09	35,35,35,35	0
82	MG	AS	3765	1/1	0.88	0.13	10,10,10,10	0
82	MG	AS	3495	1/1	0.88	0.16	12,12,12,12	0
82	MG	1	3957	1/1	0.88	0.10	22,22,22,22	0
82	MG	AS	3768	1/1	0.88	0.10	7,7,7,7	0
82	MG	1	3488	1/1	0.88	0.13	25,25,25,25	0
82	MG	AS	3436	1/1	0.88	0.07	4,4,4,4	0
82	MG	1	4089	1/1	0.88	0.14	23,23,23,23	0
82	MG	AS	3438	1/1	0.88	0.12	4,4,4,4	0
82	MG	AS	3776	1/1	0.88	0.09	22,22,22,22	0
82	MG	1	3855	1/1	0.88	0.06	9,9,9,9	0
82	MG	1	3517	1/1	0.88	0.11	8,8,8,8	0
82	MG	1	3994	1/1	0.88	0.13	14,14,14,14	0
82	MG	1	3694	1/1	0.88	0.09	37,37,37,37	0
82	MG	AS	3714	1/1	0.88	0.09	59,59,59,59	0
82	MG	AS	3861	1/1	0.88	0.38	41,41,41,41	0
82	MG	AS	3785	1/1	0.88	0.14	23,23,23,23	0
82	MG	B	1819	1/1	0.88	0.26	15,15,15,15	0
82	MG	Y	201	1/1	0.88	0.12	6,6,6,6	0
82	MG	AS	3925	1/1	0.89	0.07	26,26,26,26	0
82	MG	AS	3501	1/1	0.89	0.10	11,11,11,11	0
82	MG	AS	3929	1/1	0.89	0.08	8,8,8,8	0
82	MG	1	3923	1/1	0.89	0.08	19,19,19,19	0
82	MG	1	3925	1/1	0.89	0.12	19,19,19,19	0
82	MG	1	3410	1/1	0.89	0.24	16,16,16,16	0
82	MG	1	3513	1/1	0.89	0.12	16,16,16,16	0
82	MG	AS	3716	1/1	0.89	0.07	28,28,28,28	0
82	MG	AS	3439	1/1	0.89	0.20	67,67,67,67	0
82	MG	AS	3787	1/1	0.89	0.17	40,40,40,40	0
82	MG	AS	3788	1/1	0.89	0.20	19,19,19,19	0
82	MG	1	3609	1/1	0.89	0.09	5,5,5,5	0
82	MG	AS	3792	1/1	0.89	0.09	158,158,158,158	0
82	MG	AS	3651	1/1	0.89	0.10	31,31,31,31	0
82	MG	AS	3944	1/1	0.89	0.15	9,9,9,9	0
82	MG	1	4017	1/1	0.89	0.09	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3579	1/1	0.89	0.14	16,16,16,16	0
82	MG	1	3439	1/1	0.89	0.14	31,31,31,31	0
82	MG	AS	3798	1/1	0.89	0.10	21,21,21,21	0
82	MG	1	3899	1/1	0.89	0.17	12,12,12,12	0
82	MG	1	4021	1/1	0.89	0.10	41,41,41,41	0
82	MG	1	3632	1/1	0.89	0.08	11,11,11,11	0
82	MG	1	3475	1/1	0.89	0.22	17,17,17,17	0
82	MG	1	3693	1/1	0.89	0.11	22,22,22,22	0
82	MG	1	3935	1/1	0.89	0.20	27,27,27,27	0
82	MG	1	3655	1/1	0.89	0.12	47,47,47,47	0
82	MG	1	4074	1/1	0.89	0.31	35,35,35,35	0
82	MG	U	201	1/1	0.89	0.17	51,51,51,51	0
82	MG	1	3724	1/1	0.89	0.13	29,29,29,29	0
82	MG	1	3500	1/1	0.89	0.10	4,4,4,4	0
82	MG	CE	102	1/1	0.89	0.10	52,52,52,52	0
82	MG	AS	3814	1/1	0.89	0.18	21,21,21,21	0
82	MG	AS	3668	1/1	0.89	0.13	13,13,13,13	0
82	MG	1	3636	1/1	0.89	0.17	16,16,16,16	0
82	MG	AS	3536	1/1	0.89	0.09	48,48,48,48	0
82	MG	1	3752	1/1	0.89	0.20	4,4,4,4	0
82	MG	1	3908	1/1	0.89	0.17	12,12,12,12	0
82	MG	AS	3605	1/1	0.89	0.20	26,26,26,26	0
82	MG	1	3909	1/1	0.89	0.08	24,24,24,24	0
82	MG	B	1817	1/1	0.89	0.16	4,4,4,4	0
82	MG	1	3618	1/1	0.89	0.09	13,13,13,13	0
82	MG	1	4082	1/1	0.89	0.11	21,21,21,21	0
82	MG	AS	3413	1/1	0.89	0.15	16,16,16,16	0
82	MG	1	3426	1/1	0.89	0.15	16,16,16,16	0
82	MG	CM	1824	1/1	0.89	0.12	35,35,35,35	0
82	MG	1	3541	1/1	0.89	0.15	9,9,9,9	0
82	MG	1	3851	1/1	0.89	0.09	46,46,46,46	0
82	MG	1	3788	1/1	0.89	0.07	15,15,15,15	0
82	MG	AS	3903	1/1	0.89	0.11	30,30,30,30	0
82	MG	AS	3481	1/1	0.89	0.15	41,41,41,41	0
82	MG	1	3854	1/1	0.89	0.17	40,40,40,40	0
82	MG	AS	3554	1/1	0.89	0.17	8,8,8,8	0
82	MG	1	3954	1/1	0.89	0.28	29,29,29,29	0
82	MG	AS	3557	1/1	0.89	0.07	32,32,32,32	0
82	MG	B	1833	1/1	0.89	0.18	15,15,15,15	0
82	MG	1	3680	1/1	0.89	0.14	27,27,27,27	0
82	MG	1	4003	1/1	0.89	0.15	37,37,37,37	0
82	MG	B	1840	1/1	0.89	0.10	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	4050	1/1	0.89	0.11	11,11,11,11	0
82	MG	AS	3564	1/1	0.89	0.20	25,25,25,25	0
82	MG	1	3887	1/1	0.89	0.14	43,43,43,43	0
82	MG	1	3793	1/1	0.89	0.13	23,23,23,23	0
82	MG	AS	3848	1/1	0.89	0.08	35,35,35,35	0
82	MG	1	3662	1/1	0.89	0.09	36,36,36,36	0
83	PAR	CM	1802	42/42	0.89	0.14	26,58,74,83	0
82	MG	1	3891	1/1	0.89	0.13	8,8,8,8	0
82	MG	1	3561	1/1	0.89	0.07	3,3,3,3	0
82	MG	AS	3853	1/1	0.89	0.20	20,20,20,20	0
82	MG	AS	3922	1/1	0.89	0.23	20,20,20,20	0
82	MG	AS	3774	1/1	0.89	0.11	17,17,17,17	0
82	MG	AS	3573	1/1	0.89	0.20	24,24,24,24	0
82	MG	1	3508	1/1	0.90	0.16	12,12,12,12	0
82	MG	1	3813	1/1	0.90	0.14	29,29,29,29	0
82	MG	AS	3931	1/1	0.90	0.15	6,6,6,6	0
82	MG	AS	3932	1/1	0.90	0.18	16,16,16,16	0
82	MG	1	3815	1/1	0.90	0.18	15,15,15,15	0
82	MG	AS	3420	1/1	0.90	0.11	21,21,21,21	0
82	MG	AS	3489	1/1	0.90	0.18	20,20,20,20	0
82	MG	B	1834	1/1	0.90	0.17	8,8,8,8	0
82	MG	AS	3784	1/1	0.90	0.19	36,36,36,36	0
82	MG	AS	3938	1/1	0.90	0.10	4,4,4,4	0
82	MG	k	402	1/1	0.90	0.45	26,26,26,26	0
82	MG	AS	3423	1/1	0.90	0.16	43,43,43,43	0
82	MG	AS	3711	1/1	0.90	0.07	30,30,30,30	0
82	MG	1	3816	1/1	0.90	0.16	6,6,6,6	0
82	MG	AS	3789	1/1	0.90	0.18	29,29,29,29	0
82	MG	1	3842	1/1	0.90	0.06	14,14,14,14	0
82	MG	AS	3571	1/1	0.90	0.18	4,4,4,4	0
82	MG	AS	3717	1/1	0.90	0.05	26,26,26,26	0
82	MG	B	1845	1/1	0.90	0.08	17,17,17,17	0
82	MG	AS	3644	1/1	0.90	0.11	7,7,7,7	0
82	MG	AS	3497	1/1	0.90	0.13	18,18,18,18	0
82	MG	AS	3875	1/1	0.90	0.15	22,22,22,22	0
82	MG	1	3792	1/1	0.90	0.17	12,12,12,12	0
82	MG	AS	3877	1/1	0.90	0.10	28,28,28,28	0
82	MG	1	4063	1/1	0.90	0.06	28,28,28,28	0
82	MG	B	1851	1/1	0.90	0.20	17,17,17,17	0
82	MG	1	3872	1/1	0.90	0.11	17,17,17,17	0
82	MG	1	3531	1/1	0.90	0.11	64,64,64,64	0
82	MG	1	3606	1/1	0.90	0.09	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	B	1856	1/1	0.90	0.18	14,14,14,14	0
82	MG	AS	3730	1/1	0.90	0.16	16,16,16,16	0
82	MG	AS	3514	1/1	0.90	0.26	67,67,67,67	0
82	MG	1	3739	1/1	0.90	0.23	15,15,15,15	0
82	MG	1	3710	1/1	0.90	0.19	13,13,13,13	0
82	MG	AB	201	1/1	0.90	0.18	17,17,17,17	0
82	MG	1	3799	1/1	0.90	0.17	6,6,6,6	0
82	MG	1	4033	1/1	0.90	0.13	5,5,5,5	0
82	MG	AS	3443	1/1	0.90	0.20	20,20,20,20	0
82	MG	1	3997	1/1	0.90	0.10	21,21,21,21	0
82	MG	AS	3591	1/1	0.90	0.24	42,42,42,42	0
82	MG	1	3802	1/1	0.90	0.10	25,25,25,25	0
82	MG	1	3419	1/1	0.90	0.10	10,10,10,10	0
82	MG	1	3587	1/1	0.90	0.10	7,7,7,7	0
82	MG	1	3622	1/1	0.90	0.11	22,22,22,22	0
82	MG	CM	1821	1/1	0.90	0.14	21,21,21,21	0
82	MG	1	3781	1/1	0.90	0.09	8,8,8,8	0
82	MG	1	3912	1/1	0.90	0.14	29,29,29,29	0
82	MG	AS	3748	1/1	0.90	0.06	13,13,13,13	0
82	MG	AS	3532	1/1	0.90	0.16	16,16,16,16	0
82	MG	1	4006	1/1	0.90	0.11	24,24,24,24	0
82	MG	1	4043	1/1	0.90	0.05	10,10,10,10	0
82	MG	B	1808	1/1	0.90	0.18	8,8,8,8	0
82	MG	1	4007	1/1	0.90	0.19	43,43,43,43	0
82	MG	1	3969	1/1	0.90	0.18	23,23,23,23	0
82	MG	AS	3679	1/1	0.90	0.10	68,68,68,68	0
82	MG	1	3543	1/1	0.90	0.10	14,14,14,14	0
82	MG	1	3971	1/1	0.90	0.11	27,27,27,27	0
82	MG	B	1813	1/1	0.90	0.19	16,16,16,16	0
82	MG	1	3453	1/1	0.90	0.12	34,34,34,34	0
82	MG	1	3973	1/1	0.90	0.09	8,8,8,8	0
82	MG	1	3831	1/1	0.90	0.11	44,44,44,44	0
82	MG	AS	3408	1/1	0.90	0.06	13,13,13,13	0
82	MG	1	4090	1/1	0.90	0.12	5,5,5,5	0
82	MG	1	3496	1/1	0.90	0.23	15,15,15,15	0
82	MG	B	1822	1/1	0.90	0.16	11,11,11,11	0
82	MG	B	1823	1/1	0.90	0.14	8,8,8,8	0
82	MG	AS	3849	1/1	0.90	0.09	29,29,29,29	0
82	MG	1	3764	1/1	0.90	0.08	27,27,27,27	0
82	MG	AS	3623	1/1	0.90	0.14	33,33,33,33	0
82	MG	1	3688	1/1	0.90	0.18	14,14,14,14	0
82	MG	AS	3555	1/1	0.90	0.11	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	3	204	1/1	0.90	0.08	14,14,14,14	0
82	MG	B	1828	1/1	0.90	0.12	19,19,19,19	0
82	MG	1	3416	1/1	0.91	0.24	8,8,8,8	0
82	MG	AS	3467	1/1	0.91	0.20	39,39,39,39	0
82	MG	AS	3945	1/1	0.91	0.19	18,18,18,18	0
82	MG	1	3704	1/1	0.91	0.10	16,16,16,16	0
82	MG	1	4042	1/1	0.91	0.07	14,14,14,14	0
82	MG	AS	3702	1/1	0.91	0.08	55,55,55,55	0
82	MG	AP	203	1/1	0.91	0.12	8,8,8,8	0
82	MG	AS	3889	1/1	0.91	0.10	15,15,15,15	0
82	MG	AU	201	1/1	0.91	0.10	44,44,44,44	0
82	MG	AU	202	1/1	0.91	0.08	59,59,59,59	0
82	MG	1	3474	1/1	0.91	0.15	25,25,25,25	0
82	MG	1	3418	1/1	0.91	0.07	5,5,5,5	0
82	MG	1	3943	1/1	0.91	0.07	16,16,16,16	0
82	MG	BB	301	1/1	0.91	0.22	15,15,15,15	0
82	MG	1	4012	1/1	0.91	0.12	28,28,28,28	0
82	MG	BB	303	1/1	0.91	0.16	9,9,9,9	0
82	MG	1	3477	1/1	0.91	0.24	15,15,15,15	0
82	MG	1	4049	1/1	0.91	0.11	8,8,8,8	0
82	MG	1	3890	1/1	0.91	0.12	19,19,19,19	0
82	MG	1	4087	1/1	0.91	0.14	21,21,21,21	0
82	MG	1	3550	1/1	0.91	0.31	16,16,16,16	0
82	MG	AS	3657	1/1	0.91	0.16	19,19,19,19	0
82	MG	1	3551	1/1	0.91	0.21	15,15,15,15	0
82	MG	B	1814	1/1	0.91	0.16	13,13,13,13	0
82	MG	AS	3777	1/1	0.91	0.06	29,29,29,29	0
82	MG	1	3436	1/1	0.91	0.08	9,9,9,9	0
82	MG	AS	3546	1/1	0.91	0.14	19,19,19,19	0
82	MG	1	3785	1/1	0.91	0.14	10,10,10,10	0
82	MG	1	3654	1/1	0.91	0.14	6,6,6,6	0
82	MG	AS	3782	1/1	0.91	0.21	12,12,12,12	0
82	MG	1	3814	1/1	0.91	0.20	21,21,21,21	0
82	MG	1	3737	1/1	0.91	0.35	5,5,5,5	0
82	MG	AS	3726	1/1	0.91	0.10	17,17,17,17	0
82	MG	CM	1817	1/1	0.91	0.17	29,29,29,29	0
82	MG	AS	3552	1/1	0.91	0.10	14,14,14,14	0
82	MG	1	4022	1/1	0.91	0.09	25,25,25,25	0
82	MG	AS	3442	1/1	0.91	0.13	40,40,40,40	0
82	MG	1	4023	1/1	0.91	0.15	30,30,30,30	0
82	MG	CM	1823	1/1	0.91	0.28	18,18,18,18	0
82	MG	AS	3790	1/1	0.91	0.18	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	CM	1826	1/1	0.91	0.21	22,22,22,22	0
82	MG	1	3988	1/1	0.91	0.06	43,43,43,43	0
82	MG	AS	3500	1/1	0.91	0.07	11,11,11,11	0
82	MG	AS	3733	1/1	0.91	0.12	25,25,25,25	0
82	MG	1	3924	1/1	0.91	0.21	18,18,18,18	0
82	MG	AS	3559	1/1	0.91	0.09	31,31,31,31	0
82	MG	1	3672	1/1	0.91	0.09	10,10,10,10	0
82	MG	AS	3449	1/1	0.91	0.27	3,3,3,3	0
82	MG	AS	3507	1/1	0.91	0.18	57,57,57,57	0
82	MG	AS	3508	1/1	0.91	0.11	9,9,9,9	0
82	MG	c	201	1/1	0.91	0.27	17,17,17,17	0
82	MG	AS	3565	1/1	0.91	0.23	64,64,64,64	0
82	MG	AS	3928	1/1	0.91	0.22	17,17,17,17	0
82	MG	1	3479	1/1	0.91	0.15	8,8,8,8	0
82	MG	1	3518	1/1	0.91	0.16	7,7,7,7	0
82	MG	1	3443	1/1	0.91	0.09	16,16,16,16	0
82	MG	1	3624	1/1	0.91	0.07	18,18,18,18	0
82	MG	1	3767	1/1	0.91	0.14	23,23,23,23	0
82	MG	1	3849	1/1	0.91	0.25	12,12,12,12	0
82	MG	1	3437	1/1	0.91	0.07	7,7,7,7	0
82	MG	AS	3813	1/1	0.91	0.17	44,44,44,44	0
82	MG	1	3879	1/1	0.91	0.11	11,11,11,11	0
82	MG	1	3641	1/1	0.91	0.11	13,13,13,13	0
82	MG	AS	3635	1/1	0.91	0.06	35,35,35,35	0
82	MG	1	3967	1/1	0.91	0.12	27,27,27,27	0
82	MG	1	3642	1/1	0.91	0.11	38,38,38,38	0
82	MG	1	3774	1/1	0.91	0.19	11,11,11,11	0
82	MG	1	3608	1/1	0.92	0.07	16,16,16,16	0
82	MG	1	3990	1/1	0.92	0.10	9,9,9,9	0
82	MG	1	3441	1/1	0.92	0.07	8,8,8,8	0
82	MG	AS	3506	1/1	0.92	0.20	11,11,11,11	0
82	MG	1	3539	1/1	0.92	0.28	20,20,20,20	0
82	MG	1	3634	1/1	0.92	0.15	15,15,15,15	0
82	MG	1	3782	1/1	0.92	0.12	8,8,8,8	0
82	MG	AS	3634	1/1	0.92	0.18	48,48,48,48	0
82	MG	AS	3510	1/1	0.92	0.17	19,19,19,19	0
82	MG	1	3956	1/1	0.92	0.12	49,49,49,49	0
82	MG	AS	3637	1/1	0.92	0.13	18,18,18,18	0
82	MG	1	3613	1/1	0.92	0.17	24,24,24,24	0
82	MG	1	3755	1/1	0.92	0.16	6,6,6,6	0
82	MG	1	3852	1/1	0.92	0.20	24,24,24,24	0
82	MG	1	4001	1/1	0.92	0.08	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	3576	1/1	0.92	0.14	11,11,11,11	0
82	MG	CH	101	1/1	0.92	0.18	22,22,22,22	0
82	MG	1	3502	1/1	0.92	0.18	10,10,10,10	0
82	MG	CM	1804	1/1	0.92	0.22	12,12,12,12	0
82	MG	1	3481	1/1	0.92	0.13	17,17,17,17	0
82	MG	1	3595	1/1	0.92	0.20	4,4,4,4	0
82	MG	AS	3713	1/1	0.92	0.07	9,9,9,9	0
82	MG	1	3821	1/1	0.92	0.09	19,19,19,19	0
82	MG	1	4045	1/1	0.92	0.11	33,33,33,33	0
82	MG	1	3709	1/1	0.92	0.11	16,16,16,16	0
82	MG	CM	1813	1/1	0.92	0.08	7,7,7,7	0
82	MG	1	4088	1/1	0.92	0.15	16,16,16,16	0
82	MG	1	3495	1/1	0.92	0.24	15,15,15,15	0
82	MG	1	3516	1/1	0.92	0.17	4,4,4,4	0
82	MG	1	3505	1/1	0.92	0.27	16,16,16,16	0
82	MG	AS	3530	1/1	0.92	0.18	32,32,32,32	0
82	MG	1	4094	1/1	0.92	0.09	11,11,11,11	0
82	MG	CM	1820	1/1	0.92	0.19	11,11,11,11	0
82	MG	B	1821	1/1	0.92	0.18	13,13,13,13	0
82	MG	1	3601	1/1	0.92	0.08	15,15,15,15	0
82	MG	1	3403	1/1	0.92	0.36	16,16,16,16	0
82	MG	3	202	1/1	0.92	0.24	20,20,20,20	0
82	MG	AS	3469	1/1	0.92	0.13	16,16,16,16	0
82	MG	1	3796	1/1	0.92	0.12	8,8,8,8	0
82	MG	1	3766	1/1	0.92	0.26	16,16,16,16	0
82	MG	4	204	1/1	0.92	0.12	6,6,6,6	0
82	MG	1	3472	1/1	0.92	0.20	9,9,9,9	0
82	MG	1	3800	1/1	0.92	0.11	13,13,13,13	0
82	MG	B	1832	1/1	0.92	0.20	8,8,8,8	0
82	MG	AS	3543	1/1	0.92	0.16	34,34,34,34	0
82	MG	1	3768	1/1	0.92	0.16	8,8,8,8	0
82	MG	1	3532	1/1	0.92	0.08	15,15,15,15	0
82	MG	1	3976	1/1	0.92	0.07	13,13,13,13	0
82	MG	1	3871	1/1	0.92	0.10	23,23,23,23	0
82	MG	1	3649	1/1	0.92	0.13	7,7,7,7	0
82	MG	B	1844	1/1	0.92	0.09	16,16,16,16	0
82	MG	1	3745	1/1	0.92	0.13	18,18,18,18	0
82	MG	1	3981	1/1	0.92	0.21	15,15,15,15	0
82	MG	B	1848	1/1	0.92	0.09	5,5,5,5	0
82	MG	AS	3680	1/1	0.92	0.09	15,15,15,15	0
82	MG	z	201	1/1	0.92	0.08	14,14,14,14	0
82	MG	1	3773	1/1	0.92	0.06	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	1	3509	1/1	0.92	0.27	17,17,17,17	0
82	MG	1	3775	1/1	0.92	0.09	9,9,9,9	0
82	MG	AS	3685	1/1	0.92	0.21	9,9,9,9	0
82	MG	1	3444	1/1	0.92	0.05	3,3,3,3	0
82	MG	1	3537	1/1	0.92	0.19	8,8,8,8	0
82	MG	AD	201	1/1	0.92	0.21	11,11,11,11	0
82	MG	1	3949	1/1	0.92	0.07	28,28,28,28	0
82	MG	1	3417	1/1	0.93	0.13	11,11,11,11	0
82	MG	1	3506	1/1	0.93	0.36	44,44,44,44	0
82	MG	1	3703	1/1	0.93	0.24	16,16,16,16	0
82	MG	1	3582	1/1	0.93	0.06	8,8,8,8	0
82	MG	AS	3582	1/1	0.93	0.14	41,41,41,41	0
82	MG	1	3571	1/1	0.93	0.17	29,29,29,29	0
82	MG	1	3498	1/1	0.93	0.25	9,9,9,9	0
82	MG	1	3870	1/1	0.93	0.07	12,12,12,12	0
82	MG	AS	3480	1/1	0.93	0.16	28,28,28,28	0
82	MG	AS	3444	1/1	0.93	0.08	34,34,34,34	0
82	MG	AS	3706	1/1	0.93	0.04	14,14,14,14	0
82	MG	B	1826	1/1	0.93	0.09	8,8,8,8	0
82	MG	1	3599	1/1	0.93	0.16	6,6,6,6	0
82	MG	CM	1827	1/1	0.93	0.16	10,10,10,10	0
82	MG	B	1805	1/1	0.93	0.17	16,16,16,16	0
82	MG	1	3708	1/1	0.93	0.07	6,6,6,6	0
82	MG	1	3790	1/1	0.93	0.21	12,12,12,12	0
82	MG	AS	3526	1/1	0.93	0.13	7,7,7,7	0
82	MG	B	1831	1/1	0.93	0.07	5,5,5,5	0
82	MG	AS	3834	1/1	0.93	0.07	5,5,5,5	0
82	MG	1	3893	1/1	0.93	0.08	15,15,15,15	0
82	MG	1	3566	1/1	0.93	0.17	24,24,24,24	0
82	MG	1	3625	1/1	0.93	0.09	11,11,11,11	0
82	MG	B	1870	1/1	0.93	0.18	21,21,21,21	0
82	MG	AS	3494	1/1	0.93	0.08	8,8,8,8	0
82	MG	AS	3602	1/1	0.93	0.15	56,56,56,56	0
82	MG	AS	3799	1/1	0.93	0.09	10,10,10,10	0
82	MG	1	3626	1/1	0.93	0.16	4,4,4,4	0
82	MG	AS	3567	1/1	0.93	0.09	20,20,20,20	0
82	MG	B	1837	1/1	0.93	0.10	24,24,24,24	0
82	MG	AS	3845	1/1	0.93	0.13	23,23,23,23	0
82	MG	1	3992	1/1	0.93	0.06	39,39,39,39	0
82	MG	B	1839	1/1	0.93	0.19	8,8,8,8	0
82	MG	1	3404	1/1	0.93	0.14	9,9,9,9	0
82	MG	B	1841	1/1	0.93	0.12	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3578	1/1	0.93	0.19	11,11,11,11	0
82	MG	1	3427	1/1	0.93	0.05	3,3,3,3	0
85	ZN	AK	101	1/1	0.93	0.14	60,60,60,60	0
82	MG	B	1816	1/1	0.93	0.10	13,13,13,13	0
82	MG	1	3881	1/1	0.93	0.23	48,48,48,48	1
82	MG	3	203	1/1	0.93	0.27	12,12,12,12	0
82	MG	1	3428	1/1	0.94	0.09	5,5,5,5	0
82	MG	CM	1809	1/1	0.94	0.15	12,12,12,12	0
82	MG	1	3562	1/1	0.94	0.21	10,10,10,10	0
82	MG	4	202	1/1	0.94	0.12	19,19,19,19	0
82	MG	1	3611	1/1	0.94	0.18	77,77,77,77	0
82	MG	1	3701	1/1	0.94	0.04	5,5,5,5	0
82	MG	AS	3805	1/1	0.94	0.12	13,13,13,13	0
82	MG	1	3837	1/1	0.94	0.24	8,8,8,8	0
82	MG	1	3670	1/1	0.94	0.15	8,8,8,8	0
82	MG	1	4055	1/1	0.94	0.07	7,7,7,7	0
82	MG	1	3987	1/1	0.94	0.07	8,8,8,8	0
82	MG	AS	3645	1/1	0.94	0.11	28,28,28,28	0
82	MG	1	3644	1/1	0.94	0.12	36,36,36,36	0
82	MG	B	1869	1/1	0.94	0.25	23,23,23,23	0
82	MG	AS	3770	1/1	0.94	0.15	46,46,46,46	0
82	MG	o	303	1/1	0.94	0.21	12,12,12,12	0
82	MG	AS	3424	1/1	0.94	0.16	10,10,10,10	0
82	MG	AS	3459	1/1	0.94	0.14	13,13,13,13	0
82	MG	1	3646	1/1	0.94	0.13	25,25,25,25	0
82	MG	AS	3948	1/1	0.94	0.14	12,12,12,12	0
82	MG	AS	3775	1/1	0.94	0.08	9,9,9,9	0
82	MG	1	3480	1/1	0.94	0.08	16,16,16,16	0
82	MG	1	3801	1/1	0.94	0.09	14,14,14,14	0
82	MG	AS	3463	1/1	0.94	0.11	11,11,11,11	0
82	MG	1	3689	1/1	0.94	0.11	11,11,11,11	0
82	MG	B	1843	1/1	0.94	0.12	5,5,5,5	0
82	MG	1	3476	1/1	0.94	0.23	9,9,9,9	0
82	MG	AS	3825	1/1	0.94	0.16	18,18,18,18	0
82	MG	1	3593	1/1	0.94	0.07	11,11,11,11	0
82	MG	1	3442	1/1	0.94	0.13	9,9,9,9	0
82	MG	AS	3434	1/1	0.94	0.14	5,5,5,5	0
82	MG	B	1847	1/1	0.94	0.08	16,16,16,16	0
82	MG	AS	3471	1/1	0.94	0.14	16,16,16,16	0
82	MG	BK	201	1/1	0.94	0.11	10,10,10,10	0
82	MG	AS	3626	1/1	0.94	0.07	24,24,24,24	0
82	MG	AS	3550	1/1	0.94	0.22	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	1	3574	1/1	0.94	0.07	9,9,9,9	0
82	MG	1	3406	1/1	0.94	0.13	8,8,8,8	0
82	MG	AS	3669	1/1	0.94	0.10	7,7,7,7	0
82	MG	1	3484	1/1	0.94	0.12	25,25,25,25	0
82	MG	1	4093	1/1	0.94	0.07	17,17,17,17	0
82	MG	1	3770	1/1	0.94	0.12	5,5,5,5	0
82	MG	1	3733	1/1	0.94	0.17	22,22,22,22	0
82	MG	1	3713	1/1	0.94	0.11	6,6,6,6	0
82	MG	1	3980	1/1	0.94	0.06	6,6,6,6	0
82	MG	B	1852	1/1	0.95	0.10	4,4,4,4	0
82	MG	1	3695	1/1	0.95	0.06	3,3,3,3	0
82	MG	1	4091	1/1	0.95	0.06	5,5,5,5	0
82	MG	AS	3486	1/1	0.95	0.11	17,17,17,17	0
82	MG	1	3409	1/1	0.95	0.18	16,16,16,16	0
82	MG	AS	3488	1/1	0.95	0.06	23,23,23,23	0
82	MG	CM	1825	1/1	0.95	0.10	42,42,42,42	0
82	MG	AS	3524	1/1	0.95	0.07	17,17,17,17	0
82	MG	1	3425	1/1	0.95	0.20	26,26,26,26	0
82	MG	1	3597	1/1	0.95	0.09	11,11,11,11	0
82	MG	B	1858	1/1	0.95	0.10	6,6,6,6	0
82	MG	1	3747	1/1	0.95	0.14	15,15,15,15	0
82	MG	1	3673	1/1	0.95	0.06	20,20,20,20	0
82	MG	B	1835	1/1	0.95	0.12	8,8,8,8	0
82	MG	1	3789	1/1	0.95	0.05	9,9,9,9	0
82	MG	1	4000	1/1	0.95	0.17	12,12,12,12	0
82	MG	AS	3597	1/1	0.95	0.09	26,26,26,26	0
82	MG	AS	3598	1/1	0.95	0.13	35,35,35,35	0
82	MG	1	3700	1/1	0.95	0.23	19,19,19,19	0
82	MG	1	3865	1/1	0.95	0.05	38,38,38,38	0
82	MG	1	3454	1/1	0.95	0.06	12,12,12,12	0
82	MG	1	3725	1/1	0.95	0.09	16,16,16,16	0
82	MG	B	1842	1/1	0.95	0.15	19,19,19,19	0
82	MG	4	205	1/1	0.95	0.10	12,12,12,12	0
82	MG	AS	3505	1/1	0.95	0.16	19,19,19,19	0
82	MG	1	3950	1/1	0.95	0.09	24,24,24,24	0
82	MG	1	3884	1/1	0.95	0.30	26,26,26,26	0
82	MG	AS	3447	1/1	0.95	0.14	15,15,15,15	0
82	MG	AS	3476	1/1	0.95	0.13	31,31,31,31	0
82	MG	1	3535	1/1	0.95	0.17	13,13,13,13	0
82	MG	1	3455	1/1	0.95	0.04	4,4,4,4	0
82	MG	AS	3450	1/1	0.95	0.08	21,21,21,21	0
82	MG	AS	3613	1/1	0.95	0.10	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	ZN	h	201	1/1	0.95	0.06	126,126,126,126	0
82	MG	1	3553	1/1	0.95	0.08	14,14,14,14	0
82	MG	1	3936	1/1	0.95	0.08	17,17,17,17	0
82	MG	1	3715	1/1	0.95	0.08	8,8,8,8	0
82	MG	1	3682	1/1	0.96	0.14	4,4,4,4	0
82	MG	AS	3700	1/1	0.96	0.13	18,18,18,18	0
82	MG	1	3845	1/1	0.96	0.07	10,10,10,10	0
82	MG	1	3878	1/1	0.96	0.07	13,13,13,13	0
82	MG	1	4068	1/1	0.96	0.07	12,12,12,12	0
82	MG	BP	201	1/1	0.96	0.10	16,16,16,16	0
82	MG	L	201	1/1	0.96	0.14	8,8,8,8	0
82	MG	1	3716	1/1	0.96	0.09	9,9,9,9	0
82	MG	1	3434	1/1	0.96	0.08	12,12,12,12	0
82	MG	1	3832	1/1	0.96	0.10	6,6,6,6	0
82	MG	1	3616	1/1	0.96	0.13	6,6,6,6	0
82	MG	1	3586	1/1	0.96	0.10	12,12,12,12	0
82	MG	1	3423	1/1	0.96	0.16	9,9,9,9	0
82	MG	1	3836	1/1	0.96	0.05	14,14,14,14	0
82	MG	AS	3793	1/1	0.96	0.12	129,129,129,129	0
82	MG	AS	3616	1/1	0.96	0.06	50,50,50,50	0
82	MG	1	3411	1/1	0.96	0.25	20,20,20,20	0
82	MG	1	3657	1/1	0.96	0.16	19,19,19,19	0
82	MG	CM	1810	1/1	0.96	0.15	17,17,17,17	0
82	MG	AS	3742	1/1	0.96	0.08	10,10,10,10	0
82	MG	AS	3512	1/1	0.96	0.06	21,21,21,21	0
82	MG	1	3798	1/1	0.96	0.24	13,13,13,13	0
82	MG	1	3487	1/1	0.96	0.14	21,21,21,21	0
82	MG	AS	3801	1/1	0.96	0.09	23,23,23,23	0
82	MG	6	201	1/1	0.96	0.12	6,6,6,6	0
82	MG	AS	3694	1/1	0.96	0.11	26,26,26,26	0
82	MG	AS	3647	1/1	0.96	0.08	23,23,23,23	0
85	ZN	AH	202	1/1	0.96	0.05	75,75,75,75	0
82	MG	AS	3749	1/1	0.96	0.20	12,12,12,12	0
85	ZN	AP	201	1/1	0.96	0.05	127,127,127,127	0
82	MG	1	3430	1/1	0.96	0.12	5,5,5,5	0
82	MG	1	3577	1/1	0.96	0.07	15,15,15,15	0
82	MG	AS	3927	1/1	0.96	0.06	25,25,25,25	0
85	ZN	DQ	101	1/1	0.96	0.08	120,120,120,120	0
82	MG	1	3623	1/1	0.96	0.30	25,25,25,25	0
82	MG	AH	201	1/1	0.97	0.21	33,33,33,33	0
82	MG	1	3645	1/1	0.97	0.06	12,12,12,12	0
82	MG	1	3471	1/1	0.97	0.10	8,8,8,8	0

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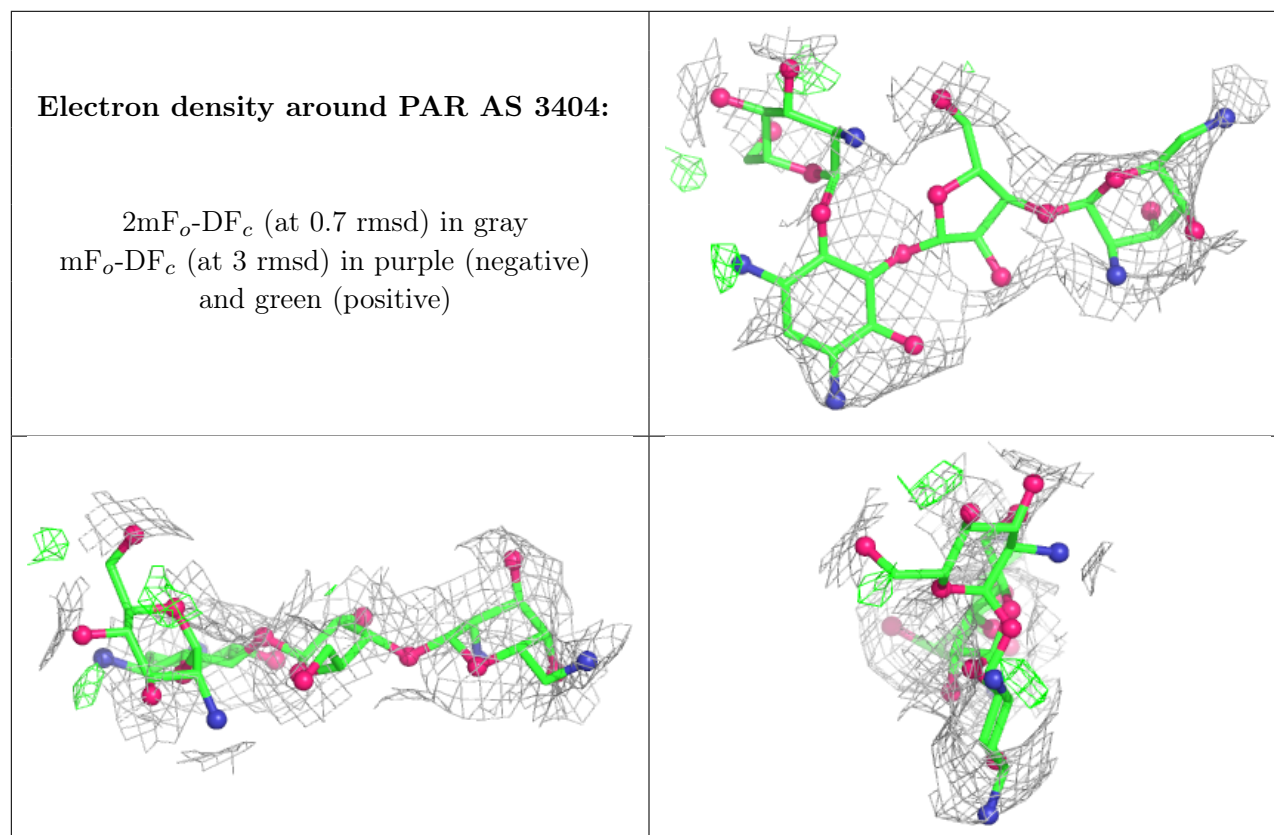
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
82	MG	BQ	202	1/1	0.97	0.11	7,7,7,7	0
82	MG	AS	3873	1/1	0.97	0.22	39,39,39,39	0
82	MG	1	3591	1/1	0.97	0.12	13,13,13,13	0
82	MG	1	3723	1/1	0.97	0.10	9,9,9,9	0
82	MG	1	3429	1/1	0.97	0.11	8,8,8,8	0
82	MG	1	3489	1/1	0.97	0.09	11,11,11,11	0
82	MG	AS	3847	1/1	0.97	0.07	27,27,27,27	0
82	MG	1	3448	1/1	0.97	0.13	20,20,20,20	0
82	MG	Z	201	1/1	0.97	0.14	8,8,8,8	0
82	MG	1	3937	1/1	0.97	0.06	11,11,11,11	0
82	MG	AS	3620	1/1	0.97	0.07	10,10,10,10	0
82	MG	AS	3621	1/1	0.97	0.05	6,6,6,6	0
82	MG	1	3470	1/1	0.97	0.36	17,17,17,17	0
82	MG	1	4024	1/1	0.97	0.07	14,14,14,14	0
82	MG	AS	3473	1/1	0.97	0.07	16,16,16,16	0
82	MG	AS	3429	1/1	0.97	0.13	17,17,17,17	0
82	MG	AS	3498	1/1	0.97	0.08	8,8,8,8	0
82	MG	AS	3654	1/1	0.97	0.16	9,9,9,9	0
82	MG	1	3522	1/1	0.97	0.04	19,19,19,19	0
82	MG	1	3610	1/1	0.97	0.06	6,6,6,6	0
82	MG	1	3573	1/1	0.97	0.06	11,11,11,11	0
82	MG	1	3585	1/1	0.97	0.05	30,30,30,30	0
82	MG	B	1849	1/1	0.97	0.08	15,15,15,15	0
82	MG	AS	3504	1/1	0.97	0.19	9,9,9,9	0
82	MG	AS	3718	1/1	0.97	0.07	20,20,20,20	0
82	MG	1	3515	1/1	0.97	0.04	5,5,5,5	0
82	MG	1	3524	1/1	0.97	0.06	4,4,4,4	0
82	MG	1	3534	1/1	0.97	0.15	6,6,6,6	0
82	MG	1	3497	1/1	0.97	0.12	7,7,7,7	0
82	MG	AS	3515	1/1	0.98	0.15	41,41,41,41	0
82	MG	1	3762	1/1	0.98	0.13	4,4,4,4	0
82	MG	AS	3712	1/1	0.98	0.06	8,8,8,8	0
82	MG	1	3744	1/1	0.98	0.11	9,9,9,9	0
85	ZN	DN	201	1/1	0.98	0.04	76,76,76,76	0
82	MG	DK	201	1/1	0.98	0.04	9,9,9,9	0
82	MG	AS	3826	1/1	0.98	0.09	24,24,24,24	0
82	MG	1	3552	1/1	0.99	0.06	6,6,6,6	0
85	ZN	CE	101	1/1	0.99	0.03	59,59,59,59	0
85	ZN	CH	102	1/1	0.99	0.06	53,53,53,53	0
85	ZN	AQ	101	1/1	0.99	0.03	35,35,35,35	0
85	ZN	CK	101	1/1	0.99	0.05	92,92,92,92	0
85	ZN	c	202	1/1	0.99	0.04	31,31,31,31	0

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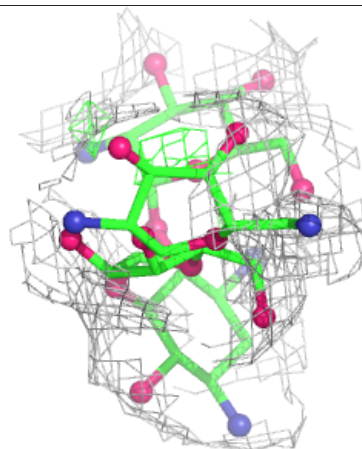
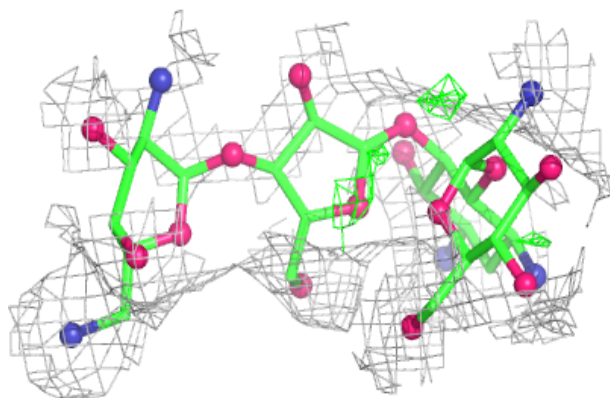
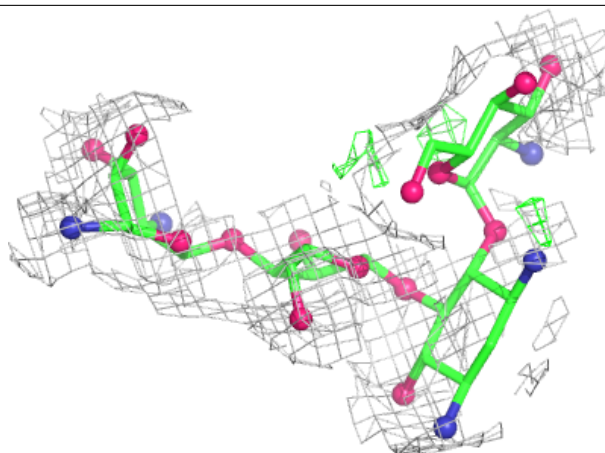
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
85	ZN	f	101	1/1	0.99	0.05	51,51,51,51	0
85	ZN	AN	101	1/1	0.99	0.02	50,50,50,50	0

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

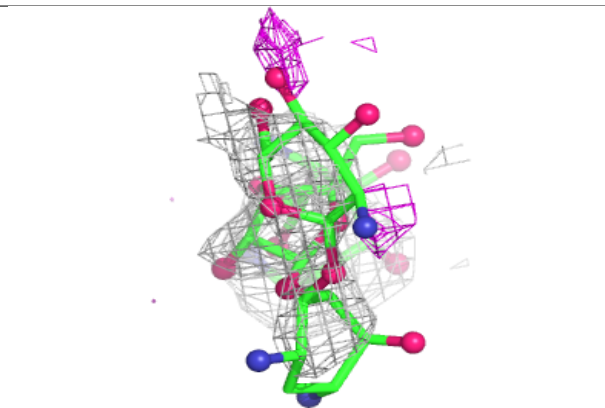
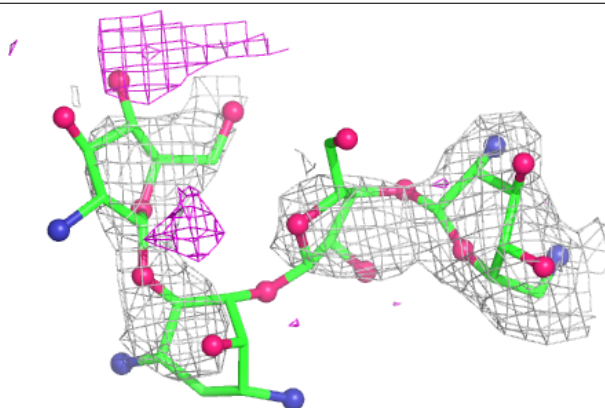


Electron density around PAR 1 3466:

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

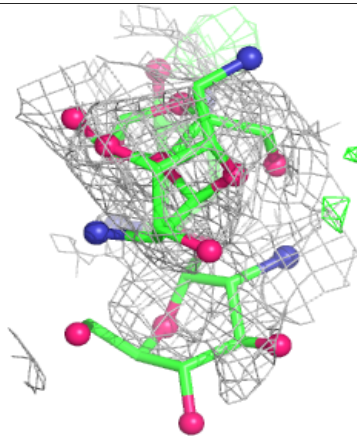
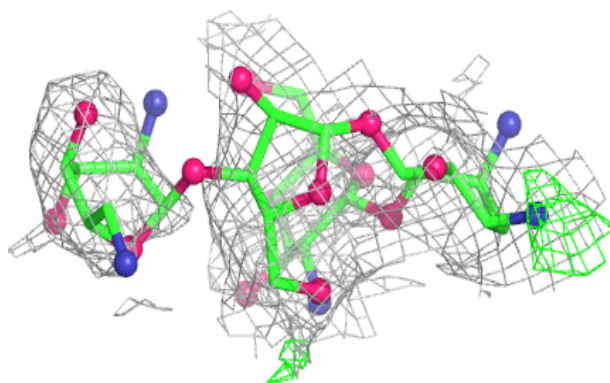
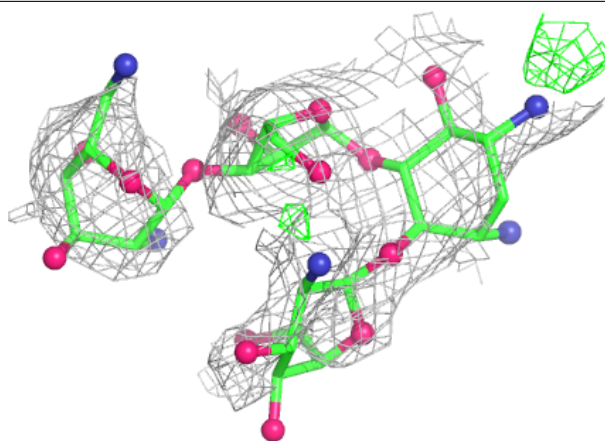
**Electron density around PAR 1 3457:**

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



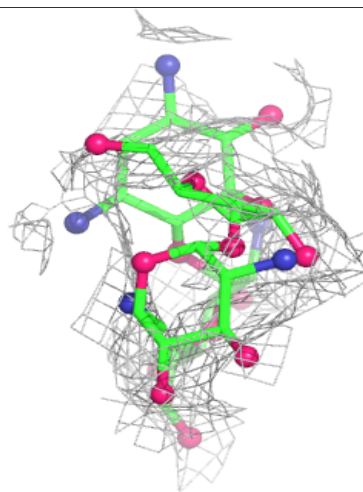
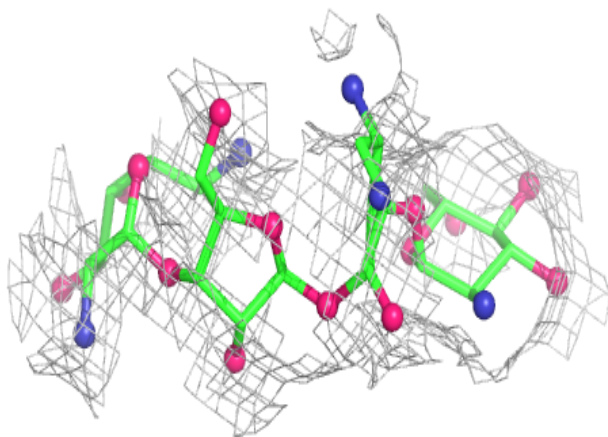
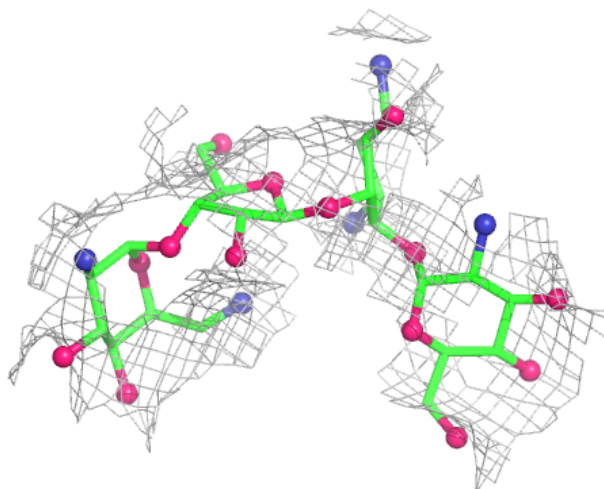
Electron density around PAR 1 3460:

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



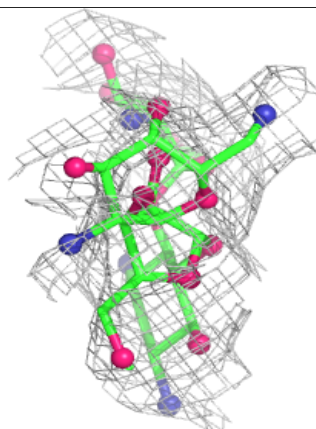
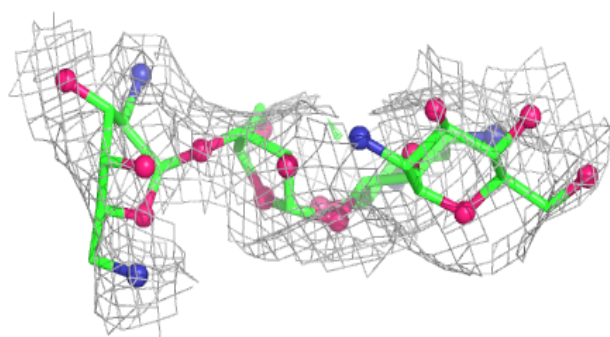
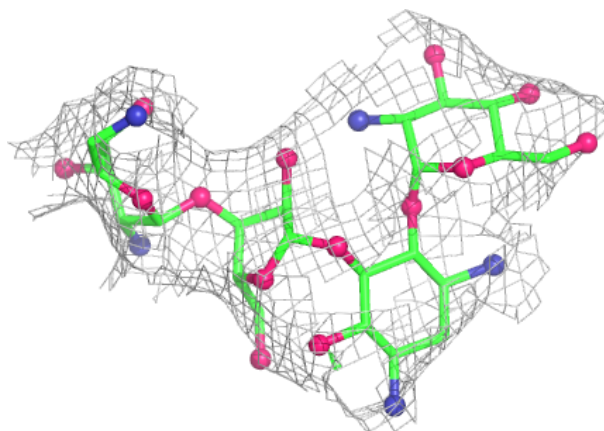
Electron density around PAR AS 3406:

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



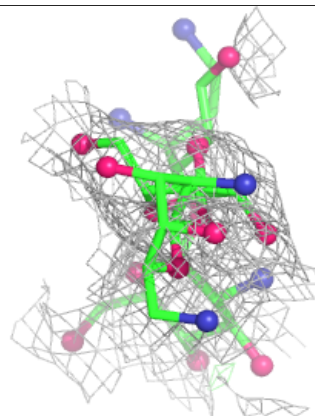
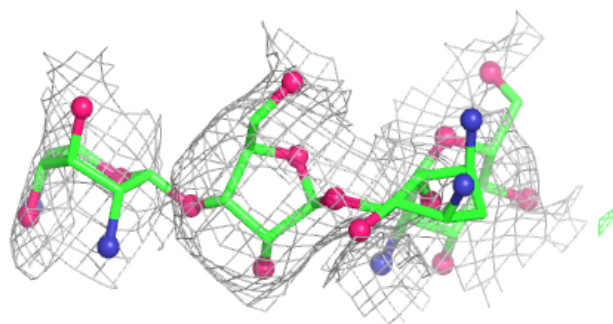
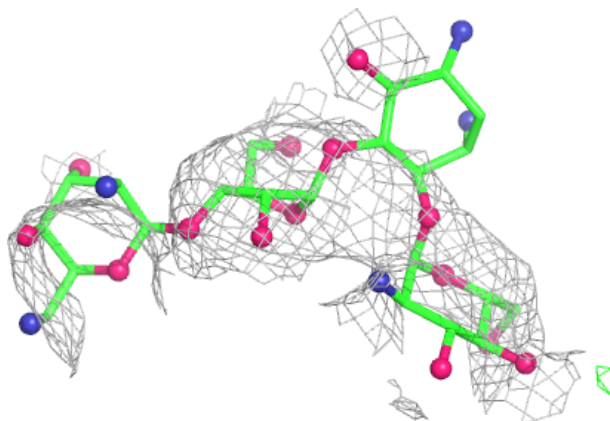
Electron density around PAR 1 3461:

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



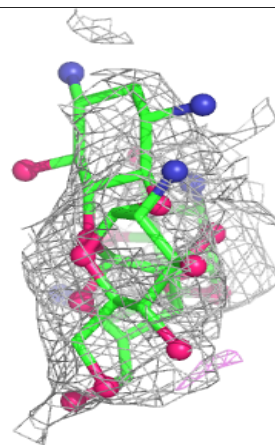
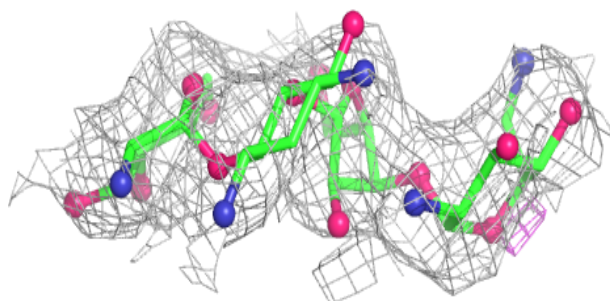
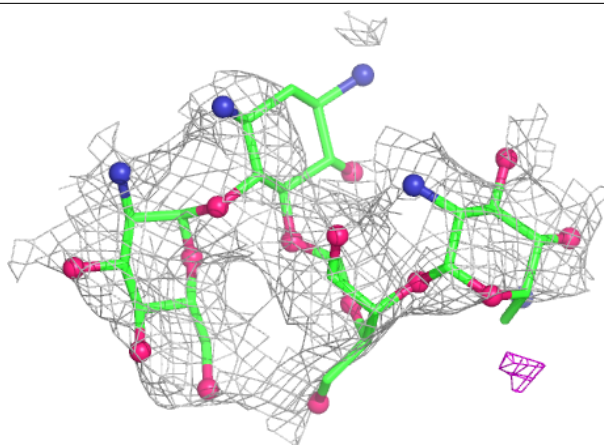
Electron density around PAR AS 3402:

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



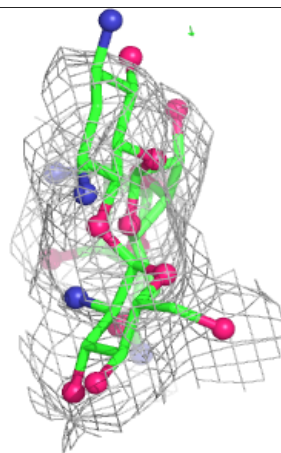
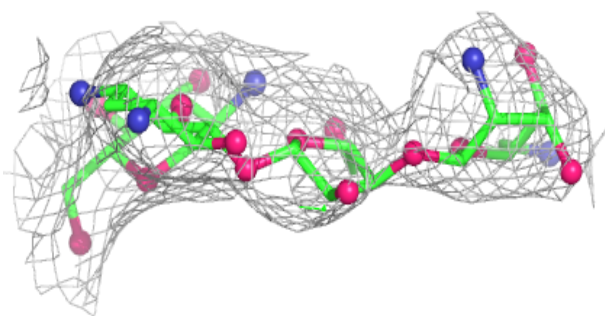
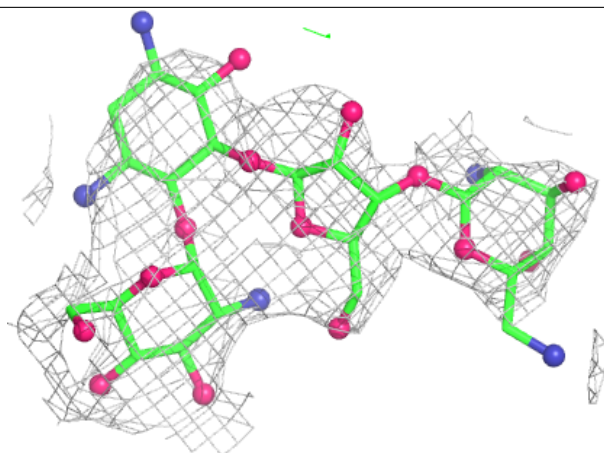
Electron density around PAR 1 3465:

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



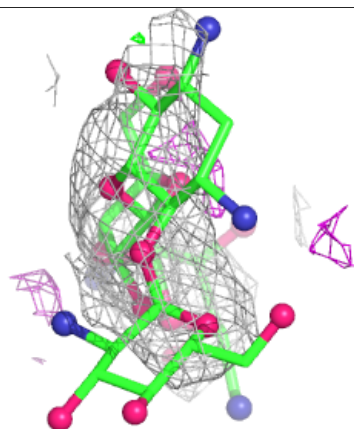
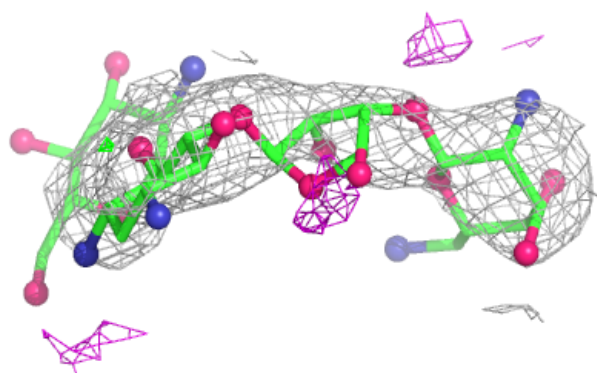
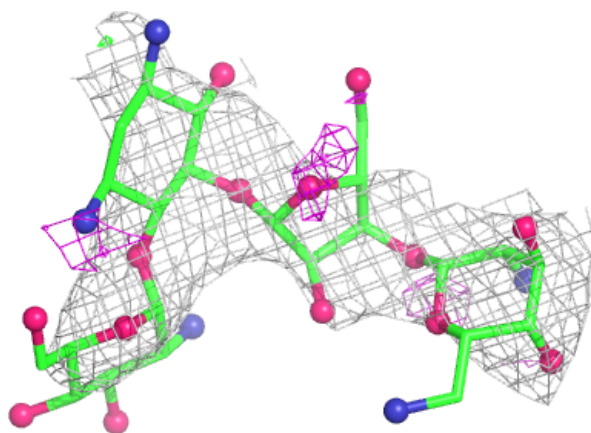
Electron density around PAR B 1803:

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



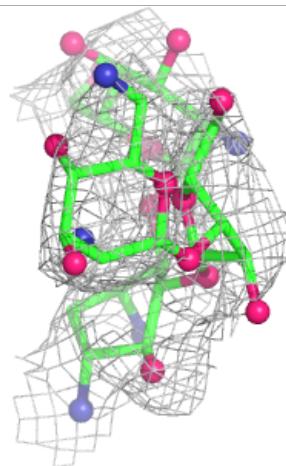
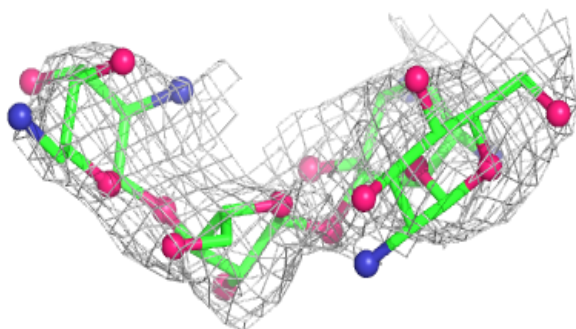
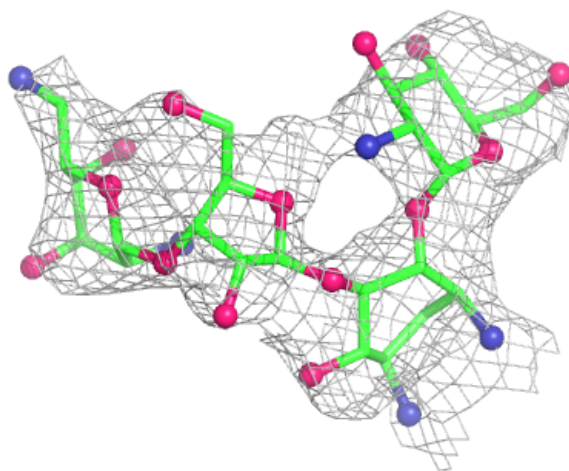
Electron density around PAR B 1801:

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



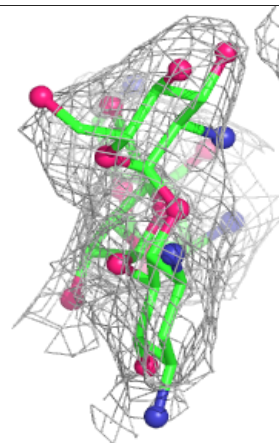
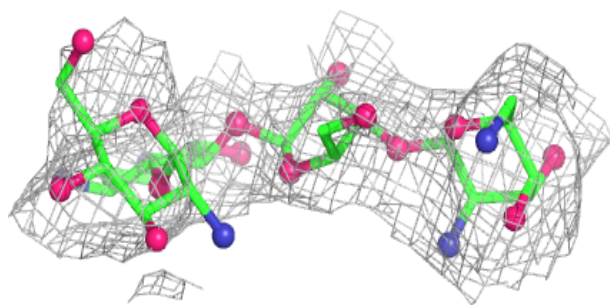
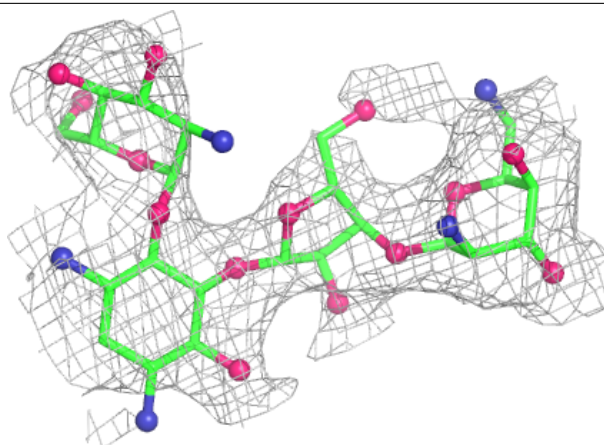
Electron density around PAR B 1802:

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



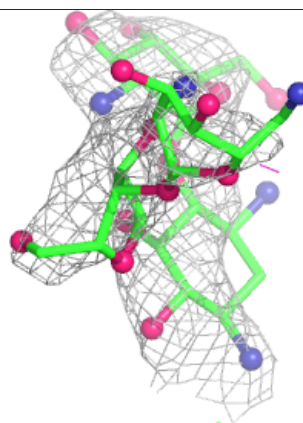
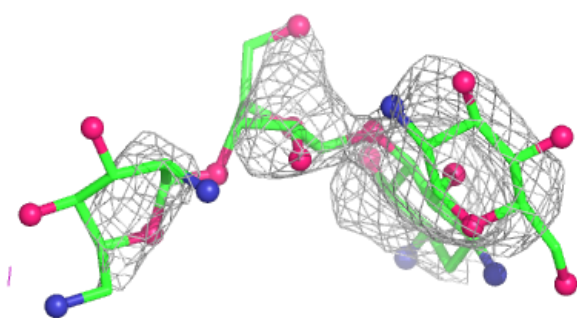
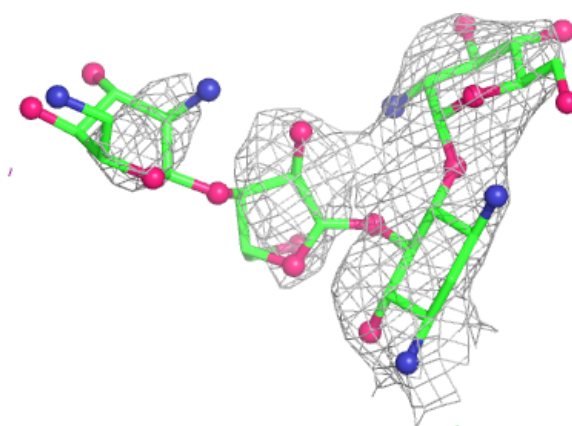
Electron density around PAR 1 3456:

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



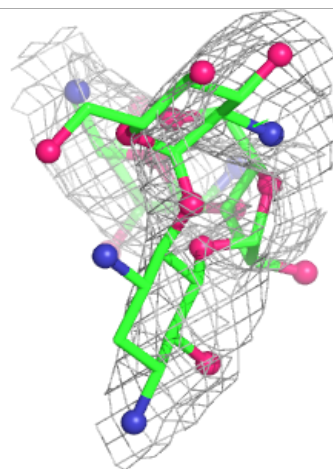
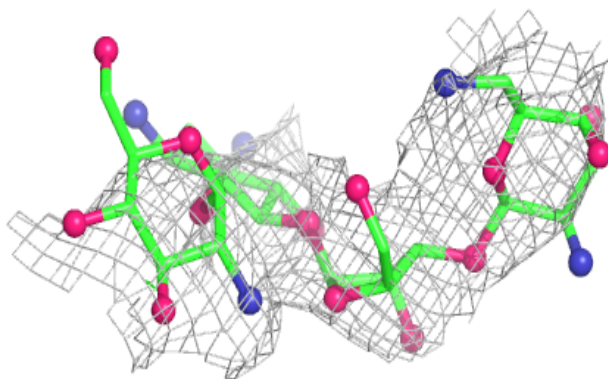
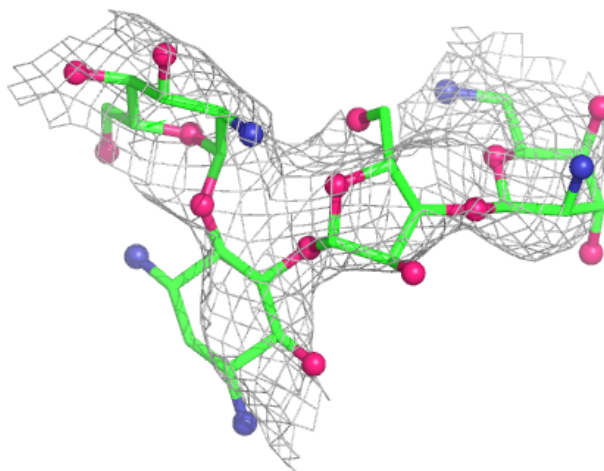
Electron density around PAR 1 3459:

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



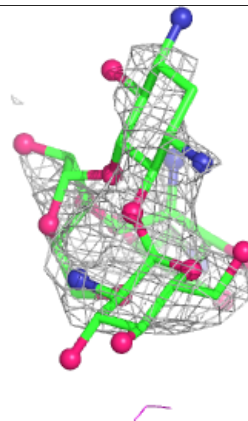
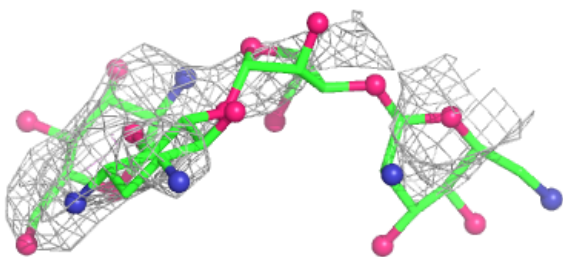
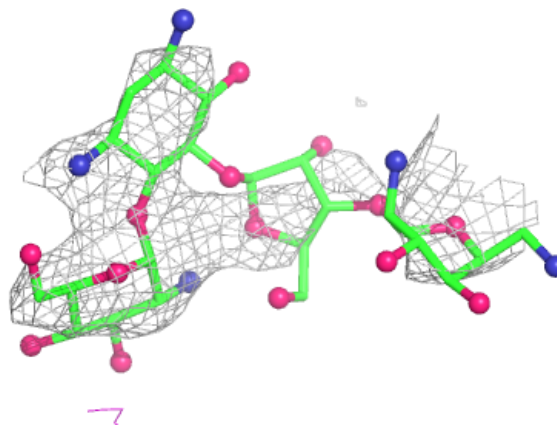
Electron density around PAR AS 3401:

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



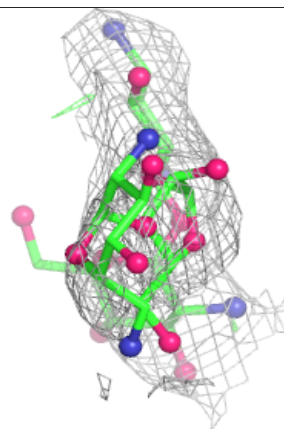
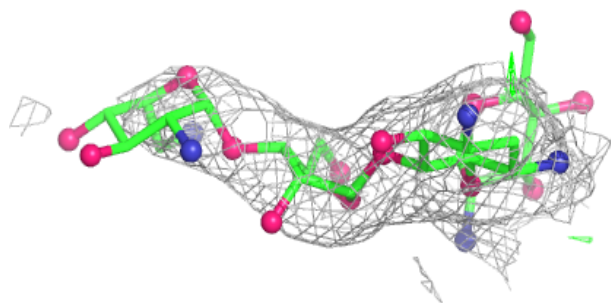
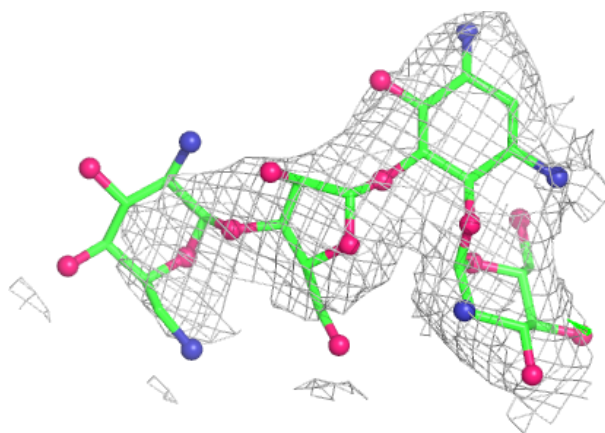
Electron density around PAR AS 3403:

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



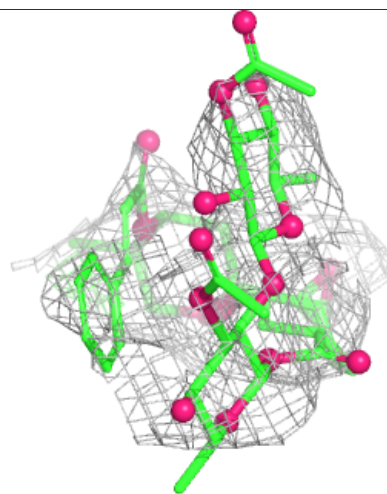
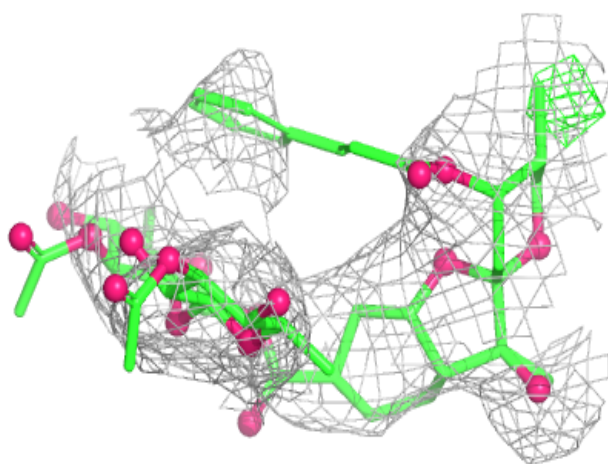
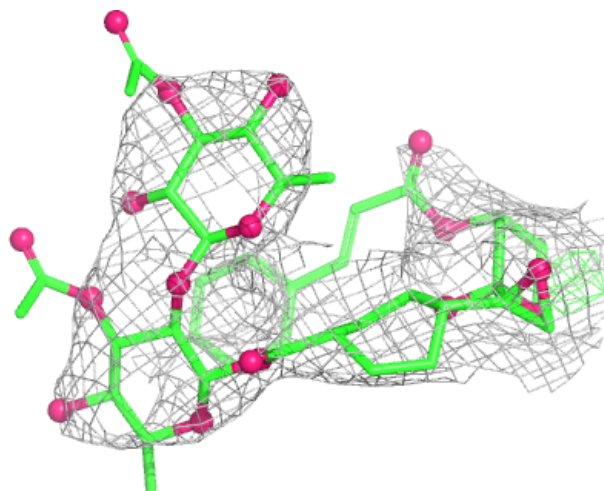
Electron density around PAR 4 201:

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



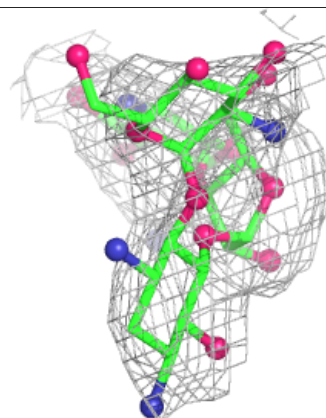
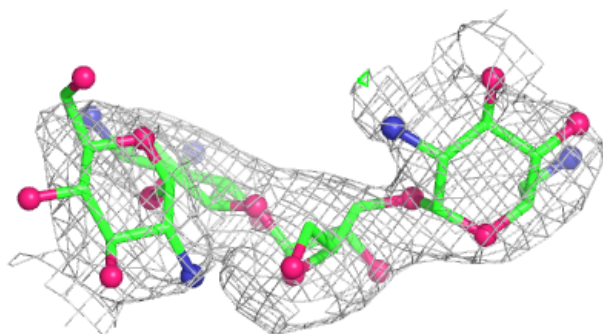
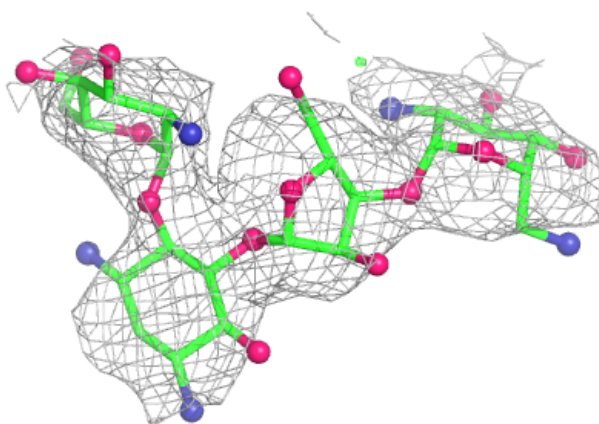
Electron density around 3K5 AS 3405:

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

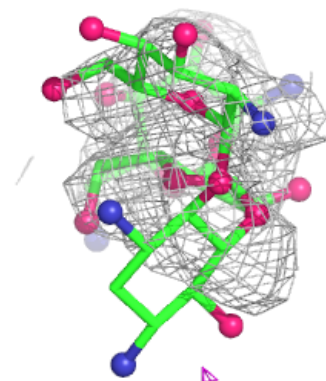
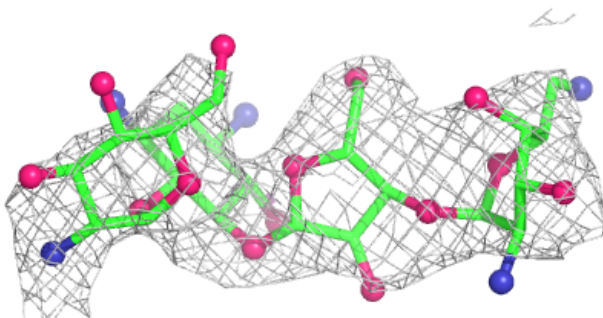
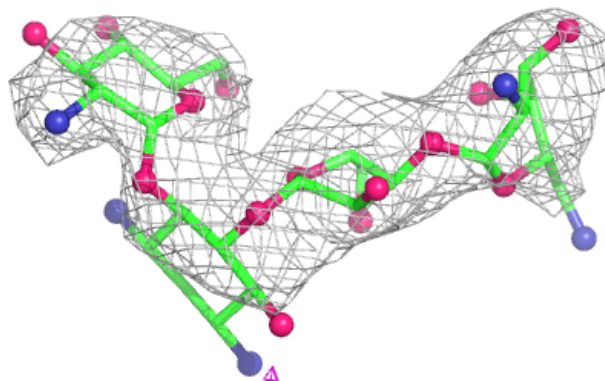


Electron density around PAR 1 3458:

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

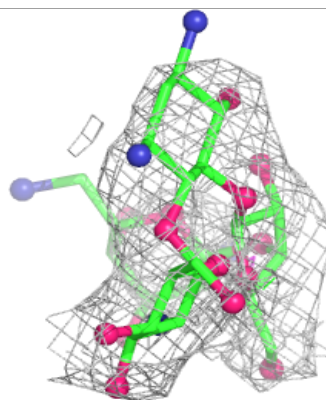
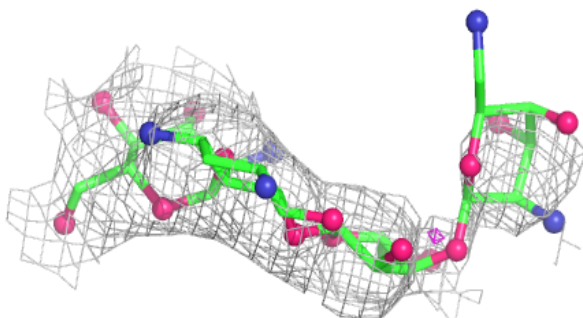
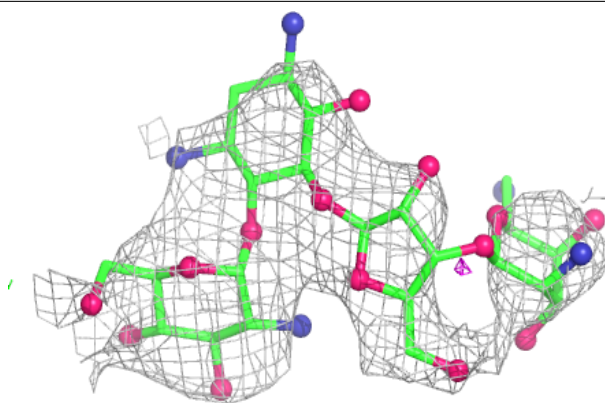
**Electron density around PAR 1 3464:**

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



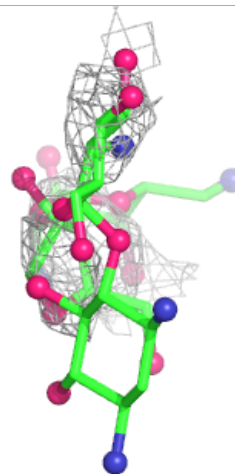
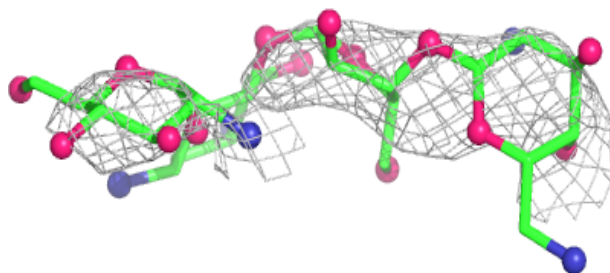
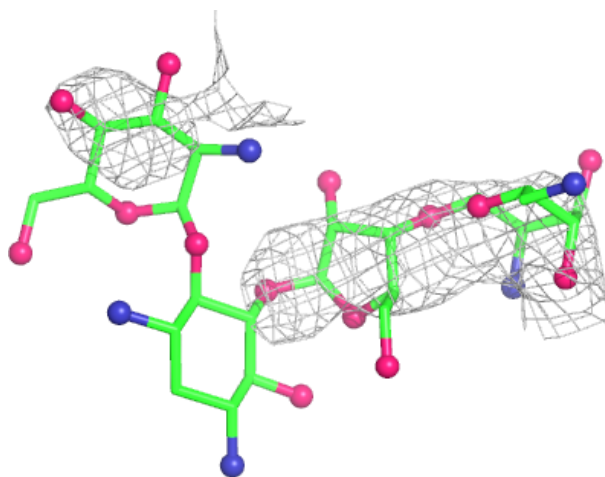
Electron density around PAR 1 3462:

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



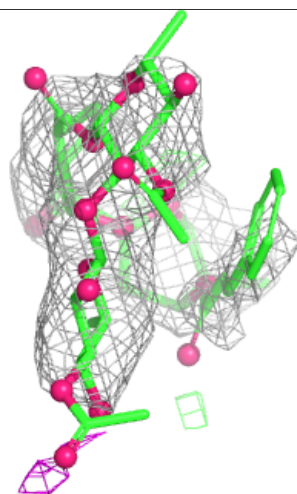
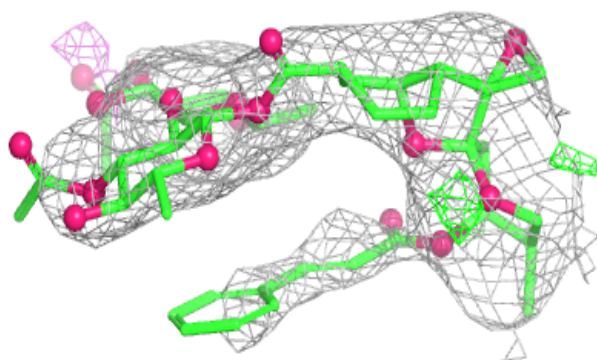
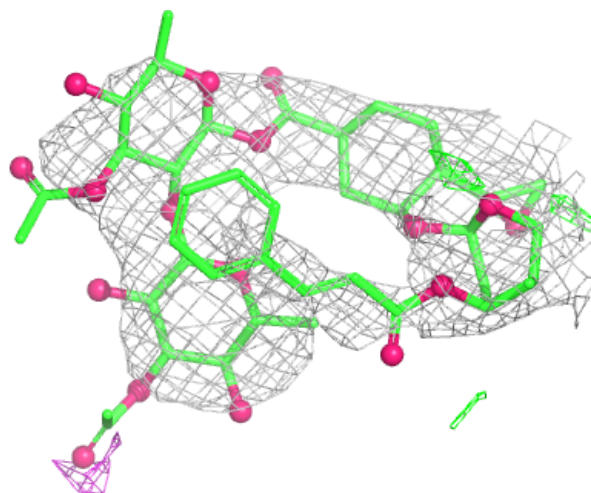
Electron density around PAR CM 1803:

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



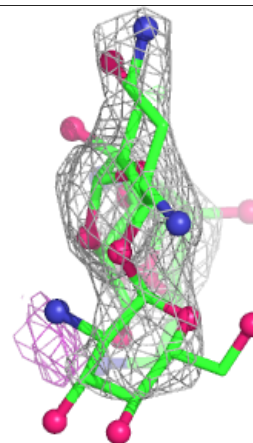
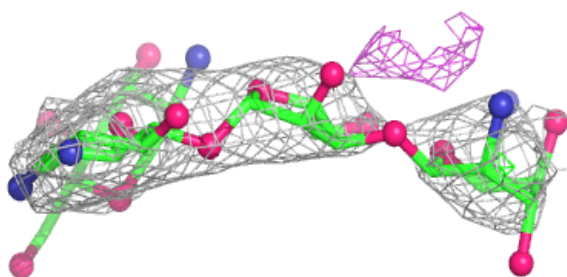
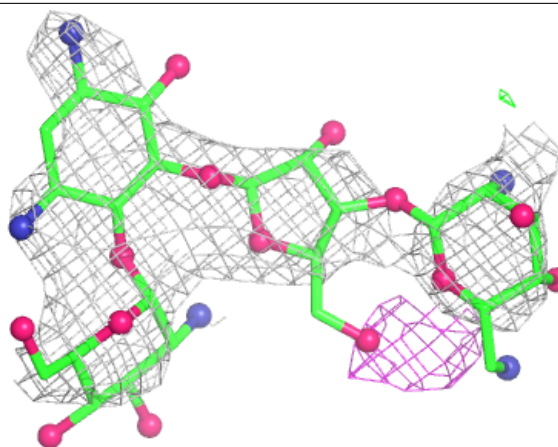
Electron density around 3K5 1 3463:

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



Electron density around PAR CM 1802:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.