



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:00 AM UTC

PDB ID : 4WOI / pdb_00004woi
Title : 4,5-linked aminoglycoside antibiotics regulate the bacterial ribosome by targeting dynamic conformational processes within intersubunit bridge B2
Authors : Pulk, A.; Cate, J.H.D.; Blanchard, S.; Wasserman, M.; Altman, R.; Zhou, Z.; Zinder, J.; Green, K.; Garneau-Tsodikova, S.
Deposited on : 2014-10-15
Resolution : 3.00 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

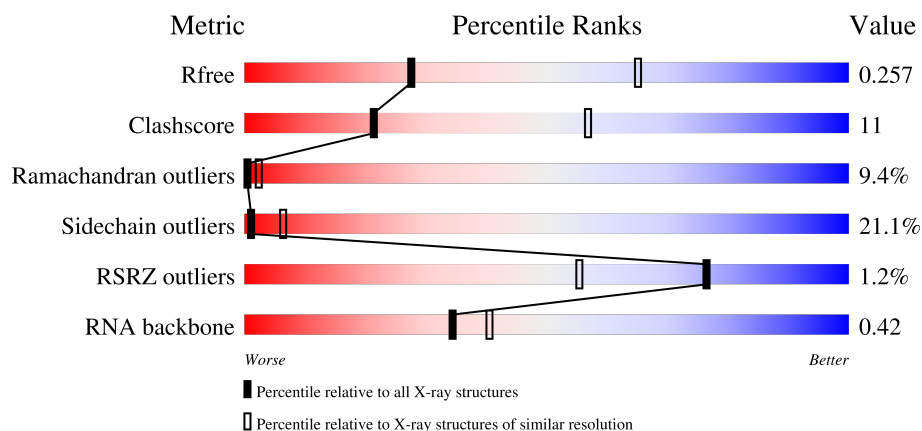
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



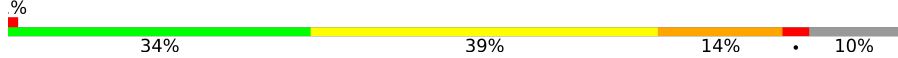
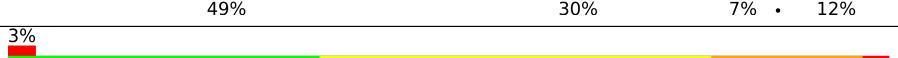
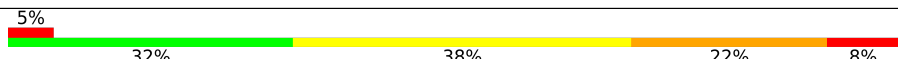
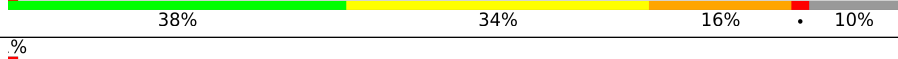
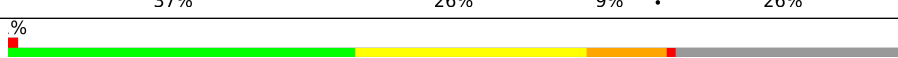
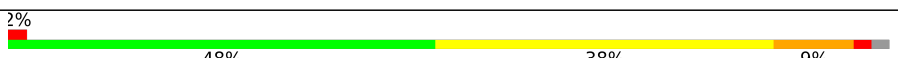
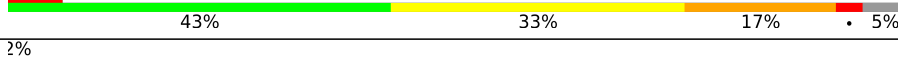
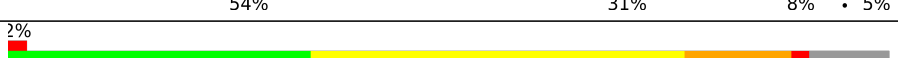
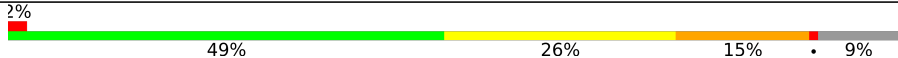
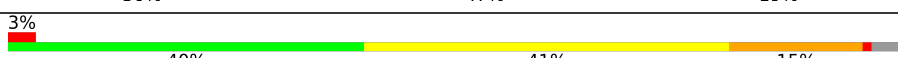
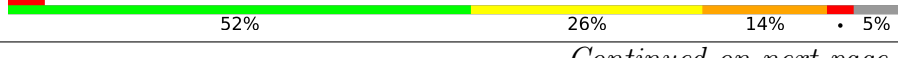
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	AA	1542	 54% 37% 9%
1	DA	1542	 56% 35% 9%
2	AB	241	 49% 27% 12% • 10%

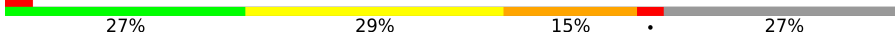
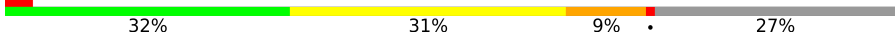
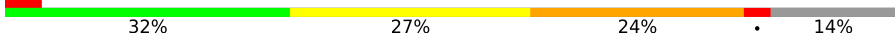
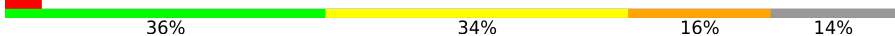
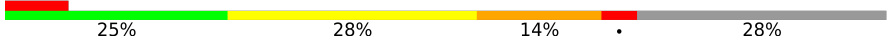
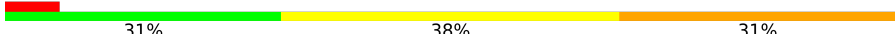
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Mol	Chain	Length	Quality of chain
2	DB	241	
3	AC	233	
3	DC	233	
4	AD	206	
4	DD	206	
5	AE	167	
5	DE	167	
6	AF	135	
6	DF	135	
7	AG	179	
7	DG	179	
8	AH	130	
8	DH	130	
9	AI	130	
9	DI	130	
10	AJ	103	
10	DJ	103	
11	AK	129	
11	DK	129	
12	AL	124	
12	DL	124	
13	AM	118	
13	DM	118	
14	AN	101	
14	DN	101	

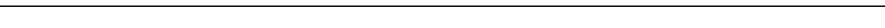
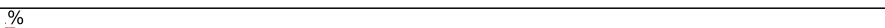
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Mol	Chain	Length	Quality of chain
15	AO	89	
15	DO	89	
16	AP	82	
16	DP	82	
17	AQ	84	
17	DQ	84	
18	AR	75	
18	DR	75	
19	AS	92	
19	DS	92	
20	AT	87	
20	DT	87	
21	AU	71	
21	DU	71	
22	AV	185	
23	AW	16	
23	DV	16	
24	AX	76	
24	DW	76	
25	BA	2904	
25	CA	2904	
26	BB	120	
26	CB	120	
27	BC	273	
27	CC	273	

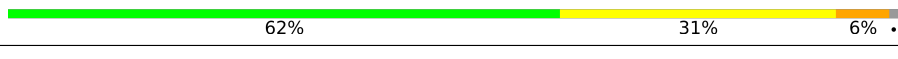
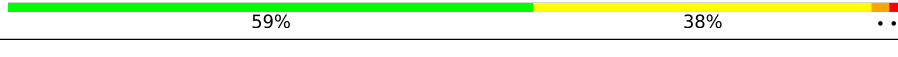
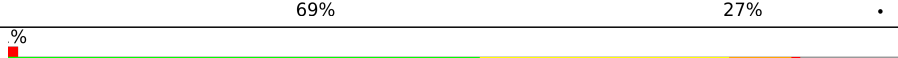
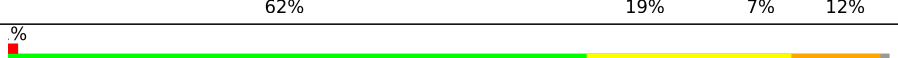
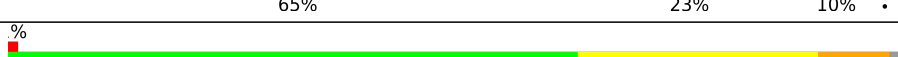
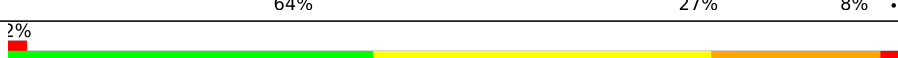
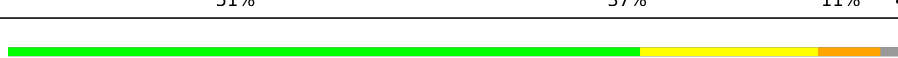
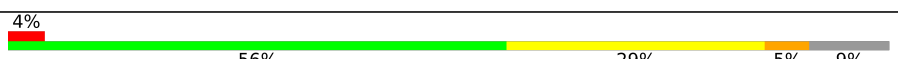
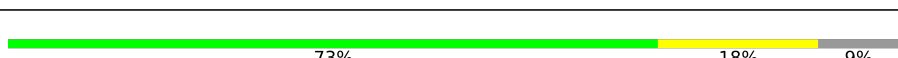
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Mol	Chain	Length	Quality of chain
28	BD	209	
28	CD	209	
29	BE	201	
29	CE	201	
30	BF	179	
30	CF	179	
31	BG	177	
31	CG	177	
32	BH	149	
32	CH	149	
33	BI	142	
33	CI	142	
34	BJ	142	
34	CJ	142	
35	BK	123	
35	CK	123	
36	BL	144	
36	CL	144	
37	BM	136	
37	CM	136	
38	BN	127	
38	CN	127	
39	BO	117	
39	CO	117	
40	BP	115	

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Mol	Chain	Length	Quality of chain
40	CP	115	
41	BQ	118	
41	CQ	118	
42	BR	103	
42	CR	103	
43	BS	110	
43	CS	110	
44	BT	100	
44	CT	100	
45	BU	104	
45	CU	104	
46	BV	94	
46	CV	94	
47	BW	85	
47	CW	85	
48	BX	78	
48	CX	78	
49	BY	63	
49	CY	63	
50	BZ	59	
50	CZ	59	
51	B0	57	
51	C0	57	
52	B1	55	
52	C1	55	

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Mol	Chain	Length	Quality of chain
53	B2	46	
53	C2	46	
54	B3	65	
54	C3	65	
55	B4	38	
55	C4	38	
56	B5	228	

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
57	MG	BA	3145	-	-	-	X
57	MG	BQ	201	-	-	-	X
58	PAR	BA	3005	-	-	X	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 294484 atoms, of which 450 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	DA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
2	DB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
3	DC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
4	DD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
5	DE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
6	DF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
7	DG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	DH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	DI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	DJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	DK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
12	DL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
13	DM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	DN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			
15	DO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	DP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
17	DQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
18	DR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
19	DS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
20	DT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
21	DU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a protein called Ribosome-recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	183	Total	C	N	O	S	0	0	0
			1419	871	260	283	5			

- Molecule 23 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	15	Total	C	N	O	P	0	0	0
			324	145	61	103	15			
23	DV	16	Total	C	N	O	P	0	0	0
			346	155	66	109	16			

- Molecule 24 is a RNA chain called Phenylalanine specific transfer RNA, tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
24	DW	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
25	CA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
26	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
27	CC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
28	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
29	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
30	CF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
31	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	149	Total	C	N	O	S	0	0	0
			1107	696	197	213	1			
32	CH	149	Total	C	N	O	S	0	0	0
			1107	696	197	213	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
33	CI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
34	CJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
35	CK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
36	CL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
38	CN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BO	116	Total	C	N	O	S	0	0	0
			892	552	178	162				
39	CO	116	Total	C	N	O	S	0	0	0
			892	552	178	162				

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
40	CP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				
41	CQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
42	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
43	CS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
44	CT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BU	102	Total	C	N	O	0	0	0
			779	492	146	141			
45	CU	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
46	CV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BW	76	Total	C	N	O	S	0	0	0
			580	359	117	103	1			
47	CW	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
48	CX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
49	CY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
50	CZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
51	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
52	C1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
54	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
55	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 56 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B5	191	Total	C	N	O		0	0	1
			1142	691	221	230				

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

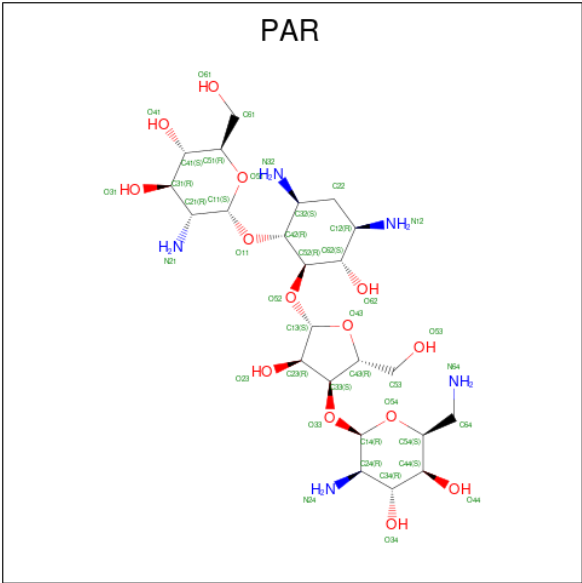
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	71	Total	Mg	0	0
			71	71		
57	AN	1	Total	Mg	0	0
			1	1		
57	BA	189	Total	Mg	0	0
			189	189		
57	BB	4	Total	Mg	0	0
			4	4		
57	BL	2	Total	Mg	0	0
			2	2		
57	BO	1	Total	Mg	0	0
			1	1		
57	BQ	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CA	165	Total	Mg	0	0
			165	165		
57	CB	3	Total	Mg	0	0
			3	3		
57	CD	1	Total	Mg	0	0
			1	1		
57	CQ	1	Total	Mg	0	0
			1	1		
57	DA	53	Total	Mg	0	0
			53	53		
57	DD	2	Total	Mg	0	0
			2	2		
57	DN	1	Total	Mg	0	0
			1	1		

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	AA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		
58	BA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		
58	BA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		
58	BA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	BA	1	Total C H N O 87 23 45 5 14	0	0
58	BA	1	Total C N O 42 23 5 14	0	0
58	CA	1	Total C N O 42 23 5 14	0	0
58	CA	1	Total C H N O 87 23 45 5 14	0	0
58	CA	1	Total C H N O 87 23 45 5 14	0	0
58	CA	1	Total C N O 42 23 5 14	0	0
58	CA	1	Total C H N O 87 23 45 5 14	0	0
58	DA	1	Total C H N O 87 23 45 5 14	0	0
58	DA	1	Total C H N O 87 23 45 5 14	0	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	B4	1	Total Zn 1 1	0	0
59	C4	1	Total Zn 1 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AA	192	Total O 192 192	0	0
60	AE	3	Total O 3 3	0	0
60	AL	1	Total O 1 1	0	0
60	AN	2	Total O 2 2	0	0
60	AT	5	Total O 5 5	0	0
60	BA	626	Total O 626 626	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BB	14	Total 14	O 14	0	0
60	BC	7	Total 7	O 7	0	0
60	BD	2	Total 2	O 2	0	0
60	BE	1	Total 1	O 1	0	0
60	BF	1	Total 1	O 1	0	0
60	BL	8	Total 8	O 8	0	0
60	BN	2	Total 2	O 2	0	0
60	BQ	1	Total 1	O 1	0	0
60	BS	1	Total 1	O 1	0	0
60	BT	3	Total 3	O 3	0	0
60	B3	1	Total 1	O 1	0	0
60	B4	1	Total 1	O 1	0	0
60	CA	608	Total 608	O 608	0	0
60	CB	14	Total 14	O 14	0	0
60	CC	10	Total 10	O 10	0	0
60	CD	5	Total 5	O 5	0	0
60	CE	3	Total 3	O 3	0	0
60	CJ	2	Total 2	O 2	0	0
60	CL	7	Total 7	O 7	0	0
60	CN	2	Total 2	O 2	0	0
60	CT	3	Total 3	O 3	0	0

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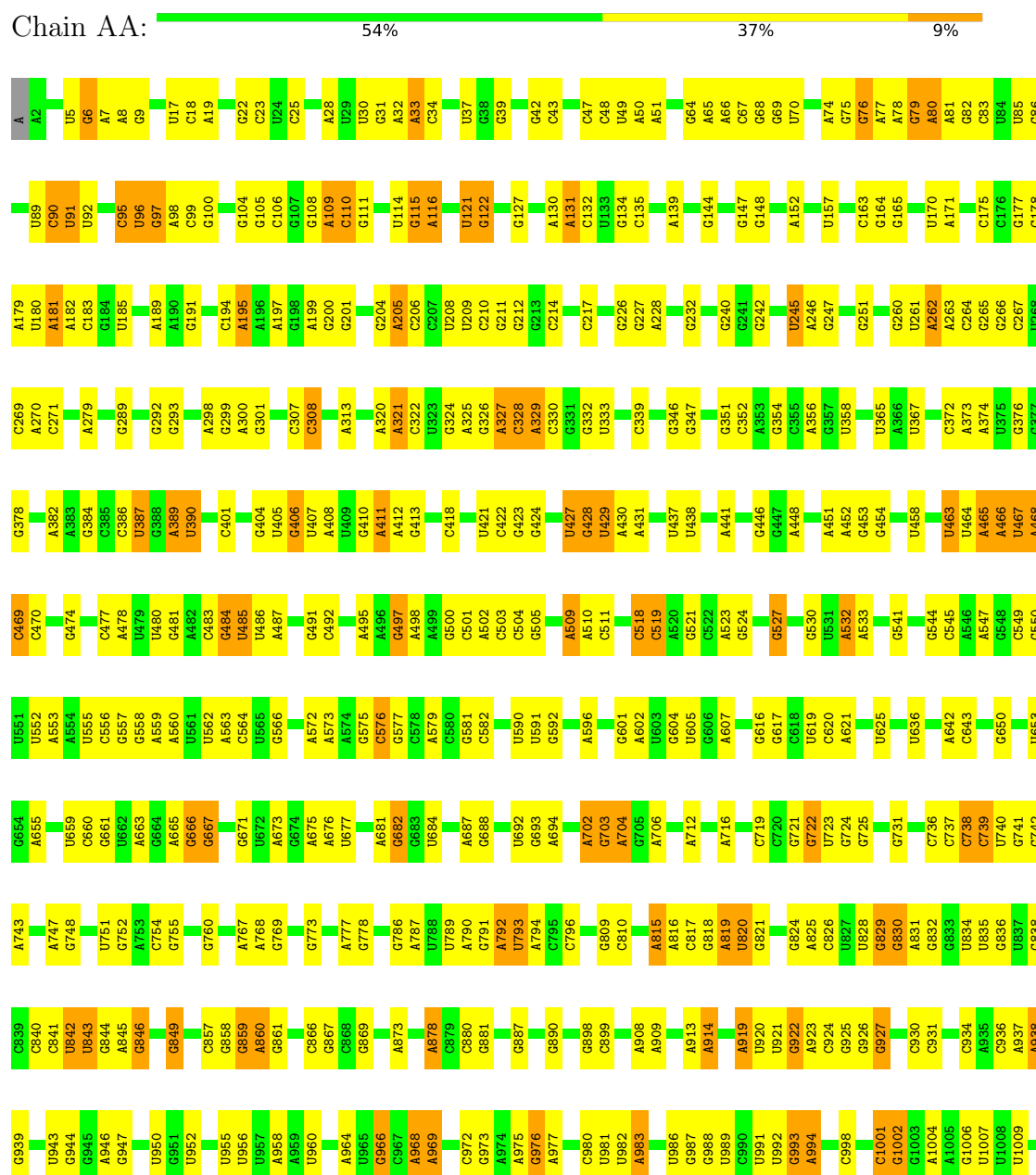
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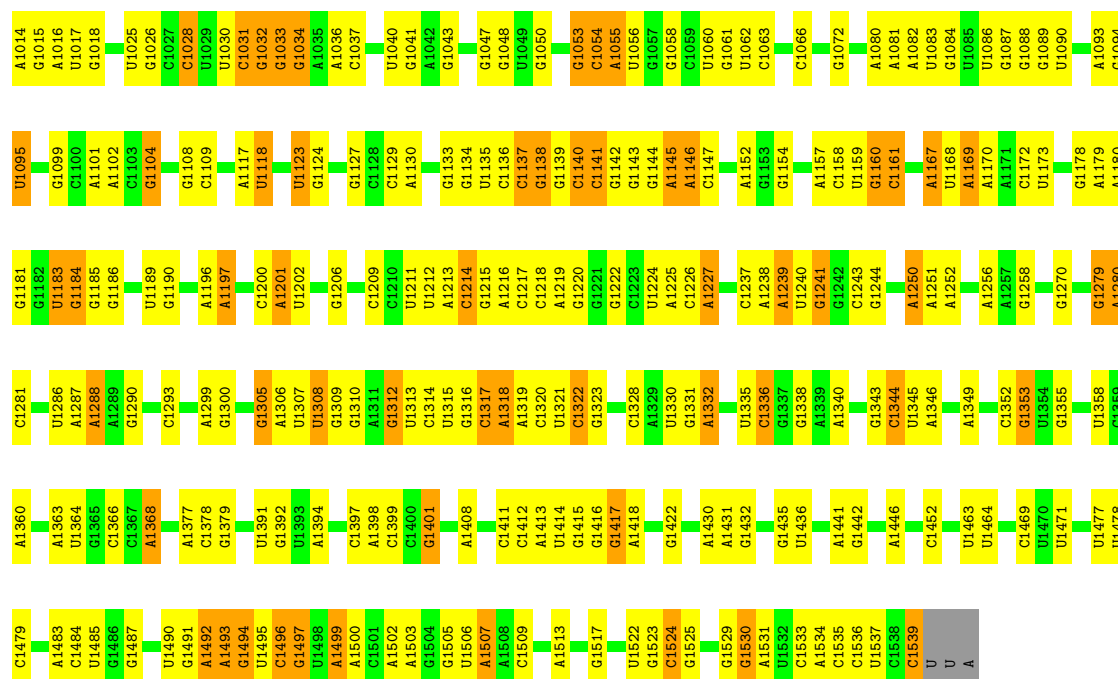
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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60	C3	1	Total 1	O 1	0	0
60	C4	2	Total 2	O 2	0	0
60	DA	184	Total 184	O 184	0	0
60	DD	2	Total 2	O 2	0	0
60	DK	2	Total 2	O 2	0	0
60	DL	2	Total 2	O 2	0	0
60	DN	4	Total 4	O 4	0	0
60	DT	3	Total 3	O 3	0	0
60	DU	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

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.

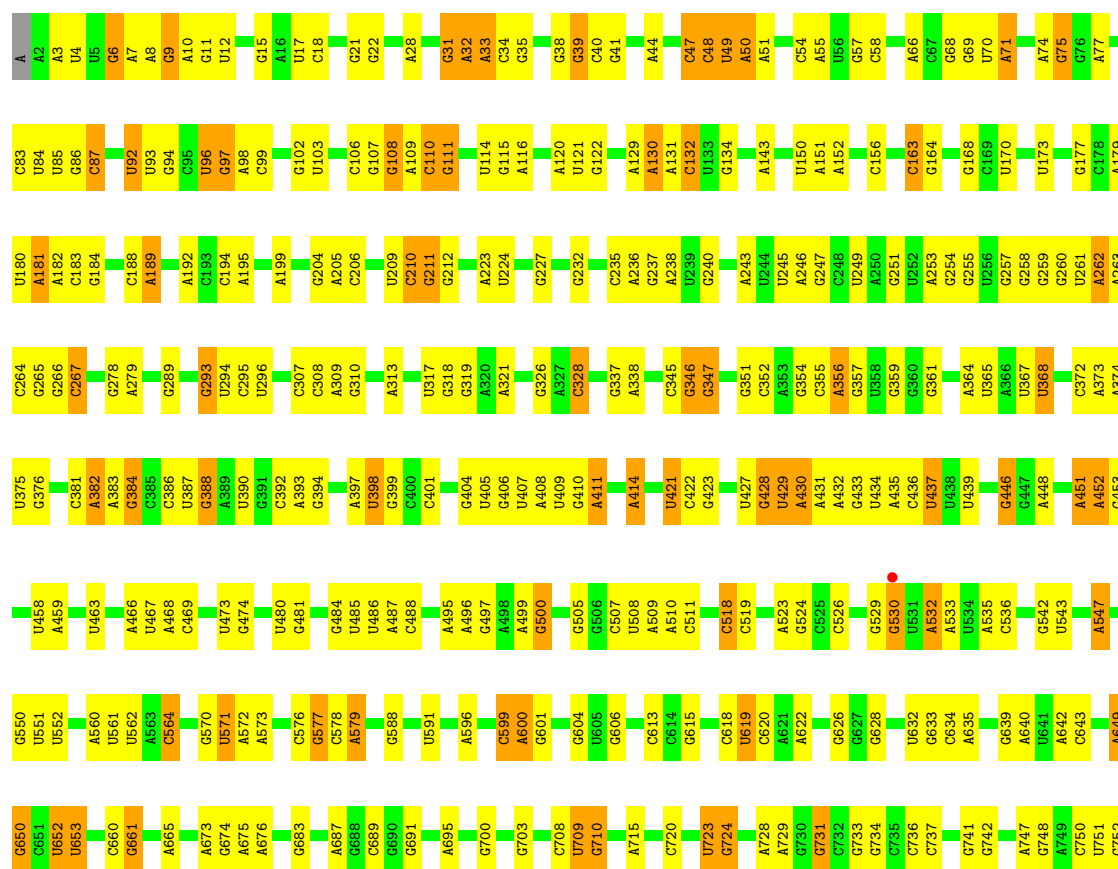
• Molecule 1: 16S ribosomal RNA

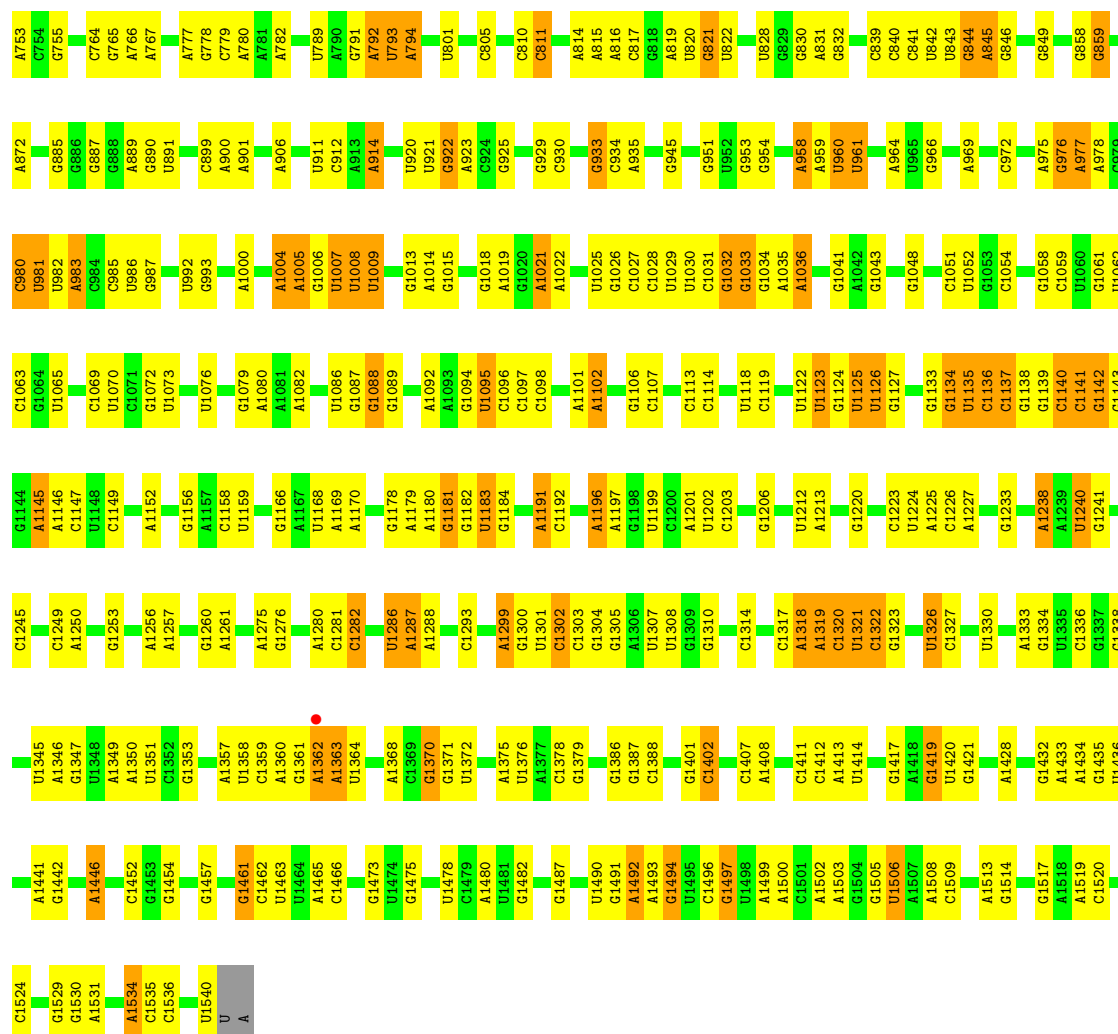


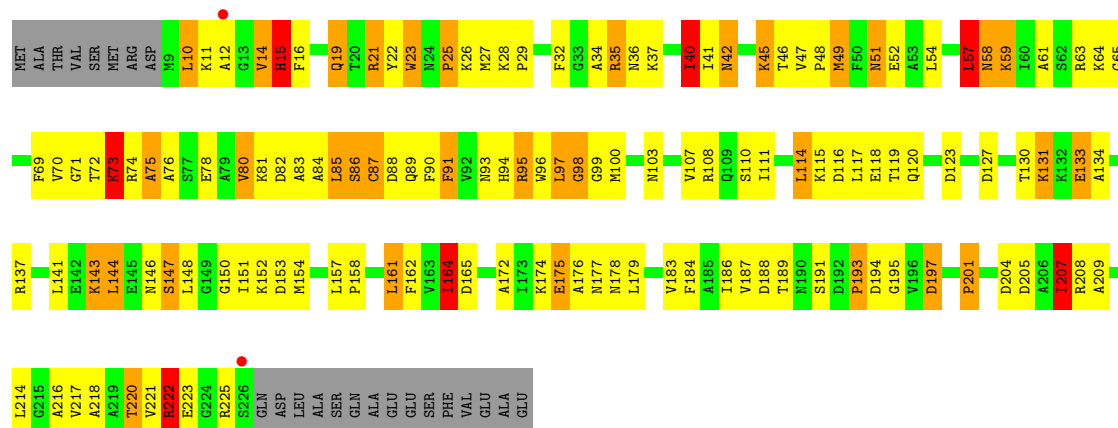


• Molecule 1: 16S ribosomal RNA

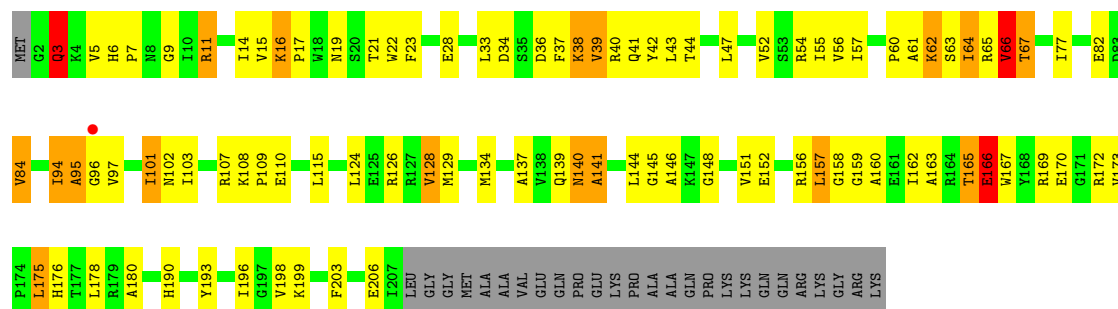
Chain DA: 56% 35% 9%



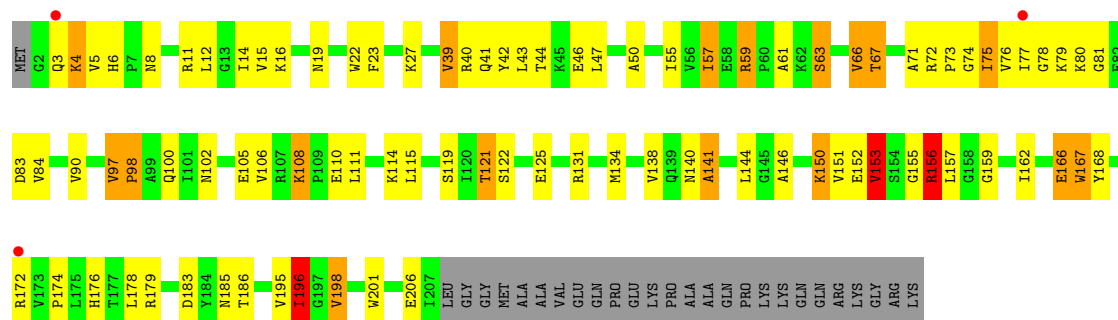




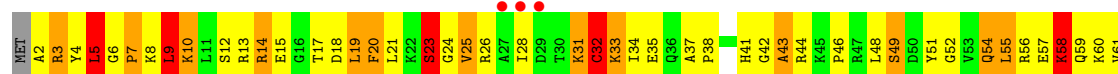
• Molecule 3: 30S ribosomal protein S3

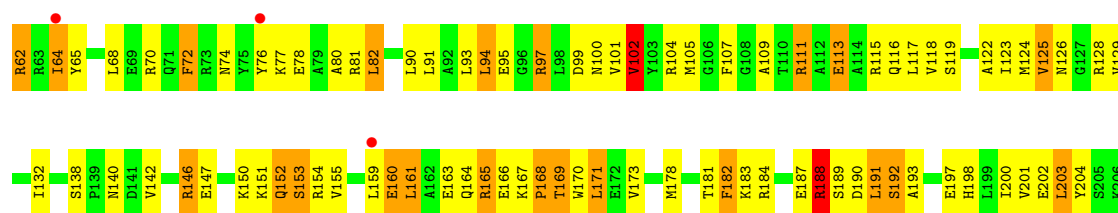


• Molecule 3: 30S ribosomal protein S3

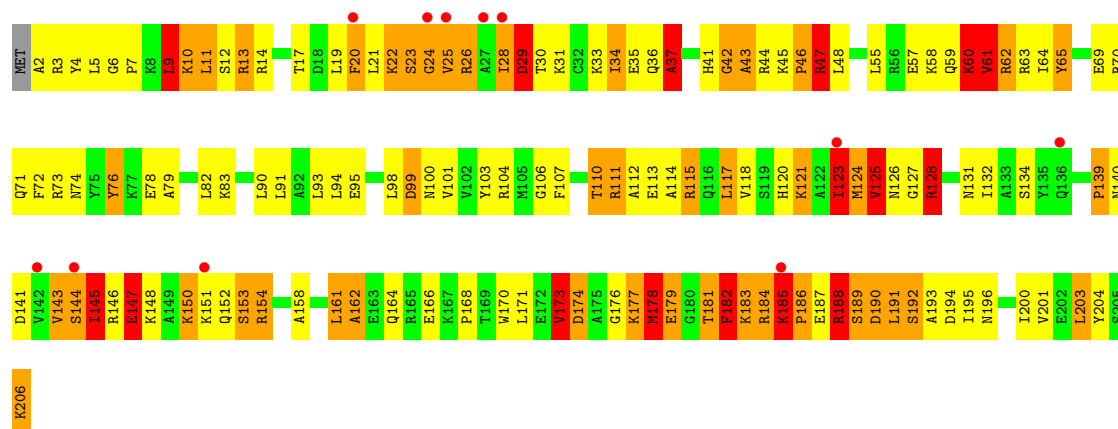


• Molecule 4: 30S ribosomal protein S4

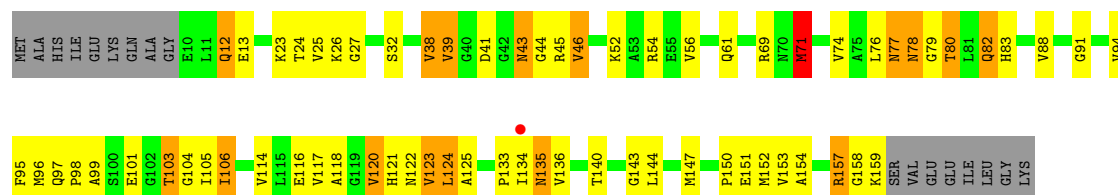




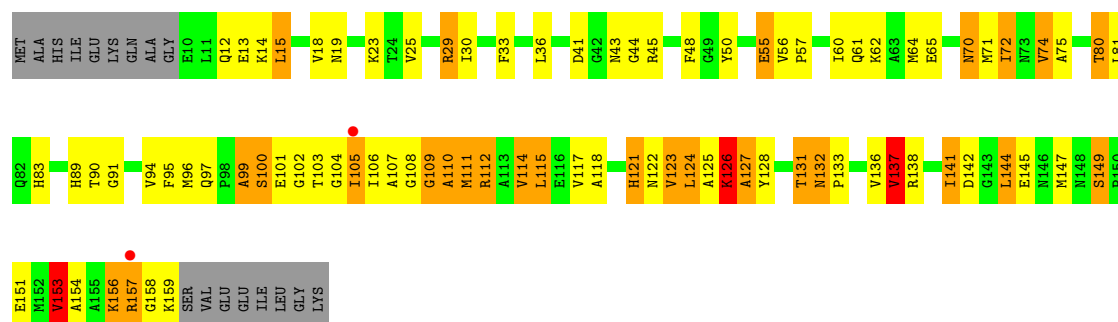
• Molecule 4: 30S ribosomal protein S4



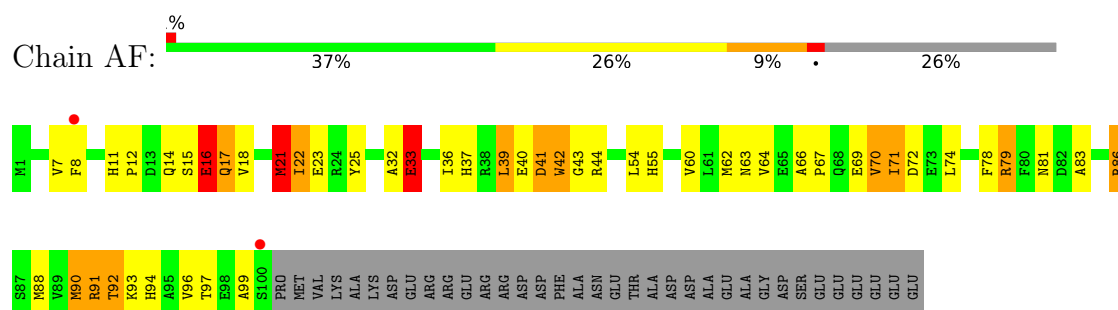
• Molecule 5: 30S ribosomal protein S5



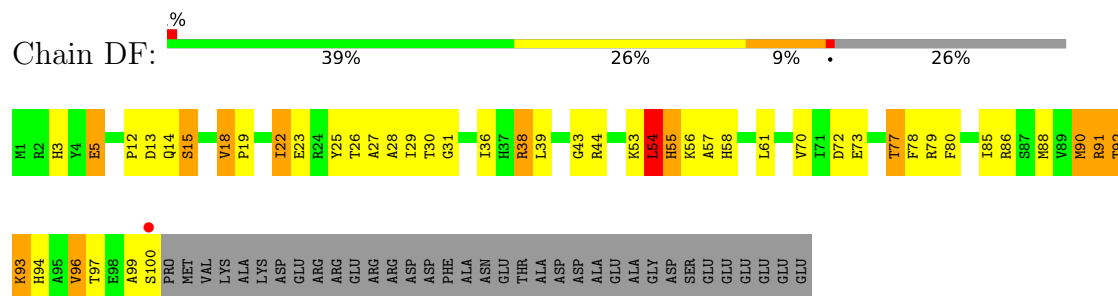
• Molecule 5: 30S ribosomal protein S5



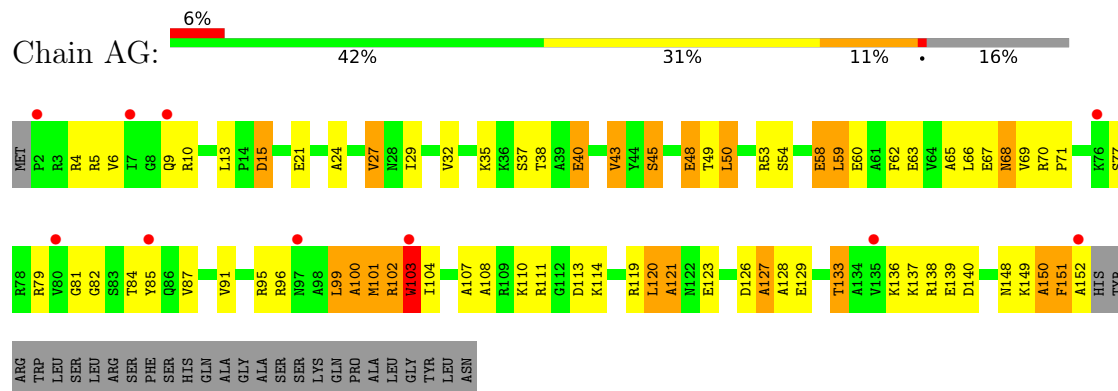
• Molecule 6: 30S ribosomal protein S6



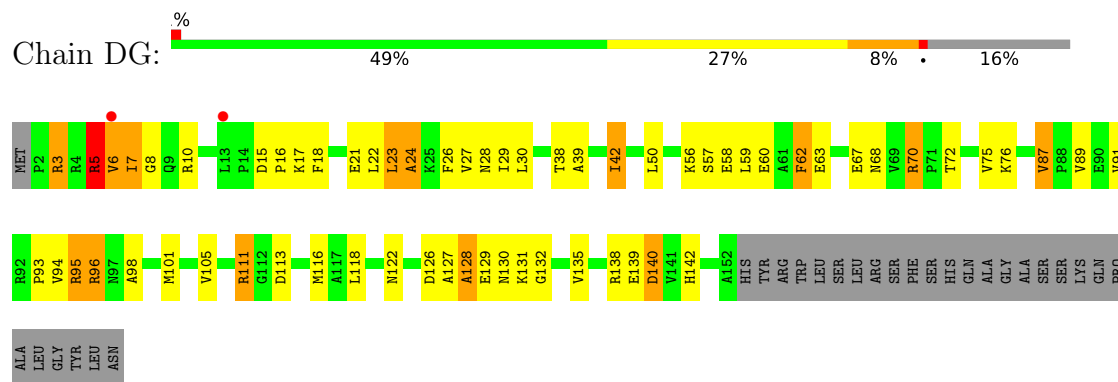
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

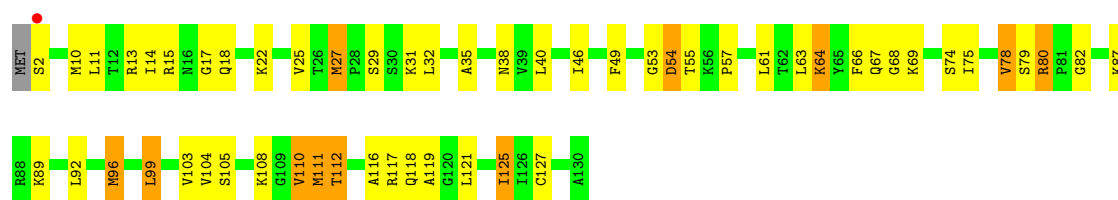


• Molecule 7: 30S ribosomal protein S7

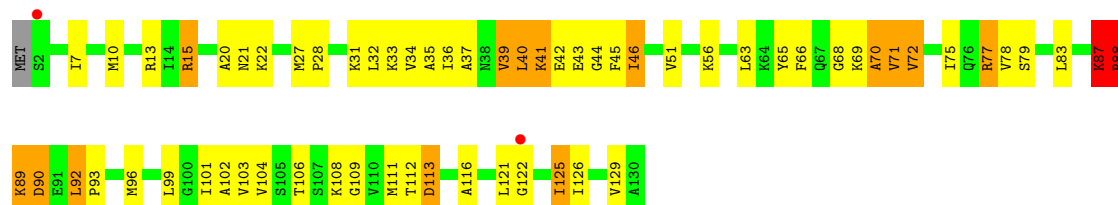


• Molecule 8: 30S ribosomal protein S8

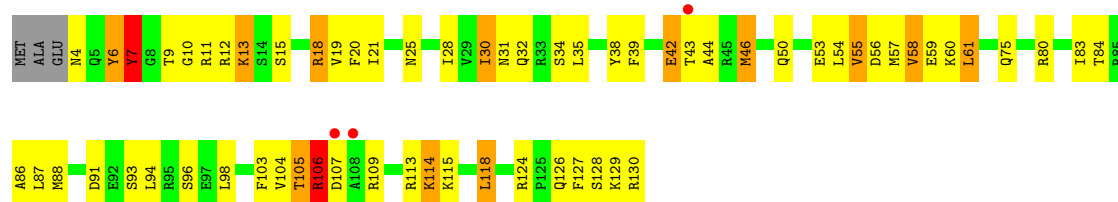




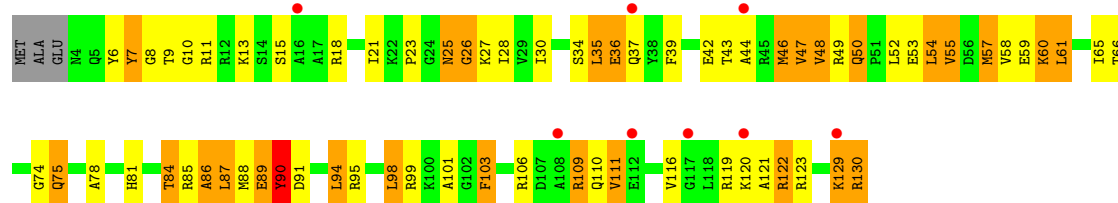
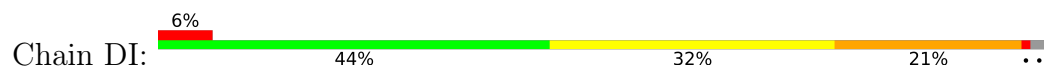
• Molecule 8: 30S ribosomal protein S8



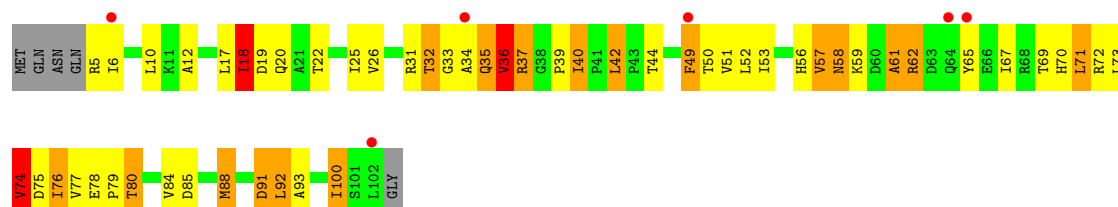
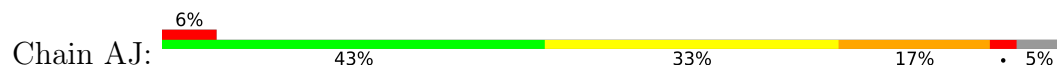
• Molecule 9: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S9

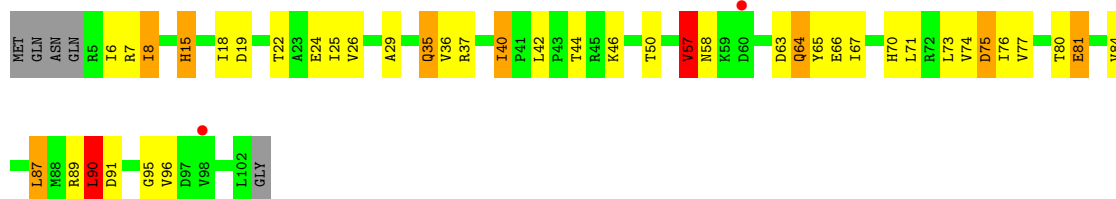


• Molecule 10: 30S ribosomal protein S10



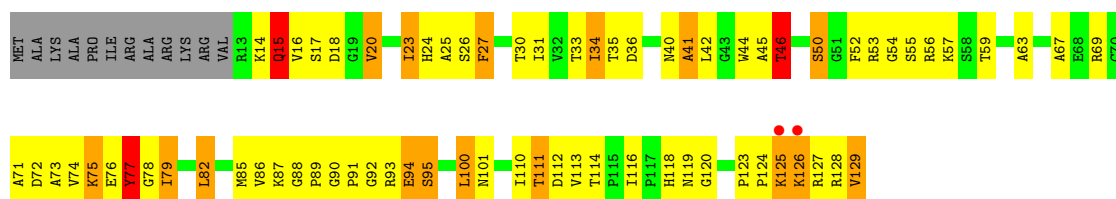
- Molecule 10: 30S ribosomal protein S10

Chain DJ: 



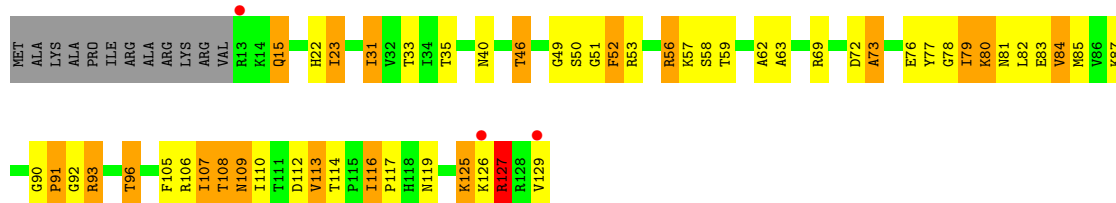
- Molecule 11: 30S ribosomal protein S11

Chain AK: 

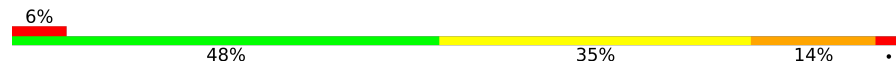


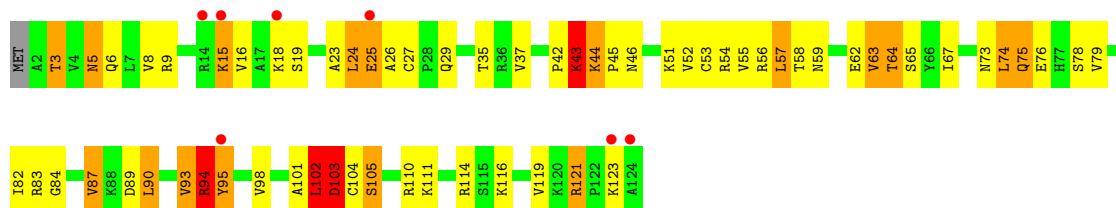
- Molecule 11: 30S ribosomal protein S11

Chain DK: 



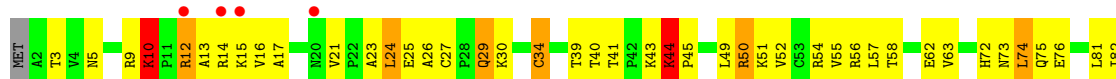
- Molecule 12: 30S ribosomal protein S12

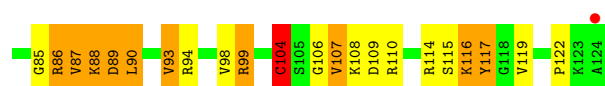
Chain AL: 



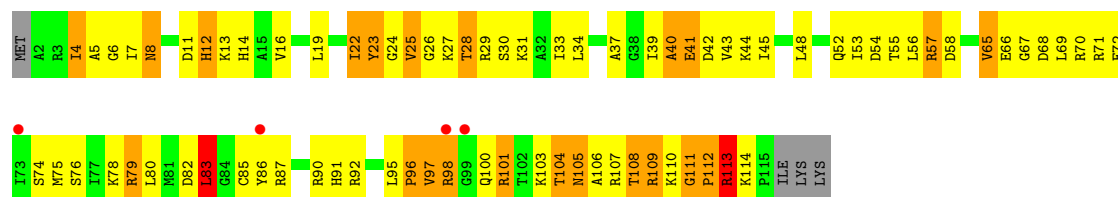
- Molecule 12: 30S ribosomal protein S12

Chain DL: 

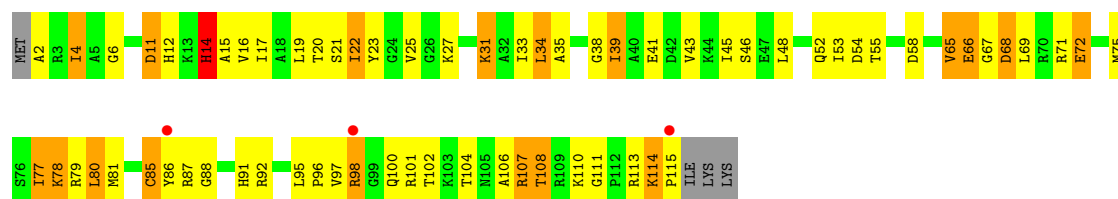
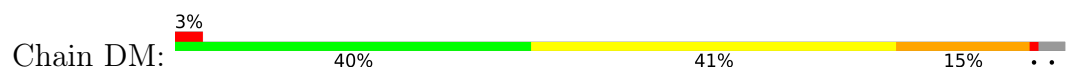




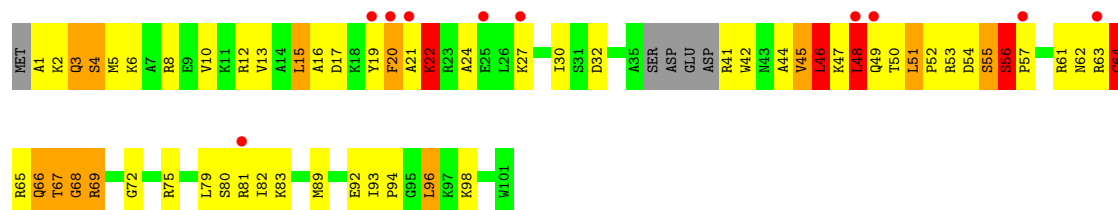
• Molecule 13: 30S ribosomal protein S13



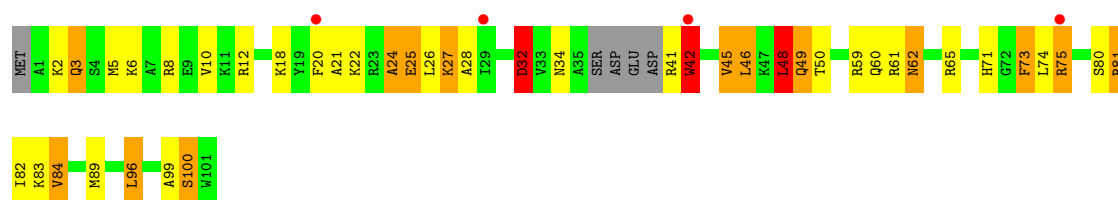
• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14

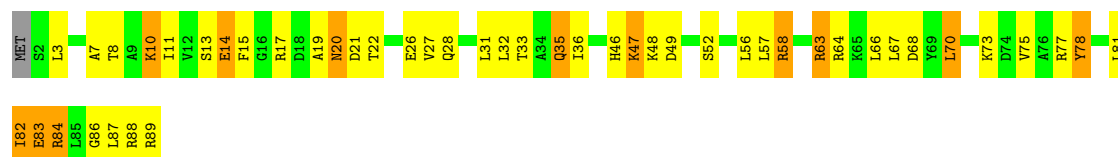


• Molecule 14: 30S ribosomal protein S14



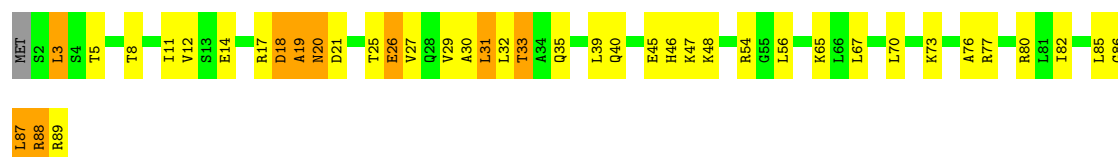
• Molecule 15: 30S ribosomal protein S15





- Molecule 15: 30S ribosomal protein S15

Chain DO: 53% 36% 10% .



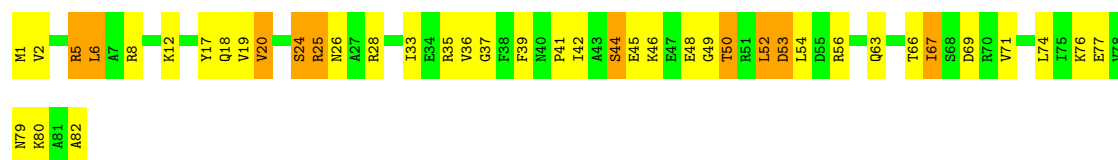
- Molecule 16: 30S ribosomal protein S16

Chain AP: 55% 29% 13% .



- Molecule 16: 30S ribosomal protein S16

Chain DP: 49% 39% 12%



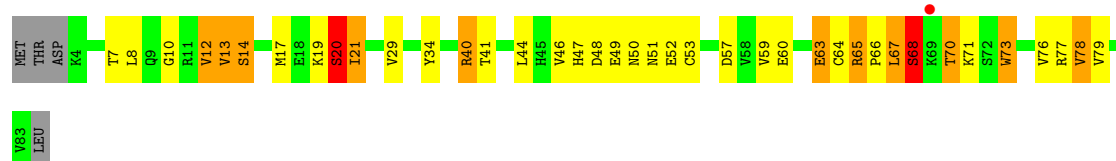
- Molecule 17: 30S ribosomal protein S17

Chain AQ: 52% 30% 13% 5%

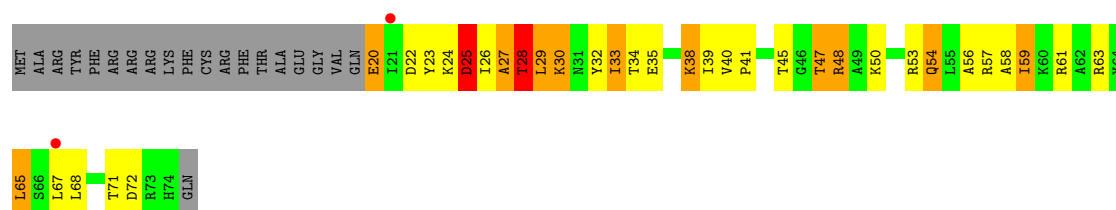
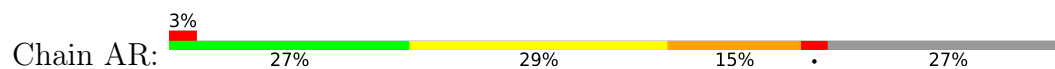


- Molecule 17: 30S ribosomal protein S17

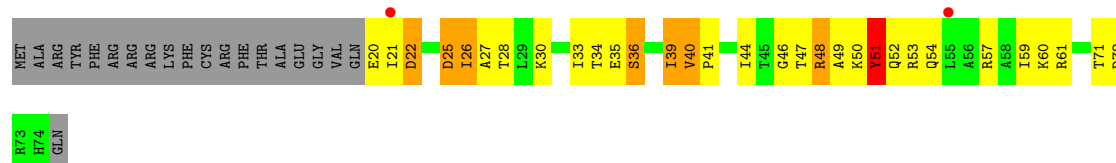
Chain DQ: 49% 31% 13% 5%



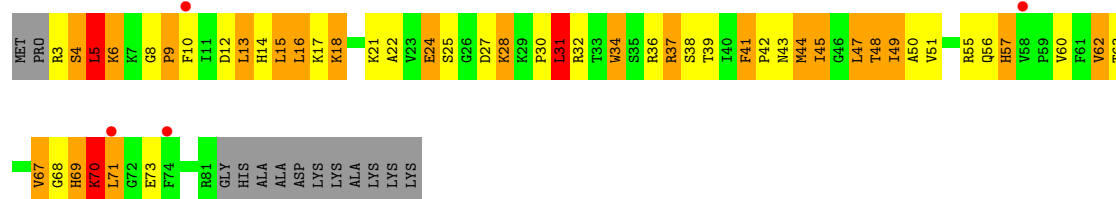
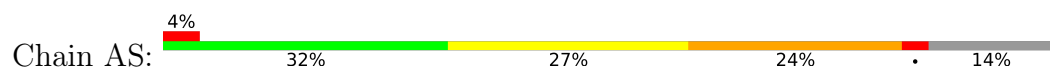
- Molecule 18: 30S ribosomal protein S18



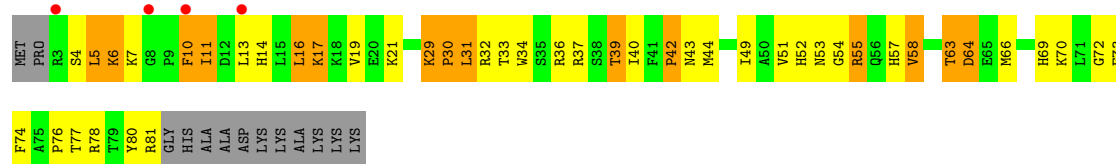
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19



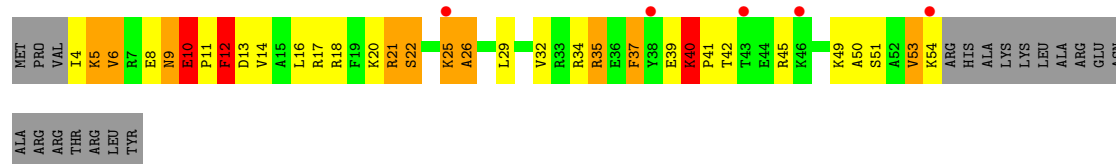
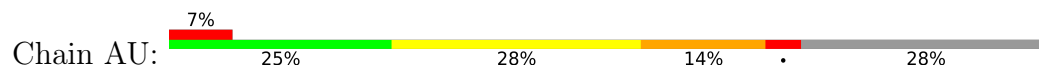
- Molecule 20: 30S ribosomal protein S20



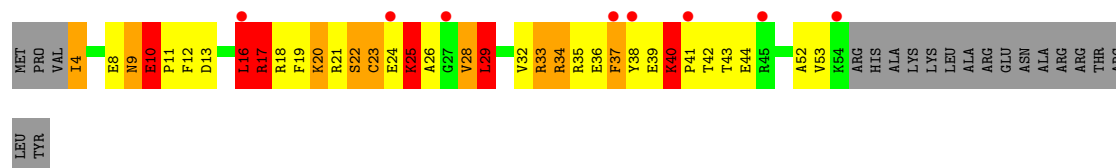
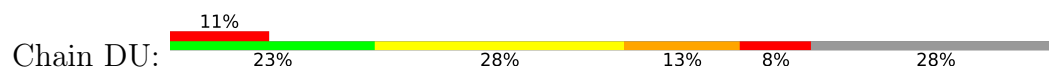
- Molecule 20: 30S ribosomal protein S20



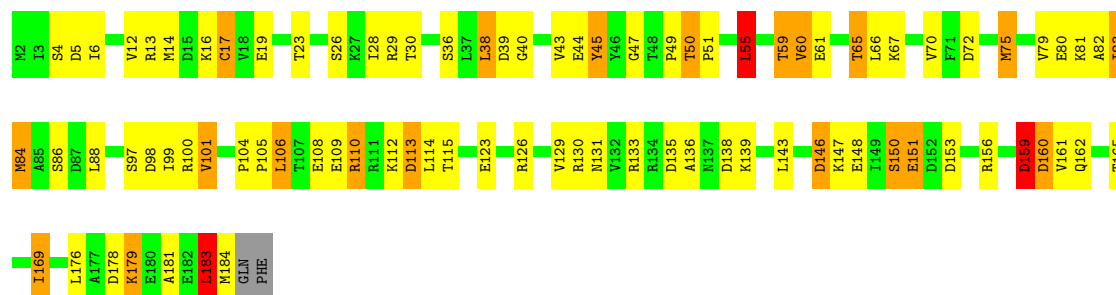
- Molecule 21: 30S ribosomal protein S21



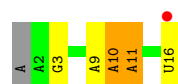
- Molecule 21: 30S ribosomal protein S21



- Molecule 22: Ribosome-recycling factor

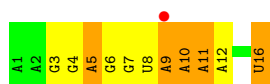


- Molecule 23: Messenger RNA

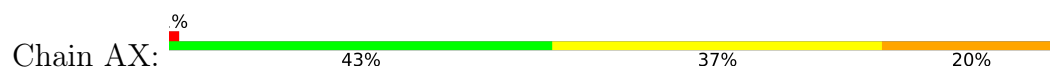


- Molecule 23: Messenger RNA

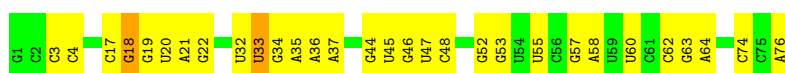




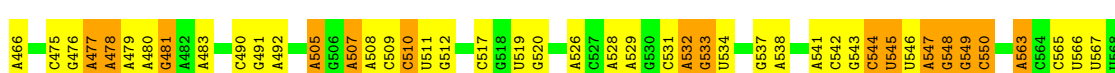
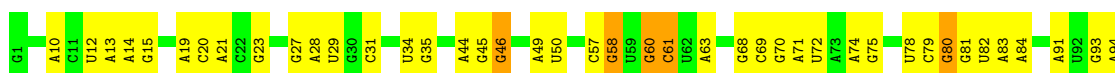
- Molecule 24: Phenylalanine specific transfer RNA, tRNA-Phe



- Molecule 24: Phenylalanine specific transfer RNA, tRNA-Phe



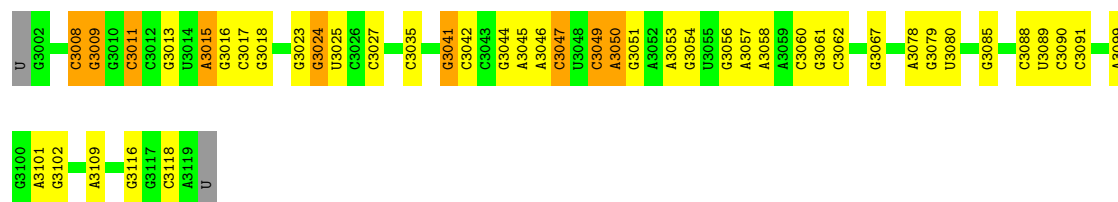
- Molecule 25: 23S ribosomal RNA







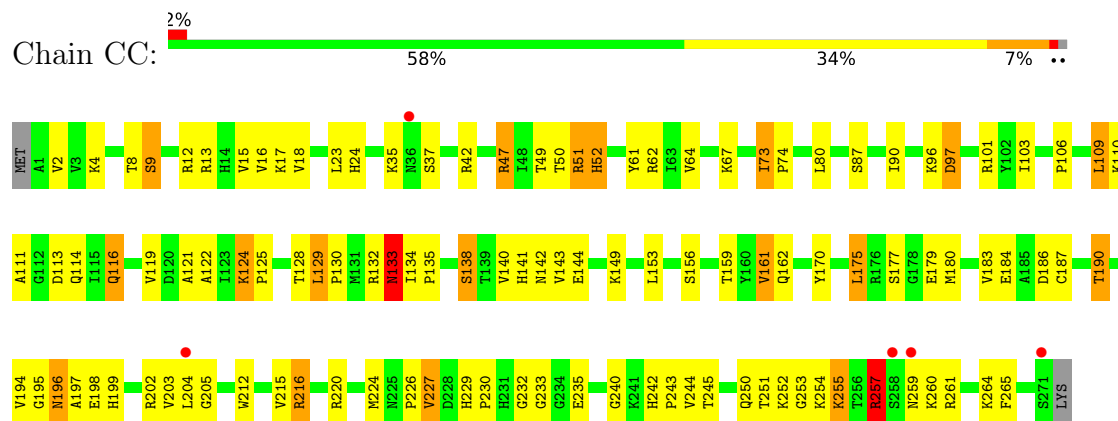
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A1927	G1930	A1936	A1937	A1938	U1939	U1940	U1943	A1948	G1949	A1952	U1955	U1961	G1964	C1965	A1966	C1967	G1968	A1969	A1970	U1971	G1972	U1979	U1980	C1986	U1991	G1992	U1993	C1994	U1995	C1996	A1998	C1999	C2000	C2001	G2004	A2005	C2006	U2011	G2012	U2016	U2017	G2018	U2019	A2101	C2104											
C1837	C1838	G1839	G1842	C1843	C1844	G1845	G1846	A1847	A1848	G1849	G1850	U1851	U1852	A1853	G1857	A1858	U1859	U1865	A1866	G1867	C1868	G1869	C1870	A1871	A1872	G1873	C1874	G1875	C1881	U1882	C1883	G1884	A1885	C1893	A1894	A1895	C1896	A1898	U1899	A1900	C1905	G1906	G1907	C1908	A1912	A1913	C1914	U1915	A1916	U1917	U1918	G1919	A1920	A1921	C1922	U1923
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G1025	G1026	A1027	A1028	U1033	C1044	G1047	G1055	G1056	U1057	U1058	U1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	C1072	A1073	G1074	C1075	U1078	C1079	U1082	A1085	A1086	G1087	A1088	A1089	A1090	C1091	C1092	G1093	U1094	A1095	A1096	U1097	C1013	A1014	C1102	A1103	C1104	U1105	G1106						
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U767	U768	C769	A761	U762	G763	A764	C765	G774	G775	G776	G777	A782	C873	G874	A785	U790	C791	A792	U793	G894	C795	C796	G797	A800	G801	G805	U810	U811	A716	C812	C817	G818	U824	A825	U826	U827	U828	A829	G830	G831	U832	A833	G834	C838	U839	G843	A844	U845	U846							



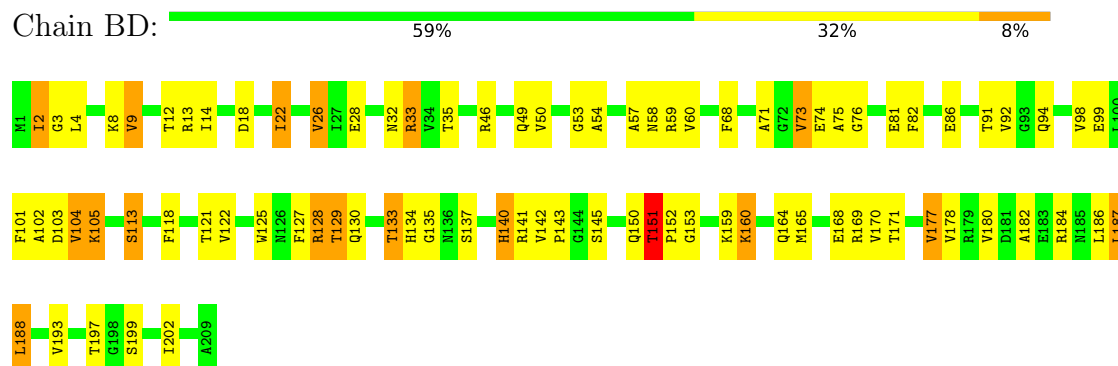
• Molecule 27: 50S ribosomal protein L2



• Molecule 27: 50S ribosomal protein L2

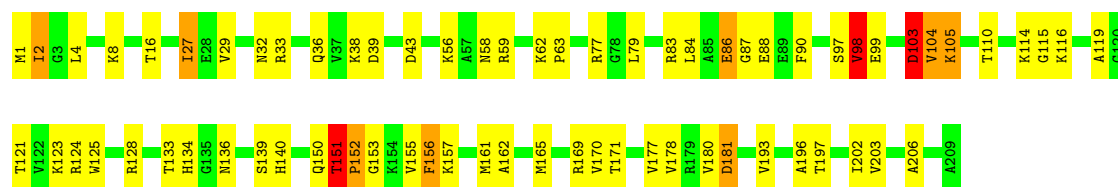


• Molecule 28: 50S ribosomal protein L3



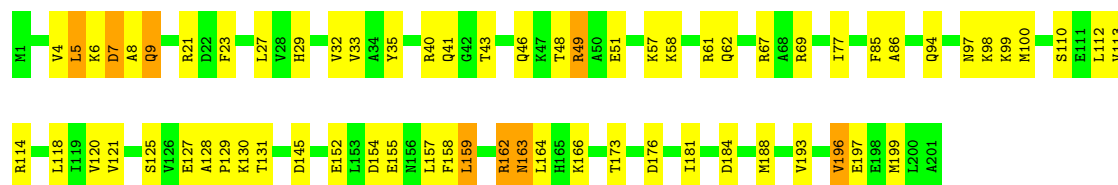
• Molecule 28: 50S ribosomal protein L3

Chain CD:  67% 28% . .



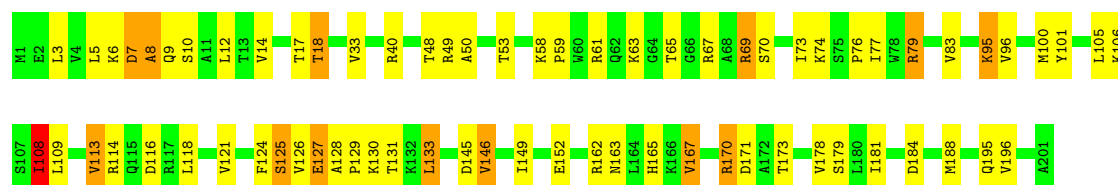
- Molecule 29: 50S ribosomal protein L4

Chain BE:  67% 29% .



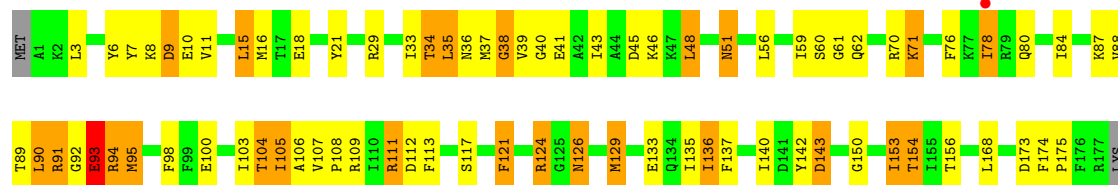
- Molecule 29: 50S ribosomal protein L4

Chain CE:  65% 28% 6%



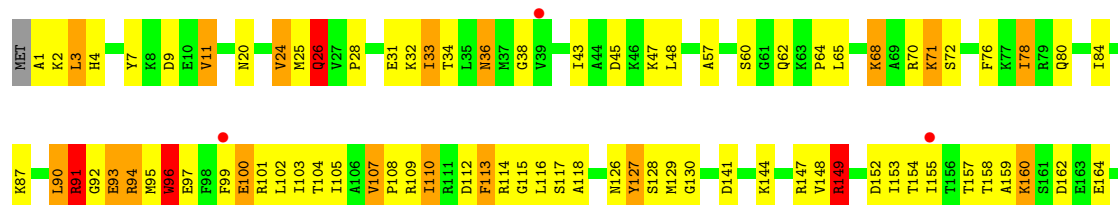
- Molecule 30: 50S ribosomal protein L5

Chain BF:  % 55% 30% 13% . .



- Molecule 30: 50S ribosomal protein L5

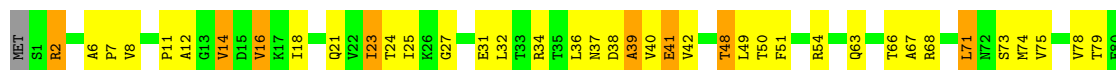
Chain CF:  2% 51% 36% 10% . .





- Molecule 31: 50S ribosomal protein L6

Chain BG: 59% 31% 9% ..



- Molecule 31: 50S ribosomal protein L6

Chain CG: 59% 36% . .



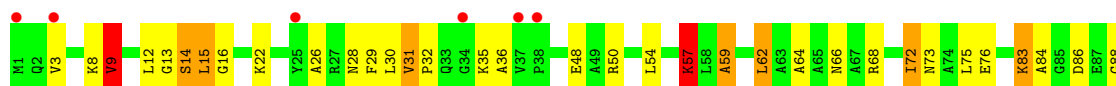
- Molecule 32: 50S ribosomal protein L9

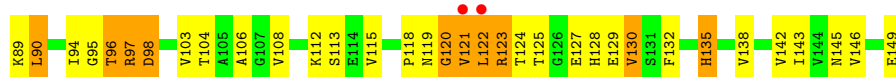
Chain BH: 42% 38% 17% .



- Molecule 32: 50S ribosomal protein L9

Chain CH: 54% 33% 11% .





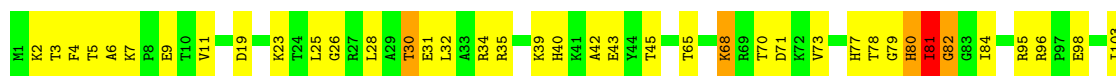
- Molecule 33: 50S ribosomal protein L11



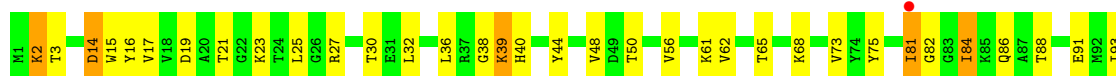
- Molecule 33: 50S ribosomal protein L11



- Molecule 34: 50S ribosomal protein L13

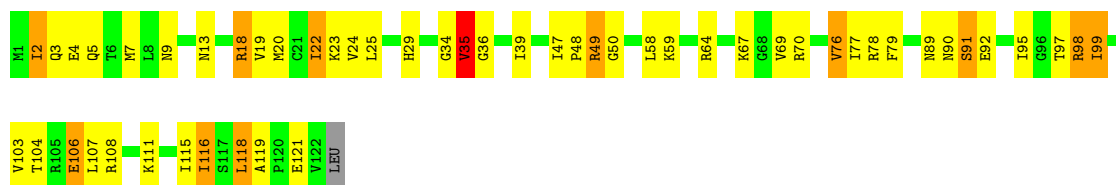


- Molecule 34: 50S ribosomal protein L13

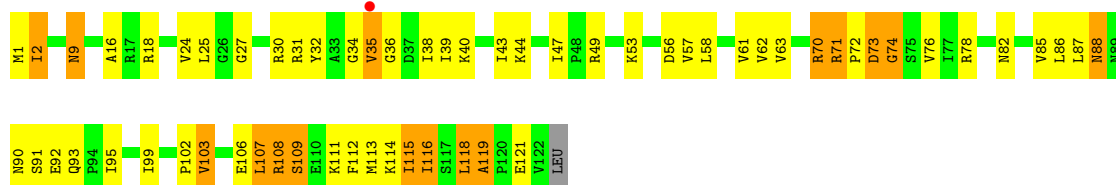


- Molecule 35: 50S ribosomal protein L14

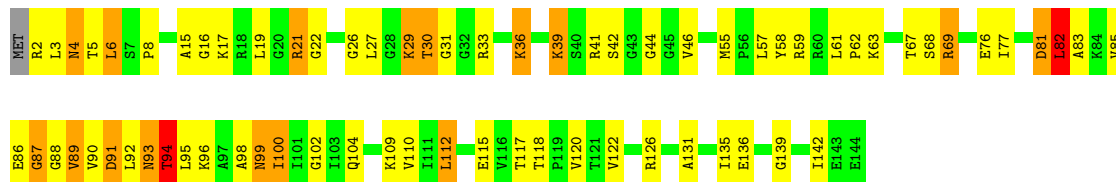




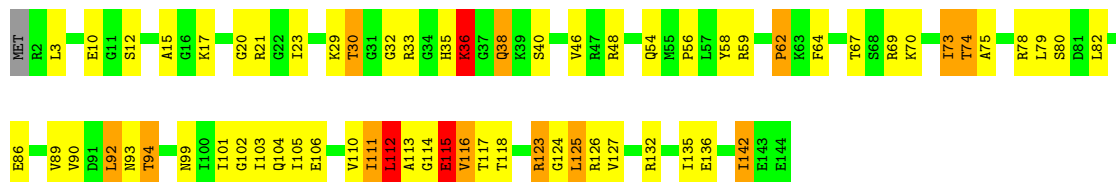
- Molecule 35: 50S ribosomal protein L14



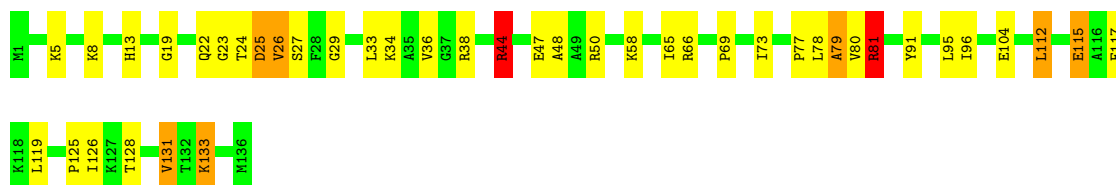
- Molecule 36: 50S ribosomal protein L15



- Molecule 36: 50S ribosomal protein L15

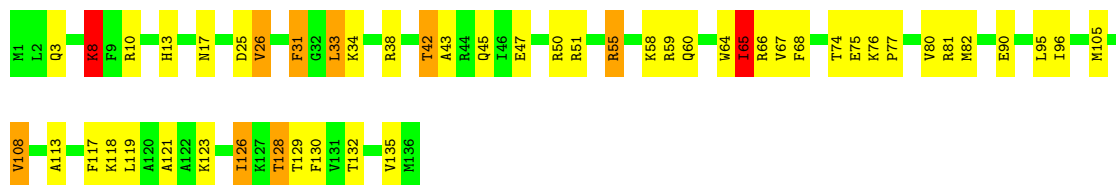


- Molecule 37: 50S ribosomal protein L16



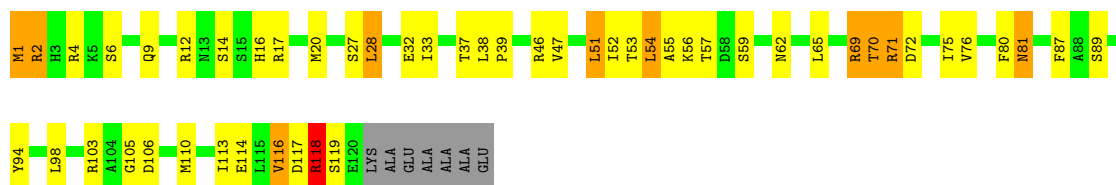
- Molecule 37: 50S ribosomal protein L16

Chain CM:  63% 29% 6% •



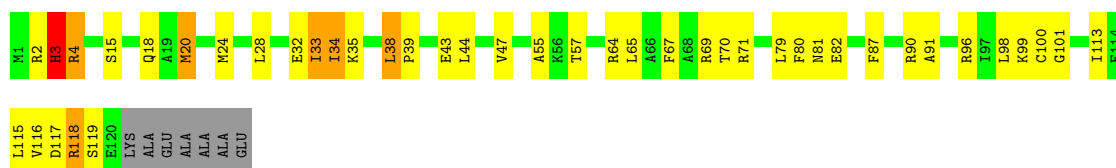
- Molecule 38: 50S ribosomal protein L17

Chain BN:  54% 31% 8% • 6%



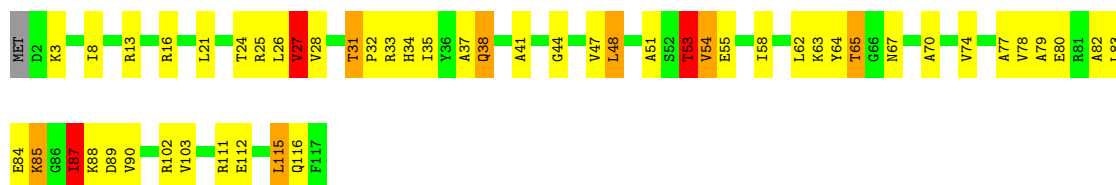
- Molecule 38: 50S ribosomal protein L17

Chain CN:  61% 28% 5% • 6%



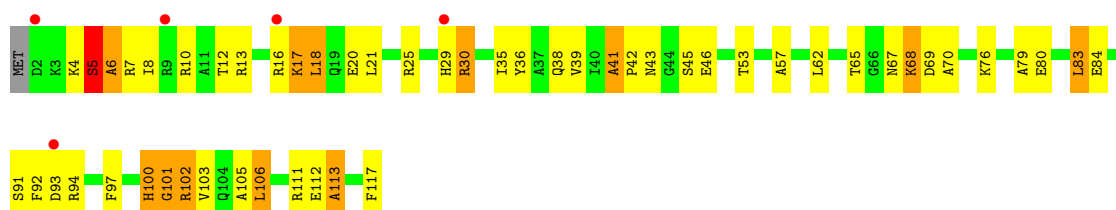
- Molecule 39: 50S ribosomal protein L18

Chain BO:  56% 35% 6% • •

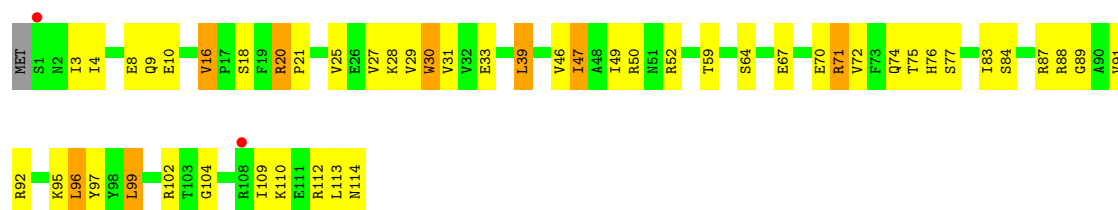


- Molecule 39: 50S ribosomal protein L18

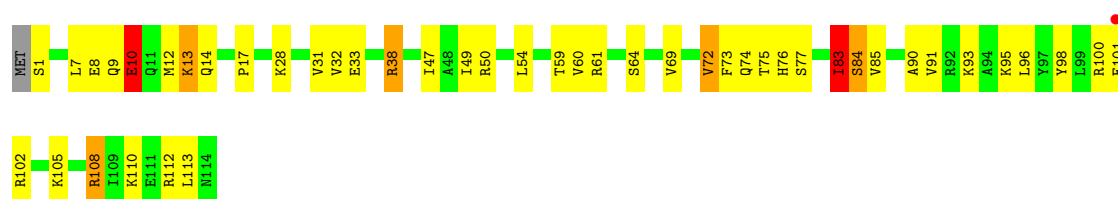
Chain CO:  4% 54% 34% 10% • •



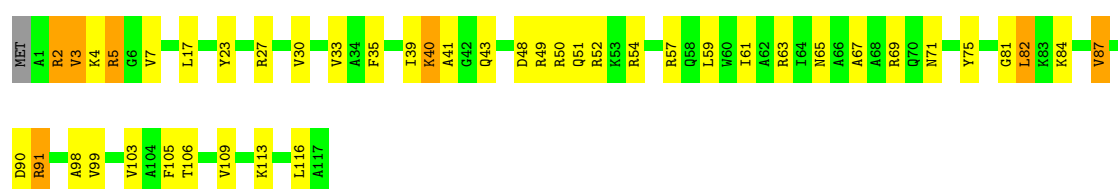
- Molecule 40: 50S ribosomal protein L19



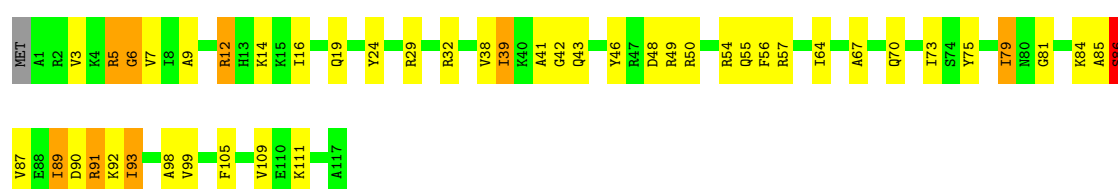
- Molecule 40: 50S ribosomal protein L19



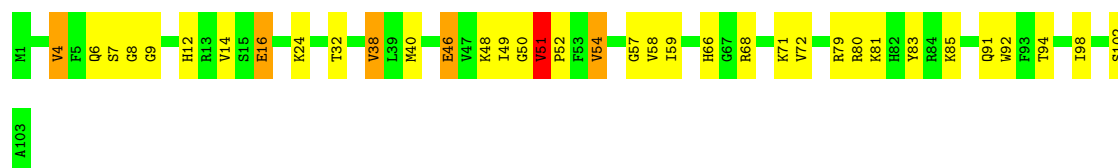
- Molecule 41: 50S ribosomal protein L20



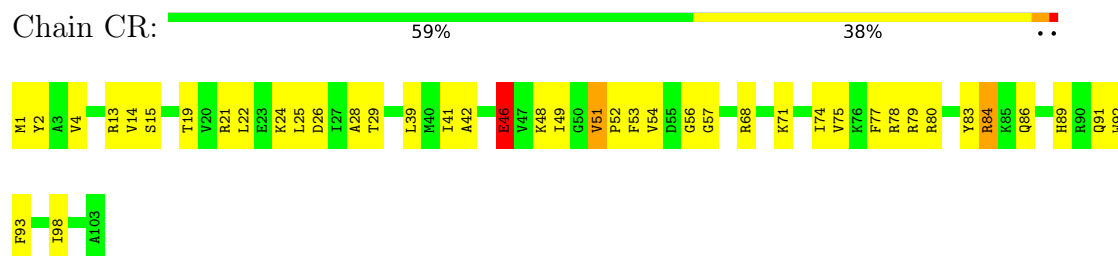
- Molecule 41: 50S ribosomal protein L20



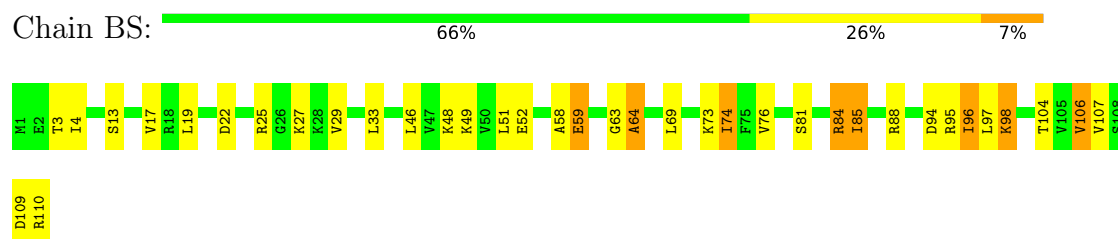
- Molecule 42: 50S ribosomal protein L21



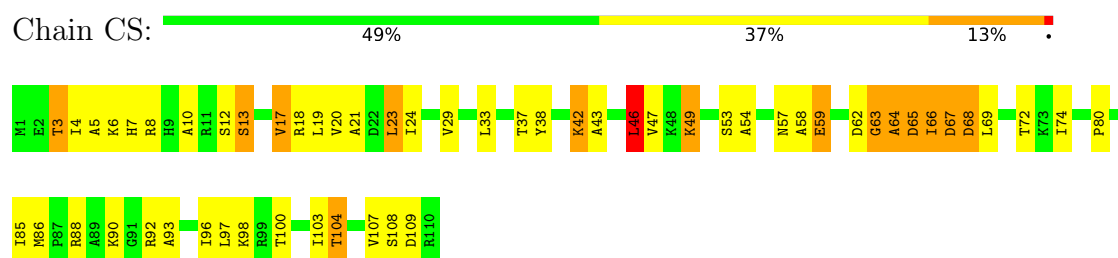
- Molecule 42: 50S ribosomal protein L21



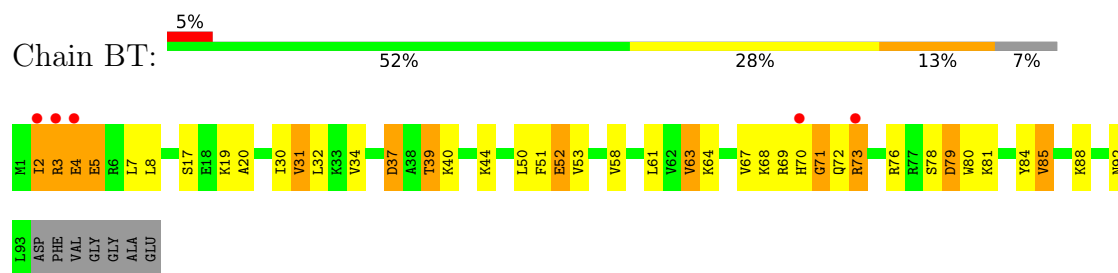
- Molecule 43: 50S ribosomal protein L22



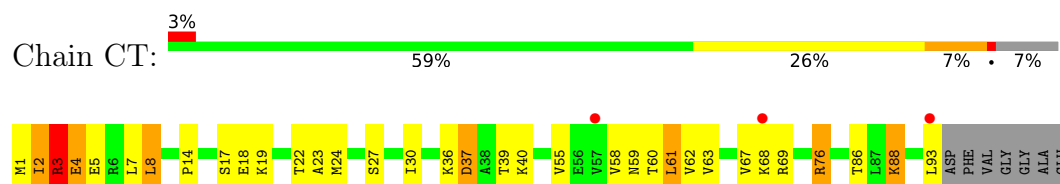
- Molecule 43: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L23

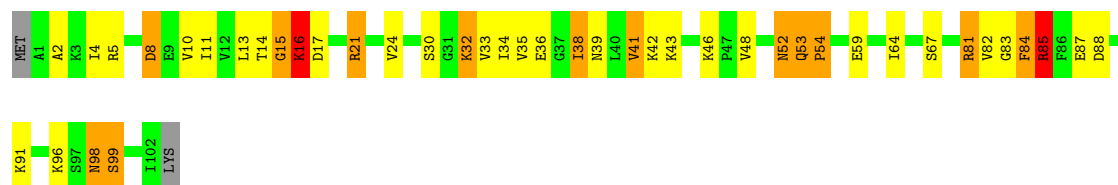


- Molecule 44: 50S ribosomal protein L23

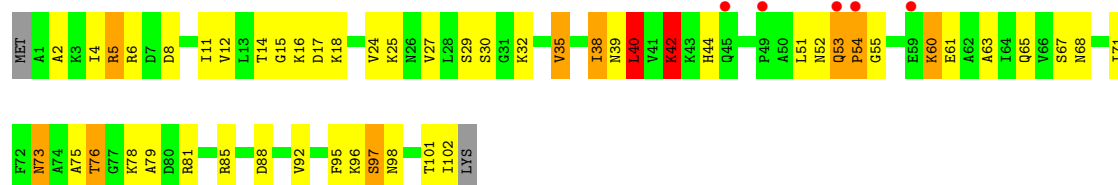


- Molecule 45: 50S ribosomal protein L24





- Molecule 45: 50S ribosomal protein L24



- Molecule 46: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L25



- Molecule 47: 50S ribosomal protein L27

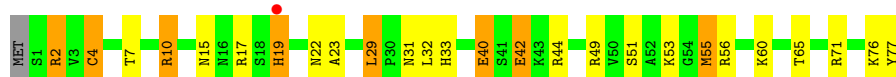


- Molecule 47: 50S ribosomal protein L27

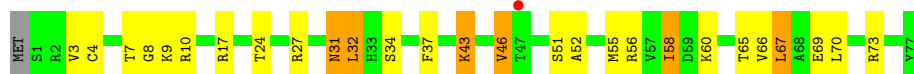


- Molecule 48: 50S ribosomal protein L28





- Molecule 48: 50S ribosomal protein L28



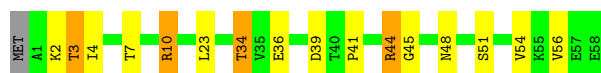
- Molecule 49: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L29



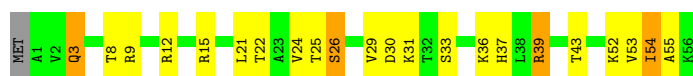
- Molecule 50: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L32

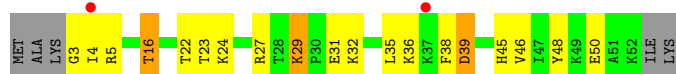


- Molecule 51: 50S ribosomal protein L32

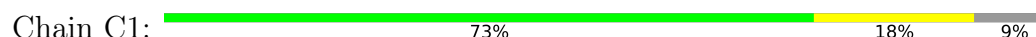




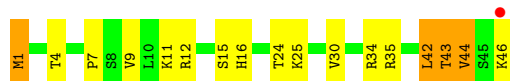
- Molecule 52: 50S ribosomal protein L33



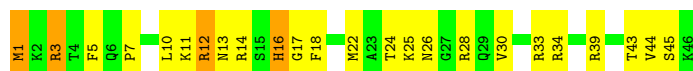
- Molecule 52: 50S ribosomal protein L33



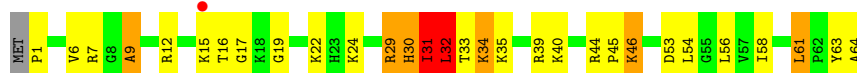
- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35

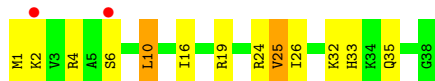


- Molecule 55: 50S ribosomal protein L36

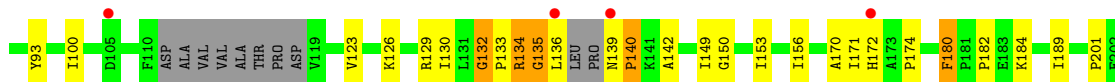
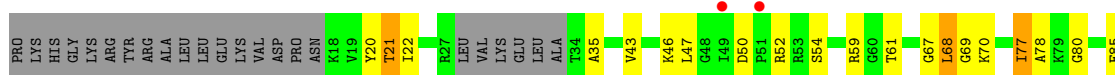




- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.10Å 435.24Å 614.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.00 70.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.1 (70.00-3.00) 81.1 (70.00-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.174 , 0.253 0.180 , 0.257	Depositor DCC
R_{free} test set	4548 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 93.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	294484	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.38% 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: PAR, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.27	0/36944	0.48	0/57632
1	DA	0.28	0/36966	0.50	0/57666
2	AB	0.53	0/1735	0.94	8/2338 (0.3%)
2	DB	0.56	0/1735	0.95	3/2338 (0.1%)
3	AC	0.59	0/1651	0.92	2/2225 (0.1%)
3	DC	0.56	0/1651	0.97	4/2225 (0.2%)
4	AD	0.58	0/1665	0.96	0/2227
4	DD	0.65	0/1665	1.12	9/2227 (0.4%)
5	AE	0.55	0/1118	0.93	0/1504
5	DE	0.62	0/1118	1.01	5/1504 (0.3%)
6	AF	0.60	0/835	0.97	1/1128 (0.1%)
6	DF	0.63	0/835	1.02	3/1128 (0.3%)
7	AG	2.57	8/1195 (0.7%)	0.99	6/1602 (0.4%)
7	DG	0.47	0/1195	0.86	2/1602 (0.1%)
8	AH	0.54	0/989	0.97	2/1326 (0.2%)
8	DH	0.58	0/989	1.03	1/1326 (0.1%)
9	AI	0.48	0/1034	0.85	1/1375 (0.1%)
9	DI	0.51	0/1034	0.88	1/1375 (0.1%)
10	AJ	0.59	0/796	0.94	2/1077 (0.2%)
10	DJ	0.55	0/796	0.85	2/1077 (0.2%)
11	AK	0.61	0/893	1.07	6/1205 (0.5%)
11	DK	0.64	0/893	0.97	3/1205 (0.2%)
12	AL	0.65	0/969	1.05	2/1300 (0.2%)
12	DL	0.70	0/969	1.10	2/1300 (0.2%)
13	AM	0.53	0/892	0.96	3/1193 (0.3%)
13	DM	0.52	0/892	0.92	0/1193
14	AN	0.57	0/785	1.08	7/1043 (0.7%)
14	DN	0.48	0/785	0.88	1/1043 (0.1%)
15	AO	0.53	0/724	0.93	1/966 (0.1%)
15	DO	0.51	0/724	0.85	1/966 (0.1%)
16	AP	0.56	1/659 (0.2%)	0.86	1/884 (0.1%)
16	DP	0.59	0/659	0.96	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.50	0/657	0.95	0/881
17	DQ	0.63	0/657	0.97	2/881 (0.2%)
18	AR	0.57	0/462	0.96	1/621 (0.2%)
18	DR	0.61	0/462	0.96	1/621 (0.2%)
19	AS	0.51	0/652	0.99	3/877 (0.3%)
19	DS	0.48	0/652	0.94	4/877 (0.5%)
20	AT	0.56	0/671	0.94	1/888 (0.1%)
20	DT	0.55	0/671	0.94	1/888 (0.1%)
21	AU	0.63	0/430	1.19	5/570 (0.9%)
21	DU	0.68	0/430	1.32	9/570 (1.6%)
22	AV	0.60	0/1430	0.93	2/1924 (0.1%)
23	AW	0.32	0/363	0.58	0/564
23	DV	0.30	0/388	0.50	0/603
24	AX	0.24	0/1813	0.47	0/2823
24	DW	0.27	0/1813	0.45	0/2823
25	BA	0.38	0/69659	0.60	3/108672 (0.0%)
25	CA	0.30	0/69659	0.52	2/108672 (0.0%)
26	BB	0.30	0/2850	0.50	0/4444
26	CB	0.23	0/2828	0.42	0/4410
27	BC	0.62	0/2121	0.99	6/2852 (0.2%)
27	CC	0.53	0/2121	0.97	6/2852 (0.2%)
28	BD	0.70	0/1586	1.04	3/2134 (0.1%)
28	CD	0.56	0/1586	1.09	5/2134 (0.2%)
29	BE	0.63	0/1571	0.94	0/2113
29	CE	0.56	0/1571	0.91	2/2113 (0.1%)
30	BF	0.52	0/1434	0.90	0/1926
30	CF	0.47	0/1434	0.87	1/1926 (0.1%)
31	BG	0.57	0/1343	0.90	5/1816 (0.3%)
31	CG	0.50	0/1343	0.83	1/1816 (0.1%)
32	BH	0.61	0/1118	0.97	3/1511 (0.2%)
32	CH	0.53	0/1118	0.85	2/1511 (0.1%)
33	BI	0.63	0/1046	0.92	3/1410 (0.2%)
33	CI	0.53	0/1046	0.94	5/1410 (0.4%)
34	BJ	0.75	1/1152 (0.1%)	0.98	0/1551
34	CJ	0.56	0/1152	0.89	2/1551 (0.1%)
35	BK	0.70	0/947	1.01	1/1268 (0.1%)
35	CK	0.60	0/947	0.93	1/1268 (0.1%)
36	BL	0.67	0/1054	1.05	2/1403 (0.1%)
36	CL	0.59	0/1054	1.00	2/1403 (0.1%)
37	BM	0.65	0/1093	1.03	2/1460 (0.1%)
37	CM	0.54	1/1093 (0.1%)	0.87	0/1460
38	BN	0.65	0/973	0.96	1/1301 (0.1%)
38	CN	0.71	4/973 (0.4%)	0.96	4/1301 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	BO	0.59	0/902	0.97	2/1209 (0.2%)
39	CO	0.48	0/902	0.93	3/1209 (0.2%)
40	BP	0.63	0/929	0.90	1/1242 (0.1%)
40	CP	0.55	0/929	0.85	0/1242
41	BQ	0.68	0/960	1.03	3/1278 (0.2%)
41	CQ	0.61	0/960	0.96	1/1278 (0.1%)
42	BR	0.69	0/829	1.05	3/1107 (0.3%)
42	CR	0.63	0/829	0.99	3/1107 (0.3%)
43	BS	0.68	0/864	0.95	0/1156
43	CS	0.63	0/864	0.98	1/1156 (0.1%)
44	BT	0.60	0/744	0.89	0/994
44	CT	0.51	0/744	0.83	1/994 (0.1%)
45	BU	0.66	0/787	1.01	3/1051 (0.3%)
45	CU	0.58	0/787	0.86	0/1051
46	BV	0.61	0/766	0.89	2/1025 (0.2%)
46	CV	0.46	0/766	0.84	0/1025
47	BW	0.66	0/587	1.01	0/776
47	CW	0.49	0/576	0.92	3/762 (0.4%)
48	BX	0.63	0/635	0.99	3/848 (0.4%)
48	CX	0.51	0/635	0.87	0/848
49	BY	0.55	0/510	0.99	2/677 (0.3%)
49	CY	0.51	0/510	0.91	0/677
50	BZ	0.73	0/453	1.02	0/605
50	CZ	0.56	0/453	0.90	0/605
51	B0	0.73	0/450	1.02	0/599
51	C0	0.63	0/450	1.05	2/599 (0.3%)
52	B1	0.51	0/416	0.80	0/554
52	C1	0.47	0/416	0.79	0/554
53	B2	0.64	0/380	0.97	0/498
53	C2	0.54	0/380	0.90	0/498
54	B3	0.71	0/513	1.07	3/676 (0.4%)
54	C3	0.57	0/513	0.93	0/676
55	B4	0.70	0/303	1.08	2/397 (0.5%)
55	C4	0.48	0/303	0.80	0/397
56	B5	0.53	0/1145	1.12	7/1556 (0.4%)
All	All	0.44	15/316403 (0.0%)	0.67	215/473109 (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
2	AB	0	1
2	DB	0	1
4	AD	0	1
4	DD	0	1
5	DE	0	2
6	AF	0	1
7	AG	0	1
9	DI	0	1
10	AJ	0	2
11	AK	0	1
12	DL	0	1
14	AN	0	2
17	DQ	0	1
19	AS	0	1
20	AT	0	1
20	DT	0	2
21	AU	0	1
27	BC	0	3
28	BD	0	1
28	CD	0	2
30	BF	0	1
36	BL	0	1
36	CL	0	1
38	BN	0	1
38	CN	0	1
40	CP	0	1
42	CR	0	1
44	BT	0	1
48	CX	0	1
All	All	0	36

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	AG	100	ALA	CA-C	75.75	2.56	1.52
7	AG	103	TRP	CE3-CZ3	22.68	2.06	1.38
7	AG	103	TRP	CZ3-CH2	18.02	1.85	1.40
7	AG	103	TRP	CE2-CZ2	17.57	1.76	1.39
7	AG	103	TRP	CZ2-CH2	13.84	1.63	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	B5	180	PHE	CA-C-N	18.56	139.49	120.38
56	B5	180	PHE	C-N-CA	18.56	139.49	120.38
28	CD	151	THR	CA-C-N	18.01	142.36	119.84
28	CD	151	THR	C-N-CA	18.01	142.36	119.84
12	DL	44	LYS	CA-C-N	-12.42	106.02	119.19

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	148	LEU	Peptide
4	AD	18	ASP	Peptide
6	AF	79	ARG	Peptide
7	AG	126	ASP	Peptide
10	AJ	17	LEU	Peptide

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	AA	32995	0	16607	444	1
1	DA	33015	0	16617	432	0
2	AB	1704	0	1732	40	0
2	DB	1704	0	1732	83	0
3	AC	1624	0	1696	49	0
3	DC	1624	0	1696	41	0
4	AD	1643	0	1707	98	0
4	DD	1643	0	1707	131	0
5	AE	1105	0	1148	33	0
5	DE	1105	0	1148	66	0
6	AF	817	0	808	23	0
6	DF	817	0	808	24	0
7	AG	1181	0	1238	77	0
7	DG	1181	0	1238	28	0
8	AH	979	0	1031	35	0
8	DH	979	0	1031	54	0
9	AI	1022	0	1070	37	0
9	DI	1022	0	1070	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	786	0	828	38	0
10	DJ	786	0	828	16	0
11	AK	877	0	887	53	0
11	DK	877	0	887	36	0
12	AL	955	0	1016	49	0
12	DL	955	0	1016	45	0
13	AM	883	0	941	63	0
13	DM	883	0	941	43	0
14	AN	774	0	827	52	0
14	DN	774	0	827	30	0
15	AO	716	0	739	35	0
15	DO	716	0	739	19	0
16	AP	649	0	666	25	0
16	DP	649	0	666	38	0
17	AQ	648	0	691	18	0
17	DQ	648	0	691	17	0
18	AR	455	0	478	22	0
18	DR	455	0	478	16	0
19	AS	637	0	665	37	0
19	DS	637	0	665	29	0
20	AT	665	0	714	16	0
20	DT	665	0	714	22	0
21	AU	425	0	449	28	0
21	DU	425	0	449	35	0
22	AV	1419	0	1465	48	0
23	AW	324	0	162	4	0
23	DV	346	0	173	15	0
24	AX	1623	0	821	20	0
24	DW	1623	0	821	8	0
25	BA	62195	0	31279	798	0
25	CA	62195	0	31280	783	0
26	BB	2549	0	1291	24	0
26	CB	2529	0	1281	20	0
27	BC	2082	0	2157	67	0
27	CC	2082	0	2157	65	0
28	BD	1565	0	1616	46	0
28	CD	1565	0	1616	33	0
29	BE	1552	0	1619	40	0
29	CE	1552	0	1619	33	0
30	BF	1410	0	1447	56	0
30	CF	1410	0	1447	51	0
31	BG	1323	0	1374	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	CG	1323	0	1374	23	0
32	BH	1107	0	1139	95	0
32	CH	1107	0	1138	64	1
33	BI	1032	0	1088	17	0
33	CI	1032	0	1088	19	0
34	BJ	1129	0	1162	27	0
34	CJ	1129	0	1162	30	0
35	BK	938	0	1012	32	0
35	CK	938	0	1012	36	0
36	BL	1045	0	1117	41	0
36	CL	1045	0	1117	41	0
37	BM	1074	0	1157	24	0
37	CM	1074	0	1157	24	0
38	BN	960	0	1000	27	0
38	CN	960	0	1000	27	0
39	BO	892	0	922	25	0
39	CO	892	0	923	34	0
40	BP	917	0	965	29	0
40	CP	917	0	965	32	0
41	BQ	947	0	1022	37	0
41	CQ	947	0	1022	36	0
42	BR	816	0	839	27	0
42	CR	816	0	839	24	0
43	BS	857	0	922	25	0
43	CS	857	0	922	23	0
44	BT	738	0	807	38	0
44	CT	738	0	806	32	0
45	BU	779	0	834	29	0
45	CU	779	0	834	35	0
46	BV	753	0	780	18	0
46	CV	753	0	780	10	0
47	BW	580	0	594	17	0
47	CW	569	0	581	11	0
48	BX	625	0	655	16	0
48	CX	625	0	655	17	0
49	BY	509	0	543	25	0
49	CY	509	0	543	23	0
50	BZ	449	0	491	6	0
50	CZ	449	0	491	10	0
51	B0	444	0	461	15	0
51	C0	444	0	461	10	0
52	B1	409	0	440	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	C1	409	0	440	5	0
53	B2	377	0	418	8	0
53	C2	377	0	418	10	0
54	B3	504	0	574	40	0
54	C3	504	0	574	11	0
55	B4	302	0	340	14	0
55	C4	302	0	340	4	0
56	B5	1142	0	865	16	0
57	AA	71	0	0	0	0
57	AN	1	0	0	0	0
57	BA	189	0	0	0	0
57	BB	4	0	0	0	0
57	BL	2	0	0	0	0
57	BO	1	0	0	0	0
57	BQ	1	0	0	0	0
57	CA	165	0	0	0	0
57	CB	3	0	0	0	0
57	CD	1	0	0	0	0
57	CQ	1	0	0	0	0
57	DA	53	0	0	0	0
57	DD	2	0	0	0	0
57	DN	1	0	0	0	0
58	AA	42	45	45	9	0
58	BA	210	180	225	33	0
58	CA	210	135	224	51	0
58	DA	84	90	90	13	0
59	B4	1	0	0	0	0
59	C4	1	0	0	0	0
60	AA	192	0	0	17	0
60	AE	3	0	0	0	0
60	AL	1	0	0	0	0
60	AN	2	0	0	1	0
60	AT	5	0	0	0	0
60	B3	1	0	0	0	0
60	B4	1	0	0	0	0
60	BA	626	0	0	93	0
60	BB	14	0	0	3	0
60	BC	7	0	0	0	0
60	BD	2	0	0	1	0
60	BE	1	0	0	0	0
60	BF	1	0	0	0	0
60	BL	8	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BN	2	0	0	0	0
60	BQ	1	0	0	0	0
60	BS	1	0	0	0	0
60	BT	3	0	0	2	0
60	C3	1	0	0	0	0
60	C4	2	0	0	0	0
60	CA	608	0	0	83	0
60	CB	14	0	0	3	0
60	CC	10	0	0	1	0
60	CD	5	0	0	1	0
60	CE	3	0	0	0	0
60	CJ	2	0	0	2	0
60	CL	7	0	0	0	0
60	CN	2	0	0	0	0
60	CT	3	0	0	1	0
60	CU	1	0	0	0	0
60	DA	184	0	0	22	0
60	DD	2	0	0	1	0
60	DK	2	0	0	0	0
60	DL	2	0	0	0	0
60	DN	4	0	0	2	0
60	DT	3	0	0	0	0
60	DU	1	0	0	0	0
All	All	294034	450	196884	5171	1

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

The worst 5 of 5171 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)
7:AG:103:TRP:CZ2	7:AG:103:TRP:CE2	1.76	1.63
7:AG:103:TRP:CH2	7:AG:103:TRP:CZ3	1.85	1.61
7:AG:100:ALA:HA	7:AG:103:TRP:CD2	1.52	1.44
7:AG:103:TRP:CZ3	7:AG:103:TRP:CE3	2.06	1.44
32:BH:124:THR:HG21	32:BH:128:HIS:NE2	1.32	1.44

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:358:U:OP1	32:CH:123:ARG:NH2[4_455]	1.91	0.29

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/241 (90%)	120 (56%)	54 (25%)	42 (19%)	0	0
2	DB	216/241 (90%)	130 (60%)	50 (23%)	36 (17%)	0	0
3	AC	204/233 (88%)	148 (72%)	34 (17%)	22 (11%)	0	1
3	DC	204/233 (88%)	154 (76%)	33 (16%)	17 (8%)	0	3
4	AD	203/206 (98%)	115 (57%)	55 (27%)	33 (16%)	0	0
4	DD	203/206 (98%)	111 (55%)	41 (20%)	51 (25%)	0	0
5	AE	148/167 (89%)	116 (78%)	19 (13%)	13 (9%)	0	3
5	DE	148/167 (89%)	106 (72%)	25 (17%)	17 (12%)	0	1
6	AF	98/135 (73%)	62 (63%)	22 (22%)	14 (14%)	0	1
6	DF	98/135 (73%)	74 (76%)	11 (11%)	13 (13%)	0	1
7	AG	149/179 (83%)	88 (59%)	43 (29%)	18 (12%)	0	1
7	DG	149/179 (83%)	112 (75%)	24 (16%)	13 (9%)	0	3
8	AH	127/130 (98%)	92 (72%)	27 (21%)	8 (6%)	1	6
8	DH	127/130 (98%)	97 (76%)	14 (11%)	16 (13%)	0	1
9	AI	125/130 (96%)	84 (67%)	28 (22%)	13 (10%)	0	2
9	DI	125/130 (96%)	83 (66%)	23 (18%)	19 (15%)	0	0
10	AJ	96/103 (93%)	60 (62%)	22 (23%)	14 (15%)	0	0
10	DJ	96/103 (93%)	71 (74%)	17 (18%)	8 (8%)	0	3
11	AK	115/129 (89%)	67 (58%)	30 (26%)	18 (16%)	0	0
11	DK	115/129 (89%)	85 (74%)	17 (15%)	13 (11%)	0	1
12	AL	121/124 (98%)	94 (78%)	14 (12%)	13 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	DL	121/124 (98%)	72 (60%)	32 (26%)	17 (14%)	0	1
13	AM	112/118 (95%)	63 (56%)	29 (26%)	20 (18%)	0	0
13	DM	112/118 (95%)	71 (63%)	26 (23%)	15 (13%)	0	1
14	AN	92/101 (91%)	65 (71%)	18 (20%)	9 (10%)	0	2
14	DN	92/101 (91%)	63 (68%)	15 (16%)	14 (15%)	0	0
15	AO	86/89 (97%)	65 (76%)	17 (20%)	4 (5%)	2	11
15	DO	86/89 (97%)	66 (77%)	14 (16%)	6 (7%)	1	4
16	AP	80/82 (98%)	48 (60%)	26 (32%)	6 (8%)	1	4
16	DP	80/82 (98%)	48 (60%)	25 (31%)	7 (9%)	0	3
17	AQ	78/84 (93%)	55 (70%)	11 (14%)	12 (15%)	0	0
17	DQ	78/84 (93%)	47 (60%)	21 (27%)	10 (13%)	0	1
18	AR	53/75 (71%)	37 (70%)	9 (17%)	7 (13%)	0	1
18	DR	53/75 (71%)	38 (72%)	7 (13%)	8 (15%)	0	0
19	AS	77/92 (84%)	45 (58%)	17 (22%)	15 (20%)	0	0
19	DS	77/92 (84%)	53 (69%)	16 (21%)	8 (10%)	0	2
20	AT	83/87 (95%)	69 (83%)	6 (7%)	8 (10%)	0	2
20	DT	83/87 (95%)	62 (75%)	15 (18%)	6 (7%)	1	4
21	AU	49/71 (69%)	20 (41%)	16 (33%)	13 (26%)	0	0
21	DU	49/71 (69%)	25 (51%)	9 (18%)	15 (31%)	0	0
22	AV	181/185 (98%)	137 (76%)	30 (17%)	14 (8%)	1	4
27	BC	269/273 (98%)	216 (80%)	37 (14%)	16 (6%)	1	7
27	CC	269/273 (98%)	214 (80%)	41 (15%)	14 (5%)	1	9
28	BD	207/209 (99%)	176 (85%)	22 (11%)	9 (4%)	2	12
28	CD	207/209 (99%)	170 (82%)	25 (12%)	12 (6%)	1	8
29	BE	199/201 (99%)	160 (80%)	30 (15%)	9 (4%)	2	12
29	CE	199/201 (99%)	156 (78%)	31 (16%)	12 (6%)	1	7
30	BF	175/179 (98%)	127 (73%)	32 (18%)	16 (9%)	0	2
30	CF	175/179 (98%)	122 (70%)	37 (21%)	16 (9%)	0	2
31	BG	174/177 (98%)	133 (76%)	29 (17%)	12 (7%)	1	5
31	CG	174/177 (98%)	135 (78%)	27 (16%)	12 (7%)	1	5
32	BH	147/149 (99%)	84 (57%)	40 (27%)	23 (16%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	CH	147/149 (99%)	93 (63%)	36 (24%)	18 (12%)	0	1
33	BI	139/142 (98%)	77 (55%)	37 (27%)	25 (18%)	0	0
33	CI	139/142 (98%)	84 (60%)	39 (28%)	16 (12%)	0	1
34	BJ	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	2	12
34	CJ	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	3	20
35	BK	120/123 (98%)	99 (82%)	10 (8%)	11 (9%)	0	2
35	CK	120/123 (98%)	92 (77%)	22 (18%)	6 (5%)	1	10
36	BL	141/144 (98%)	114 (81%)	15 (11%)	12 (8%)	0	3
36	CL	141/144 (98%)	98 (70%)	29 (21%)	14 (10%)	0	2
37	BM	134/136 (98%)	110 (82%)	16 (12%)	8 (6%)	1	7
37	CM	134/136 (98%)	109 (81%)	17 (13%)	8 (6%)	1	7
38	BN	118/127 (93%)	98 (83%)	14 (12%)	6 (5%)	1	10
38	CN	118/127 (93%)	83 (70%)	32 (27%)	3 (2%)	4	23
39	BO	114/117 (97%)	90 (79%)	18 (16%)	6 (5%)	1	9
39	CO	114/117 (97%)	80 (70%)	23 (20%)	11 (10%)	0	2
40	BP	112/115 (97%)	94 (84%)	15 (13%)	3 (3%)	4	22
40	CP	112/115 (97%)	91 (81%)	16 (14%)	5 (4%)	2	12
41	BQ	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	48
41	CQ	115/118 (98%)	99 (86%)	13 (11%)	3 (3%)	4	23
42	BR	101/103 (98%)	89 (88%)	7 (7%)	5 (5%)	1	10
42	CR	101/103 (98%)	76 (75%)	18 (18%)	7 (7%)	1	5
43	BS	108/110 (98%)	96 (89%)	10 (9%)	2 (2%)	6	30
43	CS	108/110 (98%)	82 (76%)	16 (15%)	10 (9%)	0	2
44	BT	91/100 (91%)	72 (79%)	11 (12%)	8 (9%)	0	3
44	CT	91/100 (91%)	72 (79%)	11 (12%)	8 (9%)	0	3
45	BU	100/104 (96%)	79 (79%)	14 (14%)	7 (7%)	1	4
45	CU	100/104 (96%)	67 (67%)	23 (23%)	10 (10%)	0	2
46	BV	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
46	CV	92/94 (98%)	74 (80%)	14 (15%)	4 (4%)	2	12
47	BW	74/85 (87%)	60 (81%)	9 (12%)	5 (7%)	1	5
47	CW	73/85 (86%)	60 (82%)	10 (14%)	3 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	BX	75/78 (96%)	62 (83%)	9 (12%)	4 (5%)	1	9
48	CX	75/78 (96%)	63 (84%)	10 (13%)	2 (3%)	4	22
49	BY	61/63 (97%)	46 (75%)	9 (15%)	6 (10%)	0	2
49	CY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	0	3
50	BZ	56/59 (95%)	45 (80%)	11 (20%)	0	100	100
50	CZ	56/59 (95%)	47 (84%)	9 (16%)	0	100	100
51	B0	54/57 (95%)	45 (83%)	4 (7%)	5 (9%)	0	2
51	C0	54/57 (95%)	42 (78%)	4 (7%)	8 (15%)	0	0
52	B1	48/55 (87%)	31 (65%)	12 (25%)	5 (10%)	0	2
52	C1	48/55 (87%)	37 (77%)	11 (23%)	0	100	100
53	B2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	5	25
53	C2	44/46 (96%)	38 (86%)	4 (9%)	2 (4%)	2	12
54	B3	62/65 (95%)	51 (82%)	7 (11%)	4 (6%)	1	5
54	C3	62/65 (95%)	52 (84%)	8 (13%)	2 (3%)	3	18
55	B4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	1	8
55	C4	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	4	21
56	B5	183/228 (80%)	80 (44%)	66 (36%)	37 (20%)	0	0
All	All	11599/12383 (94%)	8463 (73%)	2041 (18%)	1095 (9%)	0	2

5 of 1095 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	31	ILE
2	AB	34	ALA
2	AB	52	GLU
2	AB	73	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/199 (90%)	142 (79%)	38 (21%)	1	6
2	DB	180/199 (90%)	140 (78%)	40 (22%)	1	5
3	AC	170/190 (90%)	135 (79%)	35 (21%)	1	7
3	DC	170/190 (90%)	135 (79%)	35 (21%)	1	7
4	AD	172/173 (99%)	123 (72%)	49 (28%)	0	2
4	DD	172/173 (99%)	125 (73%)	47 (27%)	0	2
5	AE	113/126 (90%)	86 (76%)	27 (24%)	1	4
5	DE	113/126 (90%)	88 (78%)	25 (22%)	1	5
6	AF	87/116 (75%)	67 (77%)	20 (23%)	1	5
6	DF	87/116 (75%)	71 (82%)	16 (18%)	1	9
7	AG	124/147 (84%)	103 (83%)	21 (17%)	2	11
7	DG	124/147 (84%)	103 (83%)	21 (17%)	2	11
8	AH	104/105 (99%)	85 (82%)	19 (18%)	2	9
8	DH	104/105 (99%)	86 (83%)	18 (17%)	2	10
9	AI	105/107 (98%)	79 (75%)	26 (25%)	1	3
9	DI	105/107 (98%)	81 (77%)	24 (23%)	1	5
10	AJ	86/90 (96%)	64 (74%)	22 (26%)	0	3
10	DJ	86/90 (96%)	68 (79%)	18 (21%)	1	7
11	AK	90/99 (91%)	70 (78%)	20 (22%)	1	5
11	DK	90/99 (91%)	73 (81%)	17 (19%)	1	9
12	AL	103/104 (99%)	74 (72%)	29 (28%)	0	2
12	DL	103/104 (99%)	79 (77%)	24 (23%)	1	4
13	AM	92/96 (96%)	66 (72%)	26 (28%)	0	2
13	DM	92/96 (96%)	73 (79%)	19 (21%)	1	7
14	AN	79/84 (94%)	61 (77%)	18 (23%)	1	5
14	DN	79/84 (94%)	55 (70%)	24 (30%)	0	1
15	AO	76/77 (99%)	58 (76%)	18 (24%)	1	4
15	DO	76/77 (99%)	61 (80%)	15 (20%)	1	8
16	AP	65/65 (100%)	51 (78%)	14 (22%)	1	6
16	DP	65/65 (100%)	49 (75%)	16 (25%)	1	4
17	AQ	74/78 (95%)	61 (82%)	13 (18%)	2	10
17	DQ	74/78 (95%)	53 (72%)	21 (28%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	48/65 (74%)	34 (71%)	14 (29%)	0	2
18	DR	48/65 (74%)	35 (73%)	13 (27%)	0	2
19	AS	70/79 (89%)	48 (69%)	22 (31%)	0	1
19	DS	70/79 (89%)	55 (79%)	15 (21%)	1	6
20	AT	65/66 (98%)	48 (74%)	17 (26%)	0	3
20	DT	65/66 (98%)	48 (74%)	17 (26%)	0	3
21	AU	44/61 (72%)	33 (75%)	11 (25%)	0	3
21	DU	44/61 (72%)	32 (73%)	12 (27%)	0	2
22	AV	157/160 (98%)	123 (78%)	34 (22%)	1	6
27	BC	216/218 (99%)	171 (79%)	45 (21%)	1	7
27	CC	216/218 (99%)	171 (79%)	45 (21%)	1	7
28	BD	164/164 (100%)	130 (79%)	34 (21%)	1	7
28	CD	164/164 (100%)	136 (83%)	28 (17%)	2	11
29	BE	165/165 (100%)	139 (84%)	26 (16%)	2	13
29	CE	165/165 (100%)	135 (82%)	30 (18%)	2	9
30	BF	148/150 (99%)	120 (81%)	28 (19%)	1	9
30	CF	148/150 (99%)	120 (81%)	28 (19%)	1	9
31	BG	137/138 (99%)	107 (78%)	30 (22%)	1	5
31	CG	137/138 (99%)	107 (78%)	30 (22%)	1	5
32	BH	113/114 (99%)	84 (74%)	29 (26%)	0	3
32	CH	113/114 (99%)	83 (74%)	30 (26%)	0	3
33	BI	109/110 (99%)	86 (79%)	23 (21%)	1	6
33	CI	109/110 (99%)	93 (85%)	16 (15%)	3	15
34	BJ	116/116 (100%)	94 (81%)	22 (19%)	1	8
34	CJ	116/116 (100%)	98 (84%)	18 (16%)	2	13
35	BK	103/104 (99%)	83 (81%)	20 (19%)	1	8
35	CK	103/104 (99%)	78 (76%)	25 (24%)	1	4
36	BL	102/103 (99%)	74 (72%)	28 (28%)	0	2
36	CL	102/103 (99%)	82 (80%)	20 (20%)	1	8
37	BM	109/109 (100%)	96 (88%)	13 (12%)	5	22
37	CM	109/109 (100%)	90 (83%)	19 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BN	100/103 (97%)	80 (80%)	20 (20%)	1	7
38	CN	100/103 (97%)	84 (84%)	16 (16%)	2	12
39	BO	86/87 (99%)	62 (72%)	24 (28%)	0	2
39	CO	86/87 (99%)	65 (76%)	21 (24%)	1	4
40	BP	99/100 (99%)	75 (76%)	24 (24%)	1	4
40	CP	99/100 (99%)	82 (83%)	17 (17%)	2	11
41	BQ	89/90 (99%)	74 (83%)	15 (17%)	2	11
41	CQ	89/90 (99%)	72 (81%)	17 (19%)	1	8
42	BR	84/84 (100%)	72 (86%)	12 (14%)	3	16
42	CR	84/84 (100%)	73 (87%)	11 (13%)	4	19
43	BS	93/93 (100%)	78 (84%)	15 (16%)	2	12
43	CS	93/93 (100%)	66 (71%)	27 (29%)	0	2
44	BT	80/84 (95%)	61 (76%)	19 (24%)	1	4
44	CT	80/84 (95%)	67 (84%)	13 (16%)	2	12
45	BU	83/85 (98%)	62 (75%)	21 (25%)	0	3
45	CU	83/85 (98%)	64 (77%)	19 (23%)	1	5
46	BV	78/78 (100%)	65 (83%)	13 (17%)	2	12
46	CV	78/78 (100%)	63 (81%)	15 (19%)	1	8
47	BW	57/63 (90%)	45 (79%)	12 (21%)	1	6
47	CW	56/63 (89%)	47 (84%)	9 (16%)	2	12
48	BX	67/68 (98%)	55 (82%)	12 (18%)	2	10
48	CX	67/68 (98%)	55 (82%)	12 (18%)	2	10
49	BY	55/55 (100%)	40 (73%)	15 (27%)	0	2
49	CY	55/55 (100%)	43 (78%)	12 (22%)	1	6
50	BZ	48/49 (98%)	38 (79%)	10 (21%)	1	7
50	CZ	48/49 (98%)	39 (81%)	9 (19%)	1	9
51	B0	47/48 (98%)	44 (94%)	3 (6%)	16	48
51	C0	47/48 (98%)	40 (85%)	7 (15%)	3	15
52	B1	45/49 (92%)	38 (84%)	7 (16%)	2	13
52	C1	45/49 (92%)	38 (84%)	7 (16%)	2	13
53	B2	38/38 (100%)	28 (74%)	10 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	C2	38/38 (100%)	28 (74%)	10 (26%)	0	3
54	B3	51/52 (98%)	43 (84%)	8 (16%)	2	13
54	C3	51/52 (98%)	43 (84%)	8 (16%)	2	13
55	B4	34/34 (100%)	24 (71%)	10 (29%)	0	2
55	C4	34/34 (100%)	26 (76%)	8 (24%)	1	4
56	B5	61/180 (34%)	50 (82%)	11 (18%)	2	10
All	All	9543/10096 (94%)	7527 (79%)	2016 (21%)	1	6

5 of 2016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BU	34	ILE
8	DH	87	LYS
29	CE	133	LEU
7	DG	75	VAL
14	DN	45	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
52	B1	18	HIS
9	DI	5	GLN
34	CJ	135	GLN
8	DH	4	GLN
15	DO	38	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1542 (99%)	352 (22%)	15 (0%)
1	DA	1538/1542 (99%)	330 (21%)	17 (1%)
23	AW	14/16 (87%)	5 (35%)	0
23	DV	15/16 (93%)	6 (40%)	0
24	AX	75/76 (98%)	27 (36%)	6 (8%)
24	DW	75/76 (98%)	20 (26%)	0
25	BA	2896/2904 (99%)	591 (20%)	35 (1%)
25	CA	2895/2904 (99%)	618 (21%)	34 (1%)
26	BB	118/120 (98%)	16 (13%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	CB	117/120 (97%)	27 (23%)	0
All	All	9280/9316 (99%)	1992 (21%)	107 (1%)

5 of 1992 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	28	A
1	AA	30	U

5 of 107 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	CA	310	A
25	CA	1606	C
1	DA	841	C
25	CA	479	A
25	CA	784	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 510 ligands modelled in this entry, 497 are monoatomic - leaving 13 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
58	PAR	BA	3004	-	44,45,45	0.72	0	63,67,67	1.06	4 (6%)
58	PAR	BA	3002	-	44,45,45	0.79	1 (2%)	63,67,67	0.97	2 (3%)
58	PAR	CA	3169	-	44,45,45	0.47	0	63,67,67	0.96	4 (6%)
58	PAR	BA	3005	-	44,45,45	0.53	0	63,67,67	1.08	3 (4%)
58	PAR	BA	3003	-	44,45,45	0.73	0	63,67,67	1.10	7 (11%)
58	PAR	CA	3167	-	44,45,45	0.57	0	63,67,67	0.90	3 (4%)
58	PAR	CA	3168	-	44,45,45	0.52	0	63,67,67	1.36	5 (7%)
58	PAR	BA	3001	-	44,45,45	0.71	0	63,67,67	1.07	5 (7%)
58	PAR	CA	3166	-	44,45,45	0.47	0	63,67,67	0.96	4 (6%)
58	PAR	DA	1654	-	44,45,45	0.52	0	63,67,67	0.80	1 (1%)
58	PAR	CA	3170	-	44,45,45	0.49	0	63,67,67	0.95	4 (6%)
58	PAR	DA	1655	-	44,45,45	0.49	0	63,67,67	0.92	4 (6%)
58	PAR	AA	1672	-	44,45,45	0.77	0	63,67,67	1.15	3 (4%)

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
58	PAR	BA	3004	-	-	7/18/94/94	0/4/4/4
58	PAR	BA	3002	-	-	7/18/94/94	0/4/4/4
58	PAR	CA	3169	-	-	5/18/94/94	0/4/4/4
58	PAR	BA	3005	-	-	7/18/94/94	0/4/4/4
58	PAR	BA	3003	-	-	8/18/94/94	0/4/4/4
58	PAR	CA	3167	-	-	3/18/94/94	0/4/4/4
58	PAR	CA	3168	-	-	1/18/94/94	0/4/4/4
58	PAR	BA	3001	-	-	6/18/94/94	0/4/4/4
58	PAR	CA	3166	-	-	3/18/94/94	0/4/4/4
58	PAR	DA	1654	-	-	2/18/94/94	0/4/4/4
58	PAR	CA	3170	-	-	3/18/94/94	0/4/4/4
58	PAR	DA	1655	-	-	2/18/94/94	0/4/4/4
58	PAR	AA	1672	-	-	8/18/94/94	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	3002	PAR	C13-C23	-2.06	1.50	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CA	3168	PAR	C14-O33-C33	-4.73	106.77	117.98
58	CA	3168	PAR	C11-O11-C42	-4.70	106.83	117.98
58	CA	3168	PAR	C13-O52-C52	-4.68	106.88	117.98
58	BA	3004	PAR	O52-C13-O43	-3.95	107.33	111.37
58	BA	3005	PAR	C13-O52-C52	-3.78	109.03	117.98

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	PAR	C23-C13-O52-C52
58	BA	3001	PAR	C24-C14-O33-C33
58	BA	3003	PAR	C23-C13-O52-C52
58	BA	3003	PAR	O43-C13-O52-C52
58	BA	3003	PAR	C24-C14-O33-C33

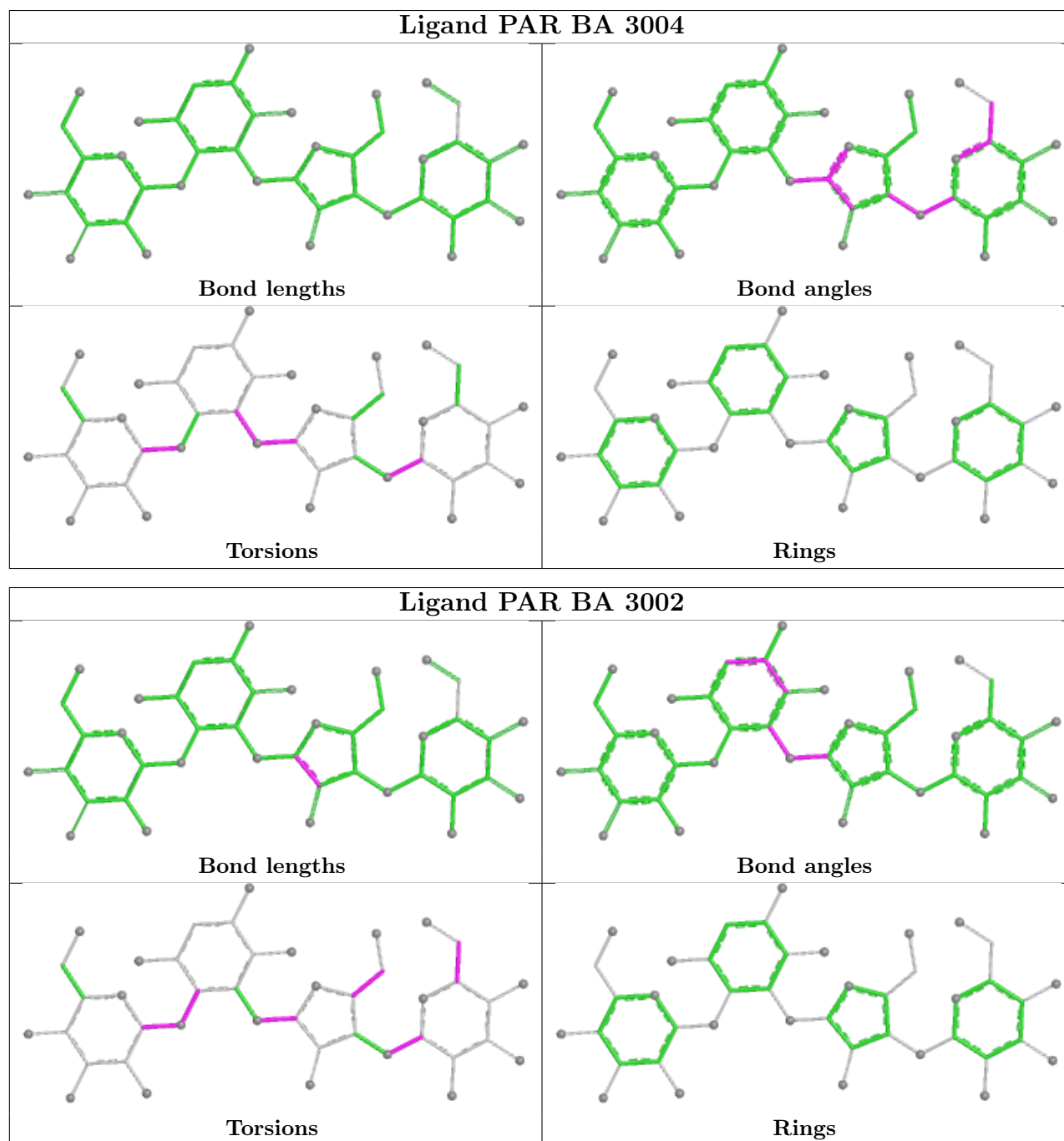
There are no ring outliers.

13 monomers are involved in 106 short contacts:

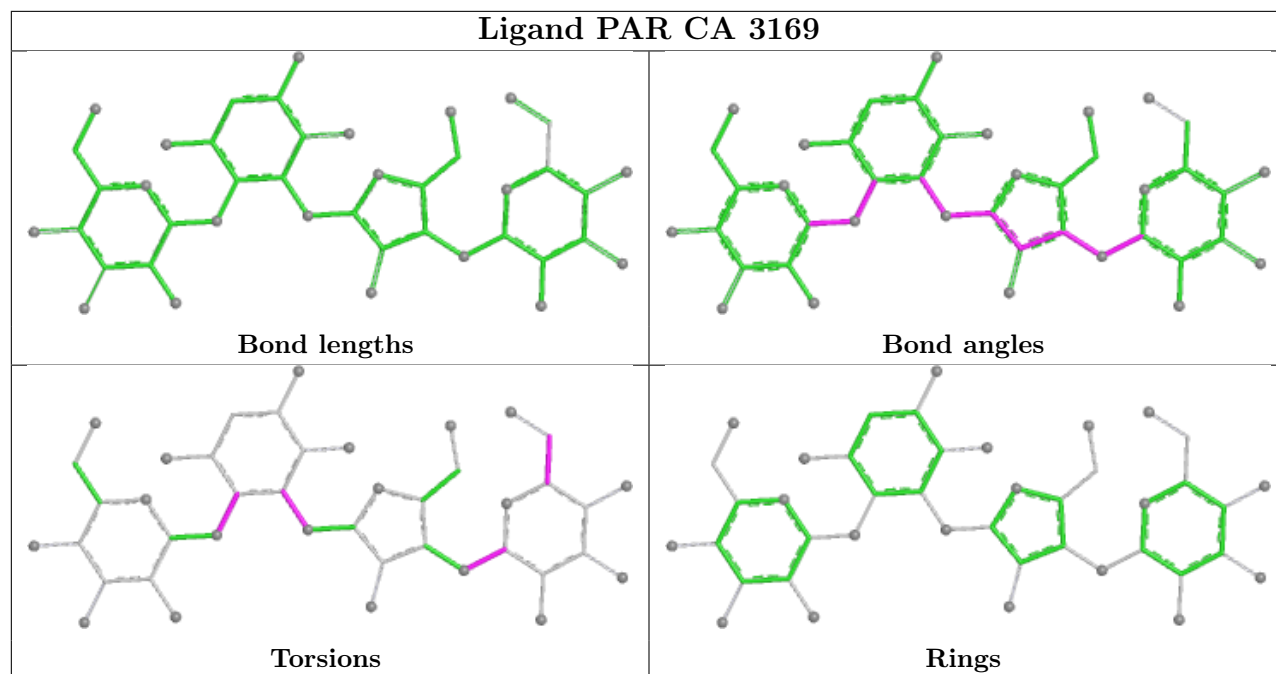
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	BA	3004	PAR	3	0
58	BA	3002	PAR	2	0
58	CA	3169	PAR	20	0
58	BA	3005	PAR	21	0
58	BA	3003	PAR	4	0
58	CA	3167	PAR	7	0
58	CA	3168	PAR	5	0
58	BA	3001	PAR	3	0
58	CA	3166	PAR	14	0
58	DA	1654	PAR	5	0
58	CA	3170	PAR	5	0
58	DA	1655	PAR	8	0
58	AA	1672	PAR	9	0

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

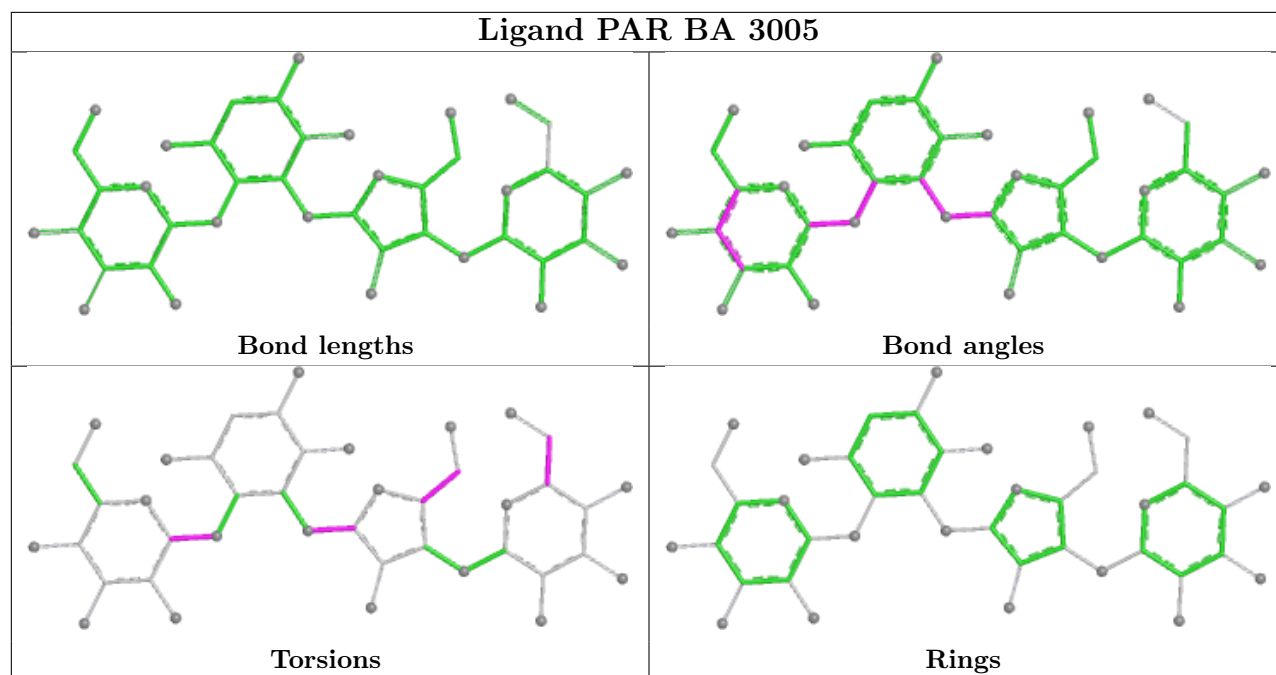
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



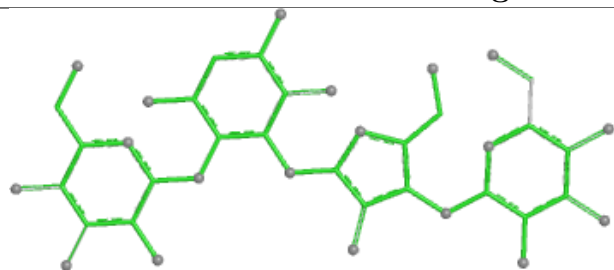
Ligand PAR CA 3169



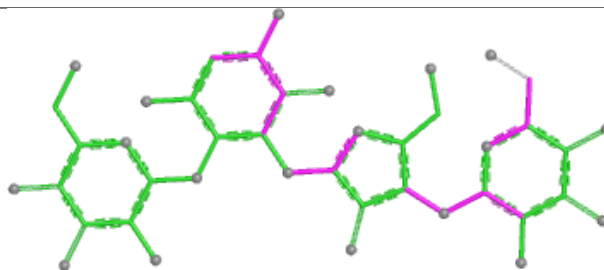
Ligand PAR BA 3005



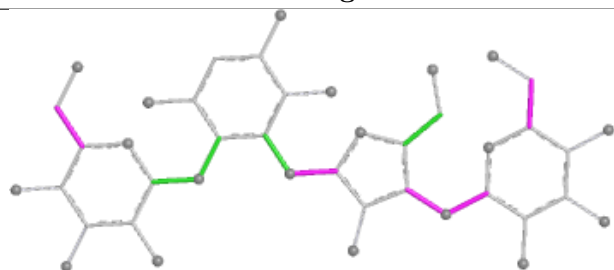
Ligand PAR BA 3003



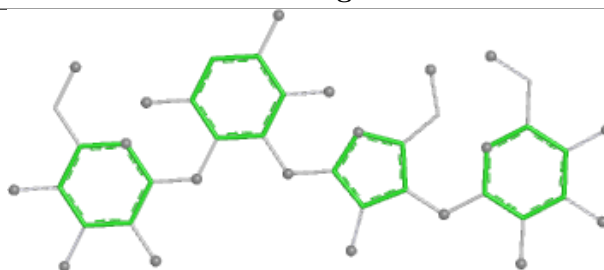
Bond lengths



Bond angles

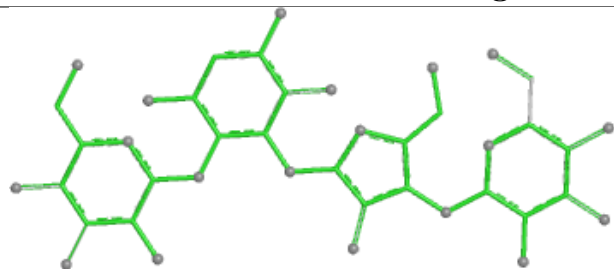


Torsions

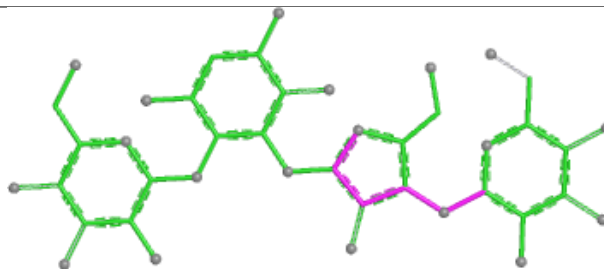


Rings

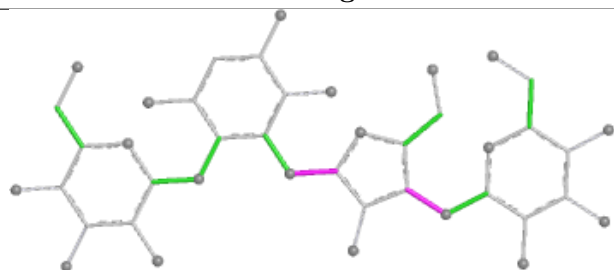
Ligand PAR CA 3167



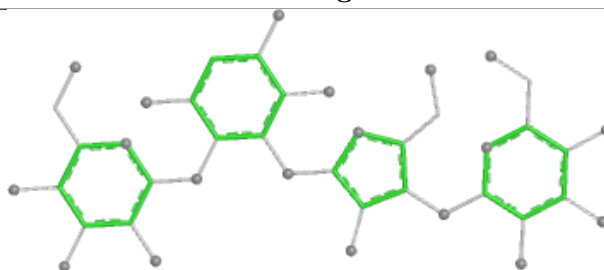
Bond lengths



Bond angles

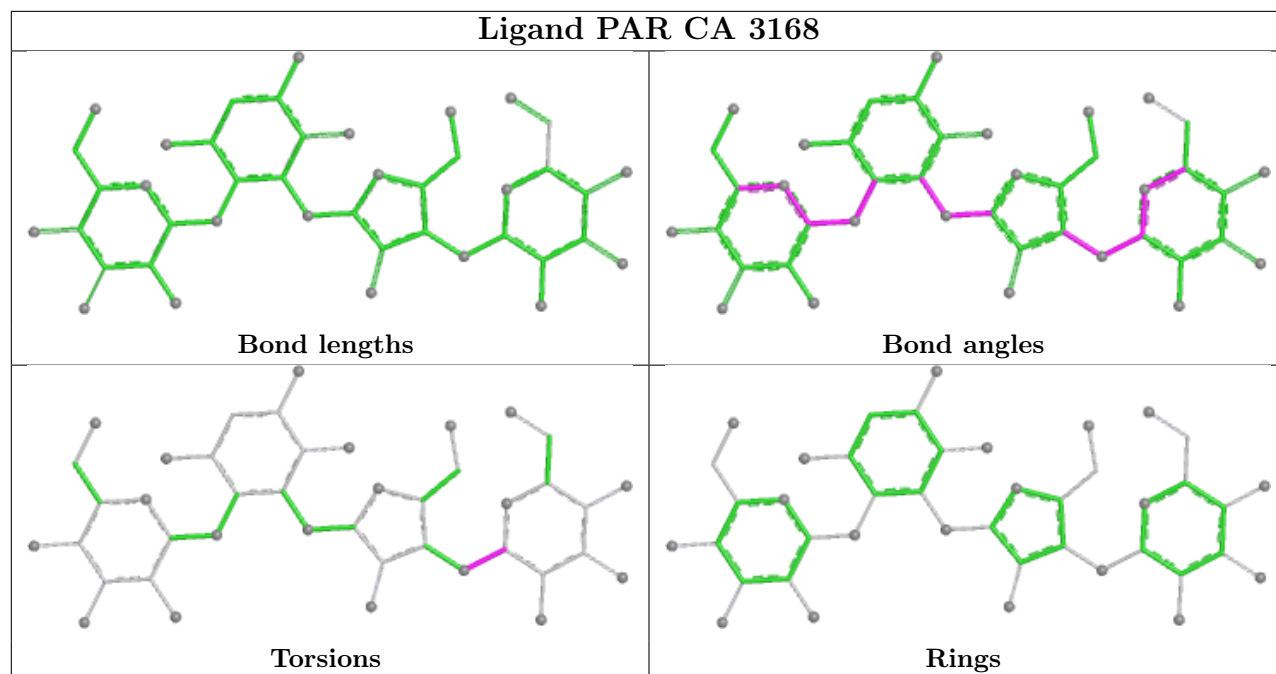


Torsions

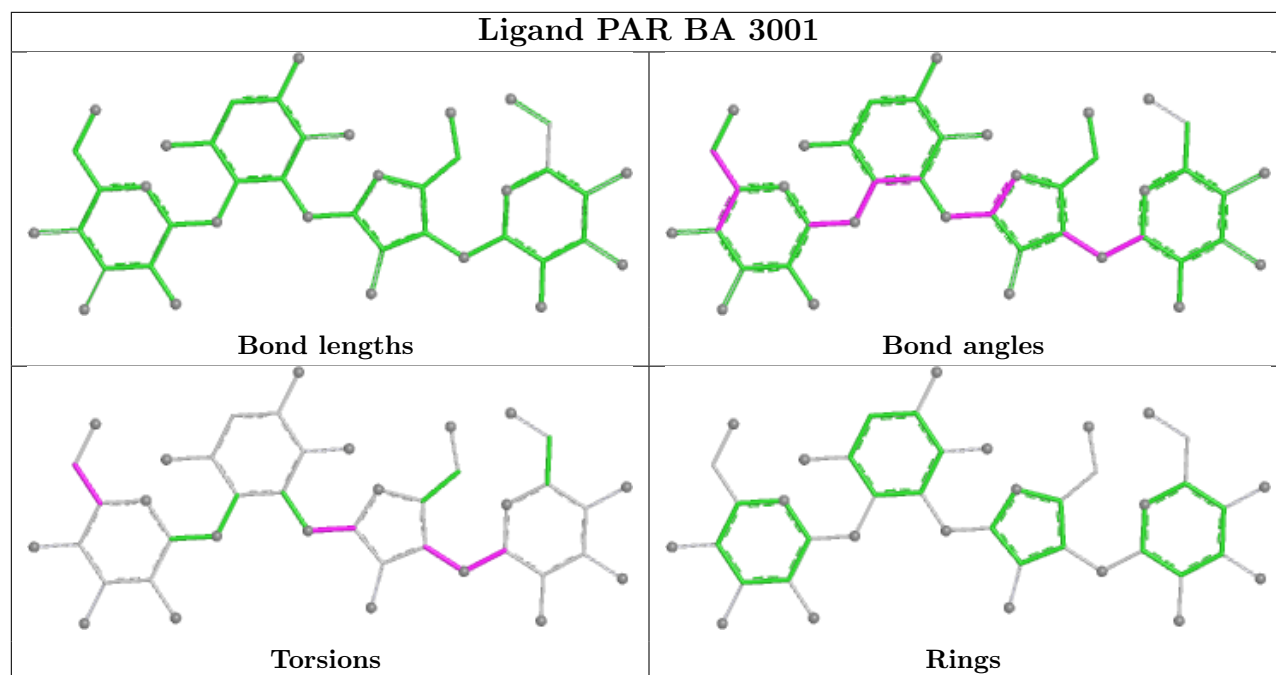


Rings

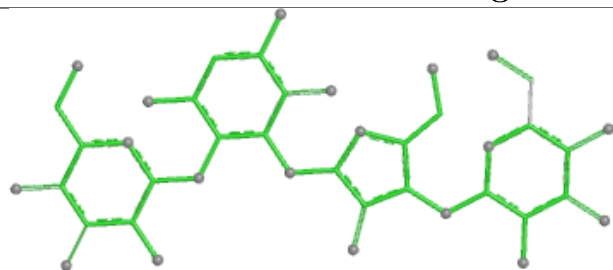
Ligand PAR CA 3168



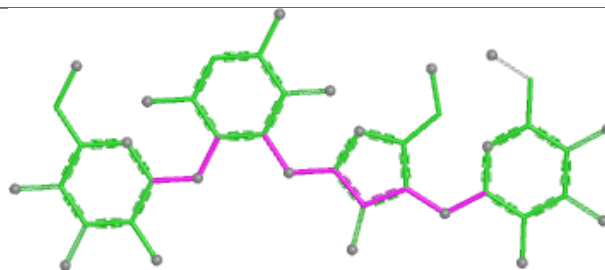
Ligand PAR BA 3001



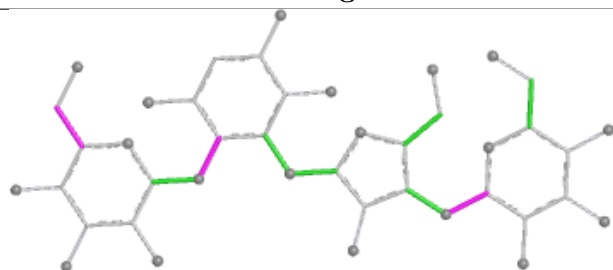
Ligand PAR CA 3166



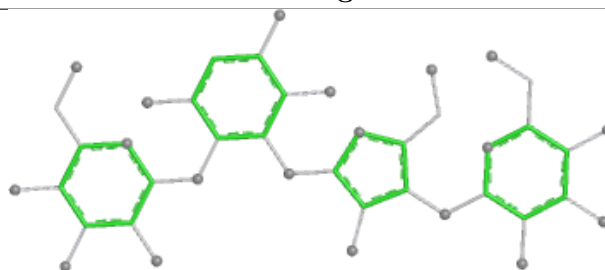
Bond lengths



Bond angles

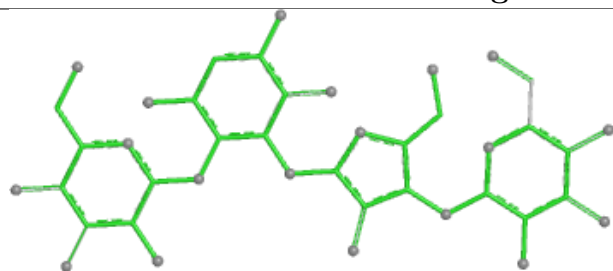


Torsions

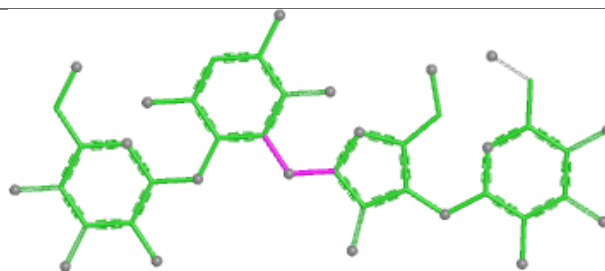


Rings

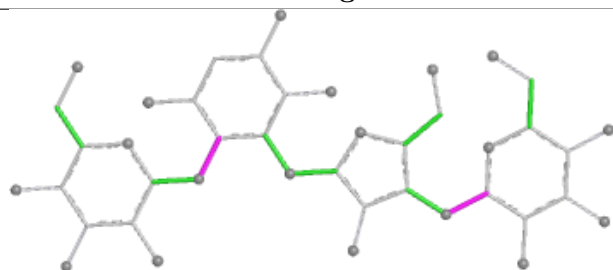
Ligand PAR DA 1654



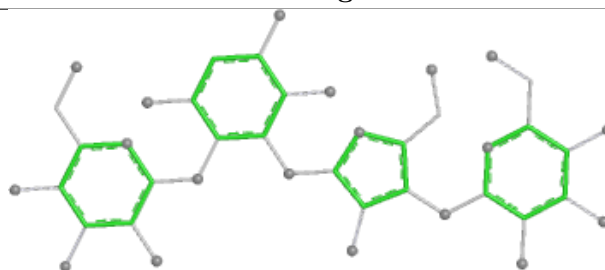
Bond lengths



Bond angles

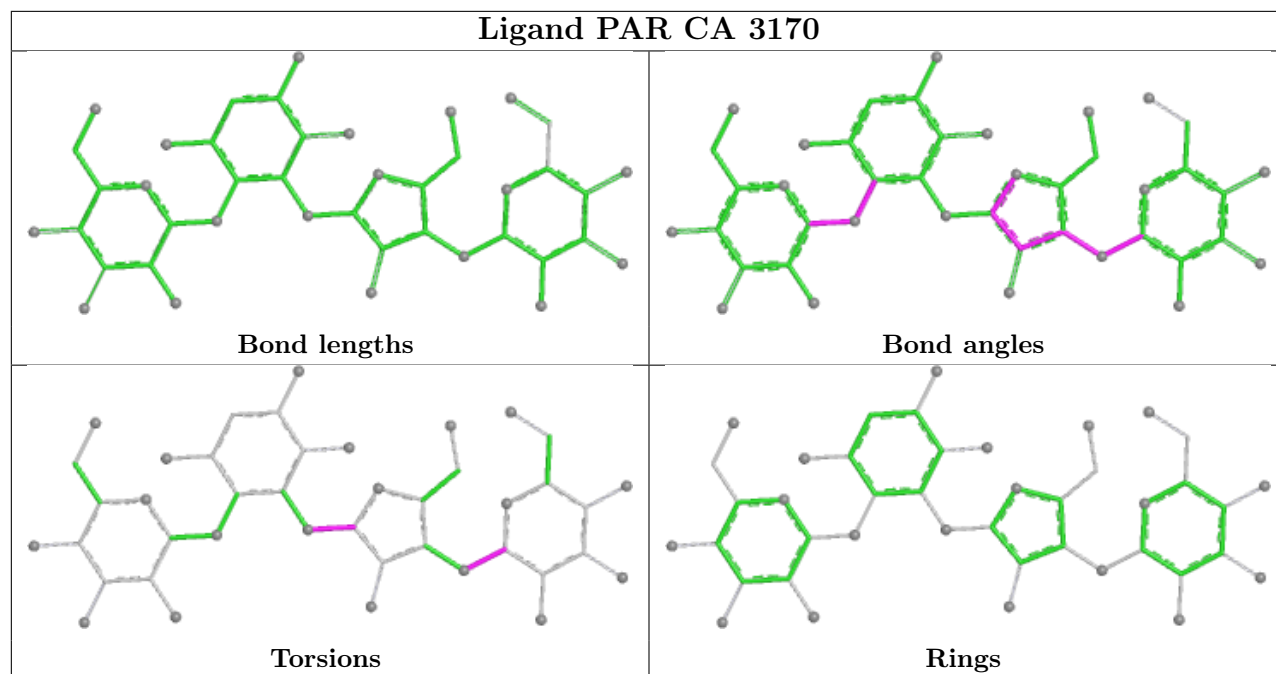


Torsions

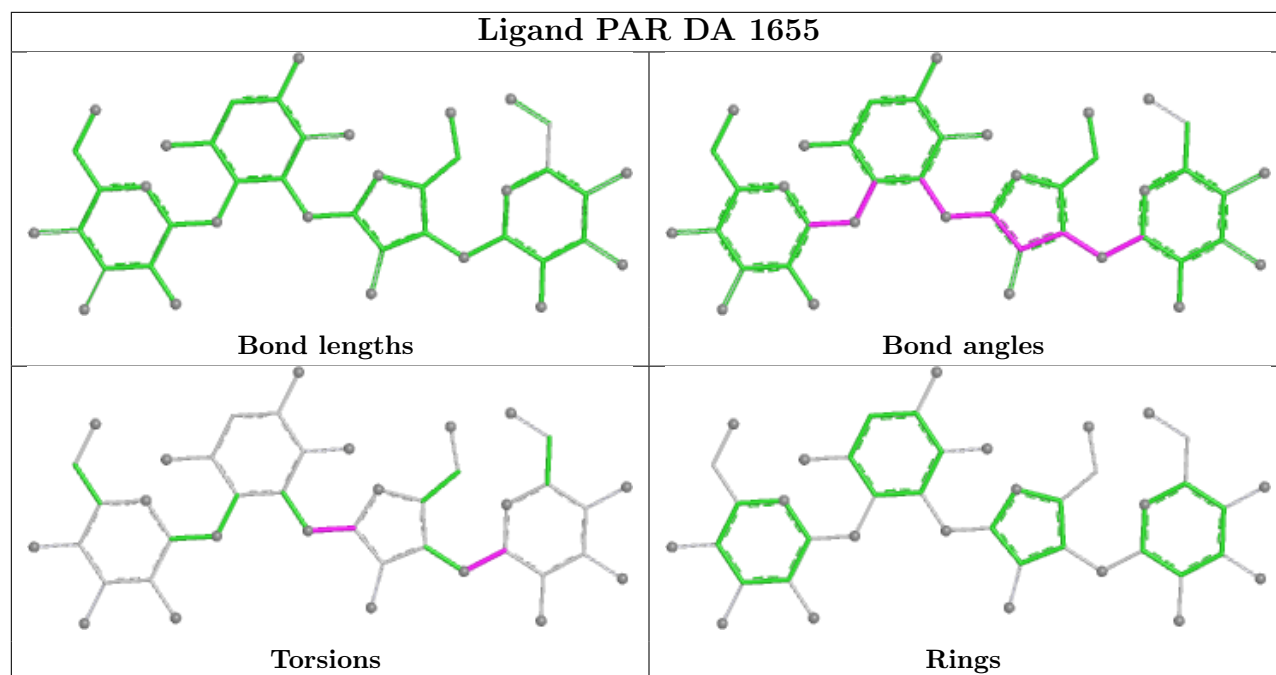


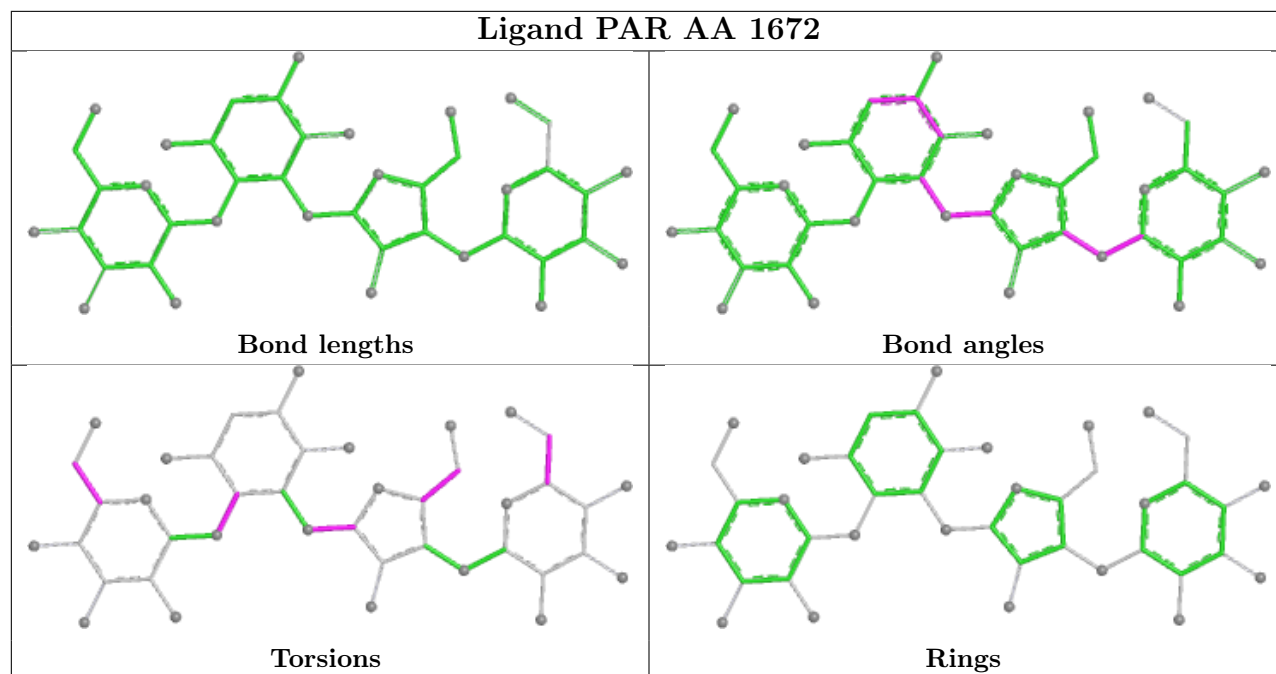
Rings

Ligand PAR CA 3170



Ligand PAR DA 1655





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	AA	1538/1542 (99%)	-0.85	0 100 100	44, 86, 166, 303	0
1	DA	1539/1542 (99%)	-0.84	2 (0%) 92 86	47, 85, 145, 285	0
2	AB	218/241 (90%)	-0.26	1 (0%) 87 72	64, 133, 196, 238	0
2	DB	218/241 (90%)	-0.05	2 (0%) 81 61	68, 115, 176, 210	0
3	AC	206/233 (88%)	-0.47	1 (0%) 87 72	44, 77, 114, 170	0
3	DC	206/233 (88%)	-0.16	3 (1%) 72 49	49, 90, 145, 213	0
4	AD	205/206 (99%)	0.17	6 (2%) 53 31	62, 104, 170, 243	0
4	DD	205/206 (99%)	0.30	11 (5%) 31 16	47, 92, 166, 215	0
5	AE	150/167 (89%)	-0.15	1 (0%) 84 66	53, 81, 124, 222	0
5	DE	150/167 (89%)	-0.20	2 (1%) 75 53	44, 79, 132, 171	0
6	AF	100/135 (74%)	0.07	2 (2%) 65 41	67, 122, 177, 211	0
6	DF	100/135 (74%)	-0.43	1 (1%) 79 59	50, 94, 135, 153	0
7	AG	151/179 (84%)	0.32	10 (6%) 24 12	62, 119, 169, 239	0
7	DG	151/179 (84%)	-0.07	2 (1%) 75 53	61, 104, 150, 211	0
8	AH	129/130 (99%)	-0.09	1 (0%) 82 64	59, 92, 136, 159	0
8	DH	129/130 (99%)	-0.28	2 (1%) 70 47	49, 84, 119, 174	0
9	AI	127/130 (97%)	0.08	3 (2%) 59 36	57, 108, 158, 215	0
9	DI	127/130 (97%)	0.39	8 (6%) 26 13	70, 116, 174, 197	0
10	AJ	98/103 (95%)	0.27	6 (6%) 27 14	57, 111, 175, 216	0
10	DJ	98/103 (95%)	0.18	2 (2%) 65 41	65, 111, 168, 200	0
11	AK	117/129 (90%)	-0.03	2 (1%) 69 45	58, 108, 177, 232	0
11	DK	117/129 (90%)	-0.31	3 (2%) 57 34	47, 75, 131, 186	0
12	AL	123/124 (99%)	-0.19	7 (5%) 29 15	33, 65, 115, 216	0
12	DL	123/124 (99%)	-0.22	5 (4%) 41 23	33, 71, 115, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/118 (96%)	0.22	4 (3%) 47 27	73, 132, 191, 263	0
13	DM	114/118 (96%)	0.16	3 (2%) 57 34	92, 135, 174, 254	0
14	AN	96/101 (95%)	0.58	10 (10%) 11 6	59, 95, 188, 237	0
14	DN	96/101 (95%)	0.30	4 (4%) 40 22	62, 104, 164, 215	0
15	AO	88/89 (98%)	-0.01	0 100 100	60, 102, 166, 216	0
15	DO	88/89 (98%)	-0.17	0 100 100	55, 85, 131, 156	0
16	AP	82/82 (100%)	0.15	2 (2%) 59 36	61, 86, 144, 198	0
16	DP	82/82 (100%)	0.07	0 100 100	53, 79, 141, 227	0
17	AQ	80/84 (95%)	-0.18	2 (2%) 58 35	52, 97, 152, 198	0
17	DQ	80/84 (95%)	-0.07	1 (1%) 75 53	58, 96, 161, 233	0
18	AR	55/75 (73%)	-0.12	2 (3%) 46 26	57, 97, 151, 178	0
18	DR	55/75 (73%)	-0.35	2 (3%) 46 26	57, 83, 134, 176	0
19	AS	79/92 (85%)	0.50	4 (5%) 33 17	91, 129, 184, 223	0
19	DS	79/92 (85%)	0.21	4 (5%) 33 17	83, 129, 181, 234	0
20	AT	85/87 (97%)	0.14	3 (3%) 47 27	54, 92, 134, 194	0
20	DT	85/87 (97%)	0.26	4 (4%) 36 19	64, 96, 132, 178	0
21	AU	51/71 (71%)	0.61	5 (9%) 13 7	67, 117, 167, 203	0
21	DU	51/71 (71%)	0.72	8 (15%) 5 3	54, 105, 159, 224	0
22	AV	183/185 (98%)	-0.28	0 100 100	20, 86, 171, 232	0
23	AW	15/16 (93%)	0.38	1 (6%) 24 12	57, 128, 176, 205	0
23	DV	16/16 (100%)	-0.11	1 (6%) 26 13	44, 99, 143, 191	0
24	AX	76/76 (100%)	-0.29	1 (1%) 75 53	44, 167, 277, 328	0
24	DW	76/76 (100%)	-0.91	0 100 100	51, 93, 135, 164	0
25	BA	2897/2904 (99%)	-1.10	20 (0%) 84 66	22, 52, 194, 368	0
25	CA	2897/2904 (99%)	-0.91	4 (0%) 92 86	37, 75, 205, 328	0
26	BB	119/120 (99%)	-1.20	0 100 100	41, 71, 101, 165	0
26	CB	118/120 (98%)	-0.82	0 100 100	63, 118, 153, 186	0
27	BC	271/273 (99%)	-0.33	1 (0%) 88 76	32, 60, 94, 149	0
27	CC	271/273 (99%)	-0.17	5 (1%) 67 44	38, 73, 106, 185	0
28	BD	209/209 (100%)	-0.68	0 100 100	21, 45, 77, 170	0
28	CD	209/209 (100%)	-0.39	0 100 100	41, 68, 109, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	BE	201/201 (100%)	-0.62	0 100 100	23, 56, 105, 161	0
29	CE	201/201 (100%)	-0.45	0 100 100	32, 79, 125, 175	0
30	BF	177/179 (98%)	-0.09	1 (0%) 85 69	44, 104, 177, 231	0
30	CF	177/179 (98%)	-0.00	3 (1%) 69 45	87, 140, 202, 243	0
31	BG	176/177 (99%)	-0.46	0 100 100	32, 72, 114, 158	0
31	CG	176/177 (99%)	-0.07	1 (0%) 85 69	72, 112, 153, 195	0
32	BH	149/149 (100%)	0.08	8 (5%) 31 16	28, 118, 177, 265	0
32	CH	149/149 (100%)	0.13	8 (5%) 31 16	28, 133, 188, 220	0
33	BI	141/142 (99%)	0.61	7 (4%) 34 18	118, 197, 266, 320	0
33	CI	141/142 (99%)	0.24	2 (1%) 73 51	137, 210, 253, 292	0
34	BJ	142/142 (100%)	-0.68	0 100 100	21, 44, 79, 102	0
34	CJ	142/142 (100%)	-0.42	1 (0%) 84 66	37, 65, 99, 167	0
35	BK	122/123 (99%)	-0.70	0 100 100	23, 49, 77, 104	0
35	CK	122/123 (99%)	-0.32	1 (0%) 82 64	42, 69, 112, 148	0
36	BL	143/144 (99%)	-0.46	0 100 100	24, 54, 83, 118	0
36	CL	143/144 (99%)	-0.17	0 100 100	39, 82, 125, 180	0
37	BM	136/136 (100%)	-0.71	0 100 100	27, 51, 89, 121	0
37	CM	136/136 (100%)	-0.26	0 100 100	44, 78, 106, 141	0
38	BN	120/127 (94%)	-0.64	0 100 100	22, 47, 71, 156	0
38	CN	120/127 (94%)	-0.34	0 100 100	46, 76, 103, 191	0
39	BO	116/117 (99%)	-0.54	0 100 100	37, 67, 99, 123	0
39	CO	116/117 (99%)	0.17	5 (4%) 40 21	70, 122, 164, 201	0
40	BP	114/115 (99%)	-0.51	2 (1%) 67 44	30, 56, 99, 206	0
40	CP	114/115 (99%)	-0.14	1 (0%) 81 61	45, 77, 116, 140	0
41	BQ	117/118 (99%)	-0.70	0 100 100	15, 39, 71, 91	0
41	CQ	117/118 (99%)	-0.48	0 100 100	32, 61, 85, 114	0
42	BR	103/103 (100%)	-0.60	0 100 100	21, 52, 87, 118	0
42	CR	103/103 (100%)	-0.31	0 100 100	32, 73, 108, 171	0
43	BS	110/110 (100%)	-0.67	0 100 100	20, 44, 76, 117	0
43	CS	110/110 (100%)	-0.49	0 100 100	31, 65, 103, 140	0
44	BT	93/100 (93%)	-0.18	5 (5%) 31 16	43, 60, 126, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CT	93/100 (93%)	0.01	3 (3%) 50 29	56, 94, 142, 202	0
45	BU	102/104 (98%)	-0.49	0 100 100	33, 61, 118, 185	0
45	CU	102/104 (98%)	0.02	5 (4%) 35 18	56, 90, 177, 215	0
46	BV	94/94 (100%)	-0.50	0 100 100	41, 71, 109, 127	0
46	CV	94/94 (100%)	-0.38	1 (1%) 78 57	66, 110, 151, 196	0
47	BW	76/85 (89%)	-0.16	1 (1%) 75 53	32, 54, 92, 126	0
47	CW	75/85 (88%)	0.02	1 (1%) 75 53	46, 82, 120, 146	0
48	BX	77/78 (98%)	-0.40	1 (1%) 75 53	38, 59, 101, 111	0
48	CX	77/78 (98%)	0.05	1 (1%) 75 53	38, 82, 121, 150	0
49	BY	63/63 (100%)	-0.32	1 (1%) 70 47	39, 69, 114, 179	0
49	CY	63/63 (100%)	-0.14	2 (3%) 50 29	66, 103, 165, 221	0
50	BZ	58/59 (98%)	-0.39	0 100 100	30, 47, 75, 106	0
50	CZ	58/59 (98%)	-0.31	0 100 100	45, 73, 112, 188	0
51	B0	56/57 (98%)	-0.53	0 100 100	22, 46, 94, 143	0
51	C0	56/57 (98%)	-0.33	1 (1%) 67 44	37, 73, 117, 194	0
52	B1	50/55 (90%)	0.19	2 (4%) 42 23	76, 105, 185, 196	0
52	C1	50/55 (90%)	-0.09	0 100 100	79, 109, 138, 164	0
53	B2	46/46 (100%)	-0.36	1 (2%) 62 39	27, 45, 76, 155	0
53	C2	46/46 (100%)	-0.21	0 100 100	39, 68, 92, 151	0
54	B3	64/65 (98%)	-0.32	1 (1%) 70 47	27, 48, 74, 122	0
54	C3	64/65 (98%)	-0.03	0 100 100	38, 69, 96, 109	0
55	B4	38/38 (100%)	-0.42	0 100 100	29, 52, 91, 122	0
55	C4	38/38 (100%)	0.23	2 (5%) 32 16	47, 83, 109, 119	0
56	B5	191/228 (83%)	0.47	7 (3%) 45 25	28, 219, 264, 311	0
All	All	21100/21699 (97%)	-0.50	249 (1%) 76 55	15, 80, 183, 368	0

The worst 5 of 249 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	DT	4	ILE	8.8
12	AL	124	ALA	7.3
4	DD	28	ILE	6.6
21	DU	27	GLY	6.4
27	CC	271	SER	6.2

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($\text{\AA}^2$)	Q<0.9
57	MG	BA	3145	1/1	0.37	0.74	164,164,164,164	0
58	PAR	CA	3169	42/42	0.54	0.24	21,68,103,144	42
57	MG	AA	1646	1/1	0.57	0.20	99,99,99,99	0
57	MG	BA	3169	1/1	0.59	0.26	88,88,88,88	0
57	MG	BQ	201	1/1	0.66	0.58	108,108,108,108	0
58	PAR	CA	3168	42/42	0.67	0.14	10,10,10,10	0
58	PAR	DA	1655	42/42	0.69	0.14	10,10,10,10	0
57	MG	BA	3029	1/1	0.73	0.21	240,240,240,240	0
57	MG	CA	3070	1/1	0.73	0.07	251,251,251,251	0
57	MG	CA	3126	1/1	0.73	0.16	146,146,146,146	0
57	MG	AA	1644	1/1	0.75	0.18	86,86,86,86	0
57	MG	CA	3123	1/1	0.75	0.24	177,177,177,177	0
57	MG	AA	1658	1/1	0.75	0.11	97,97,97,97	0
58	PAR	CA	3166	42/42	0.76	0.18	38,86,109,128	42
57	MG	AA	1648	1/1	0.76	0.06	77,77,77,77	0
57	MG	CA	3084	1/1	0.78	0.12	193,193,193,193	0
57	MG	AA	1668	1/1	0.78	0.09	70,70,70,70	0
58	PAR	CA	3167	42/42	0.78	0.12	10,10,10,10	0
57	MG	CA	3019	1/1	0.79	0.39	252,252,252,252	0
58	PAR	CA	3170	42/42	0.79	0.12	10,10,10,10	0
57	MG	AA	1654	1/1	0.79	0.23	82,82,82,82	0
57	MG	AA	1642	1/1	0.80	0.23	60,60,60,60	0
57	MG	DA	1604	1/1	0.80	0.15	166,166,166,166	0
58	PAR	BA	3005	42/42	0.80	0.14	41,100,141,152	42
57	MG	BA	3109	1/1	0.81	0.36	189,189,189,189	0
58	PAR	BA	3003	42/42	0.82	0.12	10,10,10,10	0
57	MG	CA	3165	1/1	0.82	0.23	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CD	301	1/1	0.82	0.31	234,234,234,234	0
57	MG	CA	3089	1/1	0.82	0.16	215,215,215,215	0
57	MG	DN	201	1/1	0.83	0.15	317,317,317,317	0
57	MG	AA	1655	1/1	0.83	0.28	77,77,77,77	0
57	MG	DA	1631	1/1	0.83	0.13	196,196,196,196	0
58	PAR	BA	3004	42/42	0.84	0.10	10,10,10,10	0
57	MG	AA	1663	1/1	0.85	0.21	52,52,52,52	0
57	MG	BA	3102	1/1	0.85	0.49	293,293,293,293	0
58	PAR	BA	3001	42/42	0.85	0.10	10,10,10,10	0
57	MG	AA	1609	1/1	0.85	0.20	227,227,227,227	0
57	MG	CA	3095	1/1	0.86	0.26	270,270,270,270	0
57	MG	CA	3048	1/1	0.86	0.07	157,157,157,157	0
57	MG	CA	3085	1/1	0.86	0.21	260,260,260,260	0
57	MG	DA	1652	1/1	0.86	0.18	67,67,67,67	0
57	MG	BA	3118	1/1	0.86	0.19	164,164,164,164	0
57	MG	DA	1650	1/1	0.87	0.13	81,81,81,81	0
57	MG	CA	3160	1/1	0.87	0.13	79,79,79,79	0
57	MG	DD	301	1/1	0.87	0.27	314,314,314,314	0
57	MG	BA	3154	1/1	0.87	0.21	56,56,56,56	0
57	MG	BA	3019	1/1	0.87	0.12	169,169,169,169	0
57	MG	AA	1660	1/1	0.87	0.08	67,67,67,67	0
57	MG	BA	3014	1/1	0.87	0.18	101,101,101,101	0
57	MG	DA	1628	1/1	0.88	0.17	177,177,177,177	0
57	MG	CA	3080	1/1	0.88	0.12	102,102,102,102	0
57	MG	BA	3098	1/1	0.88	0.14	157,157,157,157	0
57	MG	CA	3143	1/1	0.88	0.13	69,69,69,69	0
57	MG	AA	1651	1/1	0.88	0.20	60,60,60,60	0
57	MG	AA	1643	1/1	0.88	0.30	162,162,162,162	0
57	MG	BA	3110	1/1	0.88	0.33	89,89,89,89	0
58	PAR	DA	1654	42/42	0.88	0.09	10,10,10,10	0
57	MG	CA	3098	1/1	0.88	0.48	242,242,242,242	0
57	MG	AA	1627	1/1	0.89	0.10	111,111,111,111	0
57	MG	AA	1665	1/1	0.89	0.13	106,106,106,106	0
57	MG	CA	3071	1/1	0.89	0.15	218,218,218,218	0
58	PAR	AA	1672	42/42	0.89	0.09	10,10,10,10	0
57	MG	CA	3145	1/1	0.89	0.19	59,59,59,59	0
57	MG	AA	1653	1/1	0.89	0.18	82,82,82,82	0
57	MG	BA	3170	1/1	0.89	0.10	51,51,51,51	0
57	MG	CB	3201	1/1	0.89	0.07	216,216,216,216	0
57	MG	BA	3182	1/1	0.89	0.24	59,59,59,59	0
57	MG	BL	202	1/1	0.89	0.29	259,259,259,259	0
57	MG	DA	1626	1/1	0.89	0.10	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3067	1/1	0.89	0.18	218,218,218,218	0
57	MG	BA	3092	1/1	0.89	0.11	173,173,173,173	0
57	MG	DA	1639	1/1	0.89	0.17	161,161,161,161	0
57	MG	CA	3100	1/1	0.89	0.14	155,155,155,155	0
57	MG	CA	3083	1/1	0.90	0.09	79,79,79,79	0
57	MG	BA	3134	1/1	0.90	0.21	143,143,143,143	0
57	MG	AA	1666	1/1	0.90	0.08	44,44,44,44	0
57	MG	AA	1607	1/1	0.90	0.42	327,327,327,327	0
58	PAR	BA	3002	42/42	0.90	0.08	10,10,10,10	0
57	MG	CA	3092	1/1	0.90	0.09	134,134,134,134	0
57	MG	CA	3025	1/1	0.90	0.14	121,121,121,121	0
57	MG	CA	3028	1/1	0.90	0.30	312,312,312,312	0
57	MG	BA	3165	1/1	0.90	0.21	60,60,60,60	0
57	MG	BA	3045	1/1	0.90	0.13	217,217,217,217	0
57	MG	BA	3012	1/1	0.90	0.07	100,100,100,100	0
57	MG	DA	1641	1/1	0.90	0.17	69,69,69,69	0
57	MG	DA	1643	1/1	0.90	0.10	73,73,73,73	0
57	MG	CA	3141	1/1	0.90	0.34	68,68,68,68	0
57	MG	AA	1656	1/1	0.90	0.15	73,73,73,73	0
57	MG	BA	3095	1/1	0.91	0.06	187,187,187,187	0
57	MG	BA	3160	1/1	0.91	0.19	74,74,74,74	0
57	MG	DA	1645	1/1	0.91	0.15	57,57,57,57	0
57	MG	AA	1667	1/1	0.91	0.14	81,81,81,81	0
57	MG	AA	1604	1/1	0.91	0.08	173,173,173,173	0
57	MG	CA	3153	1/1	0.91	0.24	47,47,47,47	0
57	MG	DD	302	1/1	0.91	0.26	53,53,53,53	0
57	MG	CA	3156	1/1	0.91	0.06	45,45,45,45	0
57	MG	AA	1669	1/1	0.91	0.18	58,58,58,58	0
57	MG	CA	3162	1/1	0.91	0.12	71,71,71,71	0
57	MG	BA	3173	1/1	0.91	0.18	59,59,59,59	0
57	MG	AA	1650	1/1	0.91	0.20	55,55,55,55	0
57	MG	CB	3202	1/1	0.91	0.08	114,114,114,114	0
57	MG	BA	3082	1/1	0.91	0.09	139,139,139,139	0
57	MG	BA	3127	1/1	0.91	0.11	88,88,88,88	0
57	MG	DA	1622	1/1	0.91	0.20	331,331,331,331	0
57	MG	BA	3083	1/1	0.91	0.12	84,84,84,84	0
57	MG	AA	1637	1/1	0.91	0.12	138,138,138,138	0
57	MG	BA	3146	1/1	0.91	0.20	48,48,48,48	0
57	MG	DA	1634	1/1	0.91	0.07	128,128,128,128	0
57	MG	CA	3047	1/1	0.91	0.20	211,211,211,211	0
57	MG	CA	3159	1/1	0.92	0.11	52,52,52,52	0
57	MG	BA	3108	1/1	0.92	0.18	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3091	1/1	0.92	0.08	94,94,94,94	0
57	MG	BA	3180	1/1	0.92	0.08	48,48,48,48	0
57	MG	CA	3056	1/1	0.92	0.23	155,155,155,155	0
57	MG	CA	3061	1/1	0.92	0.12	102,102,102,102	0
57	MG	CA	3114	1/1	0.92	0.12	169,169,169,169	0
57	MG	CA	3119	1/1	0.92	0.11	215,215,215,215	0
57	MG	DA	1613	1/1	0.92	0.08	89,89,89,89	0
57	MG	CA	3068	1/1	0.92	0.09	58,58,58,58	0
57	MG	AA	1659	1/1	0.92	0.16	84,84,84,84	0
57	MG	AA	1645	1/1	0.92	0.32	75,75,75,75	0
57	MG	BA	3021	1/1	0.92	0.29	276,276,276,276	0
57	MG	BA	3167	1/1	0.92	0.21	53,53,53,53	0
57	MG	DA	1635	1/1	0.92	0.11	126,126,126,126	0
57	MG	AA	1636	1/1	0.92	0.49	313,313,313,313	0
57	MG	CA	3026	1/1	0.92	0.12	202,202,202,202	0
57	MG	CA	3158	1/1	0.92	0.25	57,57,57,57	0
57	MG	DA	1644	1/1	0.92	0.23	62,62,62,62	0
57	MG	AA	1664	1/1	0.93	0.05	67,67,67,67	0
57	MG	BA	3176	1/1	0.93	0.17	51,51,51,51	0
57	MG	BA	3178	1/1	0.93	0.07	63,63,63,63	0
57	MG	DA	1648	1/1	0.93	0.24	41,41,41,41	0
57	MG	BA	3115	1/1	0.93	0.20	133,133,133,133	0
57	MG	DA	1651	1/1	0.93	0.12	51,51,51,51	0
57	MG	CA	3055	1/1	0.93	0.12	114,114,114,114	0
57	MG	CA	3103	1/1	0.93	0.08	116,116,116,116	0
57	MG	BA	3181	1/1	0.93	0.25	106,106,106,106	0
57	MG	CA	3115	1/1	0.93	0.09	235,235,235,235	0
57	MG	AA	1614	1/1	0.93	0.09	146,146,146,146	0
57	MG	DA	1608	1/1	0.93	0.06	218,218,218,218	0
57	MG	CA	3122	1/1	0.93	0.11	88,88,88,88	0
57	MG	DA	1617	1/1	0.93	0.16	65,65,65,65	0
57	MG	AA	1608	1/1	0.93	0.07	159,159,159,159	0
57	MG	BO	201	1/1	0.93	0.08	67,67,67,67	0
57	MG	BA	3129	1/1	0.93	0.12	78,78,78,78	0
57	MG	CA	3013	1/1	0.93	0.21	362,362,362,362	0
57	MG	CA	3015	1/1	0.93	0.07	126,126,126,126	0
57	MG	CA	3147	1/1	0.93	0.16	77,77,77,77	0
57	MG	BA	3044	1/1	0.93	0.11	62,62,62,62	0
57	MG	DA	1640	1/1	0.93	0.22	66,66,66,66	0
57	MG	AA	1632	1/1	0.93	0.11	149,149,149,149	0
57	MG	DA	1630	1/1	0.94	0.08	72,72,72,72	0
57	MG	CA	3133	1/1	0.94	0.09	182,182,182,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3140	1/1	0.94	0.13	29,29,29,29	0
57	MG	CA	3079	1/1	0.94	0.07	195,195,195,195	0
57	MG	BA	3025	1/1	0.94	0.21	134,134,134,134	0
57	MG	AA	1657	1/1	0.94	0.08	78,78,78,78	0
57	MG	CA	3146	1/1	0.94	0.08	52,52,52,52	0
57	MG	AA	1628	1/1	0.94	0.08	106,106,106,106	0
57	MG	CA	3148	1/1	0.94	0.17	37,37,37,37	0
57	MG	CA	3149	1/1	0.94	0.17	69,69,69,69	0
57	MG	AA	1620	1/1	0.94	0.07	133,133,133,133	0
57	MG	DA	1649	1/1	0.94	0.09	63,63,63,63	0
57	MG	CA	3087	1/1	0.94	0.12	75,75,75,75	0
57	MG	CA	3157	1/1	0.94	0.14	54,54,54,54	0
57	MG	BA	3064	1/1	0.94	0.08	80,80,80,80	0
57	MG	DA	1653	1/1	0.94	0.18	51,51,51,51	0
57	MG	CA	3091	1/1	0.94	0.06	93,93,93,93	0
57	MG	BA	3168	1/1	0.94	0.23	39,39,39,39	0
57	MG	CA	3161	1/1	0.94	0.24	39,39,39,39	0
57	MG	AA	1633	1/1	0.94	0.06	86,86,86,86	0
57	MG	BA	3075	1/1	0.94	0.12	88,88,88,88	0
57	MG	AA	1661	1/1	0.94	0.15	53,53,53,53	0
57	MG	BA	3119	1/1	0.94	0.14	262,262,262,262	0
57	MG	CA	3108	1/1	0.94	0.16	101,101,101,101	0
57	MG	DA	1602	1/1	0.94	0.09	83,83,83,83	0
57	MG	BA	3120	1/1	0.94	0.20	91,91,91,91	0
57	MG	BA	3179	1/1	0.94	0.32	88,88,88,88	0
57	MG	AA	1635	1/1	0.94	0.17	234,234,234,234	0
57	MG	AA	1621	1/1	0.94	0.08	157,157,157,157	0
57	MG	AA	1616	1/1	0.94	0.07	118,118,118,118	0
57	MG	BA	3094	1/1	0.94	0.08	153,153,153,153	0
57	MG	CA	3131	1/1	0.94	0.09	75,75,75,75	0
57	MG	BB	3204	1/1	0.95	0.12	24,24,24,24	0
57	MG	BA	3097	1/1	0.95	0.07	91,91,91,91	0
57	MG	BA	3143	1/1	0.95	0.17	25,25,25,25	0
57	MG	DA	1636	1/1	0.95	0.07	82,82,82,82	0
57	MG	DA	1638	1/1	0.95	0.18	93,93,93,93	0
57	MG	BA	3123	1/1	0.95	0.06	115,115,115,115	0
57	MG	CA	3004	1/1	0.95	0.06	130,130,130,130	0
57	MG	CA	3086	1/1	0.95	0.06	83,83,83,83	0
57	MG	CA	3007	1/1	0.95	0.09	204,204,204,204	0
57	MG	BA	3015	1/1	0.95	0.06	58,58,58,58	0
57	MG	BA	3149	1/1	0.95	0.15	33,33,33,33	0
57	MG	DA	1647	1/1	0.95	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3171	1/1	0.95	0.15	47,47,47,47	0
57	MG	BA	3172	1/1	0.95	0.15	57,57,57,57	0
57	MG	BA	3150	1/1	0.95	0.28	38,38,38,38	0
57	MG	BA	3175	1/1	0.95	0.11	44,44,44,44	0
57	MG	CA	3029	1/1	0.95	0.27	168,168,168,168	0
57	MG	BA	3151	1/1	0.95	0.16	44,44,44,44	0
57	MG	BA	3177	1/1	0.95	0.06	86,86,86,86	0
57	MG	BA	3152	1/1	0.95	0.16	56,56,56,56	0
57	MG	AA	1631	1/1	0.95	0.10	115,115,115,115	0
57	MG	BA	3158	1/1	0.95	0.25	30,30,30,30	0
57	MG	CQ	201	1/1	0.95	0.18	32,32,32,32	0
57	MG	CA	3062	1/1	0.95	0.06	97,97,97,97	0
57	MG	CA	3125	1/1	0.95	0.06	38,38,38,38	0
57	MG	DA	1606	1/1	0.95	0.06	144,144,144,144	0
57	MG	CA	3064	1/1	0.95	0.17	118,118,118,118	0
57	MG	CA	3128	1/1	0.95	0.05	66,66,66,66	0
57	MG	DA	1616	1/1	0.95	0.06	98,98,98,98	0
57	MG	BA	3130	1/1	0.95	0.12	270,270,270,270	0
57	MG	BA	3164	1/1	0.95	0.25	54,54,54,54	0
57	MG	CA	3135	1/1	0.95	0.09	121,121,121,121	0
57	MG	CA	3137	1/1	0.95	0.18	22,22,22,22	0
57	MG	BB	3201	1/1	0.95	0.06	107,107,107,107	0
57	MG	CA	3046	1/1	0.96	0.13	130,130,130,130	0
57	MG	CA	3094	1/1	0.96	0.09	94,94,94,94	0
57	MG	BA	3188	1/1	0.96	0.10	39,39,39,39	0
57	MG	CA	3150	1/1	0.96	0.11	54,54,54,54	0
57	MG	BA	3191	1/1	0.96	0.13	43,43,43,43	0
57	MG	AA	1612	1/1	0.96	0.05	94,94,94,94	0
57	MG	BA	3074	1/1	0.96	0.07	105,105,105,105	0
57	MG	AA	1670	1/1	0.96	0.24	50,50,50,50	0
57	MG	CA	3109	1/1	0.96	0.10	74,74,74,74	0
57	MG	DA	1646	1/1	0.96	0.15	31,31,31,31	0
57	MG	CA	3110	1/1	0.96	0.06	61,61,61,61	0
57	MG	CA	3111	1/1	0.96	0.12	164,164,164,164	0
57	MG	BA	3078	1/1	0.96	0.07	86,86,86,86	0
57	MG	BA	3156	1/1	0.96	0.22	35,35,35,35	0
57	MG	CA	3116	1/1	0.96	0.12	94,94,94,94	0
57	MG	BA	3101	1/1	0.96	0.08	70,70,70,70	0
57	MG	BA	3080	1/1	0.96	0.13	75,75,75,75	0
57	MG	CA	3011	1/1	0.96	0.09	54,54,54,54	0
57	MG	CA	3074	1/1	0.96	0.07	53,53,53,53	0
57	MG	AA	1611	1/1	0.96	0.06	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3055	1/1	0.96	0.06	34,34,34,34	0
57	MG	BA	3088	1/1	0.96	0.09	147,147,147,147	0
57	MG	AA	1662	1/1	0.96	0.08	69,69,69,69	0
57	MG	BA	3065	1/1	0.96	0.09	98,98,98,98	0
57	MG	BA	3184	1/1	0.96	0.13	40,40,40,40	0
57	MG	DA	1618	1/1	0.96	0.08	51,51,51,51	0
57	MG	DA	1619	1/1	0.96	0.06	155,155,155,155	0
57	MG	CA	3138	1/1	0.96	0.19	39,39,39,39	0
57	MG	BA	3185	1/1	0.96	0.21	32,32,32,32	0
57	MG	CA	3088	1/1	0.96	0.05	98,98,98,98	0
57	MG	CA	3034	1/1	0.96	0.20	157,157,157,157	0
57	MG	CA	3090	1/1	0.96	0.06	69,69,69,69	0
57	MG	CA	3045	1/1	0.96	0.08	46,46,46,46	0
57	MG	AA	1652	1/1	0.97	0.09	50,50,50,50	0
57	MG	AA	1649	1/1	0.97	0.18	51,51,51,51	0
57	MG	BA	3017	1/1	0.97	0.07	56,56,56,56	0
57	MG	BA	3183	1/1	0.97	0.09	37,37,37,37	0
57	MG	CA	3077	1/1	0.97	0.06	131,131,131,131	0
57	MG	BA	3147	1/1	0.97	0.12	54,54,54,54	0
57	MG	BA	3148	1/1	0.97	0.21	34,34,34,34	0
57	MG	CA	3163	1/1	0.97	0.17	44,44,44,44	0
57	MG	CA	3081	1/1	0.97	0.06	48,48,48,48	0
57	MG	BA	3187	1/1	0.97	0.14	29,29,29,29	0
57	MG	BA	3060	1/1	0.97	0.07	146,146,146,146	0
57	MG	BA	3189	1/1	0.97	0.08	47,47,47,47	0
57	MG	AA	1615	1/1	0.97	0.05	123,123,123,123	0
57	MG	BA	3192	1/1	0.97	0.10	46,46,46,46	0
57	MG	AA	1671	1/1	0.97	0.09	47,47,47,47	0
57	MG	BA	3023	1/1	0.97	0.14	38,38,38,38	0
57	MG	BA	3153	1/1	0.97	0.27	34,34,34,34	0
57	MG	DA	1609	1/1	0.97	0.05	97,97,97,97	0
57	MG	DA	1612	1/1	0.97	0.05	123,123,123,123	0
57	MG	BA	3071	1/1	0.97	0.06	43,43,43,43	0
57	MG	DA	1614	1/1	0.97	0.05	96,96,96,96	0
57	MG	DA	1615	1/1	0.97	0.06	213,213,213,213	0
57	MG	BA	3155	1/1	0.97	0.10	23,23,23,23	0
57	MG	CA	3093	1/1	0.97	0.05	127,127,127,127	0
57	MG	BA	3106	1/1	0.97	0.07	71,71,71,71	0
57	MG	BA	3157	1/1	0.97	0.19	44,44,44,44	0
57	MG	CA	3008	1/1	0.97	0.09	74,74,74,74	0
57	MG	DA	1623	1/1	0.97	0.05	64,64,64,64	0
57	MG	CA	3009	1/1	0.97	0.07	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	1627	1/1	0.97	0.04	80,80,80,80	0
57	MG	BA	3073	1/1	0.97	0.05	141,141,141,141	0
57	MG	CA	3104	1/1	0.97	0.07	57,57,57,57	0
57	MG	CA	3105	1/1	0.97	0.07	44,44,44,44	0
57	MG	DA	1633	1/1	0.97	0.21	264,264,264,264	0
57	MG	CA	3107	1/1	0.97	0.13	95,95,95,95	0
57	MG	BA	3159	1/1	0.97	0.18	38,38,38,38	0
57	MG	CA	3014	1/1	0.97	0.06	82,82,82,82	0
57	MG	AN	201	1/1	0.97	0.05	109,109,109,109	0
57	MG	BA	3162	1/1	0.97	0.14	44,44,44,44	0
57	MG	CA	3112	1/1	0.97	0.14	137,137,137,137	0
57	MG	BA	3027	1/1	0.97	0.06	57,57,57,57	0
57	MG	AA	1602	1/1	0.97	0.05	107,107,107,107	0
57	MG	BA	3116	1/1	0.97	0.13	133,133,133,133	0
57	MG	BA	3079	1/1	0.97	0.04	42,42,42,42	0
57	MG	CA	3030	1/1	0.97	0.07	154,154,154,154	0
57	MG	CA	3033	1/1	0.97	0.05	56,56,56,56	0
57	MG	BA	3034	1/1	0.97	0.08	41,41,41,41	0
57	MG	CA	3036	1/1	0.97	0.05	53,53,53,53	0
57	MG	CA	3037	1/1	0.97	0.05	90,90,90,90	0
57	MG	CA	3040	1/1	0.97	0.12	98,98,98,98	0
57	MG	CA	3043	1/1	0.97	0.04	57,57,57,57	0
57	MG	BA	3037	1/1	0.97	0.09	52,52,52,52	0
57	MG	CA	3136	1/1	0.97	0.05	107,107,107,107	0
57	MG	BA	3038	1/1	0.97	0.12	73,73,73,73	0
57	MG	BA	3086	1/1	0.97	0.06	74,74,74,74	0
57	MG	BA	3128	1/1	0.97	0.09	99,99,99,99	0
57	MG	CA	3049	1/1	0.97	0.06	76,76,76,76	0
57	MG	CA	3052	1/1	0.97	0.06	54,54,54,54	0
57	MG	CA	3054	1/1	0.97	0.06	41,41,41,41	0
57	MG	BA	3039	1/1	0.97	0.08	48,48,48,48	0
57	MG	BA	3089	1/1	0.97	0.04	44,44,44,44	0
57	MG	BA	3090	1/1	0.97	0.13	71,71,71,71	0
57	MG	BA	3137	1/1	0.97	0.05	95,95,95,95	0
57	MG	BA	3141	1/1	0.97	0.10	31,31,31,31	0
57	MG	CA	3151	1/1	0.97	0.27	44,44,44,44	0
57	MG	CA	3067	1/1	0.97	0.06	64,64,64,64	0
57	MG	CA	3154	1/1	0.97	0.15	42,42,42,42	0
57	MG	CA	3155	1/1	0.97	0.17	39,39,39,39	0
59	ZN	B4	9501	1/1	0.97	0.17	386,386,386,386	0
57	MG	CA	3063	1/1	0.98	0.05	50,50,50,50	0
57	MG	BA	3081	1/1	0.98	0.04	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3136	1/1	0.98	0.05	61,61,61,61	0
57	MG	AA	1617	1/1	0.98	0.04	104,104,104,104	0
57	MG	CA	3069	1/1	0.98	0.05	63,63,63,63	0
57	MG	BA	3186	1/1	0.98	0.28	37,37,37,37	0
57	MG	BA	3138	1/1	0.98	0.15	227,227,227,227	0
57	MG	CA	3073	1/1	0.98	0.04	64,64,64,64	0
57	MG	BA	3035	1/1	0.98	0.04	43,43,43,43	0
57	MG	BA	3142	1/1	0.98	0.13	63,63,63,63	0
57	MG	CA	3078	1/1	0.98	0.04	113,113,113,113	0
57	MG	CA	3164	1/1	0.98	0.22	44,44,44,44	0
57	MG	BA	3190	1/1	0.98	0.22	68,68,68,68	0
57	MG	AA	1618	1/1	0.98	0.07	43,43,43,43	0
57	MG	BA	3144	1/1	0.98	0.18	34,34,34,34	0
57	MG	CB	3203	1/1	0.98	0.04	115,115,115,115	0
57	MG	BA	3193	1/1	0.98	0.14	28,28,28,28	0
57	MG	BA	3194	1/1	0.98	0.17	46,46,46,46	0
57	MG	DA	1601	1/1	0.98	0.04	47,47,47,47	0
57	MG	BA	3087	1/1	0.98	0.05	139,139,139,139	0
57	MG	BB	3202	1/1	0.98	0.04	34,34,34,34	0
57	MG	BA	3009	1/1	0.98	0.06	63,63,63,63	0
57	MG	BA	3010	1/1	0.98	0.05	56,56,56,56	0
57	MG	BA	3040	1/1	0.98	0.05	66,66,66,66	0
57	MG	DA	1611	1/1	0.98	0.04	60,60,60,60	0
57	MG	AA	1619	1/1	0.98	0.07	70,70,70,70	0
57	MG	CA	3003	1/1	0.98	0.05	95,95,95,95	0
57	MG	BA	3013	1/1	0.98	0.04	40,40,40,40	0
57	MG	CA	3006	1/1	0.98	0.06	83,83,83,83	0
57	MG	BA	3048	1/1	0.98	0.07	69,69,69,69	0
57	MG	BA	3049	1/1	0.98	0.05	57,57,57,57	0
57	MG	CA	3096	1/1	0.98	0.06	100,100,100,100	0
57	MG	CA	3097	1/1	0.98	0.04	63,63,63,63	0
57	MG	DA	1620	1/1	0.98	0.04	78,78,78,78	0
57	MG	BA	3050	1/1	0.98	0.03	27,27,27,27	0
57	MG	CA	3010	1/1	0.98	0.03	34,34,34,34	0
57	MG	CA	3102	1/1	0.98	0.07	123,123,123,123	0
57	MG	AA	1634	1/1	0.98	0.05	87,87,87,87	0
57	MG	BA	3056	1/1	0.98	0.07	59,59,59,59	0
57	MG	BA	3059	1/1	0.98	0.04	60,60,60,60	0
57	MG	BA	3104	1/1	0.98	0.04	37,37,37,37	0
57	MG	BA	3105	1/1	0.98	0.13	80,80,80,80	0
57	MG	CA	3024	1/1	0.98	0.06	65,65,65,65	0
57	MG	AA	1613	1/1	0.98	0.05	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3107	1/1	0.98	0.04	60,60,60,60	0
57	MG	DA	1637	1/1	0.98	0.11	158,158,158,158	0
57	MG	BA	3161	1/1	0.98	0.10	45,45,45,45	0
57	MG	CA	3113	1/1	0.98	0.08	85,85,85,85	0
57	MG	BA	3061	1/1	0.98	0.06	70,70,70,70	0
57	MG	BA	3063	1/1	0.98	0.08	93,93,93,93	0
57	MG	DA	1642	1/1	0.98	0.22	60,60,60,60	0
57	MG	CA	3031	1/1	0.98	0.07	30,30,30,30	0
57	MG	CA	3032	1/1	0.98	0.08	97,97,97,97	0
57	MG	AA	1606	1/1	0.98	0.05	102,102,102,102	0
57	MG	BA	3166	1/1	0.98	0.10	34,34,34,34	0
57	MG	CA	3124	1/1	0.98	0.06	125,125,125,125	0
57	MG	CA	3035	1/1	0.98	0.06	35,35,35,35	0
57	MG	BA	3112	1/1	0.98	0.12	29,29,29,29	0
57	MG	CA	3127	1/1	0.98	0.04	47,47,47,47	0
57	MG	BA	3114	1/1	0.98	0.05	65,65,65,65	0
57	MG	CA	3039	1/1	0.98	0.06	58,58,58,58	0
57	MG	CA	3132	1/1	0.98	0.04	67,67,67,67	0
57	MG	BA	3018	1/1	0.98	0.04	59,59,59,59	0
57	MG	BA	3066	1/1	0.98	0.06	77,77,77,77	0
57	MG	BA	3117	1/1	0.98	0.05	65,65,65,65	0
57	MG	AA	1623	1/1	0.98	0.09	67,67,67,67	0
57	MG	AA	1641	1/1	0.98	0.06	124,124,124,124	0
57	MG	CA	3139	1/1	0.98	0.19	52,52,52,52	0
57	MG	AA	1603	1/1	0.98	0.07	45,45,45,45	0
57	MG	AA	1605	1/1	0.98	0.04	122,122,122,122	0
57	MG	BA	3126	1/1	0.98	0.05	39,39,39,39	0
57	MG	CA	3144	1/1	0.98	0.10	56,56,56,56	0
57	MG	CA	3053	1/1	0.98	0.05	46,46,46,46	0
57	MG	AA	1629	1/1	0.98	0.04	54,54,54,54	0
57	MG	AA	1630	1/1	0.98	0.05	113,113,113,113	0
57	MG	BA	3031	1/1	0.98	0.04	60,60,60,60	0
57	MG	CA	3059	1/1	0.98	0.04	88,88,88,88	0
57	MG	BA	3032	1/1	0.98	0.04	33,33,33,33	0
57	MG	BA	3132	1/1	0.98	0.07	30,30,30,30	0
57	MG	CA	3001	1/1	0.99	0.03	54,54,54,54	0
57	MG	CA	3075	1/1	0.99	0.06	107,107,107,107	0
57	MG	CA	3076	1/1	0.99	0.05	77,77,77,77	0
57	MG	BA	3103	1/1	0.99	0.02	41,41,41,41	0
57	MG	BA	3016	1/1	0.99	0.03	56,56,56,56	0
57	MG	AA	1647	1/1	0.99	0.10	44,44,44,44	0
57	MG	BA	3036	1/1	0.99	0.03	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1639	1/1	0.99	0.07	59,59,59,59	0
57	MG	CA	3082	1/1	0.99	0.02	50,50,50,50	0
57	MG	BA	3068	1/1	0.99	0.03	27,27,27,27	0
57	MG	BA	3070	1/1	0.99	0.05	50,50,50,50	0
57	MG	BA	3006	1/1	0.99	0.03	40,40,40,40	0
57	MG	CA	3012	1/1	0.99	0.03	30,30,30,30	0
57	MG	BA	3111	1/1	0.99	0.09	52,52,52,52	0
57	MG	BA	3072	1/1	0.99	0.03	41,41,41,41	0
57	MG	BA	3113	1/1	0.99	0.10	96,96,96,96	0
57	MG	CA	3016	1/1	0.99	0.03	40,40,40,40	0
57	MG	CA	3018	1/1	0.99	0.02	41,41,41,41	0
57	MG	BA	3163	1/1	0.99	0.04	27,27,27,27	0
57	MG	DA	1603	1/1	0.99	0.07	37,37,37,37	0
57	MG	CA	3020	1/1	0.99	0.06	37,37,37,37	0
57	MG	DA	1605	1/1	0.99	0.06	96,96,96,96	0
57	MG	CA	3021	1/1	0.99	0.06	57,57,57,57	0
57	MG	DA	1607	1/1	0.99	0.03	63,63,63,63	0
57	MG	CA	3023	1/1	0.99	0.03	37,37,37,37	0
57	MG	BA	3020	1/1	0.99	0.02	41,41,41,41	0
57	MG	BA	3008	1/1	0.99	0.06	62,62,62,62	0
57	MG	BA	3042	1/1	0.99	0.04	32,32,32,32	0
57	MG	CA	3099	1/1	0.99	0.04	58,58,58,58	0
57	MG	CA	3027	1/1	0.99	0.04	47,47,47,47	0
57	MG	BA	3076	1/1	0.99	0.04	32,32,32,32	0
57	MG	BA	3077	1/1	0.99	0.08	63,63,63,63	0
57	MG	BA	3043	1/1	0.99	0.05	66,66,66,66	0
57	MG	AA	1622	1/1	0.99	0.06	76,76,76,76	0
57	MG	CA	3106	1/1	0.99	0.11	33,33,33,33	0
57	MG	BA	3121	1/1	0.99	0.02	34,34,34,34	0
57	MG	DA	1621	1/1	0.99	0.03	47,47,47,47	0
57	MG	BA	3122	1/1	0.99	0.04	60,60,60,60	0
57	MG	BA	3024	1/1	0.99	0.05	68,68,68,68	0
57	MG	DA	1624	1/1	0.99	0.04	30,30,30,30	0
57	MG	DA	1625	1/1	0.99	0.03	42,42,42,42	0
57	MG	BA	3174	1/1	0.99	0.12	45,45,45,45	0
57	MG	BA	3124	1/1	0.99	0.03	45,45,45,45	0
57	MG	BA	3125	1/1	0.99	0.04	36,36,36,36	0
57	MG	DA	1629	1/1	0.99	0.05	86,86,86,86	0
57	MG	CA	3038	1/1	0.99	0.04	71,71,71,71	0
57	MG	BA	3046	1/1	0.99	0.04	58,58,58,58	0
57	MG	DA	1632	1/1	0.99	0.05	71,71,71,71	0
57	MG	AA	1610	1/1	0.99	0.02	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3042	1/1	0.99	0.03	67,67,67,67	0
57	MG	CA	3117	1/1	0.99	0.03	45,45,45,45	0
57	MG	CA	3118	1/1	0.99	0.03	53,53,53,53	0
57	MG	BA	3026	1/1	0.99	0.06	47,47,47,47	0
57	MG	CA	3120	1/1	0.99	0.06	62,62,62,62	0
57	MG	CA	3121	1/1	0.99	0.03	27,27,27,27	0
57	MG	BA	3084	1/1	0.99	0.03	36,36,36,36	0
57	MG	AA	1624	1/1	0.99	0.04	99,99,99,99	0
57	MG	BA	3051	1/1	0.99	0.03	70,70,70,70	0
57	MG	BA	3133	1/1	0.99	0.04	39,39,39,39	0
57	MG	BA	3052	1/1	0.99	0.05	50,50,50,50	0
57	MG	CA	3051	1/1	0.99	0.07	24,24,24,24	0
57	MG	BA	3135	1/1	0.99	0.04	79,79,79,79	0
57	MG	CA	3129	1/1	0.99	0.03	33,33,33,33	0
57	MG	BA	3054	1/1	0.99	0.03	46,46,46,46	0
57	MG	BA	3028	1/1	0.99	0.04	35,35,35,35	0
57	MG	AA	1625	1/1	0.99	0.07	50,50,50,50	0
57	MG	CA	3134	1/1	0.99	0.03	55,55,55,55	0
57	MG	BA	3140	1/1	0.99	0.04	73,73,73,73	0
57	MG	CA	3058	1/1	0.99	0.06	55,55,55,55	0
57	MG	BA	3057	1/1	0.99	0.04	26,26,26,26	0
57	MG	CA	3060	1/1	0.99	0.04	67,67,67,67	0
57	MG	BA	3093	1/1	0.99	0.05	72,72,72,72	0
57	MG	BA	3058	1/1	0.99	0.02	25,25,25,25	0
57	MG	BA	3030	1/1	0.99	0.04	43,43,43,43	0
57	MG	CA	3142	1/1	0.99	0.08	33,33,33,33	0
57	MG	BA	3096	1/1	0.99	0.03	66,66,66,66	0
57	MG	CA	3065	1/1	0.99	0.04	76,76,76,76	0
57	MG	CA	3066	1/1	0.99	0.04	45,45,45,45	0
57	MG	AA	1601	1/1	0.99	0.03	50,50,50,50	0
57	MG	AA	1638	1/1	0.99	0.04	58,58,58,58	0
57	MG	BA	3099	1/1	0.99	0.04	96,96,96,96	0
57	MG	BA	3100	1/1	0.99	0.05	66,66,66,66	0
57	MG	BA	3062	1/1	0.99	0.07	73,73,73,73	0
57	MG	CA	3072	1/1	0.99	0.05	99,99,99,99	0
57	MG	CA	3152	1/1	0.99	0.04	44,44,44,44	0
57	MG	BA	3033	1/1	0.99	0.02	48,48,48,48	0
57	MG	BA	3007	1/1	1.00	0.03	61,61,61,61	0
57	MG	BL	201	1/1	1.00	0.03	21,21,21,21	0
57	MG	BA	3011	1/1	1.00	0.02	34,34,34,34	0
57	MG	BA	3139	1/1	1.00	0.02	47,47,47,47	0
57	MG	BA	3069	1/1	1.00	0.01	20,20,20,20	0

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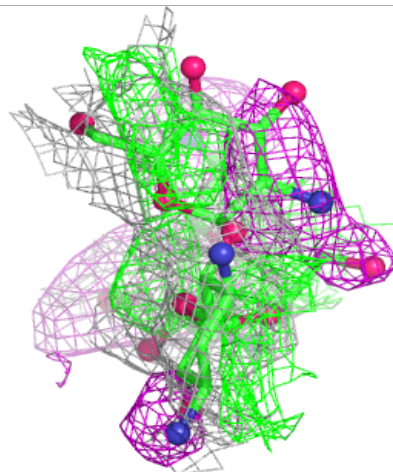
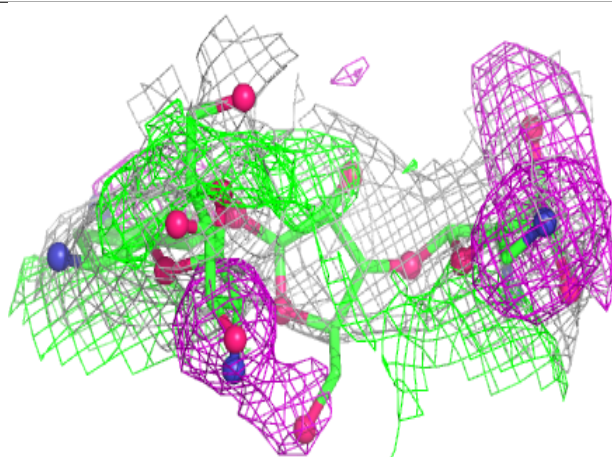
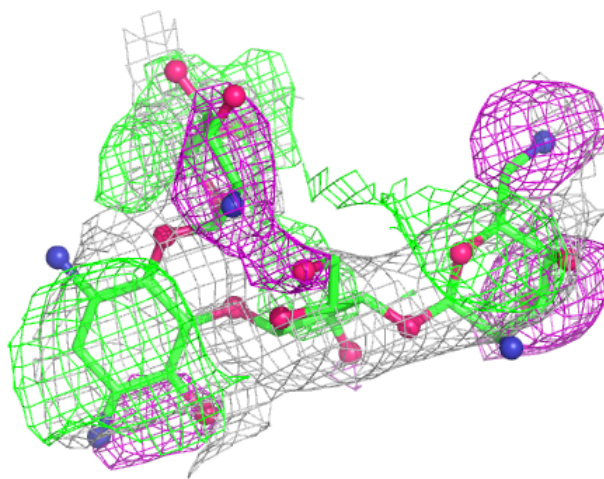
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	3017	1/1	1.00	0.02	36,36,36,36	0
57	MG	CA	3101	1/1	1.00	0.03	58,58,58,58	0
57	MG	CA	3057	1/1	1.00	0.06	46,46,46,46	0
57	MG	BA	3053	1/1	1.00	0.03	29,29,29,29	0
57	MG	CA	3002	1/1	1.00	0.05	49,49,49,49	0
57	MG	AA	1640	1/1	1.00	0.08	21,21,21,21	0
57	MG	BA	3131	1/1	1.00	0.02	39,39,39,39	0
57	MG	CA	3130	1/1	1.00	0.01	44,44,44,44	0
57	MG	CA	3022	1/1	1.00	0.03	59,59,59,59	0
57	MG	DA	1610	1/1	1.00	0.03	67,67,67,67	0
57	MG	CA	3041	1/1	1.00	0.08	36,36,36,36	0
57	MG	CA	3005	1/1	1.00	0.02	90,90,90,90	0
57	MG	BA	3047	1/1	1.00	0.02	42,42,42,42	0
57	MG	CA	3044	1/1	1.00	0.02	53,53,53,53	0
57	MG	BA	3041	1/1	1.00	0.02	32,32,32,32	0
57	MG	AA	1626	1/1	1.00	0.02	66,66,66,66	0
57	MG	BA	3022	1/1	1.00	0.02	28,28,28,28	0
57	MG	BA	3085	1/1	1.00	0.02	57,57,57,57	0
57	MG	BB	3203	1/1	1.00	0.02	52,52,52,52	0
57	MG	CA	3050	1/1	1.00	0.02	42,42,42,42	0
59	ZN	C4	9501	1/1	1.00	0.04	109,109,109,109	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.

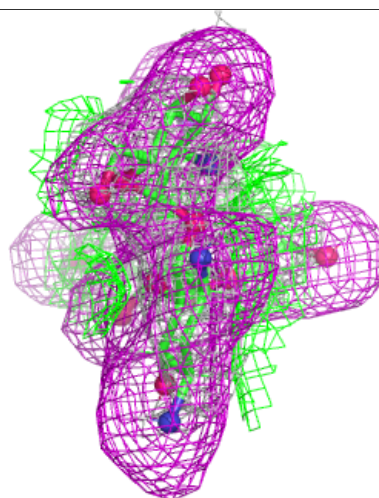
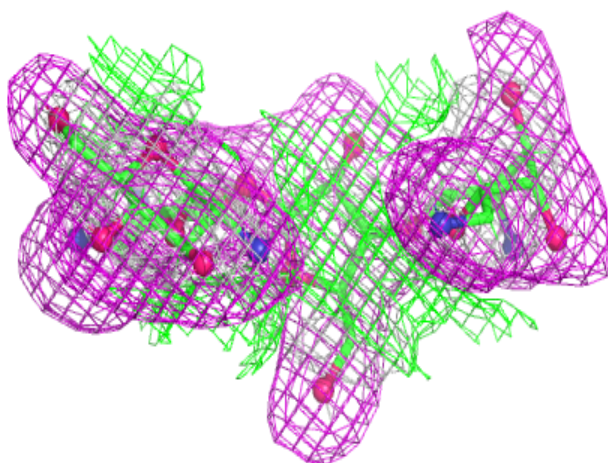
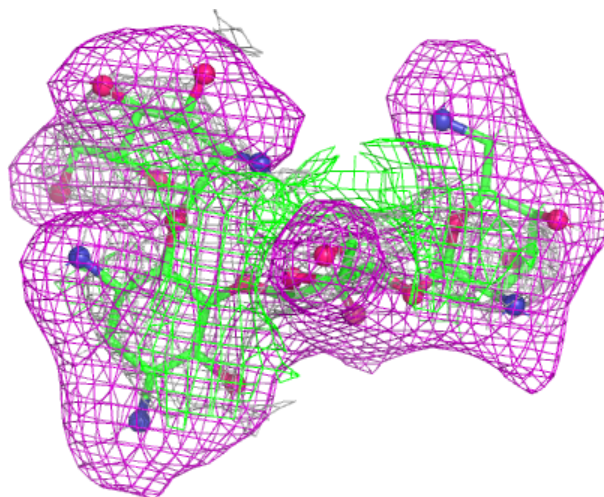
Electron density around PAR CA 3169:

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



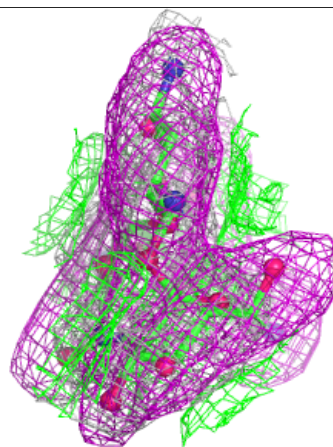
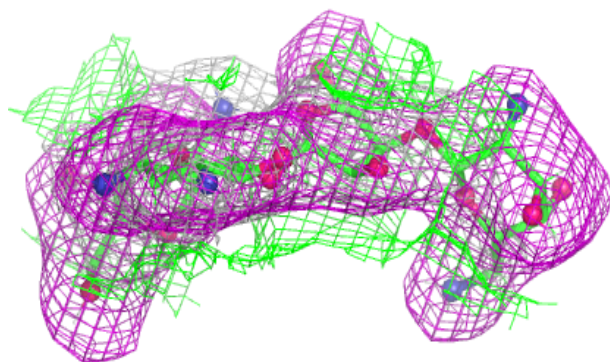
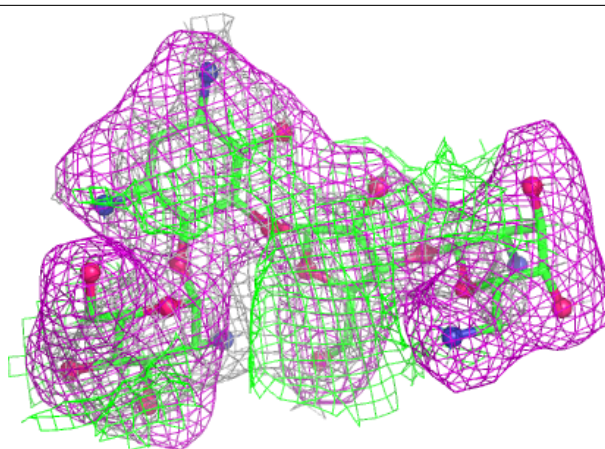
Electron density around PAR CA 3168:

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



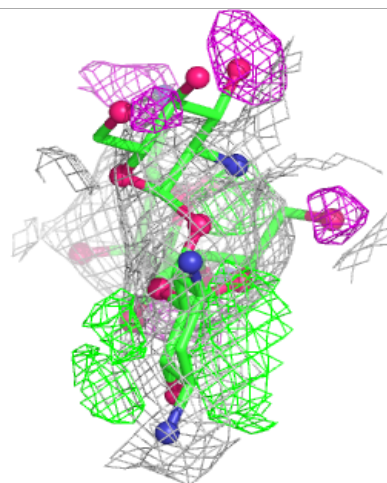
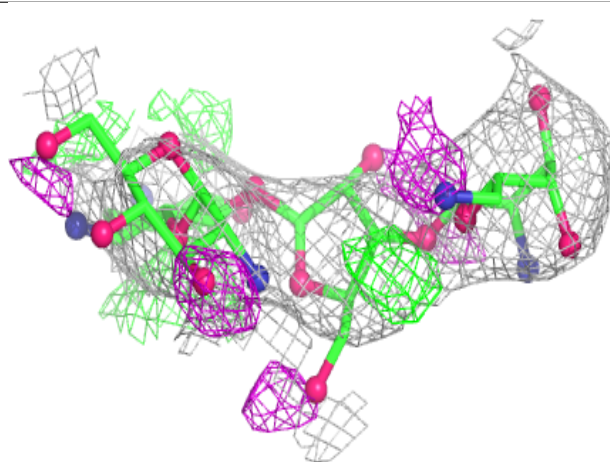
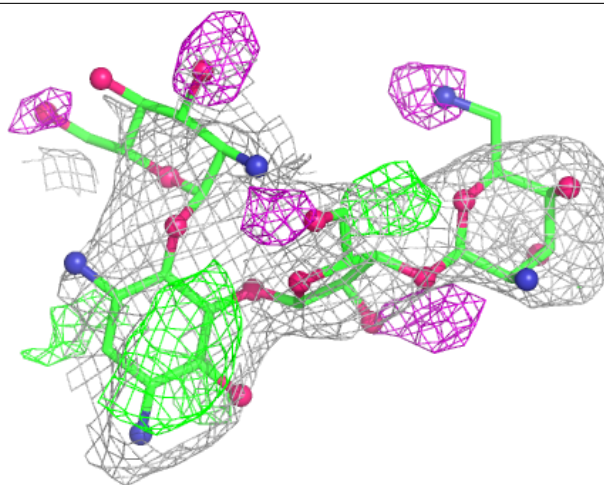
Electron density around PAR DA 1655:

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



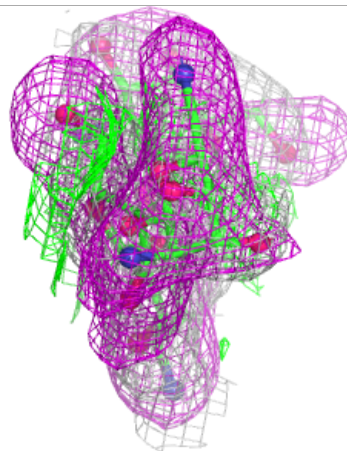
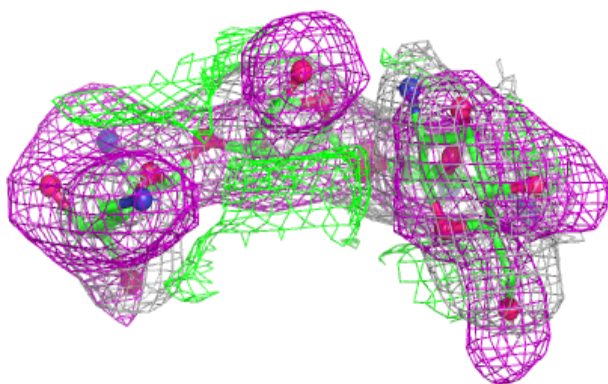
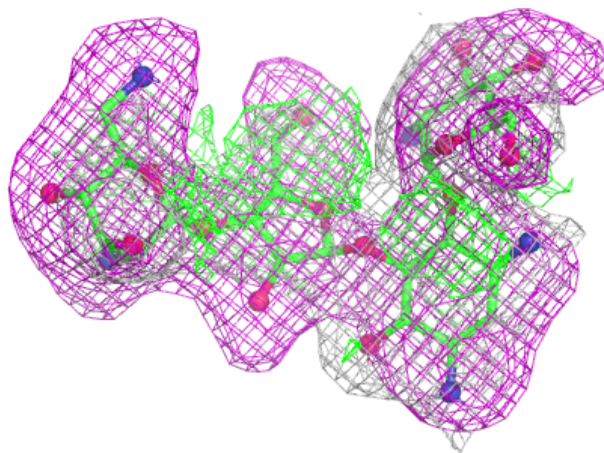
Electron density around PAR CA 3166:

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



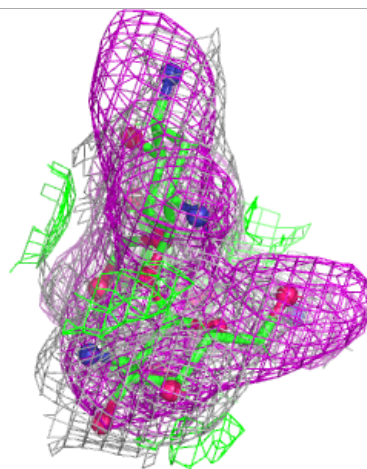
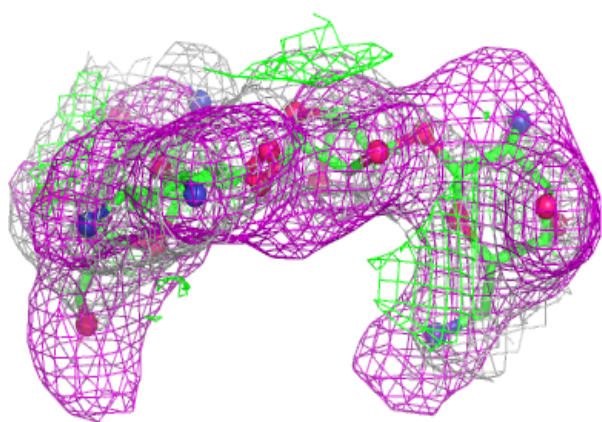
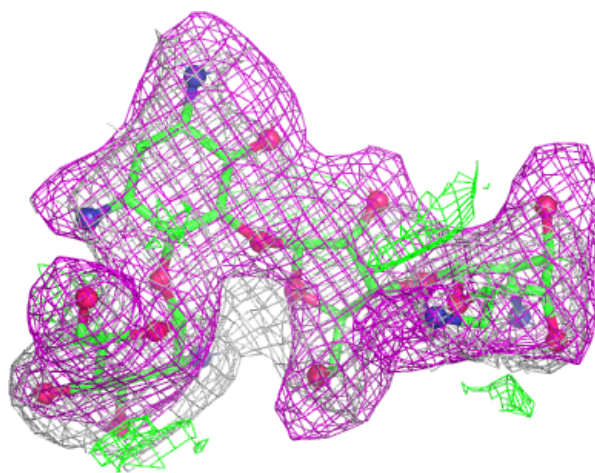
Electron density around PAR CA 3167:

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



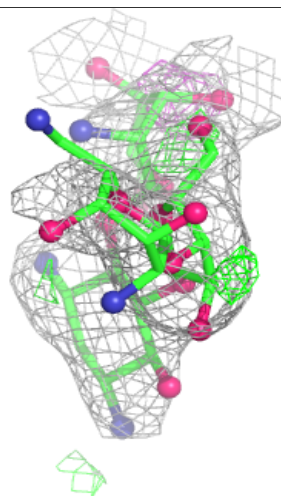
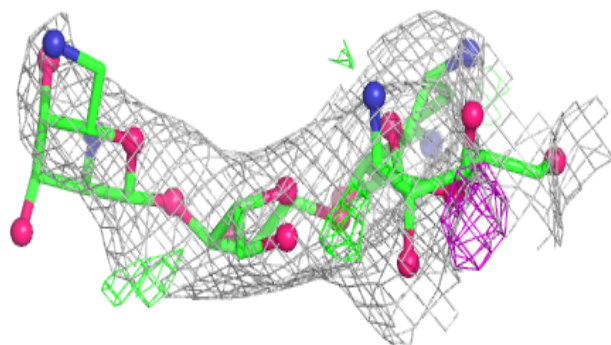
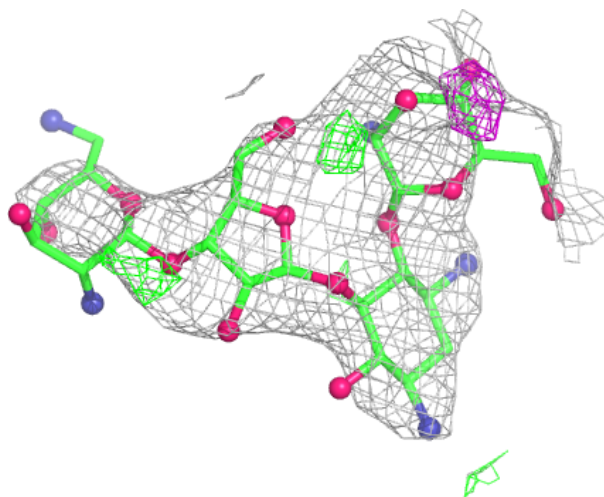
Electron density around PAR CA 3170:

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



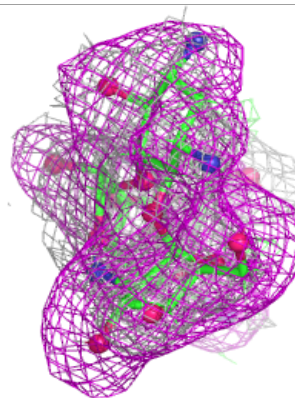
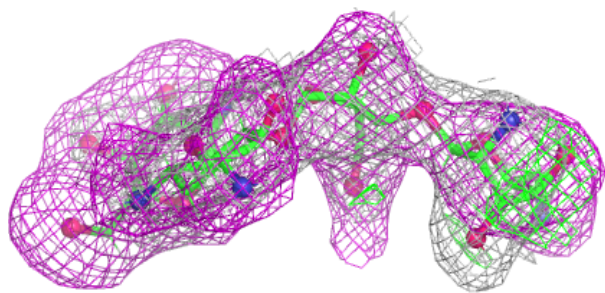
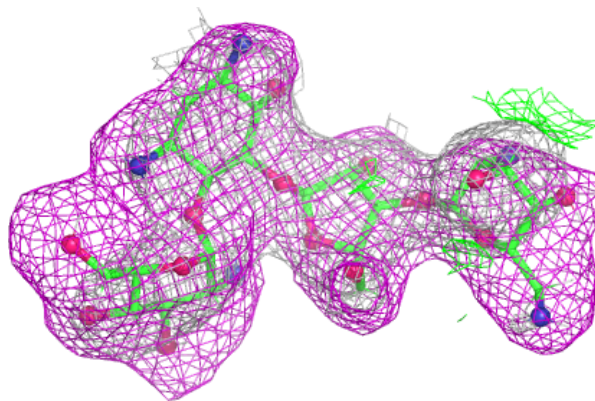
Electron density around PAR BA 3005:

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

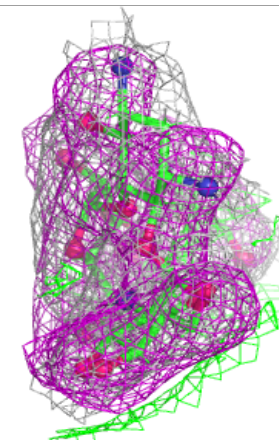
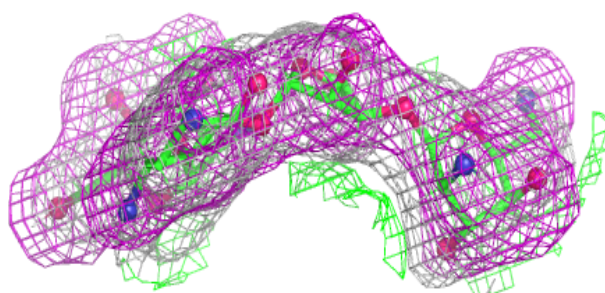
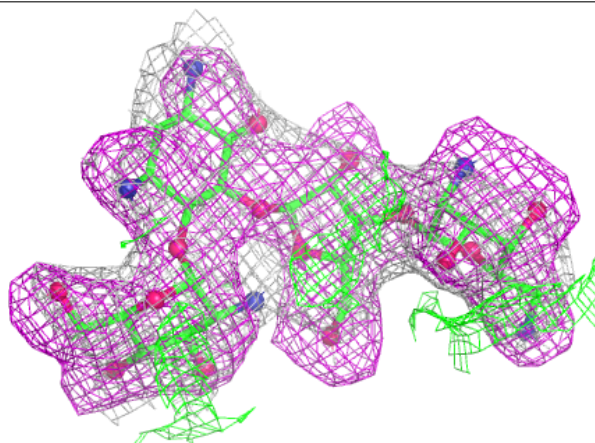


Electron density around PAR BA 3003:

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

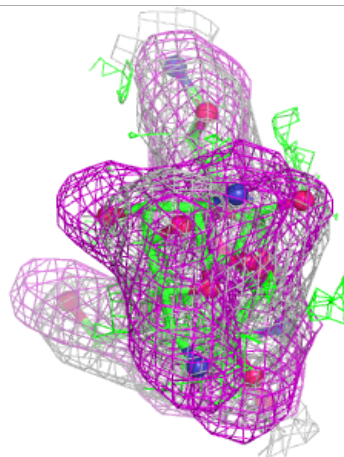
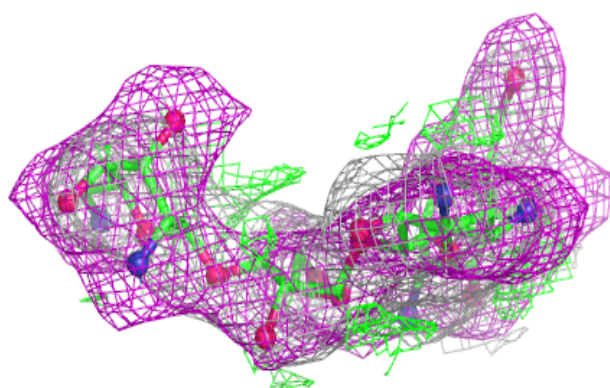
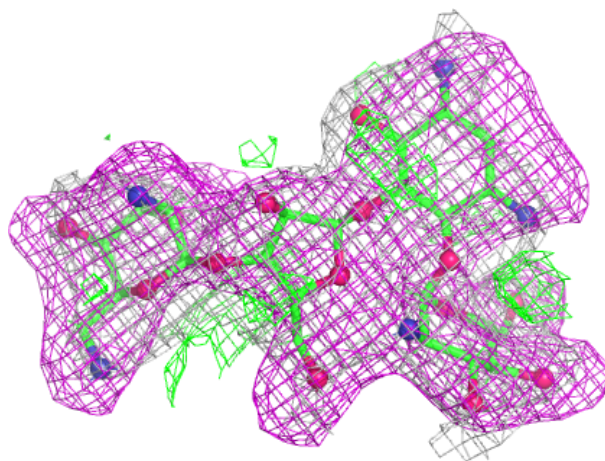
**Electron density around PAR BA 3004:**

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



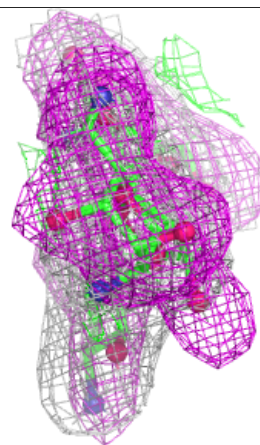
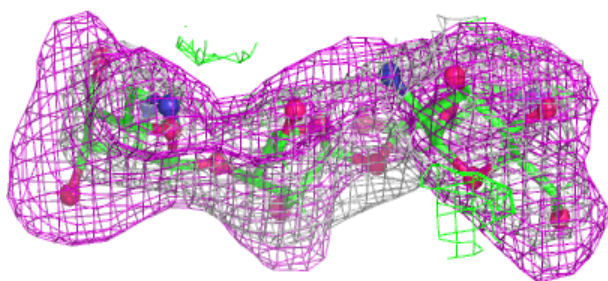
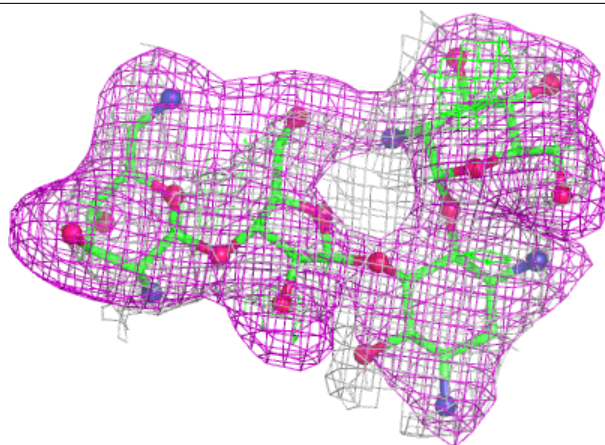
Electron density around PAR BA 3001:

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



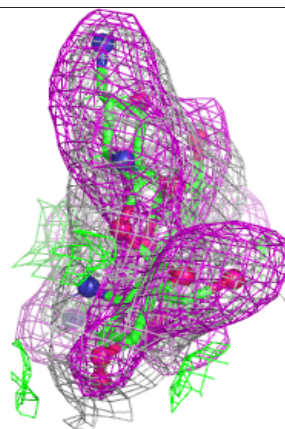
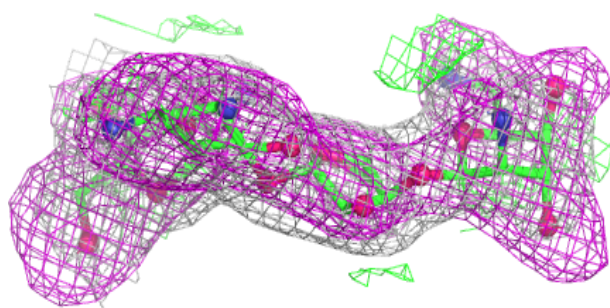
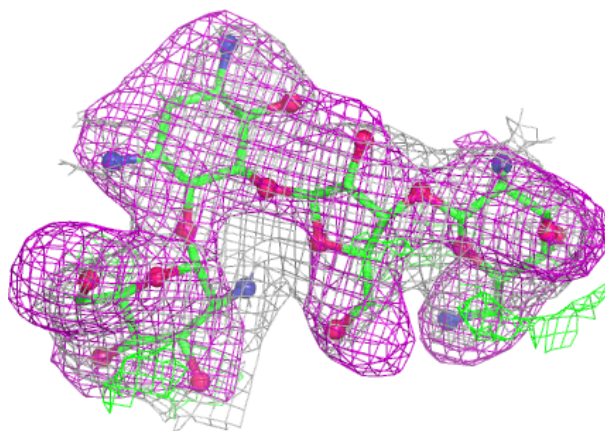
Electron density around PAR DA 1654:

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



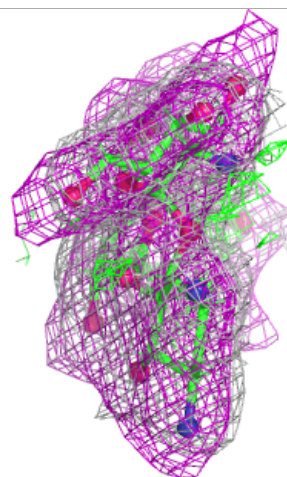
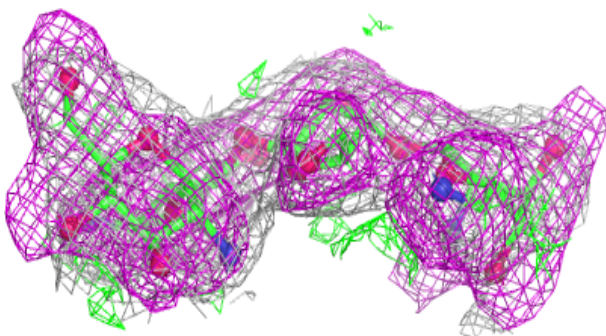
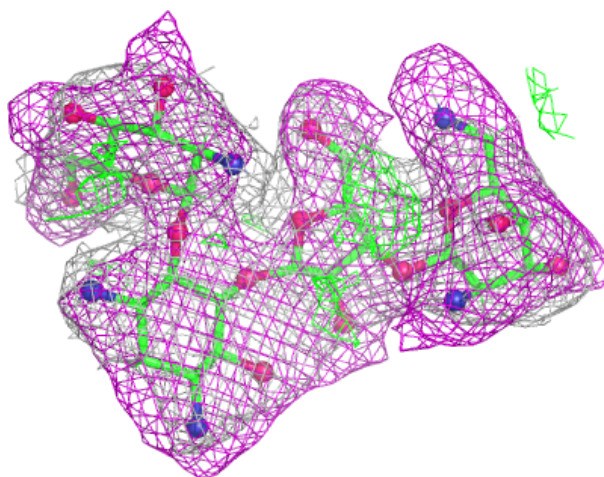
Electron density around PAR AA 1672:

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



Electron density around PAR BA 3002:

$2mF_o-DF_c$ (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.