



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:46 AM UTC

PDB ID : 4V9C / pdb_00004v9c
Title : Allosteric control of the ribosome by small-molecule antibiotics
Authors : Cate, J.H.D.; Pulk, A.; Blanchard, S.C.; Wang, L.; Feldman, M.B.; Wasserman, M.R.; Altman, R.
Deposited on : 2012-07-25
Resolution : 3.30 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

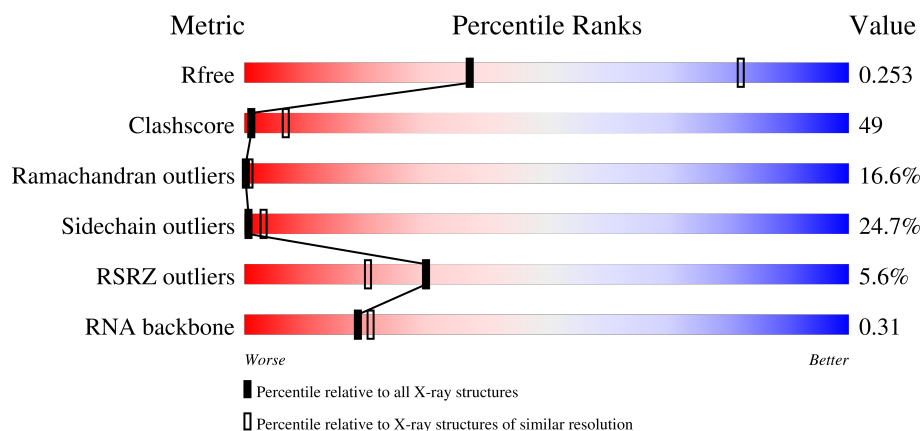
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	11% 60% 29%
1	CA	1542	14% 57% 29%
2	AB	241	5% 11% 43% 28% 8% 10%
2	CB	241	4% 16% 42% 29% 10%

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Mol	Chain	Length	Quality of chain
3	AC	233	
3	CC	233	
4	AD	206	
4	CD	206	
5	AE	167	
5	CE	167	
6	AF	135	
6	CF	135	
7	AG	179	
7	CG	179	
8	AH	130	
8	CH	130	
9	AI	130	
9	CI	130	
10	AJ	103	
10	CJ	103	
11	AK	129	
11	CK	129	
12	AL	124	
12	CL	124	
13	AM	118	
13	CM	118	
14	AN	101	
14	CN	101	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	82	
16	CP	82	
17	AQ	84	
17	CQ	84	
18	AR	75	
18	CR	75	
19	AS	92	
19	CS	92	
20	AT	87	
20	CT	87	
21	AU	71	
21	CU	71	
22	AV	76	
22	CV	76	
23	AX	24	
23	CX	24	
24	BA	2904	
24	DA	2904	
25	BB	120	
25	DB	120	
26	BC	273	
26	DC	273	
27	BD	209	
27	DD	209	

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Mol	Chain	Length	Quality of chain
28	BE	201	
28	DE	201	
29	BF	179	
29	DF	179	
30	BG	177	
30	DG	177	
31	BH	149	
31	DH	149	
32	BI	142	
32	DI	142	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	115	
39	DP	115	
40	BQ	118	

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Mol	Chain	Length	Quality of chain
40	DQ	118	
41	BR	103	
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	104	
44	DU	104	
45	BV	94	
45	DV	94	
46	BW	85	
46	DW	85	
47	BX	78	
47	DX	78	
48	BY	63	
48	DY	63	
49	BZ	59	
49	DZ	59	
50	B0	57	
50	D0	57	
51	B1	55	
51	D1	55	
52	B2	46	
52	D2	46	

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Mol	Chain	Length	Quality of chain
53	B3	65	
53	D3	65	
54	B4	38	
54	D4	38	
55	CY	185	

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
56	MG	BA	3027	-	-	-	X
56	MG	BA	3037	-	-	-	X
56	MG	BA	3059	-	-	-	X
56	MG	BA	3135	-	-	-	X
56	MG	BA	3152	-	-	-	X
56	MG	BA	3155	-	-	-	X
56	MG	BA	3157	-	-	-	X
56	MG	CA	1629	-	-	-	X
56	MG	DA	3057	-	-	-	X
56	MG	DA	3081	-	-	-	X
56	MG	DA	3095	-	-	-	X
56	MG	DA	3129	-	-	-	X
56	MG	DA	3150	-	-	-	X
56	MG	DL	201	-	-	-	X
57	NMY	AA	1655	-	-	X	-
57	NMY	BA	3165	-	-	X	-
57	NMY	DA	3190	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293103 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

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

- 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	CB	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	CC	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	CD	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	CE	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	CF	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	CG	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	CH	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	CI	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	CJ	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	CK	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	CL	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	CM	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	CN	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
			714	439	144	130	1			
15	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	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	CP	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	CQ	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	CR	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	CS	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	CT	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	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called Phenylalanine specific transfer RNA, tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
22	CV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 23 is a RNA chain called Messenger RNA, mRNA.

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

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	12	C	A	SEE REMARK 999	GB AP012306
DB	12	C	A	SEE REMARK 999	GB AP012306

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
31	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 32 is a protein called 50S ribosomal protein L11.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	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
36	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
50	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
51	D1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	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
52	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
53	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
54	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 55 is a protein called Ribosome recycling factor, RRF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	CY	183	Total	C	N	O	S	0	0	0
			1423	874	260	283	6			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	54	Total	Mg	0	0
			54	54		
56	AD	1	Total	Mg	0	0
			1	1		
56	AN	1	Total	Mg	0	0
			1	1		
56	BA	163	Total	Mg	0	0
			163	163		
56	BB	3	Total	Mg	0	0
			3	3		
56	BC	1	Total	Mg	0	0
			1	1		
56	BQ	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CA	71	Total 71	Mg 71	0	0
56	CX	1	Total 1	Mg 1	0	0
56	DA	187	Total 187	Mg 187	0	0
56	DB	4	Total 4	Mg 4	0	0
56	DE	1	Total 1	Mg 1	0	0
56	DL	1	Total 1	Mg 1	0	0
56	DO	1	Total 1	Mg 1	0	0

-
- The chemical structure of NMY is a complex polycyclic molecule. It features a central core with several fused and linked rings. Key functional groups include multiple hydroxyl groups (OH) in red, amino groups (NH₂) in blue, and ether linkages (O) in red. The structure is labeled with various atom identifiers: C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C808, C809, C810, C811, C812, C813, C814, C815, C816, C817, C818, C819, C820

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total 42	C 23	N 6	O 13	0	0
57	AA	1	Total 42	C 23	N 6	O 13	0	0
57	AA	1	Total 42	C 23	N 6	O 13	0	0
57	BA	1	Total 42	C 23	N 6	O 13	0	0



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	CA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	B4	1	Total	Zn	0	0
			1	1		
58	D4	1	Total	Zn	0	0
			1	1		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	188	Total	O	0	0
			188	188		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	2	Total 2	O 2	0	0
59	AK	1	Total 1	O 1	0	0
59	AN	4	Total 4	O 4	0	0
59	AT	2	Total 2	O 2	0	0
59	AU	1	Total 1	O 1	0	0
59	BA	616	Total 616	O 616	0	0
59	BB	13	Total 13	O 13	0	0
59	BC	10	Total 10	O 10	0	0
59	BD	4	Total 4	O 4	0	0
59	BL	4	Total 4	O 4	0	0
59	BN	1	Total 1	O 1	0	0
59	BT	3	Total 3	O 3	0	0
59	BU	3	Total 3	O 3	0	0
59	BV	1	Total 1	O 1	0	0
59	B0	1	Total 1	O 1	0	0
59	B3	1	Total 1	O 1	0	0
59	B4	1	Total 1	O 1	0	0
59	CA	192	Total 192	O 192	0	0
59	CC	1	Total 1	O 1	0	0
59	CE	1	Total 1	O 1	0	0
59	CL	1	Total 1	O 1	0	0

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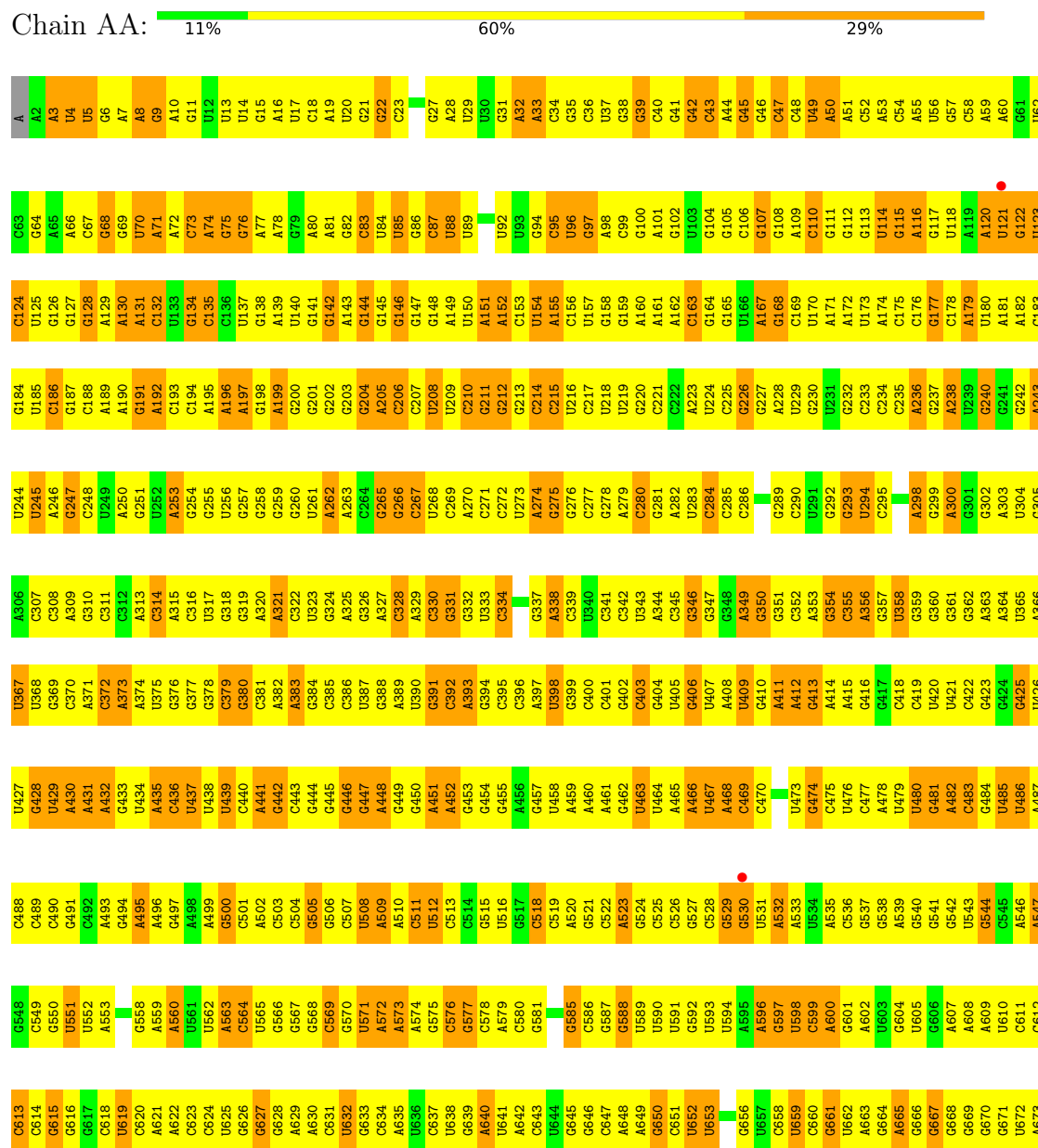
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CN	6	Total 6	O 6	0	0
59	CT	2	Total 2	O 2	0	0
59	DA	627	Total 627	O 627	0	0
59	DB	13	Total 13	O 13	0	0
59	DC	4	Total 4	O 4	0	0
59	DD	2	Total 2	O 2	0	0
59	DE	4	Total 4	O 4	0	0
59	DF	1	Total 1	O 1	0	0
59	DL	7	Total 7	O 7	0	0
59	DN	2	Total 2	O 2	0	0
59	DQ	1	Total 1	O 1	0	0
59	DS	1	Total 1	O 1	0	0
59	DT	1	Total 1	O 1	0	0
59	DU	1	Total 1	O 1	0	0
59	DV	1	Total 1	O 1	0	0
59	D3	2	Total 2	O 2	0	0
59	D4	1	Total 1	O 1	0	0

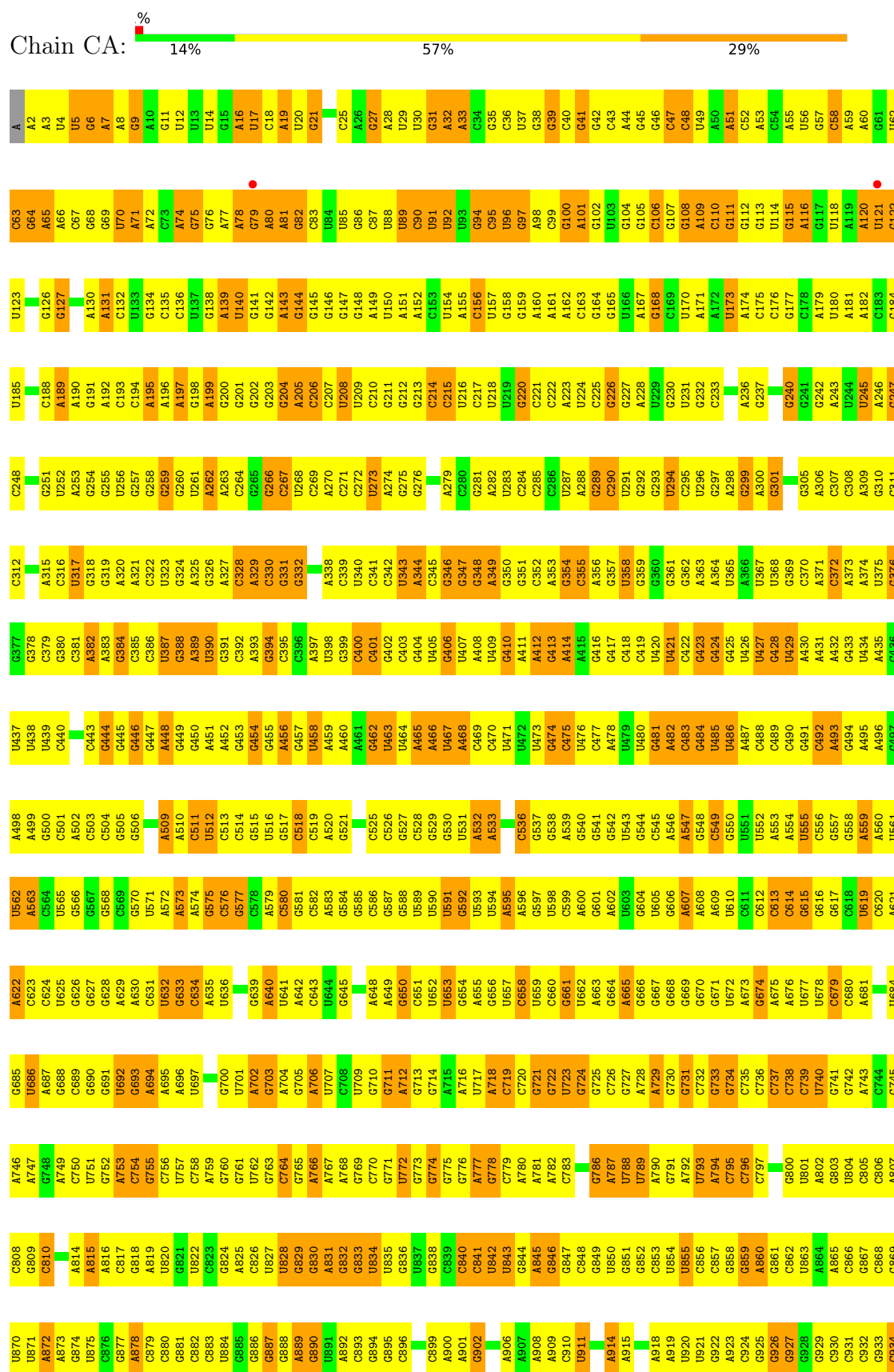
3 Residue-property plots

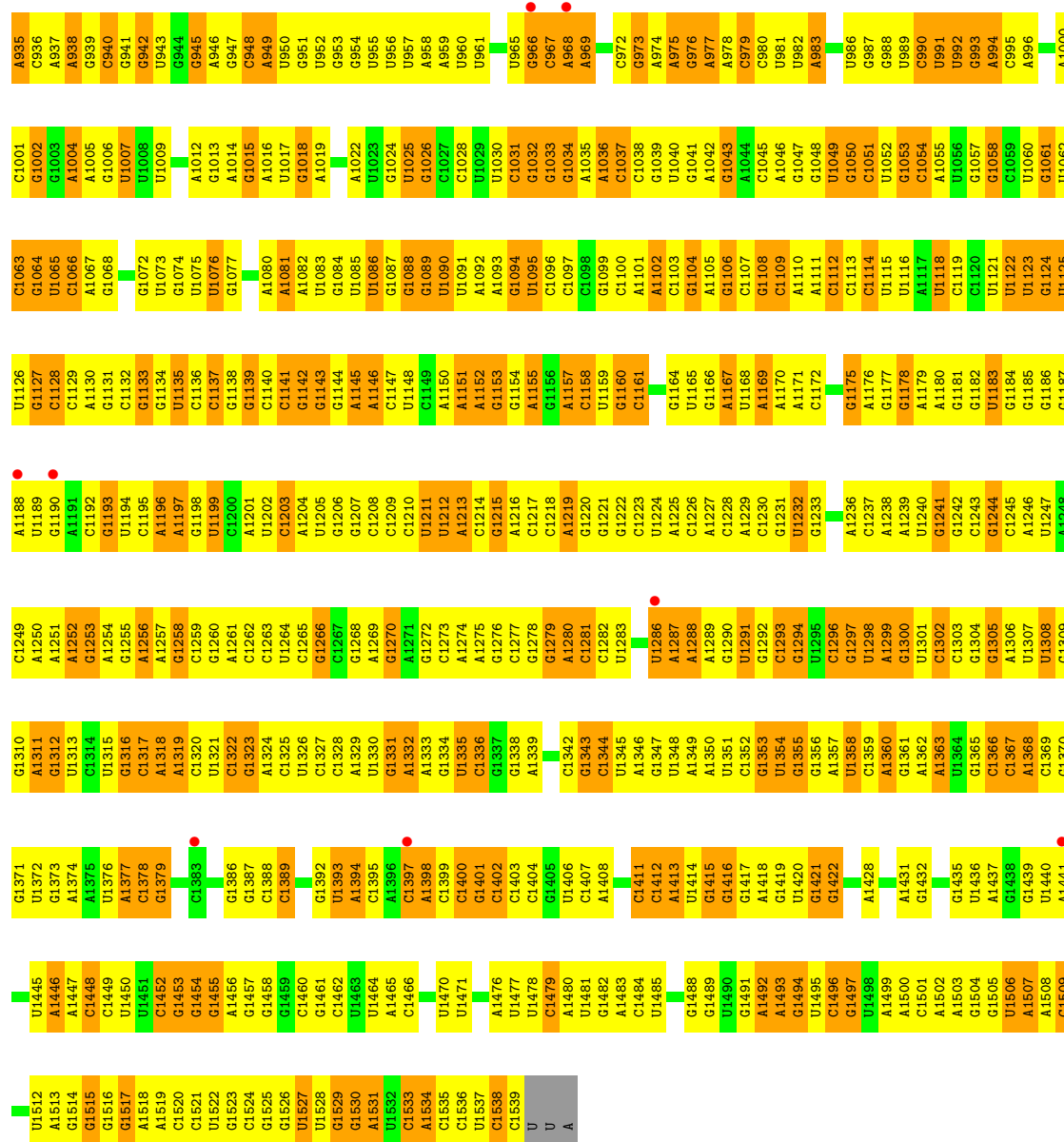
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

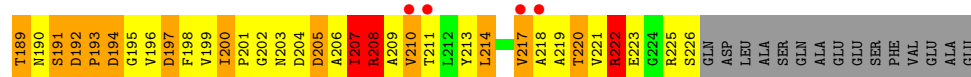
• Molecule 1: 16S ribosomal RNA



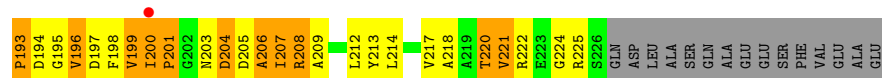
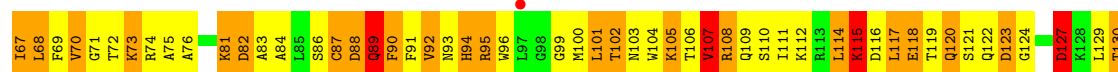
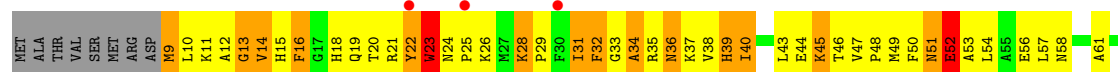
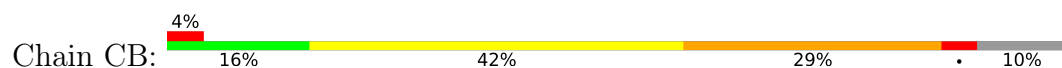
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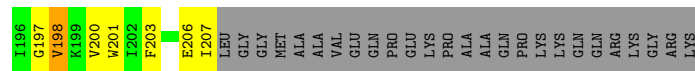
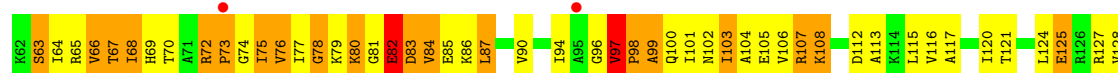
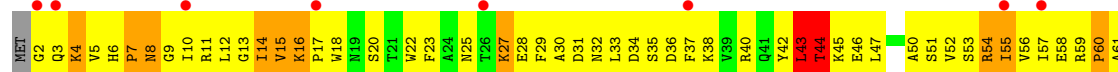
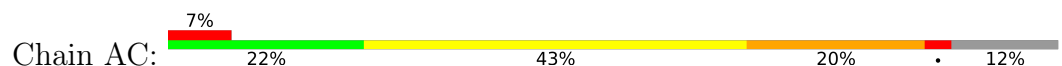




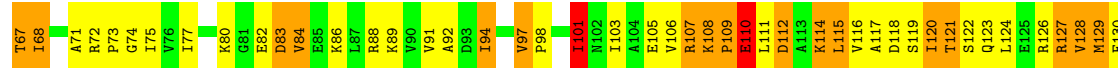
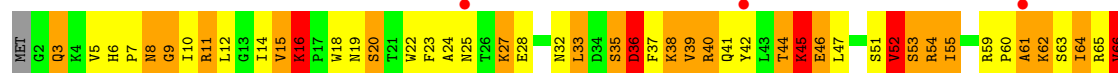
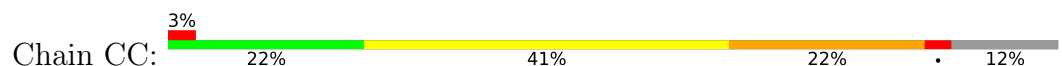
• Molecule 2: 30S ribosomal protein S2

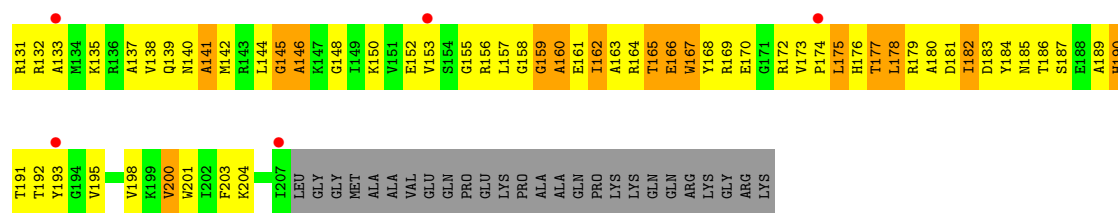


• Molecule 3: 30S ribosomal protein S3

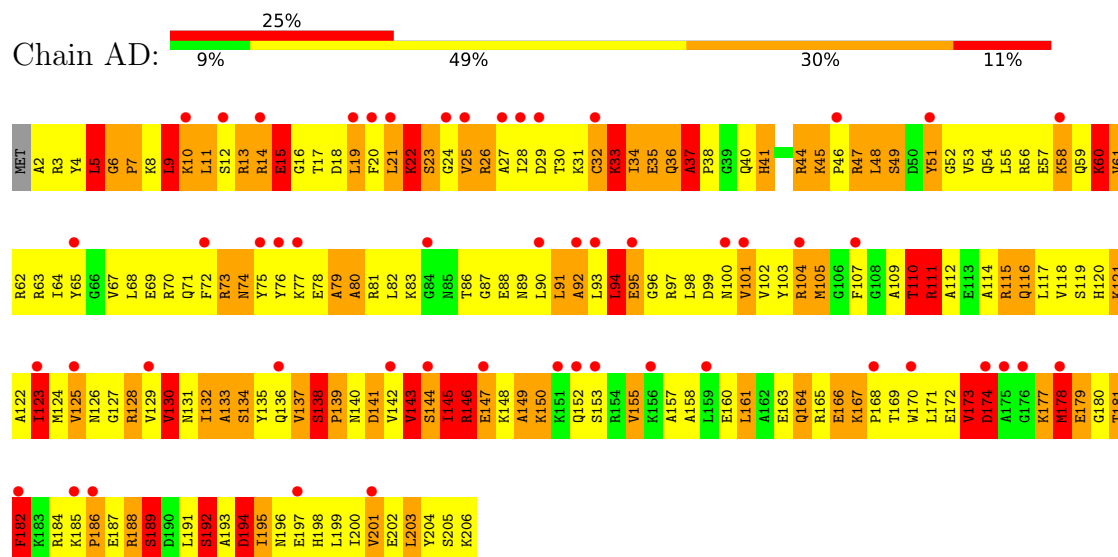


• Molecule 3: 30S ribosomal protein S3

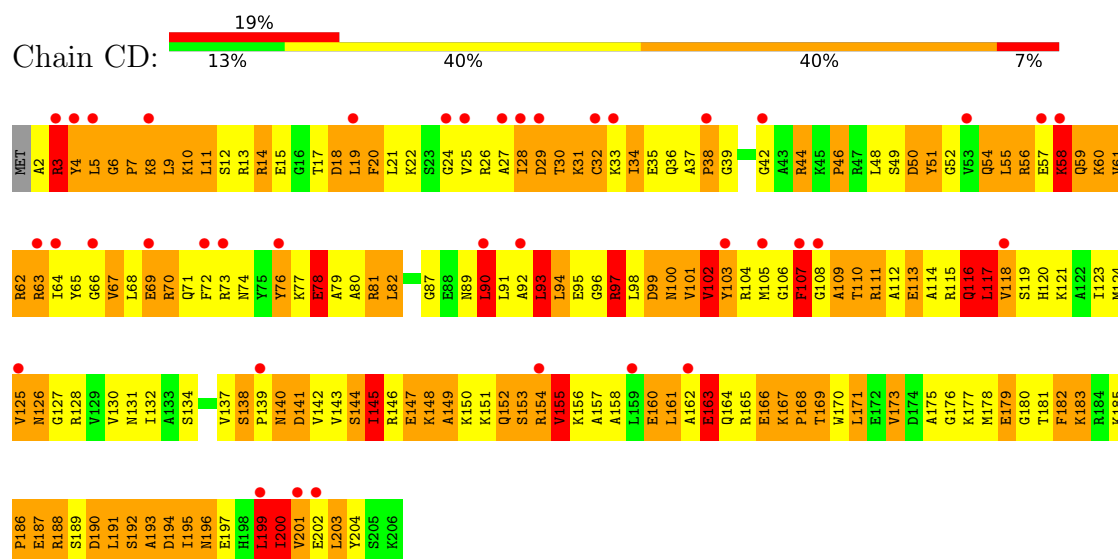




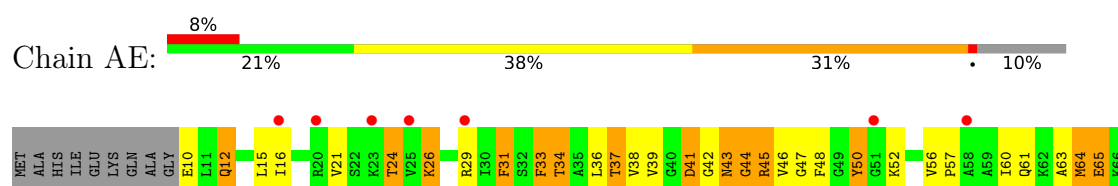
• Molecule 4: 30S ribosomal protein S4

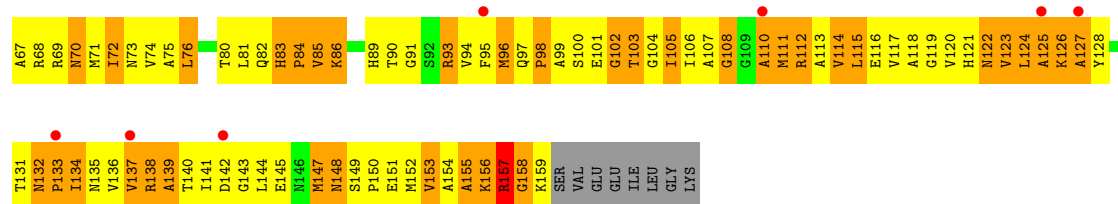


• Molecule 4: 30S ribosomal protein S4

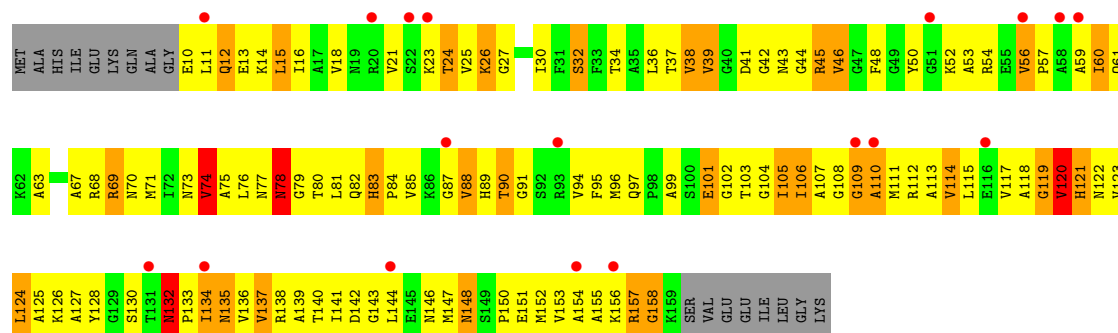
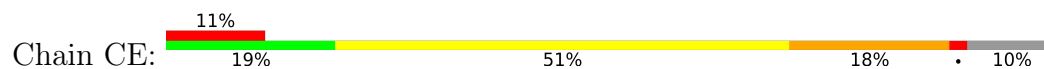


• Molecule 5: 30S ribosomal protein S5

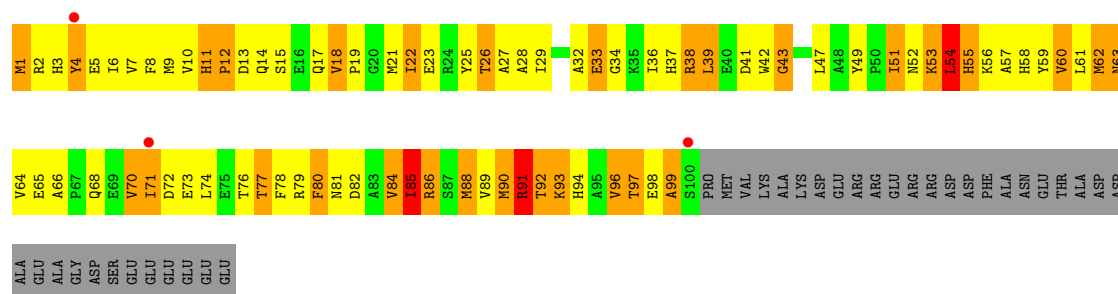




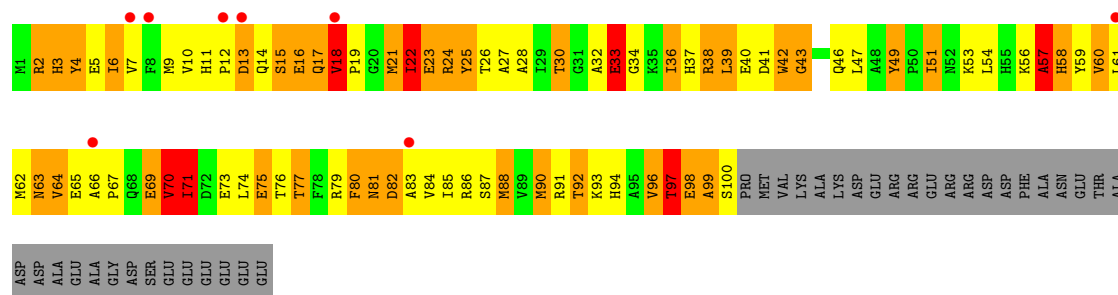
• Molecule 5: 30S ribosomal protein S5



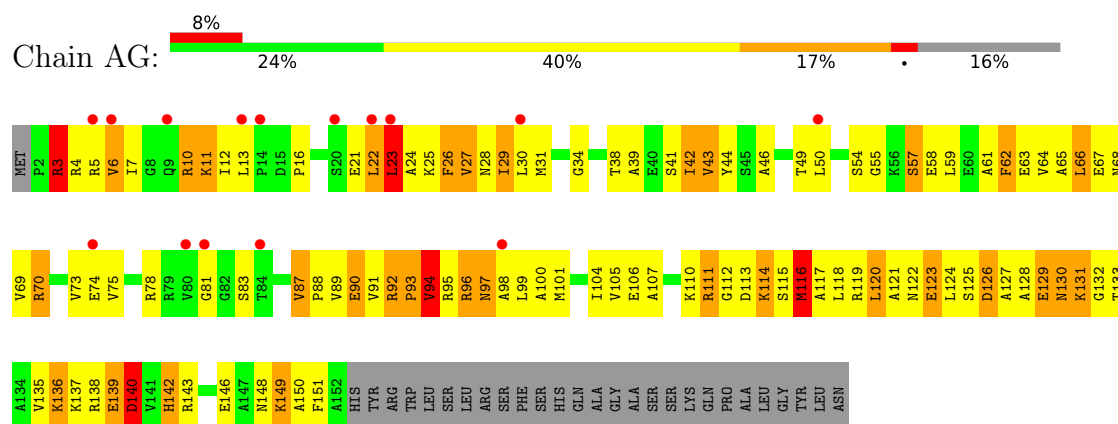
• Molecule 6: 30S ribosomal protein S6



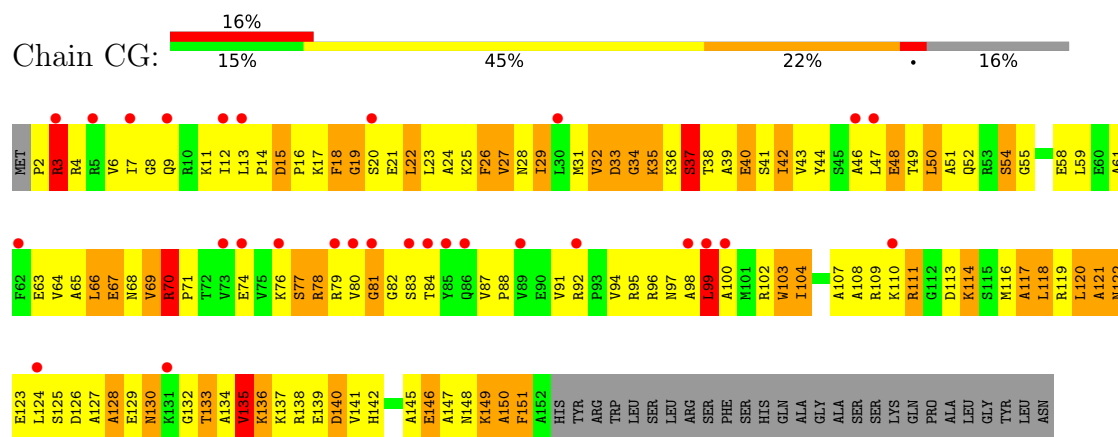
• Molecule 6: 30S ribosomal protein S6



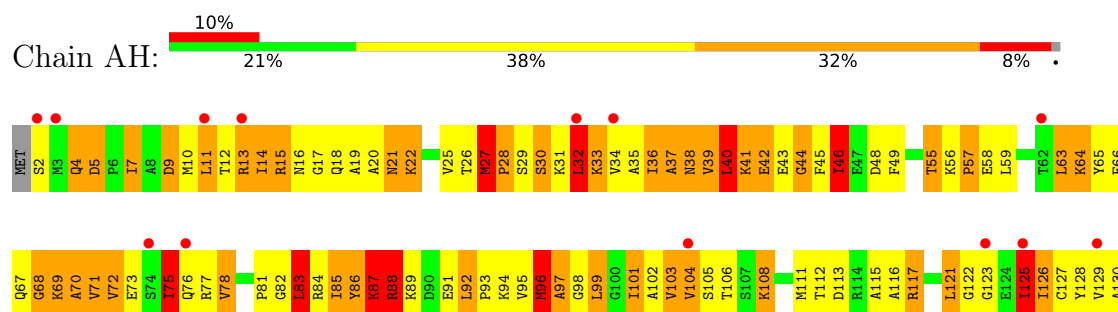
• Molecule 7: 30S ribosomal protein S7



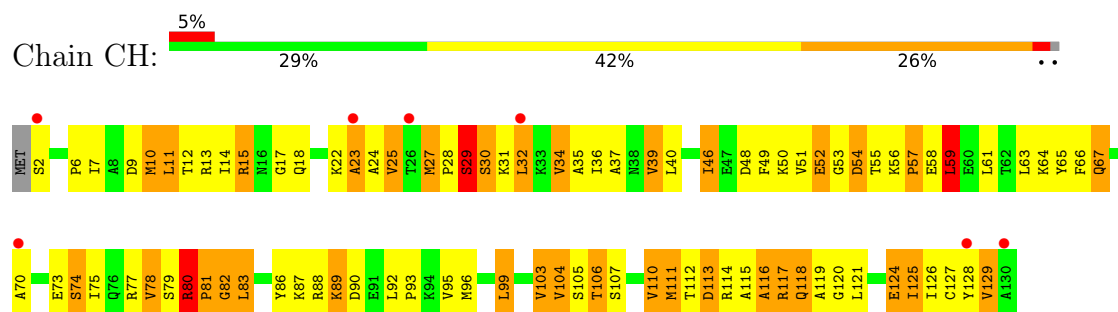
• Molecule 7: 30S ribosomal protein S7



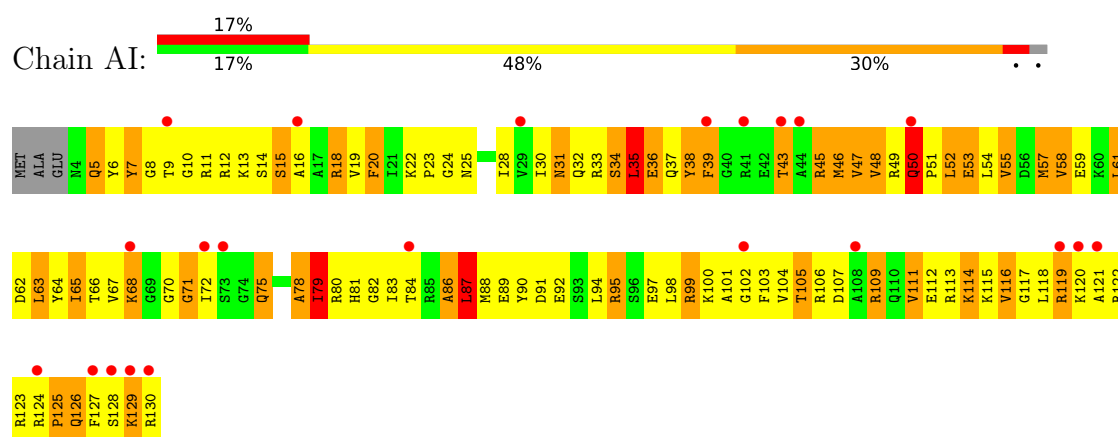
• Molecule 8: 30S ribosomal protein S8



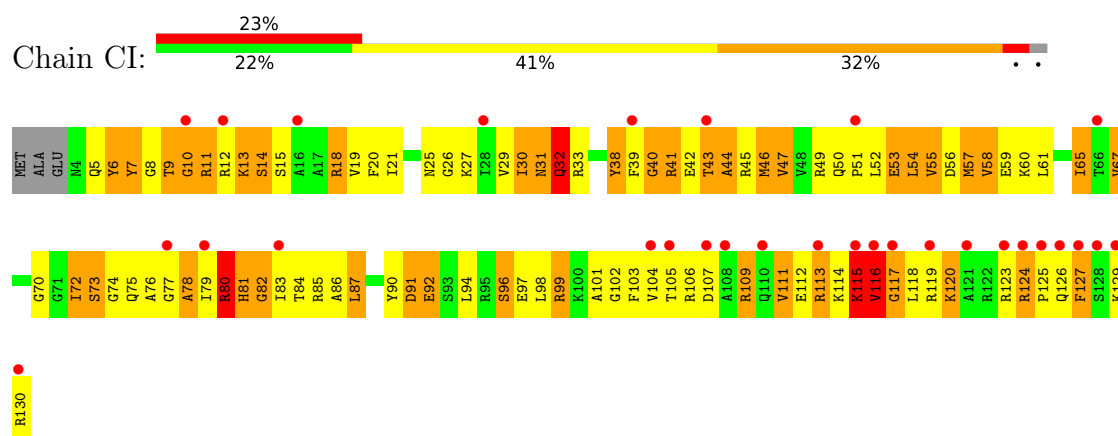
• Molecule 8: 30S ribosomal protein S8



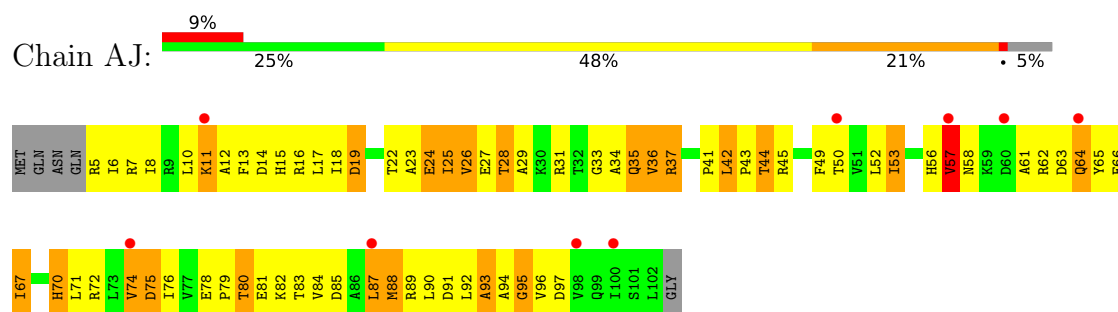
• Molecule 9: 30S ribosomal protein S9



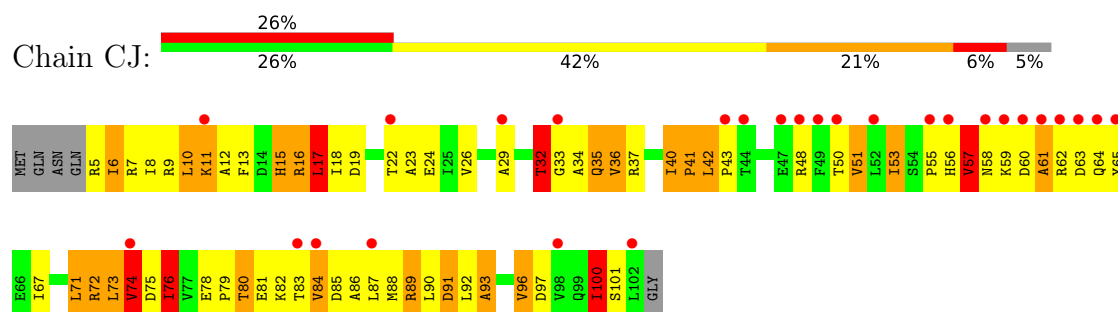
• Molecule 9: 30S ribosomal protein S9



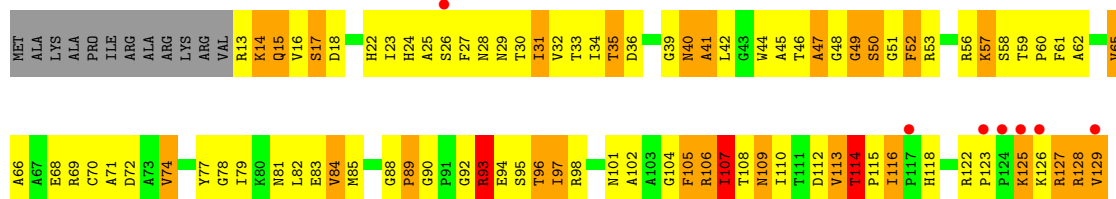
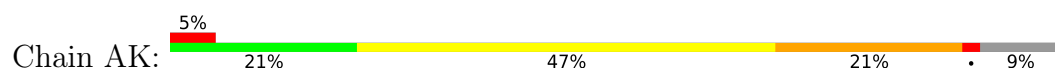
• Molecule 10: 30S ribosomal protein S10



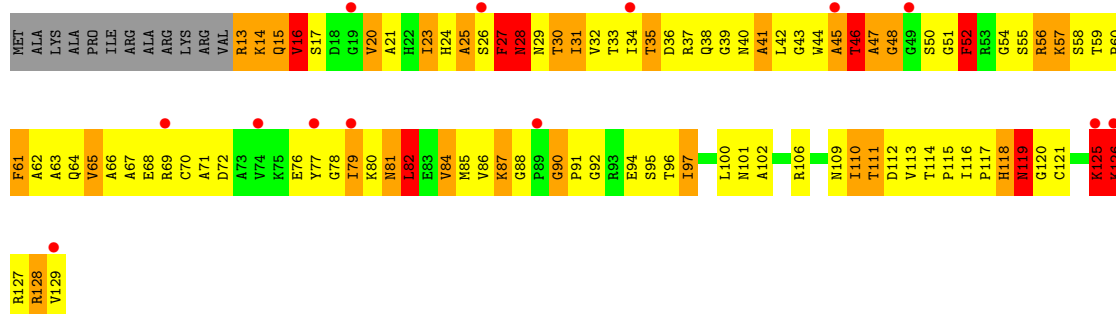
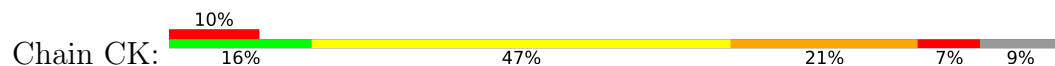
• Molecule 10: 30S ribosomal protein S10



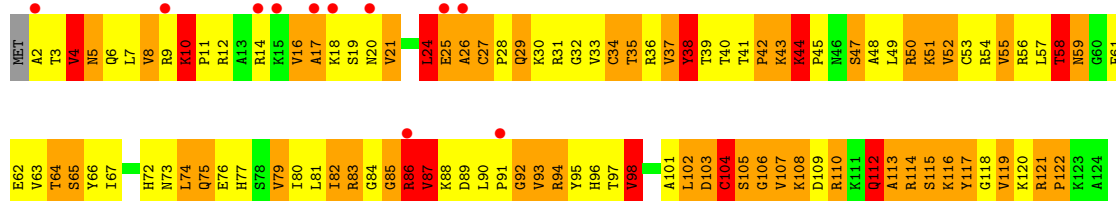
• Molecule 11: 30S ribosomal protein S11



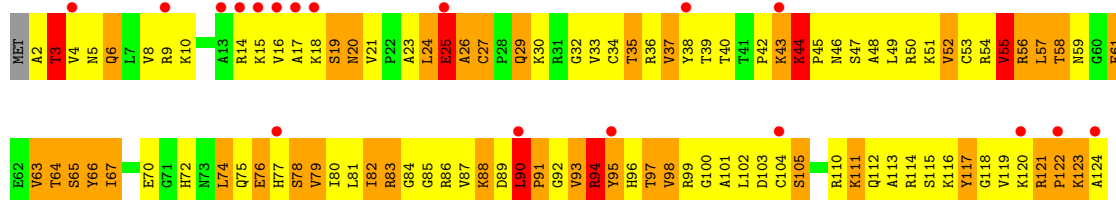
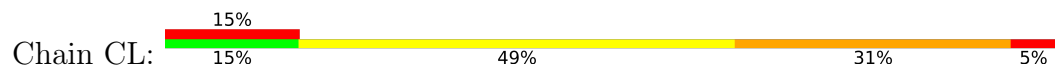
- Molecule 11: 30S ribosomal protein S11



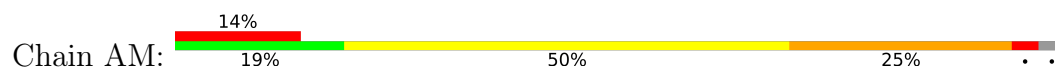
- Molecule 12: 30S ribosomal protein S12

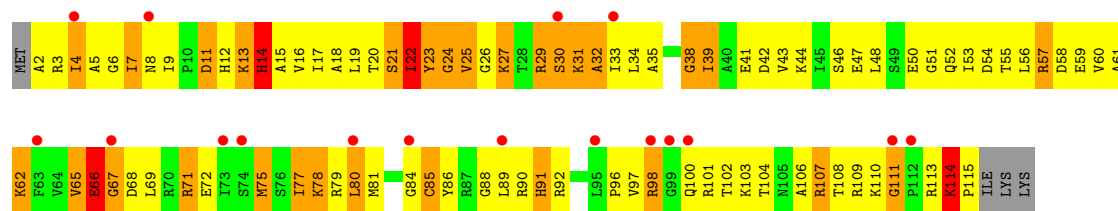


- Molecule 12: 30S ribosomal protein S12

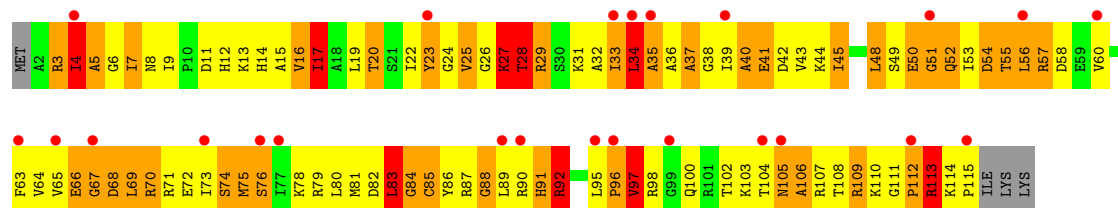
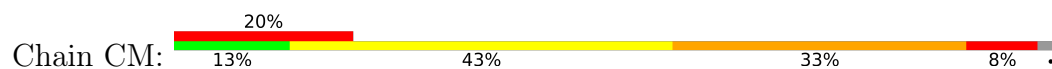


- Molecule 13: 30S ribosomal protein S13

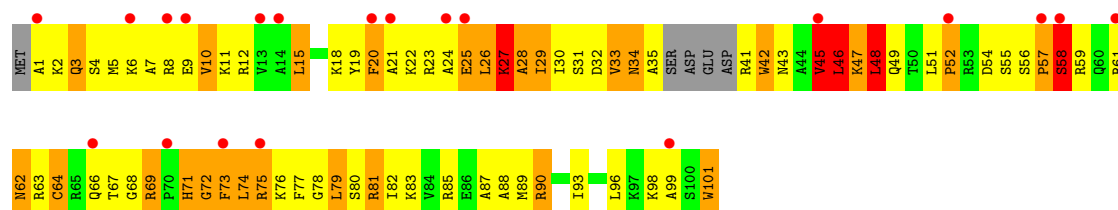
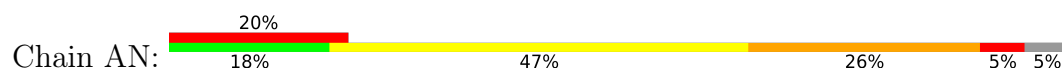




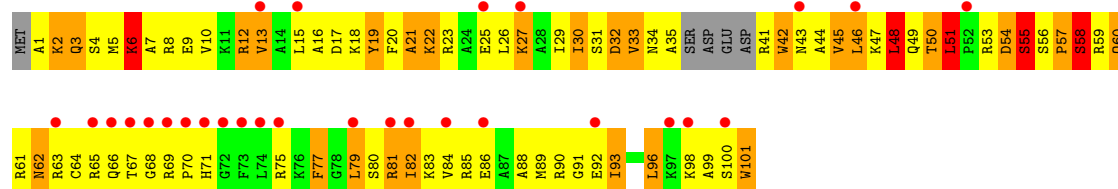
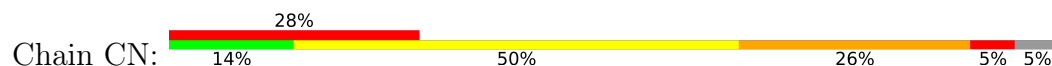
• Molecule 13: 30S ribosomal protein S13



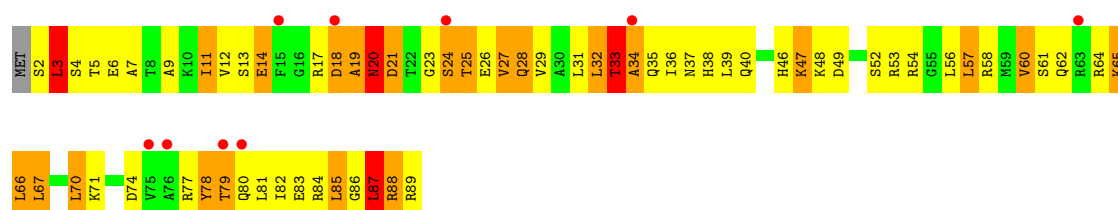
• Molecule 14: 30S ribosomal protein S14



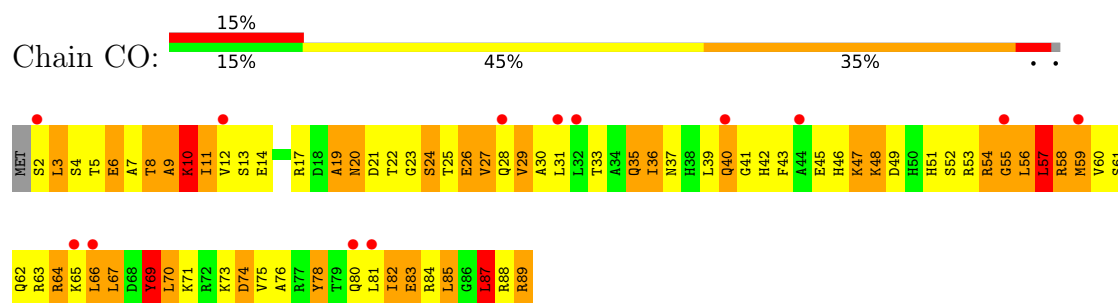
• Molecule 14: 30S ribosomal protein S14



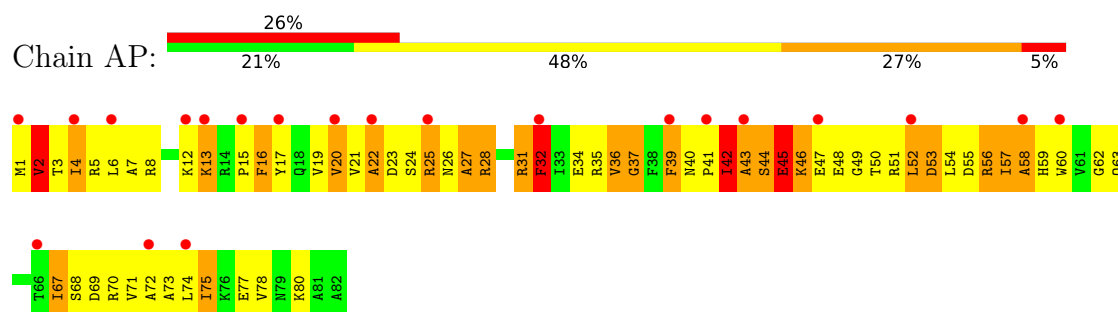
• Molecule 15: 30S ribosomal protein S15



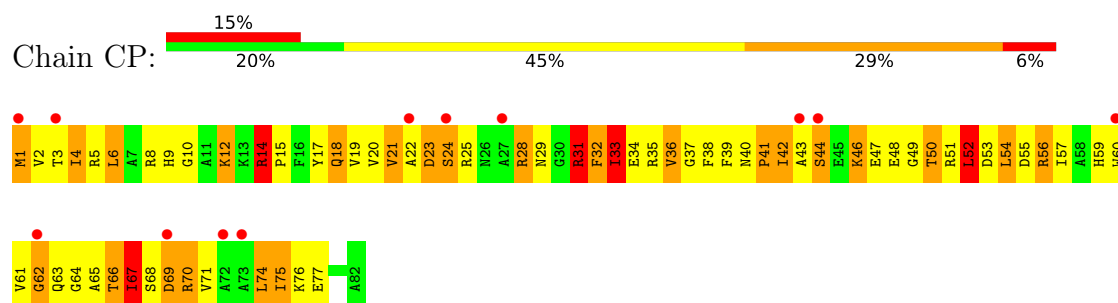
- Molecule 15: 30S ribosomal protein S15



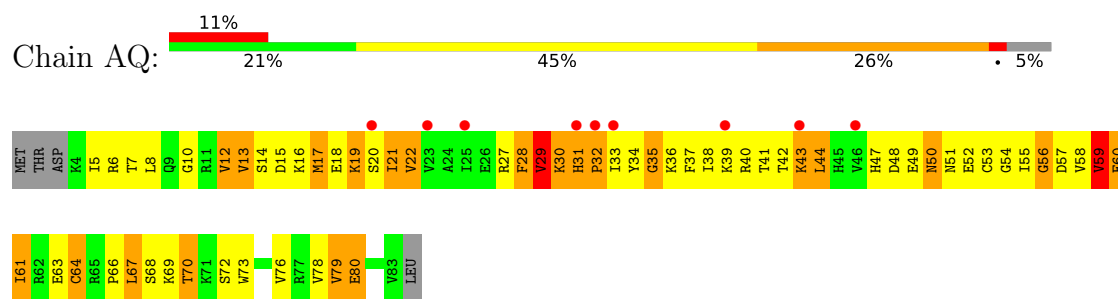
- Molecule 16: 30S ribosomal protein S16



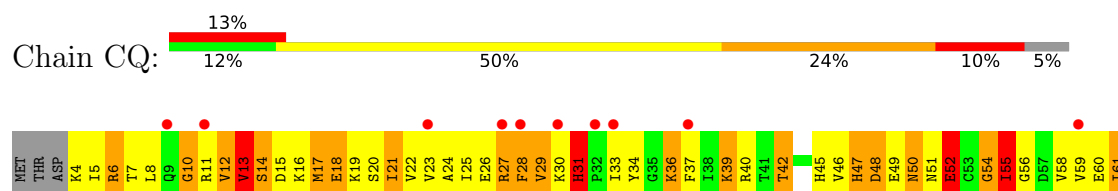
- Molecule 16: 30S ribosomal protein S16

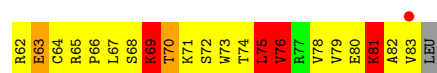


- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

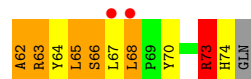




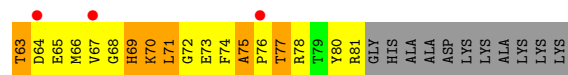
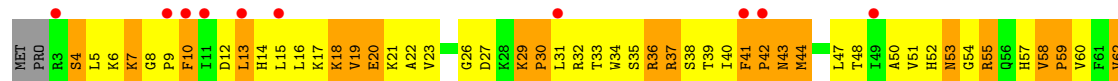
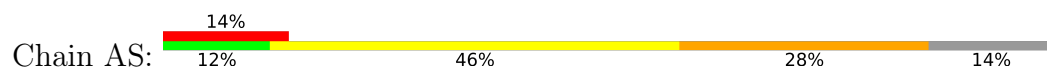
• Molecule 18: 30S ribosomal protein S18



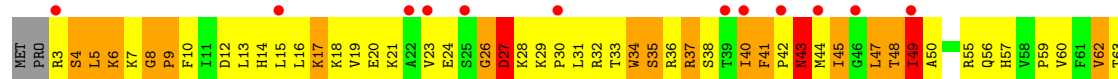
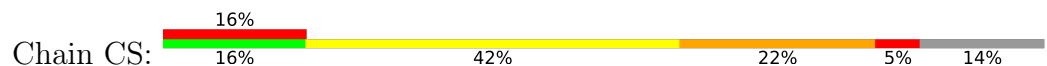
• Molecule 18: 30S ribosomal protein S18



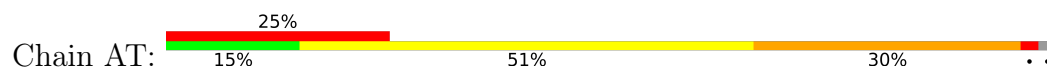
• Molecule 19: 30S ribosomal protein S19

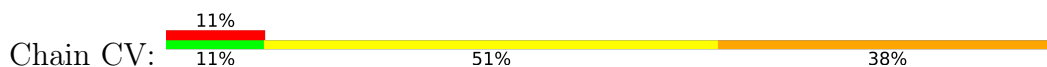


• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20







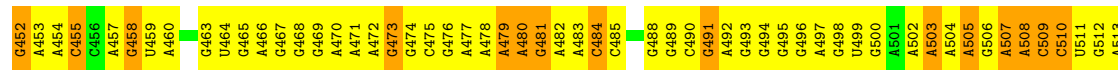
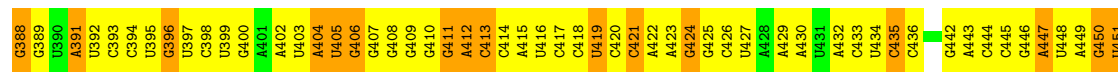
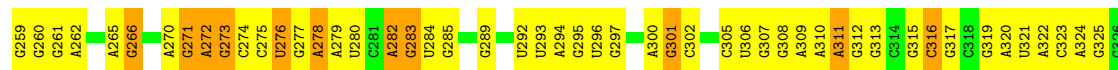
• Molecule 23: Messenger RNA, mRNA



• Molecule 23: Messenger RNA, mRNA



• Molecule 24: 23S ribosomal RNA



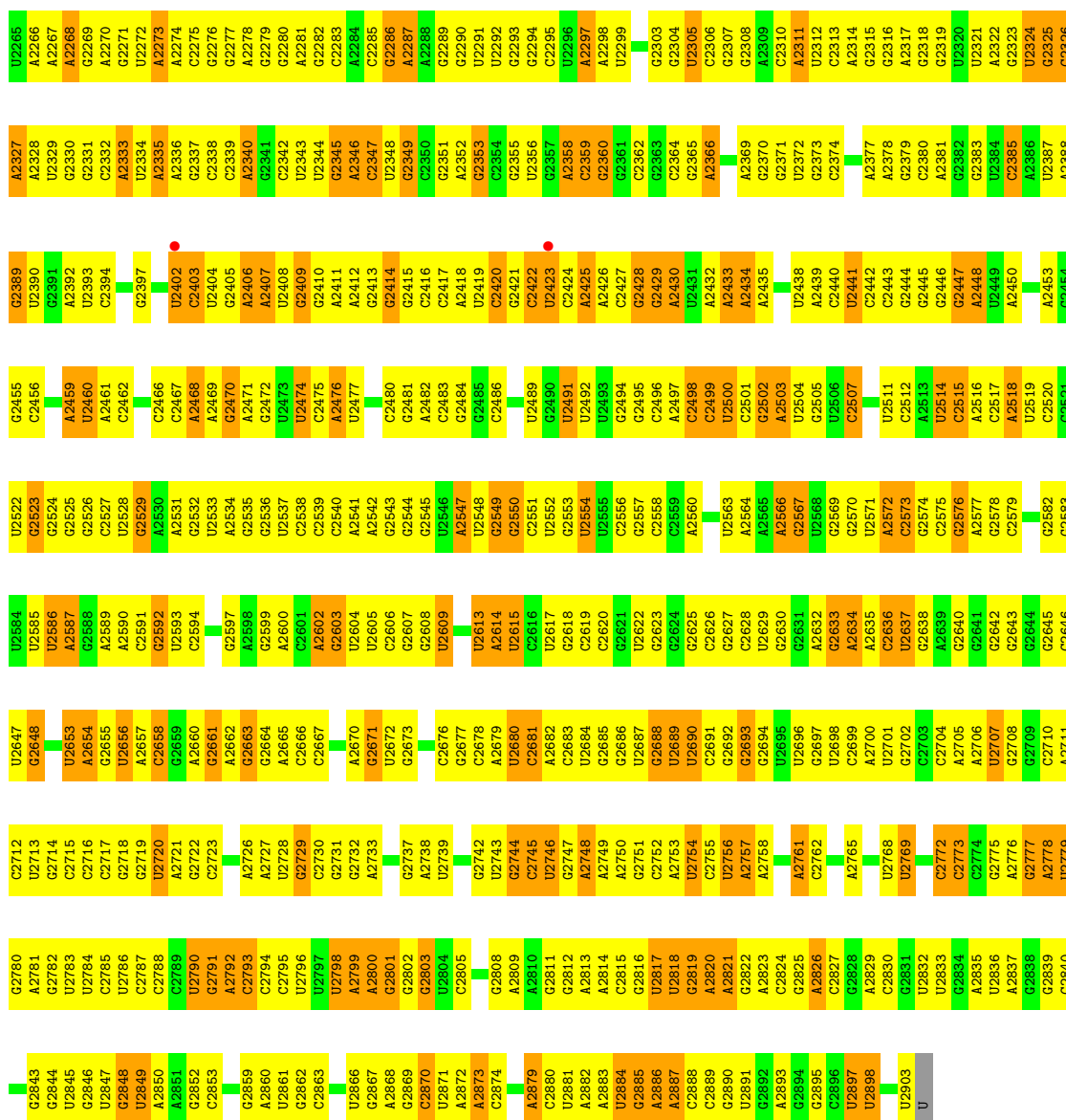
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U1325	U1326	A1327	U1328	G1329	G1332	G1333	G1334	G1335	G1336	G1337	G1338	G1339	G1340	G1341	G1342	G1343	G1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
U1203	A1204	A1205	G1206	C1207	C1208	U1209	G1210	C1211	C1212	C1213	G1214	G1215	G1216	G1217	C1218	G1219	G1220	C1221	G1222	G1223	G1224	G1225	G1226	C1227	G1228	C1229	C1230	G1231	C1232	C1233	G1234	G1235	C1236	G1237	G1238	G1239	U1240	U1241	U1242	C1243	C1244	G1245	G1246	A1247	G1248	U1249	G1250	C1251	G1252	A1253	C1254	U1255	U1256	C1257	G1258	U1259	C1260	C1261	A1262																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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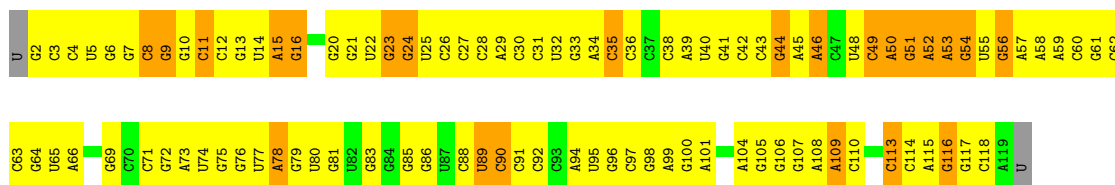


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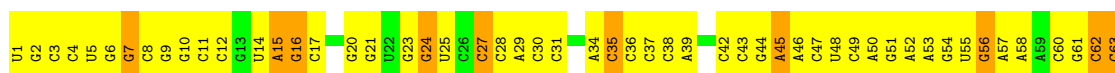
• Molecule 25: 5S ribosomal RNA

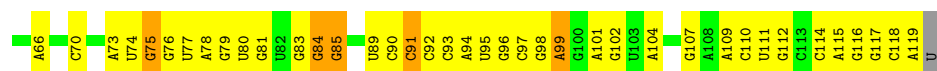
Chain BB: 14% 65% 19%



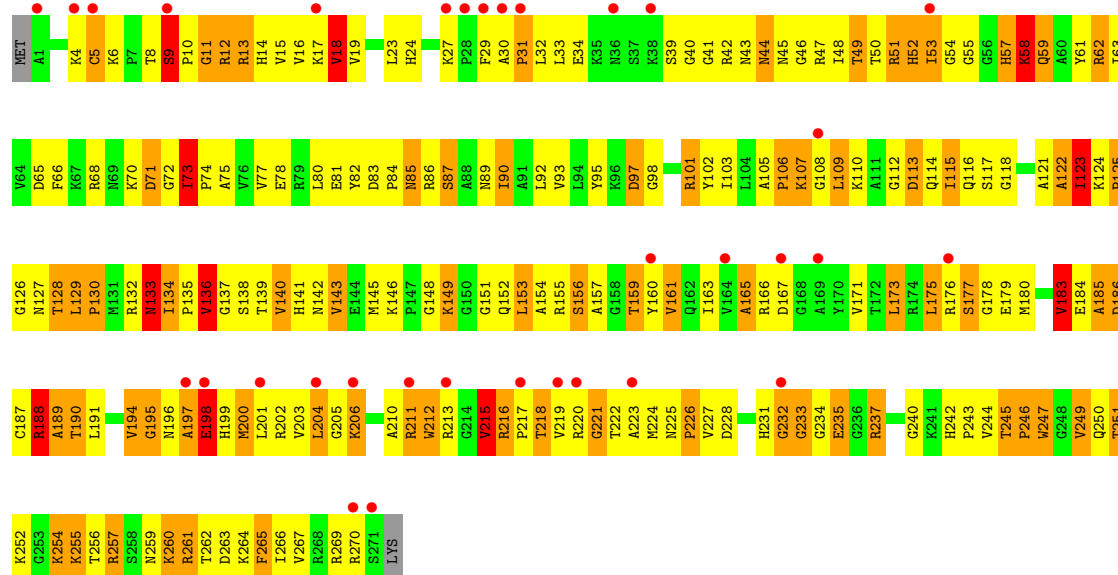
• Molecule 25: 5S ribosomal RNA

Chain DB: 22% 64% 12%

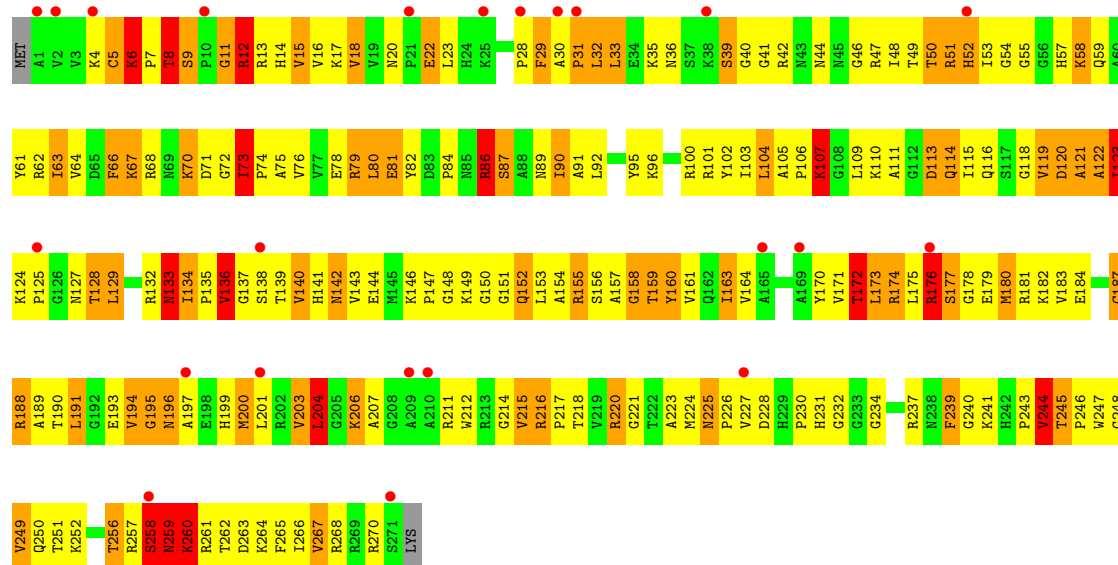




• Molecule 26: 50S ribosomal protein L2

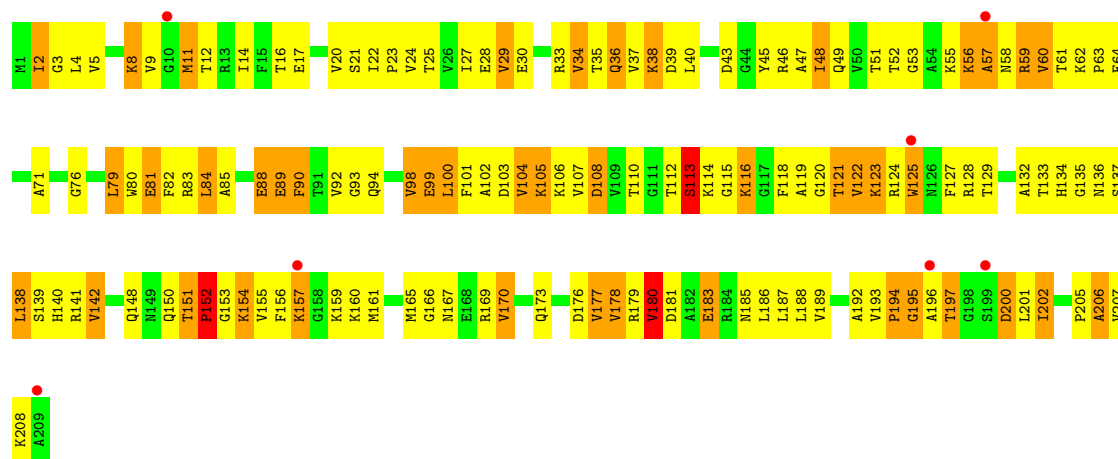


• Molecule 26: 50S ribosomal protein L2

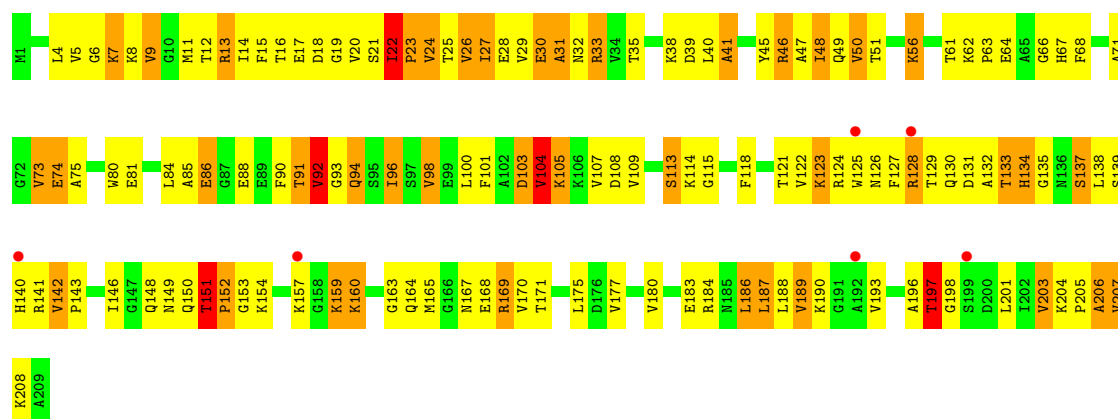


• Molecule 27: 50S ribosomal protein L3

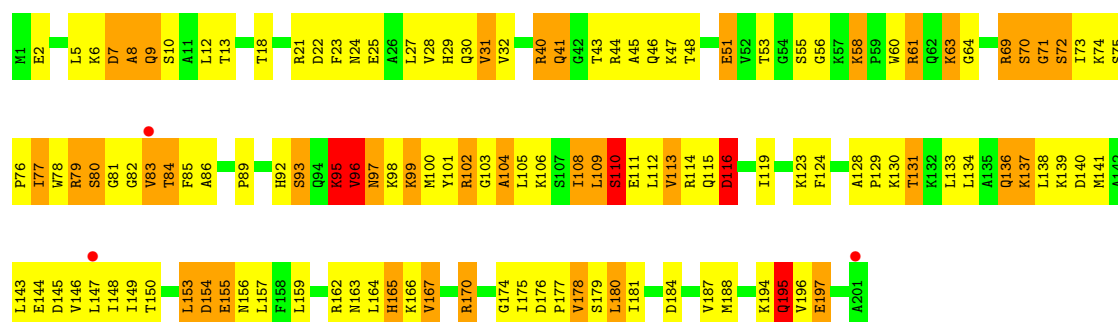




• Molecule 27: 50S ribosomal protein L3

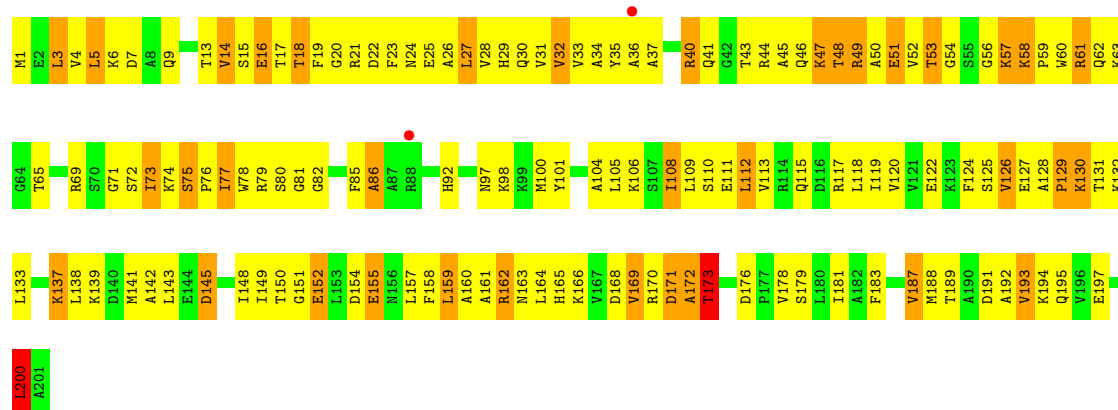


• Molecule 28: 50S ribosomal protein L4

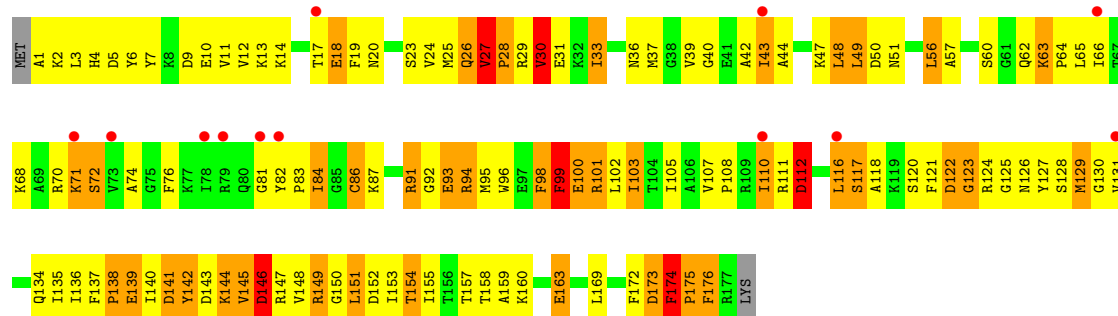


• Molecule 28: 50S ribosomal protein L4

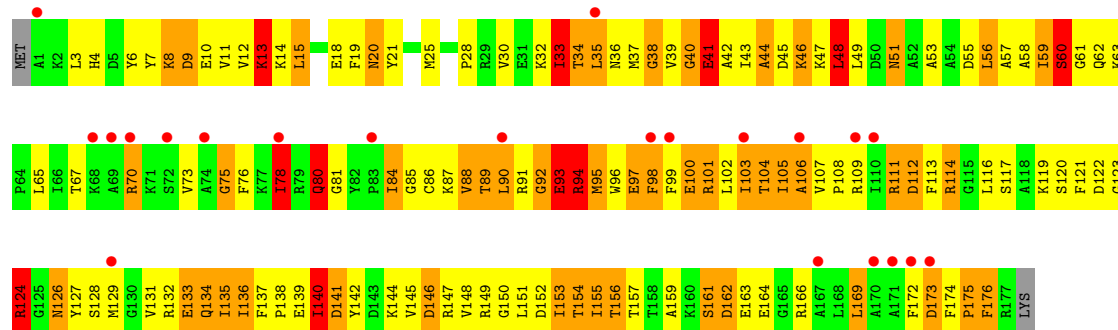
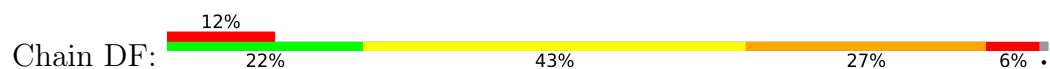




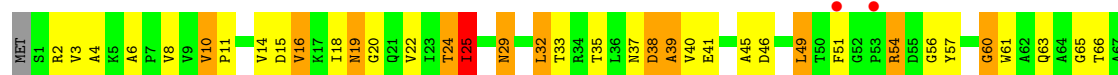
• Molecule 29: 50S ribosomal protein L5

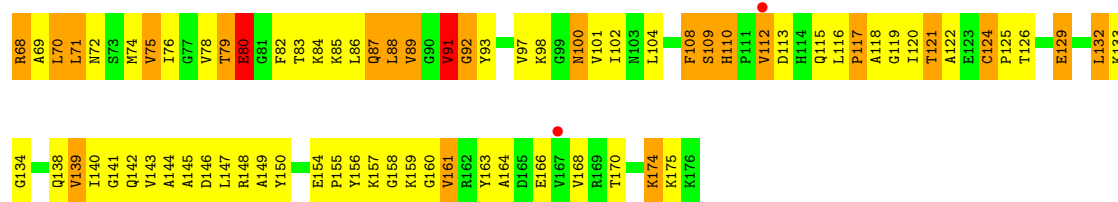


• Molecule 29: 50S ribosomal protein L5

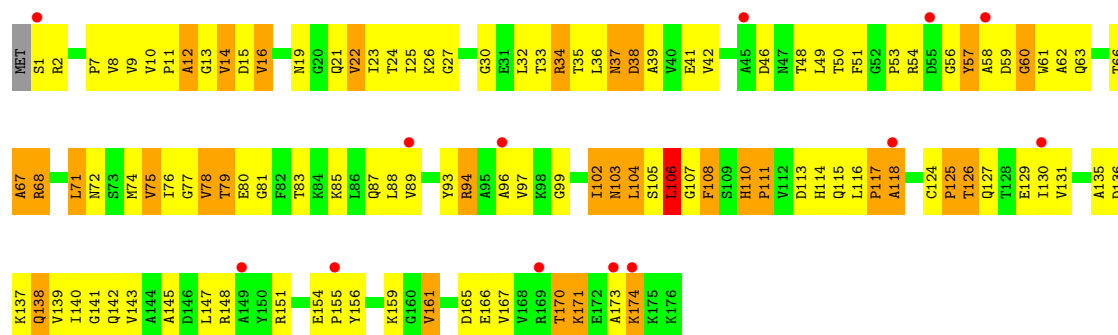


• Molecule 30: 50S ribosomal protein L6

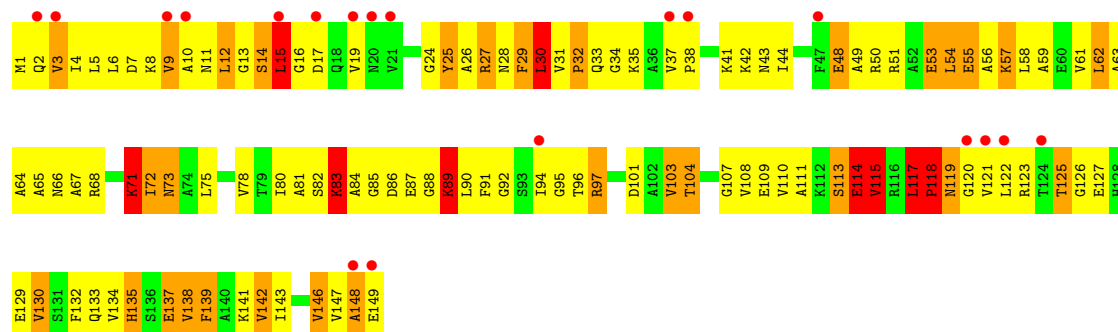




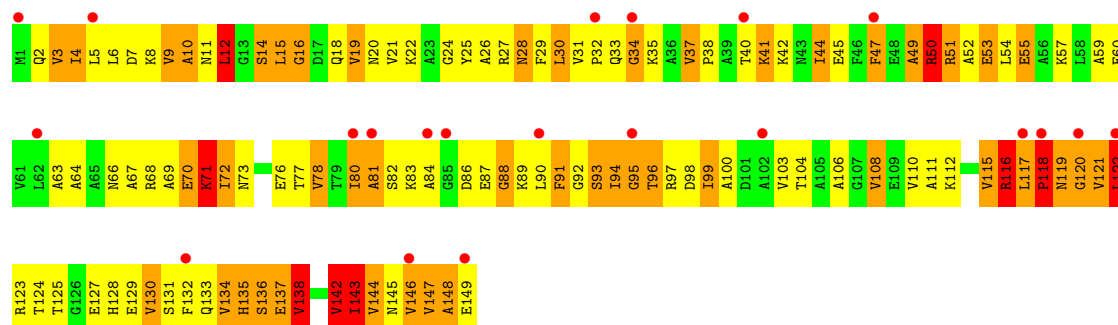
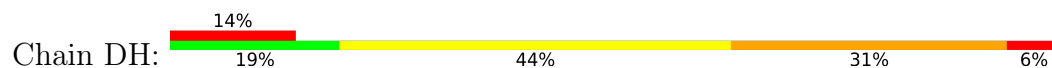
• Molecule 30: 50S ribosomal protein L6



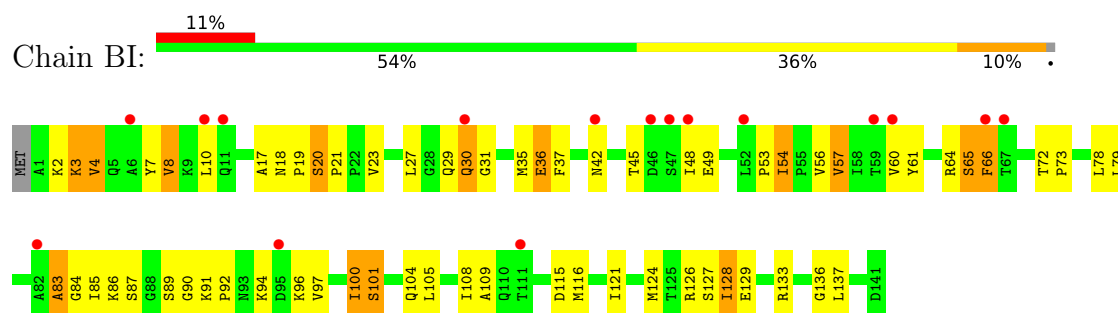
• Molecule 31: 50S ribosomal protein L9



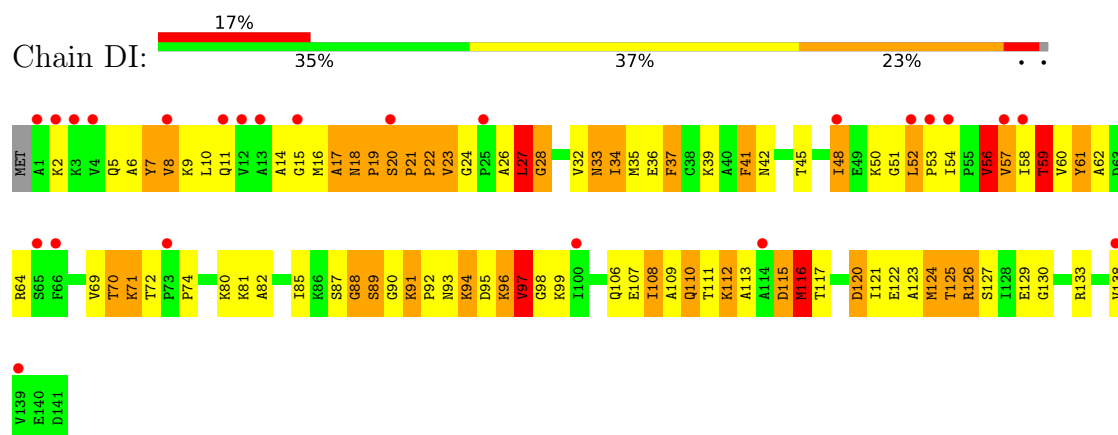
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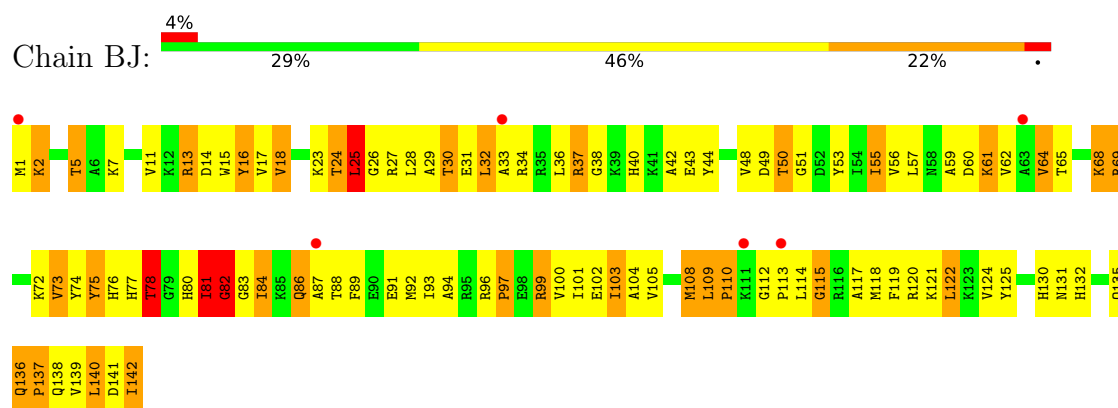
- Molecule 32: 50S ribosomal protein L11



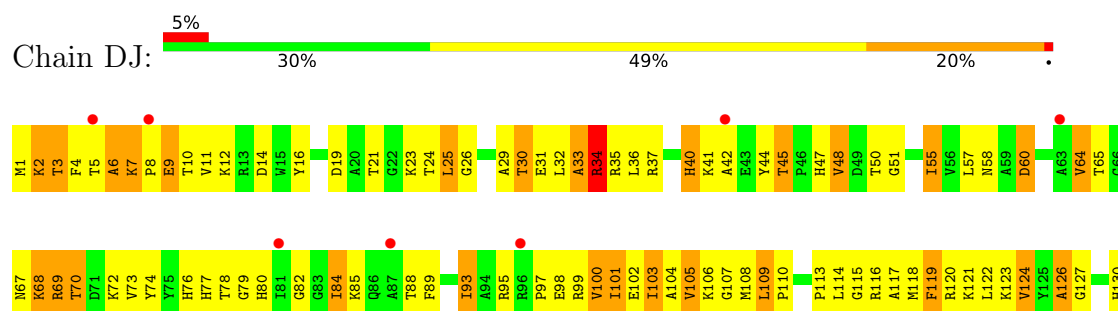
- Molecule 32: 50S ribosomal protein L11



- Molecule 33: 50S ribosomal protein L13

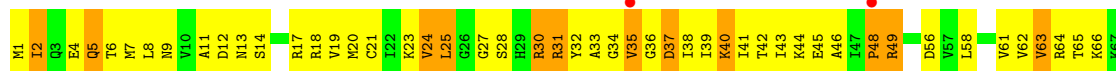


- Molecule 33: 50S ribosomal protein L13

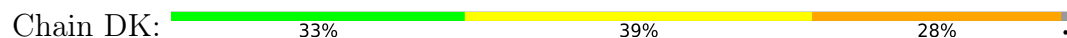




- Molecule 34: 50S ribosomal protein L14



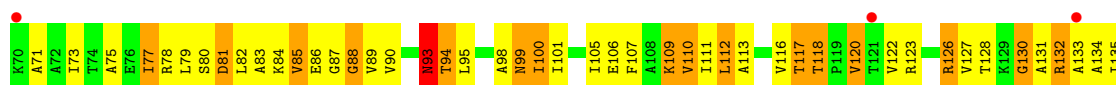
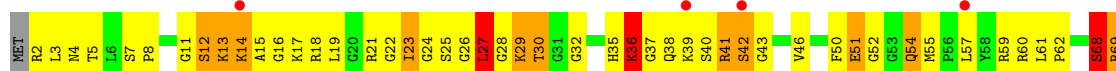
- Molecule 34: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L15

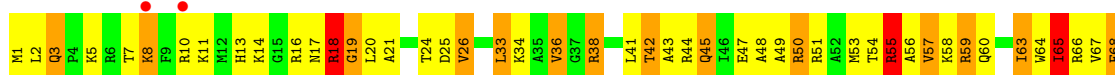


- Molecule 35: 50S ribosomal protein L15

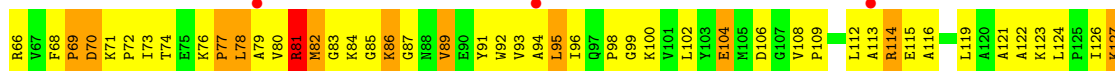




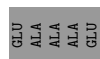
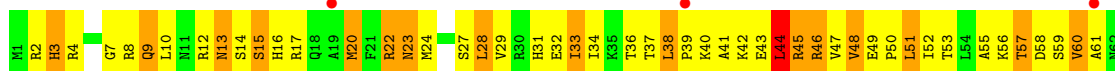
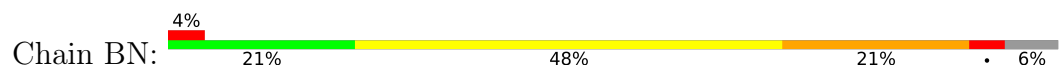
- Molecule 36: 50S ribosomal protein L16



- Molecule 36: 50S ribosomal protein L16

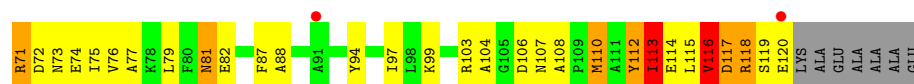


- Molecule 37: 50S ribosomal protein L17

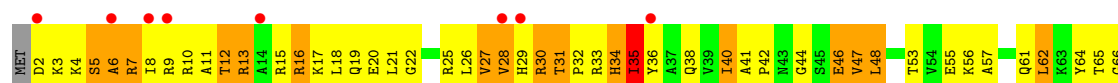


- Molecule 37: 50S ribosomal protein L17

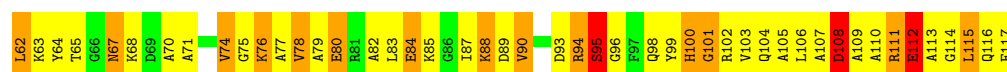
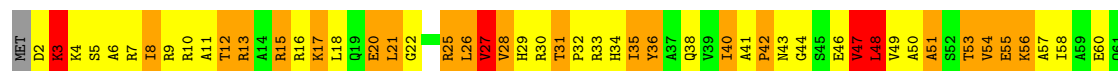
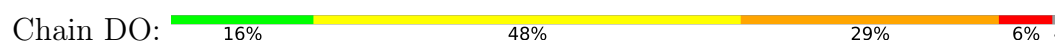




- Molecule 38: 50S ribosomal protein L18



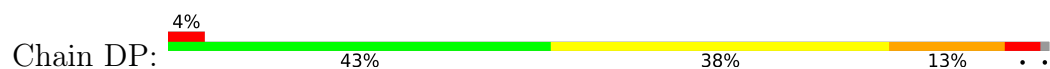
- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19

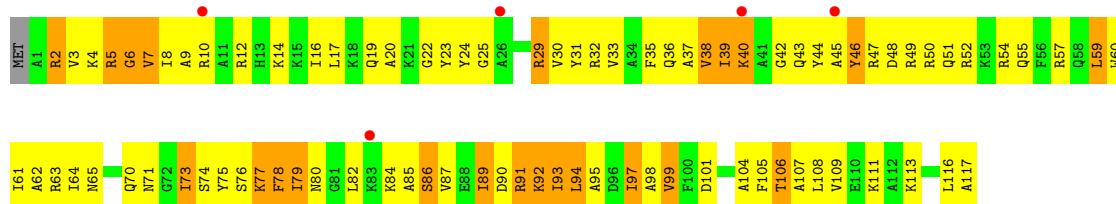


- Molecule 39: 50S ribosomal protein L19

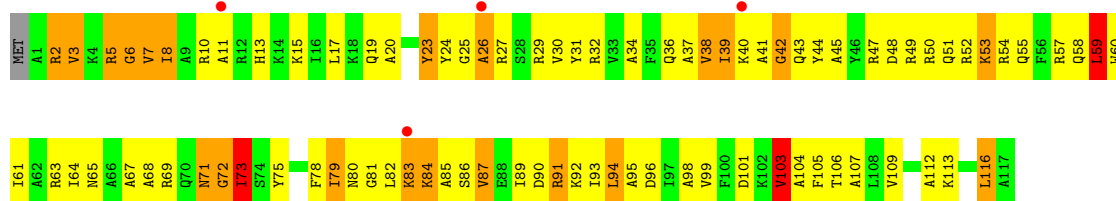


- Molecule 40: 50S ribosomal protein L20

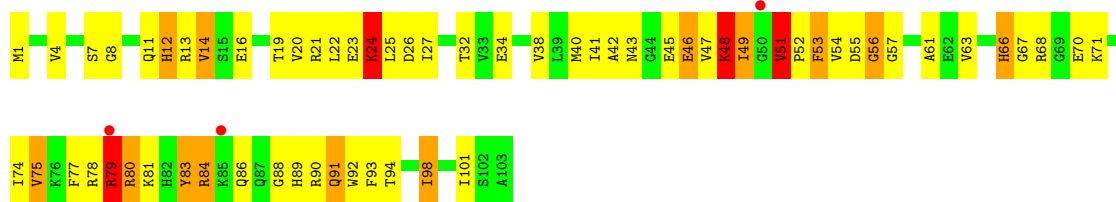




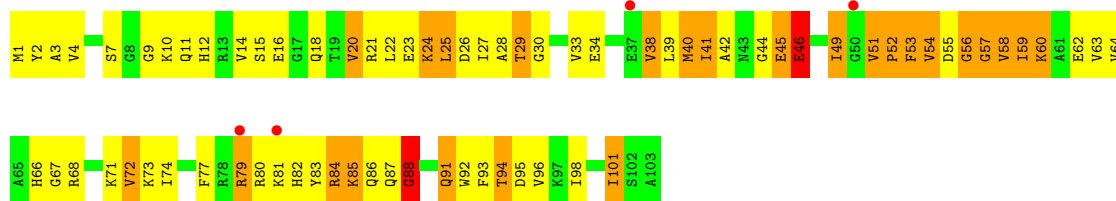
• Molecule 40: 50S ribosomal protein L20



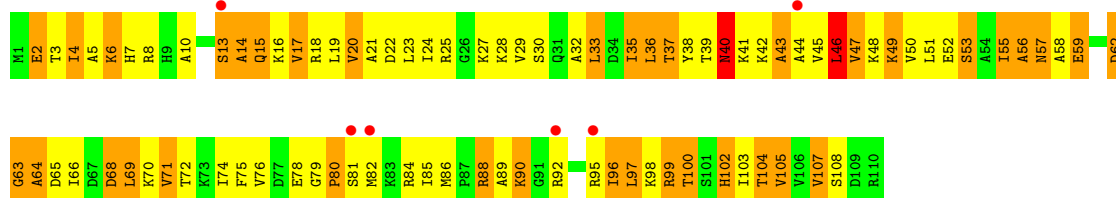
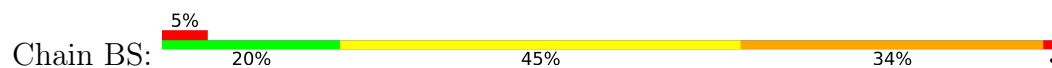
• Molecule 41: 50S ribosomal protein L21



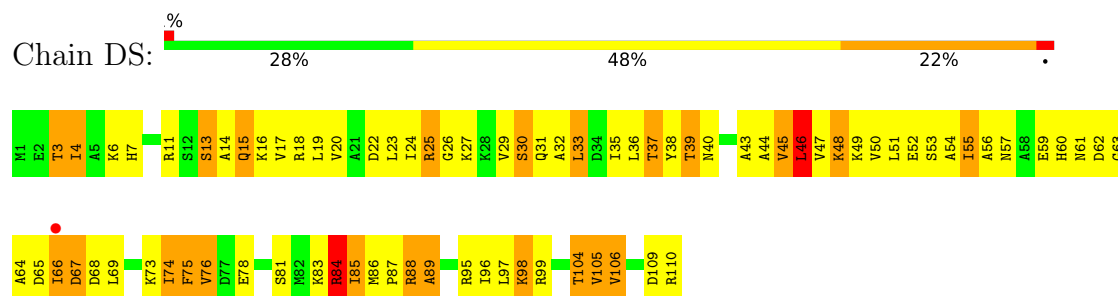
• Molecule 41: 50S ribosomal protein L21



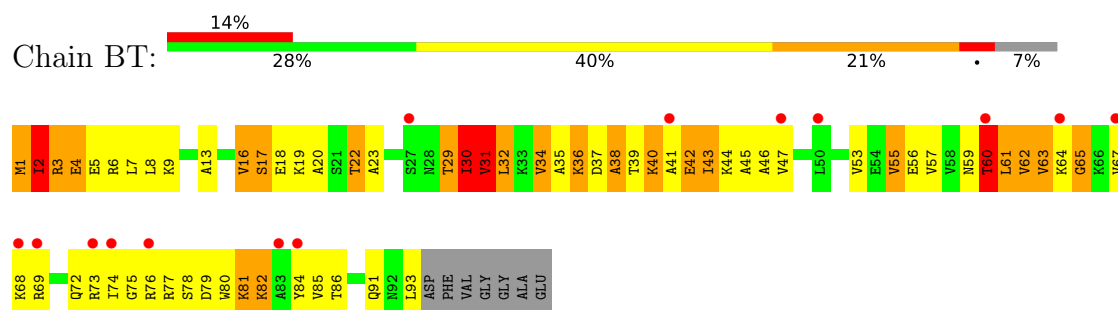
• Molecule 42: 50S ribosomal protein L22



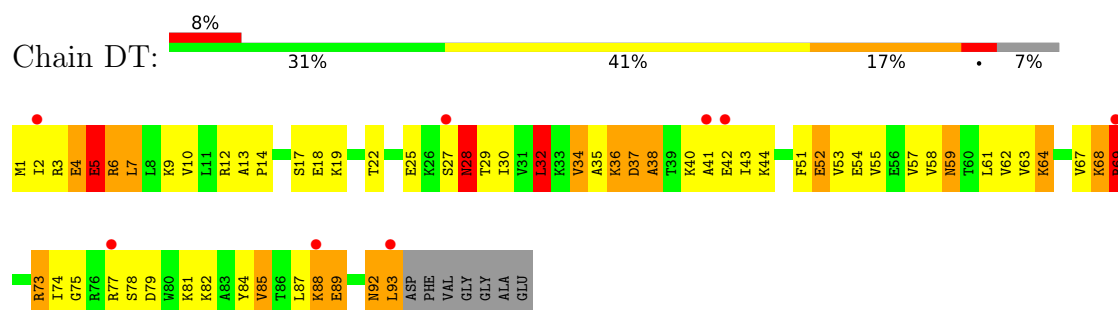
- Molecule 42: 50S ribosomal protein L22



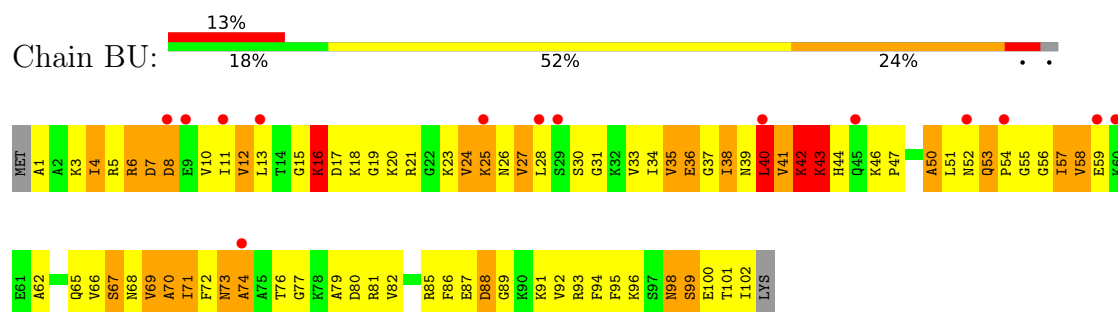
- Molecule 43: 50S ribosomal protein L23



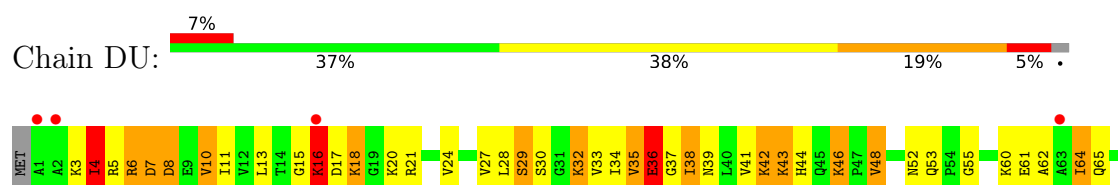
- Molecule 43: 50S ribosomal protein L23



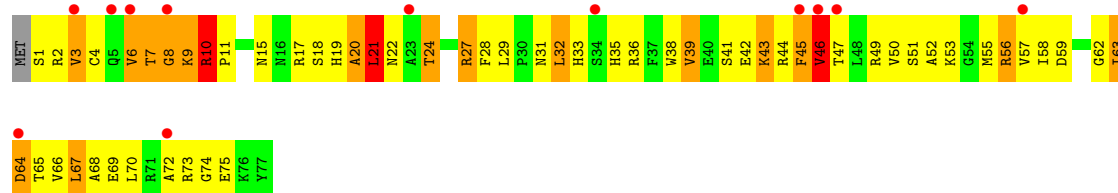
- Molecule 44: 50S ribosomal protein L24



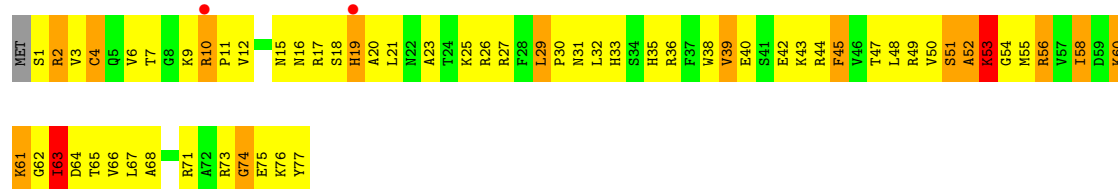
- Molecule 44: 50S ribosomal protein L24







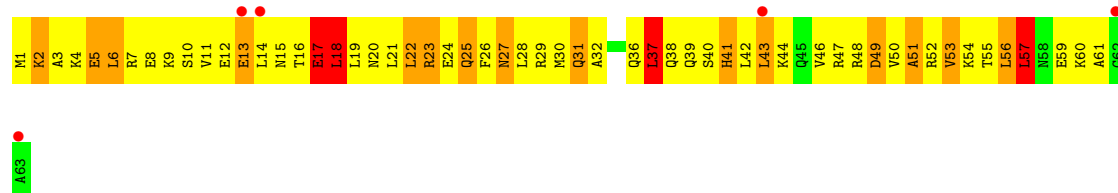
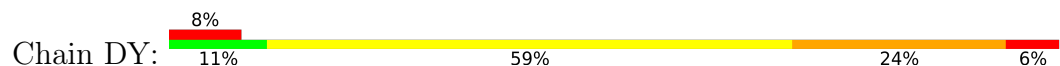
• Molecule 47: 50S ribosomal protein L28



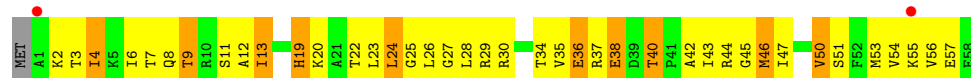
• Molecule 48: 50S ribosomal protein L29



• Molecule 48: 50S ribosomal protein L29



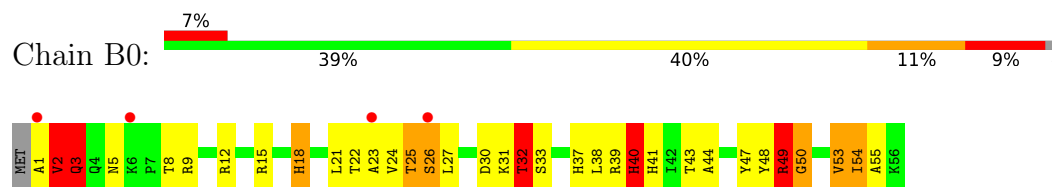
• Molecule 49: 50S ribosomal protein L30



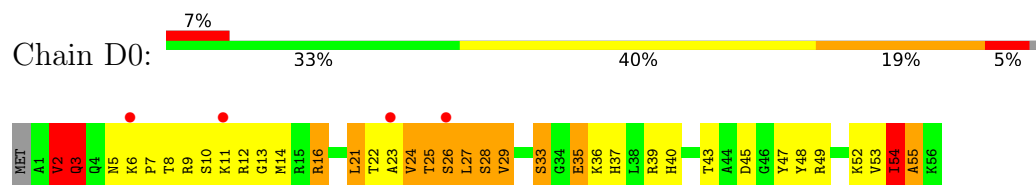
• Molecule 49: 50S ribosomal protein L30



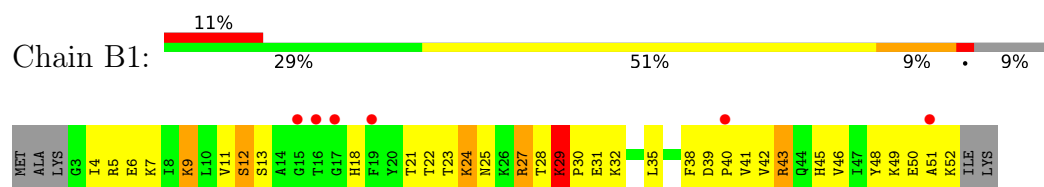
- Molecule 50: 50S ribosomal protein L32



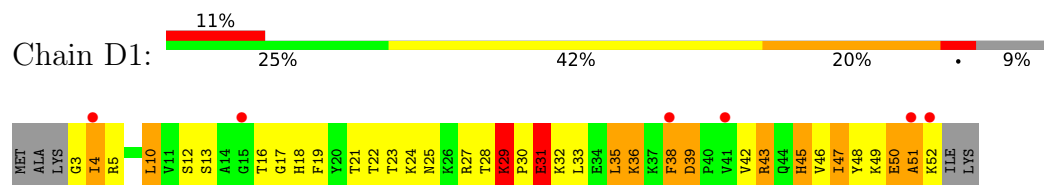
- Molecule 50: 50S ribosomal protein L32



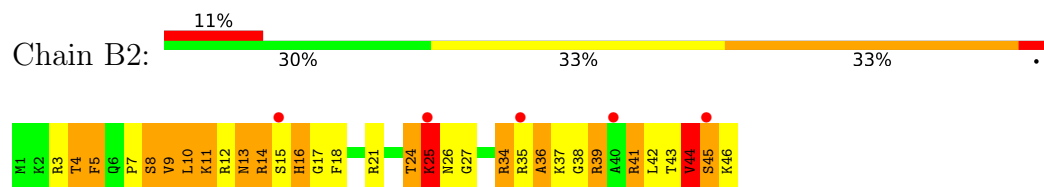
- Molecule 51: 50S ribosomal protein L33



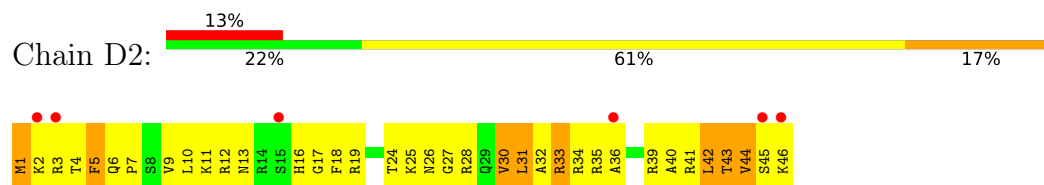
- Molecule 51: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L34

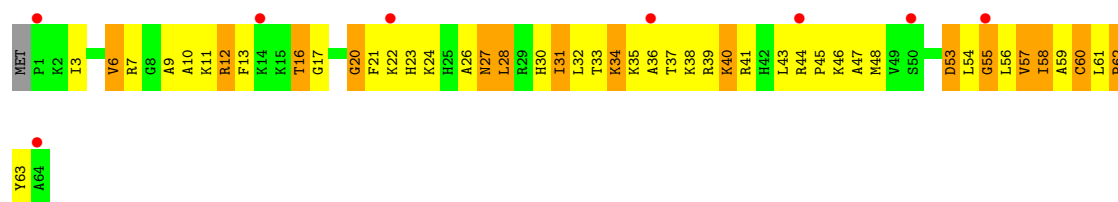


- Molecule 52: 50S ribosomal protein L34

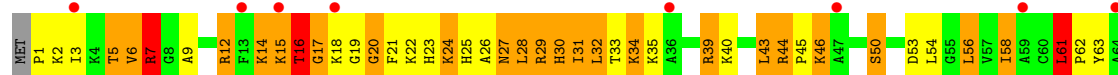
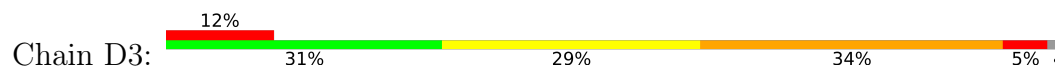


- Molecule 53: 50S ribosomal protein L35

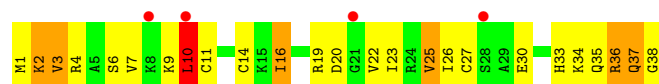




- Molecule 53: 50S ribosomal protein L35



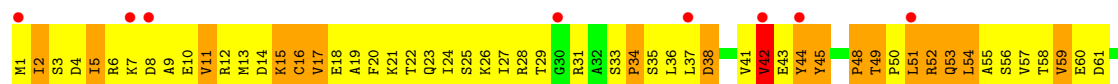
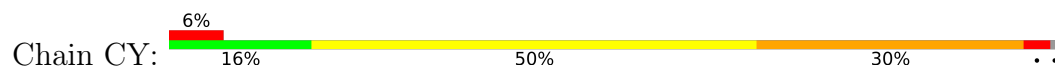
- Molecule 54: 50S ribosomal protein L36



- Molecule 54: 50S ribosomal protein L36



- Molecule 55: Ribosome recycling factor, RRF



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.18Å 433.90Å 608.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.30 70.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.30) 95.2 (70.00-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.255 0.203 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (0.24%)	wwPDB-VP
Wilson B-factor (Å ²)	96.3	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 117.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	293103	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% 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: NMY, 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	0.18	0/36966	0.44	1/57666 (0.0%)
1	CA	0.18	0/36944	0.42	0/57632
2	AB	0.40	0/1735	0.95	12/2338 (0.5%)
2	CB	0.37	0/1735	0.83	4/2338 (0.2%)
3	AC	0.40	0/1651	0.91	5/2225 (0.2%)
3	CC	0.40	0/1651	0.86	3/2225 (0.1%)
4	AD	0.46	0/1665	1.03	11/2227 (0.5%)
4	CD	0.39	0/1665	0.90	5/2227 (0.2%)
5	AE	0.39	0/1118	0.97	4/1504 (0.3%)
5	CE	0.42	0/1118	0.93	3/1504 (0.2%)
6	AF	0.46	0/835	1.00	4/1128 (0.4%)
6	CF	0.51	0/835	0.89	3/1128 (0.3%)
7	AG	0.36	0/1195	0.81	1/1602 (0.1%)
7	CG	0.39	0/1195	0.86	2/1602 (0.1%)
8	AH	0.41	0/989	0.92	4/1326 (0.3%)
8	CH	0.40	0/989	0.93	1/1326 (0.1%)
9	AI	0.34	0/1034	0.90	6/1375 (0.4%)
9	CI	0.36	0/1034	0.89	5/1375 (0.4%)
10	AJ	0.38	0/796	0.87	0/1077
10	CJ	0.36	0/796	0.83	2/1077 (0.2%)
11	AK	0.50	0/893	1.07	6/1205 (0.5%)
11	CK	0.41	0/893	0.95	8/1205 (0.7%)
12	AL	0.44	0/969	1.06	9/1300 (0.7%)
12	CL	0.50	0/969	1.06	9/1300 (0.7%)
13	AM	0.36	0/892	0.78	1/1193 (0.1%)
13	CM	0.37	0/892	0.93	3/1193 (0.3%)
14	AN	0.34	0/785	0.76	0/1043
14	CN	0.33	0/785	0.92	4/1043 (0.4%)
15	AO	0.37	0/722	0.76	1/964 (0.1%)
15	CO	0.36	0/722	0.73	1/964 (0.1%)
16	AP	0.42	0/659	0.89	0/884
16	CP	0.39	0/659	0.86	1/884 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/657	0.90	2/881 (0.2%)
17	CQ	0.41	0/657	1.04	6/881 (0.7%)
18	AR	0.44	0/462	0.89	1/621 (0.2%)
18	CR	0.35	0/462	0.80	2/621 (0.3%)
19	AS	0.36	0/652	0.97	7/877 (0.8%)
19	CS	0.34	0/652	0.91	3/877 (0.3%)
20	AT	0.42	0/671	0.80	0/888
20	CT	0.36	0/671	0.83	3/888 (0.3%)
21	AU	0.46	0/430	0.97	1/570 (0.2%)
21	CU	0.42	0/430	0.83	0/570
22	AV	0.17	0/1813	0.42	0/2823
22	CV	0.12	0/1813	0.32	0/2823
23	AX	0.17	0/388	0.40	0/603
23	CX	0.15	0/363	0.36	0/564
24	BA	0.19	0/69659	0.44	0/108672
24	DA	0.22	0/69659	0.48	0/108672
25	BB	0.15	0/2828	0.36	0/4410
25	DB	0.19	0/2850	0.43	0/4444
26	BC	0.39	0/2121	0.95	3/2852 (0.1%)
26	DC	0.47	0/2121	1.08	10/2852 (0.4%)
27	BD	0.42	0/1586	0.94	5/2134 (0.2%)
27	DD	0.49	0/1586	1.02	7/2134 (0.3%)
28	BE	0.40	0/1571	0.86	4/2113 (0.2%)
28	DE	0.43	0/1571	0.95	4/2113 (0.2%)
29	BF	0.33	0/1434	0.80	3/1926 (0.2%)
29	DF	0.40	0/1434	0.90	1/1926 (0.1%)
30	BG	0.38	0/1343	0.87	4/1816 (0.2%)
30	DG	0.42	0/1343	0.97	4/1816 (0.2%)
31	BH	0.39	1/1121 (0.1%)	0.81	3/1515 (0.2%)
31	DH	0.45	1/1121 (0.1%)	0.87	3/1515 (0.2%)
32	BI	0.33	0/1046	0.82	2/1410 (0.1%)
32	DI	0.36	0/1046	0.90	3/1410 (0.2%)
33	BJ	0.41	0/1152	0.95	2/1551 (0.1%)
33	DJ	0.43	0/1152	0.97	4/1551 (0.3%)
34	BK	0.40	0/947	0.93	1/1268 (0.1%)
34	DK	0.47	0/947	0.94	4/1268 (0.3%)
35	BL	0.39	0/1054	0.99	5/1403 (0.4%)
35	DL	0.43	0/1054	1.04	3/1403 (0.2%)
36	BM	0.39	0/1093	0.91	6/1460 (0.4%)
36	DM	0.48	0/1093	1.04	4/1460 (0.3%)
37	BN	0.39	0/973	0.90	2/1301 (0.2%)
37	DN	0.46	0/973	0.99	3/1301 (0.2%)
38	BO	0.32	0/902	0.79	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DO	0.47	0/902	0.87	1/1209 (0.1%)
39	BP	0.43	0/929	0.91	2/1242 (0.2%)
39	DP	0.48	0/929	0.93	2/1242 (0.2%)
40	BQ	0.41	0/960	0.83	1/1278 (0.1%)
40	DQ	0.43	0/960	0.96	1/1278 (0.1%)
41	BR	0.40	0/829	0.97	4/1107 (0.4%)
41	DR	0.47	0/829	0.99	3/1107 (0.3%)
42	BS	0.43	0/864	0.96	1/1156 (0.1%)
42	DS	0.50	0/864	0.98	2/1156 (0.2%)
43	BT	0.41	0/744	0.92	2/994 (0.2%)
43	DT	0.44	0/744	0.91	2/994 (0.2%)
44	BU	0.38	0/787	0.86	2/1051 (0.2%)
44	DU	0.41	0/787	0.96	2/1051 (0.2%)
45	BV	0.37	0/766	0.86	2/1025 (0.2%)
45	DV	0.42	0/766	0.90	0/1025
46	BW	0.38	0/576	0.85	2/762 (0.3%)
46	DW	0.46	0/587	1.03	2/776 (0.3%)
47	BX	0.42	0/635	0.95	2/848 (0.2%)
47	DX	0.39	0/635	0.91	0/848
48	BY	0.32	0/510	0.86	0/677
48	DY	0.37	0/510	0.97	2/677 (0.3%)
49	BZ	0.44	0/453	0.90	0/605
49	DZ	0.44	0/453	1.05	3/605 (0.5%)
50	B0	0.38	0/450	0.92	1/599 (0.2%)
50	D0	0.42	0/450	0.89	1/599 (0.2%)
51	B1	0.41	0/416	0.81	0/554
51	D1	0.37	0/416	0.88	1/554 (0.2%)
52	B2	0.38	0/380	0.95	0/498
52	D2	0.41	0/380	0.87	0/498
53	B3	0.38	0/513	0.89	1/676 (0.1%)
53	D3	0.49	0/513	1.08	4/676 (0.6%)
54	B4	0.39	0/303	0.85	0/397
54	D4	0.49	0/303	1.03	2/397 (0.5%)
55	CY	0.40	0/1434	0.97	6/1929 (0.3%)
All	All	0.28	2/315264 (0.0%)	0.61	288/471562 (0.1%)

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	CB	0	1
3	CC	0	1
4	CD	0	2
5	AE	0	1
8	AH	0	3
9	CI	0	1
12	AL	0	1
13	CM	0	1
16	AP	0	1
16	CP	0	1
26	BC	0	1
26	DC	0	3
27	BD	0	1
27	DD	0	1
31	BH	0	1
31	DH	0	2
33	DJ	0	1
37	BN	0	1
37	DN	0	1
39	DP	0	1
42	DS	0	1
50	D0	0	1
All	All	0	29

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	DH	118	PRO	N-CD	5.32	1.55	1.47
31	BH	118	PRO	N-CD	5.04	1.54	1.47

The worst 5 of 288 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AD	37	ALA	CA-C-N	10.44	132.90	119.84
4	AD	37	ALA	C-N-CA	10.44	132.90	119.84
13	CM	106	ALA	N-CA-C	-9.71	102.68	112.97
12	AL	44	LYS	CA-C-N	-9.59	109.68	120.04
12	AL	44	LYS	C-N-CA	-9.59	109.68	120.04

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	162	PHE	Peptide
5	AE	157	ARG	Peptide
8	AH	125	ILE	Peptide
8	AH	87	LYS	Peptide
8	AH	88	ARG	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	33015	0	16617	2764	0
1	CA	32995	0	16607	2608	2
2	AB	1704	0	1732	300	0
2	CB	1704	0	1732	240	0
3	AC	1624	0	1696	207	0
3	CC	1624	0	1696	194	0
4	AD	1643	0	1707	395	0
4	CD	1643	0	1707	380	0
5	AE	1105	0	1148	166	0
5	CE	1105	0	1148	137	0
6	AF	817	0	808	136	0
6	CF	817	0	808	128	0
7	AG	1181	0	1238	108	0
7	CG	1181	0	1238	158	0
8	AH	979	0	1031	212	0
8	CH	979	0	1031	140	0
9	AI	1022	0	1070	153	0
9	CI	1022	0	1070	169	0
10	AJ	786	0	828	74	0
10	CJ	786	0	828	98	0
11	AK	877	0	887	154	0
11	CK	877	0	887	213	0
12	AL	955	0	1016	160	0
12	CL	955	0	1016	188	0
13	AM	883	0	941	150	0
13	CM	883	0	941	184	0
14	AN	774	0	827	124	0
14	CN	774	0	827	148	0
15	AO	714	0	734	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	714	0	734	135	0
16	AP	649	0	666	105	0
16	CP	649	0	666	101	0
17	AQ	648	0	691	87	0
17	CQ	648	0	691	102	0
18	AR	455	0	478	75	0
18	CR	455	0	478	69	0
19	AS	637	0	665	117	0
19	CS	637	0	665	136	0
20	AT	665	0	714	133	0
20	CT	665	0	714	109	0
21	AU	425	0	449	103	0
21	CU	425	0	449	92	0
22	AV	1623	0	821	69	0
22	CV	1623	0	821	171	0
23	AX	346	0	173	39	0
23	CX	324	0	162	15	0
24	BA	62195	0	31280	4111	1
24	DA	62195	0	31280	3382	1
25	BB	2529	0	1281	204	0
25	DB	2549	0	1291	113	0
26	BC	2082	0	2157	305	0
26	DC	2082	0	2157	293	0
27	BD	1565	0	1616	190	0
27	DD	1565	0	1616	157	0
28	BE	1552	0	1619	189	0
28	DE	1552	0	1619	174	0
29	BF	1410	0	1447	229	0
29	DF	1410	0	1447	269	0
30	BG	1323	0	1374	141	0
30	DG	1323	0	1374	113	0
31	BH	1110	0	1148	145	1
31	DH	1110	0	1148	246	0
32	BI	1032	0	1088	44	0
32	DI	1032	0	1088	90	0
33	BJ	1129	0	1162	140	0
33	DJ	1129	0	1162	111	0
34	BK	938	0	1012	128	0
34	DK	938	0	1012	106	0
35	BL	1045	0	1117	149	0
35	DL	1045	0	1117	127	0
36	BM	1074	0	1157	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DM	1074	0	1157	124	0
37	BN	960	0	1000	144	0
37	DN	960	0	1000	107	0
38	BO	892	0	923	157	0
38	DO	892	0	923	131	0
39	BP	917	0	965	104	0
39	DP	917	0	965	76	0
40	BQ	947	0	1022	108	0
40	DQ	947	0	1022	140	0
41	BR	816	0	839	84	0
41	DR	816	0	839	129	0
42	BS	857	0	922	119	0
42	DS	857	0	922	98	0
43	BT	738	0	807	90	0
43	DT	738	0	807	82	0
44	BU	779	0	834	114	0
44	DU	779	0	834	112	0
45	BV	753	0	780	89	0
45	DV	753	0	780	67	1
46	BW	569	0	581	55	0
46	DW	580	0	594	83	0
47	BX	625	0	655	87	0
47	DX	625	0	655	86	0
48	BY	509	0	543	65	0
48	DY	509	0	543	81	0
49	BZ	449	0	491	60	0
49	DZ	449	0	491	36	0
50	B0	444	0	461	43	0
50	D0	444	0	461	39	0
51	B1	409	0	440	54	0
51	D1	409	0	440	41	0
52	B2	377	0	418	56	0
52	D2	377	0	418	43	0
53	B3	504	0	574	67	0
53	D3	504	0	574	71	0
54	B4	302	0	340	35	0
54	D4	302	0	340	41	0
55	CY	1423	0	1476	190	0
56	AA	54	0	0	0	0
56	AD	1	0	0	0	0
56	AN	1	0	0	0	0
56	BA	163	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BB	3	0	0	0	0
56	BC	1	0	0	0	0
56	BQ	1	0	0	0	0
56	CA	71	0	0	0	0
56	CX	1	0	0	0	0
56	DA	187	0	0	0	0
56	DB	4	0	0	0	0
56	DE	1	0	0	0	0
56	DL	1	0	0	0	0
56	DO	1	0	0	0	0
57	AA	126	0	135	48	0
57	BA	294	0	317	87	0
57	CA	42	0	46	7	0
57	DA	294	0	311	106	0
58	B4	1	0	0	0	0
58	D4	1	0	0	0	0
59	AA	188	0	0	29	0
59	AD	2	0	0	2	0
59	AK	1	0	0	1	0
59	AN	4	0	0	1	0
59	AT	2	0	0	0	0
59	AU	1	0	0	0	0
59	B0	1	0	0	0	0
59	B3	1	0	0	0	0
59	B4	1	0	0	0	0
59	BA	616	0	0	116	0
59	BB	13	0	0	2	0
59	BC	10	0	0	6	0
59	BD	4	0	0	0	0
59	BL	4	0	0	2	0
59	BN	1	0	0	0	0
59	BT	3	0	0	2	0
59	BU	3	0	0	0	0
59	BV	1	0	0	0	0
59	CA	192	0	0	32	0
59	CC	1	0	0	1	0
59	CE	1	0	0	0	0
59	CL	1	0	0	1	0
59	CN	6	0	0	0	0
59	CT	2	0	0	1	0
59	D3	2	0	0	0	0
59	D4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	DA	627	0	0	120	0
59	DB	13	0	0	4	0
59	DC	4	0	0	0	0
59	DD	2	0	0	1	0
59	DE	4	0	0	1	0
59	DF	1	0	0	0	0
59	DL	7	0	0	4	0
59	DN	2	0	0	0	0
59	DQ	1	0	0	0	0
59	DS	1	0	0	0	0
59	DT	1	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	293103	0	196267	23787	3

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 49.

The worst 5 of 23787 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)
29:BF:96:TRP:CE3	29:BF:99:PHE:CE2	1.79	1.66
29:BF:96:TRP:CZ3	29:BF:99:PHE:HE2	1.31	1.48
31:BH:121:VAL:HB	31:BH:122:LEU:CD2	1.41	1.47
29:BF:96:TRP:CD2	29:BF:99:PHE:CZ	2.03	1.47
31:BH:121:VAL:CB	31:BH:122:LEU:HD23	1.49	1.42

All (3) 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)
31:BH:123:ARG:NH2	1:CA:358:U:OP1[4_555]	2.07	0.13
24:BA:2152:G:N2	1:CA:416:G:OP1[4_555]	2.15	0.05
24:DA:544:C:OP2	45:DV:34:LYS:NZ[4_545]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/241 (90%)	106 (49%)	51 (24%)	59 (27%)	0	0
2	CB	216/241 (90%)	110 (51%)	51 (24%)	55 (26%)	0	0
3	AC	204/233 (88%)	124 (61%)	46 (22%)	34 (17%)	0	1
3	CC	204/233 (88%)	122 (60%)	48 (24%)	34 (17%)	0	1
4	AD	203/206 (98%)	100 (49%)	48 (24%)	55 (27%)	0	0
4	CD	203/206 (98%)	92 (45%)	49 (24%)	62 (30%)	0	0
5	AE	148/167 (89%)	86 (58%)	30 (20%)	32 (22%)	0	0
5	CE	148/167 (89%)	106 (72%)	22 (15%)	20 (14%)	0	1
6	AF	98/135 (73%)	53 (54%)	27 (28%)	18 (18%)	0	0
6	CF	98/135 (73%)	47 (48%)	22 (22%)	29 (30%)	0	0
7	AG	149/179 (83%)	92 (62%)	33 (22%)	24 (16%)	0	1
7	CG	149/179 (83%)	65 (44%)	46 (31%)	38 (26%)	0	0
8	AH	127/130 (98%)	62 (49%)	37 (29%)	28 (22%)	0	0
8	CH	127/130 (98%)	80 (63%)	28 (22%)	19 (15%)	0	1
9	AI	125/130 (96%)	60 (48%)	36 (29%)	29 (23%)	0	0
9	CI	125/130 (96%)	61 (49%)	36 (29%)	28 (22%)	0	0
10	AJ	96/103 (93%)	62 (65%)	22 (23%)	12 (12%)	0	1
10	CJ	96/103 (93%)	55 (57%)	21 (22%)	20 (21%)	0	0
11	AK	115/129 (89%)	76 (66%)	19 (16%)	20 (17%)	0	0
11	CK	115/129 (89%)	52 (45%)	40 (35%)	23 (20%)	0	0
12	AL	121/124 (98%)	58 (48%)	28 (23%)	35 (29%)	0	0
12	CL	121/124 (98%)	72 (60%)	26 (22%)	23 (19%)	0	0
13	AM	112/118 (95%)	65 (58%)	19 (17%)	28 (25%)	0	0
13	CM	112/118 (95%)	55 (49%)	22 (20%)	35 (31%)	0	0
14	AN	92/101 (91%)	50 (54%)	21 (23%)	21 (23%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	92/101 (91%)	64 (70%)	11 (12%)	17 (18%)	0	0
15	AO	86/89 (97%)	52 (60%)	20 (23%)	14 (16%)	0	1
15	CO	86/89 (97%)	42 (49%)	23 (27%)	21 (24%)	0	0
16	AP	80/82 (98%)	35 (44%)	27 (34%)	18 (22%)	0	0
16	CP	80/82 (98%)	39 (49%)	23 (29%)	18 (22%)	0	0
17	AQ	78/84 (93%)	40 (51%)	20 (26%)	18 (23%)	0	0
17	CQ	78/84 (93%)	51 (65%)	12 (15%)	15 (19%)	0	0
18	AR	53/75 (71%)	31 (58%)	8 (15%)	14 (26%)	0	0
18	CR	53/75 (71%)	28 (53%)	12 (23%)	13 (24%)	0	0
19	AS	77/92 (84%)	43 (56%)	23 (30%)	11 (14%)	0	1
19	CS	77/92 (84%)	35 (46%)	23 (30%)	19 (25%)	0	0
20	AT	83/87 (95%)	45 (54%)	23 (28%)	15 (18%)	0	0
20	CT	83/87 (95%)	42 (51%)	22 (26%)	19 (23%)	0	0
21	AU	49/71 (69%)	18 (37%)	16 (33%)	15 (31%)	0	0
21	CU	49/71 (69%)	23 (47%)	14 (29%)	12 (24%)	0	0
26	BC	269/273 (98%)	171 (64%)	48 (18%)	50 (19%)	0	0
26	DC	269/273 (98%)	187 (70%)	51 (19%)	31 (12%)	0	2
27	BD	207/209 (99%)	159 (77%)	29 (14%)	19 (9%)	0	3
27	DD	207/209 (99%)	159 (77%)	33 (16%)	15 (7%)	1	6
28	BE	199/201 (99%)	126 (63%)	49 (25%)	24 (12%)	0	1
28	DE	199/201 (99%)	131 (66%)	53 (27%)	15 (8%)	1	6
29	BF	175/179 (98%)	104 (59%)	44 (25%)	27 (15%)	0	1
29	DF	175/179 (98%)	96 (55%)	39 (22%)	40 (23%)	0	0
30	BG	174/177 (98%)	107 (62%)	43 (25%)	24 (14%)	0	1
30	DG	174/177 (98%)	127 (73%)	27 (16%)	20 (12%)	0	2
31	BH	147/149 (99%)	82 (56%)	39 (26%)	26 (18%)	0	0
31	DH	147/149 (99%)	67 (46%)	37 (25%)	43 (29%)	0	0
32	BI	139/142 (98%)	77 (55%)	45 (32%)	17 (12%)	0	1
32	DI	139/142 (98%)	65 (47%)	39 (28%)	35 (25%)	0	0
33	BJ	140/142 (99%)	108 (77%)	19 (14%)	13 (9%)	0	3
33	DJ	140/142 (99%)	110 (79%)	25 (18%)	5 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BK	120/123 (98%)	77 (64%)	29 (24%)	14 (12%)	0	1
34	DK	120/123 (98%)	95 (79%)	18 (15%)	7 (6%)	1	9
35	BL	141/144 (98%)	84 (60%)	35 (25%)	22 (16%)	0	1
35	DL	141/144 (98%)	98 (70%)	29 (21%)	14 (10%)	0	3
36	BM	134/136 (98%)	94 (70%)	27 (20%)	13 (10%)	0	3
36	DM	134/136 (98%)	94 (70%)	28 (21%)	12 (9%)	0	4
37	BN	118/127 (93%)	72 (61%)	30 (25%)	16 (14%)	0	1
37	DN	118/127 (93%)	84 (71%)	22 (19%)	12 (10%)	0	2
38	BO	114/117 (97%)	65 (57%)	30 (26%)	19 (17%)	0	1
38	DO	114/117 (97%)	64 (56%)	25 (22%)	25 (22%)	0	0
39	BP	112/115 (97%)	80 (71%)	18 (16%)	14 (12%)	0	1
39	DP	112/115 (97%)	92 (82%)	12 (11%)	8 (7%)	1	6
40	BQ	115/118 (98%)	98 (85%)	13 (11%)	4 (4%)	3	18
40	DQ	115/118 (98%)	89 (77%)	16 (14%)	10 (9%)	0	4
41	BR	101/103 (98%)	76 (75%)	18 (18%)	7 (7%)	1	7
41	DR	101/103 (98%)	67 (66%)	23 (23%)	11 (11%)	0	2
42	BS	108/110 (98%)	68 (63%)	22 (20%)	18 (17%)	0	1
42	DS	108/110 (98%)	77 (71%)	21 (19%)	10 (9%)	0	3
43	BT	91/100 (91%)	54 (59%)	26 (29%)	11 (12%)	0	1
43	DT	91/100 (91%)	60 (66%)	18 (20%)	13 (14%)	0	1
44	BU	100/104 (96%)	55 (55%)	21 (21%)	24 (24%)	0	0
44	DU	100/104 (96%)	73 (73%)	12 (12%)	15 (15%)	0	1
45	BV	92/94 (98%)	50 (54%)	26 (28%)	16 (17%)	0	0
45	DV	92/94 (98%)	79 (86%)	4 (4%)	9 (10%)	0	3
46	BW	73/85 (86%)	56 (77%)	9 (12%)	8 (11%)	0	2
46	DW	74/85 (87%)	51 (69%)	14 (19%)	9 (12%)	0	1
47	BX	75/78 (96%)	55 (73%)	10 (13%)	10 (13%)	0	1
47	DX	75/78 (96%)	51 (68%)	14 (19%)	10 (13%)	0	1
48	BY	61/63 (97%)	38 (62%)	17 (28%)	6 (10%)	0	3
48	DY	61/63 (97%)	31 (51%)	19 (31%)	11 (18%)	0	0
49	BZ	56/59 (95%)	42 (75%)	12 (21%)	2 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	DZ	56/59 (95%)	37 (66%)	16 (29%)	3 (5%)	1	10
50	B0	54/57 (95%)	34 (63%)	9 (17%)	11 (20%)	0	0
50	D0	54/57 (95%)	36 (67%)	10 (18%)	8 (15%)	0	1
51	B1	48/55 (87%)	29 (60%)	15 (31%)	4 (8%)	0	5
51	D1	48/55 (87%)	28 (58%)	10 (21%)	10 (21%)	0	0
52	B2	44/46 (96%)	29 (66%)	8 (18%)	7 (16%)	0	1
52	D2	44/46 (96%)	31 (70%)	10 (23%)	3 (7%)	1	7
53	B3	62/65 (95%)	47 (76%)	9 (14%)	6 (10%)	0	3
53	D3	62/65 (95%)	47 (76%)	7 (11%)	8 (13%)	0	1
54	B4	36/38 (95%)	27 (75%)	7 (19%)	2 (6%)	1	9
54	D4	36/38 (95%)	26 (72%)	7 (19%)	3 (8%)	0	5
55	CY	181/185 (98%)	99 (55%)	52 (29%)	30 (17%)	0	1
All	All	11416/12155 (94%)	7014 (61%)	2503 (22%)	1899 (17%)	0	1

5 of 1899 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	11	LYS
2	AB	16	PHE
2	AB	23	TRP
2	AB	58	ASN
2	AB	64	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%)	125 (69%)	55 (31%)	0	1
2	CB	180/199 (90%)	135 (75%)	45 (25%)	0	3
3	AC	170/190 (90%)	134 (79%)	36 (21%)	1	5
3	CC	170/190 (90%)	130 (76%)	40 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	172/173 (99%)	114 (66%)	58 (34%)	0	1
4	CD	172/173 (99%)	122 (71%)	50 (29%)	0	2
5	AE	113/126 (90%)	91 (80%)	22 (20%)	1	6
5	CE	113/126 (90%)	86 (76%)	27 (24%)	1	4
6	AF	87/116 (75%)	66 (76%)	21 (24%)	1	3
6	CF	87/116 (75%)	65 (75%)	22 (25%)	0	3
7	AG	124/147 (84%)	92 (74%)	32 (26%)	0	2
7	CG	124/147 (84%)	96 (77%)	28 (23%)	1	5
8	AH	104/105 (99%)	73 (70%)	31 (30%)	0	1
8	CH	104/105 (99%)	82 (79%)	22 (21%)	1	5
9	AI	105/107 (98%)	81 (77%)	24 (23%)	1	4
9	CI	105/107 (98%)	83 (79%)	22 (21%)	1	5
10	AJ	86/90 (96%)	71 (83%)	15 (17%)	2	9
10	CJ	86/90 (96%)	67 (78%)	19 (22%)	1	5
11	AK	90/99 (91%)	73 (81%)	17 (19%)	1	7
11	CK	90/99 (91%)	65 (72%)	25 (28%)	0	2
12	AL	103/104 (99%)	68 (66%)	35 (34%)	0	1
12	CL	103/104 (99%)	73 (71%)	30 (29%)	0	2
13	AM	92/96 (96%)	77 (84%)	15 (16%)	2	11
13	CM	92/96 (96%)	66 (72%)	26 (28%)	0	2
14	AN	79/84 (94%)	62 (78%)	17 (22%)	1	5
14	CN	79/84 (94%)	59 (75%)	20 (25%)	0	3
15	AO	76/77 (99%)	56 (74%)	20 (26%)	0	2
15	CO	76/77 (99%)	57 (75%)	19 (25%)	0	3
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	4
16	CP	65/65 (100%)	43 (66%)	22 (34%)	0	1
17	AQ	74/78 (95%)	63 (85%)	11 (15%)	3	13
17	CQ	74/78 (95%)	52 (70%)	22 (30%)	0	1
18	AR	48/65 (74%)	35 (73%)	13 (27%)	0	2
18	CR	48/65 (74%)	35 (73%)	13 (27%)	0	2
19	AS	70/79 (89%)	51 (73%)	19 (27%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	CS	70/79 (89%)	54 (77%)	16 (23%)	1	4
20	AT	65/66 (98%)	49 (75%)	16 (25%)	1	3
20	CT	65/66 (98%)	48 (74%)	17 (26%)	0	2
21	AU	44/61 (72%)	31 (70%)	13 (30%)	0	2
21	CU	44/61 (72%)	30 (68%)	14 (32%)	0	1
26	BC	216/218 (99%)	154 (71%)	62 (29%)	0	2
26	DC	216/218 (99%)	144 (67%)	72 (33%)	0	1
27	BD	164/164 (100%)	124 (76%)	40 (24%)	1	3
27	DD	164/164 (100%)	120 (73%)	44 (27%)	0	2
28	BE	165/165 (100%)	130 (79%)	35 (21%)	1	5
28	DE	165/165 (100%)	124 (75%)	41 (25%)	1	3
29	BF	148/150 (99%)	114 (77%)	34 (23%)	1	4
29	DF	148/150 (99%)	108 (73%)	40 (27%)	0	2
30	BG	137/138 (99%)	109 (80%)	28 (20%)	1	6
30	DG	137/138 (99%)	111 (81%)	26 (19%)	1	7
31	BH	114/114 (100%)	80 (70%)	34 (30%)	0	1
31	DH	114/114 (100%)	89 (78%)	25 (22%)	1	5
32	BI	109/110 (99%)	101 (93%)	8 (7%)	13	39
32	DI	109/110 (99%)	89 (82%)	20 (18%)	2	7
33	BJ	116/116 (100%)	87 (75%)	29 (25%)	0	3
33	DJ	116/116 (100%)	89 (77%)	27 (23%)	1	4
34	BK	103/104 (99%)	81 (79%)	22 (21%)	1	5
34	DK	103/104 (99%)	72 (70%)	31 (30%)	0	1
35	BL	102/103 (99%)	76 (74%)	26 (26%)	0	3
35	DL	102/103 (99%)	75 (74%)	27 (26%)	0	2
36	BM	109/109 (100%)	80 (73%)	29 (27%)	0	2
36	DM	109/109 (100%)	87 (80%)	22 (20%)	1	6
37	BN	100/103 (97%)	79 (79%)	21 (21%)	1	5
37	DN	100/103 (97%)	82 (82%)	18 (18%)	2	8
38	BO	86/87 (99%)	66 (77%)	20 (23%)	1	4
38	DO	86/87 (99%)	57 (66%)	29 (34%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BP	99/100 (99%)	80 (81%)	19 (19%)	1	7
39	DP	99/100 (99%)	79 (80%)	20 (20%)	1	6
40	BQ	89/90 (99%)	64 (72%)	25 (28%)	0	2
40	DQ	89/90 (99%)	67 (75%)	22 (25%)	1	3
41	BR	84/84 (100%)	63 (75%)	21 (25%)	0	3
41	DR	84/84 (100%)	64 (76%)	20 (24%)	1	4
42	BS	93/93 (100%)	64 (69%)	29 (31%)	0	1
42	DS	93/93 (100%)	69 (74%)	24 (26%)	0	2
43	BT	80/84 (95%)	55 (69%)	25 (31%)	0	1
43	DT	80/84 (95%)	60 (75%)	20 (25%)	0	3
44	BU	83/85 (98%)	61 (74%)	22 (26%)	0	2
44	DU	83/85 (98%)	60 (72%)	23 (28%)	0	2
45	BV	78/78 (100%)	61 (78%)	17 (22%)	1	5
45	DV	78/78 (100%)	61 (78%)	17 (22%)	1	5
46	BW	56/63 (89%)	45 (80%)	11 (20%)	1	6
46	DW	57/63 (90%)	45 (79%)	12 (21%)	1	5
47	BX	67/68 (98%)	48 (72%)	19 (28%)	0	2
47	DX	67/68 (98%)	54 (81%)	13 (19%)	1	6
48	BY	55/55 (100%)	47 (86%)	8 (14%)	3	14
48	DY	55/55 (100%)	40 (73%)	15 (27%)	0	2
49	BZ	48/49 (98%)	38 (79%)	10 (21%)	1	6
49	DZ	48/49 (98%)	40 (83%)	8 (17%)	2	11
50	B0	47/48 (98%)	37 (79%)	10 (21%)	1	5
50	D0	47/48 (98%)	37 (79%)	10 (21%)	1	5
51	B1	45/49 (92%)	37 (82%)	8 (18%)	2	8
51	D1	45/49 (92%)	37 (82%)	8 (18%)	2	8
52	B2	38/38 (100%)	26 (68%)	12 (32%)	0	1
52	D2	38/38 (100%)	31 (82%)	7 (18%)	1	7
53	B3	51/52 (98%)	38 (74%)	13 (26%)	0	3
53	D3	51/52 (98%)	32 (63%)	19 (37%)	0	0
54	B4	34/34 (100%)	26 (76%)	8 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	D4	34/34 (100%)	22 (65%)	12 (35%)	0	1
55	CY	158/160 (99%)	116 (73%)	42 (27%)	0	2
All	All	9485/9916 (96%)	7142 (75%)	2343 (25%)	1	3

5 of 2343 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	DF	105	ILE
50	D0	27	LEU
31	DH	80	ILE
29	DF	103	ILE
38	DO	60	GLU

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

Mol	Chain	Res	Type
35	DL	54	GLN
41	DR	89	HIS
50	D0	37	HIS
42	BS	61	ASN
42	BS	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1538/1542 (99%)	503 (32%)	31 (2%)
1	CA	1537/1542 (99%)	498 (32%)	37 (2%)
22	AV	75/76 (98%)	19 (25%)	1 (1%)
22	CV	75/76 (98%)	27 (36%)	6 (8%)
23	AX	15/24 (62%)	7 (46%)	0
23	CX	14/24 (58%)	6 (42%)	1 (7%)
24	BA	2896/2904 (99%)	884 (30%)	70 (2%)
24	DA	2896/2904 (99%)	828 (28%)	71 (2%)
25	BB	117/120 (97%)	29 (24%)	1 (0%)
25	DB	118/120 (98%)	24 (20%)	0
All	All	9281/9332 (99%)	2825 (30%)	218 (2%)

5 of 2825 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	3	A
1	AA	4	U
1	AA	5	U
1	AA	8	A
1	AA	9	G

5 of 218 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	575	G
22	CV	47	U
24	DA	2286	G
1	CA	737	C
1	CA	1089	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, 492 are monoatomic - leaving 18 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	$\# Z > 2$
57	NMY	AA	1656	-	43,45,45	2.31	12 (27%)	62,67,67	1.88	20 (32%)
57	NMY	BA	3161	-	43,45,45	0.49	0	62,67,67	1.03	4 (6%)
57	NMY	DA	3187	-	43,45,45	2.34	11 (25%)	62,67,67	1.51	13 (20%)
57	NMY	BA	3166	-	43,45,45	2.21	11 (25%)	62,67,67	2.22	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	NMY	DA	3190	-	43,45,45	2.29	10 (23%)	62,67,67	2.56	25 (40%)
57	NMY	AA	1655	-	43,45,45	0.56	0	62,67,67	0.97	4 (6%)
57	NMY	BA	3165	-	43,45,45	0.50	0	62,67,67	1.12	5 (8%)
57	NMY	CA	1672	-	43,45,45	0.53	0	62,67,67	0.89	2 (3%)
57	NMY	DA	3189	-	43,45,45	2.24	11 (25%)	62,67,67	2.32	23 (37%)
57	NMY	DA	3186	-	43,45,45	2.40	12 (27%)	62,67,67	2.39	15 (24%)
57	NMY	BA	3163	-	43,45,45	2.34	10 (23%)	62,67,67	2.46	28 (45%)
57	NMY	DA	3188	-	43,45,45	2.24	13 (30%)	62,67,67	2.03	24 (38%)
57	NMY	BA	3167	-	43,45,45	2.32	11 (25%)	62,67,67	1.97	14 (22%)
57	NMY	AA	1657	-	43,45,45	2.35	12 (27%)	62,67,67	1.87	18 (29%)
57	NMY	BA	3162	-	43,45,45	0.49	0	62,67,67	1.05	5 (8%)
57	NMY	DA	3185	-	43,45,45	2.36	12 (27%)	62,67,67	1.72	14 (22%)
57	NMY	DA	3184	-	43,45,45	0.57	0	62,67,67	1.26	5 (8%)
57	NMY	BA	3164	-	43,45,45	2.29	11 (25%)	62,67,67	2.44	26 (41%)

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
57	NMY	AA	1656	-	-	6/18/94/94	0/4/4/4
57	NMY	BA	3161	-	-	4/18/94/94	0/4/4/4
57	NMY	DA	3187	-	-	8/18/94/94	0/4/4/4
57	NMY	BA	3166	-	-	6/18/94/94	0/4/4/4
57	NMY	DA	3190	-	-	10/18/94/94	0/4/4/4
57	NMY	AA	1655	-	-	12/18/94/94	0/4/4/4
57	NMY	BA	3165	-	-	5/18/94/94	0/4/4/4
57	NMY	CA	1672	-	-	3/18/94/94	0/4/4/4
57	NMY	DA	3189	-	-	5/18/94/94	0/4/4/4
57	NMY	DA	3186	-	-	10/18/94/94	0/4/4/4
57	NMY	BA	3163	-	-	5/18/94/94	0/4/4/4
57	NMY	DA	3188	-	-	8/18/94/94	0/4/4/4
57	NMY	BA	3167	-	-	5/18/94/94	0/4/4/4
57	NMY	AA	1657	-	-	9/18/94/94	0/4/4/4
57	NMY	BA	3162	-	-	1/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	NMY	DA	3185	-	-	5/18/94/94	0/4/4/4
57	NMY	DA	3184	-	-	3/18/94/94	0/4/4/4
57	NMY	BA	3164	-	-	6/18/94/94	0/4/4/4

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	DA	3187	NMY	C20-C19	-10.09	1.40	1.53
57	DA	3186	NMY	C20-C19	-9.91	1.41	1.53
57	AA	1657	NMY	C20-C19	-9.88	1.41	1.53
57	DA	3190	NMY	C20-C19	-9.82	1.41	1.53
57	DA	3185	NMY	C20-C19	-9.78	1.41	1.53

The worst 5 of 261 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	DA	3186	NMY	O11-C13-O16	10.79	122.39	111.37
57	BA	3163	NMY	C1-O1-C10	-6.56	102.42	117.98
57	DA	3186	NMY	C8-C7-C12	6.53	119.85	110.08
57	DA	3190	NMY	C13-C14-C15	6.50	109.92	102.10
57	BA	3163	NMY	C8-C7-C12	6.31	119.52	110.08

There are no chirality outliers.

5 of 111 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	1655	NMY	C4-C5-C6-N6
57	AA	1655	NMY	O5-C5-C6-N6
57	AA	1655	NMY	C14-C13-O11-C11
57	AA	1655	NMY	C16-C15-O18-C18
57	AA	1655	NMY	C19-C18-O18-C15

There are no ring outliers.

18 monomers are involved in 248 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	1656	NMY	12	0
57	BA	3161	NMY	14	0
57	DA	3187	NMY	4	0
57	BA	3166	NMY	14	0

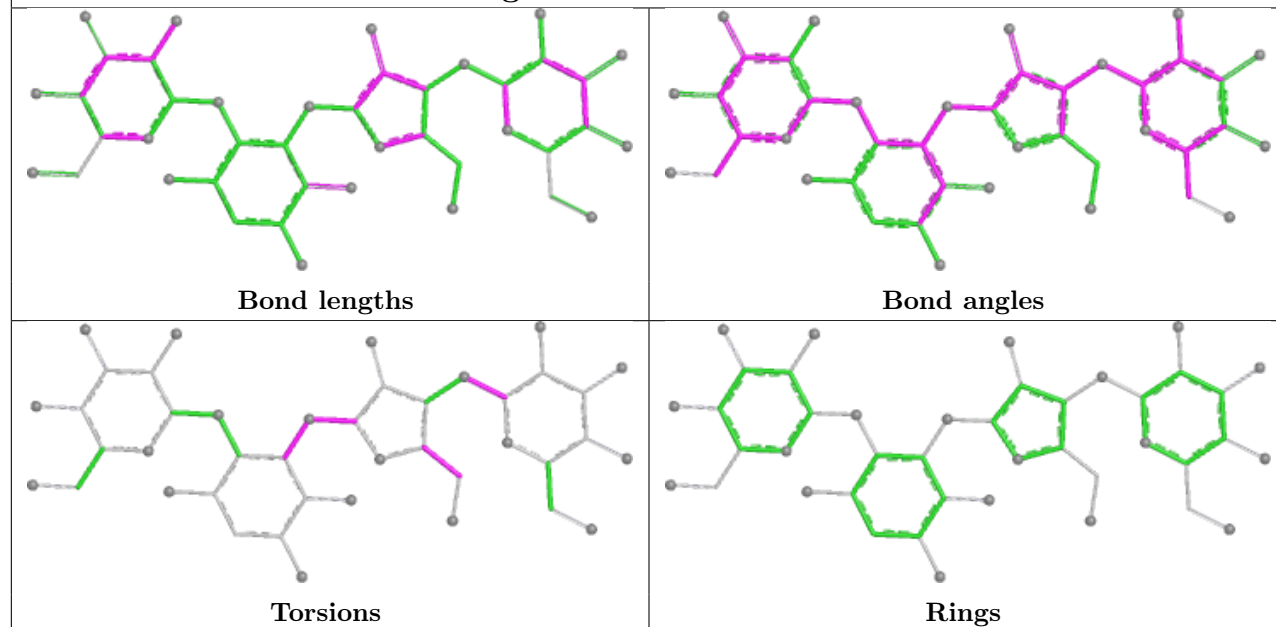
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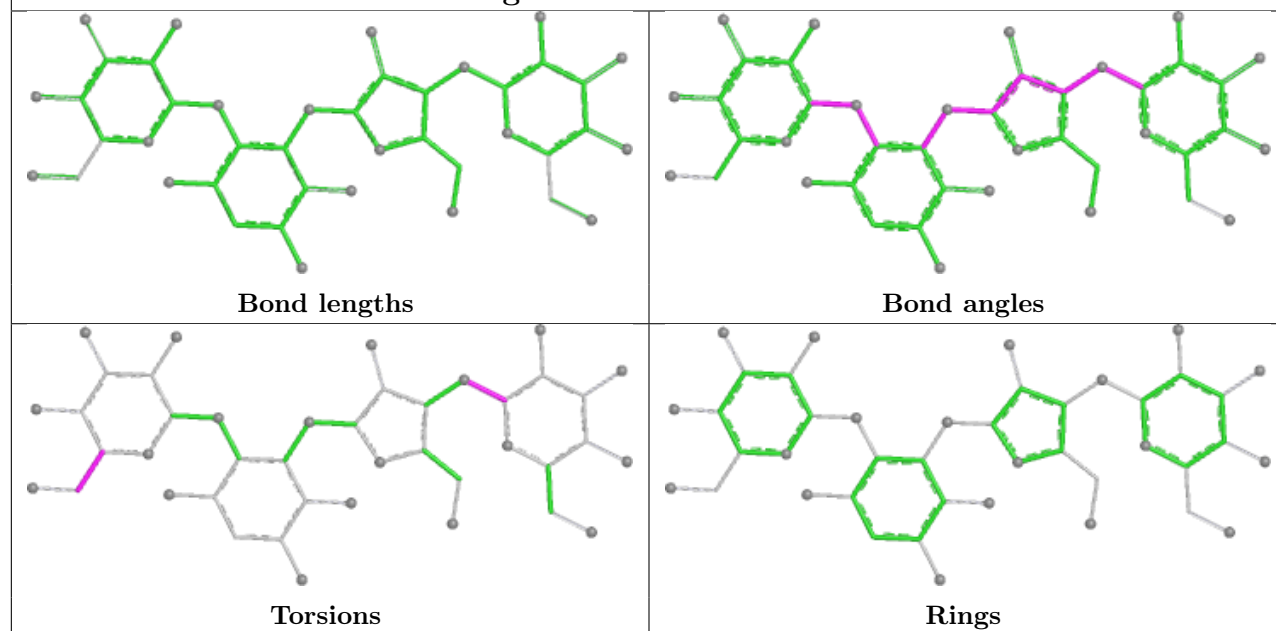
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DA	3190	NMY	32	0
57	AA	1655	NMY	26	0
57	BA	3165	NMY	24	0
57	CA	1672	NMY	7	0
57	DA	3189	NMY	9	0
57	DA	3186	NMY	19	0
57	BA	3163	NMY	11	0
57	DA	3188	NMY	12	0
57	BA	3167	NMY	5	0
57	AA	1657	NMY	10	0
57	BA	3162	NMY	16	0
57	DA	3185	NMY	13	0
57	DA	3184	NMY	17	0
57	BA	3164	NMY	3	0

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

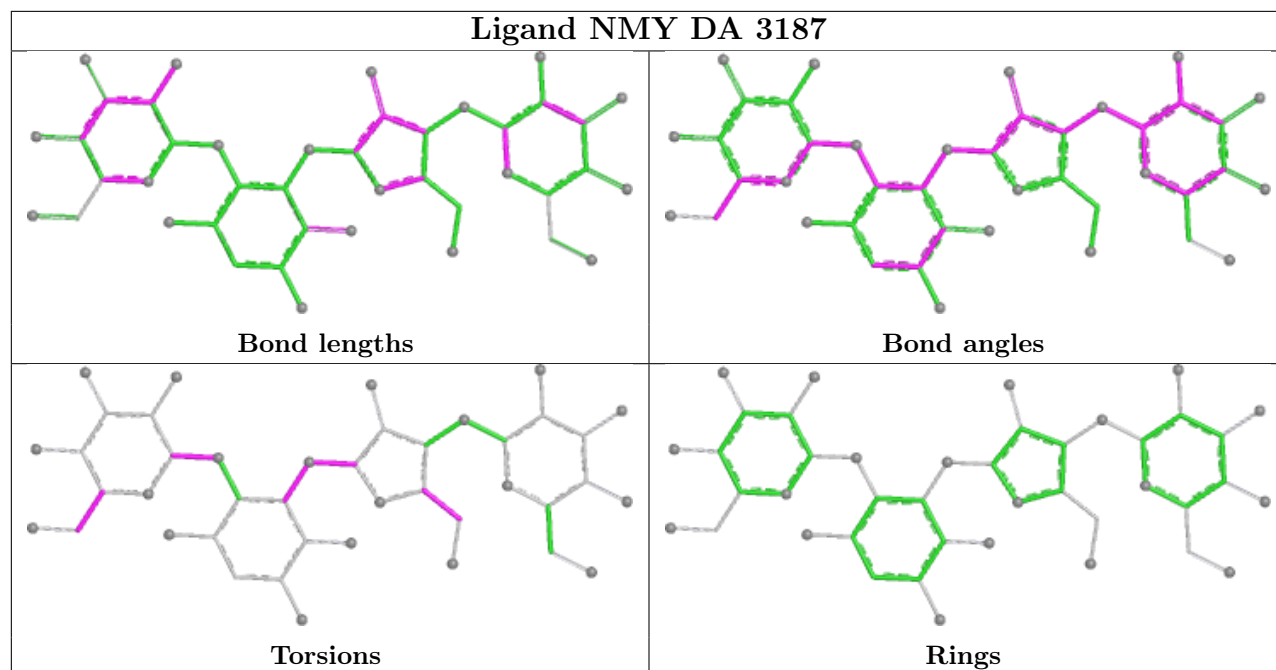
Ligand NMY AA 1656



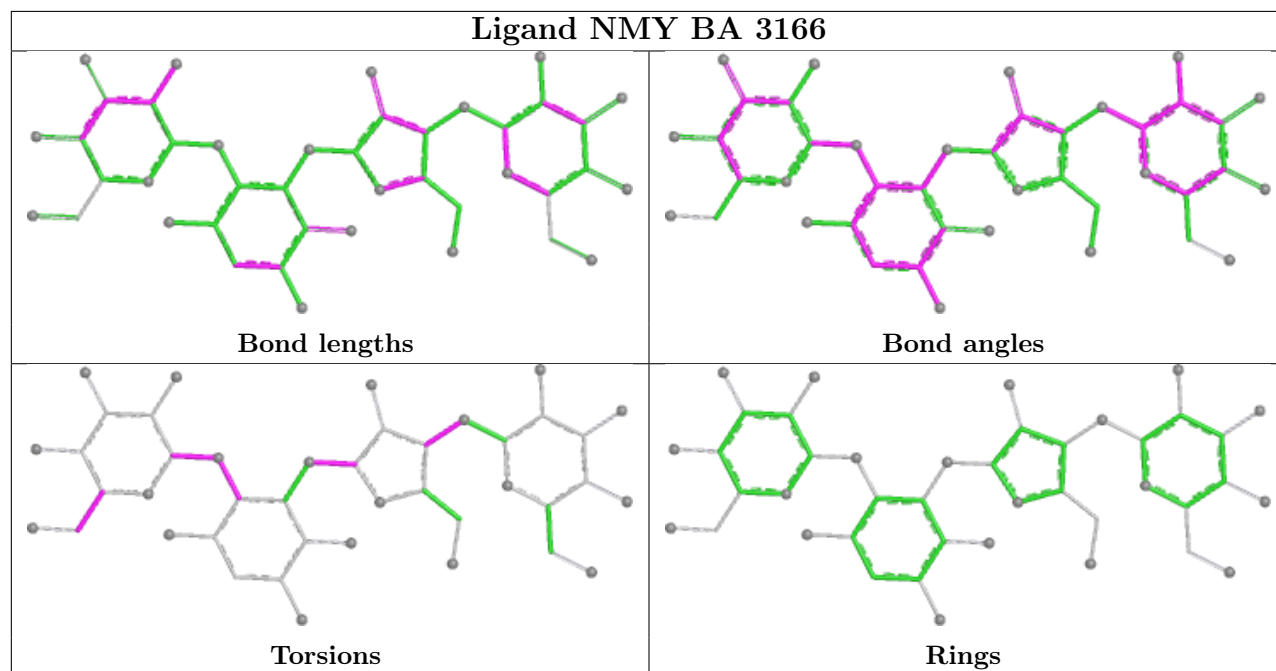
Ligand NMY BA 3161



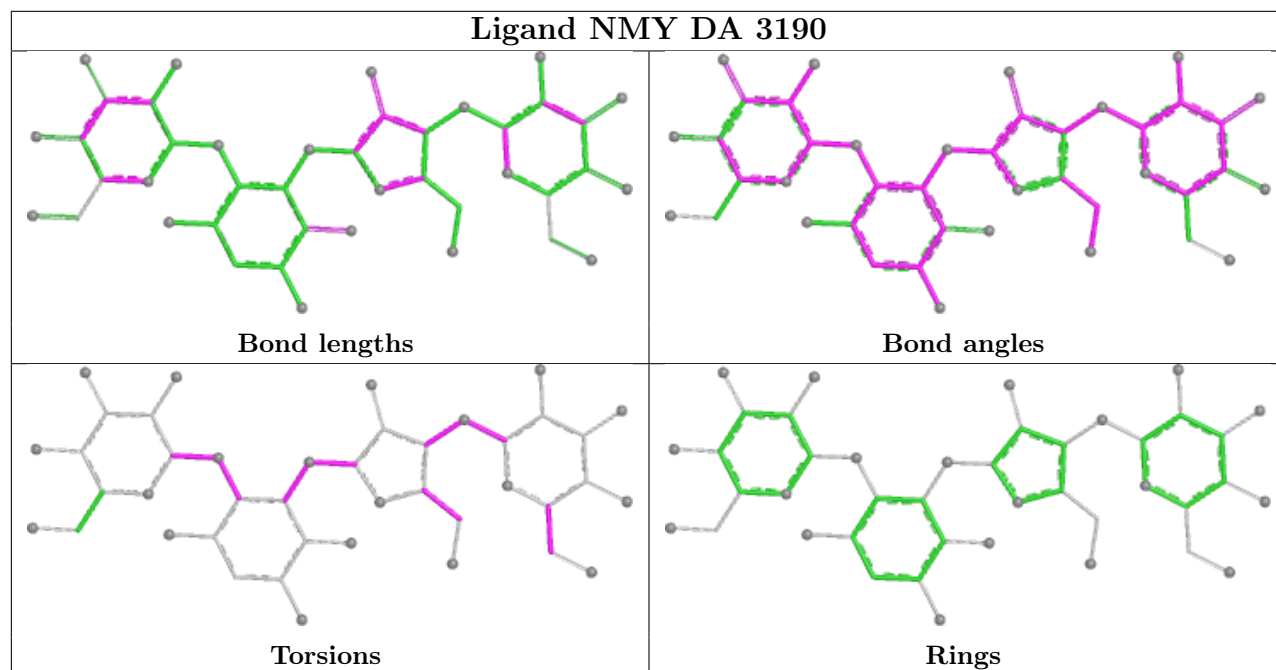
Ligand NMY DA 3187



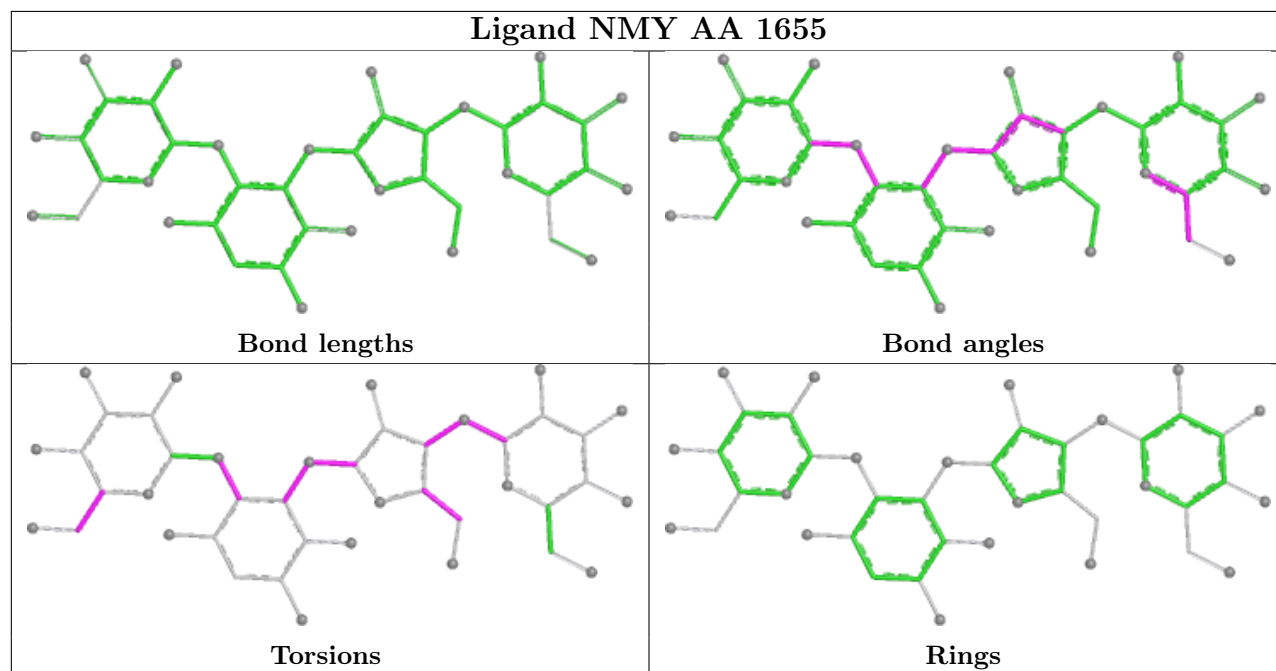
Ligand NMY BA 3166



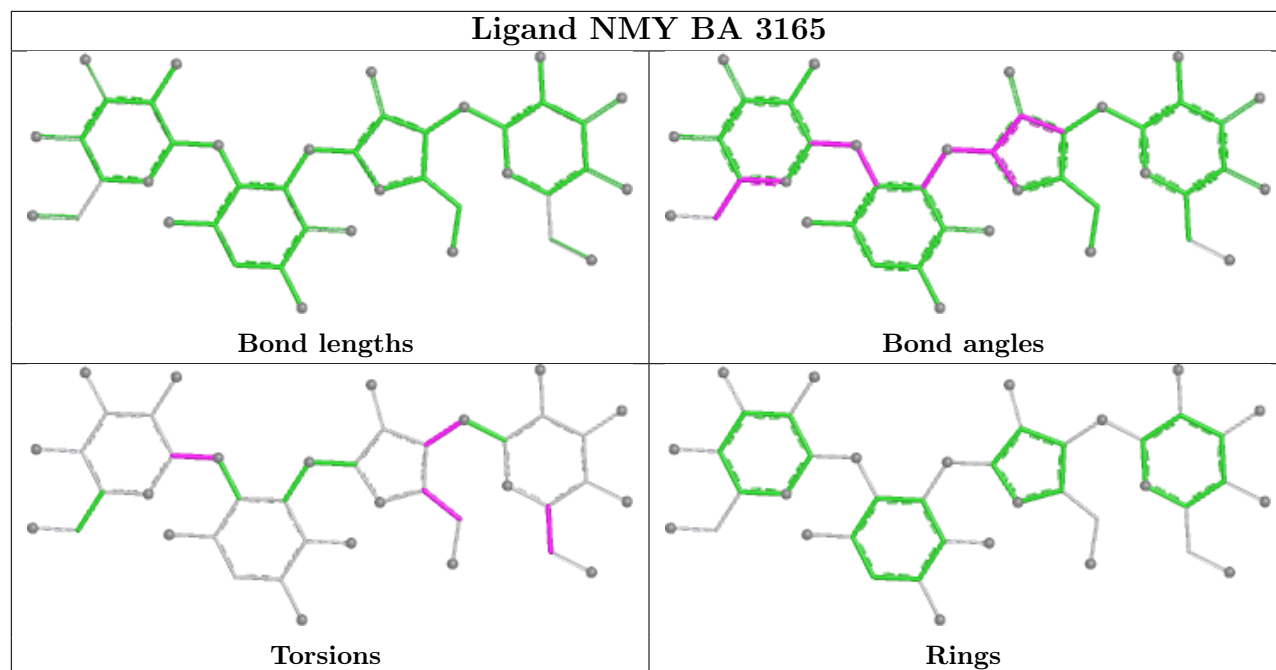
Ligand NMY DA 3190



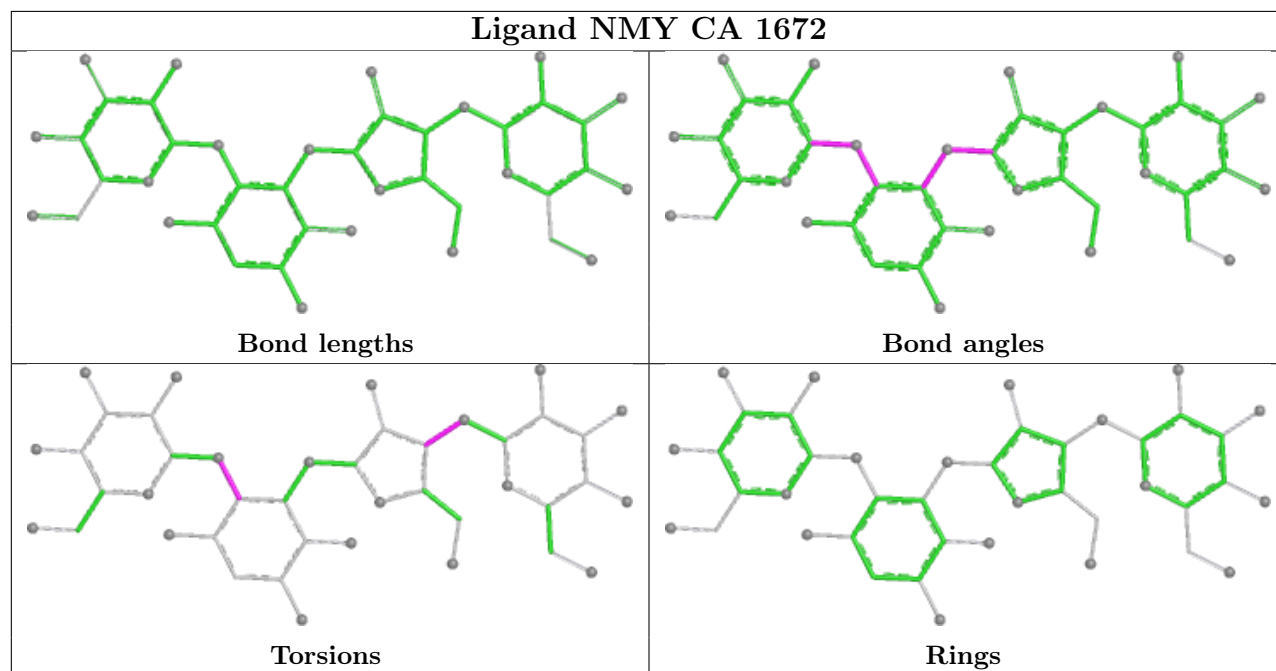
Ligand NMY AA 1655



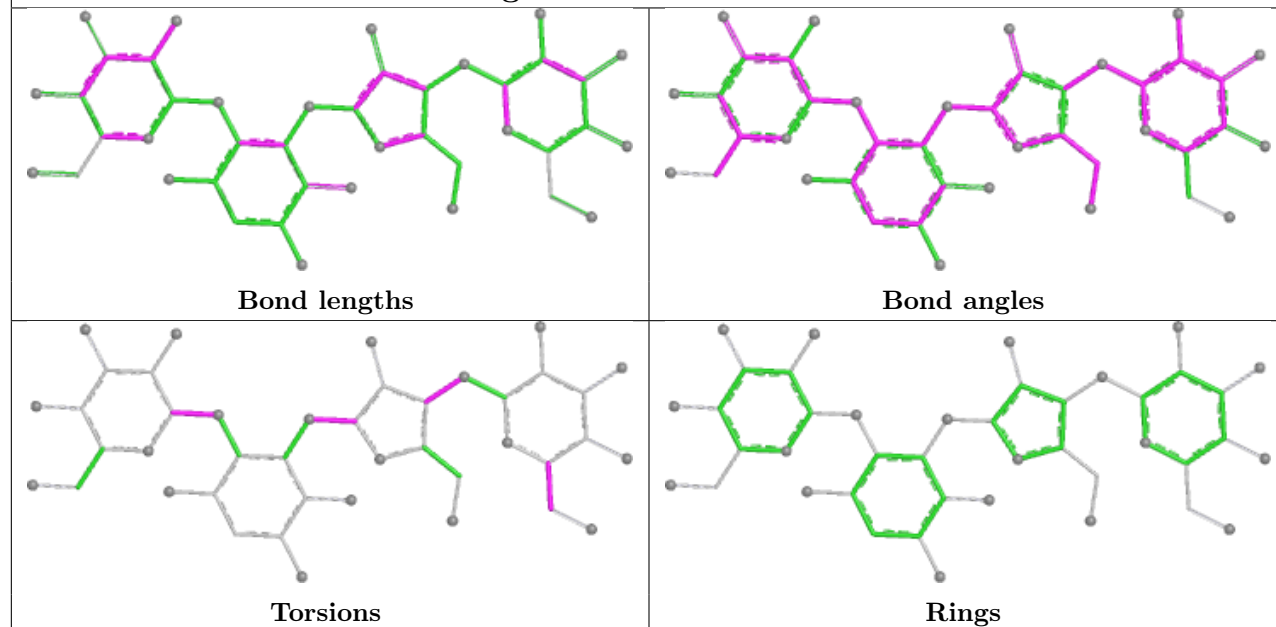
Ligand NMY BA 3165



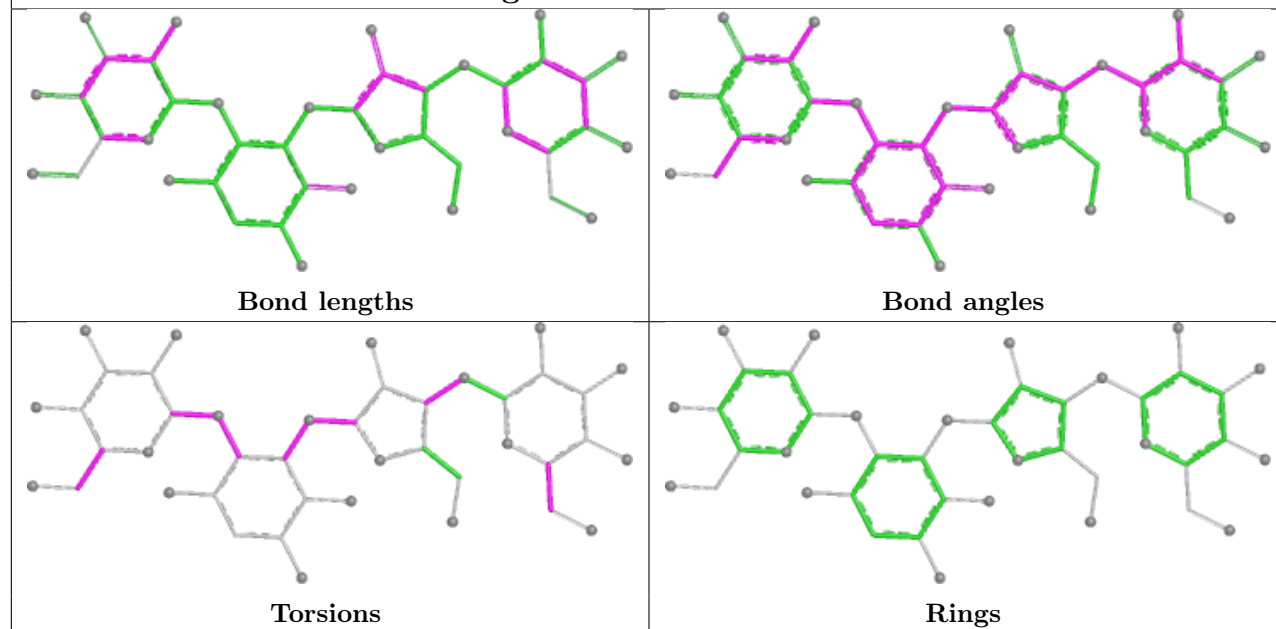
Ligand NMY CA 1672



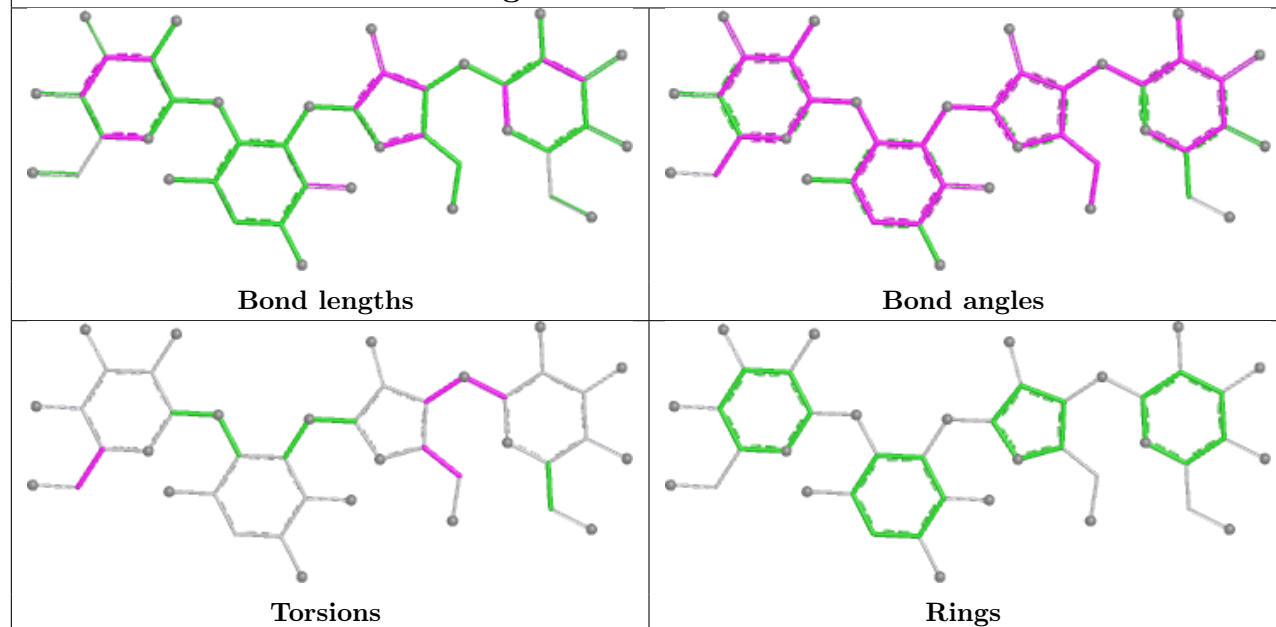
Ligand NMY DA 3189



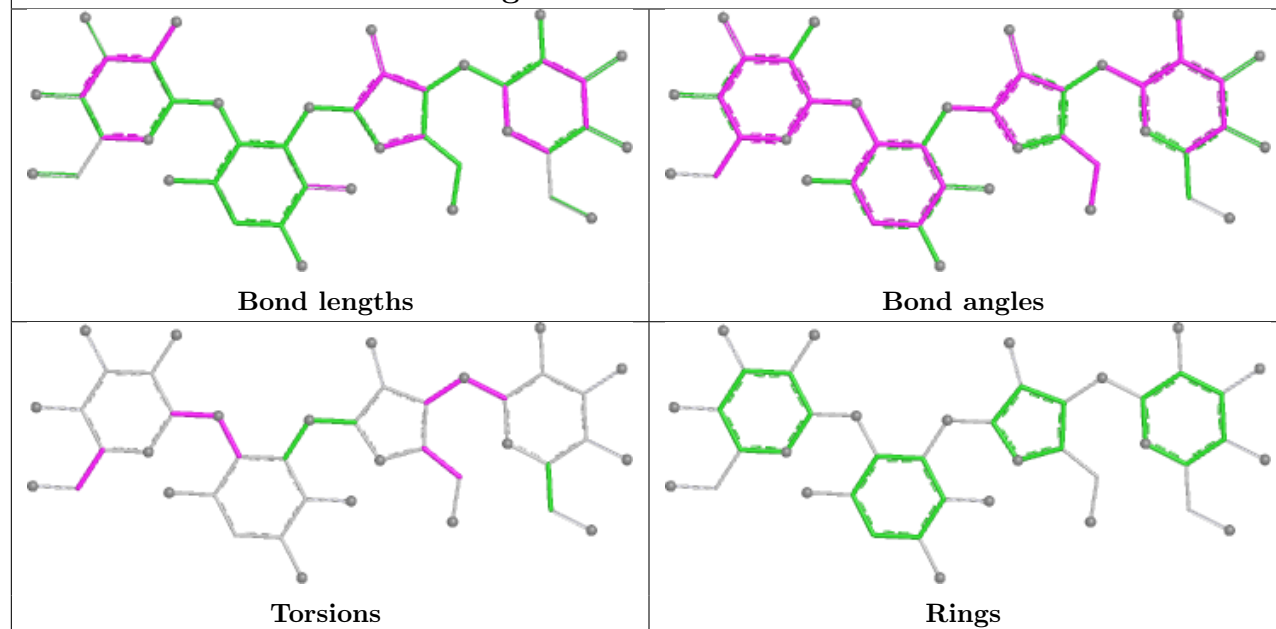
Ligand NMY DA 3186



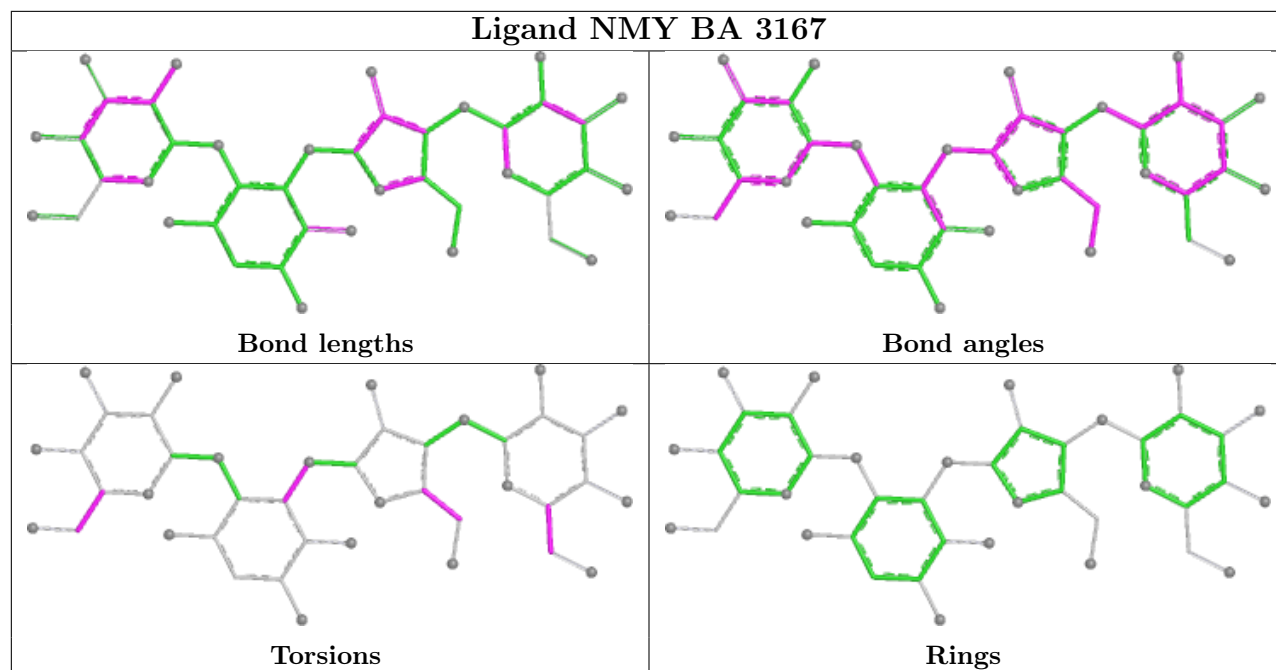
Ligand NMY BA 3163



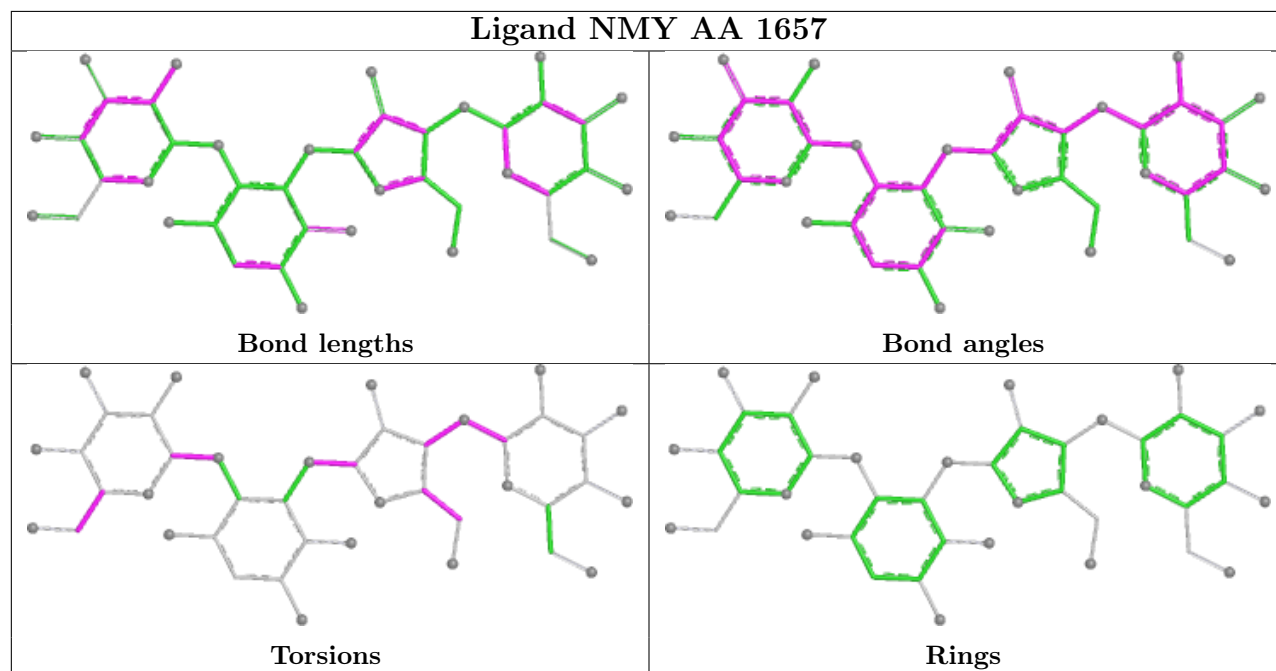
Ligand NMY DA 3188



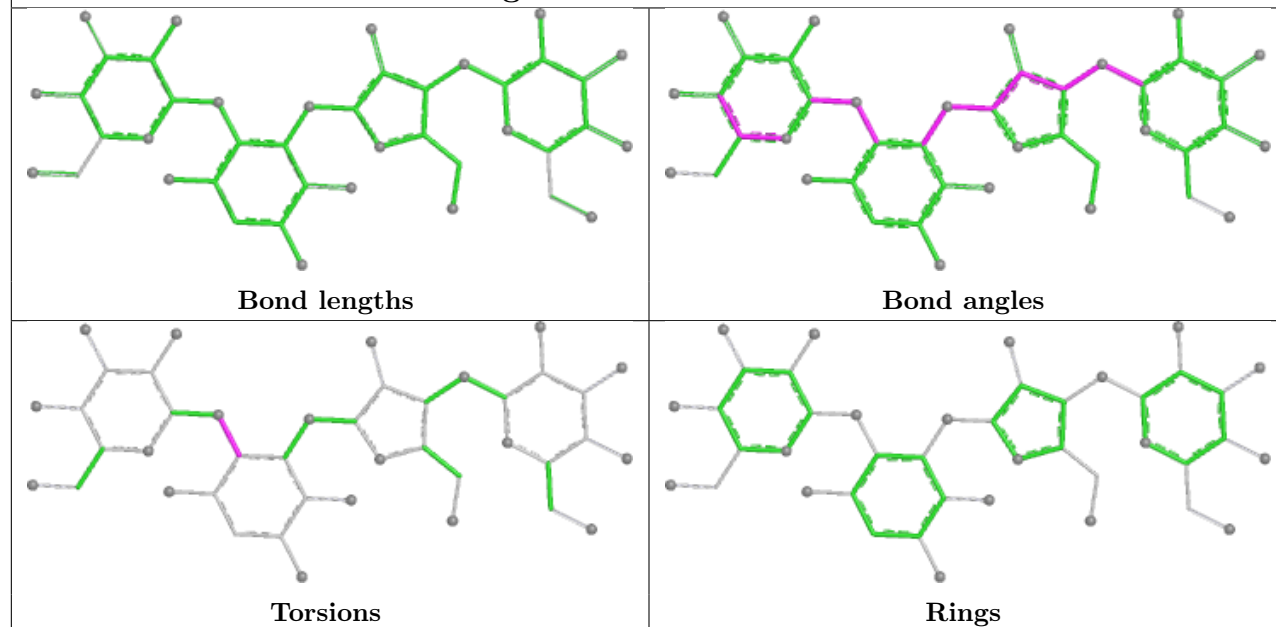
Ligand NMY BA 3167



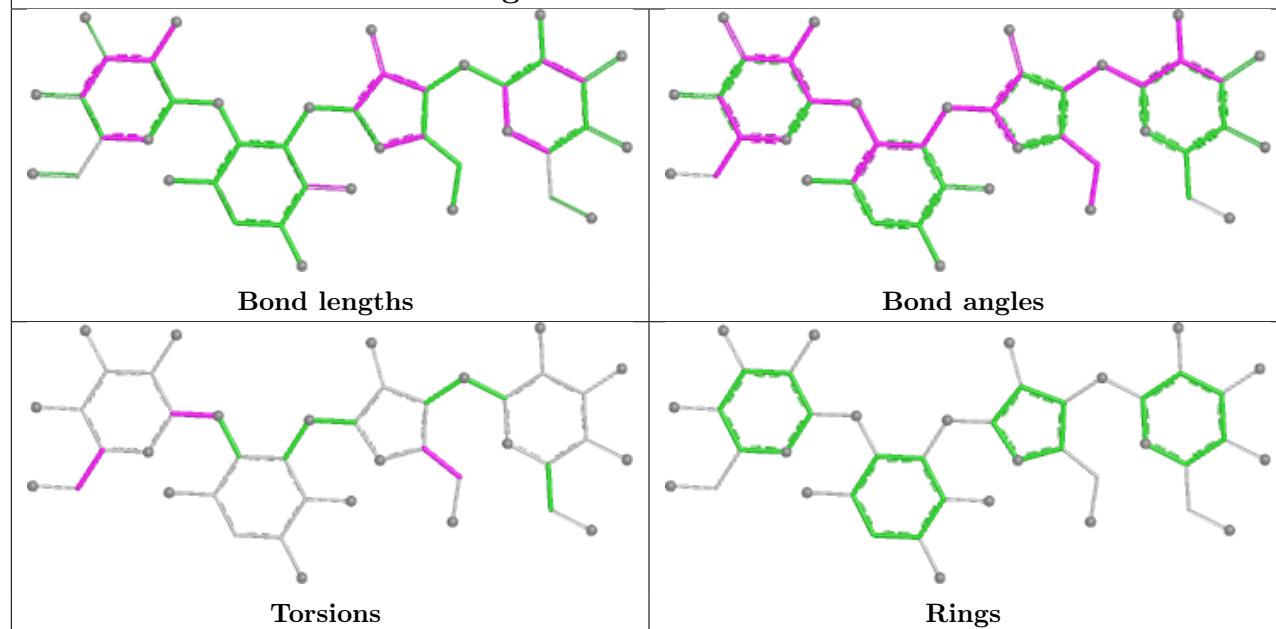
Ligand NMY AA 1657

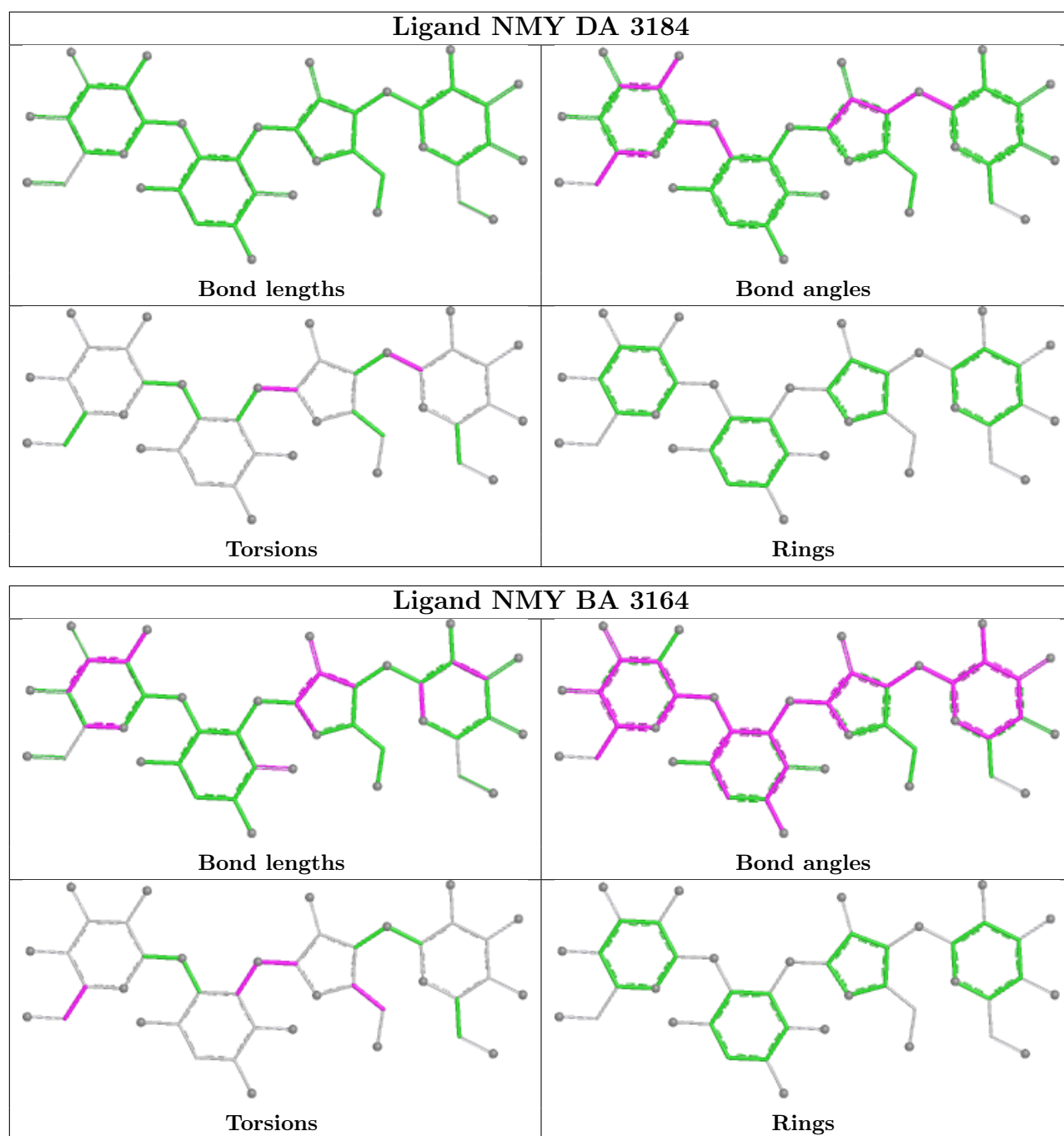


Ligand NMY BA 3162



Ligand NMY DA 3185





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	1539/1542 (99%)	-0.55	2 (0%) 92 90	67, 121, 207, 543	0
1	CA	1538/1542 (99%)	-0.57	10 (0%) 84 70	63, 120, 240, 527	0
2	AB	218/241 (90%)	0.36	13 (5%) 27 19	86, 172, 404, 542	0
2	CB	218/241 (90%)	0.26	10 (4%) 37 25	96, 215, 508, 545	0
3	AC	206/233 (88%)	0.38	16 (7%) 19 14	81, 139, 325, 514	0
3	CC	206/233 (88%)	-0.01	8 (3%) 43 29	80, 120, 286, 513	0
4	AD	205/206 (99%)	1.38	52 (25%) 1 1	83, 161, 372, 537	0
4	CD	205/206 (99%)	1.14	39 (19%) 3 3	81, 148, 442, 537	0
5	AE	150/167 (89%)	0.50	14 (9%) 14 11	79, 130, 272, 478	0
5	CE	150/167 (89%)	0.57	18 (12%) 9 7	68, 114, 292, 527	0
6	AF	100/135 (74%)	-0.04	3 (3%) 52 35	85, 142, 331, 528	0
6	CF	100/135 (74%)	0.52	8 (8%) 18 14	87, 178, 386, 531	0
7	AG	151/179 (84%)	0.44	15 (9%) 13 10	93, 161, 365, 539	0
7	CG	151/179 (84%)	0.99	29 (19%) 3 3	112, 234, 452, 540	0
8	AH	129/130 (99%)	0.45	13 (10%) 12 10	79, 145, 341, 424	0
8	CH	129/130 (99%)	0.50	7 (5%) 31 21	81, 121, 307, 437	0
9	AI	127/130 (97%)	1.01	22 (17%) 4 4	101, 180, 459, 535	0
9	CI	127/130 (97%)	1.09	30 (23%) 2 1	97, 216, 478, 540	0
10	AJ	98/103 (95%)	0.65	9 (9%) 14 11	95, 165, 363, 543	0
10	CJ	98/103 (95%)	1.38	27 (27%) 1 1	101, 202, 530, 543	0
11	AK	117/129 (90%)	0.27	7 (5%) 27 19	75, 112, 337, 492	0
11	CK	117/129 (90%)	0.73	13 (11%) 10 9	83, 243, 494, 531	0
12	AL	123/124 (99%)	0.41	11 (8%) 15 12	75, 109, 299, 403	0
12	CL	123/124 (99%)	0.58	18 (14%) 6 5	62, 93, 294, 386	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/118 (96%)	0.87	17 (14%) 5 5	106, 239, 498, 530	0
13	CM	114/118 (96%)	1.13	24 (21%) 2 2	122, 312, 536, 547	0
14	AN	96/101 (95%)	1.39	20 (20%) 2 2	89, 175, 381, 527	0
14	CN	96/101 (95%)	1.47	28 (29%) 1 1	95, 183, 535, 545	0
15	AO	88/89 (98%)	0.54	9 (10%) 12 10	90, 136, 315, 374	0
15	CO	88/89 (98%)	0.91	13 (14%) 5 5	94, 176, 350, 510	0
16	AP	82/82 (100%)	1.19	21 (25%) 1 1	76, 125, 380, 528	0
16	CP	82/82 (100%)	0.92	12 (14%) 6 5	75, 115, 387, 524	0
17	AQ	80/84 (95%)	0.71	9 (11%) 10 8	88, 162, 370, 434	0
17	CQ	80/84 (95%)	0.44	11 (13%) 6 5	75, 141, 337, 496	0
18	AR	55/75 (73%)	0.23	3 (5%) 30 21	84, 115, 320, 391	0
18	CR	55/75 (73%)	0.40	4 (7%) 21 15	107, 159, 370, 440	0
19	AS	79/92 (85%)	0.81	13 (16%) 4 4	118, 215, 454, 530	0
19	CS	79/92 (85%)	1.02	15 (18%) 3 3	133, 302, 496, 542	0
20	AT	85/87 (97%)	1.22	22 (25%) 1 1	93, 158, 363, 497	0
20	CT	85/87 (97%)	0.90	11 (12%) 7 6	82, 128, 351, 491	0
21	AU	51/71 (71%)	1.25	12 (23%) 2 2	83, 133, 326, 395	0
21	CU	51/71 (71%)	1.42	13 (25%) 1 1	108, 193, 374, 512	0
22	AV	76/76 (100%)	-0.84	0 100 100	63, 117, 160, 255	0
22	CV	76/76 (100%)	0.14	8 (10%) 11 9	61, 257, 424, 542	0
23	AX	16/24 (66%)	0.39	1 (6%) 26 17	76, 139, 214, 261	0
23	CX	15/24 (62%)	0.63	2 (13%) 7 6	83, 191, 269, 339	0
24	BA	2897/2904 (99%)	-0.68	5 (0%) 91 86	54, 96, 294, 544	0
24	DA	2897/2904 (99%)	-0.72	44 (1%) 72 53	37, 67, 231, 547	0
25	BB	118/120 (98%)	-0.80	0 100 100	78, 151, 201, 231	0
25	DB	119/120 (99%)	-0.92	0 100 100	47, 88, 129, 188	0
26	BC	271/273 (99%)	0.56	33 (12%) 8 7	56, 106, 196, 362	0
26	DC	271/273 (99%)	0.33	23 (8%) 16 13	46, 81, 188, 348	0
27	BD	209/209 (100%)	0.10	7 (3%) 49 33	58, 88, 195, 401	0
27	DD	209/209 (100%)	-0.06	6 (2%) 53 35	38, 57, 129, 253	0
28	BE	201/201 (100%)	-0.04	3 (1%) 72 53	59, 105, 224, 424	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	201/201 (100%)	-0.22	2 (0%) 79 63	40, 72, 155, 487	0
29	BF	177/179 (98%)	0.57	12 (6%) 23 16	125, 257, 446, 539	0
29	DF	177/179 (98%)	0.66	22 (12%) 8 6	76, 147, 367, 520	0
30	BG	176/177 (99%)	0.08	4 (2%) 61 42	93, 155, 360, 507	0
30	DG	176/177 (99%)	0.15	13 (7%) 20 15	54, 94, 190, 439	0
31	BH	149/149 (100%)	0.57	19 (12%) 7 6	15, 223, 436, 532	0
31	DH	149/149 (100%)	0.76	21 (14%) 6 5	25, 213, 475, 538	0
32	BI	141/142 (99%)	0.95	16 (11%) 10 8	126, 471, 546, 549	0
32	DI	141/142 (99%)	1.09	24 (17%) 4 4	123, 380, 542, 548	0
33	BJ	142/142 (100%)	0.08	6 (4%) 40 26	56, 83, 169, 348	0
33	DJ	142/142 (100%)	-0.06	7 (4%) 35 23	38, 60, 146, 265	0
34	BK	122/123 (99%)	-0.04	3 (2%) 58 39	65, 93, 197, 357	0
34	DK	122/123 (99%)	-0.23	0 100 100	43, 63, 112, 229	0
35	BL	143/144 (99%)	0.30	10 (6%) 22 15	55, 110, 265, 507	0
35	DL	143/144 (99%)	0.22	7 (4%) 35 23	41, 68, 170, 291	0
36	BM	136/136 (100%)	0.05	4 (2%) 53 35	65, 99, 208, 340	0
36	DM	136/136 (100%)	-0.02	5 (3%) 45 31	47, 67, 153, 262	0
37	BN	120/127 (94%)	0.05	5 (4%) 40 26	66, 107, 190, 466	0
37	DN	120/127 (94%)	0.07	4 (3%) 49 33	40, 61, 151, 420	0
38	BO	116/117 (99%)	0.56	13 (11%) 10 9	96, 193, 363, 537	0
38	DO	116/117 (99%)	-0.14	0 100 100	66, 94, 183, 322	0
39	BP	114/115 (99%)	0.23	7 (6%) 27 18	71, 109, 288, 356	0
39	DP	114/115 (99%)	0.01	5 (4%) 39 25	47, 69, 178, 330	0
40	BQ	117/118 (99%)	0.07	5 (4%) 40 25	55, 76, 170, 304	0
40	DQ	117/118 (99%)	-0.01	4 (3%) 48 32	38, 54, 156, 310	0
41	BR	103/103 (100%)	0.18	3 (2%) 53 35	57, 92, 180, 286	0
41	DR	103/103 (100%)	-0.06	4 (3%) 43 29	42, 68, 152, 458	0
42	BS	110/110 (100%)	0.07	6 (5%) 30 21	60, 92, 175, 299	0
42	DS	110/110 (100%)	-0.12	1 (0%) 81 65	38, 56, 115, 161	0
43	BT	93/100 (93%)	0.86	14 (15%) 5 5	93, 155, 337, 441	0
43	DT	93/100 (93%)	0.32	8 (8%) 16 12	56, 90, 192, 530	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BU	102/104 (98%)	0.61	14 (13%) 6 5	78, 133, 337, 443	0
44	DU	102/104 (98%)	0.19	7 (6%) 23 16	52, 82, 226, 299	0
45	BV	94/94 (100%)	-0.02	4 (4%) 40 25	86, 144, 310, 421	0
45	DV	94/94 (100%)	0.11	3 (3%) 50 34	60, 94, 183, 336	0
46	BW	75/85 (88%)	0.64	5 (6%) 24 16	70, 113, 202, 321	0
46	DW	76/85 (89%)	0.46	8 (10%) 11 9	46, 70, 156, 244	0
47	BX	77/78 (98%)	0.69	12 (15%) 5 4	62, 110, 268, 318	0
47	DX	77/78 (98%)	-0.08	2 (2%) 57 38	48, 83, 165, 320	0
48	BY	63/63 (100%)	0.05	2 (3%) 50 34	95, 176, 353, 521	0
48	DY	63/63 (100%)	0.19	5 (7%) 18 14	58, 106, 283, 388	0
49	BZ	58/59 (98%)	-0.08	2 (3%) 48 32	67, 93, 170, 515	0
49	DZ	58/59 (98%)	0.14	1 (1%) 69 50	44, 59, 141, 198	0
50	B0	56/57 (98%)	0.11	4 (7%) 22 15	59, 98, 294, 405	0
50	D0	56/57 (98%)	0.43	4 (7%) 22 15	33, 64, 166, 282	0
51	B1	50/55 (90%)	0.49	6 (12%) 9 7	88, 147, 326, 377	0
51	D1	50/55 (90%)	0.38	6 (12%) 9 7	78, 120, 326, 532	0
52	B2	46/46 (100%)	0.59	5 (10%) 10 9	70, 95, 239, 293	0
52	D2	46/46 (100%)	0.71	6 (13%) 7 6	54, 67, 171, 292	0
53	B3	64/65 (98%)	0.60	8 (12%) 8 6	67, 91, 201, 286	0
53	D3	64/65 (98%)	0.59	8 (12%) 8 6	47, 61, 161, 254	0
54	B4	38/38 (100%)	0.68	4 (10%) 11 9	78, 108, 174, 322	0
54	D4	38/38 (100%)	-0.02	1 (2%) 57 38	53, 67, 150, 295	0
55	CY	183/185 (98%)	0.30	11 (6%) 27 19	53, 148, 442, 539	0
All	All	20909/21487 (97%)	-0.04	1165 (5%) 30 20	15, 110, 357, 549	0

The worst 5 of 1165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	AD	24	GLY	14.3
4	CD	76	TYR	10.5
12	CL	15	LYS	10.4
9	CI	125	PRO	10.3
12	CL	25	GLU	9.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1654	1/1	-0.26	0.23	110,110,110,110	0
56	MG	BA	3159	1/1	-0.19	0.36	109,109,109,109	0
56	MG	DB	204	1/1	-0.07	0.36	109,109,109,109	0
56	MG	CA	1636	1/1	-0.05	0.19	134,134,134,134	0
56	MG	CA	1657	1/1	0.01	0.22	119,119,119,119	0
56	MG	DA	3095	1/1	0.06	0.58	116,116,116,116	0
56	MG	BA	3054	1/1	0.15	0.39	119,119,119,119	0
56	MG	CA	1652	1/1	0.16	0.25	106,106,106,106	0
56	MG	DA	3018	1/1	0.18	0.39	102,102,102,102	0
56	MG	AA	1623	1/1	0.19	0.38	119,119,119,119	0
56	MG	DA	3151	1/1	0.25	0.31	101,101,101,101	0
56	MG	CA	1637	1/1	0.25	0.36	139,139,139,139	0
56	MG	BA	3012	1/1	0.26	0.37	118,118,118,118	0
56	MG	AA	1631	1/1	0.27	0.28	126,126,126,126	0
56	MG	BA	3096	1/1	0.28	0.30	118,118,118,118	0
56	MG	AA	1640	1/1	0.29	0.26	110,110,110,110	0
56	MG	DB	202	1/1	0.30	0.32	122,122,122,122	0
56	MG	BA	3059	1/1	0.31	0.60	122,122,122,122	0
56	MG	AA	1633	1/1	0.33	0.23	128,128,128,128	0
56	MG	DA	3076	1/1	0.33	0.18	100,100,100,100	0
56	MG	BA	3026	1/1	0.33	0.28	134,134,134,134	0
56	MG	CA	1660	1/1	0.35	0.18	104,104,104,104	0
56	MG	BA	3007	1/1	0.36	0.29	127,127,127,127	0
56	MG	AA	1648	1/1	0.36	0.15	116,116,116,116	0
56	MG	AA	1646	1/1	0.37	0.23	95,95,95,95	0
56	MG	DA	3081	1/1	0.37	0.40	110,110,110,110	0
56	MG	BA	3168	1/1	0.37	0.34	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3027	1/1	0.38	0.44	108,108,108,108	0
56	MG	DA	3087	1/1	0.38	0.21	113,113,113,113	0
56	MG	BA	3142	1/1	0.40	0.25	103,103,103,103	0
56	MG	BA	3022	1/1	0.40	0.26	110,110,110,110	0
56	MG	CA	1601	1/1	0.41	0.17	140,140,140,140	0
56	MG	CA	1632	1/1	0.42	0.38	128,128,128,128	0
56	MG	DA	3134	1/1	0.44	0.25	77,77,77,77	0
56	MG	DA	3129	1/1	0.45	0.47	124,124,124,124	0
56	MG	CA	1656	1/1	0.45	0.25	106,106,106,106	0
56	MG	AN	201	1/1	0.45	0.27	133,133,133,133	0
56	MG	CA	1629	1/1	0.45	0.42	123,123,123,123	0
56	MG	AA	1639	1/1	0.45	0.40	113,113,113,113	0
56	MG	CA	1647	1/1	0.46	0.12	112,112,112,112	0
56	MG	AA	1653	1/1	0.46	0.17	106,106,106,106	0
56	MG	DA	3068	1/1	0.46	0.30	117,117,117,117	0
56	MG	BA	3066	1/1	0.47	0.21	96,96,96,96	0
56	MG	DA	3161	1/1	0.47	0.18	103,103,103,103	0
56	MG	DO	201	1/1	0.47	0.39	109,109,109,109	0
56	MG	CX	101	1/1	0.48	0.14	112,112,112,112	0
56	MG	BA	3152	1/1	0.48	0.41	115,115,115,115	0
56	MG	AA	1625	1/1	0.49	0.29	117,117,117,117	0
56	MG	BA	3125	1/1	0.49	0.26	100,100,100,100	0
56	MG	DA	3179	1/1	0.50	0.26	113,113,113,113	0
56	MG	BB	202	1/1	0.51	0.33	123,123,123,123	0
56	MG	DA	3055	1/1	0.51	0.23	94,94,94,94	0
56	MG	CA	1653	1/1	0.51	0.14	99,99,99,99	0
56	MG	AA	1608	1/1	0.52	0.26	114,114,114,114	0
56	MG	BA	3018	1/1	0.52	0.32	118,118,118,118	0
56	MG	CA	1631	1/1	0.52	0.23	120,120,120,120	0
56	MG	AA	1617	1/1	0.52	0.19	112,112,112,112	0
56	MG	CA	1607	1/1	0.53	0.29	110,110,110,110	0
56	MG	AD	301	1/1	0.53	0.28	119,119,119,119	0
56	MG	DA	3174	1/1	0.54	0.18	105,105,105,105	0
56	MG	DA	3013	1/1	0.54	0.35	107,107,107,107	0
56	MG	DA	3192	1/1	0.54	0.26	95,95,95,95	0
56	MG	CA	1665	1/1	0.54	0.11	112,112,112,112	0
56	MG	BA	3110	1/1	0.54	0.23	110,110,110,110	0
56	MG	DA	3162	1/1	0.54	0.25	95,95,95,95	0
56	MG	AA	1641	1/1	0.55	0.21	105,105,105,105	0
56	MG	DA	3057	1/1	0.55	0.41	114,114,114,114	0
56	MG	AA	1650	1/1	0.55	0.19	118,118,118,118	0
56	MG	BA	3081	1/1	0.56	0.21	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3079	1/1	0.56	0.30	99,99,99,99	0
56	MG	BA	3087	1/1	0.56	0.28	112,112,112,112	0
56	MG	BA	3030	1/1	0.56	0.20	94,94,94,94	0
56	MG	DA	3131	1/1	0.57	0.35	118,118,118,118	0
56	MG	BA	3090	1/1	0.57	0.34	130,130,130,130	0
56	MG	BC	301	1/1	0.57	0.32	122,122,122,122	0
56	MG	DA	3152	1/1	0.57	0.22	105,105,105,105	0
56	MG	BA	3160	1/1	0.58	0.23	102,102,102,102	0
56	MG	CA	1659	1/1	0.58	0.20	110,110,110,110	0
56	MG	BA	3157	1/1	0.58	0.44	97,97,97,97	0
56	MG	DA	3042	1/1	0.58	0.27	105,105,105,105	0
56	MG	BA	3141	1/1	0.58	0.13	114,114,114,114	0
56	MG	DA	3025	1/1	0.59	0.30	118,118,118,118	0
56	MG	AA	1627	1/1	0.59	0.25	121,121,121,121	0
56	MG	BA	3058	1/1	0.59	0.28	108,108,108,108	0
56	MG	BA	3107	1/1	0.59	0.21	106,106,106,106	0
56	MG	DA	3065	1/1	0.59	0.19	81,81,81,81	0
56	MG	BA	3053	1/1	0.59	0.25	98,98,98,98	0
56	MG	CA	1638	1/1	0.60	0.31	113,113,113,113	0
56	MG	AA	1628	1/1	0.60	0.22	116,116,116,116	0
56	MG	BA	3148	1/1	0.60	0.23	101,101,101,101	0
56	MG	DA	3150	1/1	0.61	0.42	78,78,78,78	0
56	MG	BA	3019	1/1	0.61	0.18	101,101,101,101	0
56	MG	BA	3144	1/1	0.61	0.31	87,87,87,87	0
56	MG	DA	3194	1/1	0.61	0.29	90,90,90,90	0
56	MG	AA	1614	1/1	0.61	0.32	123,123,123,123	0
56	MG	CA	1633	1/1	0.61	0.34	116,116,116,116	0
56	MG	DA	3172	1/1	0.61	0.21	109,109,109,109	0
56	MG	DA	3100	1/1	0.62	0.20	96,96,96,96	0
56	MG	CA	1602	1/1	0.62	0.18	105,105,105,105	0
56	MG	DA	3083	1/1	0.62	0.21	82,82,82,82	0
56	MG	CA	1644	1/1	0.62	0.31	118,118,118,118	0
56	MG	DA	3146	1/1	0.62	0.29	76,76,76,76	0
56	MG	CA	1609	1/1	0.62	0.28	117,117,117,117	0
56	MG	AA	1626	1/1	0.63	0.22	111,111,111,111	0
56	MG	BA	3077	1/1	0.63	0.22	121,121,121,121	0
56	MG	BA	3014	1/1	0.63	0.31	106,106,106,106	0
56	MG	BA	3099	1/1	0.63	0.22	112,112,112,112	0
56	MG	BA	3102	1/1	0.63	0.22	119,119,119,119	0
56	MG	CA	1643	1/1	0.63	0.22	103,103,103,103	0
56	MG	BA	3013	1/1	0.64	0.26	114,114,114,114	0
56	MG	CA	1603	1/1	0.64	0.16	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3032	1/1	0.64	0.32	110,110,110,110	0
56	MG	DA	3015	1/1	0.64	0.35	124,124,124,124	0
56	MG	BA	3044	1/1	0.64	0.28	114,114,114,114	0
56	MG	BA	3131	1/1	0.65	0.29	114,114,114,114	0
56	MG	CA	1649	1/1	0.65	0.11	107,107,107,107	0
56	MG	DA	3102	1/1	0.65	0.25	94,94,94,94	0
56	MG	AA	1629	1/1	0.65	0.27	118,118,118,118	0
56	MG	CA	1608	1/1	0.66	0.21	115,115,115,115	0
56	MG	DA	3077	1/1	0.66	0.22	98,98,98,98	0
56	MG	BA	3092	1/1	0.66	0.16	119,119,119,119	0
56	MG	DA	3176	1/1	0.66	0.36	78,78,78,78	0
56	MG	DA	3105	1/1	0.66	0.20	90,90,90,90	0
56	MG	DA	3052	1/1	0.67	0.25	95,95,95,95	0
56	MG	DA	3028	1/1	0.67	0.20	85,85,85,85	0
56	MG	DA	3023	1/1	0.67	0.26	120,120,120,120	0
56	MG	DA	3026	1/1	0.68	0.34	98,98,98,98	0
56	MG	CA	1634	1/1	0.68	0.18	120,120,120,120	0
56	MG	CA	1617	1/1	0.68	0.20	115,115,115,115	0
56	MG	DA	3097	1/1	0.68	0.28	105,105,105,105	0
56	MG	CA	1628	1/1	0.68	0.18	116,116,116,116	0
56	MG	BA	3071	1/1	0.69	0.17	104,104,104,104	0
56	MG	DA	3011	1/1	0.69	0.23	103,103,103,103	0
56	MG	BA	3136	1/1	0.69	0.37	94,94,94,94	0
56	MG	BA	3123	1/1	0.69	0.20	88,88,88,88	0
56	MG	AA	1630	1/1	0.69	0.20	105,105,105,105	0
56	MG	DA	3137	1/1	0.69	0.27	93,93,93,93	0
56	MG	CA	1627	1/1	0.69	0.21	111,111,111,111	0
56	MG	CA	1670	1/1	0.70	0.35	102,102,102,102	0
56	MG	BA	3062	1/1	0.70	0.23	91,91,91,91	0
56	MG	CA	1651	1/1	0.70	0.28	103,103,103,103	0
56	MG	CA	1623	1/1	0.70	0.33	117,117,117,117	0
56	MG	CA	1624	1/1	0.70	0.15	106,106,106,106	0
56	MG	DA	3108	1/1	0.70	0.17	100,100,100,100	0
56	MG	BA	3009	1/1	0.70	0.15	95,95,95,95	0
56	MG	BA	3070	1/1	0.70	0.19	90,90,90,90	0
56	MG	AA	1610	1/1	0.70	0.19	120,120,120,120	0
56	MG	BA	3130	1/1	0.70	0.23	103,103,103,103	0
56	MG	DA	3142	1/1	0.70	0.20	86,86,86,86	0
56	MG	BA	3105	1/1	0.70	0.18	91,91,91,91	0
56	MG	CA	1667	1/1	0.70	0.21	111,111,111,111	0
56	MG	BA	3122	1/1	0.71	0.26	112,112,112,112	0
56	MG	BA	3075	1/1	0.71	0.18	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3037	1/1	0.71	0.46	97,97,97,97	0
56	MG	DA	3183	1/1	0.71	0.26	87,87,87,87	0
56	MG	BA	3015	1/1	0.71	0.17	115,115,115,115	0
56	MG	AA	1634	1/1	0.71	0.28	120,120,120,120	0
56	MG	AA	1649	1/1	0.71	0.32	90,90,90,90	0
56	MG	AA	1636	1/1	0.71	0.16	103,103,103,103	0
56	MG	CA	1668	1/1	0.71	0.14	107,107,107,107	0
56	MG	DA	3111	1/1	0.72	0.14	102,102,102,102	0
56	MG	BA	3078	1/1	0.72	0.15	119,119,119,119	0
56	MG	DA	3169	1/1	0.72	0.22	94,94,94,94	0
56	MG	DA	3084	1/1	0.72	0.17	104,104,104,104	0
56	MG	DA	3061	1/1	0.72	0.35	106,106,106,106	0
56	MG	BA	3079	1/1	0.72	0.25	103,103,103,103	0
56	MG	BA	3023	1/1	0.72	0.22	108,108,108,108	0
56	MG	BA	3069	1/1	0.72	0.17	129,129,129,129	0
56	MG	DA	3149	1/1	0.72	0.25	107,107,107,107	0
56	MG	DA	3044	1/1	0.72	0.24	105,105,105,105	0
56	MG	AA	1622	1/1	0.72	0.19	107,107,107,107	0
56	MG	BA	3126	1/1	0.72	0.15	110,110,110,110	0
56	MG	DA	3155	1/1	0.72	0.34	115,115,115,115	0
56	MG	CA	1645	1/1	0.73	0.23	96,96,96,96	0
56	MG	DA	3115	1/1	0.73	0.15	95,95,95,95	0
56	MG	AA	1602	1/1	0.73	0.16	106,106,106,106	0
56	MG	BA	3033	1/1	0.73	0.26	98,98,98,98	0
56	MG	AA	1616	1/1	0.73	0.26	113,113,113,113	0
56	MG	BA	3040	1/1	0.73	0.15	112,112,112,112	0
56	MG	BA	3025	1/1	0.73	0.24	103,103,103,103	0
56	MG	DA	3182	1/1	0.73	0.37	96,96,96,96	0
56	MG	CA	1655	1/1	0.73	0.20	117,117,117,117	0
56	MG	BA	3124	1/1	0.73	0.11	114,114,114,114	0
56	MG	BA	3065	1/1	0.73	0.19	101,101,101,101	0
56	MG	BA	3050	1/1	0.73	0.28	101,101,101,101	0
56	MG	DA	3072	1/1	0.73	0.23	93,93,93,93	0
56	MG	BA	3155	1/1	0.73	0.48	114,114,114,114	0
56	MG	DA	3113	1/1	0.74	0.18	106,106,106,106	0
56	MG	CA	1626	1/1	0.74	0.18	99,99,99,99	0
56	MG	AA	1638	1/1	0.74	0.28	104,104,104,104	0
56	MG	BA	3156	1/1	0.75	0.17	106,106,106,106	0
56	MG	BA	3083	1/1	0.75	0.17	110,110,110,110	0
56	MG	CA	1650	1/1	0.75	0.32	102,102,102,102	0
56	MG	BA	3021	1/1	0.75	0.12	108,108,108,108	0
56	MG	DA	3139	1/1	0.75	0.26	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3039	1/1	0.75	0.17	117,117,117,117	0
56	MG	DA	3103	1/1	0.75	0.19	81,81,81,81	0
56	MG	DA	3004	1/1	0.75	0.16	99,99,99,99	0
56	MG	BA	3153	1/1	0.75	0.25	112,112,112,112	0
56	MG	DA	3109	1/1	0.75	0.16	102,102,102,102	0
56	MG	DB	201	1/1	0.75	0.13	113,113,113,113	0
56	MG	CA	1661	1/1	0.75	0.26	101,101,101,101	0
56	MG	CA	1664	1/1	0.75	0.14	112,112,112,112	0
56	MG	BA	3138	1/1	0.75	0.25	88,88,88,88	0
56	MG	DA	3092	1/1	0.76	0.16	95,95,95,95	0
56	MG	DA	3164	1/1	0.76	0.33	94,94,94,94	0
56	MG	AA	1652	1/1	0.76	0.21	101,101,101,101	0
56	MG	DA	3003	1/1	0.76	0.13	105,105,105,105	0
56	MG	DA	3098	1/1	0.76	0.14	99,99,99,99	0
56	MG	BA	3011	1/1	0.76	0.20	81,81,81,81	0
56	MG	DA	3177	1/1	0.76	0.40	96,96,96,96	0
56	MG	BA	3118	1/1	0.76	0.23	109,109,109,109	0
56	MG	AA	1642	1/1	0.76	0.20	94,94,94,94	0
56	MG	CA	1654	1/1	0.76	0.17	116,116,116,116	0
56	MG	BA	3143	1/1	0.76	0.15	103,103,103,103	0
56	MG	BA	3082	1/1	0.76	0.25	126,126,126,126	0
56	MG	DA	3059	1/1	0.76	0.19	92,92,92,92	0
56	MG	BA	3135	1/1	0.76	0.44	74,74,74,74	0
56	MG	DA	3157	1/1	0.76	0.22	96,96,96,96	0
56	MG	DA	3090	1/1	0.76	0.19	107,107,107,107	0
56	MG	DA	3040	1/1	0.77	0.13	91,91,91,91	0
56	MG	DA	3156	1/1	0.77	0.32	101,101,101,101	0
56	MG	CA	1663	1/1	0.77	0.31	82,82,82,82	0
56	MG	DA	3022	1/1	0.77	0.19	81,81,81,81	0
56	MG	BA	3095	1/1	0.77	0.16	107,107,107,107	0
56	MG	BA	3145	1/1	0.77	0.22	99,99,99,99	0
56	MG	CA	1625	1/1	0.77	0.15	107,107,107,107	0
56	MG	BA	3047	1/1	0.77	0.17	103,103,103,103	0
56	MG	DA	3082	1/1	0.77	0.16	92,92,92,92	0
56	MG	AA	1645	1/1	0.77	0.12	93,93,93,93	0
57	NMY	BA	3164	42/42	0.77	0.15	90,100,104,105	42
56	MG	DA	3060	1/1	0.78	0.22	89,89,89,89	0
56	MG	DA	3123	1/1	0.78	0.13	102,102,102,102	0
56	MG	BA	3072	1/1	0.78	0.17	103,103,103,103	0
56	MG	DA	3180	1/1	0.78	0.19	93,93,93,93	0
56	MG	DA	3101	1/1	0.78	0.20	86,86,86,86	0
56	MG	DA	3064	1/1	0.78	0.17	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3151	1/1	0.78	0.33	92,92,92,92	0
56	MG	CA	1646	1/1	0.78	0.32	95,95,95,95	0
56	MG	BA	3158	1/1	0.78	0.14	106,106,106,106	0
56	MG	BA	3097	1/1	0.78	0.39	111,111,111,111	0
56	MG	DA	3171	1/1	0.78	0.27	108,108,108,108	0
56	MG	DL	201	1/1	0.78	0.64	110,110,110,110	0
56	MG	AA	1621	1/1	0.78	0.19	116,116,116,116	0
56	MG	BA	3100	1/1	0.78	0.20	107,107,107,107	0
57	NMY	DA	3187	42/42	0.78	0.11	106,109,112,114	42
56	MG	BA	3149	1/1	0.79	0.31	85,85,85,85	0
56	MG	DA	3085	1/1	0.79	0.27	108,108,108,108	0
56	MG	BA	3061	1/1	0.79	0.14	85,85,85,85	0
56	MG	DA	3053	1/1	0.79	0.14	93,93,93,93	0
56	MG	DA	3075	1/1	0.79	0.18	106,106,106,106	0
56	MG	BA	3120	1/1	0.79	0.27	94,94,94,94	0
56	MG	AA	1601	1/1	0.79	0.20	132,132,132,132	0
56	MG	BA	3060	1/1	0.79	0.21	106,106,106,106	0
56	MG	BA	3085	1/1	0.79	0.11	95,95,95,95	0
56	MG	BA	3147	1/1	0.79	0.36	95,95,95,95	0
57	NMY	BA	3167	42/42	0.79	0.15	117,120,124,125	42
56	MG	BA	3115	1/1	0.79	0.16	105,105,105,105	0
56	MG	BA	3108	1/1	0.80	0.14	99,99,99,99	0
56	MG	DA	3071	1/1	0.80	0.14	97,97,97,97	0
56	MG	DA	3145	1/1	0.80	0.31	91,91,91,91	0
56	MG	CA	1648	1/1	0.80	0.25	103,103,103,103	0
56	MG	DA	3170	1/1	0.80	0.21	94,94,94,94	0
56	MG	BA	3074	1/1	0.80	0.15	115,115,115,115	0
56	MG	DB	203	1/1	0.80	0.16	100,100,100,100	0
56	MG	BA	3088	1/1	0.80	0.15	101,101,101,101	0
56	MG	DA	3125	1/1	0.80	0.15	113,113,113,113	0
56	MG	AA	1651	1/1	0.80	0.06	119,119,119,119	0
56	MG	DA	3006	1/1	0.80	0.12	92,92,92,92	0
56	MG	DA	3107	1/1	0.80	0.25	98,98,98,98	0
56	MG	AA	1603	1/1	0.80	0.13	117,117,117,117	0
56	MG	DA	3094	1/1	0.81	0.17	87,87,87,87	0
56	MG	DA	3120	1/1	0.81	0.19	98,98,98,98	0
56	MG	BA	3104	1/1	0.81	0.31	106,106,106,106	0
56	MG	BA	3119	1/1	0.81	0.10	106,106,106,106	0
56	MG	DA	3021	1/1	0.81	0.24	108,108,108,108	0
56	MG	AA	1615	1/1	0.81	0.10	112,112,112,112	0
56	MG	BA	3051	1/1	0.81	0.14	106,106,106,106	0
56	MG	BA	3154	1/1	0.81	0.31	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	NMY	DA	3184	42/42	0.81	0.15	57,71,80,89	42
56	MG	DA	3138	1/1	0.81	0.37	81,81,81,81	0
58	ZN	D4	101	1/1	0.81	0.49	162,162,162,162	0
56	MG	BA	3003	1/1	0.82	0.14	115,115,115,115	0
56	MG	DA	3035	1/1	0.82	0.15	94,94,94,94	0
56	MG	BA	3098	1/1	0.82	0.17	100,100,100,100	0
56	MG	CA	1606	1/1	0.82	0.11	99,99,99,99	0
56	MG	DA	3009	1/1	0.82	0.21	102,102,102,102	0
56	MG	DA	3159	1/1	0.82	0.24	90,90,90,90	0
56	MG	AA	1647	1/1	0.82	0.16	109,109,109,109	0
56	MG	DA	3045	1/1	0.82	0.11	95,95,95,95	0
56	MG	BA	3127	1/1	0.82	0.18	95,95,95,95	0
56	MG	DA	3165	1/1	0.82	0.22	78,78,78,78	0
56	MG	BA	3129	1/1	0.82	0.28	107,107,107,107	0
56	MG	CA	1615	1/1	0.82	0.13	112,112,112,112	0
56	MG	BA	3170	1/1	0.82	0.49	88,88,88,88	0
57	NMY	BA	3165	42/42	0.82	0.18	79,84,87,90	42
56	MG	CA	1618	1/1	0.82	0.15	83,83,83,83	0
56	MG	BA	3063	1/1	0.82	0.20	106,106,106,106	0
56	MG	AA	1643	1/1	0.82	0.11	110,110,110,110	0
56	MG	BA	3114	1/1	0.82	0.18	120,120,120,120	0
56	MG	BA	3137	1/1	0.83	0.23	82,82,82,82	0
56	MG	DA	3147	1/1	0.83	0.42	107,107,107,107	0
56	MG	BA	3121	1/1	0.83	0.23	110,110,110,110	0
56	MG	BA	3056	1/1	0.83	0.12	99,99,99,99	0
56	MG	DA	3073	1/1	0.83	0.18	99,99,99,99	0
56	MG	DA	3181	1/1	0.83	0.44	77,77,77,77	0
56	MG	BA	3116	1/1	0.83	0.13	99,99,99,99	0
56	MG	CA	1666	1/1	0.83	0.18	112,112,112,112	0
56	MG	DA	3127	1/1	0.83	0.12	77,77,77,77	0
56	MG	DA	3193	1/1	0.83	0.33	95,95,95,95	0
56	MG	AA	1644	1/1	0.83	0.18	106,106,106,106	0
56	MG	BA	3133	1/1	0.83	0.15	106,106,106,106	0
56	MG	BB	201	1/1	0.83	0.11	137,137,137,137	0
56	MG	DA	3135	1/1	0.83	0.18	71,71,71,71	0
56	MG	DA	3136	1/1	0.83	0.28	74,74,74,74	0
56	MG	CA	1613	1/1	0.83	0.10	103,103,103,103	0
56	MG	DA	3167	1/1	0.83	0.22	84,84,84,84	0
57	NMY	AA	1656	42/42	0.83	0.16	94,99,103,104	42
57	NMY	BA	3162	42/42	0.83	0.15	65,79,86,93	42
56	MG	DA	3168	1/1	0.83	0.15	89,89,89,89	0
56	MG	CA	1630	1/1	0.83	0.11	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3055	1/1	0.83	0.13	101,101,101,101	0
56	MG	BA	3076	1/1	0.83	0.17	120,120,120,120	0
56	MG	DA	3008	1/1	0.83	0.15	88,88,88,88	0
56	MG	DA	3173	1/1	0.83	0.17	90,90,90,90	0
56	MG	DA	3163	1/1	0.84	0.18	99,99,99,99	0
56	MG	DA	3048	1/1	0.84	0.14	96,96,96,96	0
56	MG	DA	3118	1/1	0.84	0.16	88,88,88,88	0
56	MG	DA	3119	1/1	0.84	0.14	82,82,82,82	0
56	MG	CA	1641	1/1	0.84	0.13	85,85,85,85	0
56	MG	DA	3121	1/1	0.84	0.18	86,86,86,86	0
56	MG	BA	3052	1/1	0.84	0.15	97,97,97,97	0
56	MG	DA	3020	1/1	0.84	0.16	93,93,93,93	0
56	MG	DA	3012	1/1	0.84	0.17	83,83,83,83	0
56	MG	DA	3069	1/1	0.84	0.16	81,81,81,81	0
56	MG	CA	1658	1/1	0.84	0.10	115,115,115,115	0
57	NMY	DA	3190	42/42	0.84	0.25	57,66,70,74	42
56	MG	DA	3175	1/1	0.84	0.31	75,75,75,75	0
56	MG	DA	3031	1/1	0.85	0.13	108,108,108,108	0
56	MG	BA	3112	1/1	0.85	0.19	101,101,101,101	0
56	MG	DA	3122	1/1	0.85	0.12	97,97,97,97	0
56	MG	CA	1671	1/1	0.85	0.23	96,96,96,96	0
56	MG	BA	3005	1/1	0.85	0.14	106,106,106,106	0
56	MG	DA	3104	1/1	0.85	0.13	81,81,81,81	0
56	MG	BA	3057	1/1	0.85	0.12	98,98,98,98	0
56	MG	CA	1621	1/1	0.85	0.14	111,111,111,111	0
56	MG	BA	3045	1/1	0.85	0.15	118,118,118,118	0
57	NMY	BA	3161	42/42	0.85	0.17	61,70,77,82	42
56	MG	BA	3139	1/1	0.85	0.32	83,83,83,83	0
57	NMY	BA	3163	42/42	0.85	0.19	89,98,100,101	42
56	MG	DA	3051	1/1	0.85	0.16	86,86,86,86	0
56	MG	BA	3109	1/1	0.85	0.21	106,106,106,106	0
56	MG	BA	3043	1/1	0.85	0.10	108,108,108,108	0
56	MG	BQ	201	1/1	0.85	0.30	93,93,93,93	0
56	MG	DA	3141	1/1	0.85	0.45	73,73,73,73	0
56	MG	DA	3029	1/1	0.85	0.21	84,84,84,84	0
56	MG	DA	3166	1/1	0.85	0.34	87,87,87,87	0
56	MG	BA	3001	1/1	0.86	0.13	99,99,99,99	0
56	MG	DA	3016	1/1	0.86	0.13	103,103,103,103	0
56	MG	DA	3160	1/1	0.86	0.33	92,92,92,92	0
56	MG	CA	1635	1/1	0.86	0.13	113,113,113,113	0
57	NMY	BA	3166	42/42	0.86	0.16	68,77,83,90	42
56	MG	DA	3066	1/1	0.86	0.11	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	1612	1/1	0.86	0.19	116,116,116,116	0
56	MG	CA	1669	1/1	0.86	0.29	107,107,107,107	0
56	MG	BA	3086	1/1	0.86	0.08	109,109,109,109	0
58	ZN	B4	101	1/1	0.86	0.18	186,186,186,186	0
56	MG	DA	3034	1/1	0.86	0.13	84,84,84,84	0
56	MG	DA	3093	1/1	0.87	0.22	105,105,105,105	0
56	MG	BA	3101	1/1	0.87	0.24	102,102,102,102	0
56	MG	AA	1624	1/1	0.87	0.17	110,110,110,110	0
56	MG	DA	3014	1/1	0.87	0.14	90,90,90,90	0
56	MG	DA	3056	1/1	0.87	0.11	86,86,86,86	0
56	MG	BA	3103	1/1	0.87	0.43	105,105,105,105	0
57	NMY	AA	1655	42/42	0.87	0.10	61,73,90,121	0
56	MG	BA	3089	1/1	0.87	0.10	109,109,109,109	0
56	MG	DA	3153	1/1	0.87	0.12	95,95,95,95	0
56	MG	BA	3008	1/1	0.87	0.22	107,107,107,107	0
56	MG	BA	3106	1/1	0.87	0.17	100,100,100,100	0
56	MG	DA	3062	1/1	0.87	0.13	76,76,76,76	0
56	MG	BA	3146	1/1	0.87	0.23	98,98,98,98	0
56	MG	DA	3106	1/1	0.87	0.19	100,100,100,100	0
56	MG	BA	3038	1/1	0.87	0.15	104,104,104,104	0
56	MG	CA	1614	1/1	0.87	0.10	120,120,120,120	0
56	MG	DA	3067	1/1	0.87	0.19	120,120,120,120	0
57	NMY	DA	3189	42/42	0.87	0.14	55,63,70,72	42
56	MG	DA	3088	1/1	0.87	0.11	115,115,115,115	0
56	MG	AA	1637	1/1	0.87	0.18	103,103,103,103	0
56	MG	CA	1616	1/1	0.87	0.10	98,98,98,98	0
56	MG	BA	3017	1/1	0.88	0.10	107,107,107,107	0
56	MG	CA	1620	1/1	0.88	0.17	118,118,118,118	0
56	MG	DA	3154	1/1	0.88	0.38	86,86,86,86	0
56	MG	DA	3024	1/1	0.88	0.13	73,73,73,73	0
56	MG	DA	3140	1/1	0.88	0.17	98,98,98,98	0
56	MG	AA	1632	1/1	0.88	0.15	114,114,114,114	0
56	MG	BA	3113	1/1	0.88	0.15	121,121,121,121	0
56	MG	BA	3031	1/1	0.88	0.11	87,87,87,87	0
56	MG	BA	3134	1/1	0.88	0.20	109,109,109,109	0
57	NMY	DA	3185	42/42	0.88	0.12	46,58,63,67	42
56	MG	DA	3116	1/1	0.88	0.13	107,107,107,107	0
56	MG	DA	3117	1/1	0.88	0.12	93,93,93,93	0
56	MG	BA	3169	1/1	0.88	0.13	101,101,101,101	0
56	MG	DA	3178	1/1	0.88	0.18	88,88,88,88	0
56	MG	DA	3070	1/1	0.88	0.11	56,56,56,56	0
56	MG	DA	3046	1/1	0.89	0.09	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3029	1/1	0.89	0.10	99,99,99,99	0
56	MG	DA	3049	1/1	0.89	0.18	97,97,97,97	0
56	MG	CA	1622	1/1	0.89	0.18	108,108,108,108	0
56	MG	BA	3140	1/1	0.89	0.13	101,101,101,101	0
56	MG	DA	3017	1/1	0.89	0.12	76,76,76,76	0
56	MG	DA	3007	1/1	0.89	0.09	103,103,103,103	0
56	MG	BA	3006	1/1	0.89	0.09	101,101,101,101	0
56	MG	DA	3036	1/1	0.89	0.24	90,90,90,90	0
56	MG	BA	3041	1/1	0.89	0.12	96,96,96,96	0
56	MG	DA	3112	1/1	0.89	0.18	108,108,108,108	0
57	NMY	DA	3186	42/42	0.89	0.12	53,58,64,71	42
56	MG	DA	3010	1/1	0.89	0.18	106,106,106,106	0
56	MG	DA	3096	1/1	0.89	0.11	75,75,75,75	0
56	MG	BA	3049	1/1	0.89	0.14	88,88,88,88	0
56	MG	CA	1611	1/1	0.89	0.10	110,110,110,110	0
56	MG	BA	3020	1/1	0.89	0.15	95,95,95,95	0
56	MG	AA	1618	1/1	0.90	0.14	96,96,96,96	0
56	MG	BA	3132	1/1	0.90	0.10	96,96,96,96	0
56	MG	DA	3050	1/1	0.90	0.14	86,86,86,86	0
56	MG	AA	1619	1/1	0.90	0.10	95,95,95,95	0
56	MG	DA	3041	1/1	0.90	0.10	81,81,81,81	0
56	MG	AA	1604	1/1	0.90	0.07	102,102,102,102	0
56	MG	BB	203	1/1	0.90	0.07	107,107,107,107	0
56	MG	CA	1640	1/1	0.90	0.24	114,114,114,114	0
56	MG	DA	3158	1/1	0.90	0.22	91,91,91,91	0
56	MG	BA	3039	1/1	0.90	0.08	96,96,96,96	0
56	MG	DA	3043	1/1	0.91	0.09	90,90,90,90	0
56	MG	BA	3064	1/1	0.91	0.12	96,96,96,96	0
56	MG	BA	3004	1/1	0.91	0.13	120,120,120,120	0
56	MG	CA	1610	1/1	0.91	0.17	102,102,102,102	0
56	MG	AA	1606	1/1	0.91	0.19	111,111,111,111	0
56	MG	BA	3067	1/1	0.91	0.09	89,89,89,89	0
56	MG	DA	3032	1/1	0.91	0.23	97,97,97,97	0
56	MG	AA	1609	1/1	0.91	0.17	111,111,111,111	0
56	MG	DA	3143	1/1	0.91	0.59	79,79,79,79	0
56	MG	BA	3117	1/1	0.91	0.10	89,89,89,89	0
56	MG	BA	3091	1/1	0.91	0.19	115,115,115,115	0
57	NMY	CA	1672	42/42	0.91	0.15	54,65,74,77	42
56	MG	DA	3124	1/1	0.91	0.09	78,78,78,78	0
56	MG	CA	1639	1/1	0.91	0.10	94,94,94,94	0
56	MG	BA	3024	1/1	0.91	0.25	114,114,114,114	0
56	MG	BA	3093	1/1	0.91	0.26	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	NMY	DA	3188	42/42	0.91	0.11	45,60,66,70	42
56	MG	DA	3074	1/1	0.91	0.10	95,95,95,95	0
56	MG	DA	3132	1/1	0.91	0.10	96,96,96,96	0
56	MG	BA	3111	1/1	0.91	0.10	98,98,98,98	0
56	MG	DE	301	1/1	0.91	0.08	100,100,100,100	0
56	MG	BA	3034	1/1	0.92	0.09	88,88,88,88	0
56	MG	DA	3038	1/1	0.92	0.13	81,81,81,81	0
57	NMY	AA	1657	42/42	0.92	0.34	81,84,88,90	42
56	MG	DA	3078	1/1	0.92	0.09	84,84,84,84	0
56	MG	BA	3128	1/1	0.92	0.08	94,94,94,94	0
56	MG	BA	3073	1/1	0.92	0.10	101,101,101,101	0
56	MG	DA	3144	1/1	0.92	0.11	108,108,108,108	0
56	MG	DA	3110	1/1	0.92	0.15	93,93,93,93	0
56	MG	DA	3030	1/1	0.92	0.10	76,76,76,76	0
56	MG	DA	3128	1/1	0.92	0.15	92,92,92,92	0
56	MG	AA	1605	1/1	0.93	0.14	121,121,121,121	0
56	MG	DA	3047	1/1	0.93	0.09	76,76,76,76	0
56	MG	AA	1612	1/1	0.93	0.10	107,107,107,107	0
56	MG	BA	3035	1/1	0.93	0.11	94,94,94,94	0
56	MG	DA	3130	1/1	0.93	0.15	96,96,96,96	0
56	MG	DA	3191	1/1	0.93	0.09	80,80,80,80	0
56	MG	DA	3037	1/1	0.93	0.10	72,72,72,72	0
56	MG	DA	3114	1/1	0.93	0.08	77,77,77,77	0
56	MG	DA	3099	1/1	0.93	0.08	90,90,90,90	0
56	MG	BA	3016	1/1	0.93	0.09	83,83,83,83	0
56	MG	DA	3005	1/1	0.93	0.07	88,88,88,88	0
56	MG	CA	1619	1/1	0.93	0.08	93,93,93,93	0
56	MG	DA	3054	1/1	0.93	0.14	93,93,93,93	0
56	MG	BA	3068	1/1	0.93	0.11	126,126,126,126	0
56	MG	BA	3150	1/1	0.93	0.22	95,95,95,95	0
56	MG	CA	1605	1/1	0.93	0.09	97,97,97,97	0
56	MG	BA	3048	1/1	0.93	0.06	93,93,93,93	0
56	MG	DA	3033	1/1	0.93	0.08	91,91,91,91	0
56	MG	BA	3010	1/1	0.94	0.08	85,85,85,85	0
56	MG	DA	3019	1/1	0.94	0.13	78,78,78,78	0
56	MG	BA	3036	1/1	0.94	0.07	95,95,95,95	0
56	MG	DA	3148	1/1	0.94	0.14	60,60,60,60	0
56	MG	CA	1662	1/1	0.94	0.11	114,114,114,114	0
56	MG	DA	3058	1/1	0.94	0.18	96,96,96,96	0
56	MG	AA	1635	1/1	0.94	0.17	105,105,105,105	0
56	MG	AA	1607	1/1	0.95	0.14	116,116,116,116	0
56	MG	CA	1642	1/1	0.95	0.16	106,106,106,106	0

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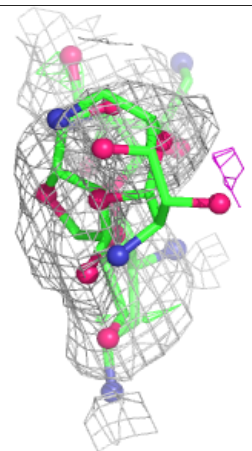
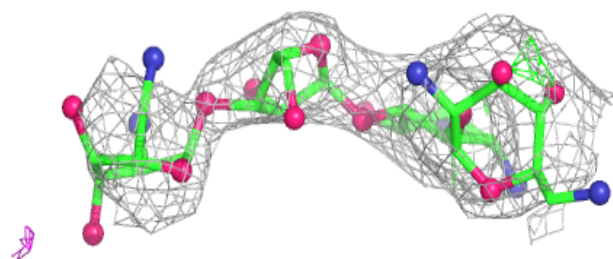
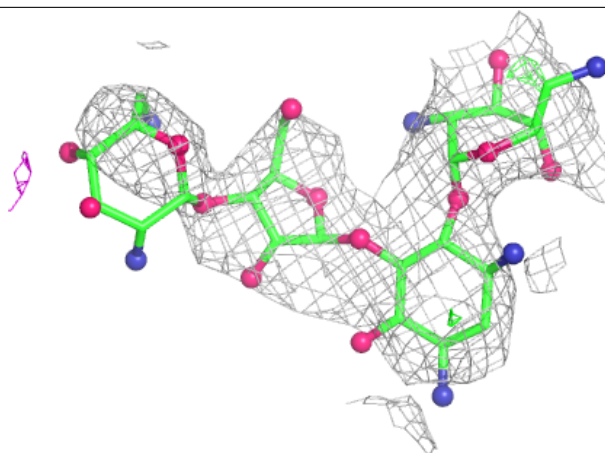
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3080	1/1	0.95	0.18	100,100,100,100	0
56	MG	DA	3133	1/1	0.95	0.13	100,100,100,100	0
56	MG	BA	3084	1/1	0.95	0.07	95,95,95,95	0
56	MG	BA	3002	1/1	0.96	0.07	89,89,89,89	0
56	MG	DA	3001	1/1	0.96	0.06	91,91,91,91	0
56	MG	DA	3126	1/1	0.96	0.07	60,60,60,60	0
56	MG	DA	3002	1/1	0.96	0.07	86,86,86,86	0
56	MG	DA	3091	1/1	0.96	0.10	104,104,104,104	0
56	MG	AA	1620	1/1	0.96	0.14	118,118,118,118	0
56	MG	DA	3086	1/1	0.96	0.06	97,97,97,97	0
56	MG	BA	3028	1/1	0.97	0.19	89,89,89,89	0
56	MG	BA	3094	1/1	0.97	0.13	92,92,92,92	0
56	MG	DA	3027	1/1	0.98	0.05	79,79,79,79	0
56	MG	DA	3063	1/1	0.98	0.05	69,69,69,69	0
56	MG	AA	1613	1/1	0.98	0.13	115,115,115,115	0
56	MG	CA	1604	1/1	0.98	0.05	86,86,86,86	0
56	MG	BA	3042	1/1	0.98	0.05	97,97,97,97	0
56	MG	BA	3046	1/1	0.98	0.07	109,109,109,109	0
56	MG	AA	1611	1/1	0.98	0.03	104,104,104,104	0
56	MG	BA	3080	1/1	0.98	0.05	73,73,73,73	0
56	MG	DA	3089	1/1	0.99	0.07	97,97,97,97	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.

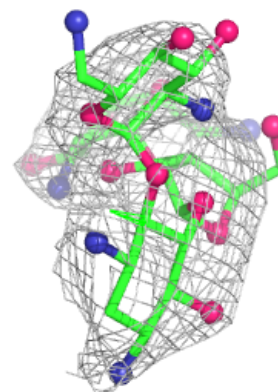
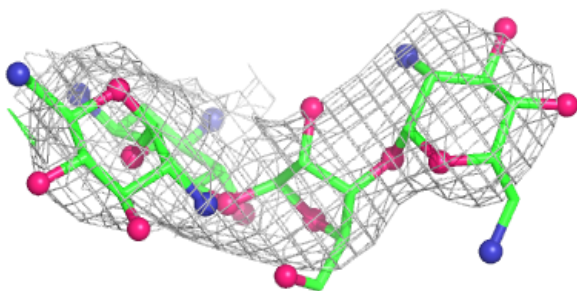
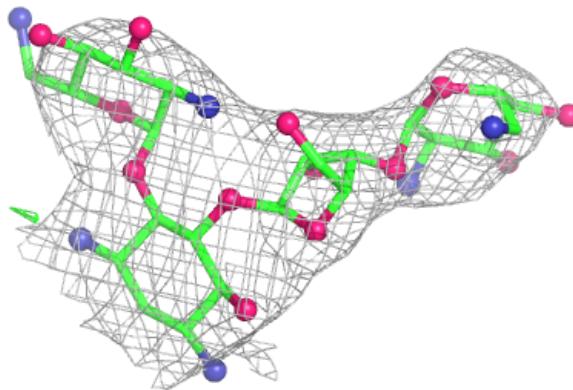
Electron density around NMY BA 3164:

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



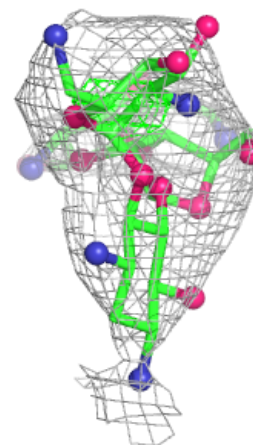
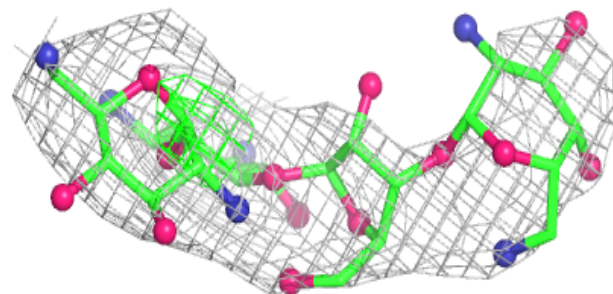
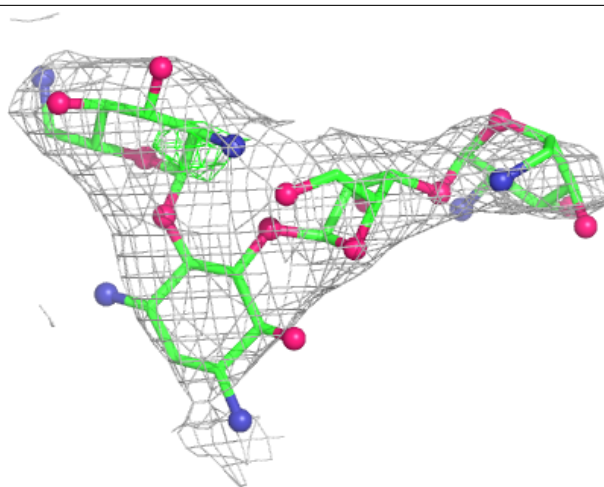
Electron density around NMY DA 3187:

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



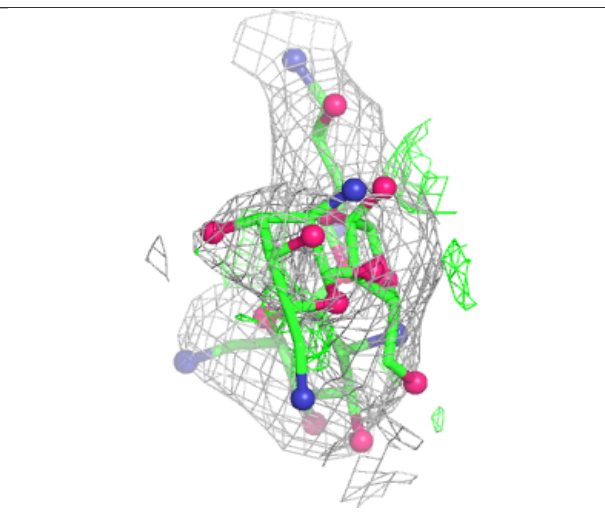
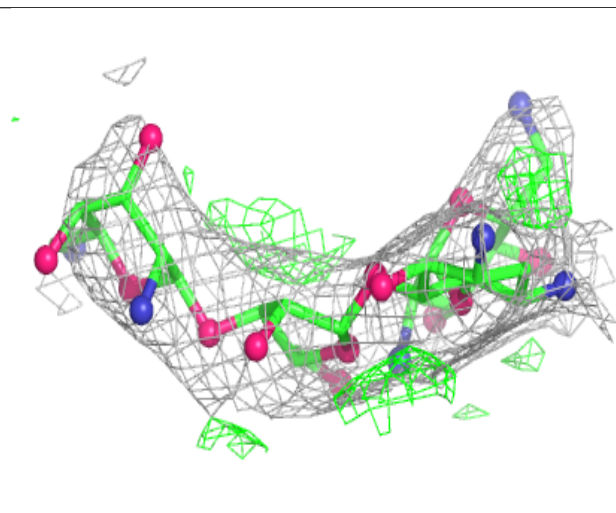
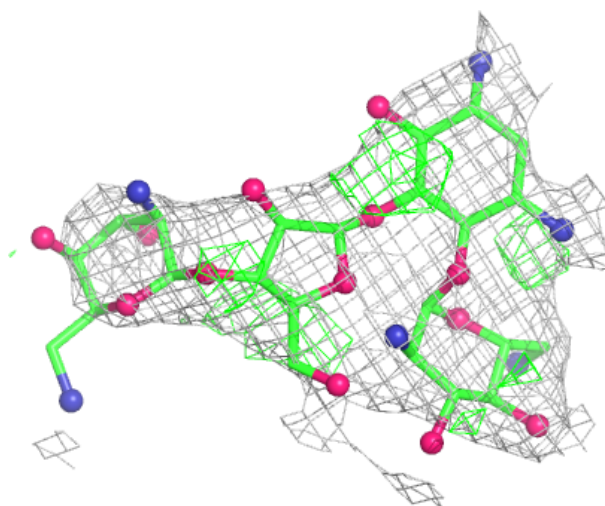
Electron density around NMY BA 3167:

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



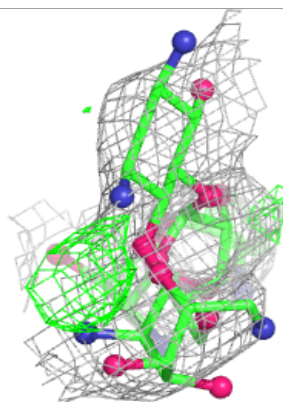
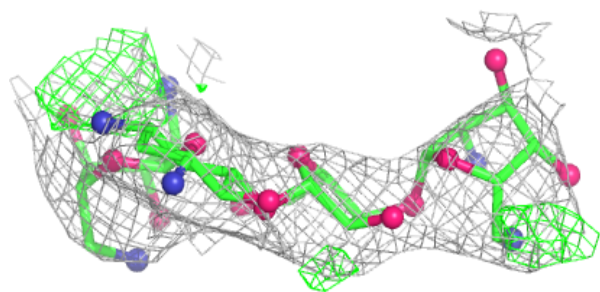
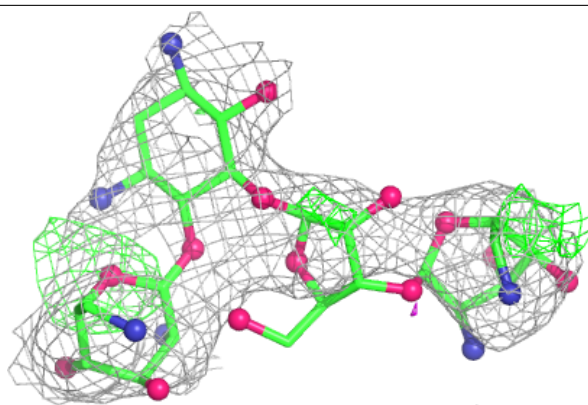
Electron density around NMY DA 3184:

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

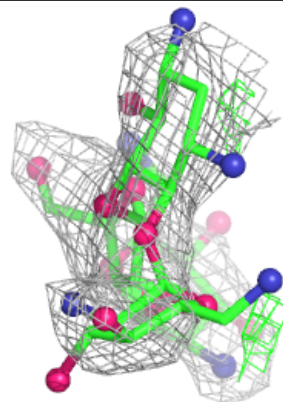
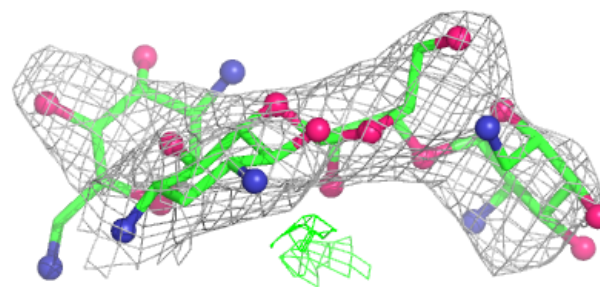
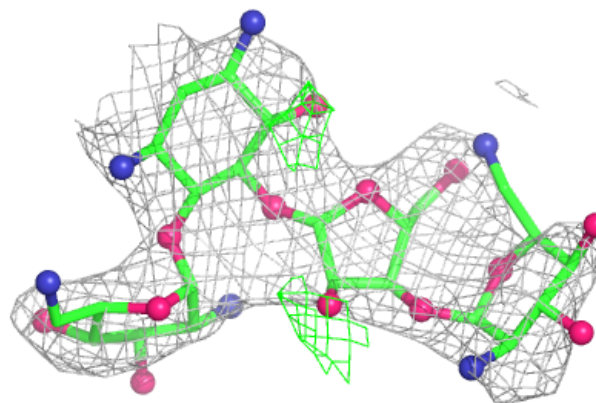


Electron density around NMY BA 3165:

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

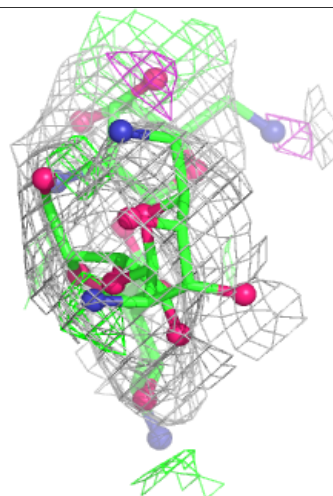
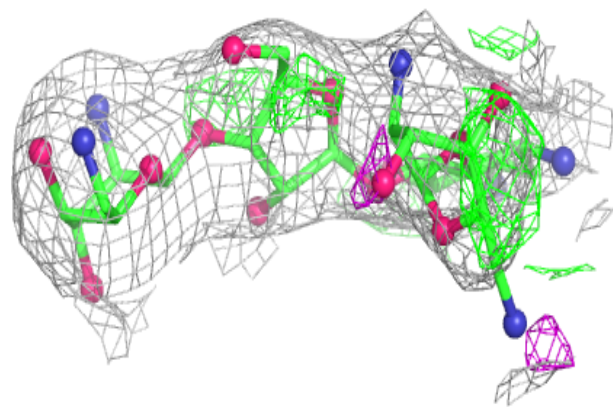
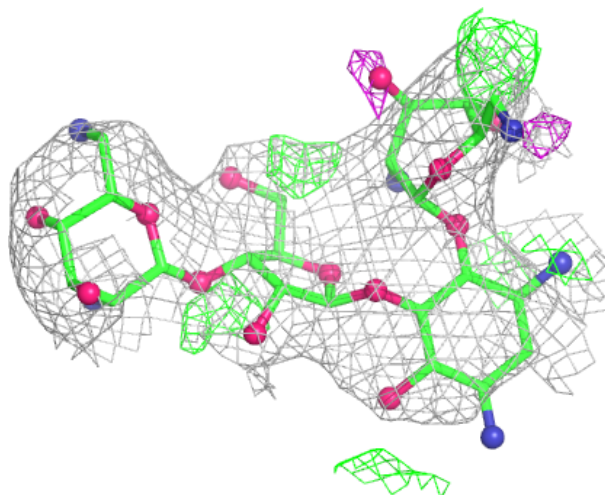
**Electron density around NMY AA 1656:**

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



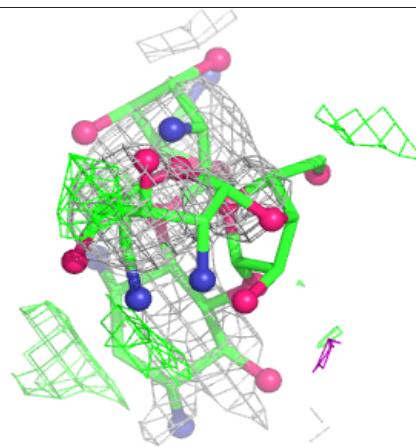
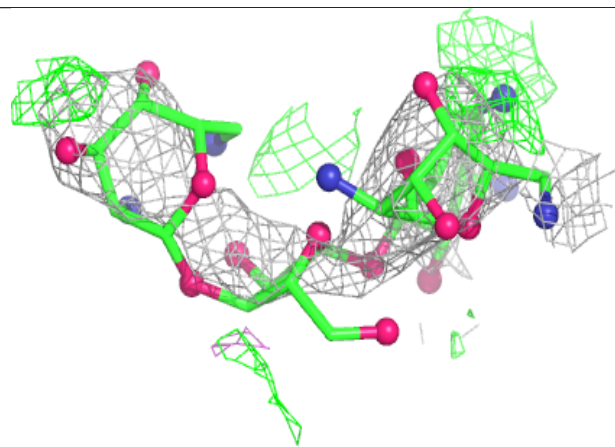
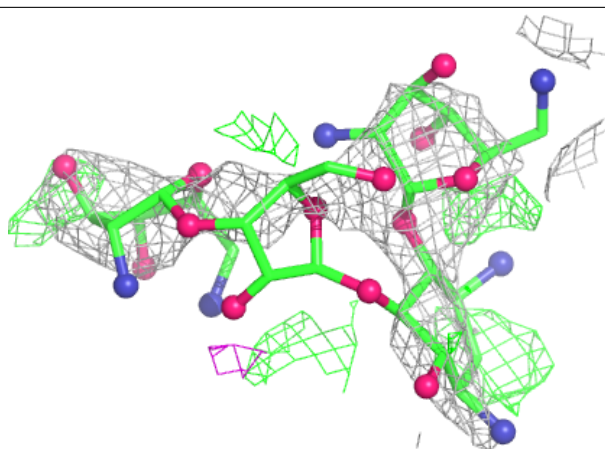
Electron density around NMY BA 3162:

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



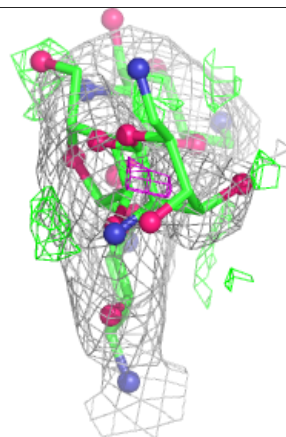
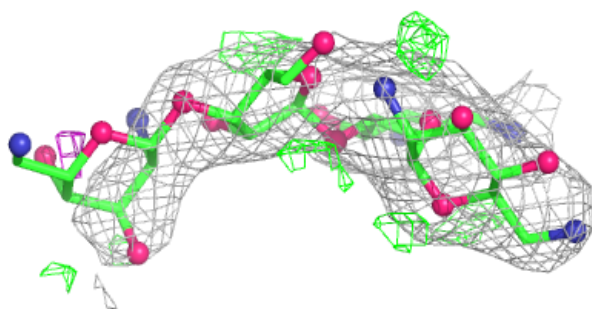
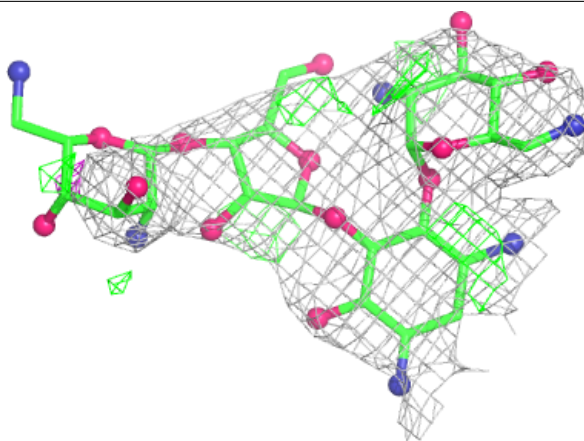
Electron density around NMY DA 3190:

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

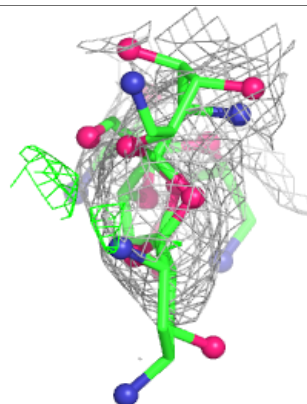
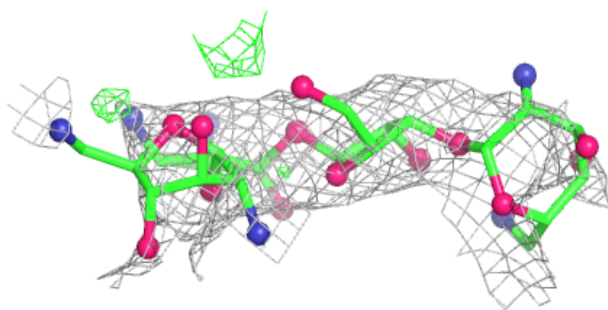
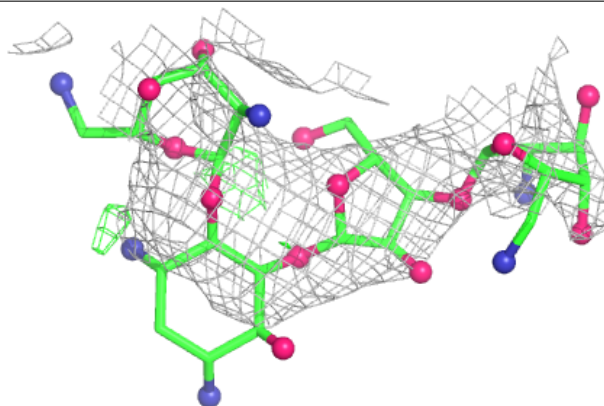


Electron density around NMY BA 3161:

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

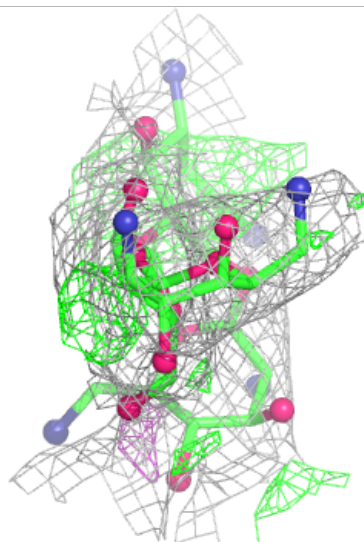
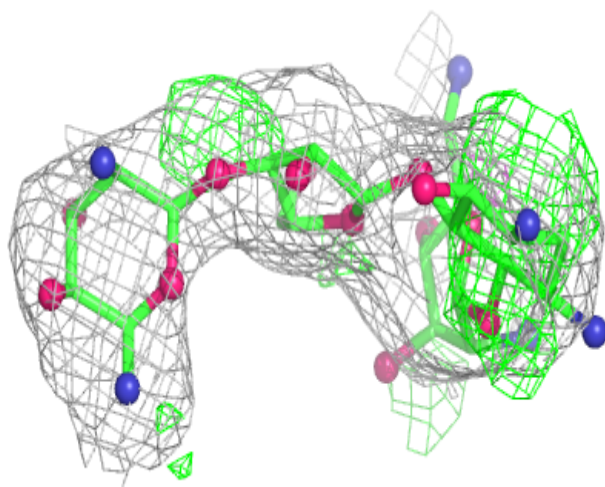
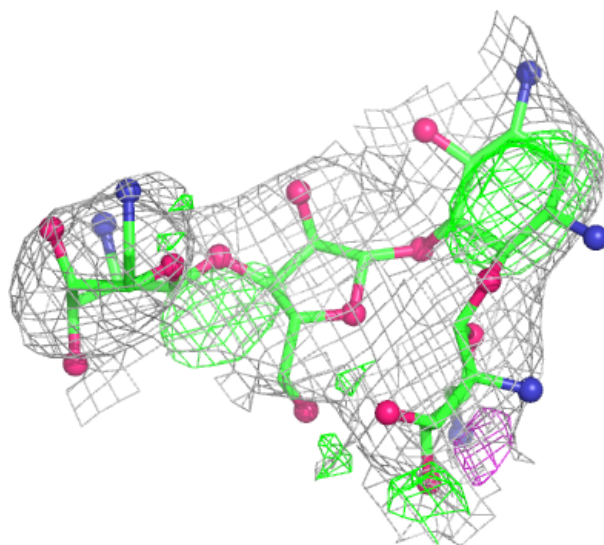
**Electron density around NMY BA 3163:**

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



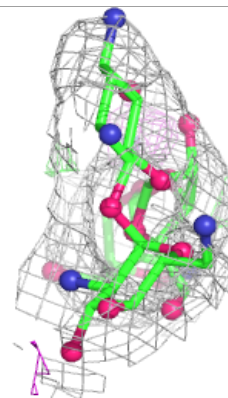
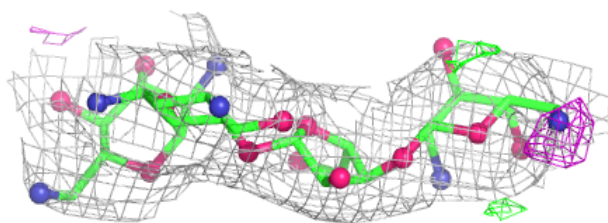
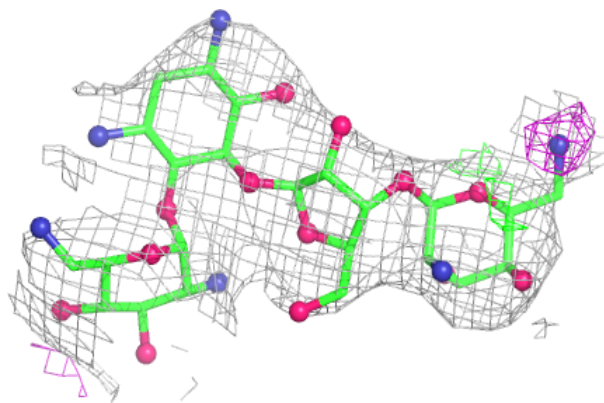
Electron density around NMY BA 3166:

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



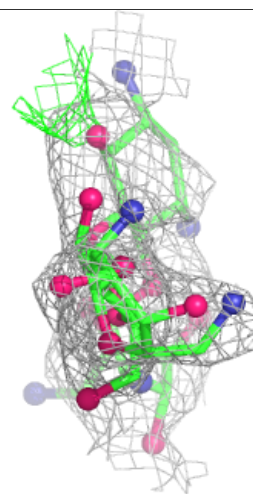
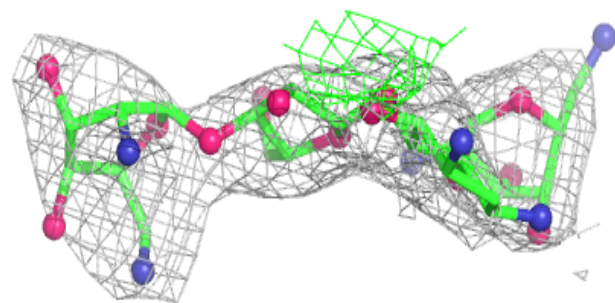
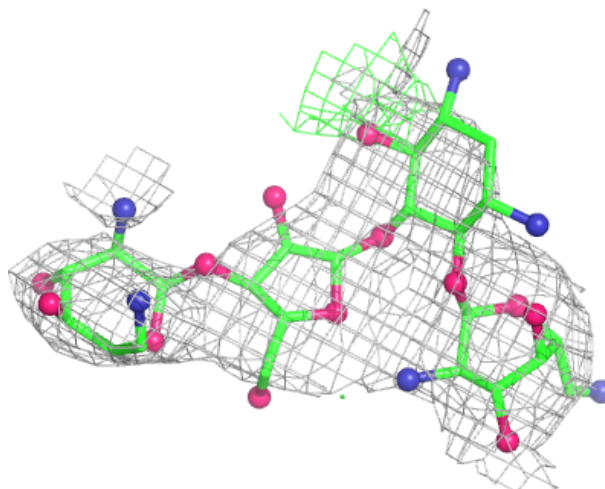
Electron density around NMY AA 1655:

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



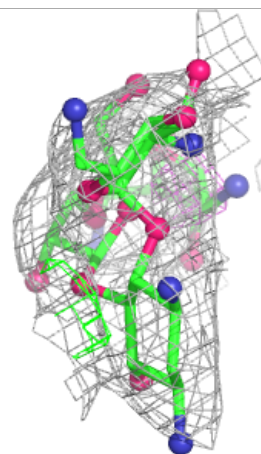
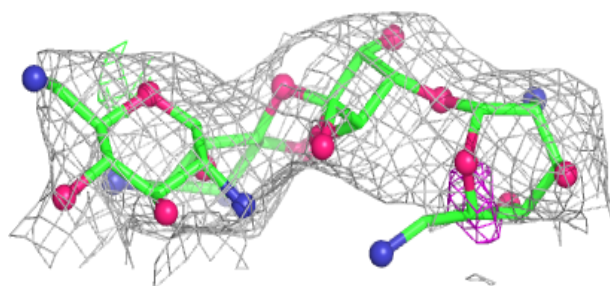
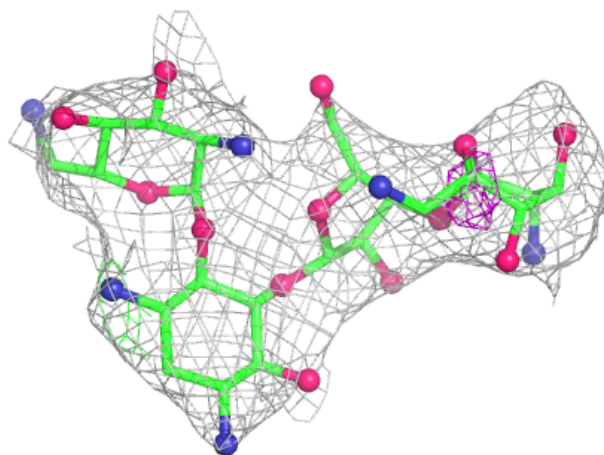
Electron density around NMY DA 3189:

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



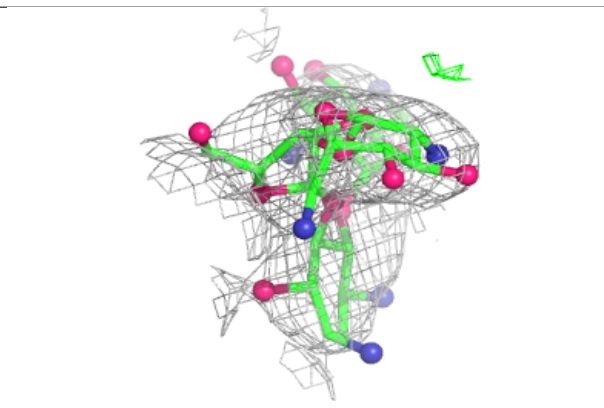
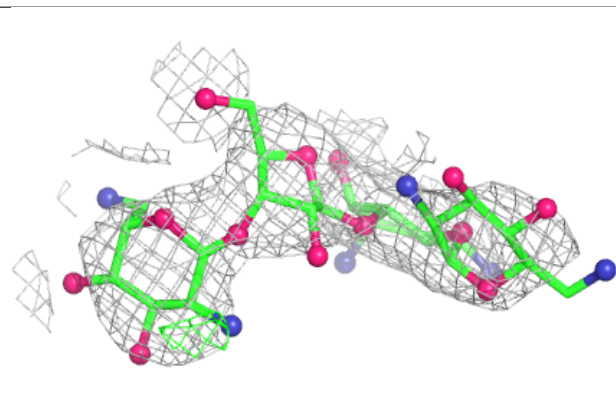
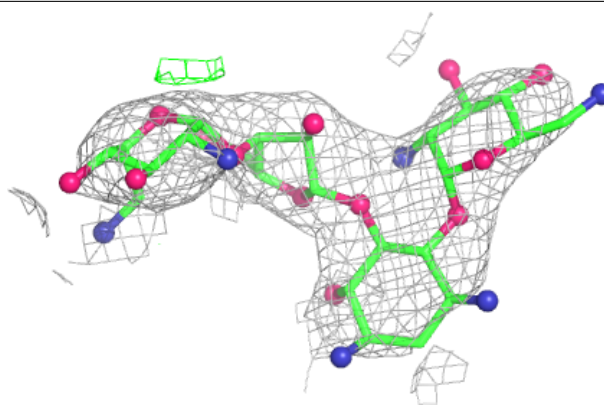
Electron density around NMY DA 3185:

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

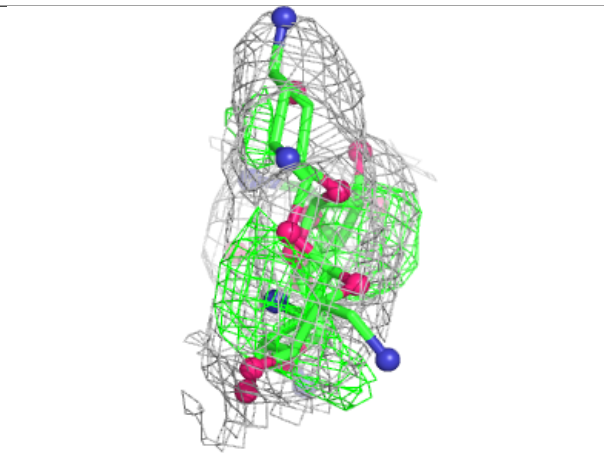
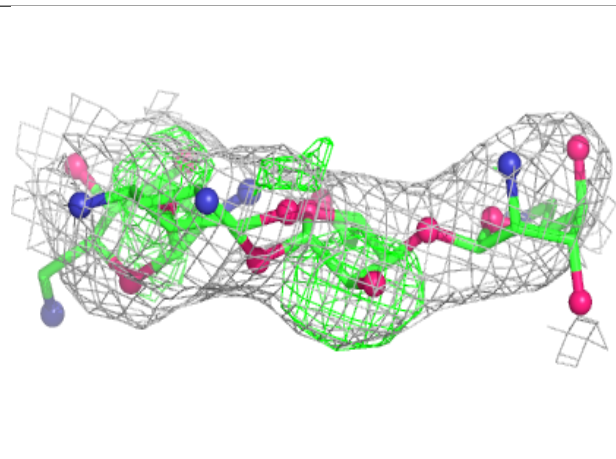
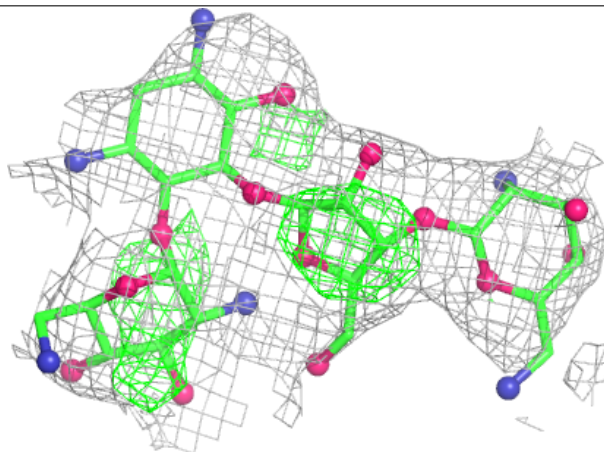


Electron density around NMY DA 3186:

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

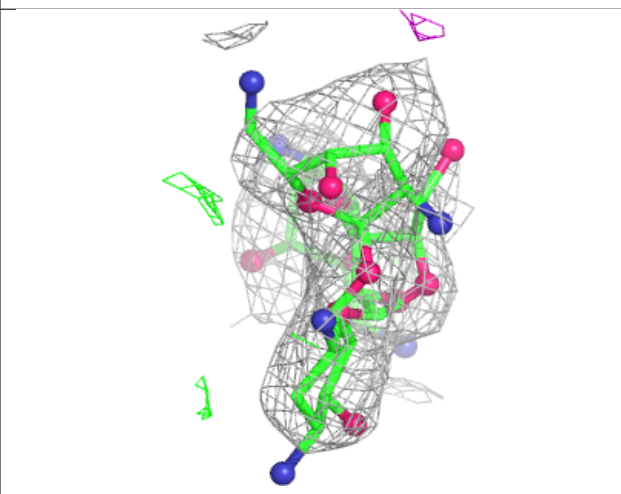
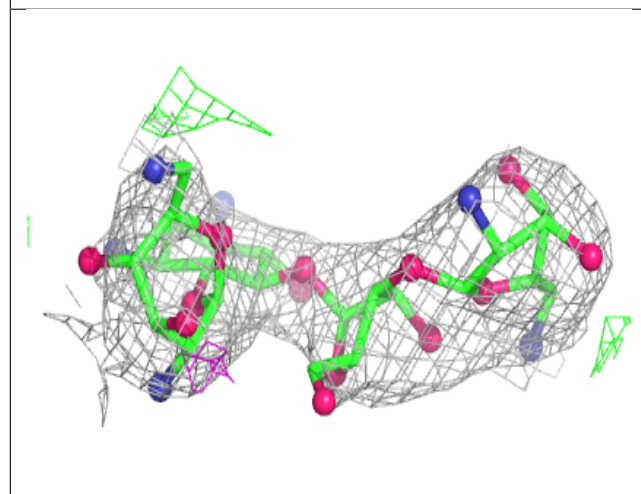
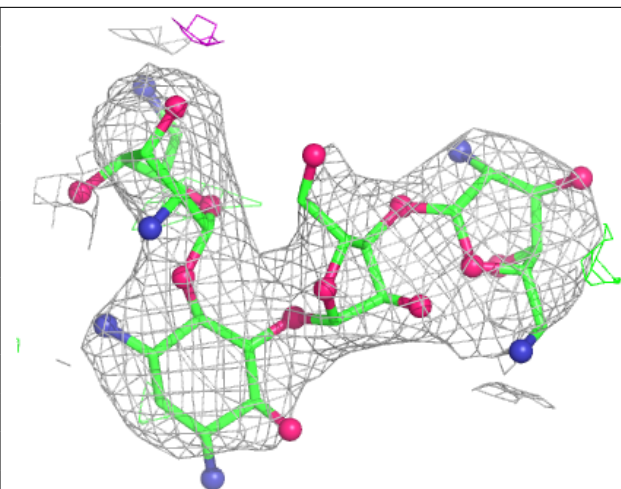
**Electron density around NMY CA 1672:**

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



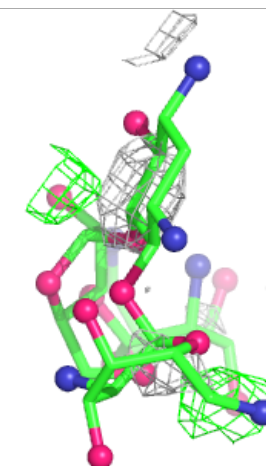
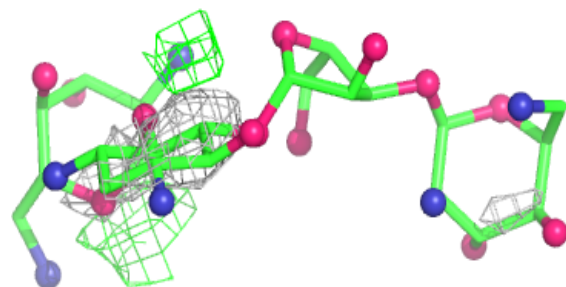
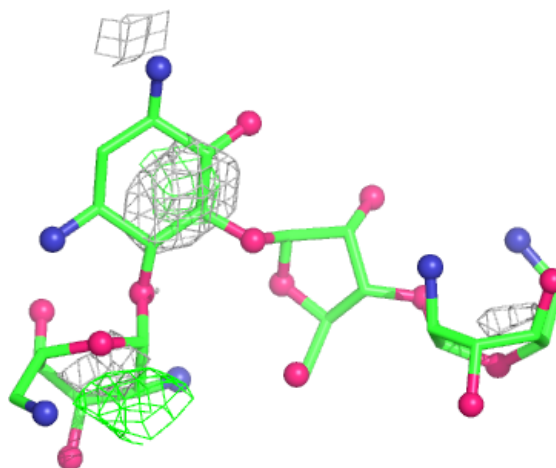
Electron density around NMY DA 3188:

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



Electron density around NMY AA 1657:

$2mF_o-DF_c$ (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.