



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 05:48 PM EDT

PDB ID : 4V9C
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

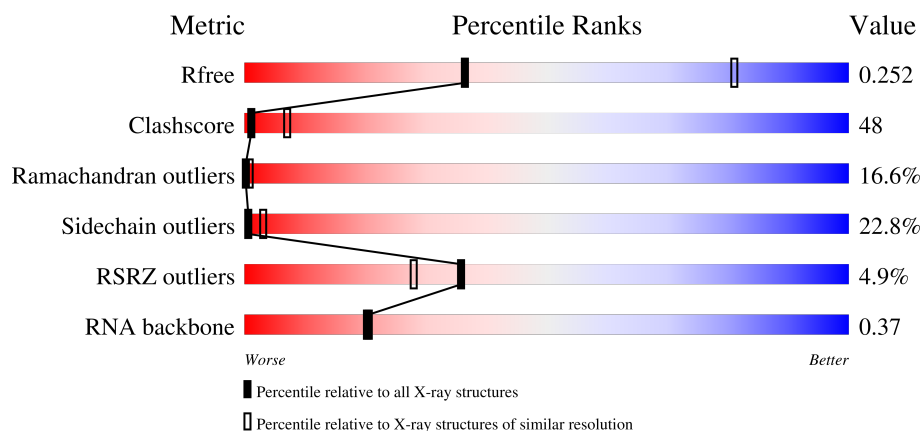
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)
RNA backbone	3690	1014 (3.64-2.96)

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	
1	CA	1542	
2	AB	241	
2	CB	241	

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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	AA	1639	-	-	-	X
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	DA	3177	-	-	-	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 (three-letter code: MG) (formula: Mg).

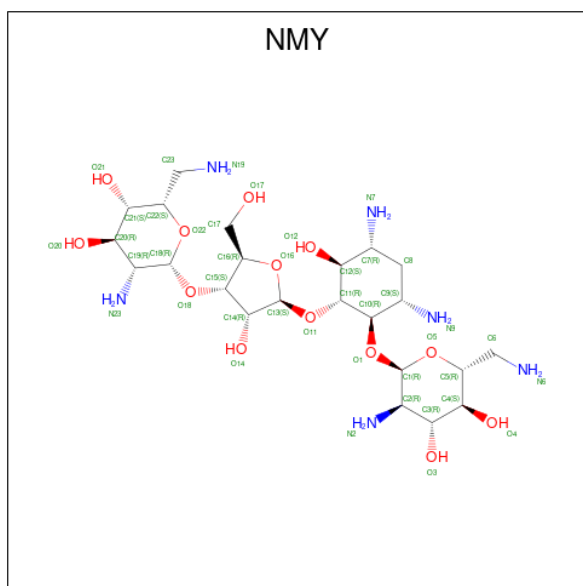
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	54	Total	Mg	0	0
			54	54		
56	AD	1	Total	Mg	0	0
			1	1		
56	AN	1	Total	Mg	0	0
			1	1		
56	BA	163	Total	Mg	0	0
			163	163		
56	BB	3	Total	Mg	0	0
			3	3		
56	BC	1	Total	Mg	0	0
			1	1		
56	BQ	1	Total	Mg	0	0
			1	1		

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

- Molecule 57 is NEOMYCIN (three-letter code: NMY) (formula: $\text{C}_{23}\text{H}_{46}\text{N}_6\text{O}_{13}$).



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 (three-letter code: 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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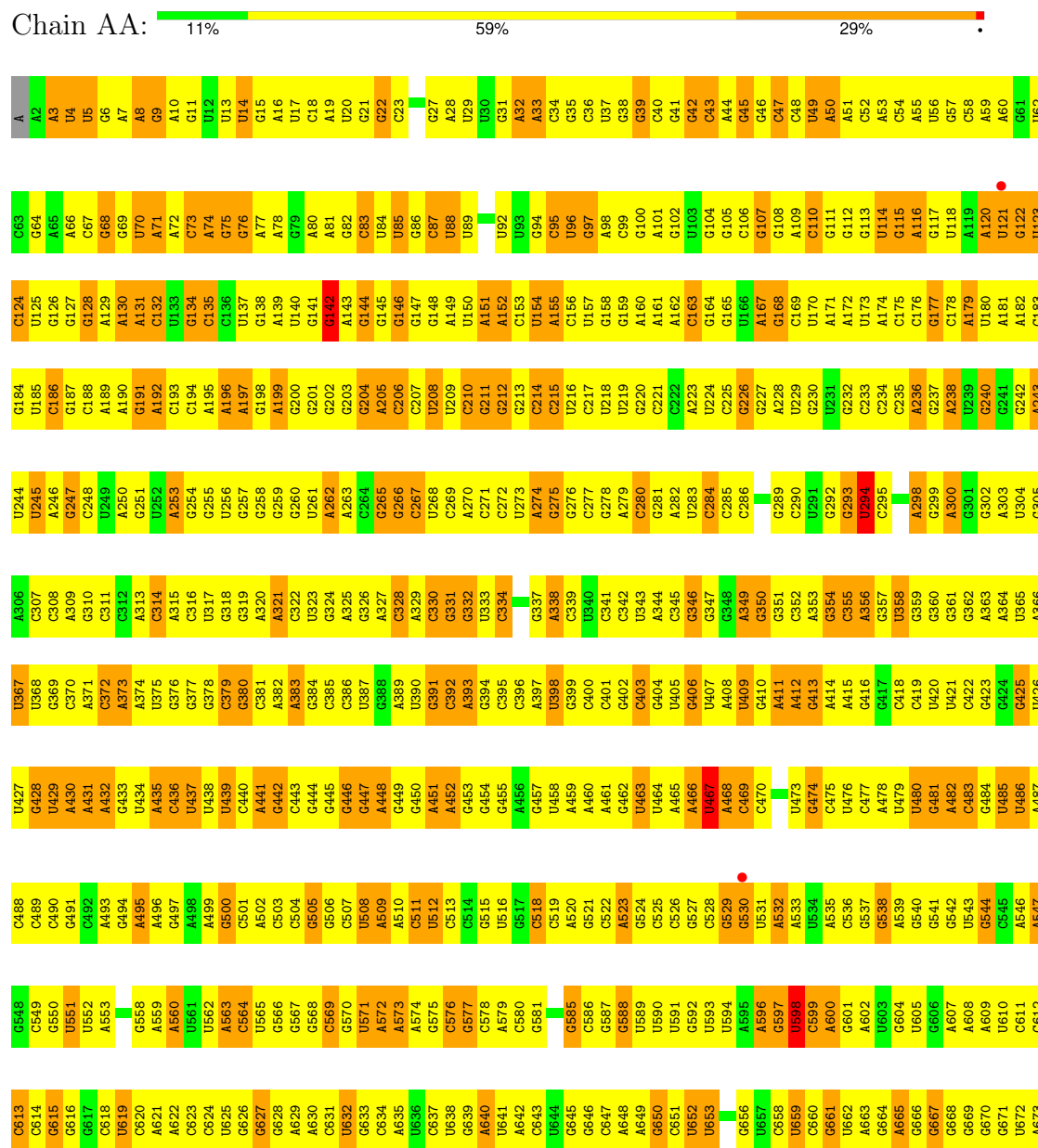
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CN	6	Total 6	O 6	0	0
59	CT	2	Total 2	O 2	0	0
59	DA	627	Total 627	O 627	0	0
59	DB	13	Total 13	O 13	0	0
59	DC	4	Total 4	O 4	0	0
59	DD	2	Total 2	O 2	0	0
59	DE	4	Total 4	O 4	0	0
59	DF	1	Total 1	O 1	0	0
59	DL	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

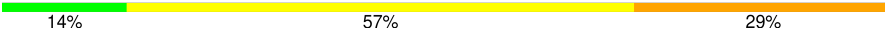
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

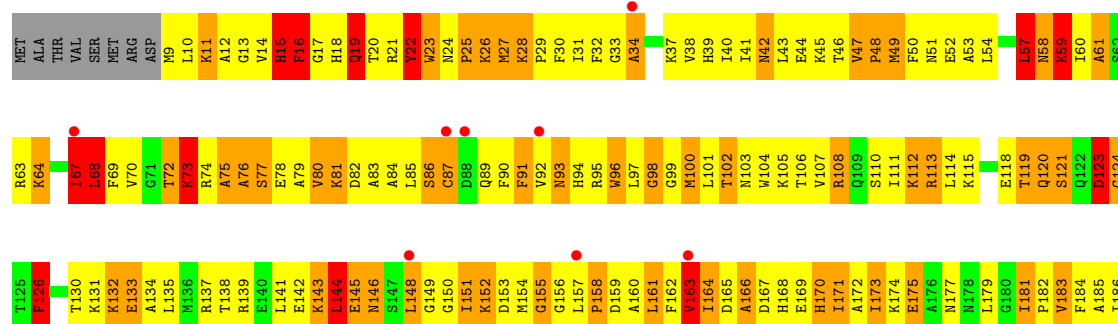


U1537	G1475	A1410	A1350	A1289	A1102	A1042	U981	U920	G859	G799	C735	G674
C1538	A1476	C1411	U1351	G1290	C1103	G1043	U982	U921	A860	G800	C736	A675
C1539	U1477	C1412	G1352	U1291	A1104	A1044	A983	G922	G861	U801	C737	A676
U1540	U1478	A1413	G1353	G1292	A1105	C1045	C984	A923	C862	A802	C738	U677
U	U1414	U1413	U1354	C1293	C1106	G1047	U986	C924	U863	G803		U678
A	G1415	G1415	G1355	G1293	C1107	G1047	U986	G925	A864	U804	G741	C679
	G1416	G1416	G1356	U1295	C1108	G1048	G987	G926	A865	C805	G742	C680
	G1417	G1417	A1357	C1296	C1109	G1050	G988	G927	C866	C806	A743	A681
	A1418	A1418	U1358	U1297	A1110	G1050	U989	G928	G867	A807	G744	G682
	G1419	C1484	C1359	U1298	A1111	U1051	C990	G929	C868	C808	G745	G683
	U1420	U1485	A1360	A1299	C1112	U1052	U991	C930	C869	G809	A746	U684
	G1421	G1486	G1361	A1238	C1113	G1053	U992	C931	U870	C810	A747	G685
	G1422	G1487	A1362	A1239	C1114	C1054	G993	C932	U871	G811	G748	U686
	G1423	G1488	A1363	U1240	U1115	A1055	A994	G933	A872	G812	A749	A687
	U1424	U1489	U1364	G1242	U1116	U1056	A995	C934	A873	U813	C750	G688
	U1425	G1490	G1365	G1243	A1117	G1057	A996	A935	G874	A814	U751	C689
	G1426	A1491	C1366	C1244	U1118	C1058	U997	C936	U875	U815	G752	G690
	C1427	A1492	C1367	G1245	U1122	G1061	C998	U943	U876	A816	G755	G691
	A1428	A1493	A1368	U1246	U1123	U1062		U944	G877	C817	G756	U692
	A1429	G1494	C1369	U1247	U1124	G1063	G1001	G945	A878	G818	C756	G693
	A1430	U1495	G1370	G1248	G1125	C1064	C1002	G946	C879	A819	C757	A694
	C1431	C1496	G1371	A1249	U1126	G1065	G1003	G947	C880	U820	C758	A695
	G1432	G1497	U1372	A1250	U1127	U1066	A1004	G942	C881	G821	A759	A696
	A1433	U1498	G1373	G1251	C1128	C1067	A1005	U943	C882	U822		U697
	A1434	A1499	A1374	U1252	U1129	A1067	G1006	G944	C883	C823	G763	G700
	G1435	A1500	A1375	G1253	A1130	G1068	U1007	G945	U884	G824	C764	U701
	U1436	C1501	U1376	G1254		C1069	U1008	A946	C885	A825	G765	A702
	A1437	A1502	A1377	U1255	G1133	C1069	U1009	G947	C886	C826	A766	G703
	G1438	A1503	G1378	A1256	G1134	U1070	C1010	C948	C887	U827	A767	A704
	A1439	G1504	C1379	A1257	C1135	C1071	C1011	A949	C888	U828	A768	A705
	U1440	U1505	U1380	G1258	U1136	G1072	A1012	U950	A889	G829	G769	G706
	A1441	U1506	A1381		C1136	U1073	G1013	G951	C890	G830	C770	
	G1442	A1507	U1382	A1261	U1137	G1074	A1014	U952	U891	U707	G771	U707
		C1508	C1383	C1262	G1138	U1075	G1015	G953	A892	G832	U772	C708
	A1446	U1509	G1384	C1263	G1139	U1076	A1016	G954	C893	U709	G773	U709
	A1447	C1510	U1385	U1264	C1140	G1077	U1017	U955	G894	G834	G774	G710
	G1448		G1386	C1265	C1141	U1078	G1018	U956	C895	U835	G775	G711
	U1449		G1387	G1266	G1142	G1079	A1019	U957	C896	G836	G776	A712
	U1450		C1388	C1267	G1143	A1080	G1020	A958	C897	U837	A777	G713
	U1451		C1389	G1268	G1144	A1081	A1021	A959	C898	G838	G778	G714
	C1452		U1390	A1269	A1145	A1082	A1022	U960	C899	C839	C779	A715
	G1453		U1391	G1270	A1146	U1083	A1023	U961	A900	C840	A780	A716
	G1454		G1392	G1271	C1147	G1084	G1024	C962	A901	C841	A781	U717
	G1455		U1393	A1272	U1148	U1085	U1025		G902	U842	A782	A718
	A1456		A1332	C1273	C1149	U1086	G1026	U965	G903	U843	C763	C719
	G1457		G1334	C1274	A1150	G1087	C1027	G966	U904	G844	A784	C720
	U1458		U1335	A1275	A1151	G1088	C1028	C967	U905	G845	G785	G721
	G1459		C1336	G1276	G1152	G1089	U1029	A968	A906	G846	G786	G722
	C1460		G1337	A1216	A1153	U1090	U1030	A969	A907	G847	A787	U723
	G1461		U1338	C1217	G1154	U1091	C1031	C970	A908	C848	U788	G724
	C1462		C1400	G1218	A1155	A1092	G1032	G971	A909	C849	U769	G725
	U1463		G1401	A1280	G1156	A1093	G1033	C972	C910	U850	A790	C726
	U1464		C1402	C1281	A1157	U1094	G1034	G973	U911	G851	G727	G727
	A1465		C1403	G1282	C1158	U1095	A1035	A974	C912	G852	A792	A728
	C1466		G1404	C1283	U1159	C1096	A1036	A975	C913	U853	A793	A729
			U1405	C1284	G1160	C1097	C1037	G976	A914	U854	A794	G730
	U1471		A1406	U1285	C1161	C1098	C1038	A977	U855	C856	C731	G731
	U1472		C1407	A1286	A1162	C1099	G1039	A978	C917	C857	C732	G732
	U1473		U1408	U1287	C1163	C1100	U1040	C979	C918	G733	C733	G734
	U1474		C1409	A1288		A1101	G1041	C980	A919	G858	U798	

• Molecule 1: 16S ribosomal RNA

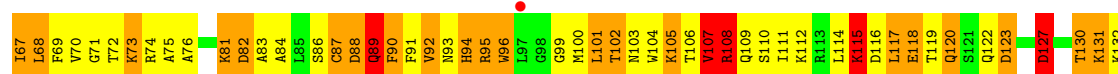
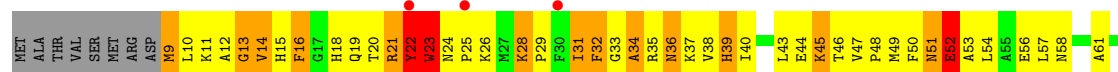
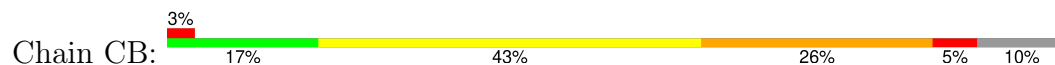
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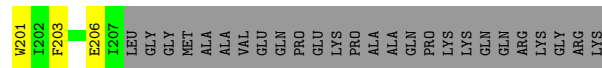
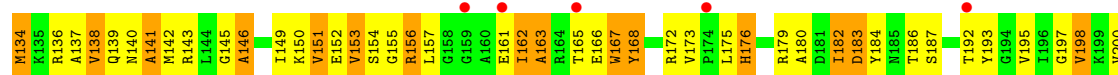
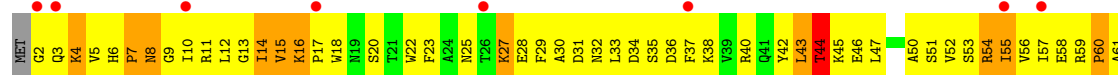




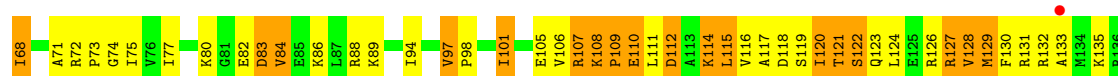
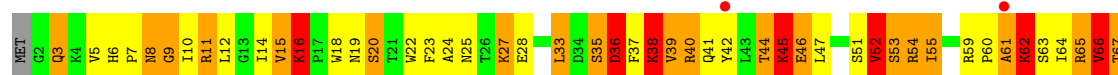
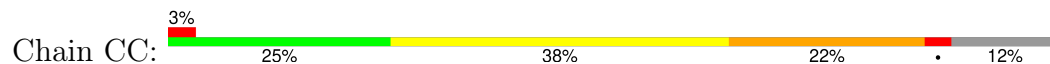
• Molecule 2: 30S ribosomal protein S2

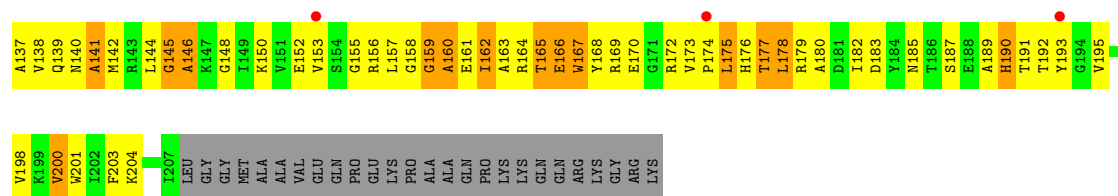


• Molecule 3: 30S ribosomal protein S3

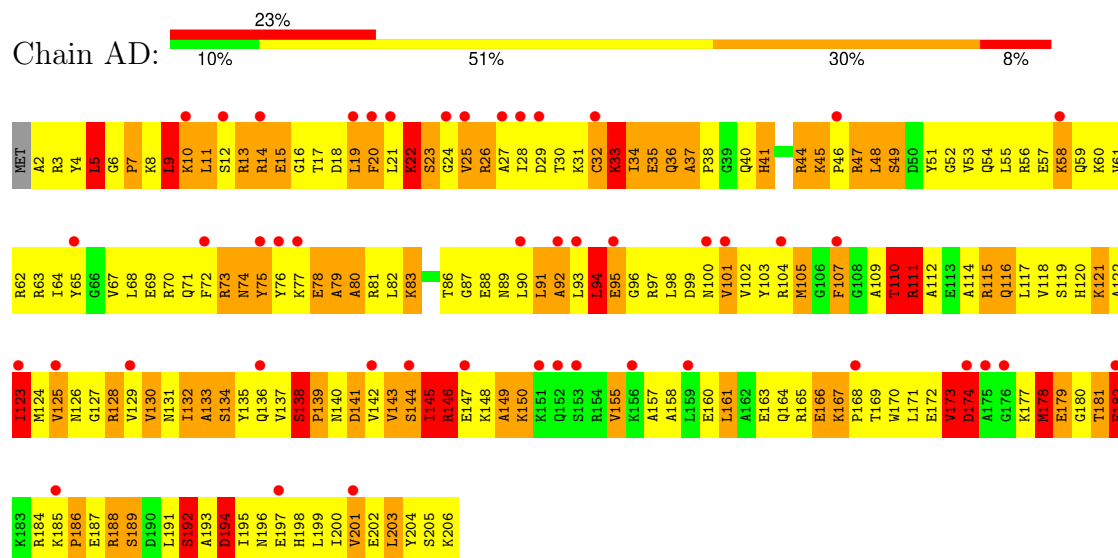


• Molecule 3: 30S ribosomal protein S3

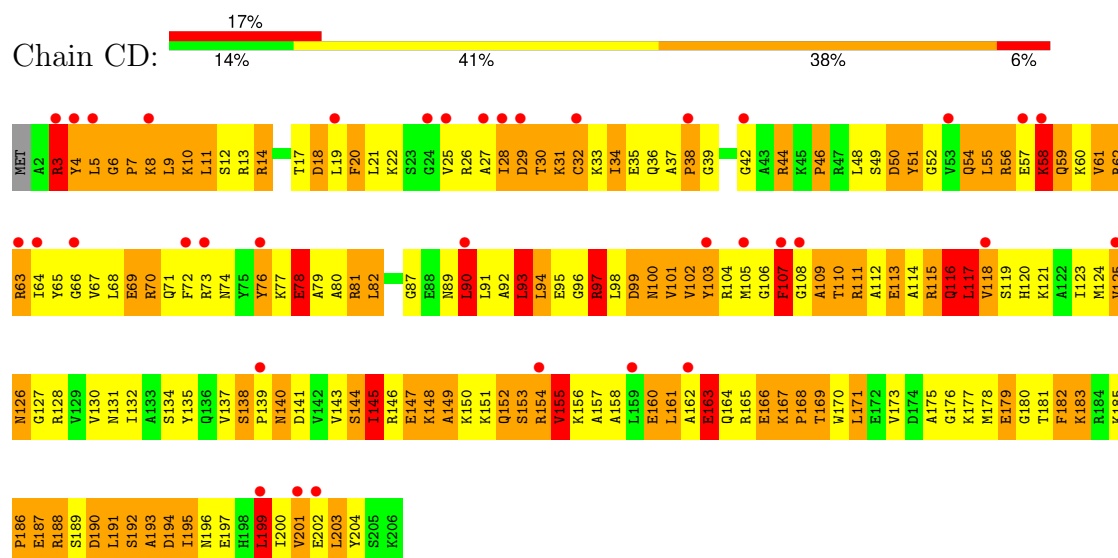




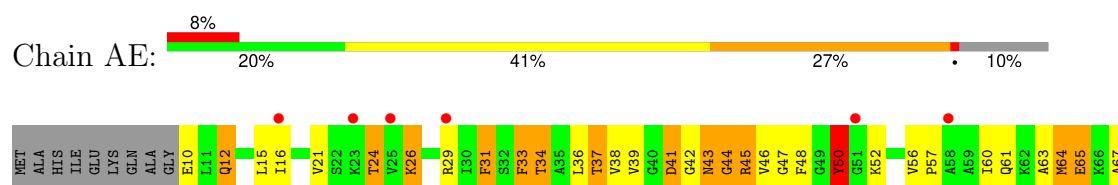
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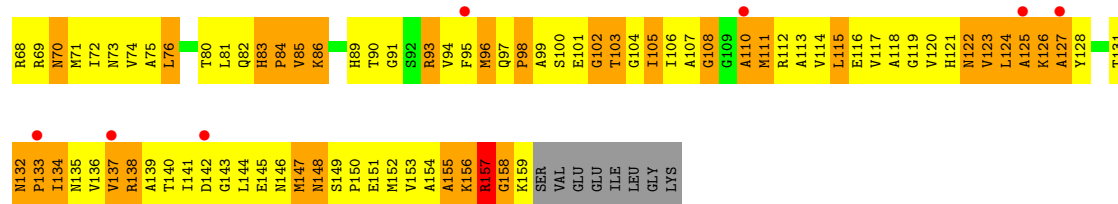


• Molecule 4: 30S ribosomal protein S4

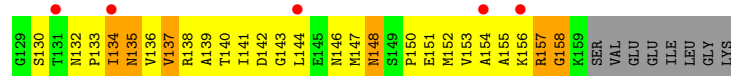
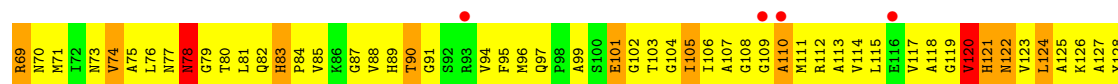
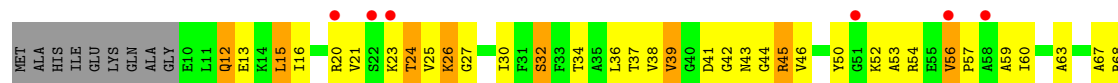


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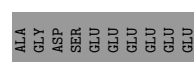
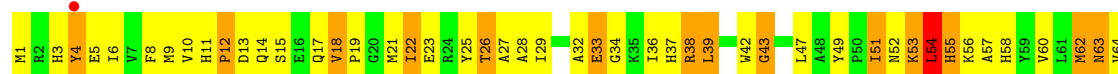
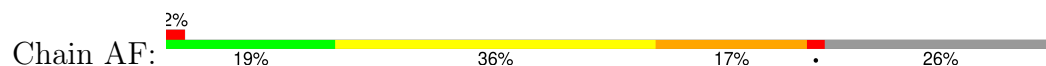




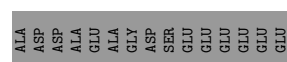
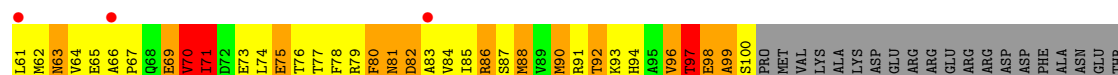
• Molecule 5: 30S ribosomal protein S5



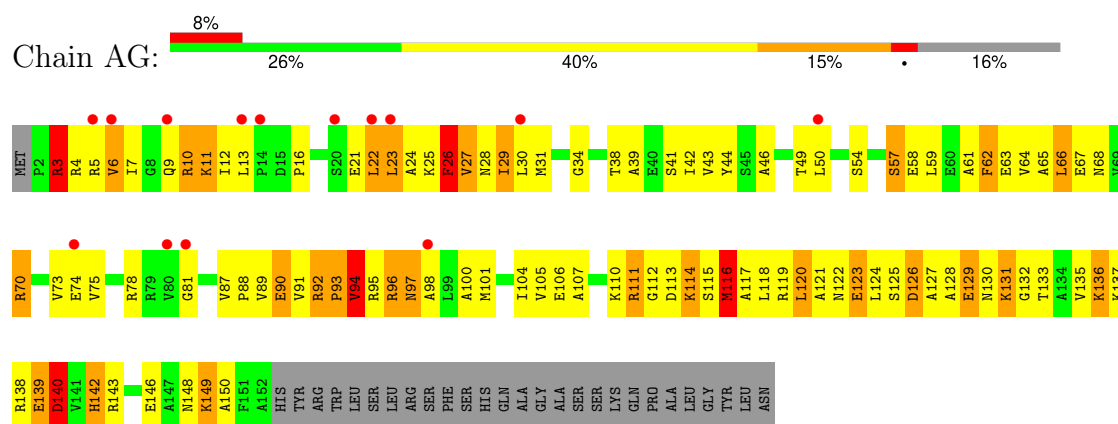
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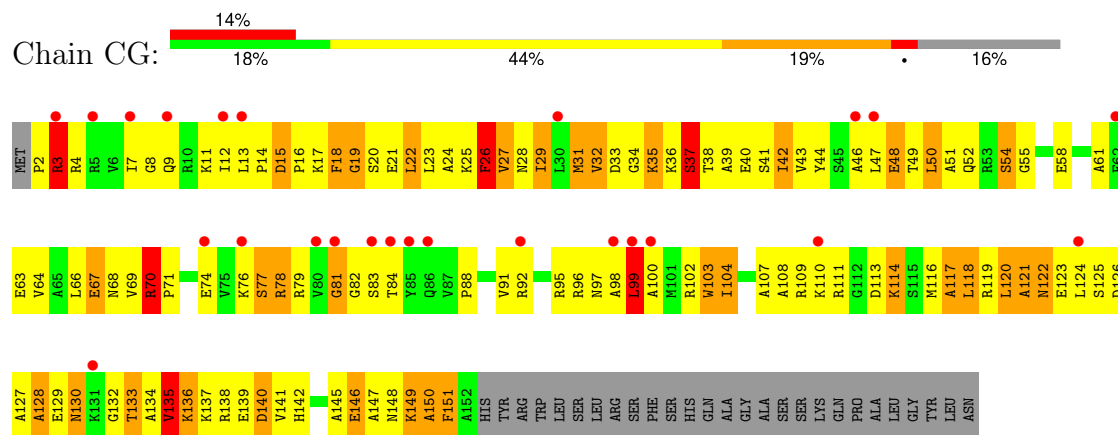
• Molecule 6: 30S ribosomal protein S6



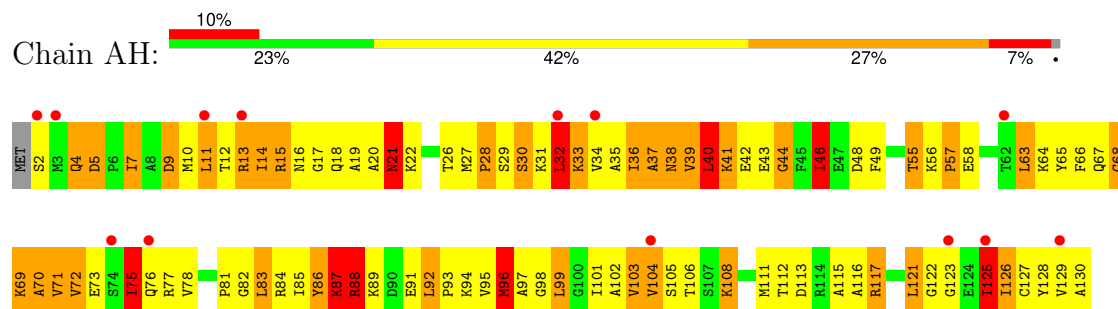
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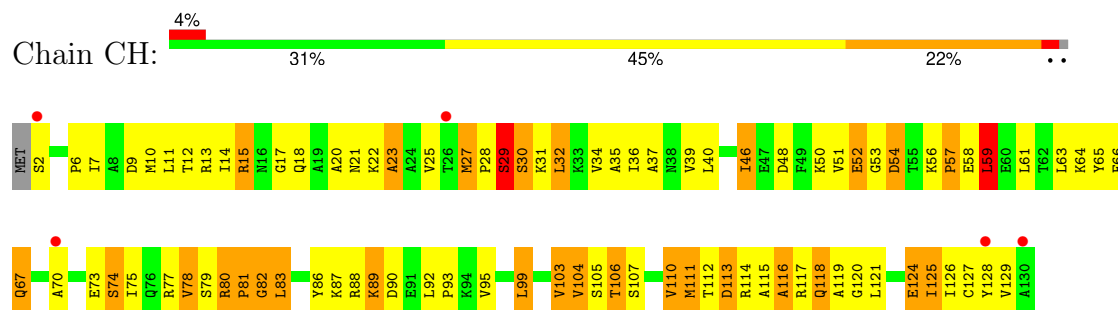
• Molecule 7: 30S ribosomal protein S7



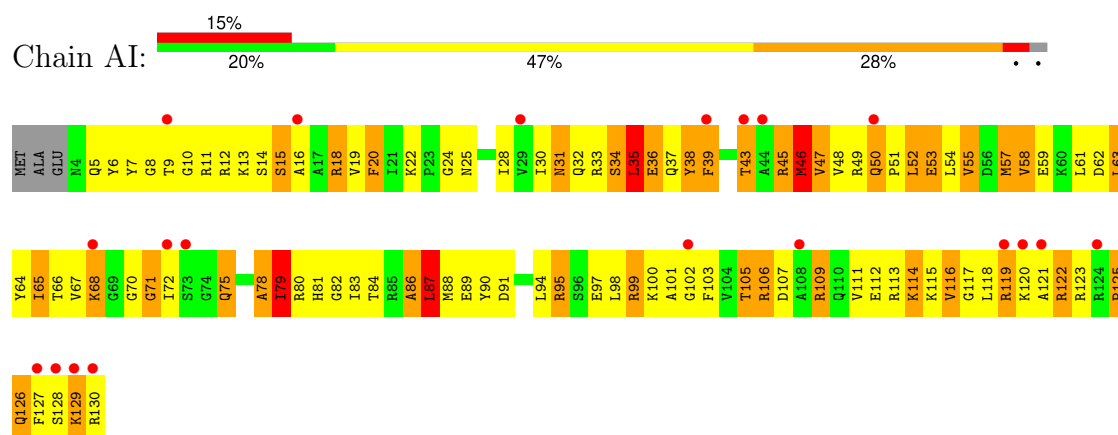
• Molecule 8: 30S ribosomal protein S8



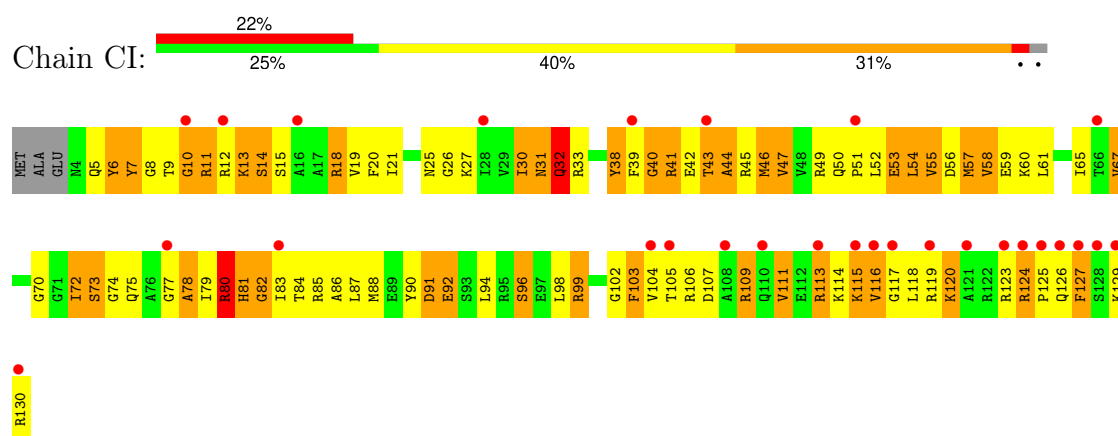
• Molecule 8: 30S ribosomal protein S8



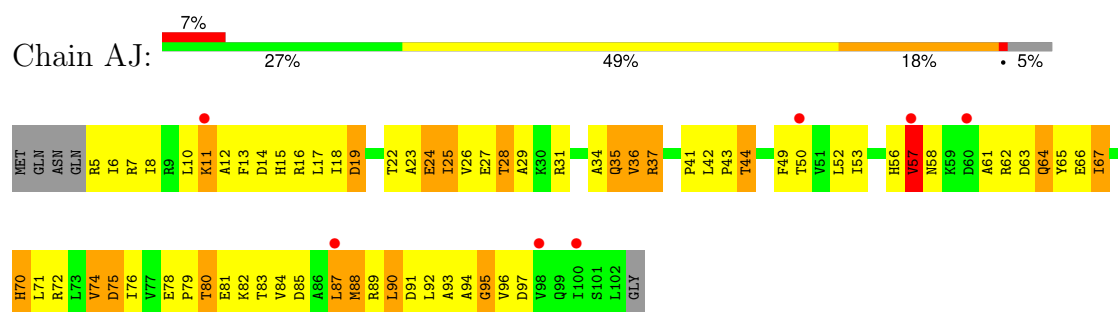
• Molecule 9: 30S ribosomal protein S9



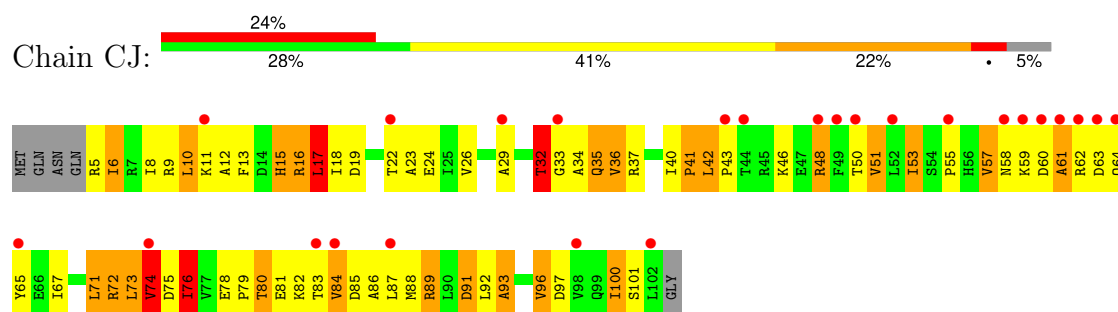
• Molecule 9: 30S ribosomal protein S9



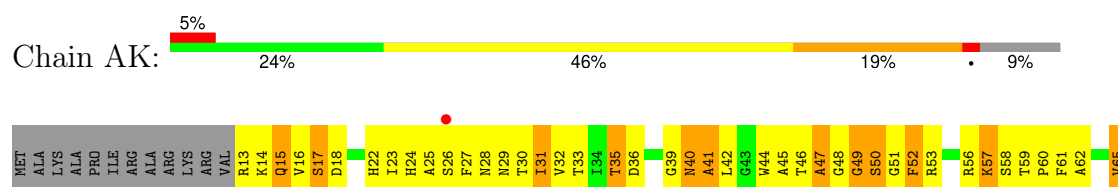
• Molecule 10: 30S ribosomal protein S10



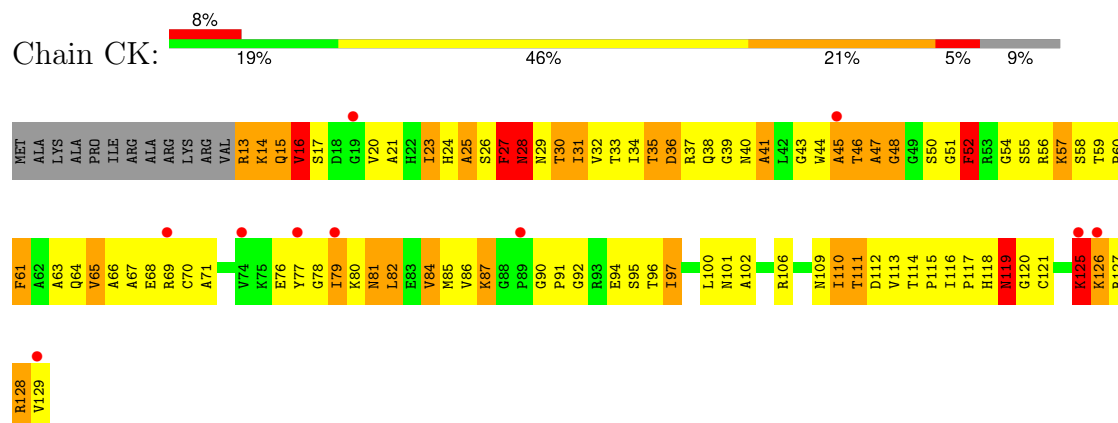
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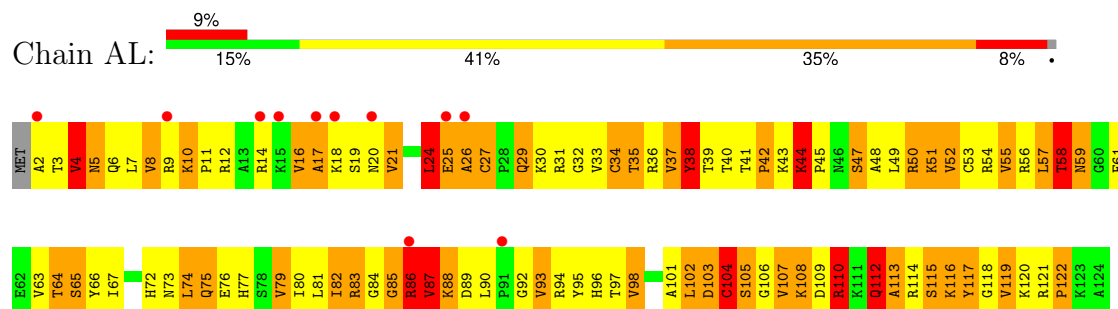
• Molecule 11: 30S ribosomal protein S11



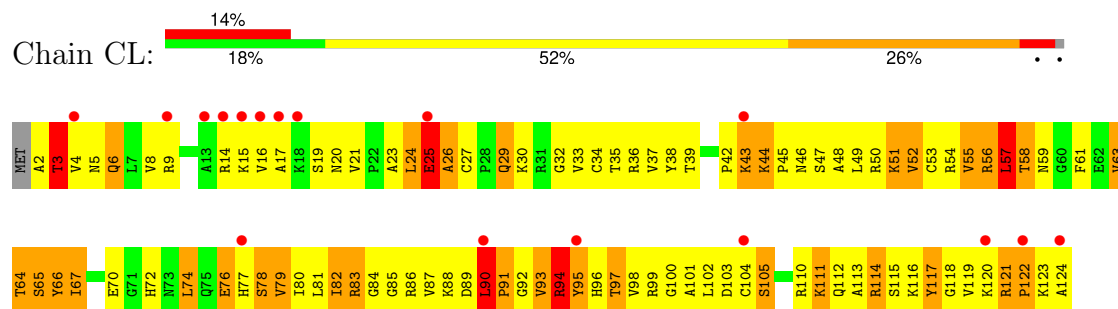
- Molecule 11: 30S ribosomal protein S11



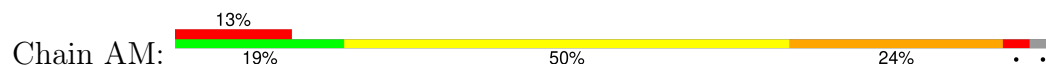
- Molecule 12: 30S ribosomal protein S12

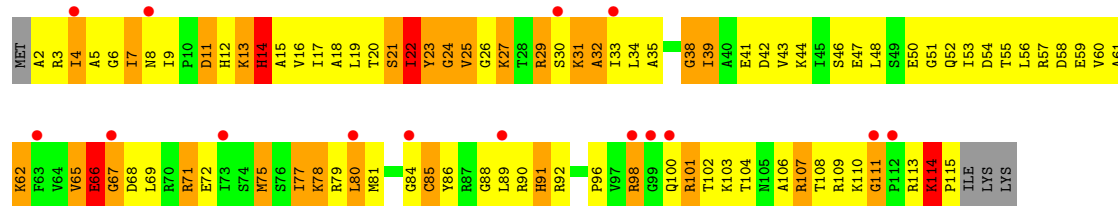


- Molecule 12: 30S ribosomal protein S12

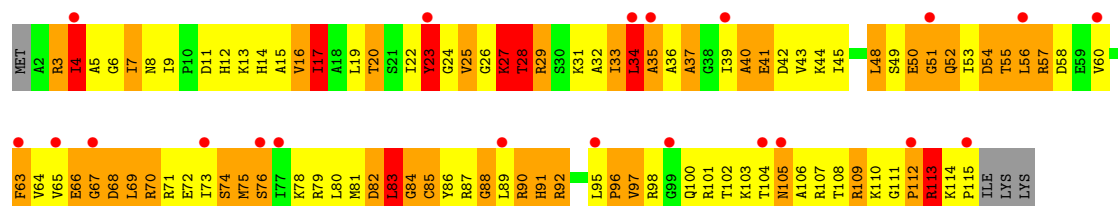


- Molecule 13: 30S ribosomal protein S13

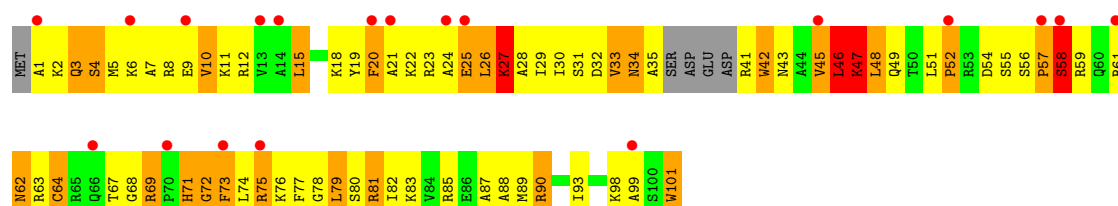
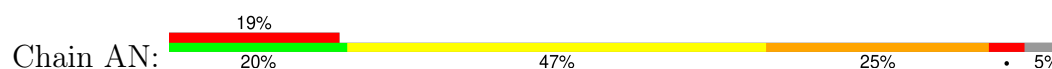




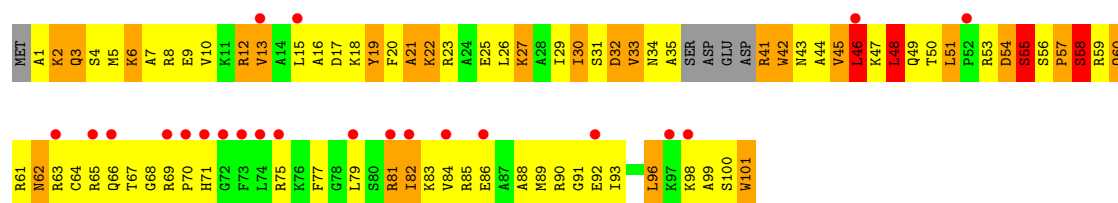
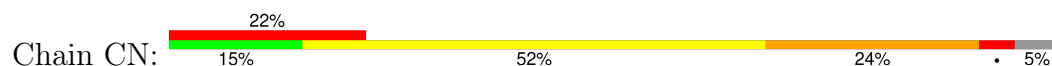
• Molecule 13: 30S ribosomal protein S13



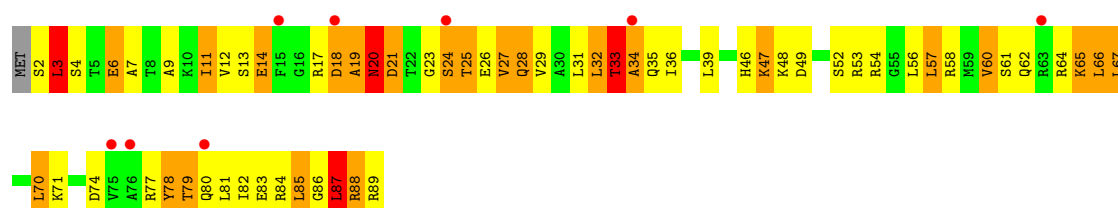
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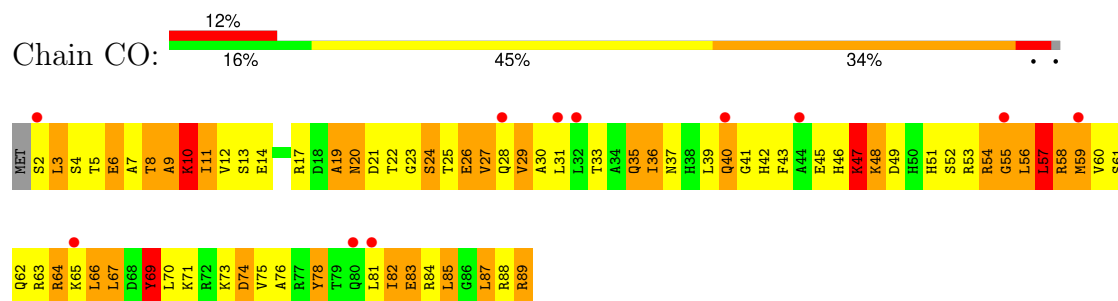
• Molecule 14: 30S ribosomal protein S14



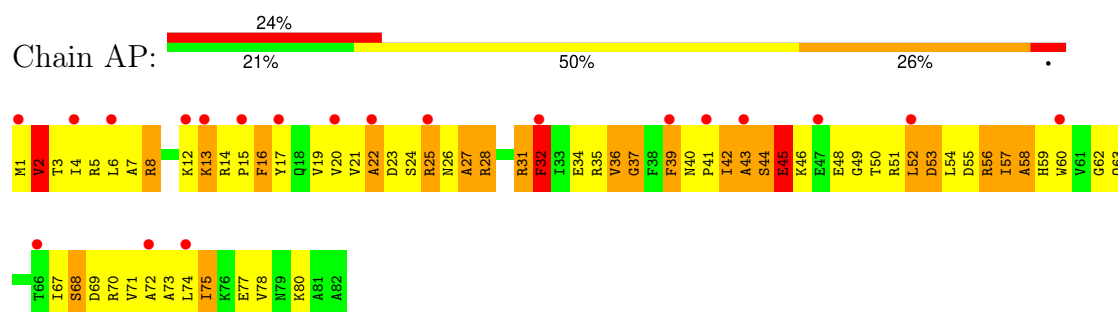
• Molecule 15: 30S ribosomal protein S15



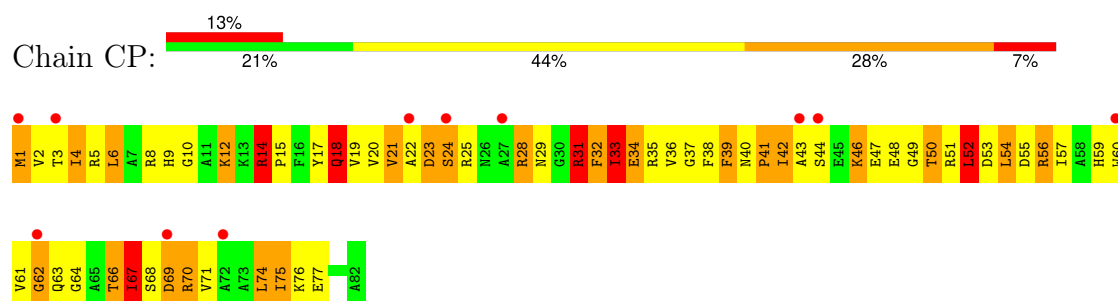
- Molecule 15: 30S ribosomal protein S15



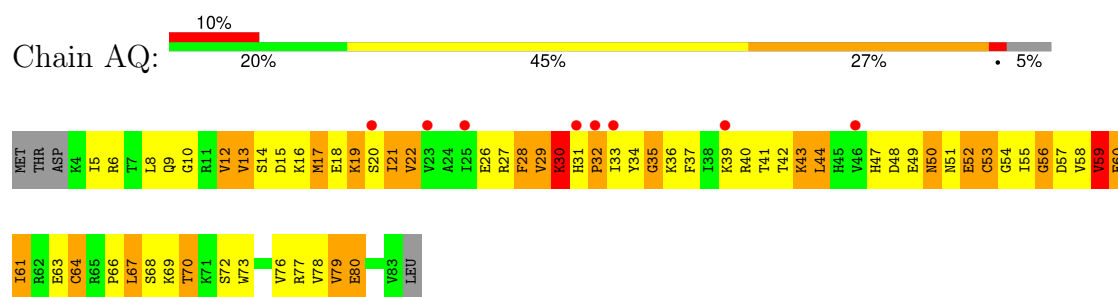
- Molecule 16: 30S ribosomal protein S16



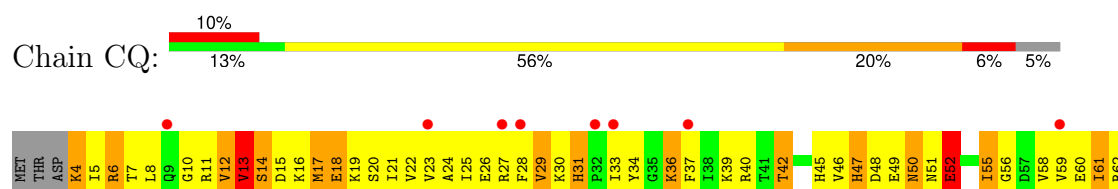
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

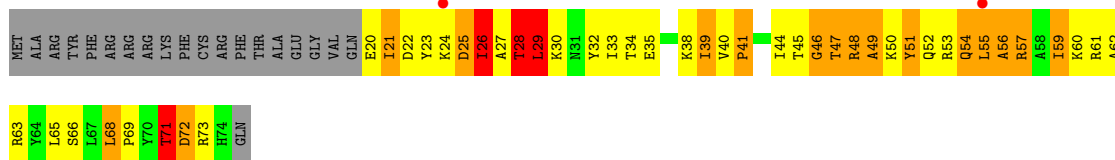


- Molecule 17: 30S ribosomal protein S17

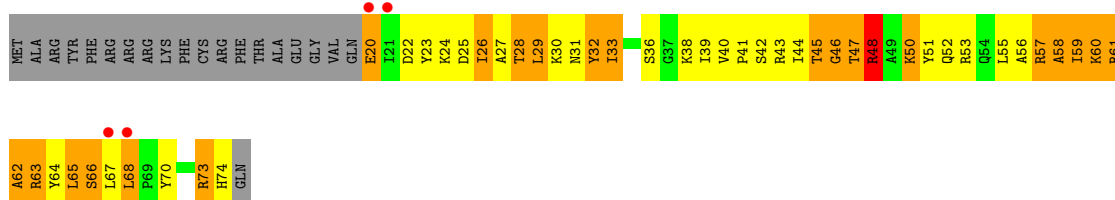




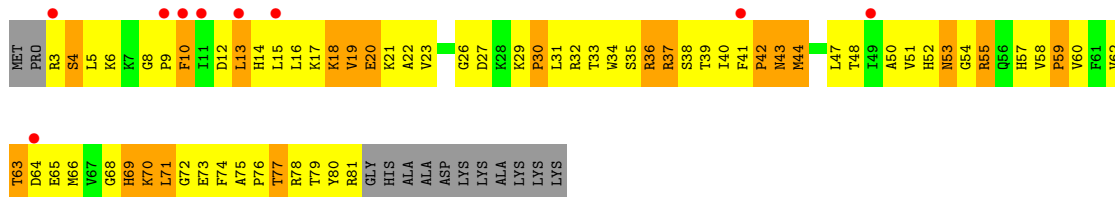
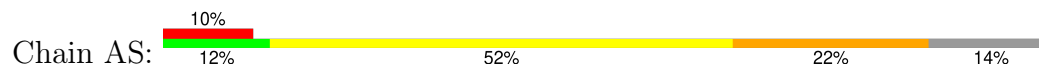
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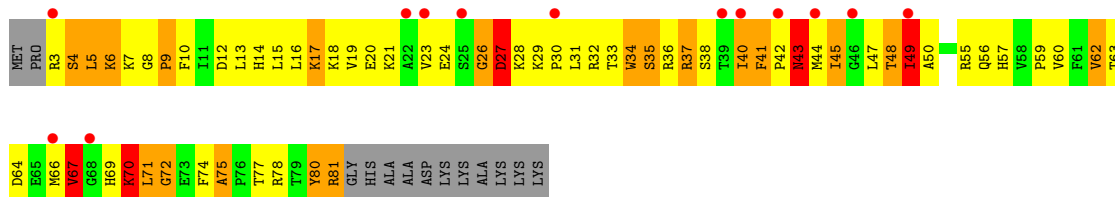
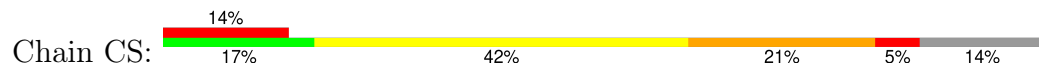
• Molecule 18: 30S ribosomal protein S18



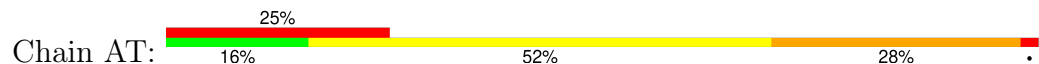
• Molecule 19: 30S ribosomal protein S19

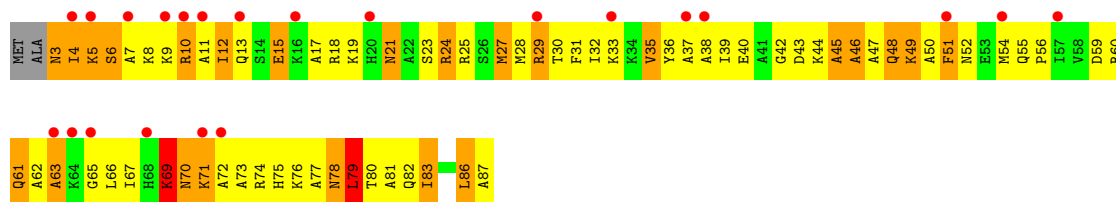


• Molecule 19: 30S ribosomal protein S19

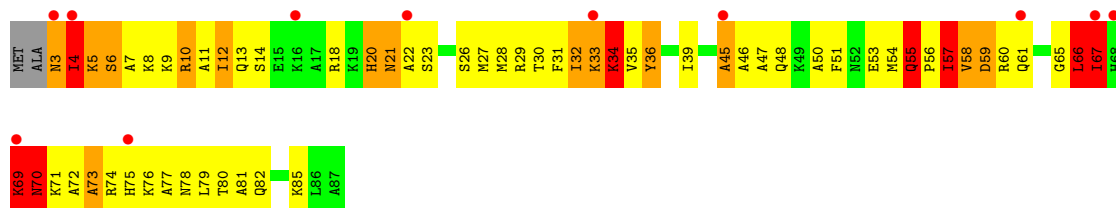


• Molecule 20: 30S ribosomal protein S20

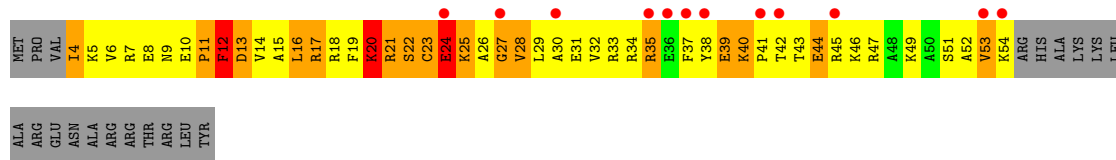




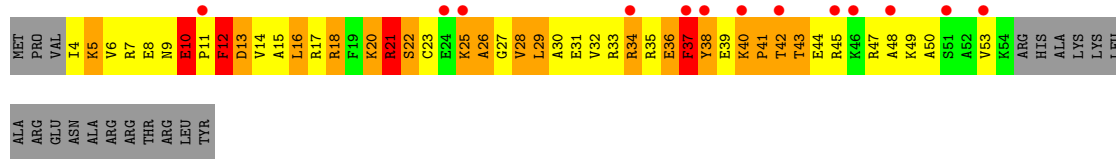
• Molecule 20: 30S ribosomal protein S20



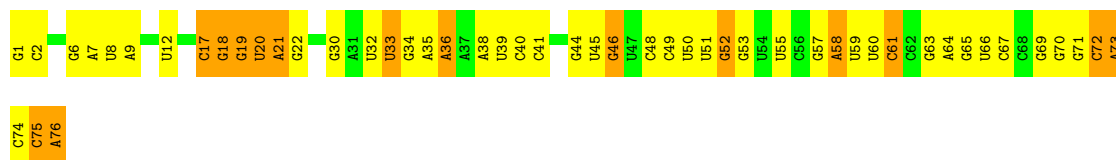
• Molecule 21: 30S ribosomal protein S21



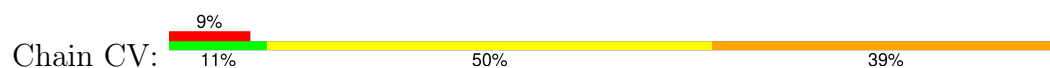
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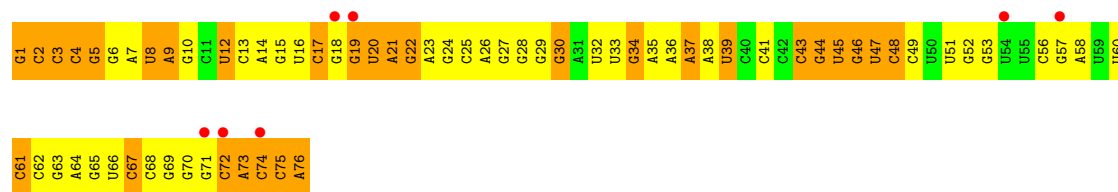


• Molecule 22: Phenylalanine specific transfer RNA, tRNA-Phe



• Molecule 22: Phenylalanine specific transfer RNA, tRNA-Phe

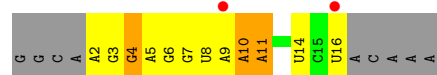




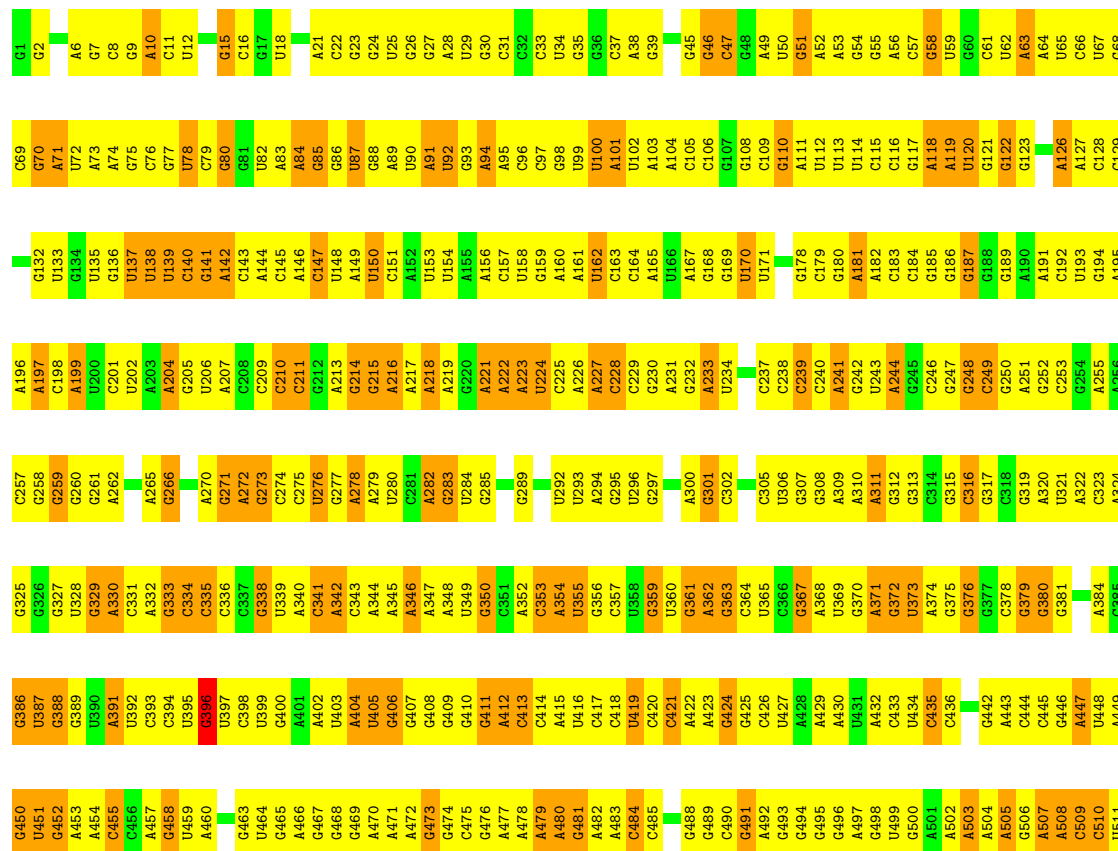
• Molecule 23: Messenger RNA, mRNA



• Molecule 23: Messenger RNA, mRNA

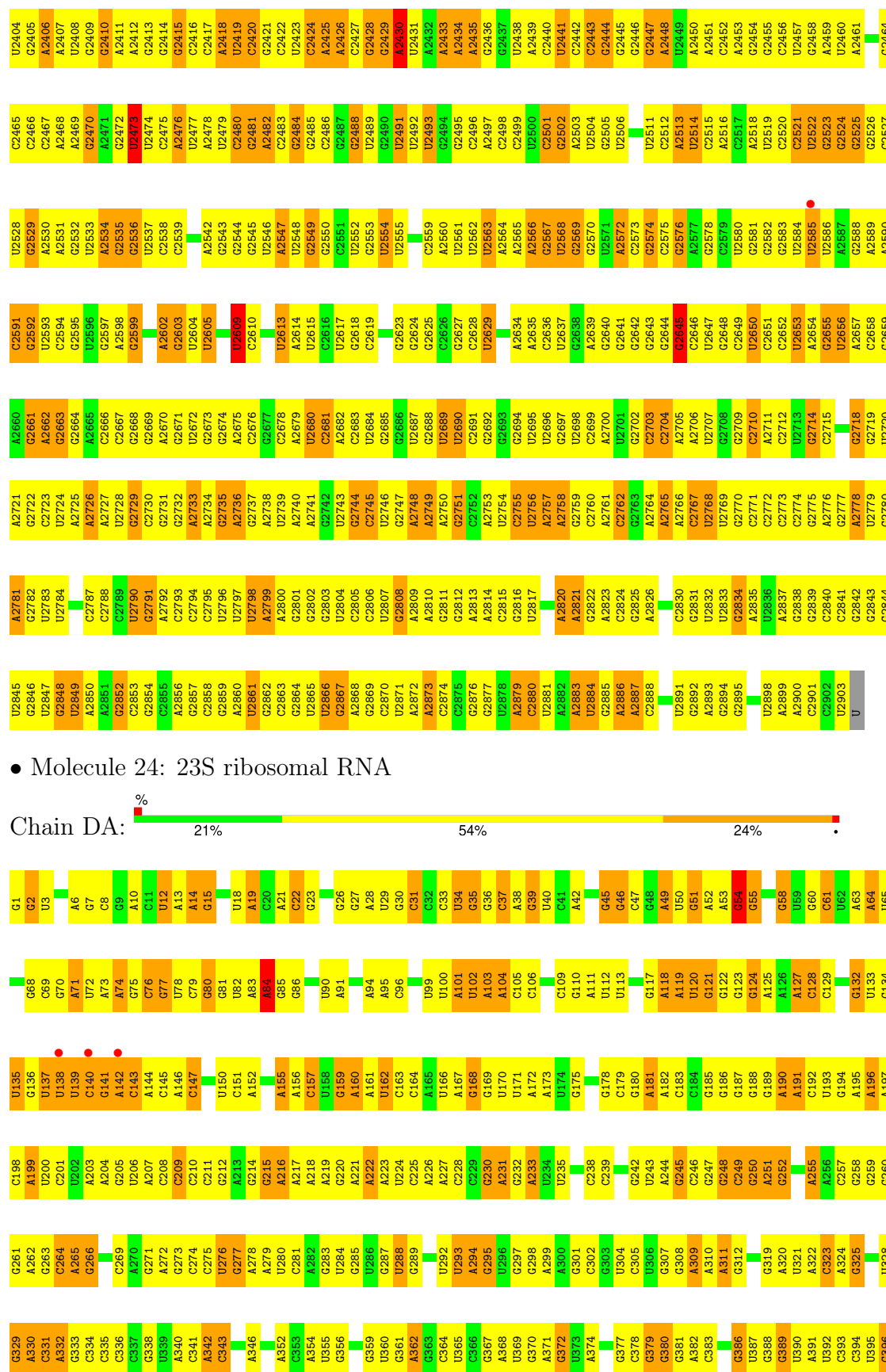


• Molecule 24: 23S ribosomal RNA



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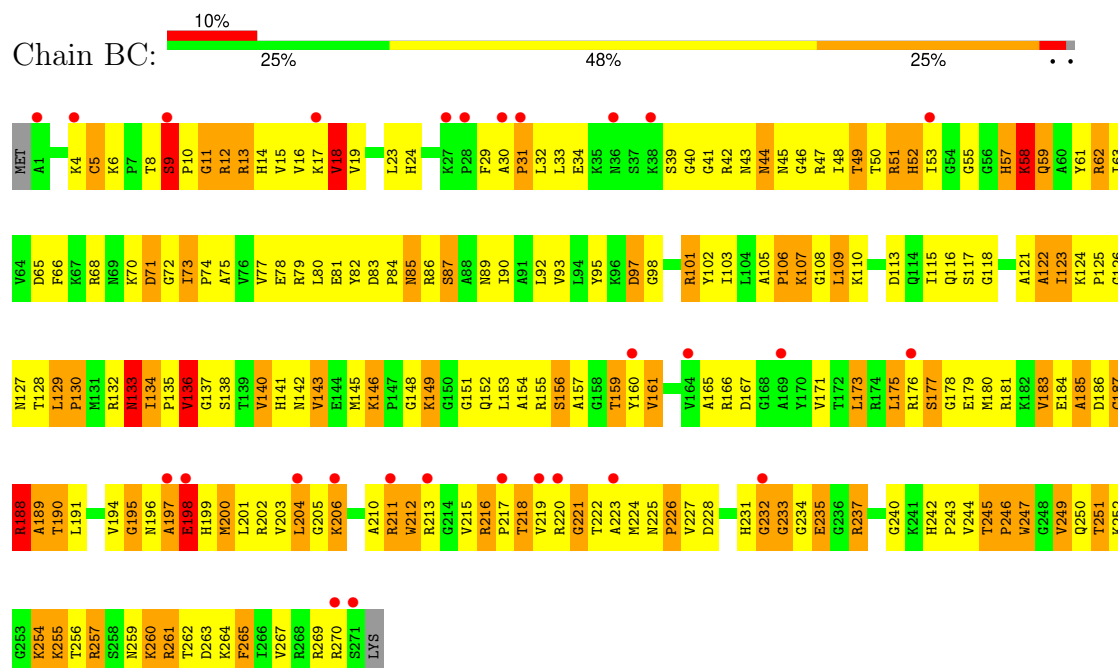
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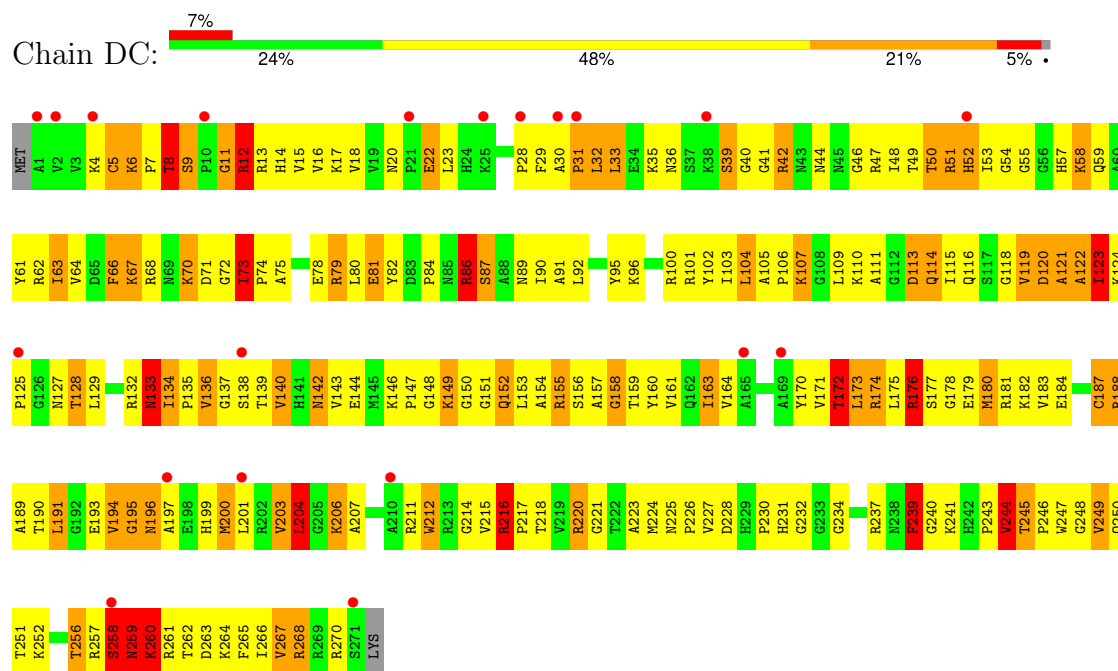
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			A943	A877	C1008	A943	A877	U813	A743	C679	G618	C557	U427	U427
			A944	A878	A1009	A944	A878	C814		C680	G619	U558	G493	G493
			A945	C879	A1010	A945	C879	C815	U746	G681	G620	G559	G494	A430
			C946	C880	G1011	C946	C880	C816	U747	C682	A621	C560	G495	U431
			A947	G881	U1012	A947	G881	C817	G748	U683	G622		G496	A432
			C948	G882	C1013	C948	G882	U818	A749	A685	C623	A563	A497	C433
				G883	A1014		G883	A819	A750	A686	C624	C564	U434	U434
			C951	U884	U1015		U884	A820	A751	U686	G625	C565	U499	C435
			G952	C885	G1016		C885	A821	A752	C687	A626	U566	G500	C436
			G953	A			A	C822	A753	U688	A627	U567	A501	U437
			G954	U			U	C823	U754	A689	G628	U568	A502	G438
			U955	C			C	U824	U755	C690	G629	U569	A503	A439
			G956	C			C	U825	A756	C691	G630	G570	A504	C440
			C957	C			C	U826	G757	C692	U571	U571	U441	U441
			U958	G			G	U827	A693	A693	A572	G506	G506	G442
			A959				A892	U828	A761	U694	C634	U573	A507	A443
			A960	C893	G1026	A960	C893	A829	U762	C695	C635	A574	A508	C444
			C961	U894	A1027	C961	U894	G830	A763	G696	G636	A575	C509	C445
			G962	U895	A1028	G962	U895	G831	A764	G697	A637	U576	C510	G446
			U963	A896	C1029	U963	A896	U832	C765	C698	G638	G577	U511	A447
			C964	C897	U1030	C964	C897	A833	G770	A699	U639	G578	G512	
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				A899	A1032		A899	C835		G704	U641	U580	A514	U451
			G969	A900	U1033	G969	A900		U773	G704	U642	C581	C517	G452
			U970	C901		U970	C901	U839	G774	G708	A643	A582	C517	A453
			G971			G971			G775	G709	A644	G583	C517	A454
			A972	G907	G1038	A972	G907	U842	G776	U709	C645	C584	G520	G455
			A973	C908	A1040	A973	C908	A844	G777	U710	U646	G585	U521	C456
			G974	A909	G1041	G974	A909	A844	G778	G711	G647	A586	A522	A457
			A975	A910	G1042	A975	A910	U846	U779	G712	G648	C587	G458	G459
			G976	A911	G1043	G976	A911	U847	G780	G713	G649	C588	C523	U459
			G977	C912	C1044	G977	C912		A781	U714	C650	U589	A526	A460

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G2264	C2200	A2076	U2012	U1946	U1884	G1823	A1759	G1624	U1562	U1497	A1435	U1372
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G2306	G2246	U2182	G2056	U1991	U1928	A1866	U1806	G1666	C1605	A1545	G1480	G1418
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C2310	U2250	G2186	G2060	U1995	A1932	C1870	U1741	C1670	U1671	A1549	U1484	G1422
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C2312	G2252	G2126	G2062	C1997	C1934	A1872	A1810	A1673	A1610	A1551	U1486	G1424
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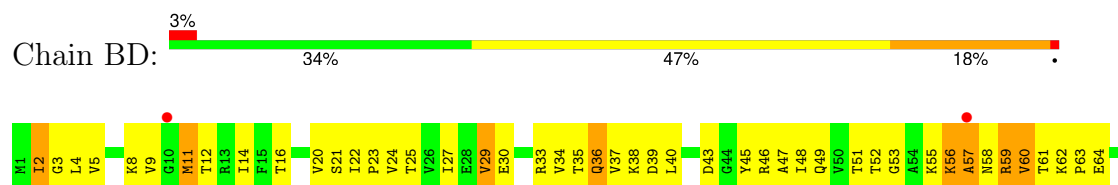
• Molecule 26: 50S ribosomal protein L2

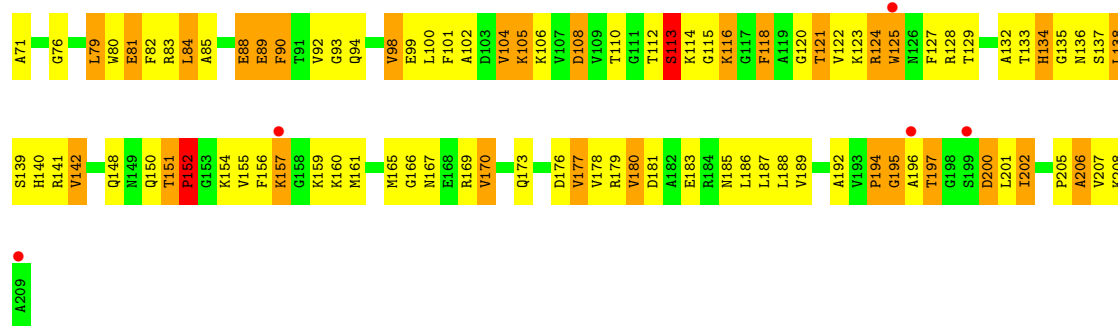


• Molecule 26: 50S ribosomal protein L2

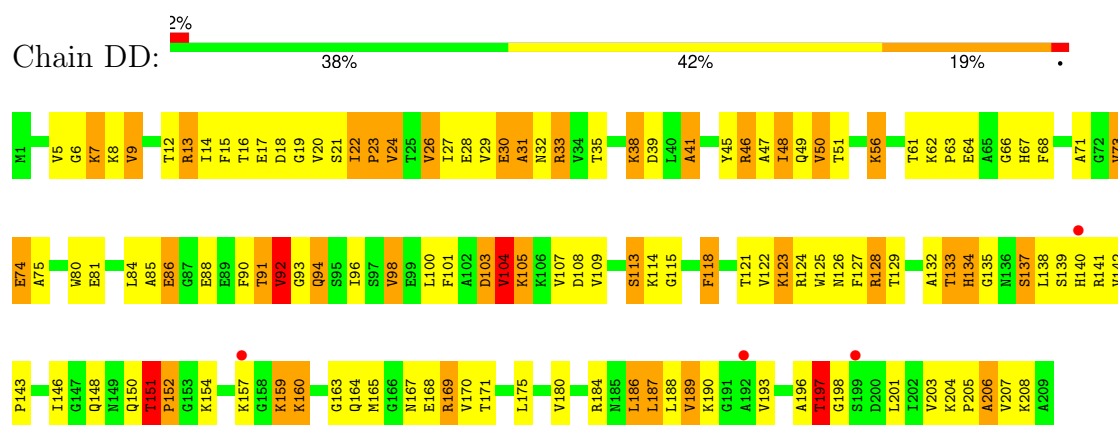


• Molecule 27: 50S ribosomal protein L3





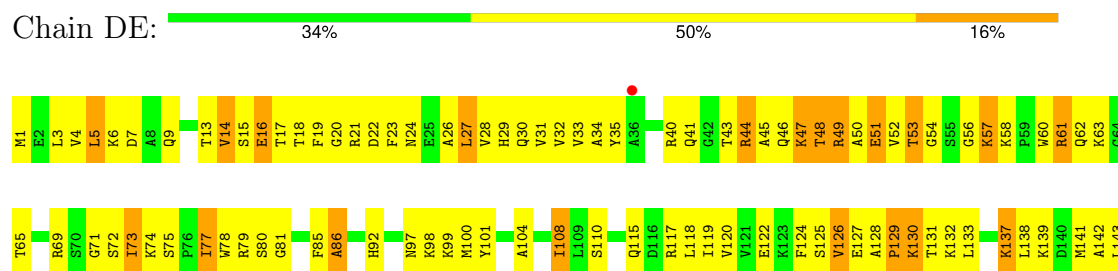
• Molecule 27: 50S ribosomal protein L3

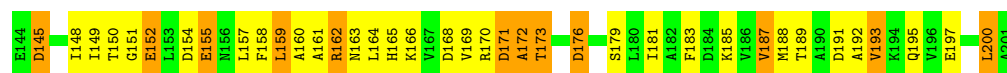


• Molecule 28: 50S ribosomal protein L4

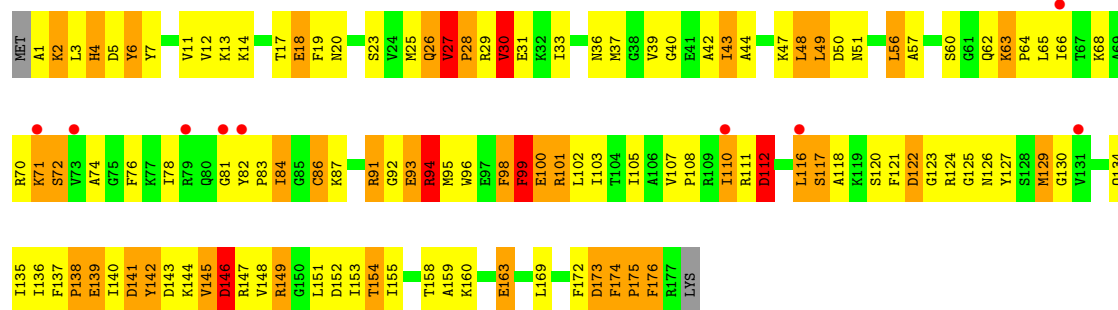


• Molecule 28: 50S ribosomal protein L4

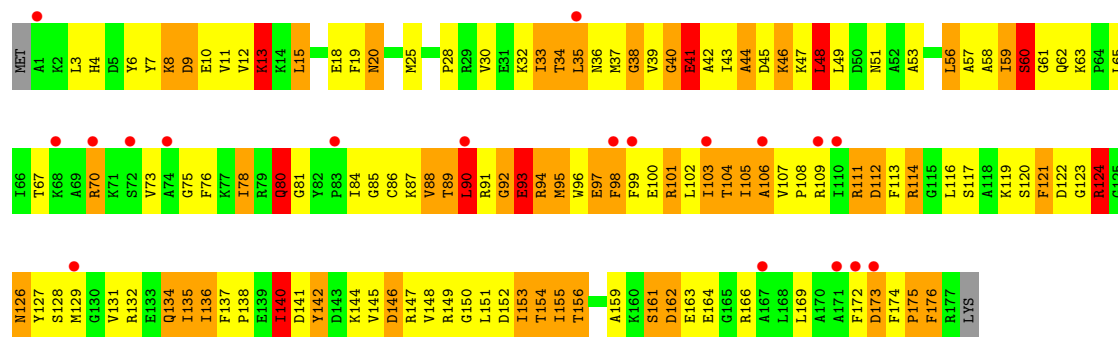




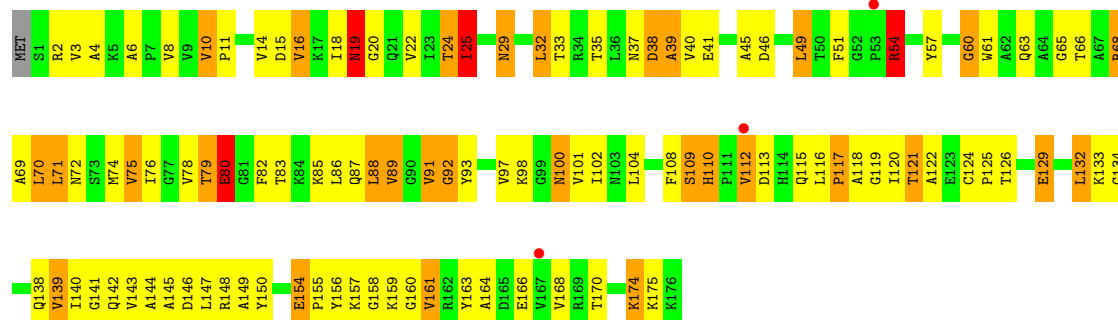
• Molecule 29: 50S ribosomal protein L5



• Molecule 29: 50S ribosomal protein L5

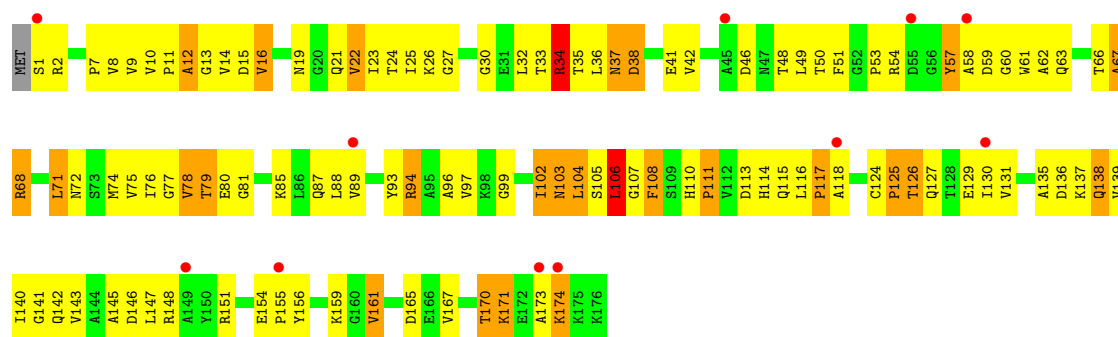


• Molecule 30: 50S ribosomal protein L6

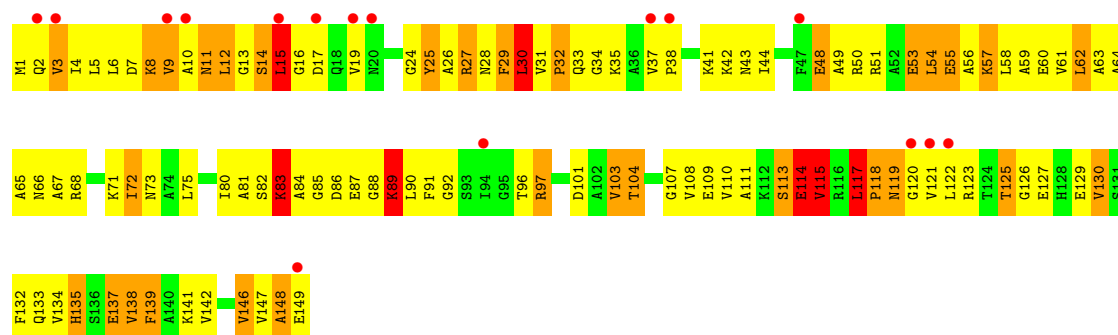


• Molecule 30: 50S ribosomal protein L6

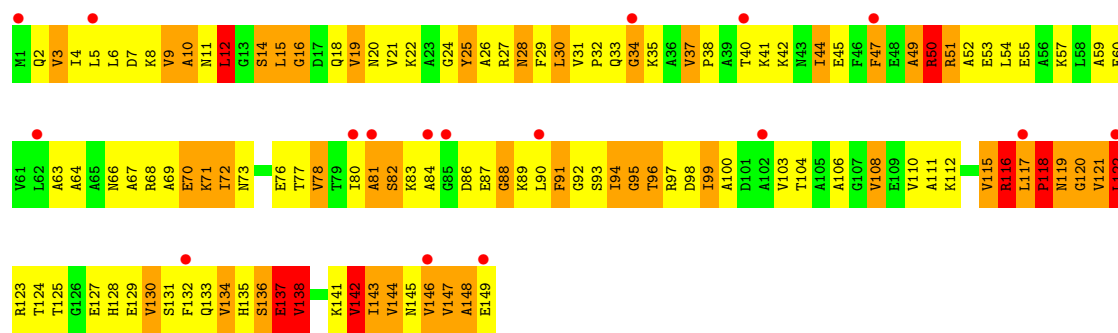
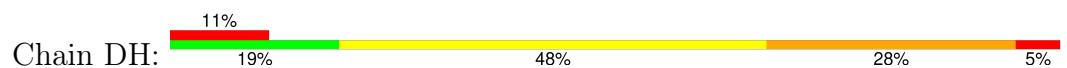




• Molecule 31: 50S ribosomal protein L9



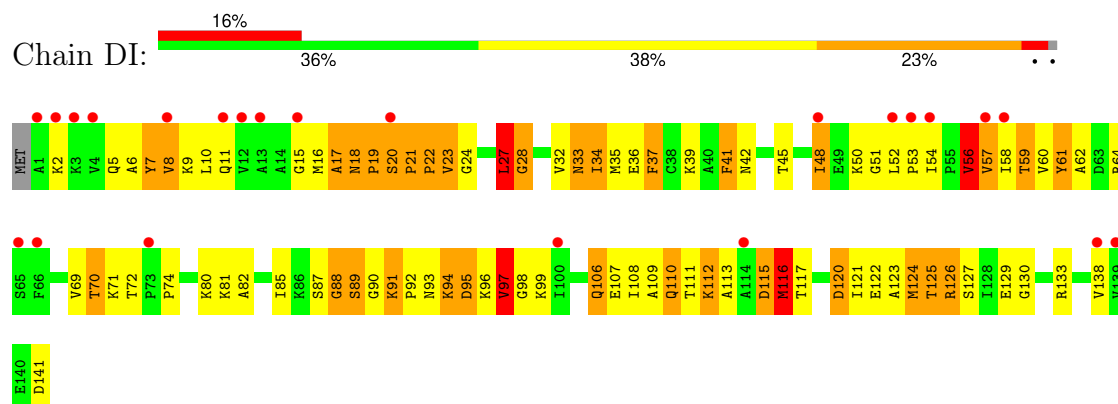
• Molecule 31: 50S ribosomal protein L9



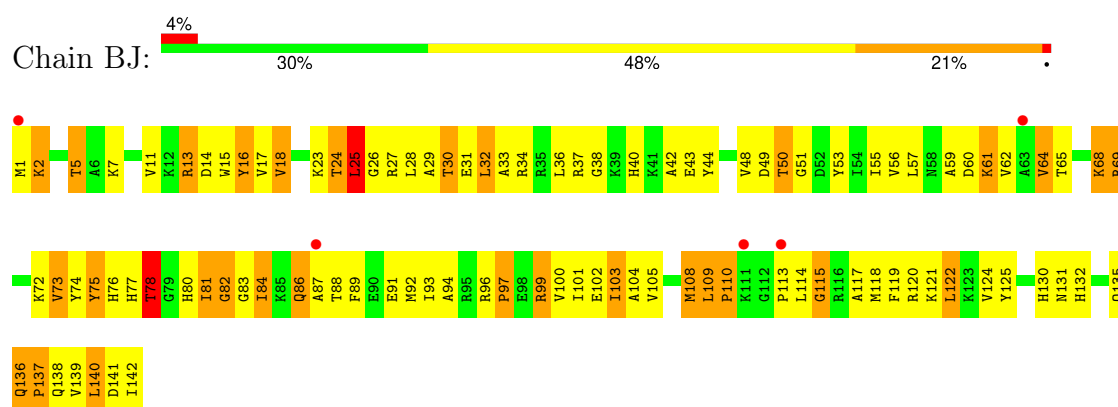
• Molecule 32: 50S ribosomal protein L11



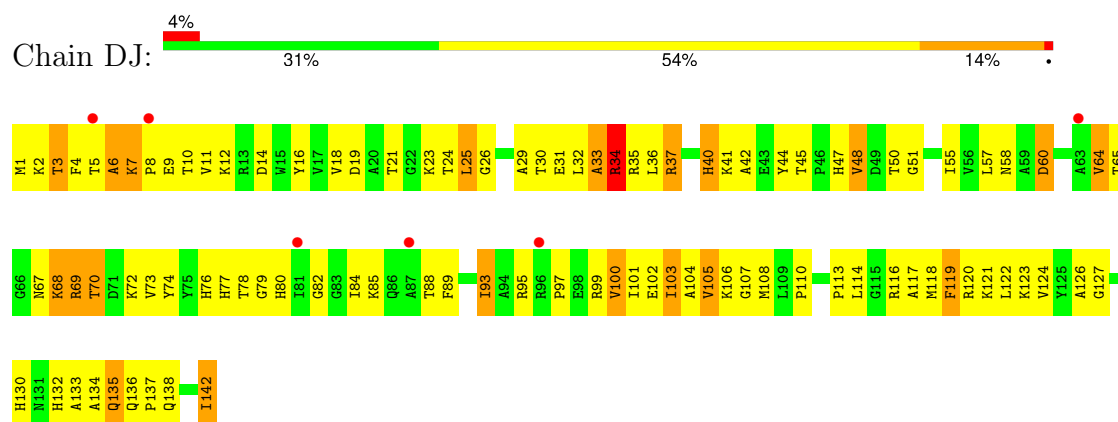
- Molecule 32: 50S ribosomal protein L11



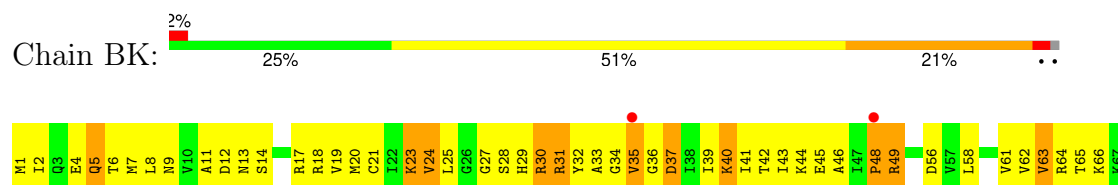
- Molecule 33: 50S ribosomal protein L13



- Molecule 33: 50S ribosomal protein L13



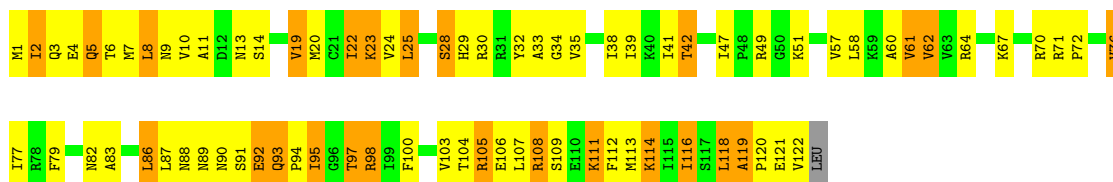
- Molecule 34: 50S ribosomal protein L14





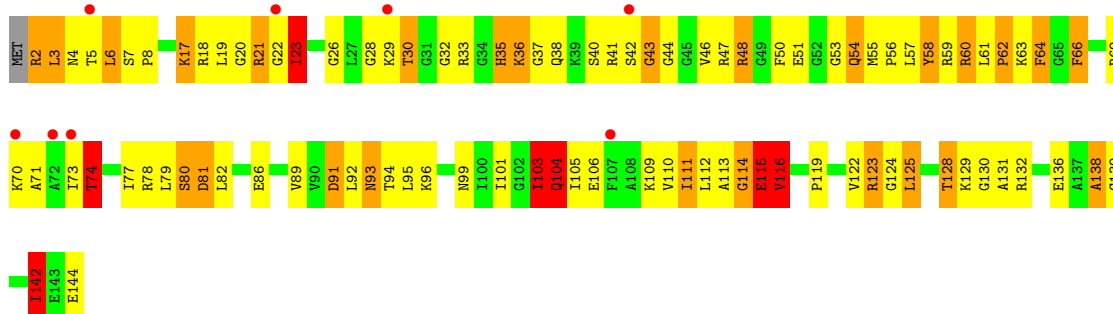
- Molecule 34: 50S ribosomal protein L14

Chain DK: 36% 43% 20%



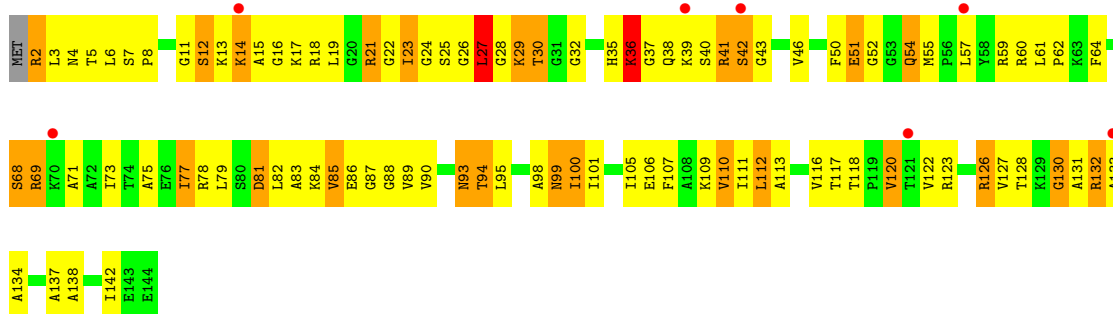
- Molecule 35: 50S ribosomal protein L15

Chain BL: 6% 33% 43% 18% 5%



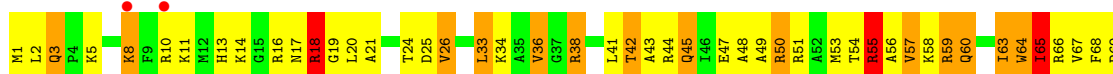
- Molecule 35: 50S ribosomal protein L15

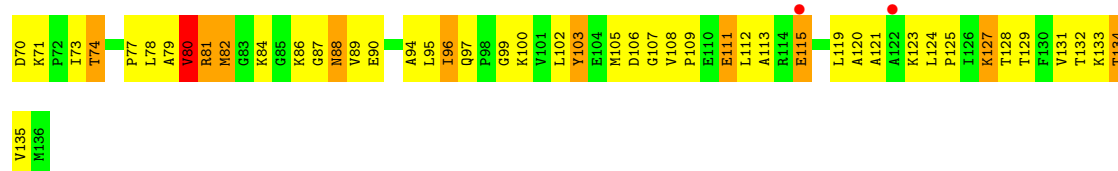
Chain DL: 5% 31% 49% 18%



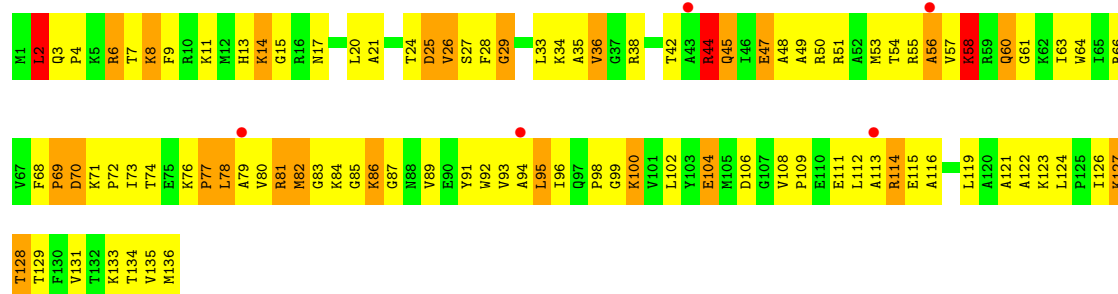
- Molecule 36: 50S ribosomal protein L16

Chain BM: 3% 31% 49% 18%

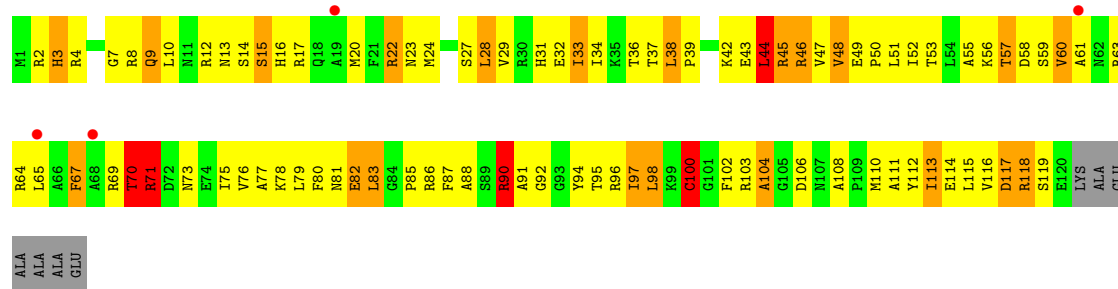




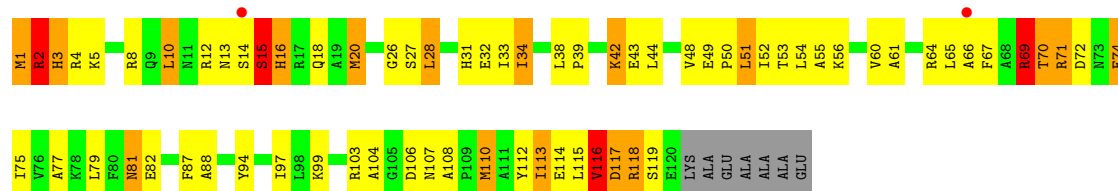
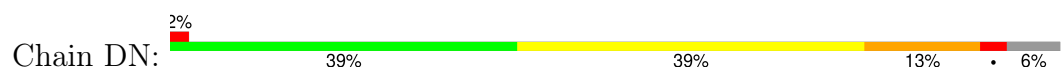
- Molecule 36: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L17

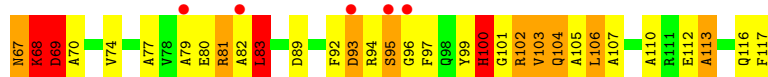


- Molecule 37: 50S ribosomal protein L17

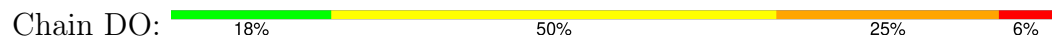


- Molecule 38: 50S ribosomal protein L18

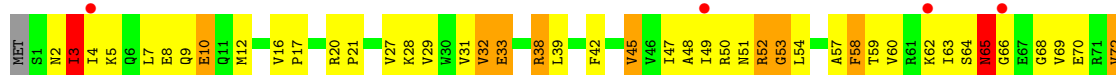




- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L19

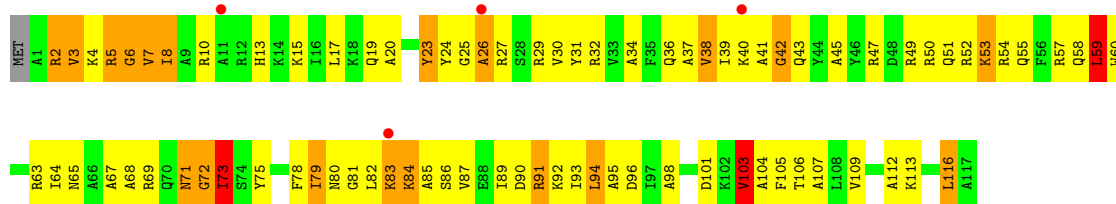


- Molecule 40: 50S ribosomal protein L20

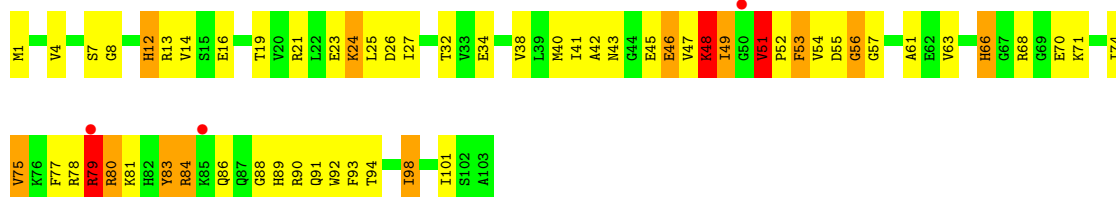
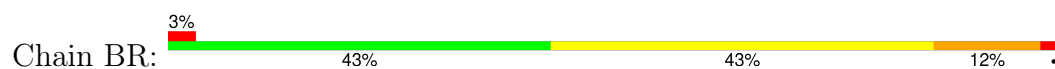


- Molecule 40: 50S ribosomal protein L20

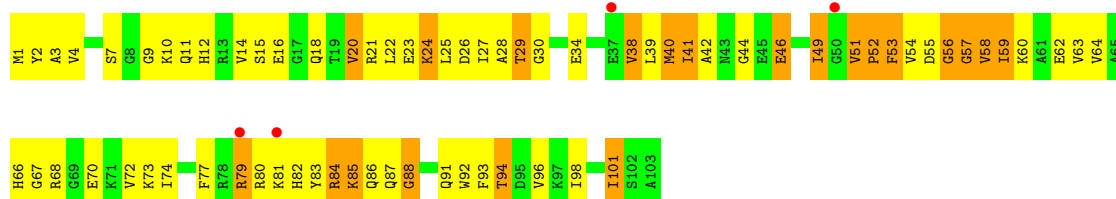




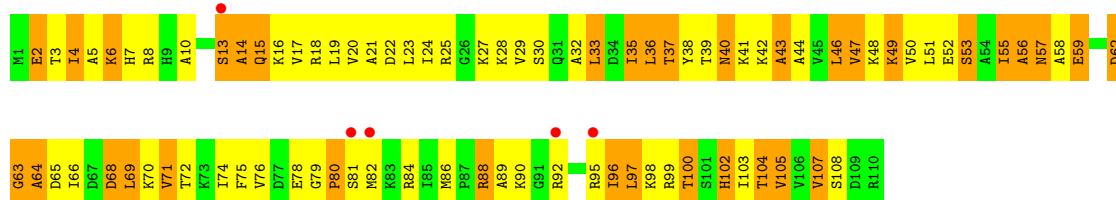
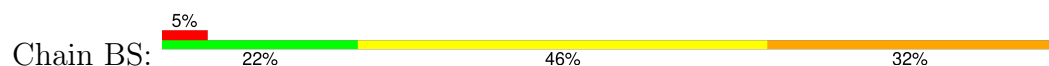
• Molecule 41: 50S ribosomal protein L21



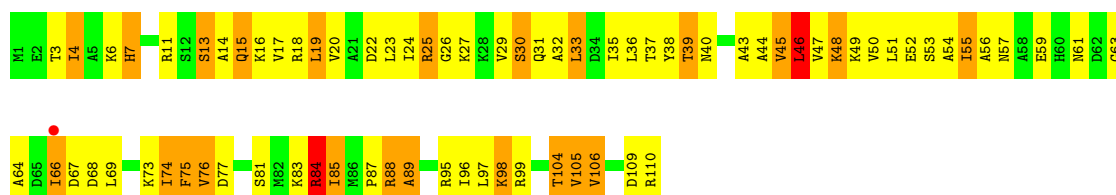
• Molecule 41: 50S ribosomal protein L21



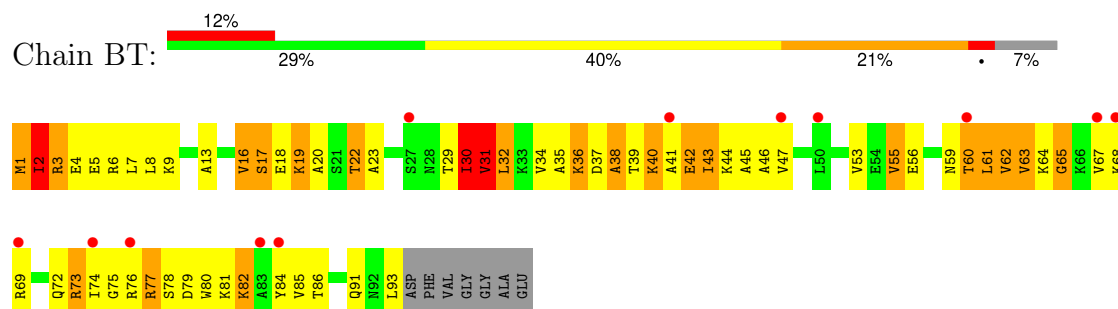
• Molecule 42: 50S ribosomal protein L22



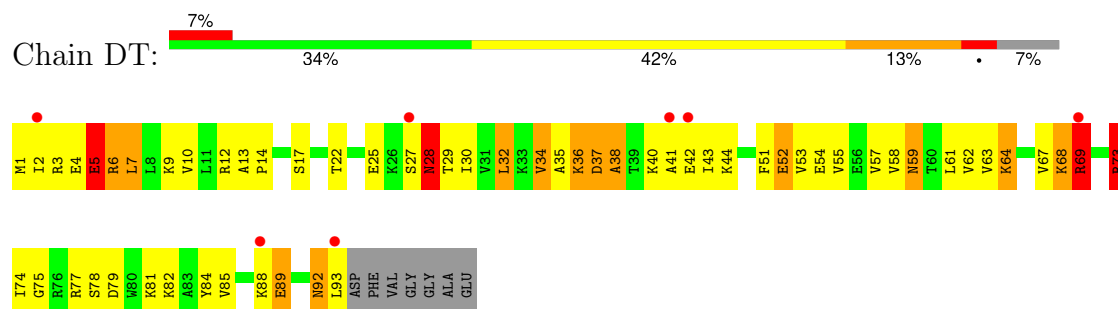
• Molecule 42: 50S ribosomal protein L22



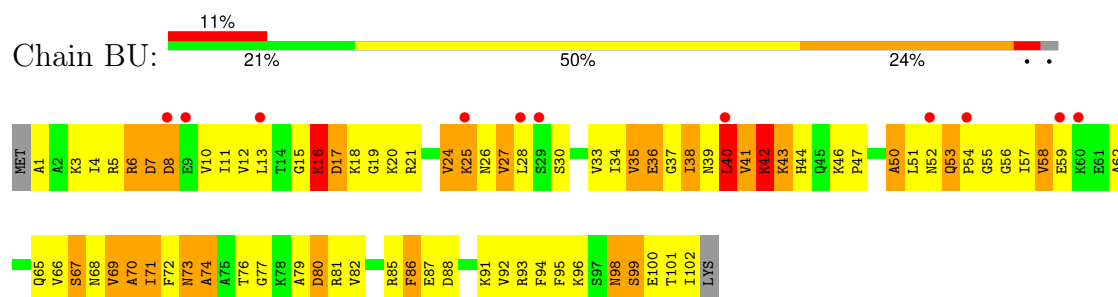
- Molecule 43: 50S ribosomal protein L23



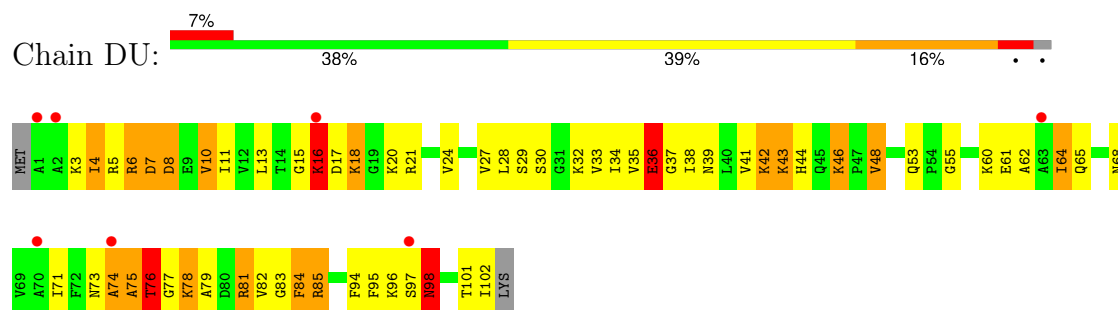
- Molecule 43: 50S ribosomal protein L23



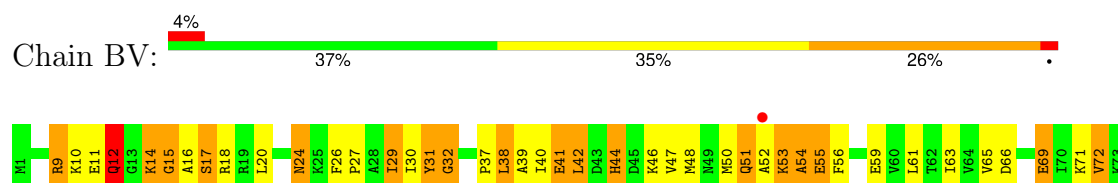
- Molecule 44: 50S ribosomal protein L24



- Molecule 44: 50S ribosomal protein L24

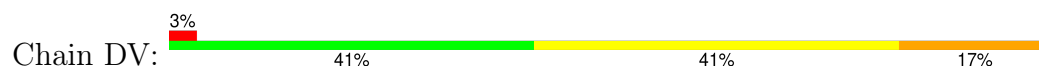


- Molecule 45: 50S ribosomal protein L25

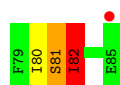
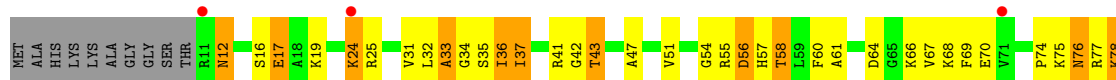
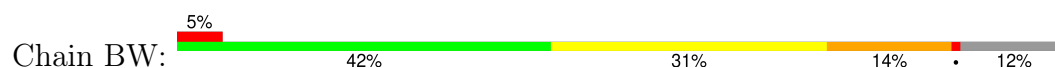




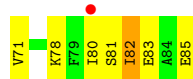
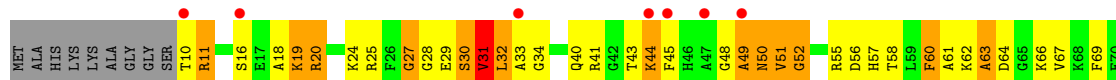
- Molecule 45: 50S ribosomal protein L25



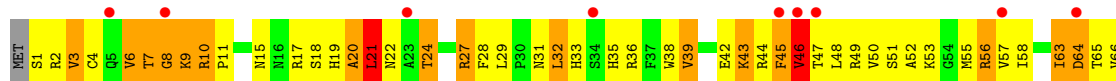
- Molecule 46: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28

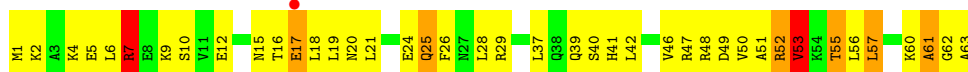


- Molecule 47: 50S ribosomal protein L28

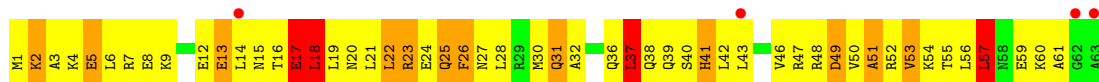
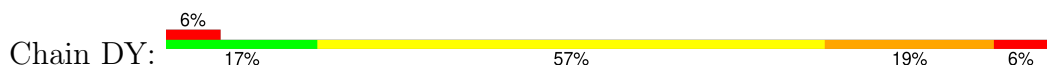




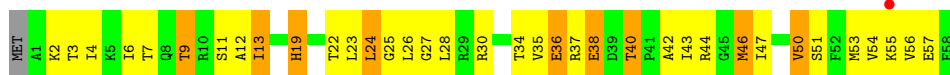
• Molecule 48: 50S ribosomal protein L29



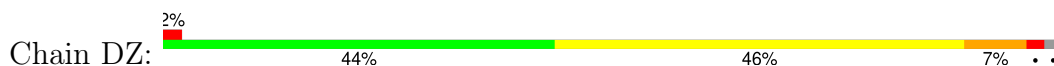
• Molecule 48: 50S ribosomal protein L29



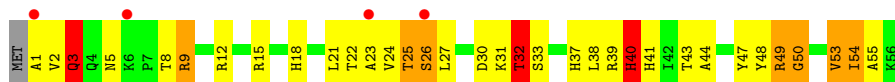
• Molecule 49: 50S ribosomal protein L30



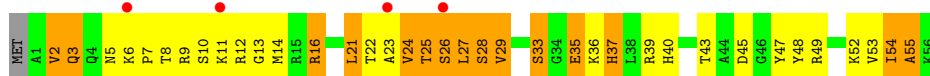
• Molecule 49: 50S ribosomal protein L30



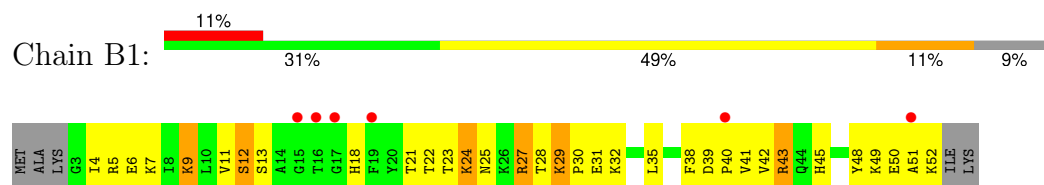
• Molecule 50: 50S ribosomal protein L32



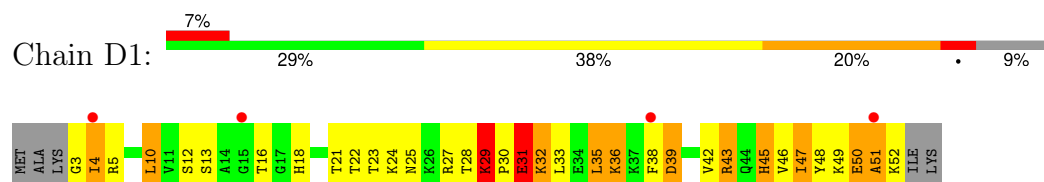
• Molecule 50: 50S ribosomal protein L32



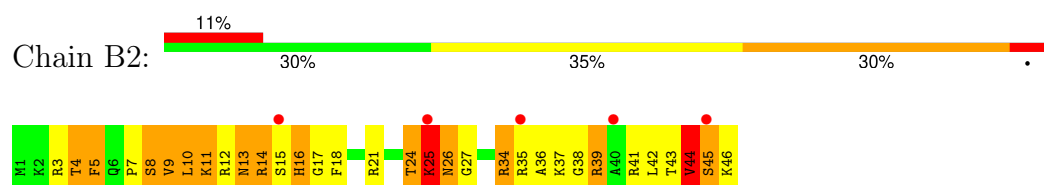
- Molecule 51: 50S ribosomal protein L33



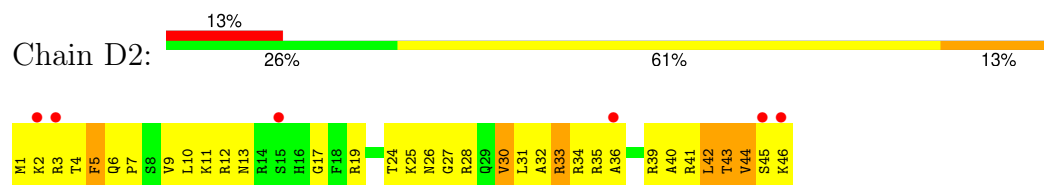
- Molecule 51: 50S ribosomal protein L33



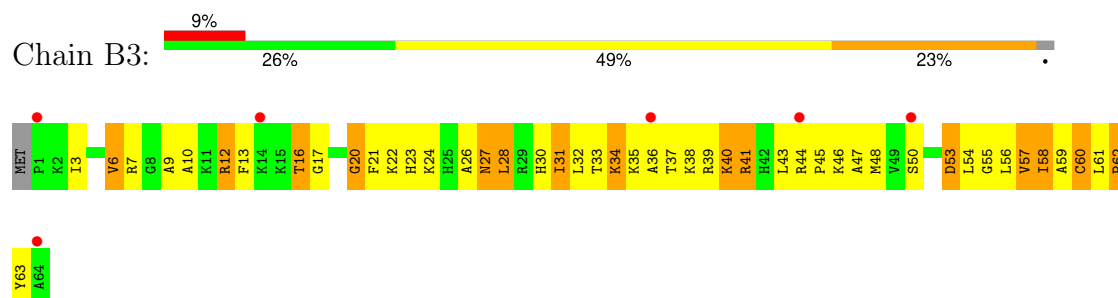
- Molecule 52: 50S ribosomal protein L34



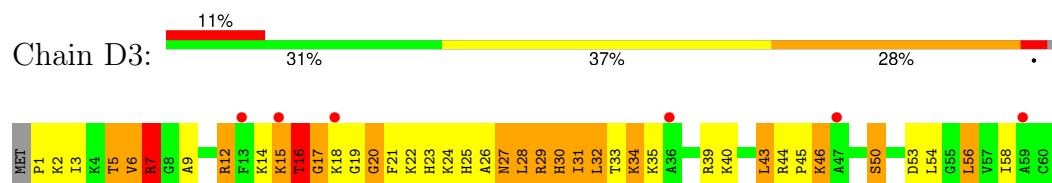
- Molecule 52: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L35



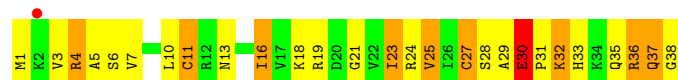
- Molecule 53: 50S ribosomal protein L35



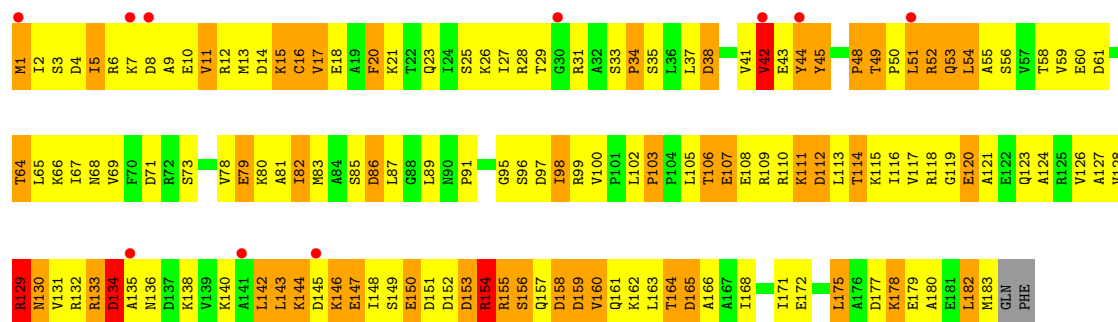
- Molecule 54: 50S ribosomal protein L36



- 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 0.204 , 0.252	Depositor DCC
R_{free} test set	1998 reflections (0.25%)	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	0.34	0/36966	0.95	39/57666 (0.1%)
1	CA	0.33	0/36944	0.93	15/57632 (0.0%)
2	AB	0.28	0/1735	0.61	0/2338
2	CB	0.26	0/1735	0.57	0/2338
3	AC	0.29	0/1651	0.61	0/2225
3	CC	0.30	0/1651	0.58	0/2225
4	AD	0.35	0/1665	0.69	0/2227
4	CD	0.29	0/1665	0.65	0/2227
5	AE	0.28	0/1118	0.66	0/1504
5	CE	0.30	0/1118	0.63	0/1504
6	AF	0.33	0/835	0.67	0/1128
6	CF	0.32	0/835	0.62	0/1128
7	AG	0.25	0/1195	0.52	0/1602
7	CG	0.27	0/1195	0.56	0/1602
8	AH	0.30	0/989	0.66	0/1326
8	CH	0.29	0/989	0.60	0/1326
9	AI	0.25	0/1034	0.59	0/1375
9	CI	0.27	0/1034	0.58	0/1375
10	AJ	0.26	0/796	0.60	0/1077
10	CJ	0.24	0/796	0.53	0/1077
11	AK	0.33	0/893	0.68	0/1205
11	CK	0.30	0/893	0.63	0/1205
12	AL	0.30	0/969	0.71	0/1300
12	CL	0.35	0/969	0.71	1/1300 (0.1%)
13	AM	0.25	0/892	0.57	0/1193
13	CM	0.26	0/892	0.64	0/1193
14	AN	0.26	0/785	0.55	0/1043
14	CN	0.25	0/785	0.56	0/1043
15	AO	0.35	0/722	0.58	0/964
15	CO	0.27	0/722	0.60	0/964
16	AP	0.32	0/659	0.74	2/884 (0.2%)
16	CP	0.29	0/659	0.63	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.28	0/657	0.61	0/881
17	CQ	0.34	0/657	0.71	0/881
18	AR	0.31	0/462	0.69	0/621
18	CR	0.30	0/462	0.60	0/621
19	AS	0.26	0/652	0.57	0/877
19	CS	0.27	0/652	0.65	0/877
20	AT	0.27	0/671	0.59	0/888
20	CT	0.25	0/671	0.58	0/888
21	AU	0.37	0/430	0.76	0/570
21	CU	0.30	0/430	0.61	0/570
22	AV	0.40	1/1813 (0.1%)	0.89	0/2823
22	CV	0.32	1/1813 (0.1%)	0.77	0/2823
23	AX	0.32	0/388	0.88	0/603
23	CX	0.28	0/363	0.85	0/564
24	BA	0.36	0/69659	0.97	72/108672 (0.1%)
24	DA	0.43	3/69659 (0.0%)	1.07	120/108672 (0.1%)
25	BB	0.28	0/2828	0.84	0/4410
25	DB	0.36	0/2850	0.96	2/4444 (0.0%)
26	BC	0.29	0/2121	0.67	0/2852
26	DC	0.34	0/2121	0.75	2/2852 (0.1%)
27	BD	0.31	0/1586	0.66	0/2134
27	DD	0.36	0/1586	0.68	0/2134
28	BE	0.29	0/1571	0.59	0/2113
28	DE	0.32	0/1571	0.67	1/2113 (0.0%)
29	BF	0.26	0/1434	0.53	0/1926
29	DF	0.29	0/1434	0.66	0/1926
30	BG	0.27	0/1343	0.57	0/1816
30	DG	0.31	0/1343	0.67	1/1816 (0.1%)
31	BH	0.31	0/1121	0.57	1/1515 (0.1%)
31	DH	0.34	1/1121 (0.1%)	0.60	1/1515 (0.1%)
32	BI	0.23	0/1046	0.47	0/1410
32	DI	0.24	0/1046	0.56	0/1410
33	BJ	0.32	0/1152	0.66	0/1551
33	DJ	0.35	0/1152	0.67	0/1551
34	BK	0.32	0/947	0.68	0/1268
34	DK	0.37	0/947	0.71	0/1268
35	BL	0.29	0/1054	0.66	0/1403
35	DL	0.33	0/1054	0.73	0/1403
36	BM	0.28	0/1093	0.61	0/1460
36	DM	0.36	0/1093	0.77	2/1460 (0.1%)
37	BN	0.28	0/973	0.63	0/1301
37	DN	0.36	0/973	0.70	0/1301
38	BO	0.27	0/902	0.55	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DO	0.33	0/902	0.62	0/1209
39	BP	0.33	0/929	0.67	0/1242
39	DP	0.37	0/929	0.74	1/1242 (0.1%)
40	BQ	0.32	0/960	0.60	0/1278
40	DQ	0.34	0/960	0.69	0/1278
41	BR	0.32	0/829	0.66	0/1107
41	DR	0.38	0/829	0.75	0/1107
42	BS	0.31	0/864	0.69	0/1156
42	DS	0.35	0/864	0.70	0/1156
43	BT	0.30	0/744	0.63	1/994 (0.1%)
43	DT	0.34	0/744	0.70	2/994 (0.2%)
44	BU	0.29	0/787	0.59	0/1051
44	DU	0.32	0/787	0.68	0/1051
45	BV	0.26	0/766	0.57	0/1025
45	DV	0.32	0/766	0.68	0/1025
46	BW	0.30	0/576	0.58	0/762
46	DW	0.35	0/587	0.72	0/776
47	BX	0.33	0/635	0.65	0/848
47	DX	0.32	0/635	0.65	0/848
48	BY	0.25	0/510	0.59	0/677
48	DY	0.28	0/510	0.70	0/677
49	BZ	0.29	0/453	0.59	0/605
49	DZ	0.29	0/453	0.73	0/605
50	B0	0.29	0/450	0.62	0/599
50	D0	0.32	0/450	0.67	0/599
51	B1	0.33	0/416	0.57	0/554
51	D1	0.29	0/416	0.63	0/554
52	B2	0.28	0/380	0.58	0/498
52	D2	0.31	0/380	0.67	0/498
53	B3	0.29	0/513	0.63	0/676
53	D3	0.33	0/513	0.71	0/676
54	B4	0.31	0/303	0.62	0/397
54	D4	0.34	0/303	0.75	0/397
55	CY	0.28	0/1434	0.66	1/1929 (0.1%)
All	All	0.36	6/315264 (0.0%)	0.91	264/471562 (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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CV	1	G	OP3-P	-10.55	1.48	1.61
22	AV	1	G	OP3-P	-10.36	1.48	1.61
24	DA	2204	G	N9-C8	7.67	1.43	1.37
24	DA	733	G	N3-C4	-5.30	1.31	1.35
31	DH	118	PRO	N-CD	5.25	1.55	1.47

The worst 5 of 264 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	DA	2204	G	C8-N9-C4	-13.18	101.13	106.40
24	DA	733	G	N3-C4-N9	-11.80	118.92	126.00
24	DA	733	G	C6-C5-N7	10.61	136.76	130.40
24	DA	733	G	N9-C4-C5	10.19	109.47	105.40
1	AA	890	G	O4'-C1'-N9	9.65	115.92	108.20

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	2761	0
1	CA	32995	0	16607	2603	2
2	AB	1704	0	1732	275	0
2	CB	1704	0	1732	227	0
3	AC	1624	0	1696	188	0
3	CC	1624	0	1696	185	0
4	AD	1643	0	1707	369	0
4	CD	1643	0	1707	356	0
5	AE	1105	0	1148	164	0
5	CE	1105	0	1148	126	0
6	AF	817	0	808	119	0
6	CF	817	0	808	113	0
7	AG	1181	0	1238	102	0
7	CG	1181	0	1238	150	0
8	AH	979	0	1031	209	0
8	CH	979	0	1031	127	0
9	AI	1022	0	1070	143	0
9	CI	1022	0	1070	161	0
10	AJ	786	0	828	71	0
10	CJ	786	0	828	89	0
11	AK	877	0	887	145	0
11	CK	877	0	887	203	0
12	AL	955	0	1016	153	0
12	CL	955	0	1016	179	0
13	AM	883	0	941	137	0
13	CM	883	0	941	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	AN	774	0	827	114	0
14	CN	774	0	827	142	0
15	AO	714	0	734	72	0
15	CO	714	0	734	128	0
16	AP	649	0	666	101	0
16	CP	649	0	666	96	0
17	AQ	648	0	691	78	0
17	CQ	648	0	691	97	0
18	AR	455	0	478	67	0
18	CR	455	0	478	65	0
19	AS	637	0	665	116	0
19	CS	637	0	665	130	0
20	AT	665	0	714	125	0
20	CT	665	0	714	103	0
21	AU	425	0	449	95	0
21	CU	425	0	449	88	0
22	AV	1623	0	821	70	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	4102	1
24	DA	62195	0	31280	3371	1
25	BB	2529	0	1281	202	0
25	DB	2549	0	1291	111	0
26	BC	2082	0	2157	284	0
26	DC	2082	0	2157	277	0
27	BD	1565	0	1616	178	0
27	DD	1565	0	1616	153	0
28	BE	1552	0	1619	176	0
28	DE	1552	0	1619	153	0
29	BF	1410	0	1447	208	0
29	DF	1410	0	1447	252	0
30	BG	1323	0	1374	137	0
30	DG	1323	0	1374	105	0
31	BH	1110	0	1148	131	1
31	DH	1110	0	1148	237	0
32	BI	1032	0	1088	42	0
32	DI	1032	0	1088	87	0
33	BJ	1129	0	1162	133	0
33	DJ	1129	0	1162	105	0
34	BK	938	0	1012	122	0
34	DK	938	0	1012	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	BL	1045	0	1117	138	0
35	DL	1045	0	1117	115	0
36	BM	1074	0	1157	117	0
36	DM	1074	0	1157	116	0
37	BN	960	0	1000	133	0
37	DN	960	0	1000	98	0
38	BO	892	0	923	147	0
38	DO	892	0	923	123	0
39	BP	917	0	965	102	0
39	DP	917	0	965	72	0
40	BQ	947	0	1022	96	0
40	DQ	947	0	1022	128	0
41	BR	816	0	839	82	0
41	DR	816	0	839	121	0
42	BS	857	0	922	116	0
42	DS	857	0	922	89	0
43	BT	738	0	807	89	0
43	DT	738	0	807	74	0
44	BU	779	0	834	108	0
44	DU	779	0	834	106	0
45	BV	753	0	780	77	0
45	DV	753	0	780	63	1
46	BW	569	0	581	55	0
46	DW	580	0	594	78	0
47	BX	625	0	655	76	0
47	DX	625	0	655	82	0
48	BY	509	0	543	59	0
48	DY	509	0	543	75	0
49	BZ	449	0	491	53	0
49	DZ	449	0	491	32	0
50	B0	444	0	461	43	0
50	D0	444	0	461	39	0
51	B1	409	0	440	50	0
51	D1	409	0	440	38	0
52	B2	377	0	418	52	0
52	D2	377	0	418	40	0
53	B3	504	0	574	66	0
53	D3	504	0	574	69	0
54	B4	302	0	340	33	0
54	D4	302	0	340	39	0
55	CY	1423	0	1476	166	0
56	AA	54	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AD	1	0	0	0	0
56	AN	1	0	0	0	0
56	BA	163	0	0	0	0
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	6	0
57	DA	294	0	311	107	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	CT	2	0	0	1	0
59	D3	2	0	0	0	0
59	D4	1	0	0	0	0
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	2	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	22971	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 48.

The worst 5 of 22971 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	1
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	1
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	1
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%)	3	18

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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	7
40	BQ	115/118 (98%)	98 (85%)	13 (11%)	4 (4%)	3	19
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	1
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	1
49	BZ	56/59 (95%)	42 (75%)	12 (21%)	2 (4%)	3	18

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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	10
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%)	128 (71%)	52 (29%)	0	1
2	CB	180/199 (90%)	137 (76%)	43 (24%)	0	3
3	AC	170/190 (90%)	138 (81%)	32 (19%)	1	6
3	CC	170/190 (90%)	130 (76%)	40 (24%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	172/173 (99%)	116 (67%)	56 (33%)	0	1
4	CD	172/173 (99%)	125 (73%)	47 (27%)	0	1
5	AE	113/126 (90%)	91 (80%)	22 (20%)	1	5
5	CE	113/126 (90%)	94 (83%)	19 (17%)	1	8
6	AF	87/116 (75%)	72 (83%)	15 (17%)	1	8
6	CF	87/116 (75%)	65 (75%)	22 (25%)	0	2
7	AG	124/147 (84%)	96 (77%)	28 (23%)	1	3
7	CG	124/147 (84%)	101 (82%)	23 (18%)	1	6
8	AH	104/105 (99%)	81 (78%)	23 (22%)	1	3
8	CH	104/105 (99%)	87 (84%)	17 (16%)	2	9
9	AI	105/107 (98%)	81 (77%)	24 (23%)	0	3
9	CI	105/107 (98%)	84 (80%)	21 (20%)	1	5
10	AJ	86/90 (96%)	73 (85%)	13 (15%)	2	10
10	CJ	86/90 (96%)	67 (78%)	19 (22%)	1	3
11	AK	90/99 (91%)	74 (82%)	16 (18%)	1	7
11	CK	90/99 (91%)	67 (74%)	23 (26%)	0	2
12	AL	103/104 (99%)	69 (67%)	34 (33%)	0	1
12	CL	103/104 (99%)	77 (75%)	26 (25%)	0	2
13	AM	92/96 (96%)	77 (84%)	15 (16%)	2	9
13	CM	92/96 (96%)	63 (68%)	29 (32%)	0	1
14	AN	79/84 (94%)	64 (81%)	15 (19%)	1	5
14	CN	79/84 (94%)	60 (76%)	19 (24%)	0	3
15	AO	76/77 (99%)	55 (72%)	21 (28%)	0	1
15	CO	76/77 (99%)	57 (75%)	19 (25%)	0	2
16	AP	65/65 (100%)	51 (78%)	14 (22%)	1	4
16	CP	65/65 (100%)	41 (63%)	24 (37%)	0	0
17	AQ	74/78 (95%)	59 (80%)	15 (20%)	1	4
17	CQ	74/78 (95%)	54 (73%)	20 (27%)	0	1
18	AR	48/65 (74%)	36 (75%)	12 (25%)	0	2
18	CR	48/65 (74%)	36 (75%)	12 (25%)	0	2
19	AS	70/79 (89%)	53 (76%)	17 (24%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	CS	70/79 (89%)	53 (76%)	17 (24%)	0	2
20	AT	65/66 (98%)	50 (77%)	15 (23%)	0	3
20	CT	65/66 (98%)	50 (77%)	15 (23%)	0	3
21	AU	44/61 (72%)	30 (68%)	14 (32%)	0	1
21	CU	44/61 (72%)	29 (66%)	15 (34%)	0	1
26	BC	216/218 (99%)	164 (76%)	52 (24%)	0	3
26	DC	216/218 (99%)	147 (68%)	69 (32%)	0	1
27	BD	164/164 (100%)	131 (80%)	33 (20%)	1	4
27	DD	164/164 (100%)	125 (76%)	39 (24%)	0	3
28	BE	165/165 (100%)	133 (81%)	32 (19%)	1	5
28	DE	165/165 (100%)	130 (79%)	35 (21%)	1	4
29	BF	148/150 (99%)	115 (78%)	33 (22%)	1	3
29	DF	148/150 (99%)	114 (77%)	34 (23%)	0	3
30	BG	137/138 (99%)	108 (79%)	29 (21%)	1	4
30	DG	137/138 (99%)	111 (81%)	26 (19%)	1	5
31	BH	114/114 (100%)	83 (73%)	31 (27%)	0	1
31	DH	114/114 (100%)	92 (81%)	22 (19%)	1	5
32	BI	109/110 (99%)	101 (93%)	8 (7%)	11	35
32	DI	109/110 (99%)	89 (82%)	20 (18%)	1	6
33	BJ	116/116 (100%)	90 (78%)	26 (22%)	1	3
33	DJ	116/116 (100%)	95 (82%)	21 (18%)	1	6
34	BK	103/104 (99%)	81 (79%)	22 (21%)	1	4
34	DK	103/104 (99%)	77 (75%)	26 (25%)	0	2
35	BL	102/103 (99%)	76 (74%)	26 (26%)	0	2
35	DL	102/103 (99%)	74 (72%)	28 (28%)	0	1
36	BM	109/109 (100%)	80 (73%)	29 (27%)	0	2
36	DM	109/109 (100%)	86 (79%)	23 (21%)	1	4
37	BN	100/103 (97%)	81 (81%)	19 (19%)	1	5
37	DN	100/103 (97%)	83 (83%)	17 (17%)	1	8
38	BO	86/87 (99%)	67 (78%)	19 (22%)	1	3
38	DO	86/87 (99%)	61 (71%)	25 (29%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
39	BP	99/100 (99%)	81 (82%)	18 (18%)	1	6	
39	DP	99/100 (99%)	80 (81%)	19 (19%)	1	5	
40	BQ	89/90 (99%)	66 (74%)	23 (26%)	0	2	
40	DQ	89/90 (99%)	69 (78%)	20 (22%)	1	3	
41	BR	84/84 (100%)	66 (79%)	18 (21%)	1	4	
41	DR	84/84 (100%)	70 (83%)	14 (17%)	2	8	
42	BS	93/93 (100%)	70 (75%)	23 (25%)	0	2	
42	DS	93/93 (100%)	68 (73%)	25 (27%)	0	1	
43	BT	80/84 (95%)	57 (71%)	23 (29%)	0	1	
43	DT	80/84 (95%)	62 (78%)	18 (22%)	1	3	
44	BU	83/85 (98%)	61 (74%)	22 (26%)	0	2	
44	DU	83/85 (98%)	63 (76%)	20 (24%)	0	3	
45	BV	78/78 (100%)	60 (77%)	18 (23%)	0	3	
45	DV	78/78 (100%)	63 (81%)	15 (19%)	1	5	
46	BW	56/63 (89%)	45 (80%)	11 (20%)	1	5	
46	DW	57/63 (90%)	48 (84%)	9 (16%)	2	10	
47	BX	67/68 (98%)	47 (70%)	20 (30%)	0	1	
47	DX	67/68 (98%)	56 (84%)	11 (16%)	2	9	
48	BY	55/55 (100%)	47 (86%)	8 (14%)	2	12	
48	DY	55/55 (100%)	43 (78%)	12 (22%)	1	3	
49	BZ	48/49 (98%)	40 (83%)	8 (17%)	2	8	
49	DZ	48/49 (98%)	42 (88%)	6 (12%)	3	16	
50	B0	47/48 (98%)	39 (83%)	8 (17%)	1	8	
50	D0	47/48 (98%)	38 (81%)	9 (19%)	1	5	
51	B1	45/49 (92%)	39 (87%)	6 (13%)	3	14	
51	D1	45/49 (92%)	36 (80%)	9 (20%)	1	5	
52	B2	38/38 (100%)	26 (68%)	12 (32%)	0	1	
52	D2	38/38 (100%)	33 (87%)	5 (13%)	3	14	
53	B3	51/52 (98%)	37 (72%)	14 (28%)	0	1	
53	D3	51/52 (98%)	36 (71%)	15 (29%)	0	1	
54	B4	34/34 (100%)	27 (79%)	7 (21%)	1	4	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	D4	34/34 (100%)	23 (68%)	11 (32%)	0	1
55	CY	158/160 (99%)	122 (77%)	36 (23%)	0	3
All	All	9485/9916 (96%)	7325 (77%)	2160 (23%)	0	3

5 of 2160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	DL	19	LEU
37	DN	43	GLU
35	DL	6	LEU
46	DW	82	ILE
37	BN	33	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
17	CQ	47	HIS
33	DJ	130	HIS
19	CS	52	HIS
26	DC	127	ASN
37	DN	3	HIS

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%)	826 (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%)	2823 (30%)	218 (2%)

5 of 2823 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	1655	-	43,45,45	0.56	0	62,67,67	0.97	4 (6%)
57	NMY	AA	1657	-	43,45,45	2.35	12 (27%)	62,67,67	1.87	18 (29%)
57	NMY	DA	3184	-	43,45,45	0.57	0	62,67,67	1.26	5 (8%)
57	NMY	DA	3187	-	43,45,45	2.34	11 (25%)	62,67,67	1.51	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	NMY	DA	3189	-	43,45,45	2.24	11 (25%)	62,67,67	2.32	23 (37%)
57	NMY	BA	3167	-	43,45,45	2.32	11 (25%)	62,67,67	1.97	14 (22%)
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	3161	-	43,45,45	0.49	0	62,67,67	1.03	4 (6%)
57	NMY	AA	1656	-	43,45,45	2.31	12 (27%)	62,67,67	1.88	20 (32%)
57	NMY	BA	3164	-	43,45,45	2.29	11 (25%)	62,67,67	2.44	26 (41%)
57	NMY	CA	1672	-	43,45,45	0.53	0	62,67,67	0.89	2 (3%)
57	NMY	DA	3190	-	43,45,45	2.29	10 (23%)	62,67,67	2.56	25 (40%)
57	NMY	DA	3186	-	43,45,45	2.40	12 (27%)	62,67,67	2.39	15 (24%)
57	NMY	DA	3185	-	43,45,45	2.36	12 (27%)	62,67,67	1.72	14 (22%)
57	NMY	BA	3165	-	43,45,45	0.50	0	62,67,67	1.12	5 (8%)
57	NMY	BA	3162	-	43,45,45	0.49	0	62,67,67	1.05	5 (8%)
57	NMY	BA	3166	-	43,45,45	2.21	11 (25%)	62,67,67	2.22	16 (25%)

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	1655	-	-	12/18/94/94	0/4/4/4
57	NMY	AA	1657	-	-	9/18/94/94	0/4/4/4
57	NMY	DA	3184	-	-	3/18/94/94	0/4/4/4
57	NMY	DA	3187	-	-	8/18/94/94	0/4/4/4
57	NMY	DA	3189	-	-	5/18/94/94	0/4/4/4
57	NMY	BA	3167	-	-	5/18/94/94	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	3161	-	-	4/18/94/94	0/4/4/4
57	NMY	AA	1656	-	-	6/18/94/94	0/4/4/4
57	NMY	BA	3164	-	-	6/18/94/94	0/4/4/4
57	NMY	CA	1672	-	-	3/18/94/94	0/4/4/4
57	NMY	DA	3190	-	-	10/18/94/94	0/4/4/4
57	NMY	DA	3186	-	-	10/18/94/94	0/4/4/4
57	NMY	DA	3185	-	-	5/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	NMY	BA	3165	-	-	5/18/94/94	0/4/4/4
57	NMY	BA	3162	-	-	1/18/94/94	0/4/4/4
57	NMY	BA	3166	-	-	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	1655	NMY	26	0
57	AA	1657	NMY	10	0
57	DA	3184	NMY	17	0
57	DA	3187	NMY	4	0

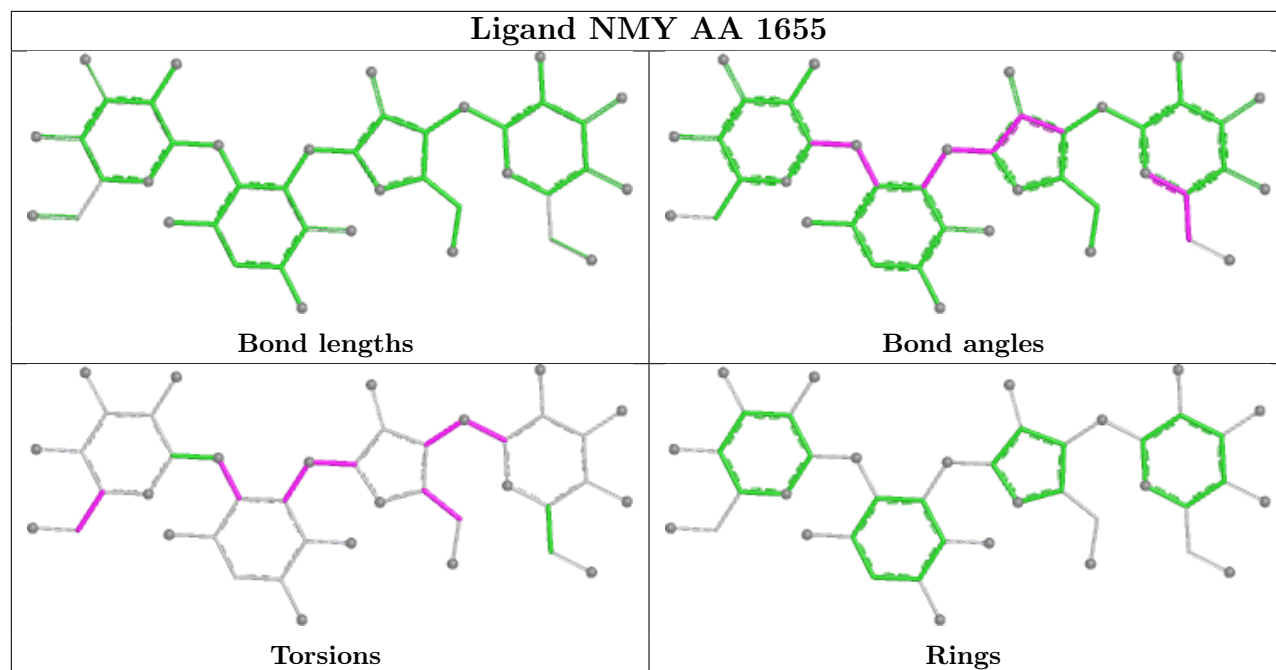
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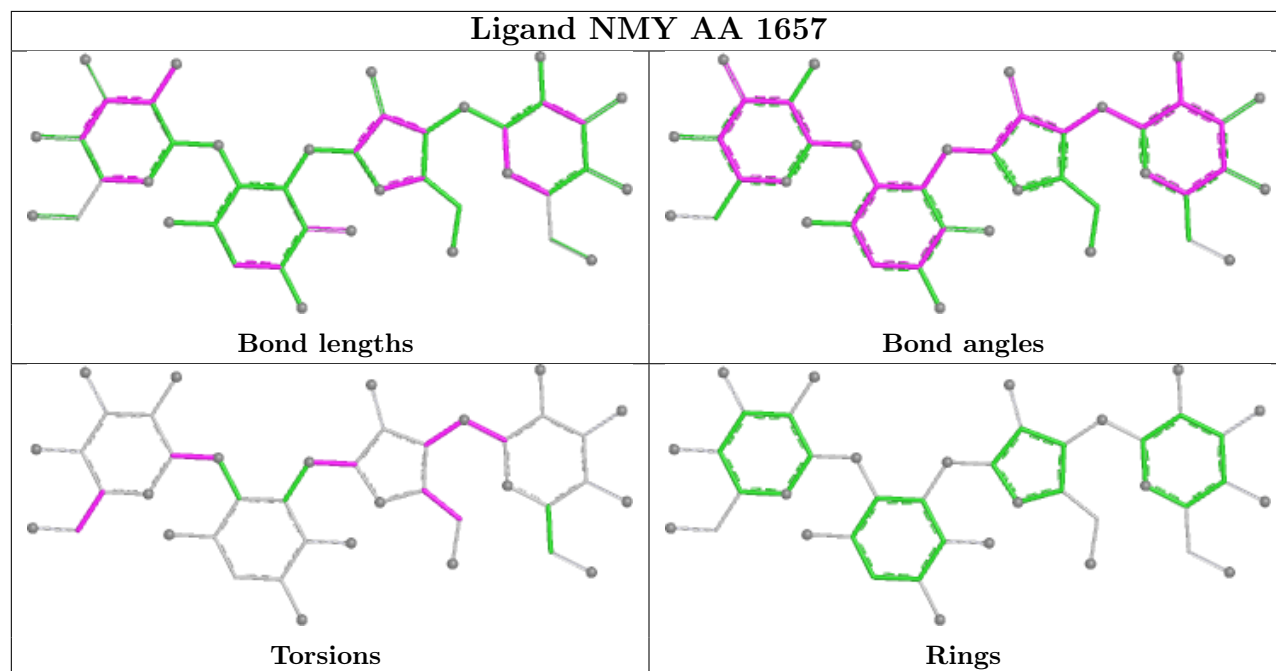
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DA	3189	NMY	10	0
57	BA	3167	NMY	5	0
57	BA	3163	NMY	11	0
57	DA	3188	NMY	12	0
57	BA	3161	NMY	14	0
57	AA	1656	NMY	12	0
57	BA	3164	NMY	3	0
57	CA	1672	NMY	6	0
57	DA	3190	NMY	32	0
57	DA	3186	NMY	19	0
57	DA	3185	NMY	13	0
57	BA	3165	NMY	25	0
57	BA	3162	NMY	16	0
57	BA	3166	NMY	13	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.

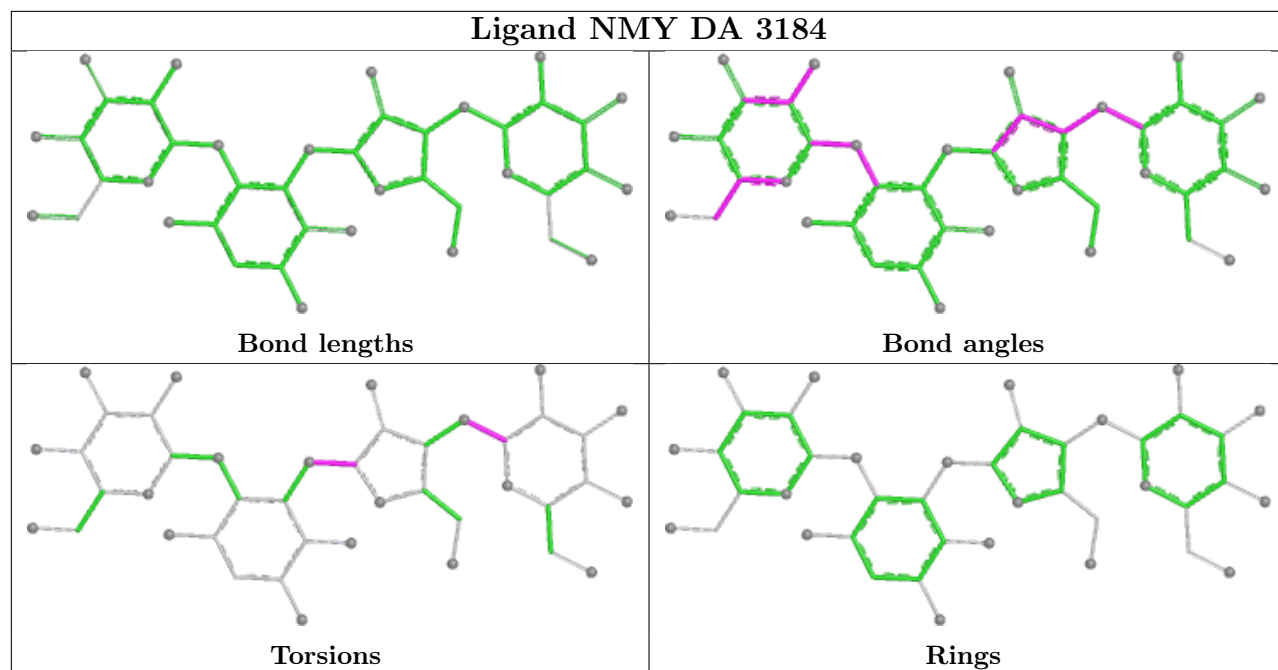
Ligand NMY AA 1655



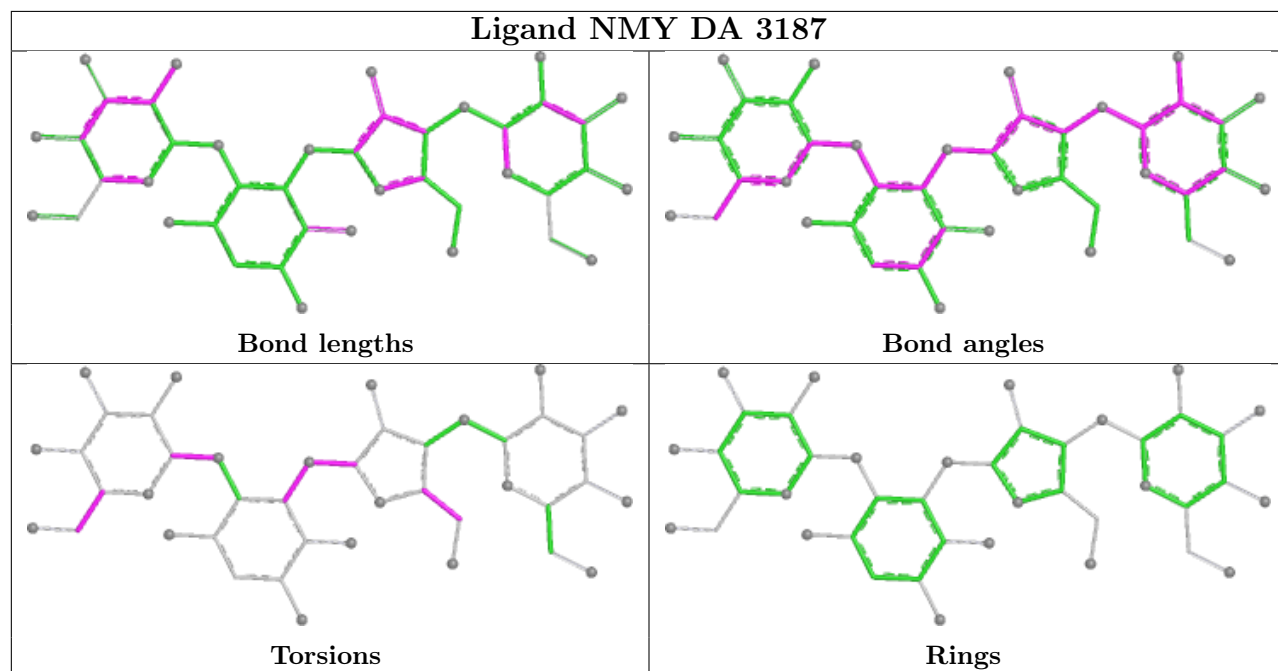
Ligand NMY AA 1657

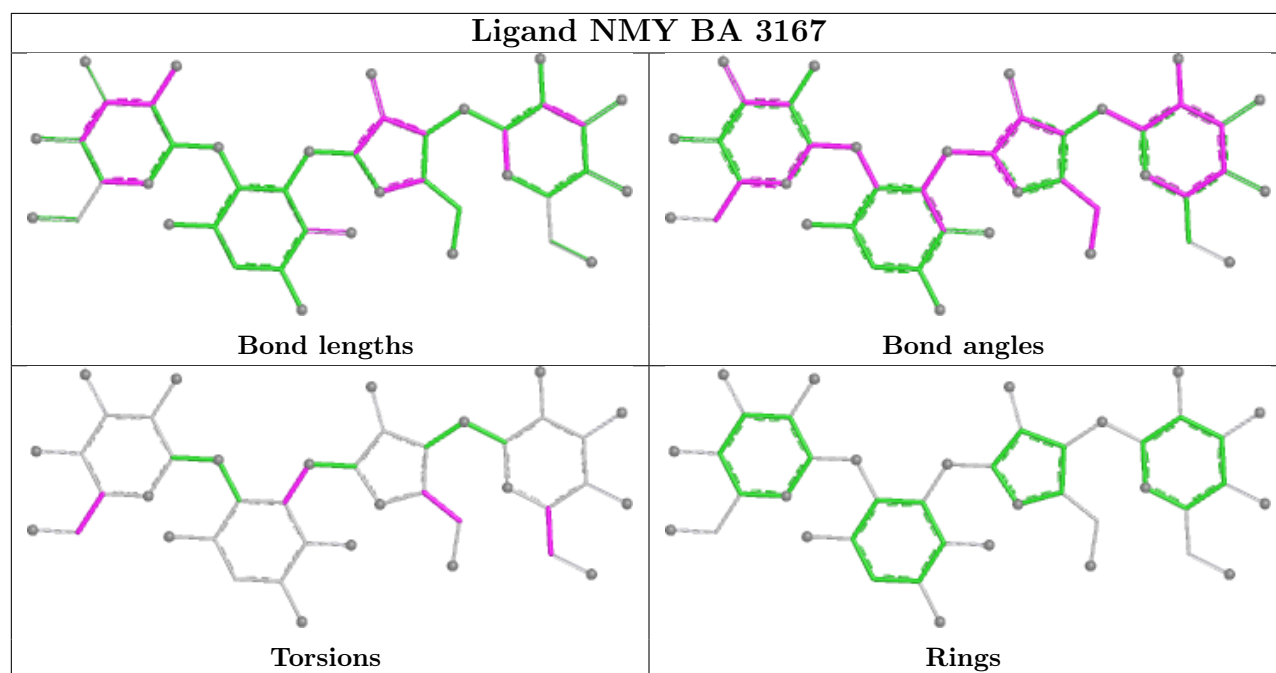
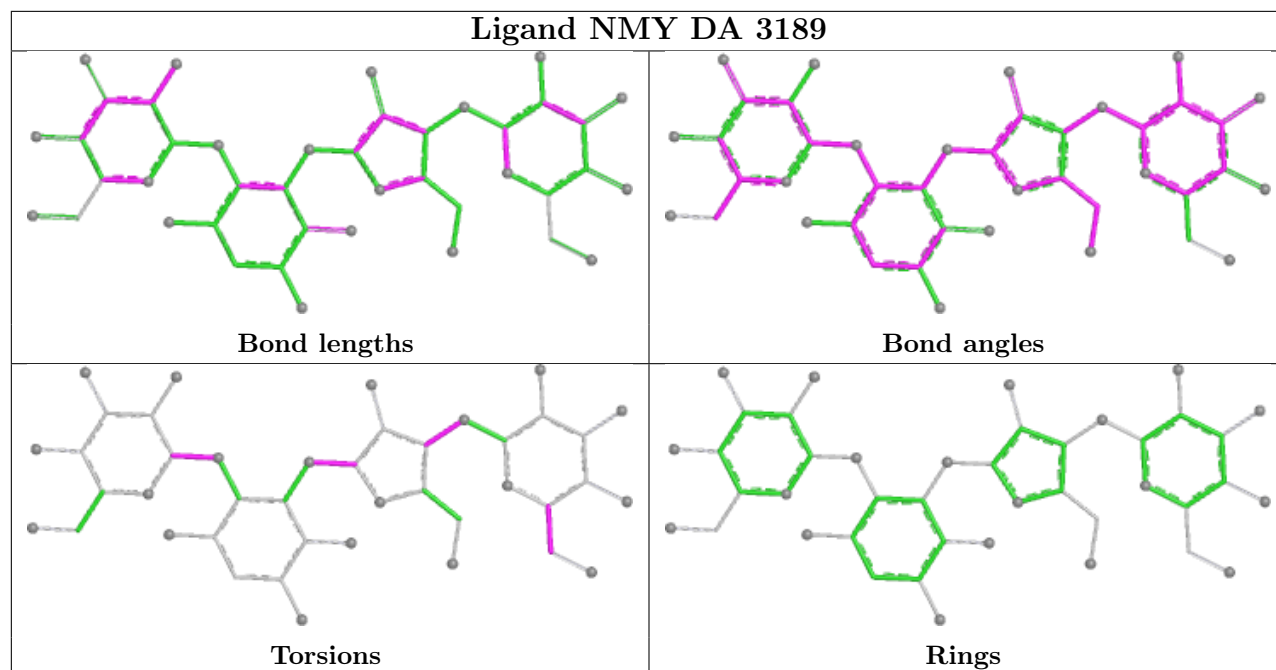


Ligand NMY DA 3184

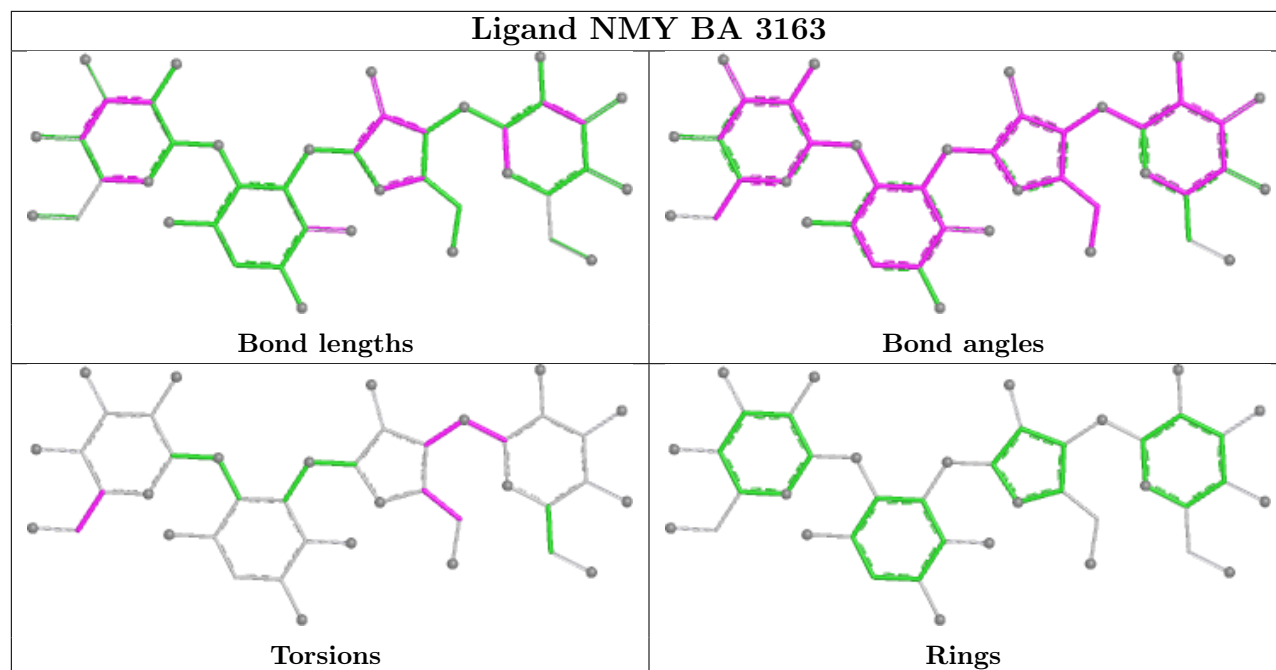


Ligand NMY DA 3187

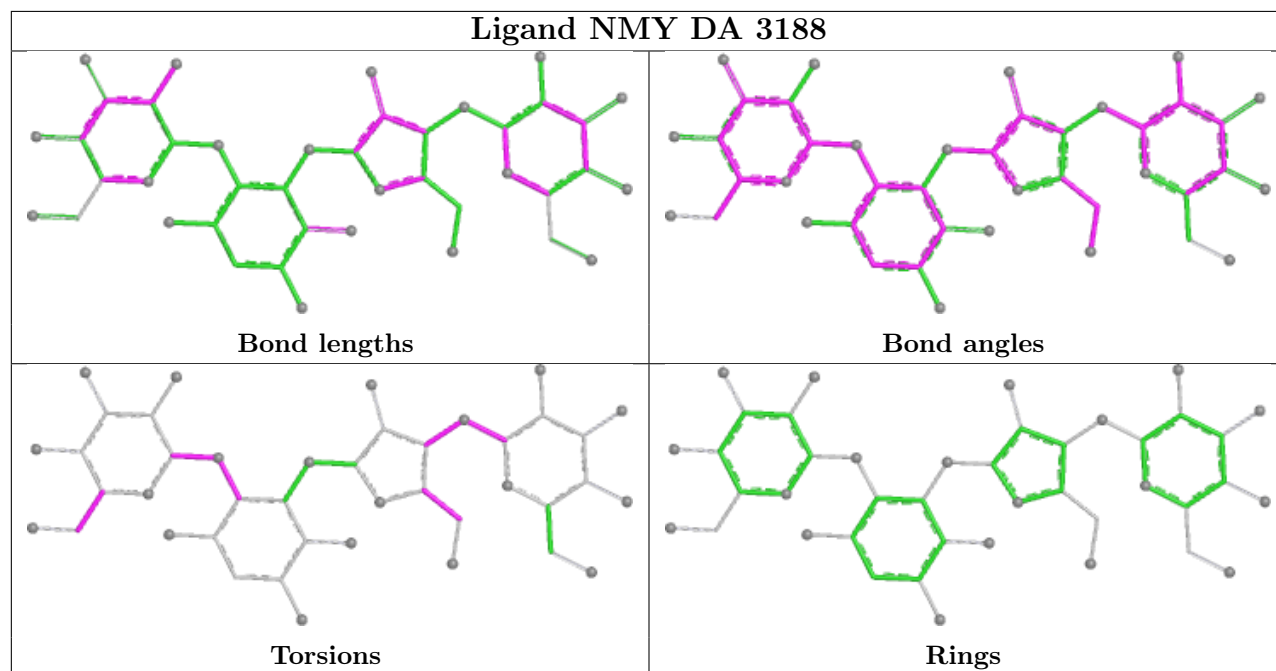




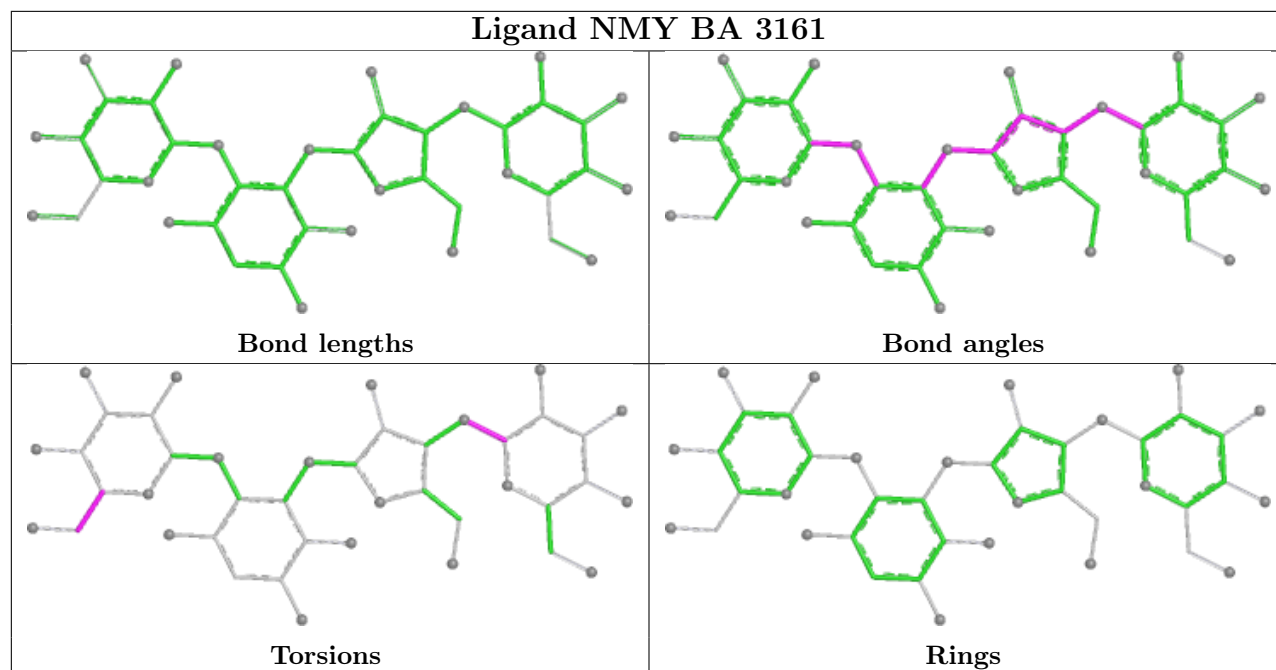
Ligand NMY BA 3163



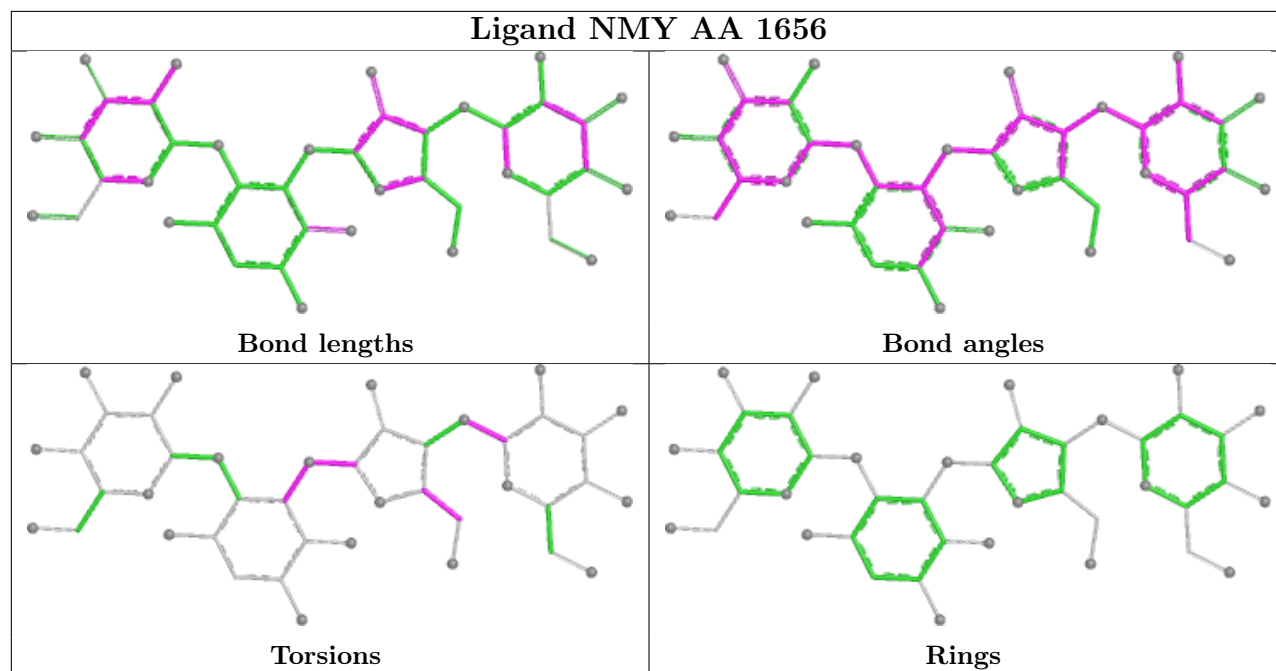
Ligand NMY DA 3188



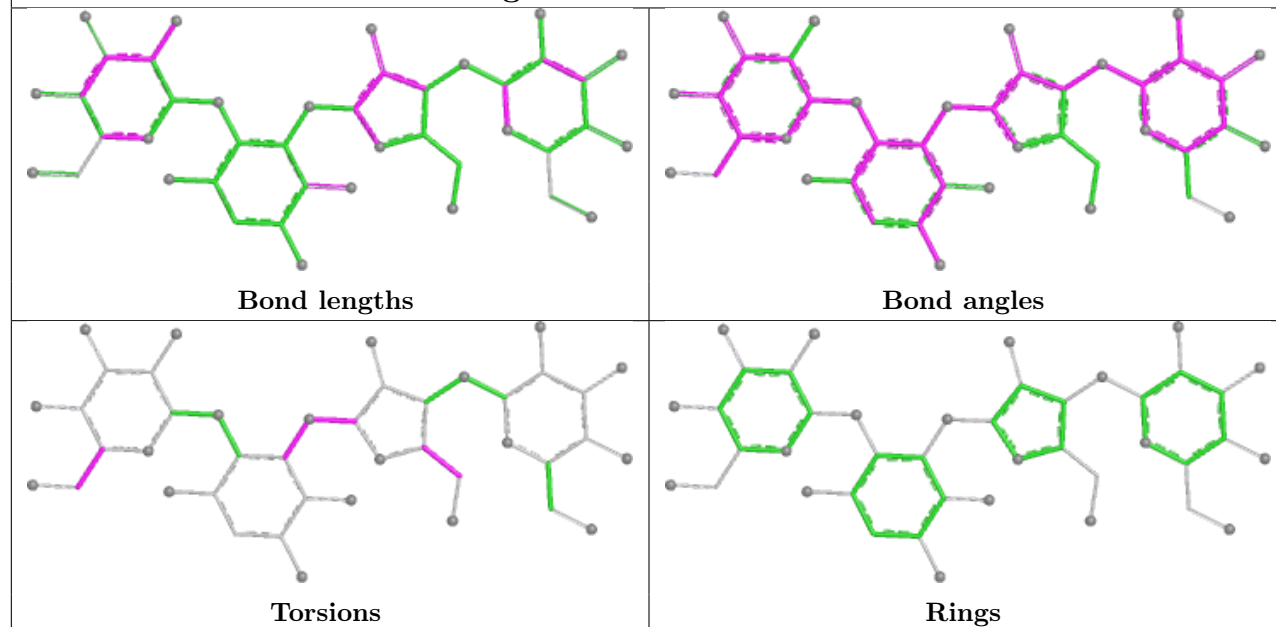
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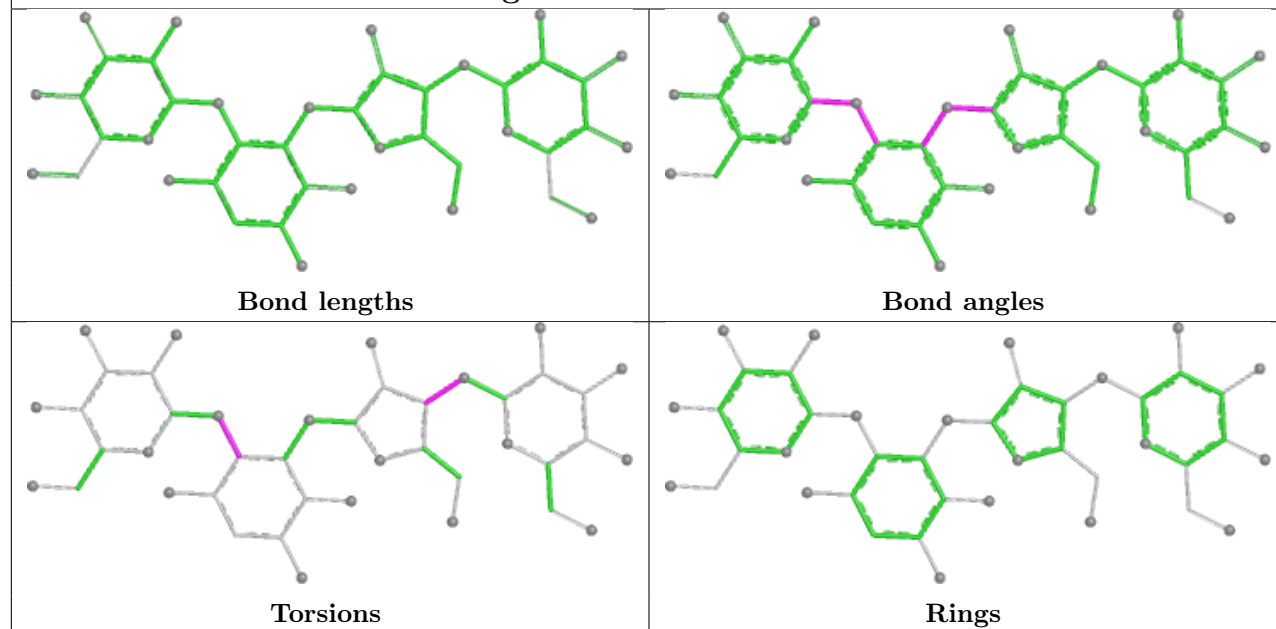
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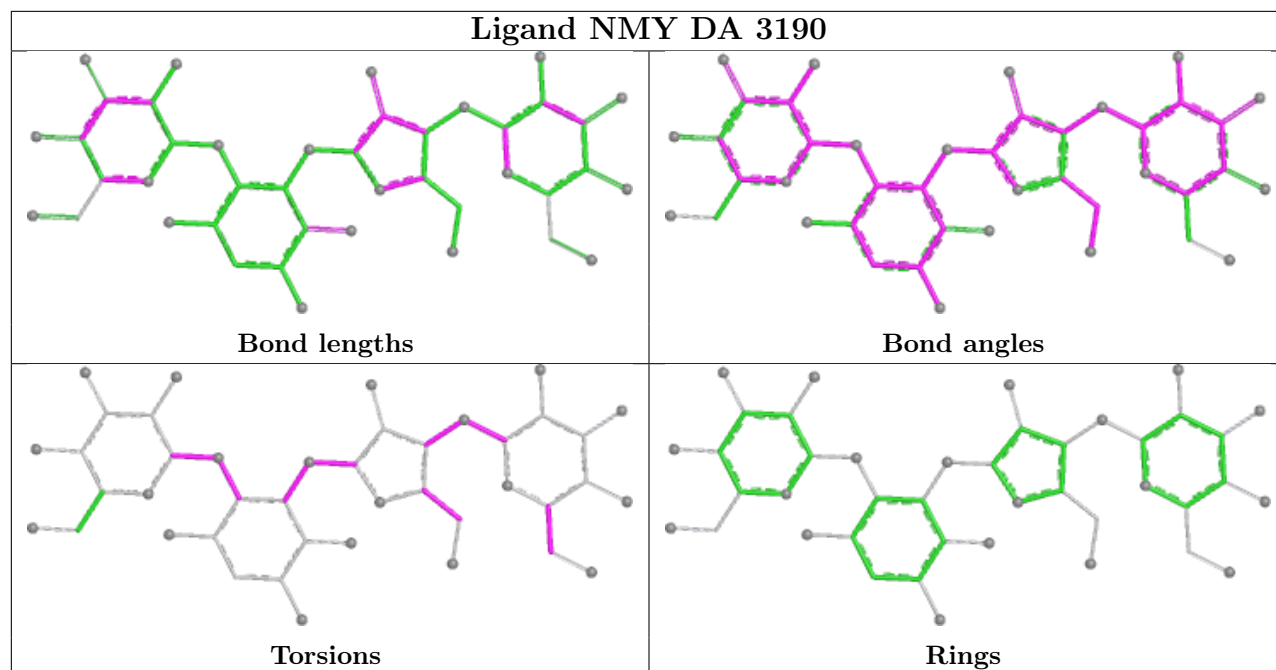
Ligand NMY BA 3164



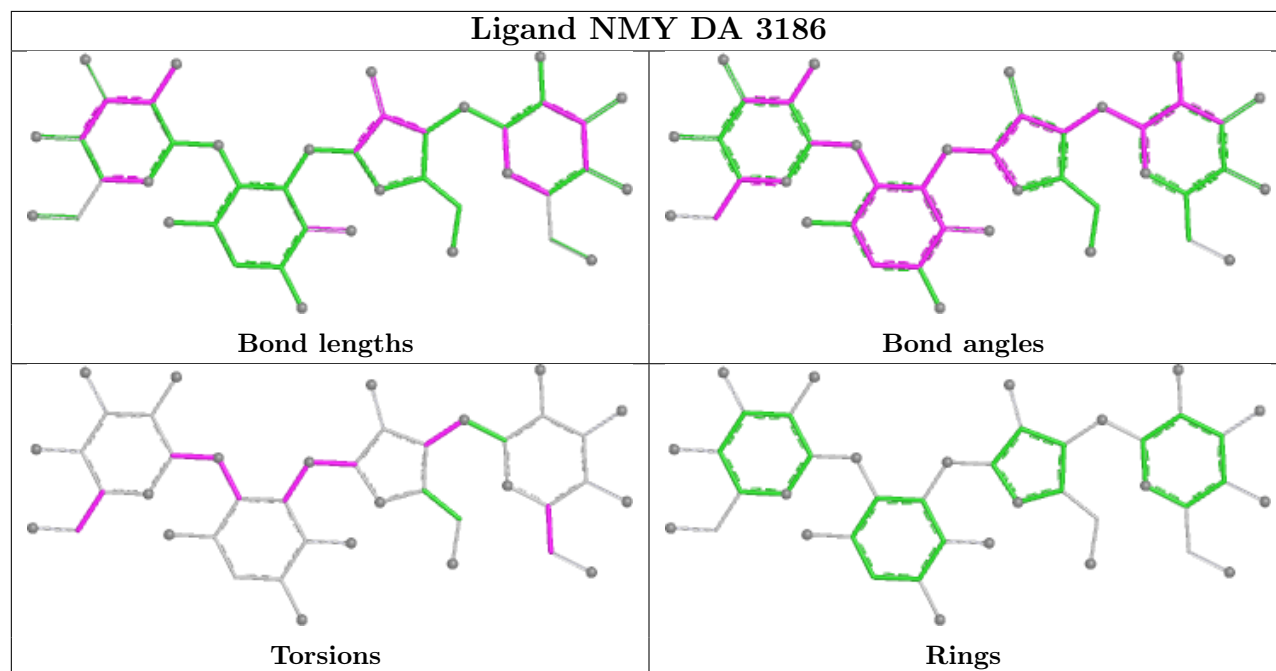
Ligand NMY CA 1672



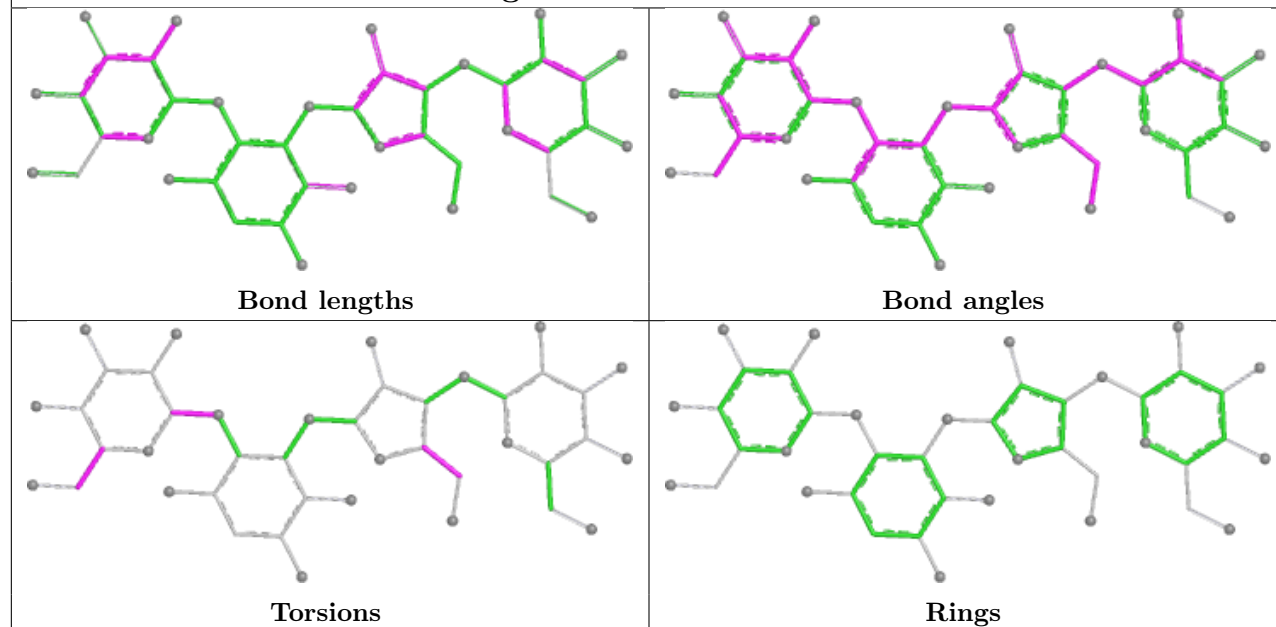
Ligand NMY DA 3190



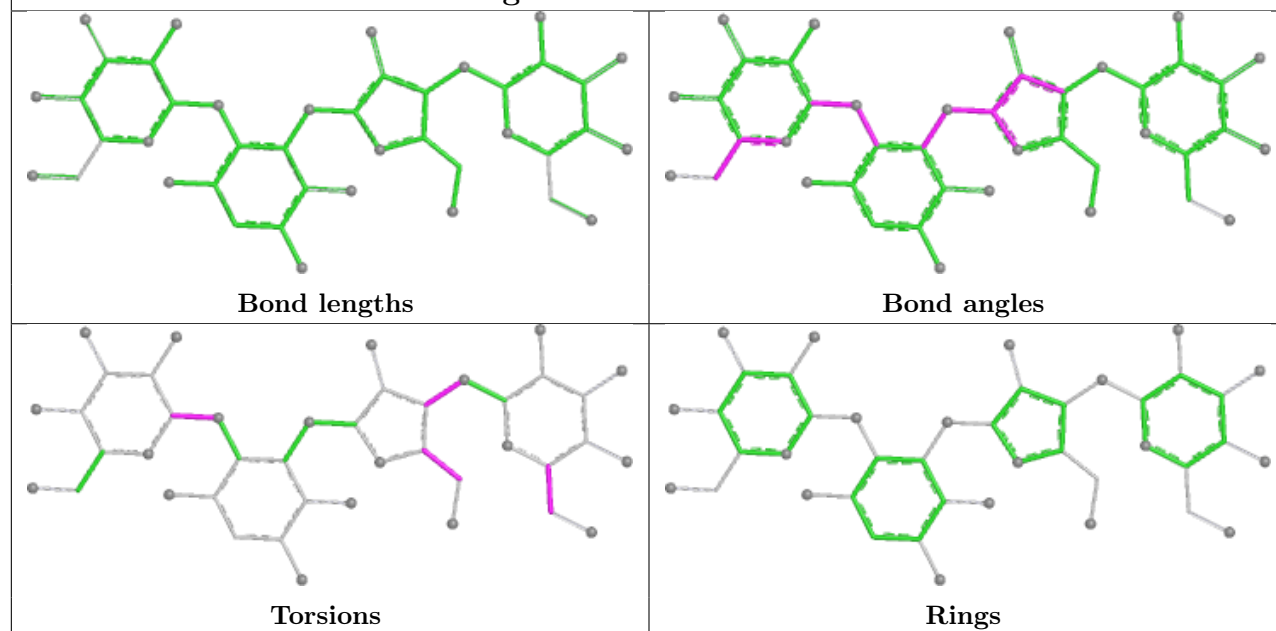
Ligand NMY DA 3186

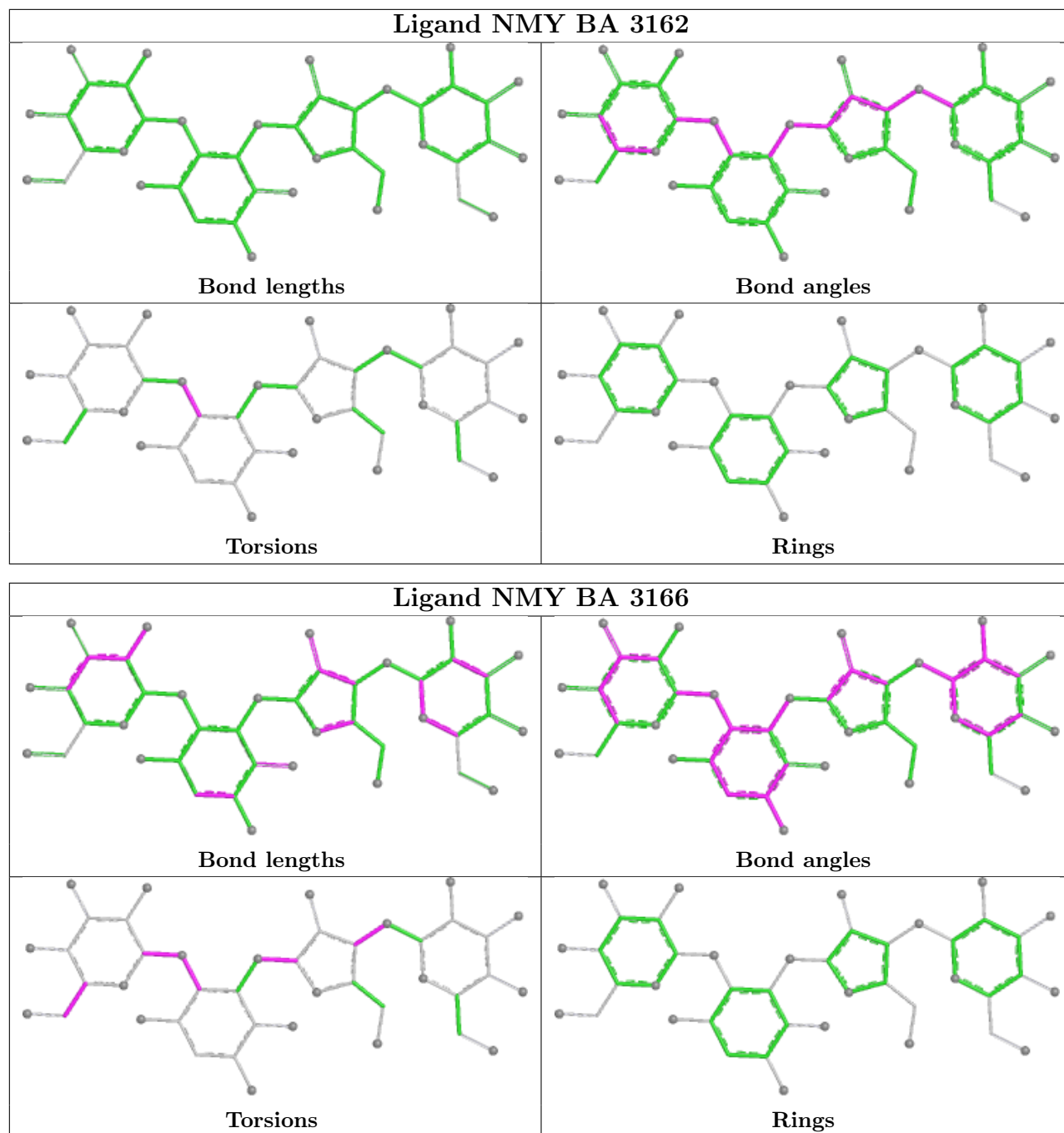


Ligand NMY DA 3185



Ligand NMY BA 3165





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%)	-0.59	2 (0%) 92 91	67, 121, 207, 543	0
1	CA	1538/1542 (99%)	-0.61	7 (0%) 87 80	63, 120, 240, 527	0
2	AB	218/241 (90%)	0.21	11 (5%) 35 28	86, 172, 404, 542	0
2	CB	218/241 (90%)	0.11	8 (3%) 45 33	96, 215, 508, 545	0
3	AC	206/233 (88%)	0.23	14 (6%) 25 20	81, 139, 325, 514	0
3	CC	206/233 (88%)	-0.16	6 (2%) 54 40	80, 120, 286, 513	0
4	AD	205/206 (99%)	1.23	47 (22%) 2 2	83, 161, 372, 537	0
4	CD	205/206 (99%)	0.99	36 (17%) 4 4	81, 148, 442, 537	0
5	AE	150/167 (89%)	0.36	13 (8%) 17 16	79, 130, 272, 478	0
5	CE	150/167 (89%)	0.42	15 (10%) 14 13	68, 114, 292, 527	0
6	AF	100/135 (74%)	-0.19	3 (3%) 52 39	85, 142, 331, 528	0
6	CF	100/135 (74%)	0.37	8 (8%) 20 18	87, 178, 386, 531	0
7	AG	151/179 (84%)	0.30	14 (9%) 16 15	93, 161, 365, 539	0
7	CG	151/179 (84%)	0.85	25 (16%) 5 5	112, 234, 452, 540	0
8	AH	129/130 (99%)	0.31	13 (10%) 14 13	79, 145, 341, 424	0
8	CH	129/130 (99%)	0.35	5 (3%) 44 33	81, 121, 307, 437	0
9	AI	127/130 (97%)	0.87	20 (15%) 6 6	101, 180, 459, 535	0
9	CI	127/130 (97%)	0.95	28 (22%) 3 2	97, 216, 478, 540	0
10	AJ	98/103 (95%)	0.51	7 (7%) 23 20	95, 165, 363, 543	0
10	CJ	98/103 (95%)	1.24	25 (25%) 2 1	101, 202, 530, 543	0
11	AK	117/129 (90%)	0.13	7 (5%) 29 23	75, 112, 337, 492	0
11	CK	117/129 (90%)	0.58	10 (8%) 18 17	83, 243, 494, 531	0
12	AL	123/124 (99%)	0.27	11 (8%) 17 16	75, 109, 299, 403	0
12	CL	123/124 (99%)	0.44	17 (13%) 8 8	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%)	0.73	15 (13%)	8 8	106, 239, 498, 530	0
13	CM	114/118 (96%)	0.98	21 (18%)	4 4	122, 312, 536, 547	0
14	AN	96/101 (95%)	1.25	19 (19%)	3 3	89, 175, 381, 527	0
14	CN	96/101 (95%)	1.33	22 (22%)	2 2	95, 183, 535, 545	0
15	AO	88/89 (98%)	0.39	8 (9%)	16 15	90, 136, 315, 374	0
15	CO	88/89 (98%)	0.76	11 (12%)	9 9	94, 176, 350, 510	0
16	AP	82/82 (100%)	1.04	20 (24%)	2 1	76, 125, 380, 528	0
16	CP	82/82 (100%)	0.77	11 (13%)	8 8	75, 115, 387, 524	0
17	AQ	80/84 (95%)	0.56	8 (10%)	14 13	88, 162, 370, 434	0
17	CQ	80/84 (95%)	0.30	8 (10%)	14 13	75, 141, 337, 496	0
18	AR	55/75 (73%)	0.09	2 (3%)	46 34	84, 115, 320, 391	0
18	CR	55/75 (73%)	0.25	4 (7%)	22 19	107, 159, 370, 440	0
19	AS	79/92 (85%)	0.66	9 (11%)	11 11	118, 215, 454, 530	0
19	CS	79/92 (85%)	0.87	13 (16%)	5 5	133, 302, 496, 542	0
20	AT	85/87 (97%)	1.08	22 (25%)	2 1	93, 158, 363, 497	0
20	CT	85/87 (97%)	0.76	11 (12%)	9 9	82, 128, 351, 491	0
21	AU	51/71 (71%)	1.11	12 (23%)	2 2	83, 133, 326, 395	0
21	CU	51/71 (71%)	1.28	13 (25%)	2 1	108, 193, 374, 512	0
22	AV	76/76 (100%)	-0.88	0	100 100	63, 117, 160, 255	0
22	CV	76/76 (100%)	0.08	7 (9%)	16 15	61, 257, 424, 542	0
23	AX	16/24 (66%)	0.31	1 (6%)	27 22	76, 139, 214, 261	0
23	CX	15/24 (62%)	0.55	2 (13%)	8 8	83, 191, 269, 339	0
24	BA	2897/2904 (99%)	-0.72	5 (0%)	92 88	54, 96, 294, 544	0
24	DA	2897/2904 (99%)	-0.76	43 (1%)	71 58	37, 67, 231, 547	0
25	BB	118/120 (98%)	-0.84	0	100 100	78, 151, 201, 231	0
25	DB	119/120 (99%)	-0.95	0	100 100	47, 88, 129, 188	0
26	BC	271/273 (99%)	0.42	28 (10%)	13 13	56, 106, 196, 362	0
26	DC	271/273 (99%)	0.18	20 (7%)	22 19	46, 81, 188, 348	0
27	BD	209/209 (100%)	-0.05	7 (3%)	49 36	58, 88, 195, 401	0
27	DD	209/209 (100%)	-0.20	4 (1%)	66 51	38, 57, 129, 253	0
28	BE	201/201 (100%)	-0.18	2 (0%)	79 68	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%)	-0.36	1 (0%) 87 80	40, 72, 155, 487	0
29	BF	177/179 (98%)	0.43	9 (5%) 34 27	125, 257, 446, 539	0
29	DF	177/179 (98%)	0.52	19 (10%) 12 12	76, 147, 367, 520	0
30	BG	176/177 (99%)	-0.06	3 (1%) 69 55	93, 155, 360, 507	0
30	DG	176/177 (99%)	0.01	11 (6%) 27 22	54, 94, 190, 439	0
31	BH	149/149 (100%)	0.43	16 (10%) 12 12	15, 223, 436, 532	0
31	DH	149/149 (100%)	0.62	17 (11%) 11 11	25, 213, 475, 538	0
32	BI	141/142 (99%)	0.80	14 (9%) 14 14	126, 471, 546, 549	0
32	DI	141/142 (99%)	0.94	23 (16%) 5 5	123, 380, 542, 548	0
33	BJ	142/142 (100%)	-0.07	5 (3%) 47 35	56, 83, 169, 348	0
33	DJ	142/142 (100%)	-0.20	6 (4%) 41 31	38, 60, 146, 265	0
34	BK	122/123 (99%)	-0.18	2 (1%) 70 57	65, 93, 197, 357	0
34	DK	122/123 (99%)	-0.37	0 100 100	43, 63, 112, 229	0
35	BL	143/144 (99%)	0.15	8 (5%) 31 25	55, 110, 265, 507	0
35	DL	143/144 (99%)	0.08	7 (4%) 36 28	41, 68, 170, 291	0
36	BM	136/136 (100%)	-0.09	4 (2%) 54 40	65, 99, 208, 340	0
36	DM	136/136 (100%)	-0.16	5 (3%) 45 33	47, 67, 153, 262	0
37	BN	120/127 (94%)	-0.09	4 (3%) 49 36	66, 107, 190, 466	0
37	DN	120/127 (94%)	-0.07	2 (1%) 69 55	40, 61, 151, 420	0
38	BO	116/117 (99%)	0.42	11 (9%) 15 14	96, 193, 363, 537	0
38	DO	116/117 (99%)	-0.28	0 100 100	66, 94, 183, 322	0
39	BP	114/115 (99%)	0.09	6 (5%) 33 26	71, 109, 288, 356	0
39	DP	114/115 (99%)	-0.13	4 (3%) 47 35	47, 69, 178, 330	0
40	BQ	117/118 (99%)	-0.07	5 (4%) 40 30	55, 76, 170, 304	0
40	DQ	117/118 (99%)	-0.15	4 (3%) 48 35	38, 54, 156, 310	0
41	BR	103/103 (100%)	0.03	3 (2%) 54 40	57, 92, 180, 286	0
41	DR	103/103 (100%)	-0.20	4 (3%) 44 33	42, 68, 152, 458	0
42	BS	110/110 (100%)	-0.07	5 (4%) 39 29	60, 92, 175, 299	0
42	DS	110/110 (100%)	-0.26	1 (0%) 81 70	38, 56, 115, 161	0
43	BT	93/100 (93%)	0.71	12 (12%) 9 9	93, 155, 337, 441	0
43	DT	93/100 (93%)	0.18	7 (7%) 22 19	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%)	0.47	11 (10%) 12 12	78, 133, 337, 443	0
44	DU	102/104 (98%)	0.05	7 (6%) 24 20	52, 82, 226, 299	0
45	BV	94/94 (100%)	-0.17	4 (4%) 40 30	86, 144, 310, 421	0
45	DV	94/94 (100%)	-0.03	3 (3%) 50 37	60, 94, 183, 336	0
46	BW	75/85 (88%)	0.50	4 (5%) 33 26	70, 113, 202, 321	0
46	DW	76/85 (89%)	0.32	8 (10%) 13 13	46, 70, 156, 244	0
47	BX	77/78 (98%)	0.54	10 (12%) 9 9	62, 110, 268, 318	0
47	DX	77/78 (98%)	-0.22	2 (2%) 57 42	48, 83, 165, 320	0
48	BY	63/63 (100%)	-0.10	1 (1%) 70 57	95, 176, 353, 521	0
48	DY	63/63 (100%)	0.05	4 (6%) 27 22	58, 106, 283, 388	0
49	BZ	58/59 (98%)	-0.22	1 (1%) 69 55	67, 93, 170, 515	0
49	DZ	58/59 (98%)	0.00	1 (1%) 69 55	44, 59, 141, 198	0
50	B0	56/57 (98%)	-0.03	4 (7%) 23 20	59, 98, 294, 405	0
50	D0	56/57 (98%)	0.29	4 (7%) 23 20	33, 64, 166, 282	0
51	B1	50/55 (90%)	0.34	6 (12%) 10 10	88, 147, 326, 377	0
51	D1	50/55 (90%)	0.23	4 (8%) 20 18	78, 120, 326, 532	0
52	B2	46/46 (100%)	0.45	5 (10%) 12 12	70, 95, 239, 293	0
52	D2	46/46 (100%)	0.57	6 (13%) 9 9	54, 67, 171, 292	0
53	B3	64/65 (98%)	0.46	6 (9%) 15 14	67, 91, 201, 286	0
53	D3	64/65 (98%)	0.45	7 (10%) 12 12	47, 61, 161, 254	0
54	B4	38/38 (100%)	0.54	4 (10%) 13 13	78, 108, 174, 322	0
54	D4	38/38 (100%)	-0.17	1 (2%) 57 42	53, 67, 150, 295	0
55	CY	183/185 (98%)	0.15	10 (5%) 32 25	53, 148, 442, 539	0
All	All	20909/21487 (97%)	-0.14	1031 (4%) 36 28	15, 110, 357, 549	0

The worst 5 of 1031 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	AD	24	GLY	14.1
12	CL	15	LYS	10.4
4	CD	76	TYR	10.3
9	CI	125	PRO	10.0
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 monosaccharides 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(\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	-0.21	0.37	109,109,109,109	0
56	MG	DB	204	1/1	-0.08	0.36	109,109,109,109	0
56	MG	CA	1636	1/1	0.00	0.18	134,134,134,134	0
56	MG	CA	1657	1/1	0.02	0.22	119,119,119,119	0
56	MG	DA	3095	1/1	0.06	0.58	116,116,116,116	0
56	MG	CA	1652	1/1	0.17	0.25	106,106,106,106	0
56	MG	DA	3018	1/1	0.18	0.38	102,102,102,102	0
56	MG	AA	1648	1/1	0.21	0.17	116,116,116,116	0
56	MG	CA	1637	1/1	0.24	0.35	139,139,139,139	0
56	MG	BA	3054	1/1	0.24	0.38	119,119,119,119	0
56	MG	BA	3007	1/1	0.27	0.28	127,127,127,127	0
56	MG	BA	3096	1/1	0.27	0.29	118,118,118,118	0
56	MG	DA	3151	1/1	0.28	0.32	101,101,101,101	0
56	MG	AA	1623	1/1	0.28	0.38	119,119,119,119	0
56	MG	BA	3026	1/1	0.31	0.28	134,134,134,134	0
56	MG	DB	202	1/1	0.32	0.32	122,122,122,122	0
56	MG	AA	1631	1/1	0.33	0.27	126,126,126,126	0
56	MG	AA	1640	1/1	0.33	0.27	110,110,110,110	0
56	MG	BA	3059	1/1	0.35	0.60	122,122,122,122	0
56	MG	AA	1633	1/1	0.35	0.23	128,128,128,128	0
56	MG	DA	3076	1/1	0.37	0.17	100,100,100,100	0
56	MG	BA	3168	1/1	0.38	0.34	114,114,114,114	0
56	MG	BA	3027	1/1	0.39	0.43	108,108,108,108	0
56	MG	CA	1632	1/1	0.39	0.37	128,128,128,128	0
56	MG	CA	1660	1/1	0.39	0.18	104,104,104,104	0
56	MG	DA	3068	1/1	0.40	0.30	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3142	1/1	0.41	0.25	103,103,103,103	0
56	MG	DA	3087	1/1	0.41	0.21	113,113,113,113	0
56	MG	CA	1601	1/1	0.41	0.17	140,140,140,140	0
56	MG	CA	1647	1/1	0.42	0.13	112,112,112,112	0
56	MG	AN	201	1/1	0.43	0.26	133,133,133,133	0
56	MG	BA	3012	1/1	0.44	0.38	118,118,118,118	0
56	MG	DA	3134	1/1	0.47	0.26	77,77,77,77	0
56	MG	DA	3081	1/1	0.47	0.42	110,110,110,110	0
56	MG	CX	101	1/1	0.47	0.14	112,112,112,112	0
56	MG	AA	1639	1/1	0.47	0.41	113,113,113,113	0
56	MG	DA	3161	1/1	0.48	0.18	103,103,103,103	0
56	MG	BA	3066	1/1	0.48	0.21	96,96,96,96	0
56	MG	AA	1646	1/1	0.48	0.23	95,95,95,95	0
56	MG	CA	1631	1/1	0.49	0.23	120,120,120,120	0
56	MG	DO	201	1/1	0.49	0.40	109,109,109,109	0
56	MG	AA	1625	1/1	0.50	0.29	117,117,117,117	0
56	MG	BB	202	1/1	0.50	0.33	123,123,123,123	0
56	MG	BA	3125	1/1	0.50	0.26	100,100,100,100	0
56	MG	AA	1650	1/1	0.50	0.19	118,118,118,118	0
56	MG	DA	3179	1/1	0.50	0.26	113,113,113,113	0
56	MG	CA	1653	1/1	0.50	0.14	99,99,99,99	0
56	MG	CA	1656	1/1	0.50	0.25	106,106,106,106	0
56	MG	AA	1653	1/1	0.50	0.18	106,106,106,106	0
56	MG	AD	301	1/1	0.51	0.28	119,119,119,119	0
56	MG	BA	3018	1/1	0.51	0.30	118,118,118,118	0
56	MG	DA	3057	1/1	0.52	0.41	114,114,114,114	0
56	MG	BA	3110	1/1	0.53	0.23	110,110,110,110	0
56	MG	DA	3192	1/1	0.53	0.27	95,95,95,95	0
56	MG	AA	1608	1/1	0.53	0.26	114,114,114,114	0
56	MG	BA	3081	1/1	0.53	0.22	109,109,109,109	0
56	MG	BA	3022	1/1	0.53	0.26	110,110,110,110	0
56	MG	AA	1617	1/1	0.54	0.19	112,112,112,112	0
56	MG	CA	1665	1/1	0.54	0.11	112,112,112,112	0
56	MG	BA	3107	1/1	0.54	0.21	106,106,106,106	0
56	MG	BA	3152	1/1	0.55	0.42	115,115,115,115	0
56	MG	DA	3162	1/1	0.55	0.25	95,95,95,95	0
56	MG	DA	3174	1/1	0.55	0.18	105,105,105,105	0
56	MG	BA	3090	1/1	0.55	0.34	130,130,130,130	0
56	MG	BC	301	1/1	0.56	0.32	122,122,122,122	0
56	MG	DA	3129	1/1	0.56	0.47	124,124,124,124	0
56	MG	DA	3079	1/1	0.57	0.30	99,99,99,99	0
56	MG	AA	1641	1/1	0.57	0.22	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1627	1/1	0.57	0.24	121,121,121,121	0
56	MG	DA	3131	1/1	0.58	0.34	118,118,118,118	0
56	MG	BA	3157	1/1	0.58	0.46	97,97,97,97	0
56	MG	CA	1659	1/1	0.58	0.20	110,110,110,110	0
56	MG	DA	3152	1/1	0.58	0.23	105,105,105,105	0
56	MG	DA	3013	1/1	0.58	0.35	107,107,107,107	0
56	MG	BA	3030	1/1	0.58	0.20	94,94,94,94	0
56	MG	AA	1628	1/1	0.59	0.22	116,116,116,116	0
56	MG	DA	3065	1/1	0.59	0.19	81,81,81,81	0
56	MG	BA	3058	1/1	0.59	0.28	108,108,108,108	0
56	MG	BA	3087	1/1	0.59	0.28	112,112,112,112	0
56	MG	DA	3194	1/1	0.59	0.29	90,90,90,90	0
56	MG	BA	3053	1/1	0.59	0.25	98,98,98,98	0
56	MG	CA	1629	1/1	0.59	0.40	123,123,123,123	0
56	MG	DA	3055	1/1	0.59	0.25	94,94,94,94	0
56	MG	AA	1614	1/1	0.60	0.31	123,123,123,123	0
56	MG	BA	3148	1/1	0.60	0.23	101,101,101,101	0
56	MG	AA	1626	1/1	0.61	0.22	111,111,111,111	0
56	MG	DA	3172	1/1	0.61	0.21	109,109,109,109	0
56	MG	CA	1649	1/1	0.61	0.12	107,107,107,107	0
56	MG	CA	1602	1/1	0.61	0.19	105,105,105,105	0
56	MG	CA	1633	1/1	0.61	0.34	116,116,116,116	0
56	MG	CA	1607	1/1	0.61	0.30	110,110,110,110	0
56	MG	BA	3019	1/1	0.61	0.18	101,101,101,101	0
56	MG	DA	3025	1/1	0.61	0.29	118,118,118,118	0
56	MG	DA	3083	1/1	0.61	0.21	82,82,82,82	0
56	MG	CA	1643	1/1	0.62	0.23	103,103,103,103	0
56	MG	BA	3141	1/1	0.62	0.13	114,114,114,114	0
56	MG	BA	3013	1/1	0.62	0.27	114,114,114,114	0
56	MG	CA	1638	1/1	0.62	0.31	113,113,113,113	0
56	MG	DA	3100	1/1	0.62	0.20	96,96,96,96	0
56	MG	DA	3146	1/1	0.63	0.30	76,76,76,76	0
56	MG	DA	3150	1/1	0.63	0.42	78,78,78,78	0
56	MG	DA	3042	1/1	0.63	0.28	105,105,105,105	0
56	MG	BA	3044	1/1	0.63	0.27	114,114,114,114	0
56	MG	BA	3160	1/1	0.63	0.24	102,102,102,102	0
56	MG	CA	1609	1/1	0.63	0.28	117,117,117,117	0
56	MG	BA	3014	1/1	0.63	0.32	106,106,106,106	0
56	MG	AA	1629	1/1	0.64	0.27	118,118,118,118	0
56	MG	CA	1603	1/1	0.64	0.17	120,120,120,120	0
56	MG	BA	3102	1/1	0.64	0.22	119,119,119,119	0
56	MG	BA	3032	1/1	0.65	0.32	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3102	1/1	0.65	0.25	94,94,94,94	0
56	MG	DA	3149	1/1	0.65	0.26	107,107,107,107	0
56	MG	DA	3015	1/1	0.65	0.35	124,124,124,124	0
56	MG	CA	1644	1/1	0.65	0.31	118,118,118,118	0
56	MG	DA	3176	1/1	0.65	0.37	78,78,78,78	0
56	MG	DA	3052	1/1	0.66	0.25	95,95,95,95	0
56	MG	BA	3092	1/1	0.66	0.17	119,119,119,119	0
56	MG	BA	3077	1/1	0.66	0.22	121,121,121,121	0
56	MG	BA	3099	1/1	0.66	0.23	112,112,112,112	0
56	MG	DA	3097	1/1	0.66	0.28	105,105,105,105	0
56	MG	CA	1634	1/1	0.66	0.18	120,120,120,120	0
56	MG	BA	3131	1/1	0.66	0.30	114,114,114,114	0
56	MG	DA	3105	1/1	0.66	0.21	90,90,90,90	0
56	MG	BA	3075	1/1	0.66	0.18	104,104,104,104	0
56	MG	DA	3077	1/1	0.67	0.22	98,98,98,98	0
56	MG	BA	3144	1/1	0.67	0.31	87,87,87,87	0
56	MG	BA	3126	1/1	0.67	0.15	110,110,110,110	0
56	MG	DA	3023	1/1	0.67	0.26	120,120,120,120	0
56	MG	DA	3011	1/1	0.67	0.24	103,103,103,103	0
56	MG	DA	3028	1/1	0.67	0.20	85,85,85,85	0
56	MG	DA	3169	1/1	0.67	0.24	94,94,94,94	0
56	MG	CA	1623	1/1	0.67	0.32	117,117,117,117	0
56	MG	CA	1617	1/1	0.68	0.20	115,115,115,115	0
56	MG	CA	1661	1/1	0.68	0.29	101,101,101,101	0
56	MG	AA	1630	1/1	0.68	0.20	105,105,105,105	0
56	MG	CA	1628	1/1	0.68	0.19	116,116,116,116	0
56	MG	DA	3009	1/1	0.68	0.24	102,102,102,102	0
56	MG	CA	1608	1/1	0.68	0.21	115,115,115,115	0
56	MG	BA	3071	1/1	0.68	0.17	104,104,104,104	0
56	MG	BA	3136	1/1	0.69	0.36	94,94,94,94	0
56	MG	AA	1610	1/1	0.69	0.19	120,120,120,120	0
56	MG	DA	3137	1/1	0.69	0.27	93,93,93,93	0
56	MG	CA	1627	1/1	0.69	0.22	111,111,111,111	0
56	MG	CA	1668	1/1	0.70	0.14	107,107,107,107	0
56	MG	BA	3069	1/1	0.70	0.17	129,129,129,129	0
56	MG	BA	3070	1/1	0.70	0.19	90,90,90,90	0
56	MG	BA	3122	1/1	0.70	0.26	112,112,112,112	0
56	MG	DA	3142	1/1	0.70	0.21	86,86,86,86	0
56	MG	BA	3123	1/1	0.70	0.21	88,88,88,88	0
56	MG	BA	3015	1/1	0.70	0.18	115,115,115,115	0
56	MG	BA	3009	1/1	0.70	0.15	95,95,95,95	0
56	MG	BA	3130	1/1	0.70	0.24	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1651	1/1	0.70	0.27	103,103,103,103	0
56	MG	DA	3127	1/1	0.70	0.14	77,77,77,77	0
56	MG	DA	3039	1/1	0.71	0.17	117,117,117,117	0
56	MG	AA	1602	1/1	0.71	0.16	106,106,106,106	0
56	MG	DA	3183	1/1	0.71	0.26	87,87,87,87	0
56	MG	BA	3072	1/1	0.71	0.18	103,103,103,103	0
56	MG	AA	1636	1/1	0.71	0.16	103,103,103,103	0
56	MG	BA	3105	1/1	0.71	0.18	91,91,91,91	0
56	MG	DA	3061	1/1	0.71	0.34	106,106,106,106	0
56	MG	BA	3062	1/1	0.71	0.23	91,91,91,91	0
56	MG	AA	1649	1/1	0.72	0.33	90,90,90,90	0
56	MG	CA	1624	1/1	0.72	0.16	106,106,106,106	0
56	MG	AA	1616	1/1	0.72	0.26	113,113,113,113	0
56	MG	BA	3078	1/1	0.72	0.15	119,119,119,119	0
56	MG	BA	3124	1/1	0.72	0.12	114,114,114,114	0
56	MG	CA	1655	1/1	0.72	0.20	117,117,117,117	0
56	MG	DA	3004	1/1	0.72	0.17	99,99,99,99	0
56	MG	DA	3111	1/1	0.72	0.14	102,102,102,102	0
56	MG	DA	3115	1/1	0.72	0.15	95,95,95,95	0
56	MG	BA	3155	1/1	0.72	0.46	114,114,114,114	0
56	MG	AA	1634	1/1	0.72	0.27	120,120,120,120	0
56	MG	BA	3023	1/1	0.73	0.21	108,108,108,108	0
56	MG	BA	3050	1/1	0.73	0.27	101,101,101,101	0
56	MG	BA	3025	1/1	0.73	0.24	103,103,103,103	0
56	MG	DA	3044	1/1	0.73	0.23	105,105,105,105	0
56	MG	DA	3084	1/1	0.73	0.17	104,104,104,104	0
56	MG	BA	3153	1/1	0.73	0.25	112,112,112,112	0
56	MG	BA	3138	1/1	0.73	0.25	88,88,88,88	0
56	MG	AA	1622	1/1	0.73	0.19	107,107,107,107	0
56	MG	CA	1663	1/1	0.73	0.31	82,82,82,82	0
56	MG	DA	3022	1/1	0.73	0.20	81,81,81,81	0
56	MG	CA	1626	1/1	0.73	0.17	99,99,99,99	0
56	MG	BA	3040	1/1	0.73	0.15	112,112,112,112	0
56	MG	DA	3155	1/1	0.73	0.33	115,115,115,115	0
56	MG	DA	3164	1/1	0.74	0.34	94,94,94,94	0
56	MG	DA	3072	1/1	0.74	0.22	93,93,93,93	0
56	MG	DA	3098	1/1	0.74	0.14	99,99,99,99	0
56	MG	BA	3033	1/1	0.74	0.27	98,98,98,98	0
56	MG	CA	1670	1/1	0.74	0.35	102,102,102,102	0
56	MG	BA	3011	1/1	0.74	0.20	81,81,81,81	0
56	MG	AA	1638	1/1	0.74	0.28	104,104,104,104	0
56	MG	DA	3113	1/1	0.74	0.17	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1650	1/1	0.74	0.34	102,102,102,102	0
56	MG	DB	201	1/1	0.74	0.13	113,113,113,113	0
56	MG	DA	3026	1/1	0.74	0.33	98,98,98,98	0
56	MG	BA	3083	1/1	0.74	0.17	110,110,110,110	0
56	MG	CA	1667	1/1	0.74	0.23	111,111,111,111	0
56	MG	DA	3109	1/1	0.75	0.17	102,102,102,102	0
56	MG	DA	3090	1/1	0.75	0.19	107,107,107,107	0
56	MG	BA	3143	1/1	0.75	0.16	103,103,103,103	0
56	MG	DA	3177	1/1	0.75	0.41	96,96,96,96	0
56	MG	BA	3118	1/1	0.75	0.23	109,109,109,109	0
56	MG	DA	3082	1/1	0.75	0.17	92,92,92,92	0
56	MG	BA	3037	1/1	0.75	0.47	97,97,97,97	0
56	MG	DA	3156	1/1	0.75	0.34	101,101,101,101	0
56	MG	BA	3082	1/1	0.75	0.25	126,126,126,126	0
56	MG	DA	3103	1/1	0.75	0.19	81,81,81,81	0
56	MG	BA	3079	1/1	0.75	0.26	103,103,103,103	0
56	MG	DA	3108	1/1	0.75	0.17	100,100,100,100	0
56	MG	DA	3003	1/1	0.76	0.14	105,105,105,105	0
56	MG	BA	3095	1/1	0.76	0.16	107,107,107,107	0
56	MG	CA	1645	1/1	0.76	0.25	96,96,96,96	0
56	MG	DA	3059	1/1	0.76	0.19	92,92,92,92	0
56	MG	DA	3040	1/1	0.76	0.13	91,91,91,91	0
56	MG	BA	3135	1/1	0.76	0.44	74,74,74,74	0
56	MG	BA	3156	1/1	0.76	0.17	106,106,106,106	0
56	MG	DA	3157	1/1	0.76	0.24	96,96,96,96	0
56	MG	CA	1625	1/1	0.77	0.15	107,107,107,107	0
56	MG	DA	3139	1/1	0.77	0.25	77,77,77,77	0
56	MG	BA	3100	1/1	0.77	0.20	107,107,107,107	0
56	MG	AA	1621	1/1	0.77	0.19	116,116,116,116	0
56	MG	CA	1654	1/1	0.77	0.18	116,116,116,116	0
56	MG	AA	1645	1/1	0.77	0.12	93,93,93,93	0
56	MG	DA	3085	1/1	0.77	0.27	108,108,108,108	0
56	MG	BA	3047	1/1	0.77	0.17	103,103,103,103	0
56	MG	BA	3145	1/1	0.77	0.22	99,99,99,99	0
57	NMY	BA	3164	42/42	0.77	0.15	90,100,104,105	42
56	MG	DA	3171	1/1	0.78	0.27	108,108,108,108	0
56	MG	BA	3115	1/1	0.78	0.16	105,105,105,105	0
56	MG	DA	3060	1/1	0.78	0.22	89,89,89,89	0
56	MG	BA	3085	1/1	0.78	0.12	95,95,95,95	0
56	MG	DA	3006	1/1	0.78	0.13	92,92,92,92	0
56	MG	BA	3051	1/1	0.78	0.14	106,106,106,106	0
56	MG	DA	3180	1/1	0.78	0.19	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3092	1/1	0.78	0.17	95,95,95,95	0
56	MG	DA	3123	1/1	0.78	0.13	102,102,102,102	0
56	MG	BA	3060	1/1	0.78	0.21	106,106,106,106	0
56	MG	BA	3151	1/1	0.78	0.33	92,92,92,92	0
56	MG	AA	1642	1/1	0.78	0.20	94,94,94,94	0
56	MG	BA	3021	1/1	0.78	0.12	108,108,108,108	0
56	MG	CA	1646	1/1	0.78	0.34	95,95,95,95	0
56	MG	AA	1601	1/1	0.78	0.20	132,132,132,132	0
57	NMY	DA	3187	42/42	0.78	0.11	106,109,112,114	42
56	MG	CA	1664	1/1	0.79	0.15	112,112,112,112	0
56	MG	BA	3097	1/1	0.79	0.39	111,111,111,111	0
56	MG	DA	3020	1/1	0.79	0.17	93,93,93,93	0
56	MG	BA	3065	1/1	0.79	0.19	101,101,101,101	0
56	MG	DA	3064	1/1	0.79	0.18	95,95,95,95	0
56	MG	DA	3101	1/1	0.79	0.20	86,86,86,86	0
56	MG	AA	1652	1/1	0.79	0.22	101,101,101,101	0
56	MG	BA	3074	1/1	0.79	0.15	115,115,115,115	0
56	MG	DA	3053	1/1	0.79	0.14	93,93,93,93	0
57	NMY	BA	3167	42/42	0.79	0.15	117,120,124,125	42
56	MG	BA	3088	1/1	0.79	0.15	101,101,101,101	0
56	MG	BA	3149	1/1	0.80	0.31	85,85,85,85	0
56	MG	DA	3182	1/1	0.80	0.35	96,96,96,96	0
56	MG	DL	201	1/1	0.80	0.64	110,110,110,110	0
56	MG	BA	3108	1/1	0.80	0.13	99,99,99,99	0
56	MG	BA	3120	1/1	0.80	0.27	94,94,94,94	0
56	MG	CA	1615	1/1	0.80	0.13	112,112,112,112	0
56	MG	DA	3075	1/1	0.80	0.18	106,106,106,106	0
56	MG	BA	3158	1/1	0.81	0.15	106,106,106,106	0
56	MG	CA	1630	1/1	0.81	0.11	118,118,118,118	0
56	MG	DA	3175	1/1	0.81	0.32	75,75,75,75	0
56	MG	CA	1648	1/1	0.81	0.25	103,103,103,103	0
56	MG	BA	3076	1/1	0.81	0.17	120,120,120,120	0
56	MG	DA	3107	1/1	0.81	0.25	98,98,98,98	0
56	MG	AA	1651	1/1	0.81	0.06	119,119,119,119	0
56	MG	DA	3021	1/1	0.81	0.24	108,108,108,108	0
56	MG	AA	1603	1/1	0.81	0.13	117,117,117,117	0
56	MG	CA	1618	1/1	0.81	0.17	83,83,83,83	0
56	MG	BA	3104	1/1	0.81	0.31	106,106,106,106	0
56	MG	BA	3061	1/1	0.81	0.15	85,85,85,85	0
56	MG	DA	3125	1/1	0.81	0.15	113,113,113,113	0
56	MG	DB	203	1/1	0.81	0.17	100,100,100,100	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(\AA^2)	Q<0.9
56	MG	BA	3121	1/1	0.81	0.23	110,110,110,110	0
56	MG	DA	3167	1/1	0.81	0.22	84,84,84,84	0
56	MG	BA	3003	1/1	0.81	0.14	115,115,115,115	0
56	MG	DA	3170	1/1	0.81	0.21	94,94,94,94	0
57	NMY	DA	3184	42/42	0.81	0.15	57,71,80,89	42
56	MG	BA	3147	1/1	0.81	0.37	95,95,95,95	0
58	ZN	D4	101	1/1	0.81	0.49	162,162,162,162	0
56	MG	DA	3094	1/1	0.82	0.18	87,87,87,87	0
56	MG	DA	3073	1/1	0.82	0.18	99,99,99,99	0
56	MG	BA	3114	1/1	0.82	0.17	120,120,120,120	0
56	MG	BA	3127	1/1	0.82	0.19	95,95,95,95	0
56	MG	BA	3129	1/1	0.82	0.28	107,107,107,107	0
56	MG	DA	3193	1/1	0.82	0.34	95,95,95,95	0
56	MG	BA	3063	1/1	0.82	0.20	106,106,106,106	0
56	MG	CA	1606	1/1	0.82	0.11	99,99,99,99	0
56	MG	DA	3165	1/1	0.82	0.22	78,78,78,78	0
56	MG	BA	3116	1/1	0.82	0.13	99,99,99,99	0
56	MG	DA	3138	1/1	0.82	0.38	81,81,81,81	0
56	MG	BA	3109	1/1	0.82	0.21	106,106,106,106	0
56	MG	BA	3098	1/1	0.82	0.17	100,100,100,100	0
56	MG	DA	3145	1/1	0.82	0.31	91,91,91,91	0
57	NMY	BA	3165	42/42	0.82	0.18	79,84,87,90	42
56	MG	DA	3045	1/1	0.82	0.11	95,95,95,95	0
56	MG	DA	3069	1/1	0.82	0.17	81,81,81,81	0
56	MG	DA	3071	1/1	0.82	0.14	97,97,97,97	0
56	MG	CA	1613	1/1	0.82	0.10	103,103,103,103	0
56	MG	BB	201	1/1	0.83	0.11	137,137,137,137	0
56	MG	CA	1641	1/1	0.83	0.13	85,85,85,85	0
56	MG	BA	3052	1/1	0.83	0.15	97,97,97,97	0
56	MG	DA	3051	1/1	0.83	0.16	86,86,86,86	0
56	MG	AA	1643	1/1	0.83	0.11	110,110,110,110	0
56	MG	DA	3147	1/1	0.83	0.42	107,107,107,107	0
56	MG	BA	3133	1/1	0.83	0.16	106,106,106,106	0
56	MG	DA	3118	1/1	0.83	0.16	88,88,88,88	0
56	MG	AA	1644	1/1	0.83	0.19	106,106,106,106	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	3008	1/1	0.83	0.16	88,88,88,88	0
56	MG	BA	3055	1/1	0.83	0.13	101,101,101,101	0
56	MG	CA	1666	1/1	0.83	0.19	112,112,112,112	0
56	MG	DA	3035	1/1	0.83	0.16	94,94,94,94	0
56	MG	DA	3012	1/1	0.83	0.17	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3170	1/1	0.83	0.49	88,88,88,88	0
56	MG	BA	3137	1/1	0.84	0.23	82,82,82,82	0
56	MG	DA	3166	1/1	0.84	0.33	87,87,87,87	0
56	MG	BQ	201	1/1	0.84	0.31	93,93,93,93	0
56	MG	DA	3168	1/1	0.84	0.15	89,89,89,89	0
56	MG	DA	3181	1/1	0.84	0.42	77,77,77,77	0
56	MG	BA	3043	1/1	0.84	0.10	108,108,108,108	0
56	MG	CA	1621	1/1	0.84	0.14	111,111,111,111	0
56	MG	DA	3119	1/1	0.84	0.15	82,82,82,82	0
56	MG	AA	1615	1/1	0.84	0.10	112,112,112,112	0
56	MG	DA	3173	1/1	0.84	0.18	90,90,90,90	0
56	MG	DA	3163	1/1	0.84	0.18	99,99,99,99	0
57	NMY	DA	3190	42/42	0.84	0.25	57,66,70,74	42
56	MG	BA	3005	1/1	0.84	0.14	106,106,106,106	0
56	MG	CA	1612	1/1	0.85	0.19	116,116,116,116	0
56	MG	DA	3120	1/1	0.85	0.19	98,98,98,98	0
56	MG	BA	3139	1/1	0.85	0.32	83,83,83,83	0
56	MG	DA	3016	1/1	0.85	0.13	103,103,103,103	0
56	MG	BA	3057	1/1	0.85	0.12	98,98,98,98	0
57	NMY	BA	3161	42/42	0.85	0.17	61,70,77,82	42
56	MG	AA	1647	1/1	0.85	0.17	109,109,109,109	0
57	NMY	BA	3163	42/42	0.85	0.19	89,98,100,101	42
56	MG	DA	3048	1/1	0.85	0.15	96,96,96,96	0
56	MG	DA	3049	1/1	0.85	0.19	97,97,97,97	0
56	MG	DA	3135	1/1	0.85	0.18	71,71,71,71	0
56	MG	DA	3029	1/1	0.85	0.21	84,84,84,84	0
56	MG	DA	3031	1/1	0.85	0.13	108,108,108,108	0
56	MG	DA	3159	1/1	0.85	0.26	90,90,90,90	0
56	MG	BA	3056	1/1	0.85	0.13	99,99,99,99	0
56	MG	DA	3136	1/1	0.86	0.29	74,74,74,74	0
56	MG	BA	3106	1/1	0.86	0.16	100,100,100,100	0
56	MG	BA	3089	1/1	0.86	0.10	109,109,109,109	0
56	MG	DA	3160	1/1	0.86	0.34	92,92,92,92	0
56	MG	AA	1624	1/1	0.86	0.17	110,110,110,110	0
56	MG	DA	3141	1/1	0.86	0.46	73,73,73,73	0
56	MG	DA	3178	1/1	0.86	0.19	88,88,88,88	0
56	MG	CA	1635	1/1	0.86	0.13	113,113,113,113	0
56	MG	DA	3121	1/1	0.86	0.19	86,86,86,86	0
56	MG	BA	3103	1/1	0.86	0.42	105,105,105,105	0
56	MG	DA	3034	1/1	0.86	0.13	84,84,84,84	0
57	NMY	BA	3166	42/42	0.86	0.16	68,77,83,90	42
56	MG	DA	3062	1/1	0.86	0.13	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3093	1/1	0.86	0.23	105,105,105,105	0
56	MG	AA	1632	1/1	0.86	0.15	114,114,114,114	0
56	MG	BA	3045	1/1	0.86	0.15	118,118,118,118	0
58	ZN	B4	101	1/1	0.86	0.18	186,186,186,186	0
56	MG	DA	3066	1/1	0.86	0.11	90,90,90,90	0
56	MG	DA	3088	1/1	0.87	0.11	115,115,115,115	0
56	MG	BA	3113	1/1	0.87	0.14	121,121,121,121	0
56	MG	DA	3116	1/1	0.87	0.13	107,107,107,107	0
56	MG	CA	1614	1/1	0.87	0.10	120,120,120,120	0
56	MG	CA	1671	1/1	0.87	0.22	96,96,96,96	0
56	MG	BA	3086	1/1	0.87	0.09	109,109,109,109	0
56	MG	CA	1616	1/1	0.87	0.10	98,98,98,98	0
57	NMY	AA	1655	42/42	0.87	0.10	61,73,90,121	0
56	MG	CA	1658	1/1	0.87	0.10	115,115,115,115	0
56	MG	BA	3001	1/1	0.87	0.13	99,99,99,99	0
56	MG	DA	3154	1/1	0.87	0.37	86,86,86,86	0
56	MG	BA	3134	1/1	0.87	0.20	109,109,109,109	0
56	MG	DA	3056	1/1	0.87	0.12	86,86,86,86	0
56	MG	CA	1620	1/1	0.87	0.17	118,118,118,118	0
56	MG	BA	3169	1/1	0.87	0.13	101,101,101,101	0
56	MG	BA	3101	1/1	0.87	0.24	102,102,102,102	0
56	MG	BA	3041	1/1	0.87	0.12	96,96,96,96	0
56	MG	DA	3014	1/1	0.87	0.14	90,90,90,90	0
57	NMY	DA	3189	42/42	0.87	0.14	55,63,70,72	42
56	MG	AA	1637	1/1	0.87	0.18	103,103,103,103	0
56	MG	BA	3038	1/1	0.87	0.15	104,104,104,104	0
56	MG	DA	3140	1/1	0.87	0.20	98,98,98,98	0
56	MG	CA	1669	1/1	0.88	0.30	107,107,107,107	0
56	MG	BA	3119	1/1	0.88	0.10	106,106,106,106	0
56	MG	DA	3117	1/1	0.88	0.12	93,93,93,93	0
56	MG	BA	3049	1/1	0.88	0.15	88,88,88,88	0
56	MG	BA	3017	1/1	0.88	0.10	107,107,107,107	0
56	MG	BA	3112	1/1	0.88	0.19	101,101,101,101	0
56	MG	DA	3153	1/1	0.88	0.12	95,95,95,95	0
57	NMY	DA	3185	42/42	0.88	0.12	46,58,63,67	42
56	MG	DA	3024	1/1	0.88	0.13	73,73,73,73	0
56	MG	DA	3067	1/1	0.88	0.19	120,120,120,120	0
56	MG	BA	3031	1/1	0.88	0.11	87,87,87,87	0
56	MG	CA	1622	1/1	0.88	0.18	108,108,108,108	0
56	MG	DA	3007	1/1	0.88	0.09	103,103,103,103	0
56	MG	DA	3070	1/1	0.89	0.11	56,56,56,56	0
56	MG	DA	3112	1/1	0.89	0.18	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3029	1/1	0.89	0.10	99,99,99,99	0
56	MG	DA	3158	1/1	0.89	0.23	91,91,91,91	0
56	MG	BA	3117	1/1	0.89	0.10	89,89,89,89	0
56	MG	DA	3036	1/1	0.89	0.25	90,90,90,90	0
56	MG	BA	3146	1/1	0.89	0.24	98,98,98,98	0
56	MG	BA	3008	1/1	0.89	0.21	107,107,107,107	0
56	MG	DA	3041	1/1	0.89	0.11	81,81,81,81	0
56	MG	BA	3132	1/1	0.89	0.10	96,96,96,96	0
56	MG	BA	3140	1/1	0.89	0.13	101,101,101,101	0
56	MG	DA	3122	1/1	0.89	0.12	97,97,97,97	0
56	MG	BA	3020	1/1	0.89	0.16	95,95,95,95	0
57	NMY	DA	3186	42/42	0.89	0.12	53,58,64,71	42
56	MG	DA	3046	1/1	0.89	0.10	86,86,86,86	0
56	MG	BA	3006	1/1	0.89	0.10	101,101,101,101	0
56	MG	DA	3017	1/1	0.89	0.12	76,76,76,76	0
56	MG	AA	1604	1/1	0.89	0.07	102,102,102,102	0
56	MG	DA	3032	1/1	0.89	0.22	97,97,97,97	0
56	MG	AA	1618	1/1	0.90	0.14	96,96,96,96	0
56	MG	BB	203	1/1	0.90	0.07	107,107,107,107	0
56	MG	BA	3064	1/1	0.90	0.12	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	0.11	95,95,95,95	0
56	MG	CA	1611	1/1	0.90	0.10	110,110,110,110	0
56	MG	AA	1606	1/1	0.90	0.19	111,111,111,111	0
56	MG	BA	3093	1/1	0.90	0.26	109,109,109,109	0
56	MG	CA	1640	1/1	0.90	0.24	114,114,114,114	0
56	MG	BA	3039	1/1	0.90	0.08	96,96,96,96	0
56	MG	DA	3096	1/1	0.90	0.12	75,75,75,75	0
56	MG	AA	1609	1/1	0.91	0.17	111,111,111,111	0
56	MG	BA	3091	1/1	0.91	0.20	115,115,115,115	0
56	MG	DE	301	1/1	0.91	0.09	100,100,100,100	0
56	MG	DA	3104	1/1	0.91	0.13	81,81,81,81	0
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	DA	3106	1/1	0.91	0.18	100,100,100,100	0
56	MG	DA	3128	1/1	0.91	0.15	92,92,92,92	0
56	MG	DA	3010	1/1	0.91	0.18	106,106,106,106	0
56	MG	DA	3037	1/1	0.91	0.12	72,72,72,72	0
56	MG	DA	3132	1/1	0.91	0.10	96,96,96,96	0
56	MG	BA	3067	1/1	0.91	0.09	89,89,89,89	0
56	MG	BA	3035	1/1	0.91	0.11	94,94,94,94	0
56	MG	CA	1610	1/1	0.91	0.17	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	NMY	CA	1672	42/42	0.91	0.15	54,65,74,77	42
56	MG	DA	3074	1/1	0.91	0.10	95,95,95,95	0
56	MG	CA	1662	1/1	0.91	0.12	114,114,114,114	0
56	MG	DA	3043	1/1	0.91	0.09	90,90,90,90	0
56	MG	BA	3024	1/1	0.91	0.25	114,114,114,114	0
57	NMY	DA	3188	42/42	0.91	0.11	45,60,66,70	42
56	MG	CA	1619	1/1	0.91	0.09	93,93,93,93	0
56	MG	DA	3030	1/1	0.91	0.11	76,76,76,76	0
56	MG	DA	3143	1/1	0.91	0.59	79,79,79,79	0
56	MG	BA	3004	1/1	0.91	0.13	120,120,120,120	0
56	MG	DA	3038	1/1	0.92	0.13	81,81,81,81	0
56	MG	AA	1605	1/1	0.92	0.14	121,121,121,121	0
56	MG	AA	1612	1/1	0.92	0.10	107,107,107,107	0
56	MG	DA	3033	1/1	0.92	0.09	91,91,91,91	0
57	NMY	AA	1657	42/42	0.92	0.34	81,84,88,90	42
56	MG	DA	3110	1/1	0.92	0.15	93,93,93,93	0
56	MG	DA	3078	1/1	0.92	0.10	84,84,84,84	0
56	MG	BA	3068	1/1	0.92	0.11	126,126,126,126	0
56	MG	BA	3073	1/1	0.92	0.10	101,101,101,101	0
56	MG	BA	3128	1/1	0.92	0.08	94,94,94,94	0
56	MG	BA	3034	1/1	0.92	0.09	88,88,88,88	0
56	MG	BA	3111	1/1	0.93	0.10	98,98,98,98	0
56	MG	CA	1605	1/1	0.93	0.09	97,97,97,97	0
56	MG	DA	3099	1/1	0.93	0.08	90,90,90,90	0
56	MG	DA	3130	1/1	0.93	0.15	96,96,96,96	0
56	MG	BA	3048	1/1	0.93	0.06	93,93,93,93	0
56	MG	DA	3144	1/1	0.93	0.11	108,108,108,108	0
56	MG	DA	3054	1/1	0.93	0.14	93,93,93,93	0
56	MG	DA	3047	1/1	0.93	0.09	76,76,76,76	0
56	MG	DA	3191	1/1	0.93	0.10	80,80,80,80	0
56	MG	BA	3016	1/1	0.93	0.09	83,83,83,83	0
56	MG	BA	3150	1/1	0.93	0.23	95,95,95,95	0
56	MG	DA	3114	1/1	0.93	0.09	77,77,77,77	0
56	MG	DA	3005	1/1	0.93	0.07	88,88,88,88	0
56	MG	BA	3036	1/1	0.94	0.07	95,95,95,95	0
56	MG	DA	3058	1/1	0.94	0.18	96,96,96,96	0
56	MG	DA	3080	1/1	0.94	0.18	100,100,100,100	0
56	MG	AA	1635	1/1	0.94	0.17	105,105,105,105	0
56	MG	DA	3019	1/1	0.94	0.14	78,78,78,78	0
56	MG	DA	3148	1/1	0.94	0.14	60,60,60,60	0
56	MG	CA	1642	1/1	0.95	0.16	106,106,106,106	0
56	MG	AA	1607	1/1	0.95	0.13	116,116,116,116	0

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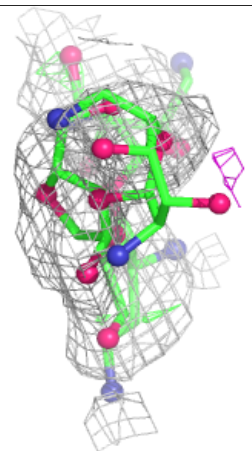
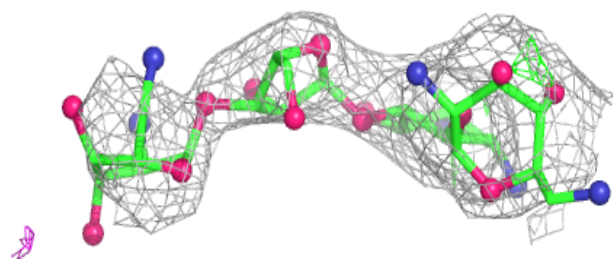
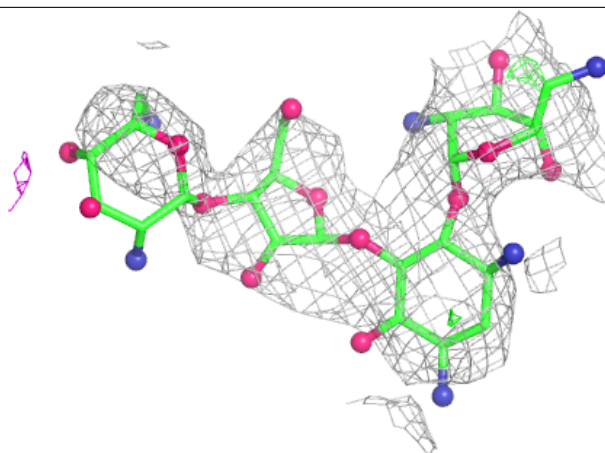
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1620	1/1	0.95	0.14	118,118,118,118	0
56	MG	DA	3133	1/1	0.95	0.14	100,100,100,100	0
56	MG	BA	3010	1/1	0.95	0.08	85,85,85,85	0
56	MG	DA	3091	1/1	0.96	0.10	104,104,104,104	0
56	MG	DA	3002	1/1	0.96	0.07	86,86,86,86	0
56	MG	BA	3002	1/1	0.96	0.07	89,89,89,89	0
56	MG	DA	3086	1/1	0.96	0.06	97,97,97,97	0
56	MG	BA	3094	1/1	0.96	0.13	92,92,92,92	0
56	MG	BA	3084	1/1	0.96	0.08	95,95,95,95	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	AA	1611	1/1	0.97	0.04	104,104,104,104	0
56	MG	BA	3028	1/1	0.97	0.19	89,89,89,89	0
56	MG	CA	1604	1/1	0.97	0.05	86,86,86,86	0
56	MG	DA	3089	1/1	0.98	0.07	97,97,97,97	0
56	MG	BA	3080	1/1	0.98	0.05	73,73,73,73	0
56	MG	BA	3042	1/1	0.98	0.05	97,97,97,97	0
56	MG	AA	1613	1/1	0.98	0.13	115,115,115,115	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	BA	3046	1/1	0.98	0.07	109,109,109,109	0

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

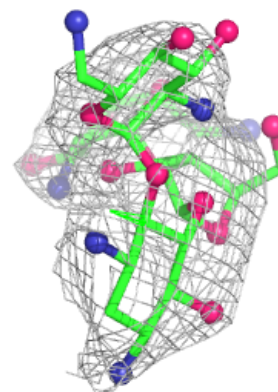
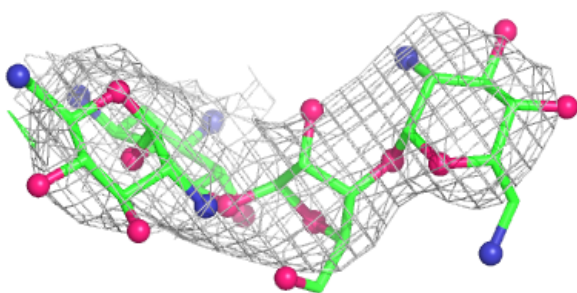
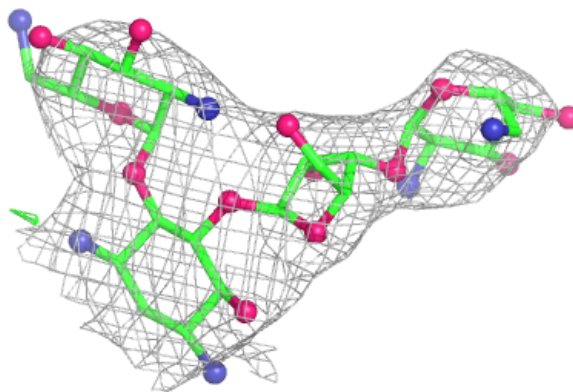
Electron density around NMY BA 3164:

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



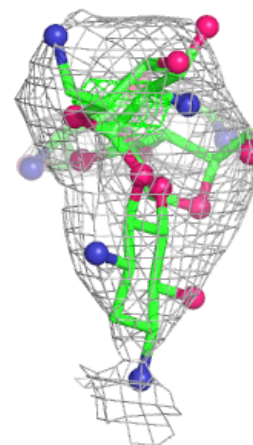
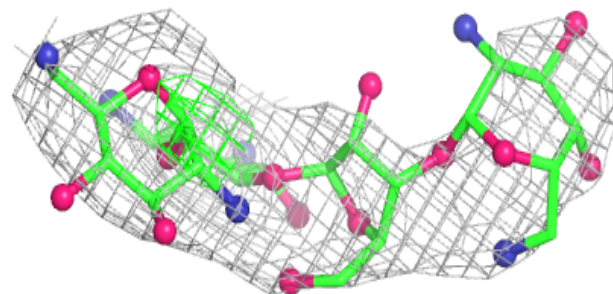
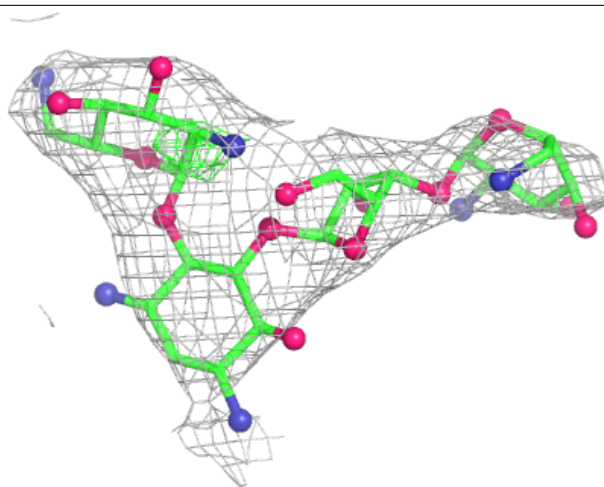
Electron density around NMY DA 3187:

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



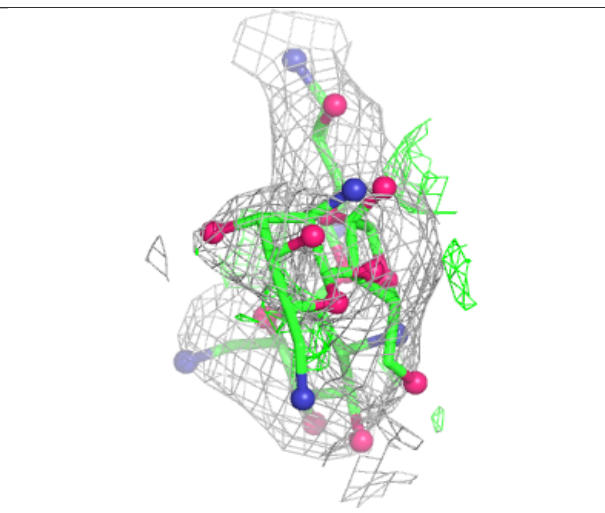
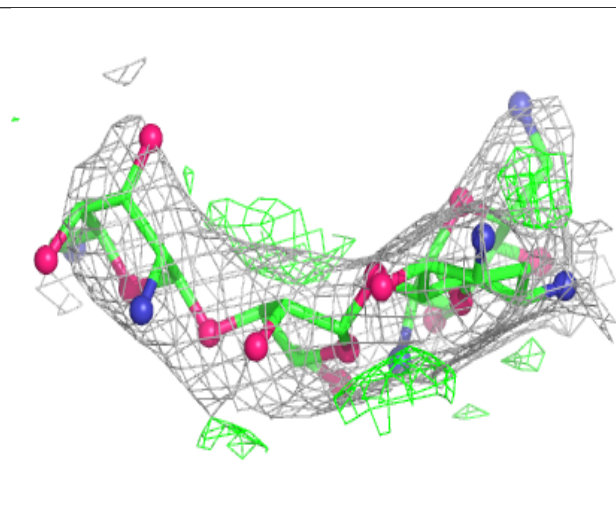
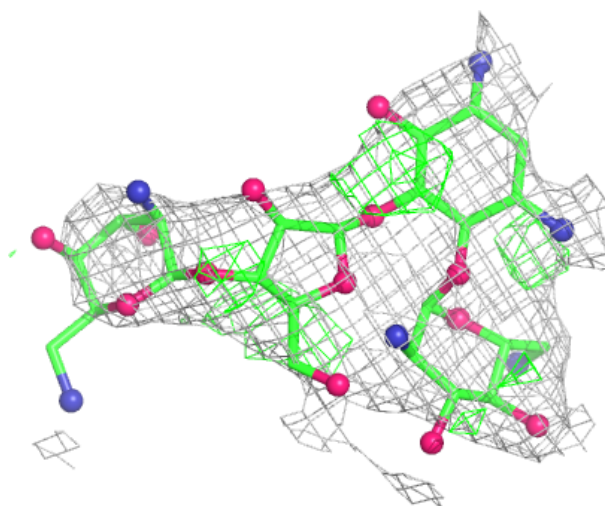
Electron density around NMY BA 3167:

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



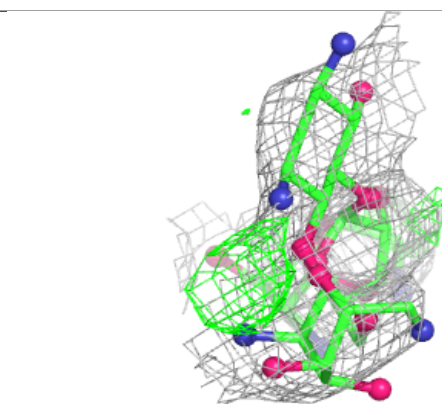
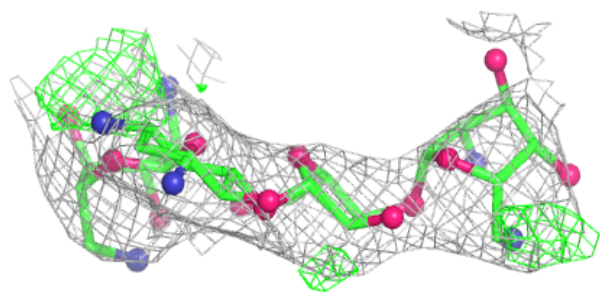
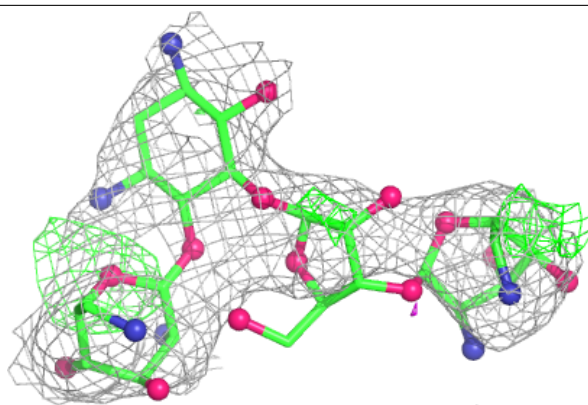
Electron density around NMY DA 3184:

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

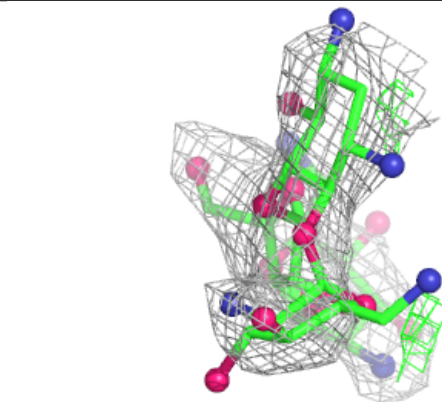
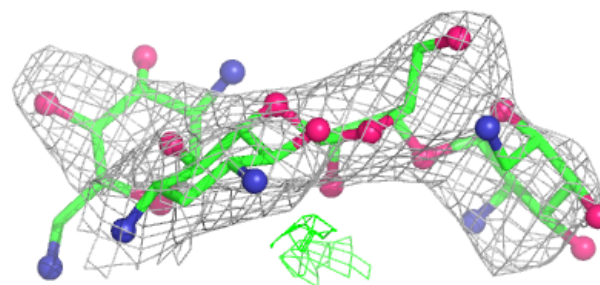
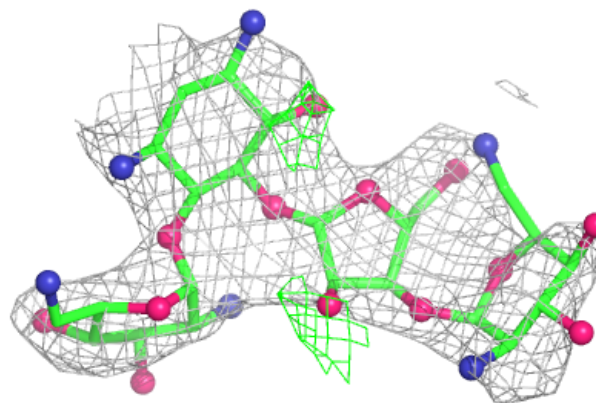


Electron density around NMY BA 3165:

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

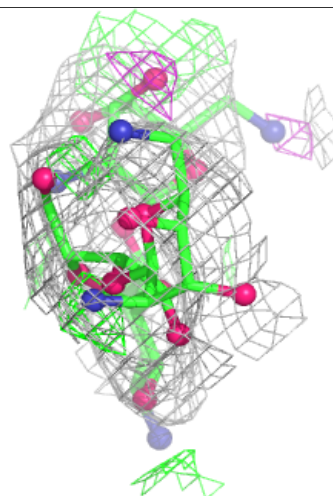
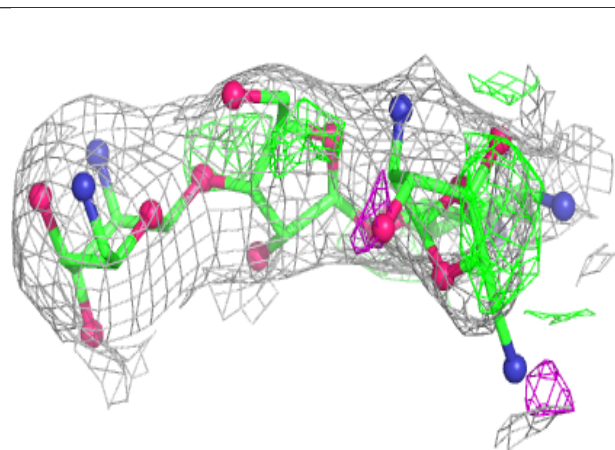
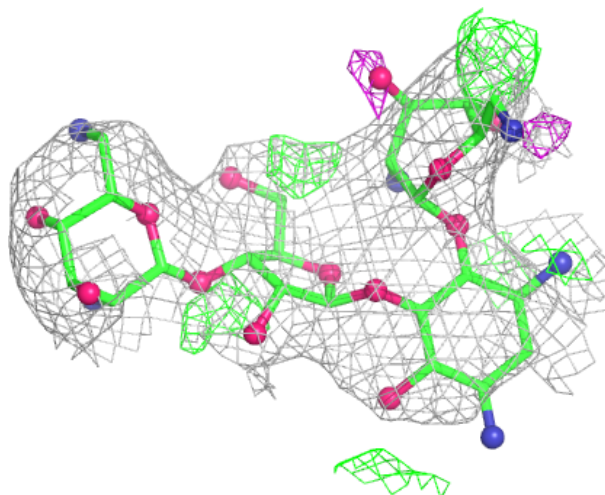
**Electron density around NMY AA 1656:**

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



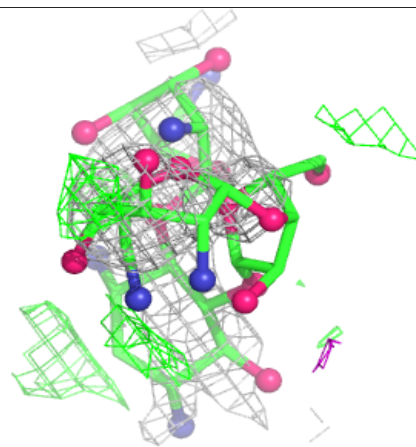
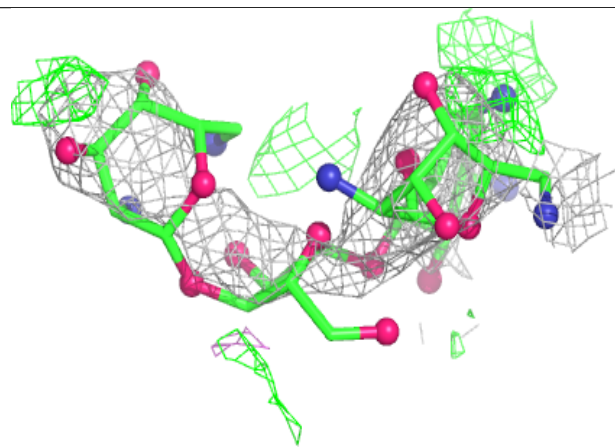
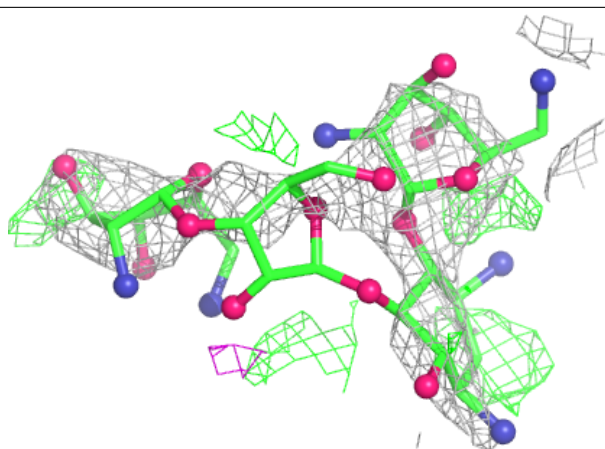
Electron density around NMY BA 3162:

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



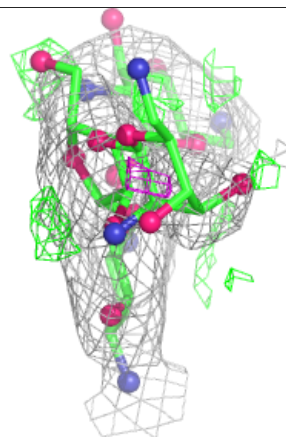
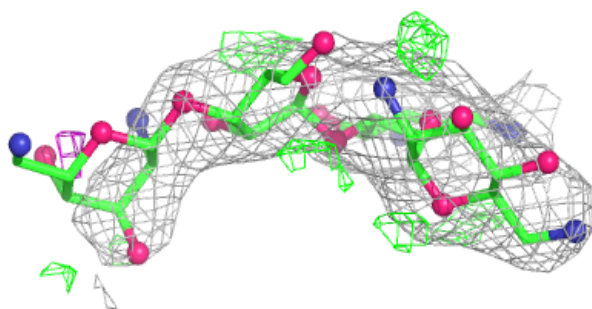
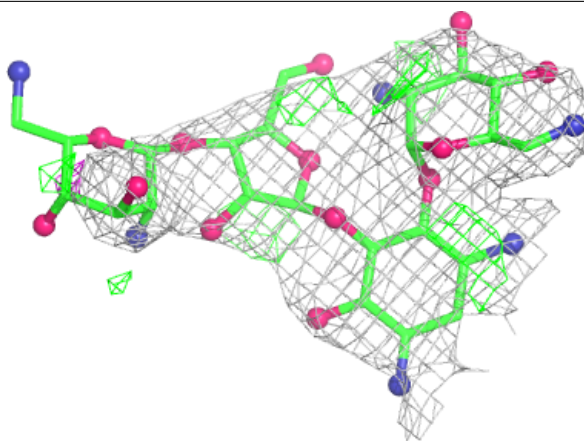
Electron density around NMY DA 3190:

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

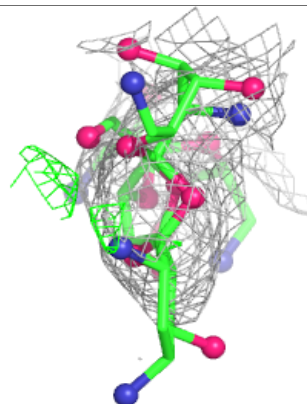
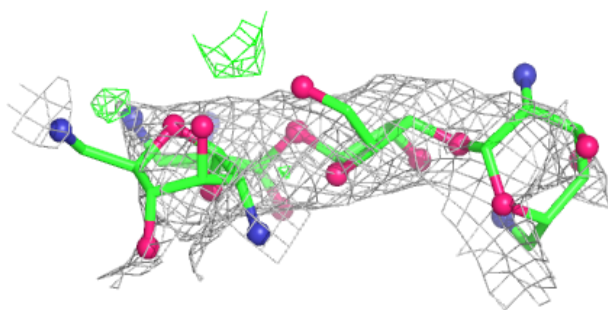
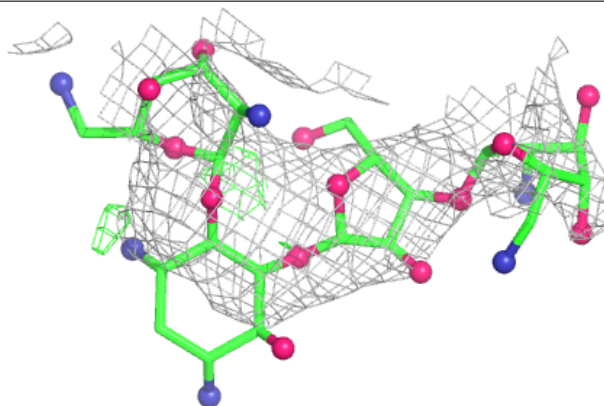


Electron density around NMY BA 3161:

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

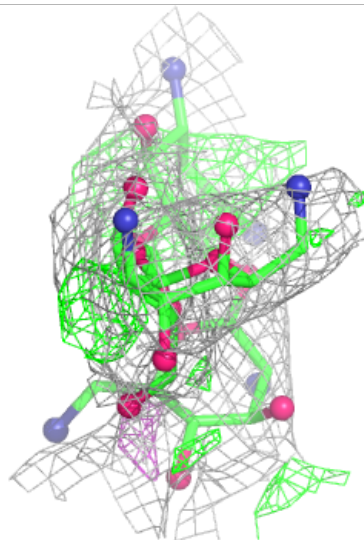
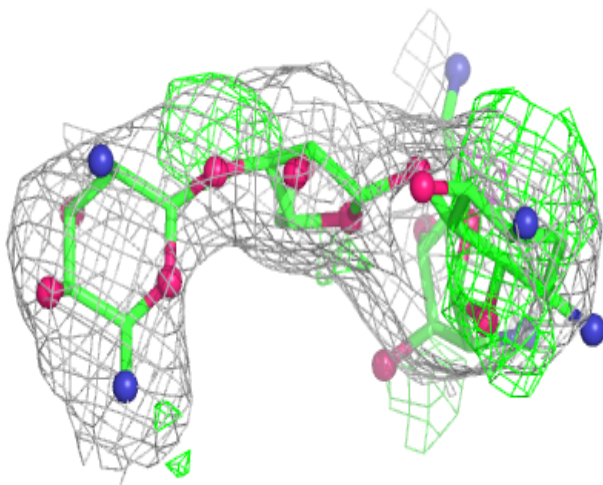
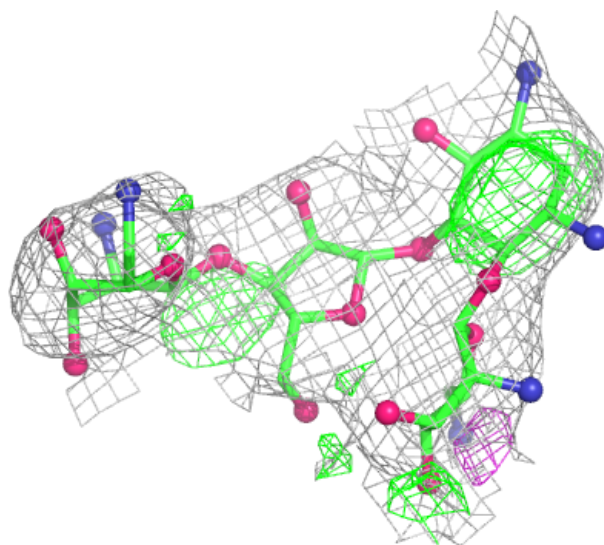
**Electron density around NMY BA 3163:**

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



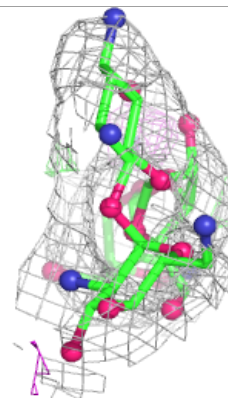
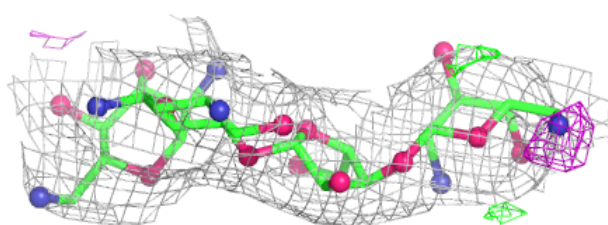
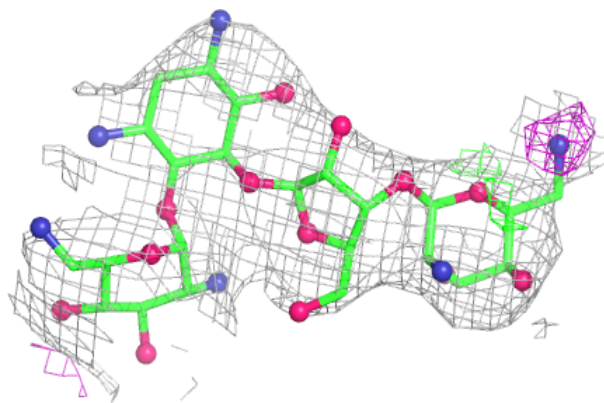
Electron density around NMY BA 3166:

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



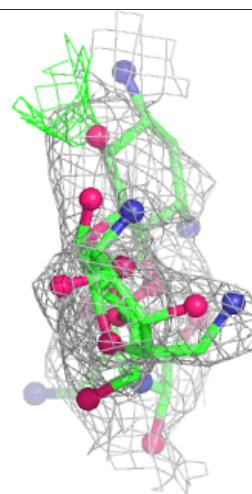
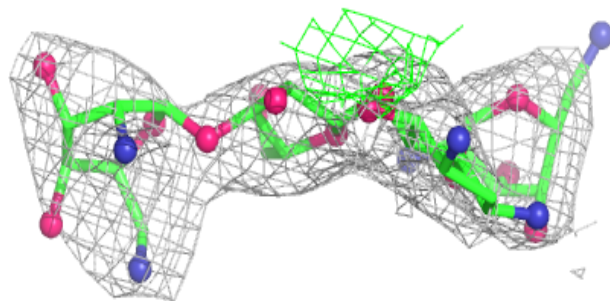
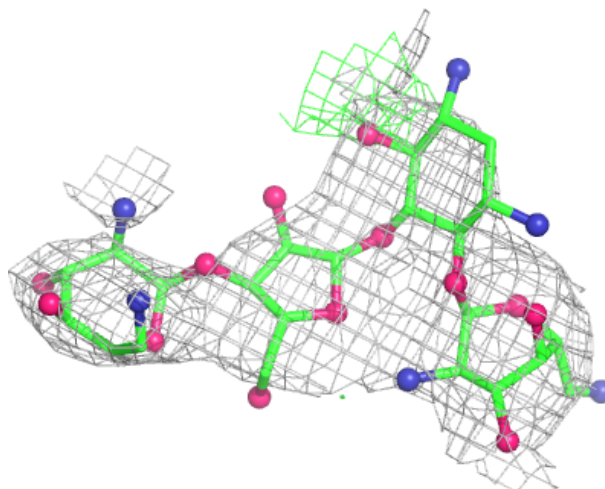
Electron density around NMY AA 1655:

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



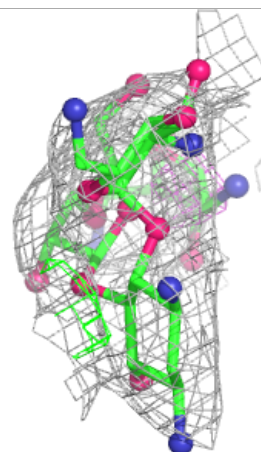
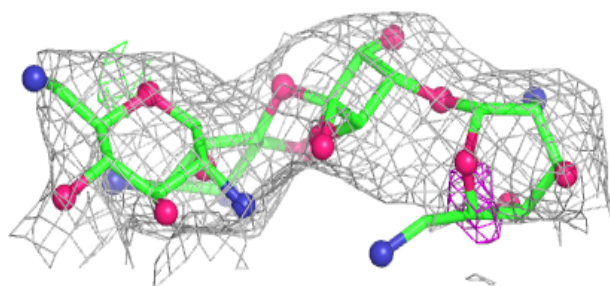
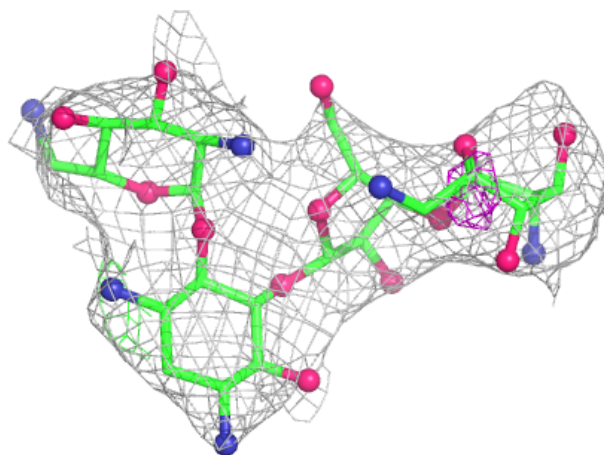
Electron density around NMY DA 3189:

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



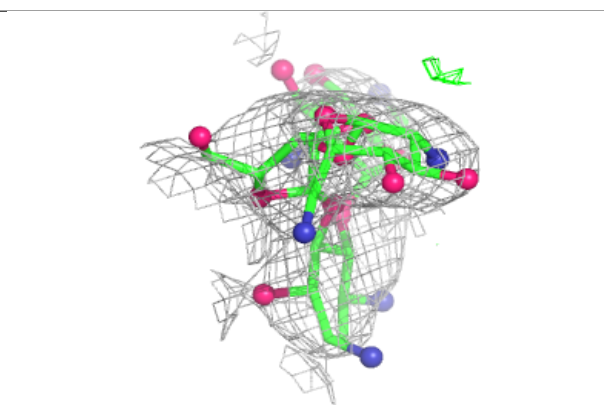
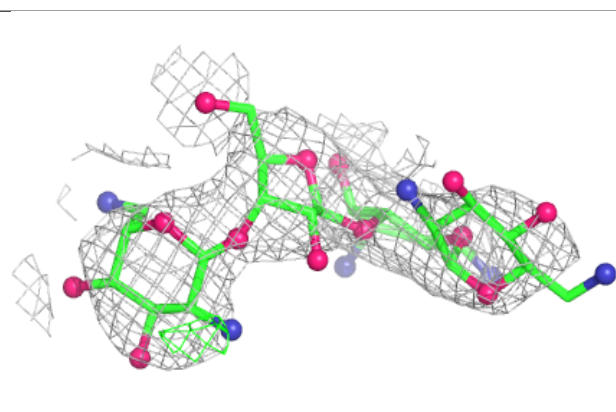
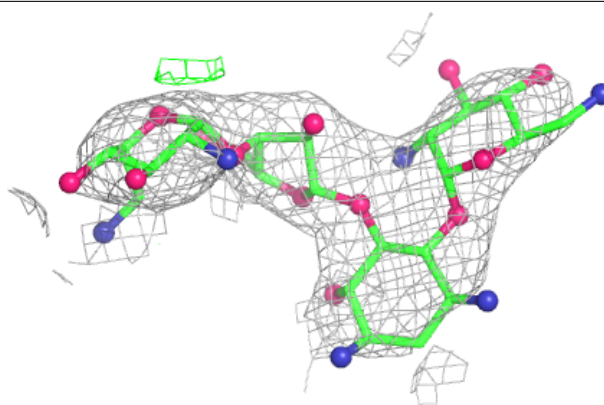
Electron density around NMY DA 3185:

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

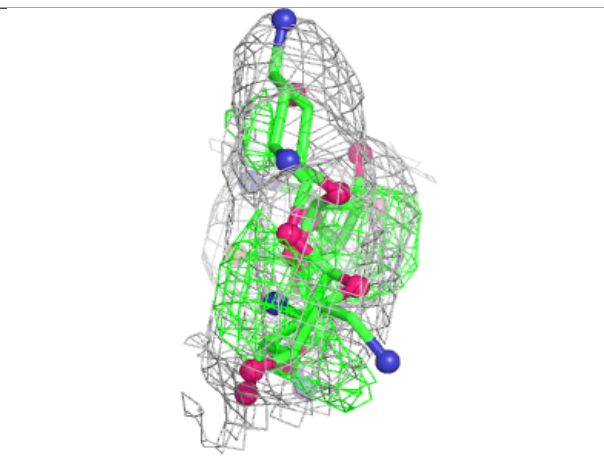
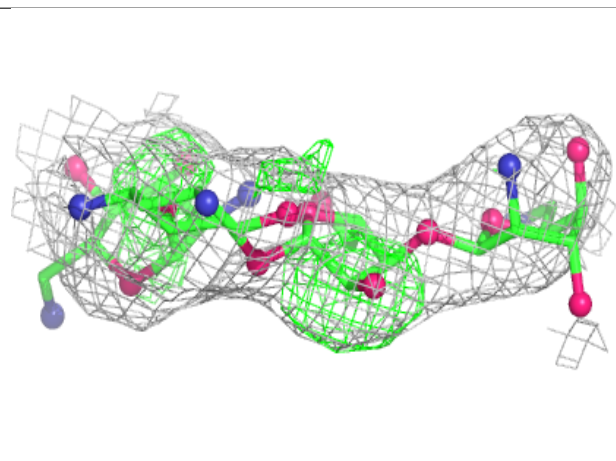
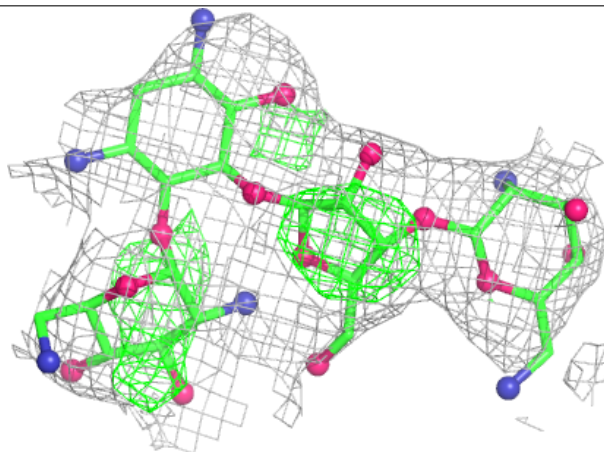


Electron density around NMY DA 3186:

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

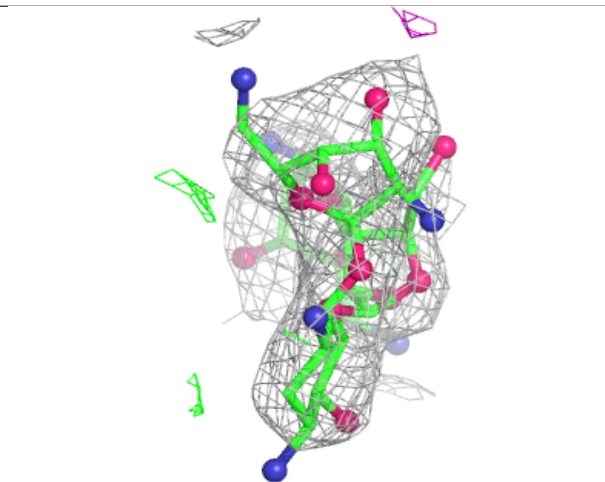
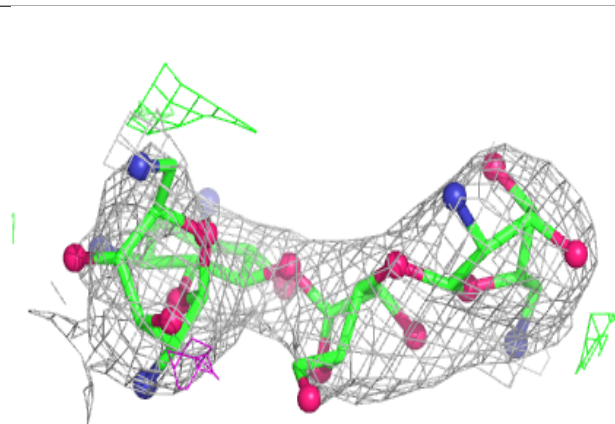
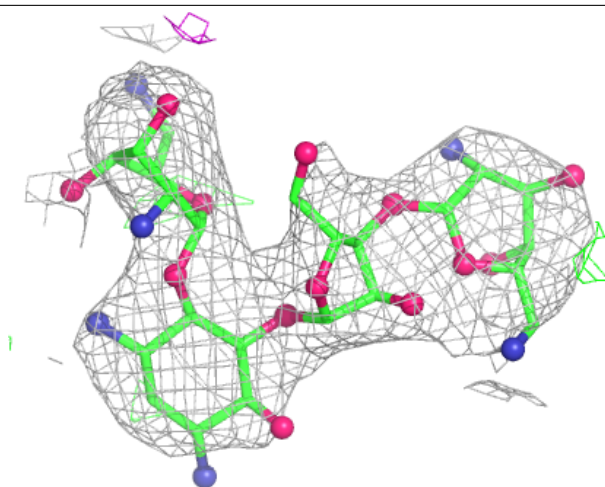
**Electron density around NMY CA 1672:**

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



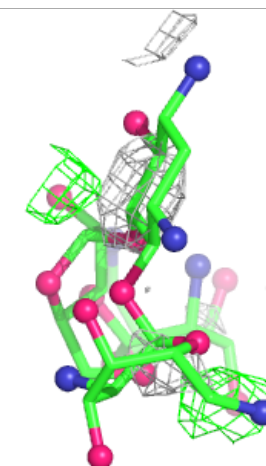
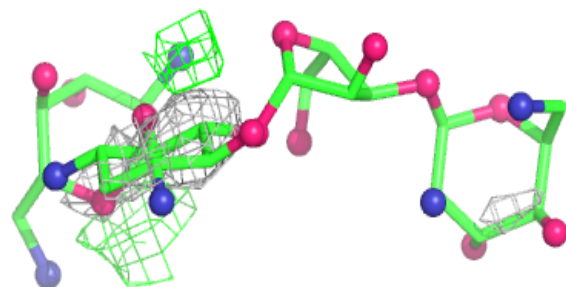
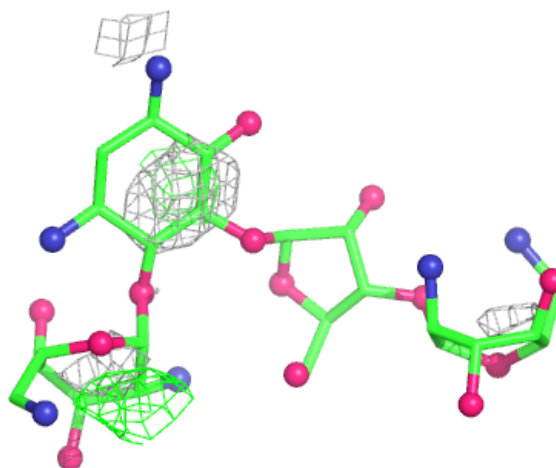
Electron density around NMY DA 3188:

$2mF_o-DF_c$ (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.