



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 07:18 AM 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

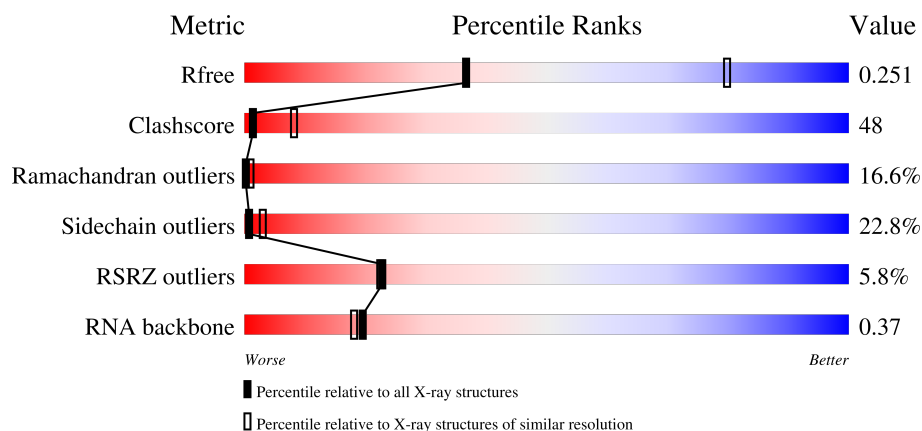
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



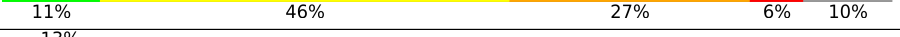
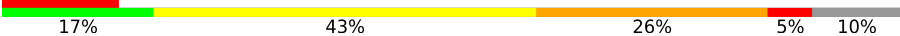
The reported resolution of this entry is 3.30 Å.

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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	




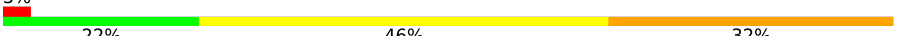
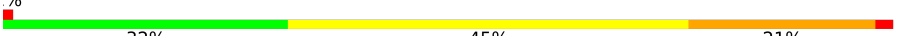
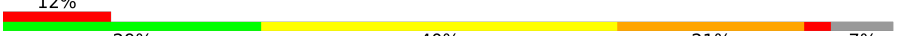



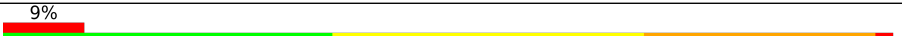

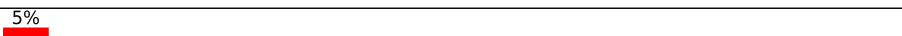

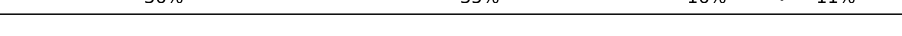
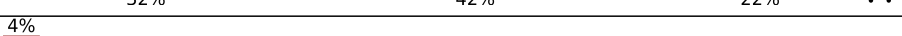
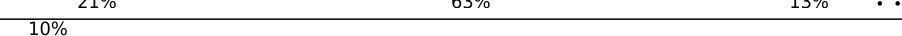





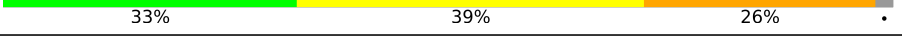

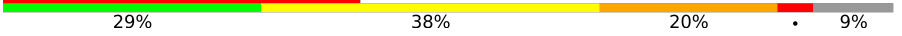
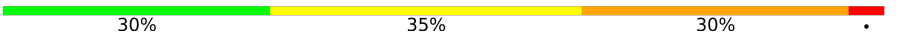
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Mol	Chain	Length	Quality of chain
28	BE	201	
28	DE	201	
29	BF	179	
29	DF	179	
30	BG	177	
30	DG	177	
31	BH	149	
31	DH	149	
32	BI	142	
32	DI	142	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN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

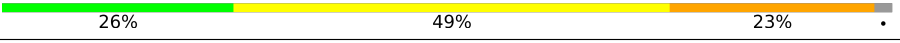
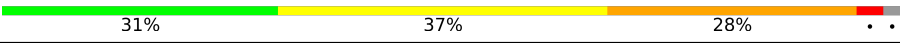
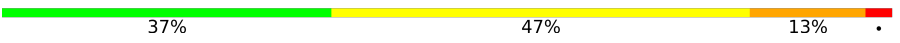
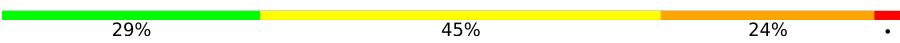
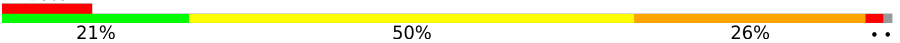
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Mol	Chain	Length	Quality of chain
40	DQ	118	
41	BR	103	
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	104	
44	DU	104	
45	BV	94	
45	DV	94	
46	BW	85	
46	DW	85	
47	BX	78	
47	DX	78	
48	BY	63	
48	DY	63	
49	BZ	59	
49	DZ	59	
50	B0	57	
50	D0	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	1602	-	-	-	X
56	MG	AA	1614	-	-	-	X
56	MG	AA	1616	-	-	-	X
56	MG	AA	1617	-	-	-	X
56	MG	AA	1623	-	-	-	X
56	MG	AA	1625	-	-	-	X
56	MG	AA	1626	-	-	-	X
56	MG	AA	1627	-	-	-	X
56	MG	AA	1629	-	-	-	X
56	MG	AA	1631	-	-	-	X
56	MG	AA	1639	-	-	-	X
56	MG	AA	1640	-	-	-	X
56	MG	AA	1641	-	-	-	X
56	MG	AA	1644	-	-	-	X
56	MG	AA	1646	-	-	-	X
56	MG	AA	1648	-	-	-	X
56	MG	AA	1649	-	-	-	X
56	MG	AA	1650	-	-	-	X
56	MG	AA	1653	-	-	-	X
56	MG	AA	1654	-	-	-	X
56	MG	AD	301	-	-	-	X
56	MG	AN	201	-	-	-	X
56	MG	BA	3007	-	-	-	X
56	MG	BA	3012	-	-	-	X
56	MG	BA	3013	-	-	-	X
56	MG	BA	3018	-	-	-	X
56	MG	BA	3022	-	-	-	X
56	MG	BA	3025	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3026	-	-	-	X
56	MG	BA	3027	-	-	-	X
56	MG	BA	3032	-	-	-	X
56	MG	BA	3053	-	-	-	X
56	MG	BA	3054	-	-	-	X
56	MG	BA	3058	-	-	-	X
56	MG	BA	3059	-	-	-	X
56	MG	BA	3069	-	-	-	X
56	MG	BA	3079	-	-	-	X
56	MG	BA	3082	-	-	-	X
56	MG	BA	3087	-	-	-	X
56	MG	BA	3090	-	-	-	X
56	MG	BA	3096	-	-	-	X
56	MG	BA	3102	-	-	-	X
56	MG	BA	3107	-	-	-	X
56	MG	BA	3110	-	-	-	X
56	MG	BA	3118	-	-	-	X
56	MG	BA	3123	-	-	-	X
56	MG	BA	3125	-	-	-	X
56	MG	BA	3129	-	-	-	X
56	MG	BA	3138	-	-	-	X
56	MG	BA	3142	-	-	-	X
56	MG	BA	3143	-	-	-	X
56	MG	BA	3145	-	-	-	X
56	MG	BA	3148	-	-	-	X
56	MG	BA	3149	-	-	-	X
56	MG	BA	3152	-	-	-	X
56	MG	BA	3153	-	-	-	X
56	MG	BA	3154	-	-	-	X
56	MG	BA	3155	-	-	-	X
56	MG	BA	3156	-	-	-	X
56	MG	BA	3157	-	-	-	X
56	MG	BA	3158	-	-	-	X
56	MG	BA	3159	-	-	-	X
56	MG	BA	3160	-	-	-	X
56	MG	BA	3168	-	-	-	X
56	MG	BC	301	-	-	-	X
56	MG	BQ	201	-	-	-	X
56	MG	CA	1601	-	-	-	X
56	MG	CA	1602	-	-	-	X
56	MG	CA	1607	-	-	-	X
56	MG	CA	1608	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	1623	-	-	-	X
56	MG	CA	1629	-	-	-	X
56	MG	CA	1631	-	-	-	X
56	MG	CA	1632	-	-	-	X
56	MG	CA	1633	-	-	-	X
56	MG	CA	1636	-	-	-	X
56	MG	CA	1637	-	-	-	X
56	MG	CA	1638	-	-	-	X
56	MG	CA	1645	-	-	-	X
56	MG	CA	1647	-	-	-	X
56	MG	CA	1649	-	-	-	X
56	MG	CA	1651	-	-	-	X
56	MG	CA	1652	-	-	-	X
56	MG	CA	1653	-	-	-	X
56	MG	CA	1654	-	-	-	X
56	MG	CA	1656	-	-	-	X
56	MG	CA	1657	-	-	-	X
56	MG	CA	1659	-	-	-	X
56	MG	CA	1660	-	-	-	X
56	MG	CA	1661	-	-	-	X
56	MG	CA	1668	-	-	-	X
56	MG	CA	1670	-	-	-	X
56	MG	CX	101	-	-	-	X
56	MG	DA	3011	-	-	-	X
56	MG	DA	3018	-	-	-	X
56	MG	DA	3023	-	-	-	X
56	MG	DA	3025	-	-	-	X
56	MG	DA	3026	-	-	-	X
56	MG	DA	3052	-	-	-	X
56	MG	DA	3057	-	-	-	X
56	MG	DA	3059	-	-	-	X
56	MG	DA	3061	-	-	-	X
56	MG	DA	3068	-	-	-	X
56	MG	DA	3071	-	-	-	X
56	MG	DA	3079	-	-	-	X
56	MG	DA	3081	-	-	-	X
56	MG	DA	3095	-	-	-	X
56	MG	DA	3097	-	-	-	X
56	MG	DA	3102	-	-	-	X
56	MG	DA	3107	-	-	-	X
56	MG	DA	3129	-	-	-	X
56	MG	DA	3131	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3137	-	-	-	X
56	MG	DA	3138	-	-	-	X
56	MG	DA	3139	-	-	-	X
56	MG	DA	3150	-	-	-	X
56	MG	DA	3151	-	-	-	X
56	MG	DA	3152	-	-	-	X
56	MG	DA	3156	-	-	-	X
56	MG	DA	3164	-	-	-	X
56	MG	DA	3165	-	-	-	X
56	MG	DA	3166	-	-	-	X
56	MG	DA	3167	-	-	-	X
56	MG	DA	3169	-	-	-	X
56	MG	DA	3170	-	-	-	X
56	MG	DA	3172	-	-	-	X
56	MG	DA	3173	-	-	-	X
56	MG	DA	3174	-	-	-	X
56	MG	DA	3176	-	-	-	X
56	MG	DA	3180	-	-	-	X
56	MG	DA	3192	-	-	-	X
56	MG	DA	3193	-	-	-	X
56	MG	DA	3194	-	-	-	X
56	MG	DB	202	-	-	-	X
56	MG	DB	204	-	-	-	X
56	MG	DO	201	-	-	-	X
57	NMY	AA	1655	-	-	X	-
57	NMY	BA	3165	-	-	X	-
57	NMY	DA	3190	-	-	X	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).

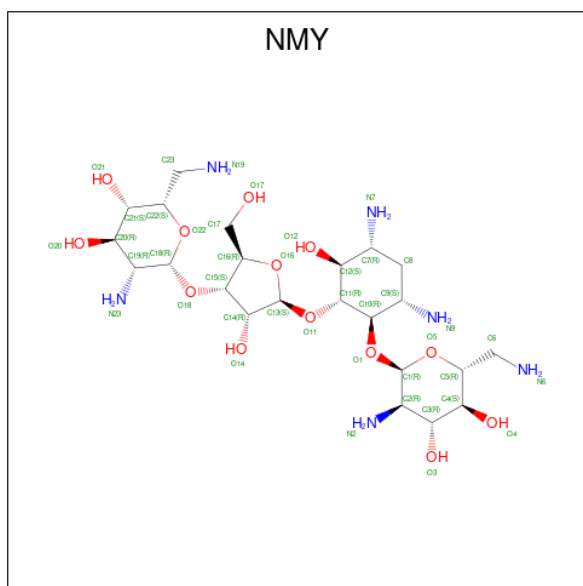
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	54	Total	Mg	0	0
			54	54		
56	AD	1	Total	Mg	0	0
			1	1		
56	AN	1	Total	Mg	0	0
			1	1		
56	BA	163	Total	Mg	0	0
			163	163		
56	BB	3	Total	Mg	0	0
			3	3		
56	BC	1	Total	Mg	0	0
			1	1		
56	BQ	1	Total	Mg	0	0
			1	1		

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

- Molecule 57 is NEOMYCIN (three-letter code: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).



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

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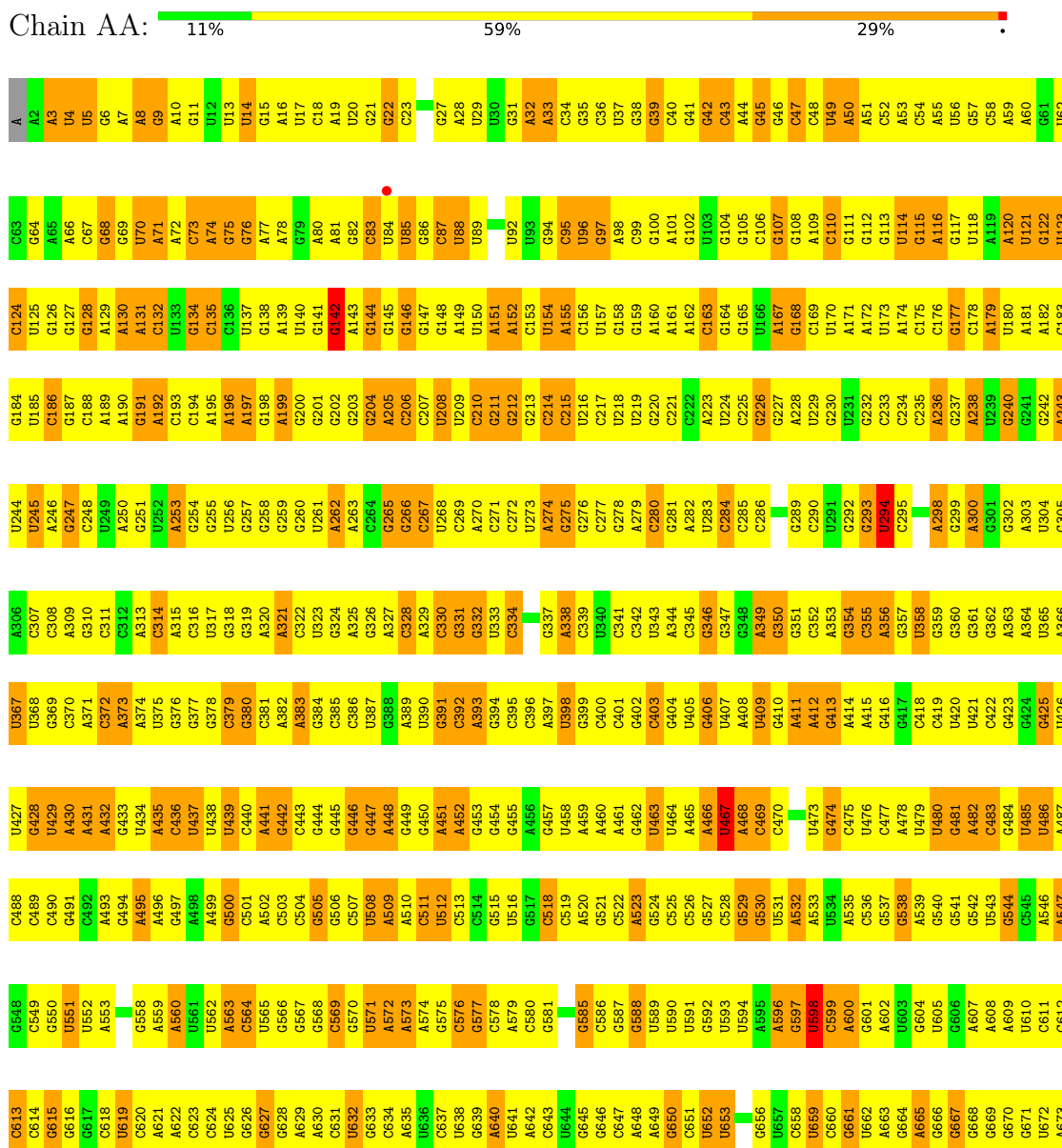
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	CN	6	Total O 6 6	0	0
59	CT	2	Total O 2 2	0	0
59	DA	627	Total O 627 627	0	0
59	DB	13	Total O 13 13	0	0
59	DC	4	Total O 4 4	0	0
59	DD	2	Total O 2 2	0	0
59	DE	4	Total O 4 4	0	0
59	DF	1	Total O 1 1	0	0
59	DL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

3 Residue-property plots

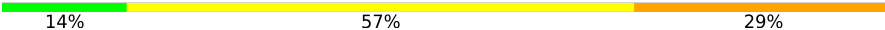
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



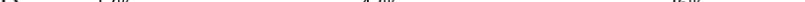
U1537	G1475	A1410	A1350	A1289	G1166	A1102	A1042	U981	U920	G859	G799	C735	G674
C1538	A1476	C1411	U1351	A1229	A1167	C1103	G1043	U952	U921	A860	G800	C736	A675
C1539	U1477	C1412	C1352	C1230	U1168	G1104	A1044	A953	G922	G861	U801	C737	A676
U1540	U1478	C1413	G1353	G1291	A1169	A1105	C1045	C984	A923	C862	A802	C738	U677
U	C1479	U1414	U1354	C1293	A1170	G1106	A1046	C985	C924	U863	G803		U678
A	A1480	G1415	G1355	G1232	A1171	C1107	G1047	U986	G925	A864	U804	G741	C679
	U1481	G1416	G1356	G1233	C1172	G1108	G1048	G987	G926	A865	C805	G742	C680
	G1482	G1417	A1357	C1234	U1173	C1109	U1049	U988	G927	C866	A806	G743	A681
	A1483	A1418	U1358	C1236	G1174	A1110	G1050	U989	G928	C867	U807	G744	G682
	C1484	G1419	A1359	C1237	U1175	A1111	C1051	C990	G929	C868	C808	G745	C683
	U1485	U1420	A1360	G1238		C1112	U1052	U991	C930	C869	C809	G746	U684
	G1486	G1421	G1361	A1239	U1178	C1113	G1053	U992	C931	U870	C810	G747	G685
	C1487	U1301	U1302	U1240	A1179	C1114	G1054	G993	C932	U871	C811	G748	U686
	G1488	C1302	C1302	G1241	A1180	U1115	A1055	A994	G933	A872	C812	A749	A687
	G1489	G1303	G1303	G1242	G1181	U1116	U1056	C995	C934	A873	U813	C750	C688
	U1490	C1304	G1365	C1243	G1182	A1117	G1057	A996	A935	G874	A814	U751	C689
	G1491	G1305	U1183	G1244	U1188	U1118	G1058	U997	C936	U875	A815	G752	G690
	C1492	C1367	G1306	C1245	G1184		C1059	C998	A937	C876	A816		G691
	A1493	U1307	U1246	G1246	G1185	U1122	U1060		A938	C877	C817	G755	U692
	G1494	C1308	U1247	G1247	G1186	U1123	G1061	C1001	G939	A878	C818	G756	G693
	U1495	G1309	A1248	G1187	G1187	U1124	U1062	G1002	C940	C879	A819	G757	A694
	C1496	G1310	C1249	A1188	U1125	U1125	G1063	G1003	C941	C880	U820	G758	A695
	G1497	A1311	A1250	U1189	U1126	G1064	G1064	A1004	G942	C881	G821	A759	A696
	U1498	G1312	A1251	U1190	G1127	U1065	G1065	A1005	U943	C882	C822		U697
	A1499	U1313	G1252	A1191	C1128	C1066	A1067	G1006	G944	C883	C823	G763	G700
	U1500	C1314	G1253	C1192	C1129	U1067	A1068	U1007	G945	U884	G824	C764	A701
	C1501	U1315	A1254	G1193	A1130		G1068	U1008	A946	C885	A825	G765	U702
	U1502	G1316	G1255	U1194		G1133	G1069	U1009	G947	C886	C826	A766	G703
	A1503	C1317	A1256	C1195	G1134	U1070	G1070	U1010	C948	C887	U827	A767	U704
	G1504	G1318	A1257	A1196	G1135	G1071	G1071	C1011	U949	C888	U828	A768	A704
	U1505	U1319	G1258	A1197	U1135	G1072	U1078	A1012	U950	A889	G829	G769	G705
	A1506	C1320		G1198	C1136	U1073	G1079	G1013	C951	C890	C830	C770	A706
	U1507	U1321	A1261	U1199	C1137	U1074	G1079	U891	U952	U891	A831	G771	U707
	A1508	C1322	C1262	C1200	G1138	U1075	A1080	A892	G953	C892	G832	U772	U708
	C1509	G1323	C1263	A1201	G1139	A1016	A1081	C893	G954	C893	G833	G773	U709
	U1510	A1324	U1264	U1202	A1140	U1017	G1077	G894	U955	C894	U834	G774	G710
	A1513	G1325	C1265	C1203	C1141	G1078	G1078	C895	U956	C895	U835	G775	G711
	G1514	U1326	G1266		G1142	G1079	G1079	C896	U957	C896	G836	A776	A712
	U1515	C1327	C1267	G1206	G1143	A1080	G1079	C897	A958	C897	U837	A777	G713
	G1516	C1328	G1268	U1207	A1144	A1081	A1081	C898	A959	C898	G838	G778	G714
	U1517	U1329	A1269	C1208	A1145	A1082	A1082	C899	U960	C899	C839	C779	A715
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	U1525	G1337	C1277	A1216	G1153	U1090	U1090	U1030	A969	A907	G847	A787	U723
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		A1339	G1279	C1218	A1155	A1092	A1092	G1032	G971	A909	C849	U789	G725
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		C1342	C1281	G1220	U1157	G1094	G1094	U911	G973	U911	C851	G791	G727
		G1343	C1282	G1221	A1158	U1095	A1095	C912	A974	C912	C852	A792	A728
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		U1345	C1284	C1223	G1160	C1097	C1097	A914	G976	A914	U854	A794	G730
		A1346	A1285	U1224	C1161	C1098	C1098	C1033	A977		U855	C795	G731
		U1286	U1286	A1225	C1162	G1099	G1099	G1039	A978		C856	C796	C732
		C1407	G1347	C1226	A1163	U1099	U1099	U1040	C979		C857	C797	G733
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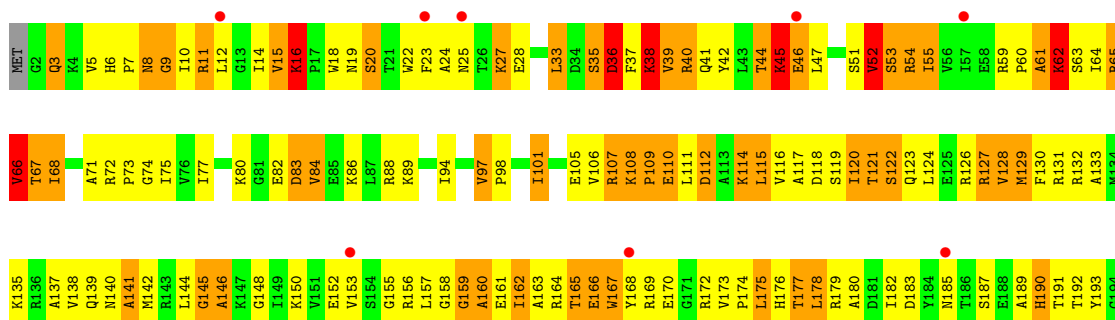
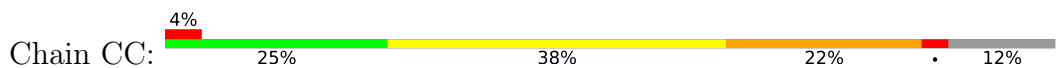
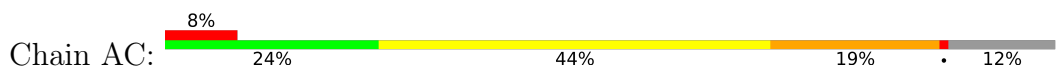
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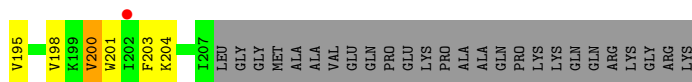
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A873	A749	G688	U625	C625	U565	C501	C440	G379	C316	U252	A189	G127	A66
G874	A814	C750	G689	G626	G566	C502		G380	U317	A253	A190	C67	
U875	A815	C751	G690	G627	G567	C503	G443	C381	G318	C254	A191	A130	G68
C876	A816	G752	G691	G628	G568	C504	G444	A382	C318	G255	A192	A131	G69
G877	A817	U692	U692	A629	C569	G505	G445	G383	G319	U256	A193	C132	U70
A878	C818	C754	G693	A630	G570	G506	G446	G384	A320	U257	C194	A133	A71
C879	A819	C755	A694	C631	U571		G447	C385	A321	G257	C195	U133	A71
C880	U820	C756	A695	U632	A572	A509	A448	C386	C322	G258	A196	G134	A72
C881	G891	U757	A696	G633	A573	A510	G449	U387	U323	G259	A197	C135	C73
C882	U822	C758	U697	C634	A574	C511	G450	G388	G324	G260	A198	C136	A74
C883	G892			A635	G575	U512	A451	A389	A325	U261	G198	U137	
U884	G824	G760		U636	C576	C513	A452	U390	G326	A262	A199	G138	G76
G885	A825	G761	U701		G577	C514	G453	G391	A327	A263	G200	A139	A77
C886	C826	U762	A702	G639	C578	G515	G454	C392	C328	C264	G201	U140	
G887	U827	G763	G703	U640	A579	U516	G455	A393	A329	G265	G202	G141	G79
C888	U828	C764	A704	U641	C580	G517	A456	G394	C330	G266	G203	G142	A80
A889	G829	G765	G705	A642	G581	C518	G457	C395	G331	C267	G204	A143	A81
C890	G830	A766	A706	C643	C582	C519	U458	U396	G332	U268	A205	G144	U20
A891	A831	A767	U707	U644	A583	A520	A459	A520		C269	C206	G145	C83
C892	C832	G768	G708	G645	G584	A521	A460	U405		A270	G207	G146	U84
G893	G833	C769	U709		G585	G521	A461	G399	A338	C271	U208	G147	U85
C894	U834	C770	G710	A648	C586		G462	C401	U340	C272	U209	G148	
A895	U835	G771		A649	C587	C525	A463	G402	C341	U273	C210	A149	C37
G896	G836	U772	G711	G650	U594	C526	U464	A403	C342	A274	G211	U150	U88
	U837	C773		C651	A595	C527	U465	C404	U343	G275	G212	A151	U89
C897	C838	G774	G714	U652	A602	G529	A466	U405	A344	C276	G213	C90	U30
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A901	C841	U777	U717	A655	U593		A469	A408	G347	C280	U216	U154	U92
G902	U842	C778	A718	G656	U594	A532	C470	U409	G348	G281	C217	A155	U93
A906	C843	C779	C719	U657	A596	A533	U471	G410	A349	A282	C218	C156	C94
U907	U844	U780	U658	C658	A597			C411	G350	U283	U218	U157	C95
A908	C845	A781	G721	U659	G597	C536	U472	A411	G351	G284	G220	G158	C96
C909	A846	C782	G722	C660	U598	G538	C474	A412	C352	C285	C221	G159	U37
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A914	C848		G724	U662	A600	G540	U476	A415		U287	C223	A161	G39
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	C852	U789	A728	C666	G604	C544	U480	C419	U358	U291	G227	G165	U103
A918	C853	A790	A729	G667	C605	C545	G481	C419	U359	G292	G227	U166	G104
C919	U854	C791	G730	C668	U606	C546	A482	U421	G360	G293	A228	A167	G105
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U921	C856	U793	C732	C670	A608	G548	C484	G423	G362	G295	G230	C169	G107
G922	C857	A794	G733	G671	A609	C549	U485	G424	A363	U296	U231	U170	G108
A923	C858	C795	G734	U672	U610	G550	U486	G425	A364	C297	G232	A171	A109
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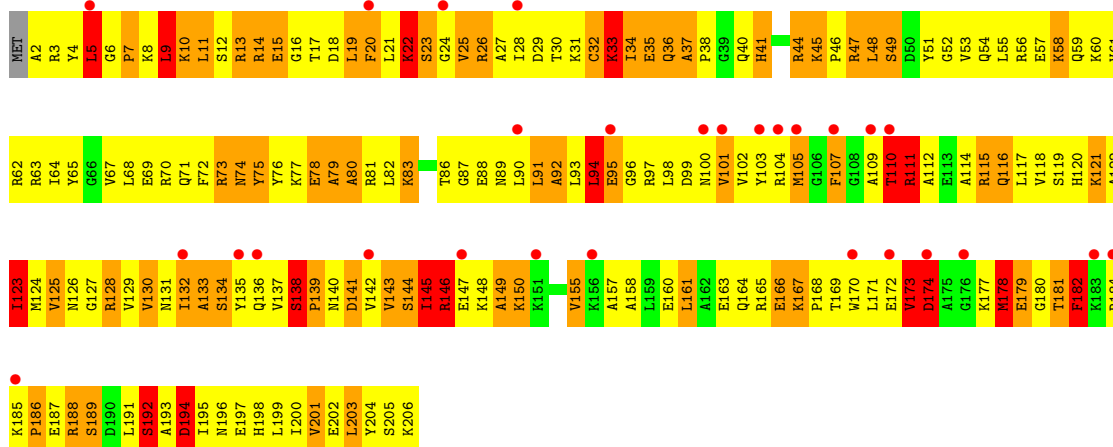
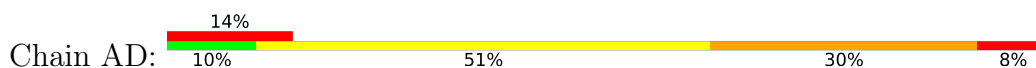
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Chain CB: 

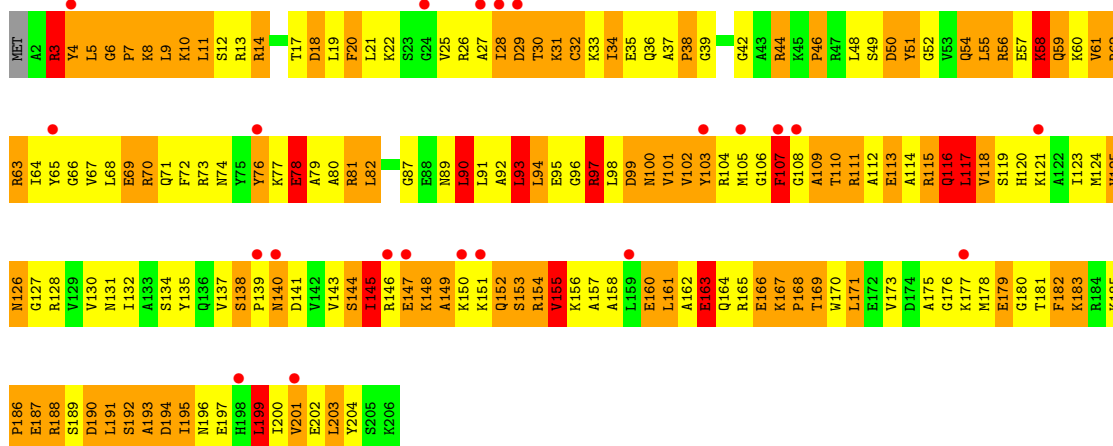
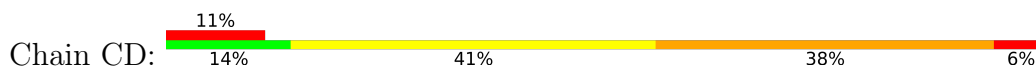




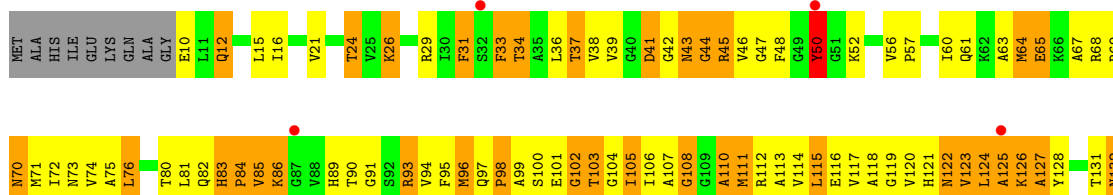
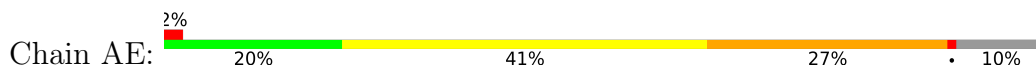
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

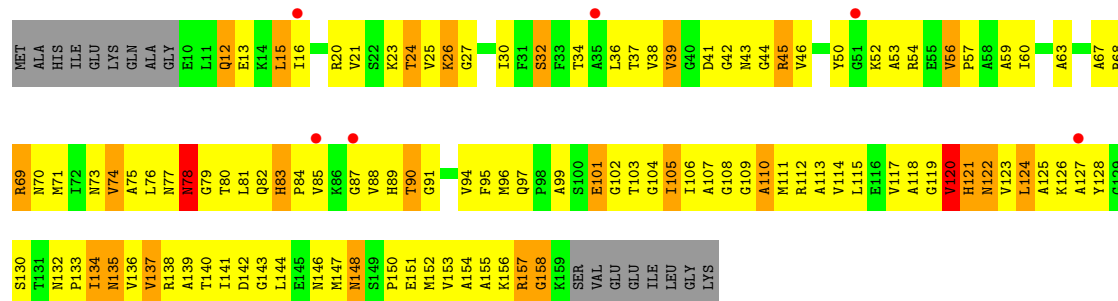


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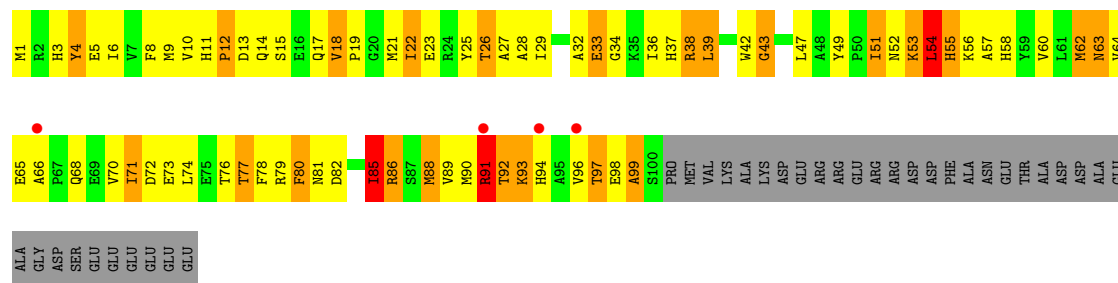
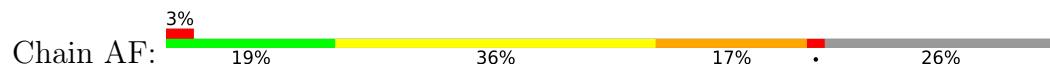




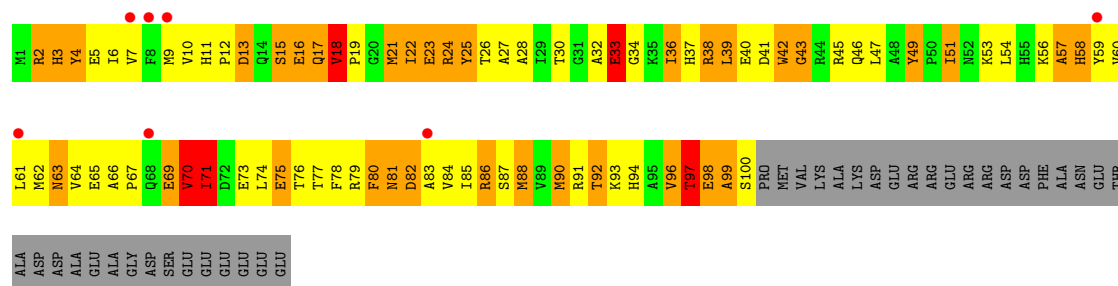
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

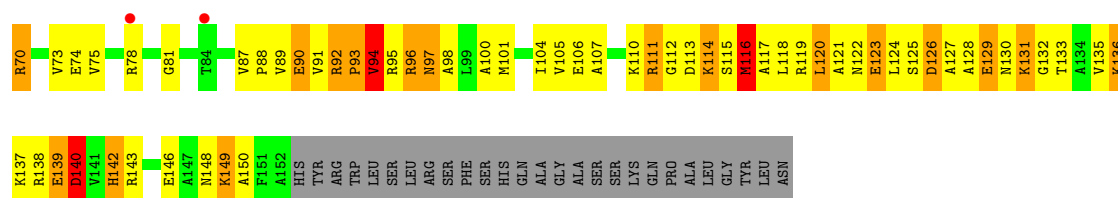


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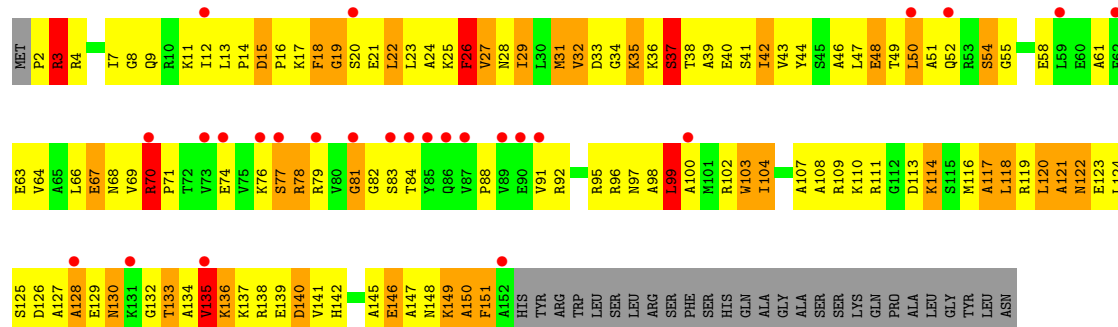
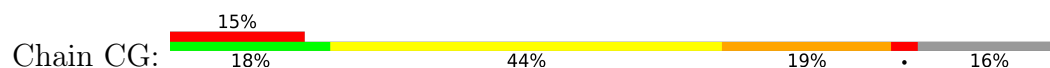


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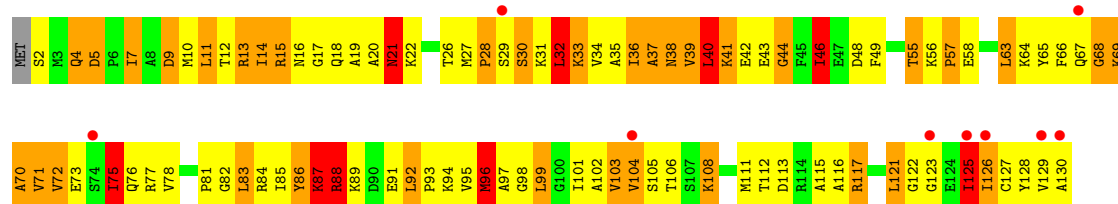
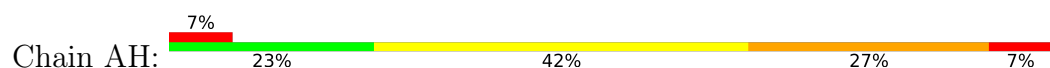




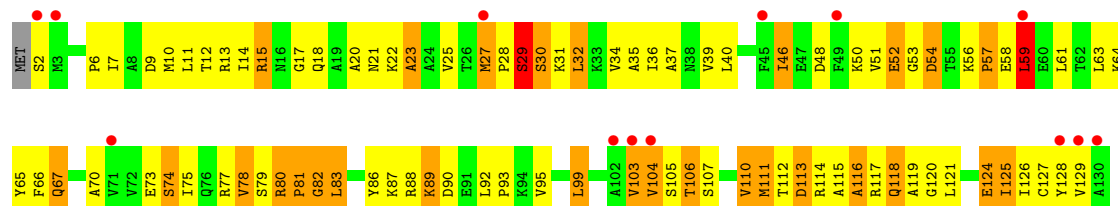
• Molecule 7: 30S ribosomal protein S7



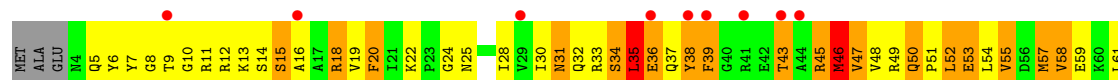
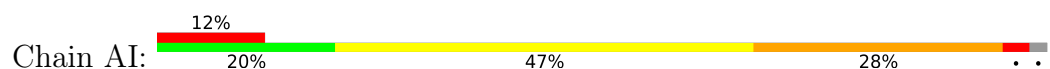
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

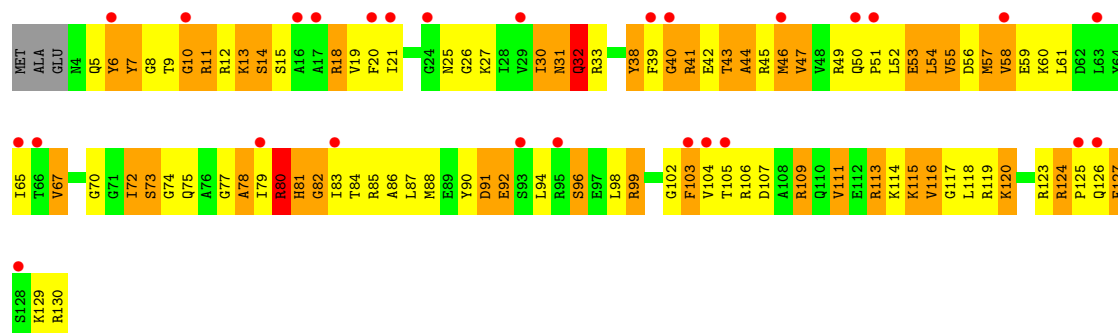
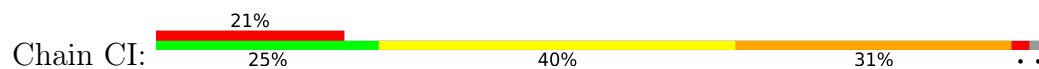


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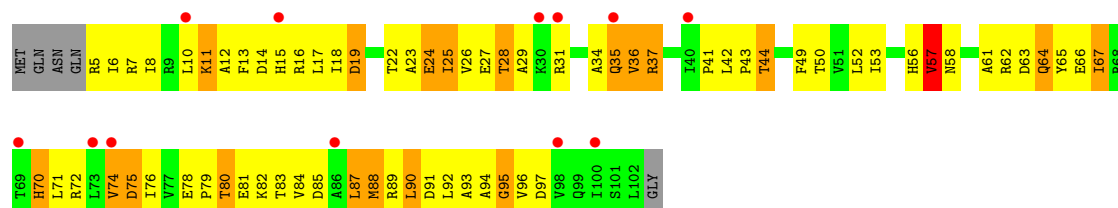




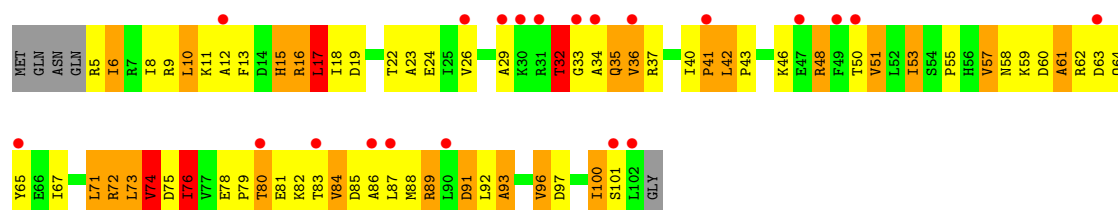
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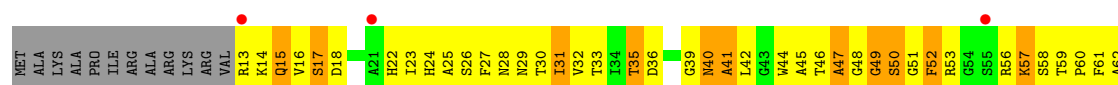
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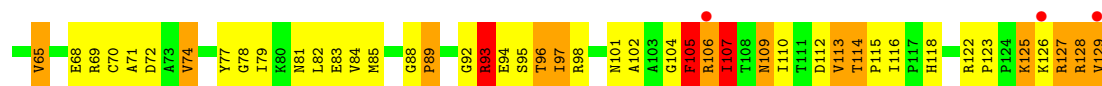


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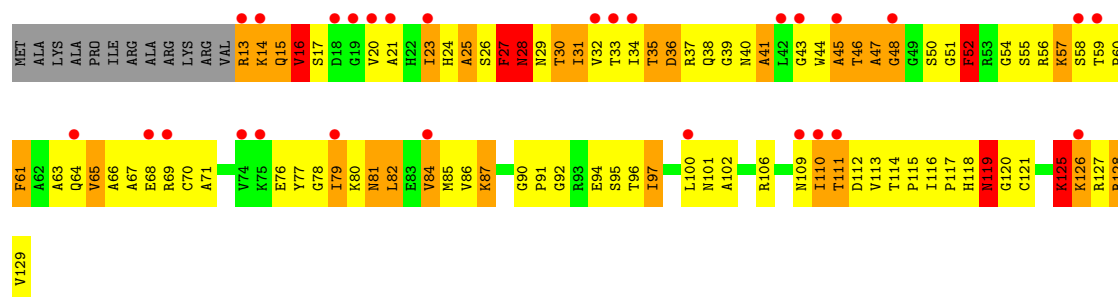
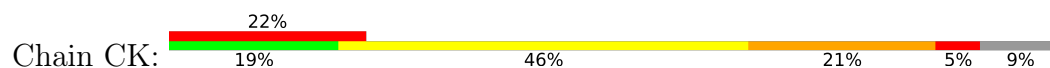


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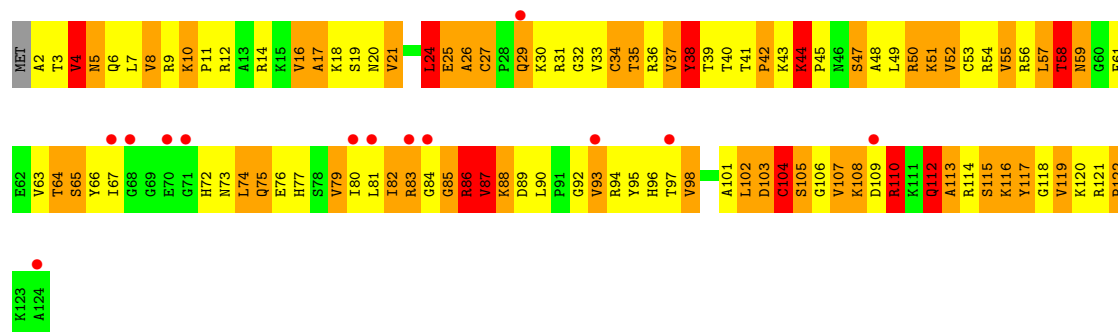
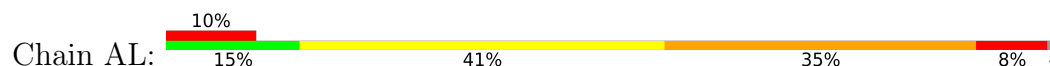




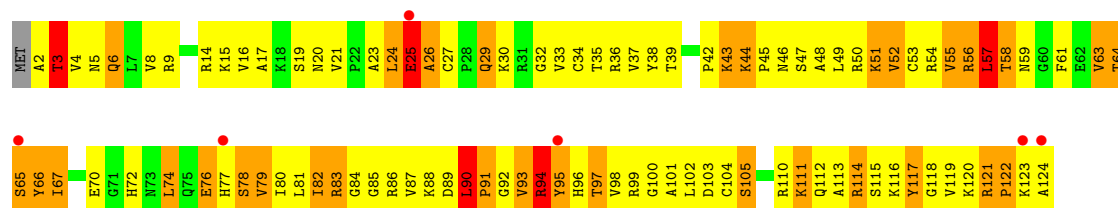
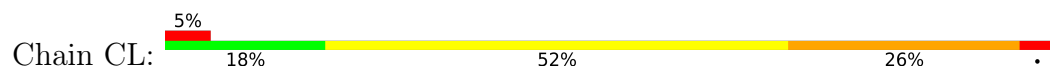
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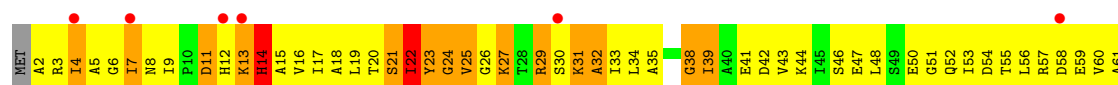
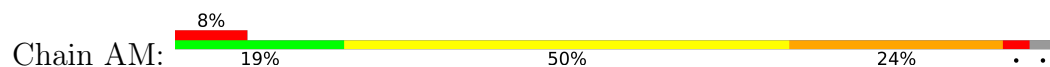
• Molecule 12: 30S ribosomal protein S12



• Molecule 12: 30S ribosomal protein S12

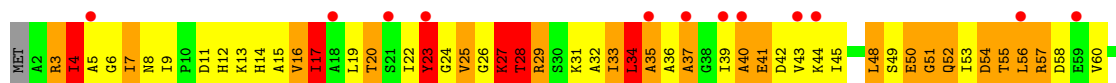
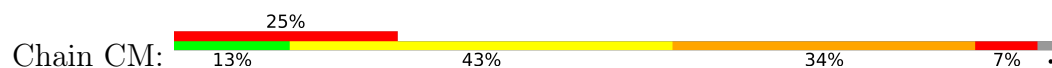


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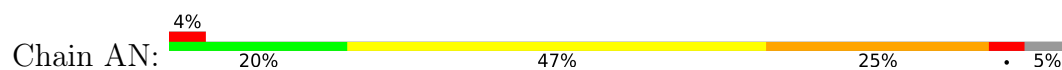




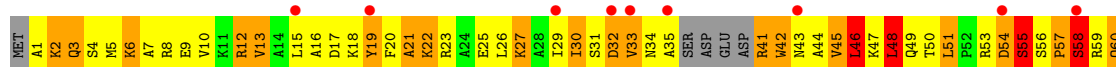
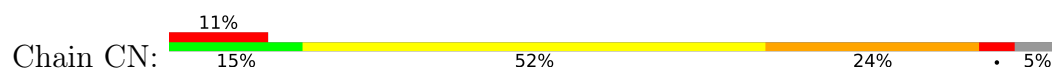
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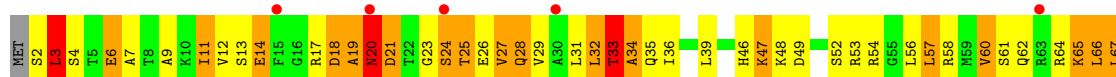
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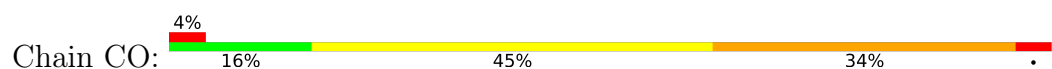
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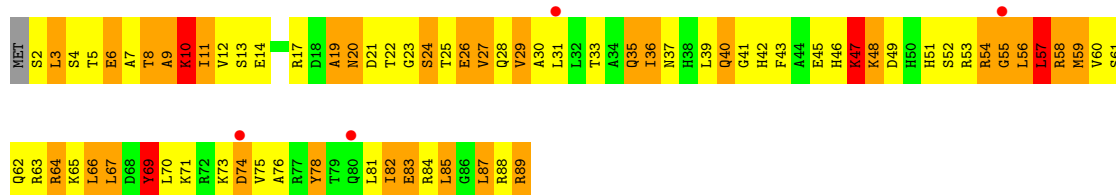


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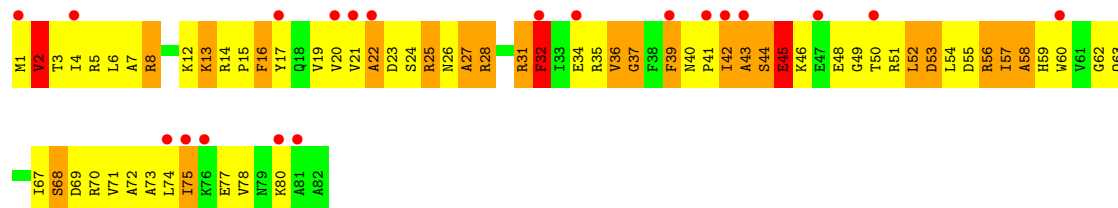
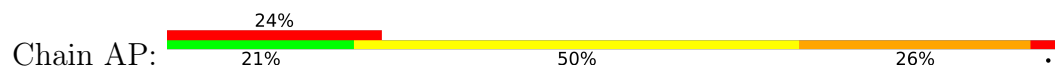


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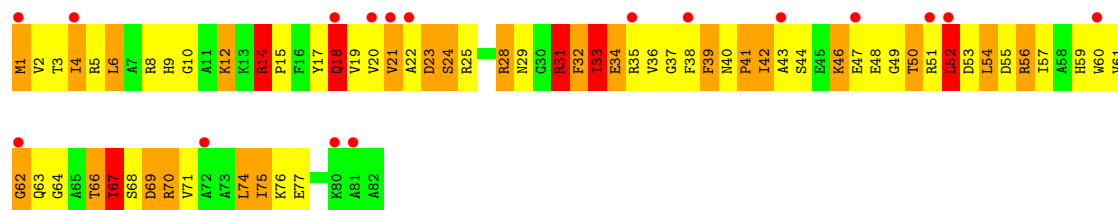
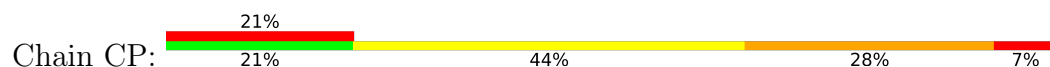




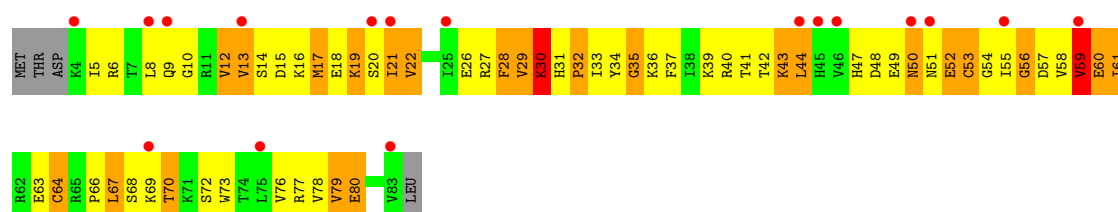
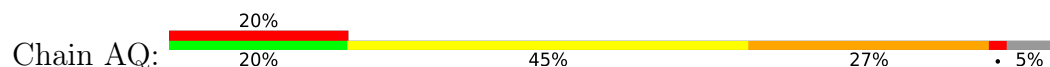
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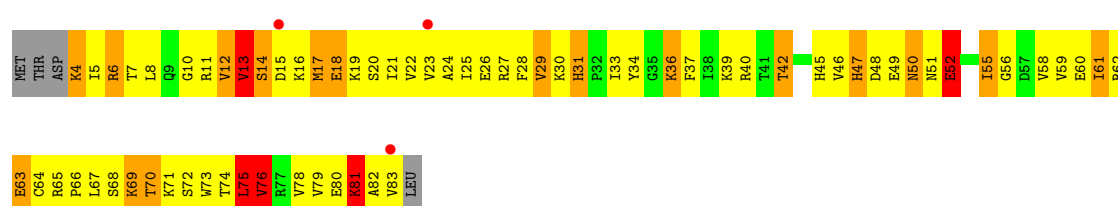
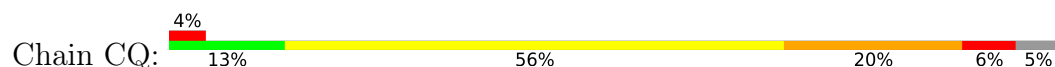
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• Molecule 17: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S17




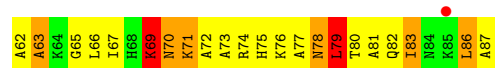
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-
- | Category | Value (%) |
|----------|-----------|
| Red | 4% |
| Green | 13% |
| Yellow | 33% |
| Orange | 21% |
| Red | 5% |
| Grey | 27% |

- Chain CR:
-
- | Amino Acid | Percentage |
|------------|------------|
| Met | 8% |
| Ala | 12% |
| Arg | 32% |
| Thr | 28% |
| Phe | 27% |
- 8% 12% 32% 28% 27%
-
- | Amino Acid | Percentage |
|------------|------------|
| Met | 8% |
| Ala | 12% |
| Arg | 32% |
| Thr | 28% |
| Phe | 27% |
- 8% 12% 32% 28% 27%

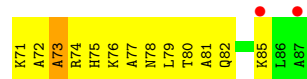
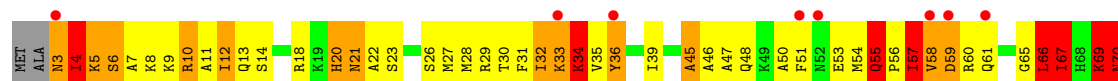
- Chain AS:
-
- | Region | Percentage |
|--------|------------|
| Red | 23% |
| Green | 12% |
| Yellow | 52% |
| Orange | 22% |
| Grey | 14% |
- Legend:
- | Region | ASes |
|--------|---|
| Red | PRO, R3, S4, K6, K7, G8, F10, I11, D12, L13, H14, L15, L16, K17, K18, V19, E20, K21, A22, V23, G26, D27, K28, K29, P30, L31, R32, W34, S35, R36, R37, S38, T39, I40, F41, P42, M43, M44, I45, G46, T48, I49, A50, V51, H52, N53, G54, R55, Q56, H57, V58, P59, V60, F61 |
| Green | V62, T63, D64, S65, M66, V67, G68, H69, K70, L71, G72, E73, F74, A75, P76, T77, R78, T79, Y80, R81, GLY, HIS, ALA, ALA, ASP, LYS, LYS, ALA, LYS, LYS, LYS |
| Yellow | |
| Orange | |
| Grey | |

- Chain CS:
-
- | Amino Acid | Percentage |
|------------|------------|
| MET | 17% |
| PRD | 17% |
| R3 | 17% |
| S4 | 17% |
| L5 | 17% |
| K6 | 17% |
| K7 | 17% |
| G8 | 17% |
| P9 | 17% |
| F10 | 17% |
| H11 | 17% |
| D12 | 17% |
| L13 | 17% |
| H14 | 17% |
| L15 | 17% |
| L16 | 17% |
| K17 | 17% |
| K18 | 17% |
| V19 | 17% |
| E20 | 17% |
| R21 | 17% |
| A22 | 17% |
| V23 | 17% |
| E24 | 17% |
| S25 | 17% |
| G26 | 17% |
| D27 | 17% |
| K28 | 17% |
| K29 | 17% |
| P30 | 17% |
| L31 | 17% |
| R32 | 17% |
| T33 | 17% |
| W34 | 17% |
| S35 | 17% |
| R36 | 17% |
| R37 | 17% |
| S38 | 17% |
| T39 | 17% |
| L40 | 17% |
| F41 | 17% |
| P42 | 17% |
| R43 | 17% |
| M44 | 17% |
| L45 | 17% |
| G46 | 17% |
| L47 | 17% |
| T48 | 17% |
| L49 | 17% |
| A50 | 17% |
| V51 | 17% |
| H52 | 17% |
| H53 | 17% |
| G54 | 17% |
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| G56 | 17% |
| H57 | 17% |
| V58 | 17% |
| P59 | 17% |
| I60 | 17% |

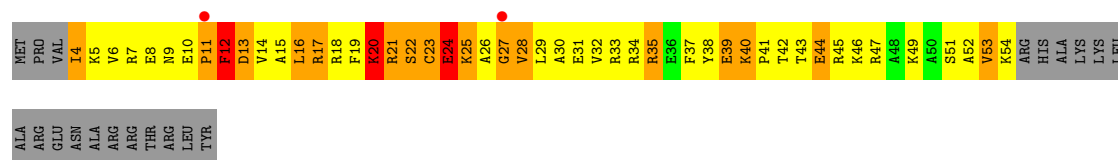
- Chain AT: 



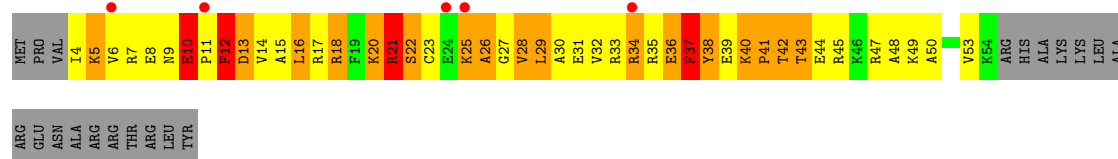
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



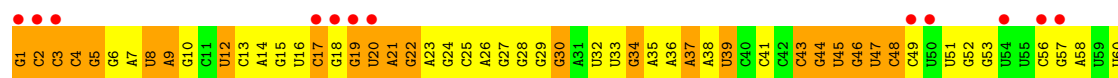
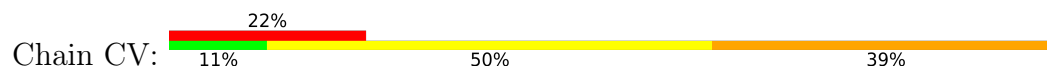
- Molecule 21: 30S ribosomal protein S21

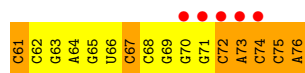


- Molecule 22: Phenylalanine specific transfer RNA, tRNA-Phe

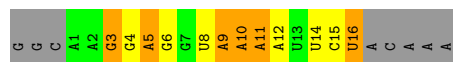


- Molecule 22: Phenylalanine specific transfer RNA, tRNA-Phe





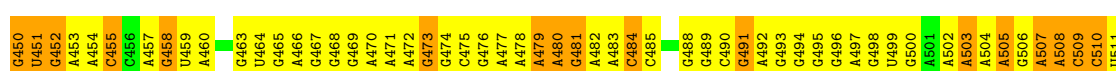
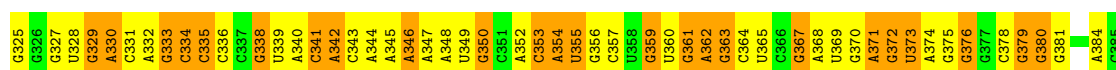
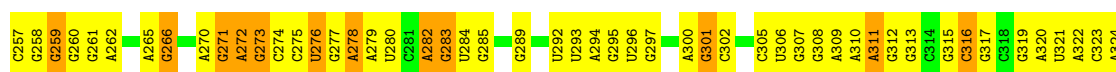
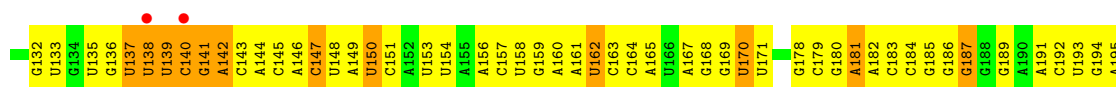
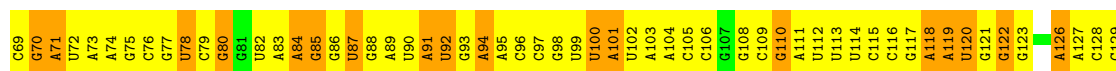
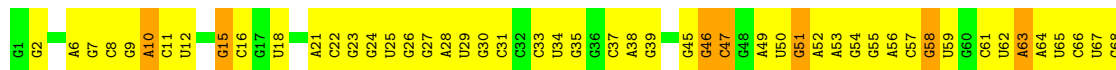
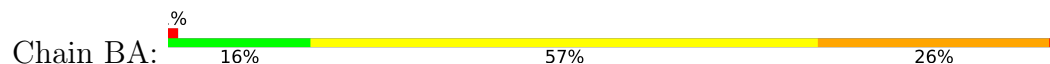
• Molecule 23: Messenger RNA, mRNA



• Molecule 23: Messenger RNA, mRNA

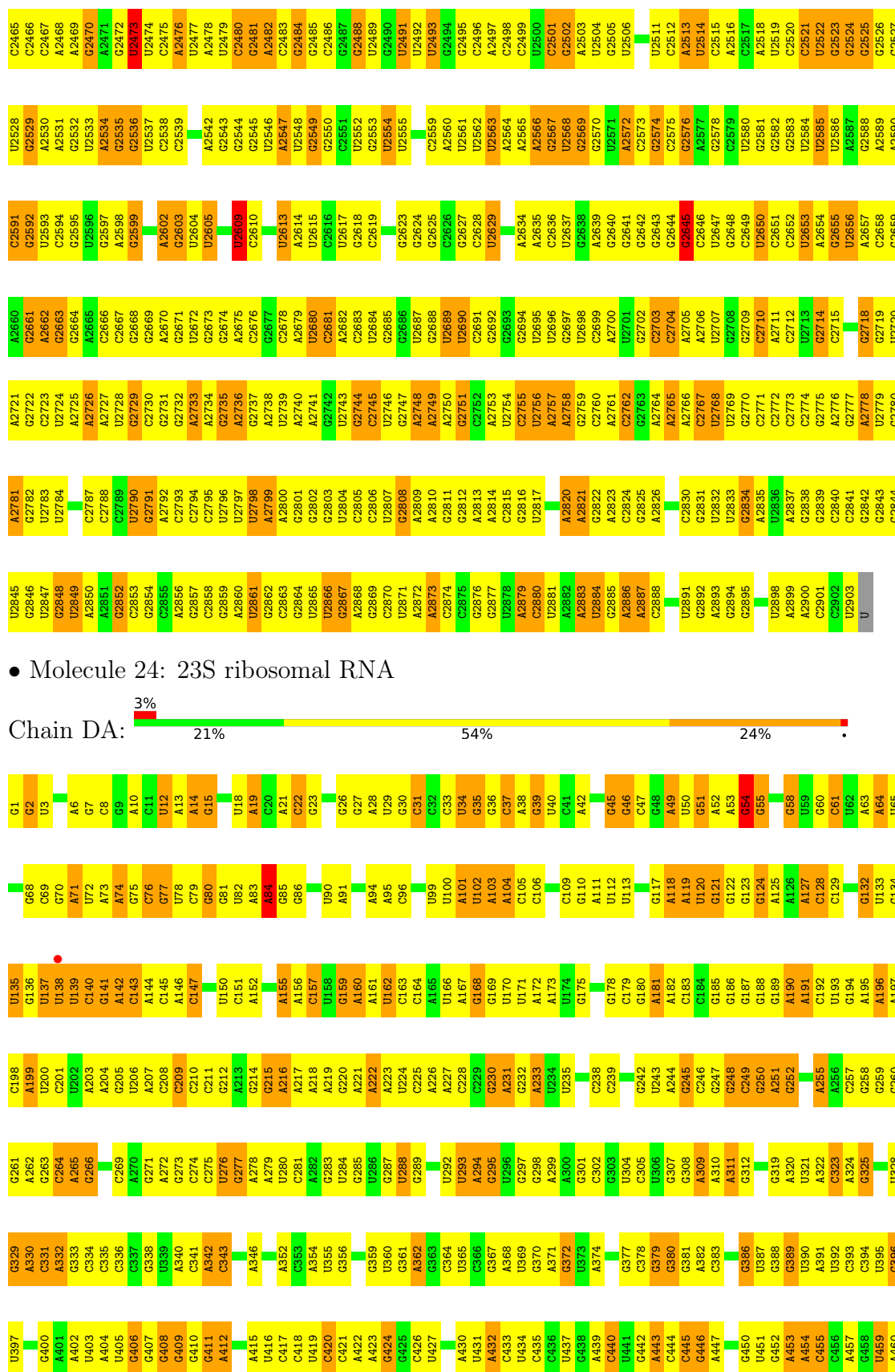


• Molecule 24: 23S ribosomal RNA



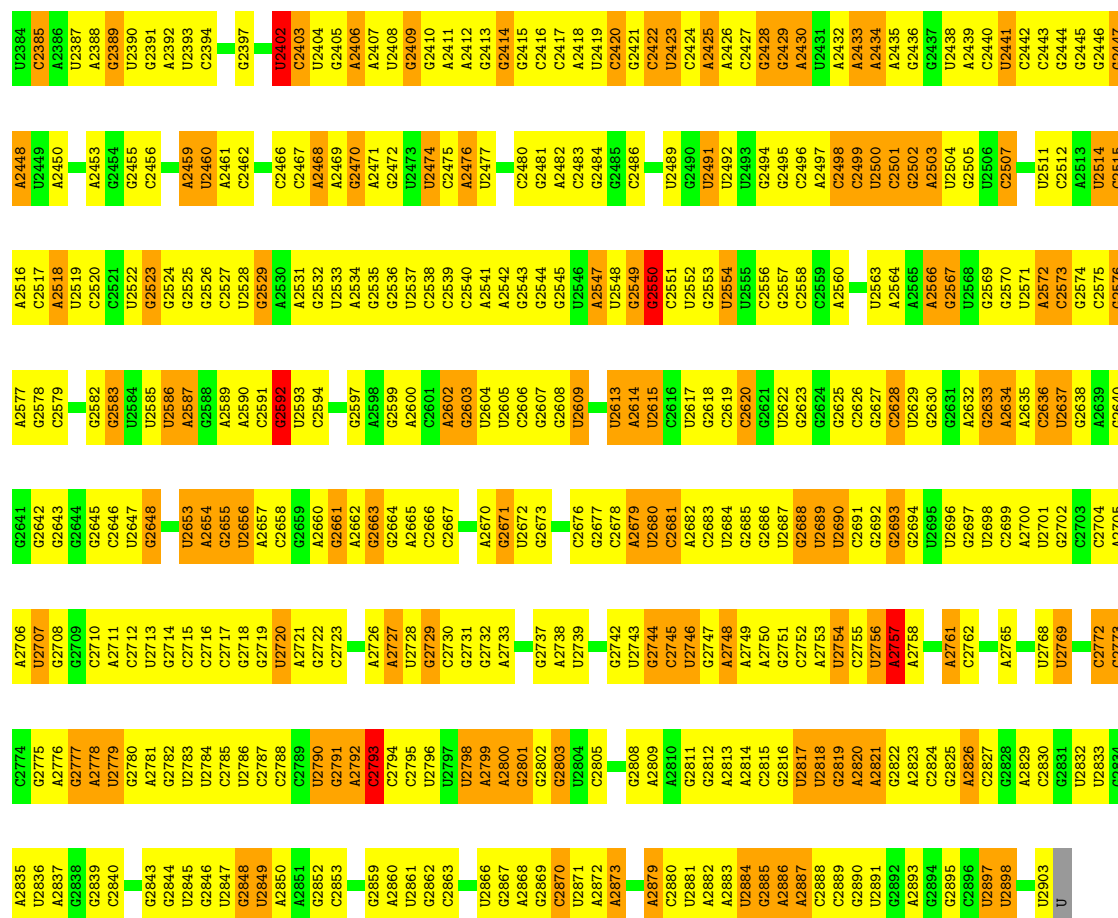
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U1443	G1382	A1321	G1259	U1199	G1139	U1078	C1013	G949	A	U824	A764	G697	A637	G577
G1444	A1383	A1322	A1260	C1200	C1140	C1079	G1016	G950	U	A825	C765	G698	G638	G578
G1445	A1384	C1323	G1261	U1201	U1141	A1080	G1017	C951	C	U826	U766	G700	U639	G579
G1446	A1385	G1324	A1262	G1202	A1142	U1081	U1018	C952	C	U827	U767	G704	G640	U580
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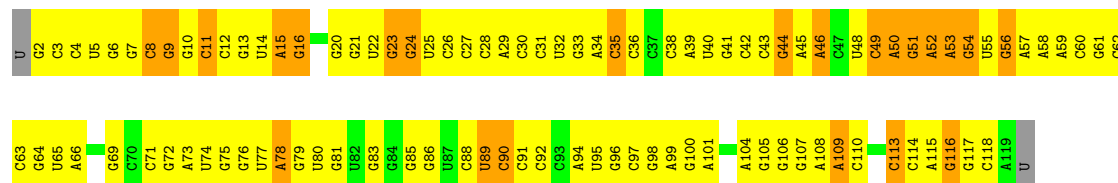
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C2365	C2303	G2055	C2119	C1990	A1927	A1927	U1865	A1802	A1665	A1603	G1543	G1478
A2366	G2304	C2056	G2120	U1991	A1928	A1928	U1866	G1802	G1666	C1604	A1544	G1479
	U2305	G2057	G2121	U1992	G1929	G1929	G1867	A1805	G1667	C1605	A1545	C1480
A2369	A2306	A2060	U2122	U1993	G1930	G1930	C1868	C1806	A1668	C1606	G1546	U1481
G2370	C2307	G2061	G2123	C1994	U1931	U1931	G1869	G1807	G1740	C1607	C1547	G1482
U2371	C2308	G2062	G2124	U1995	A1932	A1932	C1870	A1808	C1670	A1608	A1548	G1483
U2372	A2309	A2062	G2125	C1996	G1933	G1933	A1871	A1809	U1671	A1609	U1549	U1484
G2373	U2310	C2063	U2126	C1997	C1934	C1934	G1872	A1810	A1672	A1610	C1550	U1485
C2374	C2311	C2064	A2127	A1998	G1935	G1935	U1873	G1811	G1673	A1614	A1551	U1486
	U2312	C2065	U2127	C1999	U1936	U1936	C1874	G1814	G1674	C1615	A1552	U1487
A2377	A2313	C2066	C2128	U1999	A1937	A1937	G1875	U1815	C1675	C1616	A1553	C1488
A2378	G2314	G2067	G2129	C2000	A1938	A1938	C1876	A1816	A1676	C1617	U1554	A1489
C2379	C2315	G2068	U2131	G2001	A1939	A1939	U1877	G1817	G1677	C1618	G1555	C1490
A2380	G2316	C2069	U2132	A2003	U1940	U1940	G1878	G1817	A1678	A1618	G1556	C1491
U2381	U2317	G2070	G2133	G2004	C1941	C1941	U1879	U1818	A1679	G1619	C1557	U1492
G2382	C2318	A2071	U2134	A2005	C1942	C1942	U1890	A1819	U1680	G1620	C1558	C1493
C2383	U2321	C2072	A2135	C2006	U1943	U1943	C1881	U1820	G1681	U1621	U1559	A1494



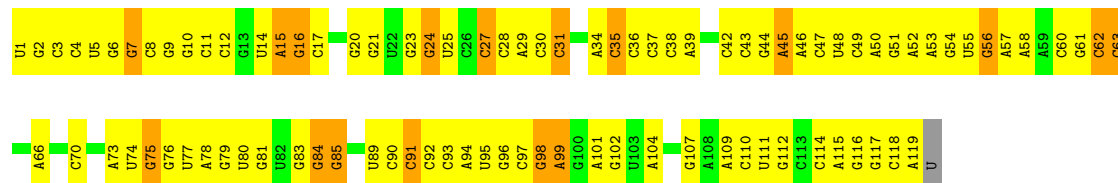
• Molecule 25: 5S ribosomal RNA

Chain BB: 14% 65% 19%



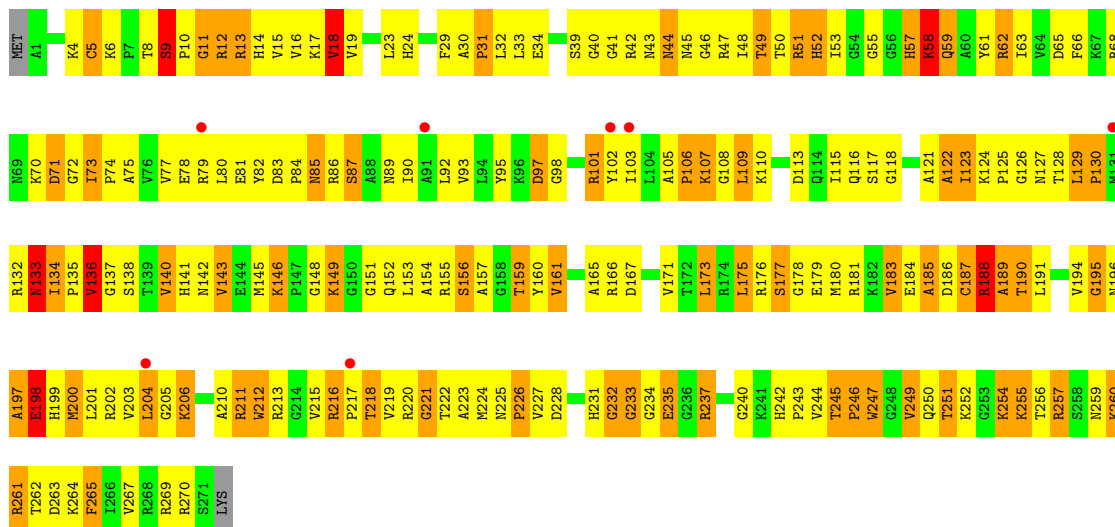
• Molecule 25: 5S ribosomal RNA

Chain DB: 22% 62% 14%

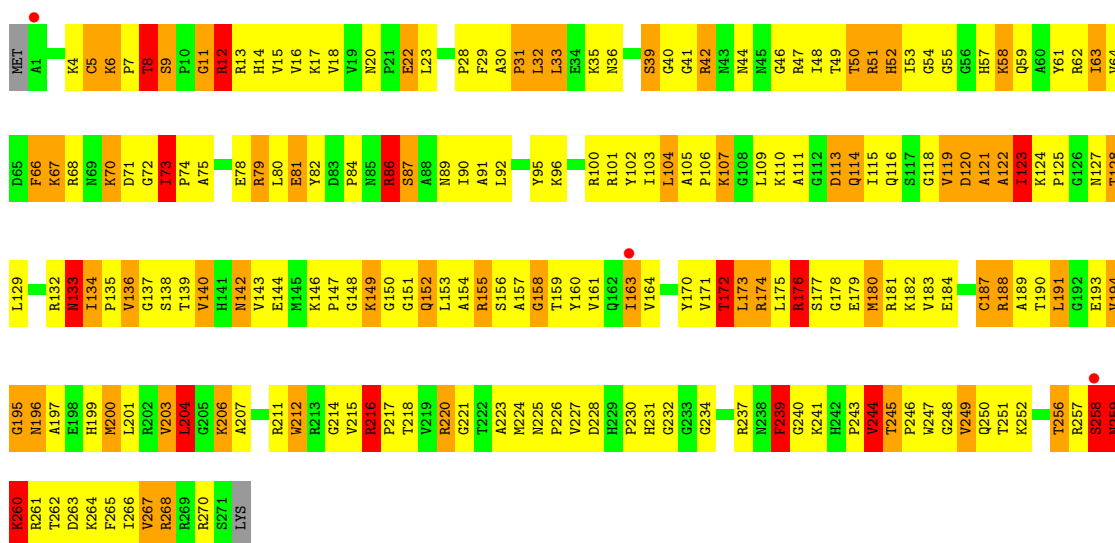


• Molecule 26: 50S ribosomal protein L2

Chain BC: 3% 25% 48% 25%



- Molecule 26: 50S ribosomal protein L2



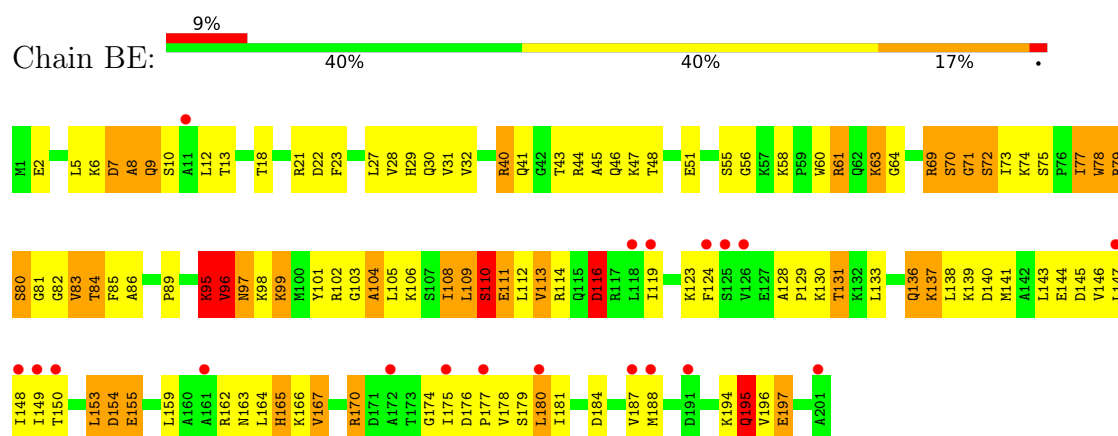
- Molecule 27: 50S ribosomal protein L3



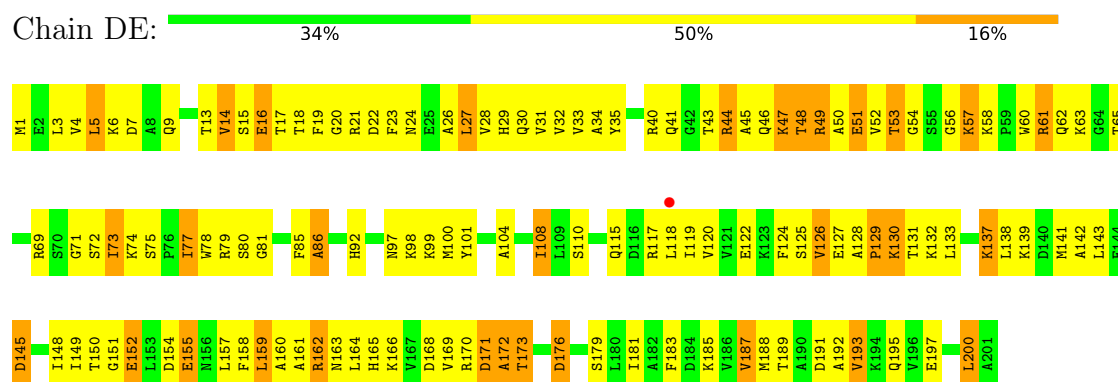
• Molecule 27: 50S ribosomal protein L3



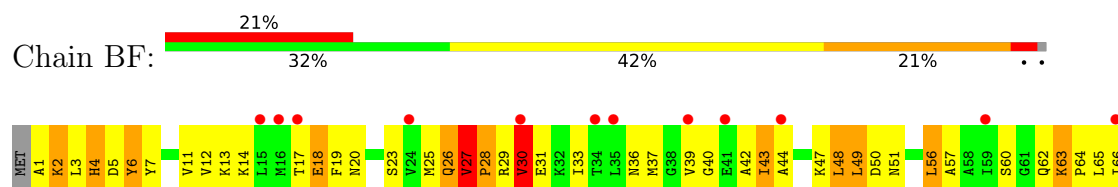
• Molecule 28: 50S ribosomal protein L4

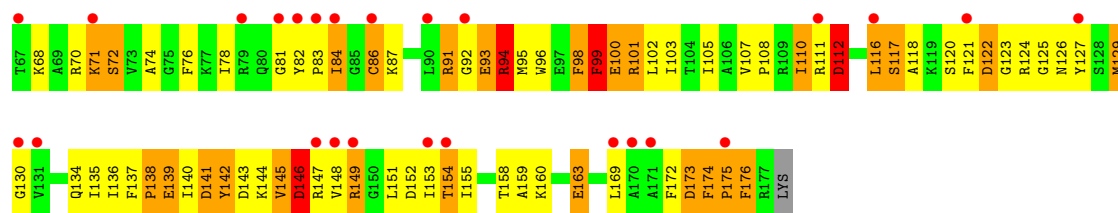


• Molecule 28: 50S ribosomal protein L4

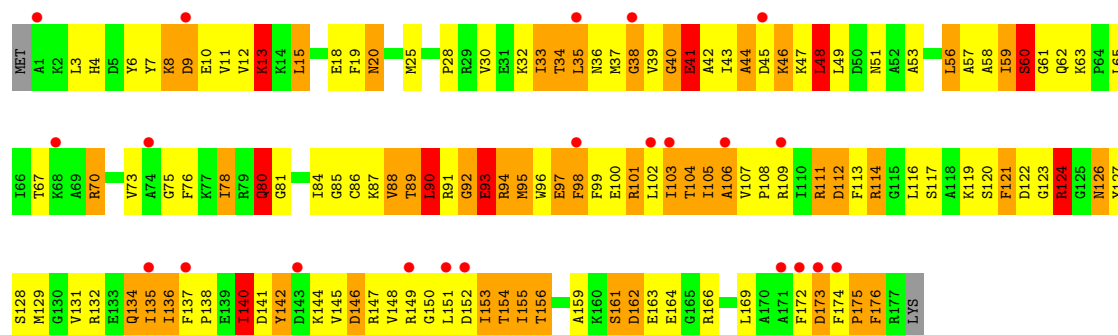


• Molecule 29: 50S ribosomal protein L5

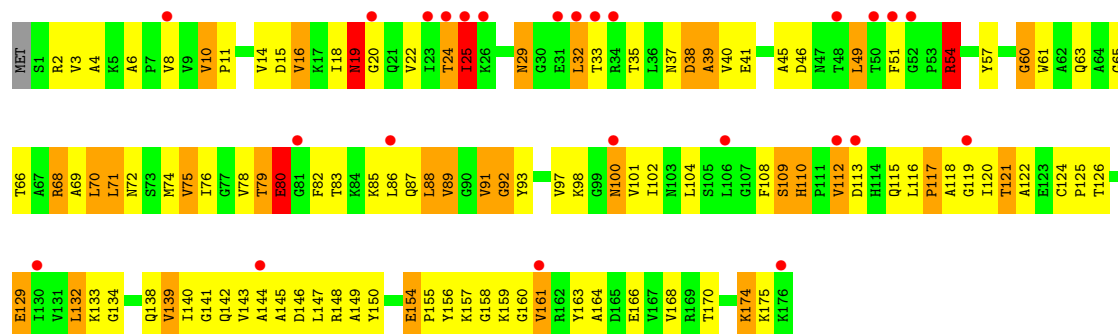




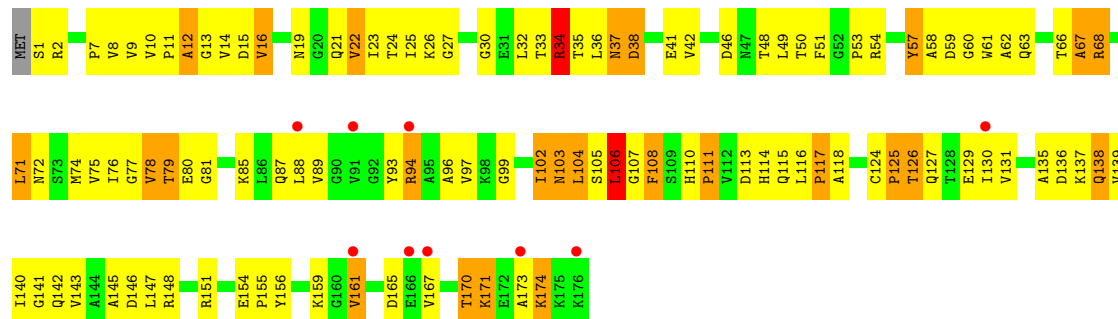
• Molecule 29: 50S ribosomal protein L5



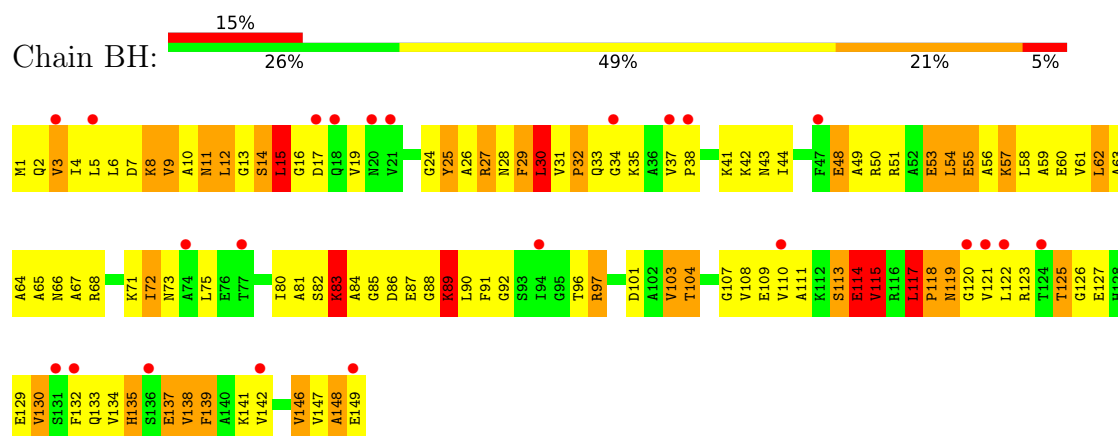
• Molecule 30: 50S ribosomal protein L6



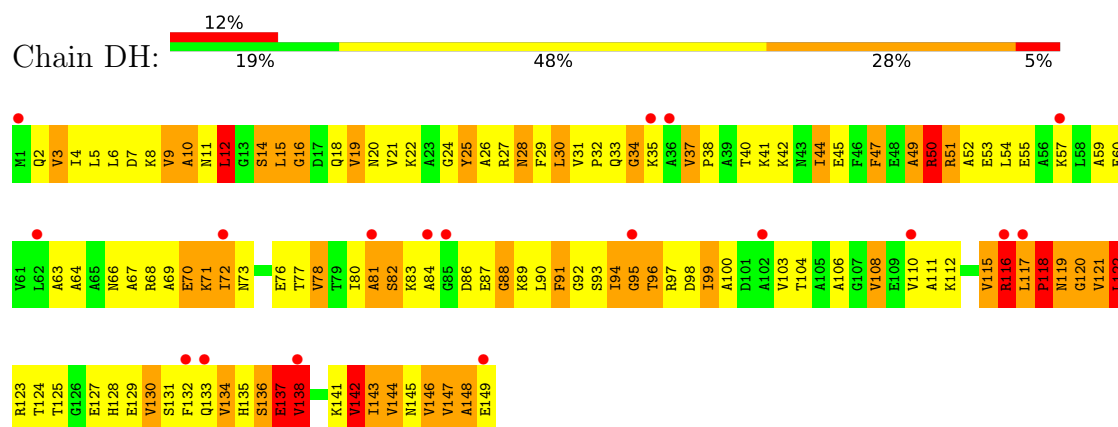
• Molecule 30: 50S ribosomal protein L6



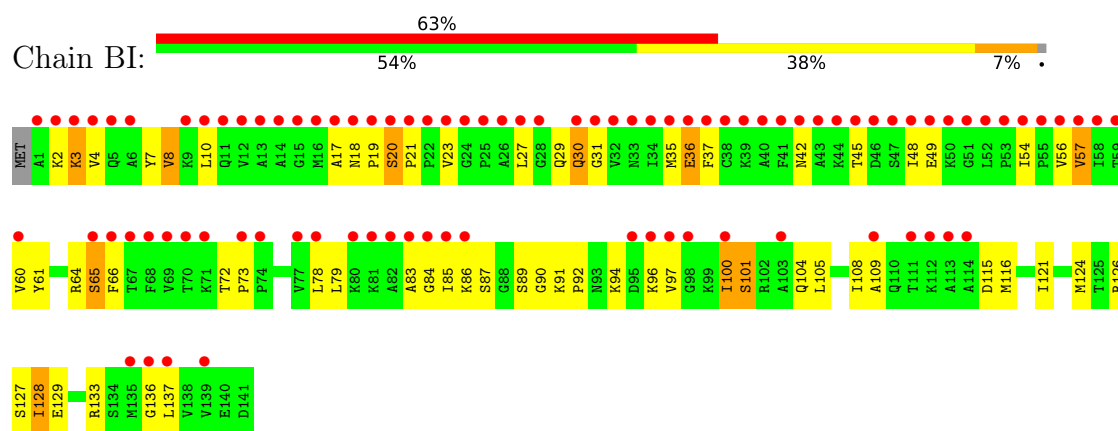
• Molecule 31: 50S ribosomal protein L9



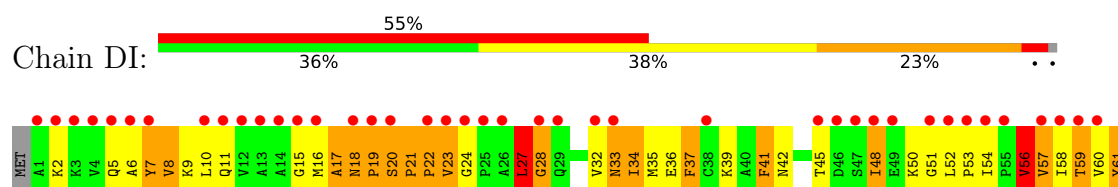
• Molecule 31: 50S ribosomal protein L9

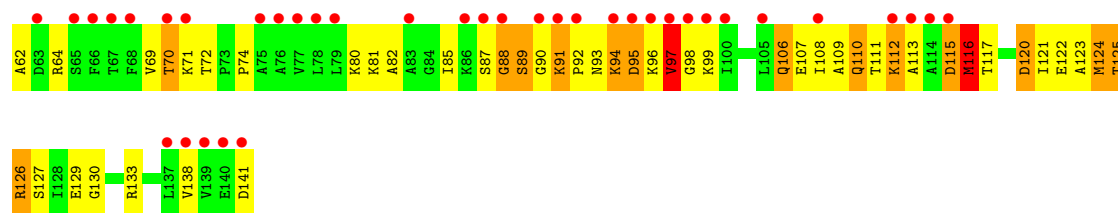


• Molecule 32: 50S ribosomal protein L11



• Molecule 32: 50S ribosomal protein L11

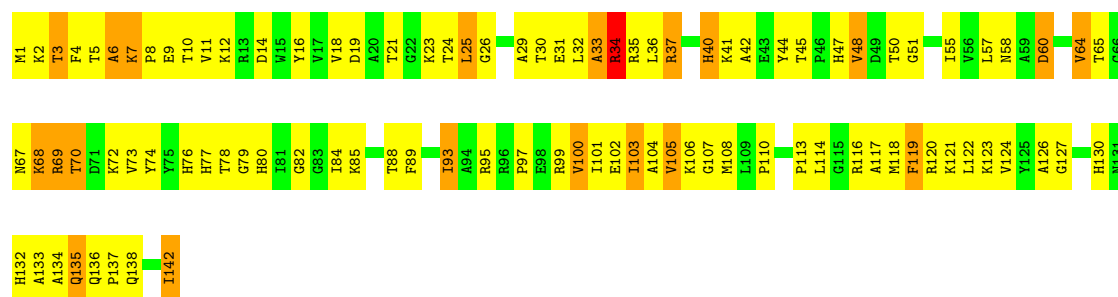
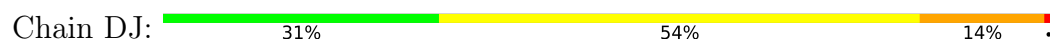




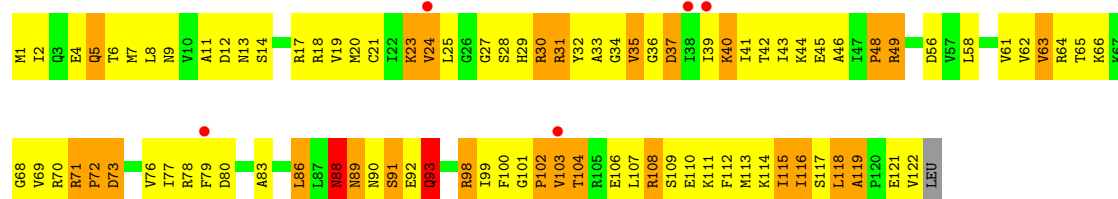
• Molecule 33: 50S ribosomal protein L13



• Molecule 33: 50S ribosomal protein L13

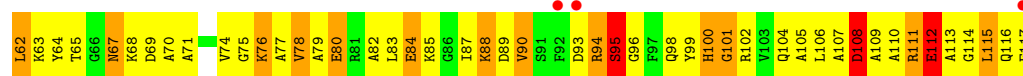
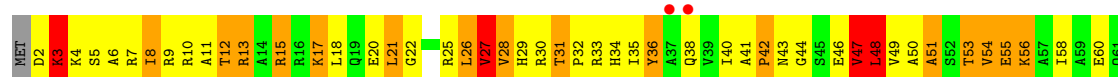


• Molecule 34: 50S ribosomal protein L14

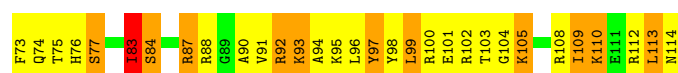
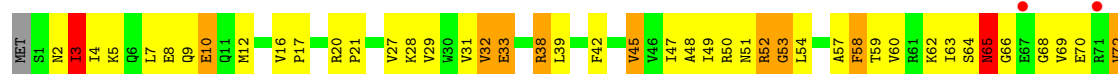


• Molecule 34: 50S ribosomal protein L14





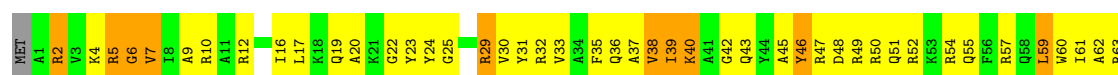
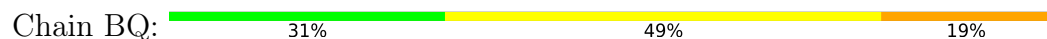
• Molecule 39: 50S ribosomal protein L19



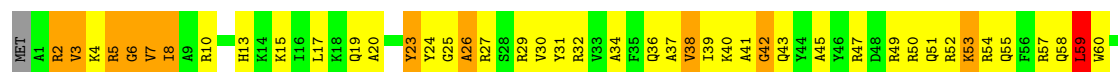
• Molecule 39: 50S ribosomal protein L19



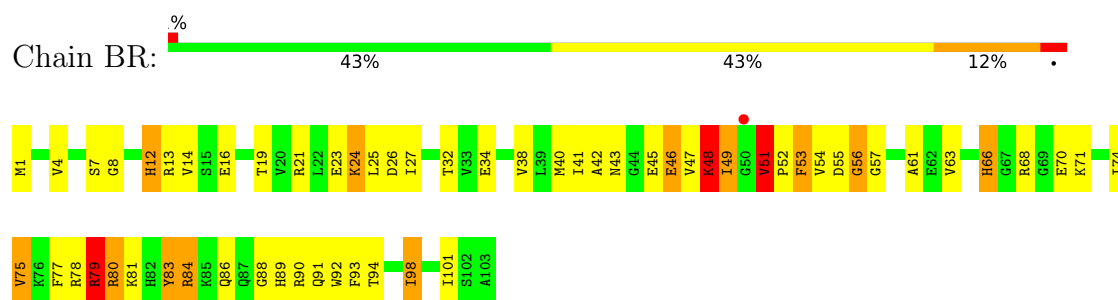
• Molecule 40: 50S ribosomal protein L20



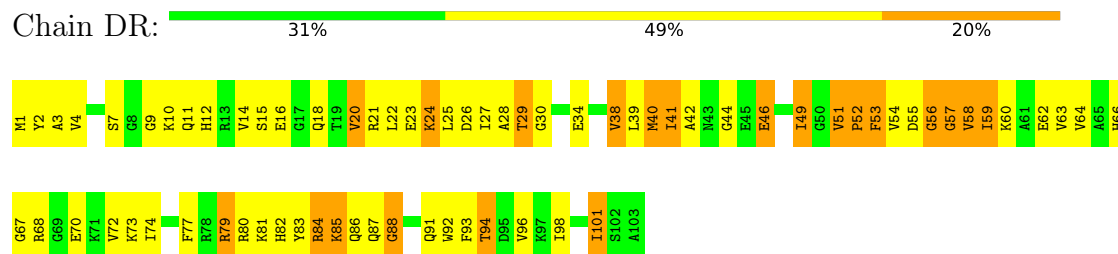
• Molecule 40: 50S ribosomal protein L20



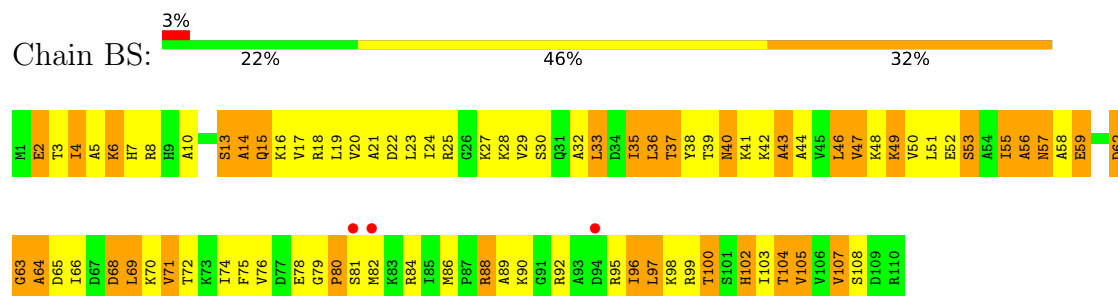
• Molecule 41: 50S ribosomal protein L21



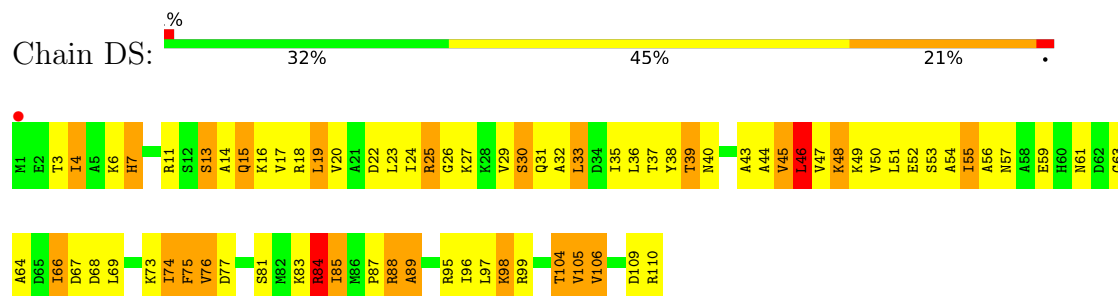
• Molecule 41: 50S ribosomal protein L21



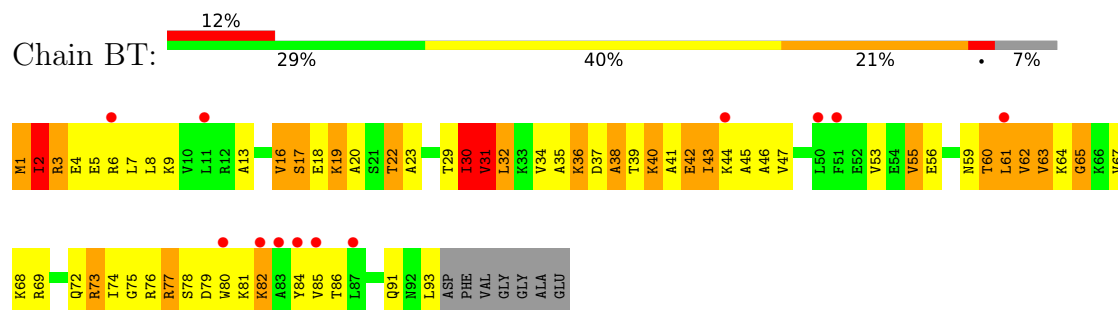
• Molecule 42: 50S ribosomal protein L22



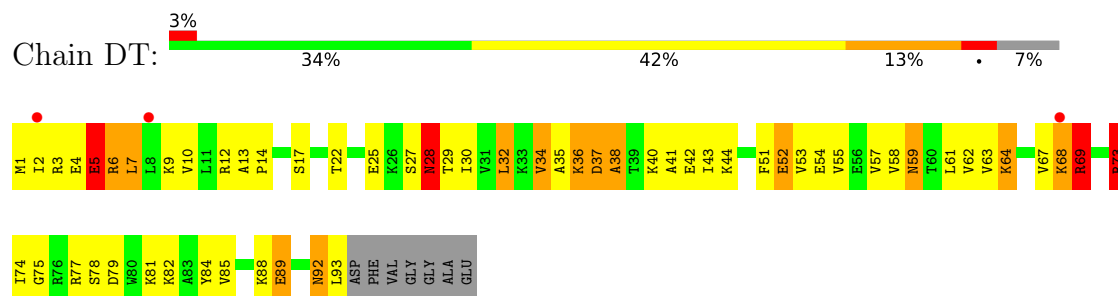
• Molecule 42: 50S ribosomal protein L22



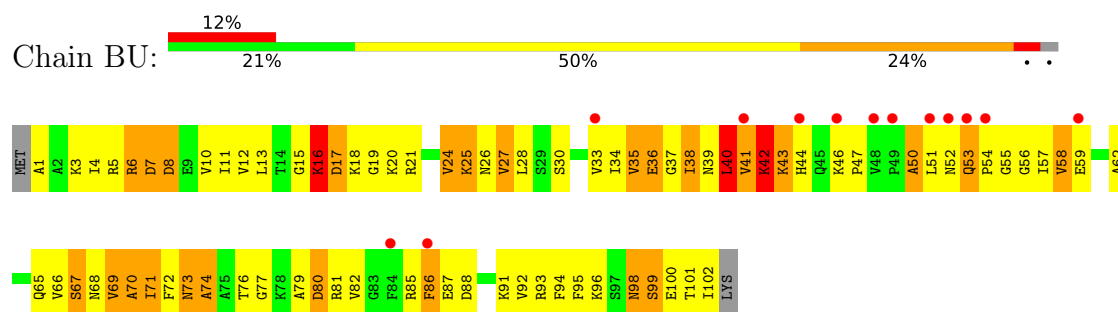
• Molecule 43: 50S ribosomal protein L23



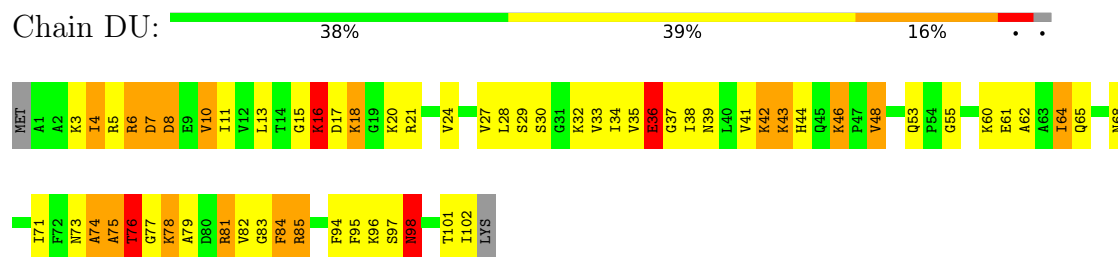
- Molecule 43: 50S ribosomal protein L23



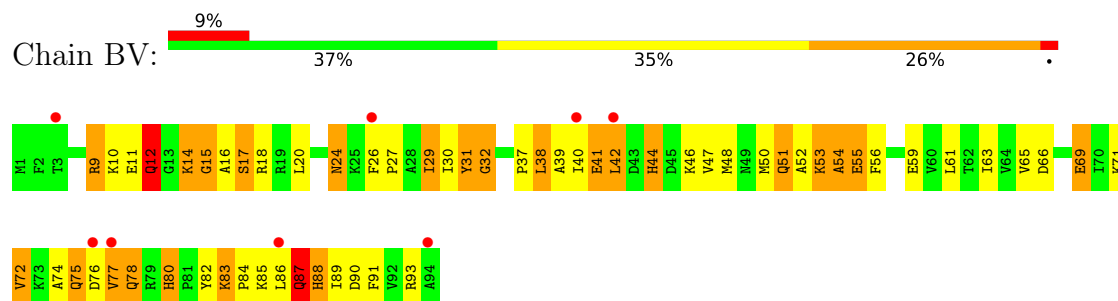
- Molecule 44: 50S ribosomal protein L24



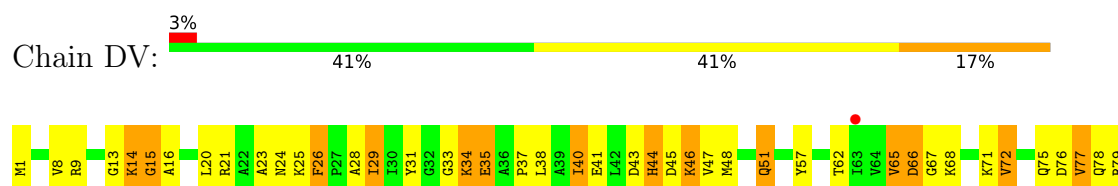
- Molecule 44: 50S ribosomal protein L24



- Molecule 45: 50S ribosomal protein L25

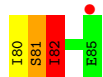
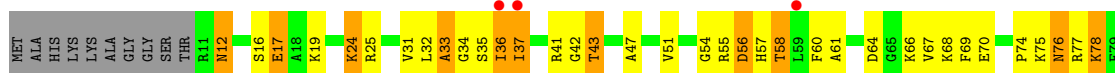
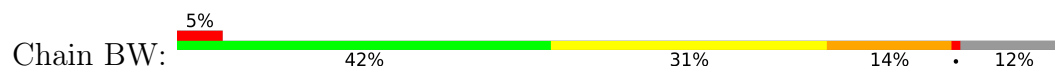


- Molecule 45: 50S ribosomal protein L25

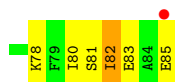
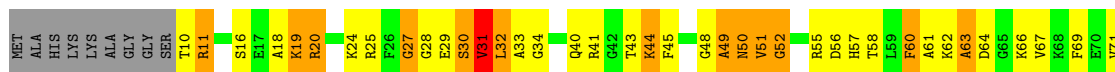




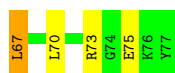
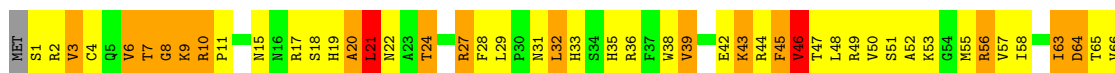
● Molecule 46: 50S ribosomal protein L27



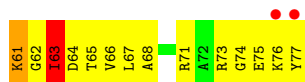
● Molecule 46: 50S ribosomal protein L27



● Molecule 47: 50S ribosomal protein L28

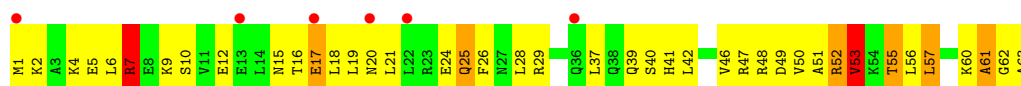


● Molecule 47: 50S ribosomal protein L28

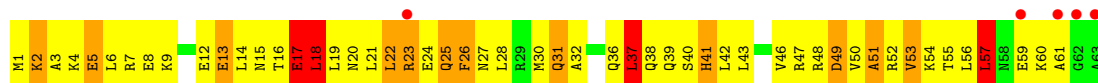


● Molecule 48: 50S ribosomal protein L29

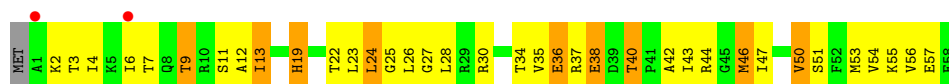




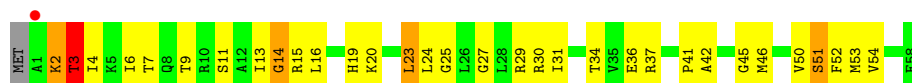
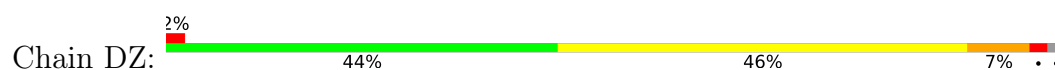
- Molecule 48: 50S ribosomal protein L29



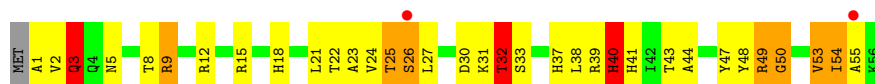
- Molecule 49: 50S ribosomal protein L30



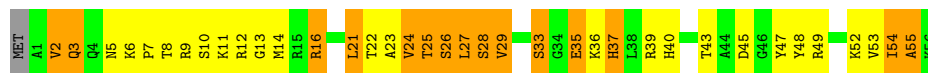
- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L32



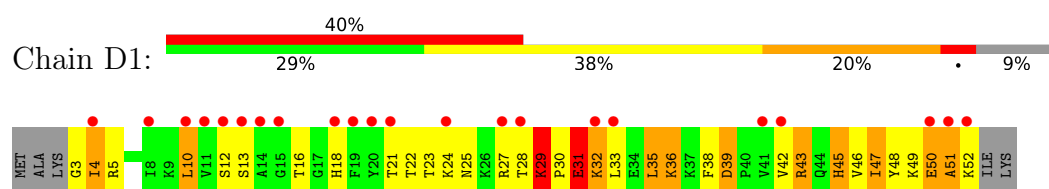
- Molecule 50: 50S ribosomal protein L32



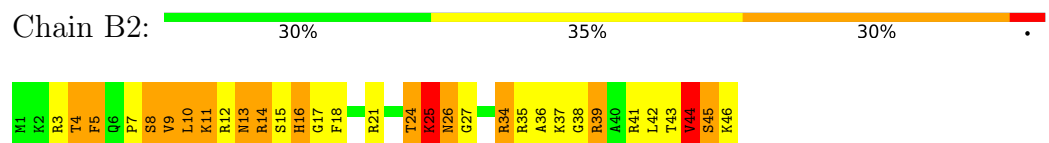
- Molecule 51: 50S ribosomal protein L33



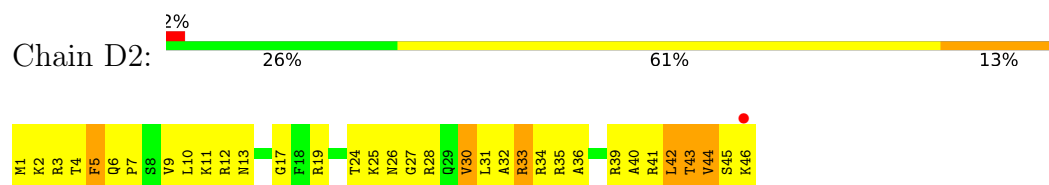
- Molecule 51: 50S ribosomal protein L33



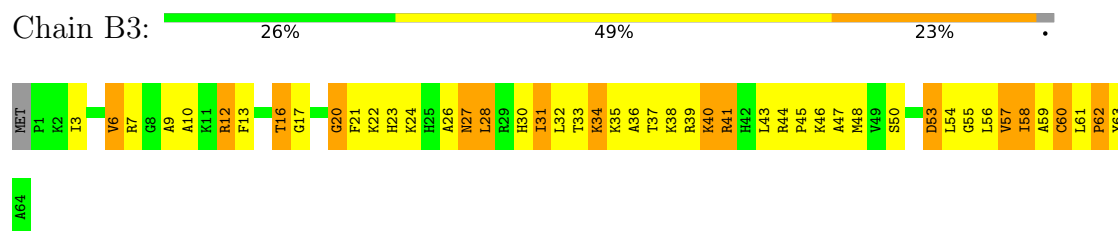
- Molecule 52: 50S ribosomal protein L34



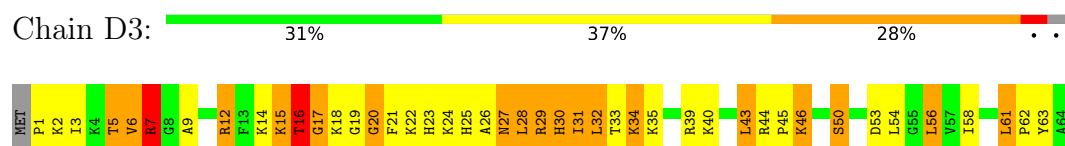
- Molecule 52: 50S ribosomal protein L34



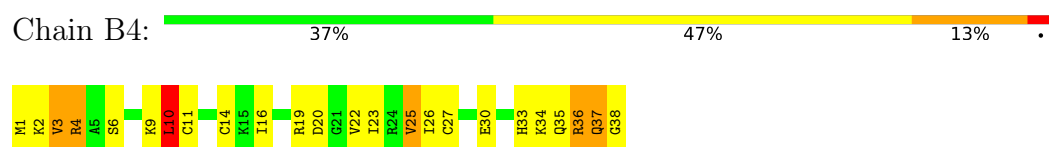
- Molecule 53: 50S ribosomal protein L35



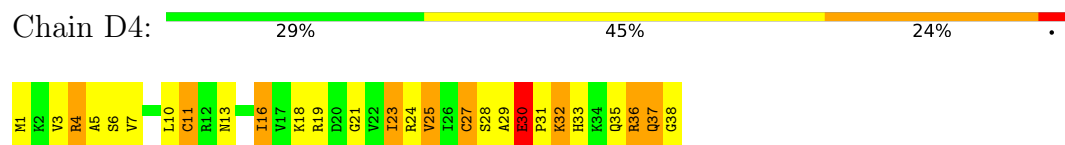
- Molecule 53: 50S ribosomal protein L35



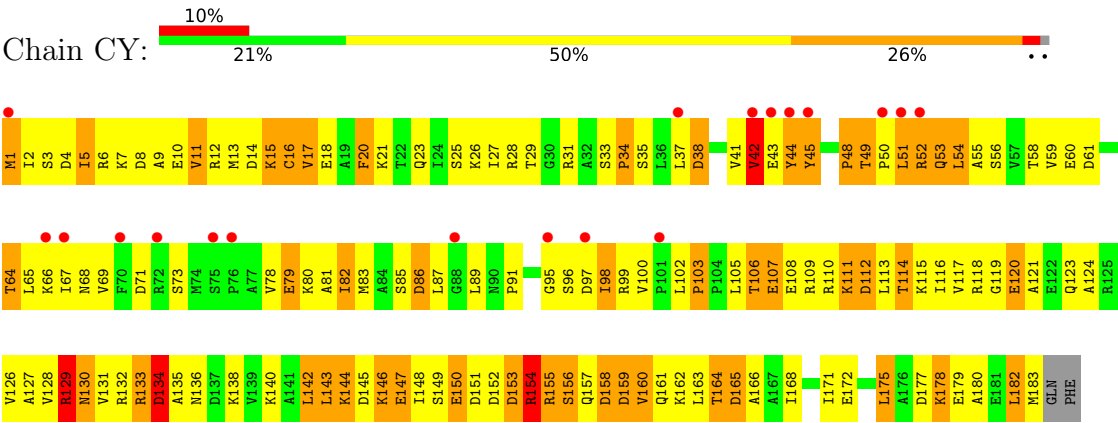
- Molecule 54: 50S ribosomal protein L36



- 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 69.81 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.30) 94.9 (69.81-3.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.255 0.203 , 0.251	Depositor DCC
R_{free} test set	2000 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)	0.24 , 110.8	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, MG, ZN

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	1
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	1
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	1
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	1
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	1
26	DC	269/273 (98%)	187 (70%)	51 (19%)	31 (12%)	0	2
27	BD	207/209 (99%)	159 (77%)	29 (14%)	19 (9%)	1	4
27	DD	207/209 (99%)	159 (77%)	33 (16%)	15 (7%)	1	7
28	BE	199/201 (99%)	126 (63%)	49 (25%)	24 (12%)	0	2
28	DE	199/201 (99%)	131 (66%)	53 (27%)	15 (8%)	1	7
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	4
33	DJ	140/142 (99%)	110 (79%)	25 (18%)	5 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BK	120/123 (98%)	77 (64%)	29 (24%)	14 (12%)	0	2
34	DK	120/123 (98%)	95 (79%)	18 (15%)	7 (6%)	1	11
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%)	1	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	3
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	21
40	DQ	115/118 (98%)	89 (77%)	16 (14%)	10 (9%)	1	5
41	BR	101/103 (98%)	76 (75%)	18 (18%)	7 (7%)	1	8
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	4
43	BT	91/100 (91%)	54 (59%)	26 (29%)	11 (12%)	0	2
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	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	DZ	56/59 (95%)	37 (66%)	16 (29%)	3 (5%)	2	12
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%)	1	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	8
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%)	2	11
54	D4	36/38 (95%)	26 (72%)	7 (19%)	3 (8%)	1	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	2
3	AC	170/190 (90%)	138 (81%)	32 (19%)	1	6
3	CC	170/190 (90%)	130 (76%)	40 (24%)	1	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%)	2	9
6	AF	87/116 (75%)	72 (83%)	15 (17%)	2	9
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	7
8	AH	104/105 (99%)	81 (78%)	23 (22%)	1	3
8	CH	104/105 (99%)	87 (84%)	17 (16%)	2	10
9	AI	105/107 (98%)	81 (77%)	24 (23%)	1	3
9	CI	105/107 (98%)	84 (80%)	21 (20%)	1	5
10	AJ	86/90 (96%)	73 (85%)	13 (15%)	3	13
10	CJ	86/90 (96%)	67 (78%)	19 (22%)	1	3
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	8
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	10
13	CM	92/96 (96%)	63 (68%)	29 (32%)	0	1
14	AN	79/84 (94%)	64 (81%)	15 (19%)	1	6
14	CN	79/84 (94%)	60 (76%)	19 (24%)	0	2
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	5
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%)	1	3
20	CT	65/66 (98%)	50 (77%)	15 (23%)	1	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	2
26	DC	216/218 (99%)	147 (68%)	69 (32%)	0	1
27	BD	164/164 (100%)	131 (80%)	33 (20%)	1	5
27	DD	164/164 (100%)	125 (76%)	39 (24%)	0	2
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%)	1	3
30	BG	137/138 (99%)	108 (79%)	29 (21%)	1	4
30	DG	137/138 (99%)	111 (81%)	26 (19%)	1	6
31	BH	114/114 (100%)	83 (73%)	31 (27%)	0	1
31	DH	114/114 (100%)	92 (81%)	22 (19%)	1	6
32	BI	109/110 (99%)	101 (93%)	8 (7%)	14	41
32	DI	109/110 (99%)	89 (82%)	20 (18%)	1	7
33	BJ	116/116 (100%)	90 (78%)	26 (22%)	1	3
33	DJ	116/116 (100%)	95 (82%)	21 (18%)	1	7
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	1
36	DM	109/109 (100%)	86 (79%)	23 (21%)	1	4
37	BN	100/103 (97%)	81 (81%)	19 (19%)	1	6
37	DN	100/103 (97%)	83 (83%)	17 (17%)	2	9
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	7
39	DP	99/100 (99%)	80 (81%)	19 (19%)	1	6
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	10
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	1
44	DU	83/85 (98%)	63 (76%)	20 (24%)	0	2
45	BV	78/78 (100%)	60 (77%)	18 (23%)	1	3
45	DV	78/78 (100%)	63 (81%)	15 (19%)	1	6
46	BW	56/63 (89%)	45 (80%)	11 (20%)	1	5
46	DW	57/63 (90%)	48 (84%)	9 (16%)	2	11
47	BX	67/68 (98%)	47 (70%)	20 (30%)	0	1
47	DX	67/68 (98%)	56 (84%)	11 (16%)	2	10
48	BY	55/55 (100%)	47 (86%)	8 (14%)	3	14
48	DY	55/55 (100%)	43 (78%)	12 (22%)	1	4
49	BZ	48/49 (98%)	40 (83%)	8 (17%)	2	10
49	DZ	48/49 (98%)	42 (88%)	6 (12%)	4	19
50	B0	47/48 (98%)	39 (83%)	8 (17%)	2	9
50	D0	47/48 (98%)	38 (81%)	9 (19%)	1	6
51	B1	45/49 (92%)	39 (87%)	6 (13%)	4	17
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%)	4	17
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%)	1	3
All	All	9485/9916 (96%)	7325 (77%)	2160 (23%)	1	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 monosaccharides 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	BA	3163	-	45,45,45	2.30	10 (22%)	63,67,67	2.41	27 (42%)
57	NMY	DA	3187	-	45,45,45	2.30	11 (24%)	63,67,67	1.51	14 (22%)
57	NMY	BA	3165	-	45,45,45	0.54	0	63,67,67	1.11	5 (7%)
57	NMY	BA	3167	-	45,45,45	2.28	11 (24%)	63,67,67	1.93	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	NMY	BA	3162	-	45,45,45	0.51	0	63,67,67	1.04	5 (7%)
57	NMY	DA	3184	-	45,45,45	0.58	0	63,67,67	1.24	5 (7%)
57	NMY	DA	3188	-	45,45,45	2.20	13 (28%)	63,67,67	2.00	24 (38%)
57	NMY	DA	3186	-	45,45,45	2.36	12 (26%)	63,67,67	2.32	16 (25%)
57	NMY	BA	3166	-	45,45,45	2.18	10 (22%)	63,67,67	2.32	17 (26%)
57	NMY	DA	3190	-	45,45,45	2.29	11 (24%)	63,67,67	2.54	26 (41%)
57	NMY	AA	1655	-	45,45,45	0.58	0	63,67,67	0.98	4 (6%)
57	NMY	DA	3189	-	45,45,45	2.20	12 (26%)	63,67,67	2.30	24 (38%)
57	NMY	BA	3161	-	45,45,45	0.51	0	63,67,67	1.01	4 (6%)
57	NMY	AA	1656	-	45,45,45	2.27	12 (26%)	63,67,67	1.86	20 (31%)
57	NMY	CA	1672	-	45,45,45	0.54	0	63,67,67	0.91	2 (3%)
57	NMY	BA	3164	-	45,45,45	2.25	11 (24%)	63,67,67	2.38	26 (41%)
57	NMY	DA	3185	-	45,45,45	2.32	13 (28%)	63,67,67	1.73	16 (25%)
57	NMY	AA	1657	-	45,45,45	2.32	13 (28%)	63,67,67	1.83	18 (28%)

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	BA	3163	-	-	5/18/94/94	0/4/4/4
57	NMY	DA	3187	-	-	8/18/94/94	0/4/4/4
57	NMY	BA	3165	-	-	6/18/94/94	0/4/4/4
57	NMY	BA	3167	-	-	5/18/94/94	0/4/4/4
57	NMY	BA	3162	-	-	1/18/94/94	0/4/4/4
57	NMY	DA	3184	-	-	4/18/94/94	0/4/4/4
57	NMY	DA	3188	-	-	8/18/94/94	0/4/4/4
57	NMY	DA	3186	-	-	11/18/94/94	0/4/4/4
57	NMY	BA	3166	-	-	7/18/94/94	0/4/4/4
57	NMY	DA	3190	-	-	10/18/94/94	0/4/4/4
57	NMY	AA	1655	-	-	12/18/94/94	0/4/4/4
57	NMY	DA	3189	-	-	5/18/94/94	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	CA	1672	-	-	4/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	NMY	BA	3164	-	-	5/18/94/94	0/4/4/4
57	NMY	DA	3185	-	-	5/18/94/94	0/4/4/4
57	NMY	AA	1657	-	-	9/18/94/94	0/4/4/4

The worst 5 of 139 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 267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	DA	3186	NMY	O11-C13-O16	10.12	122.39	111.43
57	BA	3166	NMY	O11-C13-C14	6.98	122.43	107.96
57	DA	3190	NMY	C13-C14-C15	6.50	109.92	102.10
57	DA	3186	NMY	C8-C7-C12	6.50	119.85	110.04
57	BA	3163	NMY	C1-O1-C10	-6.28	102.42	117.96

There are no chirality outliers.

5 of 115 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	BA	3163	NMY	11	0
57	DA	3187	NMY	4	0
57	BA	3165	NMY	25	0
57	BA	3167	NMY	5	0

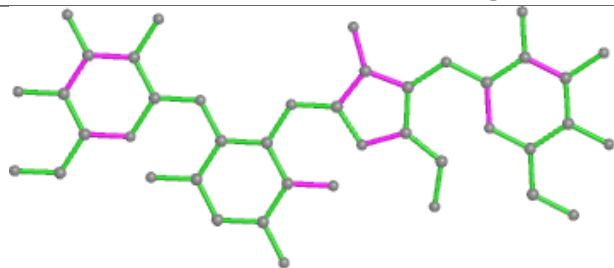
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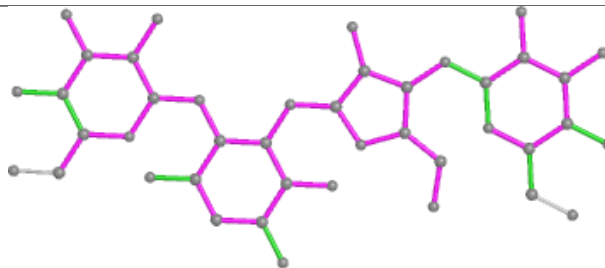
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BA	3162	NMY	16	0
57	DA	3184	NMY	17	0
57	DA	3188	NMY	12	0
57	DA	3186	NMY	19	0
57	BA	3166	NMY	13	0
57	DA	3190	NMY	32	0
57	AA	1655	NMY	26	0
57	DA	3189	NMY	10	0
57	BA	3161	NMY	14	0
57	AA	1656	NMY	12	0
57	CA	1672	NMY	6	0
57	BA	3164	NMY	3	0
57	DA	3185	NMY	13	0
57	AA	1657	NMY	10	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.

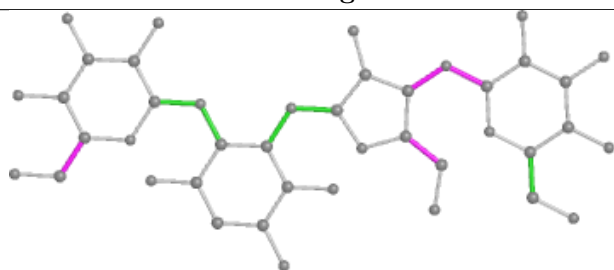
Ligand NMY BA 3163



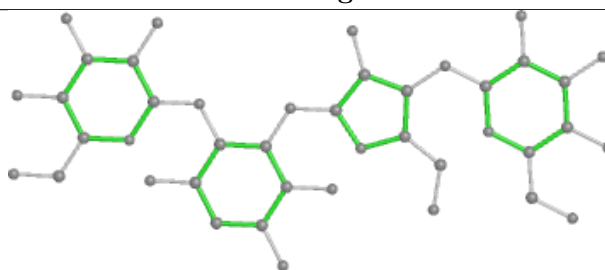
Bond lengths



Bond angles

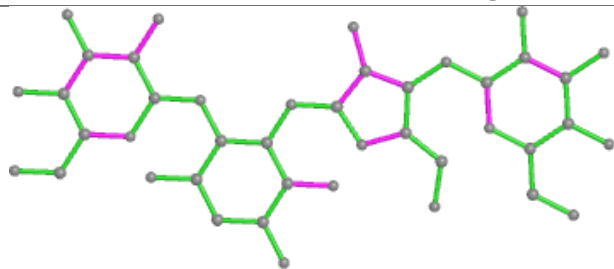


Torsions

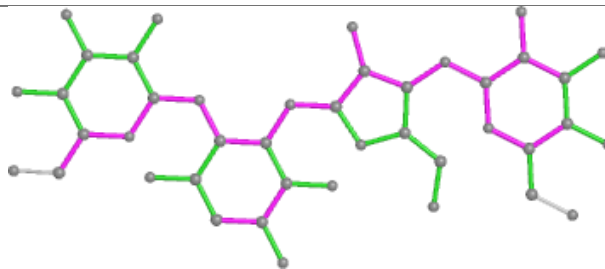


Rings

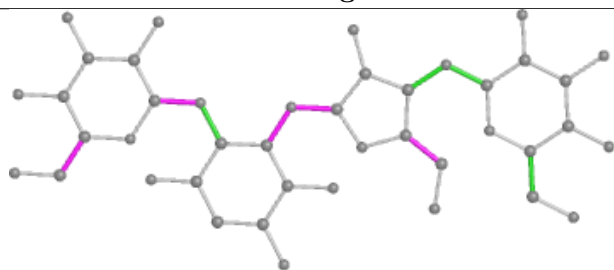
Ligand NMY DA 3187



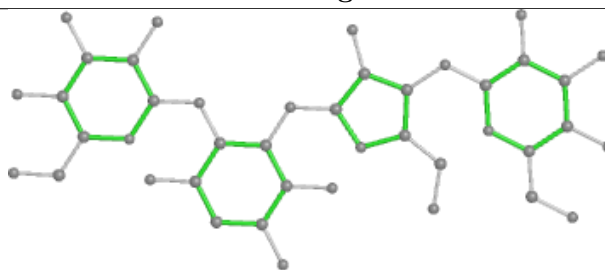
Bond lengths



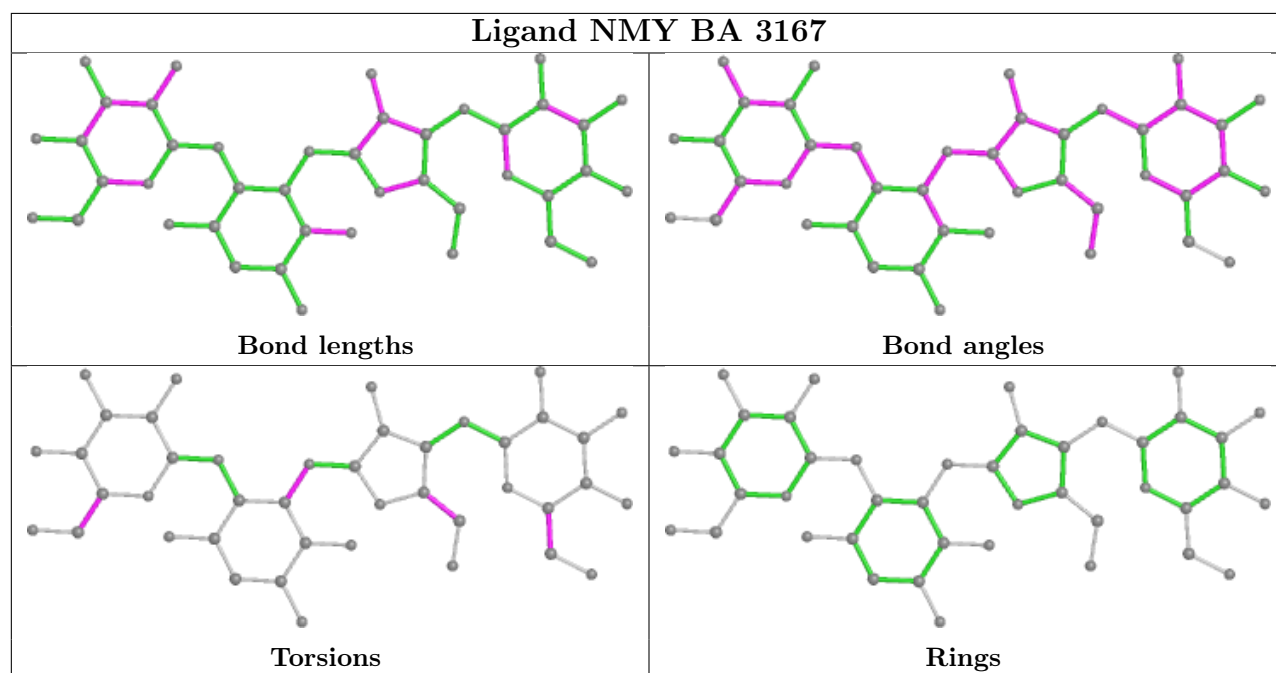
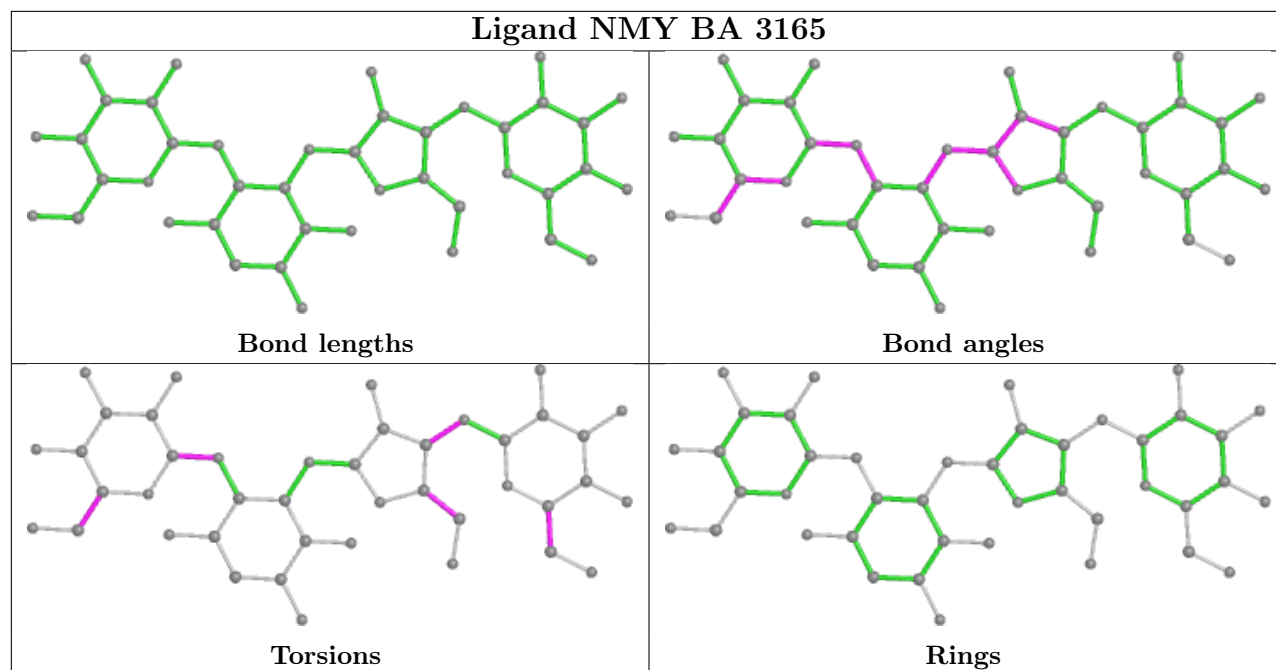
Bond angles



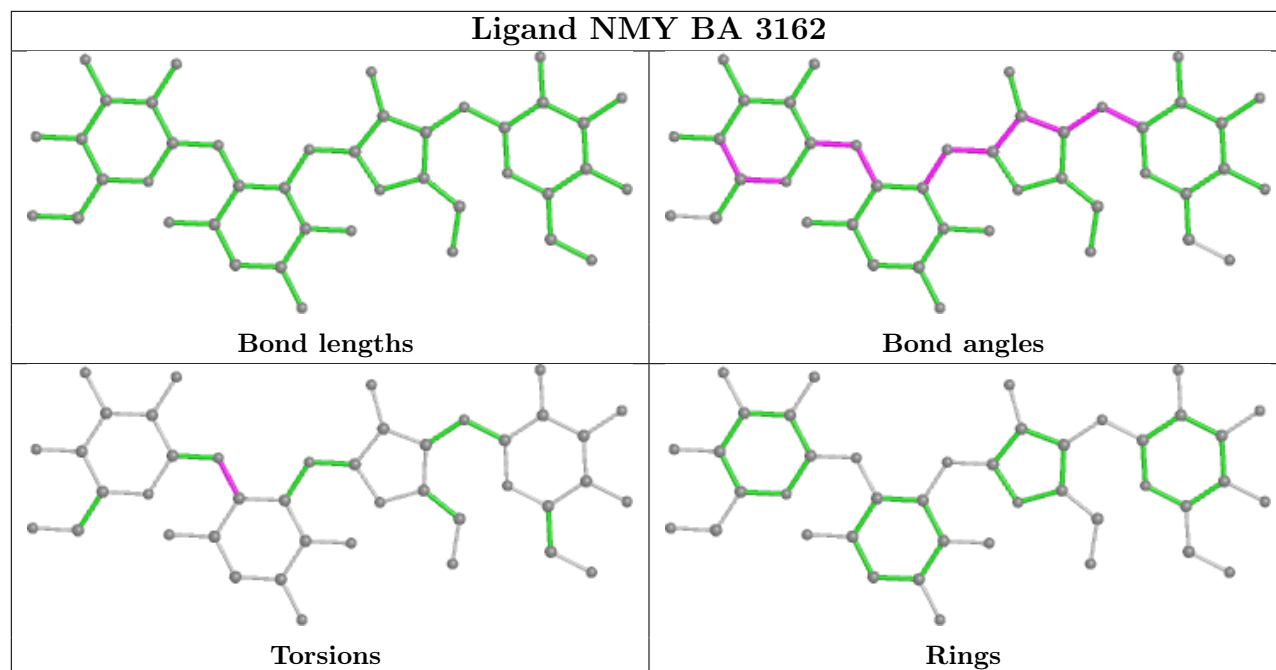
Torsions



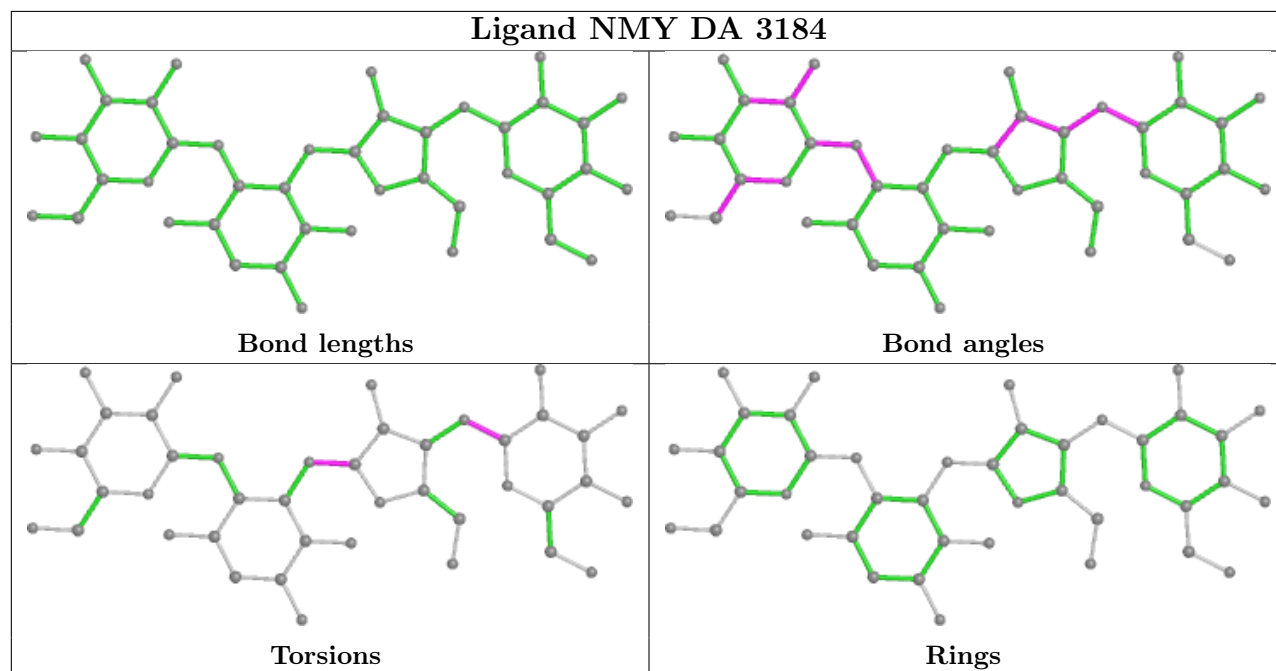
Rings



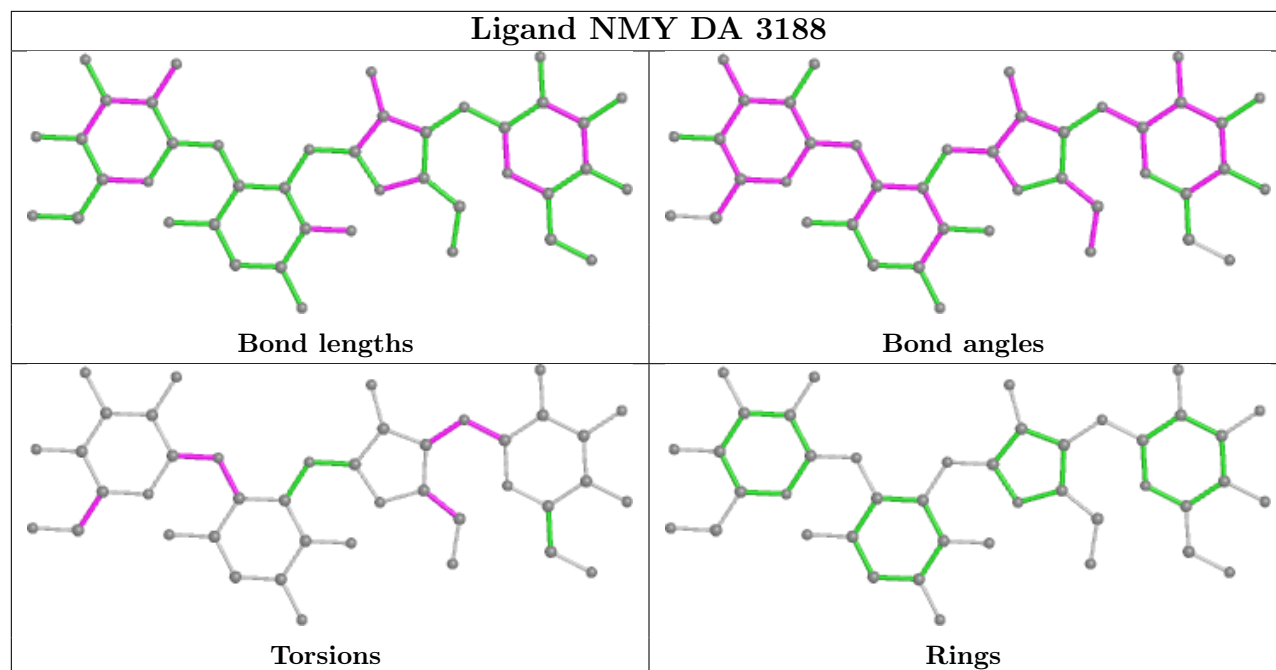
Ligand NMY BA 3162



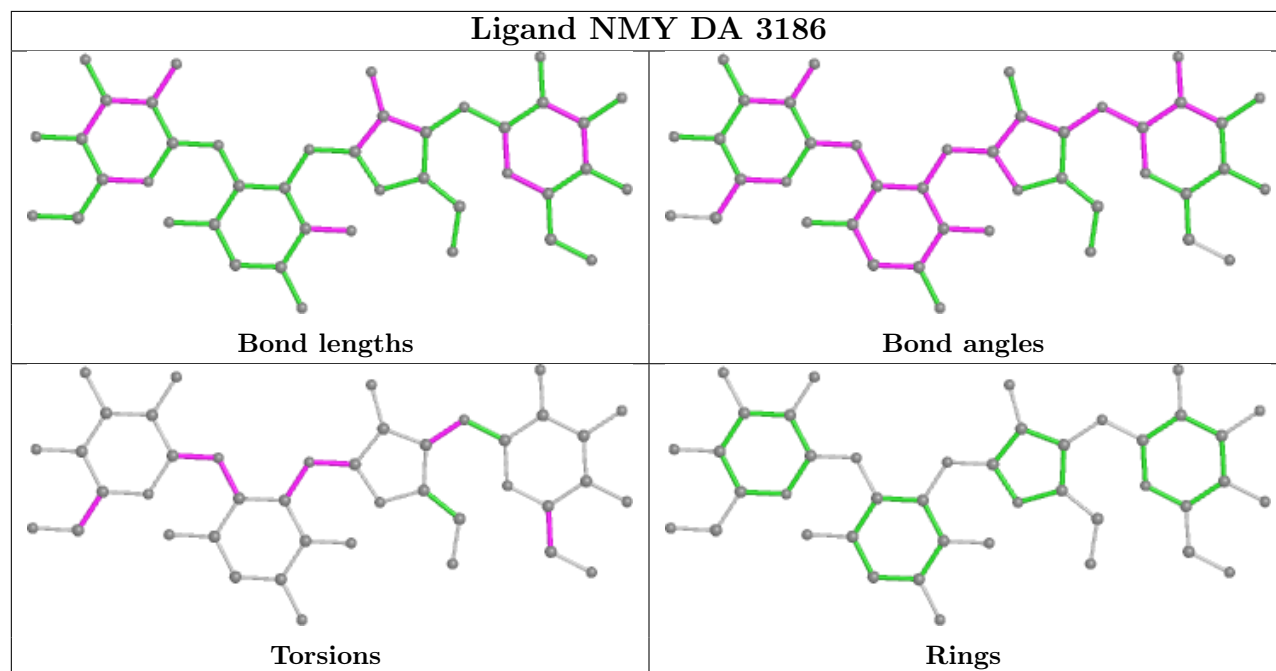
Ligand NMY DA 3184



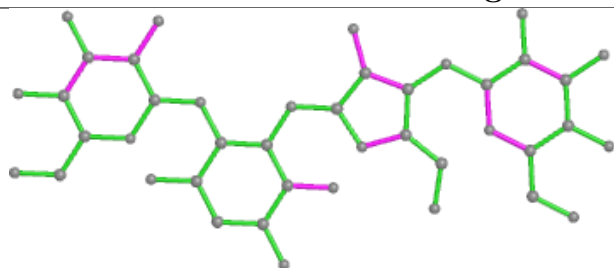
Ligand NMY DA 3188



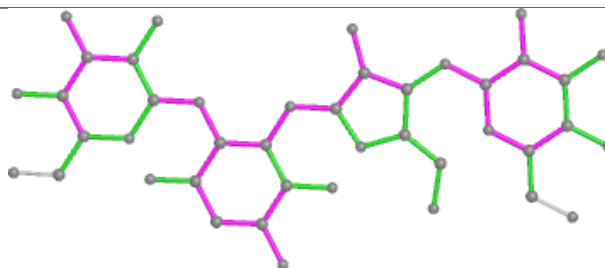
Ligand NMY DA 3186



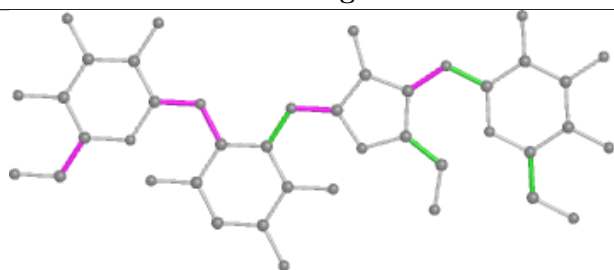
Ligand NMY BA 3166



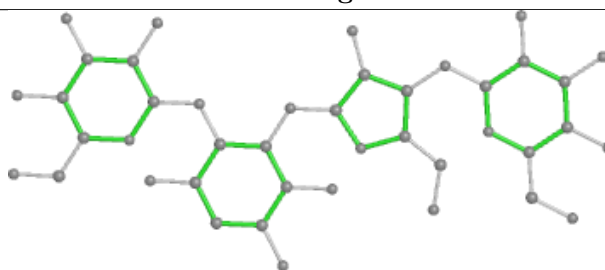
Bond lengths



Bond angles

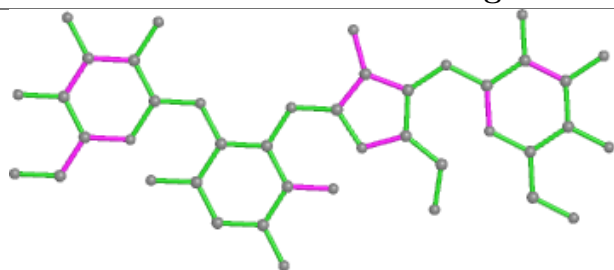


Torsions

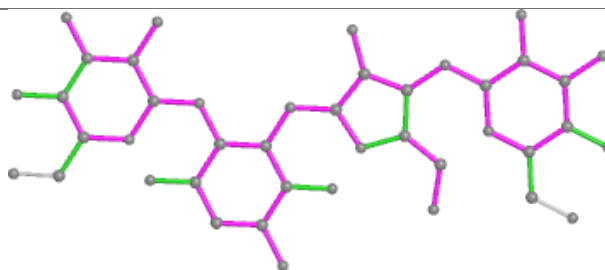


Rings

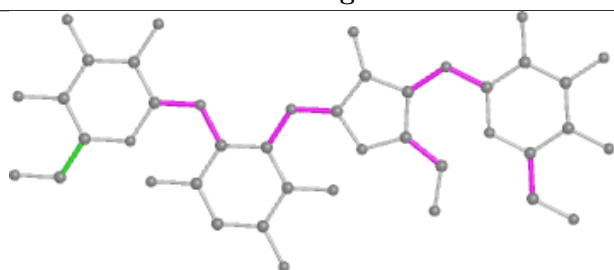
Ligand NMY DA 3190



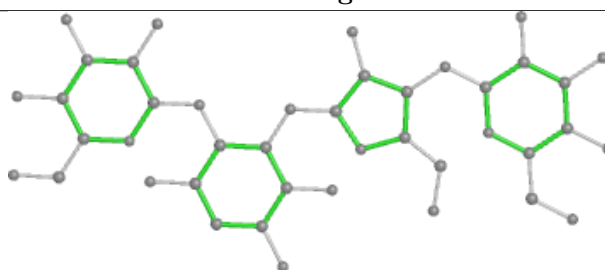
Bond lengths



Bond angles

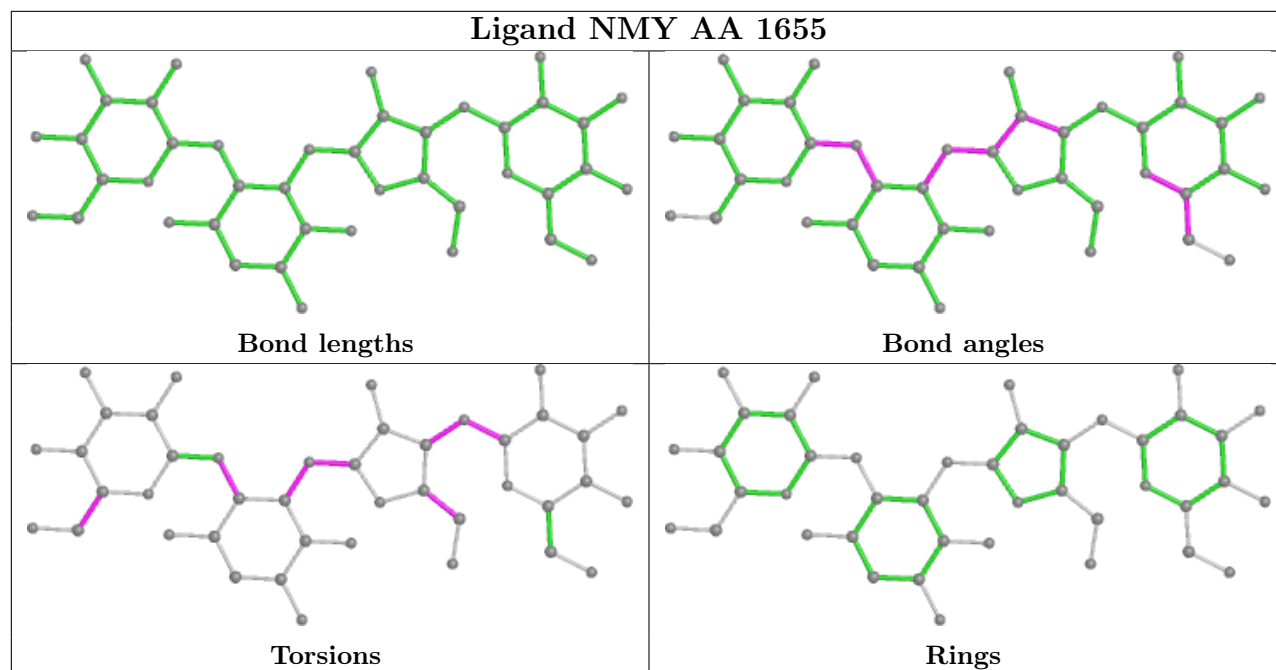


Torsions

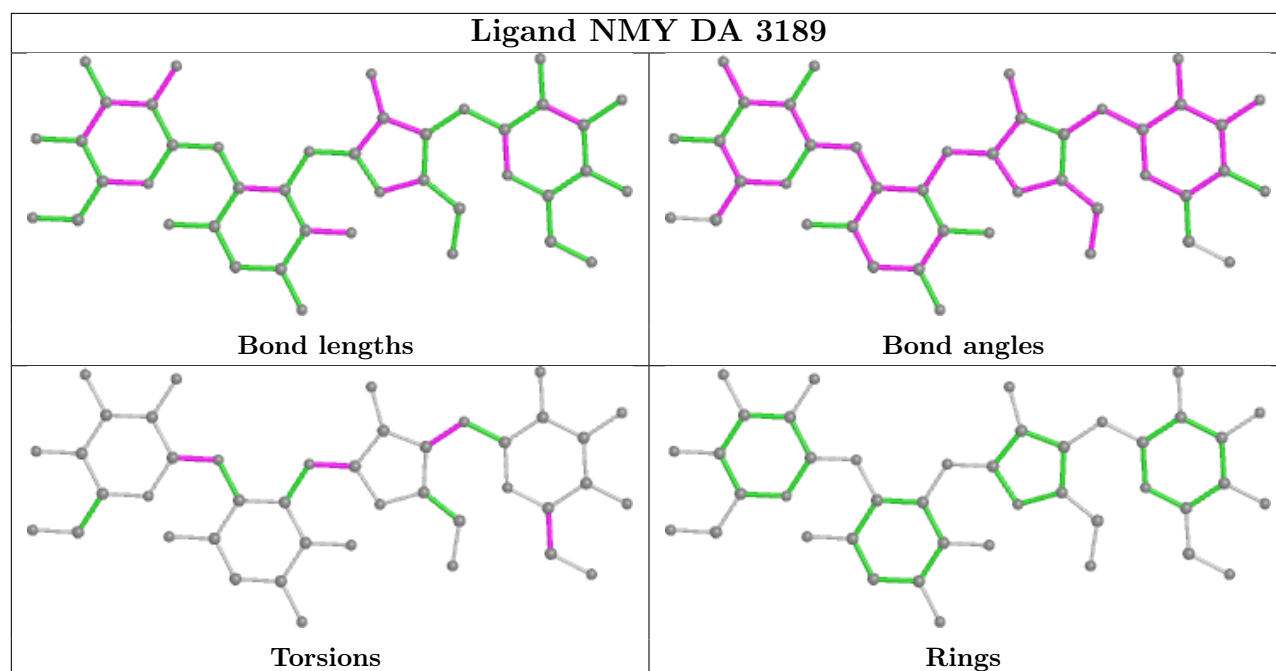


Rings

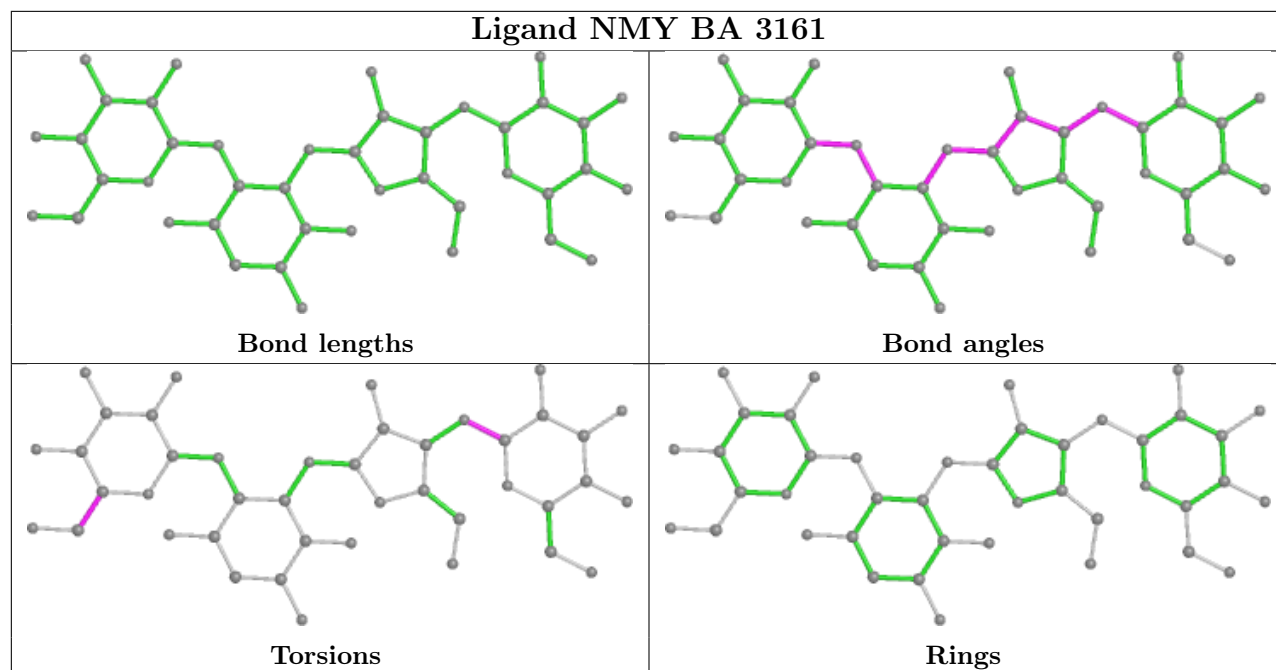
Ligand NMY AA 1655



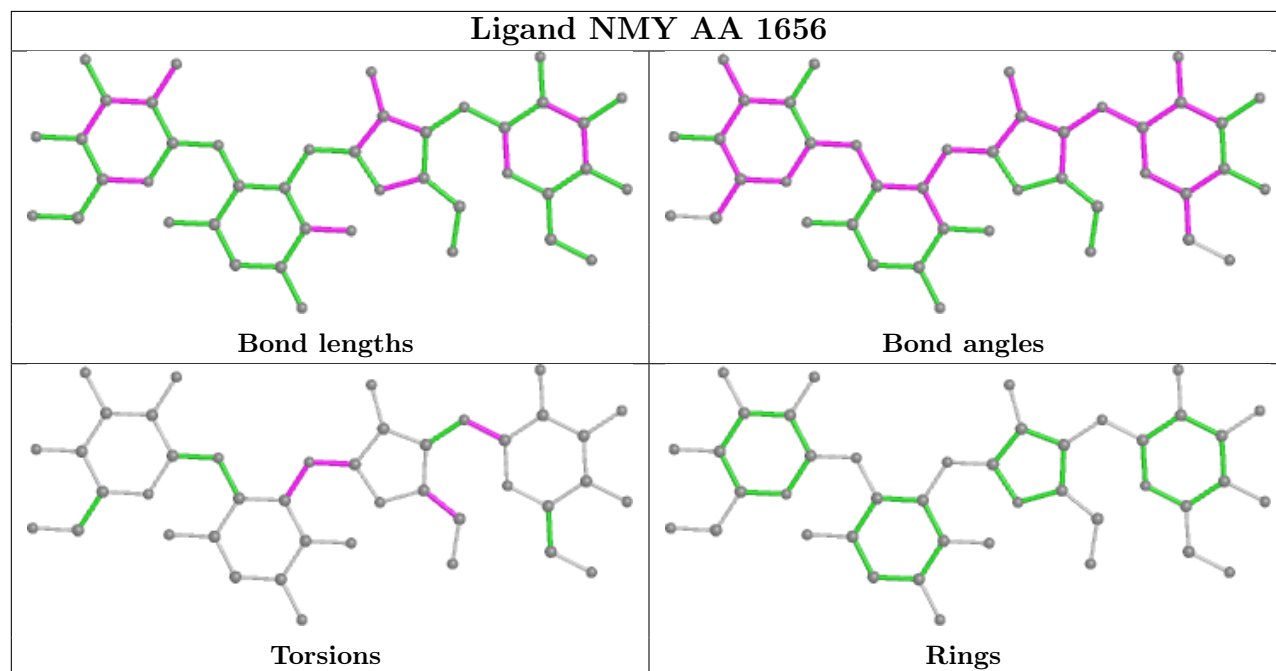
Ligand NMY DA 3189



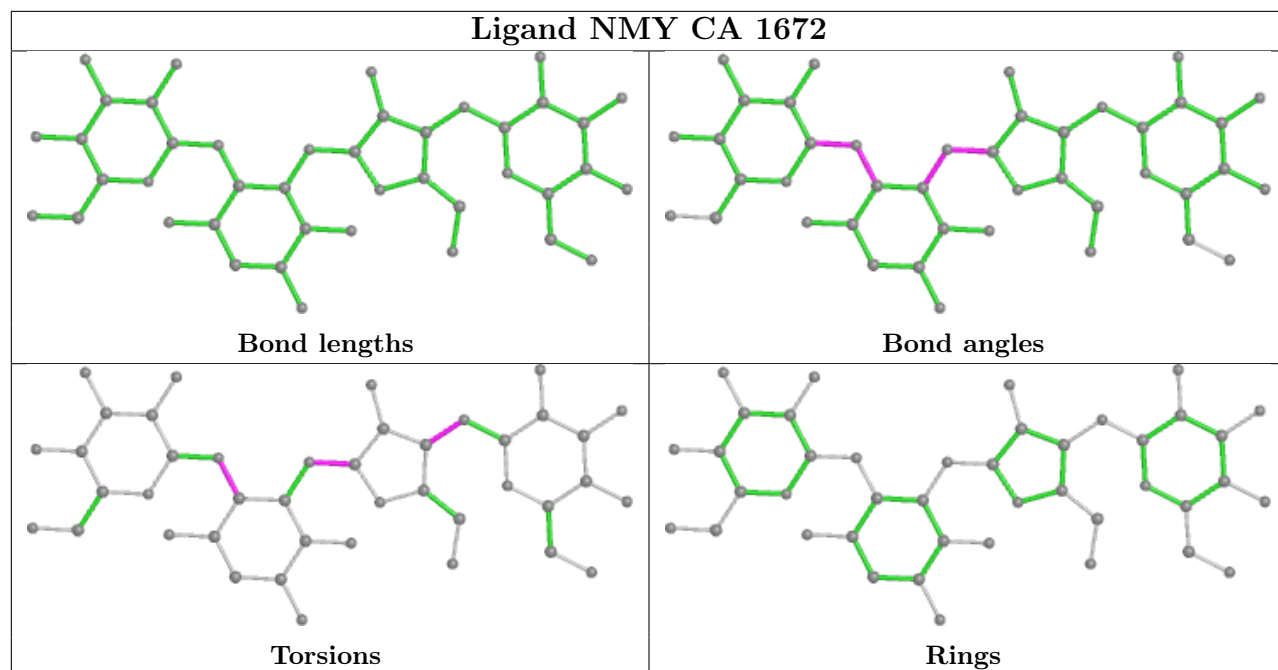
Ligand NMY BA 3161



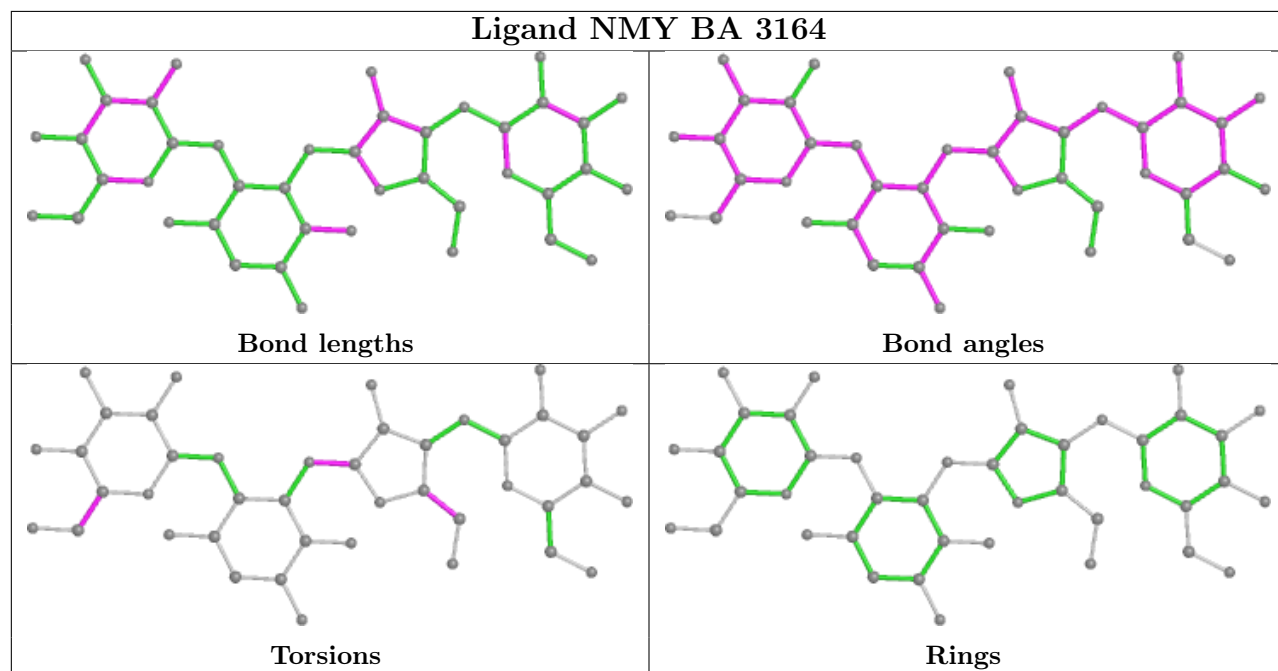
Ligand NMY AA 1656

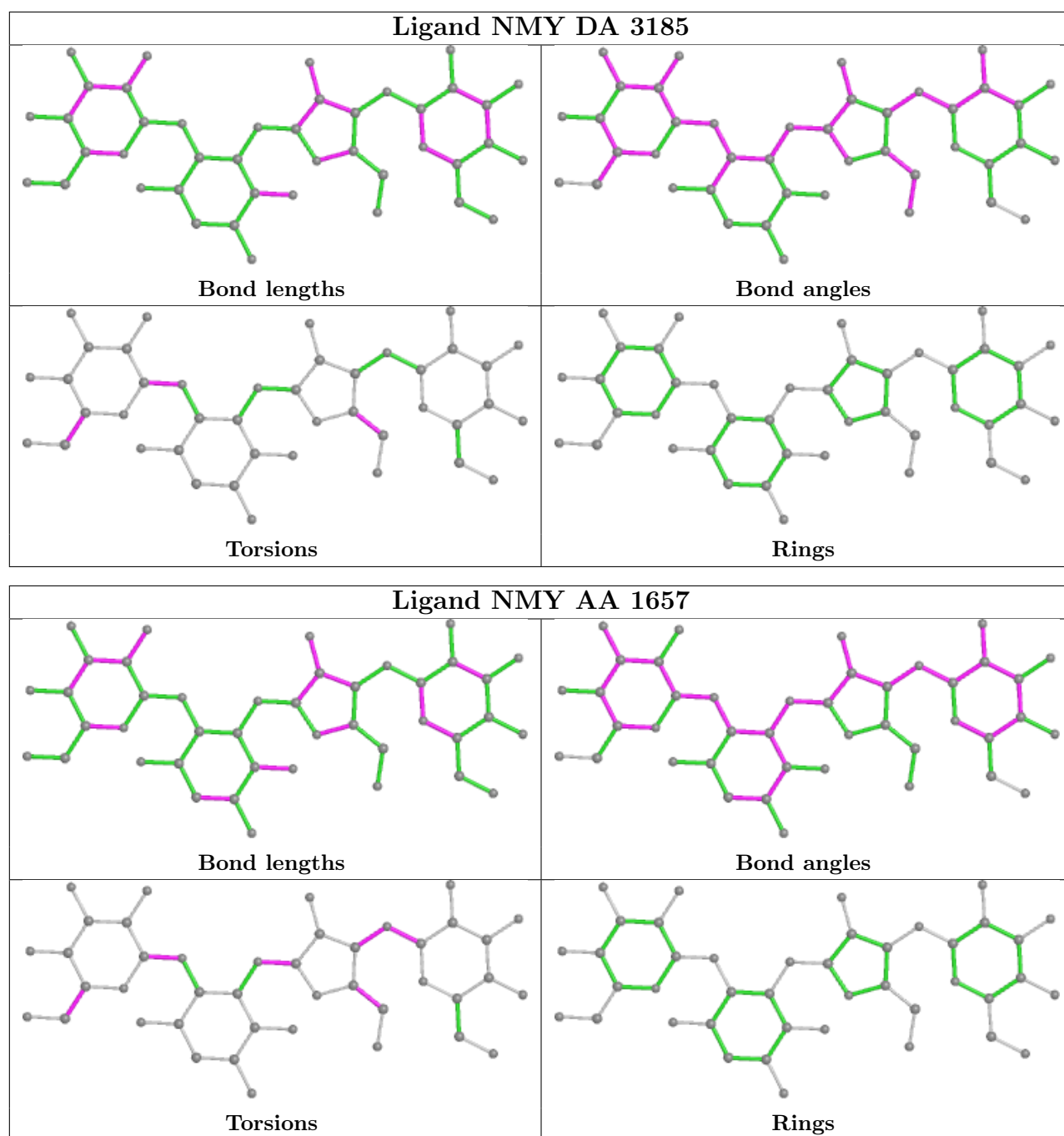


Ligand NMY CA 1672



Ligand NMY BA 3164





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%)	-0.49	3 (0%)	95 96	67, 121, 207, 543	0
1	CA	1538/1542 (99%)	-0.50	5 (0%)	94 94	63, 120, 240, 527	0
2	AB	218/241 (90%)	0.70	30 (13%)	2 2	86, 172, 404, 542	0
2	CB	218/241 (90%)	0.62	31 (14%)	2 2	96, 215, 508, 545	0
3	AC	206/233 (88%)	0.47	19 (9%)	9 9	81, 139, 325, 514	0
3	CC	206/233 (88%)	0.25	9 (4%)	34 33	80, 120, 286, 513	0
4	AD	205/206 (99%)	0.64	28 (13%)	3 2	83, 161, 372, 537	0
4	CD	205/206 (99%)	0.40	22 (10%)	6 5	81, 148, 442, 537	0
5	AE	150/167 (89%)	0.02	4 (2%)	54 52	79, 130, 272, 478	0
5	CE	150/167 (89%)	0.29	6 (4%)	38 36	68, 114, 292, 527	0
6	AF	100/135 (74%)	0.04	4 (4%)	38 36	85, 142, 331, 528	0
6	CF	100/135 (74%)	0.51	7 (7%)	16 16	87, 178, 386, 531	0
7	AG	151/179 (84%)	0.21	12 (7%)	12 12	93, 161, 365, 539	0
7	CG	151/179 (84%)	0.79	26 (17%)	1 1	112, 234, 452, 540	0
8	AH	129/130 (99%)	0.26	9 (6%)	16 16	79, 145, 341, 424	0
8	CH	129/130 (99%)	0.54	13 (10%)	7 6	81, 121, 307, 437	0
9	AI	127/130 (97%)	0.50	15 (11%)	4 4	101, 180, 459, 535	0
9	CI	127/130 (97%)	0.93	27 (21%)	0 1	97, 216, 478, 540	0
10	AJ	98/103 (95%)	0.70	12 (12%)	4 3	95, 165, 363, 543	0
10	CJ	98/103 (95%)	1.38	21 (21%)	0 1	101, 202, 530, 543	0
11	AK	117/129 (90%)	0.33	6 (5%)	28 26	75, 112, 337, 492	0
11	CK	117/129 (90%)	1.14	28 (23%)	0 0	83, 243, 494, 531	0
12	AL	123/124 (99%)	0.58	13 (10%)	6 6	75, 109, 299, 403	0
12	CL	123/124 (99%)	-0.03	6 (4%)	29 27	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%)	0.41	10 (8%)	10	106, 239, 498, 530	0
13	CM	114/118 (96%)	1.21	30 (26%)	0	122, 312, 536, 547	0
14	AN	96/101 (95%)	0.29	4 (4%)	36	89, 175, 381, 527	0
14	CN	96/101 (95%)	0.62	11 (11%)	4	95, 183, 535, 545	0
15	AO	88/89 (98%)	0.29	6 (6%)	17	90, 136, 315, 374	0
15	CO	88/89 (98%)	0.31	4 (4%)	33	94, 176, 350, 510	0
16	AP	82/82 (100%)	1.14	20 (24%)	0	76, 125, 380, 528	0
16	CP	82/82 (100%)	1.14	17 (20%)	1	75, 115, 387, 524	0
17	AQ	80/84 (95%)	1.29	17 (21%)	0	88, 162, 370, 434	0
17	CQ	80/84 (95%)	0.30	3 (3%)	40	75, 141, 337, 496	0
18	AR	55/75 (73%)	0.32	3 (5%)	25	84, 115, 320, 391	0
18	CR	55/75 (73%)	0.34	6 (10%)	5	107, 159, 370, 440	0
19	AS	79/92 (85%)	1.50	21 (26%)	0	118, 215, 454, 530	0
19	CS	79/92 (85%)	1.79	31 (39%)	0	133, 302, 496, 542	0
20	AT	85/87 (97%)	0.32	2 (2%)	59	93, 158, 363, 497	0
20	CT	85/87 (97%)	0.58	10 (11%)	4	82, 128, 351, 491	0
21	AU	51/71 (71%)	0.21	2 (3%)	39	83, 133, 326, 395	0
21	CU	51/71 (71%)	0.31	5 (9%)	7	108, 193, 374, 512	0
22	AV	76/76 (100%)	-0.20	1 (1%)	77	63, 117, 160, 255	0
22	CV	76/76 (100%)	1.24	17 (22%)	0	61, 257, 424, 542	0
23	AX	16/24 (66%)	-0.21	0	100	76, 139, 214, 261	0
23	CX	15/24 (62%)	-0.05	1 (6%)	17	83, 191, 269, 339	0
24	BA	2897/2904 (99%)	-0.43	24 (0%)	86	54, 96, 294, 544	0
24	DA	2897/2904 (99%)	-0.30	88 (3%)	50	37, 67, 231, 547	0
25	BB	118/120 (98%)	-0.81	0	100	78, 151, 201, 231	0
25	DB	119/120 (99%)	-0.68	0	100	47, 88, 129, 188	0
26	BC	271/273 (99%)	0.25	7 (2%)	56	56, 106, 196, 362	0
26	DC	271/273 (99%)	0.04	3 (1%)	80	46, 81, 188, 348	0
27	BD	209/209 (100%)	0.00	5 (2%)	59	58, 88, 195, 401	0
27	DD	209/209 (100%)	-0.16	0	100	38, 57, 129, 253	0
28	BE	201/201 (100%)	0.35	19 (9%)	8	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%)	0.04	1 (0%) 91 91	40, 72, 155, 487	0
29	BF	177/179 (98%)	1.06	37 (20%) 1 1	125, 257, 446, 539	0
29	DF	177/179 (98%)	0.78	22 (12%) 4 3	76, 147, 367, 520	0
30	BG	176/177 (99%)	0.79	25 (14%) 2 2	93, 155, 360, 507	0
30	DG	176/177 (99%)	0.28	9 (5%) 28 26	54, 94, 190, 439	0
31	BH	149/149 (100%)	0.83	23 (15%) 2 2	15, 223, 436, 532	0
31	DH	149/149 (100%)	0.61	18 (12%) 4 3	25, 213, 475, 538	0
32	BI	141/142 (99%)	3.66	90 (63%) 0 0	126, 471, 546, 549	0
32	DI	141/142 (99%)	3.08	78 (55%) 0 0	123, 380, 542, 548	0
33	BJ	142/142 (100%)	0.17	1 (0%) 87 88	56, 83, 169, 348	0
33	DJ	142/142 (100%)	-0.13	0 100 100	38, 60, 146, 265	0
34	BK	122/123 (99%)	0.33	5 (4%) 37 35	65, 93, 197, 357	0
34	DK	122/123 (99%)	0.02	1 (0%) 86 86	43, 63, 112, 229	0
35	BL	143/144 (99%)	0.04	2 (1%) 75 75	55, 110, 265, 507	0
35	DL	143/144 (99%)	-0.29	0 100 100	41, 68, 170, 291	0
36	BM	136/136 (100%)	0.67	16 (11%) 4 4	65, 99, 208, 340	0
36	DM	136/136 (100%)	0.05	1 (0%) 87 88	47, 67, 153, 262	0
37	BN	120/127 (94%)	0.21	2 (1%) 70 68	66, 107, 190, 466	0
37	DN	120/127 (94%)	-0.16	0 100 100	40, 61, 151, 420	0
38	BO	116/117 (99%)	0.61	14 (12%) 4 3	96, 193, 363, 537	0
38	DO	116/117 (99%)	0.28	5 (4%) 35 34	66, 94, 183, 322	0
39	BP	114/115 (99%)	0.17	2 (1%) 68 67	71, 109, 288, 356	0
39	DP	114/115 (99%)	-0.21	0 100 100	47, 69, 178, 330	0
40	BQ	117/118 (99%)	0.00	0 100 100	55, 76, 170, 304	0
40	DQ	117/118 (99%)	-0.32	0 100 100	38, 54, 156, 310	0
41	BR	103/103 (100%)	0.07	1 (0%) 82 82	57, 92, 180, 286	0
41	DR	103/103 (100%)	-0.06	0 100 100	42, 68, 152, 458	0
42	BS	110/110 (100%)	0.12	3 (2%) 54 52	60, 92, 175, 299	0
42	DS	110/110 (100%)	-0.01	1 (0%) 84 84	38, 56, 115, 161	0
43	BT	93/100 (93%)	0.85	12 (12%) 3 3	93, 155, 337, 441	0
43	DT	93/100 (93%)	0.36	3 (3%) 47 46	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%)	0.62	13 (12%) 3 3	78, 133, 337, 443	0
44	DU	102/104 (98%)	-0.13	0 100 100	52, 82, 226, 299	0
45	BV	94/94 (100%)	0.64	8 (8%) 10 10	86, 144, 310, 421	0
45	DV	94/94 (100%)	0.32	3 (3%) 47 46	60, 94, 183, 336	0
46	BW	75/85 (88%)	0.53	4 (5%) 26 24	70, 113, 202, 321	0
46	DW	76/85 (89%)	0.09	1 (1%) 77 77	46, 70, 156, 244	0
47	BX	77/78 (98%)	0.03	0 100 100	62, 110, 268, 318	0
47	DX	77/78 (98%)	0.27	3 (3%) 39 37	48, 83, 165, 320	0
48	BY	63/63 (100%)	0.52	6 (9%) 8 8	95, 176, 353, 521	0
48	DY	63/63 (100%)	0.31	5 (7%) 12 12	58, 106, 283, 388	0
49	BZ	58/59 (98%)	0.39	2 (3%) 45 43	67, 93, 170, 515	0
49	DZ	58/59 (98%)	-0.08	1 (1%) 70 68	44, 59, 141, 198	0
50	B0	56/57 (98%)	0.01	2 (3%) 42 40	59, 98, 294, 405	0
50	D0	56/57 (98%)	-0.38	0 100 100	33, 64, 166, 282	0
51	B1	50/55 (90%)	2.29	26 (52%) 0 0	88, 147, 326, 377	0
51	D1	50/55 (90%)	1.93	22 (44%) 0 0	78, 120, 326, 532	0
52	B2	46/46 (100%)	0.19	0 100 100	70, 95, 239, 293	0
52	D2	46/46 (100%)	0.10	1 (2%) 62 60	54, 67, 171, 292	0
53	B3	64/65 (98%)	-0.03	0 100 100	67, 91, 201, 286	0
53	D3	64/65 (98%)	-0.06	0 100 100	47, 61, 161, 254	0
54	B4	38/38 (100%)	0.06	0 100 100	78, 108, 174, 322	0
54	D4	38/38 (100%)	0.19	0 100 100	53, 67, 150, 295	0
55	CY	183/185 (98%)	0.36	19 (10%) 6 6	53, 148, 442, 539	0
All	All	20909/21487 (97%)	0.07	1211 (5%) 23 22	15, 110, 357, 549	0

The worst 5 of 1211 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	BI	66	PHE	15.7
49	BZ	1	ALA	14.3
32	DI	53	PRO	14.1
32	DI	1	ALA	13.8
51	B1	17	GLY	13.4

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	-0.38	0.66	110,110,110,110	0
56	MG	AA	1653	1/1	-0.29	0.63	106,106,106,106	0
56	MG	AA	1648	1/1	-0.09	1.12	116,116,116,116	0
56	MG	DA	3151	1/1	-0.06	1.03	101,101,101,101	0
56	MG	CA	1649	1/1	-0.01	1.11	107,107,107,107	0
56	MG	AA	1650	1/1	-0.01	3.09	118,118,118,118	0
56	MG	DA	3095	1/1	0.01	2.08	116,116,116,116	0
56	MG	DB	204	1/1	0.02	0.88	109,109,109,109	0
56	MG	CA	1617	1/1	0.03	0.39	115,115,115,115	0
56	MG	BA	3007	1/1	0.05	0.67	127,127,127,127	0
56	MG	DA	3192	1/1	0.06	0.48	95,95,95,95	0
56	MG	CA	1651	1/1	0.08	1.06	103,103,103,103	0
56	MG	AA	1633	1/1	0.09	0.37	128,128,128,128	0
56	MG	DB	203	1/1	0.12	0.27	100,100,100,100	0
56	MG	CA	1661	1/1	0.13	0.76	101,101,101,101	0
56	MG	CA	1652	1/1	0.15	0.43	106,106,106,106	0
56	MG	DA	3137	1/1	0.15	0.55	93,93,93,93	0
56	MG	CA	1606	1/1	0.18	0.16	99,99,99,99	0
56	MG	CA	1668	1/1	0.18	0.85	107,107,107,107	0
56	MG	CA	1601	1/1	0.20	0.43	140,140,140,140	0
56	MG	BA	3066	1/1	0.21	0.23	96,96,96,96	0
56	MG	DB	202	1/1	0.23	0.78	122,122,122,122	0
56	MG	BA	3040	1/1	0.23	0.23	112,112,112,112	0
56	MG	BA	3105	1/1	0.23	0.28	91,91,91,91	0
56	MG	CA	1653	1/1	0.24	0.55	99,99,99,99	0
56	MG	BA	3096	1/1	0.24	0.76	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3025	1/1	0.25	0.46	103,103,103,103	0
56	MG	BA	3125	1/1	0.27	0.43	100,100,100,100	0
56	MG	CA	1654	1/1	0.28	1.25	116,116,116,116	0
56	MG	DA	3167	1/1	0.29	0.73	84,84,84,84	0
56	MG	BA	3070	1/1	0.30	0.35	90,90,90,90	0
56	MG	DA	3152	1/1	0.31	0.78	105,105,105,105	0
56	MG	CA	1657	1/1	0.31	1.34	119,119,119,119	0
56	MG	CA	1624	1/1	0.31	0.27	106,106,106,106	0
56	MG	BA	3015	1/1	0.32	0.25	115,115,115,115	0
56	MG	DA	3161	1/1	0.33	0.30	103,103,103,103	0
56	MG	BA	3081	1/1	0.33	0.33	109,109,109,109	0
56	MG	DA	3022	1/1	0.33	0.28	81,81,81,81	0
56	MG	DA	3087	1/1	0.34	0.31	113,113,113,113	0
56	MG	BA	3152	1/1	0.35	0.83	115,115,115,115	0
56	MG	BA	3131	1/1	0.36	0.40	114,114,114,114	0
56	MG	BA	3159	1/1	0.36	0.75	109,109,109,109	0
56	MG	AN	201	1/1	0.37	0.58	133,133,133,133	0
56	MG	DA	3179	1/1	0.38	0.36	113,113,113,113	0
56	MG	DA	3059	1/1	0.38	0.47	92,92,92,92	0
56	MG	CA	1623	1/1	0.38	0.75	117,117,117,117	0
56	MG	BA	3087	1/1	0.38	0.58	112,112,112,112	0
56	MG	CA	1647	1/1	0.38	0.58	112,112,112,112	0
56	MG	AA	1629	1/1	0.39	0.53	118,118,118,118	0
56	MG	DA	3045	1/1	0.39	0.12	95,95,95,95	0
56	MG	CA	1659	1/1	0.39	0.65	110,110,110,110	0
56	MG	CA	1615	1/1	0.40	0.18	112,112,112,112	0
56	MG	BA	3156	1/1	0.40	0.68	106,106,106,106	0
56	MG	DB	201	1/1	0.40	0.22	113,113,113,113	0
56	MG	CA	1603	1/1	0.41	0.27	120,120,120,120	0
56	MG	BC	301	1/1	0.41	0.75	122,122,122,122	0
56	MG	DA	3100	1/1	0.43	0.40	96,96,96,96	0
56	MG	CA	1660	1/1	0.43	0.49	104,104,104,104	0
56	MG	DA	3081	1/1	0.43	1.05	110,110,110,110	0
56	MG	BA	3026	1/1	0.44	0.80	134,134,134,134	0
56	MG	DA	3169	1/1	0.44	0.72	94,94,94,94	0
56	MG	DA	3064	1/1	0.45	0.32	95,95,95,95	0
56	MG	BA	3099	1/1	0.45	0.38	112,112,112,112	0
56	MG	DA	3083	1/1	0.45	0.33	82,82,82,82	0
56	MG	AA	1604	1/1	0.46	0.12	102,102,102,102	0
56	MG	DA	3115	1/1	0.46	0.17	95,95,95,95	0
56	MG	DA	3018	1/1	0.47	0.76	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3097	1/1	0.47	0.64	105,105,105,105	0
56	MG	AA	1623	1/1	0.47	1.08	119,119,119,119	0
56	MG	CA	1608	1/1	0.47	0.41	115,115,115,115	0
56	MG	CA	1609	1/1	0.47	0.32	117,117,117,117	0
56	MG	DA	3171	1/1	0.47	0.38	108,108,108,108	0
56	MG	BA	3069	1/1	0.48	0.58	129,129,129,129	0
56	MG	BA	3126	1/1	0.48	0.30	110,110,110,110	0
56	MG	CA	1633	1/1	0.48	0.80	116,116,116,116	0
56	MG	DA	3012	1/1	0.49	0.26	83,83,83,83	0
56	MG	DA	3102	1/1	0.49	0.63	94,94,94,94	0
56	MG	DA	3076	1/1	0.49	0.26	100,100,100,100	0
56	MG	BA	3110	1/1	0.49	0.44	110,110,110,110	0
56	MG	BA	3124	1/1	0.49	0.19	114,114,114,114	0
56	MG	AA	1603	1/1	0.49	0.20	117,117,117,117	0
56	MG	DA	3057	1/1	0.49	0.84	114,114,114,114	0
56	MG	CA	1629	1/1	0.49	1.02	123,123,123,123	0
56	MG	DA	3073	1/1	0.50	0.27	99,99,99,99	0
56	MG	BA	3095	1/1	0.50	0.35	107,107,107,107	0
56	MG	DA	3134	1/1	0.50	0.35	77,77,77,77	0
56	MG	CA	1620	1/1	0.50	0.26	118,118,118,118	0
56	MG	BA	3123	1/1	0.50	0.49	88,88,88,88	0
56	MG	DA	3172	1/1	0.50	0.45	109,109,109,109	0
56	MG	AA	1646	1/1	0.51	0.63	95,95,95,95	0
56	MG	BA	3022	1/1	0.51	0.73	110,110,110,110	0
56	MG	DA	3003	1/1	0.51	0.15	105,105,105,105	0
56	MG	BA	3071	1/1	0.51	0.31	104,104,104,104	0
56	MG	BA	3068	1/1	0.51	0.23	126,126,126,126	0
56	MG	CA	1616	1/1	0.52	0.14	98,98,98,98	0
56	MG	BA	3075	1/1	0.52	0.40	104,104,104,104	0
56	MG	CA	1665	1/1	0.52	0.40	112,112,112,112	0
56	MG	BA	3149	1/1	0.52	0.67	85,85,85,85	0
56	MG	DA	3069	1/1	0.52	0.31	81,81,81,81	0
56	MG	DA	3061	1/1	0.53	0.63	106,106,106,106	0
56	MG	BA	3006	1/1	0.53	0.10	101,101,101,101	0
56	MG	BA	3013	1/1	0.53	0.54	114,114,114,114	0
56	MG	DA	3060	1/1	0.53	0.27	89,89,89,89	0
56	MG	DA	3182	1/1	0.54	0.34	96,96,96,96	0
56	MG	DA	3055	1/1	0.54	0.36	94,94,94,94	0
56	MG	CA	1631	1/1	0.55	0.47	120,120,120,120	0
56	MG	CA	1670	1/1	0.55	0.69	102,102,102,102	0
56	MG	BA	3107	1/1	0.56	0.45	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	BA	3058	1/1	0.56	0.95	108,108,108,108	0
56	MG	BA	3116	1/1	0.56	0.18	99,99,99,99	0
56	MG	DO	201	1/1	0.56	0.54	109,109,109,109	0
56	MG	BA	3047	1/1	0.57	0.29	103,103,103,103	0
56	MG	CA	1634	1/1	0.57	0.33	120,120,120,120	0
56	MG	CA	1655	1/1	0.57	0.31	117,117,117,117	0
56	MG	AA	1622	1/1	0.57	0.36	107,107,107,107	0
56	MG	DA	3193	1/1	0.57	0.52	95,95,95,95	0
56	MG	DA	3008	1/1	0.58	0.24	88,88,88,88	0
56	MG	BB	201	1/1	0.58	0.21	137,137,137,137	0
56	MG	CA	1627	1/1	0.58	0.32	111,111,111,111	0
56	MG	BA	3052	1/1	0.58	0.20	97,97,97,97	0
56	MG	BA	3092	1/1	0.59	0.25	119,119,119,119	0
56	MG	AA	1632	1/1	0.59	0.20	114,114,114,114	0
56	MG	DA	3123	1/1	0.59	0.33	102,102,102,102	0
56	MG	CA	1605	1/1	0.60	0.17	97,97,97,97	0
56	MG	DA	3127	1/1	0.60	0.32	77,77,77,77	0
56	MG	AD	301	1/1	0.60	0.82	119,119,119,119	0
56	MG	DA	3088	1/1	0.60	0.19	115,115,115,115	0
56	MG	AA	1610	1/1	0.60	0.25	120,120,120,120	0
56	MG	AA	1631	1/1	0.61	0.67	126,126,126,126	0
56	MG	BA	3157	1/1	0.61	1.00	97,97,97,97	0
56	MG	BA	3083	1/1	0.61	0.21	110,110,110,110	0
56	MG	AA	1649	1/1	0.61	1.03	90,90,90,90	0
56	MG	DA	3052	1/1	0.62	0.68	95,95,95,95	0
56	MG	DA	3006	1/1	0.62	0.20	92,92,92,92	0
56	MG	DA	3026	1/1	0.62	0.55	98,98,98,98	0
56	MG	DA	3065	1/1	0.62	0.28	81,81,81,81	0
56	MG	DA	3084	1/1	0.62	0.25	104,104,104,104	0
56	MG	DA	3174	1/1	0.62	0.58	105,105,105,105	0
56	MG	DA	3176	1/1	0.62	0.54	78,78,78,78	0
56	MG	BQ	201	1/1	0.62	1.42	93,93,93,93	0
56	MG	BA	3005	1/1	0.63	0.26	106,106,106,106	0
56	MG	AA	1601	1/1	0.63	0.36	132,132,132,132	0
56	MG	CA	1602	1/1	0.63	0.49	105,105,105,105	0
56	MG	BA	3168	1/1	0.63	0.91	114,114,114,114	0
56	MG	BA	3085	1/1	0.63	0.16	95,95,95,95	0
56	MG	BA	3001	1/1	0.63	0.18	99,99,99,99	0
56	MG	BA	3055	1/1	0.64	0.23	101,101,101,101	0
56	MG	DA	3074	1/1	0.64	0.13	95,95,95,95	0
56	MG	AA	1640	1/1	0.64	0.45	110,110,110,110	0
56	MG	BA	3154	1/1	0.64	0.69	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	3120	1/1	0.64	0.27	94,94,94,94	0
56	MG	BA	3054	1/1	0.64	1.62	119,119,119,119	0
56	MG	BA	3158	1/1	0.64	0.51	106,106,106,106	0
56	MG	DA	3011	1/1	0.65	0.52	103,103,103,103	0
56	MG	BA	3078	1/1	0.65	0.23	119,119,119,119	0
56	MG	DA	3068	1/1	0.65	0.88	117,117,117,117	0
56	MG	BA	3088	1/1	0.65	0.31	101,101,101,101	0
56	MG	AA	1607	1/1	0.65	0.24	116,116,116,116	0
56	MG	BA	3153	1/1	0.65	0.57	112,112,112,112	0
56	MG	DA	3010	1/1	0.65	0.39	106,106,106,106	0
56	MG	DA	3079	1/1	0.65	0.50	99,99,99,99	0
56	MG	BA	3146	1/1	0.66	0.36	98,98,98,98	0
56	MG	CA	1656	1/1	0.66	0.56	106,106,106,106	0
56	MG	DA	3094	1/1	0.66	0.35	87,87,87,87	0
56	MG	DA	3131	1/1	0.66	0.65	118,118,118,118	0
56	MG	BA	3148	1/1	0.66	0.47	101,101,101,101	0
56	MG	BA	3155	1/1	0.66	0.88	114,114,114,114	0
56	MG	BA	3009	1/1	0.66	0.30	95,95,95,95	0
56	MG	BA	3143	1/1	0.66	0.53	103,103,103,103	0
56	MG	CA	1638	1/1	0.67	0.70	113,113,113,113	0
56	MG	AA	1641	1/1	0.67	0.42	105,105,105,105	0
56	MG	DA	3142	1/1	0.67	0.19	86,86,86,86	0
56	MG	AA	1626	1/1	0.67	0.58	111,111,111,111	0
56	MG	BA	3019	1/1	0.67	0.22	101,101,101,101	0
56	MG	BA	3114	1/1	0.67	0.28	120,120,120,120	0
56	MG	BA	3012	1/1	0.67	0.99	118,118,118,118	0
56	MG	BA	3142	1/1	0.68	0.49	103,103,103,103	0
56	MG	CA	1632	1/1	0.68	1.22	128,128,128,128	0
56	MG	BA	3041	1/1	0.68	0.16	96,96,96,96	0
56	MG	DA	3023	1/1	0.68	0.69	120,120,120,120	0
56	MG	DA	3139	1/1	0.68	0.56	77,77,77,77	0
56	MG	DA	3072	1/1	0.68	0.36	93,93,93,93	0
56	MG	AA	1647	1/1	0.68	0.23	109,109,109,109	0
56	MG	BA	3003	1/1	0.68	0.23	115,115,115,115	0
56	MG	CX	101	1/1	0.69	1.13	112,112,112,112	0
56	MG	CA	1645	1/1	0.69	0.42	96,96,96,96	0
56	MG	AA	1628	1/1	0.69	0.36	116,116,116,116	0
56	MG	BA	3072	1/1	0.70	0.30	103,103,103,103	0
56	MG	AA	1614	1/1	0.70	0.47	123,123,123,123	0
56	MG	CA	1626	1/1	0.70	0.40	99,99,99,99	0
56	MG	BA	3129	1/1	0.70	0.63	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3150	1/1	0.70	0.70	78,78,78,78	0
56	MG	AA	1617	1/1	0.70	0.46	112,112,112,112	0
56	MG	DA	3035	1/1	0.70	0.24	94,94,94,94	0
56	MG	AA	1613	1/1	0.70	0.25	115,115,115,115	0
56	MG	DA	3166	1/1	0.70	0.83	87,87,87,87	0
56	MG	BA	3160	1/1	0.70	0.50	102,102,102,102	0
56	MG	DA	3129	1/1	0.70	1.85	124,124,124,124	0
56	MG	BA	3018	1/1	0.70	0.77	118,118,118,118	0
56	MG	DA	3066	1/1	0.71	0.23	90,90,90,90	0
56	MG	BA	3032	1/1	0.71	0.67	110,110,110,110	0
56	MG	CA	1628	1/1	0.71	0.34	116,116,116,116	0
56	MG	DA	3156	1/1	0.71	0.40	101,101,101,101	0
56	MG	DA	3025	1/1	0.71	0.77	118,118,118,118	0
56	MG	AA	1627	1/1	0.71	0.48	121,121,121,121	0
56	MG	CA	1637	1/1	0.71	0.97	139,139,139,139	0
56	MG	DA	3062	1/1	0.71	0.18	76,76,76,76	0
56	MG	DA	3170	1/1	0.71	0.42	94,94,94,94	0
56	MG	AA	1651	1/1	0.71	0.22	119,119,119,119	0
56	MG	CA	1639	1/1	0.71	0.12	94,94,94,94	0
56	MG	DA	3040	1/1	0.72	0.21	91,91,91,91	0
56	MG	BA	3004	1/1	0.72	0.20	120,120,120,120	0
56	MG	CA	1613	1/1	0.72	0.16	103,103,103,103	0
56	MG	BA	3030	1/1	0.72	0.32	94,94,94,94	0
56	MG	AA	1616	1/1	0.72	0.49	113,113,113,113	0
57	NMY	DA	3190	42/42	0.72	0.42	57,66,70,74	42
56	MG	DA	3046	1/1	0.73	0.15	86,86,86,86	0
56	MG	BA	3122	1/1	0.73	0.30	112,112,112,112	0
56	MG	BA	3100	1/1	0.73	0.36	107,107,107,107	0
56	MG	BA	3090	1/1	0.73	0.68	130,130,130,130	0
56	MG	DA	3130	1/1	0.73	0.27	96,96,96,96	0
56	MG	CA	1607	1/1	0.73	0.58	110,110,110,110	0
56	MG	BA	3057	1/1	0.73	0.19	98,98,98,98	0
56	MG	DA	3020	1/1	0.73	0.27	93,93,93,93	0
56	MG	BA	3021	1/1	0.73	0.29	108,108,108,108	0
56	MG	DA	3140	1/1	0.73	0.32	98,98,98,98	0
56	MG	CA	1611	1/1	0.73	0.17	110,110,110,110	0
56	MG	BA	3059	1/1	0.73	1.36	122,122,122,122	0
56	MG	BA	3098	1/1	0.73	0.36	100,100,100,100	0
56	MG	BA	3118	1/1	0.73	0.45	109,109,109,109	0
56	MG	DA	3098	1/1	0.73	0.24	99,99,99,99	0
56	MG	BA	3027	1/1	0.73	1.53	108,108,108,108	0
56	MG	DA	3007	1/1	0.73	0.23	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	1610	1/1	0.74	0.26	102,102,102,102	0
56	MG	DA	3155	1/1	0.74	0.22	115,115,115,115	0
56	MG	BA	3108	1/1	0.74	0.31	99,99,99,99	0
56	MG	BA	3121	1/1	0.74	0.34	110,110,110,110	0
56	MG	BA	3050	1/1	0.74	0.38	101,101,101,101	0
56	MG	BA	3061	1/1	0.74	0.29	85,85,85,85	0
56	MG	BA	3115	1/1	0.74	0.30	105,105,105,105	0
56	MG	DA	3108	1/1	0.74	0.29	100,100,100,100	0
56	MG	DA	3004	1/1	0.74	0.38	99,99,99,99	0
56	MG	AA	1619	1/1	0.74	0.22	95,95,95,95	0
56	MG	AA	1644	1/1	0.74	0.41	106,106,106,106	0
56	MG	CA	1612	1/1	0.75	0.40	116,116,116,116	0
56	MG	DA	3034	1/1	0.75	0.17	84,84,84,84	0
56	MG	DA	3194	1/1	0.75	0.56	90,90,90,90	0
56	MG	BA	3034	1/1	0.76	0.16	88,88,88,88	0
56	MG	DA	3092	1/1	0.76	0.33	95,95,95,95	0
56	MG	AA	1609	1/1	0.76	0.34	111,111,111,111	0
56	MG	CA	1621	1/1	0.76	0.18	111,111,111,111	0
56	MG	BA	3053	1/1	0.76	0.65	98,98,98,98	0
56	MG	AA	1625	1/1	0.76	0.79	117,117,117,117	0
56	MG	BA	3102	1/1	0.76	0.54	119,119,119,119	0
56	MG	DA	3138	1/1	0.76	0.73	81,81,81,81	0
56	MG	BA	3017	1/1	0.76	0.14	107,107,107,107	0
56	MG	BA	3117	1/1	0.76	0.15	89,89,89,89	0
56	MG	DA	3071	1/1	0.76	0.42	97,97,97,97	0
56	MG	DA	3119	1/1	0.76	0.23	82,82,82,82	0
56	MG	CA	1636	1/1	0.77	1.24	134,134,134,134	0
56	MG	BA	3138	1/1	0.77	0.71	88,88,88,88	0
56	MG	DA	3030	1/1	0.77	0.20	76,76,76,76	0
56	MG	BA	3091	1/1	0.77	0.36	115,115,115,115	0
56	MG	DA	3164	1/1	0.77	0.67	94,94,94,94	0
56	MG	DA	3110	1/1	0.77	0.26	93,93,93,93	0
56	MG	DA	3024	1/1	0.77	0.24	73,73,73,73	0
56	MG	DA	3116	1/1	0.77	0.20	107,107,107,107	0
56	MG	DA	3050	1/1	0.78	0.23	86,86,86,86	0
56	MG	DA	3107	1/1	0.78	0.44	98,98,98,98	0
56	MG	BA	3082	1/1	0.78	0.43	126,126,126,126	0
56	MG	DA	3128	1/1	0.78	0.20	92,92,92,92	0
56	MG	CA	1618	1/1	0.78	0.39	83,83,83,83	0
56	MG	CA	1635	1/1	0.78	0.20	113,113,113,113	0
56	MG	DA	3148	1/1	0.78	0.38	60,60,60,60	0
56	MG	DA	3180	1/1	0.78	0.41	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	3082	1/1	0.78	0.26	92,92,92,92	0
56	MG	BA	3056	1/1	0.79	0.18	99,99,99,99	0
56	MG	DA	3173	1/1	0.79	0.47	90,90,90,90	0
56	MG	BA	3079	1/1	0.79	0.60	103,103,103,103	0
56	MG	DA	3121	1/1	0.79	0.27	86,86,86,86	0
56	MG	AA	1639	1/1	0.79	0.94	113,113,113,113	0
56	MG	DA	3096	1/1	0.79	0.25	75,75,75,75	0
56	MG	AA	1606	1/1	0.79	0.34	111,111,111,111	0
56	MG	AA	1645	1/1	0.79	0.34	93,93,93,93	0
56	MG	BA	3024	1/1	0.80	0.60	114,114,114,114	0
56	MG	AA	1605	1/1	0.80	0.36	121,121,121,121	0
56	MG	DA	3039	1/1	0.80	0.33	117,117,117,117	0
56	MG	BA	3145	1/1	0.80	0.42	99,99,99,99	0
56	MG	DA	3021	1/1	0.80	0.37	108,108,108,108	0
56	MG	DA	3191	1/1	0.80	0.14	80,80,80,80	0
56	MG	AA	1602	1/1	0.80	0.51	106,106,106,106	0
56	MG	DA	3165	1/1	0.80	0.67	78,78,78,78	0
56	MG	DA	3109	1/1	0.80	0.24	102,102,102,102	0
56	MG	BA	3023	1/1	0.80	0.37	108,108,108,108	0
56	MG	CA	1622	1/1	0.80	0.29	108,108,108,108	0
56	MG	BA	3133	1/1	0.80	0.36	106,106,106,106	0
56	MG	DA	3056	1/1	0.80	0.16	86,86,86,86	0
56	MG	BA	3134	1/1	0.80	0.26	109,109,109,109	0
57	NMY	AA	1657	42/42	0.80	0.28	81,84,88,90	42
57	NMY	BA	3167	42/42	0.80	0.31	117,120,124,125	42
56	MG	BA	3112	1/1	0.80	0.36	101,101,101,101	0
56	MG	AA	1630	1/1	0.81	0.31	105,105,105,105	0
56	MG	DA	3042	1/1	0.81	0.71	105,105,105,105	0
56	MG	BA	3020	1/1	0.81	0.28	95,95,95,95	0
56	MG	DA	3162	1/1	0.81	0.34	95,95,95,95	0
56	MG	CA	1643	1/1	0.81	0.41	103,103,103,103	0
56	MG	BA	3151	1/1	0.81	0.66	92,92,92,92	0
56	MG	AA	1638	1/1	0.81	0.75	104,104,104,104	0
56	MG	DA	3111	1/1	0.81	0.44	102,102,102,102	0
56	MG	AA	1612	1/1	0.81	0.13	107,107,107,107	0
56	MG	BA	3109	1/1	0.81	0.38	106,106,106,106	0
56	MG	CA	1663	1/1	0.81	0.43	82,82,82,82	0
56	MG	AA	1618	1/1	0.81	0.27	96,96,96,96	0
56	MG	DA	3122	1/1	0.81	0.28	97,97,97,97	0
57	NMY	BA	3163	42/42	0.81	0.29	89,98,100,101	42
56	MG	CA	1667	1/1	0.81	0.65	111,111,111,111	0
56	MG	BA	3011	1/1	0.81	0.43	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3060	1/1	0.82	0.41	106,106,106,106	0
56	MG	DA	3085	1/1	0.82	0.48	108,108,108,108	0
56	MG	DA	3086	1/1	0.82	0.11	97,97,97,97	0
56	MG	DA	3051	1/1	0.82	0.27	86,86,86,86	0
56	MG	DA	3077	1/1	0.82	0.41	98,98,98,98	0
56	MG	DA	3177	1/1	0.82	0.51	96,96,96,96	0
56	MG	DL	201	1/1	0.82	0.81	110,110,110,110	0
56	MG	DA	3090	1/1	0.82	0.23	107,107,107,107	0
56	MG	AA	1642	1/1	0.82	0.23	94,94,94,94	0
56	MG	AA	1636	1/1	0.82	0.37	103,103,103,103	0
57	NMY	BA	3165	42/42	0.82	0.30	79,84,87,90	42
56	MG	CA	1648	1/1	0.82	0.41	103,103,103,103	0
56	MG	BA	3086	1/1	0.82	0.12	109,109,109,109	0
56	MG	DA	3118	1/1	0.83	0.28	88,88,88,88	0
56	MG	BA	3062	1/1	0.83	0.47	91,91,91,91	0
56	MG	DA	3053	1/1	0.83	0.19	93,93,93,93	0
56	MG	BA	3106	1/1	0.83	0.36	100,100,100,100	0
56	MG	BA	3048	1/1	0.83	0.09	93,93,93,93	0
56	MG	BA	3139	1/1	0.83	0.77	83,83,83,83	0
56	MG	DA	3036	1/1	0.83	0.30	90,90,90,90	0
56	MG	AA	1615	1/1	0.83	0.14	112,112,112,112	0
56	MG	BA	3073	1/1	0.83	0.15	101,101,101,101	0
56	MG	DA	3105	1/1	0.83	0.40	90,90,90,90	0
56	MG	BB	202	1/1	0.83	0.69	123,123,123,123	0
56	MG	DA	3043	1/1	0.83	0.14	90,90,90,90	0
56	MG	DA	3044	1/1	0.83	0.36	105,105,105,105	0
56	MG	CA	1619	1/1	0.83	0.13	93,93,93,93	0
56	MG	CA	1658	1/1	0.83	0.64	115,115,115,115	0
57	NMY	BA	3164	42/42	0.83	0.33	90,100,104,105	42
56	MG	DA	3112	1/1	0.83	0.26	108,108,108,108	0
56	MG	AA	1652	1/1	0.83	0.37	101,101,101,101	0
56	MG	BA	3077	1/1	0.83	0.52	121,121,121,121	0
56	MG	DA	3153	1/1	0.84	0.21	95,95,95,95	0
56	MG	DE	301	1/1	0.84	0.12	100,100,100,100	0
56	MG	BA	3016	1/1	0.84	0.17	83,83,83,83	0
56	MG	CA	1625	1/1	0.84	0.20	107,107,107,107	0
57	NMY	AA	1656	42/42	0.84	0.30	94,99,103,104	42
56	MG	DA	3104	1/1	0.84	0.20	81,81,81,81	0
56	MG	BA	3132	1/1	0.84	0.18	96,96,96,96	0
56	MG	BA	3067	1/1	0.84	0.11	89,89,89,89	0
56	MG	BA	3044	1/1	0.84	0.32	114,114,114,114	0
56	MG	CA	1669	1/1	0.84	0.35	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3029	1/1	0.84	0.24	84,84,84,84	0
56	MG	DA	3049	1/1	0.85	0.31	97,97,97,97	0
56	MG	DA	3028	1/1	0.85	0.31	85,85,85,85	0
56	MG	DA	3070	1/1	0.85	0.23	56,56,56,56	0
56	MG	BA	3049	1/1	0.85	0.28	88,88,88,88	0
56	MG	CA	1650	1/1	0.85	0.50	102,102,102,102	0
56	MG	DA	3032	1/1	0.85	0.52	97,97,97,97	0
56	MG	BA	3103	1/1	0.85	0.94	105,105,105,105	0
56	MG	BA	3144	1/1	0.85	0.40	87,87,87,87	0
56	MG	AA	1643	1/1	0.85	0.18	110,110,110,110	0
56	MG	DA	3101	1/1	0.85	0.36	86,86,86,86	0
56	MG	BA	3051	1/1	0.85	0.38	106,106,106,106	0
56	MG	DA	3103	1/1	0.85	0.35	81,81,81,81	0
56	MG	CA	1642	1/1	0.85	0.29	106,106,106,106	0
56	MG	DA	3132	1/1	0.85	0.15	96,96,96,96	0
56	MG	BA	3147	1/1	0.85	0.52	95,95,95,95	0
56	MG	BA	3089	1/1	0.85	0.19	109,109,109,109	0
57	NMY	BA	3162	42/42	0.85	0.26	65,79,86,93	42
56	MG	CA	1646	1/1	0.85	0.32	95,95,95,95	0
56	MG	AA	1624	1/1	0.85	0.40	110,110,110,110	0
56	MG	AA	1621	1/1	0.85	0.40	116,116,116,116	0
56	MG	DA	3067	1/1	0.85	0.38	120,120,120,120	0
56	MG	DA	3145	1/1	0.85	0.41	91,91,91,91	0
56	MG	DA	3031	1/1	0.86	0.28	108,108,108,108	0
56	MG	BA	3064	1/1	0.86	0.18	96,96,96,96	0
56	MG	BA	3111	1/1	0.86	0.25	98,98,98,98	0
56	MG	BA	3169	1/1	0.86	0.29	101,101,101,101	0
56	MG	CA	1664	1/1	0.86	0.30	112,112,112,112	0
56	MG	DA	3154	1/1	0.86	0.67	86,86,86,86	0
56	MG	DA	3117	1/1	0.86	0.18	93,93,93,93	0
56	MG	BA	3031	1/1	0.86	0.24	87,87,87,87	0
56	MG	DA	3157	1/1	0.86	0.38	96,96,96,96	0
57	NMY	BA	3161	42/42	0.86	0.25	61,70,77,82	42
56	MG	DA	3014	1/1	0.86	0.23	90,90,90,90	0
56	MG	DA	3078	1/1	0.86	0.19	84,84,84,84	0
56	MG	DA	3015	1/1	0.86	0.76	124,124,124,124	0
56	MG	CA	1666	1/1	0.86	0.24	112,112,112,112	0
57	NMY	BA	3166	42/42	0.86	0.25	68,77,83,90	42
56	MG	BA	3127	1/1	0.86	0.42	95,95,95,95	0
56	MG	DA	3146	1/1	0.86	0.37	76,76,76,76	0
56	MG	DA	3017	1/1	0.87	0.25	76,76,76,76	0
56	MG	DA	3135	1/1	0.87	0.21	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3009	1/1	0.87	0.36	102,102,102,102	0
56	MG	DA	3002	1/1	0.87	0.08	86,86,86,86	0
56	MG	DA	3113	1/1	0.87	0.48	106,106,106,106	0
56	MG	BA	3074	1/1	0.87	0.36	115,115,115,115	0
56	MG	DA	3016	1/1	0.87	0.21	103,103,103,103	0
56	MG	DA	3048	1/1	0.88	0.35	96,96,96,96	0
56	MG	BA	3076	1/1	0.88	0.37	120,120,120,120	0
56	MG	DA	3163	1/1	0.88	0.26	99,99,99,99	0
56	MG	DA	3037	1/1	0.88	0.25	72,72,72,72	0
56	MG	BA	3014	1/1	0.88	0.63	106,106,106,106	0
56	MG	BA	3097	1/1	0.88	1.23	111,111,111,111	0
56	MG	BA	3170	1/1	0.88	0.39	88,88,88,88	0
56	MG	BA	3043	1/1	0.88	0.19	108,108,108,108	0
56	MG	BA	3136	1/1	0.88	0.49	94,94,94,94	0
56	MG	CA	1614	1/1	0.88	0.21	120,120,120,120	0
56	MG	BA	3093	1/1	0.88	0.51	109,109,109,109	0
56	MG	DA	3047	1/1	0.88	0.20	76,76,76,76	0
57	NMY	DA	3184	42/42	0.88	0.25	57,71,80,89	42
56	MG	DA	3159	1/1	0.88	0.53	90,90,90,90	0
56	MG	BA	3036	1/1	0.89	0.14	95,95,95,95	0
56	MG	BA	3063	1/1	0.89	0.64	106,106,106,106	0
56	MG	DA	3001	1/1	0.89	0.12	91,91,91,91	0
56	MG	DA	3136	1/1	0.89	0.55	74,74,74,74	0
56	MG	DA	3106	1/1	0.89	0.52	100,100,100,100	0
57	NMY	AA	1655	42/42	0.89	0.21	61,73,90,121	0
56	MG	DA	3120	1/1	0.89	0.22	98,98,98,98	0
56	MG	AA	1620	1/1	0.89	0.25	118,118,118,118	0
56	MG	DA	3160	1/1	0.89	0.77	92,92,92,92	0
56	MG	BA	3135	1/1	0.89	0.72	74,74,74,74	0
56	MG	BB	203	1/1	0.89	0.13	107,107,107,107	0
56	MG	BA	3119	1/1	0.89	0.20	106,106,106,106	0
56	MG	BA	3065	1/1	0.89	0.31	101,101,101,101	0
56	MG	BA	3029	1/1	0.89	0.23	99,99,99,99	0
56	MG	DA	3149	1/1	0.89	0.33	107,107,107,107	0
56	MG	BA	3141	1/1	0.89	0.13	114,114,114,114	0
56	MG	BA	3010	1/1	0.89	0.12	85,85,85,85	0
56	MG	CA	1641	1/1	0.90	0.22	85,85,85,85	0
56	MG	BA	3008	1/1	0.90	0.30	107,107,107,107	0
56	MG	AA	1637	1/1	0.90	0.23	103,103,103,103	0
56	MG	DA	3005	1/1	0.90	0.16	88,88,88,88	0
56	MG	DA	3054	1/1	0.90	0.25	93,93,93,93	0
56	MG	AA	1635	1/1	0.90	0.25	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	DA	3183	1/1	0.90	0.53	87,87,87,87	0
56	MG	BA	3137	1/1	0.90	0.39	82,82,82,82	0
56	MG	DA	3075	1/1	0.90	0.42	106,106,106,106	0
57	NMY	DA	3187	42/42	0.90	0.32	106,109,112,114	42
56	MG	BA	3128	1/1	0.90	0.12	94,94,94,94	0
56	MG	BA	3130	1/1	0.91	0.59	103,103,103,103	0
56	MG	DA	3019	1/1	0.91	0.29	78,78,78,78	0
56	MG	DA	3013	1/1	0.91	0.47	107,107,107,107	0
56	MG	BA	3046	1/1	0.91	0.18	109,109,109,109	0
56	MG	DA	3147	1/1	0.91	0.82	107,107,107,107	0
56	MG	CA	1630	1/1	0.91	0.24	118,118,118,118	0
56	MG	BA	3033	1/1	0.91	0.51	98,98,98,98	0
56	MG	DA	3041	1/1	0.91	0.11	81,81,81,81	0
56	MG	CA	1640	1/1	0.91	0.99	114,114,114,114	0
56	MG	DA	3033	1/1	0.91	0.15	91,91,91,91	0
57	NMY	DA	3185	42/42	0.91	0.22	46,58,63,67	42
57	NMY	DA	3186	42/42	0.91	0.27	53,58,64,71	42
56	MG	DA	3124	1/1	0.91	0.26	78,78,78,78	0
57	NMY	DA	3189	42/42	0.91	0.23	55,63,70,72	42
56	MG	DA	3114	1/1	0.91	0.18	77,77,77,77	0
56	MG	DA	3091	1/1	0.92	0.23	104,104,104,104	0
56	MG	CA	1671	1/1	0.92	0.28	96,96,96,96	0
56	MG	DA	3093	1/1	0.92	0.62	105,105,105,105	0
56	MG	DA	3027	1/1	0.92	0.17	79,79,79,79	0
56	MG	BA	3035	1/1	0.92	0.19	94,94,94,94	0
56	MG	BA	3150	1/1	0.92	0.62	95,95,95,95	0
57	NMY	CA	1672	42/42	0.92	0.24	54,65,74,77	42
56	MG	BA	3045	1/1	0.92	0.16	118,118,118,118	0
56	MG	AA	1608	1/1	0.92	0.38	114,114,114,114	0
56	MG	BA	3094	1/1	0.92	0.23	92,92,92,92	0
56	MG	BA	3084	1/1	0.92	0.19	95,95,95,95	0
56	MG	CA	1644	1/1	0.92	1.24	118,118,118,118	0
56	MG	BA	3038	1/1	0.92	0.21	104,104,104,104	0
56	MG	DA	3133	1/1	0.93	0.22	100,100,100,100	0
56	MG	BA	3080	1/1	0.93	0.15	73,73,73,73	0
56	MG	DA	3158	1/1	0.93	0.29	91,91,91,91	0
56	MG	BA	3140	1/1	0.93	0.22	101,101,101,101	0
56	MG	DA	3181	1/1	0.93	0.39	77,77,77,77	0
56	MG	BA	3101	1/1	0.93	0.54	102,102,102,102	0
56	MG	BA	3104	1/1	0.93	0.59	106,106,106,106	0
56	MG	AA	1611	1/1	0.94	0.07	104,104,104,104	0
56	MG	DA	3125	1/1	0.94	0.19	113,113,113,113	0

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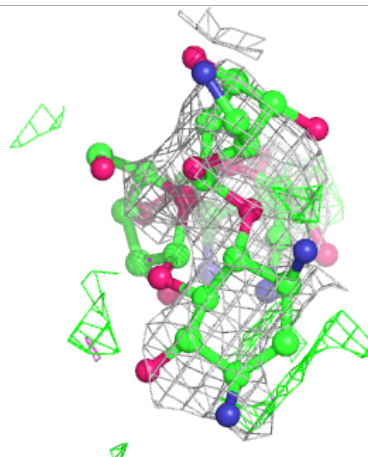
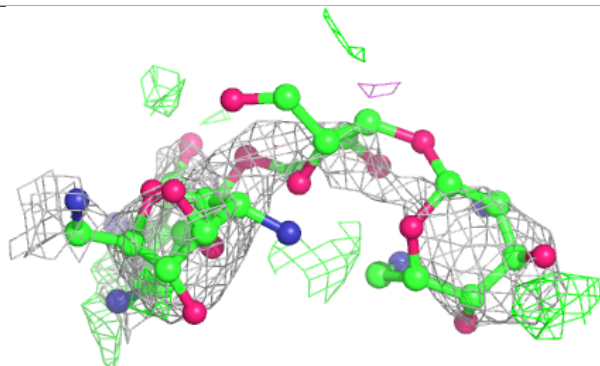
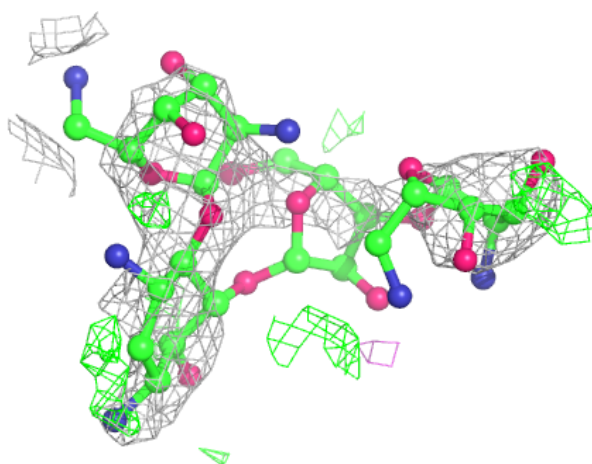
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3113	1/1	0.94	0.41	121,121,121,121	0
56	MG	DA	3080	1/1	0.94	0.31	100,100,100,100	0
56	MG	CA	1604	1/1	0.94	0.10	86,86,86,86	0
57	NMY	DA	3188	42/42	0.94	0.21	45,60,66,70	42
56	MG	DA	3168	1/1	0.94	0.20	89,89,89,89	0
56	MG	DA	3175	1/1	0.94	0.71	75,75,75,75	0
58	ZN	D4	101	1/1	0.94	0.44	162,162,162,162	0
56	MG	DA	3038	1/1	0.95	0.25	81,81,81,81	0
56	MG	BA	3037	1/1	0.95	0.75	97,97,97,97	0
56	MG	DA	3143	1/1	0.95	1.31	79,79,79,79	0
56	MG	DA	3144	1/1	0.95	0.19	108,108,108,108	0
56	MG	AA	1634	1/1	0.95	0.51	120,120,120,120	0
56	MG	BA	3042	1/1	0.95	0.10	97,97,97,97	0
56	MG	DA	3126	1/1	0.95	0.14	60,60,60,60	0
58	ZN	B4	101	1/1	0.95	0.19	186,186,186,186	0
56	MG	DA	3058	1/1	0.95	0.43	96,96,96,96	0
56	MG	DA	3089	1/1	0.96	0.12	97,97,97,97	0
56	MG	DA	3099	1/1	0.96	0.17	90,90,90,90	0
56	MG	BA	3039	1/1	0.96	0.15	96,96,96,96	0
56	MG	DA	3141	1/1	0.96	0.73	73,73,73,73	0
56	MG	BA	3028	1/1	0.96	0.28	89,89,89,89	0
56	MG	DA	3178	1/1	0.96	0.23	88,88,88,88	0
56	MG	CA	1662	1/1	0.97	0.12	114,114,114,114	0
56	MG	DA	3063	1/1	0.97	0.10	69,69,69,69	0
56	MG	BA	3002	1/1	0.97	0.16	89,89,89,89	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.

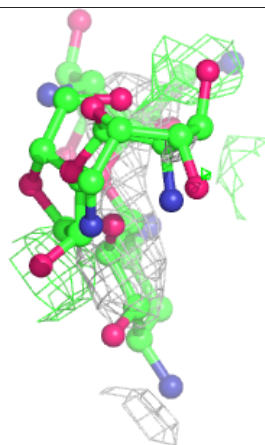
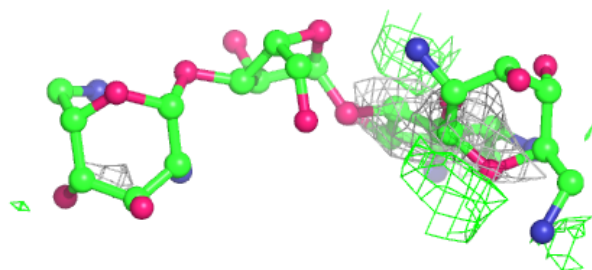
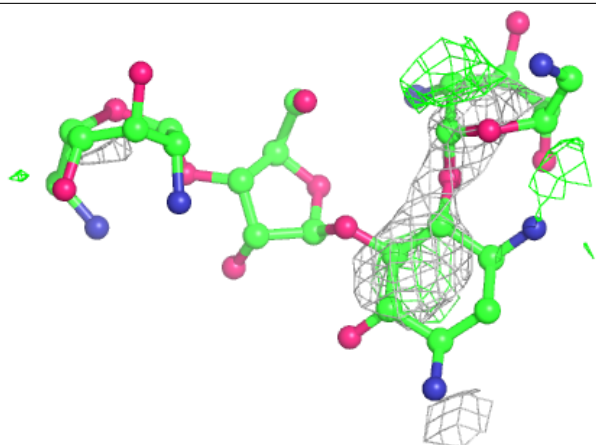
Electron density around NMY DA 3190:

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



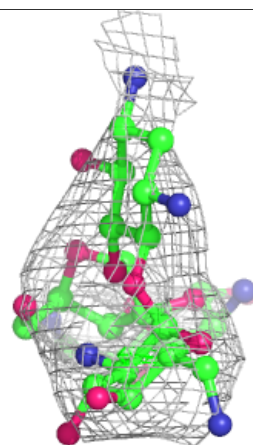
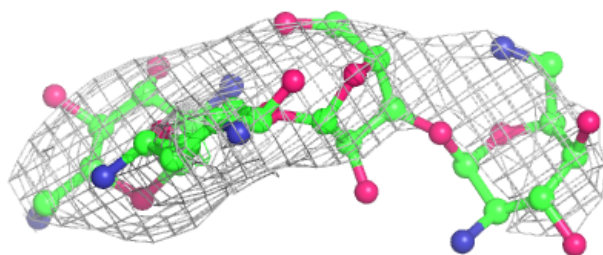
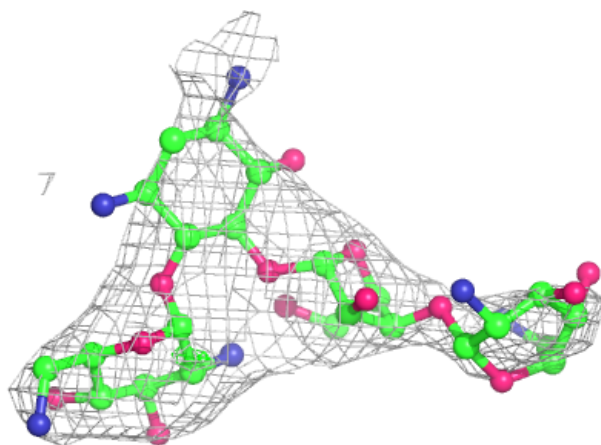
Electron density around NMY AA 1657:

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



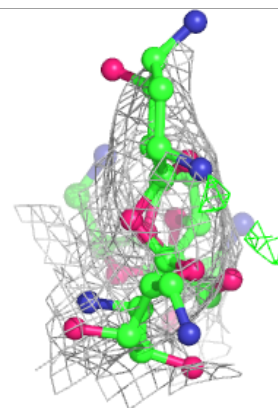
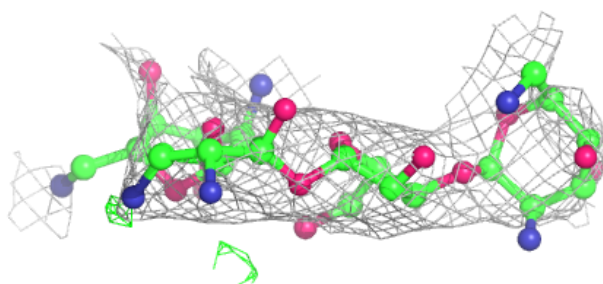
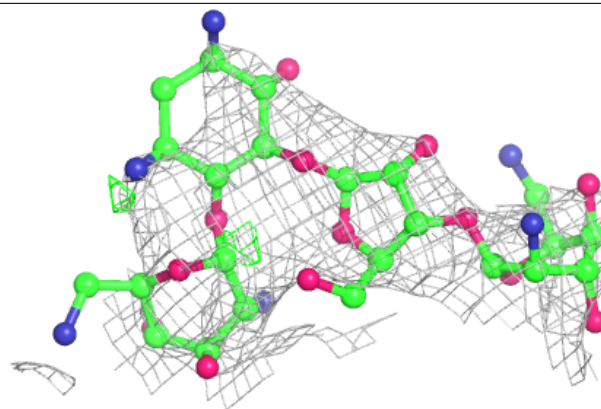
Electron density around NMY BA 3167:

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

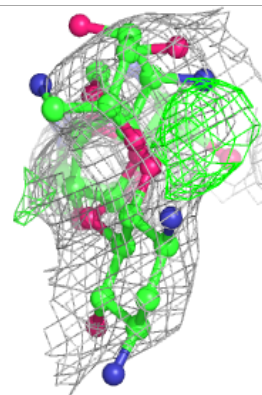
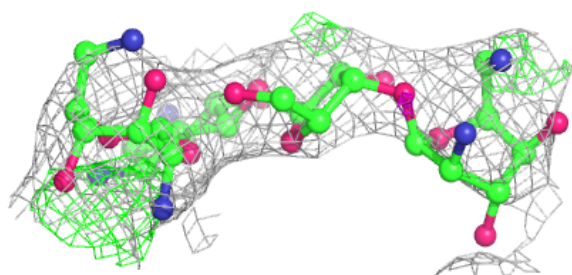
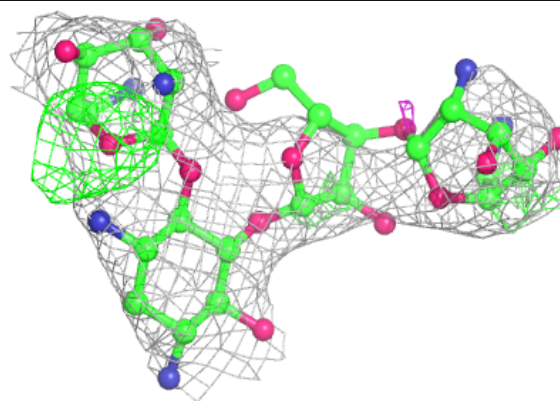


Electron density around NMY BA 3163:

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

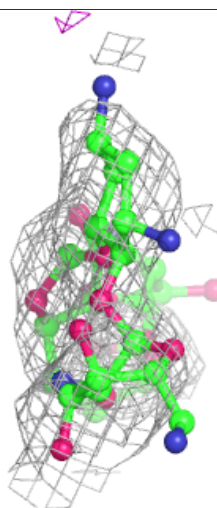
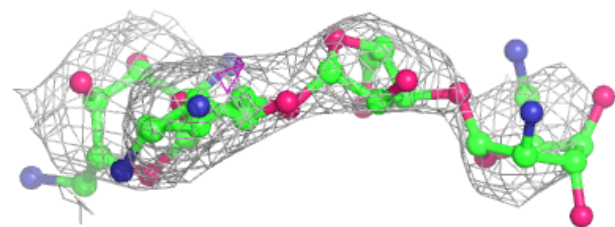
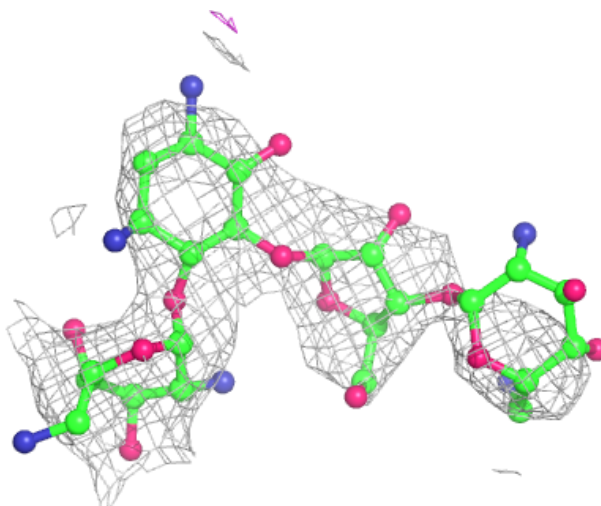
**Electron density around NMY BA 3165:**

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



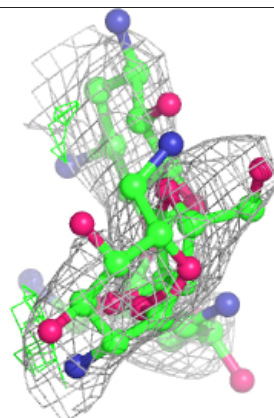
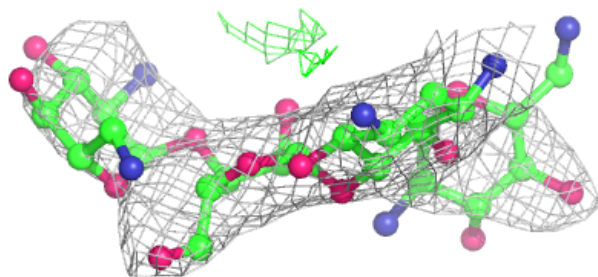
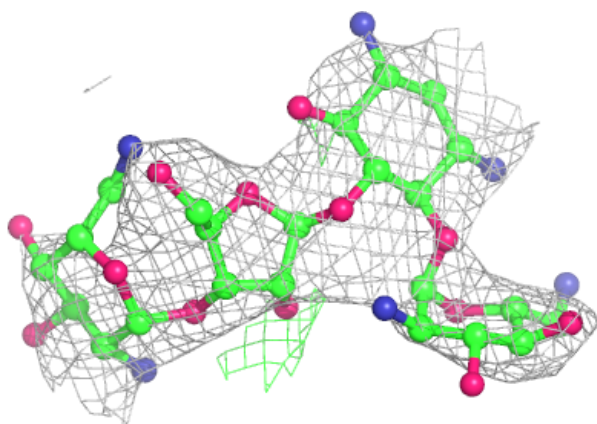
Electron density around NMY BA 3164:

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



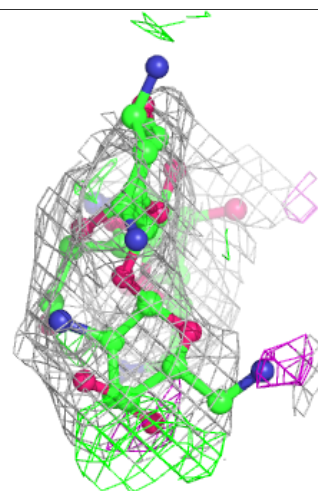
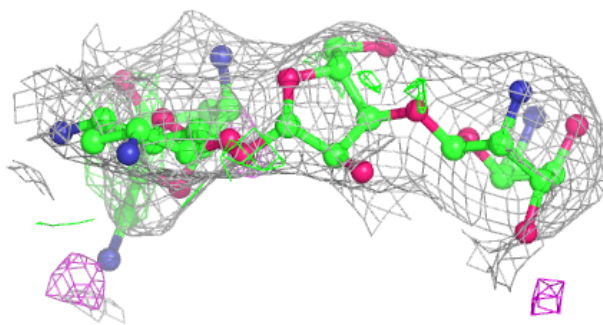
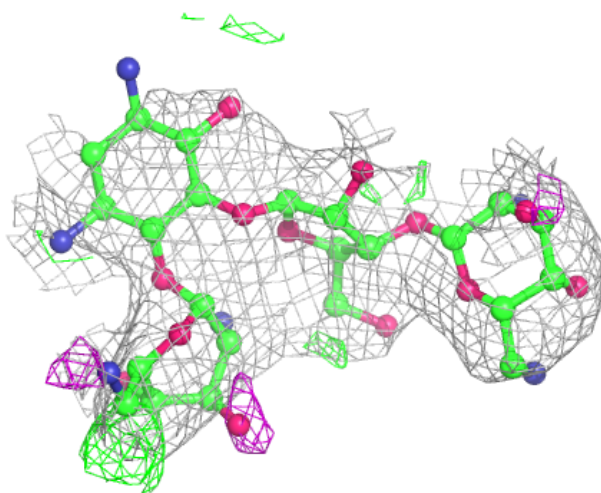
Electron density around NMY AA 1656:

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



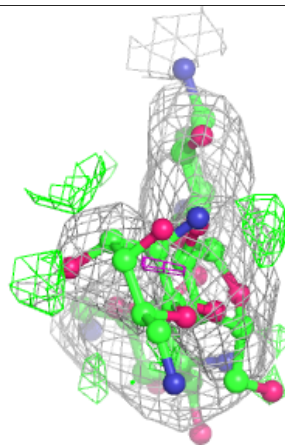
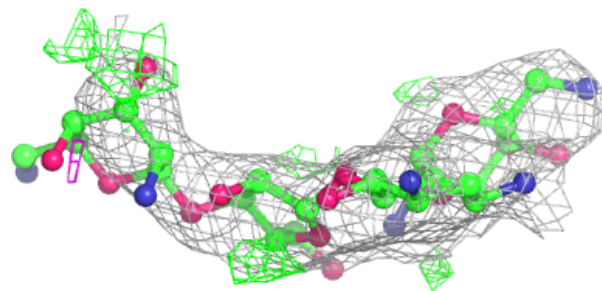
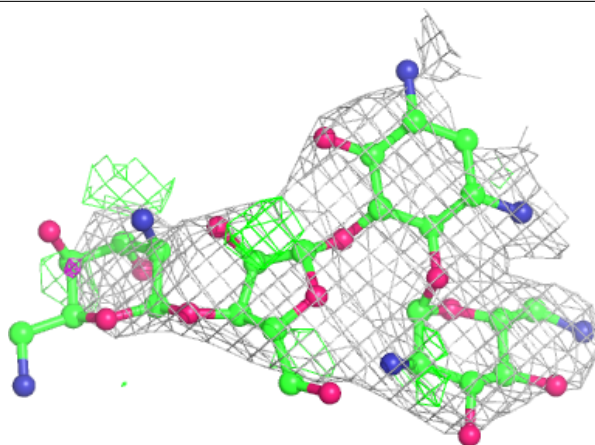
Electron density around NMY BA 3162:

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



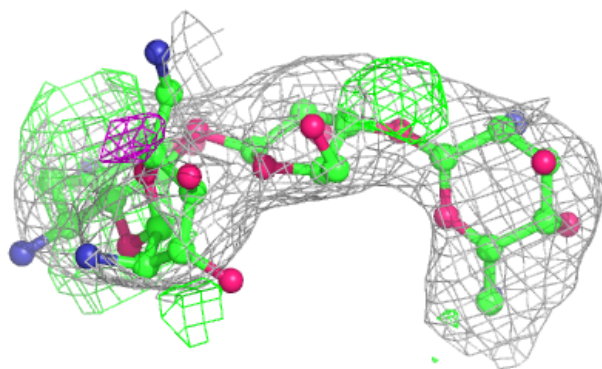
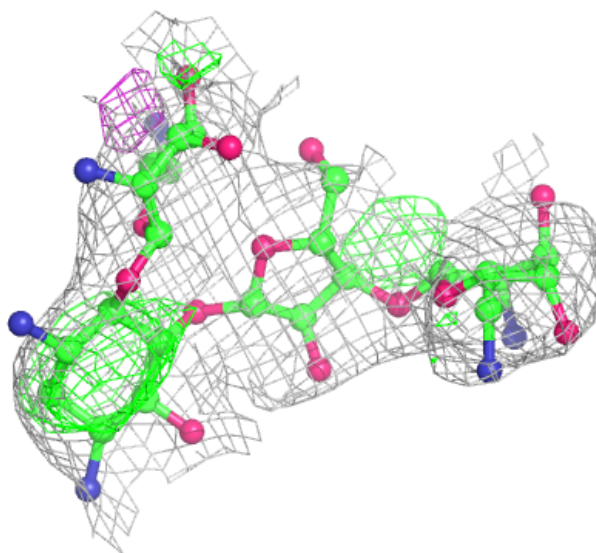
Electron density around NMY BA 3161:

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



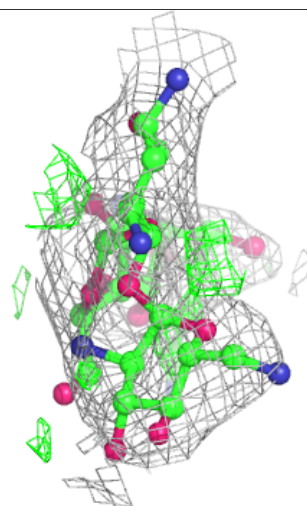
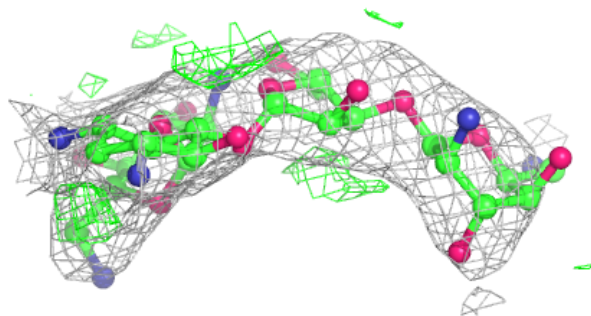
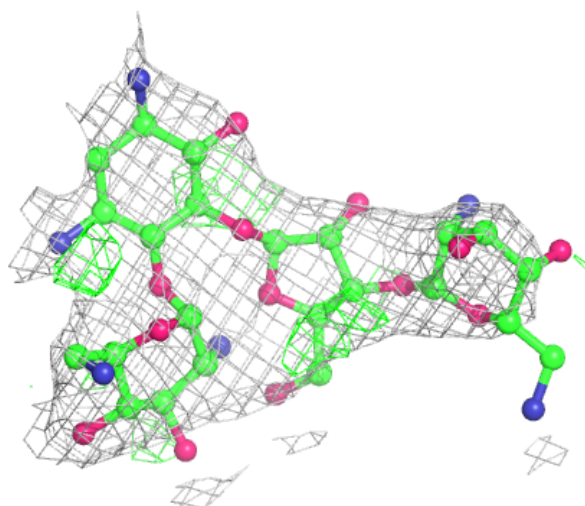
Electron density around NMY BA 3166:

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



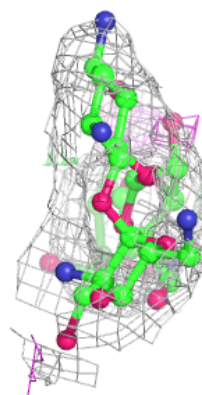
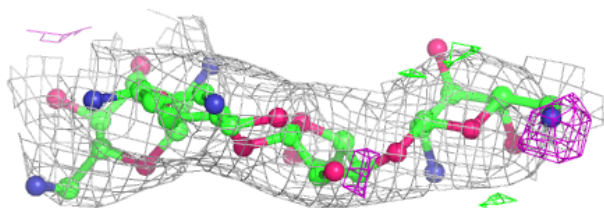
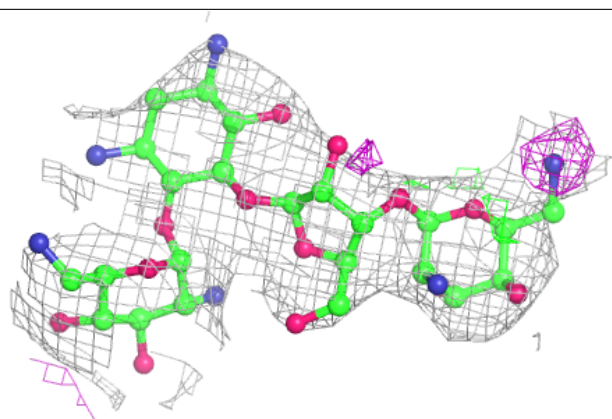
Electron density around NMY DA 3184:

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



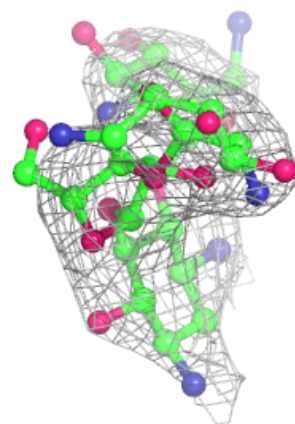
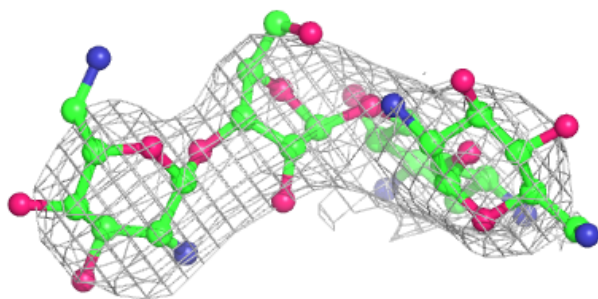
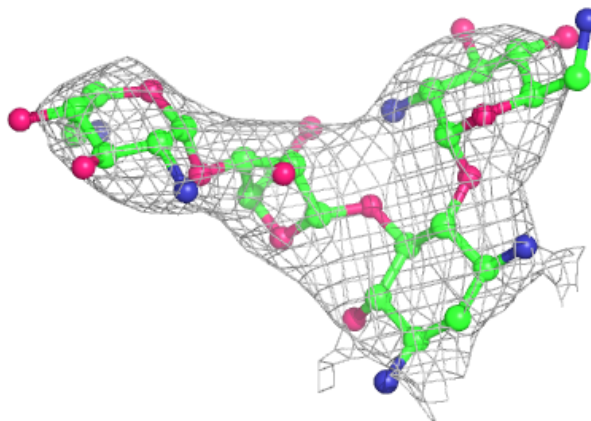
Electron density around NMY AA 1655:

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



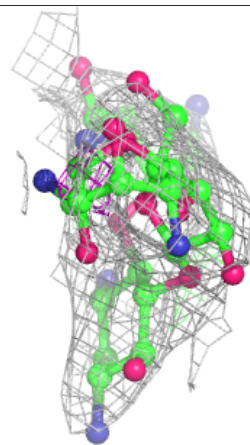
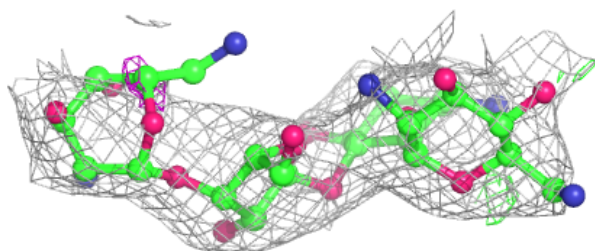
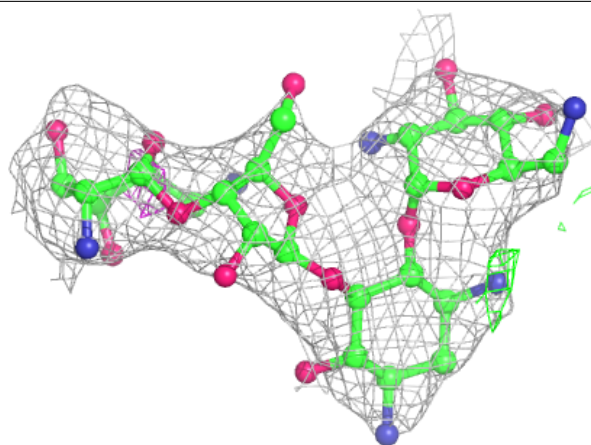
Electron density around NMY DA 3187:

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

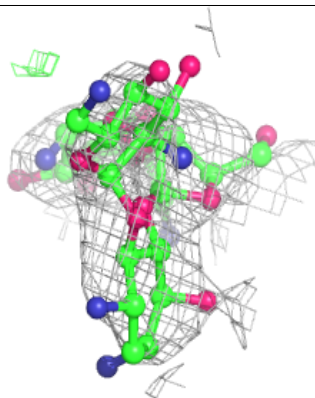
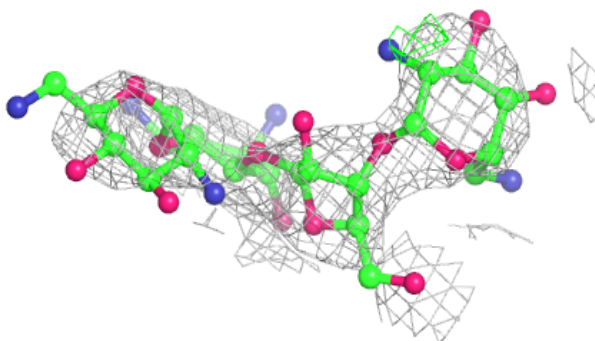
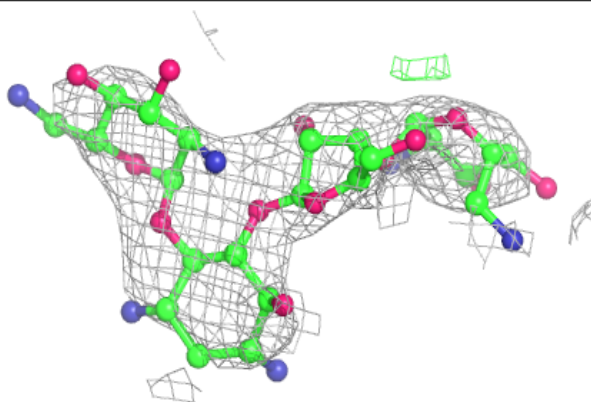


Electron density around NMY DA 3185:

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

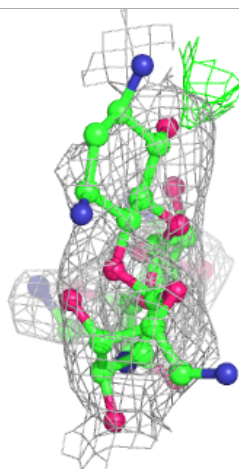
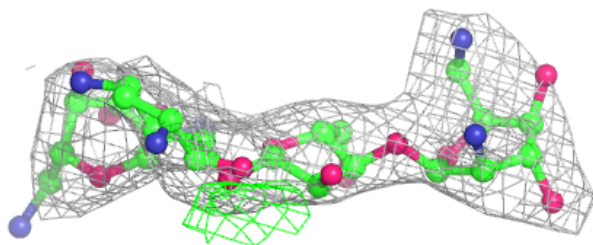
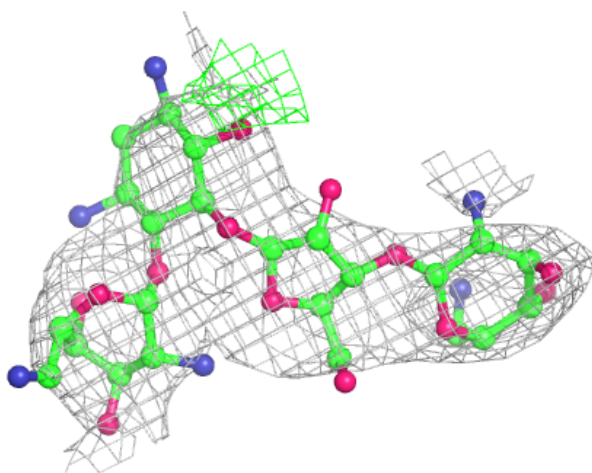
**Electron density around NMY DA 3186:**

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



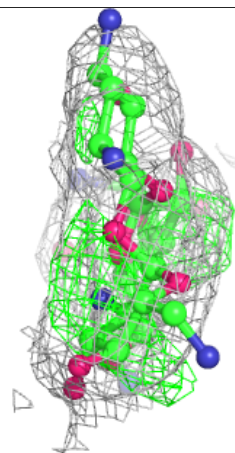
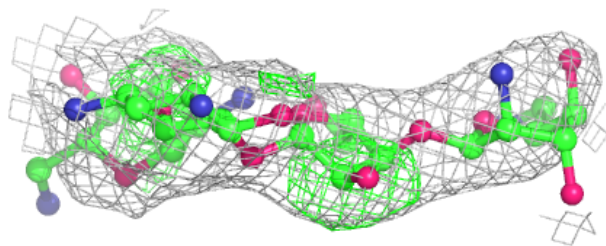
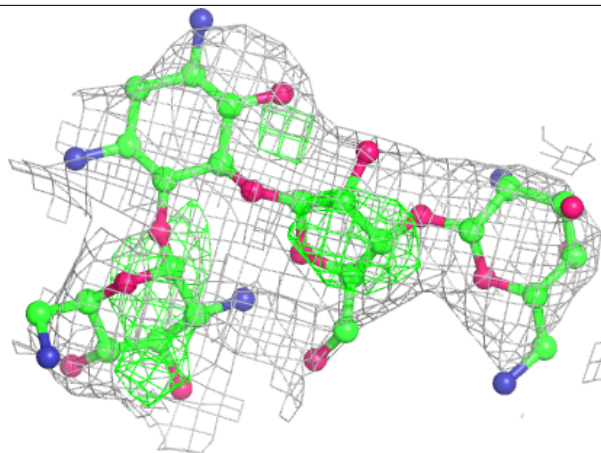
Electron density around NMY DA 3189:

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



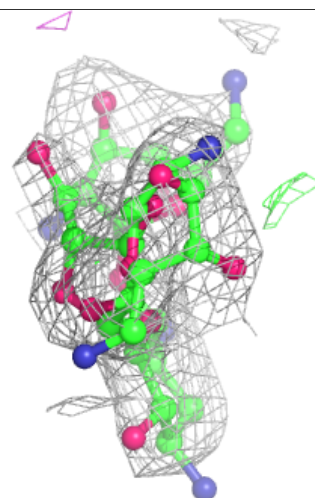
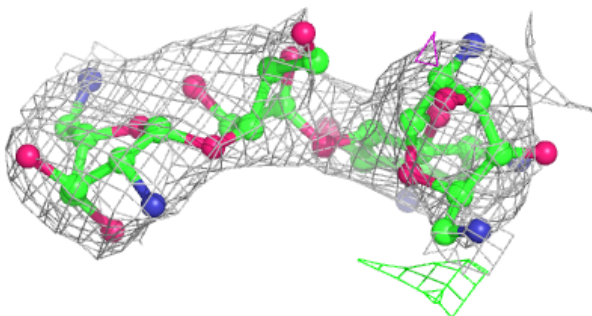
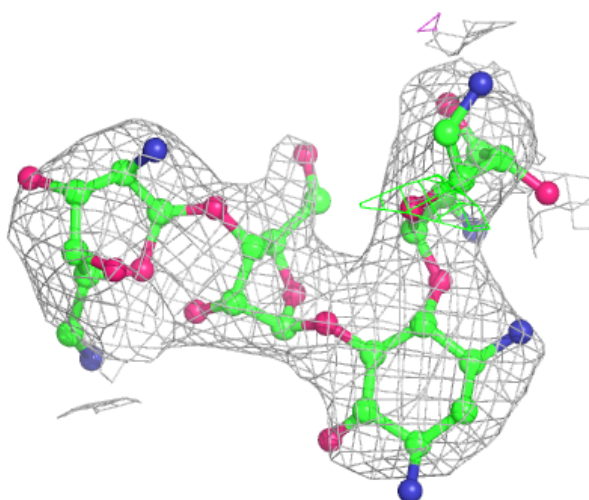
Electron density around NMY CA 1672:

$2mF_o - DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.