



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 02:16 am BST

PDB ID : 4V57
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with spectinomycin and neomycin.
Authors : Borovinskaya, M.A.; Shoji, S.; Holton, J.M.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2007-07-21
Resolution : 3.50 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 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 : 2.11
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) : 2.11

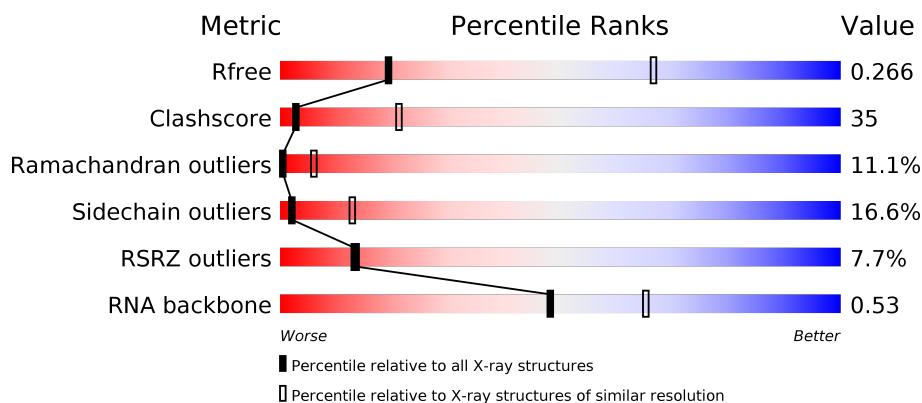
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>23%</div> <div>62%</div> <div>14%</div> <div>..</div> </div>
1	CA	1542	<div> <div>24%</div> <div>62%</div> <div>14%</div> <div>.</div> </div>
2	AC	232	<div> <div>9%</div> <div>20%</div> <div>48%</div> <div>18%</div> <div>.</div> <div>11%</div> </div>
2	CC	232	<div> <div>6%</div> <div>28%</div> <div>46%</div> <div>14%</div> <div>.</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AP	82	
13	CP	82	
14	AQ	83	
14	CQ	83	
15	AR	74	

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Mol	Chain	Length	Quality of chain
15	CR	74	
16	AS	91	
16	CS	91	
17	AT	86	
17	CT	86	
18	AB	240	
18	CB	240	
19	AU	70	
19	CU	70	
20	AO	89	
20	CO	89	
21	AN	100	
21	CN	100	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

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Mol	Chain	Length	Quality of chain
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
38	DM	136	
39	BX	63	
39	DX	63	
40	BH	149	

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Mol	Chain	Length	Quality of chain
40	DH	149	
41	BJ	142	
41	DJ	142	
42	BN	127	
42	DN	127	
43	BO	117	
43	DO	117	
44	BQ	117	
44	DQ	117	
45	BS	110	
45	DS	110	
46	BU	103	
46	DU	103	
47	BF	178	
47	DF	178	
48	BG	176	
48	DG	176	
49	BR	103	
49	DR	103	
50	BT	100	
50	DT	100	
51	BZ	78	
51	DZ	78	
52	BW	84	
52	DW	84	

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
53	NMY	BB	3001	-	-	-	X
53	NMY	DB	3001	-	-	-	X
54	MG	CA	1650	-	-	-	X
54	MG	DB	3059	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 284201 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 2 is a protein called 30S ribosomal protein S3.

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

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

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

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

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

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
12	CM	113	Total	C	N	O	S	0	0	0
			876	541	177	155	3			

- Molecule 13 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
13	CP	80	Total	C	N	O	S	0	0	0
			638	400	126	111	1			

- Molecule 14 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
14	CQ	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

- Molecule 15 is a protein called 30S ribosomal protein S18.

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

- Molecule 16 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
16	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

- Molecule 17 is a protein called 30S ribosomal protein S20.

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

- Molecule 18 is a protein called 30S ribosomal protein S2.

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

- Molecule 19 is a protein called 30S ribosomal protein S21.

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

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
20	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 21 is a protein called 30S ribosomal protein S14.

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

- Molecule 22 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
22	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	120	U	-	INSERTION	GB 85674274
DA	120	U	-	INSERTION	GB 85674274

- Molecule 23 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
23	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	2903	U	-	INSERTION	GB 85674274
BB	2904	U	-	INSERTION	GB 85674274
DB	2903	U	-	INSERTION	GB 85674274
DB	2904	U	-	INSERTION	GB 85674274

- Molecule 24 is a protein called 50S ribosomal protein L11.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

- Molecule 27 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
27	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
30	DY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
36	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
39	DX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 40 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
40	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 41 is a protein called 50S ribosomal protein L13.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
47	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 48 is a protein called 50S ribosomal protein L6.

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

- Molecule 49 is a protein called 50S ribosomal protein L21.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

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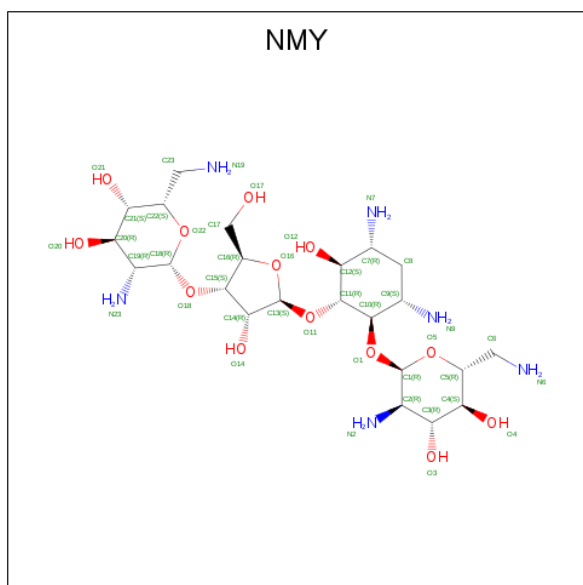
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 52 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
52	DW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 53 is NEOMYCIN (three-letter code: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).

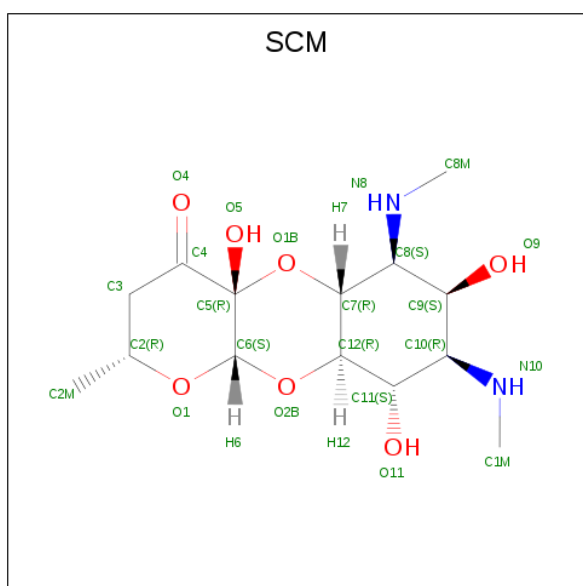


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
53	AA	1	Total	C	N	O	0	0
			42	23	6	13		
53	BB	1	Total	C	N	O	0	0
			42	23	6	13		
53	CA	1	Total	C	N	O	0	0
			42	23	6	13		
53	DB	1	Total	C	N	O	0	0
			42	23	6	13		

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	BB	110	Total Mg 110 110	0	0
54	AA	60	Total Mg 60 60	0	0
54	CA	59	Total Mg 59 59	0	0
54	DB	111	Total Mg 111 111	0	0

- Molecule 55 is SPECTINOMYCIN (three-letter code: SCM) (formula: $C_{14}H_{24}N_2O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AA	1	Total C N O 23 14 2 7	0	0
55	CA	1	Total C N O 23 14 2 7	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	290	Total O 290 290	0	0
57	AE	1	Total O 1 1	0	0
57	AK	1	Total O 1 1	0	0
57	AL	4	Total O 4 4	0	0
57	AP	1	Total O 1 1	0	0
57	AT	2	Total O 2 2	0	0
57	AN	1	Total O 1 1	0	0
57	BB	492	Total O 492 492	0	0
57	BC	7	Total O 7 7	0	0
57	BD	1	Total O 1 1	0	0
57	BE	4	Total O 4 4	0	0
57	BL	2	Total O 2 2	0	0
57	BH	1	Total O 1 1	0	0
57	CA	282	Total O 282 282	0	0
57	CE	2	Total O 2 2	0	0
57	CL	4	Total O 4 4	0	0
57	CP	1	Total O 1 1	0	0
57	CT	1	Total O 1 1	0	0
57	CI	1	Total O 1 1	0	0
57	CN	3	Total O 3 3	0	0
57	DB	501	Total O 501 501	0	0
57	DC	4	Total O 4 4	0	0

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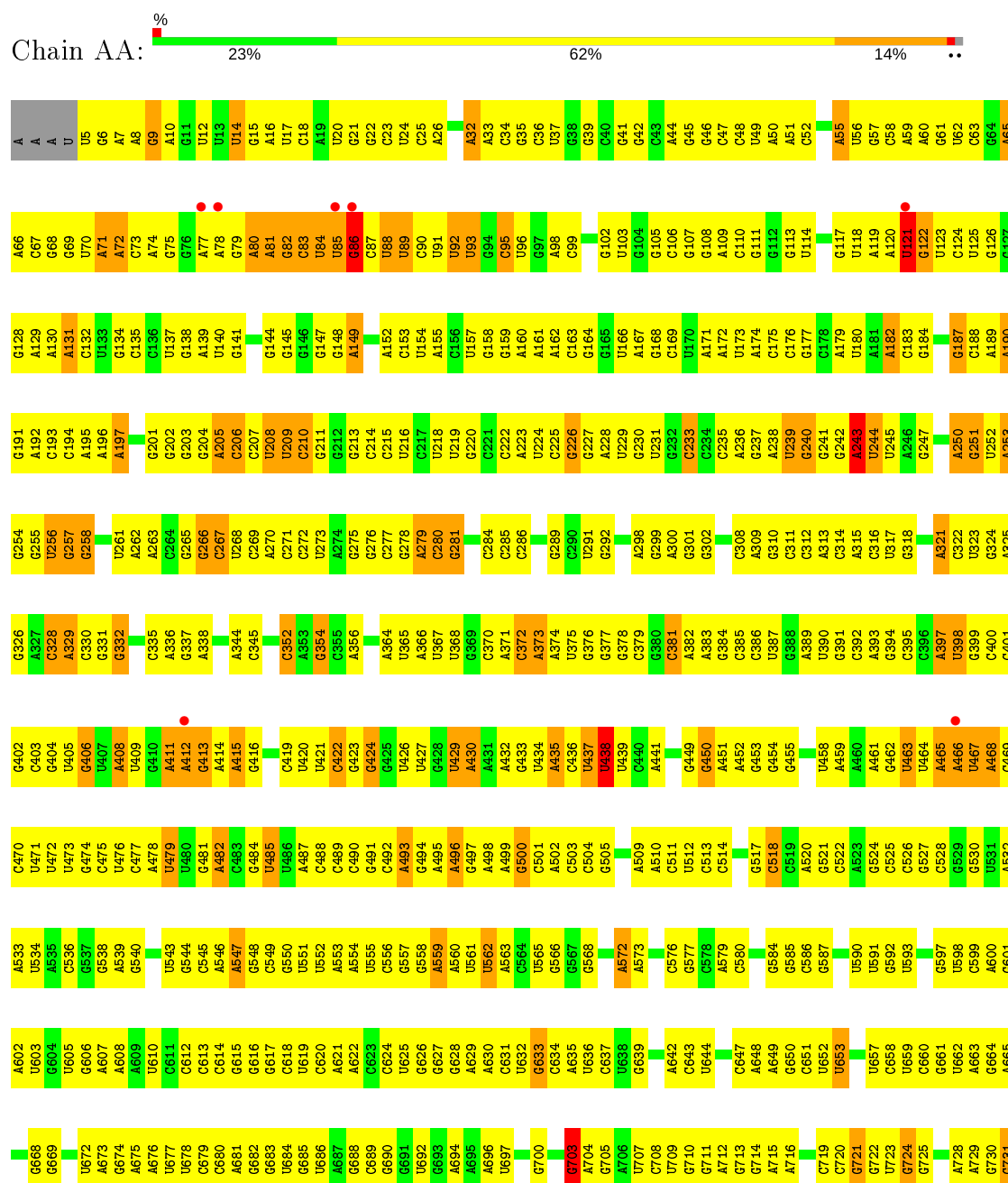
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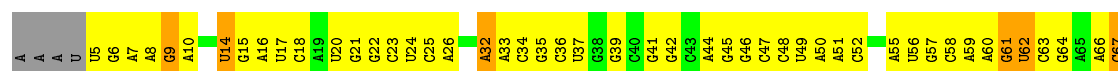
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DD	1	Total 1	O 1	0	0
57	DE	2	Total 2	O 2	0	0
57	DL	1	Total 1	O 1	0	0
57	DN	2	Total 2	O 2	0	0
57	DR	1	Total 1	O 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

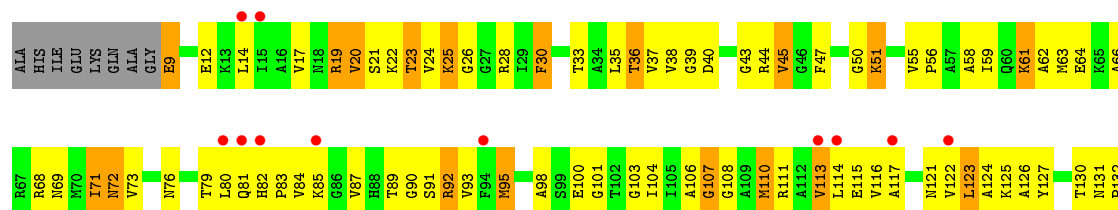
• Molecule 1: 16S rRNA

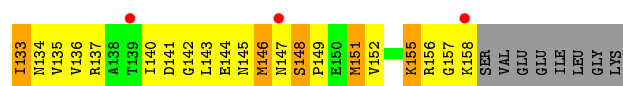




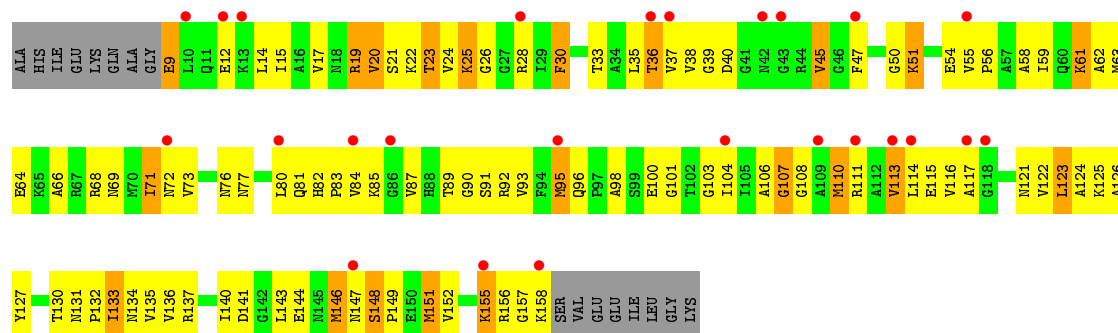
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U1090	U1023	U960	G890	C817	A747	C679	G611	C546	U480	A411	A336	A263	G201	C136	G69
U1091	G1024	U961	U891	G818	G748	C680	C612	A546	G481	A412	A337	C264	G202	U137	U70
A1092	U1025	A964	A892	A819	A749	A681	C613	A547	A482	G413	G265	G265	G203	G138	A71
A1093	G1026	U965	C893	U820	C750	G682	C614	C548	C483	A414	A338	G266	G204	U140	A72
G1094	C1027	G966	G894	G821	U751	G683	G615	C549	G484	A415	C339	C267	G205	G141	C73
U1095	U1028	C967	C895	G824	G785	U684	G616	G550	U485	G416	A344	U268	A205	A74	G75
C1096	A1029	A968	C897	A825	G786	G685	G617	U551	U486	U420	C345	C269	C206	G76	U77
C1097	U1030	A969	A900	C826	A759	U686	G618	U552	A487	U421	G346	A270	C207	A78	A78
C1098	C1031	C970	U900	U827	G760	A687	U619	A553	C488	U422	C352	C271	U208	G145	
G1099	G1032	G971	U901	U828	G761	G688	C620	A554	C489	G423	G353	G272	U209	G146	
C1100	G1033	C972	G902	U837	U762	C689	A621	U555	C490	G424	G354	U273	G210	G147	
A1101	A1036	G973	G903	G833	G763	G690	G622	G557	C492	G425	C355	G276	G211	G148	G82
A1102	C1037	A974	U904	U834	C764	U692	C624	G558	A493	U426	A356	C277	G212	A149	C83
C1103	U1040	A975	U905	U835	G765	G693	U625	A559	G494	U427		C278	C213	U84	U85
G1104	U1041	G976	A906	G836	A766	A694	U626	A560	G495	G428	A364	A279	C215	G153	G86
	A1042	A977	U907	U837	G766	G694	G627	A561	A496	U429	U365	C280	U216	U154	C87
G1107	A1043	A978	A908	C840	G769	G700	G628	U562	G497	A430	A366	G281	C217	A155	U88
C1109	U1044	C979	A909	C841	C770	G701	A629	A563	A498	A431	U367		U218	G156	U89
A1110	G1045	C980	C910	U842	G771	A702	A630	G564	A499	A432	U368	C284	U219	U157	C90
A1111	G1047	U981	U911	U843	U772	G703	C631	U565	G500	G433	G369	C285		G158	U91
A1112	G1048	U982	C912	U844	A704	A704	U632	G566	C501	U434	C370	C286	C222	G159	U92
C1113	U1049	A983	A913	G845	A777	U707	G633	G567	A502	A435	A371	U287	A223	U93	U93
G1114	G1050	C984	A914	G846	C778	C708	C634	G568	A503	C436	C372	A288	U224	A161	G94
U1115	U1051	C985	G917	C847	C779	G709	A635	A572	C504	U437	A373	G289	C225	C95	C95
U1116	U1052	U986	A918	C848	C780	U709	U636	A573	G505	U438	A374	C290	G226	U96	U96
A1117	G1053	U987	G919	G849	A781	G710	U637			U439		G291	G227	G97	G97
U1118	C1054	G988	U920	U854	A782	G711	U638	C576	A509	A440	G378	G292	U228	G165	A98
A1119	A1055	U989	U921	C858	A783	A712	G639	G577	C511	A441	C379		U229	U166	C99
C1120	U1056	C990	U922	G859	A784	G713		C578	C512		C381	A298	U230	C167	G102
U1121	G1057	U991	G923	G859	G785	G714	A642	C579	U512		A382	C299	U231	C168	G103
U1122	G1058	U992	C924	G860	U786	A715	C643	A578	C513		A383	A300	G232	C169	U103
U1123	U1059	A994	G925	G861	A787	A716	U644	C580			A384	G302	C234	U170	G104
G1124	U1060	C995	G926	C862	A790	C719	C647	G594	G517		C385		C235	A171	G105
U1125	G1061	A996	G927	U863	G791	C720	A648	G585	C518		C386	C308	A236	U172	C106
U1126	U1062	U997	G933	A864	A792	G721	A649	C586	A520		U387	A309	G237	U173	G107
C1127	C1063	C998	C934	C866	U793	G722	G650	G587	G521	U458	G388	G310	A238	C175	A109
C1128	G1064	C999	A935	G867	A794	U723	C651		G522	A459	U390	C312	U239	G176	G113
C1129	U1065	A1000	A935	U868	C795	G724	U652	U590	G523	A460	U391	A313	G240	G177	U114
A1130	C1066	C1001		C868	C796	G725	U653	U591	G524	A461	C392	C314	G241	C178	
G1131	A1067	G1002	A938	G869	C797	G726		G592	G525	G462	C393	A315	G242	A179	U118
C1132	G1068	G1003	G939	U870	U798	A728	G656	U593	C526	G463	G394	C316	A243	U180	
G1133	U1069	A1004	C940	U871	U799	A729	U657	U594	G527	U464	C395	U317	U244	A181	A119
U1134	U1070	A1005	G941		U801	G730	C658	A595	G528	A465	C396	G318	U245	A182	A120
U1135	C1071	G1006	A946	U875	A802	G731	U659	A596	G529	A466	A397		A246	C183	U121
C1136	G1072	U1007	G947	C876	G803	G732	C660	G597	G530	U467	U398	C321	G247	G184	G122
C1137	U1073	U1008	C948	G877	U804	G733	G661	G598	G531	U468	U399	C322	A250	G187	U123
G1138	G1074	U1009	C949	U878	C805	G734	U662	C599	A532	A469	C400	C323	G251	C124	C124
C1139	U1075	U1010	A949	C879	C806	C735	A663	A600	A533	C469	C401	U323	G252	U125	U125
C1140	U1076	C1011	U950	C880	A807	G736	G664	G601	U534	C470	G402	U324	U252	A189	G126
C1141	G1077	A1012	G951	C881	A808	C737	A665	A602	A535	U471	G403	A325	G254	A190	G127
G1142	U1078	G1013	U952	C882	G809	C738	U603	G603	C536	U472	C404	G326	G255	G128	G128
G1143		A1014	G953	C883	G809	C739	U672	G604	G537	U473	G405	A327	U256	A192	A129
G1144	A1081	G1015	G954	U884	C811	U740	A673	U605	G538	G474	U406	C328	G257	C193	A130
A1145	A1082	A1016	U955	G885	G812	G741	G674	G606	A539	G475	G406	A329	G258	C194	A131
C1146	G1083	U1017	U956	G886	U813	G744	A675	A607	G540	U476	U407	C330	G259	A195	C132
C1147	G1084	G1018	U957	G887	A814	C744	A676	A608	G541	U477	U408	G331		A196	U133
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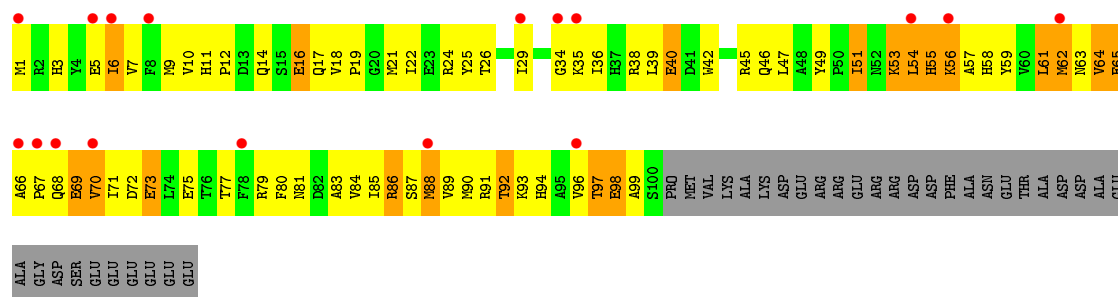
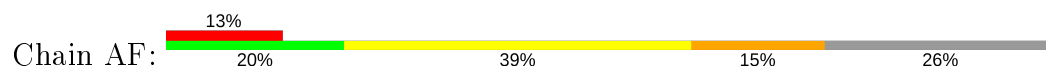




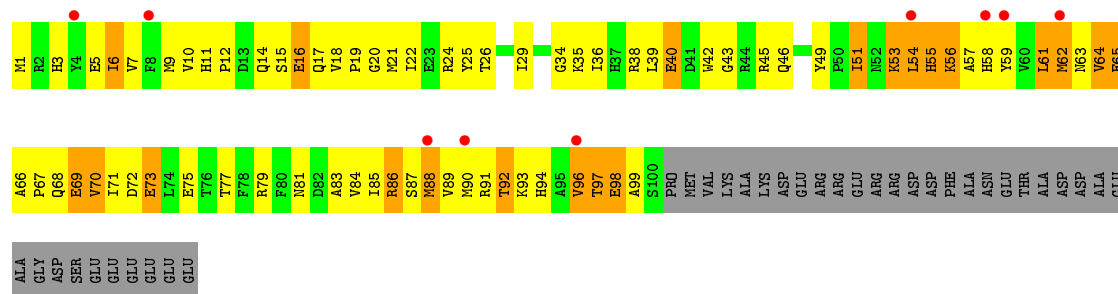
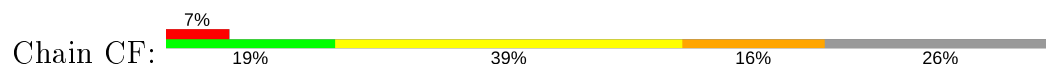
• Molecule 4: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S6

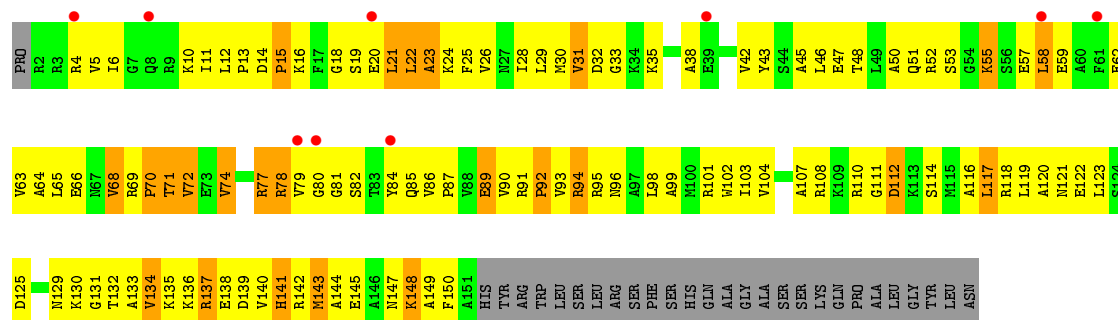


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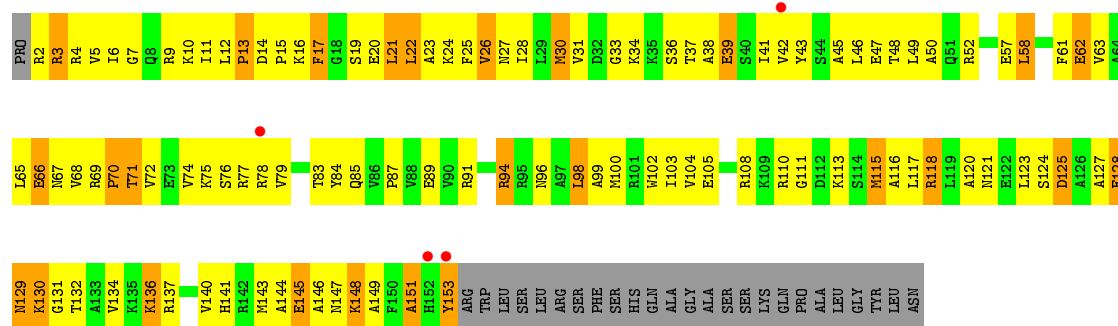


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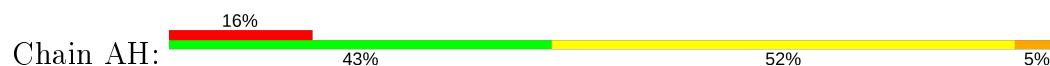




• Molecule 6: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S8

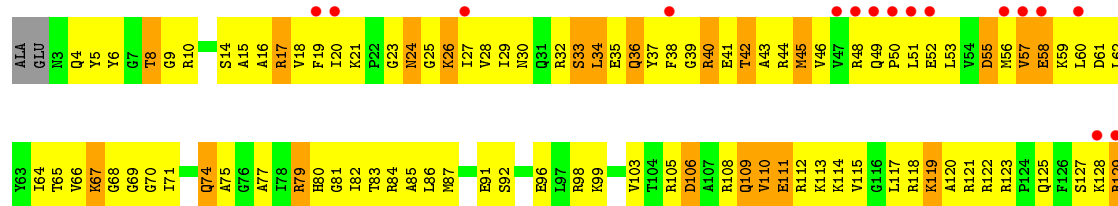


• Molecule 7: 30S ribosomal protein S8

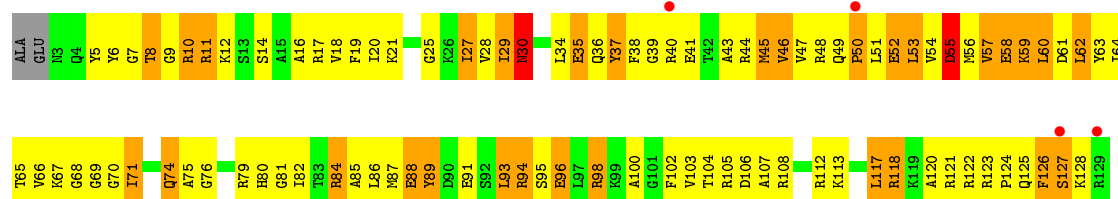


• Molecule 8: 30S ribosomal protein S9

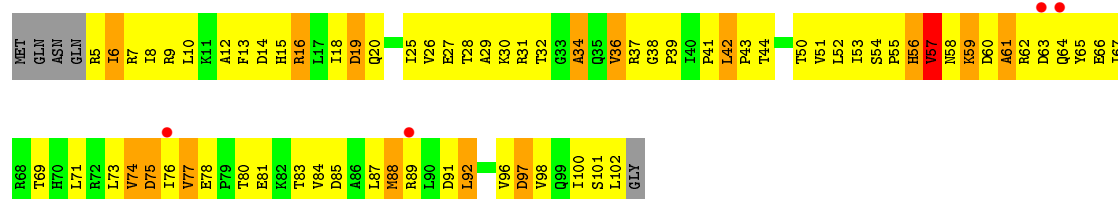




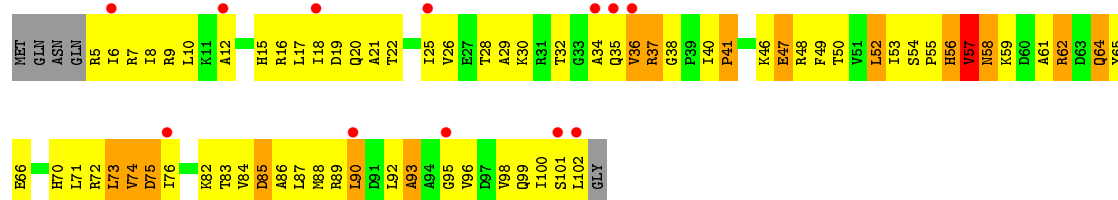
• Molecule 8: 30S ribosomal protein S9



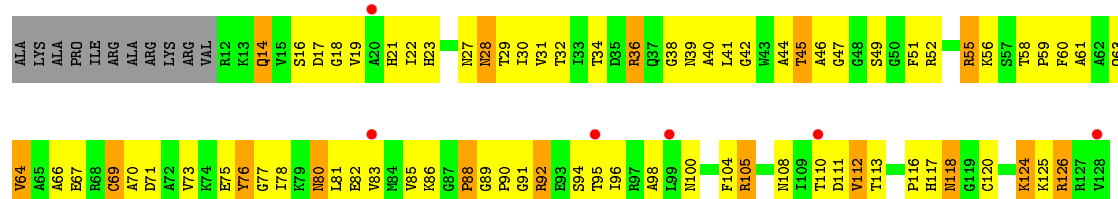
• Molecule 9: 30S ribosomal protein S10



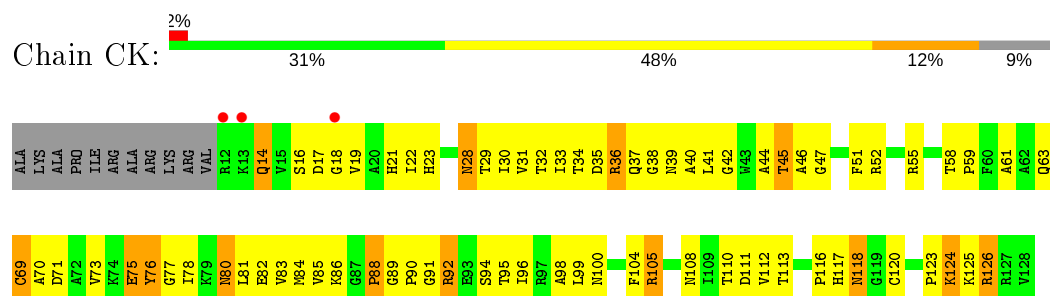
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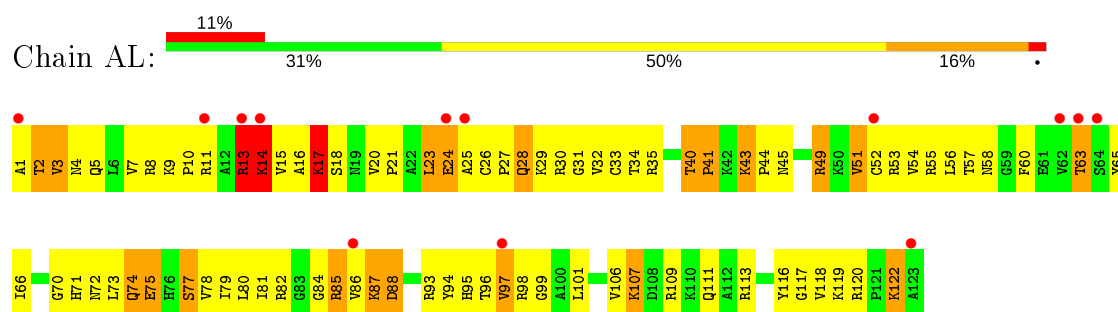
• Molecule 10: 30S ribosomal protein S11



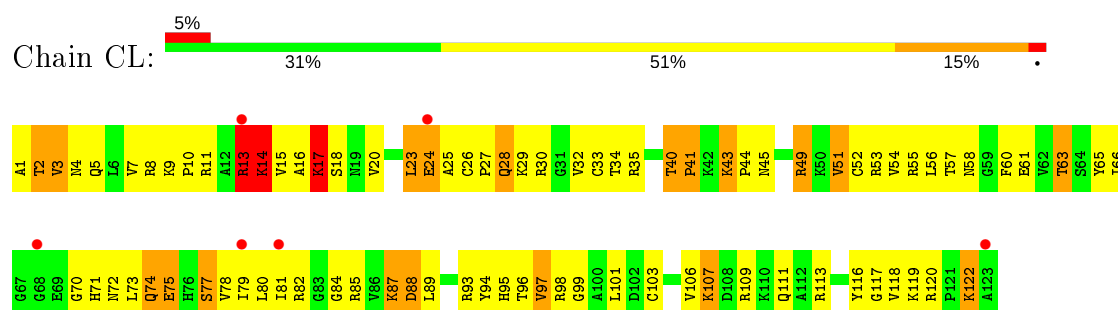
- Molecule 10: 30S ribosomal protein S11



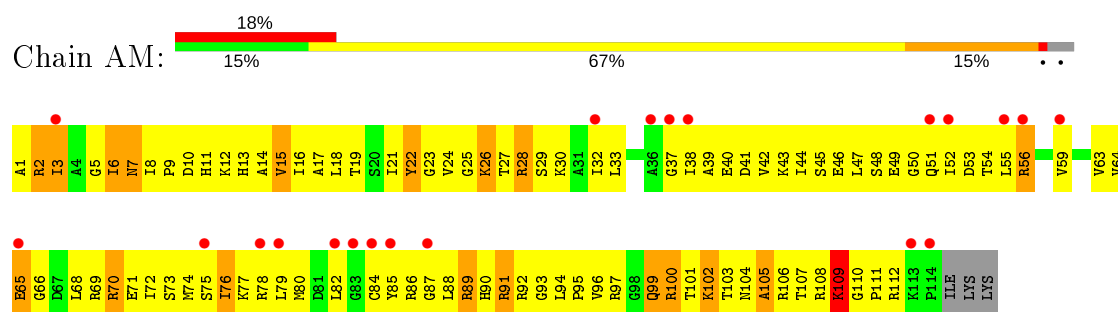
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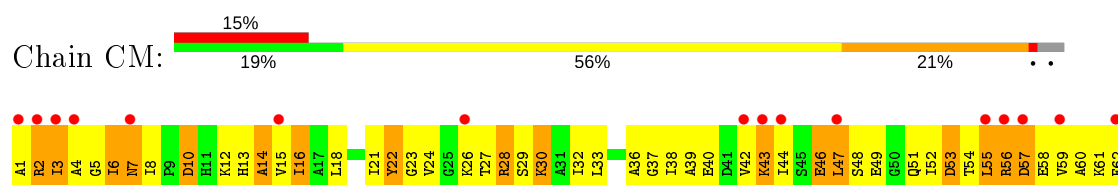
- Molecule 11: 30S ribosomal protein S12

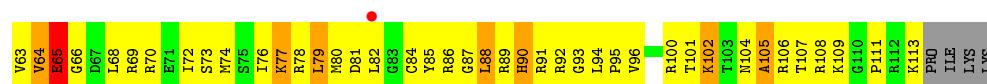


- Molecule 12: 30S ribosomal protein S13

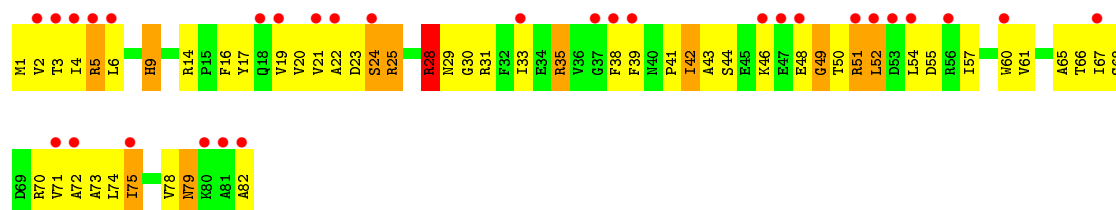


- Molecule 12: 30S ribosomal protein S13

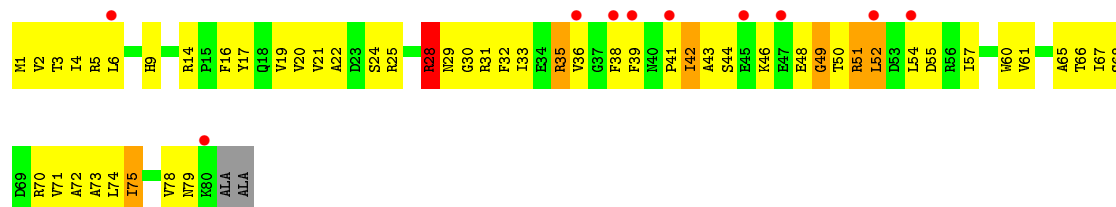




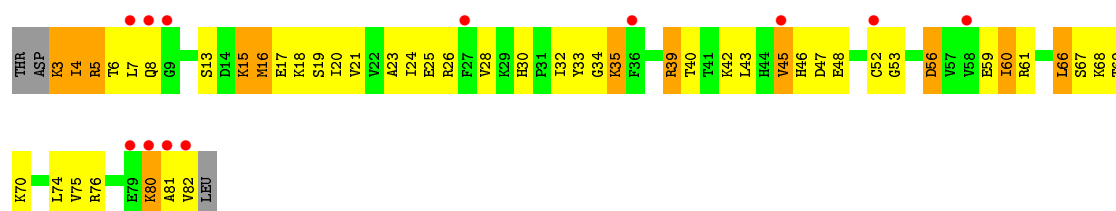
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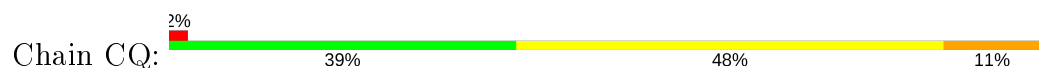
- Molecule 13: 30S ribosomal protein S16



- Molecule 14: 30S ribosomal protein S17

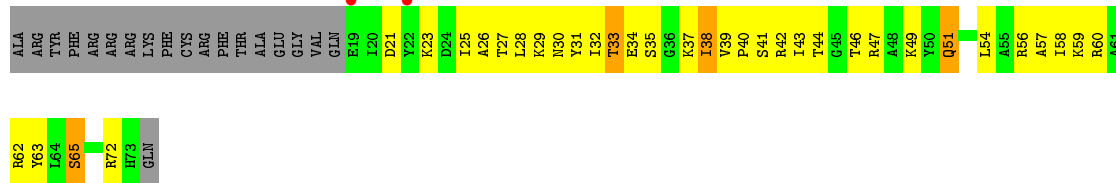


- Molecule 14: 30S ribosomal protein S17



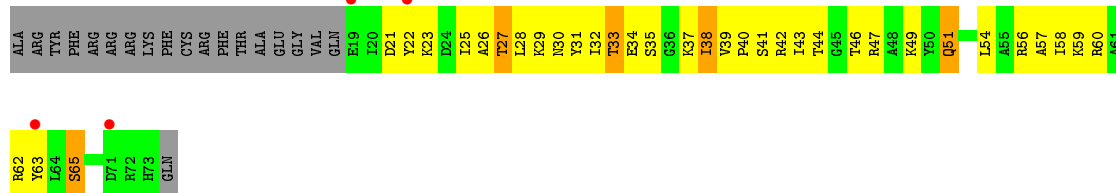
- Molecule 15: 30S ribosomal protein S18

Chain AR:



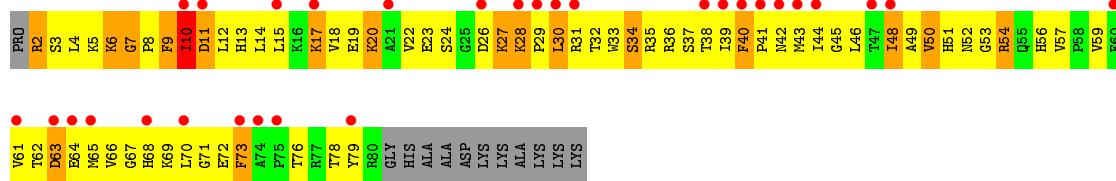
- Molecule 15: 30S ribosomal protein S18

Chain CR:



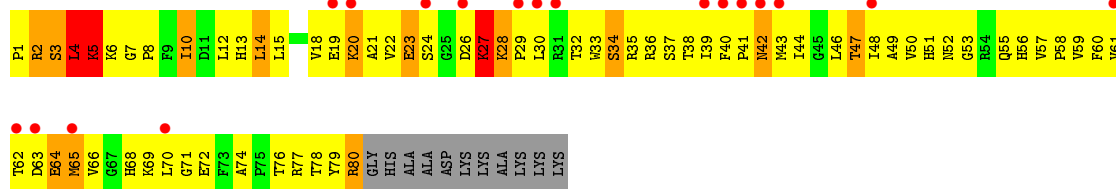
- Molecule 16: 30S ribosomal protein S19

Chain AS:



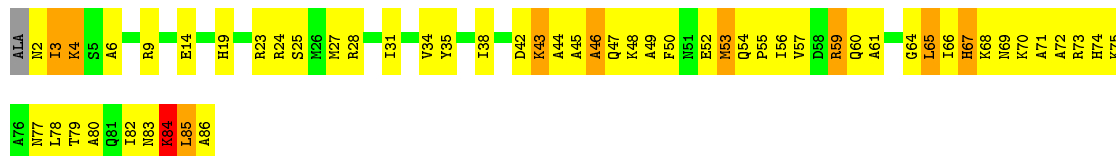
- Molecule 16: 30S ribosomal protein S19

Chain CS:

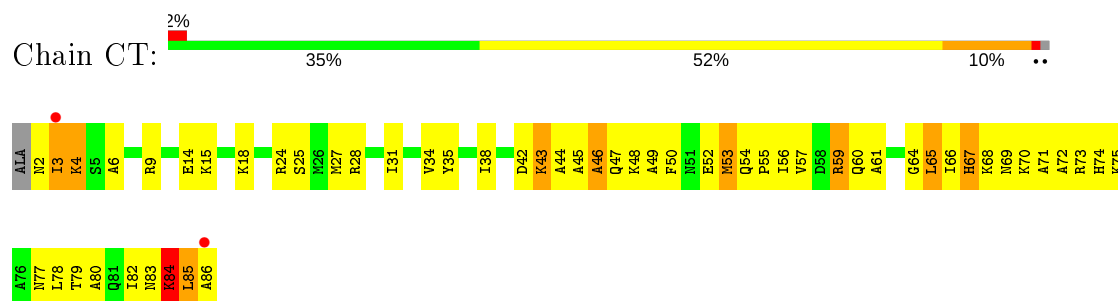


- Molecule 17: 30S ribosomal protein S20

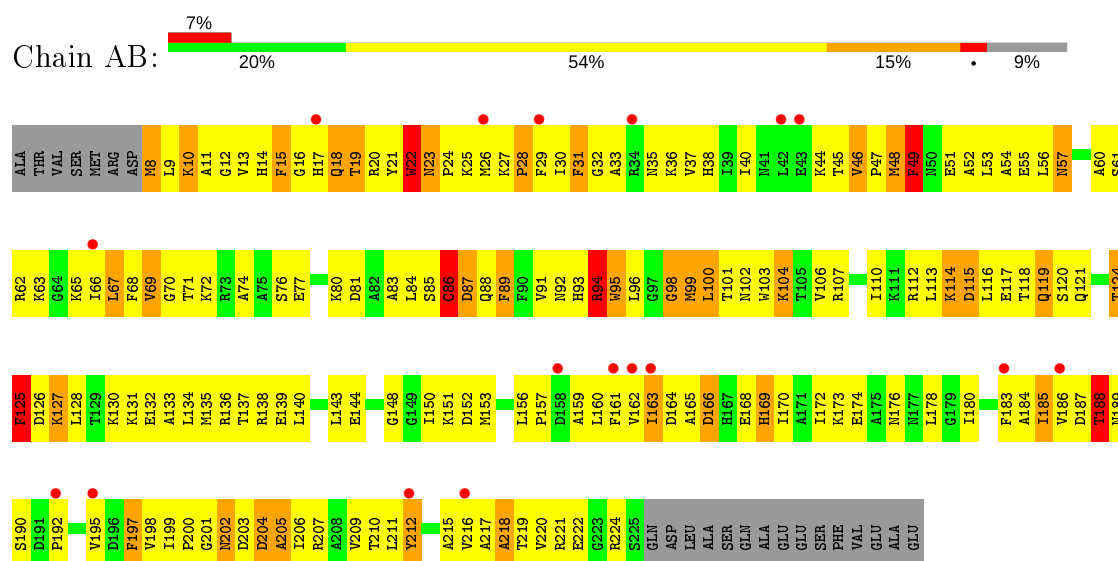
Chain AT:



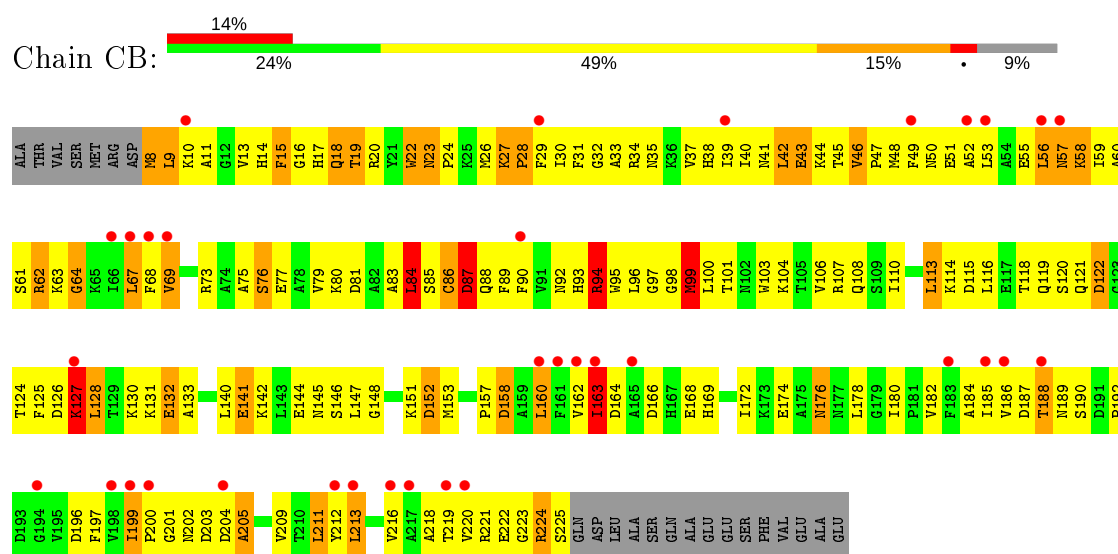
- Molecule 17: 30S ribosomal protein S20



- Molecule 18: 30S ribosomal protein S2

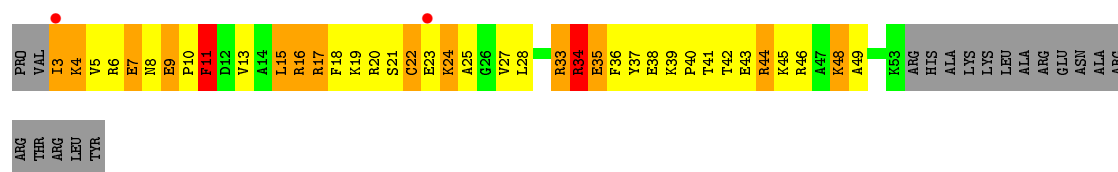


- Molecule 18: 30S ribosomal protein S2

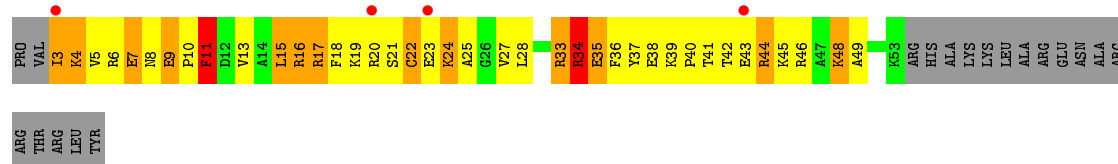


- Molecule 19: 30S ribosomal protein S21

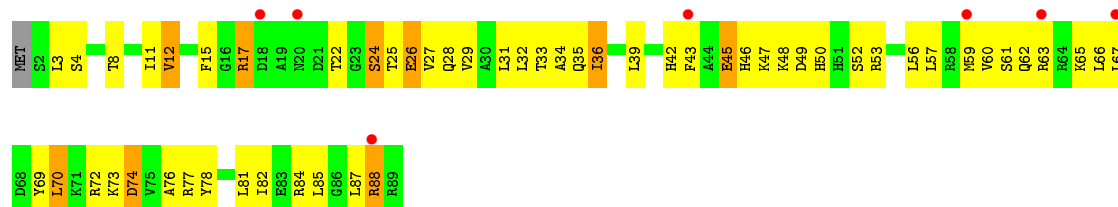




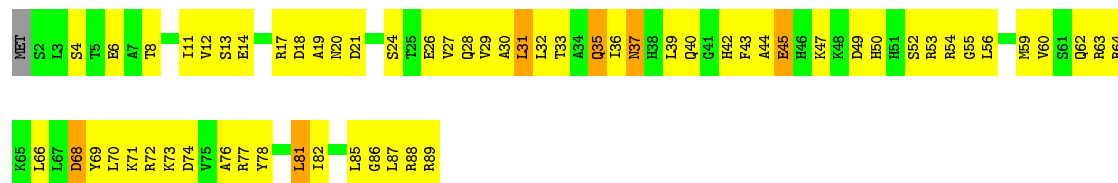
- Molecule 19: 30S ribosomal protein S21



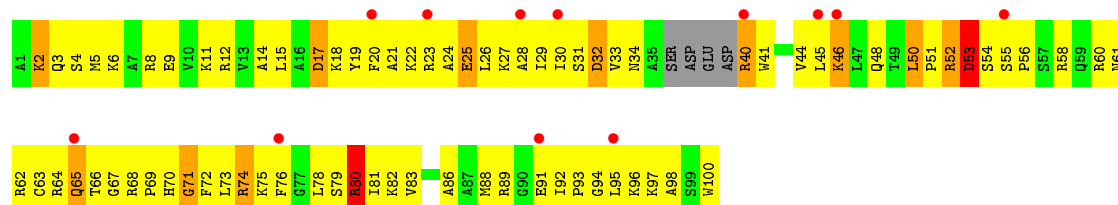
- Molecule 20: 30S ribosomal protein S15



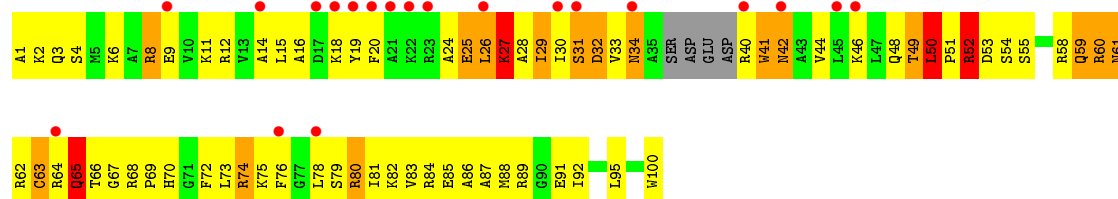
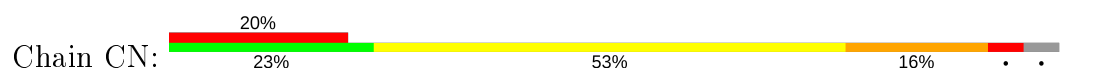
- Molecule 20: 30S ribosomal protein S15



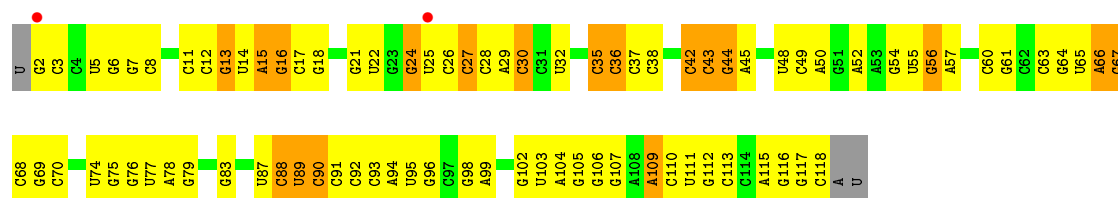
- Molecule 21: 30S ribosomal protein S14



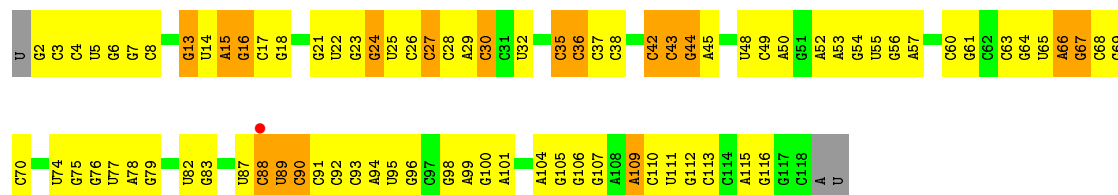
- Molecule 21: 30S ribosomal protein S14



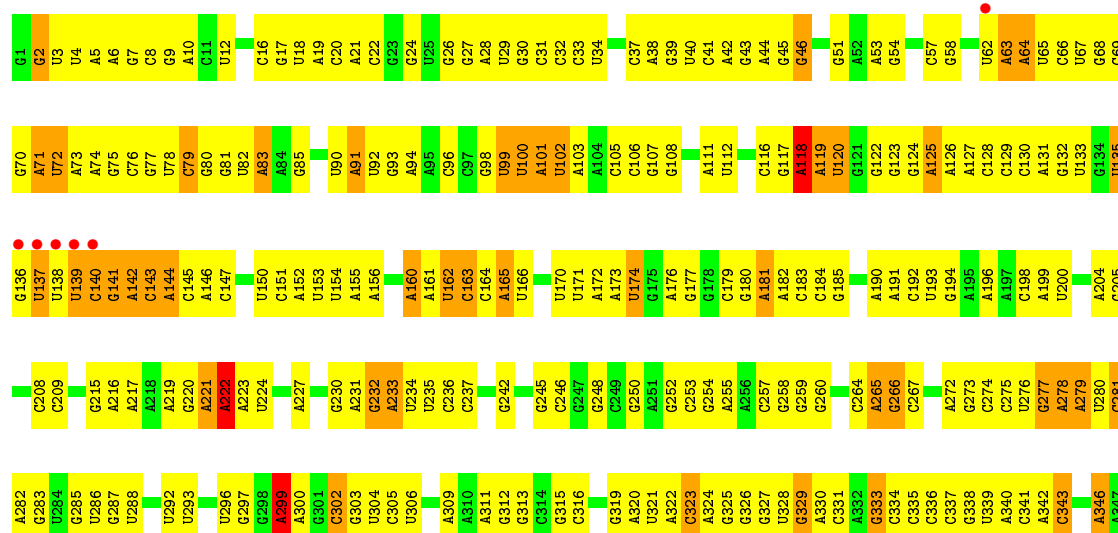
• Molecule 22: 5S rRNA



• Molecule 22: 5S rRNA

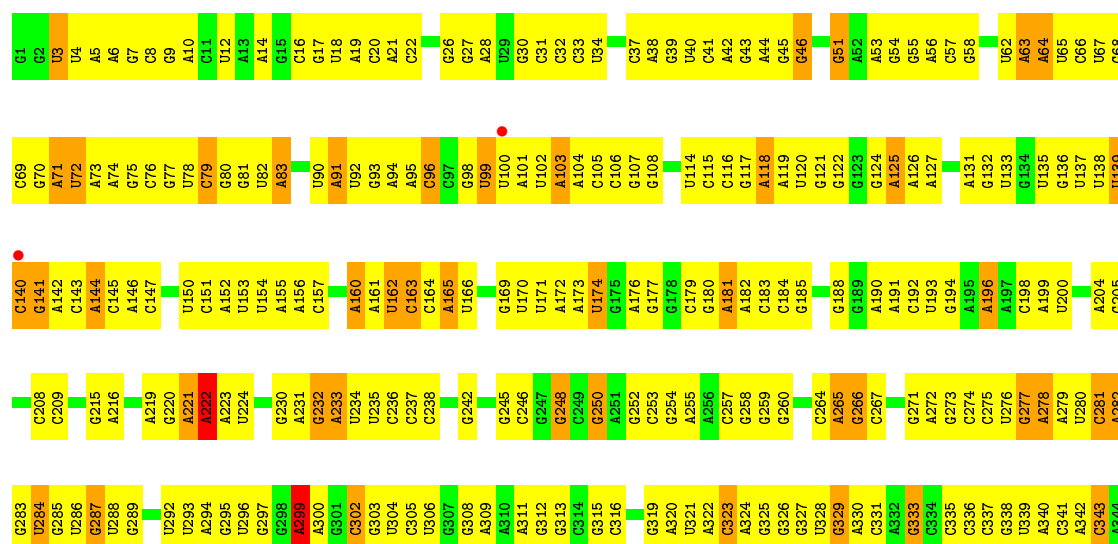


• Molecule 23: 23S rRNA



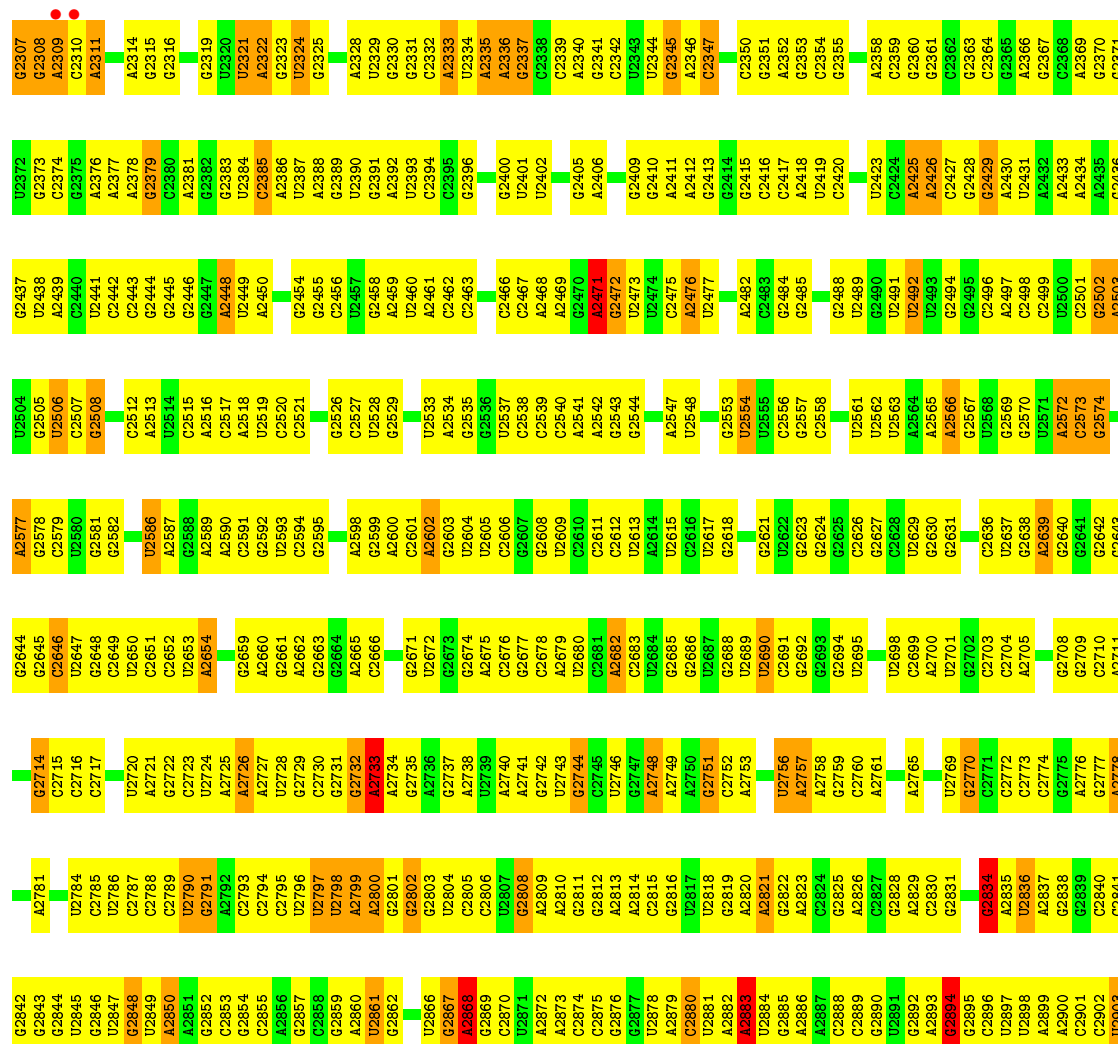


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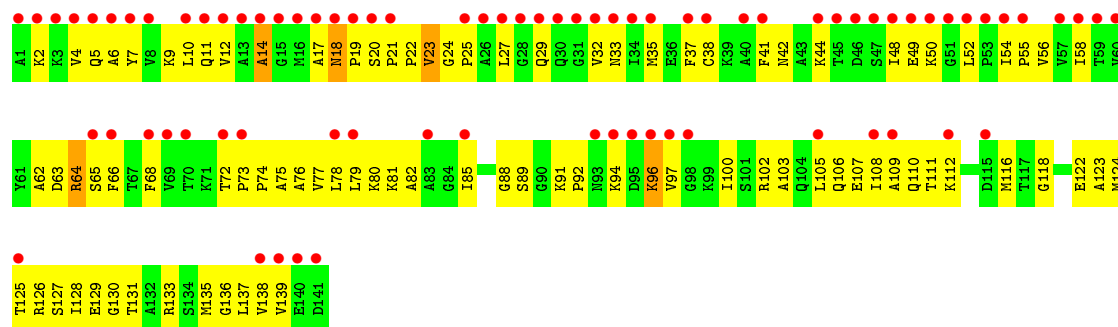


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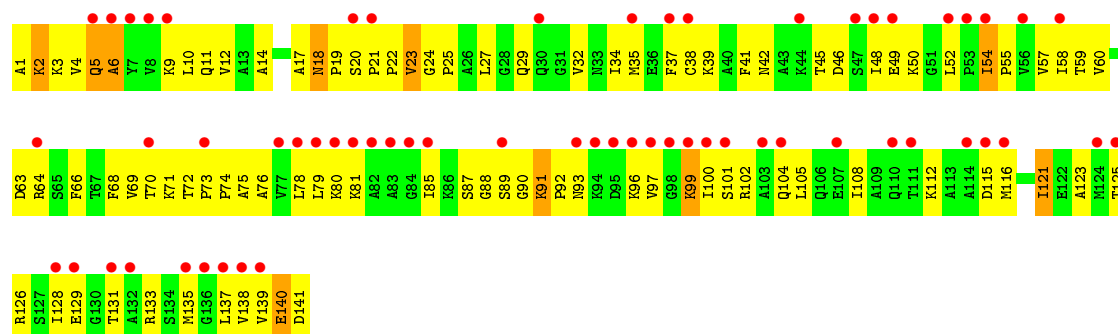


• Molecule 24: 50S ribosomal protein L11

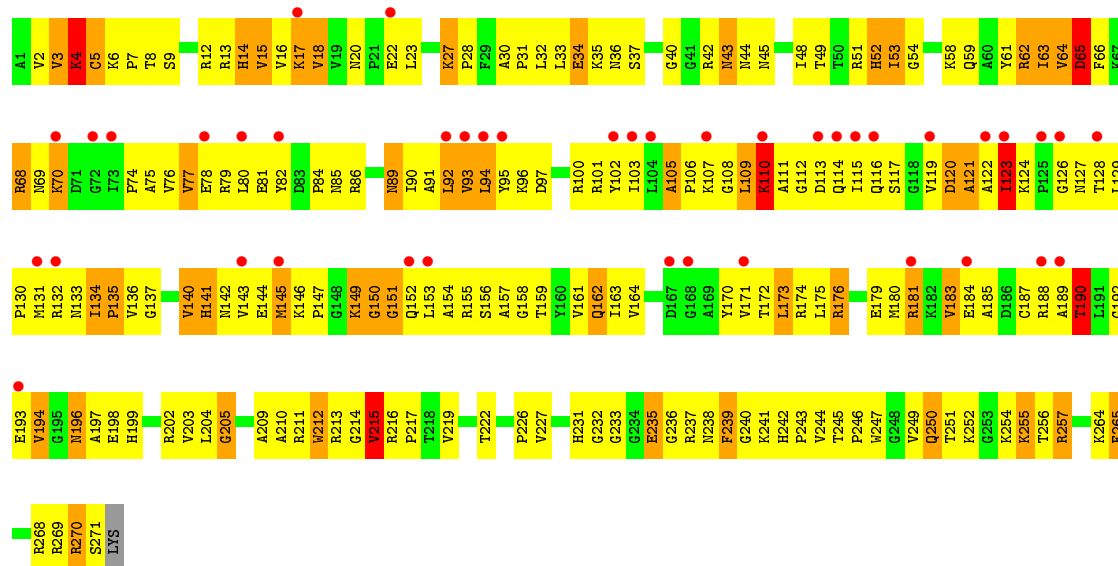


• Molecule 24: 50S ribosomal protein L11

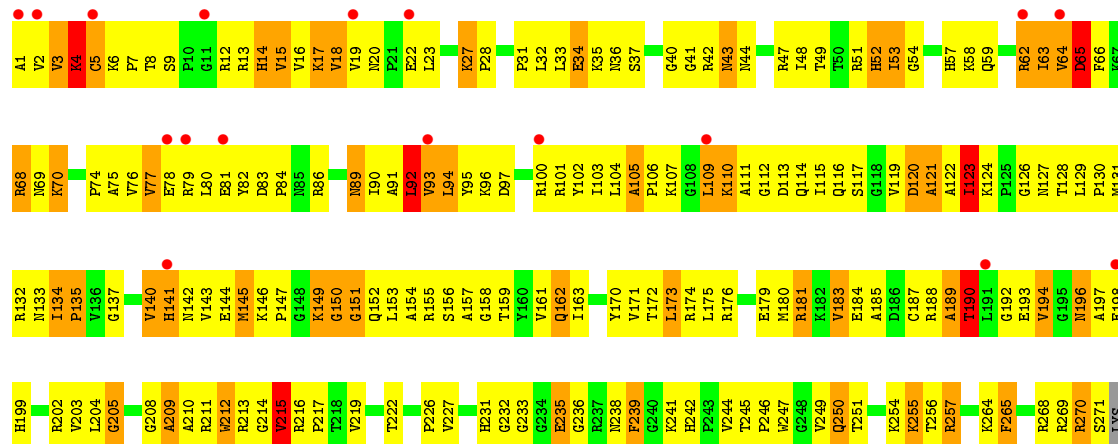




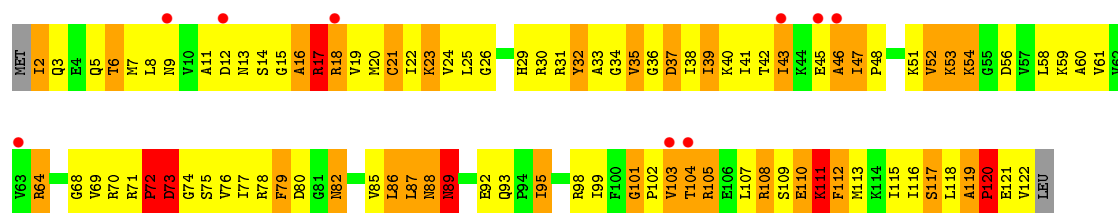
• Molecule 25: 50S ribosomal protein L2



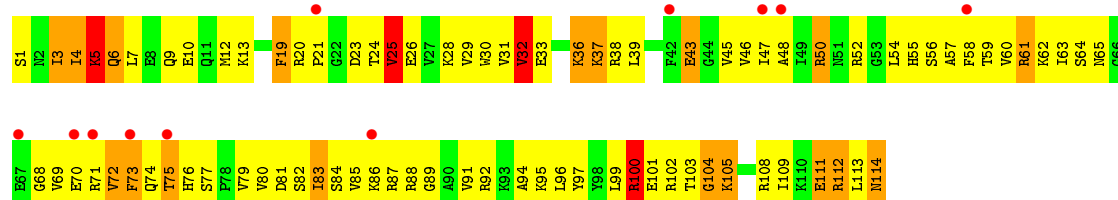
• Molecule 25: 50S ribosomal protein L2



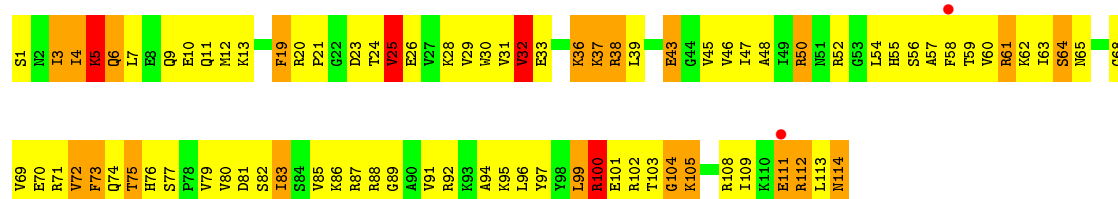
• Molecule 26: 50S ribosomal protein L3



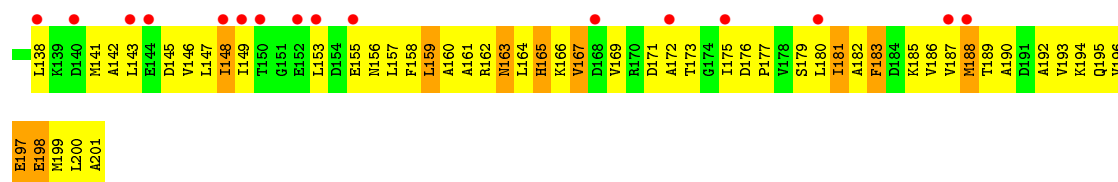
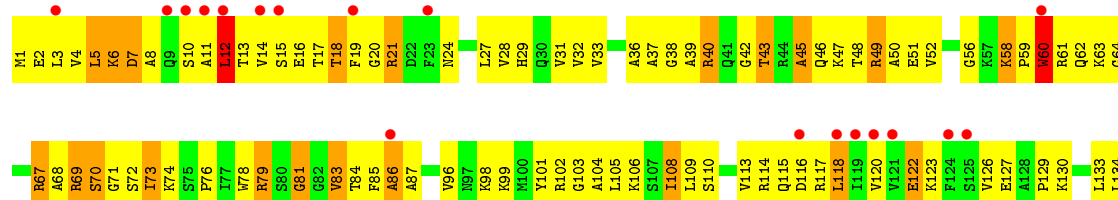
• Molecule 28: 50S ribosomal protein L19



• Molecule 28: 50S ribosomal protein L19

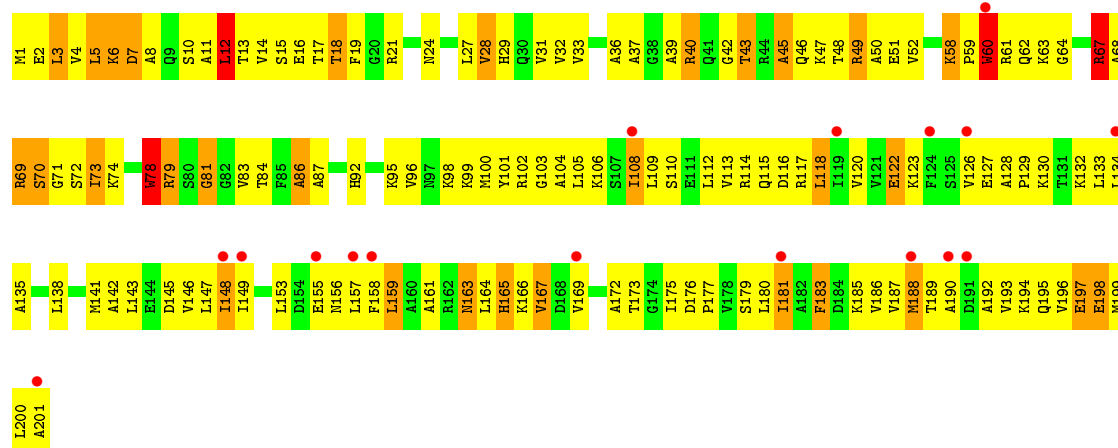


• Molecule 29: 50S ribosomal protein L4



• Molecule 29: 50S ribosomal protein L4





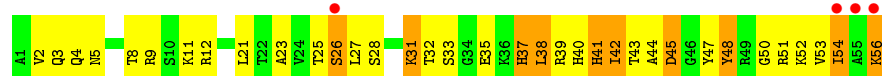
- Molecule 30: 50S ribosomal protein L30



- Molecule 30: 50S ribosomal protein L30



- Molecule 31: 50S ribosomal protein L32



- Molecule 31: 50S ribosomal protein L32



- Molecule 32: 50S ribosomal protein L36



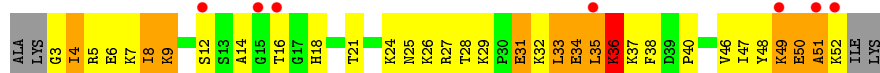
- Molecule 32: 50S ribosomal protein L36

Chain D4:  26% 53% 18% .



- Molecule 33: 50S ribosomal protein L33

Chain B1:  13% 30% 43% 19% . 7%



- Molecule 33: 50S ribosomal protein L33

Chain D1:  9% 28% 44% 19% . 7%



- Molecule 34: 50S ribosomal protein L35

Chain B3:  8% 39% 50% 11%



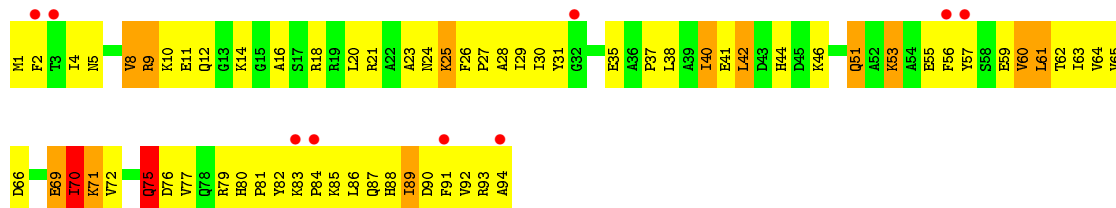
- Molecule 34: 50S ribosomal protein L35

Chain D3:  5% 41% 48% 11%

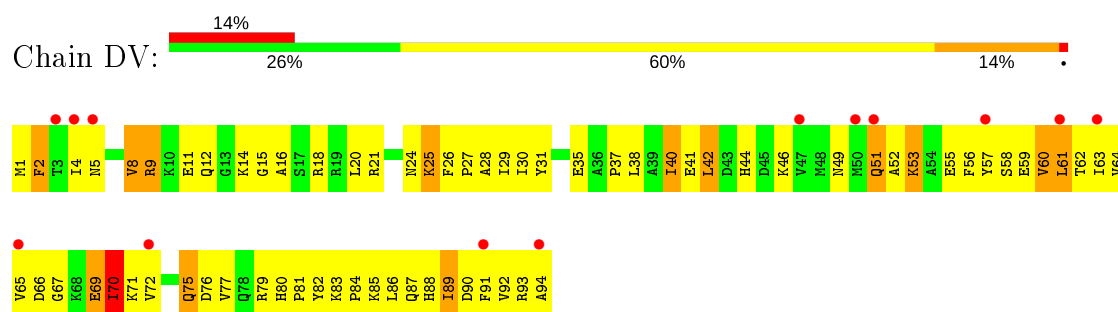


- Molecule 35: 50S ribosomal protein L25

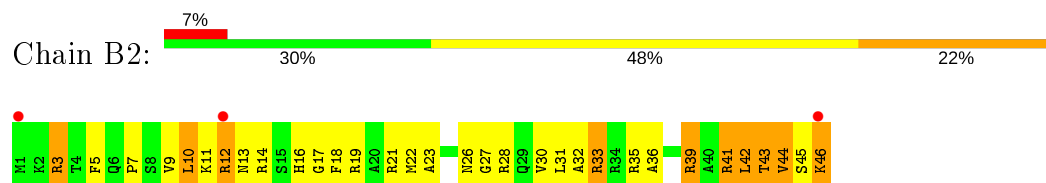
Chain BV:  10% 29% 56% 13% .



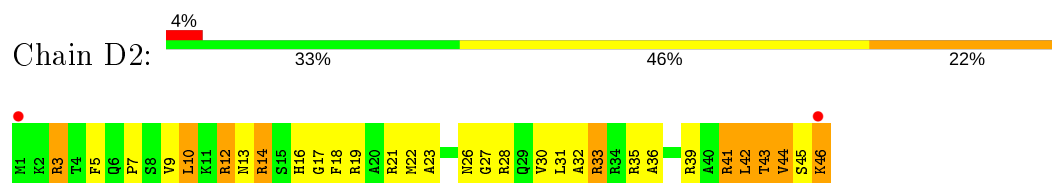
- Molecule 35: 50S ribosomal protein L25



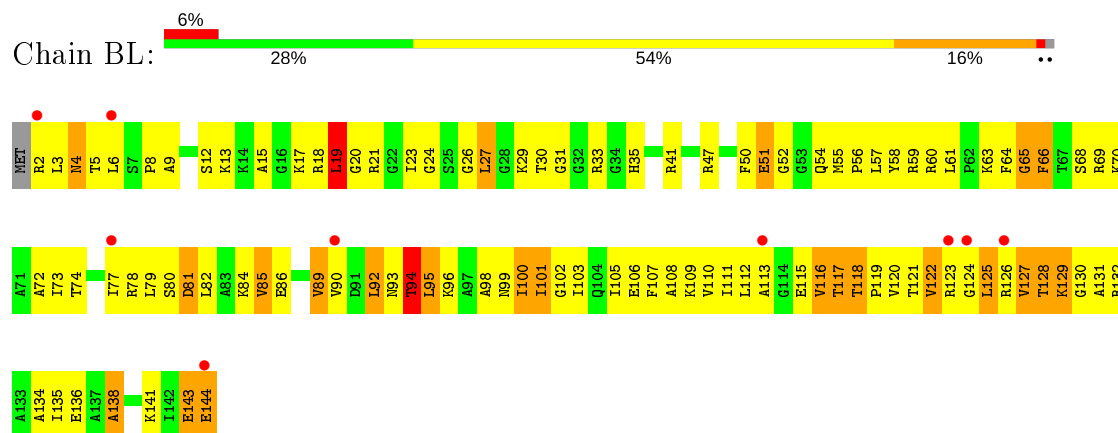
- Molecule 36: 50S ribosomal protein L34



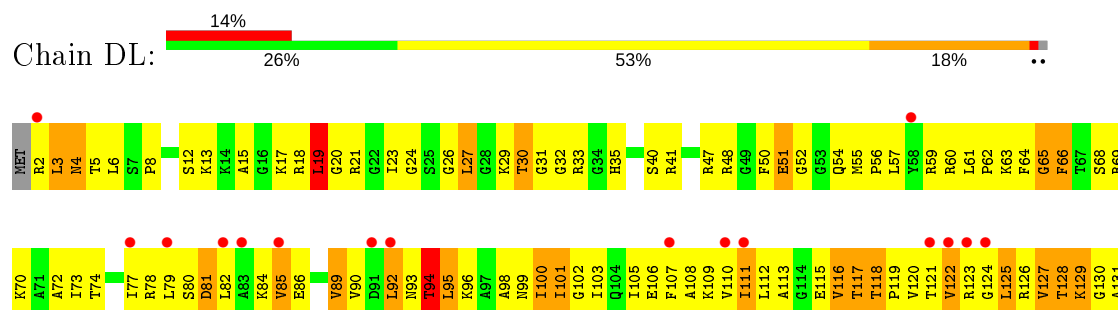
- Molecule 36: 50S ribosomal protein L34

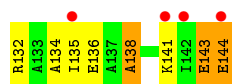


- Molecule 37: 50S ribosomal protein L15

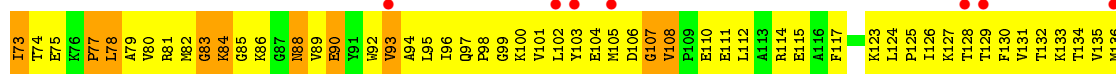
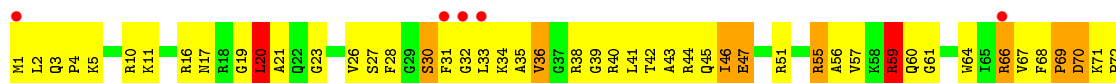


- Molecule 37: 50S ribosomal protein L15

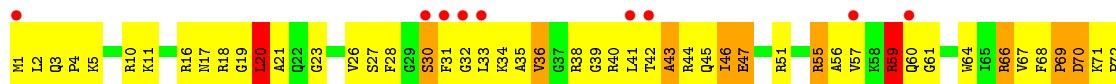




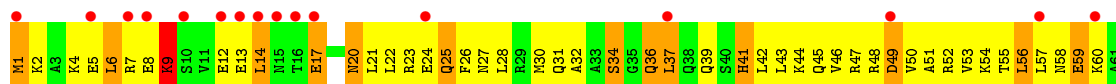
- Molecule 38: 50S ribosomal protein L16



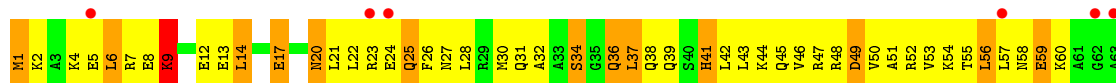
- Molecule 38: 50S ribosomal protein L16



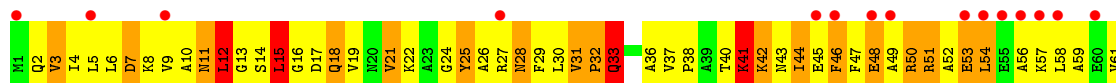
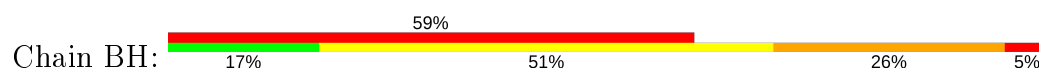
- Molecule 39: 50S ribosomal protein L29

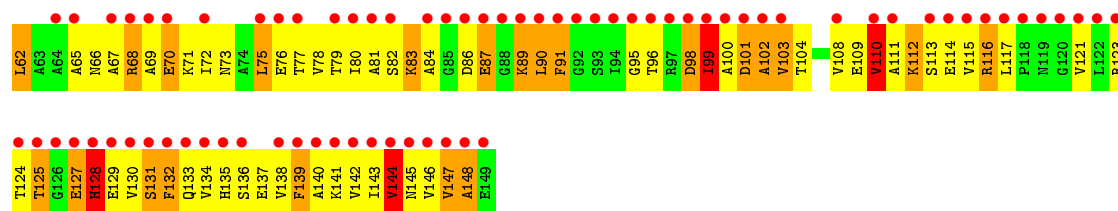


- Molecule 39: 50S ribosomal protein L29

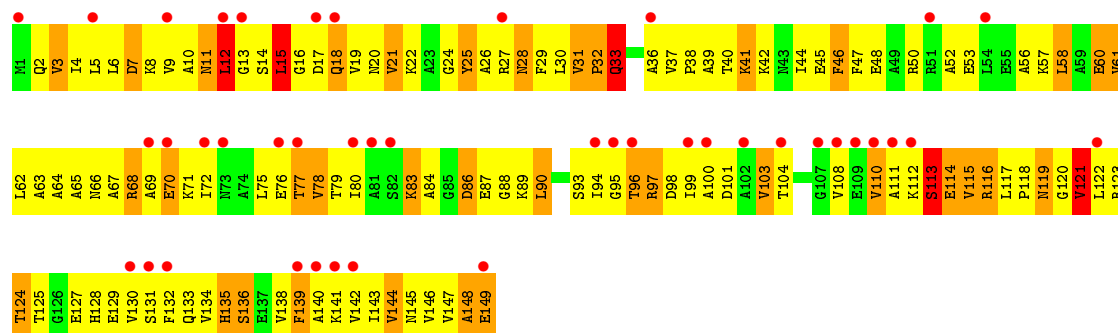
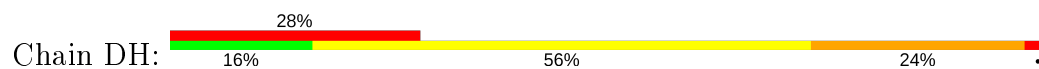


- Molecule 40: 50S ribosomal protein L9

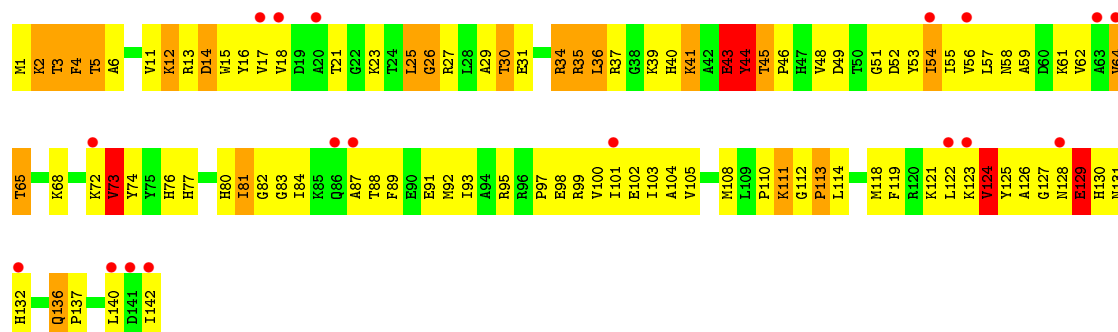




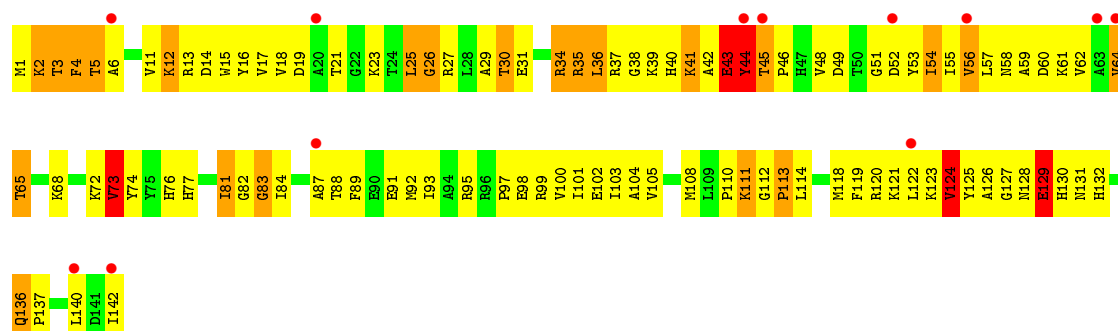
• Molecule 40: 50S ribosomal protein L9



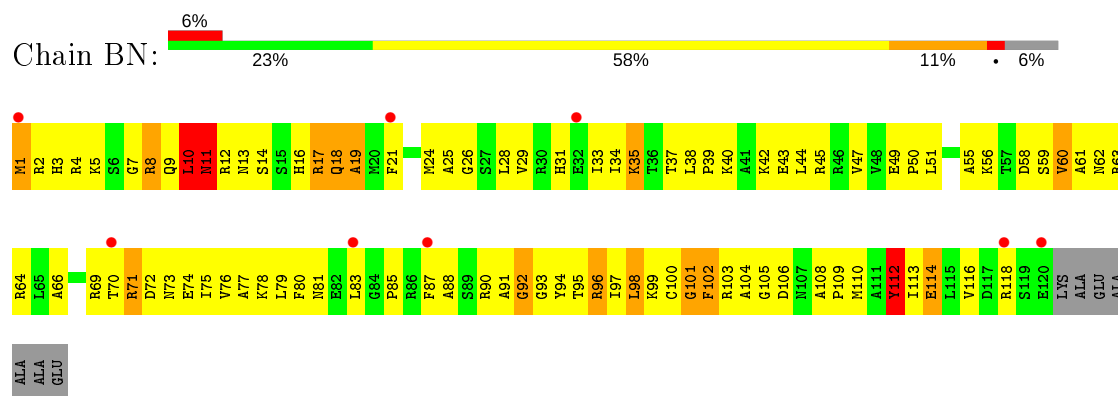
• Molecule 41: 50S ribosomal protein L13



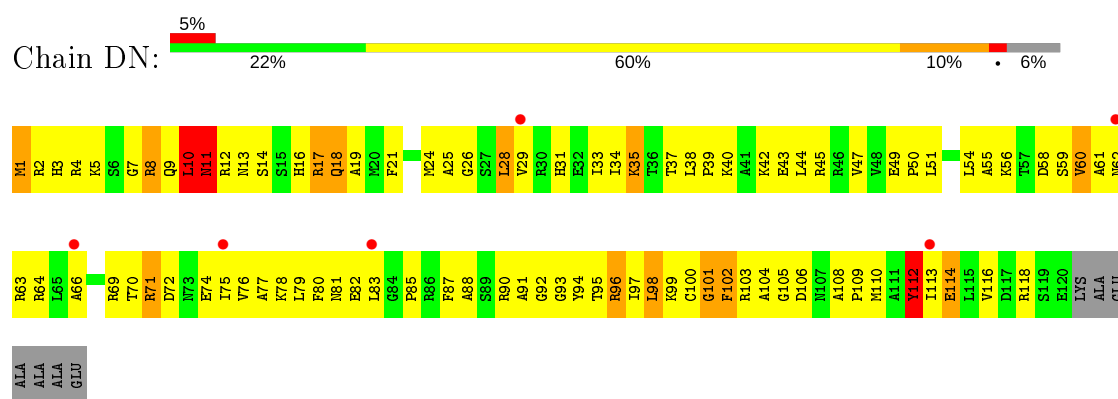
• Molecule 41: 50S ribosomal protein L13



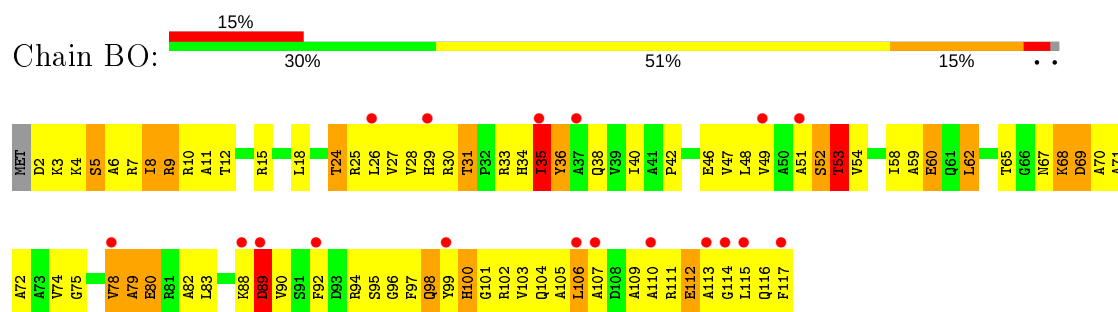
- Molecule 42: 50S ribosomal protein L17



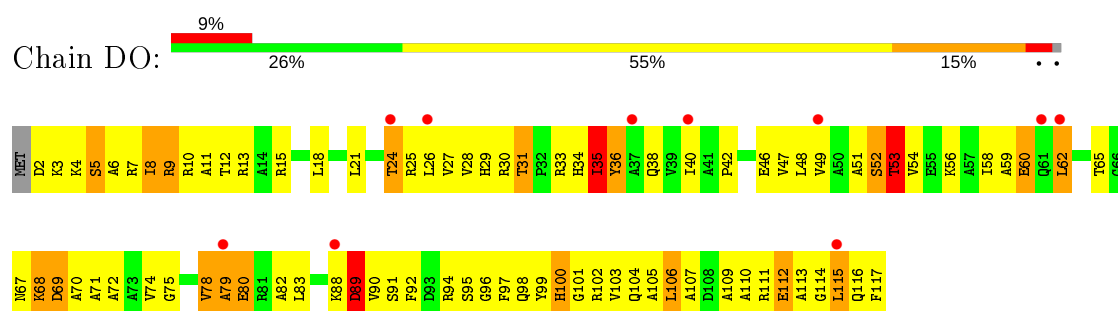
- Molecule 42: 50S ribosomal protein L17



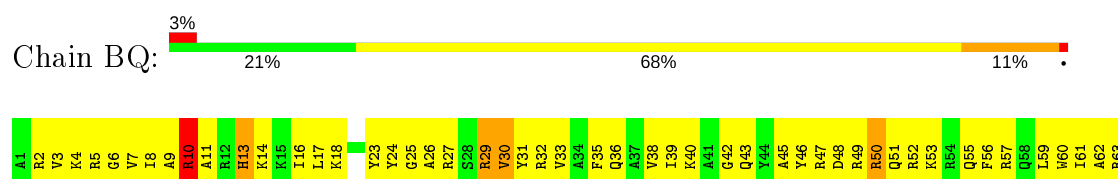
- Molecule 43: 50S ribosomal protein L18



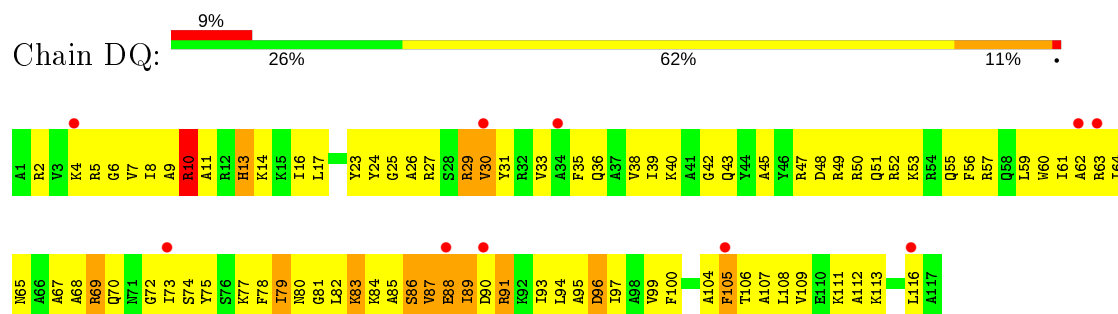
- Molecule 43: 50S ribosomal protein L18



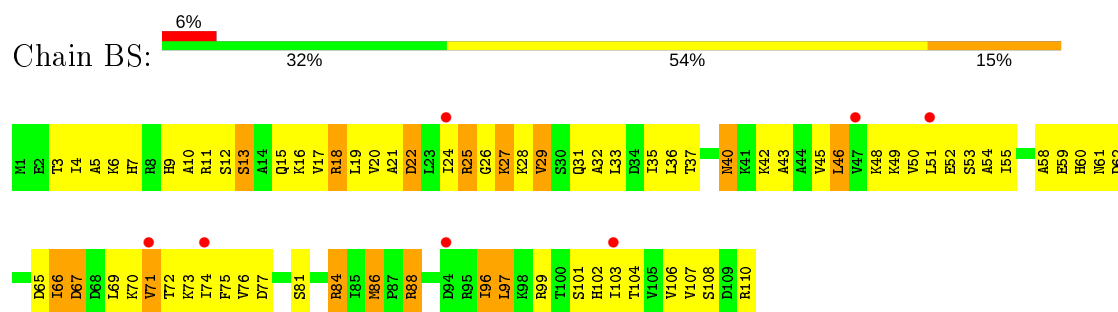
- Molecule 44: 50S ribosomal protein L20



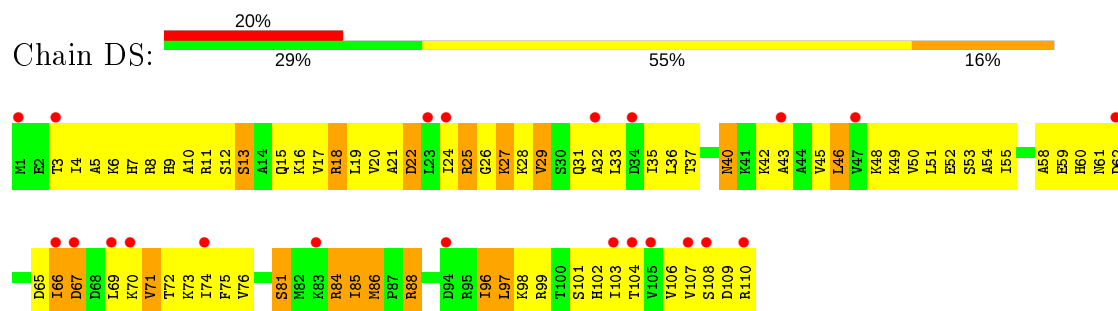
• Molecule 44: 50S ribosomal protein L20



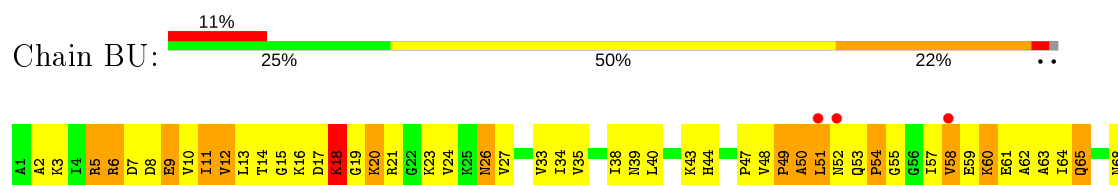
• Molecule 45: 50S ribosomal protein L22

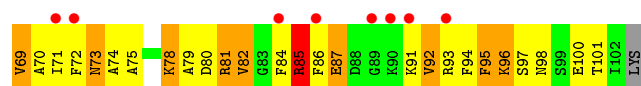


• Molecule 45: 50S ribosomal protein L22

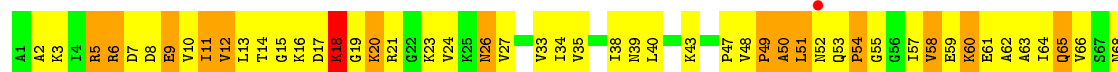


• Molecule 46: 50S ribosomal protein L24

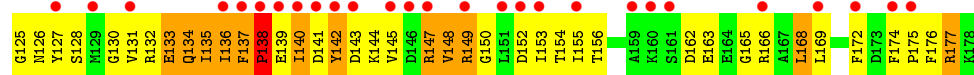
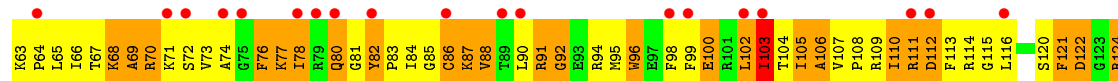
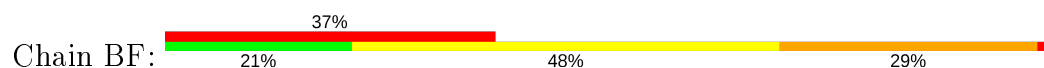




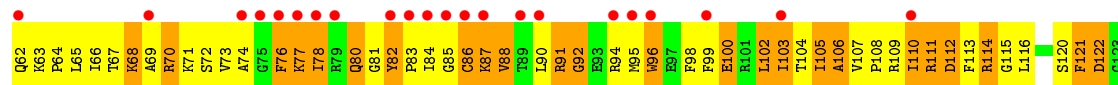
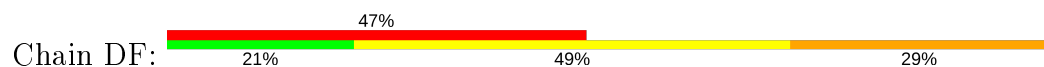
- Molecule 46: 50S ribosomal protein L24



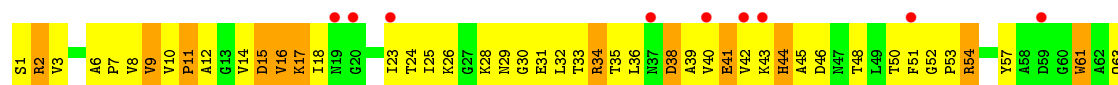
- Molecule 47: 50S ribosomal protein L5

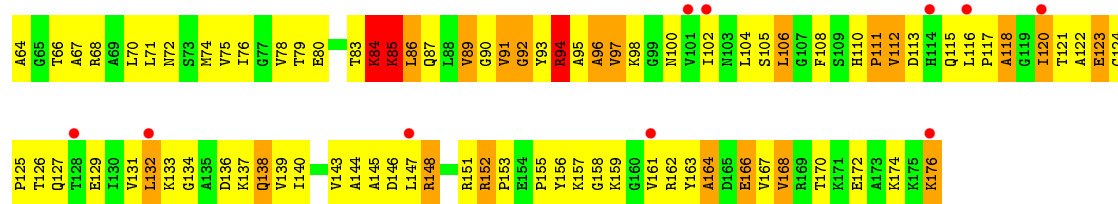


- Molecule 47: 50S ribosomal protein L5

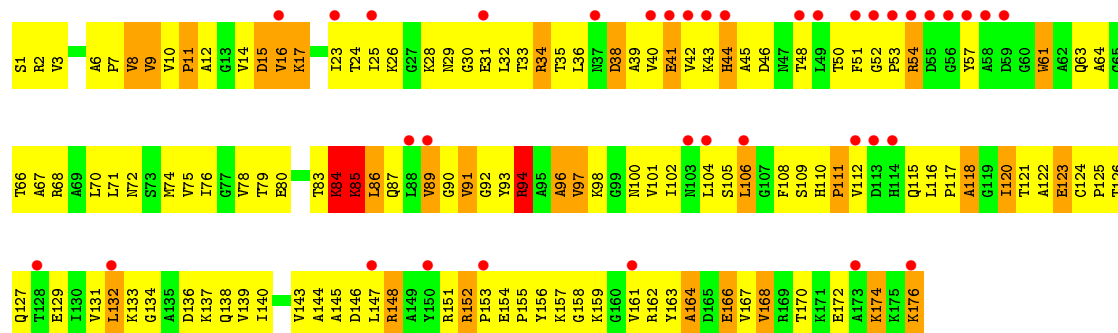


- Molecule 48: 50S ribosomal protein L6

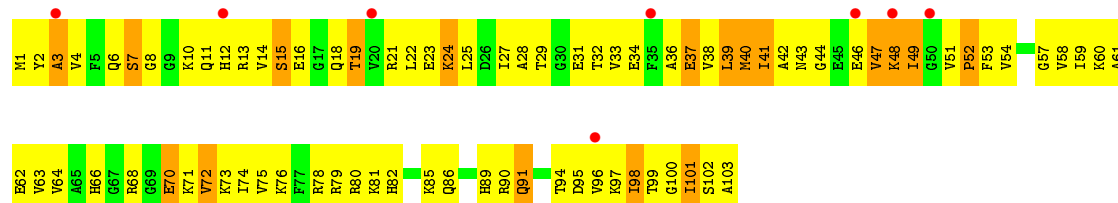




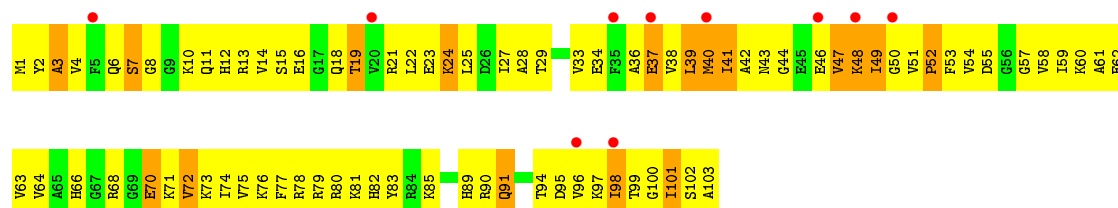
• Molecule 48: 50S ribosomal protein L6



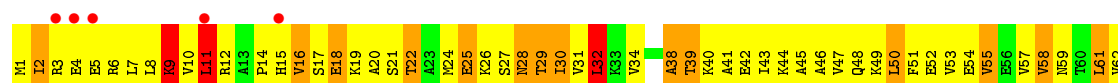
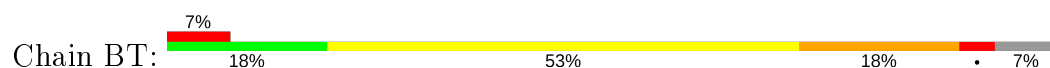
• Molecule 49: 50S ribosomal protein L21

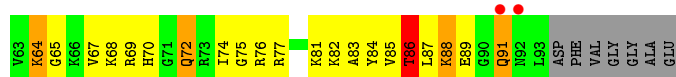


• Molecule 49: 50S ribosomal protein L21

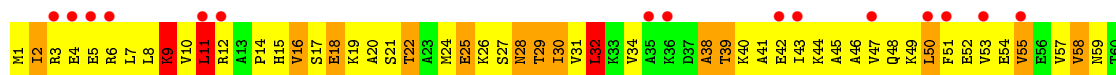
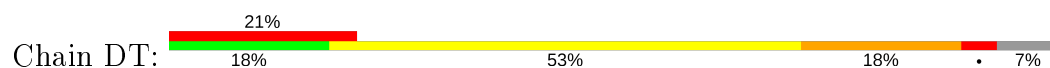


• Molecule 50: 50S ribosomal protein L23

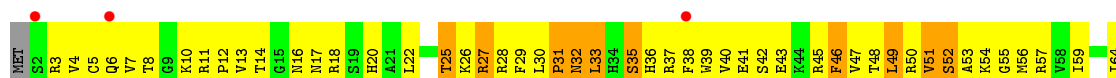




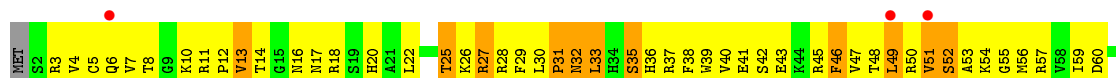
- Molecule 50: 50S ribosomal protein L23



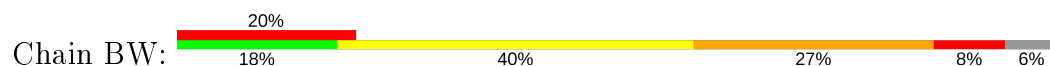
- Molecule 51: 50S ribosomal protein L28



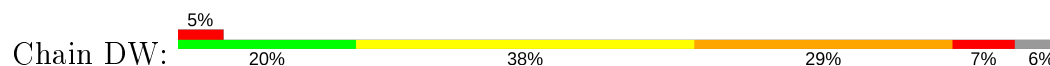
- Molecule 51: 50S ribosomal protein L28



- Molecule 52: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L27





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.50 182.94 – 3.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.50) 73.0 (182.94-3.53)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.306 0.228 , 0.266	Depositor DCC
R_{free} test set	25277 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	132.6	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 79.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284201	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% 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: SCM, ZN, MG, NMY

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	0.26	1/36762 (0.0%)	0.75	9/57350 (0.0%)
1	CA	0.32	2/36762 (0.0%)	0.77	8/57350 (0.0%)
2	AC	0.23	0/1651	0.45	0/2225
2	CC	0.23	0/1651	0.46	0/2225
3	AD	0.23	0/1665	0.43	0/2227
3	CD	0.23	0/1665	0.43	0/2227
4	AE	0.23	0/1118	0.46	0/1504
4	CE	0.23	0/1118	0.46	0/1504
5	AF	0.24	0/835	0.44	0/1128
5	CF	0.24	0/835	0.44	0/1128
6	AG	0.23	0/1187	0.44	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.45	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.44	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.48	0/1077
9	CJ	0.23	0/796	0.47	0/1077
10	AK	0.24	0/893	0.45	0/1205
10	CK	0.24	0/893	0.45	0/1205
11	AL	0.22	0/969	0.48	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AP	0.25	0/659	0.46	0/884
13	CP	0.25	0/648	0.46	0/870
14	AQ	0.24	0/657	0.46	0/881
14	CQ	0.24	0/666	0.46	0/892
15	AR	0.23	0/462	0.44	0/621
15	CR	0.23	0/462	0.45	0/621
16	AS	0.25	0/652	0.45	0/877
16	CS	0.25	0/660	0.49	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.24	0/671	0.40	0/888
17	CT	0.23	0/671	0.40	0/888
18	AB	0.25	0/1735	0.44	0/2338
18	CB	0.25	0/1735	0.45	0/2338
19	AU	0.26	0/430	0.46	0/570
19	CU	0.26	0/430	0.46	0/570
20	AO	0.23	0/722	0.44	0/964
20	CO	0.23	0/722	0.43	0/964
21	AN	0.24	0/785	0.43	0/1043
21	CN	0.24	0/785	0.45	0/1043
22	BA	0.25	0/2803	0.75	0/4371
22	DA	0.25	0/2803	0.74	0/4371
23	BB	0.28	6/68314 (0.0%)	0.77	42/106569 (0.0%)
23	DB	0.28	6/68314 (0.0%)	0.77	41/106569 (0.0%)
24	BI	0.24	0/1046	0.46	0/1410
24	DI	0.25	0/1046	0.47	0/1410
25	BC	0.22	0/2121	0.47	0/2852
25	DC	0.22	0/2121	0.47	0/2852
26	BD	0.24	0/1586	0.47	0/2134
26	DD	0.24	0/1586	0.47	0/2134
27	BK	0.23	0/939	0.52	0/1258
27	DK	0.23	0/939	0.52	0/1258
28	BP	0.24	0/929	0.49	0/1242
28	DP	0.24	0/929	0.49	0/1242
29	BE	0.24	0/1571	0.49	0/2113
29	DE	0.24	0/1571	0.49	0/2113
30	BY	0.24	0/453	0.48	0/605
30	DY	0.24	0/453	0.48	0/605
31	B0	0.22	0/450	0.51	0/599
31	D0	0.22	0/450	0.51	0/599
32	B4	0.23	0/303	0.44	0/397
32	D4	0.23	0/303	0.44	0/397
33	B1	0.27	0/416	0.47	0/554
33	D1	0.27	0/416	0.47	0/554
34	B3	0.24	0/513	0.47	0/676
34	D3	0.24	0/513	0.47	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.43	0/1025
36	B2	0.26	0/380	0.47	0/498
36	D2	0.26	0/380	0.47	0/498
37	BL	0.23	0/1054	0.47	0/1403
37	DL	0.23	0/1054	0.47	0/1403
38	BM	0.25	0/1093	0.47	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.47	0/1460
39	BX	0.24	0/510	0.52	0/677
39	DX	0.24	0/510	0.52	0/677
40	BH	0.25	0/1122	0.45	0/1515
40	DH	0.25	0/1122	0.46	0/1515
41	BJ	0.23	0/1152	0.47	0/1551
41	DJ	0.23	0/1152	0.47	0/1551
42	BN	0.24	0/973	0.49	0/1301
42	DN	0.24	0/973	0.49	0/1301
43	BO	0.23	0/902	0.47	0/1209
43	DO	0.23	0/902	0.47	0/1209
44	BQ	0.25	0/960	0.46	0/1278
44	DQ	0.25	0/960	0.46	0/1278
45	BS	0.21	0/864	0.50	0/1156
45	DS	0.21	0/864	0.50	0/1156
46	BU	0.25	0/787	0.45	0/1051
46	DU	0.25	0/787	0.45	0/1051
47	BF	0.25	0/1444	0.50	0/1937
47	DF	0.25	0/1444	0.50	0/1937
48	BG	0.23	0/1343	0.46	0/1816
48	DG	0.23	0/1343	0.46	0/1816
49	BR	0.25	0/829	0.46	0/1107
49	DR	0.25	0/829	0.46	0/1107
50	BT	0.22	0/744	0.51	0/994
50	DT	0.22	0/744	0.51	0/994
51	BZ	0.25	0/635	0.48	0/848
51	DZ	0.25	0/635	0.48	0/848
52	BW	0.28	0/603	0.48	0/797
52	DW	0.27	0/603	0.48	0/797
All	All	0.27	15/306360 (0.0%)	0.70	100/457969 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	13
1	CA	0	20
23	BB	0	44
23	DB	0	43
All	All	0	120

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-15.92	1.26	1.41
23	DB	1086	A	C5-C6	-15.80	1.26	1.41
23	BB	1088	A	C6-N1	-10.61	1.28	1.35
23	DB	1088	A	C6-N1	-10.48	1.28	1.35
23	DB	1060	U	C2-N3	7.81	1.43	1.37

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-29.68	75.09	110.70
23	BB	2204	G	O5'-P-OP2	-28.72	76.23	110.70
23	DB	2791	G	O5'-P-OP2	-27.53	77.67	110.70
23	BB	2791	G	O5'-P-OP1	-27.53	77.67	110.70
23	DB	2791	G	O5'-P-OP1	17.94	132.23	110.70

There are no chirality outliers.

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	437	U	Sidechain
1	AA	438	U	Sidechain
1	AA	86	G	Sidechain

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	32831	0	16521	1291	0
1	CA	32831	0	16521	1302	0
2	AC	1624	0	1699	189	0
2	CC	1624	0	1699	189	0
3	AD	1643	0	1710	127	0
3	CD	1643	0	1710	128	0
4	AE	1105	0	1148	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CE	1105	0	1148	93	0
5	AF	817	0	808	95	0
5	CF	817	0	808	91	0
6	AG	1174	0	1230	150	0
6	CG	1196	0	1246	114	0
7	AH	979	0	1034	68	0
7	CH	979	0	1034	70	0
8	AI	1022	0	1070	146	0
8	CI	1022	0	1070	136	0
9	AJ	786	0	828	100	0
9	CJ	786	0	828	98	0
10	AK	877	0	887	108	0
10	CK	877	0	887	97	0
11	AL	955	0	1019	96	0
11	CL	955	0	1019	97	0
12	AM	883	0	944	160	0
12	CM	876	0	937	116	0
13	AP	649	0	666	58	0
13	CP	638	0	656	50	0
14	AQ	648	0	691	63	0
14	CQ	657	0	702	59	0
15	AR	455	0	478	40	0
15	CR	455	0	478	43	0
16	AS	637	0	665	107	0
16	CS	644	0	675	106	0
17	AT	665	0	714	60	0
17	CT	665	0	714	64	0
18	AB	1704	0	1732	193	0
18	CB	1704	0	1732	210	0
19	AU	425	0	449	74	0
19	CU	425	0	449	67	0
20	AO	714	0	734	65	0
20	CO	714	0	734	50	0
21	AN	774	0	827	109	0
21	CN	774	0	827	113	0
22	BA	2507	0	1270	104	0
22	DA	2507	0	1270	107	0
23	BB	60995	0	30679	2216	0
23	DB	60995	0	30678	2313	0
24	BI	1032	0	1088	112	0
24	DI	1032	0	1088	176	0
25	BC	2082	0	2157	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DC	2082	0	2157	218	0
26	BD	1565	0	1616	206	0
26	DD	1565	0	1616	207	0
27	BK	930	0	1000	130	0
27	DK	930	0	1000	138	0
28	BP	917	0	965	115	0
28	DP	917	0	965	118	0
29	BE	1552	0	1619	199	0
29	DE	1552	0	1619	183	0
30	BY	449	0	491	58	0
30	DY	449	0	491	57	0
31	B0	444	0	461	35	0
31	D0	444	0	461	40	0
32	B4	302	0	340	42	0
32	D4	302	0	340	39	0
33	B1	409	0	440	34	0
33	D1	409	0	440	38	0
34	B3	504	0	574	50	0
34	D3	504	0	574	44	0
35	BV	753	0	780	102	0
35	DV	753	0	780	100	0
36	B2	377	0	418	48	0
36	D2	377	0	418	45	0
37	BL	1045	0	1117	139	0
37	DL	1045	0	1117	153	0
38	BM	1074	0	1157	116	0
38	DM	1074	0	1157	115	0
39	BX	509	0	543	63	0
39	DX	509	0	543	67	0
40	BH	1111	0	1148	193	0
40	DH	1111	0	1148	179	0
41	BJ	1129	0	1162	130	0
41	DJ	1129	0	1162	127	0
42	BN	960	0	1000	115	0
42	DN	960	0	1000	114	0
43	BO	892	0	923	93	0
43	DO	892	0	923	102	0
44	BQ	947	0	1022	143	0
44	DQ	947	0	1022	143	0
45	BS	857	0	922	86	0
45	DS	857	0	922	92	0
46	BU	779	0	834	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DU	779	0	834	111	0
47	BF	1420	0	1460	223	0
47	DF	1420	0	1460	216	0
48	BG	1323	0	1374	188	0
48	DG	1323	0	1374	178	0
49	BR	816	0	839	110	0
49	DR	816	0	839	105	0
50	BT	738	0	807	107	0
50	DT	738	0	807	116	0
51	BZ	625	0	652	68	0
51	DZ	625	0	652	67	0
52	BW	596	0	610	134	0
52	DW	596	0	610	127	0
53	AA	42	0	46	0	0
53	BB	42	0	46	0	0
53	CA	42	0	46	0	0
53	DB	42	0	46	1	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	59	0	0	0	0
54	DB	111	0	0	0	0
55	AA	23	0	24	5	0
55	CA	23	0	24	1	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	290	0	0	2	0
57	AE	1	0	0	0	0
57	AK	1	0	0	0	0
57	AL	4	0	0	0	0
57	AN	1	0	0	0	0
57	AP	1	0	0	0	0
57	AT	2	0	0	0	0
57	BB	492	0	0	4	0
57	BC	7	0	0	0	0
57	BD	1	0	0	0	0
57	BE	4	0	0	0	0
57	BH	1	0	0	0	0
57	BL	2	0	0	0	0
57	CA	282	0	0	2	0
57	CE	2	0	0	0	0
57	CI	1	0	0	0	0
57	CL	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CN	3	0	0	0	0
57	CP	1	0	0	0	0
57	CT	1	0	0	0	0
57	DB	501	0	0	14	0
57	DC	4	0	0	0	0
57	DD	1	0	0	0	0
57	DE	2	0	0	0	0
57	DL	1	0	0	0	0
57	DN	2	0	0	0	0
57	DR	1	0	0	0	0
All	All	284201	0	190895	16740	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

The worst 5 of 16740 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)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.32	1.27
23:BB:2305:U:H1'	47:BF:132:ARG:HA	1.33	1.10
40:BH:125:THR:HA	40:BH:146:VAL:HB	1.28	1.10
18:CB:69:VAL:HG23	18:CB:162:VAL:HB	1.34	1.09
23:DB:1098:A:H3'	24:DI:3:LYS:HA	1.32	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AC	204/232 (88%)	130 (64%)	44 (22%)	30 (15%)	0 3
2	CC	204/232 (88%)	137 (67%)	49 (24%)	18 (9%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	153 (75%)	40 (20%)	10 (5%)	2	19
3	CD	203/205 (99%)	153 (75%)	40 (20%)	10 (5%)	2	19
4	AE	148/166 (89%)	116 (78%)	24 (16%)	8 (5%)	2	17
4	CE	148/166 (89%)	114 (77%)	25 (17%)	9 (6%)	1	15
5	AF	98/135 (73%)	63 (64%)	25 (26%)	10 (10%)	0	7
5	CF	98/135 (73%)	64 (65%)	24 (24%)	10 (10%)	0	7
6	AG	148/178 (83%)	110 (74%)	30 (20%)	8 (5%)	2	17
6	CG	150/178 (84%)	111 (74%)	28 (19%)	11 (7%)	1	11
7	AH	127/129 (98%)	92 (72%)	31 (24%)	4 (3%)	4	30
7	CH	127/129 (98%)	92 (72%)	31 (24%)	4 (3%)	4	30
8	AI	125/129 (97%)	80 (64%)	35 (28%)	10 (8%)	1	10
8	CI	125/129 (97%)	80 (64%)	34 (27%)	11 (9%)	1	8
9	AJ	96/103 (93%)	59 (62%)	25 (26%)	12 (12%)	0	5
9	CJ	96/103 (93%)	64 (67%)	22 (23%)	10 (10%)	0	7
10	AK	115/128 (90%)	87 (76%)	23 (20%)	5 (4%)	2	22
10	CK	115/128 (90%)	86 (75%)	24 (21%)	5 (4%)	2	22
11	AL	121/123 (98%)	69 (57%)	37 (31%)	15 (12%)	0	5
11	CL	121/123 (98%)	72 (60%)	34 (28%)	15 (12%)	0	5
12	AM	112/117 (96%)	74 (66%)	25 (22%)	13 (12%)	0	5
12	CM	111/117 (95%)	78 (70%)	21 (19%)	12 (11%)	0	6
13	AP	80/82 (98%)	53 (66%)	20 (25%)	7 (9%)	1	8
13	CP	78/82 (95%)	52 (67%)	19 (24%)	7 (9%)	1	8
14	AQ	78/83 (94%)	59 (76%)	15 (19%)	4 (5%)	2	19
14	CQ	79/83 (95%)	57 (72%)	18 (23%)	4 (5%)	2	19
15	AR	53/74 (72%)	40 (76%)	13 (24%)	0	100	100
15	CR	53/74 (72%)	41 (77%)	11 (21%)	1 (2%)	8	40
16	AS	77/91 (85%)	49 (64%)	24 (31%)	4 (5%)	2	18
16	CS	78/91 (86%)	57 (73%)	16 (20%)	5 (6%)	1	14
17	AT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	1	15
17	CT	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	1	15
18	AB	216/240 (90%)	135 (62%)	56 (26%)	25 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CB	216/240 (90%)	145 (67%)	52 (24%)	19 (9%)	1	8
19	AU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	0	5
19	CU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	0	5
20	AO	86/89 (97%)	62 (72%)	18 (21%)	6 (7%)	1	12
20	CO	86/89 (97%)	60 (70%)	25 (29%)	1 (1%)	13	50
21	AN	92/100 (92%)	53 (58%)	30 (33%)	9 (10%)	0	7
21	CN	92/100 (92%)	49 (53%)	31 (34%)	12 (13%)	0	4
24	BI	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	4	31
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	3	26
25	BC	269/272 (99%)	163 (61%)	63 (23%)	43 (16%)	0	2
25	DC	269/272 (99%)	162 (60%)	61 (23%)	46 (17%)	0	2
26	BD	207/209 (99%)	118 (57%)	57 (28%)	32 (16%)	0	3
26	DD	207/209 (99%)	118 (57%)	58 (28%)	31 (15%)	0	3
27	BK	119/123 (97%)	70 (59%)	27 (23%)	22 (18%)	0	2
27	DK	119/123 (97%)	69 (58%)	29 (24%)	21 (18%)	0	2
28	BP	112/114 (98%)	66 (59%)	29 (26%)	17 (15%)	0	3
28	DP	112/114 (98%)	66 (59%)	29 (26%)	17 (15%)	0	3
29	BE	199/201 (99%)	124 (62%)	51 (26%)	24 (12%)	0	5
29	DE	199/201 (99%)	124 (62%)	48 (24%)	27 (14%)	0	4
30	BY	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	8
30	DY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	8
31	B0	54/56 (96%)	36 (67%)	12 (22%)	6 (11%)	0	6
31	D0	54/56 (96%)	36 (67%)	12 (22%)	6 (11%)	0	6
32	B4	36/38 (95%)	20 (56%)	9 (25%)	7 (19%)	0	2
32	D4	36/38 (95%)	21 (58%)	8 (22%)	7 (19%)	0	2
33	B1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	9
33	D1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	9
34	B3	62/64 (97%)	39 (63%)	17 (27%)	6 (10%)	0	7
34	D3	62/64 (97%)	39 (63%)	18 (29%)	5 (8%)	1	9
35	BV	92/94 (98%)	60 (65%)	22 (24%)	10 (11%)	0	6
35	DV	92/94 (98%)	59 (64%)	23 (25%)	10 (11%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	B2	44/46 (96%)	25 (57%)	16 (36%)	3 (7%)	1	13
36	D2	44/46 (96%)	24 (54%)	16 (36%)	4 (9%)	1	8
37	BL	141/144 (98%)	78 (55%)	44 (31%)	19 (14%)	0	4
37	DL	141/144 (98%)	78 (55%)	42 (30%)	21 (15%)	0	3
38	BM	134/136 (98%)	90 (67%)	28 (21%)	16 (12%)	0	5
38	DM	134/136 (98%)	91 (68%)	26 (19%)	17 (13%)	0	4
39	BX	61/63 (97%)	35 (57%)	22 (36%)	4 (7%)	1	13
39	DX	61/63 (97%)	35 (57%)	22 (36%)	4 (7%)	1	13
40	BH	147/149 (99%)	74 (50%)	42 (29%)	31 (21%)	0	1
40	DH	147/149 (99%)	86 (58%)	38 (26%)	23 (16%)	0	2
41	BJ	140/142 (99%)	88 (63%)	33 (24%)	19 (14%)	0	4
41	DJ	140/142 (99%)	88 (63%)	32 (23%)	20 (14%)	0	3
42	BN	118/127 (93%)	74 (63%)	31 (26%)	13 (11%)	0	6
42	DN	118/127 (93%)	74 (63%)	32 (27%)	12 (10%)	0	7
43	BO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	10
43	DO	114/117 (97%)	79 (69%)	25 (22%)	10 (9%)	1	8
44	BQ	115/117 (98%)	76 (66%)	32 (28%)	7 (6%)	1	15
44	DQ	115/117 (98%)	75 (65%)	33 (29%)	7 (6%)	1	15
45	BS	108/110 (98%)	67 (62%)	28 (26%)	13 (12%)	0	5
45	DS	108/110 (98%)	67 (62%)	28 (26%)	13 (12%)	0	5
46	BU	100/103 (97%)	50 (50%)	35 (35%)	15 (15%)	0	3
46	DU	100/103 (97%)	54 (54%)	31 (31%)	15 (15%)	0	3
47	BF	176/178 (99%)	102 (58%)	48 (27%)	26 (15%)	0	3
47	DF	176/178 (99%)	102 (58%)	48 (27%)	26 (15%)	0	3
48	BG	174/176 (99%)	111 (64%)	40 (23%)	23 (13%)	0	4
48	DG	174/176 (99%)	110 (63%)	40 (23%)	24 (14%)	0	3
49	BR	101/103 (98%)	59 (58%)	31 (31%)	11 (11%)	0	6
49	DR	101/103 (98%)	59 (58%)	31 (31%)	11 (11%)	0	6
50	BT	91/100 (91%)	49 (54%)	25 (28%)	17 (19%)	0	2
50	DT	91/100 (91%)	47 (52%)	27 (30%)	17 (19%)	0	2
51	BZ	75/78 (96%)	50 (67%)	17 (23%)	8 (11%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DZ	75/78 (96%)	48 (64%)	19 (25%)	8 (11%)	0	6
52	BW	77/84 (92%)	26 (34%)	26 (34%)	25 (32%)	0	0
52	DW	77/84 (92%)	26 (34%)	25 (32%)	26 (34%)	0	0
All	All	11241/11914 (94%)	7227 (64%)	2767 (25%)	1247 (11%)	0	6

5 of 1247 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	11	LEU
2	AC	14	VAL
2	AC	25	THR
2	AC	54	ILE
2	AC	83	VAL

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	AC	170/189 (90%)	137 (81%)	33 (19%)	1	7
2	CC	170/189 (90%)	139 (82%)	31 (18%)	1	9
3	AD	172/172 (100%)	153 (89%)	19 (11%)	6	29
3	CD	172/172 (100%)	154 (90%)	18 (10%)	7	31
4	AE	113/125 (90%)	90 (80%)	23 (20%)	1	6
4	CE	113/125 (90%)	91 (80%)	22 (20%)	1	7
5	AF	87/116 (75%)	75 (86%)	12 (14%)	3	20
5	CF	87/116 (75%)	74 (85%)	13 (15%)	3	17
6	AG	123/146 (84%)	104 (85%)	19 (15%)	2	16
6	CG	125/146 (86%)	102 (82%)	23 (18%)	1	8
7	AH	104/104 (100%)	96 (92%)	8 (8%)	13	42
7	CH	104/104 (100%)	97 (93%)	7 (7%)	16	48
8	AI	105/106 (99%)	88 (84%)	17 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/106 (99%)	77 (73%)	28 (27%)	0	3
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	3	19
9	CJ	86/90 (96%)	75 (87%)	11 (13%)	4	22
10	AK	90/98 (92%)	77 (86%)	13 (14%)	3	18
10	CK	90/98 (92%)	76 (84%)	14 (16%)	2	16
11	AL	103/103 (100%)	84 (82%)	19 (18%)	1	8
11	CL	103/103 (100%)	84 (82%)	19 (18%)	1	8
12	AM	92/95 (97%)	79 (86%)	13 (14%)	3	19
12	CM	91/95 (96%)	70 (77%)	21 (23%)	1	4
13	AP	65/65 (100%)	56 (86%)	9 (14%)	3	20
13	CP	65/65 (100%)	56 (86%)	9 (14%)	3	20
14	AQ	74/77 (96%)	65 (88%)	9 (12%)	5	23
14	CQ	75/77 (97%)	66 (88%)	9 (12%)	5	24
15	AR	48/64 (75%)	42 (88%)	6 (12%)	4	23
15	CR	48/64 (75%)	42 (88%)	6 (12%)	4	23
16	AS	70/78 (90%)	48 (69%)	22 (31%)	0	2
16	CS	71/78 (91%)	53 (75%)	18 (25%)	0	3
17	AT	65/65 (100%)	56 (86%)	9 (14%)	3	20
17	CT	65/65 (100%)	56 (86%)	9 (14%)	3	20
18	AB	180/198 (91%)	149 (83%)	31 (17%)	2	11
18	CB	180/198 (91%)	141 (78%)	39 (22%)	1	5
19	AU	44/60 (73%)	33 (75%)	11 (25%)	0	4
19	CU	44/60 (73%)	33 (75%)	11 (25%)	0	4
20	AO	76/77 (99%)	69 (91%)	7 (9%)	9	36
20	CO	76/77 (99%)	64 (84%)	12 (16%)	2	15
21	AN	79/83 (95%)	69 (87%)	10 (13%)	4	22
21	CN	79/83 (95%)	64 (81%)	15 (19%)	1	8
24	BI	109/109 (100%)	108 (99%)	1 (1%)	78	90
24	DI	109/109 (100%)	103 (94%)	6 (6%)	21	54
25	BC	216/217 (100%)	184 (85%)	32 (15%)	3	17
25	DC	216/217 (100%)	184 (85%)	32 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	164/164 (100%)	136 (83%)	28 (17%)	2	12
26	DD	164/164 (100%)	136 (83%)	28 (17%)	2	12
27	BK	102/104 (98%)	74 (72%)	28 (28%)	0	3
27	DK	102/104 (98%)	73 (72%)	29 (28%)	0	3
28	BP	99/99 (100%)	83 (84%)	16 (16%)	2	14
28	DP	99/99 (100%)	83 (84%)	16 (16%)	2	14
29	BE	165/165 (100%)	146 (88%)	19 (12%)	5	26
29	DE	165/165 (100%)	145 (88%)	20 (12%)	5	24
30	BY	48/48 (100%)	38 (79%)	10 (21%)	1	6
30	DY	48/48 (100%)	37 (77%)	11 (23%)	1	4
31	B0	47/47 (100%)	38 (81%)	9 (19%)	1	8
31	D0	47/47 (100%)	38 (81%)	9 (19%)	1	8
32	B4	34/34 (100%)	31 (91%)	3 (9%)	10	38
32	D4	34/34 (100%)	31 (91%)	3 (9%)	10	38
33	B1	45/48 (94%)	35 (78%)	10 (22%)	1	5
33	D1	45/48 (94%)	35 (78%)	10 (22%)	1	5
34	B3	51/51 (100%)	48 (94%)	3 (6%)	19	53
34	D3	51/51 (100%)	48 (94%)	3 (6%)	19	53
35	BV	78/78 (100%)	65 (83%)	13 (17%)	2	12
35	DV	78/78 (100%)	65 (83%)	13 (17%)	2	12
36	B2	38/38 (100%)	28 (74%)	10 (26%)	0	3
36	D2	38/38 (100%)	28 (74%)	10 (26%)	0	3
37	BL	102/103 (99%)	85 (83%)	17 (17%)	2	12
37	DL	102/103 (99%)	85 (83%)	17 (17%)	2	12
38	BM	109/109 (100%)	93 (85%)	16 (15%)	3	18
38	DM	109/109 (100%)	93 (85%)	16 (15%)	3	18
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	5
39	DX	55/55 (100%)	43 (78%)	12 (22%)	1	5
40	BH	114/114 (100%)	83 (73%)	31 (27%)	0	3
40	DH	114/114 (100%)	87 (76%)	27 (24%)	1	4
41	BJ	116/116 (100%)	100 (86%)	16 (14%)	3	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DJ	116/116 (100%)	100 (86%)	16 (14%)	3	20
42	BN	100/103 (97%)	86 (86%)	14 (14%)	3	19
42	DN	100/103 (97%)	85 (85%)	15 (15%)	3	17
43	BO	86/87 (99%)	68 (79%)	18 (21%)	1	6
43	DO	86/87 (99%)	67 (78%)	19 (22%)	1	5
44	BQ	89/89 (100%)	77 (86%)	12 (14%)	4	21
44	DQ	89/89 (100%)	77 (86%)	12 (14%)	4	21
45	BS	93/93 (100%)	85 (91%)	8 (9%)	10	38
45	DS	93/93 (100%)	83 (89%)	10 (11%)	6	30
46	BU	83/84 (99%)	68 (82%)	15 (18%)	1	9
46	DU	83/84 (99%)	68 (82%)	15 (18%)	1	9
47	BF	149/149 (100%)	111 (74%)	38 (26%)	0	3
47	DF	149/149 (100%)	112 (75%)	37 (25%)	0	4
48	BG	137/137 (100%)	114 (83%)	23 (17%)	2	12
48	DG	137/137 (100%)	113 (82%)	24 (18%)	2	10
49	BR	84/84 (100%)	71 (84%)	13 (16%)	2	16
49	DR	84/84 (100%)	72 (86%)	12 (14%)	3	19
50	BT	80/84 (95%)	66 (82%)	14 (18%)	2	10
50	DT	80/84 (95%)	66 (82%)	14 (18%)	2	10
51	BZ	67/68 (98%)	57 (85%)	10 (15%)	3	17
51	DZ	67/68 (98%)	56 (84%)	11 (16%)	2	13
52	BW	59/62 (95%)	44 (75%)	15 (25%)	0	3
52	DW	59/62 (95%)	44 (75%)	15 (25%)	0	3
All	All	9333/9700 (96%)	7780 (83%)	1553 (17%)	2	13

5 of 1553 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BG	174	LYS
15	CR	38	ILE
46	DU	78	LYS
50	BT	25	GLU
4	CE	115	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 349 such sidechains are listed below:

Mol	Chain	Res	Type
48	BG	127	GLN
10	CK	21	HIS
46	DU	26	ASN
49	BR	86	GLN
3	CD	70	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	285 (18%)	20 (1%)
1	CA	1529/1542 (99%)	255 (16%)	20 (1%)
22	BA	116/120 (96%)	21 (18%)	1 (0%)
22	DA	116/120 (96%)	20 (17%)	1 (0%)
23	BB	2837/2904 (97%)	444 (15%)	16 (0%)
23	DB	2838/2904 (97%)	437 (15%)	20 (0%)
All	All	8965/9132 (98%)	1462 (16%)	78 (0%)

5 of 1462 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	15	G
1	AA	32	A
1	AA	39	G

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2867	G
1	CA	372	C
23	DB	2336	A
23	BB	2894	G
1	CA	243	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 348 ligands modelled in this entry, 342 are monoatomic - leaving 6 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
53	NMY	BB	3001	-	45,45,45	2.05	12 (26%)	63,67,67	1.22	7 (11%)
53	NMY	AA	1601	-	45,45,45	2.11	13 (28%)	63,67,67	1.16	6 (9%)
53	NMY	CA	1601	-	45,45,45	2.03	13 (28%)	63,67,67	1.19	6 (9%)
55	SCM	AA	1662	-	23,25,25	1.65	7 (30%)	26,39,39	1.32	3 (11%)
55	SCM	CA	1661	-	23,25,25	1.66	7 (30%)	26,39,39	1.32	3 (11%)
53	NMY	DB	3001	-	45,45,45	2.07	13 (28%)	63,67,67	1.23	6 (9%)

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
53	NMY	BB	3001	-	-	6/18/94/94	0/4/4/4
53	NMY	AA	1601	-	-	4/18/94/94	0/4/4/4
53	NMY	CA	1601	-	-	4/18/94/94	0/4/4/4
55	SCM	AA	1662	-	-	2/4/57/57	0/3/3/3
55	SCM	CA	1661	-	-	2/4/57/57	0/3/3/3
53	NMY	DB	3001	-	-	5/18/94/94	0/4/4/4

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	DB	3001	NMY	C23-C22	5.18	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BB	3001	NMY	C23-C22	5.14	1.59	1.52
53	AA	1601	NMY	C23-C22	5.13	1.59	1.52
53	CA	1601	NMY	C23-C22	5.11	1.59	1.52
53	AA	1601	NMY	C3-C2	4.80	1.59	1.53

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AA	1662	SCM	C1M-N10-C10	-4.65	107.61	114.38
55	CA	1661	SCM	C1M-N10-C10	-4.63	107.64	114.38
53	DB	3001	NMY	O11-C13-O16	4.05	115.82	111.43
53	BB	3001	NMY	O18-C18-C19	3.61	114.44	108.22
53	CA	1601	NMY	O18-C18-C19	3.59	114.41	108.22

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	DB	3001	NMY	C4-C5-C6-N6
53	DB	3001	NMY	O5-C5-C6-N6
55	CA	1661	SCM	C9-C10-N10-C1M
55	CA	1661	SCM	C11-C10-N10-C1M
53	BB	3001	NMY	O16-C13-O11-C11

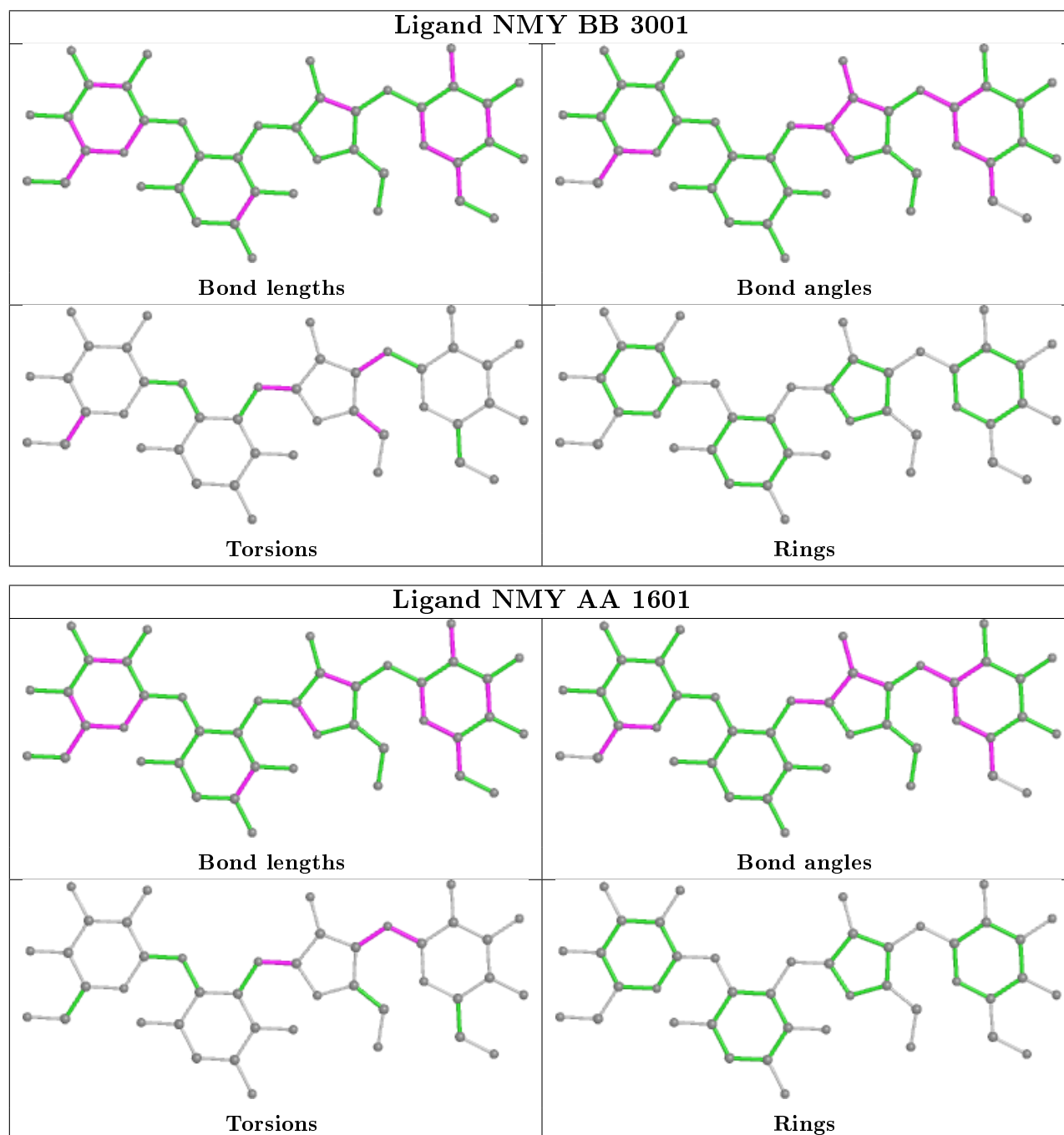
There are no ring outliers.

3 monomers are involved in 7 short contacts:

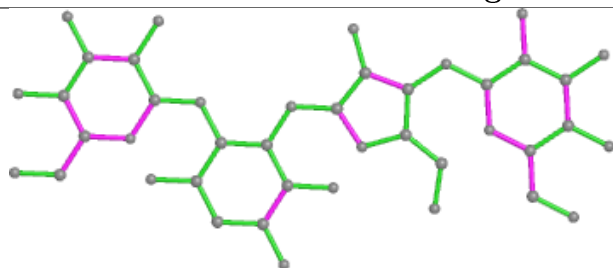
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	AA	1662	SCM	5	0
55	CA	1661	SCM	1	0
53	DB	3001	NMY	1	0

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.

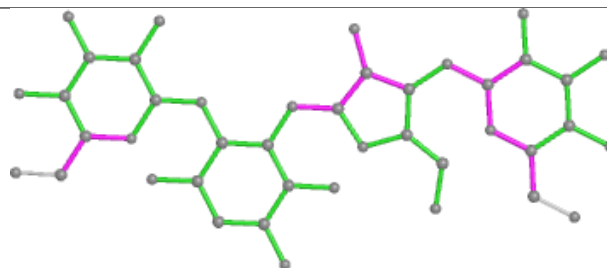
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



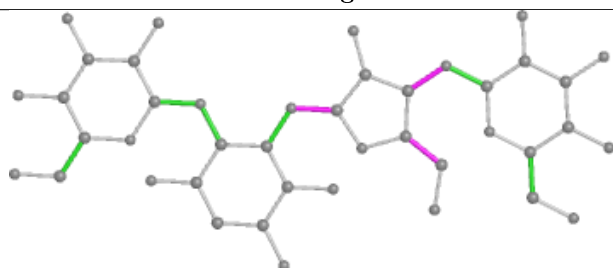
Ligand NMY CA 1601



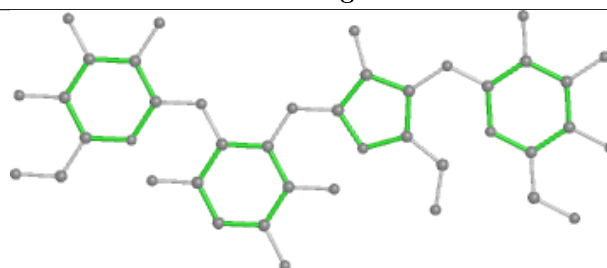
Bond lengths



Bond angles

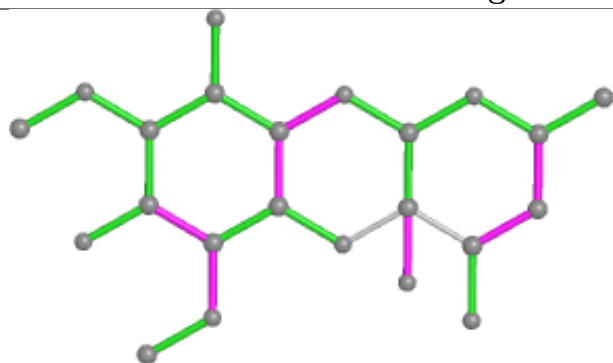


Torsions

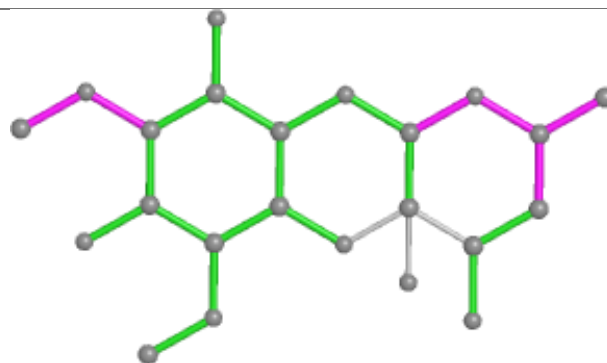


Rings

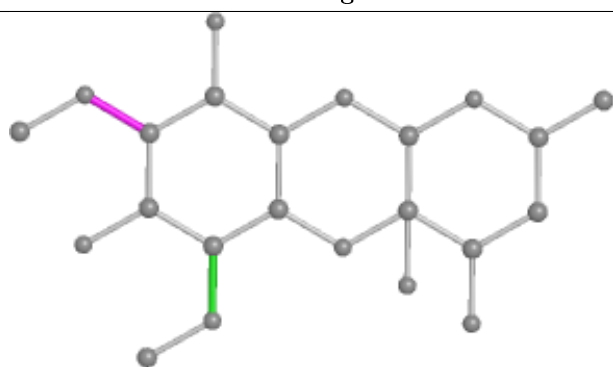
Ligand SCM AA 1662



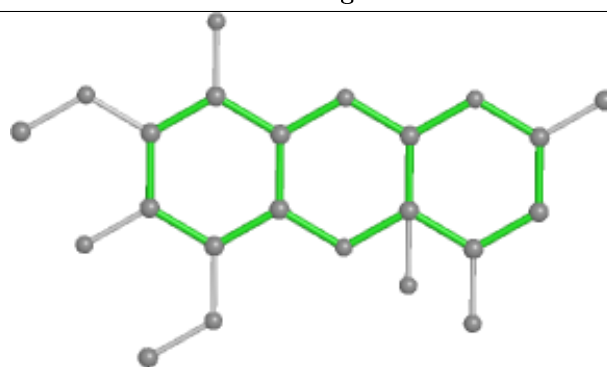
Bond lengths



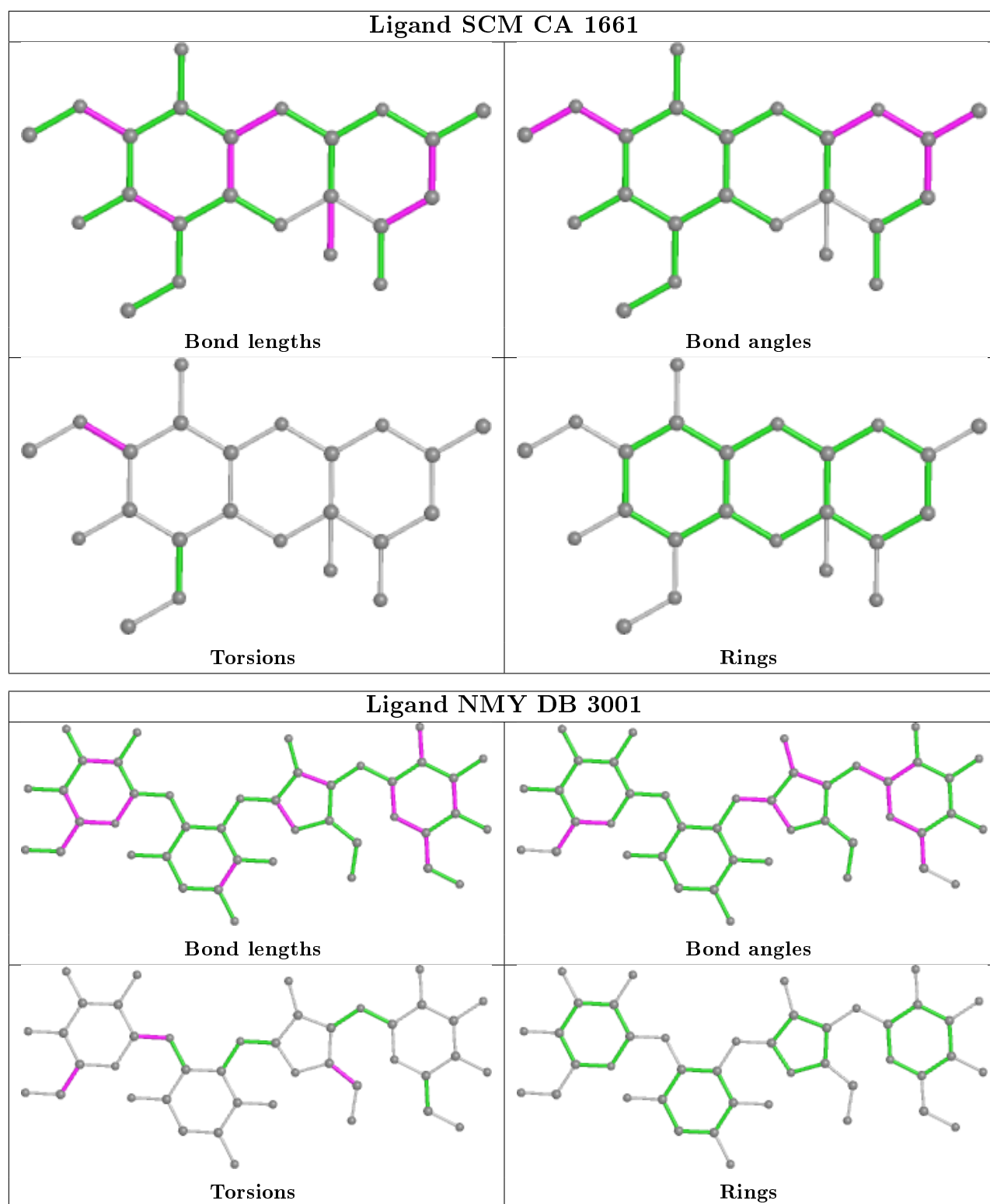
Bond angles



Torsions



Rings



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1530/1542 (99%)	-0.79	8 (0%) 91 88	16, 81, 159, 180	0
1	CA	1530/1542 (99%)	-0.72	1 (0%) 95 95	9, 57, 133, 180	0
2	AC	206/232 (88%)	0.45	20 (9%) 7 8	9, 76, 136, 180	0
2	CC	206/232 (88%)	0.28	15 (7%) 15 15	7, 75, 127, 180	0
3	AD	205/205 (100%)	0.60	25 (12%) 4 5	24, 92, 157, 180	0
3	CD	205/205 (100%)	0.50	15 (7%) 15 15	10, 64, 139, 180	0
4	AE	150/166 (90%)	0.50	14 (9%) 8 9	11, 74, 139, 176	0
4	CE	150/166 (90%)	0.80	25 (16%) 1 2	5, 61, 132, 180	0
5	AF	100/135 (74%)	1.04	17 (17%) 1 2	11, 86, 144, 172	0
5	CF	100/135 (74%)	0.56	9 (9%) 9 10	7, 83, 173, 180	0
6	AG	150/178 (84%)	0.23	9 (6%) 21 19	23, 104, 153, 180	0
6	CG	152/178 (85%)	-0.04	4 (2%) 56 49	27, 90, 147, 180	0
7	AH	129/129 (100%)	0.91	21 (16%) 1 2	13, 88, 155, 180	0
7	CH	129/129 (100%)	0.57	13 (10%) 7 7	5, 61, 127, 180	0
8	AI	127/129 (98%)	0.45	16 (12%) 3 5	36, 91, 150, 180	0
8	CI	127/129 (98%)	0.07	4 (3%) 49 43	20, 92, 148, 180	0
9	AJ	98/103 (95%)	0.40	4 (4%) 37 33	22, 94, 151, 180	0
9	CJ	98/103 (95%)	0.75	12 (12%) 4 5	17, 89, 156, 180	0
10	AK	117/128 (91%)	0.05	6 (5%) 28 25	14, 67, 125, 180	0
10	CK	117/128 (91%)	0.07	3 (2%) 56 49	5, 56, 125, 178	0
11	AL	123/123 (100%)	0.49	13 (10%) 6 7	19, 80, 133, 180	0
11	CL	123/123 (100%)	0.18	6 (4%) 29 26	7, 51, 135, 180	0
12	AM	114/117 (97%)	0.71	21 (18%) 1 1	56, 120, 166, 180	0
12	CM	113/117 (96%)	0.59	17 (15%) 2 3	38, 109, 165, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	82/82 (100%)	2.15	30 (36%) 0 0	38, 91, 152, 180	0
13	CP	80/82 (97%)	0.50	10 (12%) 3 5	6, 63, 141, 180	0
14	AQ	80/83 (96%)	0.85	12 (15%) 2 3	37, 99, 151, 180	0
14	CQ	81/83 (97%)	0.54	2 (2%) 57 51	17, 71, 129, 180	0
15	AR	55/74 (74%)	0.54	2 (3%) 42 38	16, 76, 149, 180	0
15	CR	55/74 (74%)	0.41	4 (7%) 15 15	21, 66, 126, 180	0
16	AS	79/91 (86%)	1.60	30 (37%) 0 0	55, 121, 180, 180	0
16	CS	80/91 (87%)	1.05	18 (22%) 0 0	70, 109, 174, 180	0
17	AT	85/86 (98%)	-0.22	0 100 100	49, 106, 179, 180	0
17	CT	85/86 (98%)	-0.07	2 (2%) 59 53	19, 65, 143, 159	0
18	AB	218/240 (90%)	0.23	17 (7%) 13 13	22, 94, 153, 180	0
18	CB	218/240 (90%)	0.75	34 (15%) 2 2	19, 102, 160, 180	0
19	AU	51/70 (72%)	0.25	2 (3%) 39 35	29, 101, 151, 180	0
19	CU	51/70 (72%)	0.42	4 (7%) 13 13	24, 113, 155, 180	0
20	AO	88/89 (98%)	0.52	7 (7%) 12 12	18, 83, 137, 179	0
20	CO	88/89 (98%)	-0.11	0 100 100	7, 60, 118, 161	0
21	AN	96/100 (96%)	0.71	12 (12%) 3 5	13, 98, 151, 180	0
21	CN	96/100 (96%)	0.87	20 (20%) 1 1	12, 81, 150, 180	0
22	BA	117/120 (97%)	-0.26	2 (1%) 70 64	35, 74, 117, 167	0
22	DA	117/120 (97%)	-0.56	1 (0%) 84 79	36, 86, 127, 180	0
23	BB	2841/2904 (97%)	-0.48	28 (0%) 82 77	6, 54, 148, 180	0
23	DB	2841/2904 (97%)	-0.49	15 (0%) 91 88	5, 48, 146, 180	0
24	BI	141/141 (100%)	2.72	78 (55%) 0 0	95, 172, 180, 180	0
24	DI	141/141 (100%)	2.06	61 (43%) 0 0	91, 179, 180, 180	0
25	BC	271/272 (99%)	0.80	41 (15%) 2 3	5, 50, 103, 180	0
25	DC	271/272 (99%)	0.44	17 (6%) 20 18	5, 40, 100, 146	0
26	BD	209/209 (100%)	0.08	8 (3%) 40 36	7, 68, 146, 180	0
26	DD	209/209 (100%)	0.85	41 (19%) 1 1	5, 49, 129, 180	0
27	BK	121/123 (98%)	0.68	12 (9%) 7 8	7, 69, 139, 180	0
27	DK	121/123 (98%)	0.74	9 (7%) 14 14	5, 41, 118, 180	0
28	BP	114/114 (100%)	0.51	11 (9%) 8 8	26, 85, 142, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.32	2 (1%) 68 62	5, 49, 103, 145	0
29	BE	201/201 (100%)	0.86	34 (16%) 1 2	5, 63, 143, 180	0
29	DE	201/201 (100%)	0.42	17 (8%) 10 11	5, 70, 144, 180	0
30	BY	58/58 (100%)	0.41	4 (6%) 16 16	20, 62, 140, 180	0
30	DY	58/58 (100%)	-0.17	0 100 100	5, 66, 116, 142	0
31	B0	56/56 (100%)	0.16	4 (7%) 16 15	20, 80, 163, 180	0
31	D0	56/56 (100%)	0.21	3 (5%) 25 23	12, 58, 116, 165	0
32	B4	38/38 (100%)	0.16	1 (2%) 56 49	5, 75, 120, 137	0
32	D4	38/38 (100%)	-0.35	0 100 100	7, 60, 114, 135	0
33	B1	50/54 (92%)	1.27	7 (14%) 2 3	15, 70, 135, 180	0
33	D1	50/54 (92%)	0.65	5 (10%) 7 8	20, 69, 142, 157	0
34	B3	64/64 (100%)	0.48	5 (7%) 13 13	13, 50, 102, 148	0
34	D3	64/64 (100%)	0.33	3 (4%) 31 28	5, 42, 88, 133	0
35	BV	94/94 (100%)	0.54	9 (9%) 8 8	21, 89, 143, 180	0
35	DV	94/94 (100%)	0.29	13 (13%) 2 3	9, 96, 151, 169	0
36	B2	46/46 (100%)	0.49	3 (6%) 18 17	5, 43, 120, 143	0
36	D2	46/46 (100%)	0.14	2 (4%) 35 31	11, 43, 103, 159	0
37	BL	143/144 (99%)	0.29	9 (6%) 20 18	8, 67, 133, 172	0
37	DL	143/144 (99%)	0.59	20 (13%) 2 3	5, 56, 119, 164	0
38	BM	136/136 (100%)	0.56	12 (8%) 10 10	9, 59, 117, 170	0
38	DM	136/136 (100%)	0.61	16 (11%) 4 5	7, 60, 116, 137	0
39	BX	63/63 (100%)	1.32	18 (28%) 0 0	6, 86, 135, 180	0
39	DX	63/63 (100%)	0.64	6 (9%) 8 8	38, 106, 178, 180	0
40	BH	149/149 (100%)	2.92	88 (59%) 0 0	26, 134, 177, 180	0
40	DH	149/149 (100%)	1.37	42 (28%) 0 0	11, 112, 162, 180	0
41	BJ	142/142 (100%)	0.53	18 (12%) 3 4	5, 74, 127, 180	0
41	DJ	142/142 (100%)	0.62	12 (8%) 10 11	5, 59, 125, 180	0
42	BN	120/127 (94%)	0.39	8 (6%) 17 16	20, 65, 126, 180	0
42	DN	120/127 (94%)	0.18	6 (5%) 28 25	5, 43, 103, 180	0
43	BO	116/117 (99%)	0.63	18 (15%) 2 2	12, 77, 140, 180	0
43	DO	116/117 (99%)	0.41	10 (8%) 10 11	32, 85, 152, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	-0.27	3 (2%) 56 49	6, 57, 133, 175	0
44	DQ	117/117 (100%)	0.35	10 (8%) 10 11	5, 52, 112, 161	0
45	BS	110/110 (100%)	0.48	7 (6%) 19 18	5, 50, 125, 180	0
45	DS	110/110 (100%)	0.98	22 (20%) 1 1	5, 52, 131, 180	0
46	BU	102/103 (99%)	0.82	11 (10%) 5 6	5, 70, 146, 180	0
46	DU	102/103 (99%)	0.02	1 (0%) 82 77	22, 97, 158, 180	0
47	BF	178/178 (100%)	1.52	65 (36%) 0 0	52, 123, 180, 180	0
47	DF	178/178 (100%)	2.24	84 (47%) 0 0	33, 110, 176, 180	0
48	BG	176/176 (100%)	0.61	19 (10%) 5 6	26, 104, 165, 180	0
48	DG	176/176 (100%)	0.88	37 (21%) 1 1	26, 98, 169, 180	0
49	BR	103/103 (100%)	0.35	8 (7%) 13 13	11, 76, 142, 180	0
49	DR	103/103 (100%)	0.52	10 (9%) 7 8	13, 79, 144, 180	0
50	BT	93/100 (93%)	0.60	7 (7%) 14 14	16, 75, 150, 180	0
50	DT	93/100 (93%)	1.00	21 (22%) 0 0	13, 79, 154, 180	0
51	BZ	77/78 (98%)	0.64	8 (10%) 6 7	5, 53, 122, 137	0
51	DZ	77/78 (98%)	0.20	5 (6%) 18 17	5, 47, 124, 144	0
52	BW	79/84 (94%)	1.15	17 (21%) 0 1	8, 74, 121, 180	0
52	DW	79/84 (94%)	0.10	4 (5%) 28 25	9, 77, 144, 164	0
All	All	20417/21046 (97%)	0.11	1562 (7%) 13 13	5, 69, 155, 180	0

The worst 5 of 1562 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AP	82	ALA	19.5
24	BI	49	GLU	12.0
13	AP	81	ALA	11.9
47	DF	75	GLY	11.0
40	BH	142	VAL	10.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	AA	1636	1/1	0.09	0.15	121,121,121,121	0
54	MG	DB	3061	1/1	0.28	0.17	117,117,117,117	0
54	MG	CA	1652	1/1	0.29	0.12	128,128,128,128	0
54	MG	BB	3043	1/1	0.29	0.23	145,145,145,145	0
54	MG	AA	1660	1/1	0.38	0.40	148,148,148,148	0
54	MG	CA	1650	1/1	0.39	0.50	180,180,180,180	0
54	MG	DB	3067	1/1	0.49	0.09	137,137,137,137	0
54	MG	DB	3060	1/1	0.49	0.08	96,96,96,96	0
54	MG	AA	1638	1/1	0.53	0.31	126,126,126,126	0
54	MG	AA	1626	1/1	0.53	0.24	87,87,87,87	1
53	NMY	BB	3001	42/42	0.58	0.68	89,89,89,89	42
54	MG	CA	1647	1/1	0.61	0.08	153,153,153,153	0
54	MG	DB	3059	1/1	0.63	0.80	180,180,180,180	0
54	MG	AA	1607	1/1	0.66	0.12	93,93,93,93	0
54	MG	AA	1623	1/1	0.68	0.19	157,157,157,157	0
54	MG	AA	1618	1/1	0.69	0.20	160,160,160,160	0
54	MG	CA	1633	1/1	0.69	0.07	48,48,48,48	0
53	NMY	DB	3001	42/42	0.70	0.51	68,68,68,68	42
54	MG	CA	1653	1/1	0.71	0.10	96,96,96,96	0
54	MG	AA	1621	1/1	0.73	0.05	82,82,82,82	0
54	MG	AA	1620	1/1	0.73	0.12	132,132,132,132	0
54	MG	BB	3094	1/1	0.75	0.08	75,75,75,75	0
54	MG	AA	1653	1/1	0.77	0.11	110,110,110,110	0
54	MG	DB	3014	1/1	0.77	0.15	80,80,80,80	0
54	MG	CA	1654	1/1	0.80	0.09	82,82,82,82	0
54	MG	CA	1609	1/1	0.80	0.07	110,110,110,110	0
54	MG	AA	1657	1/1	0.81	0.23	95,95,95,95	0
54	MG	AA	1640	1/1	0.81	0.15	110,110,110,110	0
54	MG	BB	3034	1/1	0.82	0.40	130,130,130,130	0
54	MG	CA	1643	1/1	0.82	0.11	75,75,75,75	0
54	MG	AA	1647	1/1	0.82	0.12	133,133,133,133	0
54	MG	CA	1617	1/1	0.82	0.07	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1614	1/1	0.82	0.34	139,139,139,139	0
54	MG	DB	3030	1/1	0.82	0.15	81,81,81,81	0
54	MG	AA	1658	1/1	0.83	0.26	120,120,120,120	0
54	MG	CA	1648	1/1	0.83	0.05	69,69,69,69	0
54	MG	BB	3081	1/1	0.83	0.09	77,77,77,77	0
54	MG	BB	3101	1/1	0.84	0.23	157,157,157,157	0
54	MG	AA	1625	1/1	0.84	0.20	102,102,102,102	0
54	MG	CA	1651	1/1	0.84	0.46	161,161,161,161	0
54	MG	DB	3054	1/1	0.84	0.11	80,80,80,80	0
54	MG	BB	3086	1/1	0.84	0.16	18,18,18,18	0
54	MG	BB	3079	1/1	0.85	0.08	68,68,68,68	0
54	MG	DB	3045	1/1	0.85	0.05	32,32,32,32	0
54	MG	AA	1634	1/1	0.85	0.10	88,88,88,88	0
54	MG	CA	1649	1/1	0.85	0.08	92,92,92,92	0
54	MG	DB	3074	1/1	0.86	0.12	29,29,29,29	0
54	MG	AA	1645	1/1	0.86	0.08	67,67,67,67	0
54	MG	DB	3084	1/1	0.86	0.16	109,109,109,109	0
54	MG	DB	3031	1/1	0.86	0.16	21,21,21,21	0
54	MG	AA	1646	1/1	0.86	0.08	89,89,89,89	0
54	MG	AA	1648	1/1	0.86	0.40	110,110,110,110	0
54	MG	DB	3027	1/1	0.86	0.12	72,72,72,72	0
54	MG	AA	1609	1/1	0.86	0.11	107,107,107,107	0
53	NMY	AA	1601	42/42	0.86	0.23	75,75,75,75	0
54	MG	DB	3035	1/1	0.86	0.09	80,80,80,80	0
54	MG	DB	3091	1/1	0.86	0.06	55,55,55,55	0
54	MG	CA	1656	1/1	0.87	0.09	135,135,135,135	0
54	MG	CA	1618	1/1	0.87	0.15	104,104,104,104	0
54	MG	AA	1659	1/1	0.87	0.05	111,111,111,111	0
54	MG	BB	3093	1/1	0.87	0.07	32,32,32,32	0
54	MG	BB	3069	1/1	0.87	0.07	41,41,41,41	0
54	MG	AA	1603	1/1	0.87	0.07	100,100,100,100	0
54	MG	CA	1613	1/1	0.88	0.18	108,108,108,108	0
54	MG	CA	1630	1/1	0.88	0.10	81,81,81,81	0
54	MG	DB	3046	1/1	0.88	0.08	104,104,104,104	0
54	MG	AA	1652	1/1	0.88	0.04	101,101,101,101	0
54	MG	AA	1651	1/1	0.88	0.07	97,97,97,97	0
54	MG	DB	3023	1/1	0.88	0.07	7,7,7,7	0
54	MG	BB	3044	1/1	0.88	0.15	118,118,118,118	0
54	MG	CA	1626	1/1	0.88	0.08	117,117,117,117	0
54	MG	AA	1615	1/1	0.89	0.10	123,123,123,123	0
54	MG	DB	3016	1/1	0.89	0.10	53,53,53,53	0
54	MG	BB	3039	1/1	0.89	0.09	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BB	3027	1/1	0.89	0.14	42,42,42,42	0
54	MG	CA	1646	1/1	0.90	0.03	52,52,52,52	0
54	MG	BB	3048	1/1	0.90	0.09	145,145,145,145	0
54	MG	DB	3051	1/1	0.90	0.11	67,67,67,67	0
54	MG	BB	3095	1/1	0.90	0.08	36,36,36,36	0
53	NMY	CA	1601	42/42	0.90	0.22	47,47,47,47	0
54	MG	CA	1645	1/1	0.90	0.08	70,70,70,70	0
54	MG	DB	3036	1/1	0.90	0.10	85,85,85,85	0
54	MG	DB	3093	1/1	0.90	0.12	98,98,98,98	0
54	MG	BB	3058	1/1	0.91	0.17	63,63,63,63	0
54	MG	AA	1650	1/1	0.91	0.06	105,105,105,105	0
54	MG	DB	3096	1/1	0.91	0.07	115,115,115,115	0
54	MG	BB	3036	1/1	0.91	0.05	26,26,26,26	0
54	MG	DB	3073	1/1	0.91	0.07	62,62,62,62	0
54	MG	CA	1635	1/1	0.91	0.07	64,64,64,64	0
54	MG	DB	3094	1/1	0.91	0.15	5,5,5,5	0
54	MG	BB	3045	1/1	0.91	0.13	42,42,42,42	0
54	MG	BB	3050	1/1	0.91	0.07	16,16,16,16	0
54	MG	BB	3029	1/1	0.91	0.22	21,21,21,21	0
54	MG	BB	3005	1/1	0.91	0.07	29,29,29,29	0
54	MG	DB	3053	1/1	0.91	0.07	90,90,90,90	0
54	MG	CA	1607	1/1	0.92	0.16	129,129,129,129	0
54	MG	BB	3082	1/1	0.92	0.11	34,34,34,34	0
54	MG	BB	3014	1/1	0.92	0.06	11,11,11,11	0
54	MG	CA	1619	1/1	0.92	0.08	53,53,53,53	0
54	MG	AA	1616	1/1	0.92	0.14	113,113,113,113	0
54	MG	BB	3024	1/1	0.92	0.15	12,12,12,12	0
54	MG	AA	1622	1/1	0.92	0.06	24,24,24,24	0
54	MG	AA	1655	1/1	0.92	0.06	73,73,73,73	0
54	MG	BB	3011	1/1	0.92	0.10	62,62,62,62	0
54	MG	BB	3038	1/1	0.92	0.13	46,46,46,46	0
54	MG	DB	3007	1/1	0.93	0.14	9,9,9,9	0
54	MG	BB	3054	1/1	0.93	0.07	46,46,46,46	0
54	MG	DB	3071	1/1	0.93	0.14	93,93,93,93	0
54	MG	DB	3056	1/1	0.93	0.11	34,34,34,34	0
54	MG	BB	3062	1/1	0.93	0.08	38,38,38,38	0
54	MG	DB	3112	1/1	0.93	0.23	87,87,87,87	0
54	MG	AA	1614	1/1	0.93	0.05	66,66,66,66	0
54	MG	AA	1654	1/1	0.93	0.09	49,49,49,49	0
54	MG	DB	3024	1/1	0.93	0.07	32,32,32,32	0
54	MG	AA	1633	1/1	0.93	0.14	65,65,65,65	0
54	MG	CA	1644	1/1	0.93	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	CA	1628	1/1	0.93	0.09	41,41,41,41	0
54	MG	BB	3080	1/1	0.93	0.10	44,44,44,44	0
54	MG	BB	3007	1/1	0.93	0.06	37,37,37,37	0
54	MG	CA	1608	1/1	0.94	0.04	31,31,31,31	0
54	MG	BB	3066	1/1	0.94	0.06	10,10,10,10	0
54	MG	BB	3072	1/1	0.94	0.08	54,54,54,54	0
54	MG	DB	3101	1/1	0.94	0.12	20,20,20,20	0
54	MG	DB	3075	1/1	0.94	0.17	58,58,58,58	0
54	MG	CA	1629	1/1	0.94	0.10	57,57,57,57	0
54	MG	BB	3052	1/1	0.94	0.12	67,67,67,67	0
55	SCM	CA	1661	23/23	0.94	0.16	37,37,37,37	0
54	MG	AA	1661	1/1	0.94	0.11	62,62,62,62	0
54	MG	BB	3083	1/1	0.94	0.13	5,5,5,5	0
54	MG	DB	3037	1/1	0.94	0.09	23,23,23,23	0
54	MG	BB	3056	1/1	0.94	0.15	23,23,23,23	0
54	MG	BB	3025	1/1	0.94	0.11	32,32,32,32	0
54	MG	AA	1643	1/1	0.94	0.13	43,43,43,43	0
54	MG	BB	3099	1/1	0.94	0.12	23,23,23,23	0
54	MG	BB	3035	1/1	0.94	0.06	41,41,41,41	0
54	MG	BB	3096	1/1	0.94	0.08	5,5,5,5	0
54	MG	AA	1624	1/1	0.95	0.32	13,13,13,13	1
54	MG	BB	3030	1/1	0.95	0.08	16,16,16,16	0
54	MG	BB	3009	1/1	0.95	0.08	80,80,80,80	0
54	MG	DB	3066	1/1	0.95	0.06	32,32,32,32	0
54	MG	DB	3028	1/1	0.95	0.10	17,17,17,17	0
54	MG	BB	3002	1/1	0.95	0.08	19,19,19,19	0
54	MG	CA	1641	1/1	0.95	0.14	61,61,61,61	0
54	MG	AA	1637	1/1	0.95	0.03	62,62,62,62	0
54	MG	DB	3049	1/1	0.95	0.06	66,66,66,66	0
54	MG	DB	3079	1/1	0.95	0.12	80,80,80,80	0
54	MG	BB	3053	1/1	0.95	0.07	30,30,30,30	0
54	MG	DB	3068	1/1	0.95	0.11	36,36,36,36	0
54	MG	AA	1606	1/1	0.95	0.19	56,56,56,56	0
54	MG	DB	3004	1/1	0.95	0.12	41,41,41,41	0
54	MG	BB	3067	1/1	0.95	0.09	26,26,26,26	0
54	MG	AA	1604	1/1	0.95	0.13	43,43,43,43	0
54	MG	CA	1659	1/1	0.95	0.06	45,45,45,45	0
54	MG	CA	1610	1/1	0.95	0.09	103,103,103,103	0
54	MG	BB	3004	1/1	0.95	0.06	31,31,31,31	0
54	MG	BB	3089	1/1	0.95	0.07	7,7,7,7	0
54	MG	CA	1604	1/1	0.95	0.07	66,66,66,66	0
56	ZN	D4	101	1/1	0.95	0.08	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BB	3032	1/1	0.95	0.12	38,38,38,38	0
54	MG	AA	1613	1/1	0.95	0.08	80,80,80,80	0
54	MG	DB	3058	1/1	0.95	0.08	39,39,39,39	0
54	MG	CA	1634	1/1	0.95	0.12	75,75,75,75	0
54	MG	DB	3029	1/1	0.95	0.04	30,30,30,30	0
54	MG	DB	3097	1/1	0.95	0.15	12,12,12,12	0
54	MG	CA	1638	1/1	0.95	0.10	123,123,123,123	0
54	MG	BB	3088	1/1	0.95	0.25	87,87,87,87	0
54	MG	CA	1606	1/1	0.95	0.06	7,7,7,7	0
54	MG	DB	3038	1/1	0.95	0.20	10,10,10,10	0
54	MG	BB	3098	1/1	0.95	0.09	85,85,85,85	0
54	MG	BB	3091	1/1	0.95	0.05	105,105,105,105	0
54	MG	DB	3033	1/1	0.95	0.07	82,82,82,82	0
54	MG	BB	3018	1/1	0.95	0.15	31,31,31,31	0
54	MG	BB	3084	1/1	0.95	0.16	61,61,61,61	0
54	MG	BB	3075	1/1	0.95	0.08	6,6,6,6	0
54	MG	BB	3031	1/1	0.95	0.06	53,53,53,53	0
54	MG	AA	1605	1/1	0.95	0.09	46,46,46,46	0
54	MG	BB	3017	1/1	0.96	0.08	43,43,43,43	0
54	MG	BB	3108	1/1	0.96	0.14	36,36,36,36	0
54	MG	DB	3095	1/1	0.96	0.05	39,39,39,39	0
54	MG	DB	3085	1/1	0.96	0.13	12,12,12,12	0
54	MG	CA	1616	1/1	0.96	0.07	15,15,15,15	0
54	MG	DB	3012	1/1	0.96	0.14	32,32,32,32	0
54	MG	BB	3040	1/1	0.96	0.18	44,44,44,44	0
54	MG	CA	1627	1/1	0.96	0.07	40,40,40,40	0
54	MG	DB	3110	1/1	0.96	0.09	17,17,17,17	0
56	ZN	B4	101	1/1	0.96	0.08	49,49,49,49	0
54	MG	DB	3032	1/1	0.96	0.14	5,5,5,5	0
54	MG	BB	3049	1/1	0.96	0.05	24,24,24,24	0
54	MG	AA	1639	1/1	0.96	0.05	65,65,65,65	0
54	MG	CA	1623	1/1	0.96	0.12	21,21,21,21	0
54	MG	BB	3015	1/1	0.96	0.03	32,32,32,32	0
54	MG	AA	1602	1/1	0.96	0.06	28,28,28,28	0
54	MG	AA	1628	1/1	0.96	0.07	53,53,53,53	0
54	MG	AA	1631	1/1	0.96	0.04	84,84,84,84	0
54	MG	AA	1629	1/1	0.96	0.09	55,55,55,55	0
54	MG	BB	3085	1/1	0.96	0.15	43,43,43,43	0
54	MG	BB	3100	1/1	0.96	0.11	34,34,34,34	0
54	MG	BB	3022	1/1	0.96	0.09	35,35,35,35	0
54	MG	DB	3005	1/1	0.96	0.14	23,23,23,23	0
54	MG	AA	1608	1/1	0.96	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DB	3100	1/1	0.96	0.15	6,6,6,6	0
55	SCM	AA	1662	23/23	0.96	0.14	23,23,23,23	0
54	MG	DB	3102	1/1	0.96	0.17	6,6,6,6	0
54	MG	AA	1617	1/1	0.96	0.11	47,47,47,47	0
54	MG	DB	3062	1/1	0.96	0.06	75,75,75,75	0
54	MG	CA	1622	1/1	0.96	0.11	44,44,44,44	0
54	MG	CA	1639	1/1	0.96	0.06	108,108,108,108	0
54	MG	AA	1641	1/1	0.96	0.15	88,88,88,88	0
54	MG	BB	3068	1/1	0.96	0.11	65,65,65,65	0
54	MG	BB	3047	1/1	0.96	0.11	66,66,66,66	0
54	MG	DB	3018	1/1	0.96	0.15	5,5,5,5	0
54	MG	BB	3078	1/1	0.96	0.15	47,47,47,47	0
54	MG	DB	3052	1/1	0.96	0.12	40,40,40,40	0
54	MG	BB	3090	1/1	0.97	0.10	54,54,54,54	0
54	MG	BB	3003	1/1	0.97	0.10	17,17,17,17	0
54	MG	AA	1627	1/1	0.97	0.11	5,5,5,5	1
54	MG	BB	3071	1/1	0.97	0.08	33,33,33,33	0
54	MG	DB	3050	1/1	0.97	0.12	6,6,6,6	0
54	MG	DB	3087	1/1	0.97	0.10	11,11,11,11	0
54	MG	DB	3022	1/1	0.97	0.09	5,5,5,5	0
54	MG	BB	3070	1/1	0.97	0.08	9,9,9,9	0
54	MG	DB	3106	1/1	0.97	0.16	53,53,53,53	0
54	MG	CA	1657	1/1	0.97	0.06	14,14,14,14	0
54	MG	DB	3006	1/1	0.97	0.14	13,13,13,13	0
54	MG	AA	1630	1/1	0.97	0.08	36,36,36,36	0
54	MG	BB	3073	1/1	0.97	0.06	35,35,35,35	0
54	MG	BB	3006	1/1	0.97	0.09	9,9,9,9	0
54	MG	BB	3107	1/1	0.97	0.07	30,30,30,30	0
54	MG	BB	3057	1/1	0.97	0.05	15,15,15,15	0
54	MG	DB	3011	1/1	0.97	0.09	9,9,9,9	0
54	MG	BB	3111	1/1	0.97	0.12	90,90,90,90	0
54	MG	DB	3057	1/1	0.97	0.09	11,11,11,11	0
54	MG	DB	3008	1/1	0.97	0.15	41,41,41,41	0
54	MG	AA	1649	1/1	0.97	0.10	31,31,31,31	0
54	MG	BB	3021	1/1	0.97	0.15	30,30,30,30	0
54	MG	BB	3105	1/1	0.97	0.17	18,18,18,18	0
54	MG	DB	3088	1/1	0.97	0.16	37,37,37,37	0
54	MG	CA	1624	1/1	0.97	0.07	21,21,21,21	0
54	MG	BB	3060	1/1	0.97	0.06	5,5,5,5	0
54	MG	DB	3043	1/1	0.97	0.09	32,32,32,32	0
54	MG	BB	3041	1/1	0.97	0.17	34,34,34,34	0
54	MG	BB	3106	1/1	0.97	0.20	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DB	3017	1/1	0.97	0.10	29,29,29,29	0
54	MG	DB	3105	1/1	0.97	0.10	41,41,41,41	0
54	MG	BB	3103	1/1	0.97	0.13	25,25,25,25	0
54	MG	DB	3092	1/1	0.97	0.16	12,12,12,12	0
54	MG	DB	3026	1/1	0.97	0.08	16,16,16,16	0
54	MG	AA	1656	1/1	0.97	0.14	95,95,95,95	0
54	MG	CA	1621	1/1	0.97	0.10	34,34,34,34	0
54	MG	DB	3098	1/1	0.97	0.17	41,41,41,41	0
54	MG	CA	1658	1/1	0.97	0.14	50,50,50,50	0
54	MG	DB	3015	1/1	0.97	0.07	37,37,37,37	0
54	MG	BB	3109	1/1	0.97	0.07	19,19,19,19	0
54	MG	DB	3040	1/1	0.97	0.08	78,78,78,78	0
54	MG	BB	3012	1/1	0.97	0.17	33,33,33,33	0
54	MG	DB	3104	1/1	0.97	0.11	31,31,31,31	0
54	MG	CA	1640	1/1	0.97	0.13	43,43,43,43	0
54	MG	CA	1655	1/1	0.97	0.06	52,52,52,52	0
54	MG	BB	3020	1/1	0.97	0.08	28,28,28,28	0
54	MG	DB	3009	1/1	0.97	0.09	49,49,49,49	0
54	MG	AA	1632	1/1	0.97	0.11	29,29,29,29	0
54	MG	DB	3039	1/1	0.97	0.11	19,19,19,19	0
54	MG	DB	3069	1/1	0.97	0.08	8,8,8,8	0
54	MG	CA	1612	1/1	0.98	0.07	25,25,25,25	0
54	MG	BB	3076	1/1	0.98	0.16	33,33,33,33	0
54	MG	DB	3111	1/1	0.98	0.09	36,36,36,36	0
54	MG	AA	1644	1/1	0.98	0.09	42,42,42,42	0
54	MG	CA	1620	1/1	0.98	0.09	62,62,62,62	0
54	MG	BB	3092	1/1	0.98	0.11	5,5,5,5	0
54	MG	DB	3025	1/1	0.98	0.11	47,47,47,47	0
54	MG	DB	3044	1/1	0.98	0.07	11,11,11,11	0
54	MG	DB	3109	1/1	0.98	0.08	33,33,33,33	0
54	MG	AA	1619	1/1	0.98	0.06	48,48,48,48	0
54	MG	DB	3070	1/1	0.98	0.15	38,38,38,38	0
54	MG	BB	3037	1/1	0.98	0.20	35,35,35,35	0
54	MG	BB	3046	1/1	0.98	0.10	50,50,50,50	0
54	MG	BB	3065	1/1	0.98	0.09	24,24,24,24	0
54	MG	DB	3089	1/1	0.98	0.10	13,13,13,13	0
54	MG	AA	1635	1/1	0.98	0.06	86,86,86,86	0
54	MG	BB	3055	1/1	0.98	0.06	46,46,46,46	0
54	MG	AA	1611	1/1	0.98	0.04	73,73,73,73	0
54	MG	CA	1615	1/1	0.98	0.07	29,29,29,29	0
54	MG	DB	3063	1/1	0.98	0.04	50,50,50,50	0
54	MG	DB	3082	1/1	0.98	0.07	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BB	3010	1/1	0.98	0.06	123,123,123,123	0
54	MG	DB	3055	1/1	0.98	0.09	22,22,22,22	0
54	MG	BB	3104	1/1	0.98	0.12	6,6,6,6	0
54	MG	BB	3051	1/1	0.98	0.05	34,34,34,34	0
54	MG	DB	3086	1/1	0.98	0.11	41,41,41,41	0
54	MG	DB	3083	1/1	0.98	0.06	37,37,37,37	0
54	MG	BB	3026	1/1	0.98	0.17	68,68,68,68	0
54	MG	BB	3008	1/1	0.98	0.18	81,81,81,81	0
54	MG	BB	3013	1/1	0.98	0.11	81,81,81,81	0
54	MG	DB	3077	1/1	0.98	0.12	28,28,28,28	0
54	MG	AA	1642	1/1	0.98	0.04	51,51,51,51	0
54	MG	BB	3028	1/1	0.98	0.05	24,24,24,24	0
54	MG	DB	3103	1/1	0.98	0.13	14,14,14,14	0
54	MG	DB	3048	1/1	0.98	0.16	14,14,14,14	0
54	MG	DB	3081	1/1	0.98	0.08	35,35,35,35	0
54	MG	CA	1660	1/1	0.98	0.07	77,77,77,77	0
54	MG	DB	3010	1/1	0.98	0.12	8,8,8,8	0
54	MG	DB	3078	1/1	0.98	0.11	24,24,24,24	0
54	MG	AA	1610	1/1	0.98	0.10	5,5,5,5	0
54	MG	DB	3020	1/1	0.98	0.10	6,6,6,6	0
54	MG	DB	3065	1/1	0.98	0.07	20,20,20,20	0
54	MG	CA	1632	1/1	0.98	0.05	31,31,31,31	0
54	MG	BB	3102	1/1	0.98	0.09	10,10,10,10	0
54	MG	DB	3080	1/1	0.98	0.09	46,46,46,46	0
54	MG	CA	1605	1/1	0.98	0.06	12,12,12,12	0
54	MG	DB	3047	1/1	0.98	0.08	27,27,27,27	0
54	MG	DB	3002	1/1	0.98	0.13	5,5,5,5	0
54	MG	BB	3110	1/1	0.98	0.15	61,61,61,61	0
54	MG	DB	3041	1/1	0.98	0.09	9,9,9,9	0
54	MG	BB	3077	1/1	0.99	0.09	5,5,5,5	0
54	MG	BB	3064	1/1	0.99	0.07	10,10,10,10	0
54	MG	DB	3108	1/1	0.99	0.06	27,27,27,27	0
54	MG	DB	3019	1/1	0.99	0.08	25,25,25,25	0
54	MG	BB	3023	1/1	0.99	0.21	12,12,12,12	0
54	MG	BB	3016	1/1	0.99	0.09	31,31,31,31	0
54	MG	DB	3072	1/1	0.99	0.08	36,36,36,36	0
54	MG	CA	1642	1/1	0.99	0.12	49,49,49,49	0
54	MG	BB	3063	1/1	0.99	0.10	7,7,7,7	0
54	MG	BB	3061	1/1	0.99	0.11	5,5,5,5	0
54	MG	AA	1612	1/1	0.99	0.06	70,70,70,70	0
54	MG	CA	1636	1/1	0.99	0.07	37,37,37,37	0
54	MG	DB	3090	1/1	0.99	0.25	99,99,99,99	0

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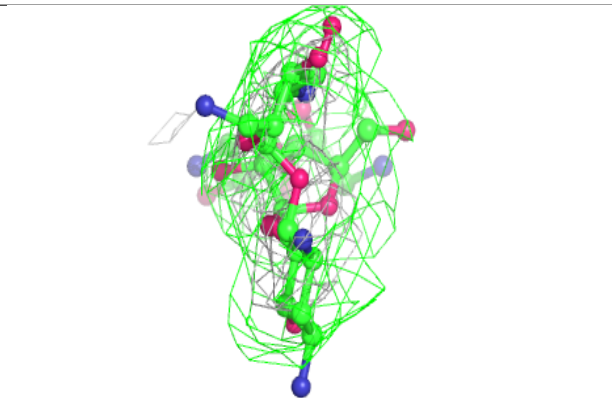
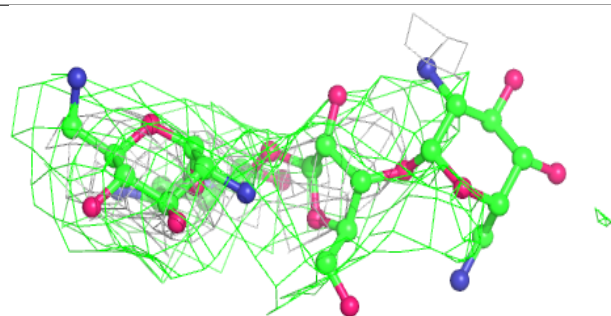
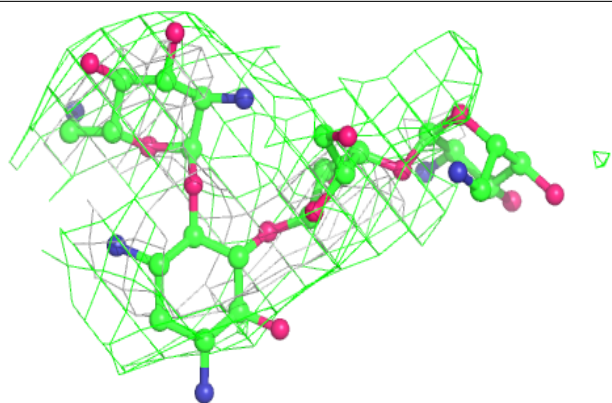
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BB	3033	1/1	0.99	0.05	25,25,25,25	0
54	MG	BB	3074	1/1	0.99	0.09	28,28,28,28	0
54	MG	DB	3042	1/1	0.99	0.09	17,17,17,17	0
54	MG	CA	1625	1/1	0.99	0.06	36,36,36,36	0
54	MG	DB	3021	1/1	0.99	0.13	5,5,5,5	0
54	MG	CA	1602	1/1	0.99	0.04	7,7,7,7	0
54	MG	DB	3013	1/1	0.99	0.17	12,12,12,12	0
54	MG	DB	3076	1/1	0.99	0.05	22,22,22,22	0
54	MG	BB	3097	1/1	0.99	0.07	5,5,5,5	0
54	MG	DB	3034	1/1	0.99	0.11	5,5,5,5	0
54	MG	DB	3003	1/1	0.99	0.07	21,21,21,21	0
54	MG	CA	1603	1/1	0.99	0.15	25,25,25,25	0
54	MG	DB	3099	1/1	0.99	0.13	9,9,9,9	0
54	MG	CA	1611	1/1	0.99	0.10	5,5,5,5	0
54	MG	CA	1631	1/1	0.99	0.15	43,43,43,43	0
54	MG	DB	3064	1/1	0.99	0.04	34,34,34,34	0
54	MG	BB	3059	1/1	0.99	0.05	13,13,13,13	0
54	MG	BB	3019	1/1	0.99	0.11	44,44,44,44	0
54	MG	CA	1637	1/1	0.99	0.08	26,26,26,26	0
54	MG	BB	3087	1/1	0.99	0.20	23,23,23,23	0
54	MG	BB	3042	1/1	1.00	0.10	10,10,10,10	0
54	MG	DB	3107	1/1	1.00	0.07	20,20,20,20	0

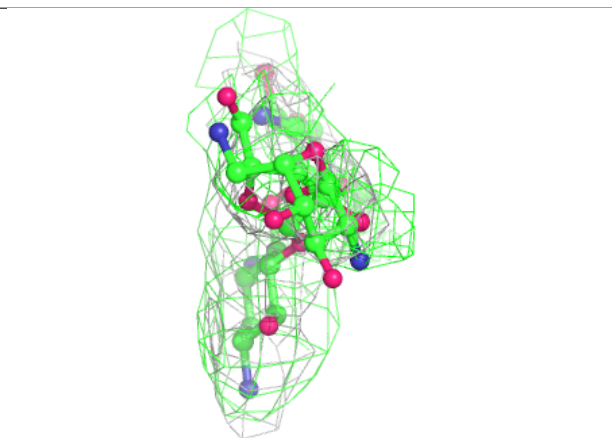
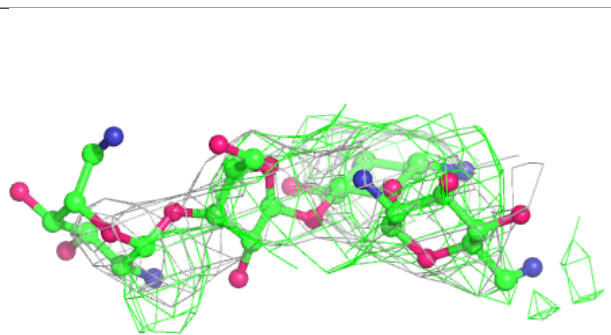
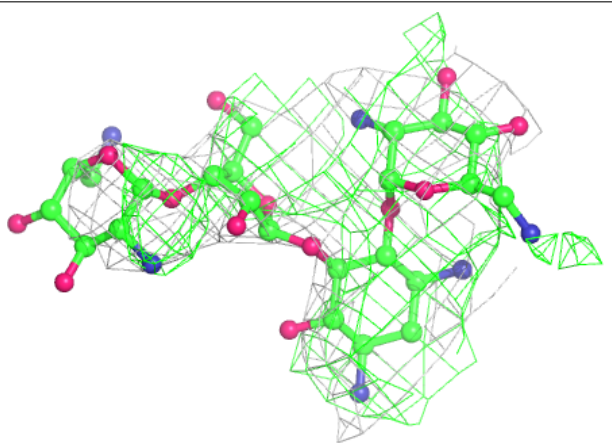
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NMY BB 3001:

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

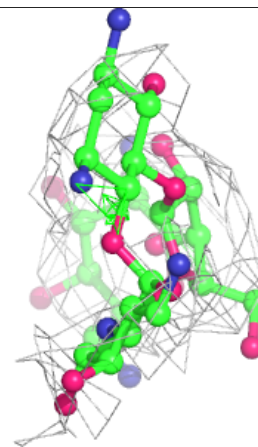
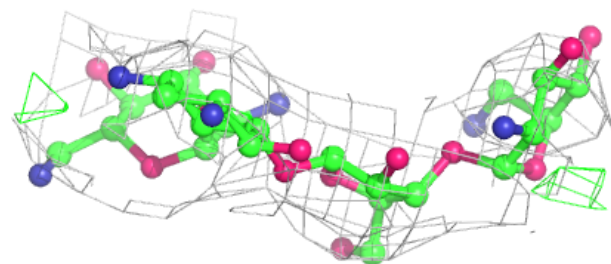
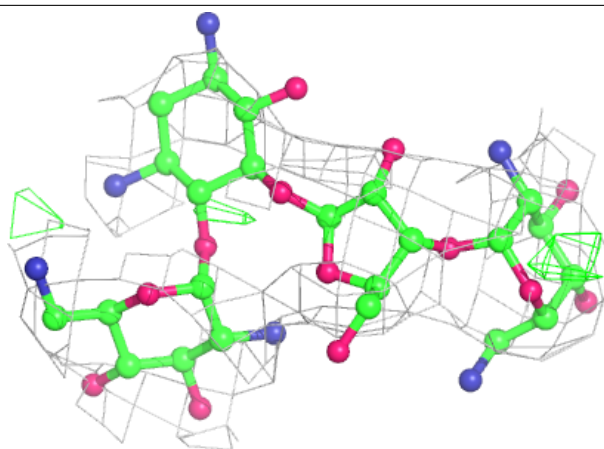
**Electron density around NMY DB 3001:**

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

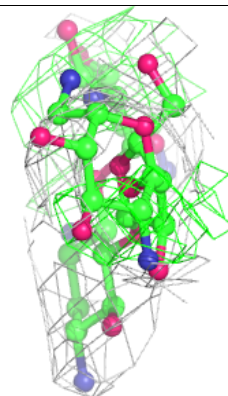
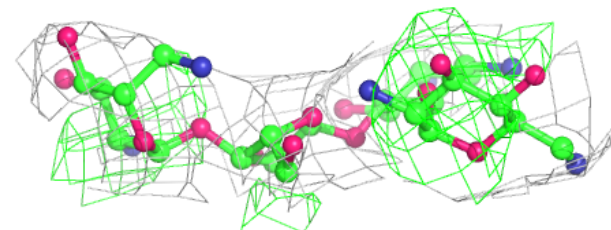
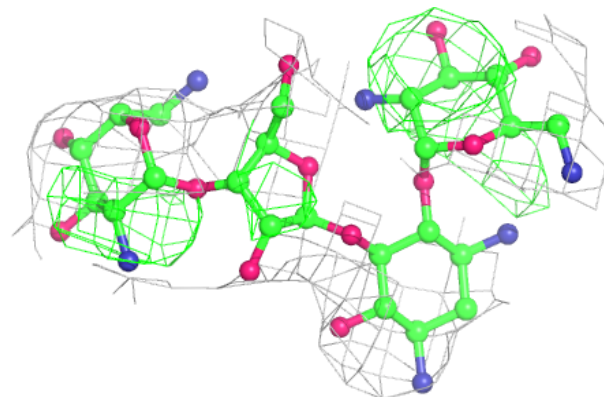


Electron density around NMY AA 1601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

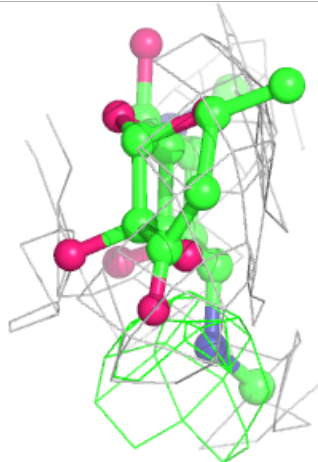
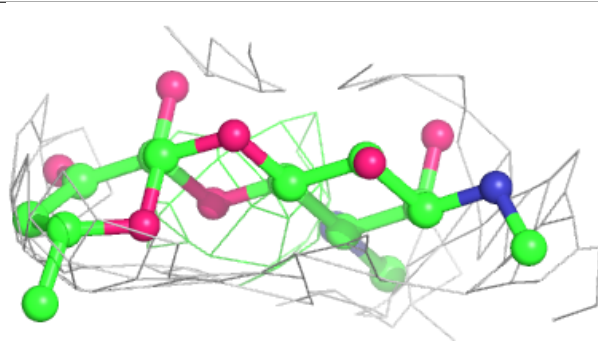
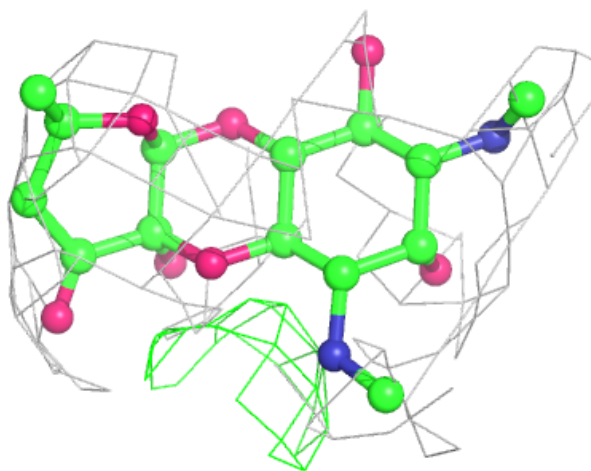
**Electron density around NMY CA 1601:**

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



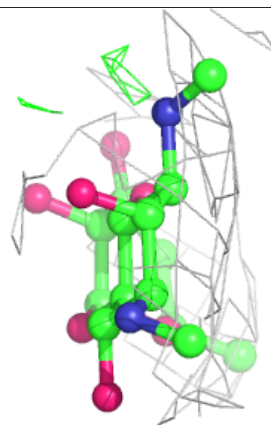
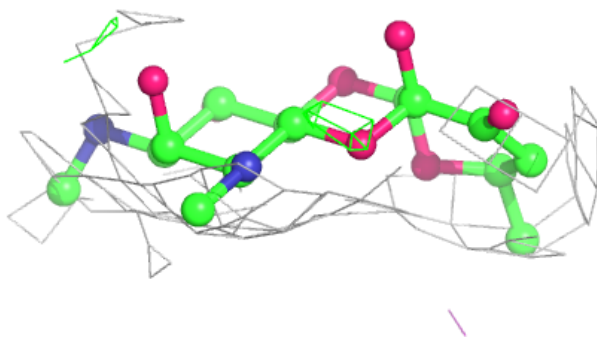
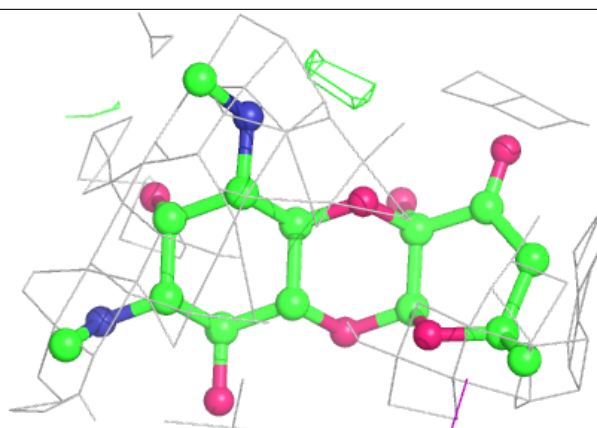
Electron density around SCM CA 1661:

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



Electron density around SCM AA 1662:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.