



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 02:36 AM UTC

PDB ID : 4V57 / pdb_00004v57
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

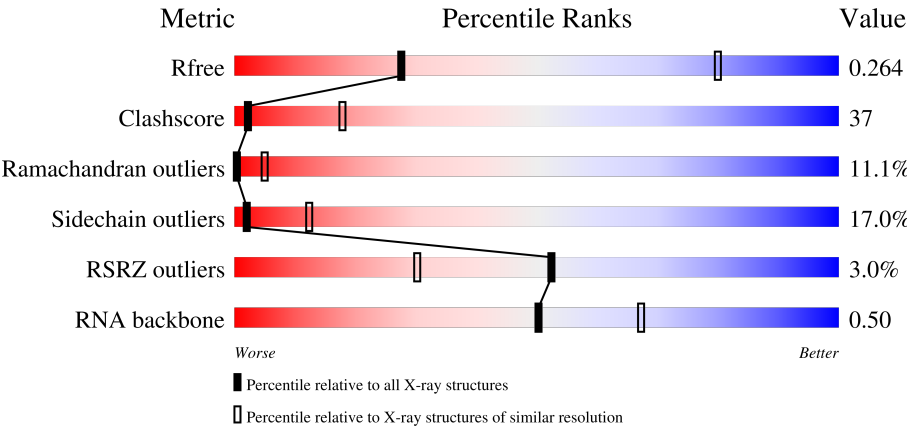
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	23% 62% 14% ..
1	CA	1542	23% 61% 13% ..
2	AC	232	18% 51% 17% • 11%
2	CC	232	27% 46% 14% • 11%

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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	

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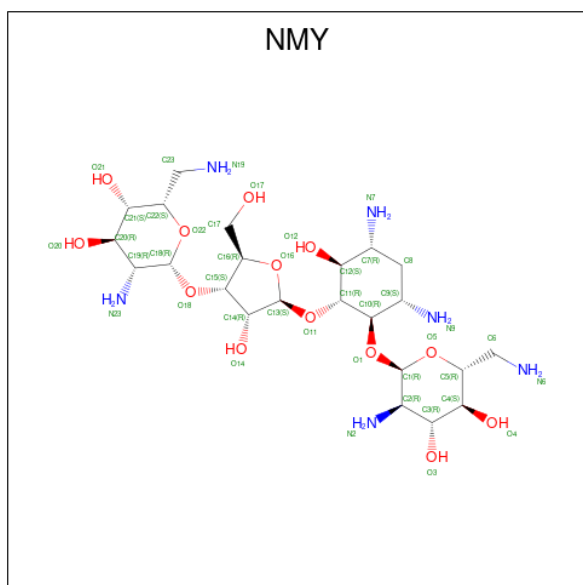
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- 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 (CCD ID: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).

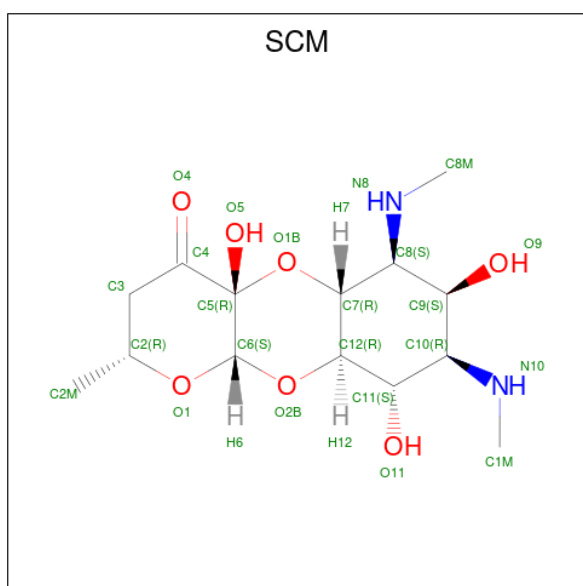


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
53	AA	1	Total	C	N	O	0	0
			42	23	6	13		
53	BB	1	Total	C	N	O	0	0
			42	23	6	13		
53	CA	1	Total	C	N	O	0	0
			42	23	6	13		
53	DB	1	Total	C	N	O	0	0
			42	23	6	13		

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 55 is SPECTINOMYCIN (CCD ID: SCM) (formula: $C_{14}H_{24}N_2O_7$).



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

- Molecule 56 is ZINC ION (CCD ID: 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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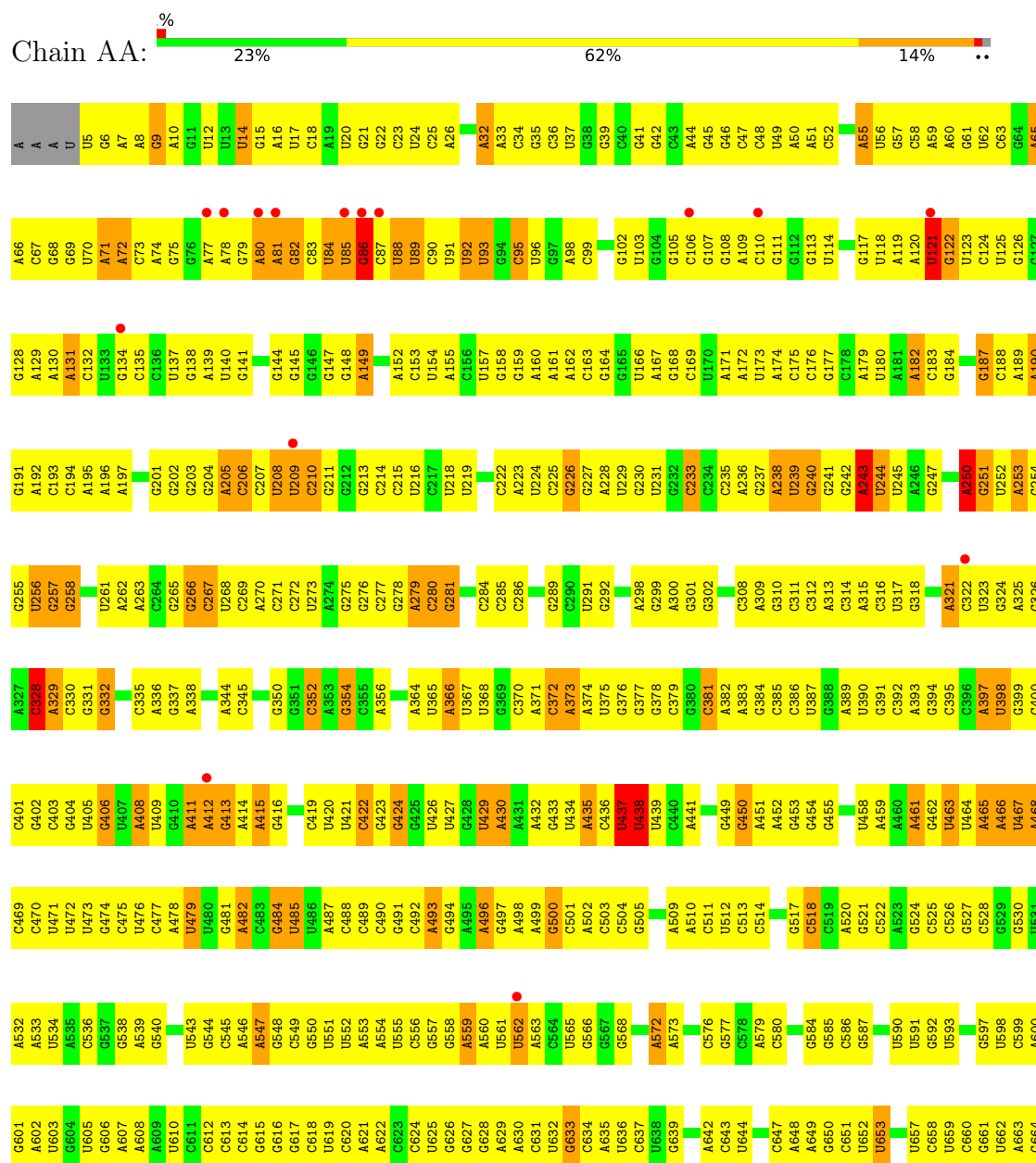
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DD	1	Total 1	O 1	0	0
57	DE	2	Total 2	O 2	0	0
57	DL	1	Total 1	O 1	0	0
57	DN	2	Total 2	O 2	0	0
57	DR	1	Total 1	O 1	0	0

3 Residue-property plots

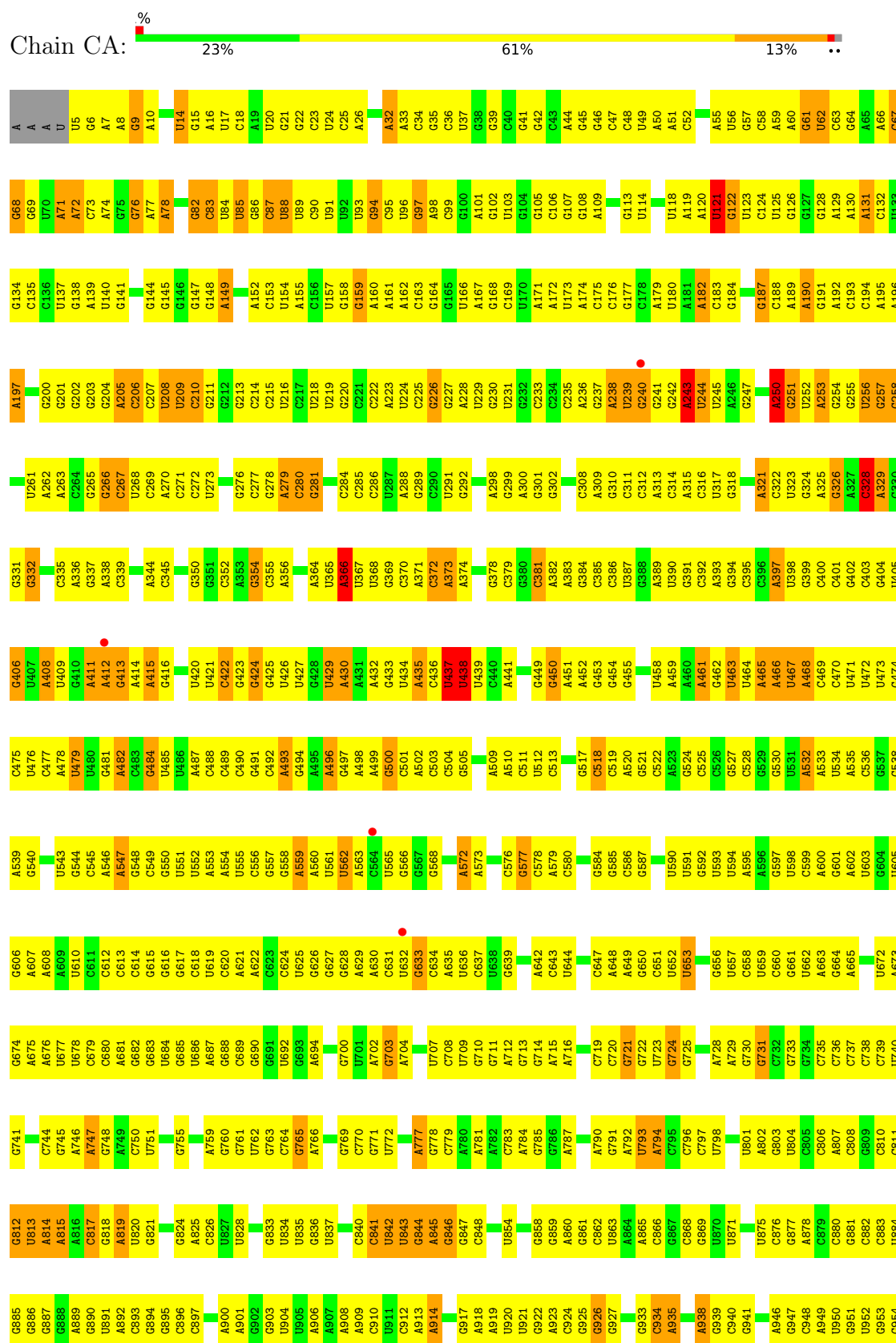
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

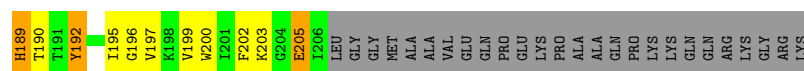
• Molecule 1: 16S rRNA



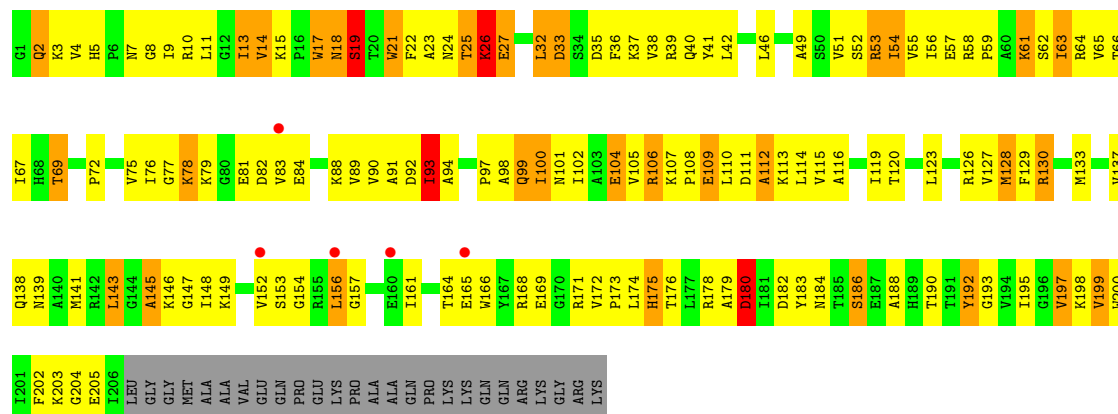
G1525	U1463	C1320	U1194	C1132	U1062	A1000	C934	U871	U801	G731	A665
G1526	U1464	U1321	C1195	G1133	C1063	C1001	C935	G874	A802	G732	G665
U1527	A1465	G1322	A1196	G1134	U1064	G1002	A935	U875	G803	G733	G668
U1528	C1466	G1323	A1197	U1135	U1065	G1003	G939	C876	U804	G734	G669
G1529	C1467	A1324	G1200	C1136	C1066	A1004	A939	C877	C805	C735	U672
G1530	A1468	C1325	G1201	G1138	U1069	A1005	A946	G877	C806	C736	U673
A1531	C1469	U1326	A1202	G1139	C1070	G1006	A947	A878	A807	C737	A674
U1532	U1470	C1327	C1203	U1142	U1071	U1007	C948	G879	C808	C738	A675
C1533	U1471	C1328	U1204	G1143	U1072	U1008	A949	G881	C809	C739	U676
A1534	U1472	A1329	U1205	G1144	U1073	U1009	U950	C882	C810	U740	U677
C	G1473	U1330	U1206	G1145	G1074	C1011	G951	C883	C811	G741	U678
C	U1474	G1331	G1207	A1146	U1075	A1012	U952	U884	U812	C744	C679
C	G1475	A1332	C1208	A1147	U1076	G1013	G953	C885	A814	G745	C680
A1476	U1477	C1333	C1209	U1148	U1077	G1014	U954	G886	A815	G746	A681
U1478	A1410	U1335	A1275	U1149	U1078	G1015	U955	G887	A816	A747	G682
U1479	C1411	C1336	U1211	C1149	G1079	A1016	U956	G888	C817	G748	U683
C1480	C1412	G1337	U1212	A1150	U1080	U1017	U957	A889	C818	U749	U684
U1481	A1413	G1338	A1213	A1151	A1081	G1018	A958	U890	A819	A753	G685
A1482	C	A1339	C1214	A1152	U1082	A1019	A959	U891	U820	C754	U686
A1483	U1418	U1340	G1215	G1153	U1083	G1020	U960	A892	G821	G755	A687
C	G1419	U1341	C1216	G1154	U1084	A1021	U961	C893	G824	A759	G688
G1486	G1422	G1343	C1217	G1155	U1085	A1022	C963	C894	A825	G760	C689
G1487	U1423	C1344	U1218	G1156	U1086	U1023	A964	C896	G826	G761	G690
G1488	U1424	U1345	G1219	C1157	G1089	U1025	U965	G897	U827	U762	G691
G1489	U1425	A1346	U1220	C1158	U1090	G1026	G966	G898	U828	G763	U692
U1490	A1429	U1347	G1221	U1159	U1091	C1027	C967	C899	G829	G764	G693
A1491	C	A1348	C1222	G1160	A1092	G1028	A968	A900	G833	G765	A695
A1492	G1429	U1349	C1223	C1161	A1093	U1029	A969	A901	U834	A766	A696
A1493	U1430	A1350	U1224	C1162	G1094	U1030	C970	G902	U835	U767	U697
G1494	G1431	U1351	C1225	A1163	U1095	C1031	G971	G903	U836	A768	C700
C	A1433	C1352	A1227	U1165	U1096	G1032	C972	U904	G837	G769	G700
G1497	U1434	G1353	C1228	G1166	C1097	G1033	G973	U905	U837	C770	G703
U1498	U1435	C1354	A1229	A1167	C1098	G1034	A974	A906	U838	G771	A704
A1499	A1436	U1355	C1230	U1168	G1099	A1035	A975	A907	C840	U772	G705
U1500	U1437	U1295	G1231	A1169	C1100	A1036	G976	A908	U841	A777	A706
G1501	G1438	C1296	G1232	A1170	A1101	C1037	A977	A909	U842	G778	U707
A1502	U1439	G1297	C1233	A1171	A1102	C1038	A978	C910	U843	G779	C708
A1503	U1440	U1298	U1234	C1172	C1103	G1039	C979	U911	G844	A780	U709
G1504	A1441	A1299	U1235	U1173	G1104	U1040	C980	C912	A845	A781	G710
G1505	C	G1300	C1237	G1174	A1105	G1041	U981	A913	G846	A782	G711
U1506	U1444	U1301	C1238	G1175	G1106	A1042	U982	A914	G847	C783	A712
A1507	U1445	A1302	A1239	A1176	C	C	A983	A915	C848	G784	G713
G1508	A1446	G1303	U1240	G1177	C1113	A1046	C984	U916	U854	A785	G714
C1509	U1447	G1304	G1241	U1178	C1114	G1047	C985	G917	C	G786	G715
G1510	C1448	G1305	U1242	A1179	U1115	G1048	U986	A918	C	A787	A716
G1511	U1449	A1306	C1243	G1180	U1116	U1049	C987	A919	G858	C	C
U1512	U1450	U1307	C1244	A1181	A1117	G1050	G988	U920	A859	A790	C719
A1513	A1451	U1308	G1245	G1182	U1118	C1051	U989	U921	G860	G791	C720
G1514	C1452	G1309	C1246	U1183	C	U1052	C990	G922	C861	A792	G721
G1515	U1453	A1310	A1247	G1184	U1121	G1053	U991	A923	C862	U793	G722
G1516	G1454	A1311	U1248	G1185	U1122	C1054	U992	C924	U863	A794	U723
G1517	U1455	U1313	C1249	G1186	U1123	A1055	G993	G925	A864	U795	G724
A1518	A1456	C1314	A1250	G1187	G1124	U1056	A994	G926	A865	C796	G725
U1519	G1457	U1315	A1251	G1188	C	G1057	C995	G927	C866	C797	C
C1520	U1458	U1316	A1252	U1189	G1127	G1058	A996	G928	C867	U798	A728
U1521	G1459	C1317	U1253	A1191	C1128	C1059	U997	G929	C868	A729	C730
U1522	C1460	A1318	A1254	A1192	C	U1060	C998	C930	C869	G799	C
G1523	G1461	C1388	G1255	G1193	G1131	G1061	C999	C931	U870	G800	G730

• Molecule 1: 16S rRNA

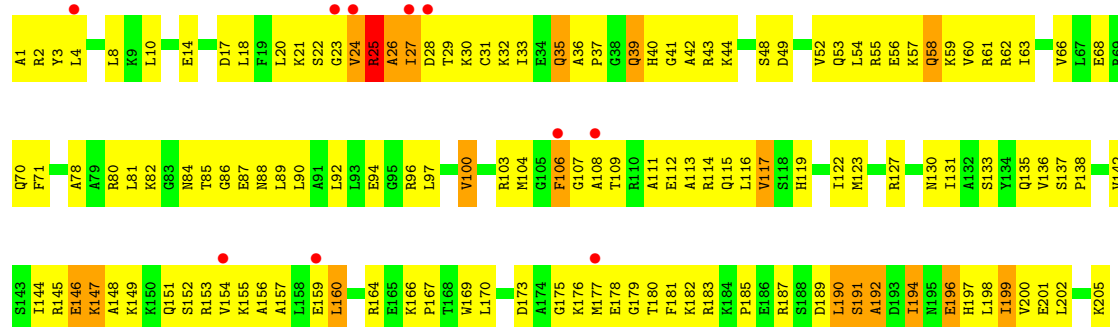




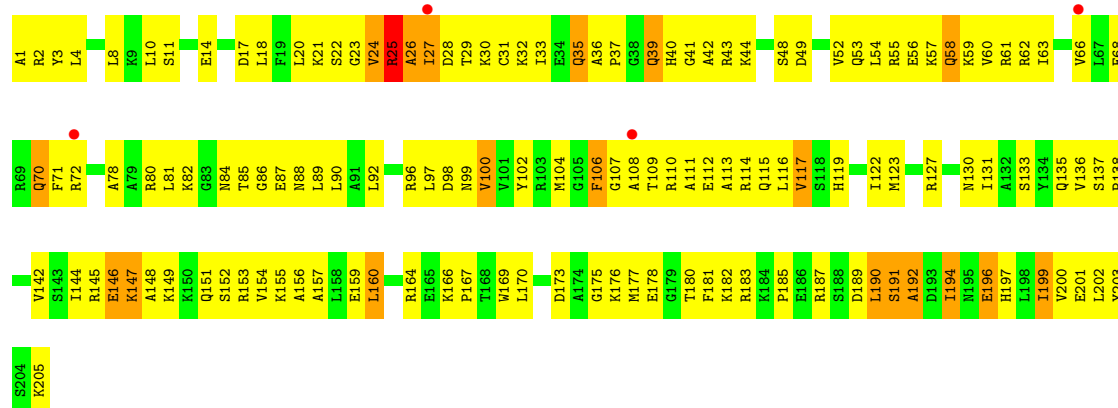
• Molecule 2: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S4



• Molecule 3: 30S ribosomal protein S4



Chain AE:

Amino Acid	Percentage
ALA	4%
HIS	28%
ILE	28%
GLU	49%
LYS	49%
GLN	49%
ALA	49%
GLY	13%
E9	10%
E12	4%
K13	28%
L14	28%
V17	49%
N18	49%
R19	49%
V20	49%
S21	49%
K22	49%
G23	49%
G26	49%
K25	49%
V24	49%
K25	49%
G26	49%
G27	49%
R28	49%
L29	49%
F30	49%
T33	49%
A34	49%
L35	49%
T36	49%
V37	49%
V38	49%
G39	49%
D40	49%
G43	49%
R44	49%
V45	49%
G46	49%
F47	49%
G50	49%
K51	49%
E54	49%
V55	49%
P56	49%
A57	49%
A58	49%
I59	49%
Q60	49%
K61	49%
A62	49%
M63	49%
E64	49%
K65	49%
A66	49%
R67	49%
R68	49%
N69	49%
M70	49%
I71	49%
N72	49%
V73	49%
N76	49%
L80	49%
Q81	49%
H82	49%
P83	49%
V84	49%
K85	49%
G86	49%
V87	49%
H88	49%
T89	49%
G90	49%
S91	49%
R92	49%
V93	49%
F94	49%
M95	49%
A98	49%
S99	49%
E100	49%
G101	49%
T102	49%
G103	49%
I104	49%
I105	49%
A106	49%
G107	49%
G108	49%
A109	49%
M110	49%
R111	49%
A112	49%
V113	49%
L114	49%
E115	49%
V116	49%
A117	49%
N121	49%
V122	49%
L123	49%
A124	49%
K125	49%
A126	49%
Y127	49%
T130	49%
N131	49%
P132	49%
T133	49%
M134	49%
V135	49%
V136	49%
R137	49%
I140	49%
D141	49%
G142	49%
L143	49%
E144	49%
M145	49%
M146	49%
N147	49%
S148	49%
P149	49%
E150	49%
M151	49%
V152	49%
K155	49%
R156	49%
G157	49%
K158	49%
SER	49%
VAL	49%
GLU	49%
GLU	49%
ILE	49%
LEU	49%
GLY	49%
LYS	49%

[illegible]

Chain AF:

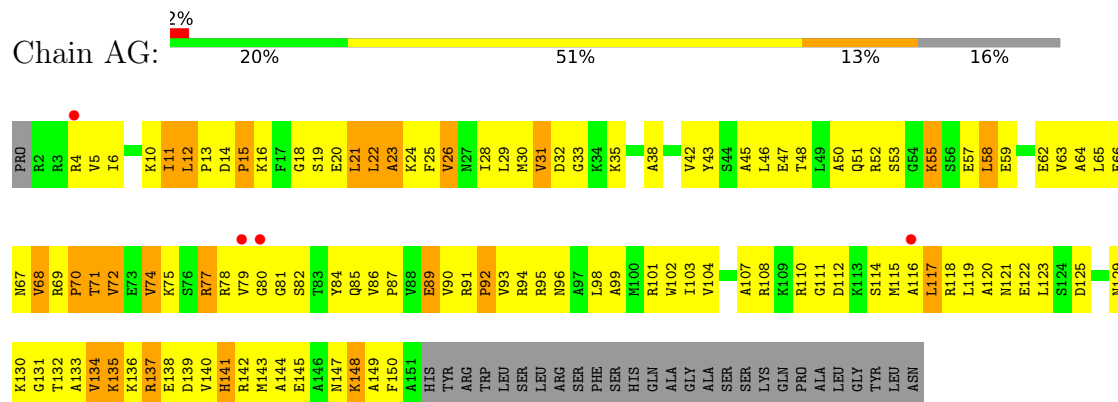
Category	Item	
GLU	M1	
	R2	
	ALA	A66
	GLY	P67
	ASP	D68
	SER	E69
	GLU	V70
	GLU	I71
	GLU	D72
	GLU	E73
	GLU	L74
	GLU	E75
	GLU	T76
	GLU	T77
	GLU	F78
	GLU	R79
	GLU	F80
	GLU	N81
	GLU	S82
	ALA	A83
H84		
R85		
R86		
S87		
H88		
H89		
M90		
R91		
T92		
K93		
H94		
A95		
V96		
T97		
E98		
A99		
S100		
PRO		
VAL		MET
VAL	W42	
LYS	G43	
ALA	R44	
LYS	R45	
ASP	Q46	
GLU	L47	
ARG	A48	
ARG	F49	
GLU	P50	
GLU	I51	
ARG	S52	
ARG	K53	
ASP	L54	
ASP	H55	
PHE	K56	
ALA	A57	
ASN	H58	
GLU	F59	
THR	V60	
ALA	L61	
ASP	M62	
ASP	N63	
ALA	V64	

Chain CF: 18% 39% 17% 26%

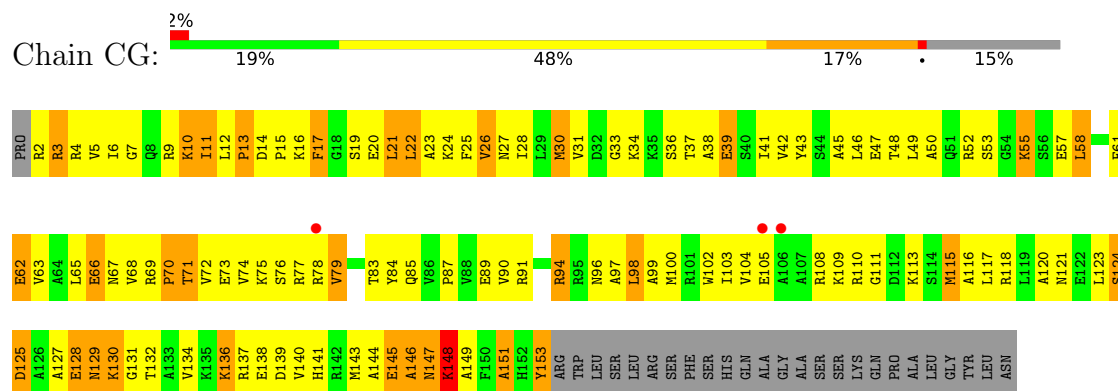
Category	Item	Value
Top 20	M1	0.0000
	R2	0.0000
	R3	0.0000
	Y4	0.0000
	E5	0.0000
	I6	0.0000
	V7	0.0000
	F8	0.0000
	N9	0.0000
	V10	0.0000
	H11	0.0000
	P12	0.0000
	D13	0.0000
	Q14	0.0000
	S15	0.0000
	E16	0.0000
	Q17	0.0000
	V18	0.0000
	P19	0.0000
	G20	0.0000
Next 20	M21	0.0000
	R22	0.0000
	F23	0.0000
	R24	0.0000
	T25	0.0000
	T26	0.0000
	T27	0.0000
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	G34	0.0000
	K35	0.0000
	I36	0.0000
	R37	0.0000
	H38	0.0000
	L39	0.0000
	E40	0.0000
	D41	0.0000
	MET42	0.0000
	VAL43	0.0000
LVS44	0.0000	
R45	0.0000	
Q46	0.0000	
L47	0.0000	
ARG48	0.0000	
Y49	0.0000	
P50	0.0000	
T51	0.0000	
N52	0.0000	
K53	0.0000	
L54	0.0000	
ASP55	0.0000	
PHE56	0.0000	
A57	0.0000	
H58	0.0000	
Y59	0.0000	
L61	0.0000	
ALA62	0.0000	
N63	0.0000	
VAL64	0.0000	
Bottom 20	E65	0.0000
	A66	0.0000
	P67	0.0000
	Q68	0.0000
	E69	0.0000
	V70	0.0000
	T71	0.0000
	D72	0.0000
	E73	0.0000
	L74	0.0000
	E75	0.0000
	T76	0.0000
	T77	0.0000
	F78	0.0000
	R79	0.0000
	F80	0.0000
	N81	0.0000
	D82	0.0000
	A83	0.0000
	V84	0.0000
I85	0.0000	
R86	0.0000	
S87	0.0000	
M88	0.0000	
V89	0.0000	
M90	0.0000	
R91	0.0000	
T92	0.0000	
K93	0.0000	
H94	0.0000	
A95	0.0000	
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T97	0.0000	
E98	0.0000	
A99	0.0000	
S100	0.0000	
PRO	0.0000	
MET	0.0000	
VAL	0.0000	
LVS	0.0000	
ALA	0.0000	
LYS	0.0000	
ASP	0.0000	
GLU	0.0000	
ARG	0.0000	
GLU	0.0000	
ARG	0.0000	
ARG	0.0000	
ASP	0.0000	
ASP	0.0000	
THR	0.0000	
ALA	0.0000	
ASP	0.0000	
ASP	0.0000	
ALA	0.0000	

GLU
ALA
GLY
ASP
SER
GLU
GLU
GLU
GLU

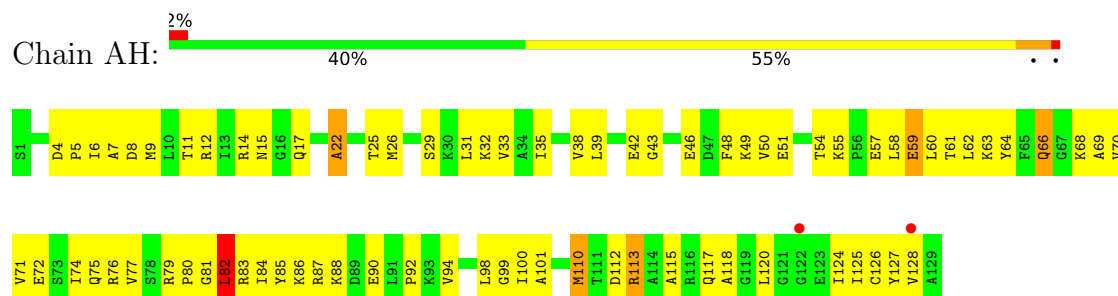
• Molecule 6: 30S ribosomal protein S7



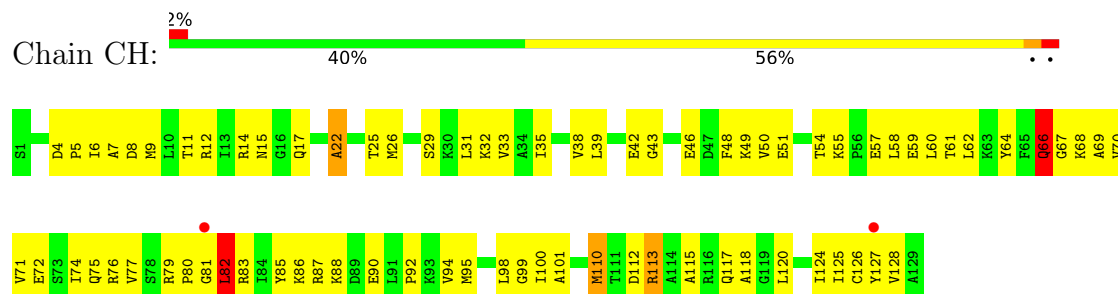
• Molecule 6: 30S ribosomal protein S7



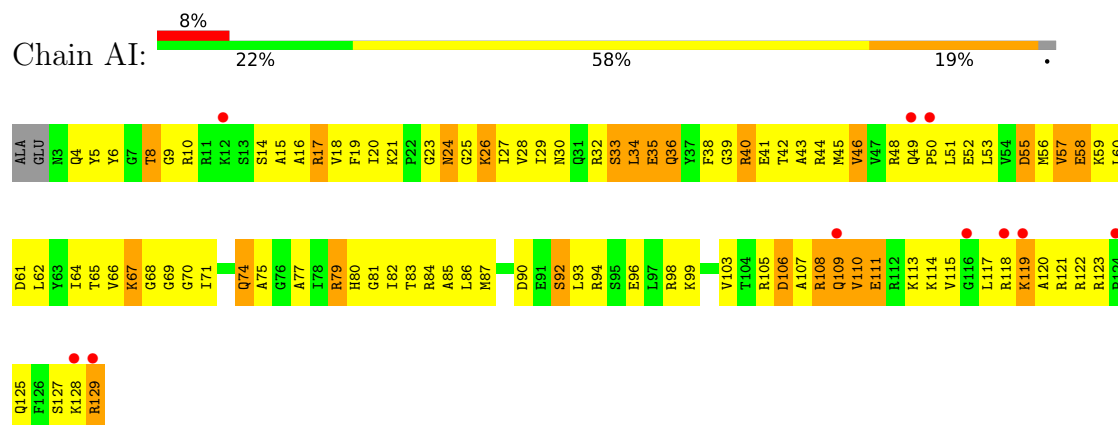
• Molecule 7: 30S ribosomal protein S8



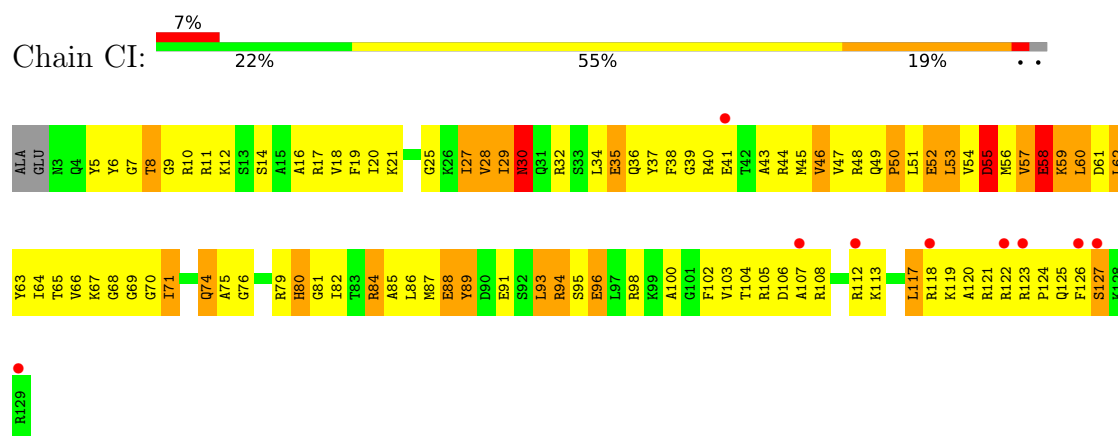
• Molecule 7: 30S ribosomal protein S8



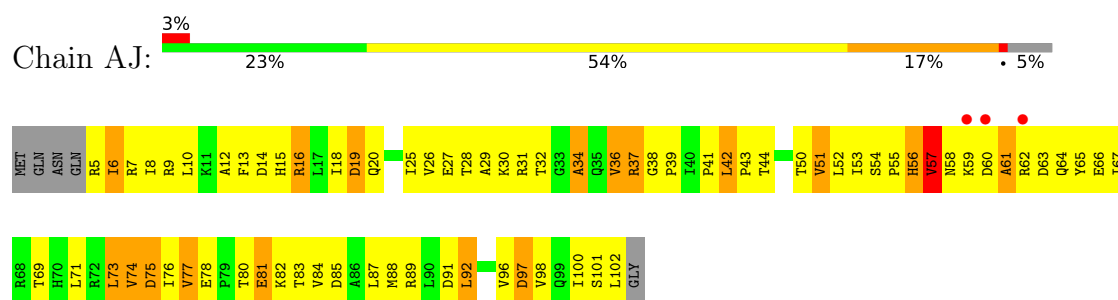
- Molecule 8: 30S ribosomal protein S9



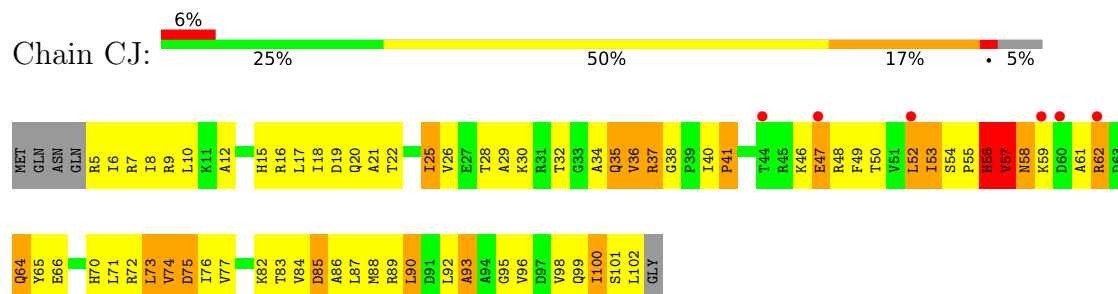
- Molecule 8: 30S ribosomal protein S9



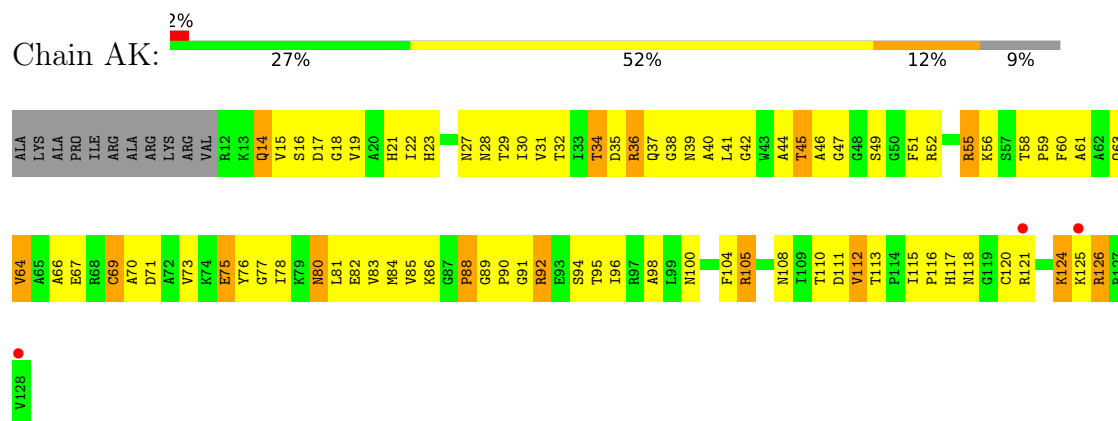
- Molecule 9: 30S ribosomal protein S10



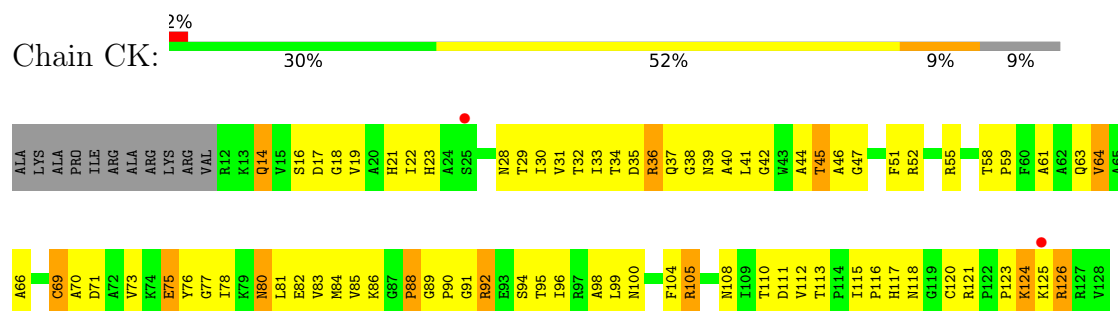
- Molecule 9: 30S ribosomal protein S10



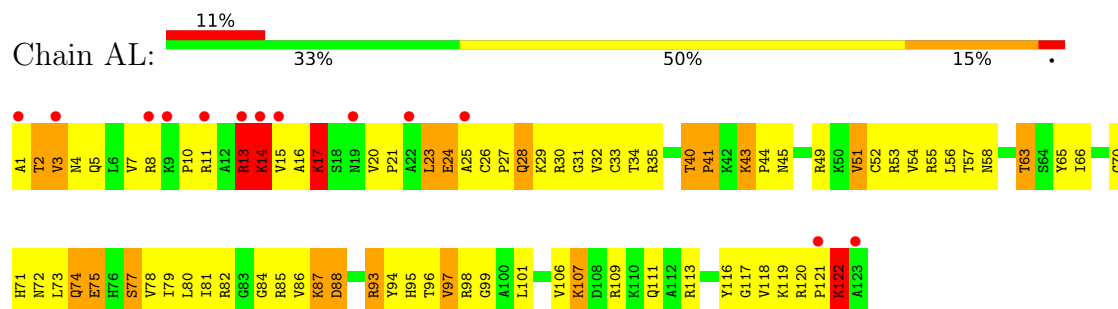
- Molecule 10: 30S ribosomal protein S11



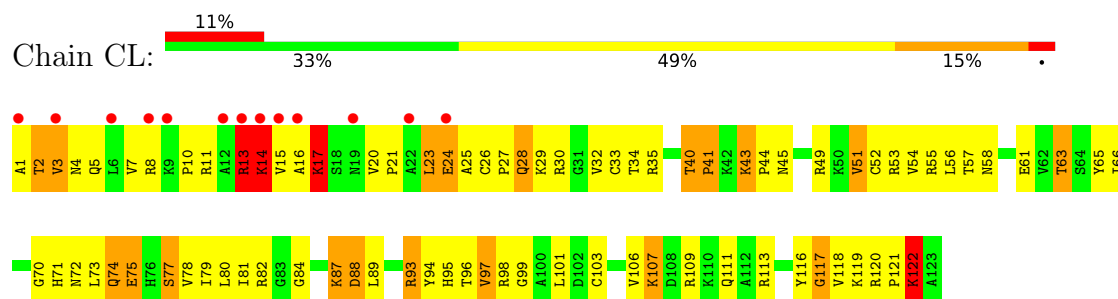
- Molecule 10: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S12

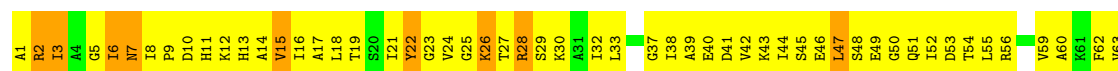


- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13

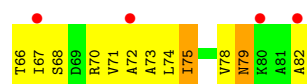
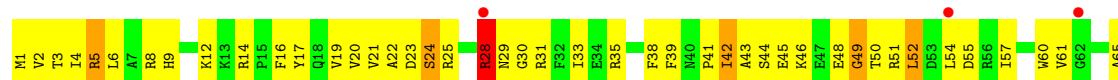




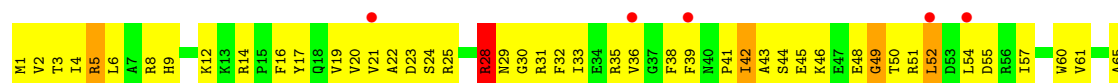
• Molecule 12: 30S ribosomal protein S13



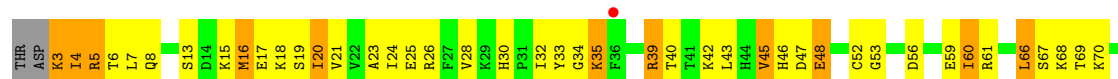
• Molecule 13: 30S ribosomal protein S16



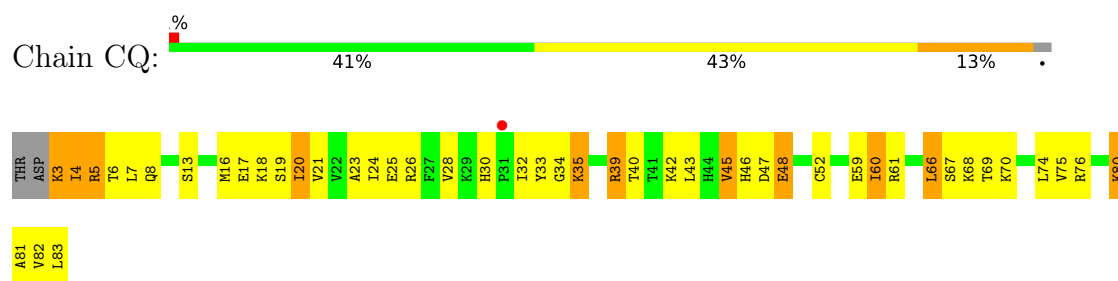
• Molecule 13: 30S ribosomal protein S16



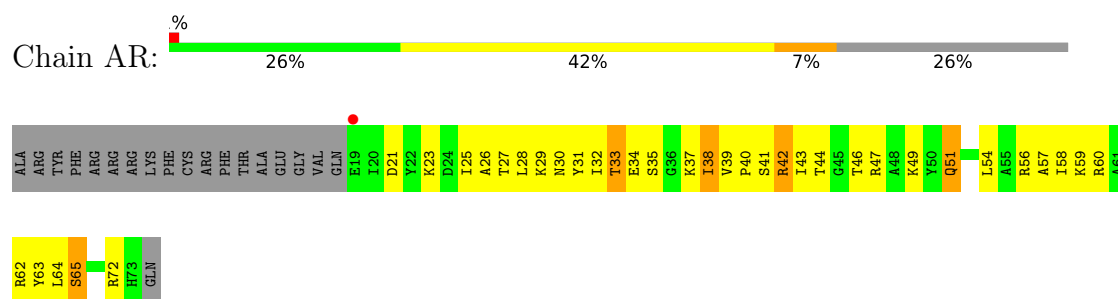
• Molecule 14: 30S ribosomal protein S17



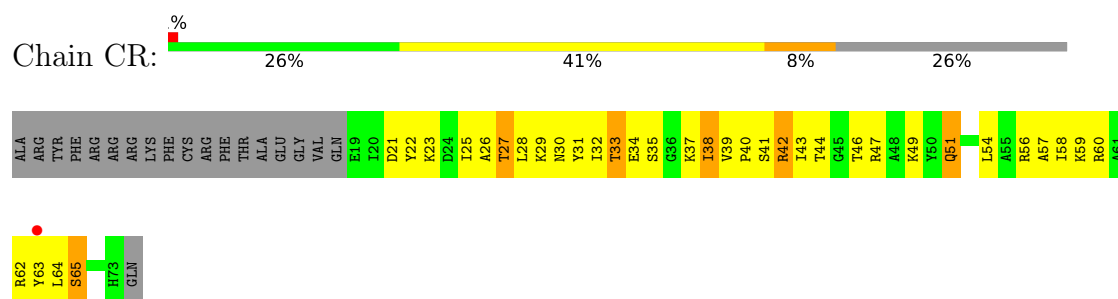
• Molecule 14: 30S ribosomal protein S17



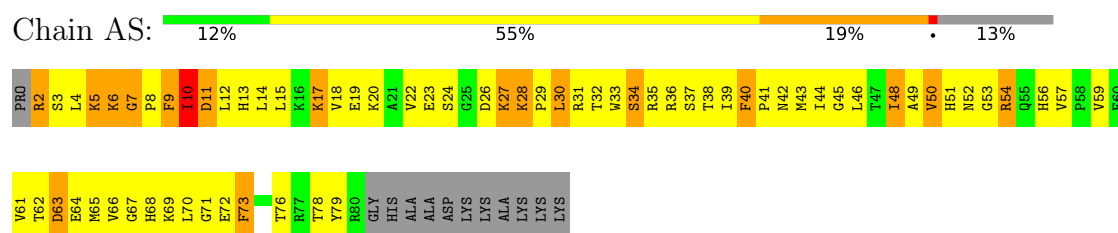
- Molecule 15: 30S ribosomal protein S18



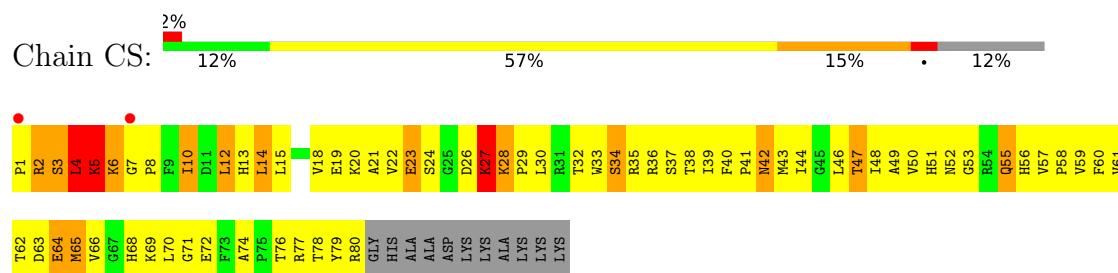
- Molecule 15: 30S ribosomal protein S18



- Molecule 16: 30S ribosomal protein S19



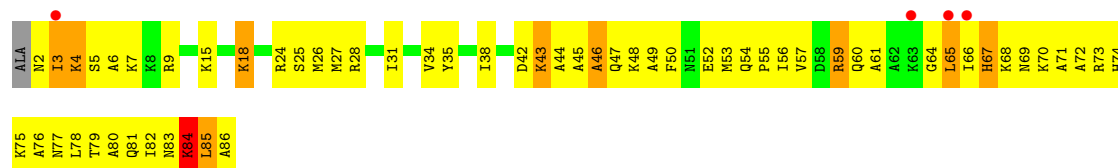
- Molecule 16: 30S ribosomal protein S19



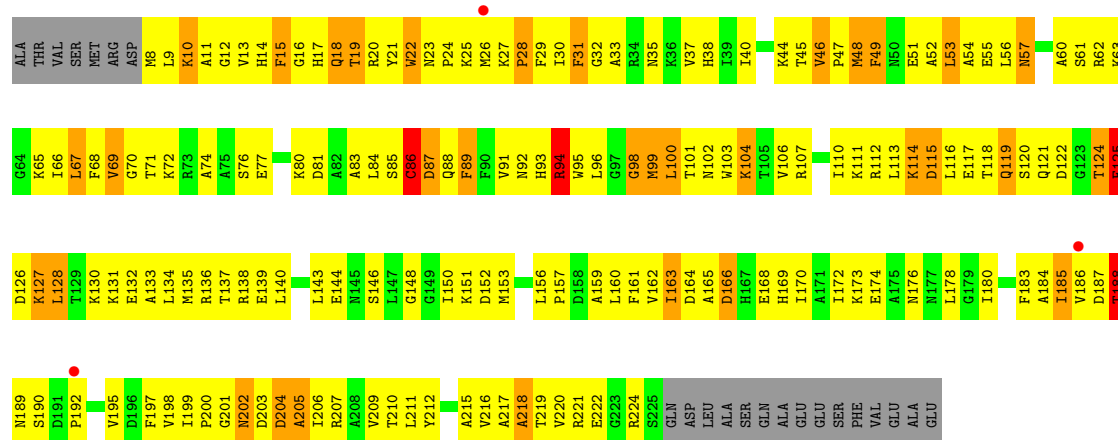
- Molecule 17: 30S ribosomal protein S20



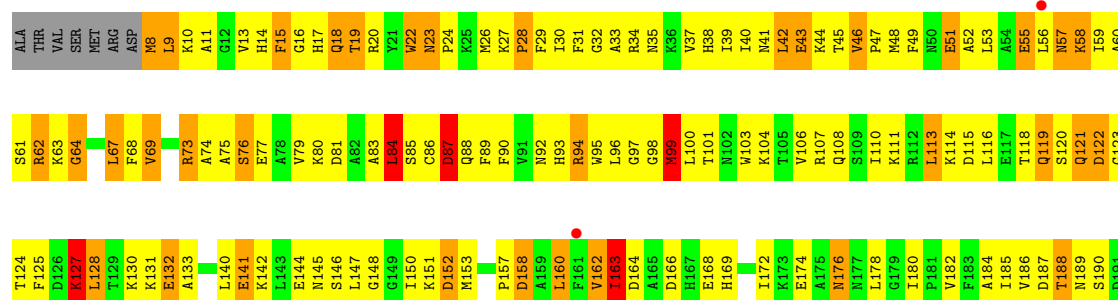
• Molecule 17: 30S ribosomal protein S20



• Molecule 18: 30S ribosomal protein S2

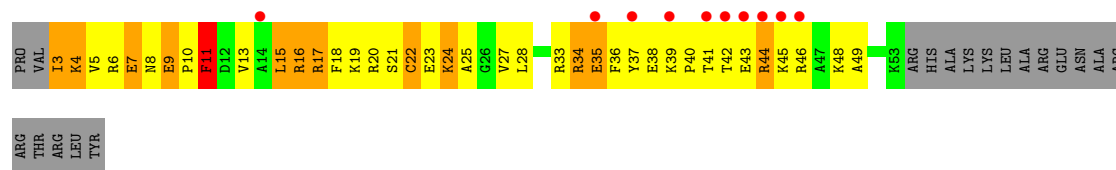
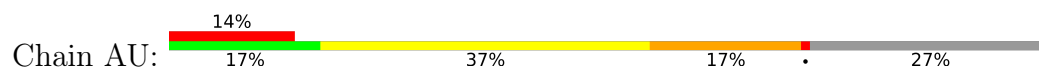


• Molecule 18: 30S ribosomal protein S2

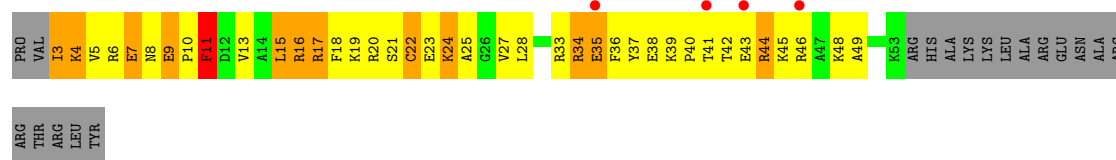
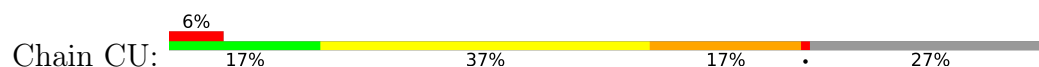




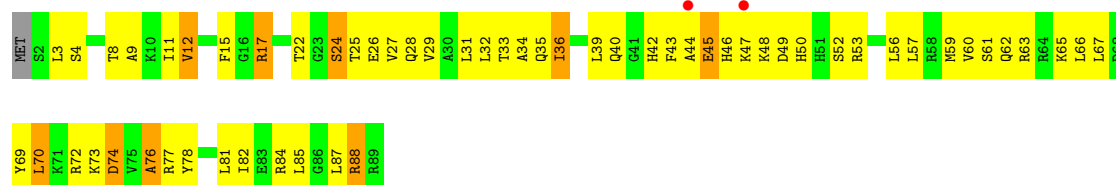
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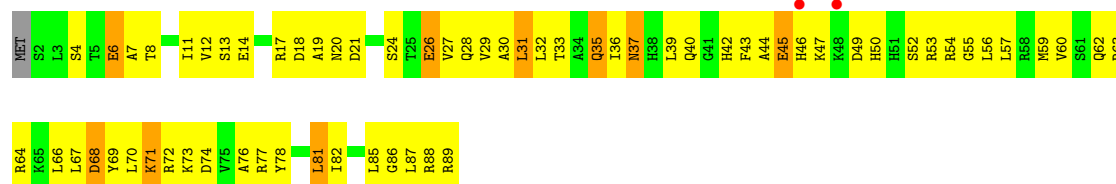
• Molecule 19: 30S ribosomal protein S21



• Molecule 20: 30S ribosomal protein S15

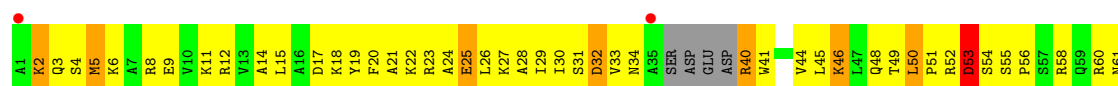


• Molecule 20: 30S ribosomal protein S15

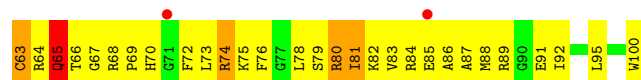
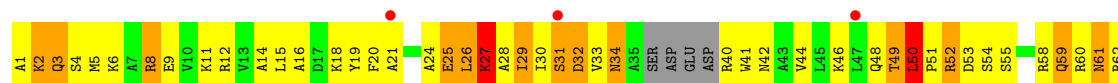


• Molecule 21: 30S ribosomal protein S14

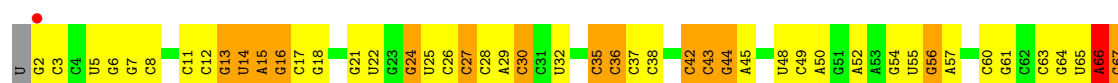




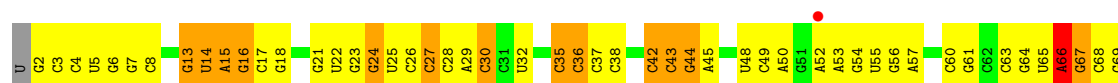
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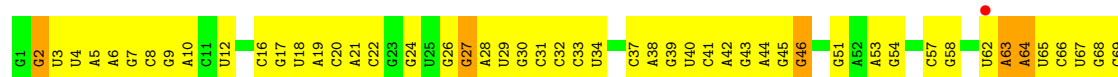
• Molecule 22: 5S rRNA



• Molecule 22: 5S rRNA

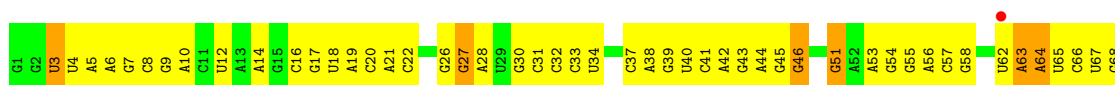


• Molecule 23: 23S rRNA



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C1102	U1035	G971	A845	U768	C697	A633	G501	A501	G425	U349	G283	C209	U138
A1103	G1036	A909	G846	U769	C698	C634	G570	A502	C426	G350	U284	G215	U139
C1104	G1037	A973	U847	G770	A699	C635	U571	A503	U427	C351	G285	G216	C140
U1105	G1038	G974	C848	G771	G700	C636	U572	A504	A428	A352	U286	A217	G141
G1106	A1039	A975	C849	G772	G701	A637	U573	A505		C353	G287	A218	A142
G1107	A1040		A849	U773	U702	G638	A574	A506		A354	U288	A219	C143
U1108	G1041	G978	U850	G774	U703	U639	A575	G507	U431	G355	U292	A220	A144
C1109	G1042	C979	C851	G775	G704	C640	U576	A508	C433	G356	U293	G221	C145
G1110	A1043	A980	U852	G776	A705	U641	U577	C509	A434	G361	A221	A222	A146
A1111	C1044	A981	C853	G777	A706	U642	U580	C510	U435	A362	A223	A223	C147
G1112	C1045	A982	C854	G778	G707	A643	C581	U511	C436	G363	G297	U224	U150
U1113	A1046	A983	G855	U779	G708	A644	C582	A512	U437	C364	G298	U225	C151
C1114	G1047	A984	G856	G780	U709	U645	U583	A513	U438	U365	A299	A227	A152
G1115	A1048	C985	U857	A781	U710	U646	C584	A514	U439	C366	A300		U153
G1116	G1049	G986	G858	A782	G711	A647	C585		C440	G370	G301	G230	U154
C1117	A1050	C987	G859	A783	G712	U648	U586		U441	A371	G302	A231	A155
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G1119		G989	G862	G785	U714	C650	C587		C443	A373	G304	G233	
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C1123	A1057	G993	A866	A794	A718	A654	A592		U451		G310	G237	C163
G1124	U1058	C994	G875	G795	G719	A655	A593		U452		A311	G242	C164
U1125	G1059	C995	C876	C796	U720	G656	U594		U453		G312	G243	U166
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U1129	U1061	G997	U878	A802	A722	U658	A528		C455		G314	G245	U171
C1130	G1062	C998	C873	U803	G725	U659	U596		C456		G315	G246	U172
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C1132	C1064	A1000	G875	G805	A727	A661	U598		C458		A391	G248	A178
U1133	U1065	A1001	C876	G806	G728	G664	G600		U459		U392	C249	A179
A1134	G1068	G1002	A877	G809	G729	U665	A603		C461		C393	G250	U174
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G1136	U1070	G1006	G	U811	C731	A666	G604		U463		U395	G252	A176
C1137	G1071	C1007	G	C812	G732	G669			U464		G396	G253	G177
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G1139			G	C814	A739	C671	A608		C466		C324	A255	C179
C1140	C1076	G1011	U	C915	G740	C672	A609		C467		G325	A256	G180
U1141	A1077	U1012	C	U816	U741	C673	C610		C468		A401	G257	A181
A1142	U1078	C1013	A	C917	A742	C674	C611		C469		G326	G258	A182
C1143	C1079	A1014	U	U818	U743	A675	C612		A470		G327	G259	C183
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G1145	U1081	U1016	C		G745	C679	A614		A472		A330		G185
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G2061	C1990	A1913	G1839	U1636	A1569	A1439	U1375	A1308	G1238	G1166
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A2053	G1907	U1981	G1766	C1704	U1566	G1633	A1499	A1367	A1302	
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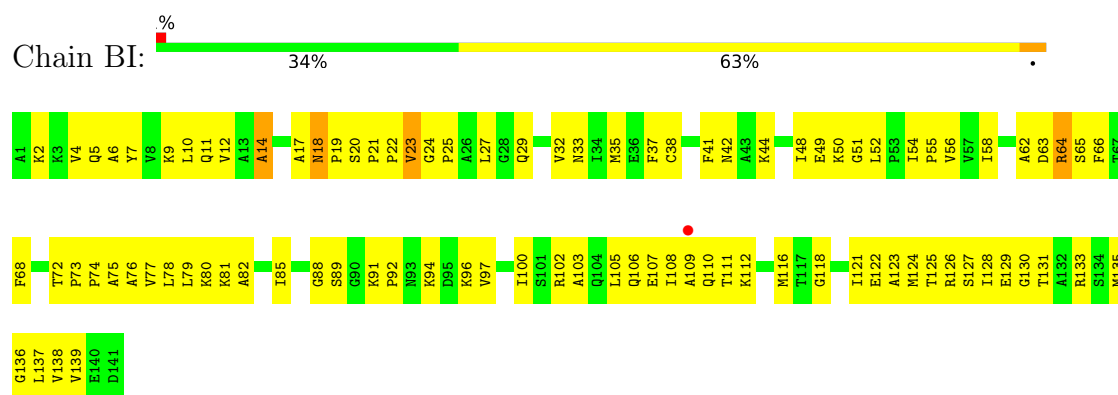


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G1024	C961	C	A833	U885	G617	C487	U416	A347	U285		A142	A71
G962	G988		G834	U886	U686		U417	A348	U286		C143	U72
U963	A899		C835	G887	G620	G491	U418	U349	G287	G215	A144	A73
C964	A900		G836	U688	A621	G492	U419	G350	U288	A216	C145	A74
	C901		C837	U689	G622	G493	C420	C351	G289		A146	G75
U967	C902		C838	G690	G623	G494		A352		A219	C147	C76
C968	C903		U839	G691	C624	G495	A423	C353	U292	G220	U150	G77
G1031	G904		G840	C692	U617	G496	C424	A354	U293		C151	U78
A1032			G841	C693	A627		C425	U355	A294	A222	A152	G80
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G1034	A910		A845	G695	A631	A501	A432	C357	U296		U154	U82
G1037	A911		U846	G696	A632	A502	A433	U358	G297	G230	A155	A83
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A1040	G914		A849	U699	C635	G505	C436	A362	A300	U234	A160	U92
G1041	C915		U850	G701	G636	A506	U437	A363	G301	U235	A161	G93
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C1043	A917		U852	U703	G638	A508	A439	U365	G303	C237	C163	A95
G1044	U918		C853	G704	U639	A509	U440	C366	U304	U238	C164	C96
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C1049	G923		U710	U580	A644	A515	A443	A371	A310	C246	A101	A101
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C994	G930		C717	C587	U651	A522	U451	U387	A320	G253	G177	G108
A996	U931		U718	U588	U652	G524	A453	G388	U321	G254	G178	U114
G997	A933		C719	U589	A654		A454	G389	A322	A255	C179	C115
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A1000	A936		C723	U593	U658	A529	C458	U392	A325	G259	C183	A118
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A1014	U950		A742	A607	G674	U546		G408	U339	U276	A197	U133
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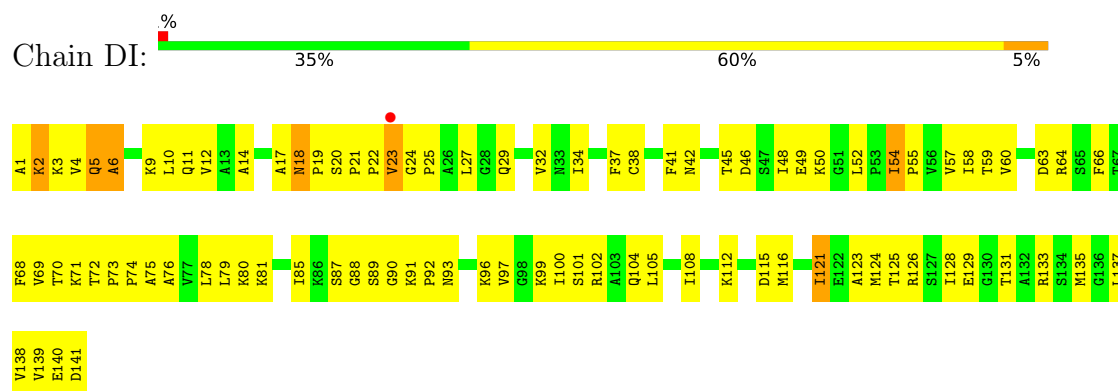
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	U2807				G2607	C2539	A2469		C2338	A2270	U	A2082
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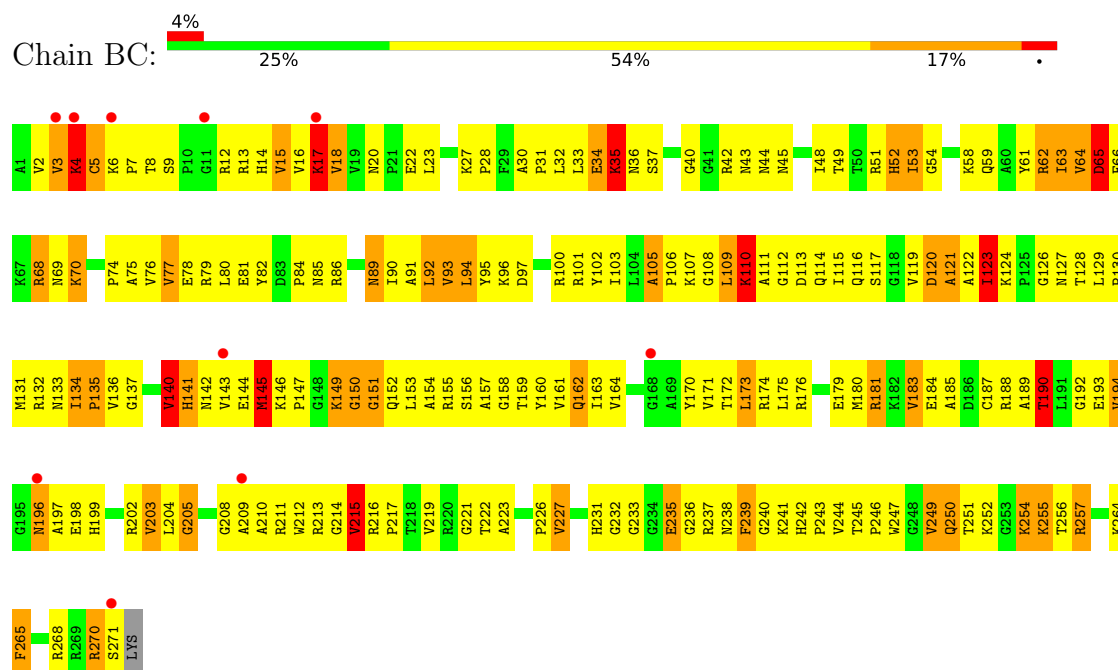
- Molecule 24: 50S ribosomal protein L11



• Molecule 24: 50S ribosomal protein L11

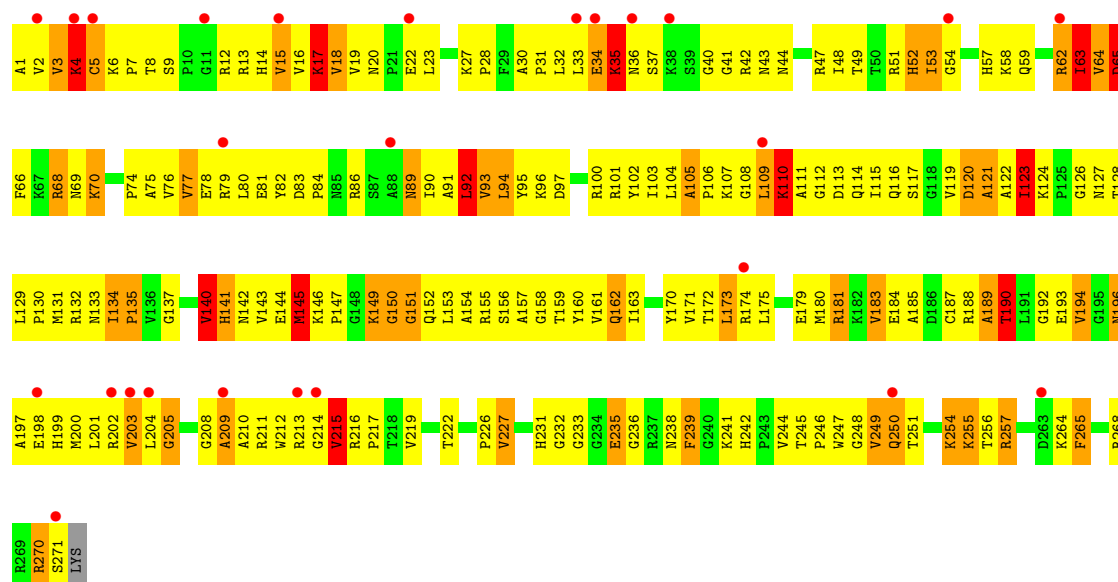


• Molecule 25: 50S ribosomal protein L2



• Molecule 25: 50S ribosomal protein L2





• Molecule 26: 50S ribosomal protein L3

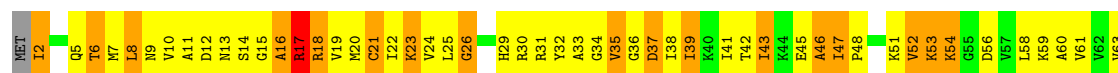
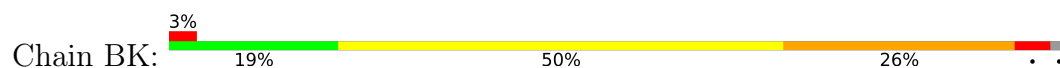


• Molecule 26: 50S ribosomal protein L3

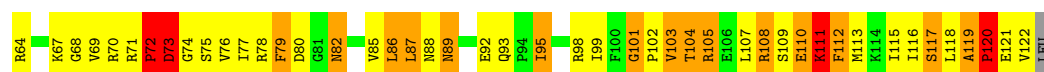
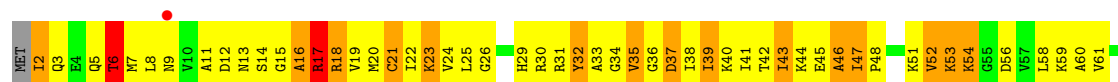
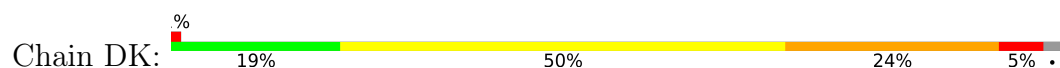




- Molecule 27: 50S ribosomal protein L14



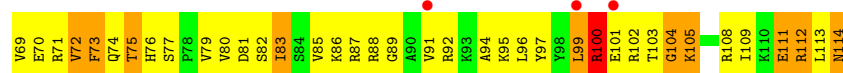
- Molecule 27: 50S ribosomal protein L14



- Molecule 28: 50S ribosomal protein L19

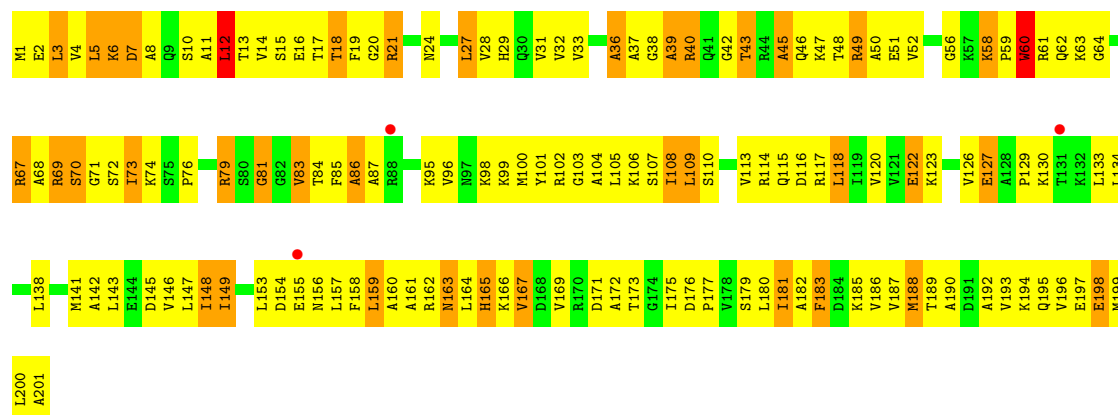


- Molecule 28: 50S ribosomal protein L19

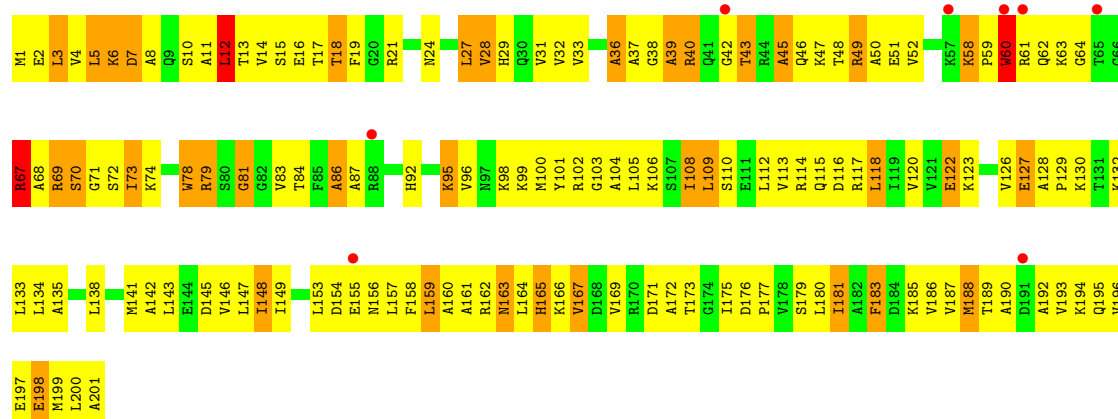


- Molecule 29: 50S ribosomal protein L4





• Molecule 29: 50S ribosomal protein L4



• Molecule 30: 50S ribosomal protein L30

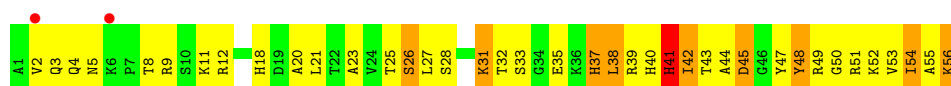


• Molecule 30: 50S ribosomal protein L30



• Molecule 31: 50S ribosomal protein L32





- Molecule 31: 50S ribosomal protein L32



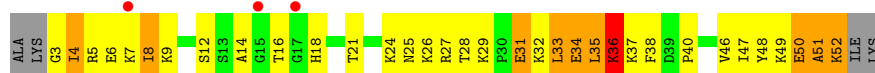
- Molecule 32: 50S ribosomal protein L36



- Molecule 32: 50S ribosomal protein L36



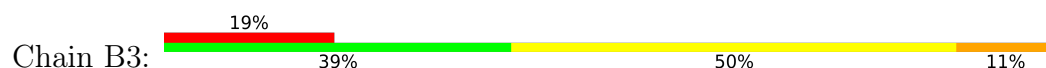
- Molecule 33: 50S ribosomal protein L33



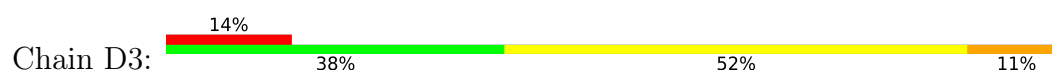
- Molecule 33: 50S ribosomal protein L33



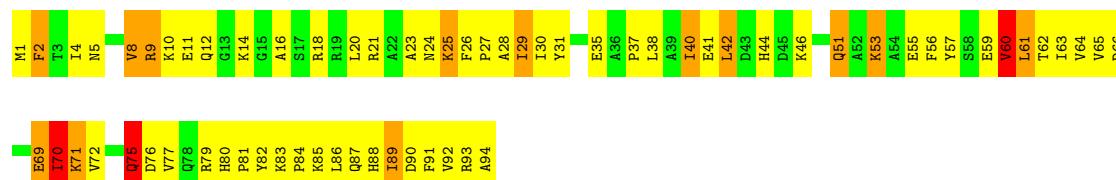
- Molecule 34: 50S ribosomal protein L35



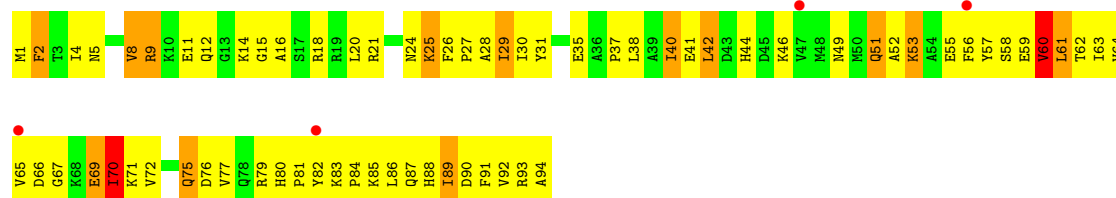
- Molecule 34: 50S ribosomal protein L35



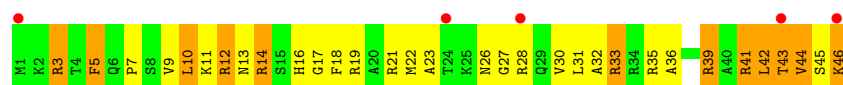
• Molecule 35: 50S ribosomal protein L25



• Molecule 35: 50S ribosomal protein L25



• Molecule 36: 50S ribosomal protein L34

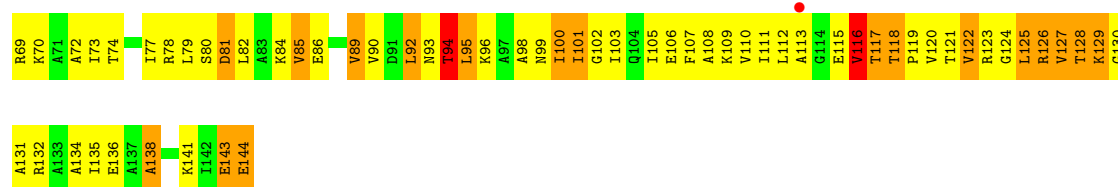


• Molecule 36: 50S ribosomal protein L34

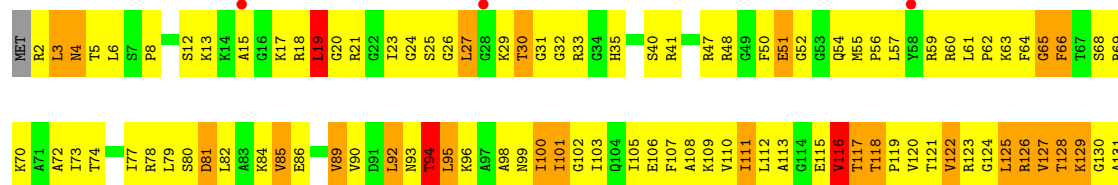


• Molecule 37: 50S ribosomal protein L15

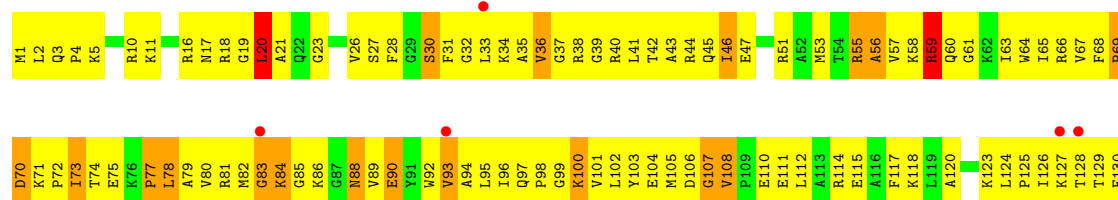




• Molecule 37: 50S ribosomal protein L15



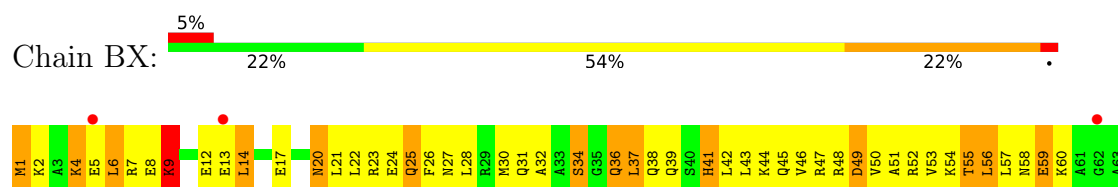
• Molecule 38: 50S ribosomal protein L16



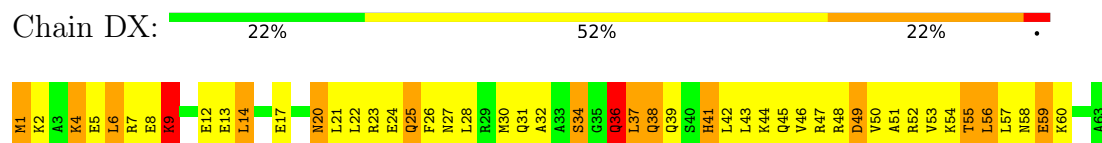
• Molecule 38: 50S ribosomal protein L16



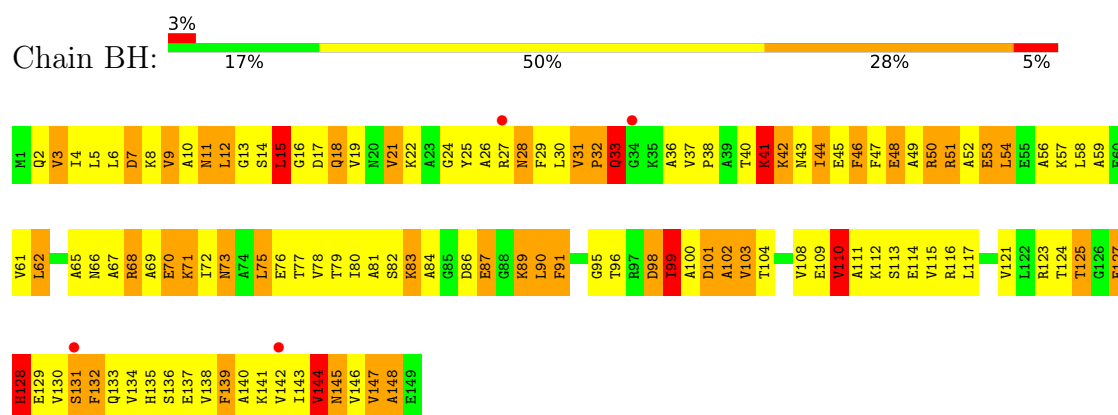
• Molecule 39: 50S ribosomal protein L29



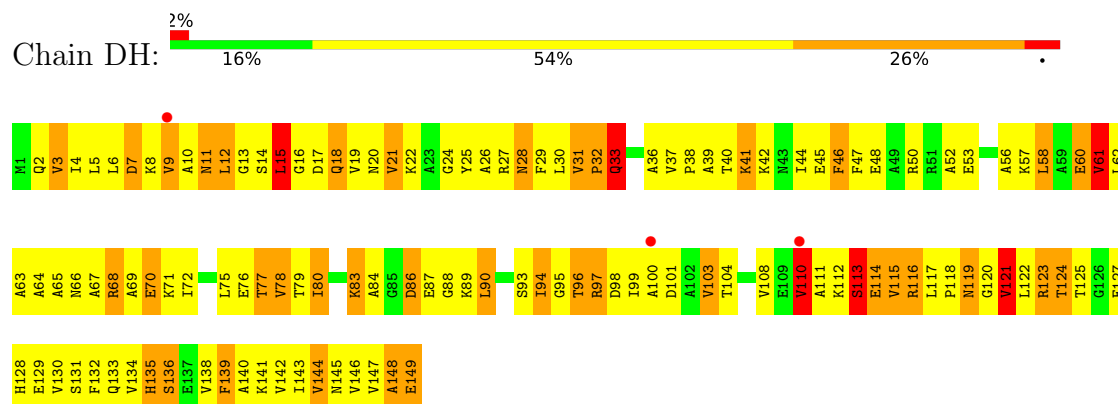
• Molecule 39: 50S ribosomal protein L29



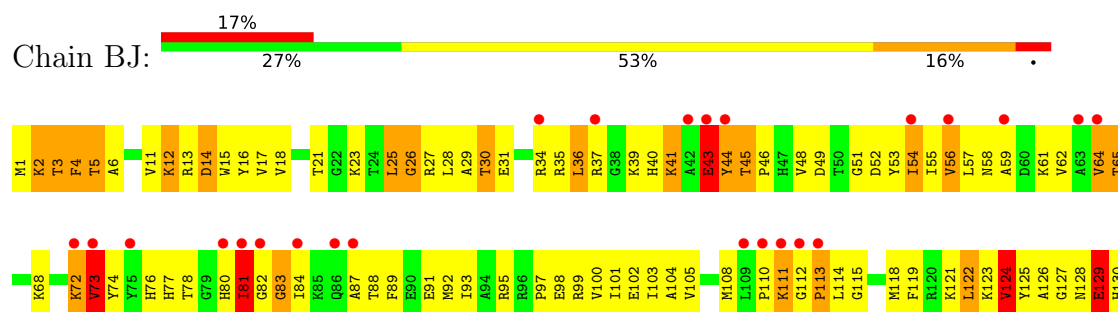
• Molecule 40: 50S ribosomal protein L9



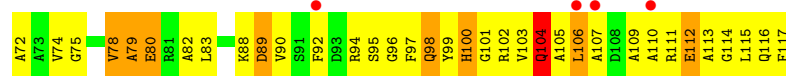
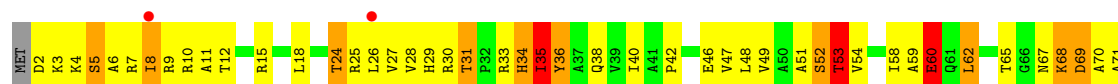
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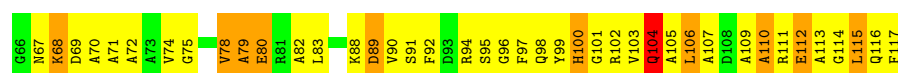
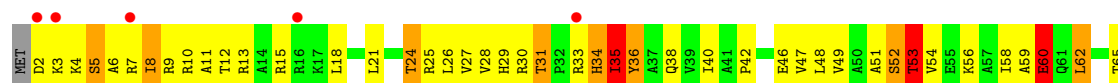
• Molecule 41: 50S ribosomal protein L13



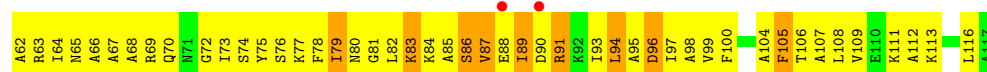




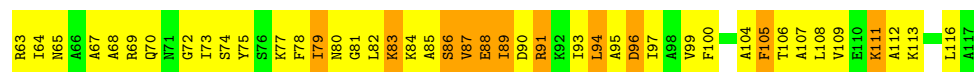
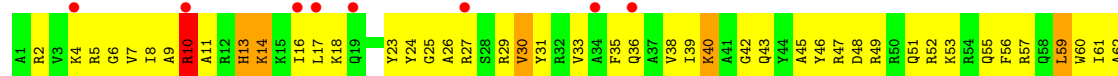
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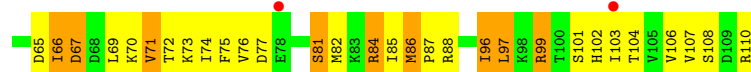
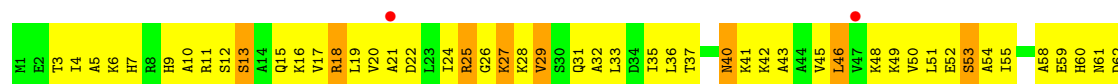
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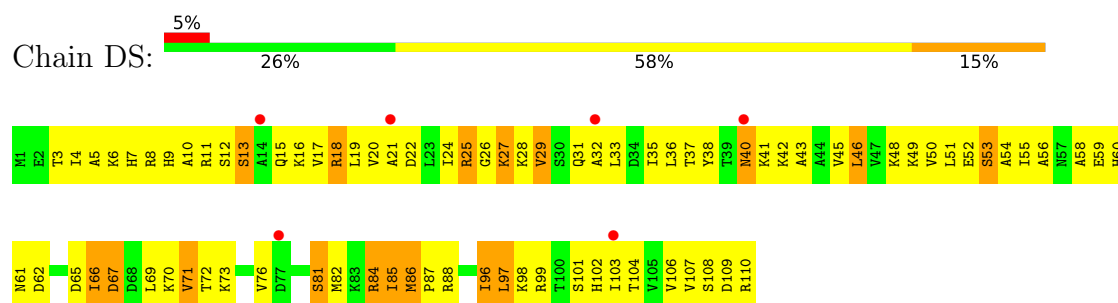
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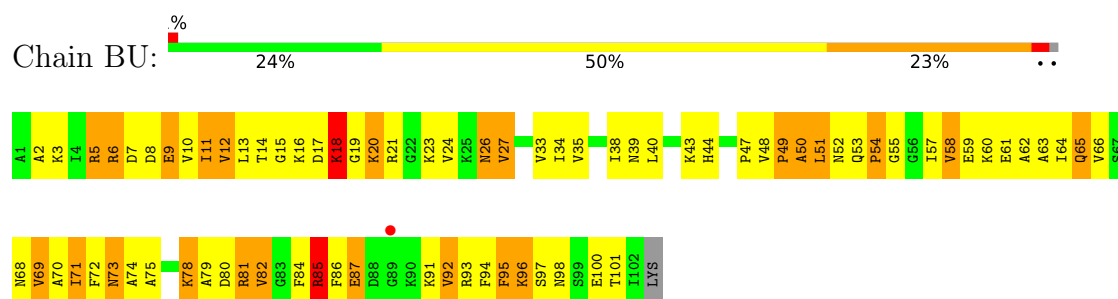
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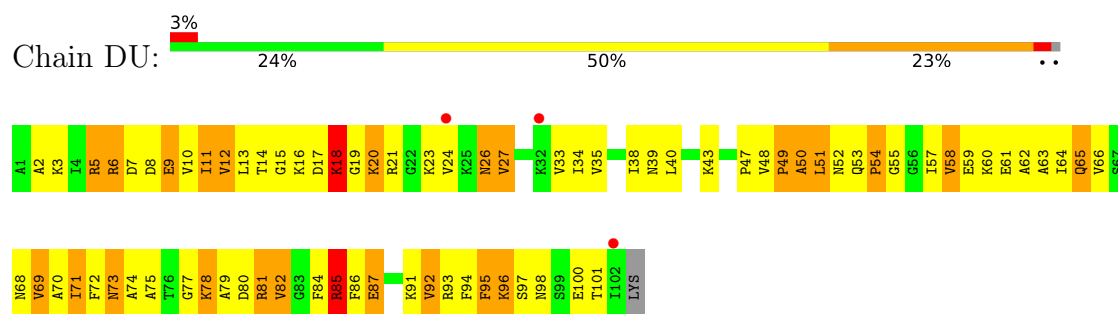
- Molecule 45: 50S ribosomal protein L22



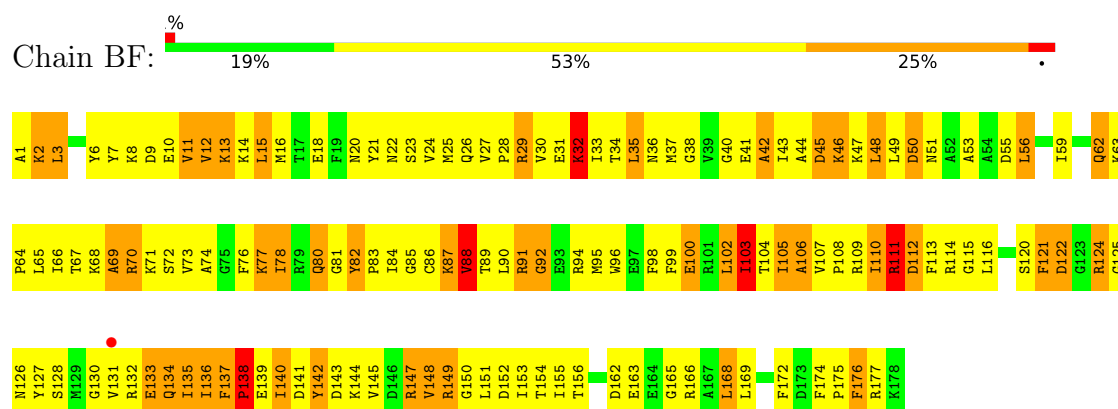
- Molecule 46: 50S ribosomal protein L24



- Molecule 46: 50S ribosomal protein L24

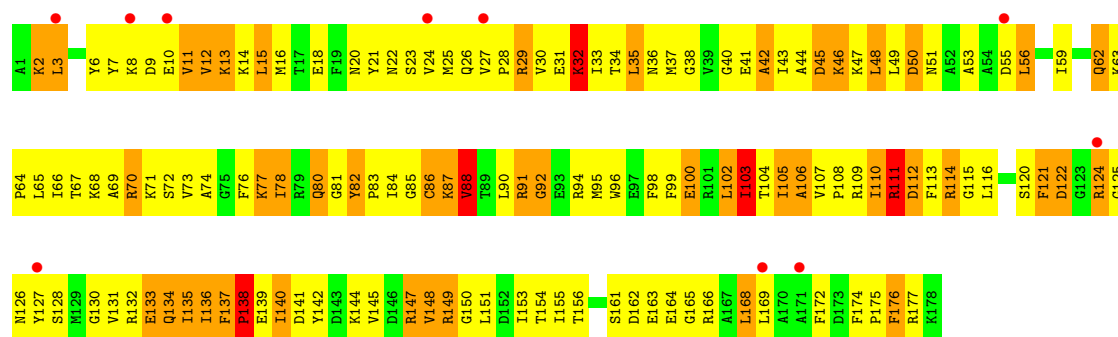


- Molecule 47: 50S ribosomal protein L5

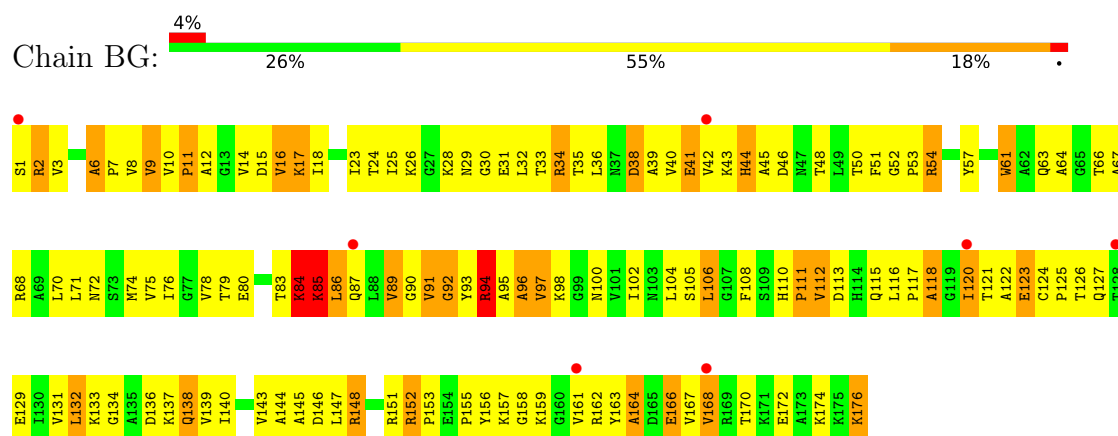


- Molecule 47: 50S ribosomal protein L5

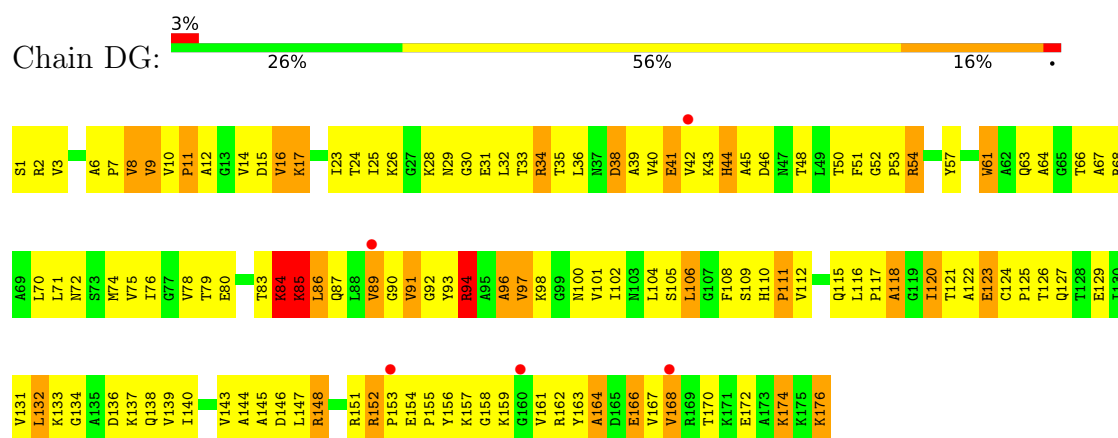




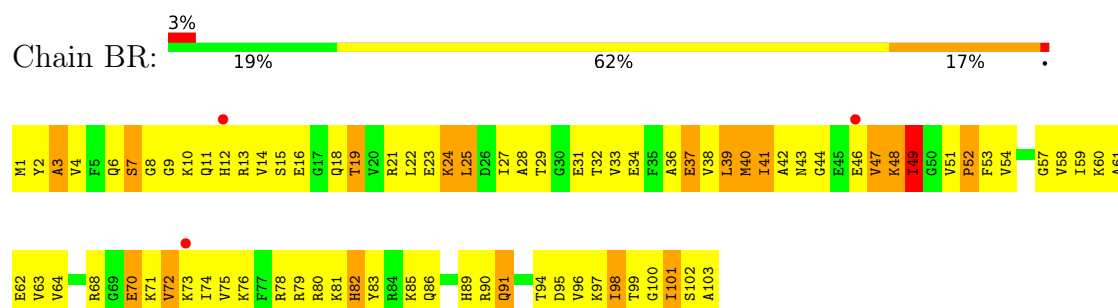
• Molecule 48: 50S ribosomal protein L6



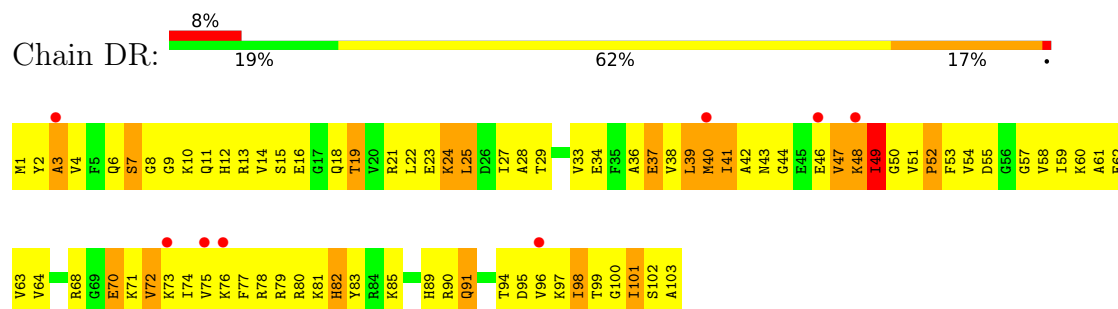
• Molecule 48: 50S ribosomal protein L6



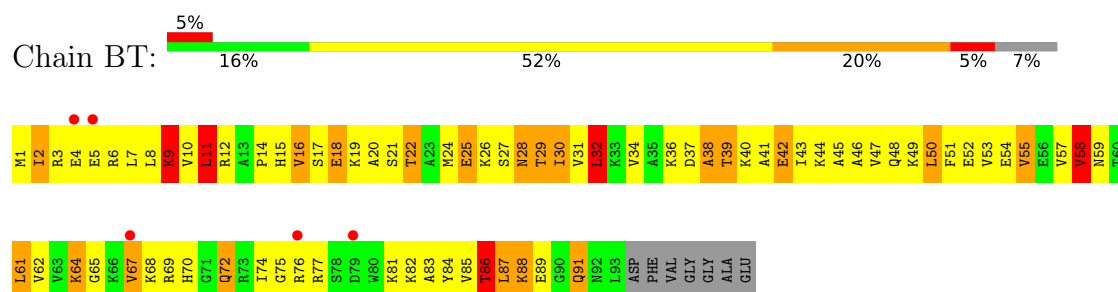
• Molecule 49: 50S ribosomal protein L21



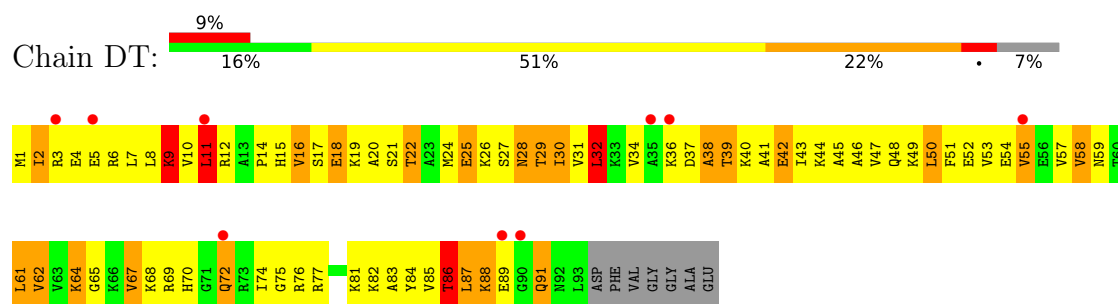
- Molecule 49: 50S ribosomal protein L21



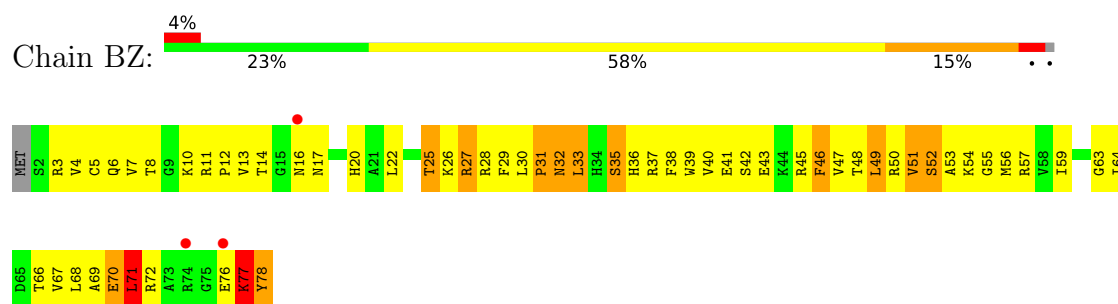
- Molecule 50: 50S ribosomal protein L23



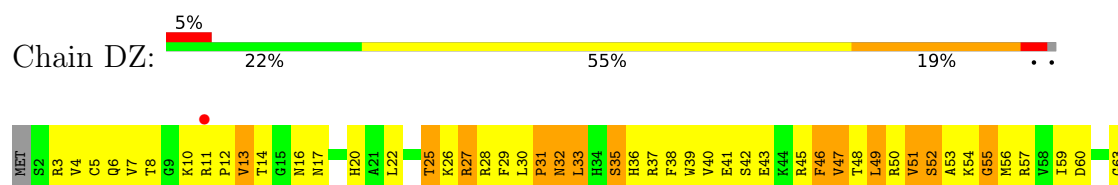
- Molecule 50: 50S ribosomal protein L23



- Molecule 51: 50S ribosomal protein L28

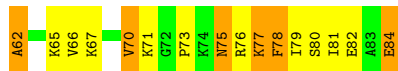
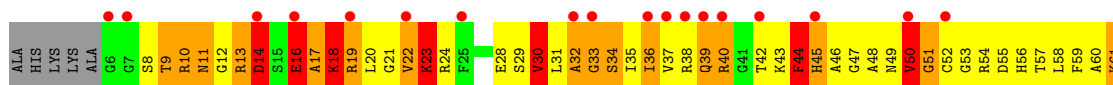
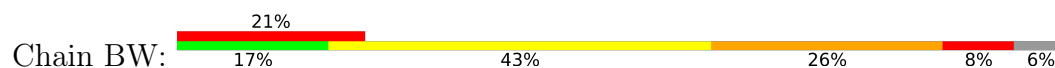


- Molecule 51: 50S ribosomal protein L28

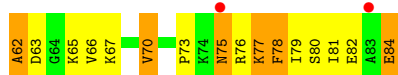
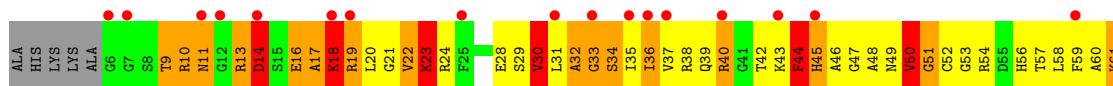
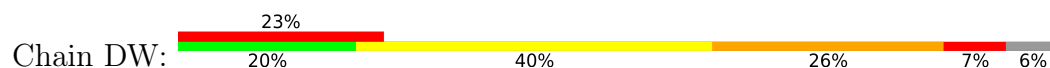




- Molecule 52: 50S ribosomal protein L27



- 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 70.00 – 3.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.50) 73.0 (70.00-3.53)	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 0.227 , 0.264	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)	0.28 , 55.6	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: ZN, MG, NMY, SCM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.27	0/36762	0.62	29/57350 (0.1%)
1	CA	0.29	0/36762	0.66	39/57350 (0.1%)
2	AC	0.28	0/1651	0.69	0/2225
2	CC	0.28	0/1651	0.73	0/2225
3	AD	0.26	0/1665	0.69	0/2227
3	CD	0.26	0/1665	0.70	0/2227
4	AE	0.28	0/1118	0.73	0/1504
4	CE	0.27	0/1118	0.74	0/1504
5	AF	0.28	0/835	0.70	0/1128
5	CF	0.28	0/835	0.70	0/1128
6	AG	0.28	0/1187	0.76	0/1591
6	CG	0.27	0/1211	0.78	2/1624 (0.1%)
7	AH	0.27	0/989	0.68	0/1326
7	CH	0.27	0/989	0.68	0/1326
8	AI	0.28	0/1034	0.68	0/1375
8	CI	0.27	0/1034	0.68	1/1375 (0.1%)
9	AJ	0.29	0/796	0.71	0/1077
9	CJ	0.29	0/796	0.72	0/1077
10	AK	0.31	0/893	0.75	0/1205
10	CK	0.31	0/893	0.75	0/1205
11	AL	0.27	0/969	0.72	0/1300
11	CL	0.27	0/969	0.73	0/1300
12	AM	0.27	0/892	0.68	0/1193
12	CM	0.26	0/884	0.71	0/1181
13	AP	0.28	0/659	0.75	1/884 (0.1%)
13	CP	0.28	0/648	0.72	1/870 (0.1%)
14	AQ	0.26	0/657	0.68	0/881
14	CQ	0.26	0/666	0.69	0/892
15	AR	0.28	0/462	0.73	0/621
15	CR	0.29	0/462	0.73	0/621
16	AS	0.28	0/652	0.76	1/877 (0.1%)
16	CS	0.27	0/660	0.71	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.28	0/671	0.68	0/888
17	CT	0.28	0/671	0.68	0/888
18	AB	0.28	0/1735	0.71	2/2338 (0.1%)
18	CB	0.29	0/1735	0.74	0/2338
19	AU	0.30	0/430	0.79	0/570
19	CU	0.29	0/430	0.78	0/570
20	AO	0.26	0/722	0.70	1/964 (0.1%)
20	CO	0.27	0/722	0.66	0/964
21	AN	0.26	0/785	0.71	0/1043
21	CN	0.27	0/785	0.71	0/1043
22	BA	0.27	0/2803	0.63	2/4371 (0.0%)
22	DA	0.27	0/2803	0.64	2/4371 (0.0%)
23	BB	0.27	1/68314 (0.0%)	0.64	72/106569 (0.1%)
23	DB	0.27	1/68314 (0.0%)	0.64	72/106569 (0.1%)
24	BI	0.32	0/1046	0.79	0/1410
24	DI	0.34	0/1046	0.82	0/1410
25	BC	0.27	0/2121	0.74	0/2852
25	DC	0.27	0/2121	0.73	0/2852
26	BD	0.29	0/1586	0.74	1/2134 (0.0%)
26	DD	0.29	0/1586	0.72	1/2134 (0.0%)
27	BK	0.29	0/939	0.78	0/1258
27	DK	0.29	0/939	0.78	0/1258
28	BP	0.28	0/929	0.78	1/1242 (0.1%)
28	DP	0.28	0/929	0.78	1/1242 (0.1%)
29	BE	0.26	0/1571	0.80	2/2113 (0.1%)
29	DE	0.27	0/1571	0.80	2/2113 (0.1%)
30	BY	0.29	0/453	0.74	0/605
30	DY	0.29	0/453	0.78	0/605
31	B0	0.25	0/450	0.79	2/599 (0.3%)
31	D0	0.25	0/450	0.79	3/599 (0.5%)
32	B4	0.29	0/303	0.81	0/397
32	D4	0.28	0/303	0.81	0/397
33	B1	0.30	0/416	0.79	0/554
33	D1	0.30	0/416	0.78	0/554
34	B3	0.28	0/513	0.77	0/676
34	D3	0.28	0/513	0.76	0/676
35	BV	0.28	0/766	0.71	0/1025
35	DV	0.28	0/766	0.70	0/1025
36	B2	0.28	0/380	0.79	0/498
36	D2	0.29	0/380	0.79	0/498
37	BL	0.28	0/1054	0.76	0/1403
37	DL	0.28	0/1054	0.76	0/1403
38	BM	0.28	0/1093	0.74	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.28	0/1093	0.73	0/1460
39	BX	0.27	0/510	0.85	2/677 (0.3%)
39	DX	0.27	0/510	0.87	2/677 (0.3%)
40	BH	0.29	0/1122	0.72	0/1515
40	DH	0.28	0/1122	0.72	2/1515 (0.1%)
41	BJ	0.28	0/1152	0.71	0/1551
41	DJ	0.28	0/1152	0.72	0/1551
42	BN	0.27	0/973	0.80	2/1301 (0.2%)
42	DN	0.27	0/973	0.82	3/1301 (0.2%)
43	BO	0.27	0/902	0.82	2/1209 (0.2%)
43	DO	0.27	0/902	0.82	3/1209 (0.2%)
44	BQ	0.27	0/960	0.82	0/1278
44	DQ	0.27	0/960	0.82	0/1278
45	BS	0.27	0/864	0.82	1/1156 (0.1%)
45	DS	0.27	0/864	0.82	1/1156 (0.1%)
46	BU	0.27	0/787	0.68	0/1051
46	DU	0.27	0/787	0.67	0/1051
47	BF	0.28	0/1444	0.83	2/1937 (0.1%)
47	DF	0.28	0/1444	0.83	2/1937 (0.1%)
48	BG	0.28	0/1343	0.75	2/1816 (0.1%)
48	DG	0.28	0/1343	0.74	0/1816
49	BR	0.26	0/829	0.63	0/1107
49	DR	0.26	0/829	0.64	0/1107
50	BT	0.26	0/744	0.80	0/994
50	DT	0.26	0/744	0.81	0/994
51	BZ	0.27	0/635	0.78	0/848
51	DZ	0.27	0/635	0.78	1/848 (0.1%)
52	BW	0.27	0/603	0.67	0/797
52	DW	0.27	0/603	0.69	0/797
All	All	0.27	2/306360 (0.0%)	0.67	263/457969 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-7.17	1.26	1.41
23	DB	1086	A	C5-C6	-7.11	1.26	1.41

The worst 5 of 263 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-10.97	75.09	108.00
23	BB	2204	G	O5'-P-OP2	-10.59	76.23	108.00
23	BB	2791	G	O5'-P-OP1	-10.11	77.67	108.00
23	DB	2791	G	O5'-P-OP2	-10.11	77.67	108.00
23	BB	2790	U	OP1-P-O3'	9.81	137.43	108.00

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	1289	0
1	CA	32831	0	16521	1305	0
2	AC	1624	0	1699	195	0
2	CC	1624	0	1699	199	0
3	AD	1643	0	1710	137	0
3	CD	1643	0	1710	134	0
4	AE	1105	0	1148	97	0
4	CE	1105	0	1148	98	0
5	AF	817	0	808	100	0
5	CF	817	0	808	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AG	1174	0	1230	155	0
6	CG	1196	0	1246	123	0
7	AH	979	0	1034	70	0
7	CH	979	0	1034	72	0
8	AI	1022	0	1070	153	0
8	CI	1022	0	1070	145	0
9	AJ	786	0	828	103	0
9	CJ	786	0	828	101	0
10	AK	877	0	887	111	0
10	CK	877	0	887	99	0
11	AL	955	0	1019	101	0
11	CL	955	0	1019	105	0
12	AM	883	0	944	168	0
12	CM	876	0	937	126	0
13	AP	649	0	666	65	0
13	CP	638	0	656	57	0
14	AQ	648	0	691	66	0
14	CQ	657	0	702	64	0
15	AR	455	0	478	41	0
15	CR	455	0	478	44	0
16	AS	637	0	665	109	0
16	CS	644	0	675	111	0
17	AT	665	0	714	70	0
17	CT	665	0	714	77	0
18	AB	1704	0	1732	209	0
18	CB	1704	0	1732	219	0
19	AU	425	0	449	78	0
19	CU	425	0	449	72	0
20	AO	714	0	734	70	0
20	CO	714	0	734	57	0
21	AN	774	0	827	118	0
21	CN	774	0	827	123	0
22	BA	2507	0	1270	105	0
22	DA	2507	0	1270	108	0
23	BB	60995	0	30679	2221	0
23	DB	60995	0	30678	2316	0
24	BI	1032	0	1088	122	0
24	DI	1032	0	1088	182	0
25	BC	2082	0	2157	235	0
25	DC	2082	0	2157	237	0
26	BD	1565	0	1616	218	0
26	DD	1565	0	1616	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	BK	930	0	1000	135	0
27	DK	930	0	1000	147	0
28	BP	917	0	965	117	0
28	DP	917	0	965	119	0
29	BE	1552	0	1619	218	0
29	DE	1552	0	1619	206	0
30	BY	449	0	491	60	0
30	DY	449	0	491	58	0
31	B0	444	0	461	39	0
31	D0	444	0	461	42	0
32	B4	302	0	340	43	0
32	D4	302	0	340	41	0
33	B1	409	0	440	36	0
33	D1	409	0	440	39	0
34	B3	504	0	574	51	0
34	D3	504	0	574	47	0
35	BV	753	0	780	104	0
35	DV	753	0	780	104	0
36	B2	377	0	418	52	0
36	D2	377	0	418	46	0
37	BL	1045	0	1117	143	0
37	DL	1045	0	1117	156	0
38	BM	1074	0	1157	125	0
38	DM	1074	0	1157	122	0
39	BX	509	0	543	66	0
39	DX	509	0	543	71	0
40	BH	1111	0	1148	202	0
40	DH	1111	0	1148	187	0
41	BJ	1129	0	1162	135	0
41	DJ	1129	0	1162	134	0
42	BN	960	0	1000	124	0
42	DN	960	0	1000	124	0
43	BO	892	0	923	96	0
43	DO	892	0	923	105	0
44	BQ	947	0	1022	154	0
44	DQ	947	0	1022	152	0
45	BS	857	0	922	90	0
45	DS	857	0	922	98	0
46	BU	779	0	834	112	0
46	DU	779	0	834	116	0
47	BF	1420	0	1460	237	0
47	DF	1420	0	1460	234	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	BG	1323	0	1374	194	0
48	DG	1323	0	1374	180	0
49	BR	816	0	839	113	0
49	DR	816	0	839	112	0
50	BT	738	0	807	113	0
50	DT	738	0	807	122	0
51	BZ	625	0	652	72	0
51	DZ	625	0	652	70	0
52	BW	596	0	610	138	0
52	DW	596	0	610	133	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
57	CN	3	0	0	0	0
57	CP	1	0	0	0	0
57	CT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	17333	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 37.

The worst 5 of 17333 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%)	0	7
3	AD	203/205 (99%)	153 (75%)	40 (20%)	10 (5%)	1	16
3	CD	203/205 (99%)	153 (75%)	40 (20%)	10 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AE	148/166 (89%)	116 (78%)	24 (16%)	8 (5%)	1	14
4	CE	148/166 (89%)	114 (77%)	25 (17%)	9 (6%)	1	12
5	AF	98/135 (73%)	63 (64%)	25 (26%)	10 (10%)	0	6
5	CF	98/135 (73%)	64 (65%)	24 (24%)	10 (10%)	0	6
6	AG	148/178 (83%)	110 (74%)	30 (20%)	8 (5%)	1	14
6	CG	150/178 (84%)	111 (74%)	28 (19%)	11 (7%)	1	9
7	AH	127/129 (98%)	92 (72%)	31 (24%)	4 (3%)	3	25
7	CH	127/129 (98%)	92 (72%)	31 (24%)	4 (3%)	3	25
8	AI	125/129 (97%)	80 (64%)	35 (28%)	10 (8%)	1	8
8	CI	125/129 (97%)	80 (64%)	34 (27%)	11 (9%)	0	7
9	AJ	96/103 (93%)	59 (62%)	25 (26%)	12 (12%)	0	4
9	CJ	96/103 (93%)	64 (67%)	22 (23%)	10 (10%)	0	5
10	AK	115/128 (90%)	87 (76%)	23 (20%)	5 (4%)	2	18
10	CK	115/128 (90%)	86 (75%)	24 (21%)	5 (4%)	2	18
11	AL	121/123 (98%)	69 (57%)	37 (31%)	15 (12%)	0	4
11	CL	121/123 (98%)	72 (60%)	34 (28%)	15 (12%)	0	4
12	AM	112/117 (96%)	74 (66%)	25 (22%)	13 (12%)	0	4
12	CM	111/117 (95%)	78 (70%)	21 (19%)	12 (11%)	0	5
13	AP	80/82 (98%)	53 (66%)	20 (25%)	7 (9%)	0	7
13	CP	78/82 (95%)	52 (67%)	19 (24%)	7 (9%)	0	7
14	AQ	78/83 (94%)	59 (76%)	15 (19%)	4 (5%)	1	15
14	CQ	79/83 (95%)	57 (72%)	18 (23%)	4 (5%)	1	15
15	AR	53/74 (72%)	40 (76%)	13 (24%)	0	100	100
15	CR	53/74 (72%)	41 (77%)	11 (21%)	1 (2%)	6	33
16	AS	77/91 (85%)	49 (64%)	24 (31%)	4 (5%)	1	14
16	CS	78/91 (86%)	57 (73%)	16 (20%)	5 (6%)	1	11
17	AT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	1	12
17	CT	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	1	12
18	AB	216/240 (90%)	135 (62%)	56 (26%)	25 (12%)	0	4
18	CB	216/240 (90%)	145 (67%)	52 (24%)	19 (9%)	0	7
19	AU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	CU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	0	4
20	AO	86/89 (97%)	62 (72%)	18 (21%)	6 (7%)	1	10
20	CO	86/89 (97%)	60 (70%)	25 (29%)	1 (1%)	10	41
21	AN	92/100 (92%)	53 (58%)	30 (33%)	9 (10%)	0	6
21	CN	92/100 (92%)	49 (53%)	31 (34%)	12 (13%)	0	3
24	BI	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	3	26
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	2	22
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	2
26	DD	207/209 (99%)	118 (57%)	58 (28%)	31 (15%)	0	2
27	BK	119/123 (97%)	70 (59%)	27 (23%)	22 (18%)	0	1
27	DK	119/123 (97%)	69 (58%)	29 (24%)	21 (18%)	0	1
28	BP	112/114 (98%)	66 (59%)	29 (26%)	17 (15%)	0	2
28	DP	112/114 (98%)	66 (59%)	29 (26%)	17 (15%)	0	2
29	BE	199/201 (99%)	124 (62%)	51 (26%)	24 (12%)	0	4
29	DE	199/201 (99%)	124 (62%)	48 (24%)	27 (14%)	0	3
30	BY	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	0	7
30	DY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	0	7
31	B0	54/56 (96%)	36 (67%)	12 (22%)	6 (11%)	0	5
31	D0	54/56 (96%)	36 (67%)	12 (22%)	6 (11%)	0	5
32	B4	36/38 (95%)	20 (56%)	9 (25%)	7 (19%)	0	1
32	D4	36/38 (95%)	21 (58%)	8 (22%)	7 (19%)	0	1
33	B1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	0	7
33	D1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	0	7
34	B3	62/64 (97%)	39 (63%)	17 (27%)	6 (10%)	0	6
34	D3	62/64 (97%)	39 (63%)	18 (29%)	5 (8%)	1	8
35	BV	92/94 (98%)	60 (65%)	22 (24%)	10 (11%)	0	5
35	DV	92/94 (98%)	59 (64%)	23 (25%)	10 (11%)	0	5
36	B2	44/46 (96%)	25 (57%)	16 (36%)	3 (7%)	1	10
36	D2	44/46 (96%)	24 (54%)	16 (36%)	4 (9%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BL	141/144 (98%)	78 (55%)	44 (31%)	19 (14%)	0	3
37	DL	141/144 (98%)	78 (55%)	42 (30%)	21 (15%)	0	2
38	BM	134/136 (98%)	90 (67%)	28 (21%)	16 (12%)	0	4
38	DM	134/136 (98%)	91 (68%)	26 (19%)	17 (13%)	0	3
39	BX	61/63 (97%)	35 (57%)	22 (36%)	4 (7%)	1	11
39	DX	61/63 (97%)	35 (57%)	22 (36%)	4 (7%)	1	11
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	3
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	5
42	DN	118/127 (93%)	74 (63%)	32 (27%)	12 (10%)	0	6
43	BO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	8
43	DO	114/117 (97%)	79 (69%)	25 (22%)	10 (9%)	0	7
44	BQ	115/117 (98%)	76 (66%)	32 (28%)	7 (6%)	1	12
44	DQ	115/117 (98%)	75 (65%)	33 (29%)	7 (6%)	1	12
45	BS	108/110 (98%)	67 (62%)	28 (26%)	13 (12%)	0	4
45	DS	108/110 (98%)	67 (62%)	28 (26%)	13 (12%)	0	4
46	BU	100/103 (97%)	50 (50%)	35 (35%)	15 (15%)	0	2
46	DU	100/103 (97%)	54 (54%)	31 (31%)	15 (15%)	0	2
47	BF	176/178 (99%)	102 (58%)	48 (27%)	26 (15%)	0	2
47	DF	176/178 (99%)	102 (58%)	48 (27%)	26 (15%)	0	2
48	BG	174/176 (99%)	111 (64%)	40 (23%)	23 (13%)	0	3
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	5
49	DR	101/103 (98%)	59 (58%)	31 (31%)	11 (11%)	0	5
50	BT	91/100 (91%)	49 (54%)	25 (28%)	17 (19%)	0	1
50	DT	91/100 (91%)	47 (52%)	27 (30%)	17 (19%)	0	1
51	BZ	75/78 (96%)	50 (67%)	17 (23%)	8 (11%)	0	5
51	DZ	75/78 (96%)	48 (64%)	19 (25%)	8 (11%)	0	5
52	BW	77/84 (92%)	26 (34%)	26 (34%)	25 (32%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	5

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%)	138 (81%)	32 (19%)	1	9
2	CC	170/189 (90%)	138 (81%)	32 (19%)	1	9
3	AD	172/172 (100%)	147 (86%)	25 (14%)	3	17
3	CD	172/172 (100%)	147 (86%)	25 (14%)	3	17
4	AE	113/125 (90%)	91 (80%)	22 (20%)	1	8
4	CE	113/125 (90%)	91 (80%)	22 (20%)	1	8
5	AF	87/116 (75%)	72 (83%)	15 (17%)	2	12
5	CF	87/116 (75%)	72 (83%)	15 (17%)	2	12
6	AG	123/146 (84%)	103 (84%)	20 (16%)	2	14
6	CG	125/146 (86%)	96 (77%)	29 (23%)	1	5
7	AH	104/104 (100%)	93 (89%)	11 (11%)	6	27
7	CH	104/104 (100%)	94 (90%)	10 (10%)	8	30
8	AI	105/106 (99%)	89 (85%)	16 (15%)	3	16
8	CI	105/106 (99%)	83 (79%)	22 (21%)	1	6
9	AJ	86/90 (96%)	72 (84%)	14 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CJ	86/90 (96%)	71 (83%)	15 (17%)	2	11
10	AK	90/98 (92%)	75 (83%)	15 (17%)	2	13
10	CK	90/98 (92%)	77 (86%)	13 (14%)	3	18
11	AL	103/103 (100%)	88 (85%)	15 (15%)	3	17
11	CL	103/103 (100%)	88 (85%)	15 (15%)	3	17
12	AM	92/95 (97%)	75 (82%)	17 (18%)	1	9
12	CM	91/95 (96%)	68 (75%)	23 (25%)	0	3
13	AP	65/65 (100%)	60 (92%)	5 (8%)	12	37
13	CP	65/65 (100%)	60 (92%)	5 (8%)	12	37
14	AQ	74/77 (96%)	65 (88%)	9 (12%)	5	22
14	CQ	75/77 (97%)	66 (88%)	9 (12%)	5	23
15	AR	48/64 (75%)	41 (85%)	7 (15%)	3	17
15	CR	48/64 (75%)	41 (85%)	7 (15%)	3	17
16	AS	70/78 (90%)	49 (70%)	21 (30%)	0	2
16	CS	71/78 (91%)	54 (76%)	17 (24%)	1	4
17	AT	65/65 (100%)	57 (88%)	8 (12%)	4	22
17	CT	65/65 (100%)	57 (88%)	8 (12%)	4	22
18	AB	180/198 (91%)	156 (87%)	24 (13%)	4	20
18	CB	180/198 (91%)	141 (78%)	39 (22%)	1	6
19	AU	44/60 (73%)	36 (82%)	8 (18%)	2	10
19	CU	44/60 (73%)	36 (82%)	8 (18%)	2	10
20	AO	76/77 (99%)	70 (92%)	6 (8%)	11	36
20	CO	76/77 (99%)	61 (80%)	15 (20%)	1	8
21	AN	79/83 (95%)	70 (89%)	9 (11%)	5	24
21	CN	79/83 (95%)	67 (85%)	12 (15%)	3	16
24	BI	109/109 (100%)	109 (100%)	0	100	100
24	DI	109/109 (100%)	106 (97%)	3 (3%)	38	61
25	BC	216/217 (100%)	182 (84%)	34 (16%)	2	15
25	DC	216/217 (100%)	181 (84%)	35 (16%)	2	14
26	BD	164/164 (100%)	133 (81%)	31 (19%)	1	9
26	DD	164/164 (100%)	134 (82%)	30 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BK	102/104 (98%)	76 (74%)	26 (26%)	0	3
27	DK	102/104 (98%)	75 (74%)	27 (26%)	0	3
28	BP	99/99 (100%)	82 (83%)	17 (17%)	2	12
28	DP	99/99 (100%)	82 (83%)	17 (17%)	2	12
29	BE	165/165 (100%)	144 (87%)	21 (13%)	4	21
29	DE	165/165 (100%)	145 (88%)	20 (12%)	5	22
30	BY	48/48 (100%)	38 (79%)	10 (21%)	1	6
30	DY	48/48 (100%)	38 (79%)	10 (21%)	1	6
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%)	29 (85%)	5 (15%)	3	17
32	D4	34/34 (100%)	30 (88%)	4 (12%)	5	23
33	B1	45/48 (94%)	36 (80%)	9 (20%)	1	7
33	D1	45/48 (94%)	36 (80%)	9 (20%)	1	7
34	B3	51/51 (100%)	48 (94%)	3 (6%)	18	44
34	D3	51/51 (100%)	48 (94%)	3 (6%)	18	44
35	BV	78/78 (100%)	63 (81%)	15 (19%)	1	8
35	DV	78/78 (100%)	63 (81%)	15 (19%)	1	8
36	B2	38/38 (100%)	27 (71%)	11 (29%)	0	2
36	D2	38/38 (100%)	27 (71%)	11 (29%)	0	2
37	BL	102/103 (99%)	83 (81%)	19 (19%)	1	9
37	DL	102/103 (99%)	83 (81%)	19 (19%)	1	9
38	BM	109/109 (100%)	92 (84%)	17 (16%)	2	15
38	DM	109/109 (100%)	92 (84%)	17 (16%)	2	15
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	6
39	DX	55/55 (100%)	42 (76%)	13 (24%)	1	4
40	BH	114/114 (100%)	83 (73%)	31 (27%)	0	3
40	DH	114/114 (100%)	85 (75%)	29 (25%)	0	3
41	BJ	116/116 (100%)	97 (84%)	19 (16%)	2	14
41	DJ	116/116 (100%)	98 (84%)	18 (16%)	2	15
42	BN	100/103 (97%)	85 (85%)	15 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	DN	100/103 (97%)	84 (84%)	16 (16%)	2	14
43	BO	86/87 (99%)	68 (79%)	18 (21%)	1	6
43	DO	86/87 (99%)	68 (79%)	18 (21%)	1	6
44	BQ	89/89 (100%)	76 (85%)	13 (15%)	3	17
44	DQ	89/89 (100%)	75 (84%)	14 (16%)	2	15
45	BS	93/93 (100%)	84 (90%)	9 (10%)	8	30
45	DS	93/93 (100%)	85 (91%)	8 (9%)	10	33
46	BU	83/84 (99%)	67 (81%)	16 (19%)	1	8
46	DU	83/84 (99%)	67 (81%)	16 (19%)	1	8
47	BF	149/149 (100%)	114 (76%)	35 (24%)	1	4
47	DF	149/149 (100%)	113 (76%)	36 (24%)	1	4
48	BG	137/137 (100%)	115 (84%)	22 (16%)	2	14
48	DG	137/137 (100%)	114 (83%)	23 (17%)	2	13
49	BR	84/84 (100%)	71 (84%)	13 (16%)	2	15
49	DR	84/84 (100%)	71 (84%)	13 (16%)	2	15
50	BT	80/84 (95%)	61 (76%)	19 (24%)	1	4
50	DT	80/84 (95%)	61 (76%)	19 (24%)	1	4
51	BZ	67/68 (98%)	57 (85%)	10 (15%)	3	17
51	DZ	67/68 (98%)	55 (82%)	12 (18%)	2	10
52	BW	59/62 (95%)	45 (76%)	14 (24%)	1	4
52	DW	59/62 (95%)	46 (78%)	13 (22%)	1	5
All	All	9333/9700 (96%)	7743 (83%)	1590 (17%)	2	12

5 of 1590 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CC	101	ASN
25	DC	257	ARG
6	CG	75	LYS
2	CC	99	GLN
21	CN	80	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 370 such sidechains are listed below:

Mol	Chain	Res	Type
2	CC	139	ASN
28	DP	76	HIS
9	CJ	20	GLN
25	DC	59	GLN
34	D3	27	ASN

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
22	DA	66	A
23	DB	2324	U
23	DB	139	U
23	DB	1301	A
23	DB	2756	U

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 oligosaccharides 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
55	SCM	AA	1662	-	23,25,25	1.70	7 (30%)	27,39,39	1.55	4 (14%)
53	NMY	AA	1601	-	43,45,45	1.93	11 (25%)	62,67,67	1.15	5 (8%)
53	NMY	CA	1601	-	43,45,45	1.84	11 (25%)	62,67,67	1.18	5 (8%)
53	NMY	BB	3001	-	43,45,45	1.85	10 (23%)	62,67,67	1.22	7 (11%)
53	NMY	DB	3001	-	43,45,45	1.89	11 (25%)	62,67,67	1.24	6 (9%)
55	SCM	CA	1661	-	23,25,25	1.71	7 (30%)	27,39,39	1.56	4 (14%)

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

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	AA	1601	NMY	C3-C2	4.80	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BB	3001	NMY	C3-C2	4.74	1.59	1.53
53	DB	3001	NMY	C3-C2	4.72	1.59	1.53
53	CA	1601	NMY	O22-C18	4.66	1.53	1.41
53	AA	1601	NMY	O22-C18	4.59	1.53	1.41

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	-5.13	107.61	114.23
55	CA	1661	SCM	C1M-N10-C10	-5.10	107.64	114.23
53	DB	3001	NMY	O11-C13-O16	4.36	115.82	111.37
53	BB	3001	NMY	O18-C18-C19	3.89	114.44	108.08
53	CA	1601	NMY	O18-C18-C19	3.87	114.41	108.08

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	AA	1601	NMY	C14-C13-O11-C11
53	AA	1601	NMY	O16-C13-O11-C11
53	BB	3001	NMY	O16-C13-O11-C11
53	BB	3001	NMY	O16-C16-C17-O17
53	DB	3001	NMY	C4-C5-C6-N6

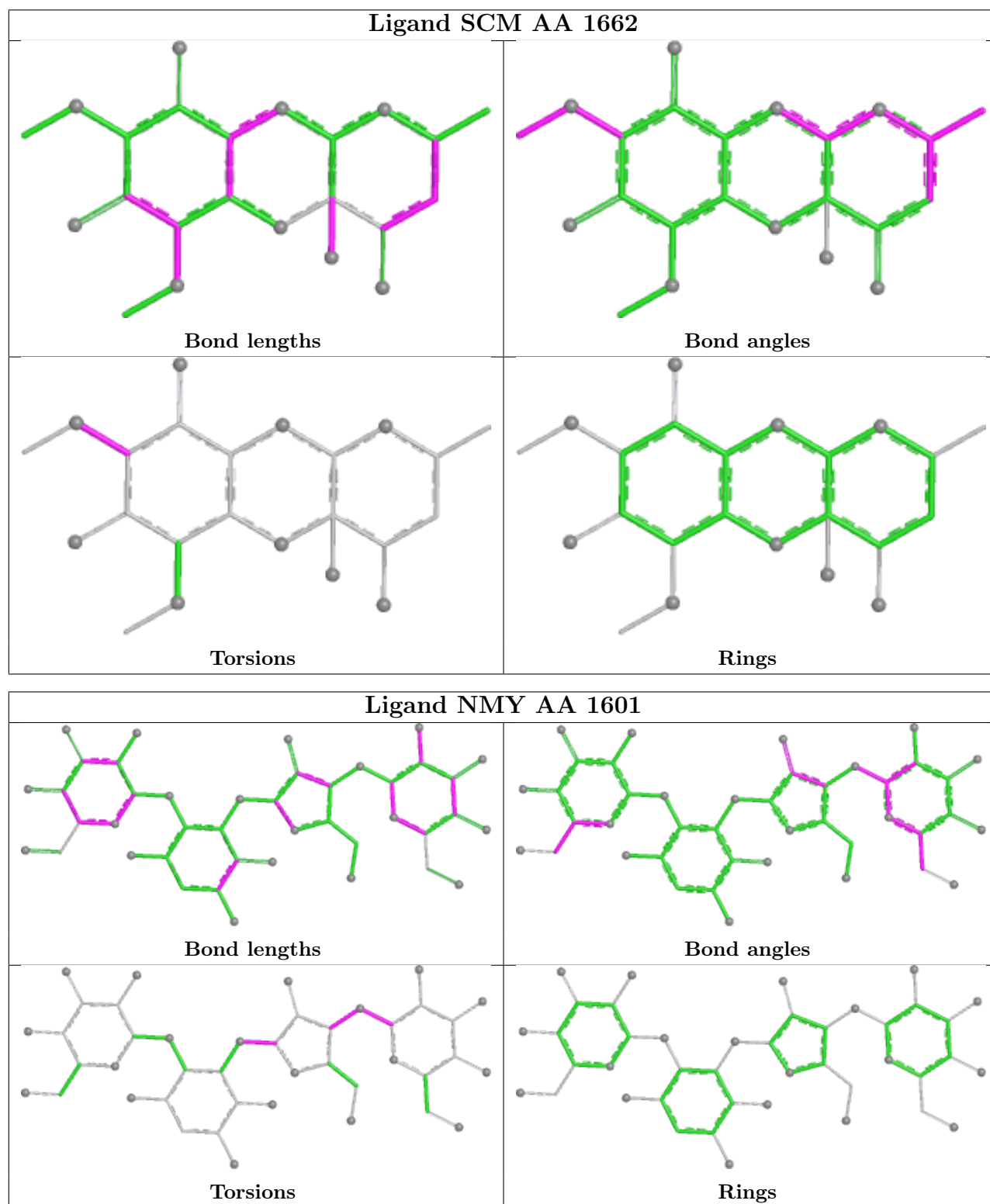
There are no ring outliers.

3 monomers are involved in 7 short contacts:

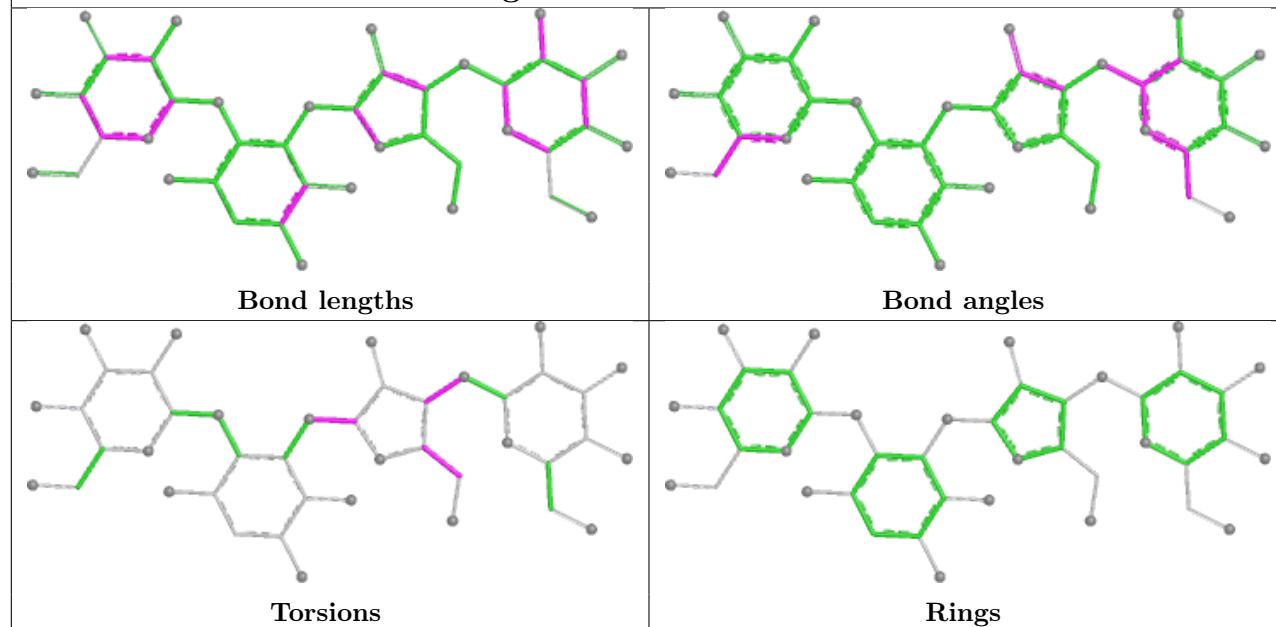
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	AA	1662	SCM	5	0
53	DB	3001	NMY	1	0
55	CA	1661	SCM	1	0

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.

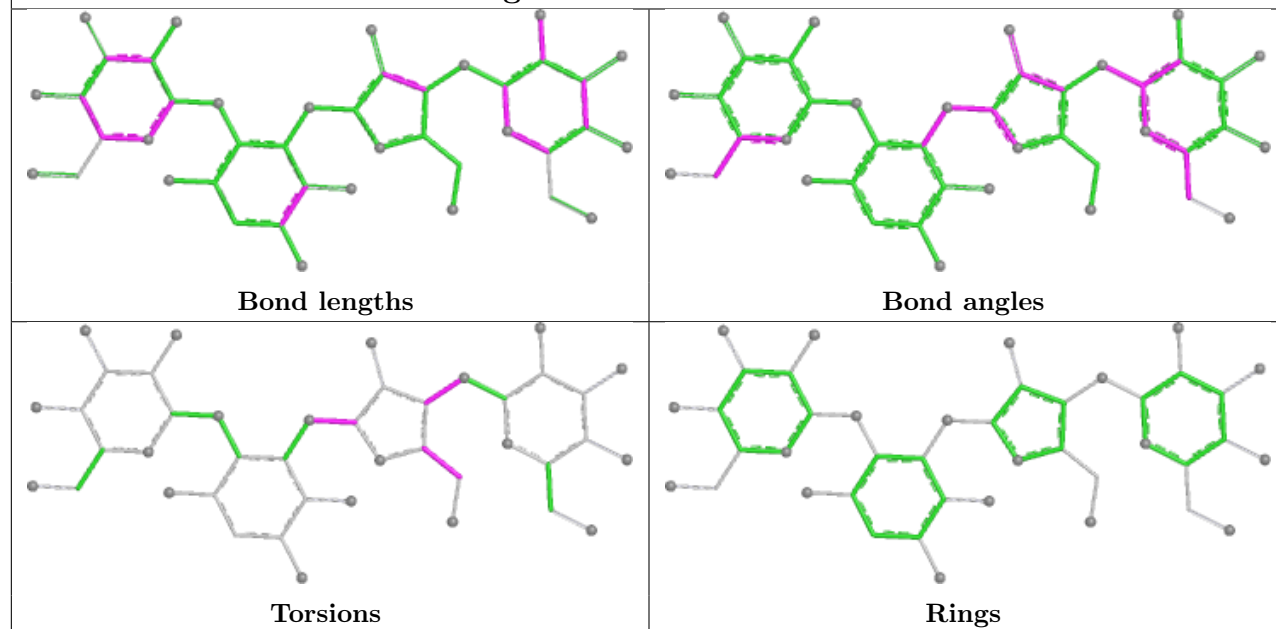
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

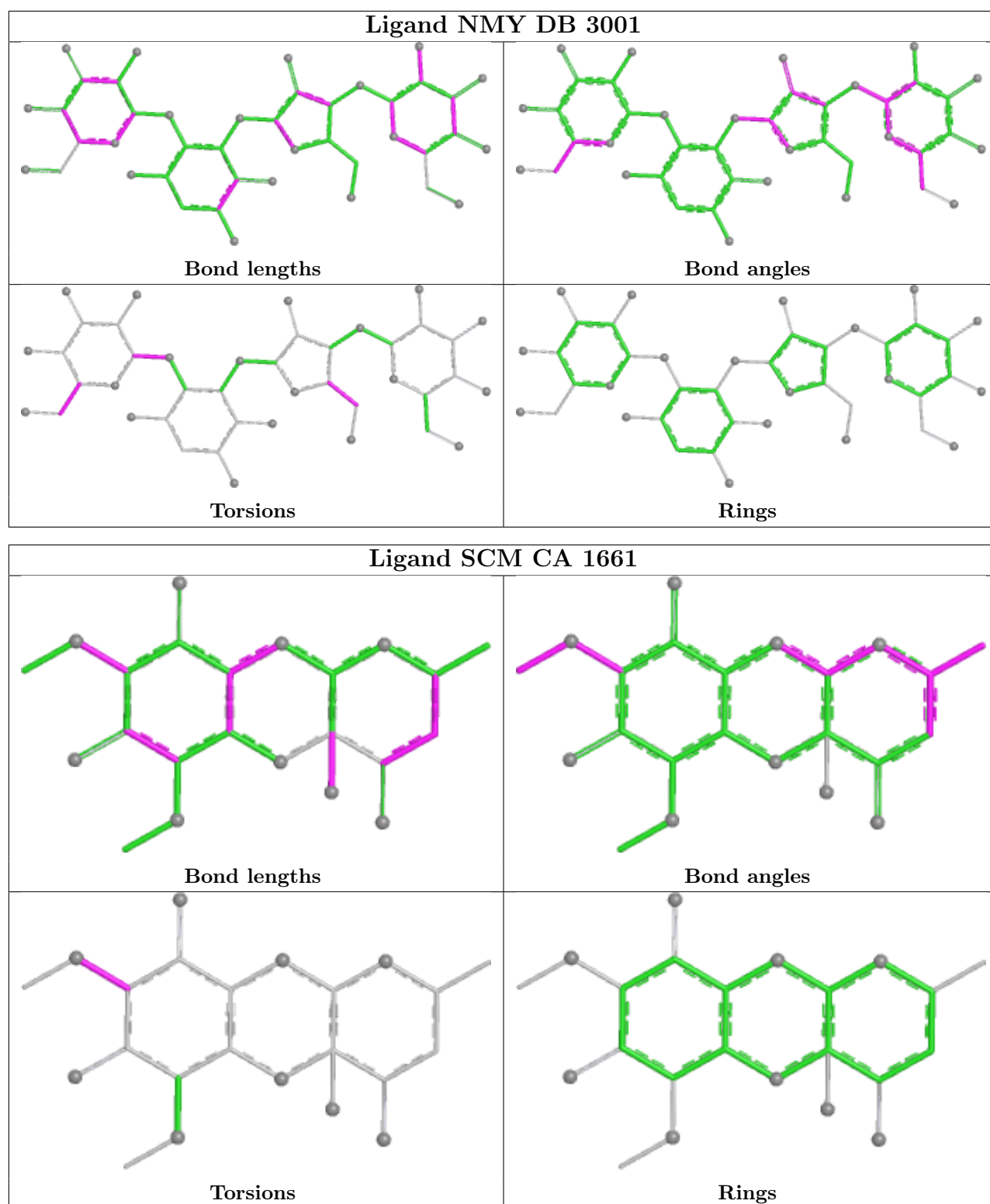


Ligand NMY CA 1601



Ligand NMY BB 3001





5.7 Other polymers ⓘ

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%)	-0.43	20 (1%) 75 50	16, 81, 159, 180	0
1	CA	1530/1542 (99%)	-0.53	10 (0%) 84 63	9, 57, 133, 180	0
2	AC	206/232 (88%)	-0.12	3 (1%) 72 47	9, 76, 136, 180	0
2	CC	206/232 (88%)	-0.17	5 (2%) 59 35	7, 75, 127, 180	0
3	AD	205/205 (100%)	0.24	10 (4%) 35 19	24, 92, 157, 180	0
3	CD	205/205 (100%)	0.00	4 (1%) 65 39	10, 64, 139, 180	0
4	AE	150/166 (90%)	0.24	7 (4%) 36 20	11, 74, 139, 176	0
4	CE	150/166 (90%)	-0.01	6 (4%) 42 23	5, 61, 132, 180	0
5	AF	100/135 (74%)	-0.13	0 100 100	11, 86, 144, 172	0
5	CF	100/135 (74%)	-0.14	0 100 100	7, 83, 173, 180	0
6	AG	150/178 (84%)	-0.12	4 (2%) 56 33	23, 104, 153, 180	0
6	CG	152/178 (85%)	-0.19	3 (1%) 65 39	27, 90, 147, 180	0
7	AH	129/129 (100%)	0.01	2 (1%) 70 45	13, 88, 155, 180	0
7	CH	129/129 (100%)	-0.07	2 (1%) 70 45	5, 61, 127, 180	0
8	AI	127/129 (98%)	0.28	10 (7%) 18 12	36, 91, 150, 180	0
8	CI	127/129 (98%)	0.30	9 (7%) 22 14	20, 92, 148, 180	0
9	AJ	98/103 (95%)	0.22	3 (3%) 51 29	22, 94, 151, 180	0
9	CJ	98/103 (95%)	0.31	6 (6%) 27 16	17, 89, 156, 180	0
10	AK	117/128 (91%)	-0.23	3 (2%) 57 33	14, 67, 124, 180	0
10	CK	117/128 (91%)	-0.22	2 (1%) 69 43	5, 56, 125, 178	0
11	AL	123/123 (100%)	0.34	13 (10%) 11 8	19, 80, 133, 180	0
11	CL	123/123 (100%)	0.36	13 (10%) 11 8	7, 51, 135, 180	0
12	AM	114/117 (97%)	-0.13	0 100 100	56, 120, 166, 180	0
12	CM	113/117 (96%)	-0.12	2 (1%) 67 42	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%)	0.59	7 (8%)	16 11	38, 91, 152, 180	0
13	CP	80/82 (97%)	0.49	5 (6%)	26 15	6, 63, 141, 180	0
14	AQ	80/83 (96%)	-0.04	1 (1%)	75 50	37, 99, 151, 180	0
14	CQ	81/83 (97%)	-0.05	1 (1%)	76 52	17, 71, 129, 180	0
15	AR	55/74 (74%)	0.01	1 (1%)	67 42	16, 76, 149, 180	0
15	CR	55/74 (74%)	-0.16	1 (1%)	67 42	21, 66, 126, 180	0
16	AS	79/91 (86%)	-0.10	0	100 100	55, 121, 180, 180	0
16	CS	80/91 (87%)	-0.10	2 (2%)	58 35	70, 109, 174, 180	0
17	AT	85/86 (98%)	0.28	8 (9%)	14 9	49, 106, 179, 180	0
17	CT	85/86 (98%)	0.23	4 (4%)	36 20	18, 65, 143, 159	0
18	AB	218/240 (90%)	-0.17	3 (1%)	73 48	22, 94, 153, 180	0
18	CB	218/240 (90%)	-0.21	4 (1%)	67 42	19, 102, 160, 180	0
19	AU	51/70 (72%)	0.96	10 (19%)	3 3	29, 101, 151, 180	0
19	CU	51/70 (72%)	0.59	4 (7%)	19 12	24, 113, 155, 180	0
20	AO	88/89 (98%)	-0.20	2 (2%)	61 37	18, 83, 137, 179	0
20	CO	88/89 (98%)	-0.17	2 (2%)	61 37	7, 60, 118, 161	0
21	AN	96/100 (96%)	0.38	5 (5%)	33 19	12, 98, 151, 180	0
21	CN	96/100 (96%)	0.40	5 (5%)	33 19	12, 81, 150, 180	0
22	BA	117/120 (97%)	-0.50	2 (1%)	69 43	35, 74, 117, 167	0
22	DA	117/120 (97%)	-0.19	3 (2%)	57 33	36, 86, 127, 180	0
23	BB	2841/2904 (97%)	-0.47	23 (0%)	82 60	6, 54, 148, 180	0
23	DB	2841/2904 (97%)	-0.50	24 (0%)	82 60	5, 48, 146, 180	0
24	BI	141/141 (100%)	0.22	1 (0%)	84 63	95, 172, 180, 180	0
24	DI	141/141 (100%)	0.02	1 (0%)	84 63	91, 179, 180, 180	0
25	BC	271/272 (99%)	0.30	10 (3%)	45 25	5, 50, 103, 180	0
25	DC	271/272 (99%)	0.41	26 (9%)	13 9	5, 40, 100, 146	0
26	BD	209/209 (100%)	0.24	11 (5%)	32 18	7, 68, 146, 180	0
26	DD	209/209 (100%)	0.36	17 (8%)	18 12	5, 49, 129, 180	0
27	BK	121/123 (98%)	0.34	4 (3%)	49 28	7, 69, 139, 180	0
27	DK	121/123 (98%)	0.08	1 (0%)	82 60	5, 41, 118, 180	0
28	BP	114/114 (100%)	0.38	9 (7%)	18 12	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%)	0.08	3 (2%)	57	33	5, 49, 103, 145	0
29	BE	201/201 (100%)	-0.07	3 (1%)	72	47	5, 63, 143, 180	0
29	DE	201/201 (100%)	-0.02	8 (3%)	42	23	5, 70, 144, 180	0
30	BY	58/58 (100%)	-0.15	0	100	100	20, 62, 140, 180	0
30	DY	58/58 (100%)	0.24	0	100	100	5, 66, 116, 142	0
31	B0	56/56 (100%)	0.28	2 (3%)	46	25	20, 80, 163, 180	0
31	D0	56/56 (100%)	0.29	2 (3%)	46	25	12, 58, 116, 165	0
32	B4	38/38 (100%)	0.65	4 (10%)	11	8	5, 75, 120, 137	0
32	D4	38/38 (100%)	0.38	0	100	100	7, 60, 114, 135	0
33	B1	50/54 (92%)	0.07	3 (6%)	27	16	15, 70, 135, 180	0
33	D1	50/54 (92%)	-0.33	0	100	100	20, 69, 142, 157	0
34	B3	64/64 (100%)	0.91	12 (18%)	3	3	13, 50, 102, 148	0
34	D3	64/64 (100%)	0.80	9 (14%)	6	5	5, 42, 88, 133	0
35	BV	94/94 (100%)	-0.22	0	100	100	21, 89, 143, 180	0
35	DV	94/94 (100%)	0.02	4 (4%)	40	21	9, 96, 151, 169	0
36	B2	46/46 (100%)	0.47	5 (10%)	10	7	5, 43, 120, 143	0
36	D2	46/46 (100%)	0.44	4 (8%)	16	10	10, 43, 103, 159	0
37	BL	143/144 (99%)	0.18	3 (2%)	63	38	8, 67, 133, 172	0
37	DL	143/144 (99%)	0.14	3 (2%)	63	38	5, 56, 119, 164	0
38	BM	136/136 (100%)	0.17	5 (3%)	45	25	9, 59, 117, 170	0
38	DM	136/136 (100%)	0.39	9 (6%)	24	15	7, 60, 116, 137	0
39	BX	63/63 (100%)	0.11	3 (4%)	35	19	6, 86, 135, 180	0
39	DX	63/63 (100%)	-0.07	0	100	100	38, 106, 178, 180	0
40	BH	149/149 (100%)	0.18	4 (2%)	56	33	26, 134, 177, 180	0
40	DH	149/149 (100%)	0.03	3 (2%)	65	39	11, 112, 162, 180	0
41	BJ	142/142 (100%)	0.70	24 (16%)	4	4	5, 74, 127, 180	0
41	DJ	142/142 (100%)	0.31	10 (7%)	22	14	5, 59, 125, 180	0
42	BN	120/127 (94%)	0.20	6 (5%)	34	19	20, 65, 126, 180	0
42	DN	120/127 (94%)	0.32	8 (6%)	24	15	5, 43, 103, 180	0
43	BO	116/117 (99%)	0.07	6 (5%)	33	19	12, 77, 140, 180	0
43	DO	116/117 (99%)	0.29	5 (4%)	40	21	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%)	0.17	7 (5%) 27 16	6, 57, 133, 175	0
44	DQ	117/117 (100%)	0.32	8 (6%) 23 14	5, 52, 112, 161	0
45	BS	110/110 (100%)	0.20	4 (3%) 46 25	5, 50, 125, 180	0
45	DS	110/110 (100%)	0.31	6 (5%) 30 18	5, 52, 131, 180	0
46	BU	102/103 (99%)	-0.10	1 (0%) 79 56	5, 70, 146, 180	0
46	DU	102/103 (99%)	0.03	3 (2%) 53 31	22, 97, 158, 180	0
47	BF	178/178 (100%)	-0.09	1 (0%) 85 65	52, 123, 180, 180	0
47	DF	178/178 (100%)	0.30	10 (5%) 30 17	33, 110, 176, 180	0
48	BG	176/176 (100%)	-0.01	7 (3%) 42 23	26, 104, 165, 180	0
48	DG	176/176 (100%)	0.11	5 (2%) 55 32	26, 98, 169, 180	0
49	BR	103/103 (100%)	0.01	3 (2%) 53 31	11, 76, 142, 180	0
49	DR	103/103 (100%)	0.36	8 (7%) 19 12	13, 79, 144, 180	0
50	BT	93/100 (93%)	0.24	5 (5%) 31 18	16, 75, 150, 180	0
50	DT	93/100 (93%)	0.56	9 (9%) 13 9	13, 79, 154, 180	0
51	BZ	77/78 (98%)	0.27	3 (3%) 43 23	5, 53, 122, 137	0
51	DZ	77/78 (98%)	0.36	4 (5%) 33 19	5, 47, 124, 144	0
52	BW	79/84 (94%)	1.05	18 (22%) 2 2	8, 74, 121, 180	0
52	DW	79/84 (94%)	1.30	19 (24%) 2 2	9, 77, 144, 164	0
All	All	20417/21046 (97%)	-0.13	603 (2%) 52 30	5, 69, 155, 180	0

The worst 5 of 603 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	CI	129	ARG	17.2
22	DA	88	C	11.8
8	AI	129	ARG	7.3
34	D3	51	LYS	6.9
11	CL	24	GLU	6.9

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 oligosaccharides 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	1660	1/1	-0.02	0.29	148,148,148,148	0
54	MG	AA	1626	1/1	0.17	0.24	87,87,87,87	1
54	MG	AA	1647	1/1	0.61	0.10	133,133,133,133	0
54	MG	AA	1623	1/1	0.62	0.10	157,157,157,157	0
54	MG	CA	1650	1/1	0.64	0.12	180,180,180,180	0
54	MG	BB	3043	1/1	0.68	0.08	145,145,145,145	0
54	MG	AA	1625	1/1	0.68	0.16	102,102,102,102	0
54	MG	DB	3059	1/1	0.70	0.35	180,180,180,180	0
54	MG	CA	1607	1/1	0.71	0.11	129,129,129,129	0
54	MG	CA	1651	1/1	0.73	0.13	161,161,161,161	0
54	MG	CA	1614	1/1	0.74	0.15	139,139,139,139	0
54	MG	CA	1652	1/1	0.75	0.10	128,128,128,128	0
54	MG	CA	1654	1/1	0.75	0.10	82,82,82,82	0
54	MG	BB	3048	1/1	0.75	0.10	145,145,145,145	0
54	MG	CA	1647	1/1	0.76	0.06	153,153,153,153	0
54	MG	DB	3014	1/1	0.77	0.12	80,80,80,80	0
53	NMY	DB	3001	42/42	0.78	0.34	68,68,68,68	42
54	MG	AA	1618	1/1	0.79	0.13	160,160,160,160	0
54	MG	DB	3067	1/1	0.79	0.07	137,137,137,137	0
54	MG	BB	3101	1/1	0.80	0.09	157,157,157,157	0
54	MG	AA	1636	1/1	0.82	0.17	121,121,121,121	0
53	NMY	BB	3001	42/42	0.82	0.90	89,89,89,89	42
54	MG	AA	1657	1/1	0.83	0.12	95,95,95,95	0
53	NMY	AA	1601	42/42	0.84	0.14	75,75,75,75	0
54	MG	DB	3030	1/1	0.84	0.10	81,81,81,81	0
54	MG	DB	3093	1/1	0.84	0.11	98,98,98,98	0
54	MG	AA	1609	1/1	0.86	0.09	107,107,107,107	0
54	MG	AA	1658	1/1	0.86	0.12	120,120,120,120	0
54	MG	AA	1653	1/1	0.86	0.07	110,110,110,110	0
54	MG	CA	1629	1/1	0.87	0.15	57,57,57,57	0
54	MG	AA	1648	1/1	0.87	0.19	110,110,110,110	0
54	MG	CA	1649	1/1	0.87	0.07	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	NMY	CA	1601	42/42	0.87	0.13	47,47,47,47	0
54	MG	AA	1638	1/1	0.89	0.17	126,126,126,126	0
54	MG	AA	1640	1/1	0.89	0.14	110,110,110,110	0
54	MG	BB	3034	1/1	0.89	0.12	130,130,130,130	0
54	MG	AA	1620	1/1	0.89	0.04	132,132,132,132	0
54	MG	AA	1603	1/1	0.90	0.06	100,100,100,100	0
54	MG	AA	1615	1/1	0.91	0.06	123,123,123,123	0
54	MG	CA	1656	1/1	0.91	0.12	135,135,135,135	0
54	MG	DB	3035	1/1	0.91	0.12	80,80,80,80	0
55	SCM	CA	1661	23/23	0.91	0.09	37,37,37,37	0
54	MG	BB	3069	1/1	0.92	0.11	41,41,41,41	0
54	MG	CA	1626	1/1	0.92	0.06	117,117,117,117	0
54	MG	BB	3044	1/1	0.92	0.06	118,118,118,118	0
54	MG	CA	1639	1/1	0.92	0.07	108,108,108,108	0
54	MG	BB	3038	1/1	0.92	0.07	46,46,46,46	0
54	MG	DB	3096	1/1	0.92	0.05	115,115,115,115	0
54	MG	CA	1609	1/1	0.92	0.07	110,110,110,110	0
54	MG	CA	1643	1/1	0.93	0.07	75,75,75,75	0
54	MG	AA	1651	1/1	0.93	0.05	97,97,97,97	0
54	MG	AA	1646	1/1	0.94	0.08	89,89,89,89	0
54	MG	DB	3084	1/1	0.94	0.09	109,109,109,109	0
54	MG	DB	3090	1/1	0.94	0.13	99,99,99,99	0
54	MG	CA	1638	1/1	0.94	0.13	123,123,123,123	0
54	MG	CA	1613	1/1	0.94	0.09	108,108,108,108	0
54	MG	DB	3112	1/1	0.94	0.15	87,87,87,87	0
54	MG	DB	3061	1/1	0.94	0.07	117,117,117,117	0
54	MG	DB	3027	1/1	0.95	0.07	72,72,72,72	0
54	MG	BB	3092	1/1	0.95	0.10	5,5,5,5	0
54	MG	BB	3094	1/1	0.95	0.06	75,75,75,75	0
54	MG	DB	3036	1/1	0.95	0.05	85,85,85,85	0
54	MG	BB	3098	1/1	0.95	0.05	85,85,85,85	0
54	MG	AA	1628	1/1	0.95	0.07	53,53,53,53	0
54	MG	BB	3010	1/1	0.95	0.05	123,123,123,123	0
54	MG	AA	1629	1/1	0.95	0.09	55,55,55,55	0
54	MG	AA	1607	1/1	0.95	0.05	93,93,93,93	0
54	MG	BB	3073	1/1	0.95	0.05	35,35,35,35	0
54	MG	CA	1619	1/1	0.95	0.10	53,53,53,53	0
54	MG	BB	3081	1/1	0.95	0.05	77,77,77,77	0
54	MG	BB	3091	1/1	0.95	0.06	105,105,105,105	0
54	MG	BB	3011	1/1	0.96	0.05	62,62,62,62	0
54	MG	CA	1641	1/1	0.96	0.09	61,61,61,61	0
54	MG	DB	3031	1/1	0.96	0.08	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1621	1/1	0.96	0.04	82,82,82,82	0
54	MG	CA	1645	1/1	0.96	0.06	70,70,70,70	0
54	MG	DB	3046	1/1	0.96	0.04	104,104,104,104	0
54	MG	DB	3049	1/1	0.96	0.04	66,66,66,66	0
54	MG	AA	1624	1/1	0.96	0.22	13,13,13,13	1
54	MG	DB	3060	1/1	0.96	0.03	96,96,96,96	0
54	MG	BB	3039	1/1	0.96	0.04	107,107,107,107	0
54	MG	AA	1659	1/1	0.96	0.03	111,111,111,111	0
54	MG	CA	1622	1/1	0.96	0.07	44,44,44,44	0
54	MG	AA	1631	1/1	0.96	0.06	84,84,84,84	0
54	MG	CA	1653	1/1	0.96	0.04	96,96,96,96	0
54	MG	AA	1634	1/1	0.96	0.11	88,88,88,88	0
54	MG	CA	1630	1/1	0.96	0.06	81,81,81,81	0
55	SCM	AA	1662	23/23	0.96	0.07	23,23,23,23	0
54	MG	BB	3068	1/1	0.96	0.06	65,65,65,65	0
54	MG	AA	1652	1/1	0.97	0.04	101,101,101,101	0
54	MG	BB	3045	1/1	0.97	0.04	42,42,42,42	0
54	MG	BB	3088	1/1	0.97	0.11	87,87,87,87	0
54	MG	CA	1648	1/1	0.97	0.04	69,69,69,69	0
54	MG	DB	3053	1/1	0.97	0.07	90,90,90,90	0
54	MG	DB	3054	1/1	0.97	0.05	80,80,80,80	0
54	MG	CA	1617	1/1	0.97	0.08	83,83,83,83	0
54	MG	CA	1618	1/1	0.97	0.07	104,104,104,104	0
54	MG	BB	3047	1/1	0.97	0.04	66,66,66,66	0
54	MG	DB	3062	1/1	0.97	0.06	75,75,75,75	0
54	MG	AA	1633	1/1	0.97	0.12	65,65,65,65	0
54	MG	DB	3074	1/1	0.97	0.05	29,29,29,29	0
54	MG	BB	3093	1/1	0.97	0.06	32,32,32,32	0
54	MG	BB	3052	1/1	0.97	0.05	67,67,67,67	0
54	MG	BB	3095	1/1	0.97	0.04	36,36,36,36	0
54	MG	CA	1633	1/1	0.97	0.06	48,48,48,48	0
54	MG	DB	3109	1/1	0.97	0.05	33,33,33,33	0
54	MG	BB	3058	1/1	0.97	0.07	63,63,63,63	0
54	MG	AA	1645	1/1	0.97	0.05	67,67,67,67	0
54	MG	AA	1613	1/1	0.97	0.04	80,80,80,80	0
54	MG	CA	1660	1/1	0.98	0.08	77,77,77,77	0
54	MG	DB	3009	1/1	0.98	0.05	49,49,49,49	0
54	MG	BB	3072	1/1	0.98	0.06	54,54,54,54	0
54	MG	BB	3027	1/1	0.98	0.05	42,42,42,42	0
54	MG	BB	3079	1/1	0.98	0.07	68,68,68,68	0
54	MG	BB	3032	1/1	0.98	0.11	38,38,38,38	0
54	MG	AA	1656	1/1	0.98	0.10	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3090	1/1	0.98	0.03	54,54,54,54	0
54	MG	DB	3040	1/1	0.98	0.04	78,78,78,78	0
54	MG	BB	3035	1/1	0.98	0.09	41,41,41,41	0
54	MG	CA	1635	1/1	0.98	0.04	64,64,64,64	0
54	MG	DB	3051	1/1	0.98	0.05	67,67,67,67	0
54	MG	DB	3052	1/1	0.98	0.04	40,40,40,40	0
54	MG	AA	1641	1/1	0.98	0.09	88,88,88,88	0
54	MG	AA	1650	1/1	0.98	0.03	105,105,105,105	0
54	MG	AA	1627	1/1	0.98	0.08	5,5,5,5	1
54	MG	AA	1616	1/1	0.98	0.04	113,113,113,113	0
54	MG	CA	1644	1/1	0.98	0.05	49,49,49,49	0
54	MG	BB	3007	1/1	0.98	0.06	37,37,37,37	0
54	MG	BB	3008	1/1	0.98	0.11	81,81,81,81	0
54	MG	DB	3071	1/1	0.98	0.05	93,93,93,93	0
54	MG	BB	3103	1/1	0.98	0.04	25,25,25,25	0
54	MG	DB	3075	1/1	0.98	0.07	58,58,58,58	0
54	MG	DB	3079	1/1	0.98	0.07	80,80,80,80	0
54	MG	BB	3111	1/1	0.98	0.05	90,90,90,90	0
54	MG	DB	3086	1/1	0.98	0.05	41,41,41,41	0
54	MG	AA	1606	1/1	0.98	0.09	56,56,56,56	0
54	MG	DB	3091	1/1	0.98	0.04	55,55,55,55	0
54	MG	AA	1655	1/1	0.98	0.03	73,73,73,73	0
54	MG	CA	1610	1/1	0.98	0.04	103,103,103,103	0
54	MG	BB	3013	1/1	0.98	0.04	81,81,81,81	0
54	MG	BB	3021	1/1	0.98	0.15	30,30,30,30	0
54	MG	BB	3026	1/1	0.98	0.05	68,68,68,68	0
54	MG	CA	1659	1/1	0.98	0.04	45,45,45,45	0
56	ZN	B4	101	1/1	0.98	0.03	49,49,49,49	0
56	ZN	D4	101	1/1	0.98	0.03	40,40,40,40	0
54	MG	CA	1623	1/1	0.99	0.05	21,21,21,21	0
54	MG	BB	3040	1/1	0.99	0.10	44,44,44,44	0
54	MG	CA	1627	1/1	0.99	0.04	40,40,40,40	0
54	MG	CA	1628	1/1	0.99	0.03	41,41,41,41	0
54	MG	BB	3041	1/1	0.99	0.06	34,34,34,34	0
54	MG	AA	1639	1/1	0.99	0.02	65,65,65,65	0
54	MG	AA	1608	1/1	0.99	0.02	53,53,53,53	0
54	MG	CA	1634	1/1	0.99	0.07	75,75,75,75	0
54	MG	AA	1617	1/1	0.99	0.02	47,47,47,47	0
54	MG	AA	1642	1/1	0.99	0.02	51,51,51,51	0
54	MG	BB	3002	1/1	0.99	0.04	19,19,19,19	0
54	MG	CA	1640	1/1	0.99	0.05	43,43,43,43	0
54	MG	BB	3050	1/1	0.99	0.07	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1642	1/1	0.99	0.02	49,49,49,49	0
54	MG	BB	3003	1/1	0.99	0.03	17,17,17,17	0
54	MG	BB	3054	1/1	0.99	0.03	46,46,46,46	0
54	MG	BB	3055	1/1	0.99	0.03	46,46,46,46	0
54	MG	CA	1646	1/1	0.99	0.04	52,52,52,52	0
54	MG	BB	3056	1/1	0.99	0.06	23,23,23,23	0
54	MG	BB	3004	1/1	0.99	0.05	31,31,31,31	0
54	MG	BB	3060	1/1	0.99	0.05	5,5,5,5	0
54	MG	BB	3062	1/1	0.99	0.04	38,38,38,38	0
54	MG	BB	3065	1/1	0.99	0.09	24,24,24,24	0
54	MG	BB	3005	1/1	0.99	0.07	29,29,29,29	0
54	MG	AA	1643	1/1	0.99	0.04	43,43,43,43	0
54	MG	BB	3071	1/1	0.99	0.04	33,33,33,33	0
54	MG	CA	1655	1/1	0.99	0.05	52,52,52,52	0
54	MG	AA	1644	1/1	0.99	0.03	42,42,42,42	0
54	MG	BB	3009	1/1	0.99	0.04	80,80,80,80	0
54	MG	BB	3075	1/1	0.99	0.03	6,6,6,6	0
54	MG	DB	3008	1/1	0.99	0.05	41,41,41,41	0
54	MG	BB	3078	1/1	0.99	0.04	47,47,47,47	0
54	MG	DB	3012	1/1	0.99	0.05	32,32,32,32	0
54	MG	AA	1605	1/1	0.99	0.03	46,46,46,46	0
54	MG	DB	3016	1/1	0.99	0.04	53,53,53,53	0
54	MG	DB	3018	1/1	0.99	0.06	5,5,5,5	0
54	MG	DB	3019	1/1	0.99	0.03	25,25,25,25	0
54	MG	DB	3023	1/1	0.99	0.04	7,7,7,7	0
54	MG	DB	3025	1/1	0.99	0.04	47,47,47,47	0
54	MG	BB	3080	1/1	0.99	0.04	44,44,44,44	0
54	MG	DB	3029	1/1	0.99	0.10	30,30,30,30	0
54	MG	AA	1611	1/1	0.99	0.03	73,73,73,73	0
54	MG	BB	3082	1/1	0.99	0.03	34,34,34,34	0
54	MG	DB	3033	1/1	0.99	0.04	82,82,82,82	0
54	MG	DB	3034	1/1	0.99	0.03	5,5,5,5	0
54	MG	BB	3083	1/1	0.99	0.03	5,5,5,5	0
54	MG	BB	3084	1/1	0.99	0.08	61,61,61,61	0
54	MG	DB	3037	1/1	0.99	0.06	23,23,23,23	0
54	MG	DB	3038	1/1	0.99	0.07	10,10,10,10	0
54	MG	DB	3039	1/1	0.99	0.03	19,19,19,19	0
54	MG	BB	3085	1/1	0.99	0.06	43,43,43,43	0
54	MG	DB	3042	1/1	0.99	0.02	17,17,17,17	0
54	MG	DB	3044	1/1	0.99	0.06	11,11,11,11	0
54	MG	DB	3045	1/1	0.99	0.04	32,32,32,32	0
54	MG	AA	1612	1/1	0.99	0.03	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3014	1/1	0.99	0.08	11,11,11,11	0
54	MG	DB	3050	1/1	0.99	0.03	6,6,6,6	0
54	MG	BB	3015	1/1	0.99	0.10	32,32,32,32	0
54	MG	BB	3016	1/1	0.99	0.03	31,31,31,31	0
54	MG	BB	3017	1/1	0.99	0.03	43,43,43,43	0
54	MG	BB	3018	1/1	0.99	0.03	31,31,31,31	0
54	MG	DB	3056	1/1	0.99	0.03	34,34,34,34	0
54	MG	DB	3058	1/1	0.99	0.03	39,39,39,39	0
54	MG	BB	3020	1/1	0.99	0.03	28,28,28,28	0
54	MG	AA	1632	1/1	0.99	0.04	29,29,29,29	0
54	MG	BB	3100	1/1	0.99	0.04	34,34,34,34	0
54	MG	BB	3022	1/1	0.99	0.03	35,35,35,35	0
54	MG	DB	3063	1/1	0.99	0.05	50,50,50,50	0
54	MG	DB	3065	1/1	0.99	0.09	20,20,20,20	0
54	MG	BB	3023	1/1	0.99	0.05	12,12,12,12	0
54	MG	DB	3068	1/1	0.99	0.10	36,36,36,36	0
54	MG	BB	3107	1/1	0.99	0.07	30,30,30,30	0
54	MG	DB	3072	1/1	0.99	0.02	36,36,36,36	0
54	MG	DB	3073	1/1	0.99	0.05	62,62,62,62	0
54	MG	BB	3108	1/1	0.99	0.02	36,36,36,36	0
54	MG	BB	3109	1/1	0.99	0.03	19,19,19,19	0
54	MG	DB	3078	1/1	0.99	0.03	24,24,24,24	0
54	MG	AA	1622	1/1	0.99	0.11	24,24,24,24	0
54	MG	DB	3080	1/1	0.99	0.03	46,46,46,46	0
54	MG	DB	3081	1/1	0.99	0.05	35,35,35,35	0
54	MG	DB	3083	1/1	0.99	0.06	37,37,37,37	0
54	MG	CA	1604	1/1	0.99	0.05	66,66,66,66	0
54	MG	DB	3085	1/1	0.99	0.05	12,12,12,12	0
54	MG	AA	1602	1/1	0.99	0.08	28,28,28,28	0
54	MG	CA	1608	1/1	0.99	0.04	31,31,31,31	0
54	MG	BB	3028	1/1	0.99	0.07	24,24,24,24	0
54	MG	BB	3029	1/1	0.99	0.08	21,21,21,21	0
54	MG	DB	3094	1/1	0.99	0.03	5,5,5,5	0
54	MG	BB	3030	1/1	0.99	0.03	16,16,16,16	0
54	MG	DB	3097	1/1	0.99	0.05	12,12,12,12	0
54	MG	DB	3098	1/1	0.99	0.03	41,41,41,41	0
54	MG	DB	3101	1/1	0.99	0.04	20,20,20,20	0
54	MG	DB	3104	1/1	0.99	0.04	31,31,31,31	0
54	MG	DB	3105	1/1	0.99	0.04	41,41,41,41	0
54	MG	DB	3106	1/1	0.99	0.06	53,53,53,53	0
54	MG	AA	1635	1/1	0.99	0.03	86,86,86,86	0
54	MG	DB	3111	1/1	0.99	0.02	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1615	1/1	0.99	0.06	29,29,29,29	0
54	MG	AA	1614	1/1	0.99	0.02	66,66,66,66	0
54	MG	AA	1654	1/1	0.99	0.03	49,49,49,49	0
54	MG	AA	1637	1/1	0.99	0.03	62,62,62,62	0
54	MG	AA	1604	1/1	0.99	0.02	43,43,43,43	0
54	MG	BB	3012	1/1	1.00	0.05	33,33,33,33	0
54	MG	DB	3017	1/1	1.00	0.02	29,29,29,29	0
54	MG	BB	3046	1/1	1.00	0.02	50,50,50,50	0
54	MG	BB	3074	1/1	1.00	0.01	28,28,28,28	0
54	MG	DB	3020	1/1	1.00	0.03	6,6,6,6	0
54	MG	DB	3021	1/1	1.00	0.08	5,5,5,5	0
54	MG	DB	3022	1/1	1.00	0.01	5,5,5,5	0
54	MG	BB	3031	1/1	1.00	0.03	53,53,53,53	0
54	MG	DB	3024	1/1	1.00	0.02	32,32,32,32	0
54	MG	CA	1611	1/1	1.00	0.05	5,5,5,5	0
54	MG	DB	3026	1/1	1.00	0.03	16,16,16,16	0
54	MG	CA	1612	1/1	1.00	0.05	25,25,25,25	0
54	MG	DB	3028	1/1	1.00	0.02	17,17,17,17	0
54	MG	BB	3076	1/1	1.00	0.07	33,33,33,33	0
54	MG	BB	3077	1/1	1.00	0.05	5,5,5,5	0
54	MG	BB	3006	1/1	1.00	0.01	9,9,9,9	0
54	MG	DB	3032	1/1	1.00	0.01	5,5,5,5	0
54	MG	CA	1616	1/1	1.00	0.05	15,15,15,15	0
54	MG	BB	3049	1/1	1.00	0.05	24,24,24,24	0
54	MG	BB	3033	1/1	1.00	0.04	25,25,25,25	0
54	MG	BB	3051	1/1	1.00	0.06	34,34,34,34	0
54	MG	CA	1620	1/1	1.00	0.02	62,62,62,62	0
54	MG	CA	1621	1/1	1.00	0.02	34,34,34,34	0
54	MG	AA	1661	1/1	1.00	0.06	62,62,62,62	0
54	MG	BB	3053	1/1	1.00	0.05	30,30,30,30	0
54	MG	DB	3041	1/1	1.00	0.02	9,9,9,9	0
54	MG	CA	1624	1/1	1.00	0.02	21,21,21,21	0
54	MG	DB	3043	1/1	1.00	0.01	32,32,32,32	0
54	MG	CA	1625	1/1	1.00	0.01	36,36,36,36	0
54	MG	AA	1649	1/1	1.00	0.03	31,31,31,31	0
54	MG	BB	3036	1/1	1.00	0.02	26,26,26,26	0
54	MG	DB	3047	1/1	1.00	0.04	27,27,27,27	0
54	MG	DB	3048	1/1	1.00	0.05	14,14,14,14	0
54	MG	BB	3086	1/1	1.00	0.03	18,18,18,18	0
54	MG	BB	3087	1/1	1.00	0.10	23,23,23,23	0
54	MG	BB	3037	1/1	1.00	0.06	35,35,35,35	0
54	MG	CA	1631	1/1	1.00	0.04	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1632	1/1	1.00	0.05	31,31,31,31	0
54	MG	BB	3089	1/1	1.00	0.05	7,7,7,7	0
54	MG	DB	3055	1/1	1.00	0.04	22,22,22,22	0
54	MG	BB	3057	1/1	1.00	0.04	15,15,15,15	0
54	MG	DB	3057	1/1	1.00	0.02	11,11,11,11	0
54	MG	BB	3024	1/1	1.00	0.01	12,12,12,12	0
54	MG	CA	1636	1/1	1.00	0.02	37,37,37,37	0
54	MG	CA	1637	1/1	1.00	0.01	26,26,26,26	0
54	MG	BB	3059	1/1	1.00	0.07	13,13,13,13	0
54	MG	BB	3025	1/1	1.00	0.04	32,32,32,32	0
54	MG	BB	3061	1/1	1.00	0.02	5,5,5,5	0
54	MG	DB	3064	1/1	1.00	0.05	34,34,34,34	0
54	MG	AA	1610	1/1	1.00	0.01	5,5,5,5	0
54	MG	DB	3066	1/1	1.00	0.09	32,32,32,32	0
54	MG	BB	3096	1/1	1.00	0.08	5,5,5,5	0
54	MG	BB	3097	1/1	1.00	0.05	5,5,5,5	0
54	MG	DB	3069	1/1	1.00	0.02	8,8,8,8	0
54	MG	DB	3070	1/1	1.00	0.05	38,38,38,38	0
54	MG	BB	3063	1/1	1.00	0.01	7,7,7,7	0
54	MG	BB	3099	1/1	1.00	0.01	23,23,23,23	0
54	MG	BB	3064	1/1	1.00	0.04	10,10,10,10	0
54	MG	AA	1619	1/1	1.00	0.03	48,48,48,48	0
54	MG	BB	3102	1/1	1.00	0.03	10,10,10,10	0
54	MG	DB	3076	1/1	1.00	0.05	22,22,22,22	0
54	MG	DB	3077	1/1	1.00	0.02	28,28,28,28	0
54	MG	BB	3066	1/1	1.00	0.02	10,10,10,10	0
54	MG	BB	3104	1/1	1.00	0.02	6,6,6,6	0
54	MG	BB	3105	1/1	1.00	0.06	18,18,18,18	0
54	MG	BB	3106	1/1	1.00	0.05	11,11,11,11	0
54	MG	DB	3082	1/1	1.00	0.04	9,9,9,9	0
54	MG	BB	3067	1/1	1.00	0.03	26,26,26,26	0
54	MG	BB	3042	1/1	1.00	0.02	10,10,10,10	0
54	MG	AA	1630	1/1	1.00	0.02	36,36,36,36	0
54	MG	BB	3110	1/1	1.00	0.06	61,61,61,61	0
54	MG	DB	3087	1/1	1.00	0.02	11,11,11,11	0
54	MG	DB	3088	1/1	1.00	0.03	37,37,37,37	0
54	MG	DB	3089	1/1	1.00	0.02	13,13,13,13	0
54	MG	CA	1657	1/1	1.00	0.04	14,14,14,14	0
54	MG	CA	1658	1/1	1.00	0.05	50,50,50,50	0
54	MG	DB	3092	1/1	1.00	0.04	12,12,12,12	0
54	MG	BB	3070	1/1	1.00	0.04	9,9,9,9	0
54	MG	CA	1602	1/1	1.00	0.12	7,7,7,7	0

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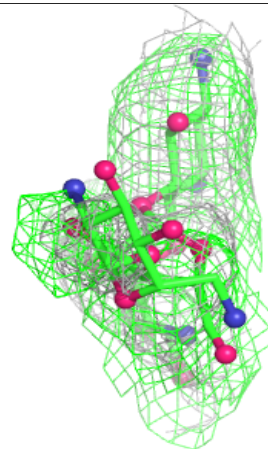
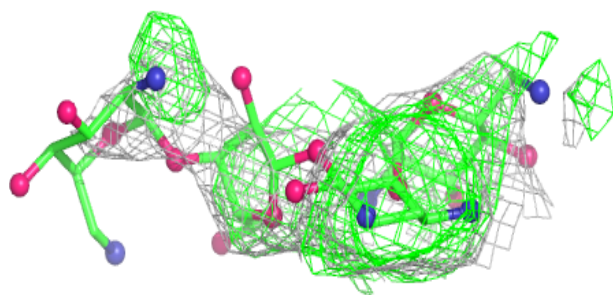
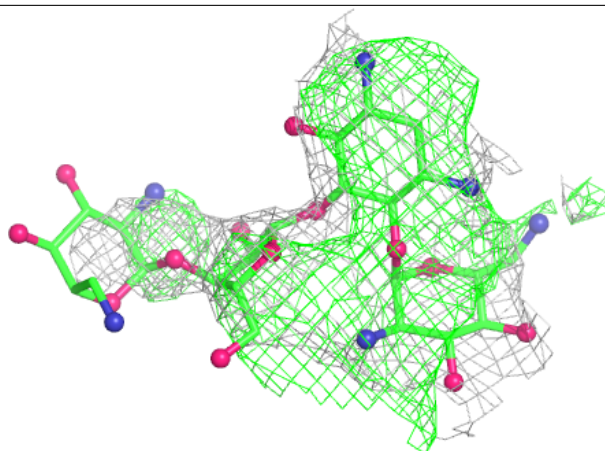
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3095	1/1	1.00	0.03	39,39,39,39	0
54	MG	DB	3002	1/1	1.00	0.03	5,5,5,5	0
54	MG	DB	3003	1/1	1.00	0.03	21,21,21,21	0
54	MG	DB	3004	1/1	1.00	0.07	41,41,41,41	0
54	MG	DB	3099	1/1	1.00	0.02	9,9,9,9	0
54	MG	DB	3100	1/1	1.00	0.02	6,6,6,6	0
54	MG	DB	3005	1/1	1.00	0.03	23,23,23,23	0
54	MG	DB	3102	1/1	1.00	0.06	6,6,6,6	0
54	MG	DB	3103	1/1	1.00	0.02	14,14,14,14	0
54	MG	DB	3006	1/1	1.00	0.01	13,13,13,13	0
54	MG	DB	3007	1/1	1.00	0.02	9,9,9,9	0
54	MG	CA	1603	1/1	1.00	0.04	25,25,25,25	0
54	MG	DB	3107	1/1	1.00	0.04	20,20,20,20	0
54	MG	DB	3108	1/1	1.00	0.03	27,27,27,27	0
54	MG	BB	3019	1/1	1.00	0.03	44,44,44,44	0
54	MG	DB	3110	1/1	1.00	0.02	17,17,17,17	0
54	MG	DB	3010	1/1	1.00	0.02	8,8,8,8	0
54	MG	DB	3011	1/1	1.00	0.01	9,9,9,9	0
54	MG	CA	1605	1/1	1.00	0.06	12,12,12,12	0
54	MG	DB	3013	1/1	1.00	0.03	12,12,12,12	0
54	MG	CA	1606	1/1	1.00	0.04	7,7,7,7	0
54	MG	DB	3015	1/1	1.00	0.03	37,37,37,37	0

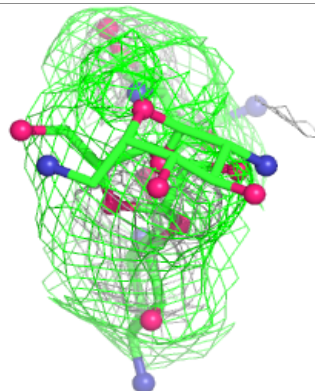
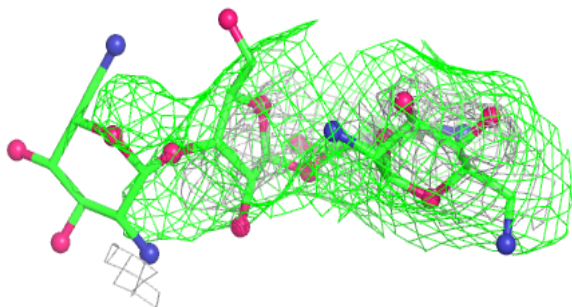
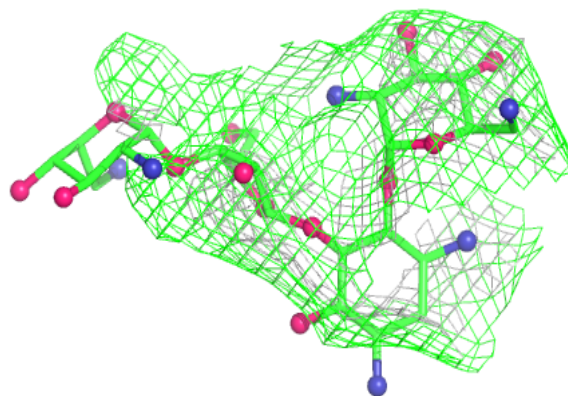
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NMY 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)

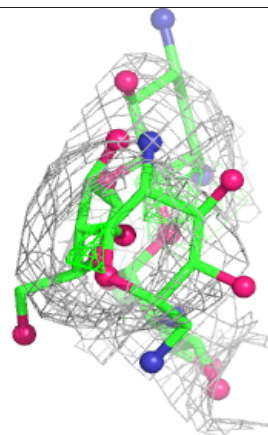
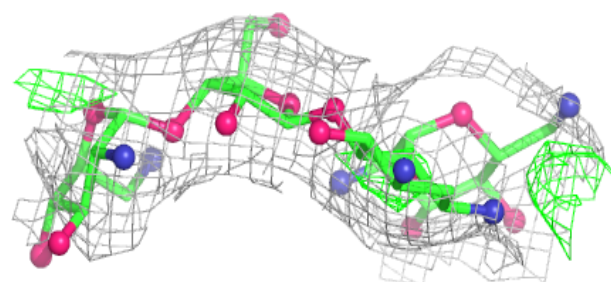
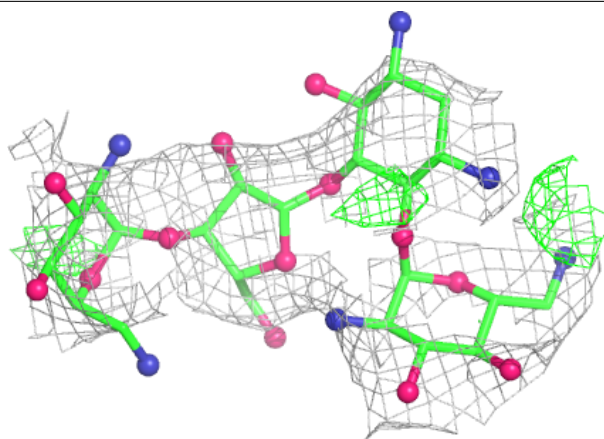
**Electron density around NMY BB 3001:**

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

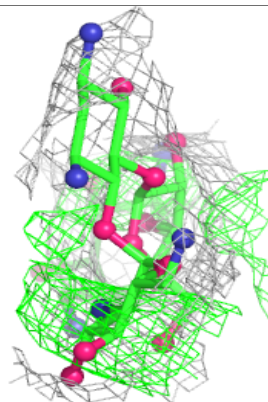
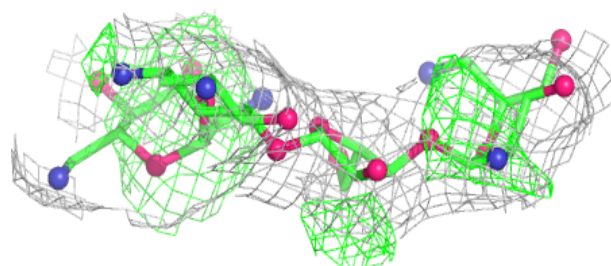
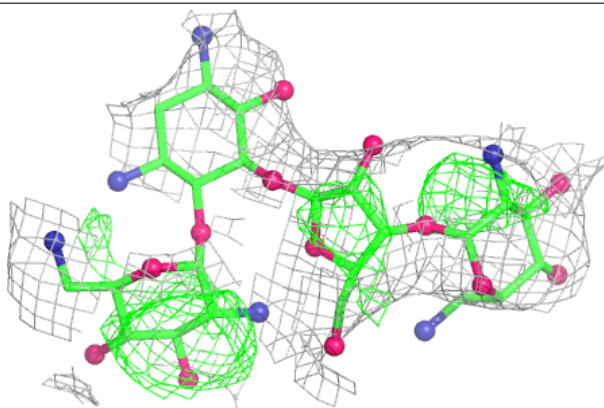


Electron density around NMY AA 1601:

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

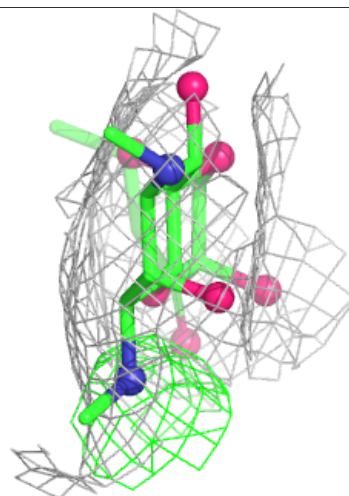
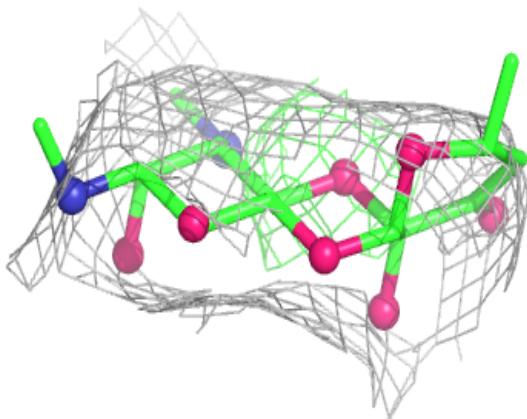
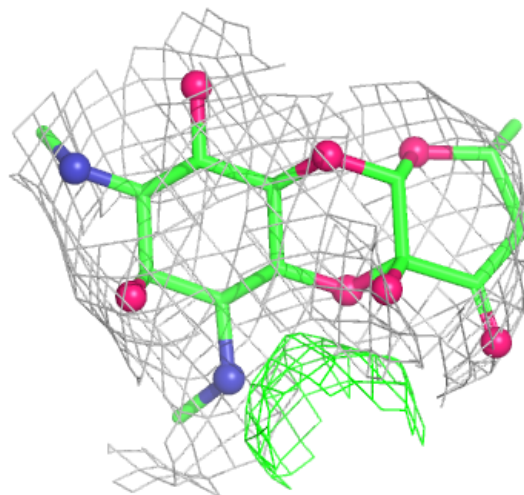
**Electron density around NMY CA 1601:**

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



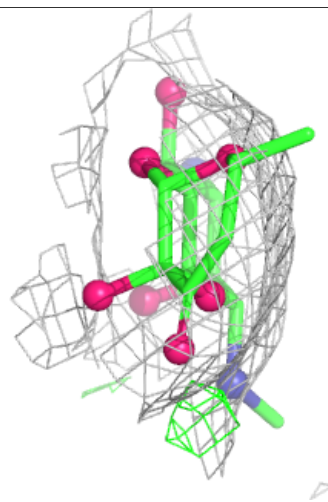
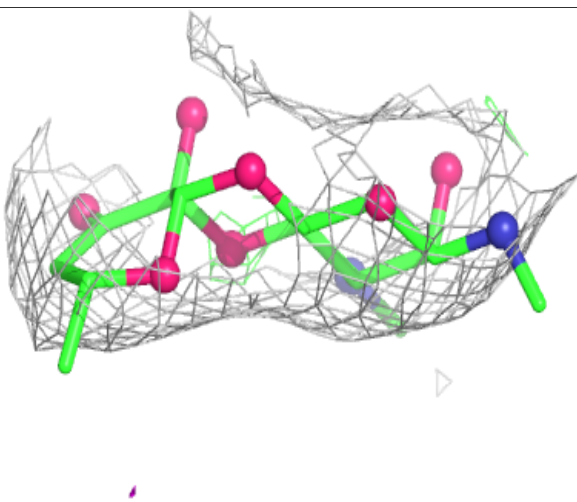
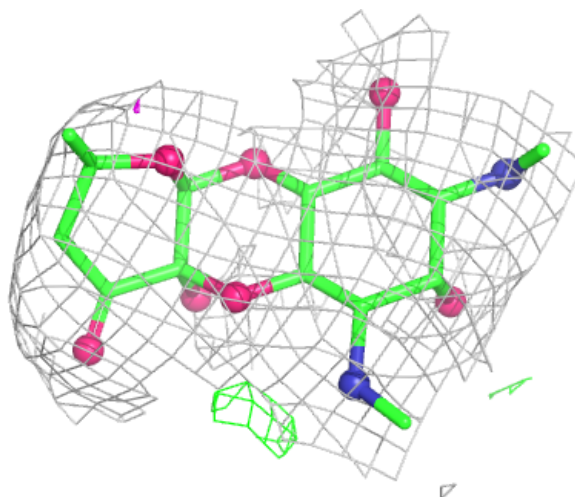
Electron density around SCM CA 1661:

$2mF_o-DF_c$ (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.