



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 03:45 PM EDT

PDB ID : 4V56 / pdb_00004v56
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with spectinomycin.
Authors : Borovinskaya, M.A.; Shoji, S.; Holton, J.M.; Fredrick, K.; Cate, J.H.D.
Deposited on : 2007-07-21
Resolution : 3.93 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:

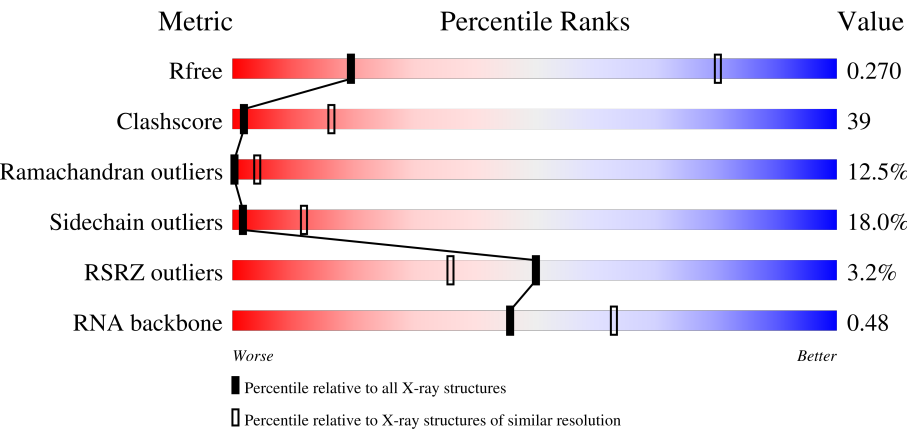
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.93 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	1022 (4.12-3.76)
Clashscore	190562	1000 (4.10-3.78)
Ramachandran outliers	187476	1009 (4.12-3.76)
Sidechain outliers	187428	1002 (4.12-3.76)
RSRZ outliers	180081	1022 (4.12-3.76)
RNA backbone	3983	1015 (4.76-3.10)

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	2% 19% 63% 16% ..
1	CA	1542	2% 20% 62% 16% ..
2	AC	232	2% 18% 45% 24% 11%
2	CC	232	2% 22% 48% 19% 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	AA	1623	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284033 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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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

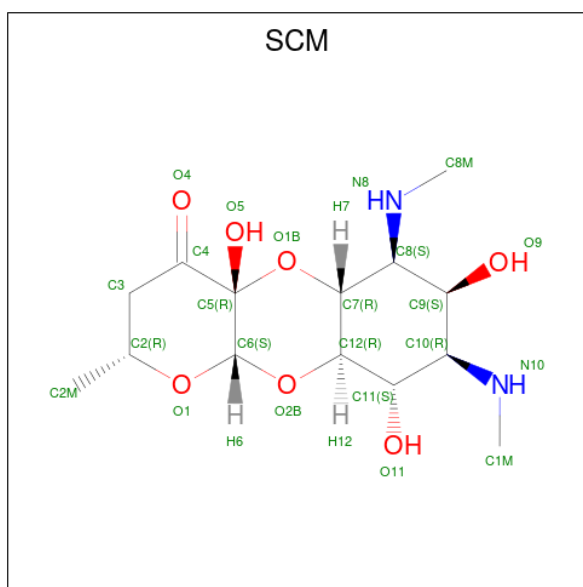
- Molecule 52 is a protein called 50S ribosomal protein L27.

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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	AA	60	Total	Mg	0	0
			60	60		
53	BB	110	Total	Mg	0	0
			110	110		
53	CA	58	Total	Mg	0	0
			58	58		
53	CE	1	Total	Mg	0	0
			1	1		
53	DB	110	Total	Mg	0	0
			110	110		
53	DN	1	Total	Mg	0	0
			1	1		

- Molecule 54 is SPECTINOMYCIN (CCD ID: SCM) (formula: C₁₄H₂₄N₂O₇).



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

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	288	Total	O	0	0
			288	288		
56	AE	3	Total	O	0	0
			3	3		
56	AK	1	Total	O	0	0
			1	1		
56	AL	4	Total	O	0	0
			4	4		
56	AP	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AT	1	Total 1	O 1	0	0
56	AN	2	Total 2	O 2	0	0
56	BB	494	Total 494	O 494	0	0
56	BC	4	Total 4	O 4	0	0
56	BE	3	Total 3	O 3	0	0
56	BL	4	Total 4	O 4	0	0
56	BH	1	Total 1	O 1	0	0
56	BT	1	Total 1	O 1	0	0
56	CA	275	Total 275	O 275	0	0
56	CE	4	Total 4	O 4	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	5	Total 5	O 5	0	0
56	CP	1	Total 1	O 1	0	0
56	CT	2	Total 2	O 2	0	0
56	CN	5	Total 5	O 5	0	0
56	DB	500	Total 500	O 500	0	0
56	DC	3	Total 3	O 3	0	0
56	DD	1	Total 1	O 1	0	0
56	DP	1	Total 1	O 1	0	0
56	DE	1	Total 1	O 1	0	0
56	DL	3	Total 3	O 3	0	0

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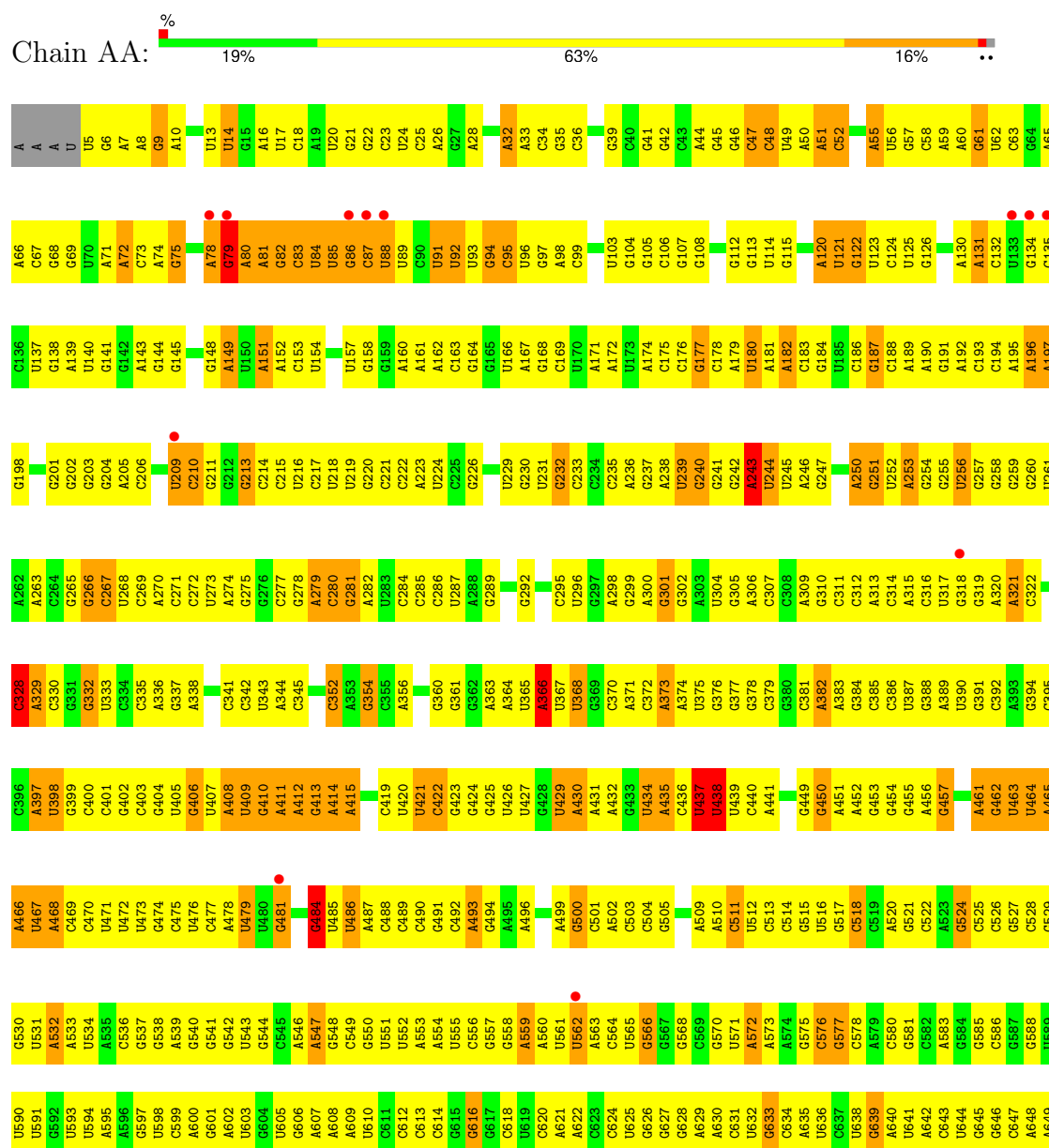
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DJ	1	Total	O	0	0
			1	1		
56	DN	2	Total	O	0	0
			2	2		
56	DR	1	Total	O	0	0
			1	1		

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

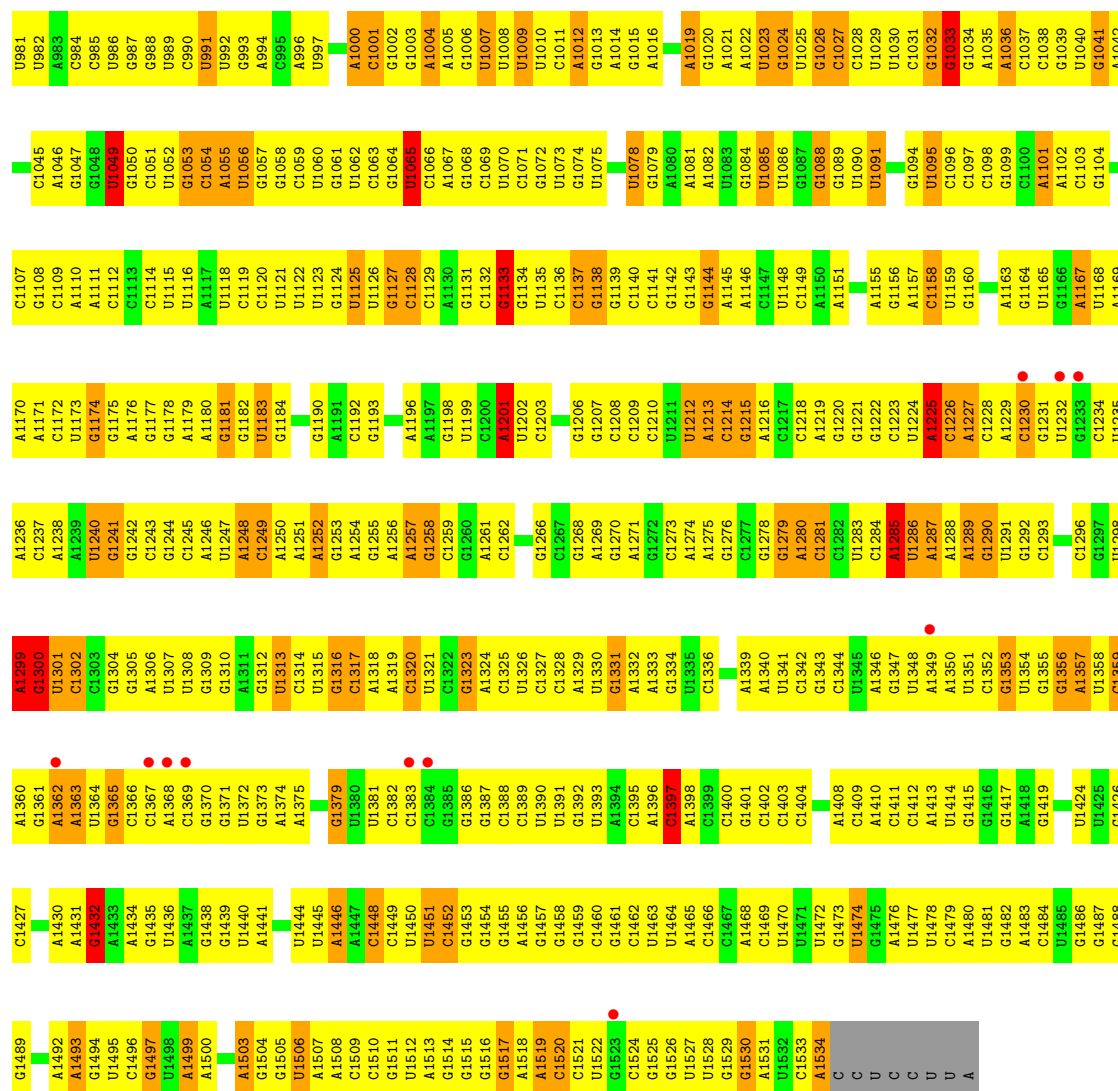


U1485	U1486	G1487	G1488	G1489	G1426	U1354	G1294	A1229	A1167	G1104	A1042	A978	A915	G847	A782	U717	G650
G1415	G1416	G1356	A1418		A1417	U1355	U1295	C1230	U1168	A1105	G1043	C979	U916	C848	C783	A718	C651
		U1356				C1355	C1296	C1231	G1296	C1106	A1044	C980	G917		A784	C719	C652
		U1357	U1418			U1358	G1297	U1232	A1170	C1107	C1045	U981	A918	G851	C785	C720	U653
		C1359				U1358	U1298	G1233	A1171	G1108	A1046	U982	A919	C852	G721		
						C1359	A1299	C1234	C1172	C1109	G1047	A983	U920	C853	G722		
						A1360	G1300	U1235	U1173	A1110	G1048	C984	U921	U854	G723		
						G1361	U1301	A1236	G1174	A1111	U1049	C985	G922		U724		
						A1362	C1302	C1237	G1175	C1112	G1050	U986	A923	C857	G725		
						A1363	C1303	A1238	A1176	C1113	C1051	G987	C924	G858	G726		
						U1364	A1239	A1239	G1177	C1114	U1052	G988	G926	G859	G727		
						G1365	G1305	U1240	G1178	U1115	G1053	U989	G926	A860	A728		
						C1366	A1306	G1241	A1179	U1116	C1054	C990	G927	A861	A729		
						U1367	U1307	G1242	A1180	U1117	A1055	U991	G927	C862	A730		
						A1368	U1308	C1243	G1181	U1118	U1056	U992	G929	C863	G731		
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						U1375	A1445	A1251		U1125	C1063	A1000	A936		C737		
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						A1377	C1317	G1253		G1127	U1065	G1002	A338	U875	C739		
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						U1380	A1513	A1257	U1193	C1129	G1068	A1005	A945	A878	G745		
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								C1328	U1202	G1138	U1076	G1013	U952				
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						U1390	A1329	A1269	C1203	C1139	G1077	G1015	G953	G890	G755		
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						C1460	G1331	A1271		C1141	U1078	A1016	G954	U891	C756		
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						A1463	C1333	C1273	C1208	G1143	A1081	G1018	U957	G894	A694		
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						U1480	C1480	A1290	U1224	C1162	U1099	C1037	C972	A909	C776		
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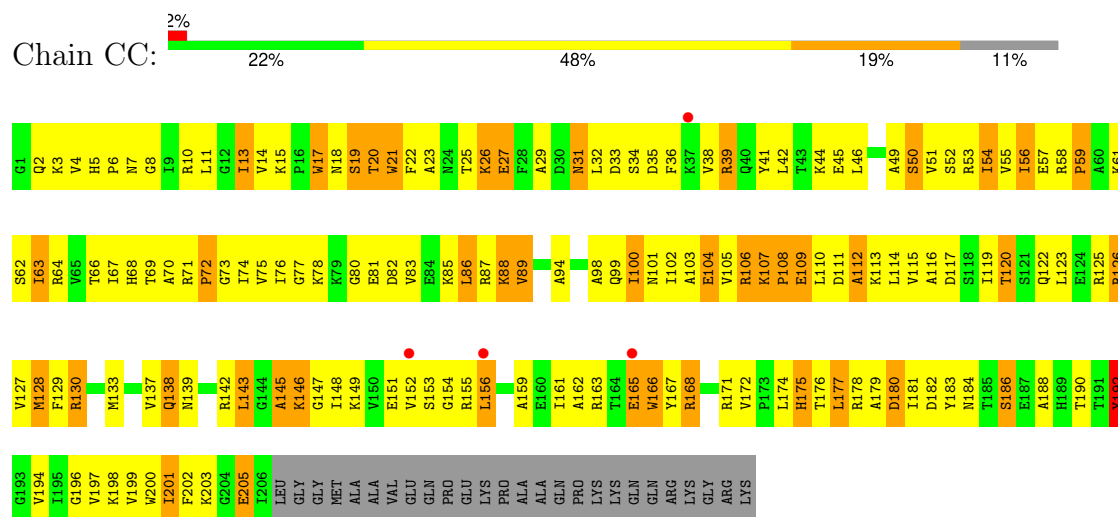
• Molecule 1: 16S rRNA



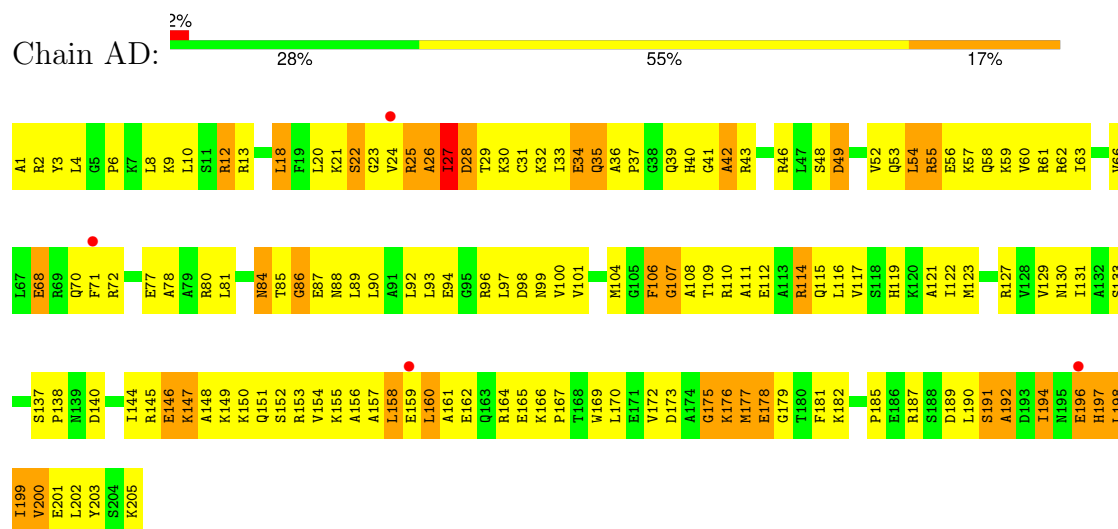
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G921	G791	C857	A792	U723	U659	A596	C536	U473	C401	A336	C267	G204	C135	A
A923	A793	G858	A793	G724	C660	G597	G537	G474	G402	G337	U268	A205	C136	U
C924	A794	G661	U793	G725	U598	U598	G538	C475	C403	A338	C269	C206	U137	U6
G925	A795	U662	C795		A663	A600	G540	U476	G404		A270		G138	U5
G926	G796	G664	C796	A728	A664	G601	G541	C477	U405	C341	C271			A7
G927	C797	A665	A665	A729	G665	A602	G542	A478	G406	C342	C272		A143	A8
G929	A864	G667	G667	G730	G666	U603	U543	U479	U407	U343	U273		G144	A9
C930	A865	G668	G668	G731	G667	G604	G544	G481	U408	A344	A274		G145	A10
C931	A866			G732		U605	G545	A482	G410	G346			G148	U13
C932	A867	U672		G733	A547	A606	A546	C483	A411	G347	A279		A149	U14
C933	C868	A673	C865	G735	G548	A608	G549	G484	A412		C280		A150	G15
C934	C869	G674	C806	G736	A673	A609	G550	U486	G413	G350	G281		A151	A16
A935	A807	A675	A807	G737	G551		G550	U487	A414	C351	A282		A152	A17
C936	C808	A676	C808	G738	G552	C612	U551	C488	A415	C352	U283		A153	A18
A937	G809	U677	G809	U740	A553	C613	U552	C489		C353	C284		U154	C18
A938	C810	U678	C810	G741	A554	C614	A553	C490	U420	G354	C285			U20
	C811	C679	C811		A555	G615	A554	G491	U421	A356	C286		U157	G21
	U812	C680	U812	G745	C556	G616	U555	G492	G422		U287		U158	G22
G941	A814	A681	U813	A746	C557	G617	C556	A493	G423	G361	A288		G159	C23
G942	A815	G682	A815	G747	G557	U618	G557	G494	G424	A363	C289		A160	U24
	A816	G683	A816	G748	A559	U619	G558	A495	G425	A364			A161	C25
	C817	U684	C817	A749	A560	C620	A559	A496	U427		G292		A162	A26
	A818	G685	A818	G750	U561	A621	A560		U428	U365			C163	G27
	A819	U686	A819		U562	A622	U561	A499	G429	U366	C295		G164	A28
	U820	A687	U820	A753	A563	C623	A562	G500	A430	U367	U296		G165	A32
	G821	G688	G821	G754	C564	U625	U564	C501	A431	U368	A298		A166	A33
	U822	G691	U822	G755	U625		U565	A502	A432	C369	C299		A167	G94
	C823	U692	C823	G756		G628	G566	C503	G433	C370	A300		G168	C34
	A824	G693	A824	U757	A629	A629	G567	C504	U434	A371	G301		C169	C35
	A825	A694	A825	C758	A630	A630	G568	G505	U435	C372	G302			C36
	C826	A695	C826	G761	C631	G631	C569	A509	U437	A374	U304		A174	G39
	U827	A696	U827	G762	U632	U632	C570	A510	U438	U375	G305		C175	C40
	U828	U697	U828	G763	G633	G633	U571	C511		G376	A306		G176	G41
	G829	G698	G829	G764	C634	C634	A572	U512	A441	G377	C307		C177	G42
		C699		G765	A635	A635	A573	C513	G449	C378	A308		U178	C43
		A700		G766	U636	U636	A574	C514	G450	C379	A309		U180	A44
		U701		G767	C637	C637	G575	C515	A451	A380	G310		A181	G45
		A702		G768	U638	U638	G576	U516	A452	C381	G311		A182	G46
		G703		G769	G639	G639	G577	G517	G453	A382	C312		C183	C47
		A704		C770	A640	A640	C578	C518	G454	A383	A313		G184	C48
		G705		G771	U641	U641	A579	C519	G455	G384	C314		U185	U49
		A706		G772	C580	A642	C580	A520	G456	C385	G315		C186	A50
		U707		G773	C643	C643	G581	G521	A456	C386	U252		A187	A51
		C708			U644	U644	C582	C522	G457	U387	A253		C188	C52
		U709			G645	G645	A583	A523		G388	G318		A189	A53
		G710			G646	G646	G584	G524	A461	A389	G255		A190	C54
		G711			C647	C647	C585	C525	G462	U390	G256		G191	A55
		A712			A648	A648	C586	C526	U463	C391	C322		C192	U56
		G713			G587	G587	C587	G527	U464	C392	G257		C193	G57
		A714			U650	U650	U589	C528	A465	G393	G258		C194	C58
		G715			C551	C551	U589	G529	A466	C394	G259		A195	A59
		A716			U590	U590	U590	G530	U467	C395	G260		A196	A60
		C719			U591	U591	G591	A531	A468	C396	U261		A197	G61
		G720			U592	U592	G592	A532	C469	A397	A262		G198	U62
					G656	G656	U593	A533	C470	U398	G264		C201	G64



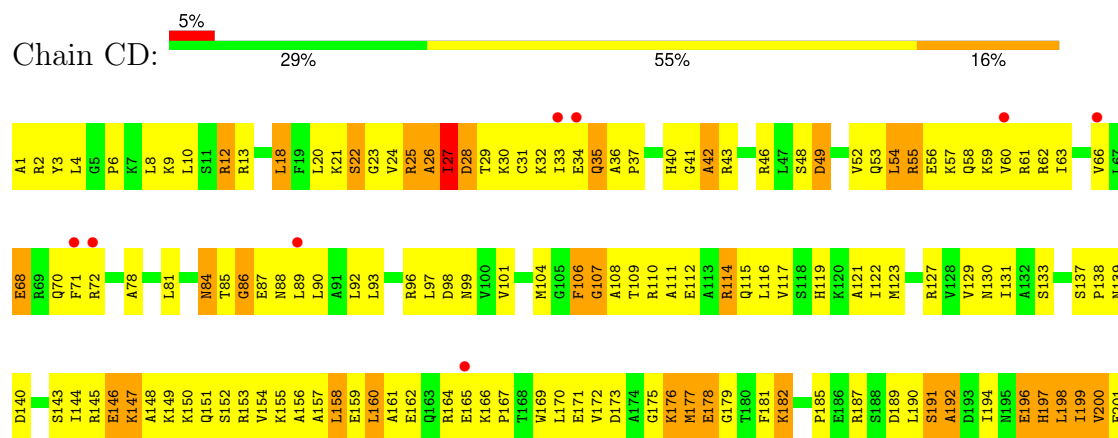
• Molecule 2: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S4

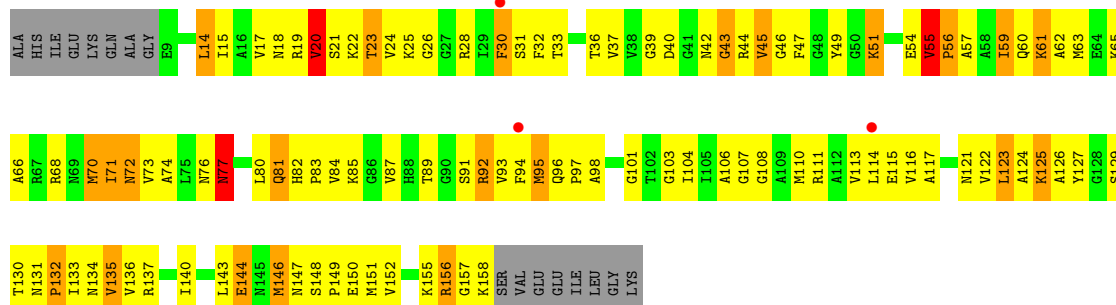


• Molecule 3: 30S ribosomal protein S4

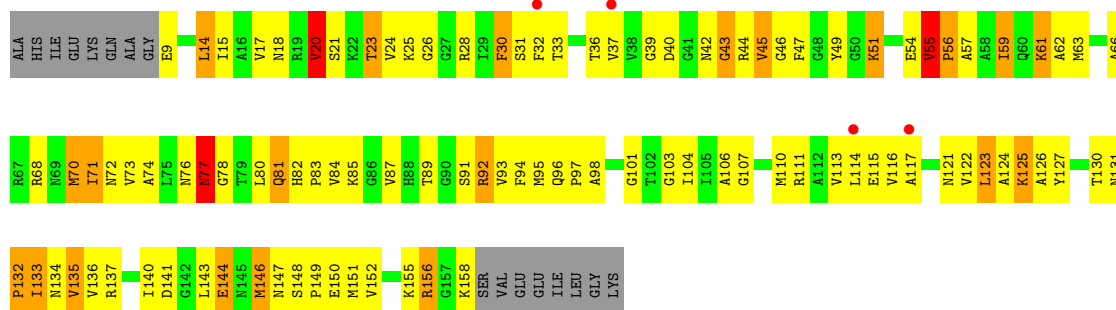




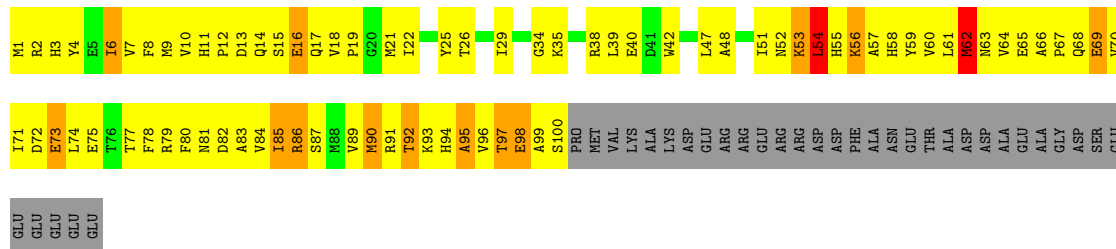
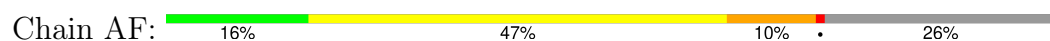
• Molecule 4: 30S ribosomal protein S5



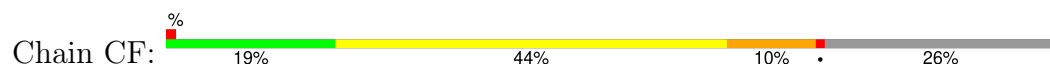
• Molecule 4: 30S ribosomal protein S5

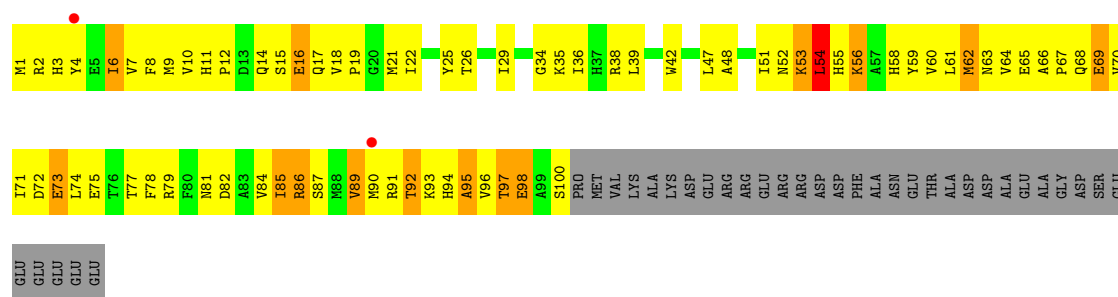


• Molecule 5: 30S ribosomal protein S6

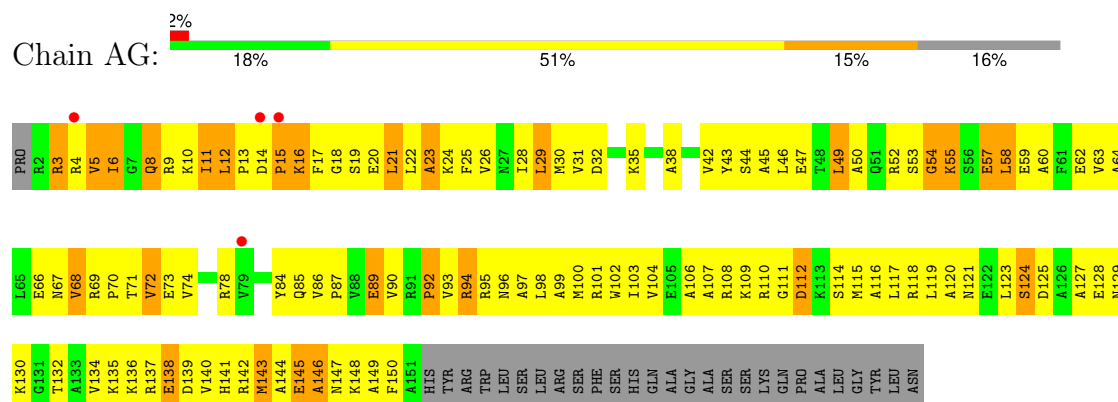


• Molecule 5: 30S ribosomal protein S6

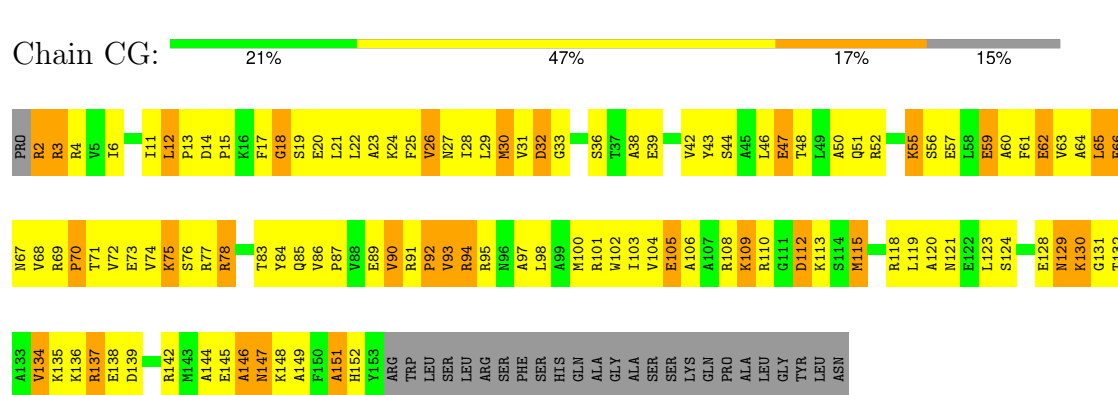




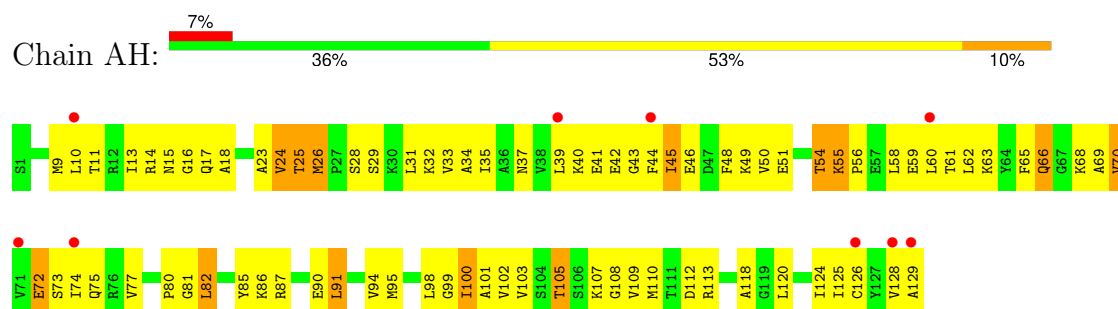
• Molecule 6: 30S ribosomal protein S7



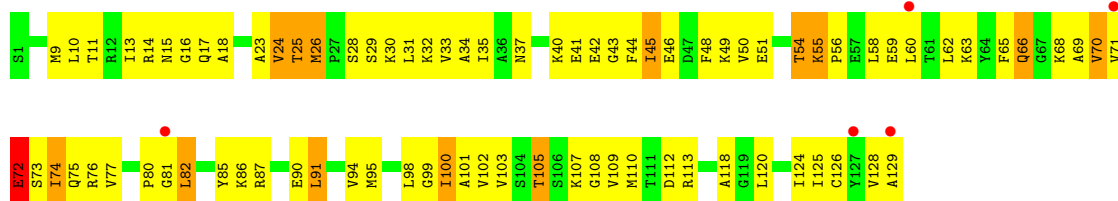
• Molecule 6: 30S ribosomal protein S7



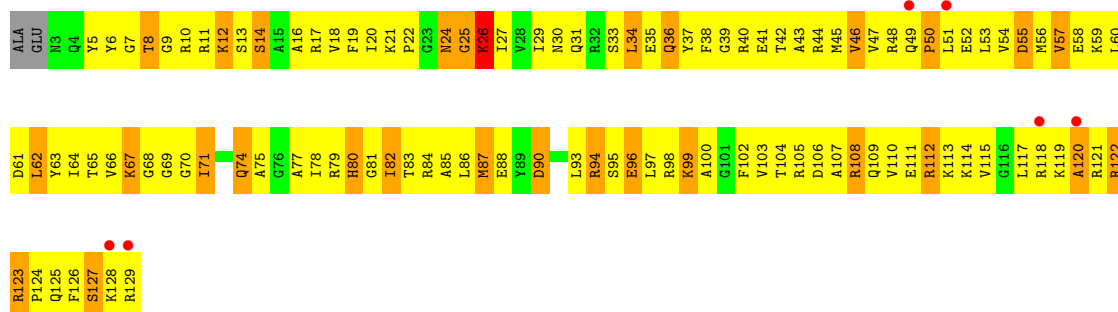
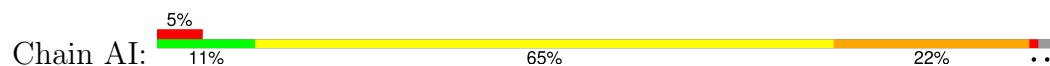
• Molecule 7: 30S ribosomal protein S8



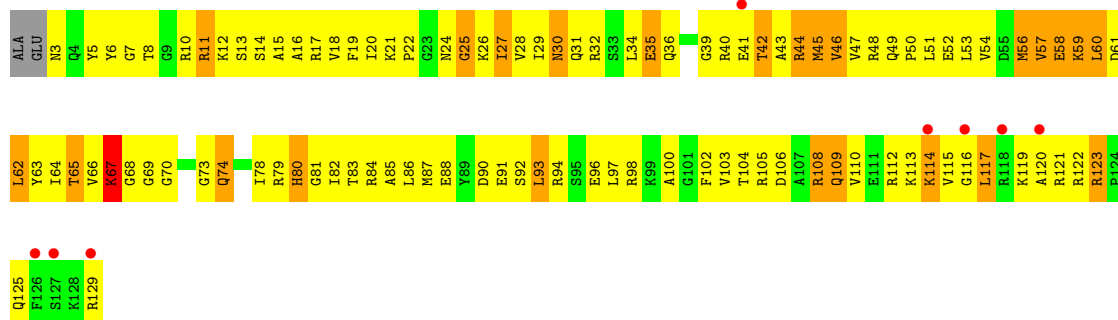
• Molecule 7: 30S ribosomal protein S8



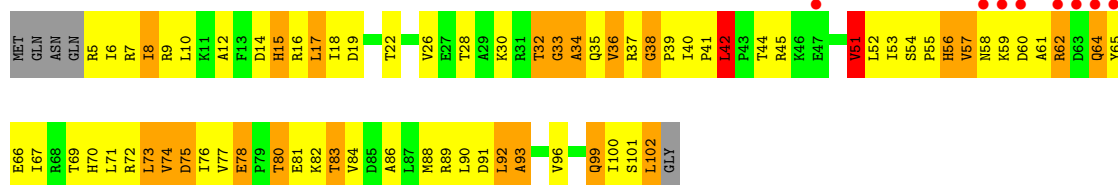
• Molecule 8: 30S ribosomal protein S9



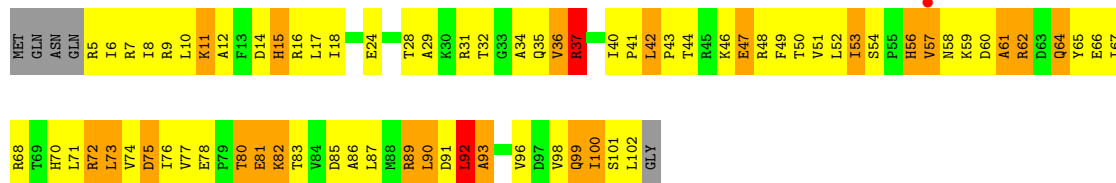
• Molecule 8: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S10



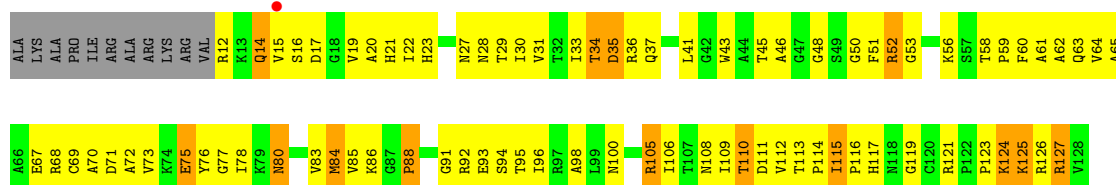
• Molecule 9: 30S ribosomal protein S10



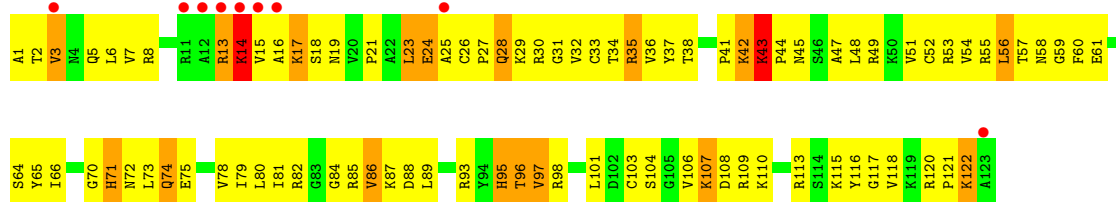
• Molecule 10: 30S ribosomal protein S11



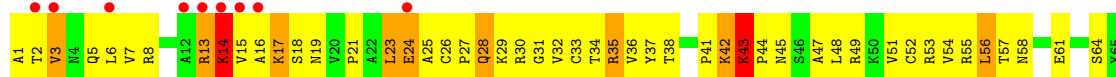
• Molecule 10: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S12



• Molecule 11: 30S ribosomal protein S12





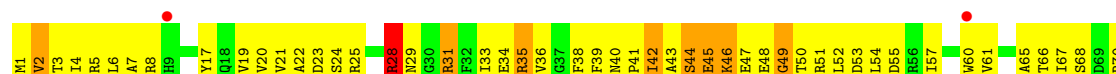
- Molecule 12: 30S ribosomal protein S13



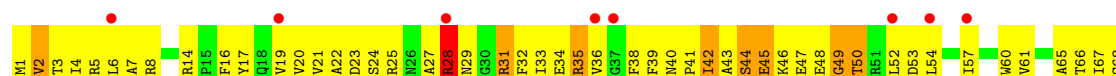
- Molecule 12: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S16

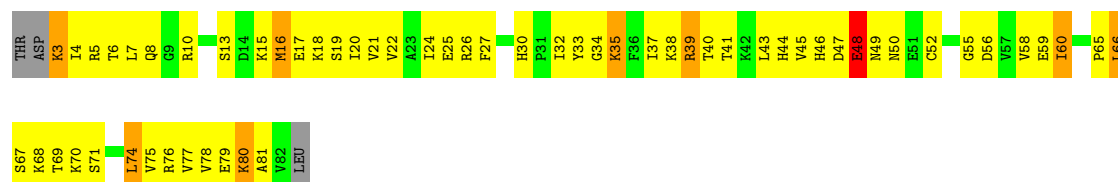


- Molecule 13: 30S ribosomal protein S16

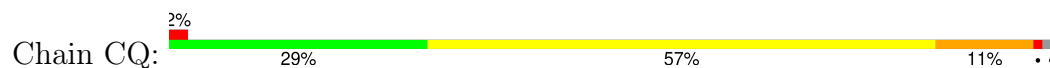


- Molecule 14: 30S ribosomal protein S17

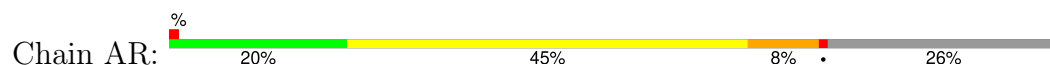




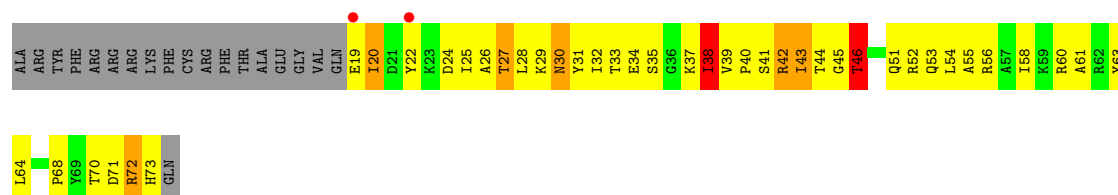
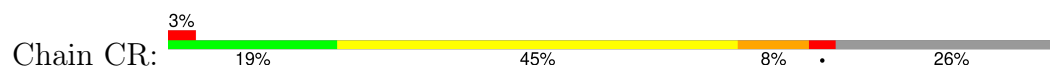
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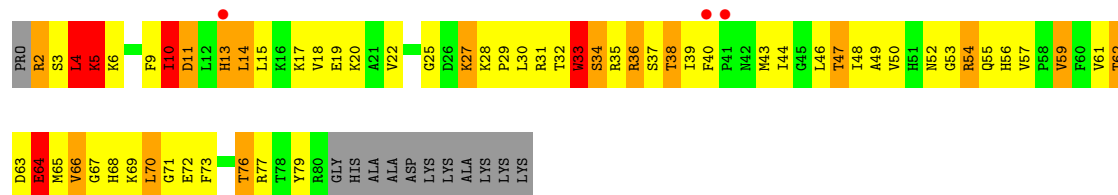
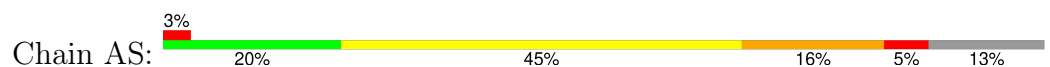
• Molecule 15: 30S ribosomal protein S18



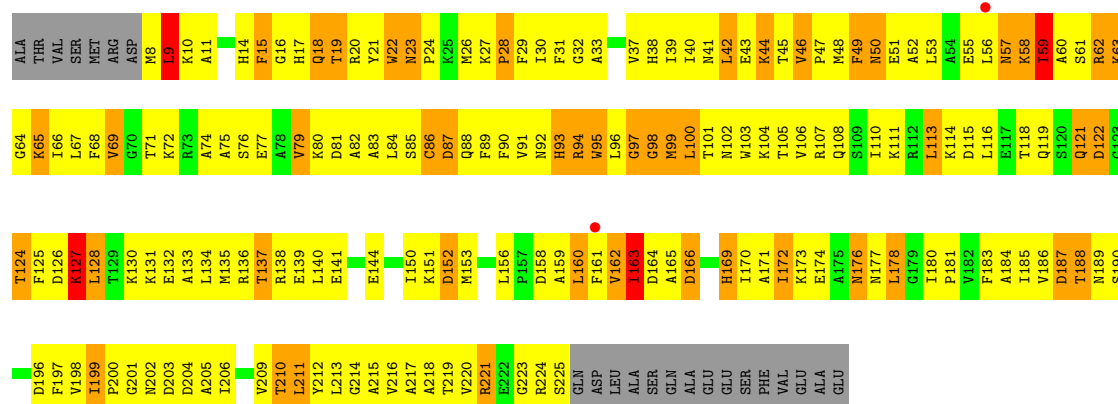
• Molecule 15: 30S ribosomal protein S18



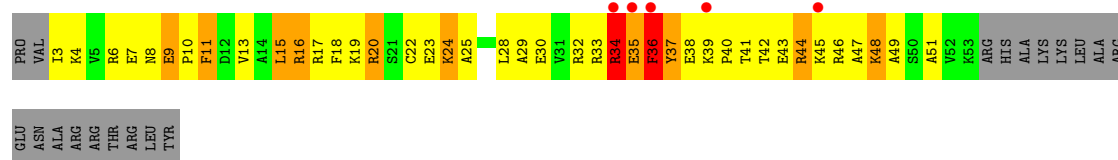
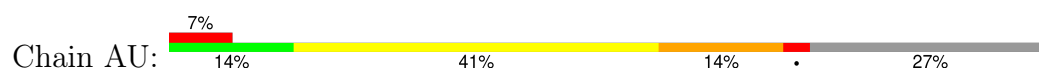
• Molecule 16: 30S ribosomal protein S19



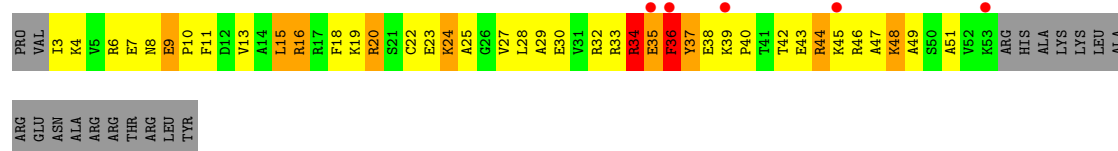
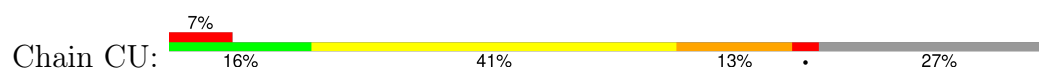
• Molecule 16: 30S ribosomal protein S19



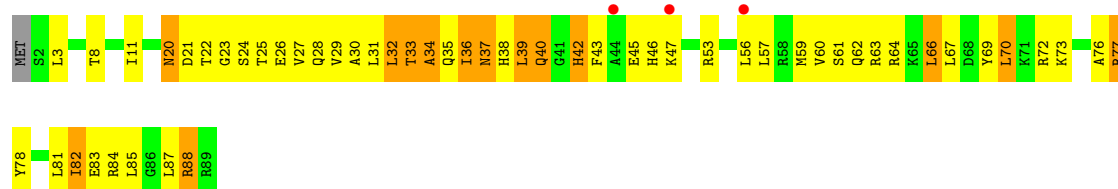
• Molecule 19: 30S ribosomal protein S21



• Molecule 19: 30S ribosomal protein S21

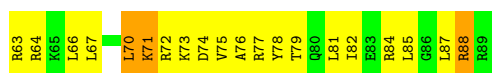


• Molecule 20: 30S ribosomal protein S15



• Molecule 20: 30S ribosomal protein S15

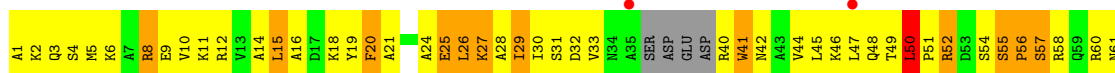
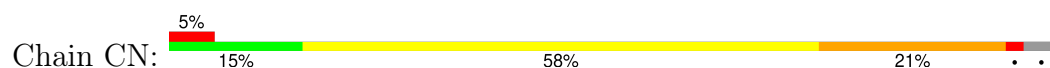




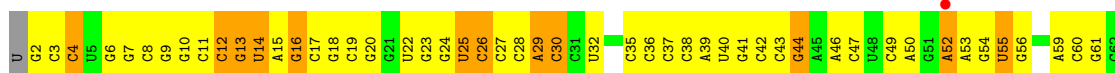
- Molecule 21: 30S ribosomal protein S14



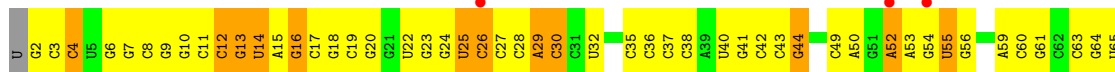
- Molecule 21: 30S ribosomal protein S14



- Molecule 22: 5S rRNA



- Molecule 22: 5S rRNA



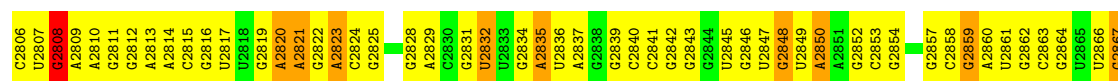
- Molecule 23: 23S rRNA





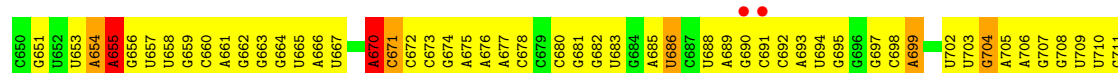
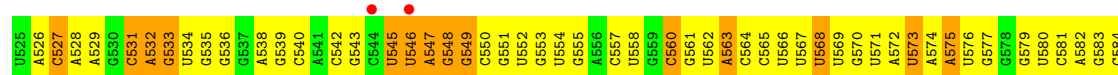
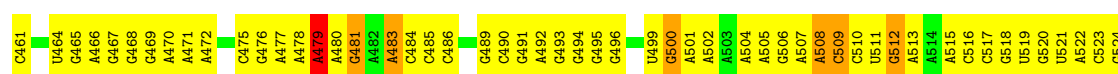
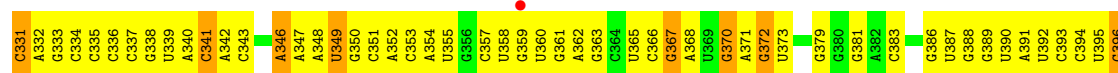
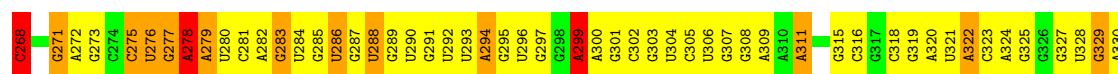
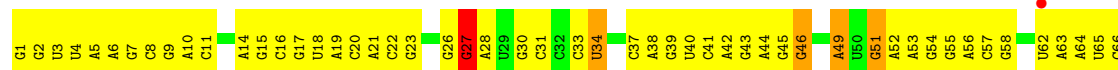
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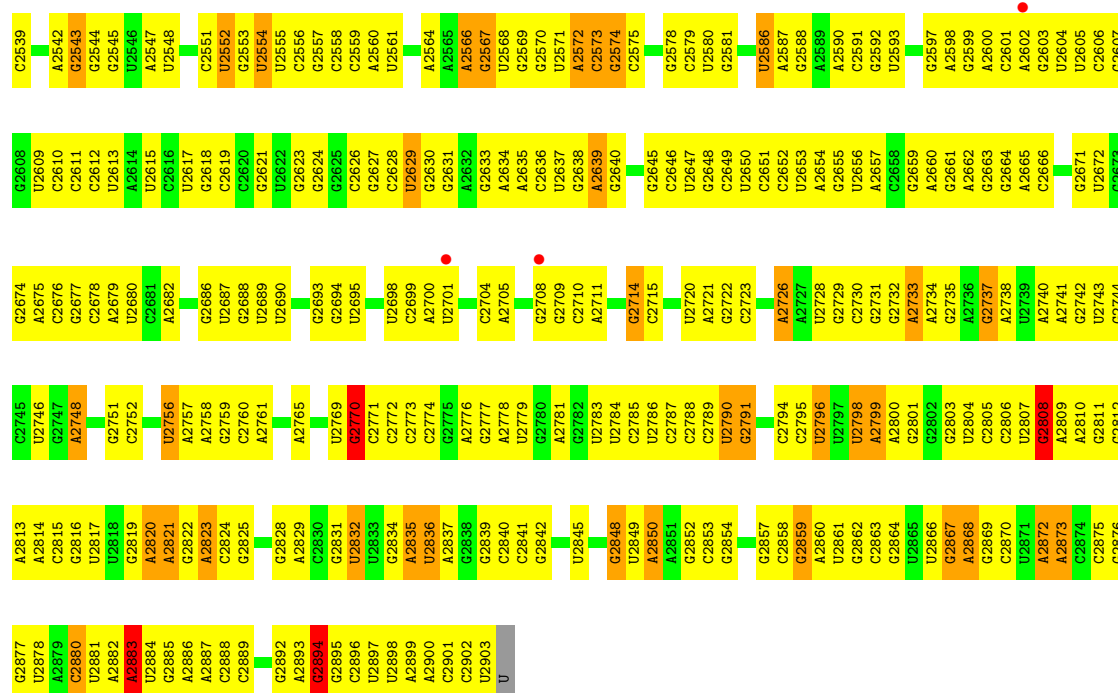
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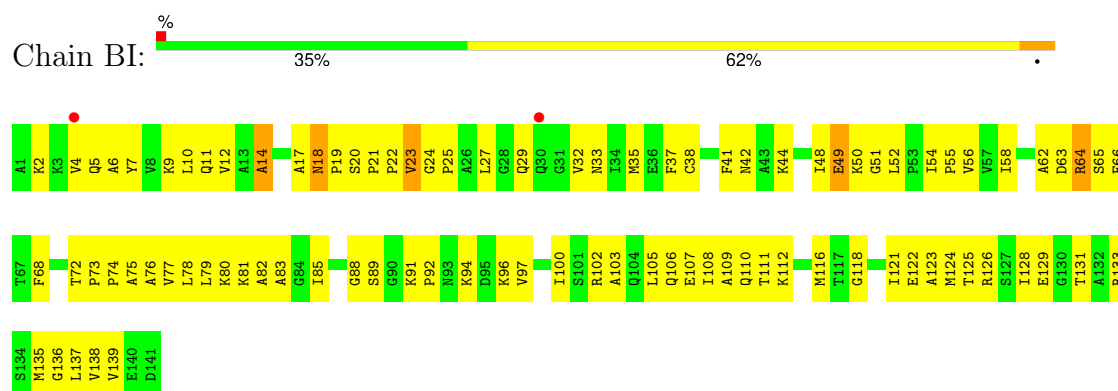


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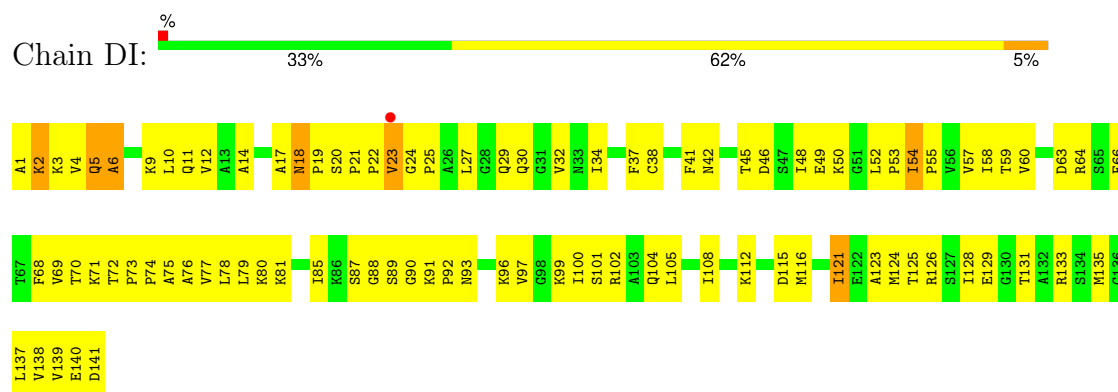
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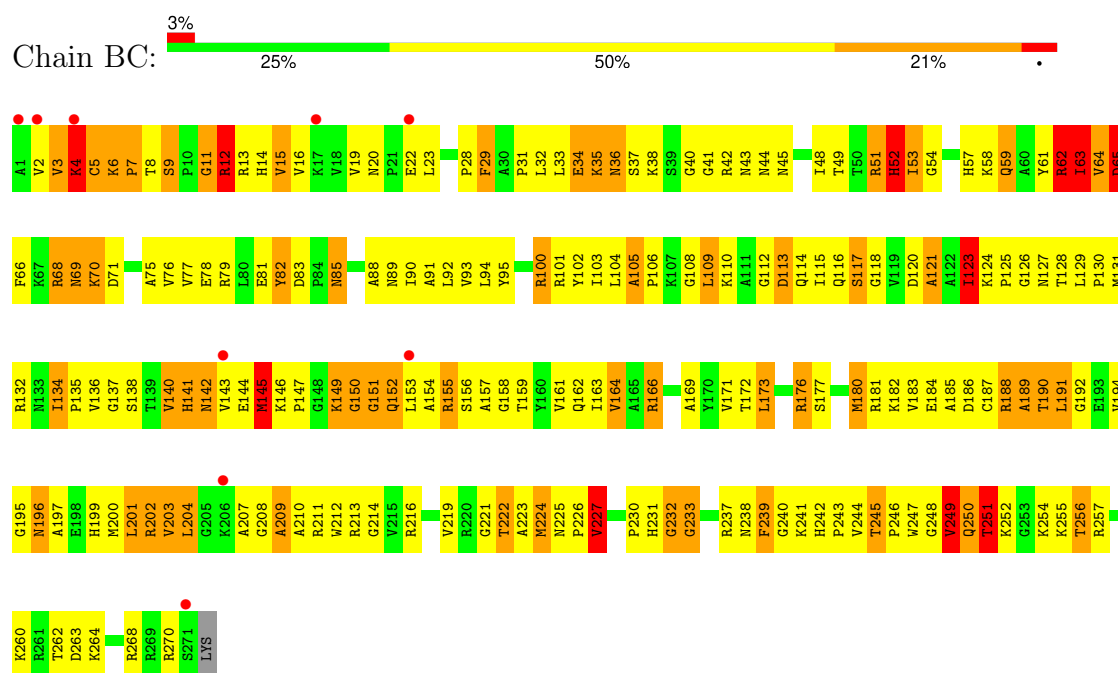
• Molecule 24: 50S ribosomal protein L11



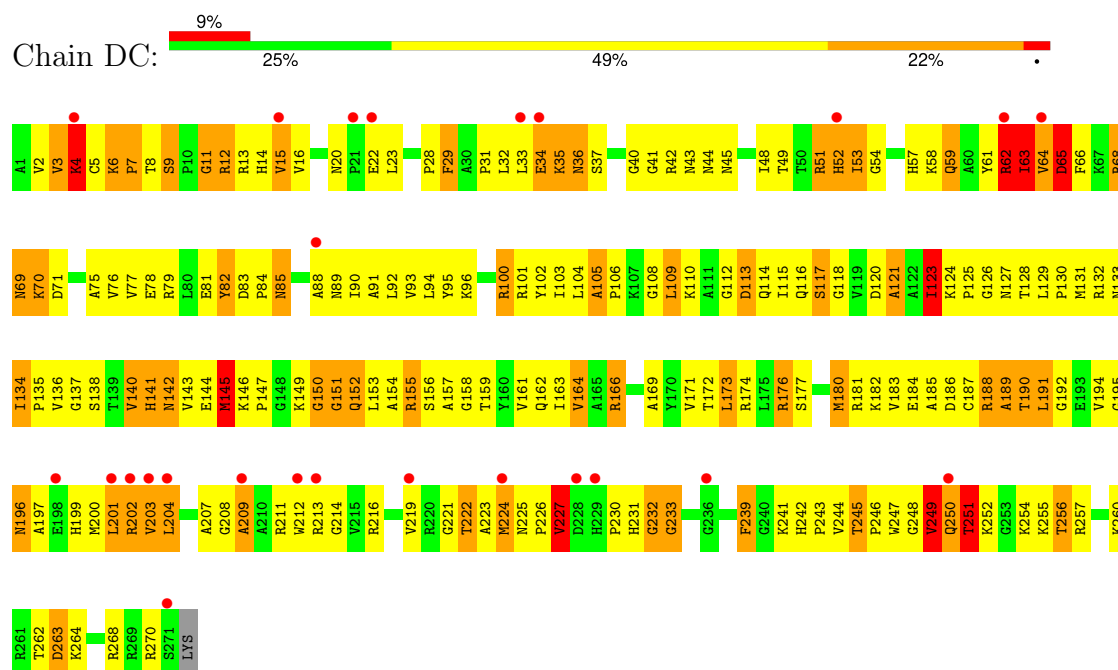
• Molecule 24: 50S ribosomal protein L11



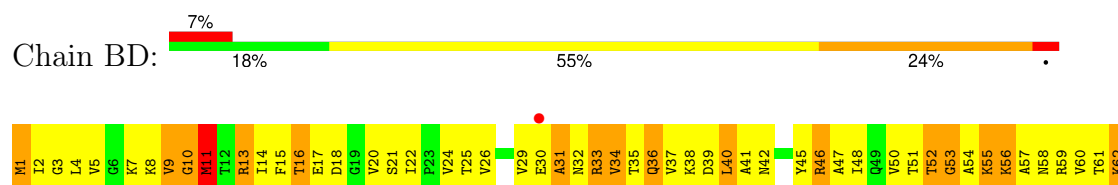
• Molecule 25: 50S ribosomal protein L2

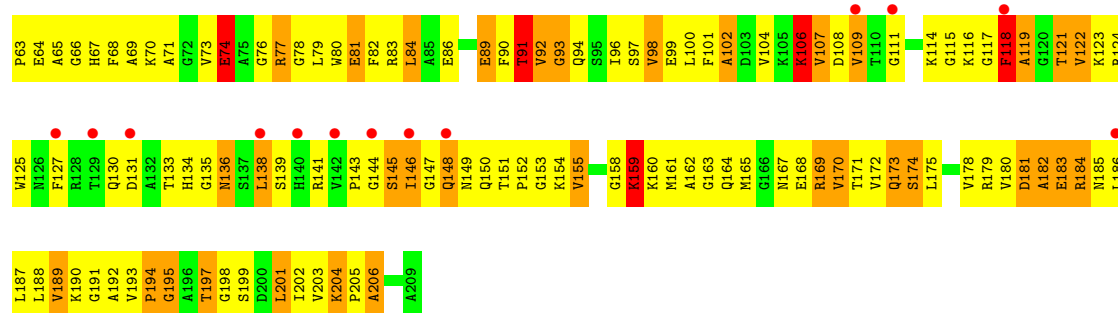


• Molecule 25: 50S ribosomal protein L2

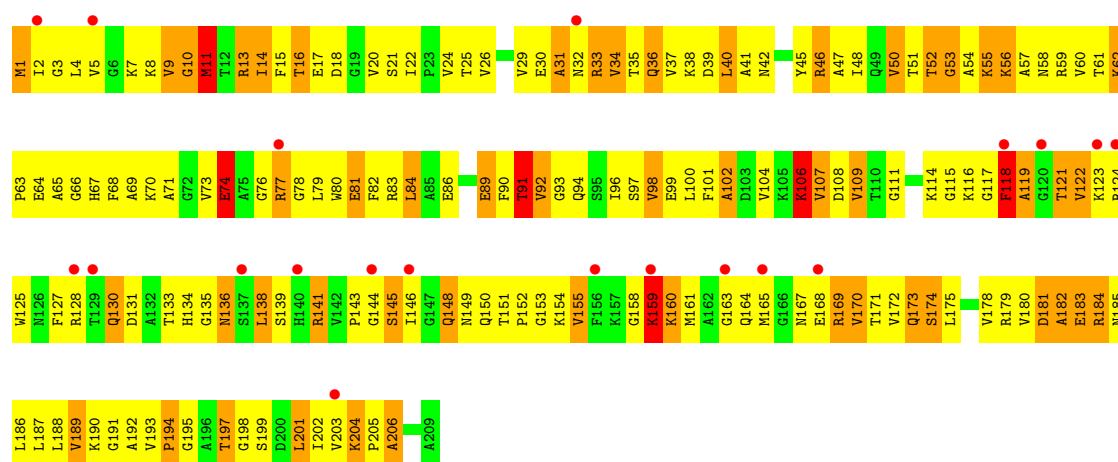


• Molecule 26: 50S ribosomal protein L3

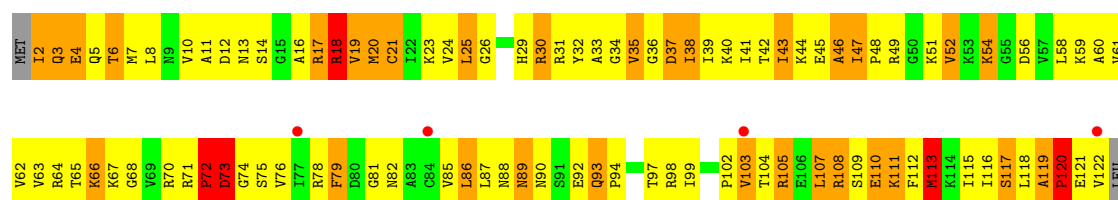
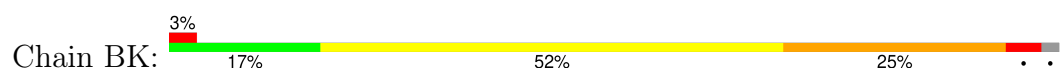




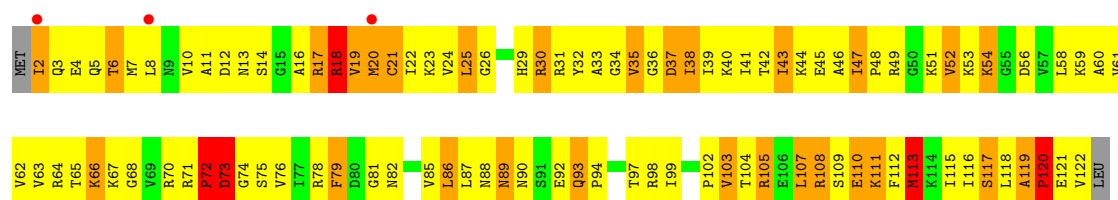
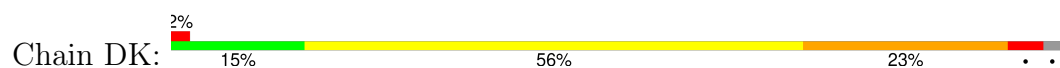
• Molecule 26: 50S ribosomal protein L3



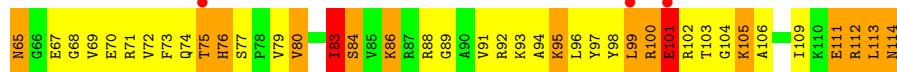
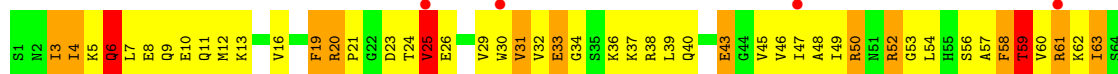
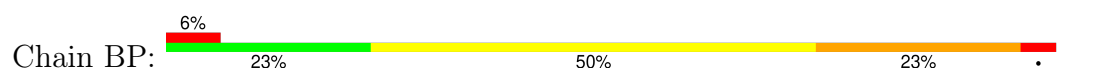
• Molecule 27: 50S ribosomal protein L14



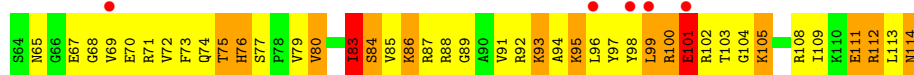
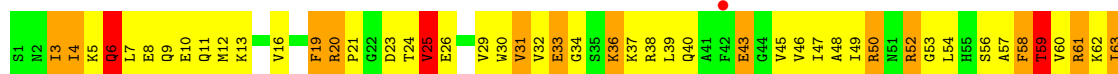
• Molecule 27: 50S ribosomal protein L14



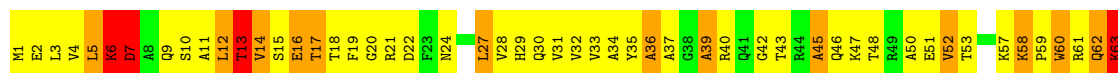
• Molecule 28: 50S ribosomal protein L19



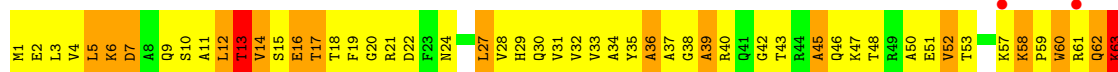
• Molecule 28: 50S ribosomal protein L19

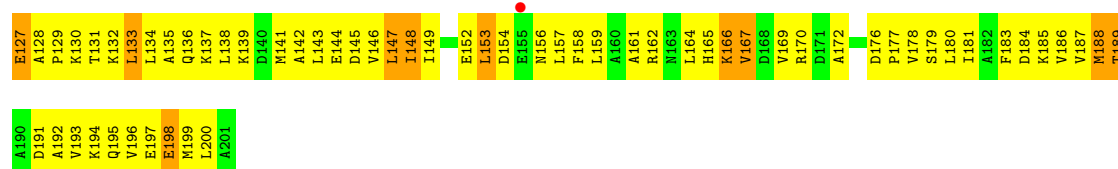


• Molecule 29: 50S ribosomal protein L4



• Molecule 29: 50S ribosomal protein L4





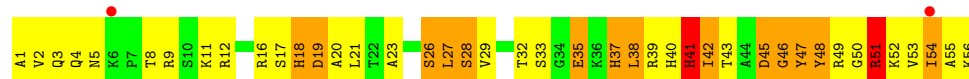
• Molecule 30: 50S ribosomal protein L30



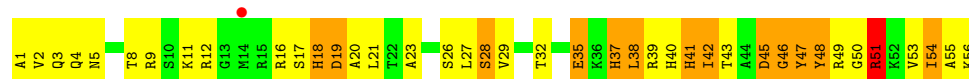
• Molecule 30: 50S ribosomal protein L30



• Molecule 31: 50S ribosomal protein L32



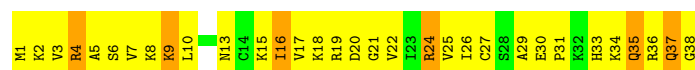
• Molecule 31: 50S ribosomal protein L32



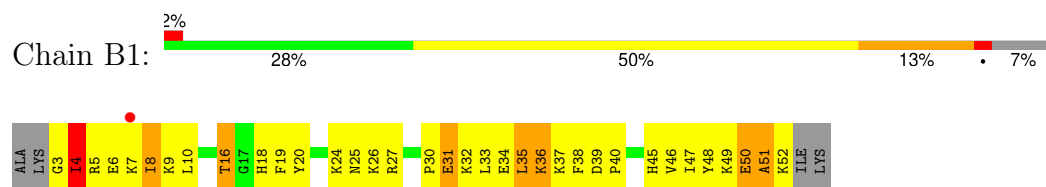
• Molecule 32: 50S ribosomal protein L36



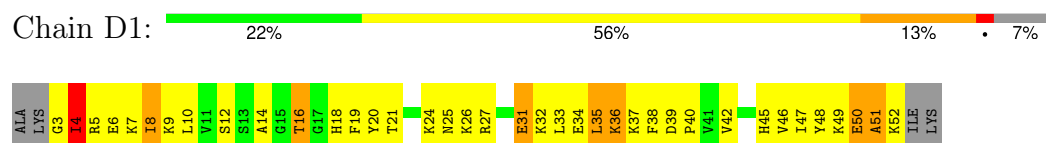
• Molecule 32: 50S ribosomal protein L36



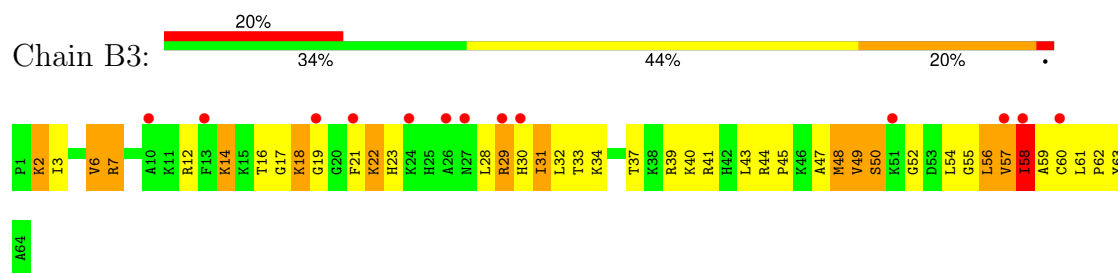
- Molecule 33: 50S ribosomal protein L33



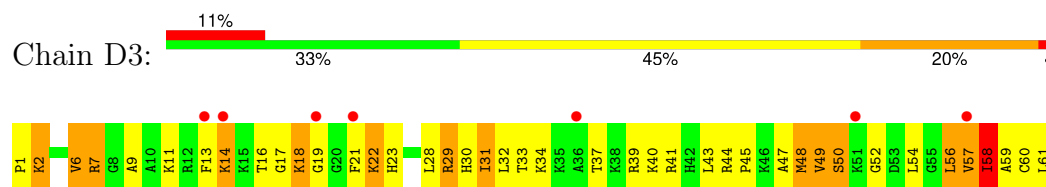
- Molecule 33: 50S ribosomal protein L33



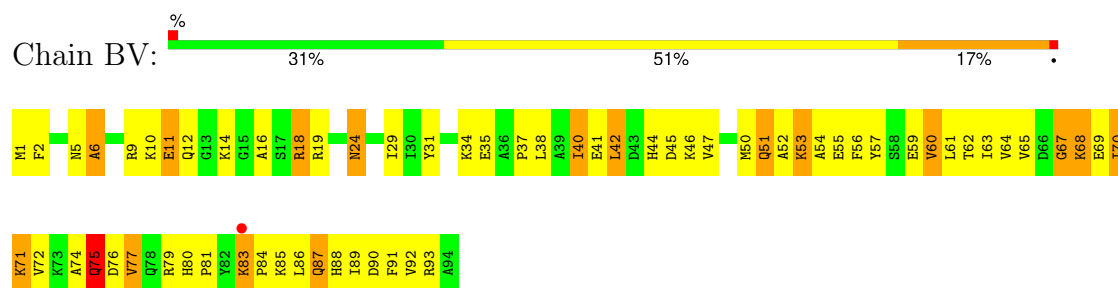
- Molecule 34: 50S ribosomal protein L35



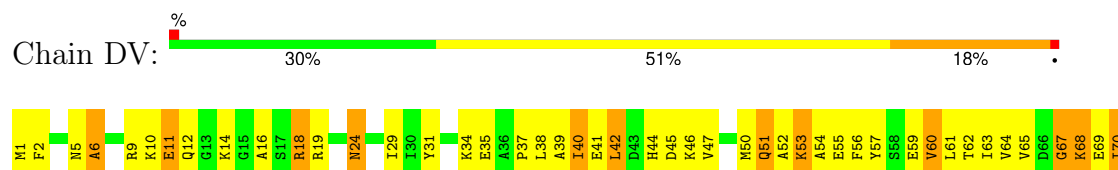
- Molecule 34: 50S ribosomal protein L35

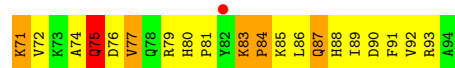


- Molecule 35: 50S ribosomal protein L25



- Molecule 35: 50S ribosomal protein L25

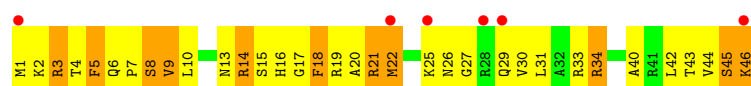




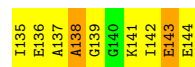
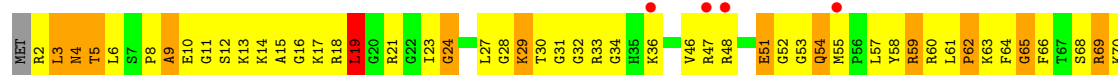
• Molecule 36: 50S ribosomal protein L34



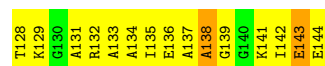
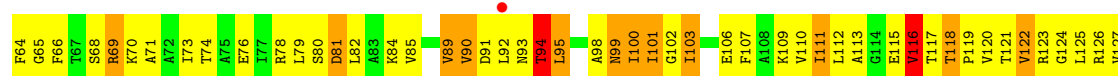
• Molecule 36: 50S ribosomal protein L34



• Molecule 37: 50S ribosomal protein L15

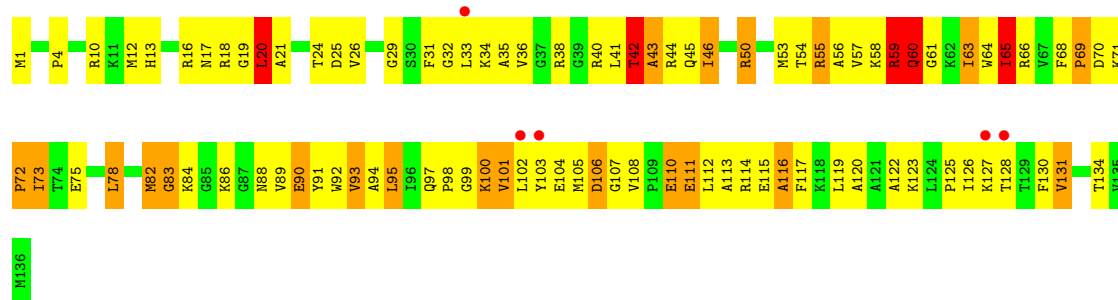


• Molecule 37: 50S ribosomal protein L15

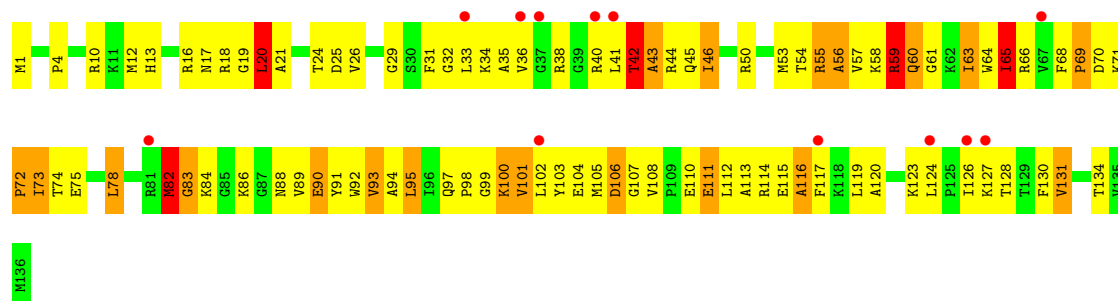


• Molecule 38: 50S ribosomal protein L16





• Molecule 38: 50S ribosomal protein L16



• Molecule 39: 50S ribosomal protein L29



• Molecule 39: 50S ribosomal protein L29

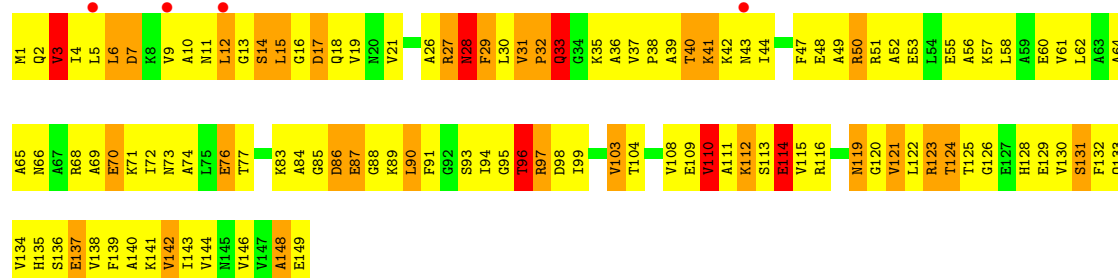


• Molecule 40: 50S ribosomal protein L9





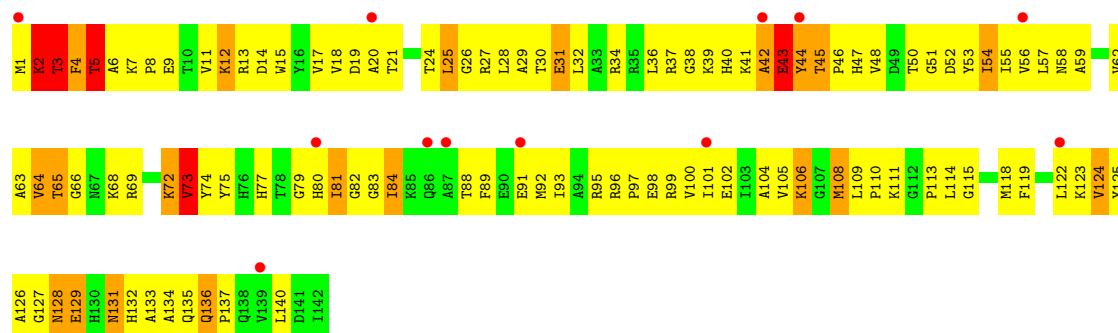
• Molecule 40: 50S ribosomal protein L9



• Molecule 41: 50S ribosomal protein L13

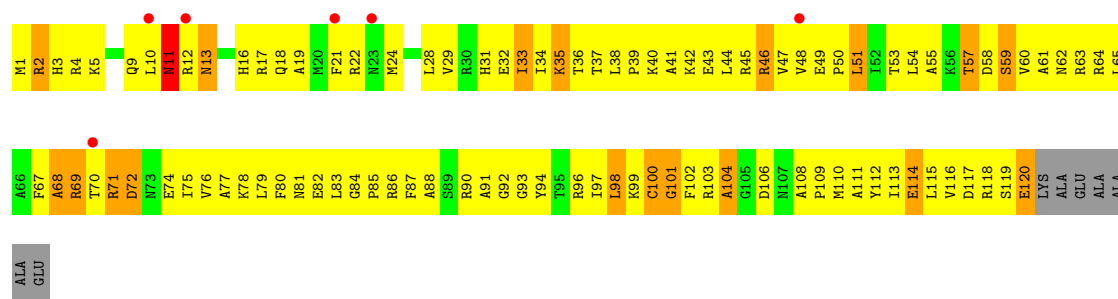


• Molecule 41: 50S ribosomal protein L13

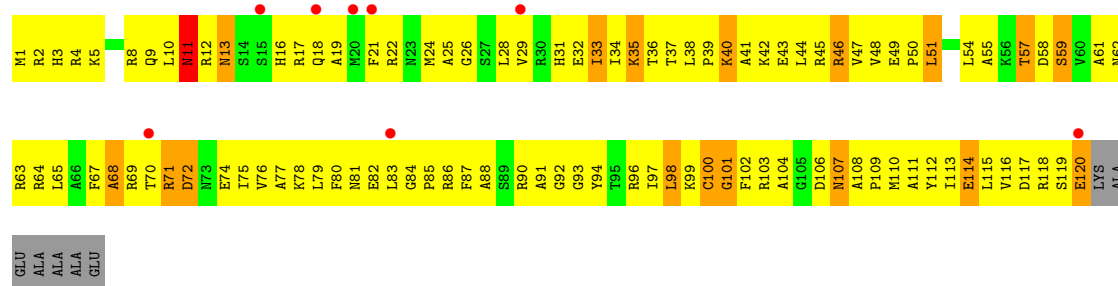


• Molecule 42: 50S ribosomal protein L17

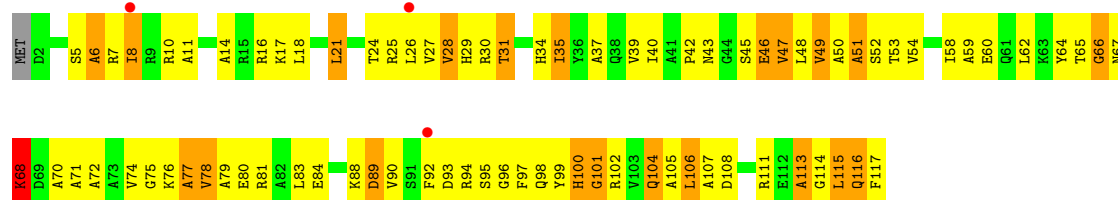




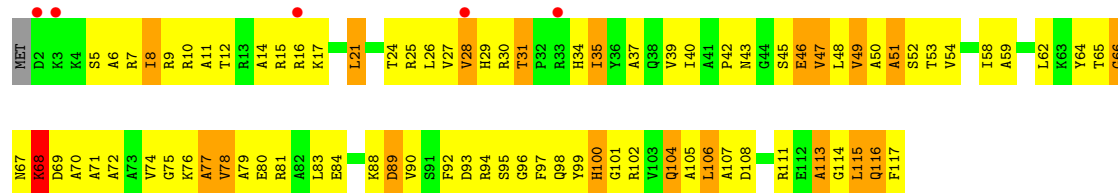
• Molecule 42: 50S ribosomal protein L17



• Molecule 43: 50S ribosomal protein L18

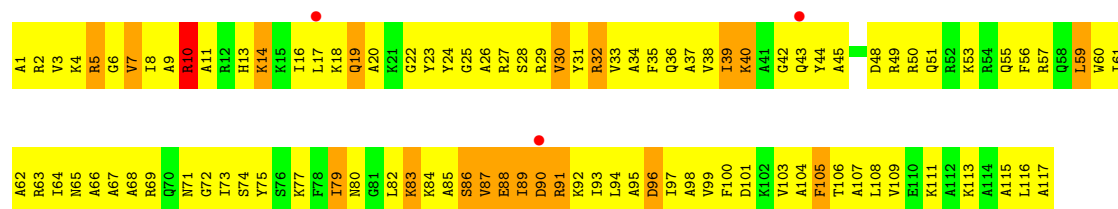


• Molecule 43: 50S ribosomal protein L18

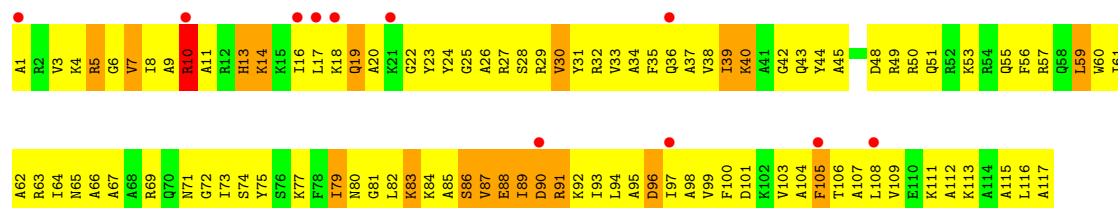


• Molecule 44: 50S ribosomal protein L20

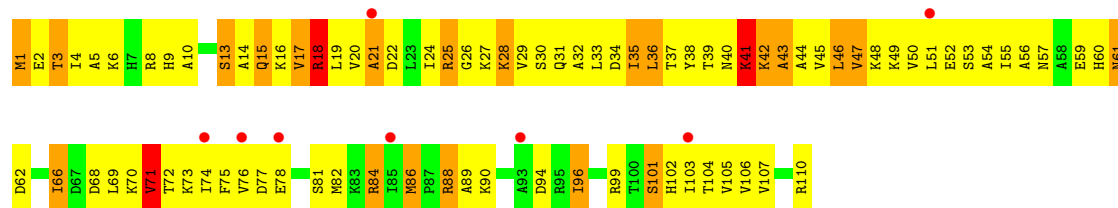




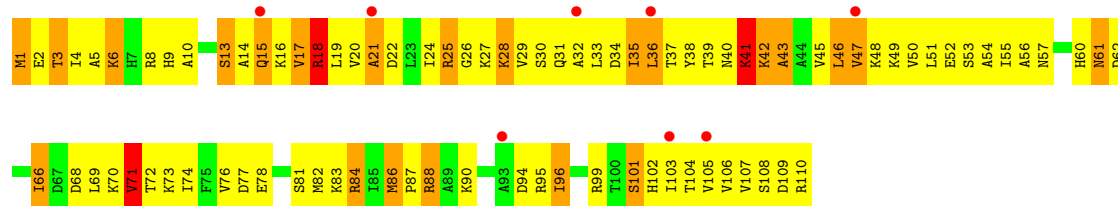
• Molecule 44: 50S ribosomal protein L20



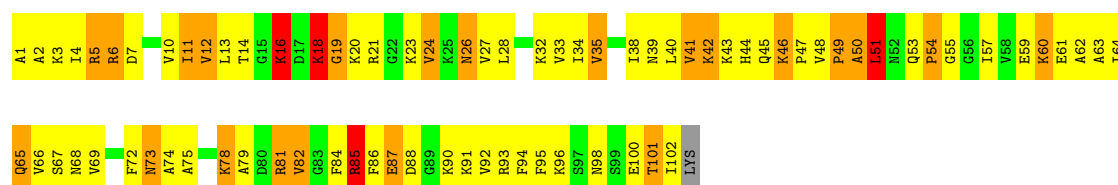
• Molecule 45: 50S ribosomal protein L22



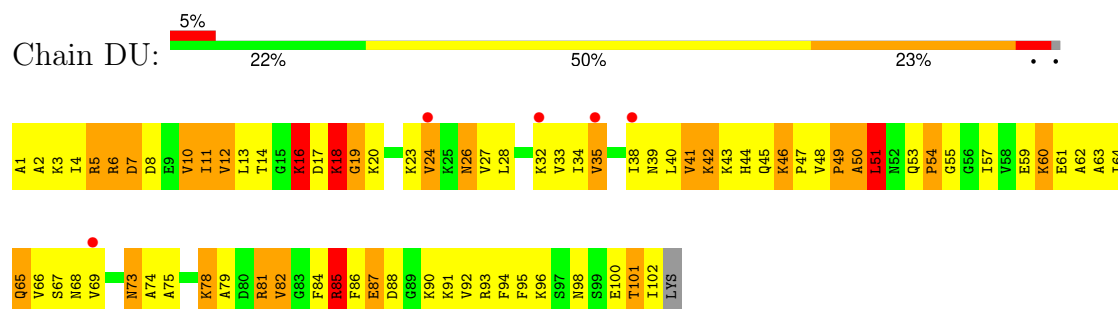
• Molecule 45: 50S ribosomal protein L22



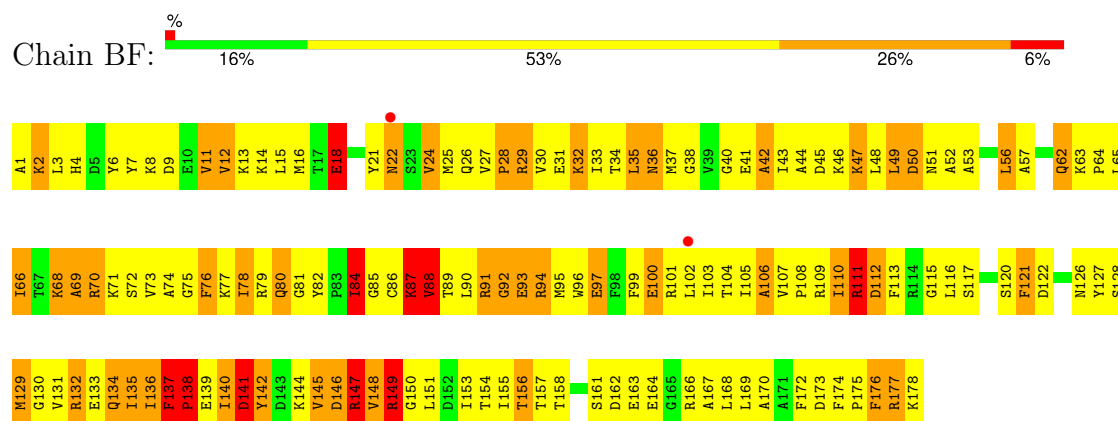
• Molecule 46: 50S ribosomal protein L24



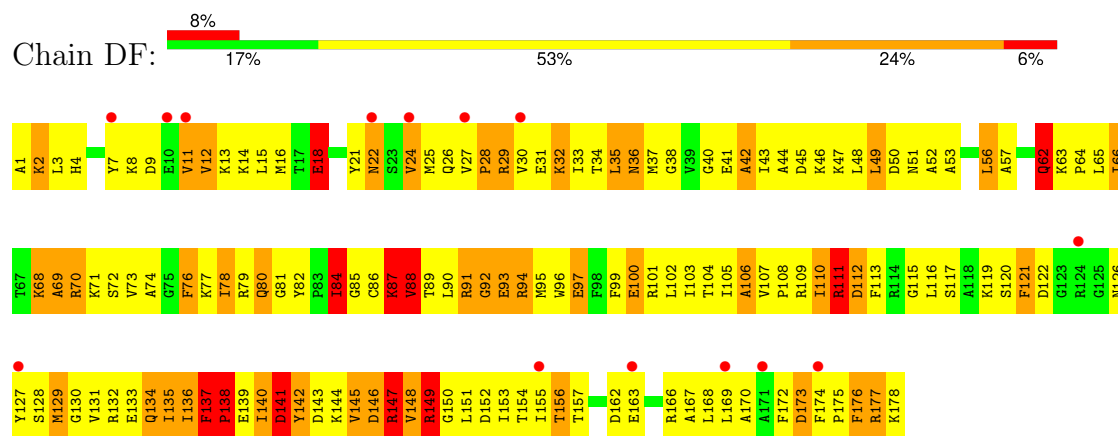
- Molecule 46: 50S ribosomal protein L24



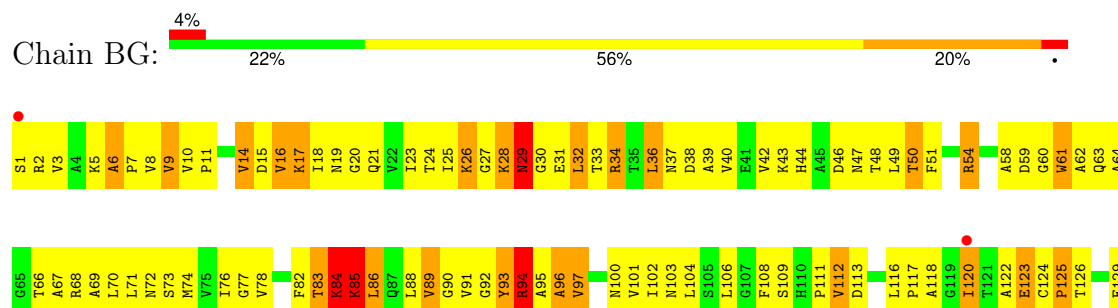
- Molecule 47: 50S ribosomal protein L5

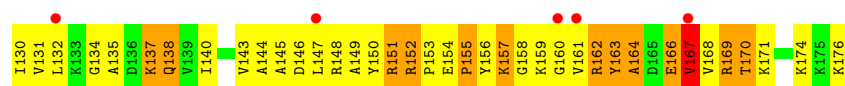


- Molecule 47: 50S ribosomal protein L5

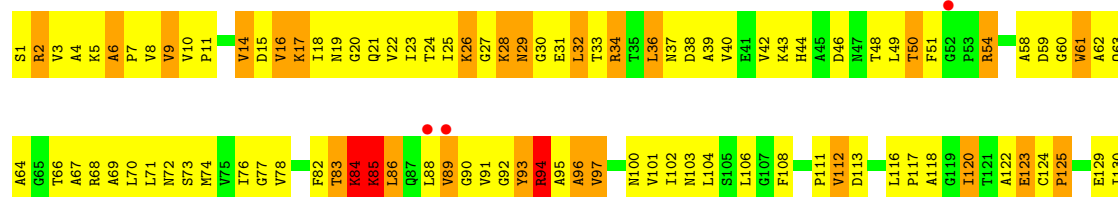


- Molecule 48: 50S ribosomal protein L6

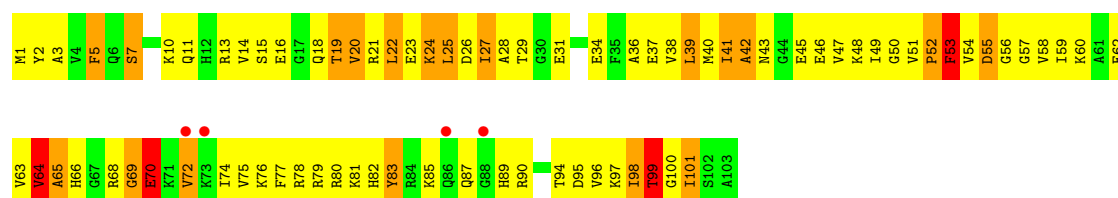




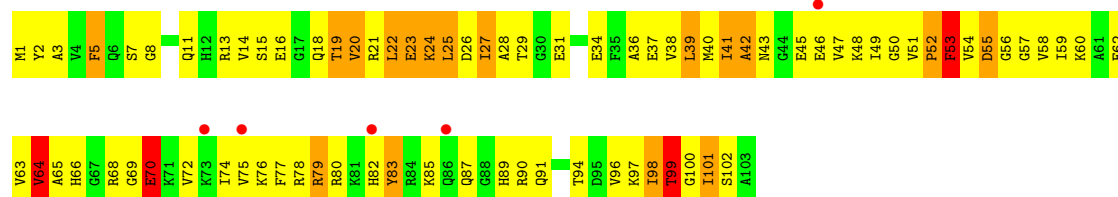
• Molecule 48: 50S ribosomal protein L6



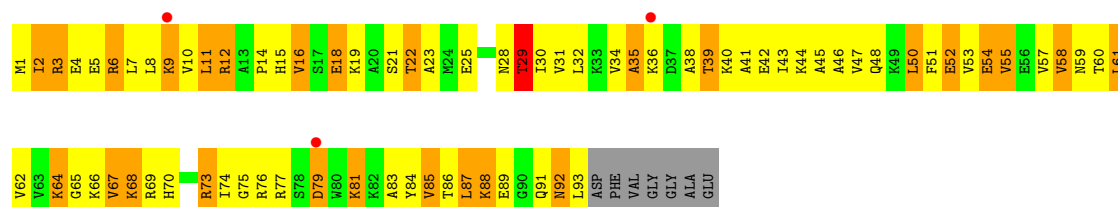
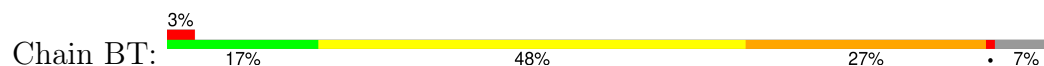
• Molecule 49: 50S ribosomal protein L21



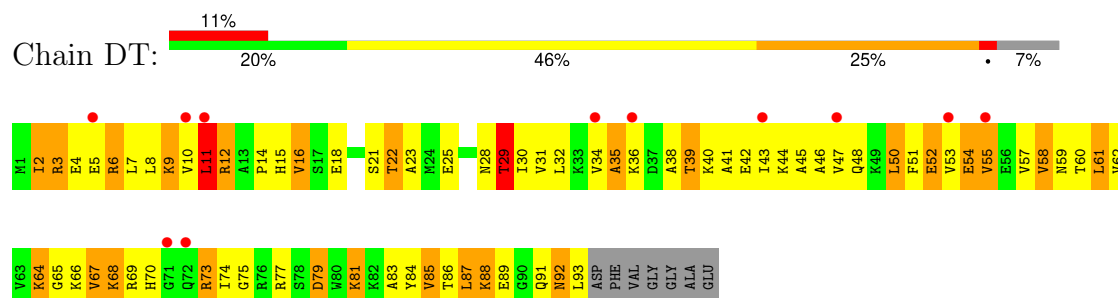
• Molecule 49: 50S ribosomal protein L21



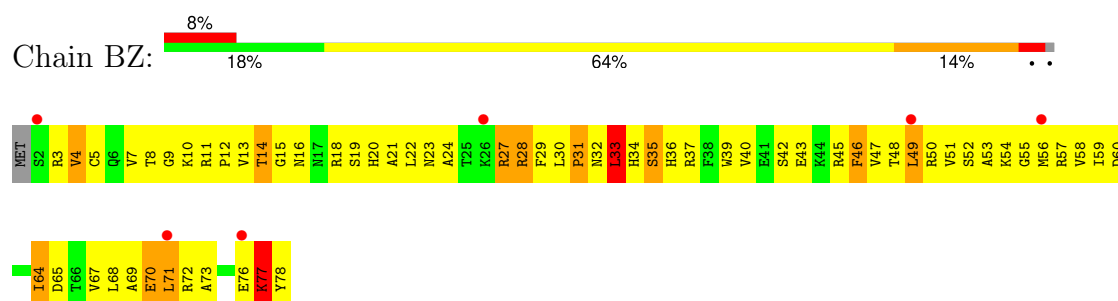
• Molecule 50: 50S ribosomal protein L23



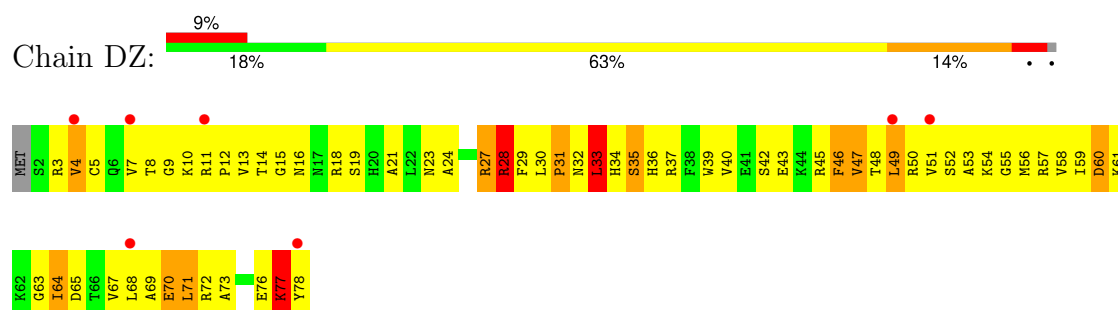
- Molecule 50: 50S ribosomal protein L23



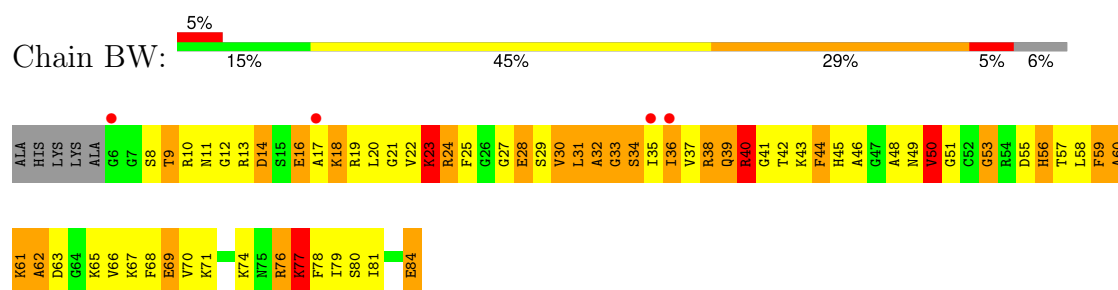
- Molecule 51: 50S ribosomal protein L28



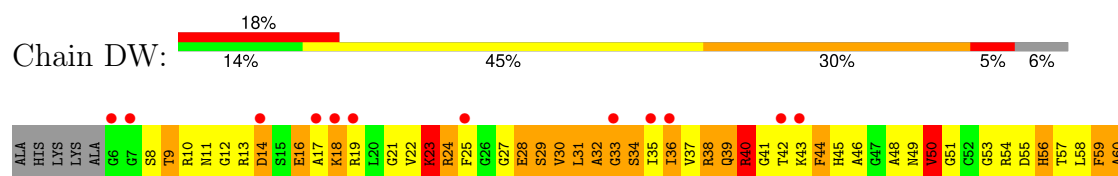
- Molecule 51: 50S ribosomal protein L28



- Molecule 52: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L27





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.93 70.00 – 3.94	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.93) 76.0 (70.00-3.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.311 0.223 , 0.270	Depositor DCC
R_{free} test set	19247 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	149.7	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 37.2	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	284033	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: MG, SCM, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.27	0/36762	0.65	37/57350 (0.1%)
1	CA	0.29	0/36762	0.66	51/57350 (0.1%)
2	AC	0.29	0/1651	0.69	0/2225
2	CC	0.28	0/1651	0.70	0/2225
3	AD	0.26	0/1665	0.71	0/2227
3	CD	0.26	0/1665	0.71	0/2227
4	AE	0.28	0/1118	0.75	2/1504 (0.1%)
4	CE	0.28	0/1118	0.75	2/1504 (0.1%)
5	AF	0.29	0/835	0.73	0/1128
5	CF	0.29	0/835	0.73	0/1128
6	AG	0.27	0/1187	0.77	2/1591 (0.1%)
6	CG	0.28	0/1211	0.78	2/1624 (0.1%)
7	AH	0.28	0/989	0.70	0/1326
7	CH	0.28	0/989	0.69	0/1326
8	AI	0.27	0/1034	0.68	0/1375
8	CI	0.28	0/1034	0.70	0/1375
9	AJ	0.29	0/796	0.68	0/1077
9	CJ	0.28	0/796	0.69	0/1077
10	AK	0.31	0/893	0.75	0/1205
10	CK	0.31	0/893	0.74	0/1205
11	AL	0.27	0/969	0.75	0/1300
11	CL	0.27	0/969	0.76	0/1300
12	AM	0.27	0/892	0.73	1/1193 (0.1%)
12	CM	0.27	0/884	0.72	0/1181
13	AP	0.28	0/659	0.74	1/884 (0.1%)
13	CP	0.27	0/648	0.74	1/870 (0.1%)
14	AQ	0.26	0/657	0.71	0/881
14	CQ	0.27	0/666	0.71	0/892
15	AR	0.29	0/462	0.76	0/621
15	CR	0.29	0/462	0.75	0/621
16	AS	0.28	0/652	0.70	1/877 (0.1%)
16	CS	0.27	0/660	0.76	1/888 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.28	0/671	0.72	1/888 (0.1%)
17	CT	0.28	0/671	0.71	1/888 (0.1%)
18	AB	0.29	0/1735	0.72	0/2338
18	CB	0.29	0/1735	0.72	0/2338
19	AU	0.28	0/430	0.79	0/570
19	CU	0.28	0/430	0.79	0/570
20	AO	0.25	0/722	0.68	0/964
20	CO	0.26	0/722	0.64	0/964
21	AN	0.27	0/785	0.72	0/1043
21	CN	0.28	0/785	0.77	1/1043 (0.1%)
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	60/106569 (0.1%)
23	DB	0.27	1/68314 (0.0%)	0.65	62/106569 (0.1%)
24	BI	0.31	0/1046	0.80	0/1410
24	DI	0.35	0/1046	0.82	0/1410
25	BC	0.26	0/2121	0.75	3/2852 (0.1%)
25	DC	0.26	0/2121	0.74	1/2852 (0.0%)
26	BD	0.28	0/1586	0.72	1/2134 (0.0%)
26	DD	0.28	0/1586	0.73	1/2134 (0.0%)
27	BK	0.30	0/939	0.81	2/1258 (0.2%)
27	DK	0.30	0/939	0.81	2/1258 (0.2%)
28	BP	0.28	0/929	0.85	2/1242 (0.2%)
28	DP	0.29	0/929	0.86	2/1242 (0.2%)
29	BE	0.27	0/1571	0.81	4/2113 (0.2%)
29	DE	0.27	0/1571	0.82	4/2113 (0.2%)
30	BY	0.30	0/453	0.75	0/605
30	DY	0.30	0/453	0.76	0/605
31	B0	0.26	0/450	0.76	1/599 (0.2%)
31	D0	0.26	0/450	0.76	1/599 (0.2%)
32	B4	0.27	0/303	0.76	0/397
32	D4	0.27	0/303	0.75	0/397
33	B1	0.31	0/416	0.80	0/554
33	D1	0.31	0/416	0.80	0/554
34	B3	0.28	0/513	0.71	0/676
34	D3	0.27	0/513	0.71	0/676
35	BV	0.27	0/766	0.73	0/1025
35	DV	0.27	0/766	0.73	0/1025
36	B2	0.29	0/380	0.77	0/498
36	D2	0.29	0/380	0.78	0/498
37	BL	0.27	0/1054	0.76	2/1403 (0.1%)
37	DL	0.27	0/1054	0.76	2/1403 (0.1%)
38	BM	0.29	0/1093	0.75	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.29	0/1093	0.74	0/1460
39	BX	0.26	0/510	0.83	2/677 (0.3%)
39	DX	0.25	0/510	0.84	2/677 (0.3%)
40	BH	0.28	0/1122	0.75	1/1515 (0.1%)
40	DH	0.28	0/1122	0.76	1/1515 (0.1%)
41	BJ	0.28	0/1152	0.70	0/1551
41	DJ	0.28	0/1152	0.72	1/1551 (0.1%)
42	BN	0.29	0/973	0.81	0/1301
42	DN	0.29	0/973	0.82	0/1301
43	BO	0.26	0/902	0.76	1/1209 (0.1%)
43	DO	0.27	0/902	0.77	1/1209 (0.1%)
44	BQ	0.26	0/960	0.87	1/1278 (0.1%)
44	DQ	0.26	0/960	0.86	1/1278 (0.1%)
45	BS	0.27	0/864	0.80	1/1156 (0.1%)
45	DS	0.27	0/864	0.81	1/1156 (0.1%)
46	BU	0.27	0/787	0.71	1/1051 (0.1%)
46	DU	0.27	0/787	0.71	1/1051 (0.1%)
47	BF	0.28	0/1444	0.82	2/1937 (0.1%)
47	DF	0.27	0/1444	0.83	2/1937 (0.1%)
48	BG	0.27	0/1343	0.74	2/1816 (0.1%)
48	DG	0.27	0/1343	0.74	2/1816 (0.1%)
49	BR	0.27	0/829	0.67	0/1107
49	DR	0.27	0/829	0.68	0/1107
50	BT	0.26	0/744	0.80	1/994 (0.1%)
50	DT	0.26	0/744	0.80	1/994 (0.1%)
51	BZ	0.27	0/635	0.80	0/848
51	DZ	0.28	0/635	0.80	0/848
52	BW	0.28	0/603	0.70	0/797
52	DW	0.28	0/603	0.69	0/797
All	All	0.27	2/306360 (0.0%)	0.68	283/457969 (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	15
1	CA	0	19
23	BB	0	37
23	DB	0	37
All	All	0	108

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	1086	A	C5-C6	-7.29	1.26	1.41
23	BB	1086	A	C5-C6	-7.24	1.26	1.41

The worst 5 of 283 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-11.11	74.68	108.00
23	BB	2204	G	O5'-P-OP2	-10.49	76.52	108.00
23	DB	2791	G	O5'-P-OP2	-10.47	76.59	108.00
23	DB	2790	U	OP2-P-O3'	10.13	138.40	108.00
23	BB	2791	G	O5'-P-OP1	-10.07	77.80	108.00

There are no chirality outliers.

5 of 108 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	450	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	1448	0
1	CA	32831	0	16521	1413	0
2	AC	1624	0	1699	214	0
2	CC	1624	0	1699	198	0
3	AD	1643	0	1710	186	0
3	CD	1643	0	1710	189	0
4	AE	1105	0	1148	133	0
4	CE	1105	0	1148	121	0
5	AF	817	0	808	96	0
5	CF	817	0	808	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AG	1174	0	1230	157	0
6	CG	1196	0	1246	140	0
7	AH	979	0	1034	94	0
7	CH	979	0	1034	94	0
8	AI	1022	0	1070	188	0
8	CI	1022	0	1070	153	0
9	AJ	786	0	828	87	0
9	CJ	786	0	828	107	0
10	AK	877	0	887	116	0
10	CK	877	0	887	105	0
11	AL	955	0	1019	99	0
11	CL	955	0	1019	99	0
12	AM	883	0	944	144	0
12	CM	876	0	937	148	0
13	AP	649	0	666	71	0
13	CP	638	0	656	73	0
14	AQ	648	0	691	66	0
14	CQ	657	0	702	67	0
15	AR	455	0	478	38	0
15	CR	455	0	478	41	0
16	AS	637	0	665	102	0
16	CS	644	0	675	120	0
17	AT	665	0	714	64	0
17	CT	665	0	714	68	0
18	AB	1704	0	1732	228	0
18	CB	1704	0	1732	246	0
19	AU	425	0	449	62	0
19	CU	425	0	449	59	0
20	AO	714	0	734	68	0
20	CO	714	0	734	70	0
21	AN	774	0	827	111	0
21	CN	774	0	827	120	0
22	BA	2507	0	1270	119	0
22	DA	2507	0	1270	113	0
23	BB	60995	0	30679	2411	0
23	DB	60995	0	30678	2456	0
24	BI	1032	0	1088	120	0
24	DI	1032	0	1088	179	0
25	BC	2082	0	2157	251	0
25	DC	2082	0	2157	253	0
26	BD	1565	0	1616	253	0
26	DD	1565	0	1616	255	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	BK	930	0	1000	163	0
27	DK	930	0	1000	162	0
28	BP	917	0	965	129	0
28	DP	917	0	965	136	0
29	BE	1552	0	1619	215	0
29	DE	1552	0	1619	211	0
30	BY	449	0	491	61	0
30	DY	449	0	491	55	0
31	B0	444	0	461	50	0
31	D0	444	0	461	46	0
32	B4	302	0	340	44	0
32	D4	302	0	340	45	0
33	B1	409	0	440	54	0
33	D1	409	0	440	54	0
34	B3	504	0	574	53	0
34	D3	504	0	574	57	0
35	BV	753	0	780	88	0
35	DV	753	0	780	90	0
36	B2	377	0	418	41	0
36	D2	377	0	418	46	0
37	BL	1045	0	1117	147	0
37	DL	1045	0	1117	151	0
38	BM	1074	0	1157	128	0
38	DM	1074	0	1157	125	0
39	BX	509	0	543	54	0
39	DX	509	0	543	59	0
40	BH	1111	0	1148	184	0
40	DH	1111	0	1148	153	0
41	BJ	1129	0	1162	145	0
41	DJ	1129	0	1162	152	0
42	BN	960	0	1000	143	0
42	DN	960	0	1000	141	0
43	BO	892	0	923	99	0
43	DO	892	0	923	98	0
44	BQ	947	0	1022	161	0
44	DQ	947	0	1022	156	0
45	BS	857	0	922	107	0
45	DS	857	0	922	105	0
46	BU	779	0	834	123	0
46	DU	779	0	834	120	0
47	BF	1420	0	1460	277	0
47	DF	1420	0	1460	260	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	BG	1323	0	1374	193	0
48	DG	1323	0	1374	184	0
49	BR	816	0	839	114	0
49	DR	816	0	839	120	0
50	BT	738	0	807	120	0
50	DT	738	0	807	113	0
51	BZ	625	0	652	79	0
51	DZ	625	0	652	76	0
52	BW	596	0	610	125	0
52	DW	596	0	610	135	0
53	AA	60	0	0	0	0
53	BB	110	0	0	0	0
53	CA	58	0	0	0	0
53	CE	1	0	0	0	0
53	DB	110	0	0	0	0
53	DN	1	0	0	0	0
54	AA	23	0	24	2	0
54	CA	23	0	24	1	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	288	0	0	6	0
56	AE	3	0	0	1	0
56	AK	1	0	0	0	0
56	AL	4	0	0	0	0
56	AN	2	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	BB	494	0	0	4	0
56	BC	4	0	0	0	0
56	BE	3	0	0	0	0
56	BH	1	0	0	0	0
56	BL	4	0	0	0	0
56	BT	1	0	0	0	0
56	CA	275	0	0	4	0
56	CE	4	0	0	0	0
56	CK	1	0	0	0	0
56	CL	5	0	0	0	0
56	CN	5	0	0	0	0
56	CP	1	0	0	0	0
56	CT	2	0	0	0	0
56	DB	500	0	0	9	0
56	DC	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DD	1	0	0	0	0
56	DE	1	0	0	0	0
56	DJ	1	0	0	0	0
56	DL	3	0	0	0	0
56	DN	2	0	0	0	0
56	DP	1	0	0	0	0
56	DR	1	0	0	0	0
All	All	284033	0	190711	18514	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 39.

The worst 5 of 18514 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	1.36	1.21
23:BB:855:G:H21	52:BW:23:LYS:HG2	1.11	1.13
23:DB:322:A:H5'	23:DB:340:A:H1'	1.32	1.12
2:AC:70:ALA:HA	2:AC:105:VAL:HG21	1.26	1.11
23:BB:1205:A:H62	29:BE:165:HIS:HB2	1.11	1.10

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%)	112 (55%)	56 (28%)	36 (18%)	0	2
2	CC	204/232 (88%)	134 (66%)	48 (24%)	22 (11%)	0	6
3	AD	203/205 (99%)	133 (66%)	58 (29%)	12 (6%)	1	16
3	CD	203/205 (99%)	132 (65%)	58 (29%)	13 (6%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AE	148/166 (89%)	109 (74%)	30 (20%)	9 (6%)	1	16
4	CE	148/166 (89%)	108 (73%)	31 (21%)	9 (6%)	1	16
5	AF	98/135 (73%)	62 (63%)	27 (28%)	9 (9%)	0	10
5	CF	98/135 (73%)	64 (65%)	25 (26%)	9 (9%)	0	10
6	AG	148/178 (83%)	98 (66%)	44 (30%)	6 (4%)	2	21
6	CG	150/178 (84%)	101 (67%)	36 (24%)	13 (9%)	0	10
7	AH	127/129 (98%)	86 (68%)	35 (28%)	6 (5%)	2	19
7	CH	127/129 (98%)	85 (67%)	36 (28%)	6 (5%)	2	19
8	AI	125/129 (97%)	84 (67%)	25 (20%)	16 (13%)	0	4
8	CI	125/129 (97%)	89 (71%)	30 (24%)	6 (5%)	2	19
9	AJ	96/103 (93%)	61 (64%)	18 (19%)	17 (18%)	0	2
9	CJ	96/103 (93%)	62 (65%)	21 (22%)	13 (14%)	0	3
10	AK	115/128 (90%)	85 (74%)	26 (23%)	4 (4%)	3	23
10	CK	115/128 (90%)	84 (73%)	25 (22%)	6 (5%)	1	18
11	AL	121/123 (98%)	71 (59%)	34 (28%)	16 (13%)	0	3
11	CL	121/123 (98%)	72 (60%)	33 (27%)	16 (13%)	0	3
12	AM	112/117 (96%)	69 (62%)	36 (32%)	7 (6%)	1	15
12	CM	111/117 (95%)	77 (69%)	23 (21%)	11 (10%)	0	8
13	AP	80/82 (98%)	53 (66%)	18 (22%)	9 (11%)	0	5
13	CP	78/82 (95%)	53 (68%)	19 (24%)	6 (8%)	1	12
14	AQ	78/83 (94%)	61 (78%)	14 (18%)	3 (4%)	2	22
14	CQ	79/83 (95%)	62 (78%)	15 (19%)	2 (2%)	4	29
15	AR	53/74 (72%)	33 (62%)	17 (32%)	3 (6%)	1	17
15	CR	53/74 (72%)	33 (62%)	16 (30%)	4 (8%)	1	13
16	AS	77/91 (85%)	49 (64%)	21 (27%)	7 (9%)	0	10
16	CS	78/91 (86%)	51 (65%)	20 (26%)	7 (9%)	0	10
17	AT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	1	16
17	CT	83/86 (96%)	63 (76%)	14 (17%)	6 (7%)	1	14
18	AB	216/240 (90%)	140 (65%)	53 (24%)	23 (11%)	0	6
18	CB	216/240 (90%)	135 (62%)	59 (27%)	22 (10%)	0	8
19	AU	49/70 (70%)	29 (59%)	13 (26%)	7 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	CU	49/70 (70%)	29 (59%)	15 (31%)	5 (10%)	0	8
20	AO	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	11
20	CO	86/89 (97%)	50 (58%)	29 (34%)	7 (8%)	1	11
21	AN	92/100 (92%)	54 (59%)	29 (32%)	9 (10%)	0	8
21	CN	92/100 (92%)	45 (49%)	31 (34%)	16 (17%)	0	2
24	BI	139/141 (99%)	118 (85%)	16 (12%)	5 (4%)	2	23
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	2	23
25	BC	269/272 (99%)	149 (55%)	68 (25%)	52 (19%)	0	1
25	DC	269/272 (99%)	147 (55%)	70 (26%)	52 (19%)	0	1
26	BD	207/209 (99%)	113 (55%)	58 (28%)	36 (17%)	0	2
26	DD	207/209 (99%)	114 (55%)	58 (28%)	35 (17%)	0	2
27	BK	119/123 (97%)	73 (61%)	24 (20%)	22 (18%)	0	2
27	DK	119/123 (97%)	73 (61%)	25 (21%)	21 (18%)	0	2
28	BP	112/114 (98%)	67 (60%)	28 (25%)	17 (15%)	0	3
28	DP	112/114 (98%)	66 (59%)	31 (28%)	15 (13%)	0	3
29	BE	199/201 (99%)	120 (60%)	49 (25%)	30 (15%)	0	3
29	DE	199/201 (99%)	123 (62%)	47 (24%)	29 (15%)	0	3
30	BY	56/58 (97%)	36 (64%)	16 (29%)	4 (7%)	1	14
30	DY	56/58 (97%)	36 (64%)	14 (25%)	6 (11%)	0	6
31	B0	54/56 (96%)	34 (63%)	10 (18%)	10 (18%)	0	2
31	D0	54/56 (96%)	35 (65%)	9 (17%)	10 (18%)	0	2
32	B4	36/38 (95%)	19 (53%)	13 (36%)	4 (11%)	0	6
32	D4	36/38 (95%)	19 (53%)	13 (36%)	4 (11%)	0	6
33	B1	48/54 (89%)	36 (75%)	8 (17%)	4 (8%)	0	11
33	D1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	0	11
34	B3	62/64 (97%)	34 (55%)	20 (32%)	8 (13%)	0	4
34	D3	62/64 (97%)	35 (56%)	19 (31%)	8 (13%)	0	4
35	BV	92/94 (98%)	60 (65%)	25 (27%)	7 (8%)	1	13
35	DV	92/94 (98%)	61 (66%)	24 (26%)	7 (8%)	1	13
36	B2	44/46 (96%)	23 (52%)	16 (36%)	5 (11%)	0	5
36	D2	44/46 (96%)	23 (52%)	12 (27%)	9 (20%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BL	141/144 (98%)	76 (54%)	37 (26%)	28 (20%)	0	1
37	DL	141/144 (98%)	76 (54%)	39 (28%)	26 (18%)	0	2
38	BM	134/136 (98%)	79 (59%)	39 (29%)	16 (12%)	0	4
38	DM	134/136 (98%)	82 (61%)	35 (26%)	17 (13%)	0	4
39	BX	61/63 (97%)	35 (57%)	20 (33%)	6 (10%)	0	8
39	DX	61/63 (97%)	35 (57%)	20 (33%)	6 (10%)	0	8
40	BH	147/149 (99%)	78 (53%)	42 (29%)	27 (18%)	0	2
40	DH	147/149 (99%)	91 (62%)	30 (20%)	26 (18%)	0	2
41	BJ	140/142 (99%)	85 (61%)	37 (26%)	18 (13%)	0	4
41	DJ	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	3
42	BN	118/127 (93%)	73 (62%)	33 (28%)	12 (10%)	0	8
42	DN	118/127 (93%)	74 (63%)	33 (28%)	11 (9%)	0	10
43	BO	114/117 (97%)	68 (60%)	28 (25%)	18 (16%)	0	3
43	DO	114/117 (97%)	66 (58%)	30 (26%)	18 (16%)	0	3
44	BQ	115/117 (98%)	76 (66%)	29 (25%)	10 (9%)	0	10
44	DQ	115/117 (98%)	76 (66%)	30 (26%)	9 (8%)	1	12
45	BS	108/110 (98%)	59 (55%)	34 (32%)	15 (14%)	0	3
45	DS	108/110 (98%)	60 (56%)	33 (31%)	15 (14%)	0	3
46	BU	100/103 (97%)	58 (58%)	25 (25%)	17 (17%)	0	2
46	DU	100/103 (97%)	57 (57%)	24 (24%)	19 (19%)	0	2
47	BF	176/178 (99%)	91 (52%)	51 (29%)	34 (19%)	0	1
47	DF	176/178 (99%)	93 (53%)	49 (28%)	34 (19%)	0	1
48	BG	174/176 (99%)	100 (58%)	42 (24%)	32 (18%)	0	2
48	DG	174/176 (99%)	101 (58%)	42 (24%)	31 (18%)	0	2
49	BR	101/103 (98%)	57 (56%)	26 (26%)	18 (18%)	0	2
49	DR	101/103 (98%)	58 (57%)	26 (26%)	17 (17%)	0	3
50	BT	91/100 (91%)	40 (44%)	40 (44%)	11 (12%)	0	4
50	DT	91/100 (91%)	41 (45%)	39 (43%)	11 (12%)	0	4
51	BZ	75/78 (96%)	53 (71%)	16 (21%)	6 (8%)	1	12
51	DZ	75/78 (96%)	54 (72%)	14 (19%)	7 (9%)	0	10
52	BW	77/84 (92%)	29 (38%)	24 (31%)	24 (31%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	DW	77/84 (92%)	27 (35%)	26 (34%)	24 (31%)	0	0
All	All	11241/11914 (94%)	6932 (62%)	2908 (26%)	1401 (12%)	0	4

5 of 1401 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	19	SER
2	AC	26	LYS
2	AC	47	ALA
2	AC	54	ILE

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%)	129 (76%)	41 (24%)	1	5
2	CC	170/189 (90%)	135 (79%)	35 (21%)	1	8
3	AD	172/172 (100%)	142 (83%)	30 (17%)	2	12
3	CD	172/172 (100%)	143 (83%)	29 (17%)	2	13
4	AE	113/125 (90%)	90 (80%)	23 (20%)	1	8
4	CE	113/125 (90%)	93 (82%)	20 (18%)	2	12
5	AF	87/116 (75%)	74 (85%)	13 (15%)	3	16
5	CF	87/116 (75%)	76 (87%)	11 (13%)	4	20
6	AG	123/146 (84%)	100 (81%)	23 (19%)	1	10
6	CG	125/146 (86%)	95 (76%)	30 (24%)	1	5
7	AH	104/104 (100%)	92 (88%)	12 (12%)	5	22
7	CH	104/104 (100%)	91 (88%)	13 (12%)	4	20
8	AI	105/106 (99%)	85 (81%)	20 (19%)	1	10
8	CI	105/106 (99%)	79 (75%)	26 (25%)	1	4
9	AJ	86/90 (96%)	71 (83%)	15 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CJ	86/90 (96%)	68 (79%)	18 (21%)	1	7
10	AK	90/98 (92%)	77 (86%)	13 (14%)	3	17
10	CK	90/98 (92%)	77 (86%)	13 (14%)	3	17
11	AL	103/103 (100%)	88 (85%)	15 (15%)	3	16
11	CL	103/103 (100%)	88 (85%)	15 (15%)	3	16
12	AM	92/95 (97%)	75 (82%)	17 (18%)	1	11
12	CM	91/95 (96%)	74 (81%)	17 (19%)	1	10
13	AP	65/65 (100%)	62 (95%)	3 (5%)	24	48
13	CP	65/65 (100%)	61 (94%)	4 (6%)	16	42
14	AQ	74/77 (96%)	63 (85%)	11 (15%)	3	16
14	CQ	75/77 (97%)	63 (84%)	12 (16%)	2	14
15	AR	48/64 (75%)	40 (83%)	8 (17%)	2	13
15	CR	48/64 (75%)	39 (81%)	9 (19%)	1	10
16	AS	70/78 (90%)	51 (73%)	19 (27%)	0	3
16	CS	71/78 (91%)	50 (70%)	21 (30%)	0	2
17	AT	65/65 (100%)	54 (83%)	11 (17%)	2	13
17	CT	65/65 (100%)	54 (83%)	11 (17%)	2	13
18	AB	180/198 (91%)	140 (78%)	40 (22%)	1	6
18	CB	180/198 (91%)	135 (75%)	45 (25%)	0	4
19	AU	44/60 (73%)	33 (75%)	11 (25%)	0	4
19	CU	44/60 (73%)	33 (75%)	11 (25%)	0	4
20	AO	76/77 (99%)	66 (87%)	10 (13%)	4	19
20	CO	76/77 (99%)	63 (83%)	13 (17%)	2	13
21	AN	79/83 (95%)	63 (80%)	16 (20%)	1	8
21	CN	79/83 (95%)	63 (80%)	16 (20%)	1	8
24	BI	109/109 (100%)	109 (100%)	0	100	100
24	DI	109/109 (100%)	106 (97%)	3 (3%)	38	60
25	BC	216/217 (100%)	180 (83%)	36 (17%)	2	13
25	DC	216/217 (100%)	182 (84%)	34 (16%)	2	15
26	BD	164/164 (100%)	128 (78%)	36 (22%)	1	6
26	DD	164/164 (100%)	124 (76%)	40 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BK	102/104 (98%)	77 (76%)	25 (24%)	1	4
27	DK	102/104 (98%)	77 (76%)	25 (24%)	1	4
28	BP	99/99 (100%)	77 (78%)	22 (22%)	1	6
28	DP	99/99 (100%)	77 (78%)	22 (22%)	1	6
29	BE	165/165 (100%)	145 (88%)	20 (12%)	5	21
29	DE	165/165 (100%)	145 (88%)	20 (12%)	5	21
30	BY	48/48 (100%)	40 (83%)	8 (17%)	2	13
30	DY	48/48 (100%)	40 (83%)	8 (17%)	2	13
31	B0	47/47 (100%)	35 (74%)	12 (26%)	0	4
31	D0	47/47 (100%)	38 (81%)	9 (19%)	1	10
32	B4	34/34 (100%)	30 (88%)	4 (12%)	5	21
32	D4	34/34 (100%)	31 (91%)	3 (9%)	9	33
33	B1	45/48 (94%)	39 (87%)	6 (13%)	4	18
33	D1	45/48 (94%)	39 (87%)	6 (13%)	4	18
34	B3	51/51 (100%)	43 (84%)	8 (16%)	2	15
34	D3	51/51 (100%)	43 (84%)	8 (16%)	2	15
35	BV	78/78 (100%)	63 (81%)	15 (19%)	1	10
35	DV	78/78 (100%)	63 (81%)	15 (19%)	1	10
36	B2	38/38 (100%)	32 (84%)	6 (16%)	2	15
36	D2	38/38 (100%)	34 (90%)	4 (10%)	6	24
37	BL	102/103 (99%)	91 (89%)	11 (11%)	6	24
37	DL	102/103 (99%)	90 (88%)	12 (12%)	5	21
38	BM	109/109 (100%)	86 (79%)	23 (21%)	1	7
38	DM	109/109 (100%)	88 (81%)	21 (19%)	1	9
39	BX	55/55 (100%)	44 (80%)	11 (20%)	1	9
39	DX	55/55 (100%)	44 (80%)	11 (20%)	1	9
40	BH	114/114 (100%)	79 (69%)	35 (31%)	0	2
40	DH	114/114 (100%)	86 (75%)	28 (25%)	1	4
41	BJ	116/116 (100%)	96 (83%)	20 (17%)	2	13
41	DJ	116/116 (100%)	97 (84%)	19 (16%)	2	13
42	BN	100/103 (97%)	88 (88%)	12 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	DN	100/103 (97%)	88 (88%)	12 (12%)	5	21
43	BO	86/87 (99%)	74 (86%)	12 (14%)	3	17
43	DO	86/87 (99%)	74 (86%)	12 (14%)	3	17
44	BQ	89/89 (100%)	75 (84%)	14 (16%)	2	15
44	DQ	89/89 (100%)	75 (84%)	14 (16%)	2	15
45	BS	93/93 (100%)	77 (83%)	16 (17%)	2	13
45	DS	93/93 (100%)	77 (83%)	16 (17%)	2	13
46	BU	83/84 (99%)	67 (81%)	16 (19%)	1	9
46	DU	83/84 (99%)	67 (81%)	16 (19%)	1	9
47	BF	149/149 (100%)	114 (76%)	35 (24%)	1	5
47	DF	149/149 (100%)	114 (76%)	35 (24%)	1	5
48	BG	137/137 (100%)	116 (85%)	21 (15%)	3	15
48	DG	137/137 (100%)	117 (85%)	20 (15%)	3	16
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%)	60 (75%)	20 (25%)	0	4
50	DT	80/84 (95%)	61 (76%)	19 (24%)	1	5
51	BZ	67/68 (98%)	52 (78%)	15 (22%)	1	6
51	DZ	67/68 (98%)	52 (78%)	15 (22%)	1	6
52	BW	59/62 (95%)	46 (78%)	13 (22%)	1	6
52	DW	59/62 (95%)	46 (78%)	13 (22%)	1	6
All	All	9333/9700 (96%)	7655 (82%)	1678 (18%)	2	12

5 of 1678 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	CL	43	LYS
16	CS	65	MET
48	DG	17	LYS
15	CR	20	ILE
11	CL	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 338 such sidechains are listed below:

Mol	Chain	Res	Type
12	CM	13	HIS
38	DM	88	ASN
18	CB	108	GLN
27	DK	88	ASN
40	DH	119	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	295 (19%)	25 (1%)
1	CA	1529/1542 (99%)	282 (18%)	21 (1%)
22	BA	116/120 (96%)	21 (18%)	1 (0%)
22	DA	116/120 (96%)	19 (16%)	1 (0%)
23	BB	2837/2904 (97%)	456 (16%)	18 (0%)
23	DB	2837/2904 (97%)	469 (16%)	20 (0%)
All	All	8964/9132 (98%)	1542 (17%)	86 (0%)

5 of 1542 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G

5 of 86 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1049	U
23	DB	1210	G
1	CA	1067	A
22	DA	25	U
23	DB	1847	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 344 ligands modelled in this entry, 342 are monoatomic - leaving 2 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
54	SCM	AA	1661	-	23,25,25	1.71	8 (34%)	27,39,39	1.57	4 (14%)
54	SCM	CA	1659	-	23,25,25	1.66	6 (26%)	27,39,39	1.59	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
54	SCM	AA	1661	-	-	2/4/57/57	0/3/3/3
54	SCM	CA	1659	-	-	2/4/57/57	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	AA	1661	SCM	C3-C2	3.25	1.58	1.51
54	CA	1659	SCM	C9-C8	3.22	1.59	1.53
54	CA	1659	SCM	C3-C2	3.03	1.57	1.51
54	AA	1661	SCM	C9-C8	3.02	1.58	1.53
54	AA	1661	SCM	C3-C4	2.64	1.54	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AA	1661	SCM	C1M-N10-C10	-5.38	107.28	114.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CA	1659	SCM	C1M-N10-C10	-5.01	107.76	114.23
54	CA	1659	SCM	O1-C2-C3	3.76	113.86	108.62
54	AA	1661	SCM	O1-C2-C3	3.67	113.73	108.62
54	CA	1659	SCM	C2M-C2-C3	-2.87	108.11	113.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	AA	1661	SCM	C9-C10-N10-C1M
54	AA	1661	SCM	C11-C10-N10-C1M
54	CA	1659	SCM	C11-C10-N10-C1M
54	CA	1659	SCM	C9-C10-N10-C1M

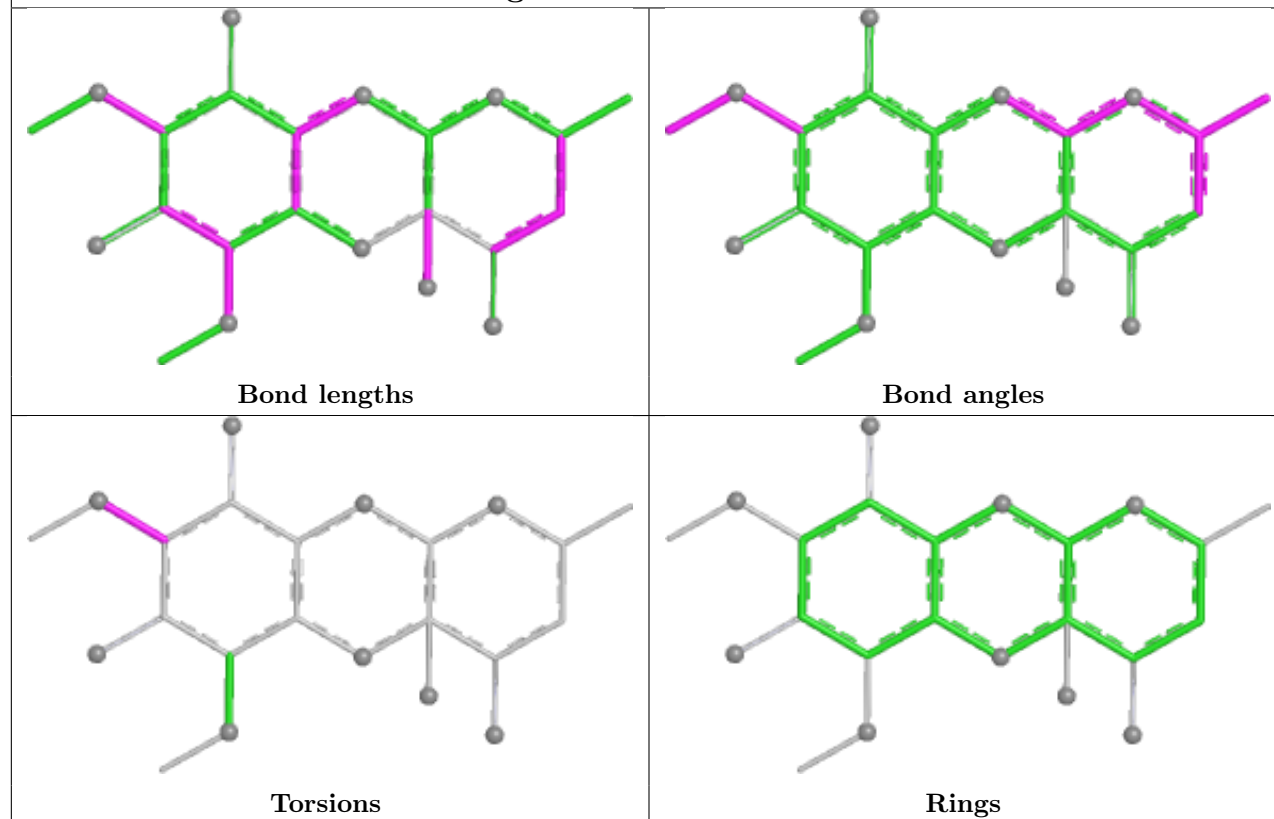
There are no ring outliers.

2 monomers are involved in 3 short contacts:

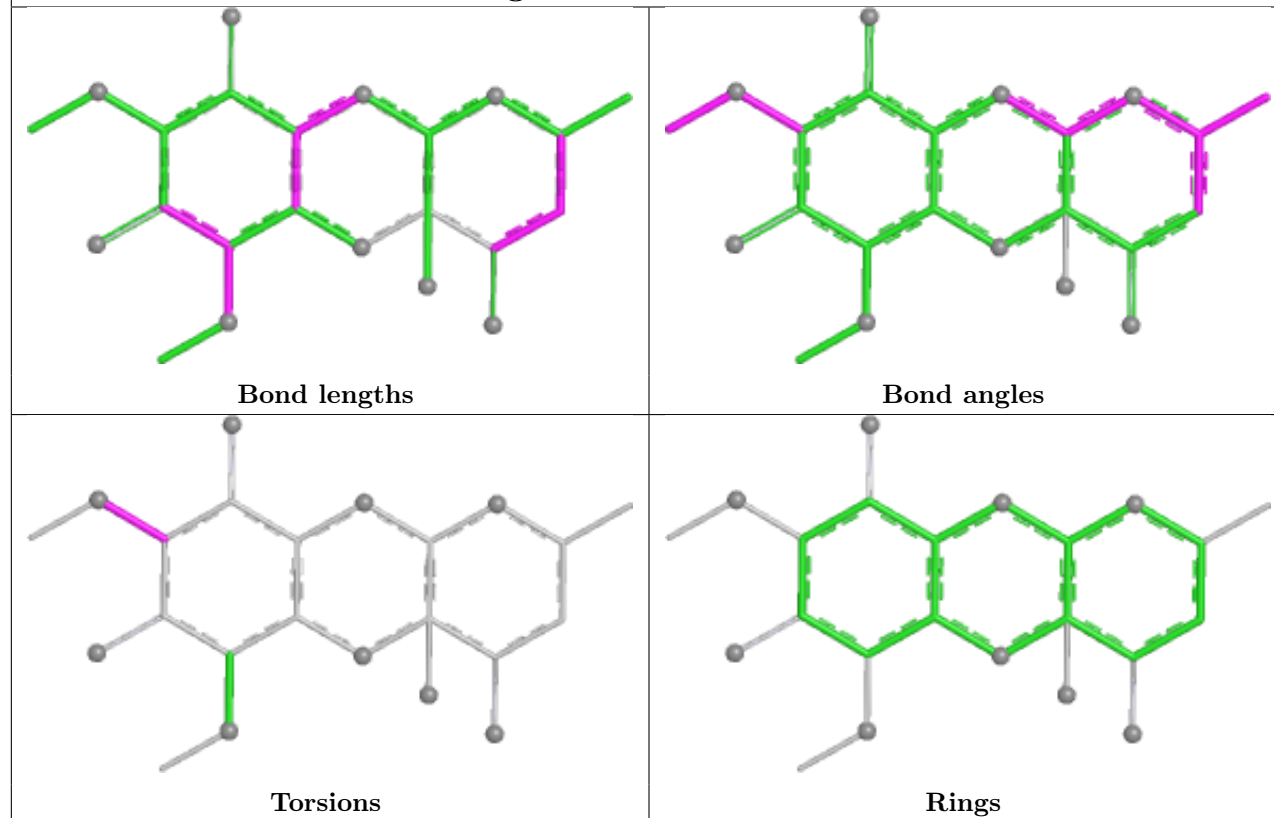
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	AA	1661	SCM	2	0
54	CA	1659	SCM	1	0

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 SCM AA 1661



Ligand SCM CA 1659



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	-0.47	17 (1%) 78 58	12, 77, 142, 179	0
1	CA	1530/1542 (99%)	-0.51	27 (1%) 67 48	5, 57, 124, 180	0
2	AC	206/232 (88%)	-0.09	5 (2%) 59 43	5, 70, 115, 162	0
2	CC	206/232 (88%)	-0.32	4 (1%) 66 47	5, 71, 111, 150	0
3	AD	205/205 (100%)	0.03	4 (1%) 65 46	5, 79, 127, 173	0
3	CD	205/205 (100%)	-0.04	10 (4%) 35 27	5, 66, 125, 166	0
4	AE	150/166 (90%)	0.08	3 (2%) 65 46	5, 68, 122, 157	0
4	CE	150/166 (90%)	-0.03	4 (2%) 56 39	5, 67, 121, 180	0
5	AF	100/135 (74%)	-0.25	0 100 100	10, 81, 133, 147	0
5	CF	100/135 (74%)	-0.15	2 (2%) 65 46	5, 73, 131, 172	0
6	AG	150/178 (84%)	-0.21	4 (2%) 56 39	16, 89, 125, 143	0
6	CG	152/178 (85%)	-0.42	0 100 100	6, 79, 125, 172	0
7	AH	129/129 (100%)	0.02	9 (6%) 22 20	19, 77, 130, 158	0
7	CH	129/129 (100%)	0.04	5 (3%) 43 31	5, 62, 116, 158	0
8	AI	127/129 (98%)	-0.02	6 (4%) 36 28	6, 83, 117, 155	0
8	CI	127/129 (98%)	0.03	8 (6%) 26 22	5, 80, 122, 157	0
9	AJ	98/103 (95%)	0.10	8 (8%) 17 18	9, 79, 126, 147	0
9	CJ	98/103 (95%)	0.08	1 (1%) 79 59	16, 82, 113, 137	0
10	AK	117/128 (91%)	-0.25	3 (2%) 57 40	5, 72, 117, 155	0
10	CK	117/128 (91%)	-0.31	1 (0%) 81 62	5, 67, 123, 136	0
11	AL	123/123 (100%)	0.05	9 (7%) 21 19	6, 79, 123, 158	0
11	CL	123/123 (100%)	0.30	9 (7%) 21 19	5, 54, 103, 151	0
12	AM	114/117 (97%)	-0.19	1 (0%) 81 62	23, 96, 137, 169	0
12	CM	113/117 (96%)	-0.19	1 (0%) 81 62	22, 96, 142, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	82/82 (100%)	0.40	3 (3%) 45 32	15, 82, 130, 163	0
13	CP	80/82 (97%)	0.54	9 (11%) 10 13	5, 58, 126, 180	0
14	AQ	80/83 (96%)	-0.26	0 100 100	15, 92, 145, 154	0
14	CQ	81/83 (97%)	-0.27	2 (2%) 58 41	5, 72, 119, 149	0
15	AR	55/74 (74%)	-0.19	1 (1%) 67 48	5, 73, 129, 164	0
15	CR	55/74 (74%)	-0.25	2 (3%) 46 33	5, 66, 127, 143	0
16	AS	79/91 (86%)	-0.17	3 (3%) 44 32	52, 98, 142, 167	0
16	CS	80/91 (87%)	-0.18	1 (1%) 75 55	41, 95, 133, 159	0
17	AT	85/86 (98%)	-0.07	2 (2%) 59 43	19, 88, 126, 156	0
17	CT	85/86 (98%)	0.04	5 (5%) 28 24	5, 66, 113, 154	0
18	AB	218/240 (90%)	-0.34	5 (2%) 61 43	12, 81, 120, 160	0
18	CB	218/240 (90%)	-0.31	2 (0%) 81 62	5, 87, 133, 163	0
19	AU	51/70 (72%)	0.65	5 (9%) 13 15	20, 94, 139, 153	0
19	CU	51/70 (72%)	0.36	5 (9%) 13 15	57, 96, 137, 171	0
20	AO	88/89 (98%)	-0.24	3 (3%) 48 34	5, 73, 118, 177	0
20	CO	88/89 (98%)	0.01	7 (7%) 18 18	5, 56, 108, 135	0
21	AN	96/100 (96%)	0.17	3 (3%) 51 36	5, 84, 128, 155	0
21	CN	96/100 (96%)	0.22	5 (5%) 33 26	5, 75, 129, 145	0
22	BA	117/120 (97%)	-0.35	4 (3%) 48 34	35, 77, 125, 167	0
22	DA	117/120 (97%)	-0.03	6 (5%) 33 26	31, 87, 133, 176	0
23	BB	2841/2904 (97%)	-0.49	36 (1%) 75 55	5, 60, 136, 180	0
23	DB	2841/2904 (97%)	-0.49	43 (1%) 72 51	5, 51, 136, 180	0
24	BI	141/141 (100%)	0.13	2 (1%) 73 53	60, 135, 178, 180	0
24	DI	141/141 (100%)	-0.01	1 (0%) 84 68	66, 135, 180, 180	0
25	BC	271/272 (99%)	0.17	9 (3%) 49 35	5, 61, 109, 132	0
25	DC	271/272 (99%)	0.30	25 (9%) 14 16	5, 45, 99, 144	0
26	BD	209/209 (100%)	0.17	14 (6%) 24 21	5, 71, 118, 148	0
26	DD	209/209 (100%)	0.34	20 (9%) 13 15	5, 60, 110, 168	0
27	BK	121/123 (98%)	0.11	4 (3%) 49 35	5, 75, 125, 159	0
27	DK	121/123 (98%)	0.07	3 (2%) 58 41	5, 45, 112, 150	0
28	BP	114/114 (100%)	0.32	7 (6%) 27 23	7, 82, 125, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.14	6 (5%)	32	26	5, 64, 118, 139	0
29	BE	201/201 (100%)	-0.09	4 (1%)	65	46	5, 65, 128, 164	0
29	DE	201/201 (100%)	-0.10	9 (4%)	38	29	5, 73, 123, 160	0
30	BY	58/58 (100%)	-0.13	2 (3%)	48	34	5, 75, 129, 160	0
30	DY	58/58 (100%)	-0.05	2 (3%)	48	34	5, 72, 116, 147	0
31	B0	56/56 (100%)	0.04	2 (3%)	46	33	5, 78, 118, 147	0
31	D0	56/56 (100%)	0.16	1 (1%)	67	48	5, 62, 129, 153	0
32	B4	38/38 (100%)	0.44	3 (7%)	18	18	27, 81, 131, 145	0
32	D4	38/38 (100%)	0.21	0	100	100	5, 67, 106, 117	0
33	B1	50/54 (92%)	-0.20	1 (2%)	65	46	17, 70, 120, 134	0
33	D1	50/54 (92%)	-0.42	0	100	100	17, 73, 116, 137	0
34	B3	64/64 (100%)	1.01	13 (20%)	3	5	5, 68, 103, 129	0
34	D3	64/64 (100%)	0.86	7 (10%)	10	13	5, 55, 86, 122	0
35	BV	94/94 (100%)	-0.43	1 (1%)	78	58	5, 81, 126, 152	0
35	DV	94/94 (100%)	-0.25	1 (1%)	78	58	5, 88, 120, 160	0
36	B2	46/46 (100%)	0.71	5 (10%)	10	13	5, 53, 104, 141	0
36	D2	46/46 (100%)	0.61	6 (13%)	7	10	9, 48, 110, 141	0
37	BL	143/144 (99%)	0.12	4 (2%)	55	39	5, 67, 121, 145	0
37	DL	143/144 (99%)	0.22	10 (6%)	22	20	5, 63, 111, 145	0
38	BM	136/136 (100%)	0.02	5 (3%)	45	32	7, 68, 121, 179	0
38	DM	136/136 (100%)	0.36	12 (8%)	15	16	5, 65, 117, 144	0
39	BX	63/63 (100%)	-0.09	3 (4%)	35	28	16, 79, 128, 159	0
39	DX	63/63 (100%)	-0.39	0	100	100	16, 91, 144, 169	0
40	BH	149/149 (100%)	0.19	4 (2%)	56	39	7, 104, 149, 180	0
40	DH	149/149 (100%)	-0.05	4 (2%)	56	39	5, 91, 131, 162	0
41	BJ	142/142 (100%)	0.46	20 (14%)	6	9	5, 77, 118, 140	0
41	DJ	142/142 (100%)	0.23	12 (8%)	16	17	5, 70, 119, 173	0
42	BN	120/127 (94%)	-0.01	6 (5%)	34	26	5, 69, 111, 154	0
42	DN	120/127 (94%)	0.29	8 (6%)	24	21	5, 51, 94, 163	0
43	BO	116/117 (99%)	0.09	3 (2%)	57	40	6, 80, 109, 172	0
43	DO	116/117 (99%)	0.06	5 (4%)	40	30	5, 83, 136, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	-0.11	3 (2%) 57 40	5, 62, 115, 144	0
44	DQ	117/117 (100%)	0.22	11 (9%) 14 16	5, 60, 111, 154	0
45	BS	110/110 (100%)	0.26	8 (7%) 21 19	5, 62, 121, 148	0
45	DS	110/110 (100%)	0.31	8 (7%) 21 19	5, 64, 127, 156	0
46	BU	102/103 (99%)	-0.29	0 100 100	12, 80, 125, 157	0
46	DU	102/103 (99%)	-0.09	5 (4%) 35 27	8, 94, 127, 149	0
47	BF	178/178 (100%)	-0.14	2 (1%) 78 58	29, 100, 146, 180	0
47	DF	178/178 (100%)	0.13	14 (7%) 18 18	12, 93, 142, 163	0
48	BG	176/176 (100%)	-0.18	7 (3%) 42 31	18, 94, 133, 171	0
48	DG	176/176 (100%)	0.00	9 (5%) 33 26	8, 90, 136, 166	0
49	BR	103/103 (100%)	-0.06	4 (3%) 43 31	5, 83, 123, 133	0
49	DR	103/103 (100%)	0.11	5 (4%) 35 27	10, 76, 135, 149	0
50	BT	93/100 (93%)	0.13	3 (3%) 50 36	8, 83, 130, 165	0
50	DT	93/100 (93%)	0.58	11 (11%) 9 12	5, 84, 144, 172	0
51	BZ	77/78 (98%)	0.38	6 (7%) 19 18	5, 63, 120, 142	0
51	DZ	77/78 (98%)	0.42	7 (9%) 15 16	5, 56, 106, 120	0
52	BW	79/84 (94%)	0.46	4 (5%) 33 26	5, 75, 124, 180	0
52	DW	79/84 (94%)	1.06	15 (18%) 3 6	5, 71, 121, 166	0
All	All	20417/21046 (97%)	-0.19	659 (3%) 50 36	5, 70, 134, 180	0

The worst 5 of 659 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	DA	88	C	23.0
8	CI	129	ARG	13.3
52	DW	18	LYS	9.0
22	BA	88	C	8.8
23	BB	140	C	8.7

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($\text{\AA}^2$)	Q<0.9
53	MG	AA	1623	1/1	-0.58	0.41	33,33,33,33	1
53	MG	CA	1616	1/1	-0.02	0.23	58,58,58,58	1
53	MG	AA	1625	1/1	0.53	0.16	79,79,79,79	1
53	MG	AA	1622	1/1	0.56	0.16	130,130,130,130	0
53	MG	AA	1626	1/1	0.60	0.22	36,36,36,36	1
53	MG	CA	1649	1/1	0.73	0.18	123,123,123,123	0
53	MG	CA	1637	1/1	0.76	0.16	98,98,98,98	0
53	MG	AA	1659	1/1	0.76	0.27	108,108,108,108	0
53	MG	AA	1608	1/1	0.78	0.08	123,123,123,123	0
53	MG	AA	1624	1/1	0.79	0.24	83,83,83,83	0
53	MG	CA	1613	1/1	0.82	0.15	126,126,126,126	0
53	MG	AA	1614	1/1	0.82	0.07	119,119,119,119	0
53	MG	BB	3097	1/1	0.83	0.06	113,113,113,113	0
53	MG	BB	3051	1/1	0.84	0.09	107,107,107,107	0
53	MG	AA	1647	1/1	0.88	0.19	113,113,113,113	0
53	MG	CA	1646	1/1	0.90	0.04	139,139,139,139	0
53	MG	CA	1650	1/1	0.90	0.07	105,105,105,105	0
53	MG	DB	3029	1/1	0.90	0.07	87,87,87,87	0
53	MG	DB	3094	1/1	0.90	0.06	100,100,100,100	0
53	MG	AA	1652	1/1	0.91	0.08	84,84,84,84	0
53	MG	DB	3051	1/1	0.91	0.08	75,75,75,75	0
53	MG	DB	3058	1/1	0.91	0.05	139,139,139,139	0
53	MG	DB	3065	1/1	0.91	0.05	128,128,128,128	0
53	MG	CA	1606	1/1	0.91	0.08	106,106,106,106	0
53	MG	DB	3052	1/1	0.92	0.12	105,105,105,105	0
53	MG	BB	3093	1/1	0.92	0.05	108,108,108,108	0
53	MG	DB	3063	1/1	0.92	0.08	72,72,72,72	0
53	MG	DB	3034	1/1	0.92	0.14	57,57,57,57	0
53	MG	CA	1618	1/1	0.92	0.09	73,73,73,73	0
53	MG	DN	201	1/1	0.92	0.21	145,145,145,145	0
53	MG	BB	3049	1/1	0.93	0.06	67,67,67,67	0
53	MG	CA	1648	1/1	0.93	0.04	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3110	1/1	0.93	0.15	84,84,84,84	0
53	MG	CA	1651	1/1	0.93	0.06	101,101,101,101	0
54	SCM	CA	1659	23/23	0.93	0.10	18,18,18,18	0
53	MG	AA	1615	1/1	0.94	0.13	96,96,96,96	0
53	MG	DB	3091	1/1	0.94	0.06	90,90,90,90	0
53	MG	AA	1602	1/1	0.94	0.06	85,85,85,85	0
53	MG	AA	1637	1/1	0.94	0.11	99,99,99,99	0
53	MG	BB	3100	1/1	0.94	0.11	116,116,116,116	0
53	MG	AA	1646	1/1	0.94	0.05	84,84,84,84	0
53	MG	BB	3090	1/1	0.95	0.10	88,88,88,88	0
53	MG	DB	3066	1/1	0.95	0.12	65,65,65,65	0
53	MG	DB	3045	1/1	0.95	0.07	110,110,110,110	0
53	MG	BB	3034	1/1	0.95	0.07	86,86,86,86	0
53	MG	BB	3042	1/1	0.95	0.08	92,92,92,92	0
53	MG	BB	3004	1/1	0.95	0.05	80,80,80,80	0
53	MG	BB	3033	1/1	0.95	0.16	102,102,102,102	0
53	MG	AA	1649	1/1	0.96	0.06	89,89,89,89	0
53	MG	AA	1619	1/1	0.96	0.04	111,111,111,111	0
53	MG	AA	1655	1/1	0.96	0.10	88,88,88,88	0
53	MG	BB	3046	1/1	0.96	0.04	89,89,89,89	0
53	MG	DB	3013	1/1	0.96	0.06	52,52,52,52	0
53	MG	DB	3028	1/1	0.96	0.13	70,70,70,70	0
53	MG	AA	1657	1/1	0.96	0.16	91,91,91,91	0
53	MG	AA	1617	1/1	0.96	0.04	112,112,112,112	0
53	MG	AA	1630	1/1	0.96	0.07	88,88,88,88	0
54	SCM	AA	1661	23/23	0.96	0.06	13,13,13,13	0
53	MG	BB	3009	1/1	0.96	0.05	98,98,98,98	0
55	ZN	B4	101	1/1	0.96	0.04	67,67,67,67	0
53	MG	BB	3043	1/1	0.97	0.06	107,107,107,107	0
53	MG	DB	3031	1/1	0.97	0.05	46,46,46,46	0
53	MG	DB	3032	1/1	0.97	0.04	73,73,73,73	0
53	MG	AA	1632	1/1	0.97	0.16	96,96,96,96	0
53	MG	DB	3035	1/1	0.97	0.04	79,79,79,79	0
53	MG	AA	1635	1/1	0.97	0.13	80,80,80,80	0
53	MG	CA	1621	1/1	0.97	0.11	80,80,80,80	0
53	MG	CA	1632	1/1	0.97	0.06	76,76,76,76	0
53	MG	AA	1628	1/1	0.97	0.07	70,70,70,70	0
53	MG	CA	1640	1/1	0.97	0.05	62,62,62,62	0
53	MG	CA	1644	1/1	0.97	0.06	57,57,57,57	0
53	MG	BB	3064	1/1	0.97	0.05	78,78,78,78	0
53	MG	DB	3088	1/1	0.97	0.10	87,87,87,87	0
53	MG	BB	3070	1/1	0.97	0.05	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BB	3010	1/1	0.97	0.06	53,53,53,53	0
53	MG	BB	3026	1/1	0.97	0.07	65,65,65,65	0
53	MG	AA	1645	1/1	0.97	0.06	70,70,70,70	0
53	MG	CA	1652	1/1	0.97	0.04	49,49,49,49	0
53	MG	AA	1656	1/1	0.97	0.05	87,87,87,87	0
53	MG	AA	1627	1/1	0.97	0.04	63,63,63,63	0
53	MG	BB	3081	1/1	0.98	0.06	30,30,30,30	0
53	MG	BB	3089	1/1	0.98	0.03	72,72,72,72	0
53	MG	BB	3037	1/1	0.98	0.04	45,45,45,45	0
53	MG	BB	3092	1/1	0.98	0.04	46,46,46,46	0
53	MG	BB	3038	1/1	0.98	0.04	92,92,92,92	0
53	MG	CA	1654	1/1	0.98	0.15	105,105,105,105	0
53	MG	CE	201	1/1	0.98	0.03	109,109,109,109	0
53	MG	AA	1621	1/1	0.98	0.12	36,36,36,36	0
53	MG	BB	3099	1/1	0.98	0.04	41,41,41,41	0
53	MG	AA	1650	1/1	0.98	0.04	94,94,94,94	0
53	MG	DB	3030	1/1	0.98	0.13	47,47,47,47	0
53	MG	BB	3102	1/1	0.98	0.04	43,43,43,43	0
53	MG	BB	3012	1/1	0.98	0.03	67,67,67,67	0
53	MG	CA	1608	1/1	0.98	0.04	76,76,76,76	0
53	MG	CA	1609	1/1	0.98	0.03	85,85,85,85	0
53	MG	DB	3036	1/1	0.98	0.04	87,87,87,87	0
53	MG	CA	1612	1/1	0.98	0.16	93,93,93,93	0
53	MG	DB	3050	1/1	0.98	0.10	80,80,80,80	0
53	MG	BB	3047	1/1	0.98	0.03	104,104,104,104	0
53	MG	CA	1614	1/1	0.98	0.04	83,83,83,83	0
53	MG	BB	3014	1/1	0.98	0.10	37,37,37,37	0
53	MG	DB	3059	1/1	0.98	0.08	99,99,99,99	0
53	MG	DB	3060	1/1	0.98	0.10	83,83,83,83	0
53	MG	DB	3061	1/1	0.98	0.03	66,66,66,66	0
53	MG	DB	3062	1/1	0.98	0.04	58,58,58,58	0
53	MG	CA	1617	1/1	0.98	0.05	88,88,88,88	0
53	MG	DB	3064	1/1	0.98	0.12	49,49,49,49	0
53	MG	AA	1658	1/1	0.98	0.04	120,120,120,120	0
53	MG	AA	1620	1/1	0.98	0.04	60,60,60,60	0
53	MG	CA	1628	1/1	0.98	0.13	52,52,52,52	0
53	MG	CA	1629	1/1	0.98	0.07	67,67,67,67	0
53	MG	BB	3068	1/1	0.98	0.14	13,13,13,13	0
53	MG	DB	3095	1/1	0.98	0.07	92,92,92,92	0
53	MG	DB	3099	1/1	0.98	0.09	58,58,58,58	0
53	MG	DB	3103	1/1	0.98	0.07	36,36,36,36	0
53	MG	DB	3104	1/1	0.98	0.09	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3108	1/1	0.98	0.04	43,43,43,43	0
53	MG	AA	1642	1/1	0.98	0.09	49,49,49,49	0
53	MG	CA	1638	1/1	0.98	0.03	86,86,86,86	0
53	MG	BB	3071	1/1	0.98	0.06	68,68,68,68	0
53	MG	BB	3072	1/1	0.98	0.03	35,35,35,35	0
53	MG	BB	3077	1/1	0.98	0.04	53,53,53,53	0
55	ZN	D4	101	1/1	0.98	0.04	62,62,62,62	0
53	MG	CA	1634	1/1	0.99	0.03	74,74,74,74	0
53	MG	BB	3057	1/1	0.99	0.02	53,53,53,53	0
53	MG	BB	3063	1/1	0.99	0.03	33,33,33,33	0
53	MG	BB	3007	1/1	0.99	0.09	68,68,68,68	0
53	MG	CA	1641	1/1	0.99	0.03	42,42,42,42	0
53	MG	CA	1642	1/1	0.99	0.02	79,79,79,79	0
53	MG	BB	3067	1/1	0.99	0.03	63,63,63,63	0
53	MG	CA	1645	1/1	0.99	0.02	55,55,55,55	0
53	MG	BB	3008	1/1	0.99	0.04	82,82,82,82	0
53	MG	AA	1633	1/1	0.99	0.03	65,65,65,65	0
53	MG	AA	1634	1/1	0.99	0.03	72,72,72,72	0
53	MG	AA	1605	1/1	0.99	0.04	50,50,50,50	0
53	MG	BB	3075	1/1	0.99	0.04	40,40,40,40	0
53	MG	AA	1651	1/1	0.99	0.10	35,35,35,35	0
53	MG	CA	1653	1/1	0.99	0.03	48,48,48,48	0
53	MG	BB	3078	1/1	0.99	0.17	27,27,27,27	0
53	MG	BB	3080	1/1	0.99	0.04	53,53,53,53	0
53	MG	DB	3006	1/1	0.99	0.03	10,10,10,10	0
53	MG	DB	3007	1/1	0.99	0.06	62,62,62,62	0
53	MG	DB	3008	1/1	0.99	0.07	13,13,13,13	0
53	MG	DB	3010	1/1	0.99	0.03	5,5,5,5	0
53	MG	BB	3015	1/1	0.99	0.03	25,25,25,25	0
53	MG	DB	3015	1/1	0.99	0.04	42,42,42,42	0
53	MG	DB	3025	1/1	0.99	0.10	44,44,44,44	0
53	MG	DB	3026	1/1	0.99	0.06	45,45,45,45	0
53	MG	BB	3082	1/1	0.99	0.04	18,18,18,18	0
53	MG	BB	3084	1/1	0.99	0.03	32,32,32,32	0
53	MG	BB	3086	1/1	0.99	0.05	5,5,5,5	0
53	MG	BB	3087	1/1	0.99	0.09	80,80,80,80	0
53	MG	BB	3017	1/1	0.99	0.04	50,50,50,50	0
53	MG	BB	3022	1/1	0.99	0.04	32,32,32,32	0
53	MG	BB	3091	1/1	0.99	0.10	5,5,5,5	0
53	MG	BB	3024	1/1	0.99	0.03	55,55,55,55	0
53	MG	DB	3039	1/1	0.99	0.02	62,62,62,62	0
53	MG	AA	1606	1/1	0.99	0.05	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3046	1/1	0.99	0.04	23,23,23,23	0
53	MG	DB	3047	1/1	0.99	0.08	43,43,43,43	0
53	MG	DB	3048	1/1	0.99	0.04	38,38,38,38	0
53	MG	BB	3095	1/1	0.99	0.02	62,62,62,62	0
53	MG	BB	3096	1/1	0.99	0.03	58,58,58,58	0
53	MG	BB	3027	1/1	0.99	0.03	50,50,50,50	0
53	MG	DB	3053	1/1	0.99	0.03	65,65,65,65	0
53	MG	BB	3031	1/1	0.99	0.04	60,60,60,60	0
53	MG	AA	1654	1/1	0.99	0.03	67,67,67,67	0
53	MG	AA	1638	1/1	0.99	0.05	51,51,51,51	0
53	MG	BB	3106	1/1	0.99	0.11	10,10,10,10	0
53	MG	BB	3107	1/1	0.99	0.03	46,46,46,46	0
53	MG	BB	3110	1/1	0.99	0.07	80,80,80,80	0
53	MG	CA	1604	1/1	0.99	0.12	20,20,20,20	0
53	MG	AA	1639	1/1	0.99	0.04	93,93,93,93	0
53	MG	AA	1601	1/1	0.99	0.09	36,36,36,36	0
53	MG	DB	3069	1/1	0.99	0.04	64,64,64,64	0
53	MG	DB	3071	1/1	0.99	0.04	57,57,57,57	0
53	MG	DB	3073	1/1	0.99	0.04	50,50,50,50	0
53	MG	DB	3075	1/1	0.99	0.03	44,44,44,44	0
53	MG	DB	3077	1/1	0.99	0.03	45,45,45,45	0
53	MG	DB	3081	1/1	0.99	0.08	41,41,41,41	0
53	MG	DB	3082	1/1	0.99	0.13	83,83,83,83	0
53	MG	DB	3083	1/1	0.99	0.03	27,27,27,27	0
53	MG	AA	1644	1/1	0.99	0.02	75,75,75,75	0
53	MG	DB	3089	1/1	0.99	0.03	79,79,79,79	0
53	MG	DB	3090	1/1	0.99	0.05	14,14,14,14	0
53	MG	AA	1610	1/1	0.99	0.02	78,78,78,78	0
53	MG	DB	3093	1/1	0.99	0.04	59,59,59,59	0
53	MG	BB	3044	1/1	0.99	0.05	45,45,45,45	0
53	MG	BB	3001	1/1	0.99	0.04	5,5,5,5	0
53	MG	DB	3096	1/1	0.99	0.04	26,26,26,26	0
53	MG	DB	3097	1/1	0.99	0.09	41,41,41,41	0
53	MG	BB	3003	1/1	0.99	0.03	53,53,53,53	0
53	MG	DB	3100	1/1	0.99	0.07	19,19,19,19	0
53	MG	AA	1613	1/1	0.99	0.03	58,58,58,58	0
53	MG	BB	3050	1/1	0.99	0.03	53,53,53,53	0
53	MG	DB	3105	1/1	0.99	0.06	40,40,40,40	0
53	MG	BB	3006	1/1	0.99	0.06	61,61,61,61	0
53	MG	CA	1625	1/1	0.99	0.02	70,70,70,70	0
53	MG	CA	1627	1/1	0.99	0.04	27,27,27,27	0
53	MG	BB	3052	1/1	0.99	0.03	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	BB	3053	1/1	0.99	0.06	60,60,60,60	0
53	MG	CA	1631	1/1	0.99	0.05	41,41,41,41	0
53	MG	BB	3054	1/1	0.99	0.06	49,49,49,49	0
53	MG	BB	3018	1/1	1.00	0.04	39,39,39,39	0
53	MG	CA	1635	1/1	1.00	0.02	30,30,30,30	0
53	MG	CA	1636	1/1	1.00	0.04	5,5,5,5	0
53	MG	BB	3065	1/1	1.00	0.03	32,32,32,32	0
53	MG	BB	3066	1/1	1.00	0.01	5,5,5,5	0
53	MG	CA	1639	1/1	1.00	0.02	35,35,35,35	0
53	MG	BB	3019	1/1	1.00	0.01	21,21,21,21	0
53	MG	BB	3020	1/1	1.00	0.14	6,6,6,6	0
53	MG	BB	3069	1/1	1.00	0.04	5,5,5,5	0
53	MG	CA	1643	1/1	1.00	0.03	36,36,36,36	0
53	MG	BB	3021	1/1	1.00	0.03	52,52,52,52	0
53	MG	AA	1640	1/1	1.00	0.08	46,46,46,46	0
53	MG	BB	3023	1/1	1.00	0.02	5,5,5,5	0
53	MG	CA	1647	1/1	1.00	0.07	75,75,75,75	0
53	MG	BB	3073	1/1	1.00	0.04	44,44,44,44	0
53	MG	BB	3074	1/1	1.00	0.03	10,10,10,10	0
53	MG	AA	1641	1/1	1.00	0.02	32,32,32,32	0
53	MG	BB	3076	1/1	1.00	0.02	35,35,35,35	0
53	MG	BB	3025	1/1	1.00	0.03	30,30,30,30	0
53	MG	AA	1629	1/1	1.00	0.01	12,12,12,12	0
53	MG	BB	3079	1/1	1.00	0.02	38,38,38,38	0
53	MG	CA	1655	1/1	1.00	0.02	32,32,32,32	0
53	MG	CA	1656	1/1	1.00	0.05	38,38,38,38	0
53	MG	CA	1657	1/1	1.00	0.02	73,73,73,73	0
53	MG	CA	1658	1/1	1.00	0.02	37,37,37,37	0
53	MG	AA	1643	1/1	1.00	0.02	40,40,40,40	0
53	MG	DB	3001	1/1	1.00	0.01	5,5,5,5	0
53	MG	DB	3002	1/1	1.00	0.05	11,11,11,11	0
53	MG	DB	3003	1/1	1.00	0.07	30,30,30,30	0
53	MG	DB	3004	1/1	1.00	0.01	8,8,8,8	0
53	MG	DB	3005	1/1	1.00	0.08	25,25,25,25	0
53	MG	BB	3028	1/1	1.00	0.12	9,9,9,9	0
53	MG	BB	3029	1/1	1.00	0.01	5,5,5,5	0
53	MG	BB	3083	1/1	1.00	0.05	30,30,30,30	0
53	MG	DB	3009	1/1	1.00	0.02	9,9,9,9	0
53	MG	BB	3030	1/1	1.00	0.03	51,51,51,51	0
53	MG	DB	3011	1/1	1.00	0.03	5,5,5,5	0
53	MG	DB	3012	1/1	1.00	0.01	9,9,9,9	0
53	MG	BB	3085	1/1	1.00	0.01	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3014	1/1	1.00	0.01	21,21,21,21	0
53	MG	AA	1660	1/1	1.00	0.04	56,56,56,56	0
53	MG	DB	3016	1/1	1.00	0.04	5,5,5,5	0
53	MG	DB	3017	1/1	1.00	0.11	5,5,5,5	0
53	MG	DB	3018	1/1	1.00	0.02	7,7,7,7	0
53	MG	DB	3019	1/1	1.00	0.07	5,5,5,5	0
53	MG	DB	3020	1/1	1.00	0.09	5,5,5,5	0
53	MG	DB	3021	1/1	1.00	0.02	16,16,16,16	0
53	MG	DB	3022	1/1	1.00	0.02	11,11,11,11	0
53	MG	DB	3023	1/1	1.00	0.08	69,69,69,69	0
53	MG	DB	3024	1/1	1.00	0.03	40,40,40,40	0
53	MG	BB	3032	1/1	1.00	0.03	22,22,22,22	0
53	MG	BB	3088	1/1	1.00	0.03	11,11,11,11	0
53	MG	DB	3027	1/1	1.00	0.05	13,13,13,13	0
53	MG	AA	1607	1/1	1.00	0.02	57,57,57,57	0
53	MG	BB	3002	1/1	1.00	0.01	23,23,23,23	0
53	MG	BB	3035	1/1	1.00	0.04	13,13,13,13	0
53	MG	BB	3036	1/1	1.00	0.07	51,51,51,51	0
53	MG	AA	1631	1/1	1.00	0.05	5,5,5,5	0
53	MG	DB	3033	1/1	1.00	0.06	11,11,11,11	0
53	MG	BB	3094	1/1	1.00	0.02	36,36,36,36	0
53	MG	AA	1603	1/1	1.00	0.07	57,57,57,57	0
53	MG	BB	3039	1/1	1.00	0.05	41,41,41,41	0
53	MG	DB	3037	1/1	1.00	0.10	8,8,8,8	0
53	MG	DB	3038	1/1	1.00	0.02	5,5,5,5	0
53	MG	BB	3040	1/1	1.00	0.01	12,12,12,12	0
53	MG	DB	3040	1/1	1.00	0.03	5,5,5,5	0
53	MG	DB	3041	1/1	1.00	0.07	40,40,40,40	0
53	MG	DB	3042	1/1	1.00	0.01	37,37,37,37	0
53	MG	DB	3043	1/1	1.00	0.06	7,7,7,7	0
53	MG	DB	3044	1/1	1.00	0.06	18,18,18,18	0
53	MG	BB	3098	1/1	1.00	0.02	14,14,14,14	0
53	MG	BB	3041	1/1	1.00	0.00	5,5,5,5	0
53	MG	BB	3005	1/1	1.00	0.02	5,5,5,5	0
53	MG	BB	3101	1/1	1.00	0.03	19,19,19,19	0
53	MG	DB	3049	1/1	1.00	0.05	42,42,42,42	0
53	MG	AA	1609	1/1	1.00	0.03	40,40,40,40	0
53	MG	BB	3103	1/1	1.00	0.06	11,11,11,11	0
53	MG	BB	3104	1/1	1.00	0.05	26,26,26,26	0
53	MG	BB	3105	1/1	1.00	0.06	5,5,5,5	0
53	MG	DB	3054	1/1	1.00	0.03	21,21,21,21	0
53	MG	DB	3055	1/1	1.00	0.02	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3056	1/1	1.00	0.02	5,5,5,5	0
53	MG	DB	3057	1/1	1.00	0.05	48,48,48,48	0
53	MG	AA	1648	1/1	1.00	0.03	6,6,6,6	0
53	MG	BB	3045	1/1	1.00	0.02	72,72,72,72	0
53	MG	BB	3108	1/1	1.00	0.05	10,10,10,10	0
53	MG	BB	3109	1/1	1.00	0.02	11,11,11,11	0
53	MG	AA	1616	1/1	1.00	0.02	5,5,5,5	0
53	MG	CA	1601	1/1	1.00	0.05	5,5,5,5	0
53	MG	CA	1602	1/1	1.00	0.02	5,5,5,5	0
53	MG	CA	1603	1/1	1.00	0.03	56,56,56,56	0
53	MG	AA	1604	1/1	1.00	0.04	38,38,38,38	0
53	MG	DB	3067	1/1	1.00	0.01	5,5,5,5	0
53	MG	DB	3068	1/1	1.00	0.09	5,5,5,5	0
53	MG	CA	1605	1/1	1.00	0.04	12,12,12,12	0
53	MG	DB	3070	1/1	1.00	0.02	33,33,33,33	0
53	MG	BB	3048	1/1	1.00	0.06	12,12,12,12	0
53	MG	DB	3072	1/1	1.00	0.03	20,20,20,20	0
53	MG	CA	1607	1/1	1.00	0.02	5,5,5,5	0
53	MG	DB	3074	1/1	1.00	0.01	26,26,26,26	0
53	MG	AA	1636	1/1	1.00	0.04	64,64,64,64	0
53	MG	DB	3076	1/1	1.00	0.01	33,33,33,33	0
53	MG	BB	3011	1/1	1.00	0.05	5,5,5,5	0
53	MG	DB	3078	1/1	1.00	0.03	25,25,25,25	0
53	MG	DB	3079	1/1	1.00	0.03	7,7,7,7	0
53	MG	DB	3080	1/1	1.00	0.05	62,62,62,62	0
53	MG	CA	1610	1/1	1.00	0.02	5,5,5,5	0
53	MG	CA	1611	1/1	1.00	0.03	28,28,28,28	0
53	MG	AA	1618	1/1	1.00	0.04	38,38,38,38	0
53	MG	DB	3084	1/1	1.00	0.07	29,29,29,29	0
53	MG	DB	3085	1/1	1.00	0.02	38,38,38,38	0
53	MG	DB	3086	1/1	1.00	0.01	18,18,18,18	0
53	MG	DB	3087	1/1	1.00	0.01	5,5,5,5	0
53	MG	BB	3013	1/1	1.00	0.02	45,45,45,45	0
53	MG	AA	1653	1/1	1.00	0.04	21,21,21,21	0
53	MG	CA	1615	1/1	1.00	0.07	13,13,13,13	0
53	MG	AA	1611	1/1	1.00	0.01	43,43,43,43	0
53	MG	DB	3092	1/1	1.00	0.06	10,10,10,10	0
53	MG	BB	3055	1/1	1.00	0.07	6,6,6,6	0
53	MG	BB	3056	1/1	1.00	0.04	5,5,5,5	0
53	MG	CA	1619	1/1	1.00	0.02	36,36,36,36	0
53	MG	CA	1620	1/1	1.00	0.03	72,72,72,72	0
53	MG	BB	3016	1/1	1.00	0.02	55,55,55,55	0

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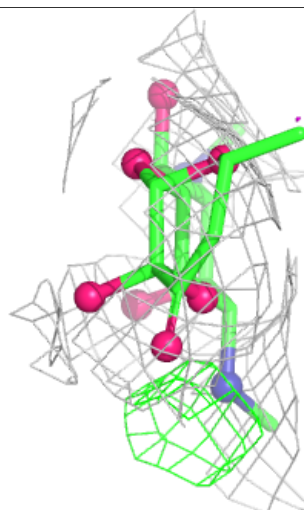
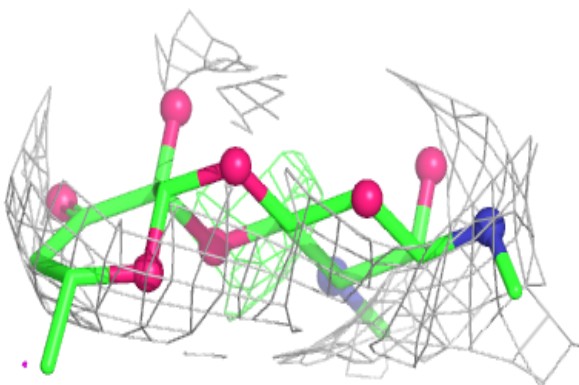
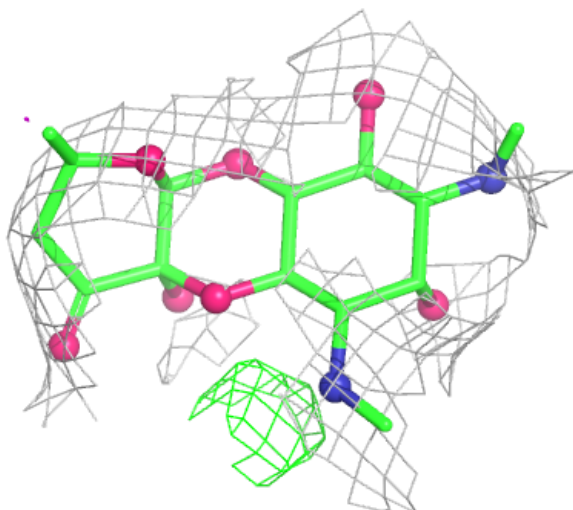
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	DB	3098	1/1	1.00	0.06	5,5,5,5	0
53	MG	CA	1622	1/1	1.00	0.09	5,5,5,5	0
53	MG	CA	1623	1/1	1.00	0.03	11,11,11,11	0
53	MG	DB	3101	1/1	1.00	0.04	26,26,26,26	0
53	MG	DB	3102	1/1	1.00	0.07	28,28,28,28	0
53	MG	CA	1624	1/1	1.00	0.02	38,38,38,38	0
53	MG	BB	3058	1/1	1.00	0.05	15,15,15,15	0
53	MG	CA	1626	1/1	1.00	0.02	8,8,8,8	0
53	MG	DB	3106	1/1	1.00	0.01	61,61,61,61	0
53	MG	DB	3107	1/1	1.00	0.01	5,5,5,5	0
53	MG	BB	3059	1/1	1.00	0.02	10,10,10,10	0
53	MG	DB	3109	1/1	1.00	0.05	9,9,9,9	0
53	MG	BB	3060	1/1	1.00	0.04	30,30,30,30	0
53	MG	BB	3061	1/1	1.00	0.07	24,24,24,24	0
53	MG	CA	1630	1/1	1.00	0.02	37,37,37,37	0
53	MG	BB	3062	1/1	1.00	0.01	7,7,7,7	0
53	MG	AA	1612	1/1	1.00	0.06	61,61,61,61	0
53	MG	CA	1633	1/1	1.00	0.01	23,23,23,23	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.

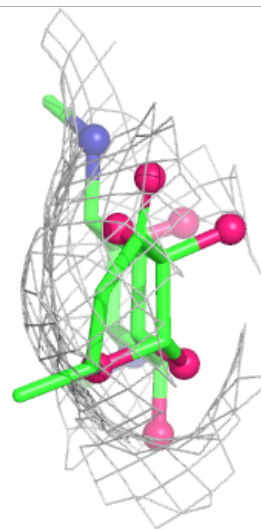
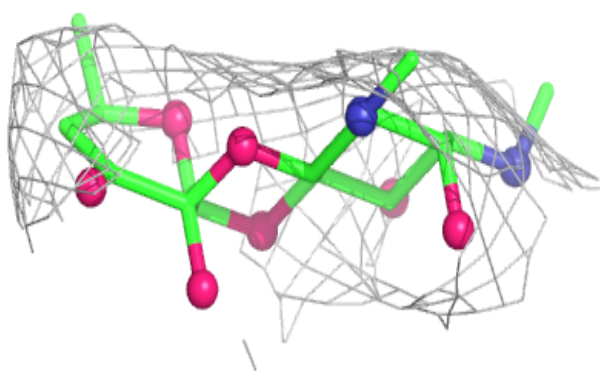
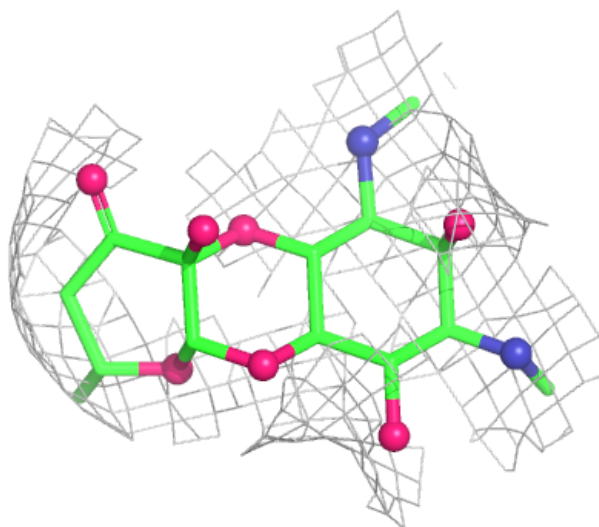
Electron density around SCM CA 1659:

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



Electron density around SCM AA 1661:

$2mF_o-DF_c$ (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.