



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:36 PM GMT

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

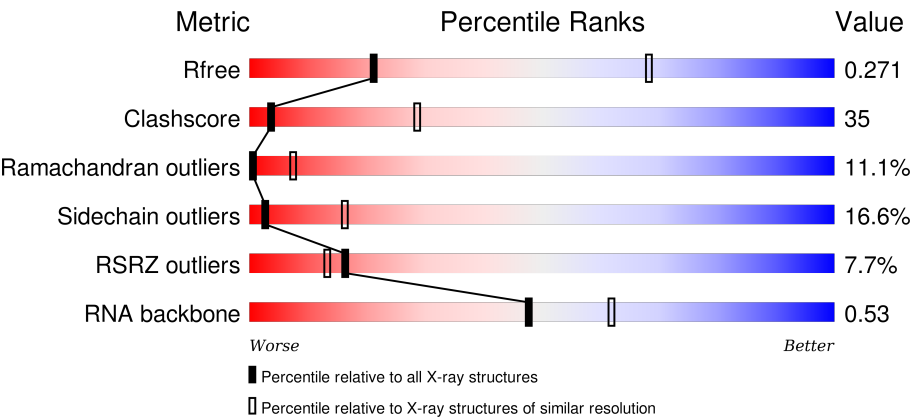
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



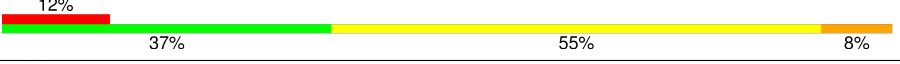
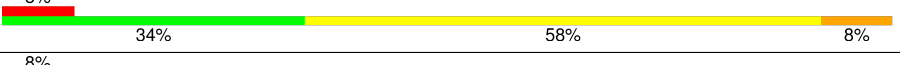
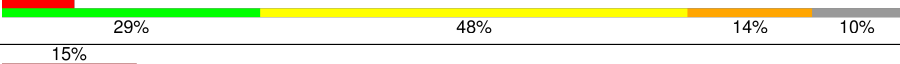
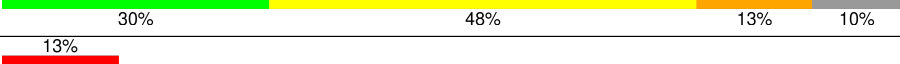
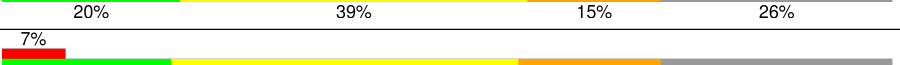
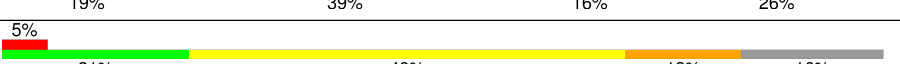
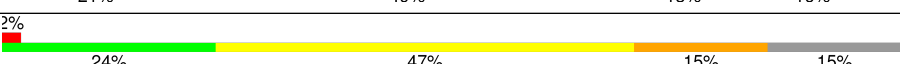
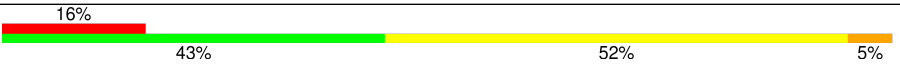

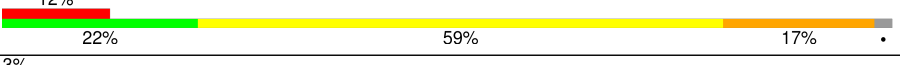
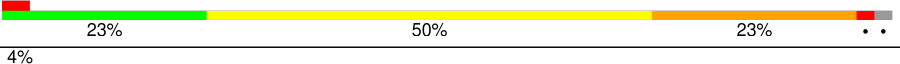
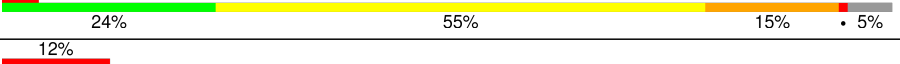
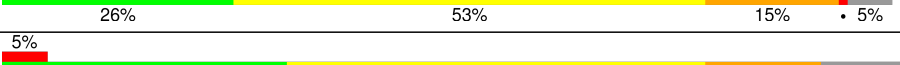
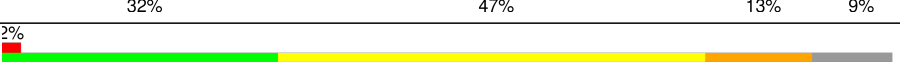
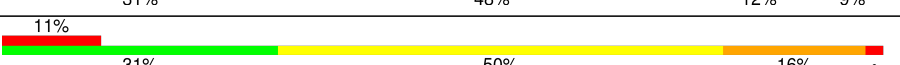
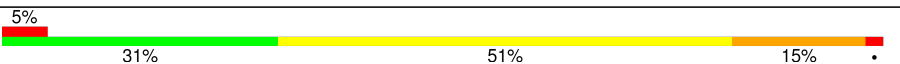
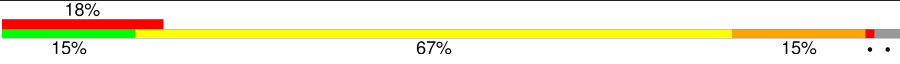
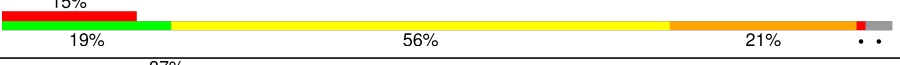
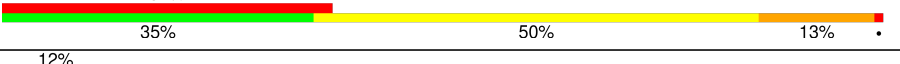


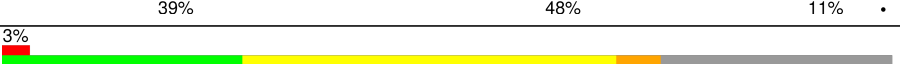
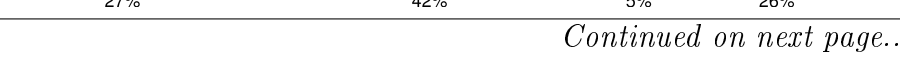


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	<div><div></div><div><div>23%</div><div>62%</div><div>14%</div><div>..</div></div></div>
1	CA	1542	<div><div></div><div><div>24%</div><div>62%</div><div>14%</div><div>.</div></div></div>
2	AC	232	<div><div>9%</div><div><div>20%</div><div>48%</div><div>18%</div><div>11%</div><div>.</div></div></div>
2	CC	232	<div><div>7%</div><div><div>28%</div><div>46%</div><div>14%</div><div>11%</div><div>.</div></div></div>

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	NMY	AA	1601	-	-	-	X
53	NMY	BB	3001	-	-	-	X
53	NMY	CA	1601	-	-	-	X
53	NMY	DB	3001	-	-	-	X
54	MG	AA	1658	-	-	-	X
54	MG	BB	3088	-	-	-	X
54	MG	DB	3090	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 284201 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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			

Continued on next page...

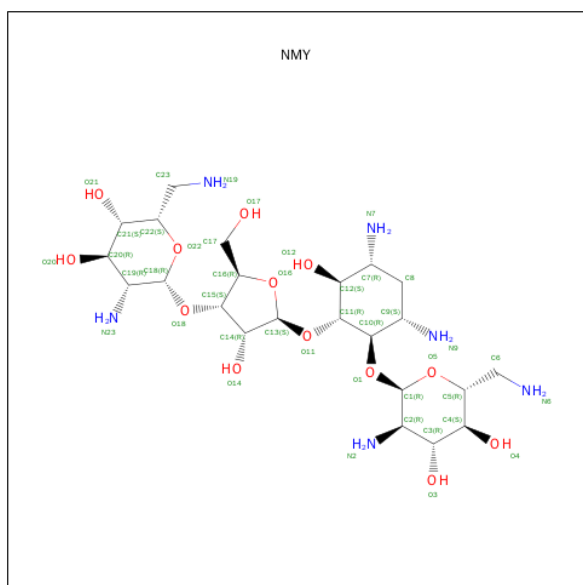
Continued from previous page...

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

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

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

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

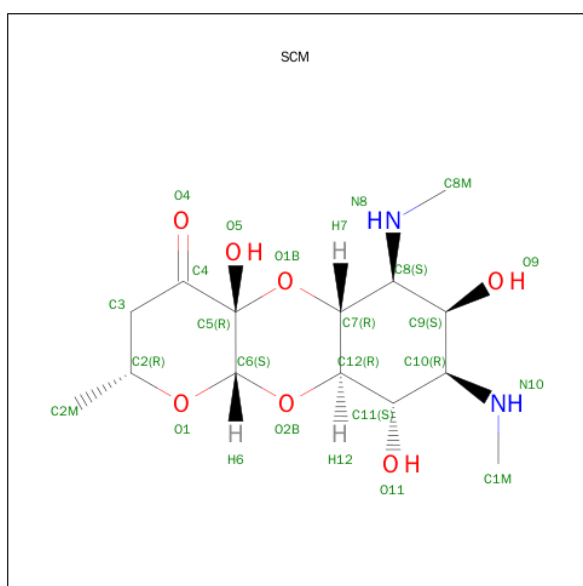


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
53	AA	1	Total	C	N	O	0	0
			42	23	6	13		
53	BB	1	Total	C	N	O	0	0
			42	23	6	13		
53	CA	1	Total	C	N	O	0	0
			42	23	6	13		
53	DB	1	Total	C	N	O	0	0
			42	23	6	13		

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

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

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



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

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

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

- Molecule 57 is water.

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

Continued on next page...

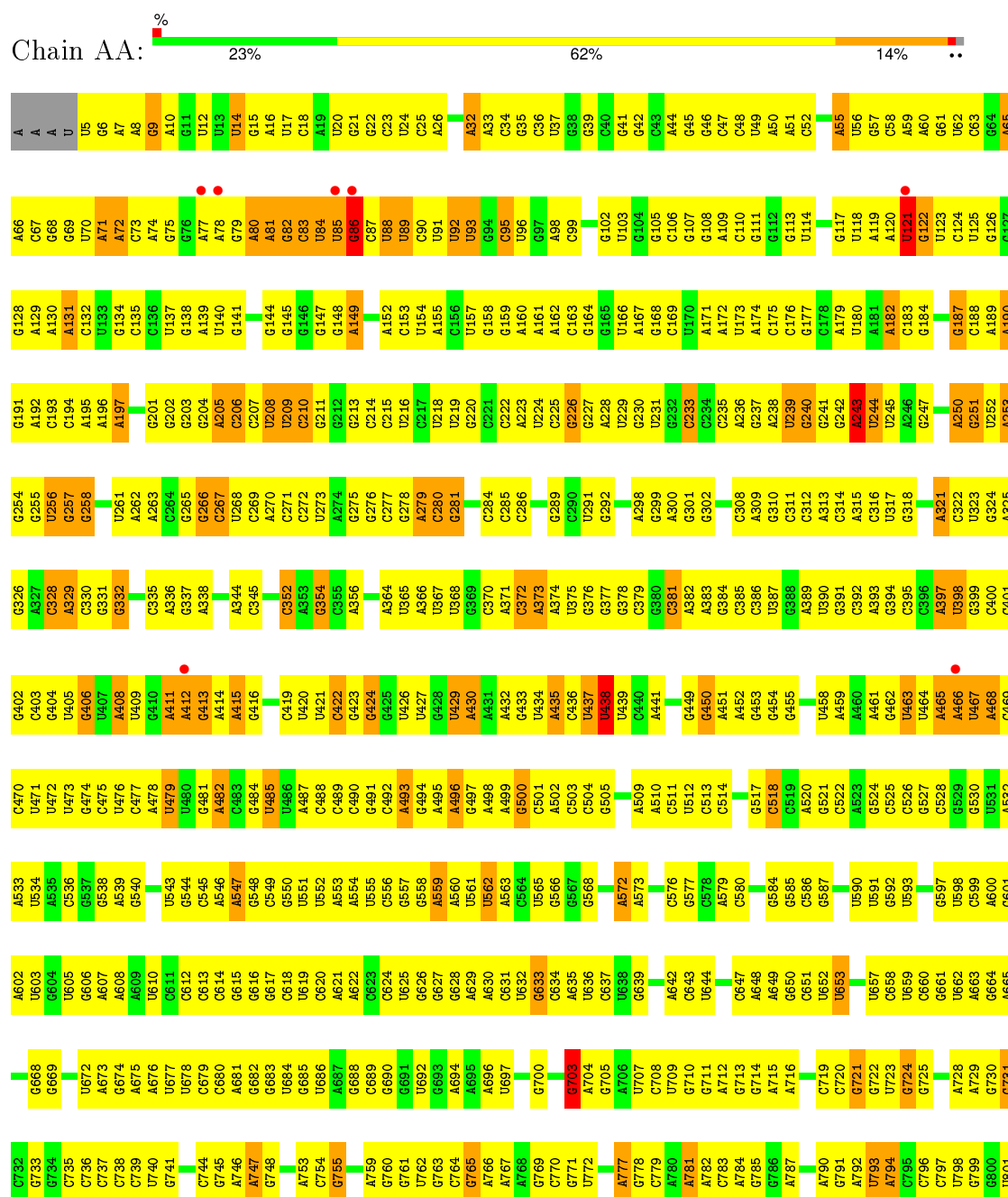
Continued from previous page...

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

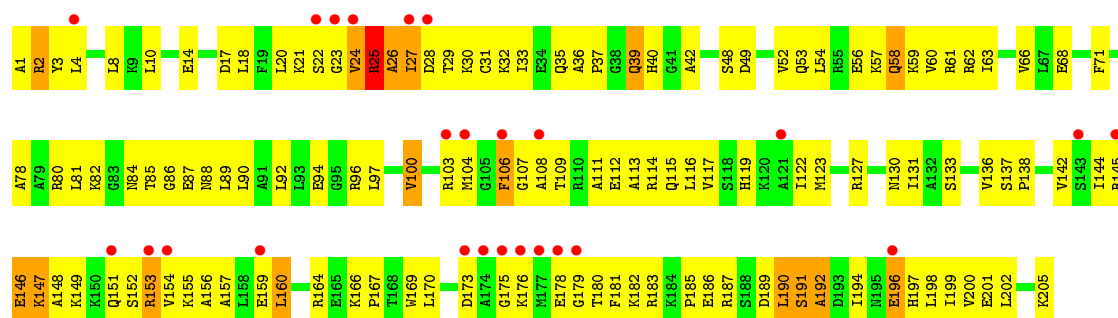
3 Residue-property plots

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

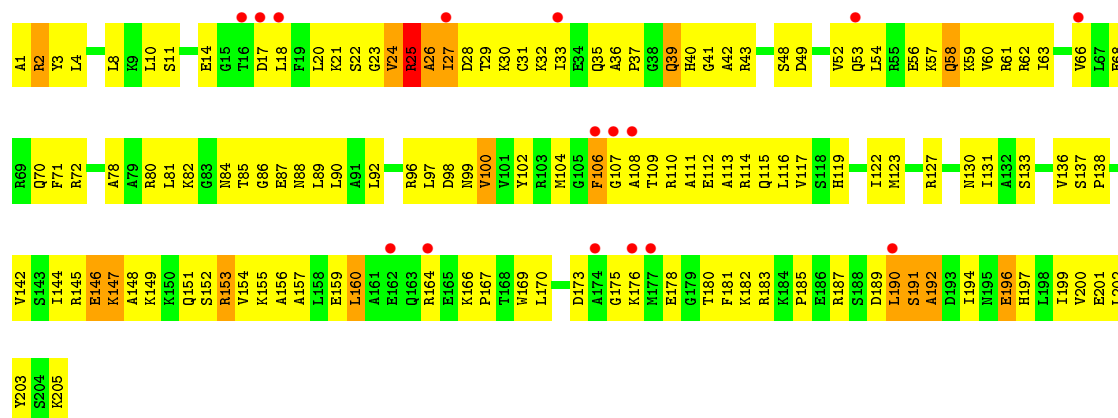
• Molecule 1: 16S rRNA



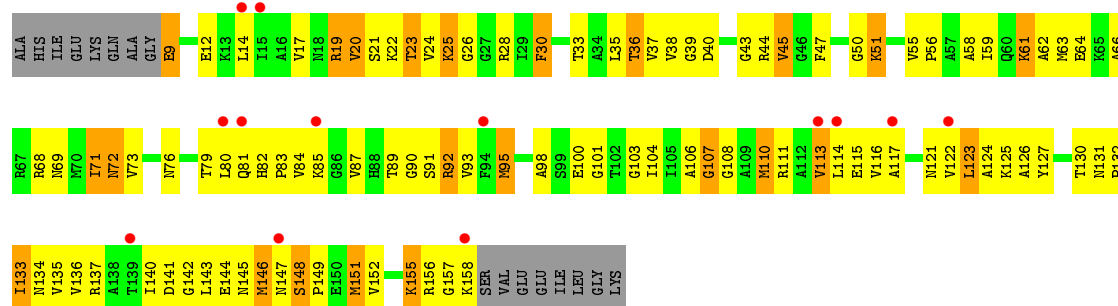
G1279	A1216	C1149	U1086	A1022	A959	A889	A816	A746	U678	U610	G544	U479	G410	C335	A262	G200
A1280	C1217	A1150	U1090	A1023	U960	G890	C817	A747	C679	C611	C545	U480	A411	C336	A263	G201
C1281	A1218	A1151	U1091	G1024	U961	U891	G818	G748	C680	C613	A547	G481	A412	A337	C264	G202
U1283	C1219	A1152	U1092	A1025	U965	C893	A819	A749	G682	C614	A548	C482	A413	G338	G265	G203
U1284	G1221	A1093	A1093	G1026	U966	G894	U820	C750	G683	G615	C549	C483	A414	A339	G266	G204
A1285	G1222	A1157	G1094	C1027	G966	G895	G824	G755	U684	G616	G550	U485	A415	C339	C267	G205
U1286	C1223	C1158	U1095	C1028	G967	C896	G825	G756	G685	G617	U551	U486	A416	A344	U268	A205
U1287	U1224	U1159	C1096	U1029	A968	C897	A826	A759	U686	G618	U552	A487	U420	C345	C269	C206
A1288	C1225	G1160	C1097	U1030	A969	A900	C826	A759	A687	U619	A553	C488	U421	C352	C271	U208
A1289	C1226	C1161	C1098	C1031	C970	U901	U827	G760	G688	C620	A554	C489	U422	A353	C272	U209
G1290	A1227	G1162	G1099	G1032	G971	A902	U828	G761	G689	A621	U555	C490	G423	G354	U273	G210
U1291	C1228	A1163	G1100	G1033	C972	G903	G833	G763	G691	C623	G557	C492	G425	C355	G212	G211
G1292	A1229	G1164	A1101	A1036	G973	U904	U834	G765	U692	C624	A558	A493	U426	A356	G276	G213
C1293	C1230	U1165	A1102	C1037	A974	U905	U835	G766	G693	U625	A559	A494	U427	A357	C277	G214
U1295	G1232	G1166	C1103	G1037	G976	A906	U836	A766	A694	G626	A560	A495	U428	A364	A279	C215
C1296	U1233	U1167	G1104	U1040	A977	U907	U837	A767	A694	G627	A561	A496	U429	A365	C280	U216
U1297	G1234	U1168	G1107	U1041	A978	A908	G840	G769	G700	G628	U562	A497	A430	A366	G281	C217
G1298	C1235	A1169	G1108	A1042	C979	A909	C841	C770	U701	A629	A563	A498	A431	U367	U218	U219
U1299	A1236	A1171	C1109	G1043	C980	C910	C842	G771	A702	C630	C564	A499	A432	U368	C284	C222
G1300	C1237	U1172	A1110	G1047	U981	U911	U842	U772	G703	C631	U565	C500	G433	C369	C285	A223
U1301	A1238	U1173	A1111	G1048	U982	C912	U843	U773	A704	U632	G566	C501	U434	C370	C286	A224
C1302	G1239	G1174	C1112	U1049	A983	A913	G844	A777	U707	C633	G567	A502	C435	A371	U287	A225
G1303	U1240	G1175	G1113	U1049	C984	A914	A845	G778	C708	A634	G568	C503	C436	C372	A288	U224
G1304	G1241	A1176	C1114	G1050	C985	A914	G846	C779	C708	A635	U572	C504	U437	A373	C289	C225
A1305	G1242	G1177	U1115	C1051	U986	G917	G847	A780	U709	C636	A573	G505	U438	A374	C290	G226
G1306	C1243	U1178	U1116	U1052	G987	A918	C848	A781	U710	U637	A573	G505	U439	U367	U291	G227
U1307	G1244	A1179	A1117	G1053	U987	A919	U854	A782	G711	U638	C576	A510	A441	C378	G292	A228
C1308	C1245	A1180	U1118	C1054	U988	A919	U855	A783	A712	G639	C577	A511	A442	C379	U229	G230
G1309	A1246	G1181	C1119	U1055	C990	U921	G856	A784	G713	U640	C578	C512	U449	C380	A298	U231
G1310	U1247	G1182	C1120	U1056	U991	G922	G858	G785	G714	C643	A579	C513	G450	C381	C299	G232
A1311	A1248	U1183	U1121	G1057	U992	A923	G859	G786	A715	U644	C580	C514	G451	A382	A300	G233
C1312	C1249	G1184	U1122	G1058	G993	C924	A860	A787	A716	U644	C580	C514	A452	A383	G301	C234
U1313	U1250	G1185	U1123	C1059	A994	G925	A861	A787	A716	U644	C580	C514	A453	A384	G302	G235
C1314	A1251	G1186	G1124	U1060	C995	G926	C862	A790	C719	C647	G584	C515	U488	C385	A308	A236
U1315	C1252	A1187	U1125	G1061	A996	G927	U863	G791	C720	A648	G585	C516	A460	C386	A309	G237
G1316	G1253	A1188	U1126	U1062	U997	G933	A864	A792	G721	A649	C586	A520	G454	U387	G310	G238
C1317	A1254	U1189	C1127	C1063	C998	G934	A865	U793	G722	C650	G587	C521	U489	G388	C311	U239
G1318	G1255	G1190	U1128	C1064	C999	A935	C866	A794	U723	C651	G587	C522	A461	U390	C312	G240
A1319	U1256	U1191	C1129	U1065	A1000	A935	C867	C795	G724	U652	U590	A523	A462	C391	C313	G241
C1320	A1257	A1196	A1130	C1066	C1001	A938	C868	C796	G725	U653	G592	C524	A463	C392	C314	G242
U1321	G1258	A1197	G1131	A1067	G1002	G939	C869	C797	G726	U654	G593	C525	U464	A393	A315	C243
C1322	C1259	U1198	C1132	U1068	G1003	C940	U870	C797	U798	G656	U594	C526	U465	C394	C316	U244
G1323	U1260	U1199	G1133	C1069	A1004	G941	U871	U798	A728	U657	A595	C527	A466	C395	U317	U245
A1324	C1262	C1200	G1134	U1070	A1005	G941	U872	U801	C735	G658	A596	C528	A467	C396	G318	G247
C1325	G1263	A1201	U1135	C1071	G1006	A946	U873	A802	G731	U659	G597	A529	A468	A397	A321	A250
U1326	U1264	C1202	C1136	G1072	U1007	G947	C876	G803	G732	C660	G598	A530	U469	U398	C322	G251
C1327	G1265	U1203	G1137	U1073	U1008	C948	G877	U804	G733	C661	U599	A531	A470	C399	U323	U252
G1328	U1266	U1204	G1138	G1074	U1009	C948	A878	C805	G734	U662	C600	A532	A471	C400	A324	A253
U1329	C1267	G1206	G1139	U1075	U1010	A949	C879	C806	C735	A663	A600	A533	A472	C401	A325	G254
G1331	G1268	G1207	U1140	U1076	C1011	U950	C880	A807	C736	G664	G601	A534	U473	C402	G326	G255
A1332	A1269	C1208	C1141	G1077	A1012	G951	C881	G808	C737	A665	A602	A535	U474	C403	A327	U256
C1333	U1270	C1209	G1142	U1078	G1013	U952	C882	G809	C738	U672	U603	A536	U475	C404	A328	G257
G1334	A1271	C1210	G1143	U1079	C1014	G953	C883	C810	C739	U673	G604	A537	U476	C405	A329	G258
U1335	U1272	U1211	G1144	U1080	G1015	G954	U884	C811	U740	A673	U605	A538	U477	U405	A330	U261
C1336	G1273	U1212	A1145	A1082	A1016	U955	U885	G812	G741	G674	G606	A539	U478	G406	A331	G332
G1337	A1274	C1213	A1146	U1083	U1017	U956	G886	U813	G742	A675	A607	G540	U479	U407	G333	G332
U1338	U1275	U1214	C1147	G1084	U1018	U957	G887	U814	C744	A676	A608	G541	A478	A408	G334	G332
A1339	G1278	G1215	U1148	U1085	A1019	A958	G888	A815	G745	U677	A609	U543	A479	U409	G335	G332



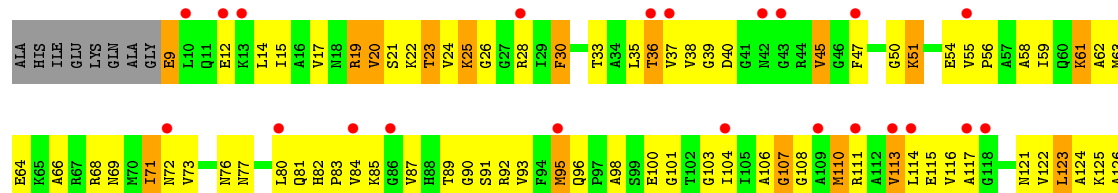
• Molecule 3: 30S ribosomal protein S4

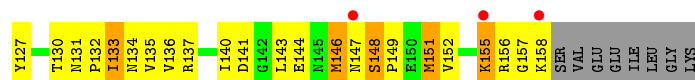


• Molecule 4: 30S ribosomal protein S5

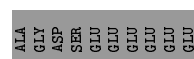
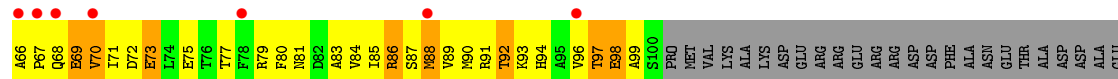
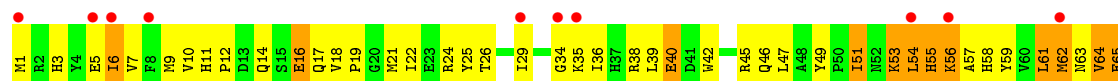
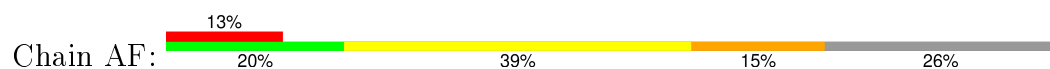


• Molecule 4: 30S ribosomal protein S5

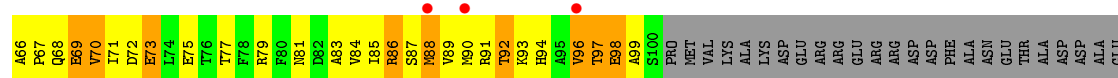
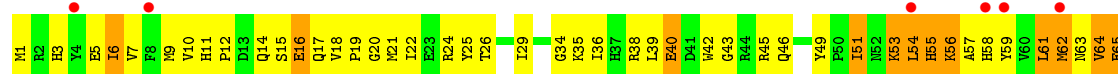
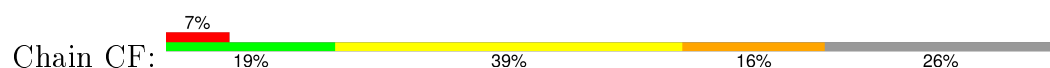




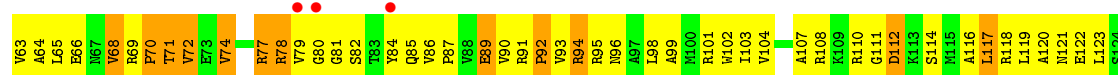
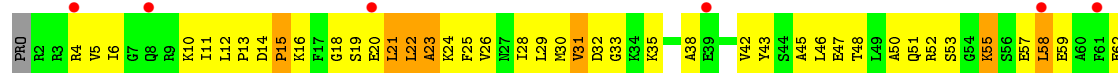
• Molecule 5: 30S ribosomal protein S6



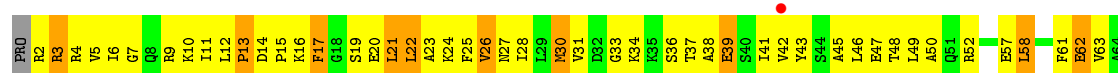
• Molecule 5: 30S ribosomal protein S6

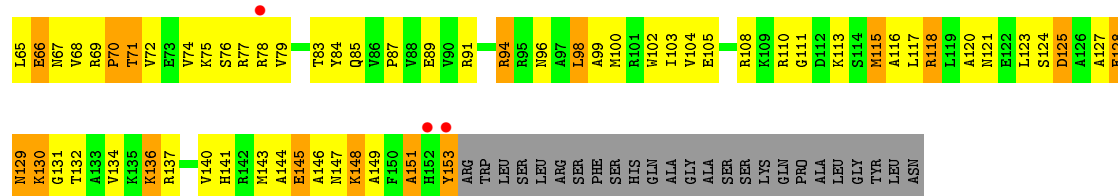


• Molecule 6: 30S ribosomal protein S7

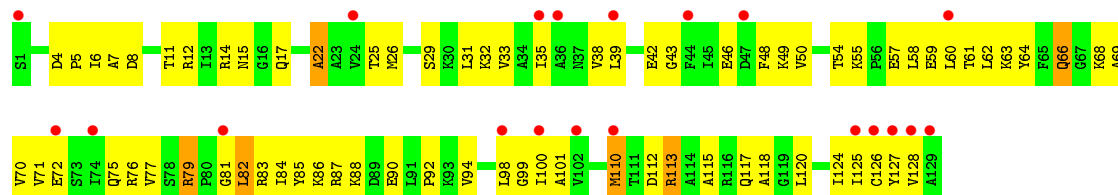
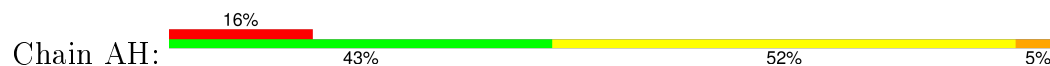


• Molecule 6: 30S ribosomal protein S7

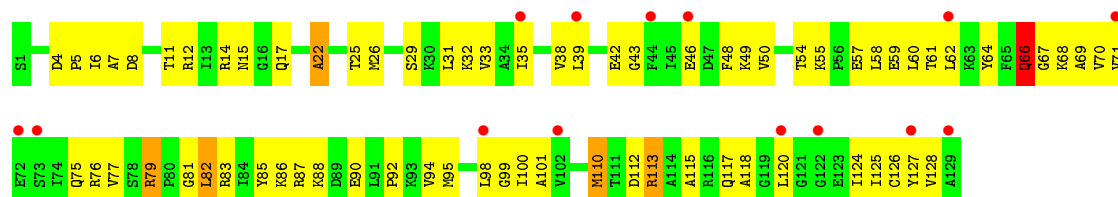




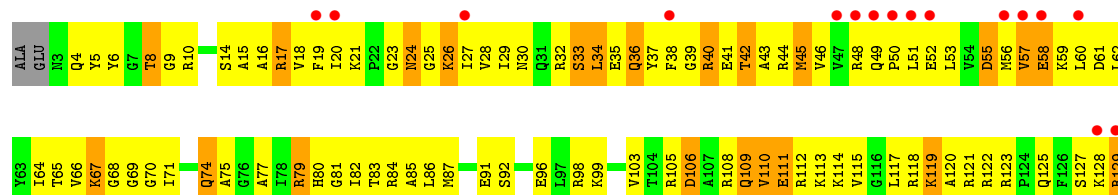
• Molecule 7: 30S ribosomal protein S8



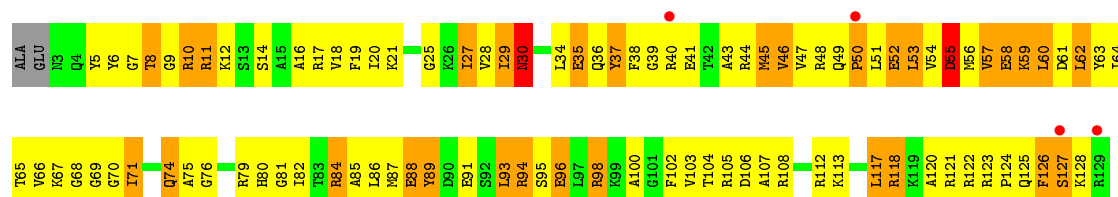
• Molecule 7: 30S ribosomal protein S8



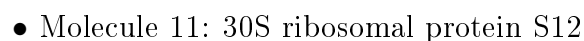
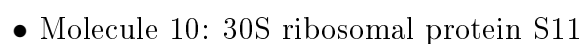
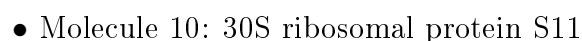
• Molecule 8: 30S ribosomal protein S9



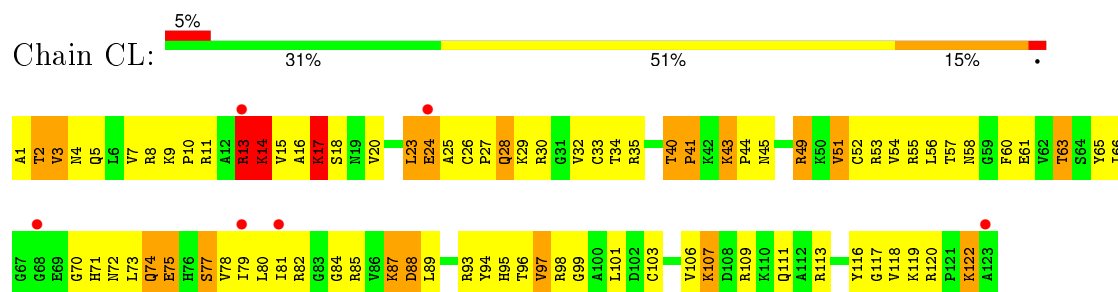
• Molecule 8: 30S ribosomal protein S9



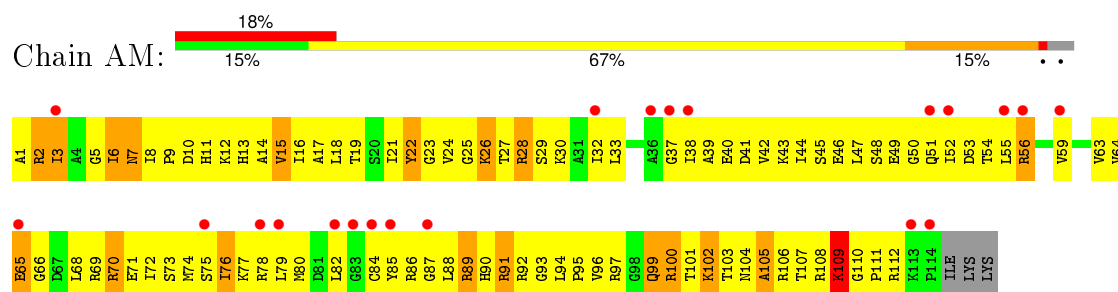
• Molecule 9: 30S ribosomal protein S10



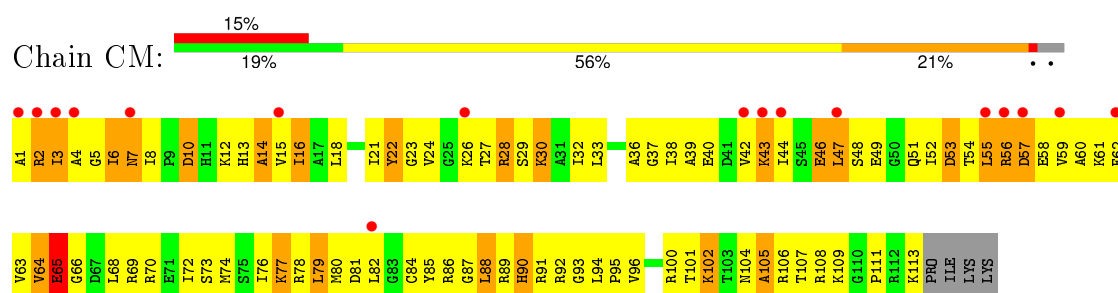
- Molecule 11: 30S ribosomal protein S12



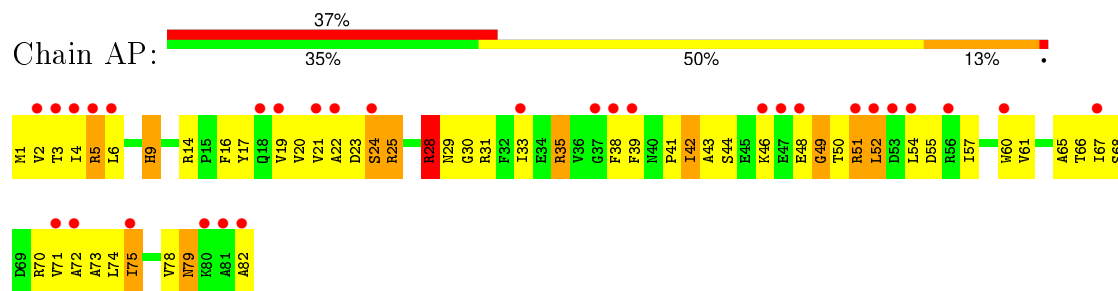
- Molecule 12: 30S ribosomal protein S13



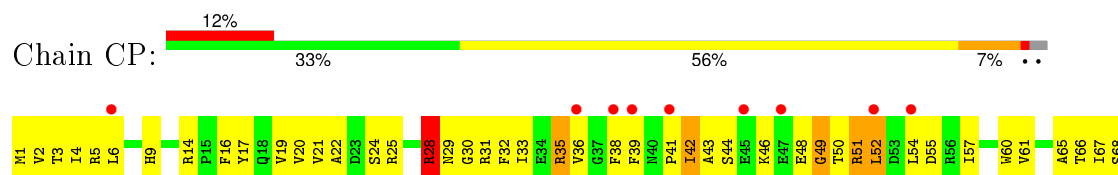
- Molecule 12: 30S ribosomal protein S13

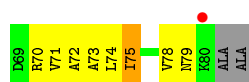


- Molecule 13: 30S ribosomal protein S16

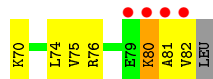


- Molecule 13: 30S ribosomal protein S16

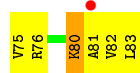
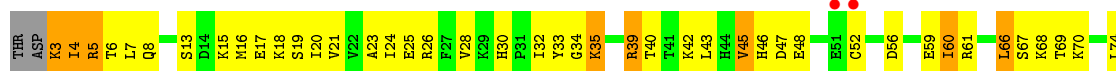
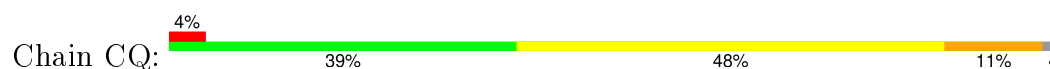




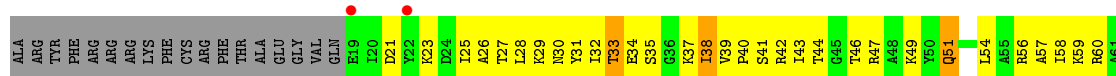
- Molecule 14: 30S ribosomal protein S17



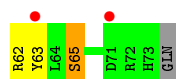
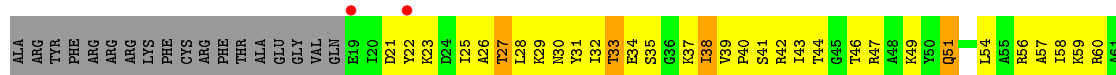
- Molecule 14: 30S ribosomal protein S17



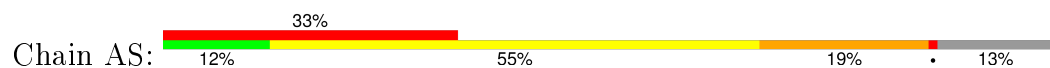
- Molecule 15: 30S ribosomal protein S18

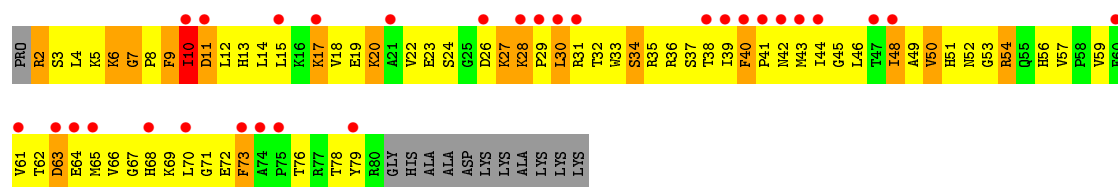


- Molecule 15: 30S ribosomal protein S18

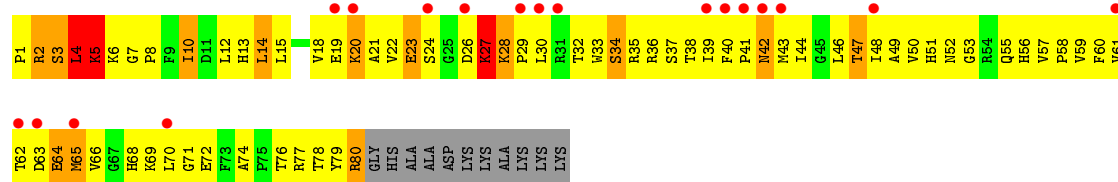
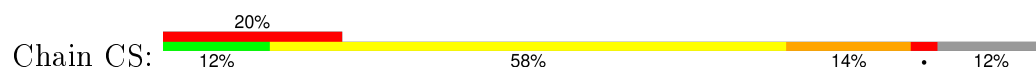


- Molecule 16: 30S ribosomal protein S19

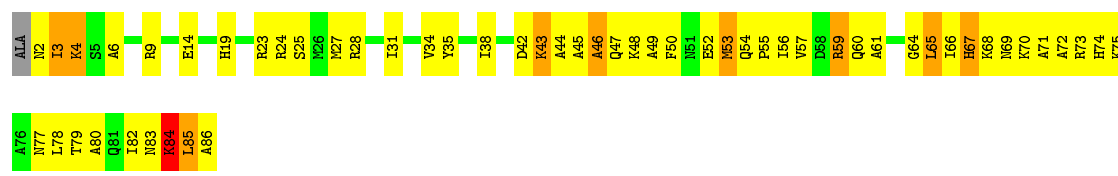
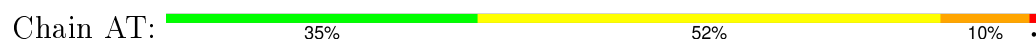




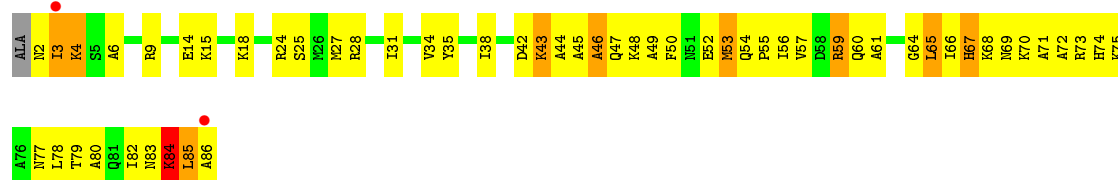
• Molecule 16: 30S ribosomal protein S19



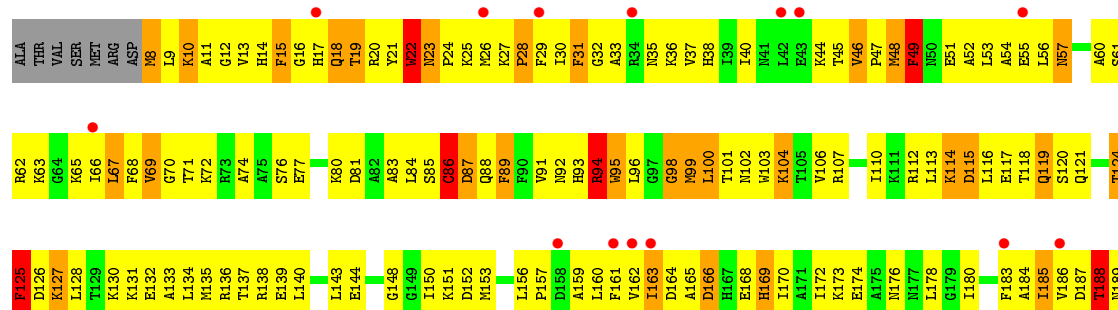
• Molecule 17: 30S ribosomal protein S20

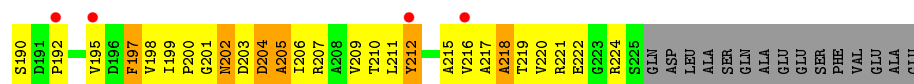


• Molecule 17: 30S ribosomal protein S20

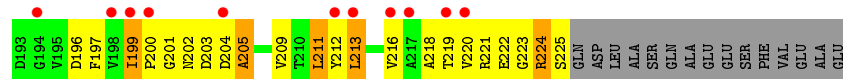
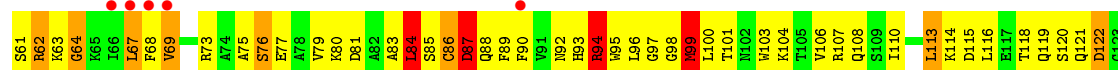
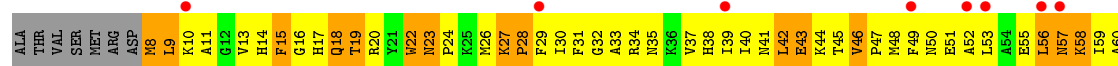


• Molecule 18: 30S ribosomal protein S2

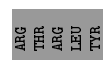
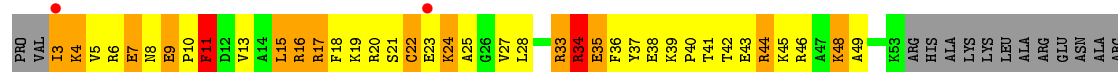




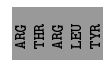
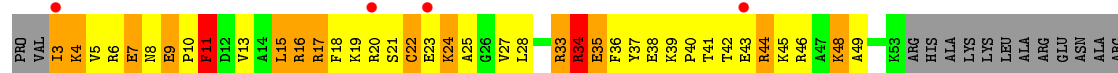
• Molecule 18: 30S ribosomal protein S2



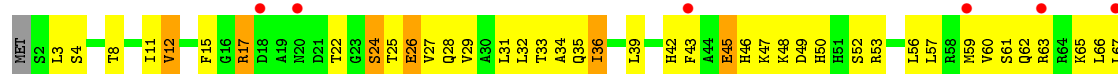
• Molecule 19: 30S ribosomal protein S21



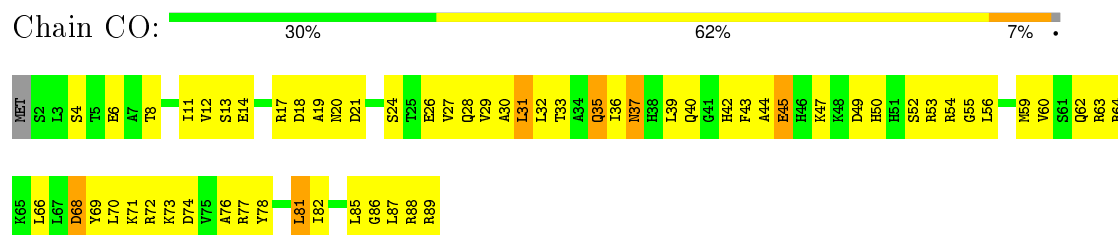
• Molecule 19: 30S ribosomal protein S21



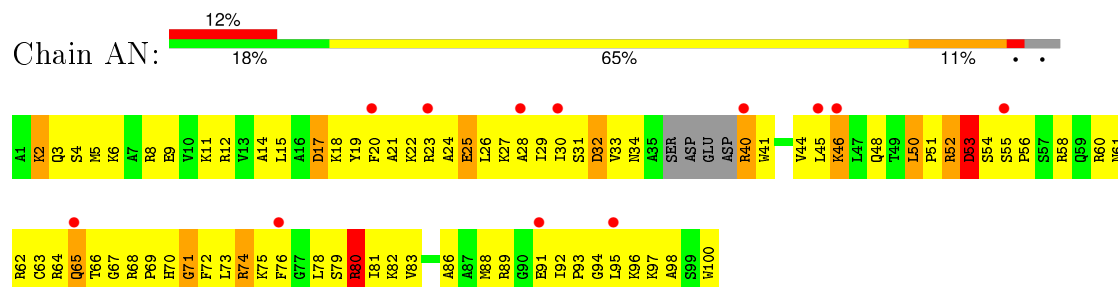
• Molecule 20: 30S ribosomal protein S15



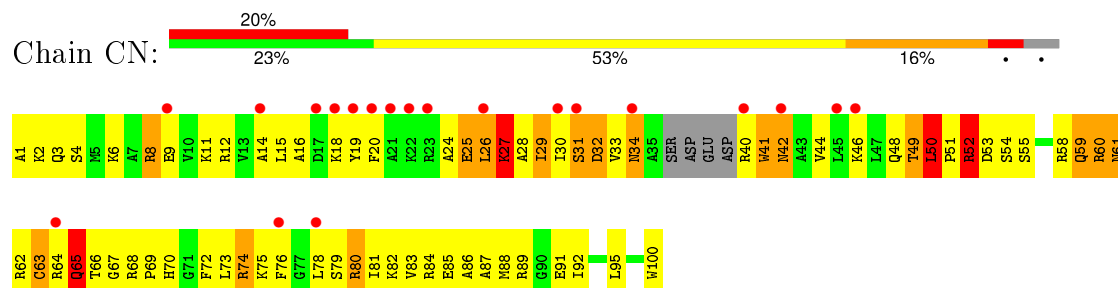
- Molecule 20: 30S ribosomal protein S15



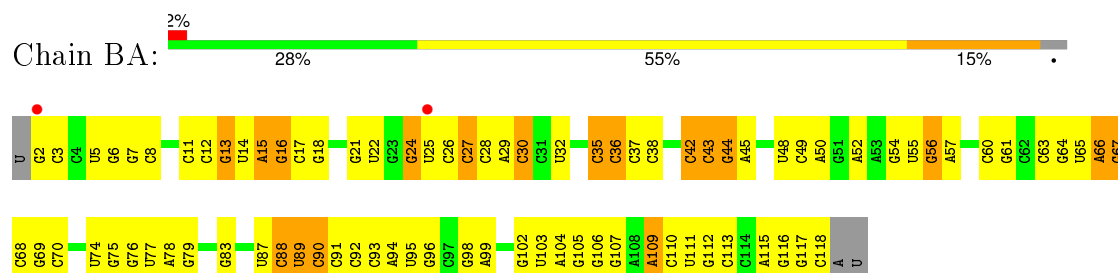
- Molecule 21: 30S ribosomal protein S14



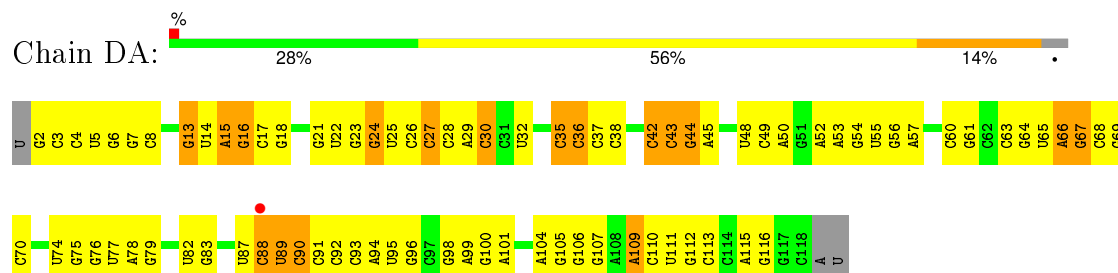
- Molecule 21: 30S ribosomal protein S14



- Molecule 22: 5S rRNA

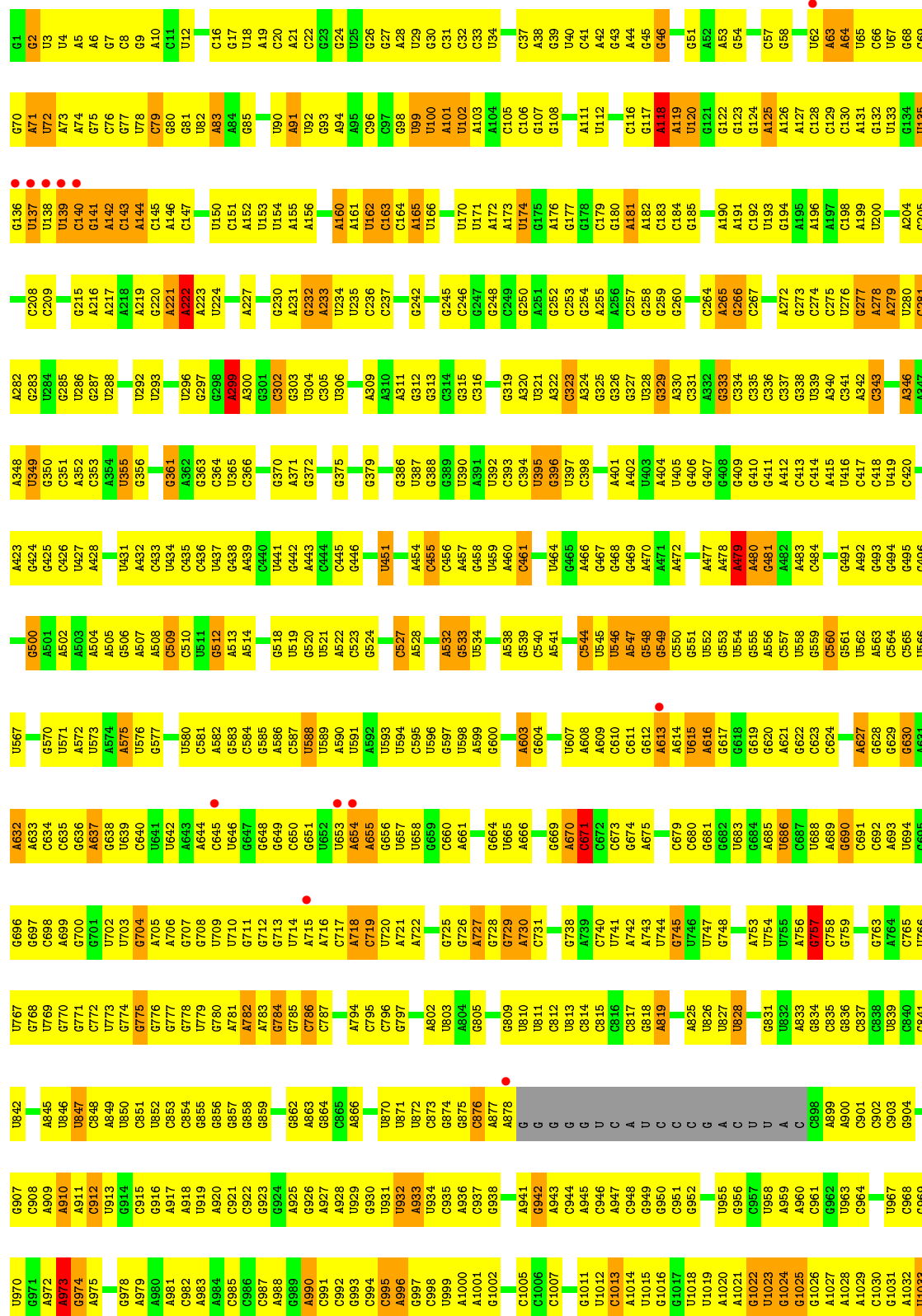


- Molecule 22: 5S rRNA

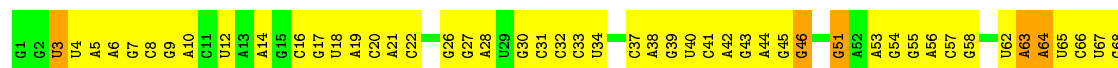


● Molecule 23: 23S rRNA

Chain BB: 



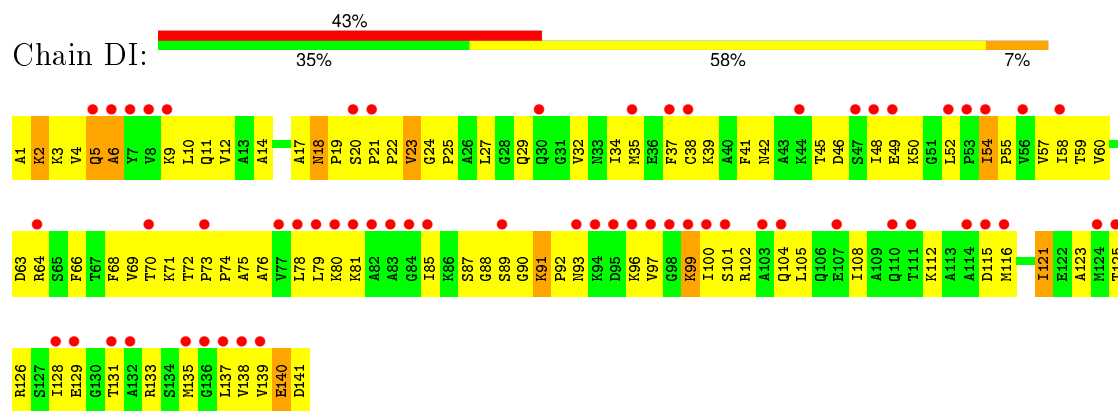




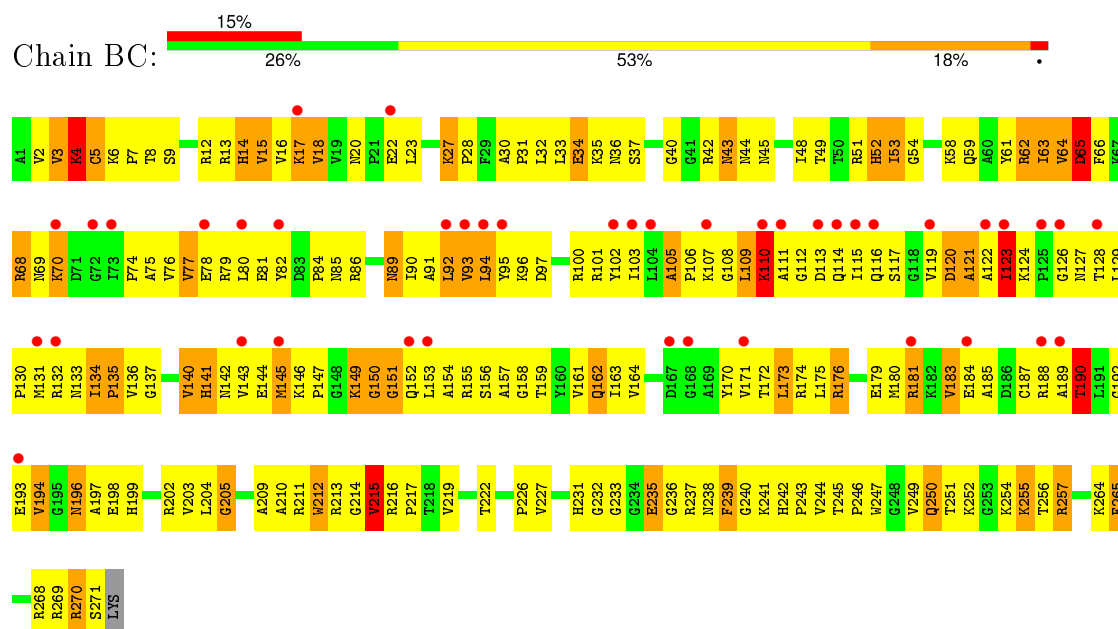
U1097	U1023	A960	A	U832	U683	U615	U552	C485	C414	A345	G283	C208	C140	C69
A1098	G1024	C961	C	A833	G884	A616	G553	C486	A415	A346	U284	C209	G141	G70
G1099	G1025	G962		G834	U885	G617	U554	C487	A416	A347	U285	C210	A142	A71
C1100	G1026	U963	A899	C835	U886		U555		C417	A348	U286		C143	U72
U1101	A1027	A900	A900	G836	G887	G620	A556	G491	C418	A349	U287	G215	A144	A73
C1102	A1028	C901	C901	G837	U888	G621	C557	G492	U419	G350	U288	A216	C145	A74
A1103	A1029	C902	C902	C838	U889	G622	U558	G493	C420	C351	U289		A146	G75
C1104	C1030	C903	C903	U839	G890	G623	G559	G494		A352		A219	A147	G76
U1105	G1031	G969	G904	C840	C891	C624	C560	G495	A423	C353	U292	G220	U150	G77
C1106	A1032	U970		G841	C892	C625	U561	G496	A424	A354	U293	A221	C151	U78
G1107	U1033	U971	C908	U842	C893		A562		G425	U355	A294	A222	C152	C79
U1108	G1034	A972	A909	U843	U694	A627	A563	G500	U426	G356	U295	A223	A152	G80
G1109		A973	A910	A845	G895	G630	A564	A501	U427	C357	U296	U224	U153	G81
G1110	G1037	A974	A911	U846	G896	A631	C565	A502	A428	U358	G297		U154	U82
A1111	G1038	A975		U847	G897	A632	U567	A503		G359	G298	G230	A155	A83
G1112	A1039	U912	U912	U848	G898	A633	U567	A504	U431	U360	A299	A231	A156	
U1113	A1040	C913	C913	C848	C899	C634	U570	A505	A432	G361	A300	G232	C157	U90
C1114	A1041	A979	C915	U850	G700	C635	U571	G506	C433	A362	A301	A233	A160	A91
G1115	G1042	U980	U916	C851	G701	G636	A572	A507	U434	G363	C302	U234	U161	U92
A1116	C1043	A981	A917	U852	U702	A637	A573	A508	C435	G364	G303	U235	U162	G93
G1117	G1044	A918	A918	C853	U703	G638	U574	A509	C436	U365	U304	U236	C163	A94
C1118	C1045	A983	U919	G854	U704	U639	A575	C510	U437	G366	U305	C237	C164	A95
U1119	A1046	A984	A920	G855	A705	C640	U576	U511	U438	G367	U306	C238	C165	C96
G1125	G1047	C985	C922	G856	G706	U641	U577	G512	A439	U368	G307	G242	A165	C97
A1126	A1048	C986	C922	G857	U707	U642	U577	A513	C440	U369	G308		U166	G98
A1129	C1049	C987	G923	C858	U709	A643	U580	A514	U441	G370	A309	G245	U169	U99
	G1050	A988	G924	G859	U710	A644	U581	C515	A442	A371	A310	C246	G170	U100
C1132	A1051	G989	U925	G860	G711	C645	C582	C516	A443	G372	A311	C247	U171	U102
A1133	C1052	A990	G926	A862	G712	U646	A583	C517	C444		G313	G248	A172	A103
C1134	A1057	C991	A927	A863	G713	G647	C584	G518	C445	G375	G314	C249	A173	A104
G1135	U1058	C992	A928	G864	U714	G648	C585	U519	U446	G379	G315	G250	U174	C105
C1136	G1060	G993	U929	C865	A715	G649	U586	U521	A447		C316	G251	G175	C106
G1137	U1061	C994	G930	A866	A716	C650	U587	A522	U451	G386	G319	C252	A176	G107
A1138	G1062	A996	U931	U870	C717	U653	U588	C523	G452	U387	A320	C253	G177	G108
C1139	U1063	C997	A933	U871	C718	A654	U589	G524	A453	G388	U321	G254	C179	U114
U1140	C1064	U999	U934	U872	U720	A655	A590		A454	G389	A322	A255	G180	C115
A1141	U1065	A1000	C935	C873	A721	C656	U591	C527	C455	A391	C323	A256	A181	C116
C1142		A1001	C937	G874	A722	U657	A592	A528	C456	U392	A324	C257	A182	G117
A1143	A1070	G1002	G938	G875	C723	U658	U593	A529	A457	C393	G325	G258	C183	A118
C1144				A877	U724	G659	C594	G530	U458	C394	G326	G259	C184	A119
C1145				A878	G725	C660	U595	C531	U459	U395	G327	G260	G185	U120
C1146				G805	G726	A661	U597	A532	A460	G396	U328	C264	G121	G122
G1149	U1076	C1005	A941	G	A727	G664	U598	U534	U464	U397	G329	A265	G188	G123
C1150	U1077	C1006	A942	G	G728	U665	A599		G465	C398	A330	G266	G189	G124
A1151	C1078	C1007	A943	G	U729	U666	G600	A538		A401	A332	C267	A191	A125
C1152	U1081	A1008	C944	G	A730	A666		G539	A466	U403	G334	G271	C192	A126
G1153	U1082	G1010	A945	G	C731			C540	G467	A404	C335	A272	G193	A127
C1154	U1083	A1011	C946	G	G738	G669	A603	C542	U468	U405	C336	G273	A194	A131
A1155	A1084	U1012	A947	C	A739	C671	G604	G543	G469	U406	C337	C274	A195	G132
G1156	U1085	C1013	C948	C	U740	C672	G605	U544	A470	G407	G338	U275	A196	G133
	A1086	A1014	C951	A	A741	C673	U606	U545	A471	G408	U339	G277	A197	U133
G1159	G1087	G1016	G952	C	U742	G674	A609	U546	A472	G409	A340	A278	C198	U134
C1160	A1088	U1017	C	C	A743	A675	C610	A547	A477	G410	C341	A279	A199	G136
G1163		U1018	G	G	U744		C611	G548	A478	G411	A342	U280	U200	U137
C1164	U1093	U1019	A	C	G745	C679	G612	G549	A479	A412	C343	A281	A204	G138
A1165	U1094	A1021	C	U	U746	C680	A613	C550	A480	A413	C344	G282	G205	U139
		G1022	U	U	G748	G682	A614	G551	G481	C413	A344			



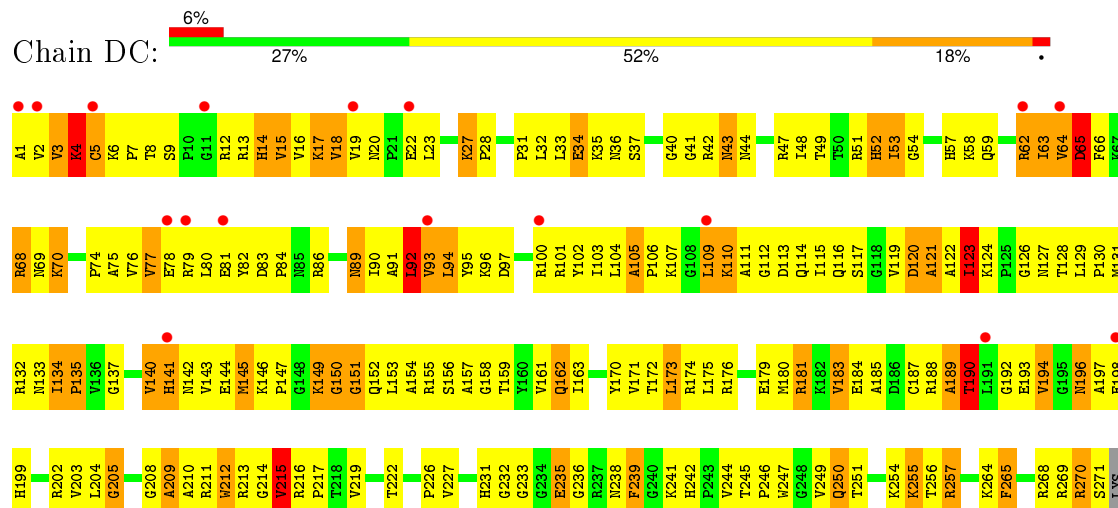
Chain DI:



Chain BC:



Chain DC:



Chain BD:

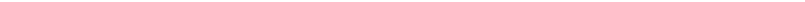
Category	Percentage
M1	4%
I2	4%
G3	4%
L4	4%
V5	4%
K8	4%
V9	4%
G10	4%
M11	4%
T12	4%
R13	4%
I14	4%
E17	4%
D18	4%
G19	4%
V20	4%
S21	4%
P23	4%
V24	4%
T25	4%
V26	4%
I27	4%
V29	4%
E30	4%
A31	4%
N32	4%
R33	4%
V34	4%
T35	4%
Q36	4%
V37	4%
K38	4%
D39	4%
L40	4%
A41	4%
N42	4%
Y45	4%
R46	4%
A47	4%
I48	4%
Q49	4%
V50	4%
T51	4%
T52	4%
G53	4%
A54	4%
K55	4%
K56	4%
A57	4%
N58	4%
R59	4%
V60	4%
T61	4%
L62	4%
R63	4%
E64	4%
A65	4%
F68	4%
A69	4%
K70	4%
G71	4%
G72	4%
V73	4%
E74	4%
A75	4%
G76	4%
R77	4%
G78	4%
L79	4%
R80	4%
E81	4%
F82	4%
A83	4%
L84	4%
A85	4%
E88	4%
E89	4%
F90	4%
T91	4%
E92	4%
V92	4%
G93	4%
Q94	4%
S95	4%
I96	4%
S97	4%
V98	4%
E99	4%
A102	4%
D103	4%
V104	4%
K105	4%
K106	4%
V107	4%
D108	4%
V109	4%
T110	4%
G111	4%
T112	4%
S113	4%
K114	4%
G115	4%
K116	4%
G117	4%
F118	4%
A119	4%
G120	4%
T121	4%
V122	4%
K123	4%
R124	4%
V125	4%
A126	4%
F127	4%
Q130	4%
D131	4%
A132	4%
T133	4%
H134	4%
G135	4%
N136	4%
S137	4%
L138	4%
S139	4%
H140	4%
R141	4%
V142	4%
P143	4%
G144	4%
S145	4%
I146	4%
G147	4%
Q148	4%
N149	4%
Q150	4%
T151	4%
P152	4%
G153	4%
K154	4%
V155	4%
F156	4%
K157	4%
G158	4%
K159	4%
K160	4%
M161	4%
A162	4%
G163	4%
Q164	4%
M165	4%
G166	4%
M167	4%
E168	4%
R169	4%
V170	4%
T171	4%
V172	4%
Q173	4%
S174	4%
L175	4%
D176	4%
V177	4%
F178	4%
R179	4%
A182	4%
E183	4%
R184	4%
N185	4%
L186	4%
L187	4%
L189	4%

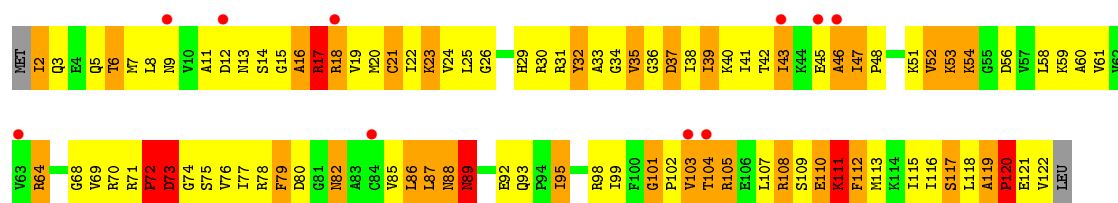
Chain DD:

Category	Percentage
M1	20%
I2	25%
G3	56%
L4	17%
V5	
R8	
V9	
G10	
M11	
T12	
R13	
I14	
E17	
D18	
G19	
V20	
S21	
I22	
P23	
V24	
T25	
V26	
I27	
E28	
V29	
E30	
A31	
N32	
R33	
V34	
T35	
Q36	
V37	
K38	
D39	
L40	
A41	
M42	
Y45	
R46	
A47	
I48	
Q49	
V50	
T51	
T52	
G53	
A54	
K55	
K56	
A57	
R58	
R59	
V60	
T61	
K62	
R63	
E64	
A65	
G66	
H67	
R68	
A69	
K70	
A71	
G72	
V73	
E74	
A75	
G76	
R77	
R80	
E81	
R82	
R83	
L84	
A85	
E86	
G87	
E88	
E89	
F90	
T91	
V92	
G93	
Q94	
S95	
I96	
S97	
V98	
E99	
L100	
F101	
A102	
D103	
V104	
K105	
K106	
V107	
D108	
V109	
T110	
G111	
T112	
S113	
K114	
G115	
K116	
G117	
F118	
A119	
G120	
T121	
V122	
K123	
R124	
N125	
M126	
F127	
R128	
T129	
K130	
D131	
Q132	
T133	
H134	
G135	
N136	
S137	
L138	
S139	
H140	
R141	
V142	
P143	
G144	
S145	
I146	
G147	
Q148	
N149	
Q150	
T151	
P152	
G153	
K154	
V155	
F156	
K157	
G158	
K159	
K160	
M161	
A162	
G163	
Q164	
M165	
G166	
V167	
E168	
R169	
V170	
T171	
V172	
Q173	
S174	
L175	
D176	
V177	
V178	
R179	
V180	
L181	
A182	
R183	
R184	
N185	
L186	
L187	
L188	
V189	
K190	
G191	
A192	
V193	
P194	
T197	
G198	
S199	
L201	
I202	
V203	
K204	
P205	
A206	
A209	

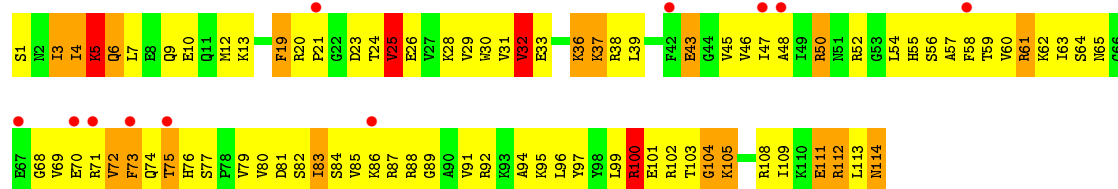
Chain BK:

Category	Percentage
MET	
12	
9%	9%
19%	19%
49%	49%
26%	26%
5%	5%

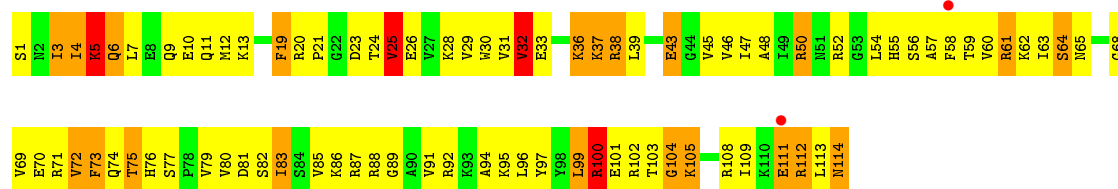
Chain DK: 



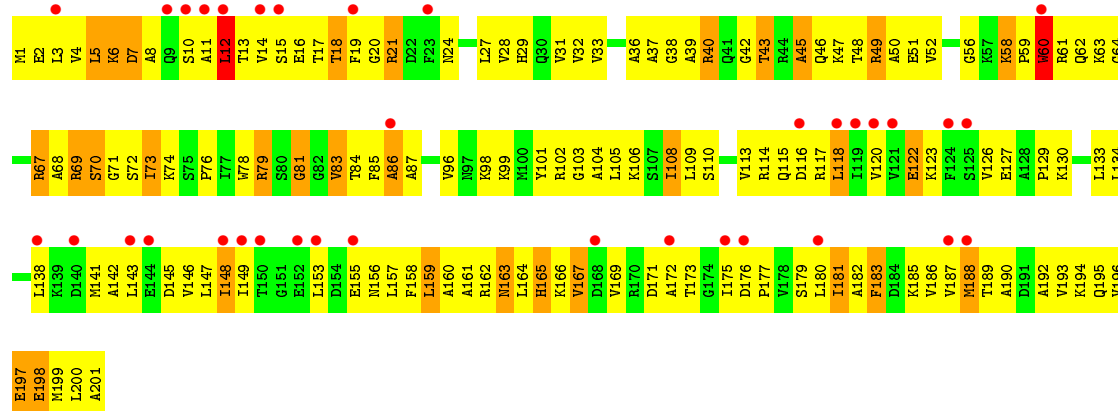
• Molecule 28: 50S ribosomal protein L19



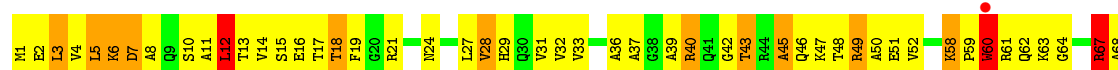
• Molecule 28: 50S ribosomal protein L19

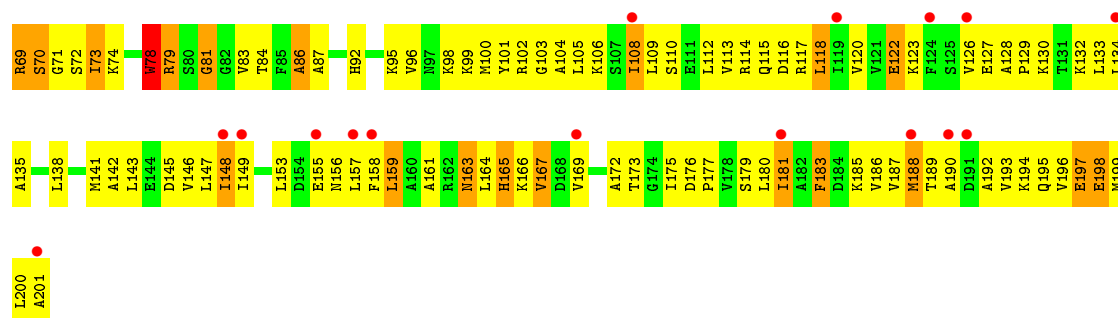


• Molecule 29: 50S ribosomal protein L4

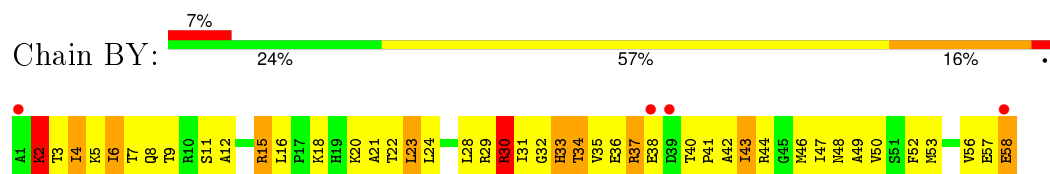


• Molecule 29: 50S ribosomal protein L4

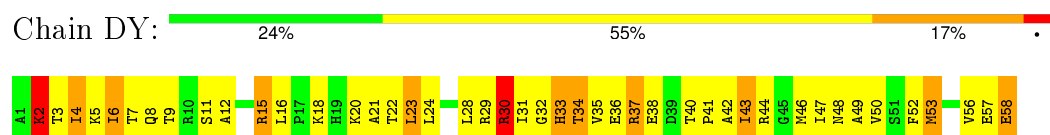




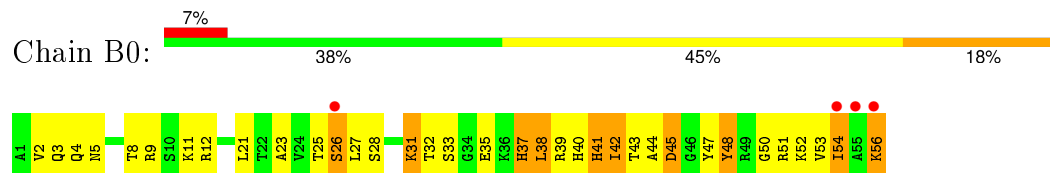
- Molecule 30: 50S ribosomal protein L30



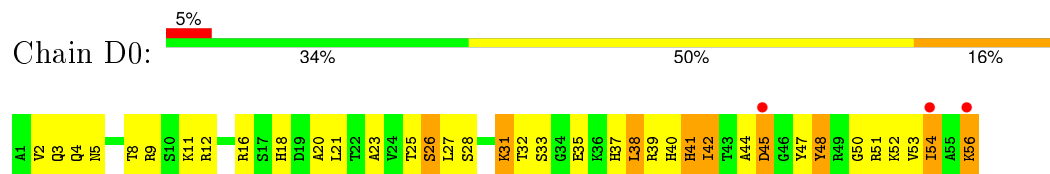
- Molecule 30: 50S ribosomal protein L30



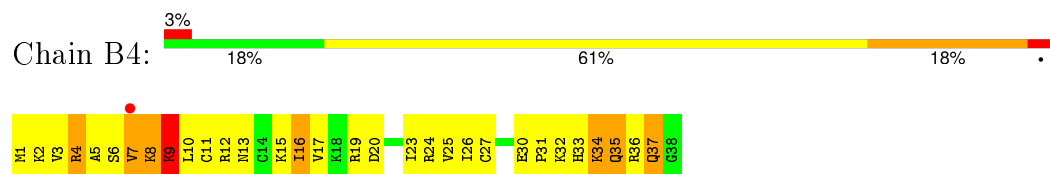
- Molecule 31: 50S ribosomal protein L32



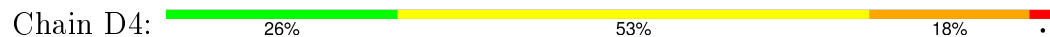
- Molecule 31: 50S ribosomal protein L32



- Molecule 32: 50S ribosomal protein L36



- Molecule 32: 50S ribosomal protein L36

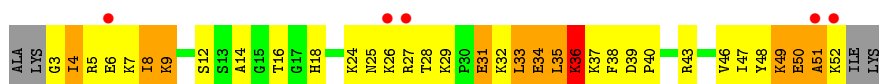




- Molecule 33: 50S ribosomal protein L33



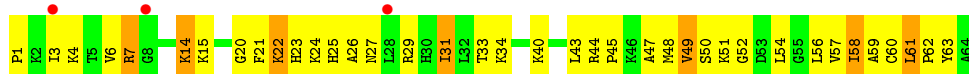
- Molecule 33: 50S ribosomal protein L33



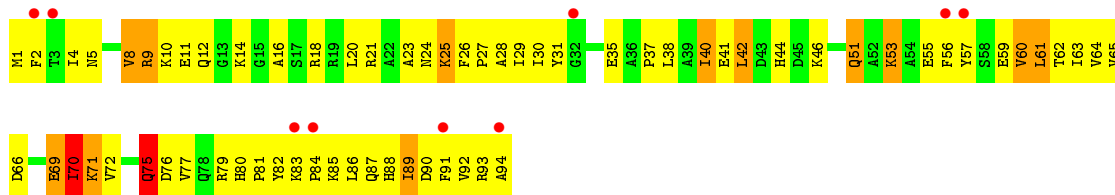
- Molecule 34: 50S ribosomal protein L35



- Molecule 34: 50S ribosomal protein L35

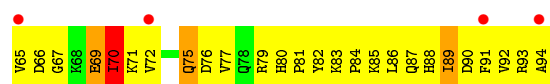


- Molecule 35: 50S ribosomal protein L25



- Molecule 35: 50S ribosomal protein L25





- Molecule 36: 50S ribosomal protein L34



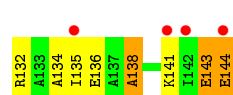
- Molecule 36: 50S ribosomal protein L34



- Molecule 37: 50S ribosomal protein L15

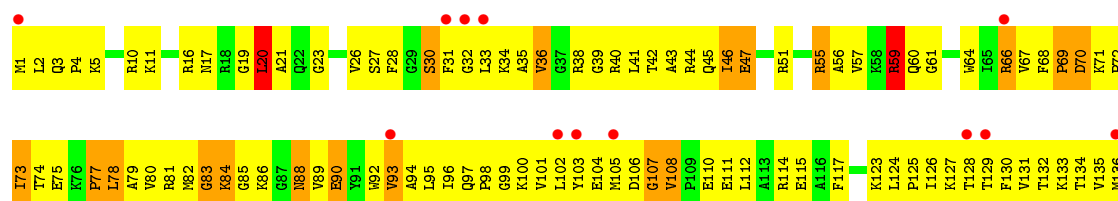


- Molecule 37: 50S ribosomal protein L15

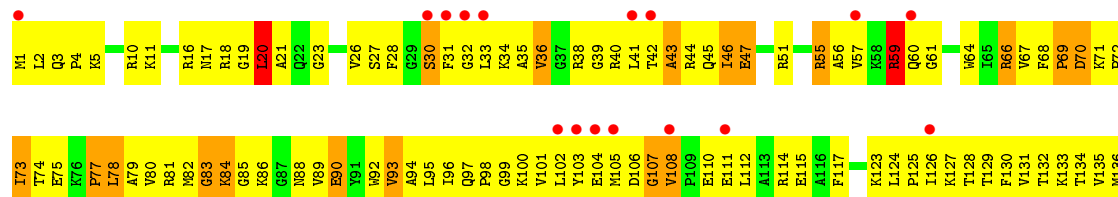


- Molecule 38: 50S ribosomal protein L16

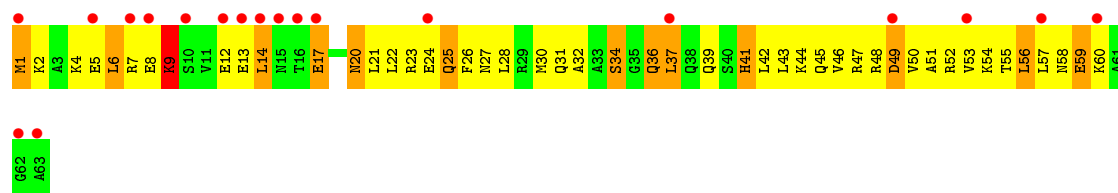




• Molecule 38: 50S ribosomal protein L16



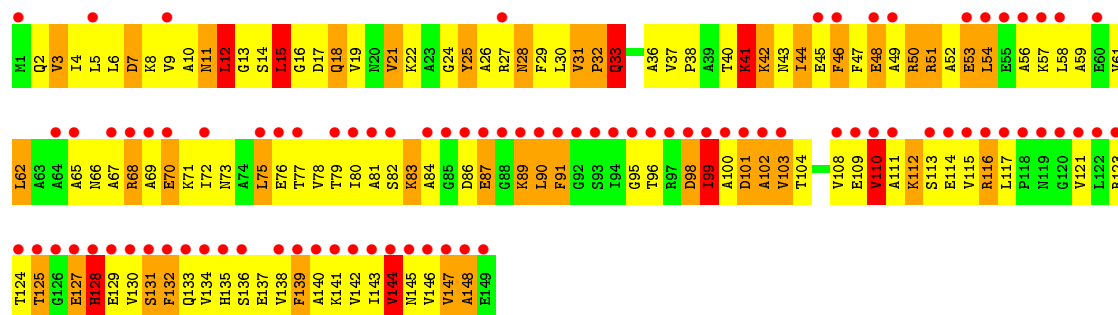
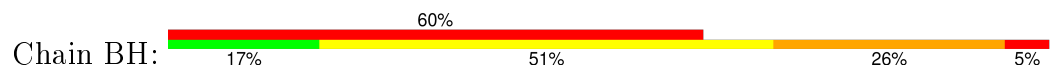
• Molecule 39: 50S ribosomal protein L29



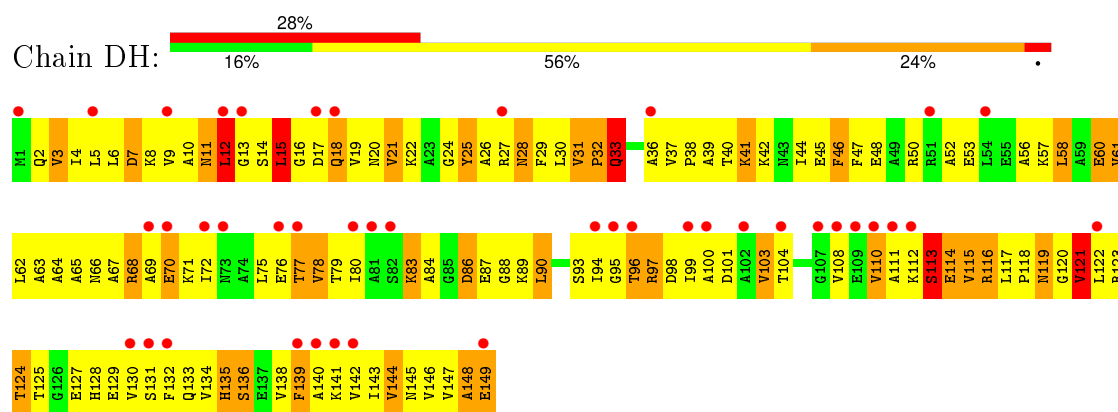
• Molecule 39: 50S ribosomal protein L29



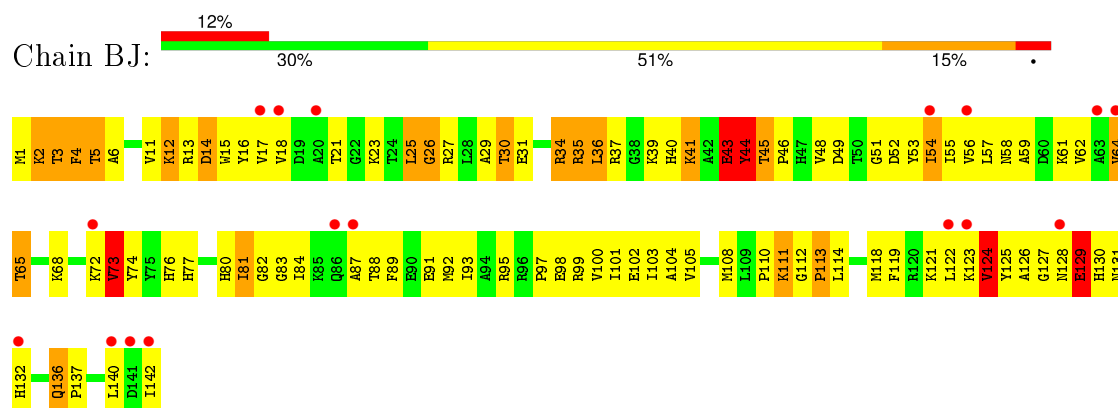
• Molecule 40: 50S ribosomal protein L9



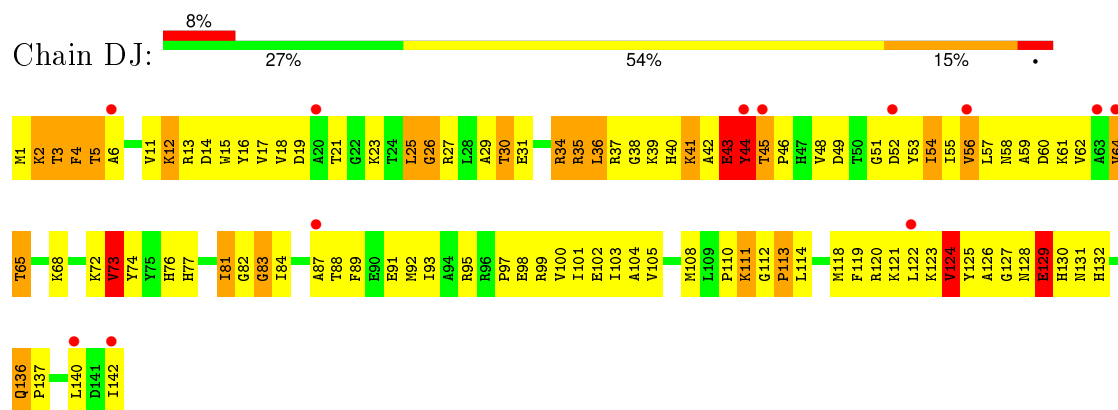
• Molecule 40: 50S ribosomal protein L9



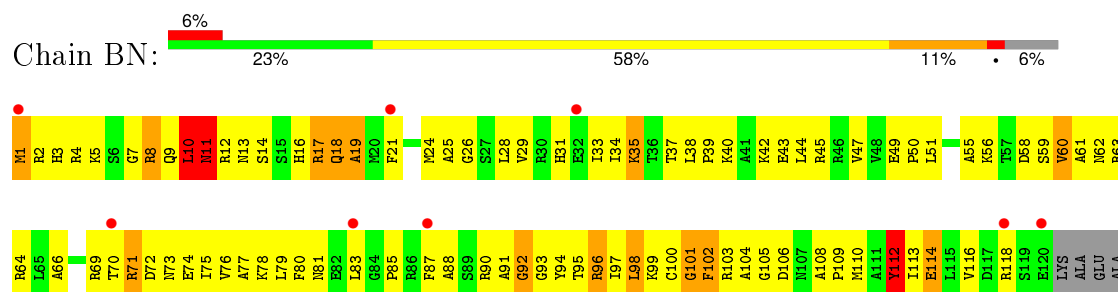
• Molecule 41: 50S ribosomal protein L13



• Molecule 41: 50S ribosomal protein L13



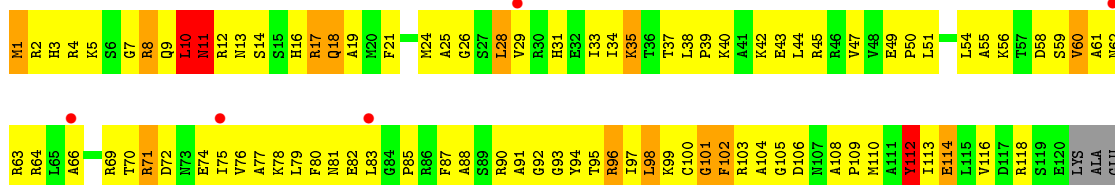
• Molecule 42: 50S ribosomal protein L17



ALA
ALA
GLU

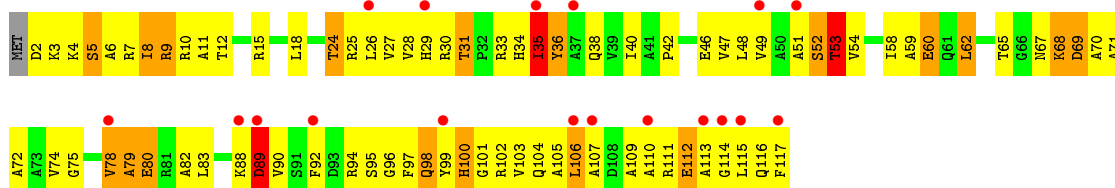
- Molecule 42: 50S ribosomal protein L17

Chain DN: 

ALA
ALA
GLU

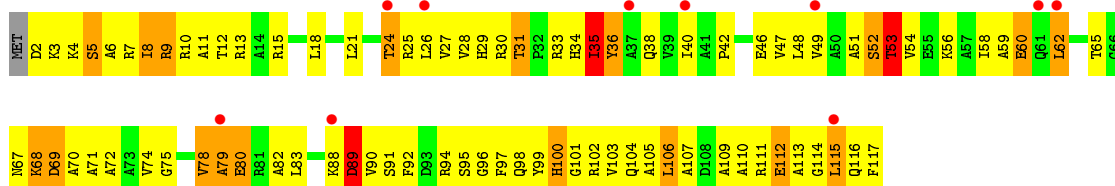
- Molecule 43: 50S ribosomal protein L18

Chain BO: 



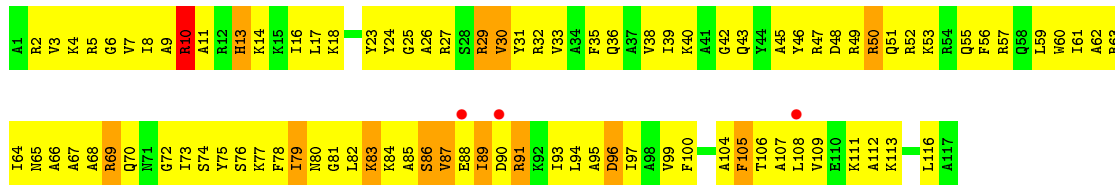
- Molecule 43: 50S ribosomal protein L18

Chain DO: 



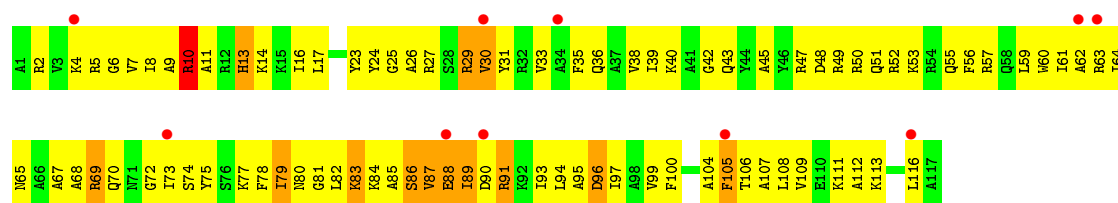
- Molecule 44: 50S ribosomal protein L20

Chain BQ: 

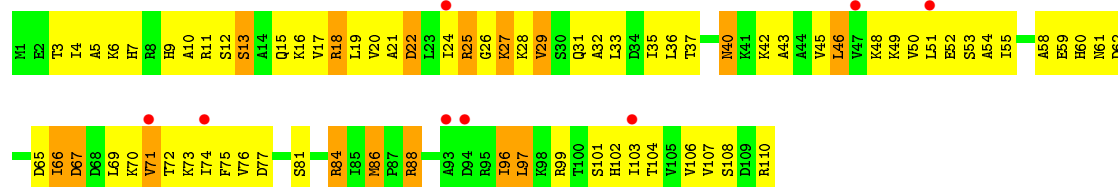


- Molecule 44: 50S ribosomal protein L20

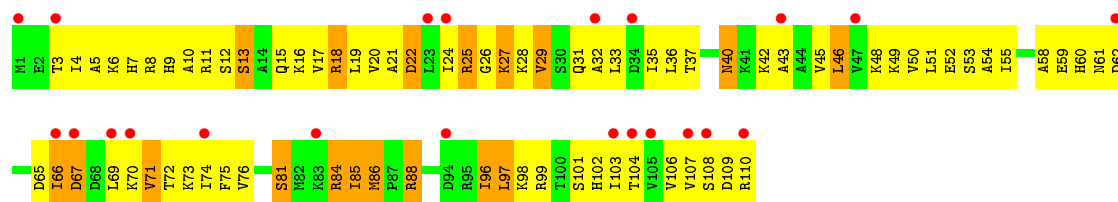
Chain DQ: 



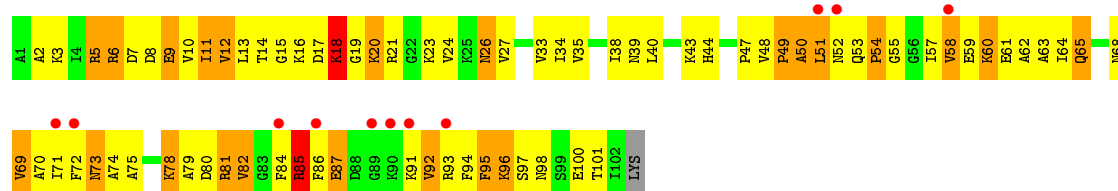
• Molecule 45: 50S ribosomal protein L22



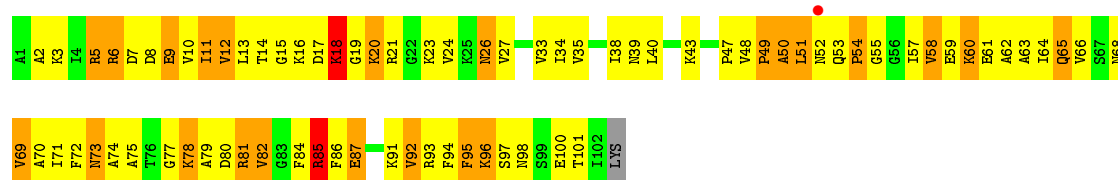
• Molecule 45: 50S ribosomal protein L22



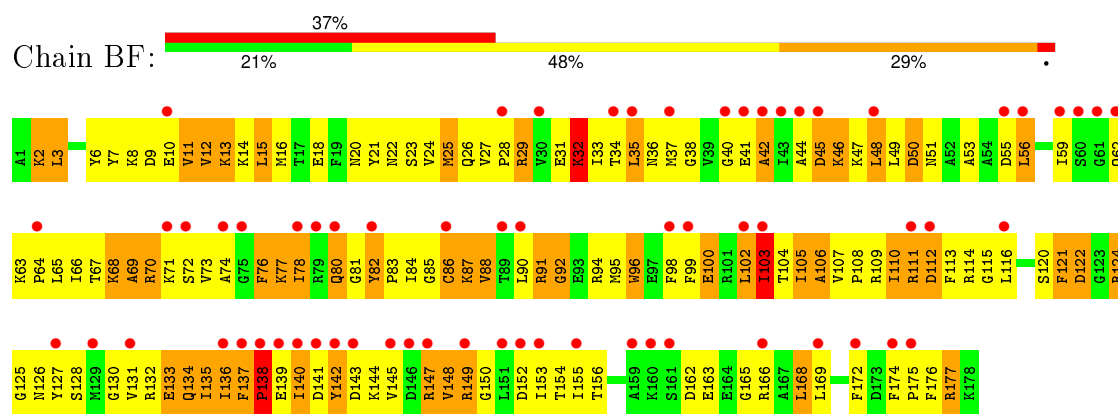
• Molecule 46: 50S ribosomal protein L24



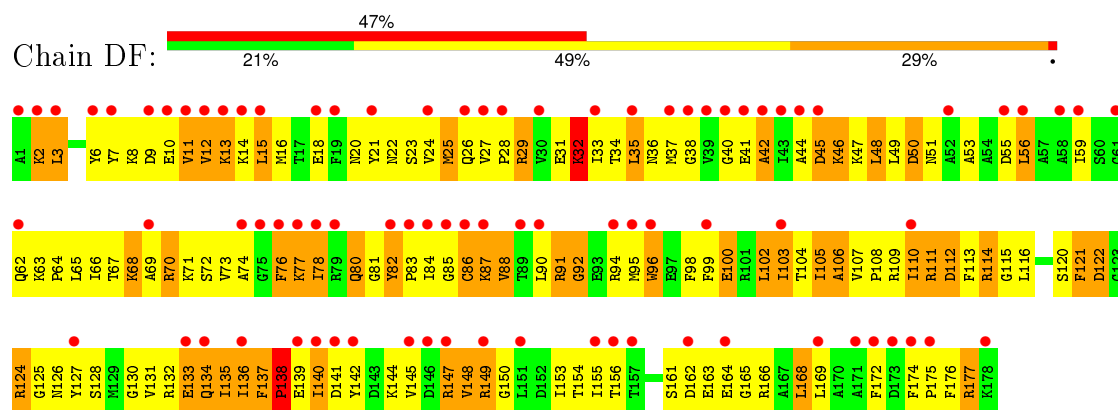
• Molecule 46: 50S ribosomal protein L24



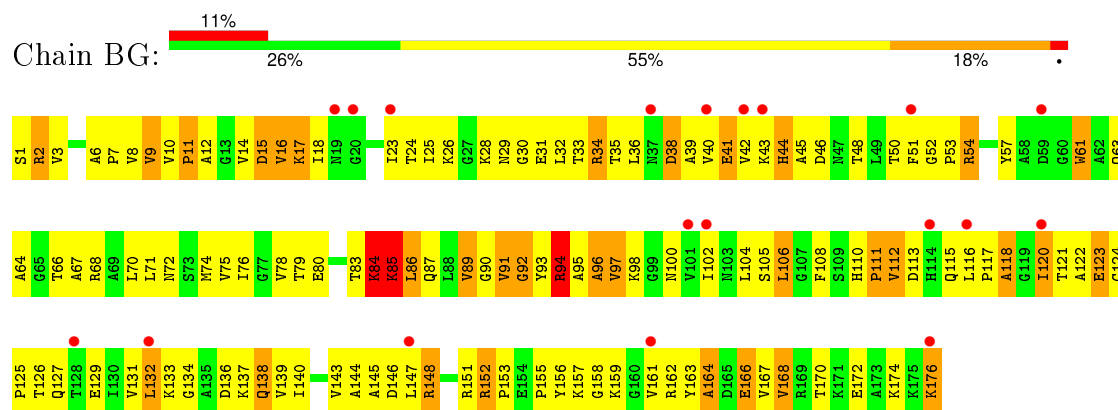
• Molecule 47: 50S ribosomal protein L5



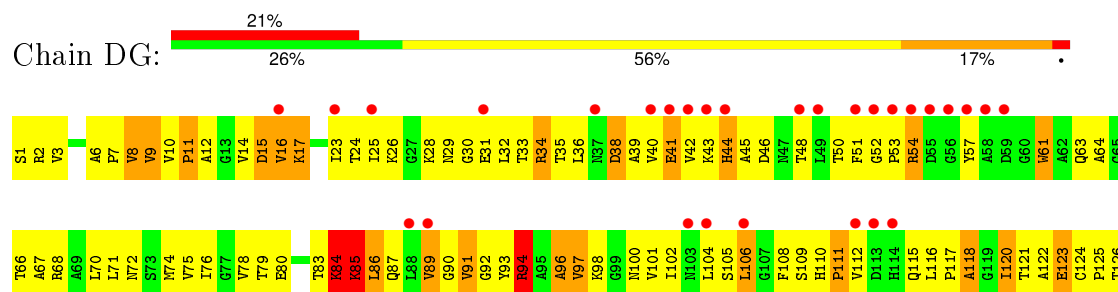
• Molecule 47: 50S ribosomal protein L5

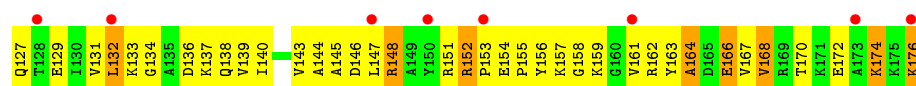


• Molecule 48: 50S ribosomal protein L6

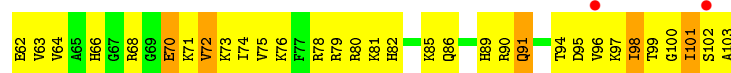


• Molecule 48: 50S ribosomal protein L6

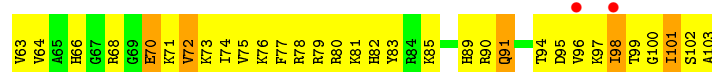
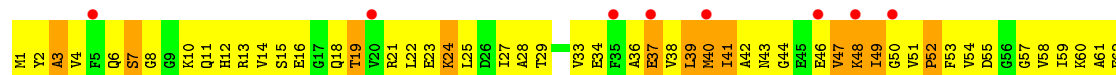




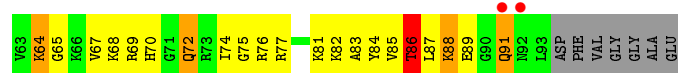
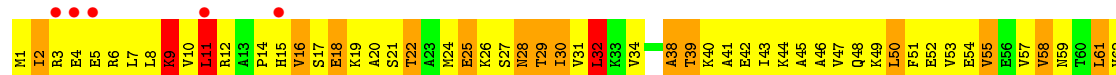
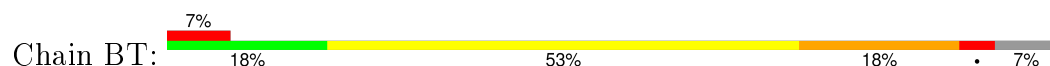
- Molecule 49: 50S ribosomal protein L21



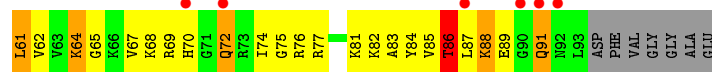
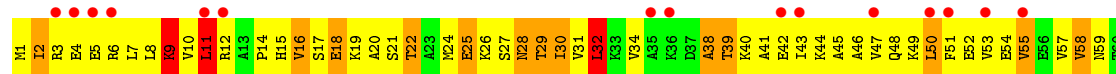
- Molecule 49: 50S ribosomal protein L21



- Molecule 50: 50S ribosomal protein L23

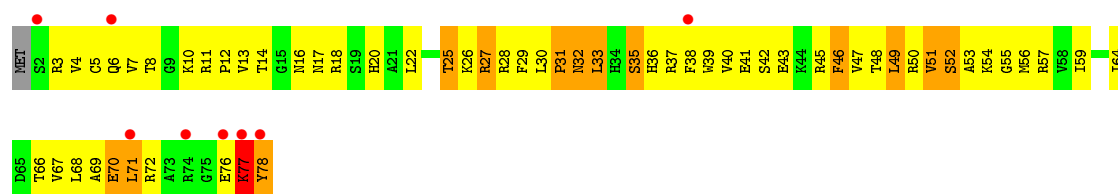


- Molecule 50: 50S ribosomal protein L23

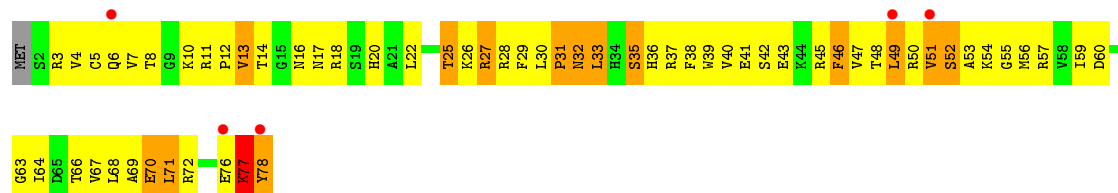


- Molecule 51: 50S ribosomal protein L28

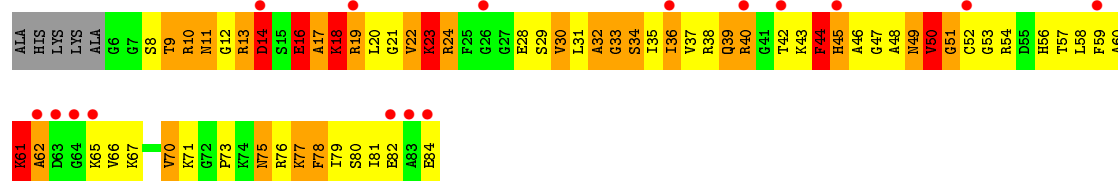
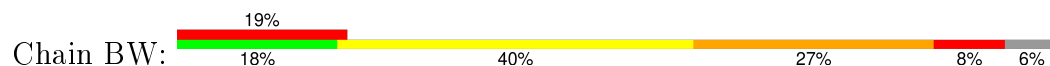




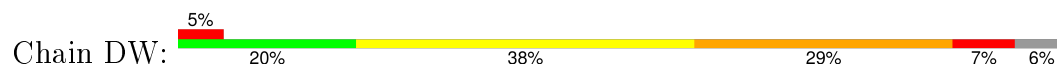
- Molecule 51: 50S ribosomal protein L28



- Molecule 52: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L27



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.50 182.94 – 3.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.50) 73.0 (182.94-3.53)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.264 , 0.306 0.232 , 0.271	Depositor DCC
R_{free} test set	25274 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	132.6	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 79.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 521228 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284201	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SCM, ZN, MG, NMY

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 120 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1291	0
1	CA	32831	0	16521	1302	0
2	AC	1624	0	1699	189	0
2	CC	1624	0	1699	189	0
3	AD	1643	0	1710	127	0
3	CD	1643	0	1710	128	0
4	AE	1105	0	1148	94	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

The worst 5 of 16740 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.32	1.27
23:BB:2305:U:H1'	47:BF:132:ARG:HA	1.33	1.10
40:BH:125:THR:HA	40:BH:146:VAL:HB	1.28	1.10
18:CB:69:VAL:HG23	18:CB:162:VAL:HB	1.34	1.09
23:DB:1098:A:H3'	24:DI:3:LYS:HA	1.32	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AC	204/232 (88%)	130 (64%)	44 (22%)	30 (15%)	0 4
2	CC	204/232 (88%)	137 (67%)	49 (24%)	18 (9%)	1 12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/205 (99%)	153 (75%)	40 (20%)	10 (5%)	3	27
3	CD	203/205 (99%)	153 (75%)	40 (20%)	10 (5%)	3	27
4	AE	148/166 (89%)	116 (78%)	24 (16%)	8 (5%)	2	25
4	CE	148/166 (89%)	114 (77%)	25 (17%)	9 (6%)	2	21
5	AF	98/135 (73%)	63 (64%)	25 (26%)	10 (10%)	1	9
5	CF	98/135 (73%)	64 (65%)	24 (24%)	10 (10%)	1	9
6	AG	148/178 (83%)	110 (74%)	30 (20%)	8 (5%)	2	25
6	CG	150/178 (84%)	111 (74%)	28 (19%)	11 (7%)	1	16
7	AH	127/129 (98%)	92 (72%)	31 (24%)	4 (3%)	5	41
7	CH	127/129 (98%)	92 (72%)	31 (24%)	4 (3%)	5	41
8	AI	125/129 (97%)	80 (64%)	35 (28%)	10 (8%)	1	13
8	CI	125/129 (97%)	80 (64%)	34 (27%)	11 (9%)	1	12
9	AJ	96/103 (93%)	59 (62%)	25 (26%)	12 (12%)	0	6
9	CJ	96/103 (93%)	64 (67%)	22 (23%)	10 (10%)	1	8
10	AK	115/128 (90%)	87 (76%)	23 (20%)	5 (4%)	3	31
10	CK	115/128 (90%)	86 (75%)	24 (21%)	5 (4%)	3	31
11	AL	121/123 (98%)	69 (57%)	37 (31%)	15 (12%)	0	6
11	CL	121/123 (98%)	72 (60%)	34 (28%)	15 (12%)	0	6
12	AM	112/117 (96%)	74 (66%)	25 (22%)	13 (12%)	0	7
12	CM	111/117 (95%)	78 (70%)	21 (19%)	12 (11%)	0	8
13	AP	80/82 (98%)	53 (66%)	20 (25%)	7 (9%)	1	12
13	CP	78/82 (95%)	52 (67%)	19 (24%)	7 (9%)	1	11
14	AQ	78/83 (94%)	59 (76%)	15 (19%)	4 (5%)	2	26
14	CQ	79/83 (95%)	57 (72%)	18 (23%)	4 (5%)	2	26
15	AR	53/74 (72%)	40 (76%)	13 (24%)	0	100	100
15	CR	53/74 (72%)	41 (77%)	11 (21%)	1 (2%)	10	51
16	AS	77/91 (85%)	49 (64%)	24 (31%)	4 (5%)	2	25
16	CS	78/91 (86%)	57 (73%)	16 (20%)	5 (6%)	2	20
17	AT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	2	21
17	CT	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	2	21
18	AB	216/240 (90%)	135 (62%)	56 (26%)	25 (12%)	0	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CB	216/240 (90%)	145 (67%)	52 (24%)	19 (9%)	1	12
19	AU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	0	6
19	CU	49/70 (70%)	29 (59%)	14 (29%)	6 (12%)	0	6
20	AO	86/89 (97%)	62 (72%)	18 (21%)	6 (7%)	1	18
20	CO	86/89 (97%)	60 (70%)	25 (29%)	1 (1%)	16	61
21	AN	92/100 (92%)	53 (58%)	30 (33%)	9 (10%)	1	10
21	CN	92/100 (92%)	49 (53%)	31 (34%)	12 (13%)	0	5
24	BI	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	6	42
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	4	37
25	BC	269/272 (99%)	163 (61%)	63 (23%)	43 (16%)	0	3
25	DC	269/272 (99%)	162 (60%)	61 (23%)	46 (17%)	0	3
26	BD	207/209 (99%)	118 (57%)	57 (28%)	32 (16%)	0	3
26	DD	207/209 (99%)	118 (57%)	58 (28%)	31 (15%)	0	3
27	BK	119/123 (97%)	70 (59%)	27 (23%)	22 (18%)	0	2
27	DK	119/123 (97%)	69 (58%)	29 (24%)	21 (18%)	0	2
28	BP	112/114 (98%)	66 (59%)	29 (26%)	17 (15%)	0	3
28	DP	112/114 (98%)	66 (59%)	29 (26%)	17 (15%)	0	3
29	BE	199/201 (99%)	124 (62%)	51 (26%)	24 (12%)	0	6
29	DE	199/201 (99%)	124 (62%)	48 (24%)	27 (14%)	0	4
30	BY	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	11
30	DY	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	11
31	B0	54/56 (96%)	36 (67%)	12 (22%)	6 (11%)	0	7
31	D0	54/56 (96%)	36 (67%)	12 (22%)	6 (11%)	0	7
32	B4	36/38 (95%)	20 (56%)	9 (25%)	7 (19%)	0	2
32	D4	36/38 (95%)	21 (58%)	8 (22%)	7 (19%)	0	2
33	B1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	13
33	D1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	13
34	B3	62/64 (97%)	39 (63%)	17 (27%)	6 (10%)	1	10
34	D3	62/64 (97%)	39 (63%)	18 (29%)	5 (8%)	1	13
35	BV	92/94 (98%)	60 (65%)	22 (24%)	10 (11%)	0	8
35	DV	92/94 (98%)	59 (64%)	23 (25%)	10 (11%)	0	8

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	DZ	75/78 (96%)	48 (64%)	19 (25%)	8 (11%)	0	8
52	BW	77/84 (92%)	26 (34%)	26 (34%)	25 (32%)	0	0
52	DW	77/84 (92%)	26 (34%)	25 (32%)	26 (34%)	0	0
All	All	11241/11914 (94%)	7227 (64%)	2767 (25%)	1247 (11%)	0	7

5 of 1247 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	137 (81%)	33 (19%)	2	10
2	CC	170/189 (90%)	139 (82%)	31 (18%)	2	12
3	AD	172/172 (100%)	153 (89%)	19 (11%)	8	36
3	CD	172/172 (100%)	154 (90%)	18 (10%)	8	38
4	AE	113/125 (90%)	90 (80%)	23 (20%)	1	8
4	CE	113/125 (90%)	91 (80%)	22 (20%)	2	10
5	AF	87/116 (75%)	75 (86%)	12 (14%)	4	25
5	CF	87/116 (75%)	74 (85%)	13 (15%)	4	22
6	AG	123/146 (84%)	104 (85%)	19 (15%)	3	20
6	CG	125/146 (86%)	102 (82%)	23 (18%)	2	11
7	AH	104/104 (100%)	96 (92%)	8 (8%)	16	54
7	CH	104/104 (100%)	97 (93%)	7 (7%)	20	61
8	AI	105/106 (99%)	88 (84%)	17 (16%)	3	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/106 (99%)	77 (73%)	28 (27%)	0	4
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	4	24
9	CJ	86/90 (96%)	75 (87%)	11 (13%)	5	28
10	AK	90/98 (92%)	77 (86%)	13 (14%)	4	23
10	CK	90/98 (92%)	76 (84%)	14 (16%)	3	20
11	AL	103/103 (100%)	84 (82%)	19 (18%)	2	11
11	CL	103/103 (100%)	84 (82%)	19 (18%)	2	11
12	AM	92/95 (97%)	79 (86%)	13 (14%)	4	24
12	CM	91/95 (96%)	70 (77%)	21 (23%)	1	5
13	AP	65/65 (100%)	56 (86%)	9 (14%)	4	25
13	CP	65/65 (100%)	56 (86%)	9 (14%)	4	25
14	AQ	74/77 (96%)	65 (88%)	9 (12%)	6	29
14	CQ	75/77 (97%)	66 (88%)	9 (12%)	6	30
15	AR	48/64 (75%)	42 (88%)	6 (12%)	6	29
15	CR	48/64 (75%)	42 (88%)	6 (12%)	6	29
16	AS	70/78 (90%)	48 (69%)	22 (31%)	0	3
16	CS	71/78 (91%)	53 (75%)	18 (25%)	1	4
17	AT	65/65 (100%)	56 (86%)	9 (14%)	4	25
17	CT	65/65 (100%)	56 (86%)	9 (14%)	4	25
18	AB	180/198 (91%)	149 (83%)	31 (17%)	2	15
18	CB	180/198 (91%)	141 (78%)	39 (22%)	1	7
19	AU	44/60 (73%)	33 (75%)	11 (25%)	1	4
19	CU	44/60 (73%)	33 (75%)	11 (25%)	1	4
20	AO	76/77 (99%)	69 (91%)	7 (9%)	11	45
20	CO	76/77 (99%)	64 (84%)	12 (16%)	3	19
21	AN	79/83 (95%)	69 (87%)	10 (13%)	5	28
21	CN	79/83 (95%)	64 (81%)	15 (19%)	2	10
24	BI	109/109 (100%)	108 (99%)	1 (1%)	84	94
24	DI	109/109 (100%)	103 (94%)	6 (6%)	27	67
25	BC	216/217 (100%)	184 (85%)	32 (15%)	4	22
25	DC	216/217 (100%)	184 (85%)	32 (15%)	4	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	164/164 (100%)	136 (83%)	28 (17%)	2	15
26	DD	164/164 (100%)	136 (83%)	28 (17%)	2	15
27	BK	102/104 (98%)	74 (72%)	28 (28%)	0	3
27	DK	102/104 (98%)	73 (72%)	29 (28%)	0	3
28	BP	99/99 (100%)	83 (84%)	16 (16%)	3	17
28	DP	99/99 (100%)	83 (84%)	16 (16%)	3	17
29	BE	165/165 (100%)	146 (88%)	19 (12%)	7	33
29	DE	165/165 (100%)	145 (88%)	20 (12%)	6	30
30	BY	48/48 (100%)	38 (79%)	10 (21%)	1	8
30	DY	48/48 (100%)	37 (77%)	11 (23%)	1	6
31	B0	47/47 (100%)	38 (81%)	9 (19%)	2	10
31	D0	47/47 (100%)	38 (81%)	9 (19%)	2	10
32	B4	34/34 (100%)	31 (91%)	3 (9%)	12	48
32	D4	34/34 (100%)	31 (91%)	3 (9%)	12	48
33	B1	45/48 (94%)	35 (78%)	10 (22%)	1	6
33	D1	45/48 (94%)	35 (78%)	10 (22%)	1	6
34	B3	51/51 (100%)	48 (94%)	3 (6%)	24	65
34	D3	51/51 (100%)	48 (94%)	3 (6%)	24	65
35	BV	78/78 (100%)	65 (83%)	13 (17%)	3	16
35	DV	78/78 (100%)	65 (83%)	13 (17%)	3	16
36	B2	38/38 (100%)	28 (74%)	10 (26%)	0	4
36	D2	38/38 (100%)	28 (74%)	10 (26%)	0	4
37	BL	102/103 (99%)	85 (83%)	17 (17%)	3	16
37	DL	102/103 (99%)	85 (83%)	17 (17%)	3	16
38	BM	109/109 (100%)	93 (85%)	16 (15%)	4	22
38	DM	109/109 (100%)	93 (85%)	16 (15%)	4	22
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	7
39	DX	55/55 (100%)	43 (78%)	12 (22%)	1	7
40	BH	114/114 (100%)	83 (73%)	31 (27%)	0	3
40	DH	114/114 (100%)	87 (76%)	27 (24%)	1	5
41	BJ	116/116 (100%)	100 (86%)	16 (14%)	4	25

Continued on next page...

Continued from previous page...

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

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

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

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

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

5.3.3 RNA ⓘ

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

5 of 1462 RNA backbone outliers are listed below:

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

5 of 78 RNA pucker outliers are listed below:

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

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 348 ligands modelled in this entry, 342 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	NMY	AA	1601	-	45,45,45	1.93	13 (28%)	58,67,67	1.17	6 (10%)
55	SCM	AA	1662	-	23,25,25	1.67	8 (34%)	22,39,39	1.03	1 (4%)
53	NMY	BB	3001	-	45,45,45	1.86	12 (26%)	58,67,67	1.20	6 (10%)
53	NMY	CA	1601	-	45,45,45	1.85	13 (28%)	58,67,67	1.21	6 (10%)
55	SCM	CA	1661	-	23,25,25	1.67	7 (30%)	22,39,39	1.04	1 (4%)
53	NMY	DB	3001	-	45,45,45	1.90	13 (28%)	58,67,67	1.15	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	NMY	AA	1601	-	-	0/18/94/94	0/4/4/4
55	SCM	AA	1662	-	-	0/4/57/57	0/3/3/3
53	NMY	BB	3001	-	-	0/18/94/94	0/4/4/4
53	NMY	CA	1601	-	-	0/18/94/94	0/4/4/4
55	SCM	CA	1661	-	-	0/4/57/57	0/3/3/3
53	NMY	DB	3001	-	-	0/18/94/94	0/4/4/4

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	AA	1662	SCM	C5-C4	-2.03	1.52	1.54
53	DB	3001	NMY	C6-C5	2.01	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	CA	1601	NMY	C6-C5	2.04	1.57	1.52
53	AA	1601	NMY	C6-C5	2.05	1.57	1.52
53	CA	1601	NMY	C20-C21	2.07	1.57	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	CA	1661	SCM	C2M-C2-C3	-2.96	108.15	113.45
55	AA	1662	SCM	C2M-C2-C3	-2.88	108.28	113.45
53	DB	3001	NMY	O11-C13-C14	2.08	112.07	107.75
53	CA	1601	NMY	O11-C13-C14	2.14	112.21	107.75
53	CA	1601	NMY	O14-C14-C15	2.18	117.45	111.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

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

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%)	-0.72	8 (0%) 91 88	16, 81, 159, 180	0
1	CA	1530/1542 (99%)	-0.66	1 (0%) 95 94	9, 57, 133, 180	0
2	AC	206/232 (88%)	0.47	20 (9%) 10 9	9, 76, 136, 180	0
2	CC	206/232 (88%)	0.30	16 (7%) 16 13	7, 75, 127, 180	0
3	AD	205/205 (100%)	0.63	25 (12%) 5 6	24, 92, 157, 180	0
3	CD	205/205 (100%)	0.52	16 (7%) 16 13	10, 64, 139, 180	0
4	AE	150/166 (90%)	0.52	13 (8%) 13 12	11, 74, 139, 176	0
4	CE	150/166 (90%)	0.82	25 (16%) 2 2	5, 61, 132, 180	0
5	AF	100/135 (74%)	1.06	17 (17%) 2 2	11, 86, 144, 172	0
5	CF	100/135 (74%)	0.58	9 (9%) 12 10	7, 83, 173, 180	0
6	AG	150/178 (84%)	0.25	9 (6%) 25 19	23, 104, 153, 180	0
6	CG	152/178 (85%)	-0.02	4 (2%) 59 49	27, 90, 147, 180	0
7	AH	129/129 (100%)	0.93	20 (15%) 3 3	13, 88, 155, 180	0
7	CH	129/129 (100%)	0.59	14 (10%) 7 7	5, 61, 127, 180	0
8	AI	127/129 (98%)	0.47	16 (12%) 5 6	36, 91, 150, 180	0
8	CI	127/129 (98%)	0.09	4 (3%) 52 43	20, 92, 148, 180	0
9	AJ	98/103 (95%)	0.42	4 (4%) 41 32	22, 94, 151, 180	0
9	CJ	98/103 (95%)	0.77	12 (12%) 5 6	17, 89, 156, 180	0
10	AK	117/128 (91%)	0.07	6 (5%) 32 24	14, 67, 125, 180	0
10	CK	117/128 (91%)	0.09	3 (2%) 59 49	5, 56, 125, 178	0
11	AL	123/123 (100%)	0.51	14 (11%) 7 7	19, 80, 133, 180	0
11	CL	123/123 (100%)	0.20	6 (4%) 33 25	7, 51, 135, 180	0
12	AM	114/117 (97%)	0.72	21 (18%) 2 2	56, 120, 166, 180	0
12	CM	113/117 (96%)	0.61	17 (15%) 3 3	38, 109, 165, 180	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	82/82 (100%)	2.17	30 (36%) 0 0	38, 91, 152, 180	0
13	CP	80/82 (97%)	0.53	10 (12%) 5 6	6, 63, 141, 180	0
14	AQ	80/83 (96%)	0.87	12 (15%) 3 3	37, 99, 151, 180	0
14	CQ	81/83 (97%)	0.56	3 (3%) 45 36	17, 71, 129, 180	0
15	AR	55/74 (74%)	0.57	2 (3%) 46 37	16, 76, 149, 180	0
15	CR	55/74 (74%)	0.43	4 (7%) 18 14	21, 66, 126, 180	0
16	AS	79/91 (86%)	1.61	30 (37%) 0 0	55, 121, 180, 180	0
16	CS	80/91 (87%)	1.06	18 (22%) 1 1	70, 109, 174, 180	0
17	AT	85/86 (98%)	-0.19	0 100 100	49, 106, 179, 180	0
17	CT	85/86 (98%)	-0.05	2 (2%) 62 52	19, 65, 143, 159	0
18	AB	218/240 (90%)	0.25	18 (8%) 14 12	22, 94, 153, 180	0
18	CB	218/240 (90%)	0.77	35 (16%) 3 3	19, 102, 160, 180	0
19	AU	51/70 (72%)	0.27	2 (3%) 43 35	29, 101, 151, 180	0
19	CU	51/70 (72%)	0.44	4 (7%) 16 13	24, 113, 155, 180	0
20	AO	88/89 (98%)	0.54	7 (7%) 15 12	18, 83, 137, 179	0
20	CO	88/89 (98%)	-0.08	0 100 100	7, 60, 118, 161	0
21	AN	96/100 (96%)	0.73	12 (12%) 5 6	13, 98, 151, 180	0
21	CN	96/100 (96%)	0.89	20 (20%) 1 1	12, 81, 150, 180	0
22	BA	117/120 (97%)	-0.21	2 (1%) 73 64	35, 74, 117, 167	0
22	DA	117/120 (97%)	-0.50	1 (0%) 85 78	36, 86, 127, 180	0
23	BB	2841/2904 (97%)	-0.43	28 (0%) 84 76	6, 54, 148, 180	0
23	DB	2841/2904 (97%)	-0.43	15 (0%) 91 88	5, 48, 146, 180	0
24	BI	141/141 (100%)	2.72	78 (55%) 0 0	95, 172, 180, 180	0
24	DI	141/141 (100%)	2.07	61 (43%) 0 0	91, 179, 180, 180	0
25	BC	271/272 (99%)	0.82	42 (15%) 3 3	5, 50, 103, 180	0
25	DC	271/272 (99%)	0.46	17 (6%) 23 18	5, 40, 100, 146	0
26	BD	209/209 (100%)	0.10	8 (3%) 44 36	7, 68, 146, 180	0
26	DD	209/209 (100%)	0.87	41 (19%) 1 2	5, 49, 129, 180	0
27	BK	121/123 (98%)	0.70	11 (9%) 11 10	7, 69, 139, 180	0
27	DK	121/123 (98%)	0.76	10 (8%) 14 12	5, 41, 118, 180	0
28	BP	114/114 (100%)	0.53	11 (9%) 10 9	26, 85, 142, 175	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.34	2 (1%) 71 62	5, 49, 103, 145	0
29	BE	201/201 (100%)	0.88	35 (17%) 2 2	5, 63, 143, 180	0
29	DE	201/201 (100%)	0.44	17 (8%) 13 12	5, 70, 144, 180	0
30	BY	58/58 (100%)	0.43	4 (6%) 20 16	20, 62, 140, 180	0
30	DY	58/58 (100%)	-0.14	0 100 100	5, 66, 116, 142	0
31	B0	56/56 (100%)	0.18	4 (7%) 19 15	20, 80, 163, 180	0
31	D0	56/56 (100%)	0.24	3 (5%) 29 23	12, 58, 116, 165	0
32	B4	38/38 (100%)	0.17	1 (2%) 59 49	5, 75, 120, 137	0
32	D4	38/38 (100%)	-0.32	0 100 100	7, 60, 114, 135	0
33	B1	50/54 (92%)	1.28	7 (14%) 4 4	15, 70, 135, 180	0
33	D1	50/54 (92%)	0.67	5 (10%) 9 9	20, 69, 142, 157	0
34	B3	64/64 (100%)	0.50	5 (7%) 16 13	13, 50, 102, 148	0
34	D3	64/64 (100%)	0.35	3 (4%) 35 28	5, 42, 88, 133	0
35	BV	94/94 (100%)	0.56	9 (9%) 10 9	21, 89, 143, 180	0
35	DV	94/94 (100%)	0.31	13 (13%) 4 4	9, 96, 151, 169	0
36	B2	46/46 (100%)	0.50	3 (6%) 22 17	5, 43, 120, 143	0
36	D2	46/46 (100%)	0.16	2 (4%) 39 30	11, 43, 103, 159	0
37	BL	143/144 (99%)	0.31	9 (6%) 23 18	8, 67, 133, 172	0
37	DL	143/144 (99%)	0.61	21 (14%) 3 3	5, 56, 119, 164	0
38	BM	136/136 (100%)	0.58	12 (8%) 12 11	9, 59, 117, 170	0
38	DM	136/136 (100%)	0.63	16 (11%) 6 6	7, 60, 116, 137	0
39	BX	63/63 (100%)	1.35	19 (30%) 1 1	6, 86, 135, 180	0
39	DX	63/63 (100%)	0.66	6 (9%) 10 10	38, 106, 178, 180	0
40	BH	149/149 (100%)	2.93	89 (59%) 0 0	26, 134, 177, 180	0
40	DH	149/149 (100%)	1.38	42 (28%) 1 1	11, 112, 162, 180	0
41	BJ	142/142 (100%)	0.55	17 (11%) 6 6	5, 74, 127, 180	0
41	DJ	142/142 (100%)	0.64	12 (8%) 13 12	5, 59, 125, 180	0
42	BN	120/127 (94%)	0.41	8 (6%) 21 16	20, 65, 126, 180	0
42	DN	120/127 (94%)	0.20	5 (4%) 40 31	5, 43, 103, 180	0
43	BO	116/117 (99%)	0.65	18 (15%) 3 3	12, 77, 140, 180	0
43	DO	116/117 (99%)	0.43	10 (8%) 13 12	32, 85, 152, 180	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	-0.24	3 (2%) 59 49	6, 57, 133, 175	0
44	DQ	117/117 (100%)	0.37	10 (8%) 13 12	5, 52, 112, 161	0
45	BS	110/110 (100%)	0.50	8 (7%) 18 14	5, 50, 125, 180	0
45	DS	110/110 (100%)	1.00	22 (20%) 1 2	5, 52, 131, 180	0
46	BU	102/103 (99%)	0.84	11 (10%) 8 7	5, 70, 146, 180	0
46	DU	102/103 (99%)	0.04	1 (0%) 84 76	22, 97, 158, 180	0
47	BF	178/178 (100%)	1.53	65 (36%) 0 0	52, 123, 180, 180	0
47	DF	178/178 (100%)	2.25	84 (47%) 0 0	33, 110, 176, 180	0
48	BG	176/176 (100%)	0.63	19 (10%) 8 7	26, 104, 165, 180	0
48	DG	176/176 (100%)	0.89	37 (21%) 1 1	26, 98, 169, 180	0
49	BR	103/103 (100%)	0.37	9 (8%) 13 12	11, 76, 142, 180	0
49	DR	103/103 (100%)	0.54	10 (9%) 10 9	13, 79, 144, 180	0
50	BT	93/100 (93%)	0.62	7 (7%) 17 14	16, 75, 150, 180	0
50	DT	93/100 (93%)	1.02	21 (22%) 1 1	13, 79, 154, 180	0
51	BZ	77/78 (98%)	0.66	8 (10%) 8 8	5, 53, 122, 137	0
51	DZ	77/78 (98%)	0.22	5 (6%) 22 17	5, 47, 124, 144	0
52	BW	79/84 (94%)	1.17	16 (20%) 1 2	8, 74, 121, 180	0
52	DW	79/84 (94%)	0.12	4 (5%) 32 24	9, 77, 144, 164	0
All	All	20417/21046 (97%)	0.15	1571 (7%) 16 13	5, 69, 155, 180	0

The worst 5 of 1571 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AP	82	ALA	19.5
24	BI	49	GLU	12.2
13	AP	81	ALA	11.9
47	DF	75	GLY	10.9
40	BH	142	VAL	10.7

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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
53	NMY	BB	3001	42/42	0.58	0.68	17.78	89,89,89,89	42
53	NMY	DB	3001	42/42	0.70	0.51	13.07	68,68,68,68	42
54	MG	AA	1658	1/1	0.83	0.26	7.04	120,120,120,120	0
54	MG	DB	3090	1/1	0.99	0.25	7.04	99,99,99,99	0
54	MG	BB	3088	1/1	0.95	0.25	5.98	87,87,87,87	0
53	NMY	CA	1601	42/42	0.90	0.22	2.78	47,47,47,47	0
53	NMY	AA	1601	42/42	0.86	0.23	2.55	75,75,75,75	0
54	MG	BB	3087	1/1	0.99	0.20	1.80	23,23,23,23	0
54	MG	CA	1613	1/1	0.88	0.17	1.37	108,108,108,108	0
54	MG	AA	1636	1/1	0.09	0.15	1.13	121,121,121,121	0
55	SCM	CA	1661	23/23	0.94	0.16	0.99	37,37,37,37	0
54	MG	BB	3041	1/1	0.97	0.17	0.53	34,34,34,34	0
54	MG	BB	3111	1/1	0.97	0.12	0.38	90,90,90,90	0
55	SCM	AA	1662	23/23	0.96	0.15	0.37	23,23,23,23	0
54	MG	DB	3013	1/1	0.99	0.17	0.29	12,12,12,12	0
54	MG	BB	3012	1/1	0.97	0.17	0.19	33,33,33,33	0
54	MG	CA	1634	1/1	0.95	0.12	-0.31	75,75,75,75	0
54	MG	BB	3086	1/1	0.83	0.16	-0.32	18,18,18,18	0
54	MG	BB	3084	1/1	0.95	0.16	-0.34	61,61,61,61	0
54	MG	BB	3076	1/1	0.98	0.16	-0.51	33,33,33,33	0
54	MG	AA	1616	1/1	0.92	0.14	-0.63	113,113,113,113	0
54	MG	AA	1634	1/1	0.85	0.10	-0.65	88,88,88,88	0
54	MG	AA	1653	1/1	0.78	0.11	-0.79	110,110,110,110	0
54	MG	DB	3111	1/1	0.98	0.09	-0.82	36,36,36,36	0
54	MG	DB	3091	1/1	0.86	0.06	-0.83	55,55,55,55	0
54	MG	DB	3015	1/1	0.97	0.07	-0.99	37,37,37,37	0
54	MG	DB	3031	1/1	0.86	0.16	-1.01	21,21,21,21	0
54	MG	DB	3100	1/1	0.96	0.15	-1.05	6,6,6,6	0
54	MG	CA	1654	1/1	0.80	0.09	-1.10	82,82,82,82	0
54	MG	DB	3088	1/1	0.97	0.16	-1.16	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3097	1/1	0.95	0.15	-1.18	12,12,12,12	0
54	MG	DB	3093	1/1	0.90	0.12	-1.18	98,98,98,98	0
54	MG	DB	3079	1/1	0.95	0.12	-1.22	80,80,80,80	0
54	MG	DB	3026	1/1	0.97	0.08	-1.27	16,16,16,16	0
54	MG	AA	1654	1/1	0.93	0.09	-1.31	49,49,49,49	0
54	MG	CA	1648	1/1	0.83	0.05	-1.38	69,69,69,69	0
54	MG	AA	1614	1/1	0.93	0.05	-1.41	66,66,66,66	0
56	ZN	B4	101	1/1	0.96	0.08	-1.47	49,49,49,49	0
54	MG	BB	3013	1/1	0.98	0.11	-1.51	81,81,81,81	0
54	MG	DB	3095	1/1	0.96	0.05	-1.58	39,39,39,39	0
56	ZN	D4	101	1/1	0.95	0.08	-1.59	40,40,40,40	0
54	MG	BB	3024	1/1	0.92	0.15	-1.65	12,12,12,12	0
54	MG	DB	3008	1/1	0.97	0.15	-1.65	41,41,41,41	0
54	MG	CA	1611	1/1	0.99	0.10	-1.70	5,5,5,5	0
54	MG	AA	1644	1/1	0.98	0.09	-1.71	42,42,42,42	0
54	MG	BB	3006	1/1	0.97	0.09	-1.72	9,9,9,9	0
54	MG	BB	3093	1/1	0.86	0.07	-1.79	32,32,32,32	0
54	MG	BB	3002	1/1	0.95	0.08	-1.81	19,19,19,19	0
54	MG	AA	1604	1/1	0.95	0.13	-1.82	43,43,43,43	0
54	MG	BB	3099	1/1	0.94	0.12	-1.84	23,23,23,23	0
54	MG	DB	3048	1/1	0.98	0.16	-1.92	14,14,14,14	0
54	MG	CA	1656	1/1	0.87	0.09	-1.92	135,135,135,135	0
54	MG	DB	3007	1/1	0.93	0.14	-1.98	9,9,9,9	0
54	MG	DB	3110	1/1	0.96	0.09	-2.02	17,17,17,17	0
54	MG	AA	1608	1/1	0.96	0.07	-2.05	53,53,53,53	0
54	MG	CA	1646	1/1	0.90	0.03	-2.08	52,52,52,52	0
54	MG	DB	3010	1/1	0.98	0.12	-2.08	8,8,8,8	0
54	MG	AA	1610	1/1	0.98	0.10	-2.15	5,5,5,5	0
54	MG	DB	3021	1/1	0.99	0.13	-2.36	5,5,5,5	0
54	MG	AA	1611	1/1	0.98	0.04	-2.41	73,73,73,73	0
54	MG	BB	3083	1/1	0.94	0.13	-2.51	5,5,5,5	0
54	MG	CA	1622	1/1	0.96	0.11	-2.53	44,44,44,44	0
54	MG	DB	3036	1/1	0.90	0.10	-2.61	85,85,85,85	0
54	MG	DB	3004	1/1	0.95	0.12	-2.62	41,41,41,41	0
54	MG	BB	3050	1/1	0.91	0.07	-2.67	16,16,16,16	0
54	MG	BB	3003	1/1	0.97	0.10	-2.72	17,17,17,17	0
54	MG	BB	3104	1/1	0.98	0.12	-2.72	6,6,6,6	0
54	MG	DB	3070	1/1	0.98	0.15	-2.77	38,38,38,38	0
54	MG	AA	1652	1/1	0.88	0.04	-2.91	101,101,101,101	0
54	MG	DB	3104	1/1	0.97	0.11	-2.91	31,31,31,31	0
54	MG	DB	3023	1/1	0.88	0.07	-2.93	7,7,7,7	0
54	MG	AA	1645	1/1	0.86	0.08	-2.94	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3056	1/1	0.93	0.11	-2.97	34,34,34,34	0
54	MG	BB	3066	1/1	0.94	0.06	-2.98	10,10,10,10	0
54	MG	DB	3071	1/1	0.93	0.14	-2.98	93,93,93,93	0
54	MG	DB	3086	1/1	0.98	0.11	-3.01	41,41,41,41	0
54	MG	DB	3073	1/1	0.91	0.07	-3.08	62,62,62,62	0
54	MG	DB	3011	1/1	0.97	0.09	-3.08	9,9,9,9	0
54	MG	DB	3089	1/1	0.98	0.10	-3.28	13,13,13,13	0
54	MG	BB	3030	1/1	0.95	0.08	-3.32	16,16,16,16	0
54	MG	DB	3069	1/1	0.97	0.08	-3.40	8,8,8,8	0
54	MG	CA	1628	1/1	0.93	0.09	-3.48	41,41,41,41	0
54	MG	CA	1612	1/1	0.98	0.07	-3.49	25,25,25,25	0
54	MG	DB	3052	1/1	0.96	0.12	-3.56	40,40,40,40	0
54	MG	CA	1621	1/1	0.97	0.10	-3.59	34,34,34,34	0
54	MG	AA	1642	1/1	0.98	0.04	-3.61	51,51,51,51	0
54	MG	CA	1635	1/1	0.91	0.07	-3.62	64,64,64,64	0
54	MG	BB	3022	1/1	0.96	0.09	-3.63	35,35,35,35	0
54	MG	AA	1631	1/1	0.96	0.04	-3.64	84,84,84,84	0
54	MG	BB	3082	1/1	0.92	0.11	-3.67	34,34,34,34	0
54	MG	AA	1639	1/1	0.96	0.05	-3.83	65,65,65,65	0
54	MG	BB	3089	1/1	0.95	0.07	-3.83	7,7,7,7	0
54	MG	BB	3091	1/1	0.95	0.05	-3.91	105,105,105,105	0
54	MG	DB	3057	1/1	0.97	0.09	-4.00	11,11,11,11	0
54	MG	AA	1637	1/1	0.95	0.03	-4.09	62,62,62,62	0
54	MG	CA	1637	1/1	0.99	0.08	-4.18	26,26,26,26	0
54	MG	BB	3095	1/1	0.90	0.08	-4.20	36,36,36,36	0
54	MG	DB	3002	1/1	0.98	0.13	-4.27	5,5,5,5	0
54	MG	DB	3085	1/1	0.96	0.13	-4.53	12,12,12,12	0
54	MG	BB	3075	1/1	0.95	0.08	-4.57	6,6,6,6	0
54	MG	CA	1625	1/1	0.99	0.06	-4.65	36,36,36,36	0
54	MG	DB	3109	1/1	0.98	0.08	-4.65	33,33,33,33	0
54	MG	CA	1636	1/1	0.99	0.07	-4.81	37,37,37,37	0
54	MG	AA	1655	1/1	0.92	0.06	-4.85	73,73,73,73	0
54	MG	AA	1602	1/1	0.96	0.06	-4.91	28,28,28,28	0
54	MG	BB	3063	1/1	0.99	0.10	-4.99	7,7,7,7	0
54	MG	BB	3014	1/1	0.92	0.06	-5.20	11,11,11,11	0
54	MG	BB	3080	1/1	0.93	0.10	-5.24	44,44,44,44	0
54	MG	DB	3003	1/1	0.99	0.07	-5.98	21,21,21,21	0
54	MG	BB	3070	1/1	0.97	0.08	-6.05	9,9,9,9	0
54	MG	BB	3033	1/1	0.99	0.05	-6.17	25,25,25,25	0
54	MG	CA	1602	1/1	0.99	0.04	-6.36	7,7,7,7	0
54	MG	CA	1606	1/1	0.95	0.06	-6.46	7,7,7,7	0
54	MG	BB	3057	1/1	0.97	0.05	-6.62	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3109	1/1	0.97	0.07	-6.66	19,19,19,19	0
54	MG	DB	3045	1/1	0.85	0.05	-6.69	32,32,32,32	0
54	MG	DB	3076	1/1	0.99	0.05	-6.86	22,22,22,22	0
54	MG	BB	3020	1/1	0.97	0.08	-8.07	28,28,28,28	0
54	MG	DB	3035	1/1	0.86	0.09	-9.10	80,80,80,80	0
54	MG	BB	3060	1/1	0.97	0.06	-9.57	5,5,5,5	0
54	MG	BB	3036	1/1	0.91	0.05	-11.17	26,26,26,26	0
54	MG	BB	3053	1/1	0.95	0.07	-14.14	30,30,30,30	0
54	MG	DB	3081	1/1	0.98	0.08	-15.48	35,35,35,35	0
54	MG	CA	1605	1/1	0.98	0.06	-17.16	12,12,12,12	0
54	MG	BB	3049	1/1	0.96	0.05	-27.29	24,24,24,24	0
54	MG	DB	3046	1/1	0.88	0.08	-	104,104,104,104	0
54	MG	BB	3034	1/1	0.82	0.40	-	130,130,130,130	0
54	MG	BB	3061	1/1	0.99	0.11	-	5,5,5,5	0
54	MG	DB	3055	1/1	0.98	0.09	-	22,22,22,22	0
54	MG	DB	3032	1/1	0.96	0.14	-	5,5,5,5	0
54	MG	CA	1640	1/1	0.97	0.13	-	43,43,43,43	0
54	MG	DB	3051	1/1	0.90	0.11	-	67,67,67,67	0
54	MG	BB	3032	1/1	0.95	0.12	-	38,38,38,38	0
54	MG	BB	3077	1/1	0.99	0.09	-	5,5,5,5	0
54	MG	BB	3039	1/1	0.89	0.09	-	107,107,107,107	0
54	MG	DB	3072	1/1	0.99	0.08	-	36,36,36,36	0
54	MG	BB	3069	1/1	0.87	0.07	-	41,41,41,41	0
54	MG	BB	3044	1/1	0.88	0.15	-	118,118,118,118	0
54	MG	BB	3027	1/1	0.89	0.14	-	42,42,42,42	0
54	MG	BB	3102	1/1	0.98	0.09	-	10,10,10,10	0
54	MG	DB	3024	1/1	0.93	0.07	-	32,32,32,32	0
54	MG	DB	3068	1/1	0.95	0.11	-	36,36,36,36	0
54	MG	DB	3060	1/1	0.49	0.08	-	96,96,96,96	0
54	MG	BB	3081	1/1	0.83	0.09	-	77,77,77,77	0
54	MG	AA	1620	1/1	0.73	0.12	-	132,132,132,132	0
54	MG	CA	1657	1/1	0.97	0.06	-	14,14,14,14	0
54	MG	BB	3015	1/1	0.96	0.03	-	32,32,32,32	0
54	MG	AA	1630	1/1	0.97	0.08	-	36,36,36,36	0
54	MG	DB	3019	1/1	0.99	0.08	-	25,25,25,25	0
54	MG	CA	1653	1/1	0.71	0.10	-	96,96,96,96	0
54	MG	BB	3046	1/1	0.98	0.10	-	50,50,50,50	0
54	MG	BB	3055	1/1	0.98	0.06	-	46,46,46,46	0
54	MG	BB	3097	1/1	0.99	0.07	-	5,5,5,5	0
54	MG	CA	1638	1/1	0.95	0.10	-	123,123,123,123	0
54	MG	BB	3010	1/1	0.98	0.06	-	123,123,123,123	0
54	MG	BB	3064	1/1	0.99	0.07	-	10,10,10,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1638	1/1	0.53	0.31	-	126,126,126,126	0
54	MG	DB	3099	1/1	0.99	0.13	-	9,9,9,9	0
54	MG	AA	1649	1/1	0.97	0.10	-	31,31,31,31	0
54	MG	CA	1627	1/1	0.96	0.07	-	40,40,40,40	0
54	MG	AA	1609	1/1	0.86	0.11	-	107,107,107,107	0
54	MG	CA	1660	1/1	0.98	0.07	-	77,77,77,77	0
54	MG	BB	3096	1/1	0.94	0.08	-	5,5,5,5	0
54	MG	CA	1658	1/1	0.97	0.14	-	50,50,50,50	0
54	MG	BB	3042	1/1	1.00	0.10	-	10,10,10,10	0
54	MG	DB	3105	1/1	0.97	0.10	-	41,41,41,41	0
54	MG	AA	1621	1/1	0.73	0.05	-	82,82,82,82	0
54	MG	AA	1647	1/1	0.82	0.12	-	133,133,133,133	0
54	MG	DB	3018	1/1	0.96	0.15	-	5,5,5,5	0
54	MG	DB	3047	1/1	0.98	0.08	-	27,27,27,27	0
54	MG	AA	1656	1/1	0.97	0.14	-	95,95,95,95	0
54	MG	AA	1626	1/1	0.53	0.24	-	87,87,87,87	1
54	MG	DB	3059	1/1	0.63	0.80	-	180,180,180,180	0
54	MG	AA	1643	1/1	0.94	0.13	-	43,43,43,43	0
54	MG	CA	1647	1/1	0.61	0.08	-	153,153,153,153	0
54	MG	CA	1633	1/1	0.69	0.07	-	48,48,48,48	0
54	MG	DB	3038	1/1	0.95	0.20	-	10,10,10,10	0
54	MG	BB	3079	1/1	0.85	0.08	-	68,68,68,68	0
54	MG	BB	3071	1/1	0.97	0.08	-	33,33,33,33	0
54	MG	DB	3050	1/1	0.97	0.12	-	6,6,6,6	0
54	MG	BB	3065	1/1	0.98	0.09	-	24,24,24,24	0
54	MG	AA	1635	1/1	0.98	0.06	-	86,86,86,86	0
54	MG	DB	3108	1/1	0.99	0.06	-	27,27,27,27	0
54	MG	CA	1644	1/1	0.93	0.08	-	49,49,49,49	0
54	MG	DB	3042	1/1	0.99	0.09	-	17,17,17,17	0
54	MG	DB	3016	1/1	0.89	0.10	-	53,53,53,53	0
54	MG	CA	1610	1/1	0.95	0.09	-	103,103,103,103	0
54	MG	BB	3085	1/1	0.96	0.15	-	43,43,43,43	0
54	MG	BB	3100	1/1	0.96	0.11	-	34,34,34,34	0
54	MG	DB	3077	1/1	0.98	0.12	-	28,28,28,28	0
54	MG	BB	3052	1/1	0.93	0.12	-	67,67,67,67	0
54	MG	BB	3098	1/1	0.95	0.09	-	85,85,85,85	0
54	MG	CA	1619	1/1	0.92	0.08	-	53,53,53,53	0
54	MG	CA	1609	1/1	0.79	0.07	-	110,110,110,110	0
54	MG	BB	3101	1/1	0.84	0.23	-	157,157,157,157	0
54	MG	BB	3068	1/1	0.96	0.11	-	65,65,65,65	0
54	MG	DB	3033	1/1	0.95	0.07	-	82,82,82,82	0
54	MG	CA	1632	1/1	0.98	0.05	-	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1648	1/1	0.86	0.40	-	110,110,110,110	0
54	MG	CA	1614	1/1	0.82	0.34	-	139,139,139,139	0
54	MG	BB	3056	1/1	0.94	0.14	-	23,23,23,23	0
54	MG	DB	3067	1/1	0.49	0.09	-	137,137,137,137	0
54	MG	DB	3043	1/1	0.97	0.09	-	32,32,32,32	0
54	MG	CA	1642	1/1	0.99	0.12	-	49,49,49,49	0
54	MG	DB	3030	1/1	0.82	0.15	-	81,81,81,81	0
54	MG	BB	3040	1/1	0.96	0.18	-	44,44,44,44	0
54	MG	DB	3084	1/1	0.86	0.16	-	109,109,109,109	0
54	MG	CA	1652	1/1	0.29	0.12	-	128,128,128,128	0
54	MG	DB	3005	1/1	0.96	0.14	-	23,23,23,23	0
54	MG	DB	3098	1/1	0.97	0.17	-	41,41,41,41	0
54	MG	AA	1659	1/1	0.87	0.05	-	111,111,111,111	0
54	MG	DB	3101	1/1	0.94	0.12	-	20,20,20,20	0
54	MG	DB	3040	1/1	0.97	0.08	-	78,78,78,78	0
54	MG	AA	1651	1/1	0.88	0.07	-	97,97,97,97	0
54	MG	BB	3025	1/1	0.94	0.11	-	32,32,32,32	0
54	MG	CA	1649	1/1	0.85	0.08	-	92,92,92,92	0
54	MG	BB	3009	1/1	0.95	0.08	-	80,80,80,80	0
54	MG	DB	3066	1/1	0.95	0.06	-	32,32,32,32	0
54	MG	CA	1623	1/1	0.96	0.12	-	21,21,21,21	0
54	MG	DB	3082	1/1	0.98	0.07	-	9,9,9,9	0
54	MG	AA	1660	1/1	0.38	0.40	-	148,148,148,148	0
54	MG	BB	3045	1/1	0.91	0.13	-	42,42,42,42	0
54	MG	BB	3110	1/1	0.98	0.15	-	61,61,61,61	0
54	MG	CA	1641	1/1	0.95	0.14	-	61,61,61,61	0
54	MG	BB	3090	1/1	0.97	0.10	-	54,54,54,54	0
54	MG	CA	1608	1/1	0.94	0.04	-	31,31,31,31	0
54	MG	BB	3028	1/1	0.98	0.05	-	24,24,24,24	0
54	MG	DB	3103	1/1	0.98	0.13	-	14,14,14,14	0
54	MG	DB	3106	1/1	0.97	0.16	-	53,53,53,53	0
54	MG	AA	1627	1/1	0.97	0.11	-	5,5,5,5	1
54	MG	DB	3006	1/1	0.97	0.14	-	13,13,13,13	0
54	MG	BB	3062	1/1	0.93	0.08	-	38,38,38,38	0
54	MG	DB	3061	1/1	0.28	0.17	-	117,117,117,117	0
54	MG	BB	3008	1/1	0.98	0.18	-	81,81,81,81	0
54	MG	CA	1618	1/1	0.87	0.15	-	104,104,104,104	0
54	MG	AA	1661	1/1	0.94	0.11	-	62,62,62,62	0
54	MG	AA	1633	1/1	0.93	0.14	-	65,65,65,65	0
54	MG	CA	1659	1/1	0.95	0.06	-	45,45,45,45	0
54	MG	CA	1639	1/1	0.96	0.06	-	108,108,108,108	0
54	MG	BB	3073	1/1	0.97	0.06	-	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3092	1/1	0.97	0.16	-	12,12,12,12	0
54	MG	DB	3078	1/1	0.98	0.11	-	24,24,24,24	0
54	MG	AA	1650	1/1	0.91	0.06	-	105,105,105,105	0
54	MG	BB	3048	1/1	0.90	0.09	-	145,145,145,145	0
54	MG	CA	1630	1/1	0.88	0.10	-	81,81,81,81	0
54	MG	DB	3094	1/1	0.91	0.15	-	5,5,5,5	0
54	MG	AA	1612	1/1	0.99	0.06	-	70,70,70,70	0
54	MG	BB	3017	1/1	0.96	0.08	-	43,43,43,43	0
54	MG	BB	3092	1/1	0.98	0.11	-	5,5,5,5	0
54	MG	DB	3029	1/1	0.95	0.04	-	30,30,30,30	0
54	MG	BB	3004	1/1	0.96	0.06	-	31,31,31,31	0
54	MG	CA	1616	1/1	0.96	0.07	-	15,15,15,15	0
54	MG	CA	1655	1/1	0.97	0.06	-	52,52,52,52	0
54	MG	CA	1643	1/1	0.82	0.11	-	75,75,75,75	0
54	MG	DB	3012	1/1	0.96	0.14	-	32,32,32,32	0
54	MG	CA	1603	1/1	0.99	0.15	-	25,25,25,25	0
54	MG	CA	1650	1/1	0.39	0.50	-	180,180,180,180	0
54	MG	DB	3075	1/1	0.94	0.17	-	58,58,58,58	0
54	MG	BB	3106	1/1	0.97	0.20	-	11,11,11,11	0
54	MG	CA	1620	1/1	0.98	0.09	-	62,62,62,62	0
54	MG	CA	1615	1/1	0.98	0.07	-	29,29,29,29	0
54	MG	BB	3103	1/1	0.97	0.13	-	25,25,25,25	0
54	MG	AA	1625	1/1	0.84	0.20	-	102,102,102,102	0
54	MG	AA	1618	1/1	0.69	0.20	-	160,160,160,160	0
54	MG	DB	3027	1/1	0.87	0.11	-	72,72,72,72	0
54	MG	AA	1629	1/1	0.96	0.09	-	55,55,55,55	0
54	MG	BB	3051	1/1	0.98	0.05	-	34,34,34,34	0
54	MG	BB	3018	1/1	0.95	0.15	-	31,31,31,31	0
54	MG	BB	3026	1/1	0.98	0.17	-	68,68,68,68	0
54	MG	DB	3020	1/1	0.98	0.10	-	6,6,6,6	0
54	MG	AA	1622	1/1	0.92	0.06	-	24,24,24,24	0
54	MG	AA	1613	1/1	0.95	0.08	-	80,80,80,80	0
54	MG	BB	3021	1/1	0.97	0.15	-	30,30,30,30	0
54	MG	BB	3054	1/1	0.93	0.07	-	46,46,46,46	0
54	MG	BB	3031	1/1	0.95	0.06	-	53,53,53,53	0
54	MG	DB	3107	1/1	1.00	0.07	-	20,20,20,20	0
54	MG	BB	3011	1/1	0.92	0.10	-	62,62,62,62	0
54	MG	BB	3058	1/1	0.91	0.17	-	63,63,63,63	0
54	MG	DB	3034	1/1	0.99	0.11	-	5,5,5,5	0
54	MG	DB	3014	1/1	0.77	0.15	-	80,80,80,80	0
54	MG	CA	1629	1/1	0.94	0.10	-	57,57,57,57	0
54	MG	CA	1624	1/1	0.97	0.07	-	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3065	1/1	0.98	0.07	-	20,20,20,20	0
54	MG	BB	3059	1/1	0.99	0.05	-	13,13,13,13	0
54	MG	BB	3043	1/1	0.29	0.23	-	145,145,145,145	0
54	MG	DB	3009	1/1	0.97	0.09	-	49,49,49,49	0
54	MG	DB	3074	1/1	0.86	0.12	-	29,29,29,29	0
54	MG	BB	3038	1/1	0.92	0.13	-	46,46,46,46	0
54	MG	DB	3049	1/1	0.95	0.06	-	66,66,66,66	0
54	MG	DB	3087	1/1	0.97	0.10	-	11,11,11,11	0
54	MG	AA	1624	1/1	0.95	0.32	-	13,13,13,13	1
54	MG	BB	3016	1/1	0.99	0.09	-	31,31,31,31	0
54	MG	DB	3028	1/1	0.95	0.10	-	17,17,17,17	0
54	MG	AA	1607	1/1	0.66	0.12	-	93,93,93,93	0
54	MG	BB	3108	1/1	0.96	0.14	-	36,36,36,36	0
54	MG	DB	3054	1/1	0.84	0.10	-	80,80,80,80	0
54	MG	AA	1606	1/1	0.95	0.19	-	56,56,56,56	0
54	MG	BB	3007	1/1	0.93	0.06	-	37,37,37,37	0
54	MG	BB	3067	1/1	0.95	0.09	-	26,26,26,26	0
54	MG	AA	1615	1/1	0.89	0.10	-	123,123,123,123	0
54	MG	BB	3029	1/1	0.91	0.22	-	21,21,21,21	0
54	MG	AA	1646	1/1	0.86	0.08	-	89,89,89,89	0
54	MG	BB	3037	1/1	0.98	0.20	-	35,35,35,35	0
54	MG	DB	3112	1/1	0.93	0.23	-	87,87,87,87	0
54	MG	CA	1631	1/1	0.99	0.15	-	43,43,43,43	0
54	MG	DB	3083	1/1	0.98	0.06	-	37,37,37,37	0
54	MG	BB	3072	1/1	0.94	0.08	-	54,54,54,54	0
54	MG	CA	1617	1/1	0.81	0.07	-	83,83,83,83	0
54	MG	CA	1604	1/1	0.95	0.07	-	66,66,66,66	0
54	MG	BB	3094	1/1	0.75	0.08	-	75,75,75,75	0
54	MG	DB	3064	1/1	0.99	0.04	-	34,34,34,34	0
54	MG	BB	3105	1/1	0.96	0.17	-	18,18,18,18	0
54	MG	AA	1605	1/1	0.95	0.09	-	46,46,46,46	0
54	MG	DB	3096	1/1	0.91	0.07	-	115,115,115,115	0
54	MG	AA	1657	1/1	0.81	0.24	-	95,95,95,95	0
54	MG	DB	3058	1/1	0.95	0.08	-	39,39,39,39	0
54	MG	CA	1651	1/1	0.84	0.46	-	161,161,161,161	0
54	MG	BB	3019	1/1	0.99	0.11	-	44,44,44,44	0
54	MG	CA	1607	1/1	0.92	0.16	-	129,129,129,129	0
54	MG	BB	3023	1/1	0.99	0.21	-	12,12,12,12	0
54	MG	DB	3017	1/1	0.97	0.11	-	29,29,29,29	0
54	MG	AA	1640	1/1	0.81	0.15	-	110,110,110,110	0
54	MG	AA	1628	1/1	0.96	0.07	-	53,53,53,53	0
54	MG	AA	1619	1/1	0.98	0.06	-	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3022	1/1	0.97	0.09	-	5,5,5,5	0
54	MG	AA	1603	1/1	0.87	0.07	-	100,100,100,100	0
54	MG	DB	3063	1/1	0.98	0.04	-	50,50,50,50	0
54	MG	DB	3037	1/1	0.94	0.09	-	23,23,23,23	0
54	MG	CA	1645	1/1	0.90	0.08	-	70,70,70,70	0
54	MG	BB	3074	1/1	0.99	0.09	-	28,28,28,28	0
54	MG	BB	3107	1/1	0.97	0.07	-	30,30,30,30	0
54	MG	AA	1641	1/1	0.96	0.15	-	88,88,88,88	0
54	MG	DB	3102	1/1	0.96	0.17	-	6,6,6,6	0
54	MG	AA	1617	1/1	0.96	0.11	-	47,47,47,47	0
54	MG	DB	3062	1/1	0.96	0.06	-	75,75,75,75	0
54	MG	BB	3047	1/1	0.96	0.11	-	66,66,66,66	0
54	MG	DB	3025	1/1	0.98	0.11	-	47,47,47,47	0
54	MG	DB	3044	1/1	0.98	0.07	-	11,11,11,11	0
54	MG	CA	1626	1/1	0.88	0.08	-	117,117,117,117	0
54	MG	AA	1623	1/1	0.68	0.19	-	157,157,157,157	0
54	MG	BB	3005	1/1	0.91	0.07	-	29,29,29,29	0
54	MG	BB	3035	1/1	0.94	0.06	-	41,41,41,41	0
54	MG	DB	3080	1/1	0.98	0.09	-	46,46,46,46	0
54	MG	BB	3078	1/1	0.96	0.15	-	47,47,47,47	0
54	MG	AA	1632	1/1	0.97	0.11	-	29,29,29,29	0
54	MG	DB	3039	1/1	0.97	0.11	-	19,19,19,19	0
54	MG	DB	3053	1/1	0.91	0.07	-	90,90,90,90	0
54	MG	DB	3041	1/1	0.98	0.09	-	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.