



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 08:20 PM BST

PDB ID : 4V80
Title : Crystal structure of the E. coli ribosome bound to CEM-101.
Authors : Dunkle, J.A.; Zhang, W.; Cate, J.H.D.; Mankin, A.S.
Deposited on : 2010-09-06
Resolution : 3.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

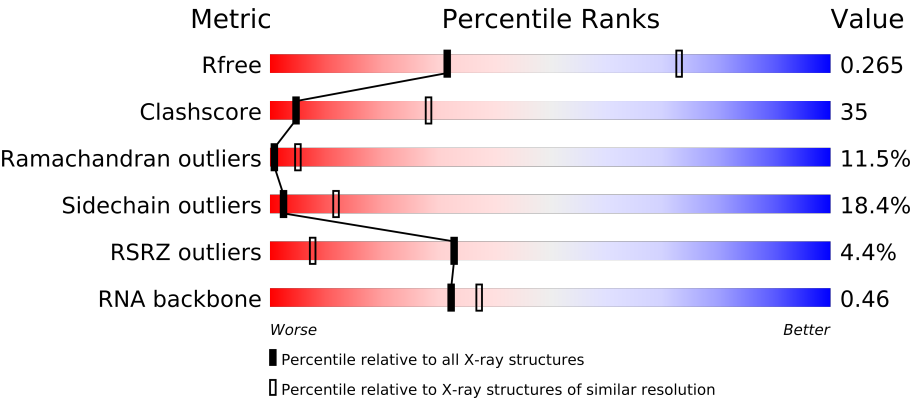
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable23397
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23397

1 Overall quality at a glance i

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1533	<div><div></div><div></div></div>
1	CA	1533	<div><div></div><div></div></div>
2	AB	241	<div><div></div><div></div></div>
2	CB	241	<div><div></div><div></div></div>
3	AC	233	<div><div></div><div></div></div>
3	CC	233	<div><div></div><div></div></div>
4	AD	206	<div><div></div><div></div></div>
4	CD	206	<div><div></div><div></div></div>
5	AE	167	<div><div></div><div></div></div>
5	CE	167	<div><div></div><div></div></div>
6	AF	135	<div><div></div><div></div></div>
6	CF	135	<div><div></div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	AG	179	
7	CG	179	
8	AH	130	
8	CH	130	
9	AI	130	
9	CI	130	
10	AJ	103	
10	CJ	103	
11	AK	129	
11	CK	129	
12	AL	124	
12	CL	124	
13	AM	118	
13	CM	118	
14	AN	101	
14	CN	101	
15	AO	89	
15	CO	89	
16	AP	82	
16	CP	82	
17	AQ	84	
17	CQ	84	
18	AR	75	
18	CR	75	
19	AS	92	
19	CS	92	
20	AT	87	
20	CT	87	
21	AU	71	
21	CU	71	
22	BA	2904	
22	DA	2904	
23	BB	120	
23	DB	120	
24	BC	273	
24	DC	273	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	179	
27	DF	179	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BG	177	
28	DG	177	
29	BH	149	
29	DH	149	
30	BI	142	
30	DI	142	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	115	
37	DP	115	
38	BQ	118	
38	DQ	118	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	100	
41	DT	100	
42	BU	104	
42	DU	104	
43	BV	94	
43	DV	94	
44	BW	85	
44	DW	85	
45	BX	78	
45	DX	78	
46	BY	63	
46	DY	63	
47	BZ	59	
47	DZ	59	
48	B0	57	
48	D0	57	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
49	B1	55	
49	D1	55	
50	B2	46	
50	D2	46	
51	B3	65	
51	D3	65	
52	B4	38	
52	D4	38	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
53	MG	AA	1608	-	X
53	MG	AA	1614	-	X
53	MG	AA	1619	-	X
53	MG	AA	1626	-	X
53	MG	AA	1628	-	X
53	MG	AA	1631	-	X
53	MG	AA	1636	-	X
53	MG	AA	1639	-	X
53	MG	AA	1641	-	X
53	MG	BA	3018	-	X
53	MG	BA	3020	-	X
53	MG	BA	3024	-	X
53	MG	BA	3035	-	X
53	MG	BA	3036	-	X
53	MG	BA	3039	-	X
53	MG	BA	3043	-	X
53	MG	BA	3054	-	X
53	MG	BA	3055	-	X
53	MG	BA	3058	-	X
53	MG	BA	3059	-	X
53	MG	BA	3060	-	X
53	MG	BA	3069	-	X
53	MG	BA	3070	-	X
53	MG	BA	3073	-	X
53	MG	BA	3081	-	X
53	MG	BA	3085	-	X
53	MG	BA	3089	-	X
53	MG	BA	3096	-	X
53	MG	BA	3099	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
53	MG	BA	3100	-	X
53	MG	BA	3105	-	X
53	MG	BA	3107	-	X
53	MG	BA	3114	-	X
53	MG	BA	3117	-	X
53	MG	BA	3120	-	X
53	MG	BA	3122	-	X
53	MG	BA	3124	-	X
53	MG	BA	3129	-	X
53	MG	BA	3131	-	X
53	MG	BA	3133	-	X
53	MG	BA	3134	-	X
53	MG	BB	201	-	X
53	MG	CA	1608	-	X
53	MG	CA	1614	-	X
53	MG	CA	1615	-	X
53	MG	CA	1616	-	X
53	MG	CA	1624	-	X
53	MG	CA	1625	-	X
53	MG	CA	1626	-	X
53	MG	CA	1627	-	X
53	MG	CA	1628	-	X
53	MG	CA	1640	-	X
53	MG	DA	3002	-	X
53	MG	DA	3003	-	X
53	MG	DA	3005	-	X
53	MG	DA	3007	-	X
53	MG	DA	3008	-	X
53	MG	DA	3019	-	X
53	MG	DA	3021	-	X
53	MG	DA	3022	-	X
53	MG	DA	3026	-	X
53	MG	DA	3031	-	X
53	MG	DA	3033	-	X
53	MG	DA	3049	-	X
53	MG	DA	3053	-	X
53	MG	DA	3057	-	X
53	MG	DA	3058	-	X
53	MG	DA	3060	-	X
53	MG	DA	3062	-	X
53	MG	DA	3063	-	X
53	MG	DA	3064	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
53	MG	DA	3074	-	X
53	MG	DA	3075	-	X
53	MG	DA	3078	-	X
53	MG	DA	3079	-	X
53	MG	DA	3088	-	X
53	MG	DA	3105	-	X
53	MG	DA	3108	-	X
53	MG	DA	3109	-	X
53	MG	DA	3120	-	X
53	MG	DA	3123	-	X
53	MG	DA	3127	-	X
53	MG	DA	3128	-	X
53	MG	DA	3129	-	X
53	MG	DA	3130	-	X
53	MG	DA	3132	-	X
53	MG	DC	301	-	X
53	MG	DE	301	-	X
53	MG	DJ	201	-	X
54	EM1	BA	3135	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284464 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
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 S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
7	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

Continued on next page...

Continued from previous page...

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	CN	91	Total	C	N	O	S	0	0	0
			735	461	151	120	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
19	CS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
22	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
23	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

Continued on next page...

Continued from previous page...

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
27	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
32	DK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

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

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

Continued on next page...

Continued from previous page...

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

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

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BX	77	Total	C	N	O	S		
			625	388	129	106	2	0	0
45	DX	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BY	63	Total	C	N	O	S		
			509	313	99	95	2	0	0
46	DY	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	BZ	58	Total	C	N	O	S		
			449	281	87	79	2	0	0
47	DZ	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

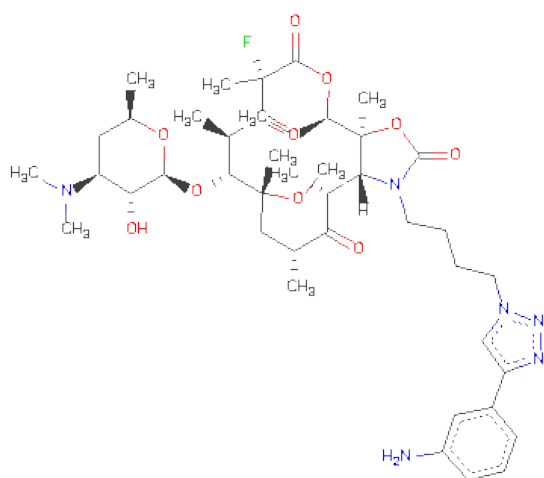
- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	BB	4	Total Mg 4 4	0	0
53	DE	1	Total Mg 1 1	0	0
53	BA	134	Total Mg 134 134	0	0
53	CA	42	Total Mg 42 42	0	0
53	DJ	1	Total Mg 1 1	0	0
53	BL	1	Total Mg 1 1	0	0
53	AA	43	Total Mg 43 43	0	0
53	DA	133	Total Mg 133 133	0	0
53	DC	1	Total Mg 1 1	0	0
53	DB	1	Total Mg 1 1	0	0

- Molecule 54 is (3a*S*,4*R*,7*S*,9*R*,10*R*,11*R*,13*R*,15*R*,15a*R*)-1-{4-[4-(3-aminophenyl)-1*H*-1,2,3-triazol-1-yl]butyl}-4-ethyl-7-fluoro-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,8,14-tetraoxotetradecahydro-2*H*-oxacyclotetradecino[4,3-*d*][1,3]oxazol-10-yl3,4,6-trideoxy-3-(dimethylamino)-β-D-xylo-hexopyranoside (three-letter code: EM1) (formula: C₄₃H₆₅FN₆O₁₀).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
54	BA	1	Total	C	F	N	O	0	0
			60	43	1	6	10		

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	200	Total	O	0	0
			200	200		
56	AL	1	Total	O	0	0
			1	1		
56	AN	5	Total	O	0	0
			5	5		
56	AT	1	Total	O	0	0
			1	1		
56	AU	1	Total	O	0	0
			1	1		
56	BA	606	Total	O	0	0
			606	606		
56	BB	20	Total	O	0	0
			20	20		
56	BC	9	Total	O	0	0
			9	9		
56	BD	1	Total	O	0	0
			1	1		
56	BL	4	Total	O	0	0
			4	4		
56	BN	3	Total	O	0	0
			3	3		
56	BT	2	Total	O	0	0
			2	2		
56	B2	1	Total	O	0	0
			1	1		
56	B3	2	Total	O	0	0
			2	2		
56	B4	2	Total	O	0	0
			2	2		

Continued on next page...

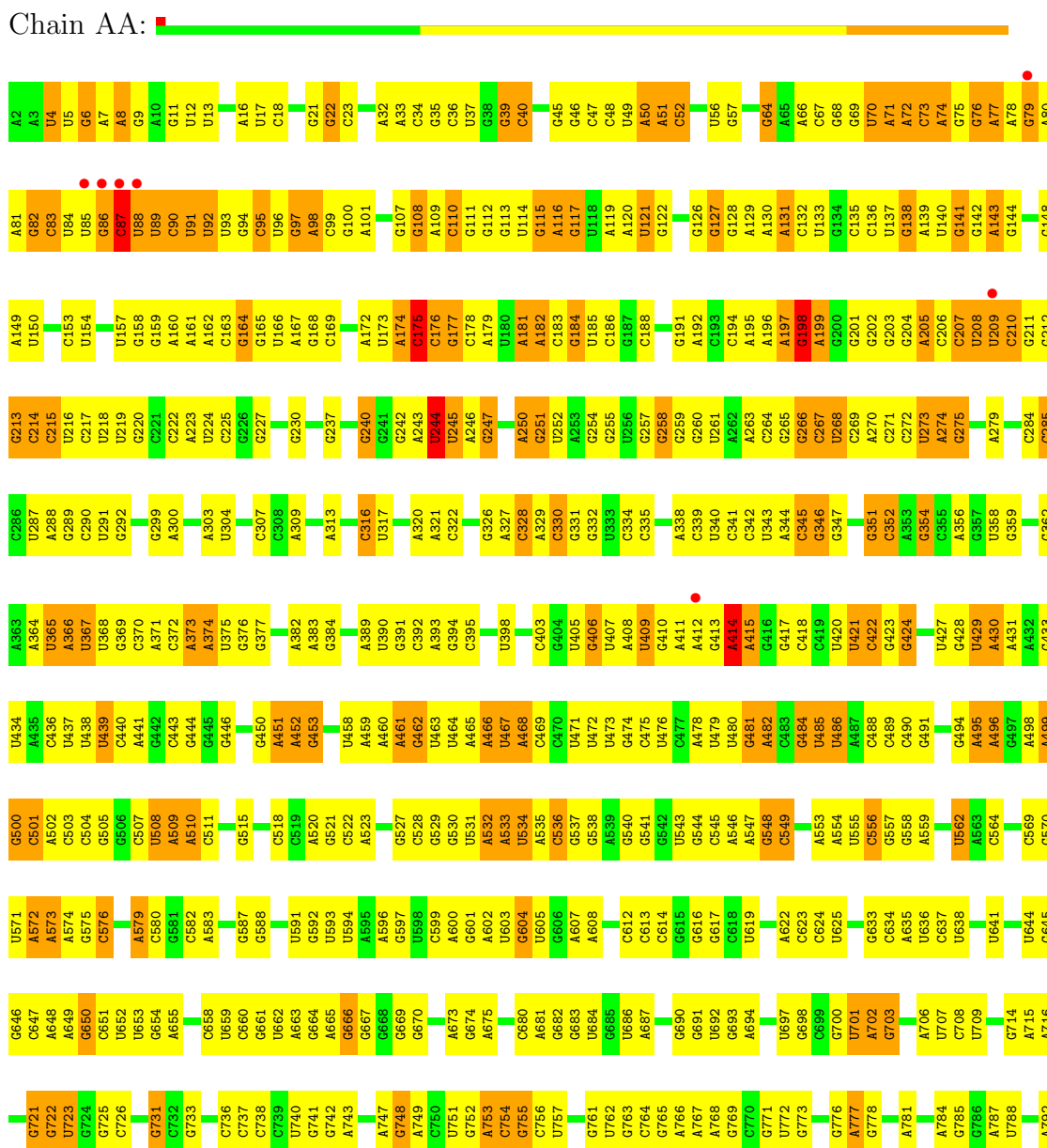
Continued from previous page...

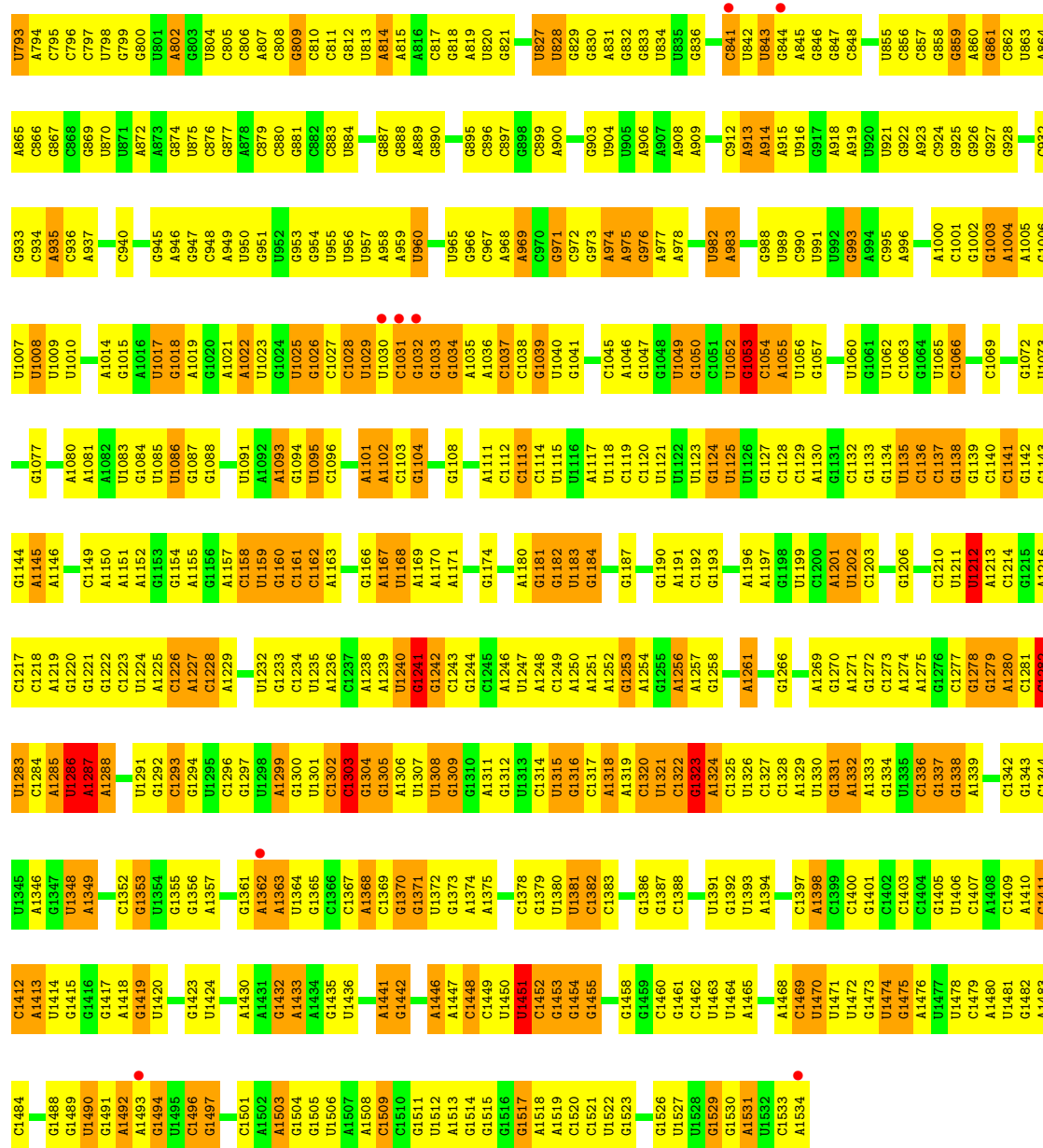
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CA	194	Total 194	O 194	0	0
56	CE	5	Total 5	O 5	0	0
56	CI	1	Total 1	O 1	0	0
56	CL	1	Total 1	O 1	0	0
56	CN	3	Total 3	O 3	0	0
56	CT	2	Total 2	O 2	0	0
56	CU	1	Total 1	O 1	0	0
56	DA	605	Total 605	O 605	0	0
56	DB	4	Total 4	O 4	0	0
56	DC	8	Total 8	O 8	0	0
56	DD	3	Total 3	O 3	0	0
56	DE	3	Total 3	O 3	0	0
56	DJ	3	Total 3	O 3	0	0
56	DL	4	Total 4	O 4	0	0
56	DN	1	Total 1	O 1	0	0
56	DT	2	Total 2	O 2	0	0
56	DU	2	Total 2	O 2	0	0
56	DV	1	Total 1	O 1	0	0
56	D2	1	Total 1	O 1	0	0
56	D3	1	Total 1	O 1	0	0
56	D4	5	Total 5	O 5	0	0

3 Residue-property plots

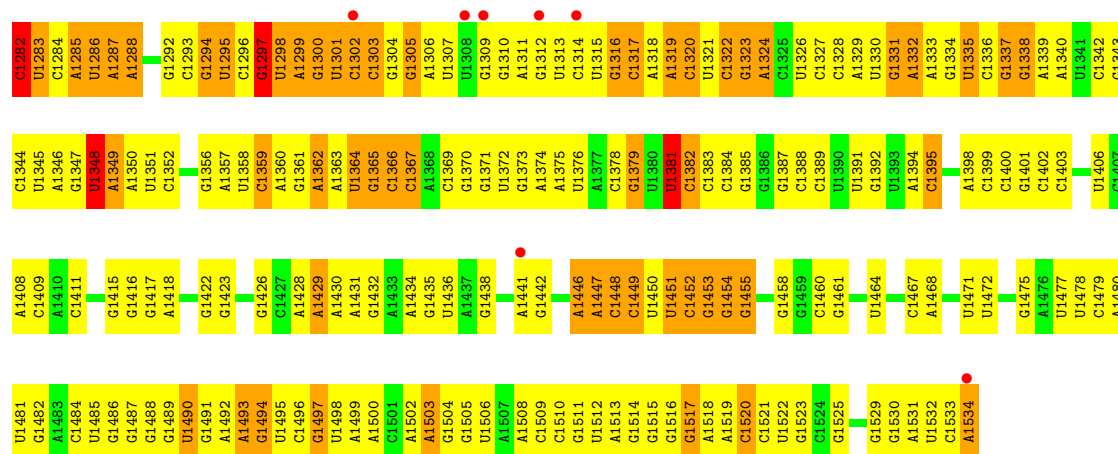
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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



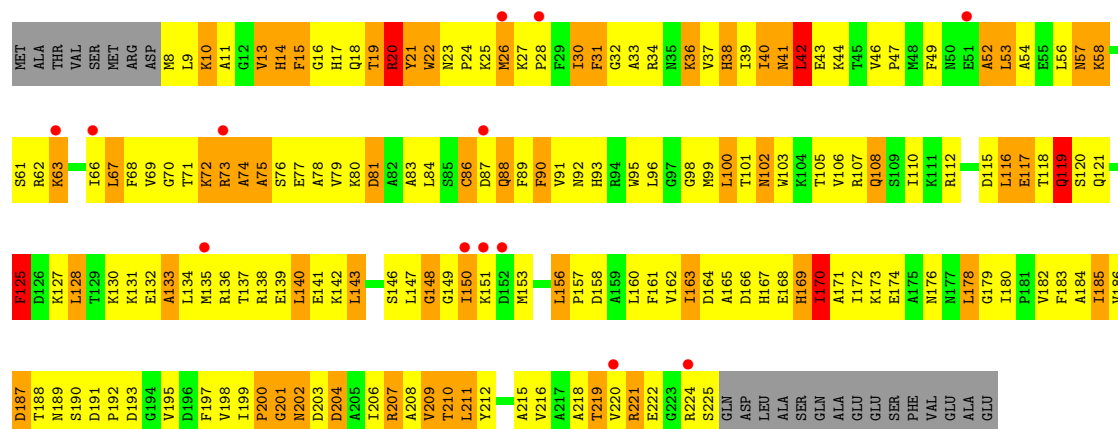


A1213	A1146	A1080	A1019	A959	G881	A814	U751	C679	A609	A532	C469	C403	G337	C267	G200
C1214	C1147	A1081	G1020	U960	C882	A815	G752	C680	U610	A533	C470	G404	A338	U268	G201
G1215	U1148	A1082	A1021	U961	C883	A816	A753	A681	G615	U534	U471	U406	C339	C269	G202
A1216	C1149	U1083	A1022	C962	G884	G818	G754	G682	G616	A535	U472	G406	G344	A270	G203
C1217	A1150	G1084	U1023	G963	G885	G819	G755	G683	G617	C536	U473	U407	U343	C271	G204
A1218	A1151	U1085	G1024	A964	G889	A819	G756	U684	G618	C537	G474	A408	A344	A205	G205
A1219	A1152	U1086	U1025	U965	G890	U820	U757	G685	C618	C538	C475	U409	C345	C206	G206
G1220	G1153	G1089	G1026	G966	U891	G821	C758	U686	U619	C542	U476	C410	C346	C207	G207
G1221	G1154	C967	C1027	C967	A892	U822	A759	A687	C620	U543	U477	C411	G347	C208	G208
C1222	A1157	U1090	C1028	A968	C893	C923	G760	G688	A621	U544	C478	A411	C348	C277	U209
C1223	C1158	U1091	U1029	A969	C894	G824	G761	C689	A622	A547	U479	C413	A349	C278	C210
U1224	U1159	A1092	U1030	C970	G898	A825	U762	G690	C623	C549	U480	A414	G350	G211	G211
A1225	G1160	A1093	C1031	C971	C899	C826	G763	G691	C624	C550	G481	A415	G351	C280	G212
C1226	C1161	G1094	G1032	C972	A900	U827	C764	U692	U625	C551	C482	G416	C352	G281	G213
A1227	C1162	U1095	G1033	G973	A901	U828	A766	G693	G626	A554	G484	G417	A353	A282	C214
C1228	C1096	C1096	G1034	A974	G906	G829	G765	A694	G627	U555	U485	C418	G354	C215	C215
A1229	U1167	C1097	A1035	A975	A906	G830	G766	A695	G628	C556	C566	C419	C355	C284	U216
U1232	A1169	U1098	A1036	G976	A907	A831	G769	A696	A629	C557	U487	U421	A356	C285	C217
G1233	A1170	G1099	C1037	A977	A908	G832	C770	G705	A630	C558	C488	C422	G357	C286	U218
A1238	A1171	C1100	C1038	A978	A909	U834	G771	A706	C631	A559	C489	G423	U358	U287	U219
A1239	C1172	A1101	U1039	C979	C910	U835	U772	U701	U632	U561	C490	G424	G359	A288	G220
C1243	A1178	A1102	G1040	C980	G836	G836	G773	A702	G633	U562	G491	G425	G360	C289	C221
C1245	U1173	C1103	G1041	U981	U837	U837	G774	G703	C633	U563	C492	U426	G361	C290	C222
A1246	G1174	G1104	A1042	U982	A914	C841	G775	A704	U636	C564	G494	U427	G362	U291	A223
G1247	G1175	A1105	G1043	A983	G917	U842	C776	G705	C637	C565	G495	U428	G366	U292	U224
G1248	A1176	G1106	G1046	C984	C917	U843	A777	A706	U638	C566	A496	U429	A366	G227	G227
C1249	G1177	C1107	U1047	C985	A918	U844	G778	U707	G639	C567	U496	A430	U367	C295	A228
A1250	C1178	G1108	G1048	U986	A919	G844	C779	C708	A640	U568	C497	A435	U368	U296	U229
A1251	A1179	A1109	U1049	C987	U920	A845	A780	U709	U641	C569	A498	C436	C369	G297	G230
G1252	C1180	G1110	G1050	G988	U921	G846	A781	G710	A642	C570	A499	C437	C370	A298	G231
C1253	G1181	G1112	C1051	U989	G926	G847	U782	G711	C643	U571	G500	U437	A371	G299	G232
A1254	G1182	C1113	C1052	C990	G927	C848	C783	A712	U644	A572	C501	U438	C372	A300	G237
C1255	U1183	C1114	U1052	U991	C927	G849	A784	G713	G645	A573	A502	U439	A373	G301	A238
A1256	G1185	G1115	C1053	U992	C932	C853	G785	U717	G650	A574	C503	G442	A374	G302	U239
C1257	G1186	C1116	A1054	A994	C933	U854	A787	C718	C653	C575	G504	C443	U375	G306	G240
A1258	A1187	U1123	U1056	C995	C934	U855	A790	C720	U654	C576	A509	C444	G376	A306	A243
G1259	C1188	G1124	G1057	A996	A935	C856	G791	G721	G654	C577	A510	C445	G377	U244	U244
C1260	U1189	G1125	C1058	U997	C936	C857	A792	G722	C659	C578	C511	G446	G378	U245	U245
A1261	A1190	U1126	U1060	C998	G939	G858	U793	G723	U659	U580	U512	G447	C312	A246	A246
G1262	C1192	G1127	G1061	C999	C940	G861	A794	U724	C660	U581	C513	A448	C381	C247	G247
U1263	G1193	C1128	U1062	C1001	G941	C862	C795	G725	G661	C582	C514	A451	A382	C248	C248
C1264	U1194	G1129	G1063	G1002	G942	C863	C796	U726	U662	C587	G515	A452	A383	U249	U249
C1265	C1195	A1130	G1064	G1003	U943	A865	C797	A729	A663	C588	U516	G453	G384	A250	A250
G1266	A1196	G1131	U1065	A1004	G944	C866	U798	G730	C664	C589	G517	G454	C385	G251	G251
C1267	A1197	C1132	C1066	A1005	G945	C867	G799	G731	A665	U590	C518	G455	C386	U252	U252
G1268	G1198	G1133	A1067	G1006	A946	C868	G800	C732	G666	U591	C519	A456	U387	A253	A253
A1269	U1199	G1134	G1068	U1007	G947	G869	U801	C733	C667	C595	A520	G457	C388	G254	G254
C1270	G1200	U1135	C1069	U1008	C948	U870	A802	C736	G668	A595	G521	U458	A389	G255	G255
A1271	A1201	C1136	U1070	U1009	A949	U871	G803	C737	G669	A596	G522	A459	U390	U256	U256
G1272	U1202	C1137	C1071	U1010	U950	A872	U804	C738	C670	C597	C523	A460	C391	G257	G257
C1273	C1203	G1138	G1072	C1011	G951	A873	C805	C739	U671	C598	A524	A461	C392	C328	G258
U1274	G1206	G1139	U1073	A1012	U952	G874	C806	U740	G672	C599	C525	G462	A393	C329	G259
C1275	C1207	C1140	G1074	G1013	G953	U875	A807	G741	A673	C602	C526	U463	C394	C330	G260
G1276	U1207	G1141	U1075	A1014	G954	C876	C808	G741	C674	U603	G527	U464	C395	G331	U261
C1277	G1208	G1142	U1076	G1015	U955	G877	C811	A747	A675	G604	C528	A465	C396	G332	A262
G1278	C1209	G1143	U1077	A1016	U956	A878	C812	G749	A676	U605	G529	A466	A397	U333	A263
A1280	U1017	G1144	U1078	U1017	U957	C879	G812	A749	U677	C606	G530	U467	U398	C334	C265
C1281	U1212	A1145	G1079	G1018	A958	C880	U813	C750	U678	A608	U531	A468	C399	A336	G266



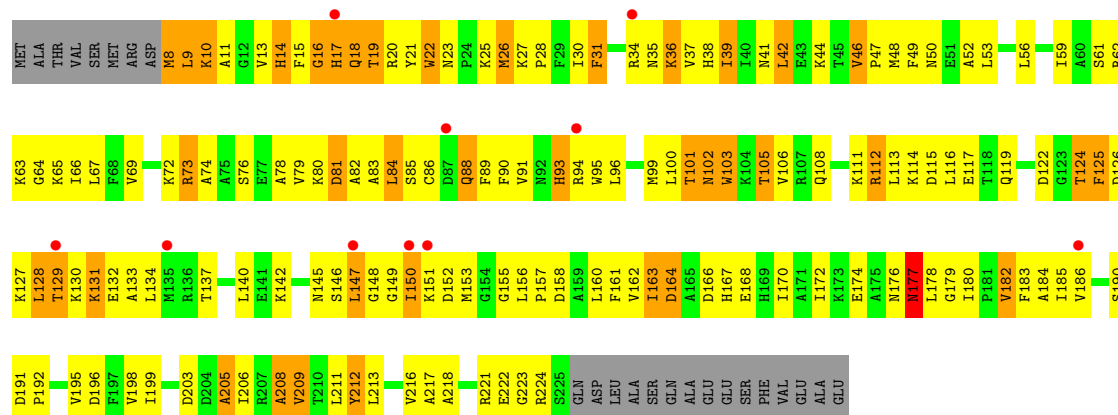
• Molecule 2: 30S ribosomal protein S2

Chain AB:



• Molecule 2: 30S ribosomal protein S2

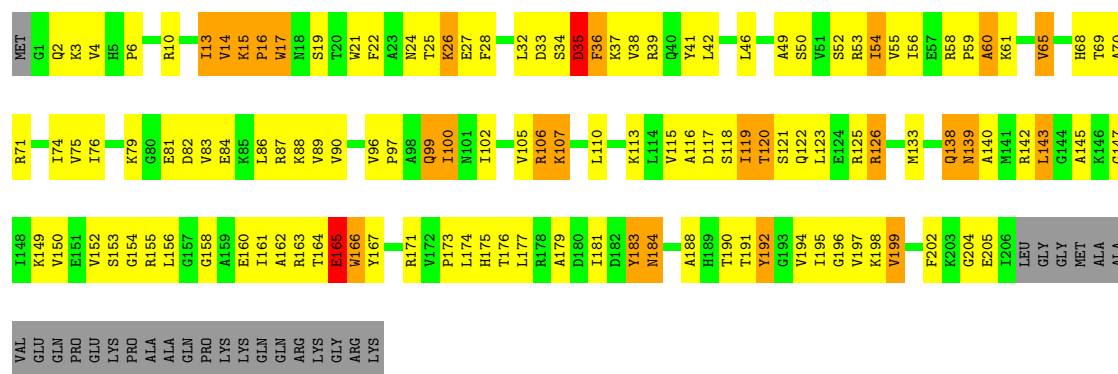
Chain CB:



• Molecule 3: 30S ribosomal protein S3

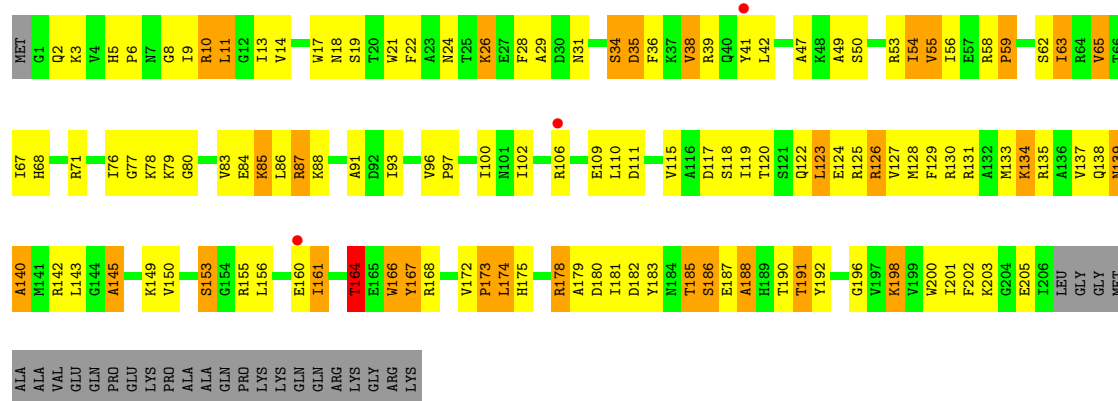
Chain AC:





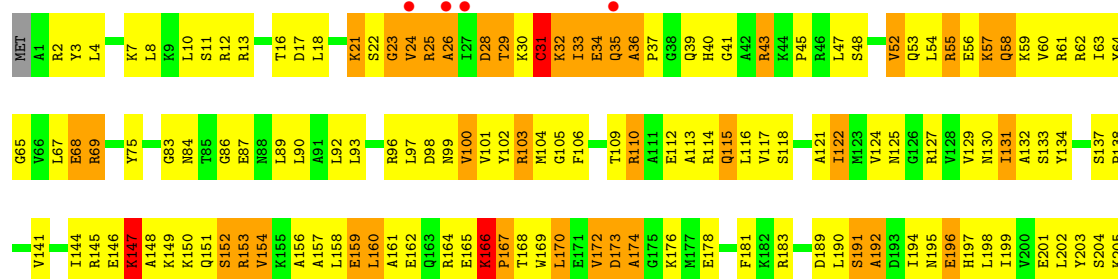
• Molecule 3: 30S ribosomal protein S3

Chain CC:



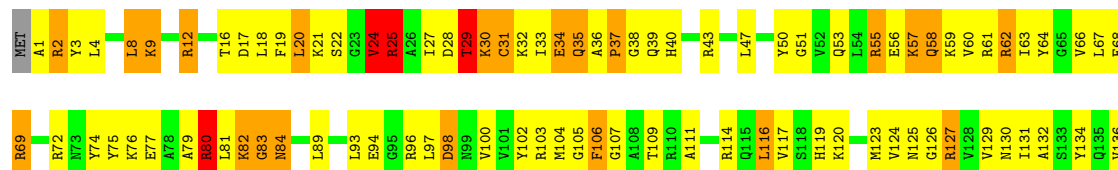
• Molecule 4: 30S ribosomal protein S4

Chain AD:



• Molecule 4: 30S ribosomal protein S4

Chain CD:

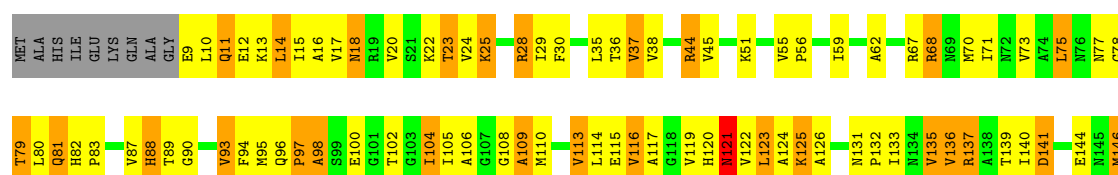




S204
K205

• Molecule 5: 30S ribosomal protein S5

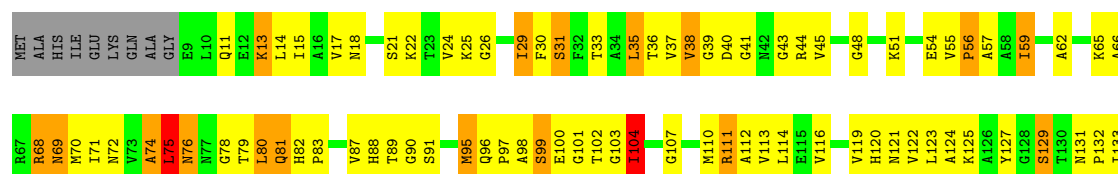
Chain AE:



N147, S148, P149, M150, M151, V152, A153, K154, K155, R156, G157, S158, VAL, GLU, ILE, LEU, GLY, LYS

• Molecule 5: 30S ribosomal protein S5

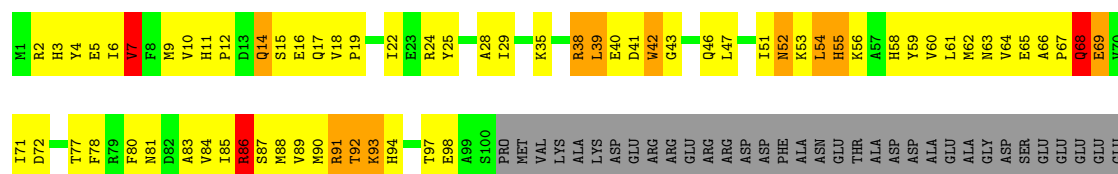
Chain CE:



N134, V135, R136, R137, M138, T139, L143, E144, N145, M146, N147, S148, P149, E150, M151, V152, A153, K154, K155, R156, G157, S158, VAL, GLU, ILE, LEU, GLY, LYS

• Molecule 6: 30S ribosomal protein S6

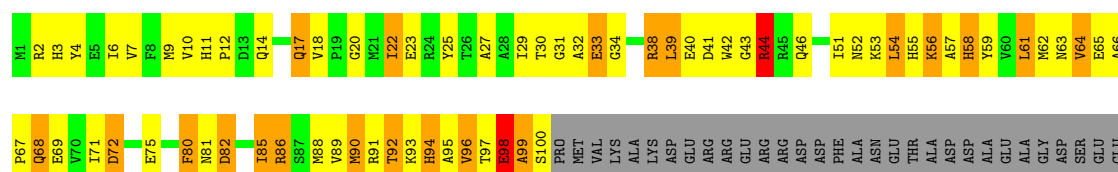
Chain AF:



GLU

• Molecule 6: 30S ribosomal protein S6

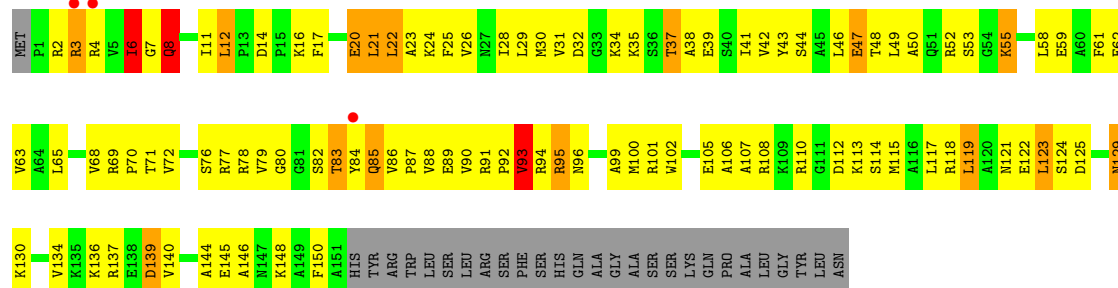
Chain CF:



GLU
GLU
GLU

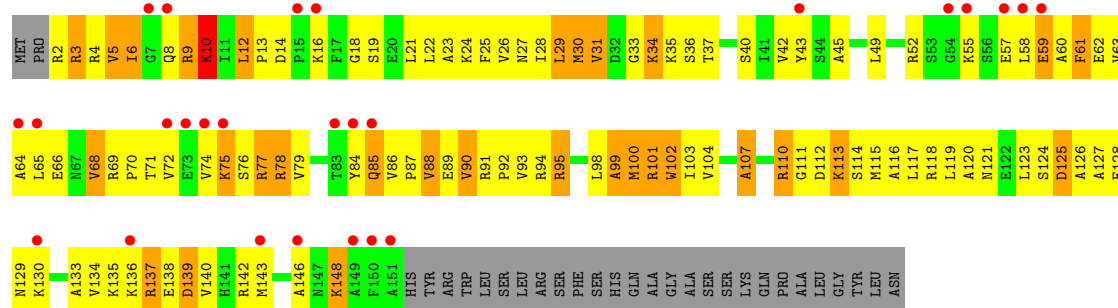
• Molecule 7: 30S ribosomal protein S7

Chain AG:



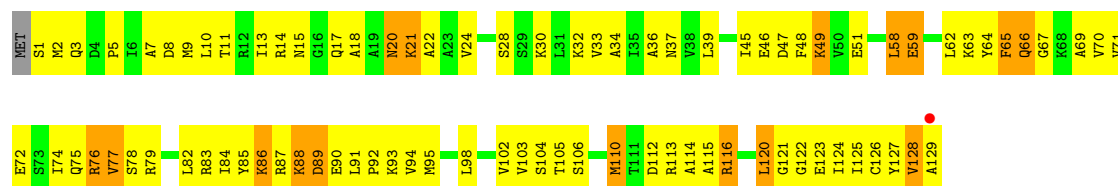
• Molecule 7: 30S ribosomal protein S7

Chain CG:



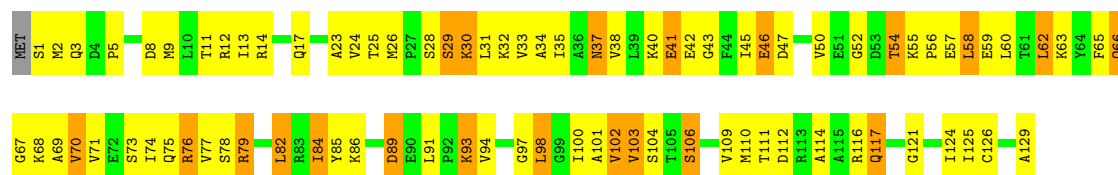
• Molecule 8: 30S ribosomal protein S8

Chain AH:



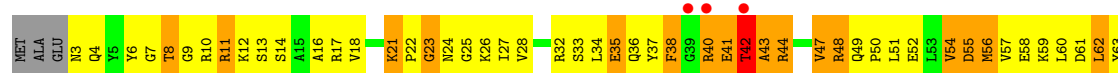
• Molecule 8: 30S ribosomal protein S8

Chain CH:



• Molecule 9: 30S ribosomal protein S9

Chain AI:



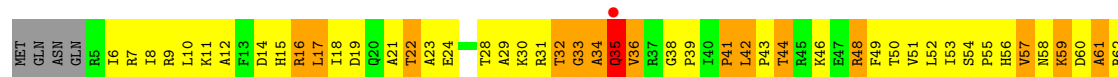
• Molecule 9: 30S ribosomal protein S9

Chain CI:



• Molecule 10: 30S ribosomal protein S10

Chain AJ:



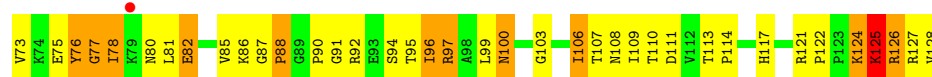
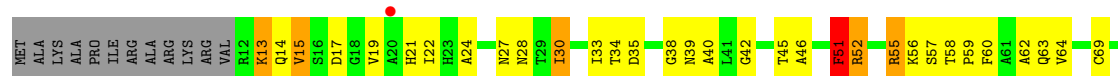
• Molecule 10: 30S ribosomal protein S10

Chain CJ:



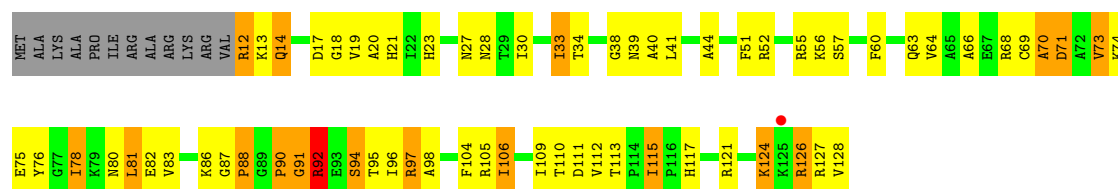
• Molecule 11: 30S ribosomal protein S11

Chain AK:



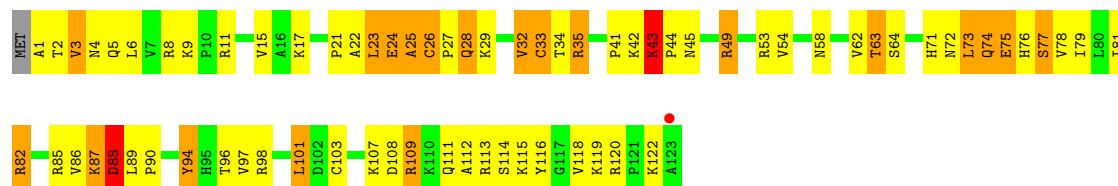
• Molecule 11: 30S ribosomal protein S11

Chain CK:



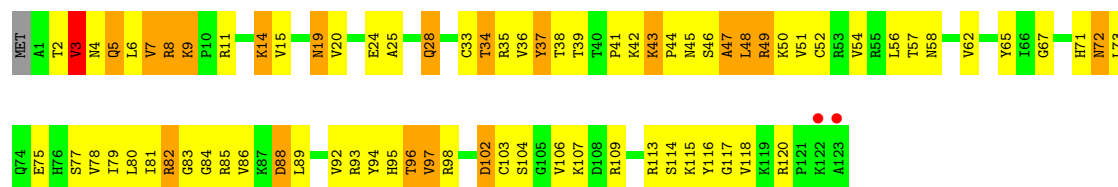
- Molecule 12: 30S ribosomal protein S12

Chain AL:



- Molecule 12: 30S ribosomal protein S12

Chain CL:



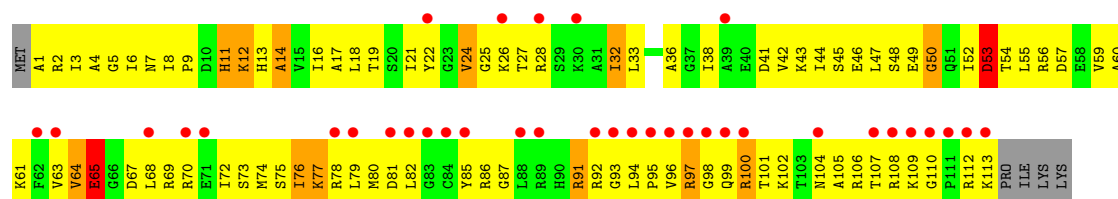
- Molecule 13: 30S ribosomal protein S13

Chain AM:



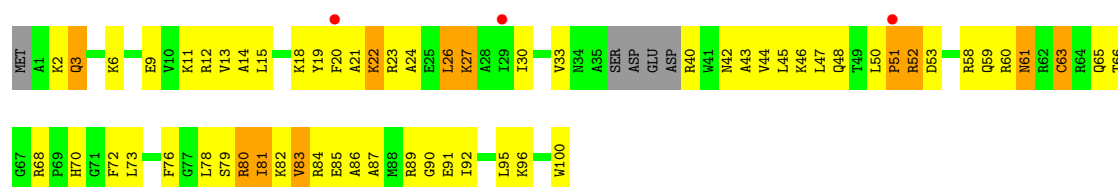
- Molecule 13: 30S ribosomal protein S13

Chain CM:



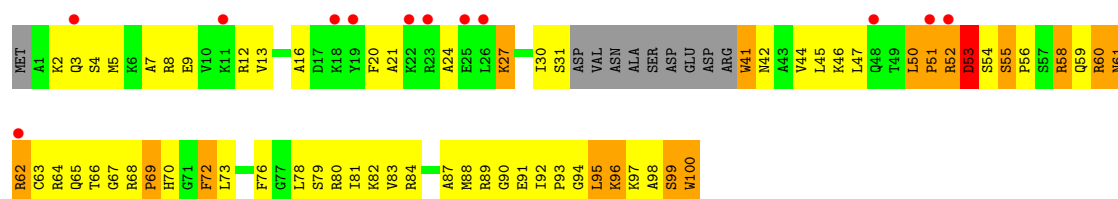
- Molecule 14: 30S ribosomal protein S14

Chain AN:



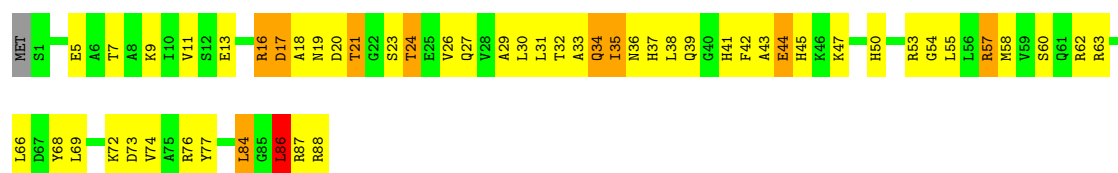
• Molecule 14: 30S ribosomal protein S14

Chain CN:



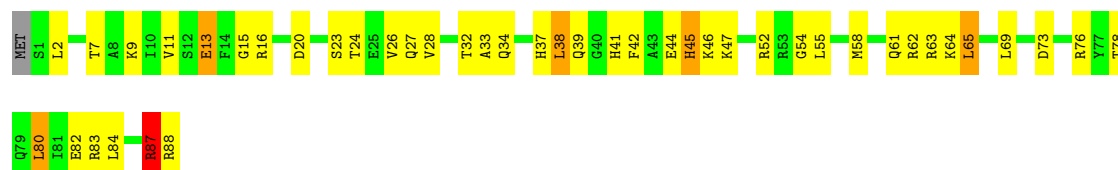
• Molecule 15: 30S ribosomal protein S15

Chain AO:



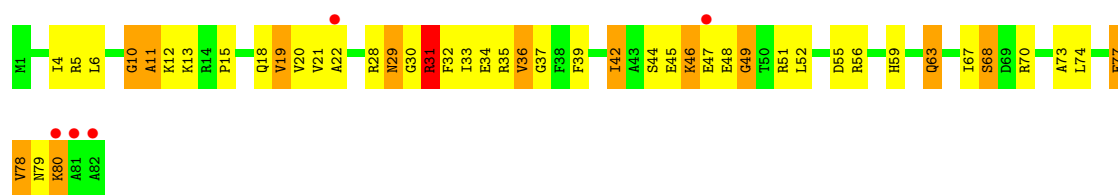
• Molecule 15: 30S ribosomal protein S15

Chain CO:



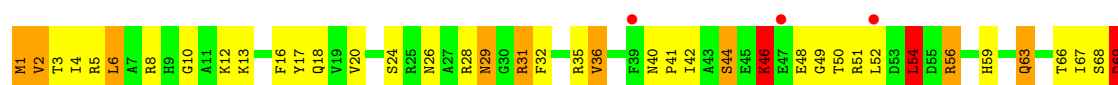
• Molecule 16: 30S ribosomal protein S16

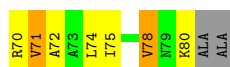
Chain AP:



• Molecule 16: 30S ribosomal protein S16

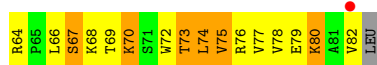
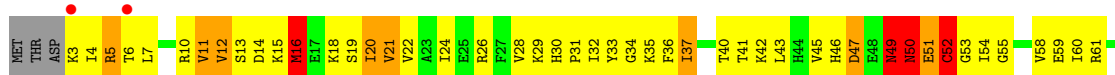
Chain CP:





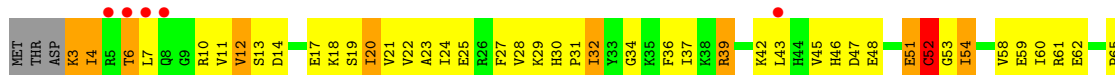
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



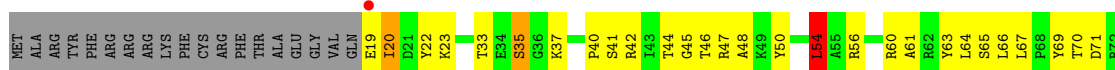
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



- Molecule 18: 30S ribosomal protein S18

Chain AR:



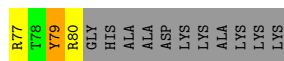
- Molecule 18: 30S ribosomal protein S18

Chain CR:



- Molecule 19: 30S ribosomal protein S19

Chain AS:



- Molecule 19: 30S ribosomal protein S19

- Molecule 20: 30S ribosomal protein S20

- Molecule 20: 30S ribosomal protein S20

- Molecule 21: 30S ribosomal protein S21

- Molecule 21: 30S ribosomal protein S21

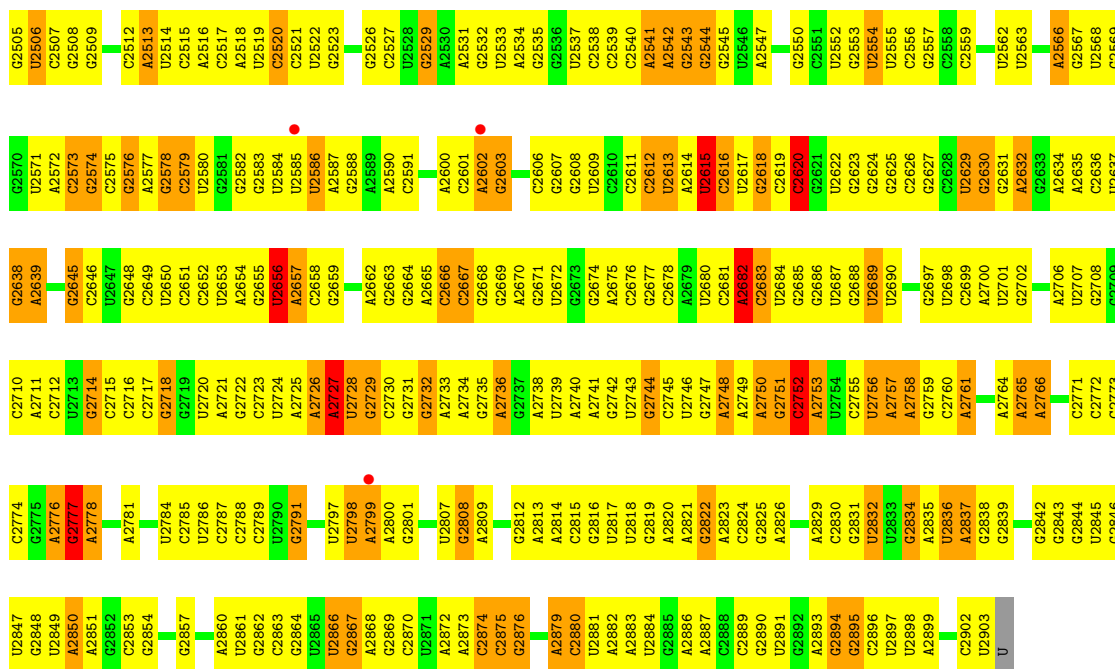
- Molecule 22: 23S rRNA



U2438	G2357	U2291	A2198	U1995	A1927	G1849	A1783	U1716	A1626	G1546	U1467	A1392
A2439	A2358	U2292	A2199	C1996	A1928	G1850	A1784	A1717	G1627	G1546	U1468	A1393
G2440	G2361	U2293	C2200	C1997	G1929	U1851	A1785	U1720	G1628	U1554	U1470	A1395
G2444	G2364	G2294	G2203	C1999	A1930	A1852	A1786	G1721	U1635	G1555	U1474	C1399
G2445	G2365	G2295	G2204	C2000	A1932	A1853	A1789	A1722	U1636	C1558	U1475	U1402
G2446	A2366	U2296	U2210	C2006	A1933	U1855	C1790	G1723	U1637	U1562	U1476	A1403
G2447	A2367	A2297	A2211	G2012	A1936	U1856	A1791	G1724	C1638	U1563	A1477	C1404
A2448	U2298	A2212	A2212	U2075	A1937	A1858	C1792	C1726	C1644	U1564	G1478	U1405
A2450	U2299	U2213	G2214	U2076	A1938	U1859	A1794	G1727	U1647	C1565	G1479	
	U2305	A2214		A2080	A1939	U1864	C1795	G1728	U1648	U1566		
	G2306	U2149			U1939	U1865	C1796	U1729	U1649	U1567	G1482	G1408
G2454	G2307	U2151	U2086	U2086	U1940	U1866	C1797	C1730	G1649	G1567	G1483	U1409
G2455	G2308	G2152	G2087	G2087	C1941	G1867	C1799	G1731	A1650	G1568	U1484	G1410
G2456	G2309	G2153	U2092	U2092	U1943	U1868	C1799	C1732	G1651	A1569	U1485	U1411
A2459	G2310	A2154	G2093	G2093	U1944	G1869	A1801	G1733	G1652	A1570	U1486	U1412
G2460	A2311	U2155	A2094	A2094	U1945	U1870	A1802	G1734	G1653	A1571	U1487	A1413
U2461	G2312	U2156	A2095	A2095	G1946	A1871	A1802	A1735	A1654	A1572	U1488	C1414
	G2313	G2157	A2096	A2096	U1947	A1872	A1805	U1736	A1655	G1573	C1489	U1415
G2466	A2314	A	G2097	G2097	U2022	G1873	A1808	U1737	C1656	U1576	C1489	G1416
	G2315	G	U2097	U2097	G2023	C1874	A1809	G1738	G1663	U1577	C1493	C1417
	G2316	C	U2098	U2098	G1948	G1875	A1810	A1739	G1664	U1578	A1494	A1418
	A2317	C			A1952	A1876	A1810	G1743	A1665	A1495	A1495	A1419
G2472	G2338	G	G2102	G2102	C2025	G1876	C1811	A1744	G1666	G1581	A1496	A1420
U2473	G2339	A	C2103	C2103	G1954	C1881	U1812	A1745	G1667	C1582	U1497	G1421
U2474	G2340	C	U2104	U2104	U1955	U1882	C1812	A1746	G1668	C1583	C1498	G1422
G2475	U2243	C	C2105	C2105	U1956	U1883	G1814	U1747	G1669	U1584	C1499	G1423
G2476	U2244	U	U2106	U2106	C1957	G1884	A1815	G1748	C1670	C1585	G1500	
G2477	G2324	U	G2107	G2107	G1958	U1885	C1816	A1749		A1586	G1501	A1427
G2478	G2325	G	A2108	A2108	G1959	U1886	G1817		G1674	A1587	A1502	C1428
U2479	G2326	A	U2109	U2109	A1960	U1886	U1818	A1754	C1675	G1588	A1503	G1429
G2480	G2327	A	G2110	G2110	C1961	A1889	A1819	A1755	A1676	U1589	A1504	G1430
G2481	G2328	A	U	U	C1962	A1890	U1820	G1756	A1677	A1590	A1505	A1431
	U2257	U	G	G	G1963	A1891	A1821	U1757		A1591	U1506	G1432
G2484	G2258	A	U	U	C1964	G1897	C1822	U1758	U1680	C1592	A1433	A1433
G2485	U2259	C	A	A	A1965	U1898		A1759	G1681	A1593	A1434	A1434
G2486		C	G	G	C1966	A1899	G1826	C1760	G1682	U1594	A1508	A1435
	U2262	A	A2042	A2042	C1967	A1900	U1827	C1761	U1683	U1599	C1510	G1436
G2487	U2263	C	C2043	C2043	U1968	A1901	G1828	A1762	G1684	U1599	C1511	U1437
U2488	G2263	C	C2044	C2044	A1969	G1902	A1829	G1763		C1600	U1512	U1438
U2489	A2267	C	G2045	G2045	A1970	C1902	C1830	G1764	U1688		U1513	A1439
G2490	A2268	U	G2046	G2046	U1971	G1906	C1831			A1603	U1514	U1440
G2491	G2269	G			G1972	G1907	C1832	G1767	U1692	C1604	A1515	G1441
U2419	G2269	U	G2049	G2049	G1973	G1907	C1833	C1768	U1693	C1605	U1516	U1442
G2420		U	C2050	C2050	A1977	A1913	U1834	U1769	C1694	C1606	U1443	U1443
G2421	U2272	A	A2051	A2051		C1914	C1835	G1770	G1695	C1607	U1520	G1444
G2422	A2273	G	G2052	G2052	G1983	U1915	C1836	C1771	G1696	A1608		
U2423	A2274	G	G2053	G2053	G1984	A1916	C1837	A1772	G1697	A1609	U1528	G1450
G2424	G2275	A	C2055	C2055	C1985	U1917	C1838	A1773		A1610	G1529	C1451
A2425	G2276	G	G2056	G2056	C1986	A1918	C1839	C1774	A1700	C1611	G1533	G1452
A2426	G2277	C	G2057	G2057	U1987	A1919	U1840	U1775	A1701	C1612	U1534	A1453
G2347	G2278	U	A2058	A2058	G1988	C1920	U1841	G1776	G1701	C1613	U1535	C1454
G2348	G2279	U	A2059	A2059	U1989	G1921	G1842	U1777	A1705	A1614	C1455	G1455
G2349	G2279	U	A2060	A2060	C1990	G1922	C1843	U1778	G1706		C1536	G1456
G2350	G2280	U	G2061	G2061	U1991	U1923	C1844	U1779	G1707	A1618	U1457	U1457
G2351	G2281	G	A2062	A2062	G1992	C1924	A1847	A1780	U1714	G1622	U1458	U1458
A2352	G2282	C	C2063	C2063	U1993	C1925	A1847	U1781	G1715		U1539	G1459
G2353	A2284	U	G2064	G2064	C1994	U1926	A1848	U1782			G1540	U1460
G2354	G2285	U	C2065	C2065								
G2355	G2286	U	U2137	U2137								
G2356	A2287	U										

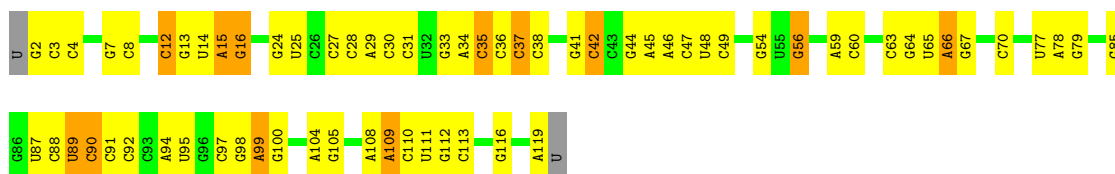
G1444	A1383	U1263	C1196	A1126	C1064	G993	A928	G864	U803	U741	C671	G549
G1447	A1384	A1264	G1197	A1127	U1065	C994	U929	C865	A804	A742	C672	C550
C1448	C1386	A1265	U1198	G1128	U1066	C995	G930	A866	G805	A743	C673	G551
G1387	A1387	G1266	U1199	A1129	A996	A996	U931	C867	C806	U744	G674	U552
G1388	G1388	U1267	C1200	G1130	G1068	G997	U932	U868	U807	G745	A675	G553
G1389	G1389	A1268	U1201	U1131	A1069	C998	A933	G869	G808	U746	A676	U554
U1390	U1390	C1269	G1202	G1132	A1070	U999	U934	U870	G809	U747	A677	G555
G1331	G1331	C1270	U1203	U1133	G1071	A1000	C935	U871	U810	G748		
A1392	A1392	G1271	A1204	A1134	C1072	A1001	A936	U872	U811	A749	G682	U558
G1333	G1333	A1205	U1205	C1135	A1073	C1005	A941	G873	U812	A750	U683	G559
A1393	A1393	G1206	G1206	G1136	G1074	C1006	G942	G874	U813	A751	G884	C560
U1394	U1394	C1207	C1207	G1137	C1075	C1007	A943	G875	C814	A752	A685	G561
A1395	A1395	A1275	G1208	U1138	C1076	C1007	A943	C876	C815	A753	U686	U562
U1396	U1396	A1276	U1209	G1139	A1077	A1008	C944	A877	C816	U754	C687	A563
G1337	G1337	C1277	G1210	C1140	U1078	A1009	A945	A878	C817	U755		C564
C1338	C1338	C1278	C1211	U1141	U1079	A1010	A946	G	G818	A756	G689	C565
G1339	G1339	G1279	G1212	A1142	A1080	G1011	A947	G	A819	G757	U689	U566
U1340	U1340	G1280	A1213	A1143	U1081	U1012	C948	G	A820	G758	A627	U567
G1341	G1341	G1281	A1214		U1082	C1013	G949	G	A821	G759	G628	U568
A1342	A1342	U1282		A1147	U1083	C1014	G950	G	C822	G760	G629	U569
G1343	G1343	G1283	U1222	U1148	A1084	U1015	C951	U		A761	G630	U570
C1344	C1344	A1284	G1223	G1149	A1085	G1016	G952	C		G631	A632	U571
G1345	G1345	A1285			A1086		G953	A	U826	G632	G598	A572
G1346	G1346	A1286	A1226	C1152	A1087	U1019	G954	U	U827	A633	A699	U573
A1347	A1347	A1287	G1227	C1153	A1088	A1020	U955	C	U828	C634	G700	A574
G1348	G1348	G1288	G1228	G1154	A1089	A1021	G956	C	A829	C635	G701	A575
C1349	C1349	C1289	C1229	A1155	A1090	G1022	G957	C		G636		U576
G1350	G1350	G1290	A1230	A1156	A1091	U1023	U958	G	G830	A637	A705	G577
C1351	C1351	G1291	G1231	G1157	C1092	G1024	G959	A	U832	A638	A706	G578
U1412	U1412	C1292	U1232	C1158	C1093	G1025	A960	C	A833	G639	G579	G579
A1353	A1353	C1293	C1233		U1094	G1026	C961	U	G834	G708	G708	U580
A1354	A1354	U1294	C1234	G1166	A1095	A1027	G962	U	C835	U709	U709	C581
G1355	G1355	C1295	G1235	C1167	A1096		U963		G836	G775	U710	C582
C1356	C1356	G1296	G1236	G1168	U1097	U1032	C964	C	U837	G776	A643	G583
G1357	G1357	A1297	A1237	A1169	A1098	C1033	C965	C	U838	G777	G644	C584
C1358	C1358	G1298	G1238	C1170	G1099	G1034	G966	A899	U839	G778	C645	G585
A1359	A1359	G1299	G1239	G1171	C1100	U1035	U967		C840	U779	C646	A586
G1360	G1360	G1300	U1240	C1172	U1101		C968		G841	U780	G647	C587
G1361	G1361	A1301	A1241	U1173	C1102	G1042	G969	C902	U842	A716	A716	A588
C1362	C1362	A1302	U1242	U1174	A1103	C1043	U970	C903	U843	C717	C717	U589
G1363	G1363	G1303	C1243	A1175	C1104	C1044	G971	G904	A844	A718	A718	C590
A1364	A1364	A1304	A1244	U1176	U1105	C1045	A972	A905	A845	C719	C719	U591
A1365	A1365	C1305	G1245	G1177	G1106	A1046	A973	A910	U846	A721	A721	A592
A1366	A1366	C1306	C1246	C1178		G1047	G974	C912	U847	C786	C786	U593
A1367	A1367	A1307	A1247	G1179	C1109	A1048	A975	U913	C848	U724	U724	U594
G1368	G1368	A1308	G1248	U1180	G1110	C1049	G976	U914	A849	G725	G725	C595
C1369	C1369	G1309	U1249	U1181	A1111	U1050	G977	G913	U850	G726	G726	U596
C1370	C1370	G1310	G1250	G1182	G1112	G1051	G978	C915	C851	A727	A727	G597
G1371	G1371	G1311	C1251	U1183	U1113	C1052	A979	G916	U852	G728	G728	U598
U1372	U1372	U1312	G1252	U1184	C1114	C1053	U980	A917	C853	G729	G729	A599
A1373	A1373	U1313	A1253	G1185	G1115	A1054	A981	A918	C854	A730	A730	G600
G1374	G1374	C1314	C1254	U1186	G1116	C1055	C982	U919	G855	C661	C661	C601
U1375	U1375	C1315	U1255	G1187		G1056	A983	A920	C856	C662	C662	A602
C1376	C1376	U1316	G1256	U1188	U1119	A1057	A984	C921	C857	G732	G732	A603
G1377	G1377	G1317	C1257	A1189	G1120	U1058	C985	C922	G858	G733	G733	G604
A1378	A1378	U1318	U1258	G1190	C1121	G1059		C923	C859	C736	C736	G605
C1379	C1379	C1319	G1259	G1191	G1122	U1060	G989	G924	U860	C737	C737	U606
G1380	G1380	C1320	A1260	G1192	C1123	U1061	A990	A925	A861	G738	G738	U607
A1381	A1381	A1321	G1261	G1193	G1124	G1062	C991	G926	G862	A739	A739	A608
G1382	G1382	A1322	A1262	G1195	G1125	G1063	C992	A927	A863	C740	C740	A609

A2435	U2243	U2305	U2243	U2180	G	G2053	U1915	G1831	G1767	A1705	U1636	G1568	C1507
G2436	U2244	C2306	U2244	U2181	G	A2054	A1916	C1832	C1768	C1706	A1637	A1569	A1508
A2437	U2245	G2307	U2245	U2182	U	G2055	U1917	C1833	U1769	C1707	C1638	A1570	A1509
A2438	U2246	G2308	U2246	A2183	G	G2056	U1918	U1834		C1708	C1639	A1571	G1510
A2439	A2247	A2309	A2247	A2184	G	A2057	A1919	G1835	C1773	U1709	A1640	A1572	G1511
G2440		C2310		U2185	G	G2058	C1920	C1836	A1774	G1710	G1645	C1573	C1512
U2441	G2250	A2311	G2250	G2186	A	A2059		C1837	U1775	A1711	G1646	C1574	U1513
A2442		U2312		U2187	G	A2060	C1924	C1838	U1776	U1712	C1647		U1514
C2443	G2253	U2313	G2253	U2188	G	G2061	C1925	U1839	U1777	A1713	C1648	C1577	A1515
G2444	C2254	A2314	C2254	U2189	C	A2062	U1926	G1840	U1778	U1714	U1649	A1578	G1516
G2445	G2255	G2315	G2255	U2190	U		U1927	G1842	U1779	G1715		A1579	G1517
G2446	G2256	A2316	G2256	A2191	U	C2066	A1928	C1843	A1780	U1716	A1650		C1518
G2447	U2257	G2317	U2257	U2192	U	G2067	G1929	C1844	U1781	U1717	G1651		G1519
A2448	C2258	G2318	C2258	G2193	G	U2068	G1930	U1845	U1782	G1718	A1652	A1583	U1520
U2449	U2259	U2194	U2259	U2195	A	G2069	U1931	G1846	A1783	G1719	G1653	U1584	A1521
	C2260	U2196	C2260	U2197	G	A2070	A1932	A1847	A1784		U1654	C1586	A1522
A2453	C2261	C2196	C2261	C2197	G	G2071		U1848	A1785		A1655	G1587	U1523
A2454	G2262	U2197	G2262	U2198	U	C2072	G1935	A1854	A1786	G1723	C1656	G1588	G1524
	C2263	A2198	C2263	A2199	G	C2073	A1936	U1855	A1787	G1724		U1589	A1525
A2457	C2264	A2199	C2264	U2200	G	U2074	A1937	U1856	C1788	U1725	G1661	A1590	C1526
G2458	U2265	C2200	U2265	G2201	G	U2075	U1938	U1857	A1789	C1726	U1662	A1591	G1527
A2459	A2266	G2201	A2266	U2202	G	A2076	U1939	A1858	C1790	C1727	G1663	C1592	A1528
U2460	A2267	U2202	A2267	A2203	G	U2077	C1941	U1859	A1791	C1728	A1664	A1593	G1529
A2461	G2268	G2203	G2268	G2204	G	C2078	C1942	U1940		U1729	A1665	U1594	G1530
C2462	A2269	U2204	A2269	A2205	G	U2079	U1943	U1860	A1794	C1730	G1666	C1595	C1531
G2463	A2270	A2205	A2270		G	A2080	U1944	U1861	C1795	U1731	G1667	A1596	A1532
C2464	G2271	C2206	G2271	C2207	G		G1945	U1862	U1796	C1732	A1668	A1597	C1533
A2465	U2272	U2207	U2272	U2208	G	G2081		U1863	U1797	G1733	A1669	U1598	U1534
A2466	A2273	C2208	A2273	C2209	G	C2084	G1946	U1864	U1798	C1734	G1670	U1599	A1535
C2467	G2274	U2210	G2274	U2211	G	U2087	G1948	U1865	C1799	A1735	U1671	C1600	C1536
A2468	C2275	A2211	C2275	A2212	G		U1951	C1870	C1800	U1736	A1672	G1601	G1537
A2469	G2276	U2212	G2276	U2213	G	C2091	A1952	A1871	A1801	U1737	G1673	U1602	G1538
	G2277	C2213	G2277	C2214	G	U2092	U1953	A1872	A1802	G1738	G1674	A1603	U1539
C2470	A2278	G2214	A2278	C2215	G	G2093	G1954	C1874	A1803	A1739	C1675	C1604	G1540
C2471	G2279	C2215	G2279	A2216	G	C2094	U1955	G1875	A1804	G1740	A1676	G1605	C1541
A2472	G2280	G2216	G2280	G2217	G	U2095	U1956	A1876	A1805	C1741	A1677	U1542	U1542
U2473	A2281	G2217	A2281	G2218	G	A2096	U1957	A1877	G1806	U1742	C1607	C1606	G1543
A2478	G2282	U2218	G2282	U2219	G	C2096	C1957	A1877	G1807	G1743	A1608	A1544	A1544
	C2283	U2220	C2283	U2221	A	A2097	C1958	G1878	A1808	A1744	G1681	A1609	A1545
A2482	A2284	C2221	A2284	C2222	G	U2098	G1959	C1879	A1809	A1745	U1682	A1610	G1546
	C2285	G2222	C2285	G2223	C	U2099		U1880	A1810	A1746	U1683	C1611	
G2485	G2286	C2223	G2286	G2224	C	G2100	U1963	U1883	U1812	U1747	G1684	C1612	A1549
A2488	A2287	G2223	A2287	G2224	G		G1964	U1884	U1813		C1685	G1613	C1550
U2489	G2288	A2225	G2288	A2226	C		A1965				C1686	A1614	A1551
G2490	C2289	C2226	C2289	C2227	G	U2105	C1966	A1889	C1816	U1751	G1687	C1615	A1552
U2491	U2290	U2106	U2290	U2107	U	G2038	C1967	A1890	G1817	G1752	U1688	A1616	U1553
U2492	U2291	U2107	U2291	U2108	U	G2039	A1968	A1891	U1818	A1754			
U2493	G2292	G2228	G2292	G2229	G	U2040	A1969	A1900	A1819	A1755	C1691	U1554	U1554
U2494	G2293	U2229	G2293	U2230	A	U2041	U1971	A1901	U1820	G1756	U1692	G1555	C1556
G2495	C2294	G2230	C2294	G2231	A	G2110	G1972	C1902	U1821	U1757	U1693	C1557	C1557
U2496	U2295	U2232	U2295	U2233	A		G1973	G1903	A1822	U1758	G1695	U1621	U1559
A2497	C2296	C2233	A2497	C2234	U	U	C1974	G1904	G1823	A1759	G1696	G1560	G1560
C2498	A2297	U2234	A2297	U2235	U	G	G1975	G1905	G1824	C1760		C1561	C1561
G2499	U2298	G2235	U2298	G2236	C	A		G1906	U1825	C1761	G1699	U1562	U1562
U2500	C2300	U2236	C2300	U2237	C	G		G1907	U1826	U1762	A1700	U1629	U1563
C2501	C2301	G2237	C2301	G2238	A		A1981		U1827	A1763	A1701	C1564	C1564
G2502	U2302	G2238	U2302	G2239	C	U	U1982	G1983	G1828	U1765	G1702	C1565	C1565
A2503	C2303	A2239	A2503	A2240	C	A	G1983	A1912	G1829	C1766	A1634	A1566	A1566
U2504	G2304		G2304		A		C1985	C1914	C1830		C1704	A1635	G1567



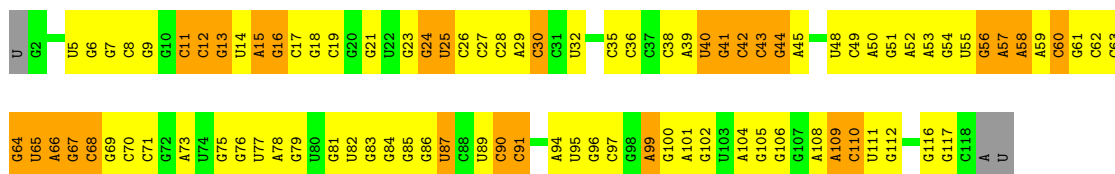
• Molecule 23: 5S rRNA

Chain BB:



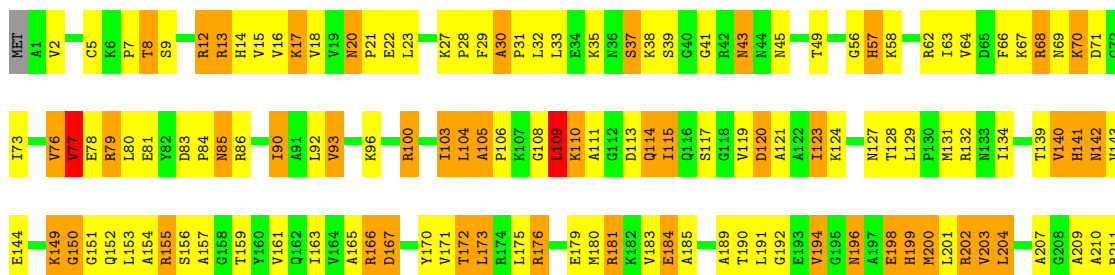
• Molecule 23: 5S rRNA

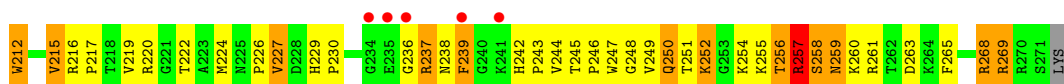
Chain DB:



• Molecule 24: 50S ribosomal protein L2

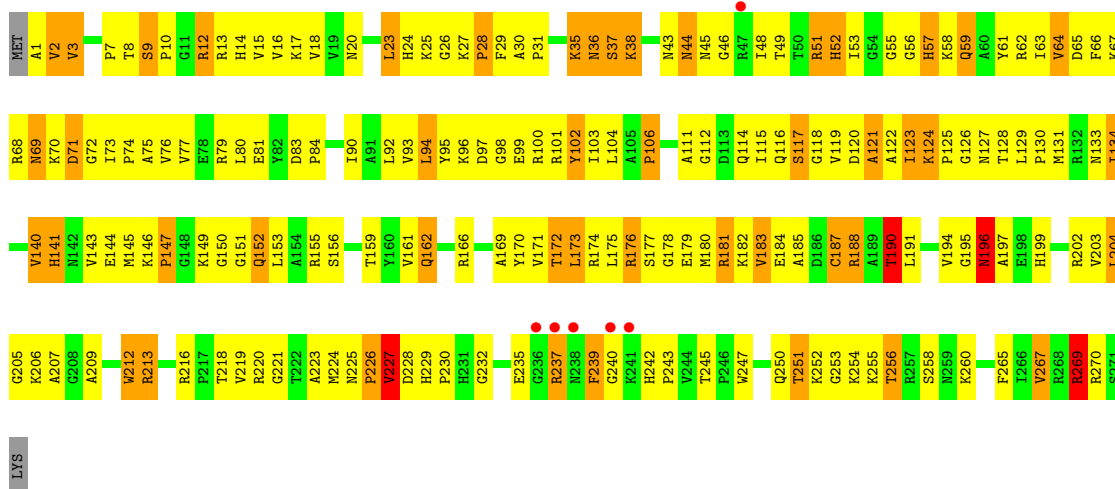
Chain BC:





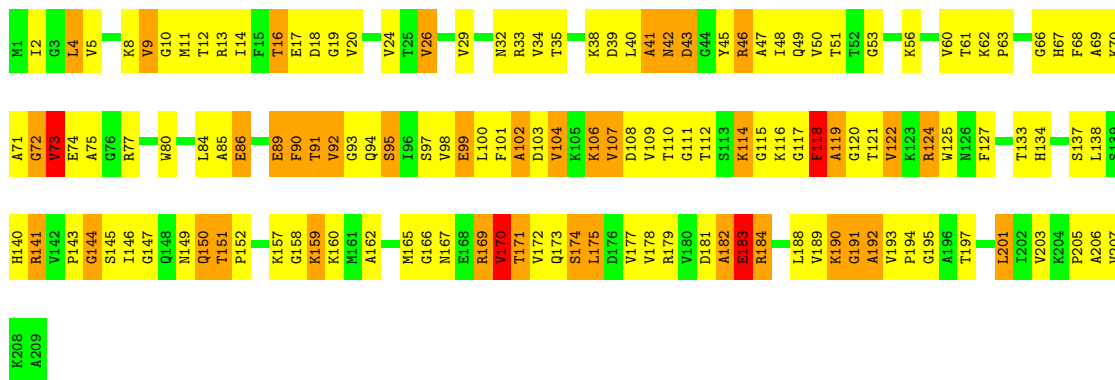
• Molecule 24: 50S ribosomal protein L2

Chain DC:



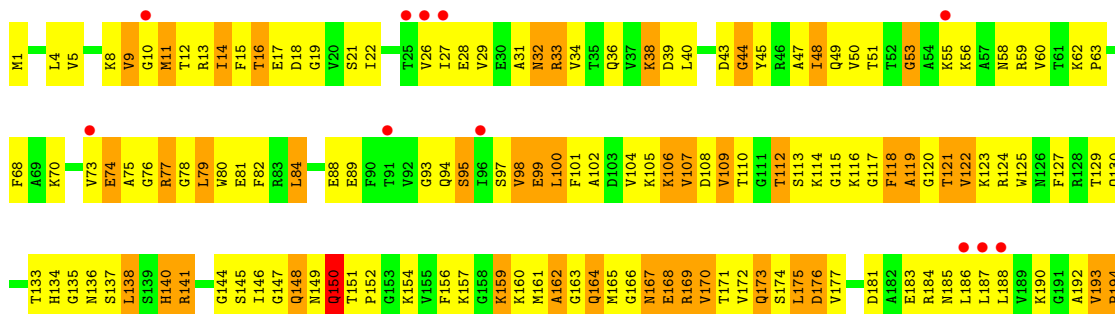
• Molecule 25: 50S ribosomal protein L3

Chain BD:



• Molecule 25: 50S ribosomal protein L3

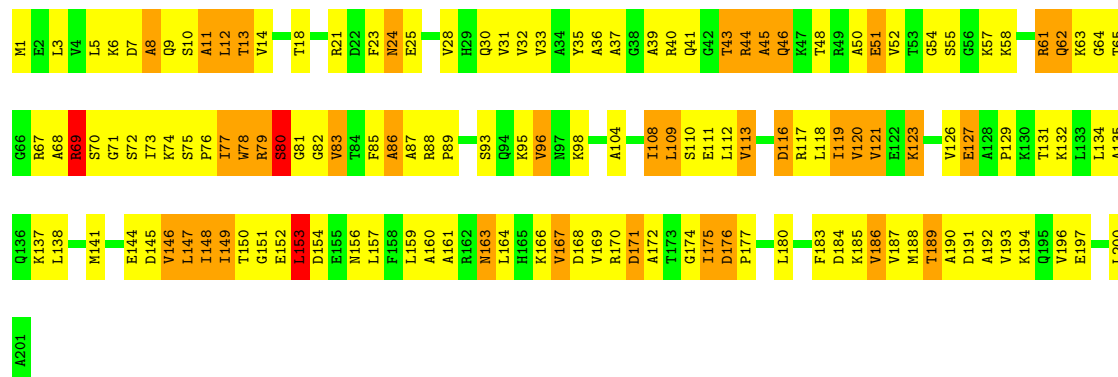
Chain DD:





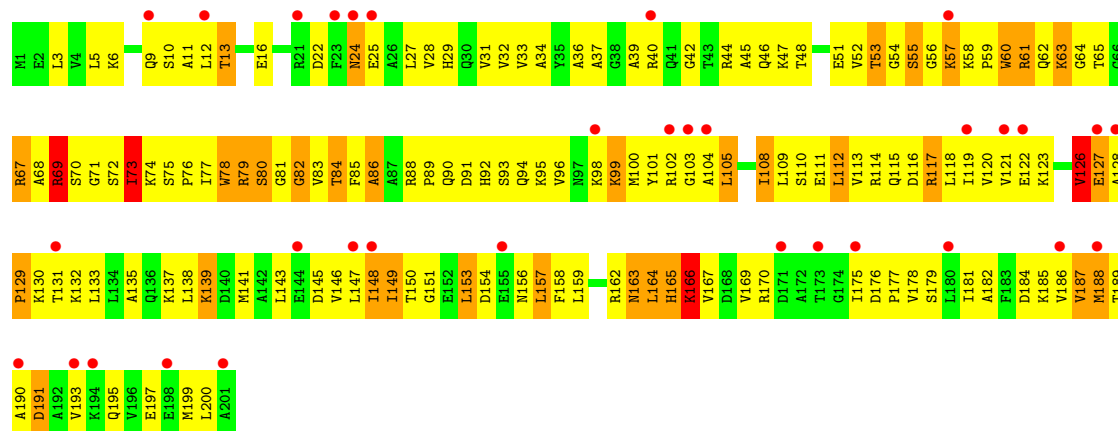
- Molecule 26: 50S ribosomal protein L4

Chain BE:



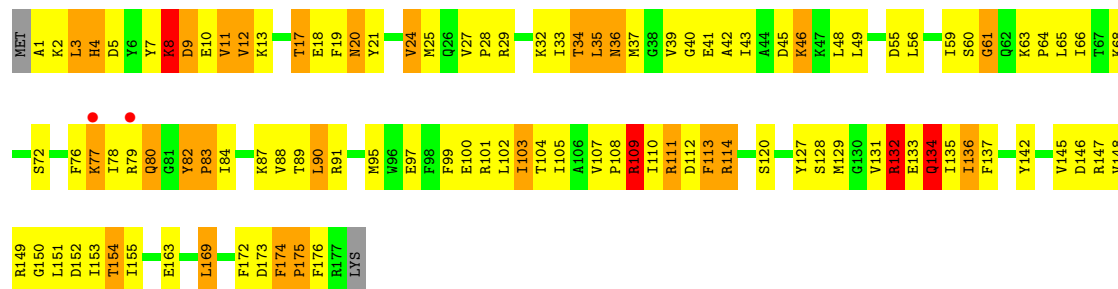
- Molecule 26: 50S ribosomal protein L4

Chain DE:



- Molecule 27: 50S ribosomal protein L5

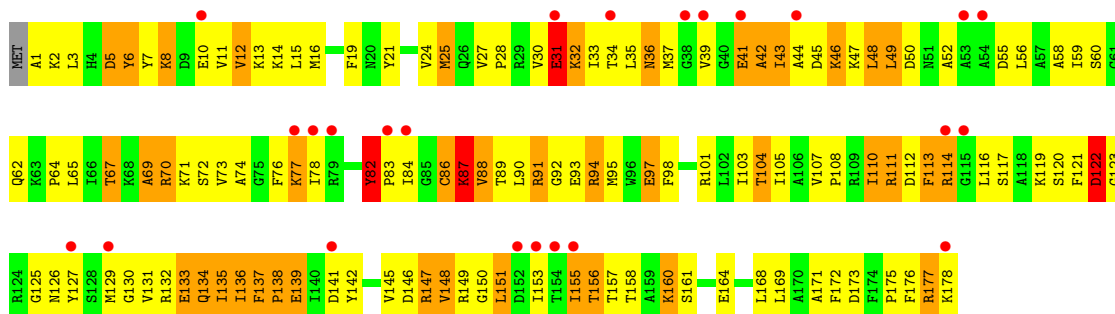
Chain BF:



- Molecule 27: 50S ribosomal protein L5

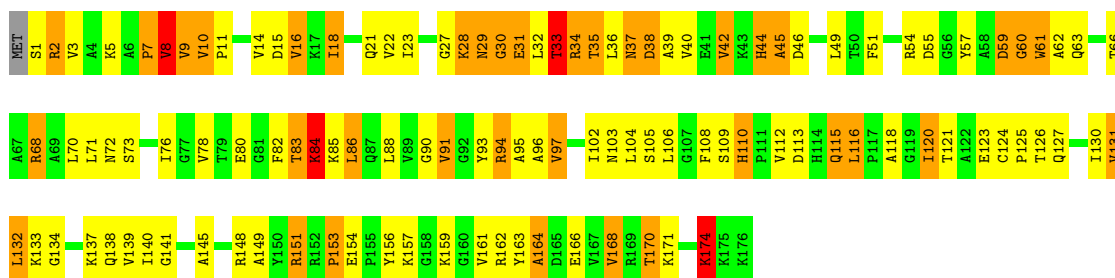
Chain DF:





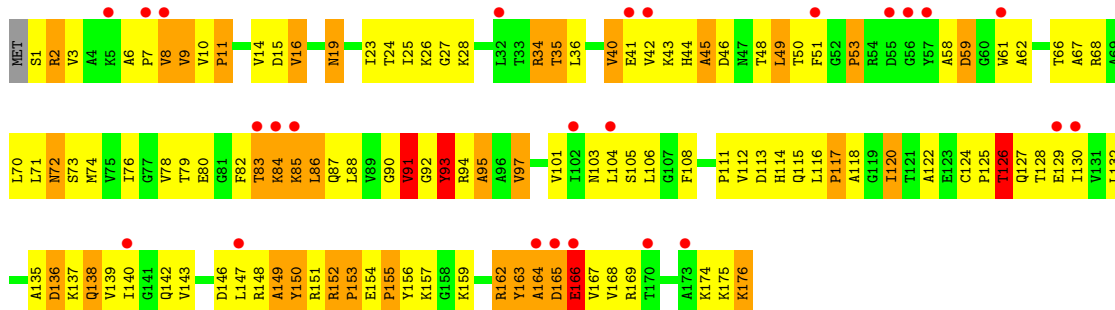
- Molecule 28: 50S ribosomal protein L6

Chain BG:



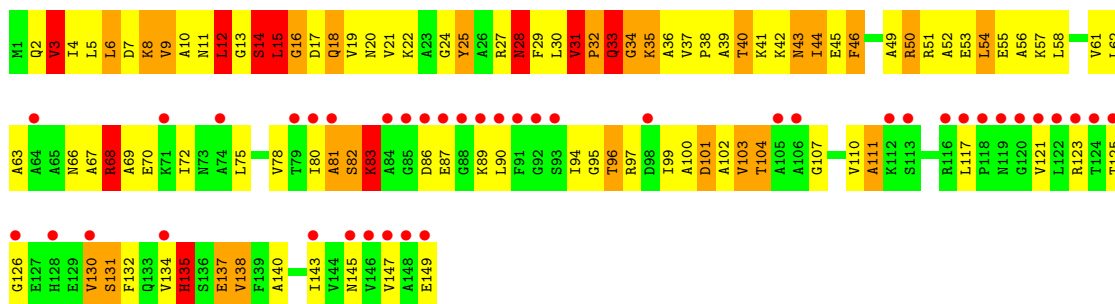
- Molecule 28: 50S ribosomal protein L6

Chain DG:



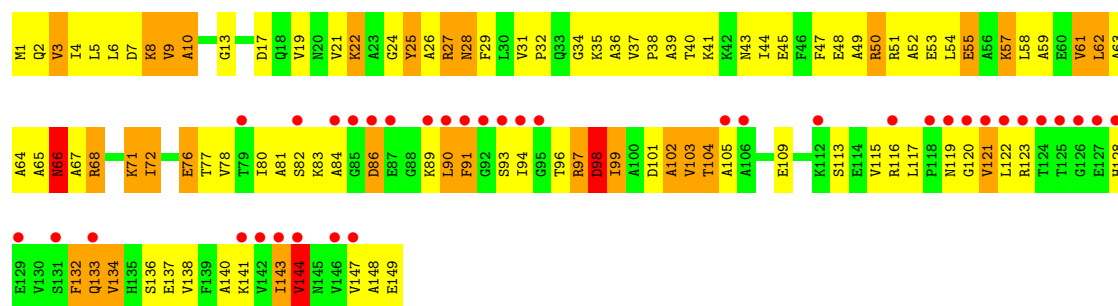
- Molecule 29: 50S ribosomal protein L9

Chain BH:



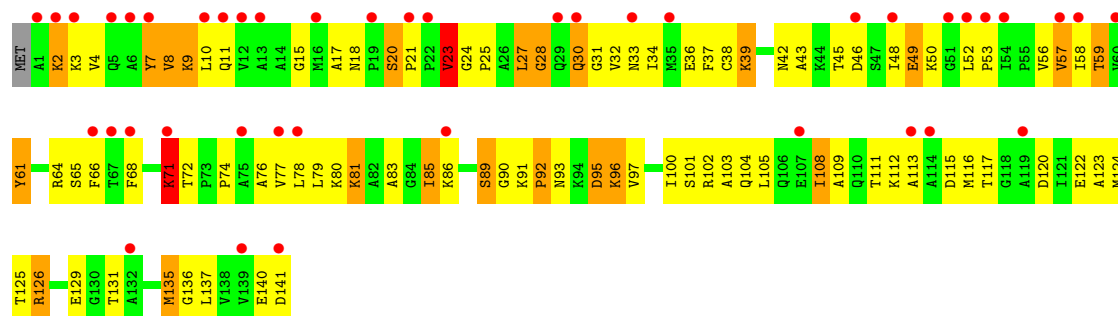
- Molecule 29: 50S ribosomal protein L9

Chain DH:



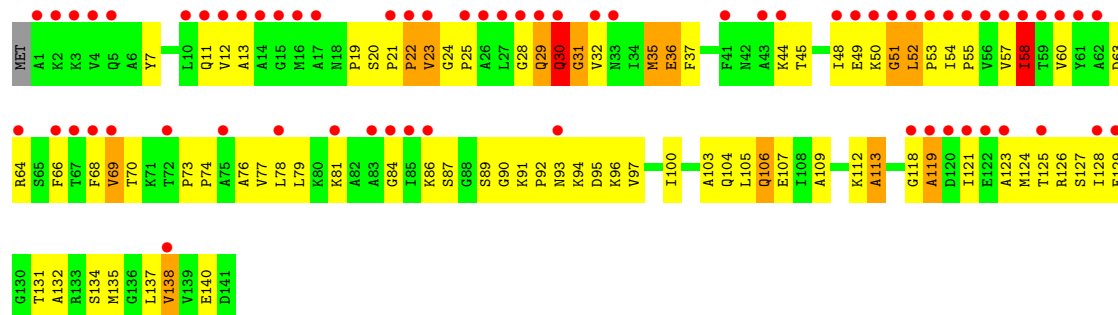
- Molecule 30: 50S ribosomal protein L11

Chain BI:



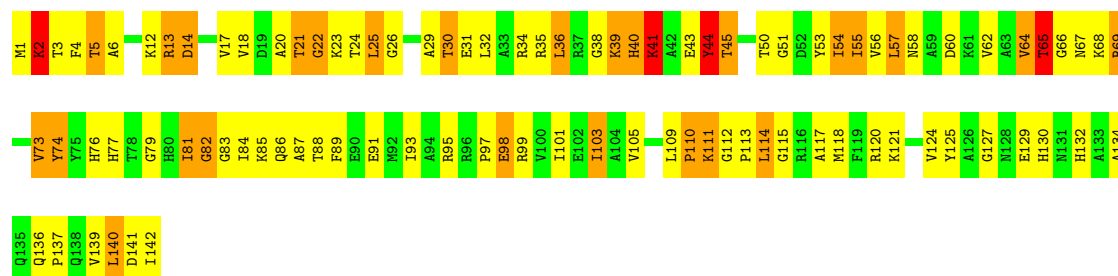
- Molecule 30: 50S ribosomal protein L11

Chain DI:



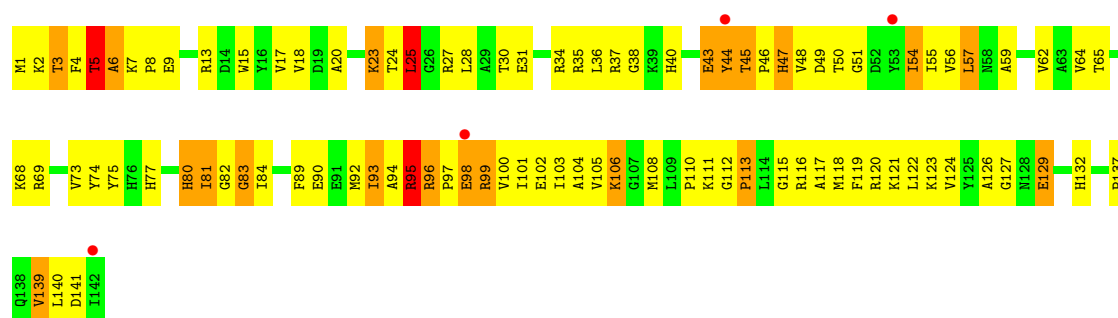
- Molecule 31: 50S ribosomal protein L13

Chain BJ:



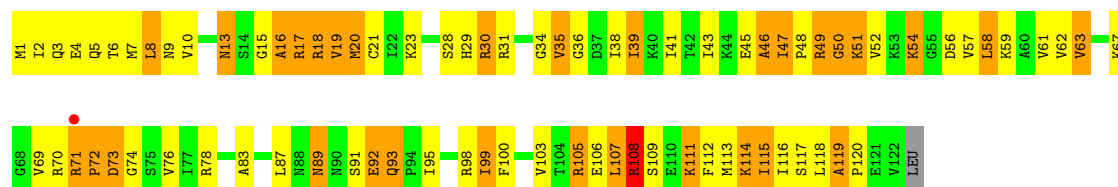
- Molecule 31: 50S ribosomal protein L13

Chain DJ:



- Molecule 32: 50S ribosomal protein L14

Chain BK:



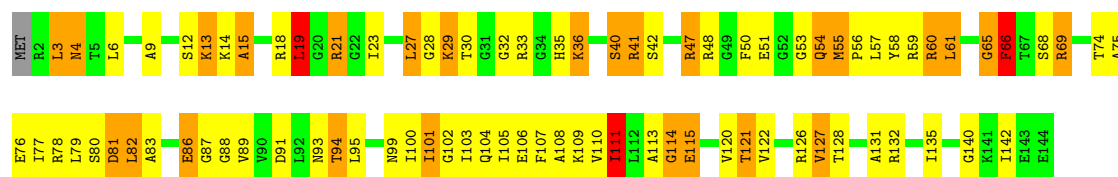
- Molecule 32: 50S ribosomal protein L14

Chain DK:



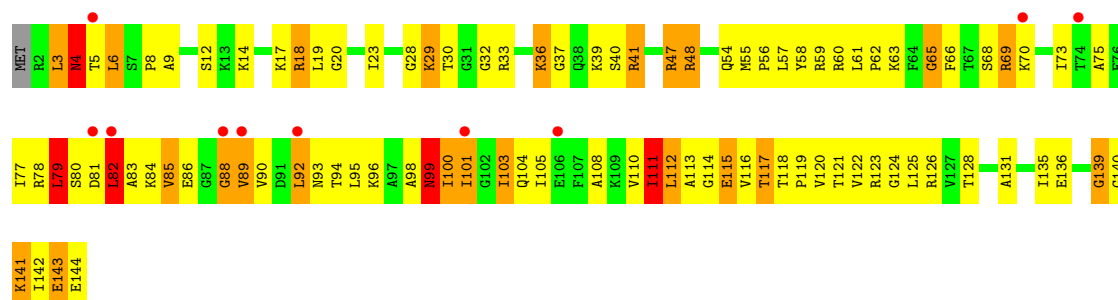
- Molecule 33: 50S ribosomal protein L15

Chain BL:



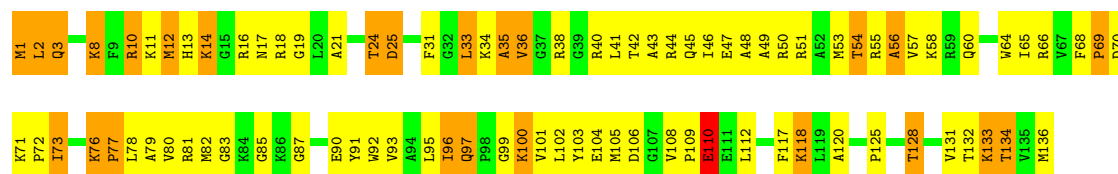
- Molecule 33: 50S ribosomal protein L15

Chain DL:



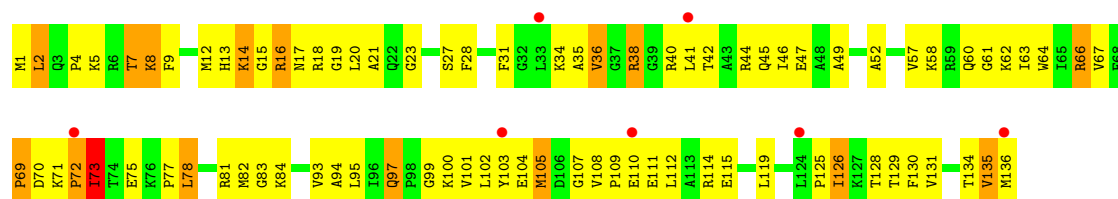
- Molecule 34: 50S ribosomal protein L16

Chain BM:



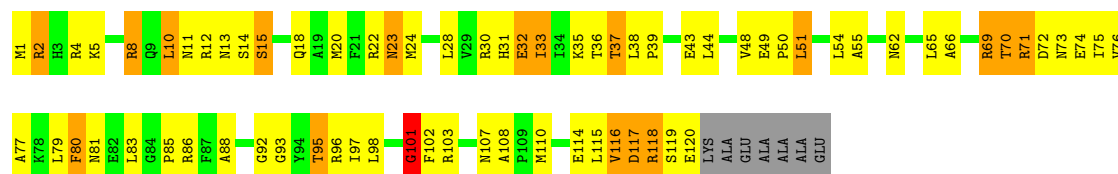
- Molecule 34: 50S ribosomal protein L16

Chain DM:



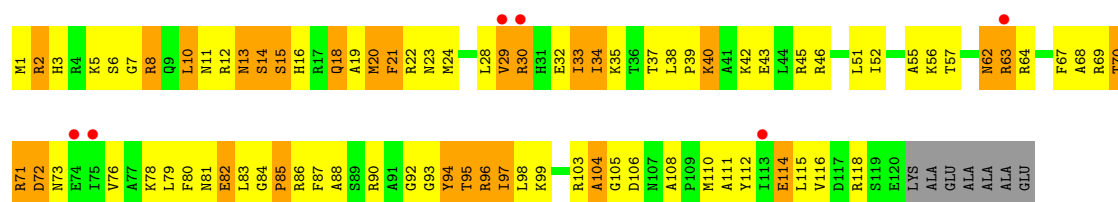
- Molecule 35: 50S ribosomal protein L17

Chain BN:



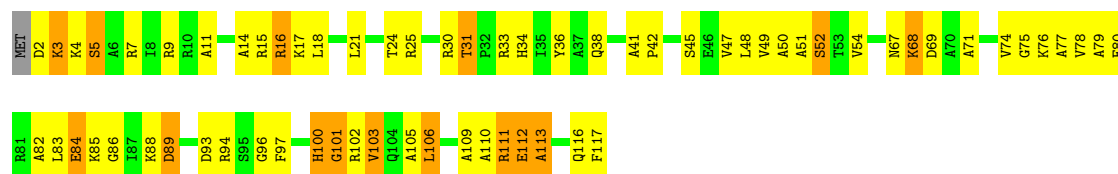
- Molecule 35: 50S ribosomal protein L17

Chain DN:



- Molecule 36: 50S ribosomal protein L18

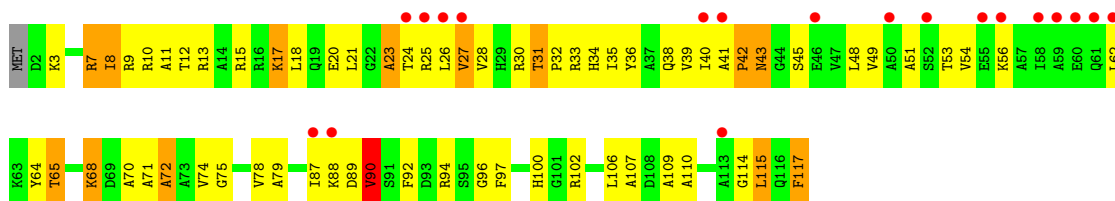
Chain BO:



- Molecule 36: 50S ribosomal protein L18

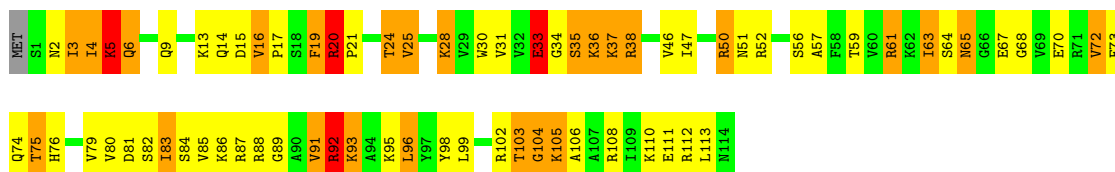
Chain DO:





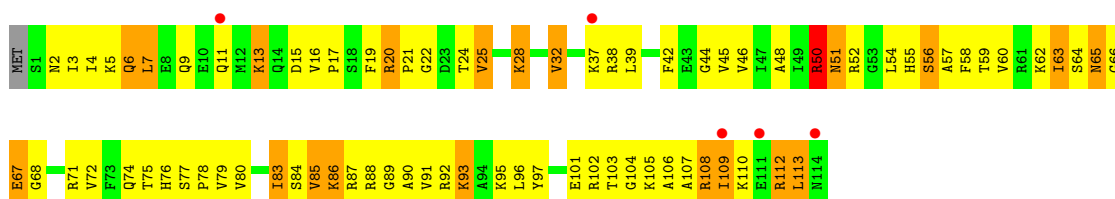
• Molecule 37: 50S ribosomal protein L19

Chain BP:



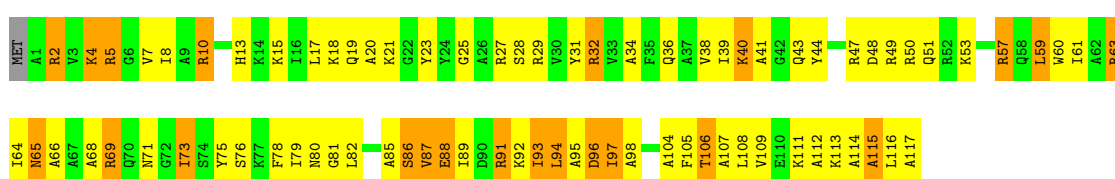
• Molecule 37: 50S ribosomal protein L19

Chain DP:



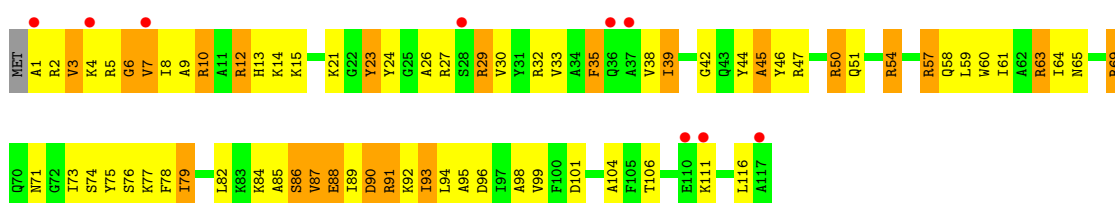
• Molecule 38: 50S ribosomal protein L20

Chain BQ:



• Molecule 38: 50S ribosomal protein L20

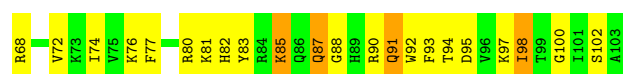
Chain DQ:



• Molecule 39: 50S ribosomal protein L21

Chain BR:





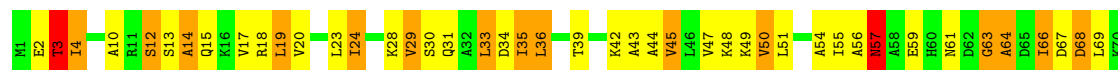
• Molecule 39: 50S ribosomal protein L21

Chain DR:



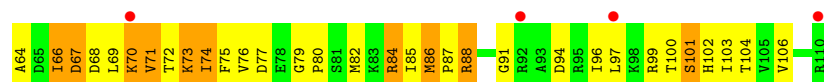
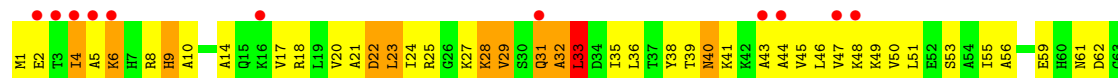
• Molecule 40: 50S ribosomal protein L22

Chain BS:



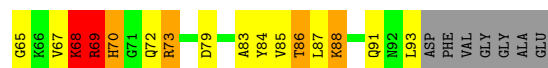
• Molecule 40: 50S ribosomal protein L22

Chain DS:



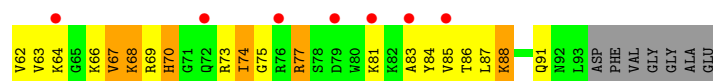
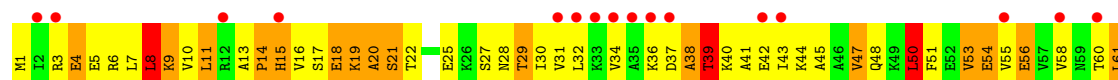
• Molecule 41: 50S ribosomal protein L23

Chain BT:



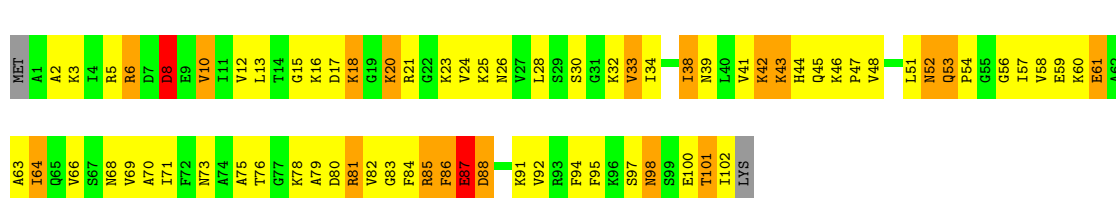
• Molecule 41: 50S ribosomal protein L23

Chain DT:



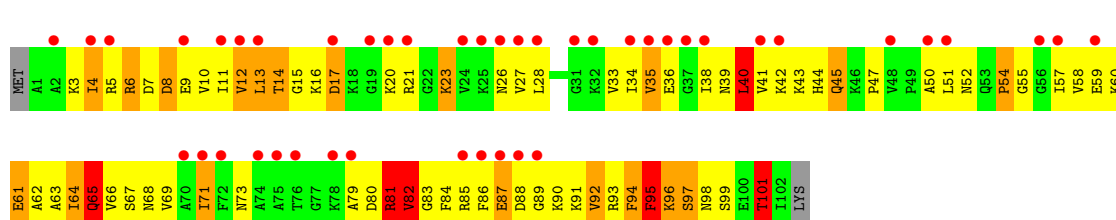
- Molecule 42: 50S ribosomal protein L24

Chain BU:



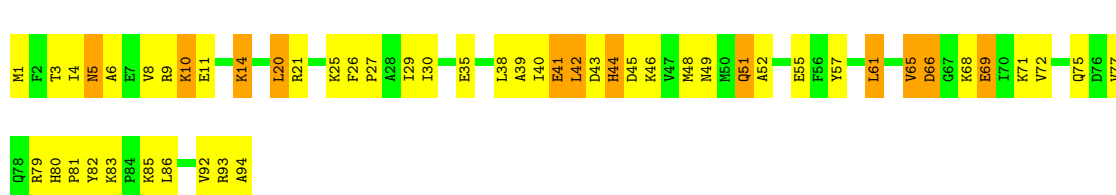
- Molecule 42: 50S ribosomal protein L24

Chain DU:



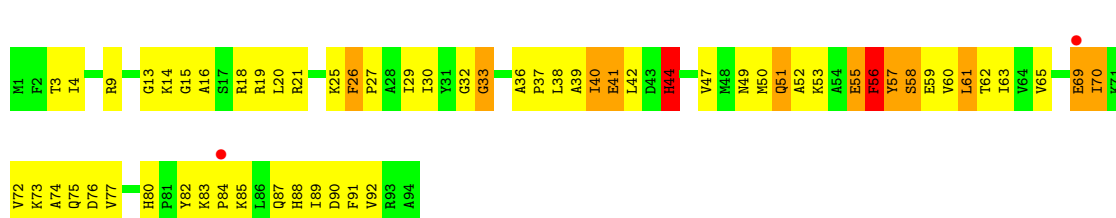
- Molecule 43: 50S ribosomal protein L25

Chain BV:



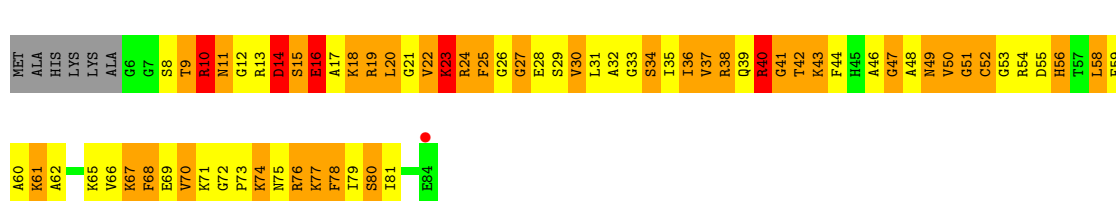
- Molecule 43: 50S ribosomal protein L25

Chain DV:



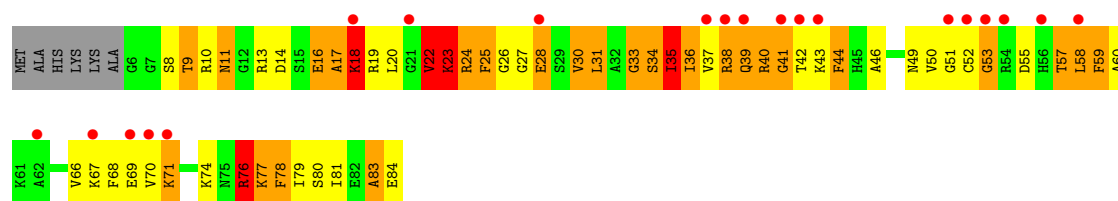
- Molecule 44: 50S ribosomal protein L27

Chain BW:



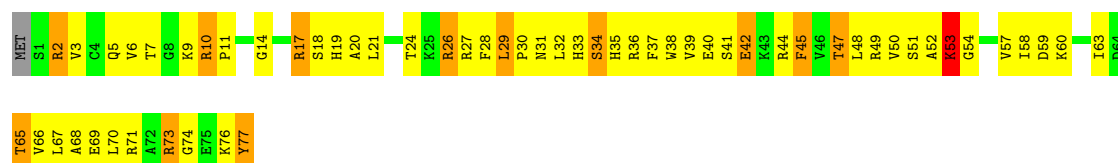
- Molecule 44: 50S ribosomal protein L27

Chain DW:



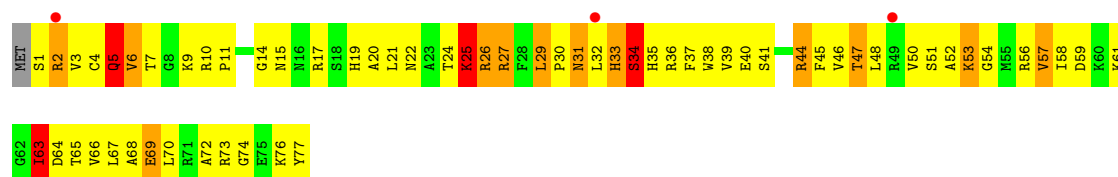
• Molecule 45: 50S ribosomal protein L28

Chain BX:



• Molecule 45: 50S ribosomal protein L28

Chain DX:



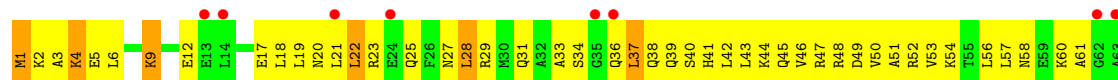
• Molecule 46: 50S ribosomal protein L29

Chain BY:



• Molecule 46: 50S ribosomal protein L29

Chain DY:



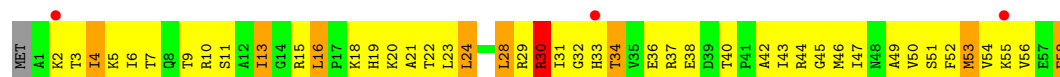
• Molecule 47: 50S ribosomal protein L30

Chain BZ:



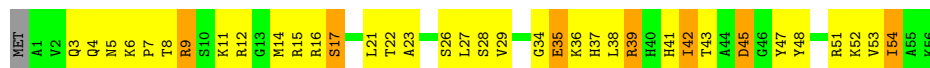
• Molecule 47: 50S ribosomal protein L30

Chain DZ:



- Molecule 48: 50S ribosomal protein L32

Chain B0:



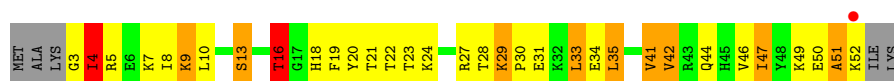
- Molecule 48: 50S ribosomal protein L32

Chain D0:



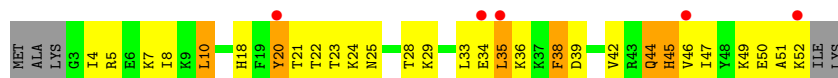
- Molecule 49: 50S ribosomal protein L33

Chain B1:



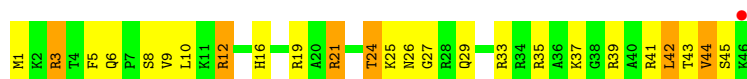
- Molecule 49: 50S ribosomal protein L33

Chain D1:



- Molecule 50: 50S ribosomal protein L34

Chain B2:



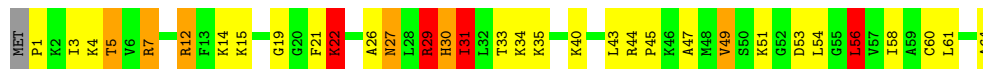
- Molecule 50: 50S ribosomal protein L34

Chain D2:



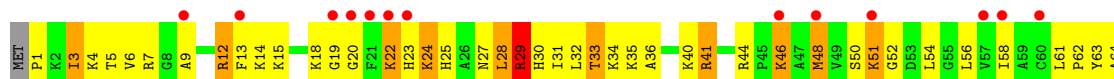
- Molecule 51: 50S ribosomal protein L35

Chain B3:

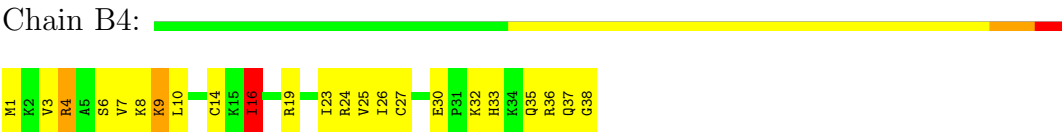


- Molecule 51: 50S ribosomal protein L35

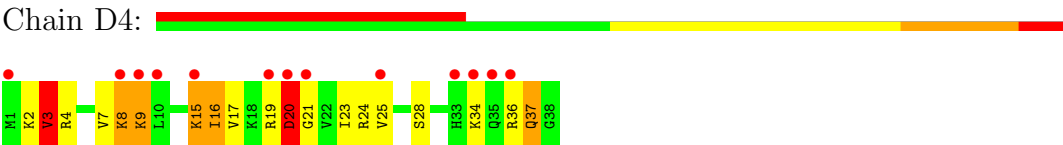
Chain D3:



● Molecule 52: 50S ribosomal protein L36



● Molecule 52: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.76Å 433.27Å 618.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.78 – 3.30 69.78 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (69.78-3.30) 95.9 (69.78-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_501)	Depositor
R, R_{free}	0.187 , 0.244 0.216 , 0.265	Depositor DCC
R_{free} test set	19581 reflections (2.06%)	DCC
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 971020 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284464	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EM1, MG

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	0.43	0/36834	0.82	31/57462 (0.1%)
1	CA	0.39	0/36762	0.80	29/57350 (0.1%)
2	AB	0.30	0/1735	0.55	0/2338
2	CB	0.26	0/1735	0.49	0/2338
3	AC	0.30	0/1651	0.53	1/2225 (0.0%)
3	CC	0.26	0/1651	0.48	0/2225
4	AD	0.32	0/1665	0.54	0/2227
4	CD	0.40	0/1665	0.63	0/2227
5	AE	0.38	0/1118	0.63	0/1504
5	CE	0.35	0/1118	0.60	0/1504
6	AF	0.31	0/835	0.51	0/1128
6	CF	0.30	0/835	0.54	0/1128
7	AG	0.27	0/1195	0.47	0/1602
7	CG	0.25	0/1187	0.48	0/1591
8	AH	0.35	0/989	0.56	0/1326
8	CH	0.30	0/989	0.51	0/1326
9	AI	0.27	0/1034	0.51	0/1375
9	CI	0.26	0/1034	0.48	0/1375
10	AJ	0.30	0/796	0.52	0/1077
10	CJ	0.26	0/796	0.50	0/1077
11	AK	0.29	0/893	0.54	0/1205
11	CK	0.29	0/893	0.55	0/1205
12	AL	0.35	0/969	0.67	0/1300
12	CL	0.34	0/969	0.58	0/1300
13	AM	0.26	0/892	0.50	0/1193
13	CM	0.22	0/884	0.44	0/1181
14	AN	0.29	0/785	0.51	0/1043
14	CN	0.23	0/746	0.42	0/990
15	AO	0.31	0/722	0.49	0/964
15	CO	0.27	0/722	0.46	0/964
16	AP	0.29	0/659	0.51	0/884
16	CP	0.31	0/648	0.53	0/870

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.39	0/657	0.63	0/881
17	CQ	0.32	0/657	0.53	0/881
18	AR	0.30	0/462	0.52	0/621
18	CR	0.35	0/462	0.50	0/621
19	AS	0.26	0/652	0.48	0/877
19	CS	0.22	0/652	0.45	0/877
20	AT	0.38	0/671	0.58	0/888
20	CT	0.27	0/671	0.52	0/888
21	AU	0.33	0/430	0.50	0/570
21	CU	0.38	0/430	0.64	0/570
22	BA	0.73	7/68626 (0.0%)	1.08	288/107056 (0.3%)
22	DA	0.38	0/68314	0.83	60/106569 (0.1%)
23	BB	0.64	0/2828	0.94	1/4410 (0.0%)
23	DB	0.30	0/2803	0.76	1/4371 (0.0%)
24	BC	0.47	0/2121	0.72	1/2852 (0.0%)
24	DC	0.32	0/2121	0.55	0/2852
25	BD	0.56	0/1586	0.80	1/2134 (0.0%)
25	DD	0.31	0/1586	0.57	0/2134
26	BE	0.43	0/1571	0.66	0/2113
26	DE	0.27	0/1571	0.51	0/2113
27	BF	0.32	0/1434	0.53	0/1926
27	DF	0.24	0/1444	0.50	0/1937
28	BG	0.40	0/1343	0.65	0/1816
28	DG	0.24	0/1343	0.50	0/1816
29	BH	0.32	0/1122	0.56	0/1515
29	DH	0.29	0/1122	0.52	0/1515
30	BI	0.23	0/1046	0.48	0/1410
30	DI	0.22	0/1046	0.47	0/1410
31	BJ	0.57	0/1152	0.82	1/1551 (0.1%)
31	DJ	0.29	0/1152	0.60	1/1551 (0.1%)
32	BK	0.54	0/947	0.80	0/1268
32	DK	0.34	0/947	0.58	0/1268
33	BL	0.44	0/1054	0.75	1/1403 (0.1%)
33	DL	0.28	0/1054	0.56	0/1403
34	BM	0.50	0/1093	0.71	0/1460
34	DM	0.29	0/1093	0.50	0/1460
35	BN	0.49	0/973	0.72	0/1301
35	DN	0.30	0/973	0.53	0/1301
36	BO	0.41	0/902	0.63	0/1209
36	DO	0.24	0/902	0.45	0/1209
37	BP	0.48	0/929	0.73	0/1242
37	DP	0.32	0/929	0.52	0/1242
38	BQ	0.58	0/960	0.75	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.30	0/960	0.47	0/1278
39	BR	0.59	0/829	0.80	0/1107
39	DR	0.30	0/829	0.52	0/1107
40	BS	0.54	0/864	0.76	0/1156
40	DS	0.29	0/864	0.54	1/1156 (0.1%)
41	BT	0.47	0/744	0.72	0/994
41	DT	0.26	0/744	0.54	0/994
42	BU	0.43	0/787	0.68	0/1051
42	DU	0.26	0/787	0.51	0/1051
43	BV	0.42	0/766	0.61	0/1025
43	DV	0.24	0/766	0.44	0/1025
44	BW	0.67	1/603 (0.2%)	0.96	2/797 (0.3%)
44	DW	0.29	0/603	0.54	0/797
45	BX	0.44	0/635	0.69	0/848
45	DX	0.28	0/635	0.58	0/848
46	BY	0.35	0/510	0.61	0/677
46	DY	0.23	0/510	0.50	0/677
47	BZ	0.56	0/453	0.77	0/605
47	DZ	0.28	0/453	0.53	0/605
48	B0	0.45	0/450	0.74	0/599
48	D0	0.30	0/450	0.52	0/599
49	B1	0.39	0/416	0.63	0/554
49	D1	0.27	0/416	0.49	0/554
50	B2	0.52	0/380	0.76	0/498
50	D2	0.30	0/380	0.54	0/498
51	B3	0.46	0/513	0.73	1/676 (0.1%)
51	D3	0.29	0/513	0.56	0/676
52	B4	0.52	0/303	0.73	0/397
52	D4	0.33	0/303	0.53	0/397
All	All	0.48	8/306703 (0.0%)	0.84	420/458519 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
25	BD	0	1
31	BJ	0	1
35	BN	0	1
51	B3	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	984	A	N9-C4	-8.71	1.32	1.37
22	BA	1142	A	N9-C4	-8.61	1.32	1.37
22	BA	1936	A	N9-C4	-6.89	1.33	1.37
44	BW	32	ALA	CA-CB	5.66	1.64	1.52
22	BA	984	A	C5-C6	-5.54	1.36	1.41

The worst 5 of 420 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	974	G	C5-N7-C8	-11.14	98.73	104.30
22	BA	1142	A	C2-N3-C4	-10.75	105.23	110.60
22	BA	974	G	N7-C8-N9	10.43	118.31	113.10
22	BA	1990	C	C6-N1-C2	10.42	124.47	120.30
22	BA	560	C	N3-C4-C5	10.30	126.02	121.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	B3	29	ARG	Peptide
25	BD	9	VAL	Peptide
31	BJ	110	PRO	Peptide
35	BN	101	GLY	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32895	0	16553	1244	0
1	CA	32831	0	16521	1591	0
2	AB	1704	0	1732	225	0
2	CB	1704	0	1732	160	0
3	AC	1624	0	1699	109	0
3	CC	1624	0	1699	125	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AD	1643	0	1710	153	0
4	CD	1643	0	1710	156	0
5	AE	1105	0	1148	135	0
5	CE	1105	0	1148	106	0
6	AF	817	0	808	83	0
6	CF	817	0	808	85	0
7	AG	1181	0	1240	93	0
7	CG	1174	0	1230	130	0
8	AH	979	0	1034	86	0
8	CH	979	0	1034	97	0
9	AI	1022	0	1070	99	0
9	CI	1022	0	1070	127	0
10	AJ	786	0	828	93	0
10	CJ	786	0	828	96	0
11	AK	877	0	887	83	0
11	CK	877	0	887	74	0
12	AL	955	0	1019	88	0
12	CL	955	0	1019	86	0
13	AM	883	0	944	67	0
13	CM	876	0	937	106	0
14	AN	774	0	827	78	0
14	CN	735	0	790	97	0
15	AO	714	0	737	54	0
15	CO	714	0	737	43	0
16	AP	649	0	666	48	0
16	CP	638	0	656	51	0
17	AQ	648	0	691	89	0
17	CQ	648	0	691	56	0
18	AR	455	0	478	21	0
18	CR	455	0	478	39	0
19	AS	637	0	665	54	0
19	CS	637	0	665	87	0
20	AT	665	0	714	85	0
20	CT	665	0	714	40	0
21	AU	425	0	449	79	0
21	CU	425	0	449	76	0
22	BA	61274	0	30819	1807	0
22	DA	60995	0	30679	3669	0
23	BB	2529	0	1281	57	0
23	DB	2507	0	1270	166	0
24	BC	2082	0	2157	207	0
24	DC	2082	0	2157	227	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	BD	1565	0	1616	201	0
25	DD	1565	0	1616	202	0
26	BE	1552	0	1619	151	0
26	DE	1552	0	1619	188	0
27	BF	1410	0	1447	128	0
27	DF	1420	0	1460	158	0
28	BG	1323	0	1374	138	0
28	DG	1323	0	1374	144	0
29	BH	1111	0	1148	97	0
29	DH	1111	0	1148	119	0
30	BI	1032	0	1088	108	0
30	DI	1032	0	1088	83	0
31	BJ	1129	0	1162	151	0
31	DJ	1129	0	1162	132	0
32	BK	938	0	1012	91	0
32	DK	938	0	1012	107	0
33	BL	1045	0	1117	110	0
33	DL	1045	0	1117	136	0
34	BM	1074	0	1157	94	0
34	DM	1074	0	1157	91	0
35	BN	960	0	1000	77	0
35	DN	960	0	1000	141	0
36	BO	892	0	923	50	0
36	DO	892	0	923	76	0
37	BP	917	0	965	122	0
37	DP	917	0	965	123	0
38	BQ	947	0	1022	139	0
38	DQ	947	0	1022	124	0
39	BR	816	0	839	102	0
39	DR	816	0	839	94	0
40	BS	857	0	922	83	0
40	DS	857	0	922	69	0
41	BT	738	0	807	107	0
41	DT	738	0	807	104	0
42	BU	779	0	834	61	0
42	DU	779	0	834	98	0
43	BV	753	0	780	47	0
43	DV	753	0	780	62	0
44	BW	596	0	610	191	0
44	DW	596	0	610	127	0
45	BX	625	0	655	53	0
45	DX	625	0	655	77	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	BY	509	0	543	40	0
46	DY	509	0	543	76	0
47	BZ	449	0	491	33	0
47	DZ	449	0	491	42	0
48	B0	444	0	461	29	0
48	D0	444	0	461	54	0
49	B1	409	0	440	42	0
49	D1	409	0	440	39	0
50	B2	377	0	418	25	0
50	D2	377	0	418	52	0
51	B3	504	0	574	42	0
51	D3	504	0	574	52	0
52	B4	302	0	340	29	0
52	D4	302	0	342	22	0
53	AA	43	0	0	0	0
53	BA	134	0	0	0	0
53	BB	4	0	0	0	0
53	BL	1	0	0	0	0
53	CA	42	0	0	0	0
53	DA	133	0	0	0	0
53	DB	1	0	0	0	0
53	DC	1	0	0	0	0
53	DE	1	0	0	0	0
53	DJ	1	0	0	0	0
54	BA	60	0	64	7	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	200	0	0	4	0
56	AL	1	0	0	0	0
56	AN	5	0	0	1	0
56	AT	1	0	0	0	0
56	AU	1	0	0	0	0
56	B2	1	0	0	0	0
56	B3	2	0	0	0	0
56	B4	2	0	0	0	0
56	BA	606	0	0	39	0
56	BB	20	0	0	0	0
56	BC	9	0	0	0	0
56	BD	1	0	0	0	0
56	BL	4	0	0	0	0
56	BN	3	0	0	0	0
56	BT	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CA	194	0	0	7	0
56	CE	5	0	0	1	0
56	CI	1	0	0	0	0
56	CL	1	0	0	0	0
56	CN	3	0	0	0	0
56	CT	2	0	0	0	0
56	CU	1	0	0	0	0
56	D2	1	0	0	1	0
56	D3	1	0	0	0	0
56	D4	5	0	0	0	0
56	DA	605	0	0	35	0
56	DB	4	0	0	1	0
56	DC	8	0	0	0	0
56	DD	3	0	0	0	0
56	DE	3	0	0	0	0
56	DJ	3	0	0	0	0
56	DL	4	0	0	0	0
56	DN	1	0	0	0	0
56	DT	2	0	0	0	0
56	DU	2	0	0	0	0
56	DV	1	0	0	0	0
All	All	284464	0	190872	16438	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 35.

The worst 5 of 16438 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:BQ:63:ARG:NH1	38:BQ:96:ASP:HA	1.42	1.33
12:CL:43:LYS:HB3	12:CL:44:PRO:HD2	1.18	1.17
22:BA:1073:A:H3'	22:BA:1074:G:H5''	1.20	1.17
1:CA:120:A:C3'	1:CA:121:U:H5''	1.75	1.17
6:AF:16:GLU:HG2	4:CD:191:SER:HB2	1.20	1.17

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/241 (90%)	129 (60%)	51 (24%)	36 (17%)	0	1
2	CB	216/241 (90%)	146 (68%)	49 (23%)	21 (10%)	1	8
3	AC	204/233 (88%)	159 (78%)	26 (13%)	19 (9%)	1	9
3	CC	204/233 (88%)	137 (67%)	44 (22%)	23 (11%)	1	5
4	AD	203/206 (98%)	135 (66%)	39 (19%)	29 (14%)	0	2
4	CD	203/206 (98%)	141 (70%)	44 (22%)	18 (9%)	1	10
5	AE	148/167 (89%)	108 (73%)	25 (17%)	15 (10%)	1	8
5	CE	148/167 (89%)	110 (74%)	24 (16%)	14 (10%)	1	9
6	AF	98/135 (73%)	62 (63%)	28 (29%)	8 (8%)	1	13
6	CF	98/135 (73%)	59 (60%)	28 (29%)	11 (11%)	1	5
7	AG	149/179 (83%)	108 (72%)	33 (22%)	8 (5%)	3	26
7	CG	148/179 (83%)	86 (58%)	46 (31%)	16 (11%)	1	6
8	AH	127/130 (98%)	95 (75%)	25 (20%)	7 (6%)	3	25
8	CH	127/130 (98%)	92 (72%)	25 (20%)	10 (8%)	1	13
9	AI	125/130 (96%)	88 (70%)	25 (20%)	12 (10%)	1	9
9	CI	125/130 (96%)	91 (73%)	25 (20%)	9 (7%)	2	16
10	AJ	96/103 (93%)	64 (67%)	17 (18%)	15 (16%)	0	1
10	CJ	96/103 (93%)	61 (64%)	22 (23%)	13 (14%)	0	3
11	AK	115/129 (89%)	83 (72%)	22 (19%)	10 (9%)	1	11
11	CK	115/129 (89%)	87 (76%)	18 (16%)	10 (9%)	1	11
12	AL	121/124 (98%)	87 (72%)	23 (19%)	11 (9%)	1	10
12	CL	121/124 (98%)	90 (74%)	22 (18%)	9 (7%)	2	15
13	AM	112/118 (95%)	83 (74%)	20 (18%)	9 (8%)	1	13
13	CM	111/118 (94%)	64 (58%)	33 (30%)	14 (13%)	0	3
14	AN	92/101 (91%)	57 (62%)	25 (27%)	10 (11%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	87/101 (86%)	58 (67%)	18 (21%)	11 (13%)	0	3
15	AO	86/89 (97%)	55 (64%)	26 (30%)	5 (6%)	3	23
15	CO	86/89 (97%)	64 (74%)	18 (21%)	4 (5%)	4	30
16	AP	80/82 (98%)	55 (69%)	17 (21%)	8 (10%)	1	8
16	CP	78/82 (95%)	52 (67%)	18 (23%)	8 (10%)	1	7
17	AQ	78/84 (93%)	55 (70%)	11 (14%)	12 (15%)	0	1
17	CQ	78/84 (93%)	63 (81%)	6 (8%)	9 (12%)	1	5
18	AR	53/75 (71%)	41 (77%)	10 (19%)	2 (4%)	5	37
18	CR	53/75 (71%)	37 (70%)	15 (28%)	1 (2%)	12	60
19	AS	77/92 (84%)	57 (74%)	14 (18%)	6 (8%)	1	14
19	CS	77/92 (84%)	47 (61%)	25 (32%)	5 (6%)	2	19
20	AT	83/87 (95%)	61 (74%)	16 (19%)	6 (7%)	2	16
20	CT	83/87 (95%)	59 (71%)	18 (22%)	6 (7%)	2	16
21	AU	49/71 (69%)	25 (51%)	14 (29%)	10 (20%)	0	1
21	CU	49/71 (69%)	21 (43%)	12 (24%)	16 (33%)	0	0
24	BC	269/273 (98%)	198 (74%)	43 (16%)	28 (10%)	1	7
24	DC	269/273 (98%)	180 (67%)	60 (22%)	29 (11%)	1	6
25	BD	207/209 (99%)	147 (71%)	31 (15%)	29 (14%)	0	2
25	DD	207/209 (99%)	128 (62%)	45 (22%)	34 (16%)	0	1
26	BE	199/201 (99%)	146 (73%)	32 (16%)	21 (11%)	1	6
26	DE	199/201 (99%)	117 (59%)	55 (28%)	27 (14%)	0	3
27	BF	175/179 (98%)	138 (79%)	22 (13%)	15 (9%)	1	11
27	DF	176/179 (98%)	102 (58%)	42 (24%)	32 (18%)	0	1
28	BG	174/177 (98%)	121 (70%)	26 (15%)	27 (16%)	0	1
28	DG	174/177 (98%)	104 (60%)	36 (21%)	34 (20%)	0	1
29	BH	147/149 (99%)	64 (44%)	49 (33%)	34 (23%)	0	0
29	DH	147/149 (99%)	73 (50%)	59 (40%)	15 (10%)	1	7
30	BI	139/142 (98%)	84 (60%)	42 (30%)	13 (9%)	1	9
30	DI	139/142 (98%)	85 (61%)	37 (27%)	17 (12%)	1	4
31	BJ	140/142 (99%)	107 (76%)	19 (14%)	14 (10%)	1	8
31	DJ	140/142 (99%)	98 (70%)	28 (20%)	14 (10%)	1	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BK	120/123 (98%)	87 (72%)	16 (13%)	17 (14%)	0	2
32	DK	120/123 (98%)	83 (69%)	20 (17%)	17 (14%)	0	2
33	BL	141/144 (98%)	98 (70%)	27 (19%)	16 (11%)	1	5
33	DL	141/144 (98%)	77 (55%)	45 (32%)	19 (14%)	0	3
34	BM	134/136 (98%)	97 (72%)	22 (16%)	15 (11%)	1	5
34	DM	134/136 (98%)	92 (69%)	28 (21%)	14 (10%)	1	7
35	BN	118/127 (93%)	96 (81%)	14 (12%)	8 (7%)	2	18
35	DN	118/127 (93%)	72 (61%)	30 (25%)	16 (14%)	0	3
36	BO	114/117 (97%)	89 (78%)	17 (15%)	8 (7%)	2	17
36	DO	114/117 (97%)	74 (65%)	29 (25%)	11 (10%)	1	9
37	BP	112/115 (97%)	78 (70%)	18 (16%)	16 (14%)	0	2
37	DP	112/115 (97%)	70 (62%)	25 (22%)	17 (15%)	0	1
38	BQ	115/118 (98%)	93 (81%)	17 (15%)	5 (4%)	4	34
38	DQ	115/118 (98%)	77 (67%)	27 (24%)	11 (10%)	1	9
39	BR	101/103 (98%)	82 (81%)	11 (11%)	8 (8%)	1	13
39	DR	101/103 (98%)	66 (65%)	22 (22%)	13 (13%)	0	3
40	BS	108/110 (98%)	88 (82%)	10 (9%)	10 (9%)	1	9
40	DS	108/110 (98%)	75 (69%)	22 (20%)	11 (10%)	1	7
41	BT	91/100 (91%)	51 (56%)	25 (28%)	15 (16%)	0	1
41	DT	91/100 (91%)	42 (46%)	27 (30%)	22 (24%)	0	0
42	BU	100/104 (96%)	69 (69%)	16 (16%)	15 (15%)	0	2
42	DU	100/104 (96%)	53 (53%)	23 (23%)	24 (24%)	0	0
43	BV	92/94 (98%)	81 (88%)	9 (10%)	2 (2%)	10	55
43	DV	92/94 (98%)	61 (66%)	23 (25%)	8 (9%)	1	11
44	BW	77/85 (91%)	34 (44%)	16 (21%)	27 (35%)	0	0
44	DW	77/85 (91%)	30 (39%)	27 (35%)	20 (26%)	0	0
45	BX	75/78 (96%)	58 (77%)	14 (19%)	3 (4%)	5	36
45	DX	75/78 (96%)	45 (60%)	22 (29%)	8 (11%)	1	6
46	BY	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	3
46	DY	61/63 (97%)	37 (61%)	20 (33%)	4 (7%)	2	19
47	BZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	5	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DZ	56/59 (95%)	34 (61%)	16 (29%)	6 (11%)	1	6
48	B0	54/57 (95%)	42 (78%)	9 (17%)	3 (6%)	3	25
48	D0	54/57 (95%)	38 (70%)	7 (13%)	9 (17%)	0	1
49	B1	48/55 (87%)	36 (75%)	8 (17%)	4 (8%)	1	12
49	D1	48/55 (87%)	33 (69%)	10 (21%)	5 (10%)	1	7
50	B2	44/46 (96%)	37 (84%)	5 (11%)	2 (4%)	4	32
50	D2	44/46 (96%)	29 (66%)	9 (20%)	6 (14%)	0	3
51	B3	62/65 (95%)	50 (81%)	8 (13%)	4 (6%)	2	19
51	D3	62/65 (95%)	43 (69%)	13 (21%)	6 (10%)	1	8
52	B4	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	3	25
52	D4	36/38 (95%)	22 (61%)	8 (22%)	6 (17%)	0	1
All	All	11234/11970 (94%)	7596 (68%)	2346 (21%)	1292 (12%)	1	5

5 of 1292 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	20	ARG
2	AB	33	ALA
2	AB	40	ILE
2	AB	58	LYS
2	AB	72	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/199 (90%)	138 (77%)	42 (23%)	1	5
2	CB	180/199 (90%)	148 (82%)	32 (18%)	2	13
3	AC	170/190 (90%)	142 (84%)	28 (16%)	3	16
3	CC	170/190 (90%)	148 (87%)	22 (13%)	6	29
4	AD	172/173 (99%)	142 (83%)	30 (17%)	3	14
4	CD	172/173 (99%)	133 (77%)	39 (23%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	113/126 (90%)	86 (76%)	27 (24%)	1	4
5	CE	113/126 (90%)	89 (79%)	24 (21%)	1	7
6	AF	87/116 (75%)	71 (82%)	16 (18%)	2	12
6	CF	87/116 (75%)	69 (79%)	18 (21%)	2	8
7	AG	124/147 (84%)	105 (85%)	19 (15%)	4	20
7	CG	123/147 (84%)	94 (76%)	29 (24%)	1	4
8	AH	104/105 (99%)	85 (82%)	19 (18%)	2	12
8	CH	104/105 (99%)	84 (81%)	20 (19%)	2	10
9	AI	105/107 (98%)	82 (78%)	23 (22%)	1	7
9	CI	105/107 (98%)	82 (78%)	23 (22%)	1	7
10	AJ	86/90 (96%)	69 (80%)	17 (20%)	2	9
10	CJ	86/90 (96%)	70 (81%)	16 (19%)	2	11
11	AK	90/99 (91%)	73 (81%)	17 (19%)	2	11
11	CK	90/99 (91%)	76 (84%)	14 (16%)	4	19
12	AL	103/104 (99%)	85 (82%)	18 (18%)	3	14
12	CL	103/104 (99%)	84 (82%)	19 (18%)	2	12
13	AM	92/96 (96%)	85 (92%)	7 (8%)	19	61
13	CM	91/96 (95%)	81 (89%)	10 (11%)	9	38
14	AN	79/84 (94%)	74 (94%)	5 (6%)	25	70
14	CN	75/84 (89%)	64 (85%)	11 (15%)	4	22
15	AO	76/77 (99%)	66 (87%)	10 (13%)	6	28
15	CO	76/77 (99%)	69 (91%)	7 (9%)	13	48
16	AP	65/65 (100%)	55 (85%)	10 (15%)	4	20
16	CP	65/65 (100%)	51 (78%)	14 (22%)	1	7
17	AQ	74/78 (95%)	57 (77%)	17 (23%)	1	5
17	CQ	74/78 (95%)	57 (77%)	17 (23%)	1	5
18	AR	48/65 (74%)	44 (92%)	4 (8%)	16	56
18	CR	48/65 (74%)	42 (88%)	6 (12%)	7	31
19	AS	70/79 (89%)	61 (87%)	9 (13%)	6	29
19	CS	70/79 (89%)	60 (86%)	10 (14%)	5	23
20	AT	65/66 (98%)	48 (74%)	17 (26%)	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	CT	65/66 (98%)	48 (74%)	17 (26%)	1	2
21	AU	44/61 (72%)	32 (73%)	12 (27%)	0	2
21	CU	44/61 (72%)	36 (82%)	8 (18%)	2	12
24	BC	216/218 (99%)	164 (76%)	52 (24%)	1	4
24	DC	216/218 (99%)	181 (84%)	35 (16%)	3	17
25	BD	164/164 (100%)	138 (84%)	26 (16%)	4	18
25	DD	164/164 (100%)	142 (87%)	22 (13%)	6	27
26	BE	165/165 (100%)	126 (76%)	39 (24%)	1	4
26	DE	165/165 (100%)	140 (85%)	25 (15%)	4	20
27	BF	148/150 (99%)	121 (82%)	27 (18%)	2	12
27	DF	149/150 (99%)	120 (80%)	29 (20%)	2	9
28	BG	137/138 (99%)	108 (79%)	29 (21%)	1	7
28	DG	137/138 (99%)	119 (87%)	18 (13%)	6	28
29	BH	114/114 (100%)	93 (82%)	21 (18%)	2	12
29	DH	114/114 (100%)	91 (80%)	23 (20%)	2	8
30	BI	109/110 (99%)	89 (82%)	20 (18%)	2	12
30	DI	109/110 (99%)	102 (94%)	7 (6%)	25	69
31	BJ	116/116 (100%)	86 (74%)	30 (26%)	1	3
31	DJ	116/116 (100%)	99 (85%)	17 (15%)	4	22
32	BK	103/104 (99%)	81 (79%)	22 (21%)	1	7
32	DK	103/104 (99%)	84 (82%)	19 (18%)	2	12
33	BL	102/103 (99%)	80 (78%)	22 (22%)	1	7
33	DL	102/103 (99%)	85 (83%)	17 (17%)	3	16
34	BM	109/109 (100%)	89 (82%)	20 (18%)	2	12
34	DM	109/109 (100%)	98 (90%)	11 (10%)	11	42
35	BN	100/103 (97%)	82 (82%)	18 (18%)	2	13
35	DN	100/103 (97%)	85 (85%)	15 (15%)	4	21
36	BO	86/87 (99%)	67 (78%)	19 (22%)	1	6
36	DO	86/87 (99%)	79 (92%)	7 (8%)	17	58
37	BP	99/100 (99%)	76 (77%)	23 (23%)	1	5
37	DP	99/100 (99%)	89 (90%)	10 (10%)	11	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BQ	89/90 (99%)	69 (78%)	20 (22%)	1	6
38	DQ	89/90 (99%)	75 (84%)	14 (16%)	4	19
39	BR	84/84 (100%)	70 (83%)	14 (17%)	3	16
39	DR	84/84 (100%)	67 (80%)	17 (20%)	2	8
40	BS	93/93 (100%)	70 (75%)	23 (25%)	1	3
40	DS	93/93 (100%)	73 (78%)	20 (22%)	1	7
41	BT	80/84 (95%)	62 (78%)	18 (22%)	1	6
41	DT	80/84 (95%)	71 (89%)	9 (11%)	9	36
42	BU	83/85 (98%)	63 (76%)	20 (24%)	1	4
42	DU	83/85 (98%)	68 (82%)	15 (18%)	2	12
43	BV	78/78 (100%)	62 (80%)	16 (20%)	2	8
43	DV	78/78 (100%)	67 (86%)	11 (14%)	5	24
44	BW	59/63 (94%)	37 (63%)	22 (37%)	0	0
44	DW	59/63 (94%)	41 (70%)	18 (30%)	0	1
45	BX	67/68 (98%)	50 (75%)	17 (25%)	1	3
45	DX	67/68 (98%)	52 (78%)	15 (22%)	1	6
46	BY	55/55 (100%)	44 (80%)	11 (20%)	2	9
46	DY	55/55 (100%)	51 (93%)	4 (7%)	20	63
47	BZ	48/49 (98%)	33 (69%)	15 (31%)	0	1
47	DZ	48/49 (98%)	37 (77%)	11 (23%)	1	5
48	B0	47/48 (98%)	38 (81%)	9 (19%)	2	10
48	D0	47/48 (98%)	34 (72%)	13 (28%)	0	2
49	B1	45/49 (92%)	34 (76%)	11 (24%)	1	3
49	D1	45/49 (92%)	41 (91%)	4 (9%)	14	51
50	B2	38/38 (100%)	30 (79%)	8 (21%)	1	7
50	D2	38/38 (100%)	32 (84%)	6 (16%)	4	18
51	B3	51/52 (98%)	42 (82%)	9 (18%)	3	13
51	D3	51/52 (98%)	38 (74%)	13 (26%)	1	3
52	B4	34/34 (100%)	30 (88%)	4 (12%)	8	34
52	D4	34/34 (100%)	27 (79%)	7 (21%)	2	8
All	All	9327/9756 (96%)	7607 (82%)	1720 (18%)	2	12

5 of 1720 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	BT	30	ILE
2	CB	209	VAL
40	DS	84	ARG
42	BU	42	LYS
46	BY	56	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 309 such sidechains are listed below:

Mol	Chain	Res	Type
40	BS	61	ASN
2	CB	38	HIS
40	DS	9	HIS
42	BU	26	ASN
46	BY	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	372 (24%)	56 (3%)
1	CA	1529/1533 (99%)	442 (28%)	70 (4%)
22	BA	2850/2904 (98%)	547 (19%)	74 (2%)
22	DA	2837/2904 (97%)	870 (30%)	153 (5%)
23	BB	117/120 (97%)	22 (18%)	0
23	DB	116/120 (96%)	31 (26%)	6 (5%)
All	All	8981/9114 (98%)	2284 (25%)	359 (3%)

5 of 2284 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	22	G

5 of 359 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	451	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	DA	14	A
22	DA	2497	A
1	CA	519	C
1	CA	1101	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 364 ligands modelled in this entry, 363 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
54	EM1	BA	3135	-	64,64,64	2.13	11 (17%)	97,97,97	3.88	38 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	EM1	BA	3135	-	-	0/77/112/112	0/5/5/5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	3135	EM1	O16-C10	10.30	1.37	1.21
54	BA	3135	EM1	C10-N6	7.51	1.50	1.35
54	BA	3135	EM1	F25-C21	-3.82	1.34	1.40
54	BA	3135	EM1	N82-N81	-3.73	1.28	1.34
54	BA	3135	EM1	O5-C10	3.58	1.41	1.35

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	3135	EM1	C3-N6-C10	-14.86	93.81	111.97
54	BA	3135	EM1	C4-C2-C3	12.24	123.77	110.26
54	BA	3135	EM1	C7-C3-N6	11.57	132.88	112.50
54	BA	3135	EM1	O5-C10-N6	-11.01	100.69	109.87
54	BA	3135	EM1	O5-C10-O16	-10.08	109.74	122.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1533/1533 (100%)	-0.63	15 (0%) 79 33	46, 97, 198, 345	0
1	CA	1530/1533 (99%)	-0.27	24 (1%) 68 22	55, 113, 259, 356	0
2	AB	218/241 (90%)	0.42	13 (5%) 21 5	82, 141, 198, 243	0
2	CB	218/241 (90%)	0.61	10 (4%) 31 7	93, 145, 201, 251	0
3	AC	206/233 (88%)	-0.01	0 100 100	71, 107, 156, 198	0
3	CC	206/233 (88%)	0.24	3 (1%) 70 24	86, 136, 185, 215	0
4	AD	205/206 (99%)	0.11	4 (1%) 62 19	57, 114, 174, 236	0
4	CD	205/206 (99%)	-0.17	0 100 100	41, 78, 132, 212	0
5	AE	150/167 (89%)	-0.12	0 100 100	59, 90, 147, 217	0
5	CE	150/167 (89%)	-0.19	0 100 100	55, 92, 141, 191	0
6	AF	100/135 (74%)	-0.05	0 100 100	80, 126, 168, 190	0
6	CF	100/135 (74%)	0.02	0 100 100	82, 119, 176, 211	0
7	AG	151/179 (84%)	0.13	3 (1%) 62 19	98, 138, 186, 203	0
7	CG	150/179 (83%)	0.99	26 (17%) 2 1	121, 195, 245, 277	0
8	AH	129/130 (99%)	0.00	1 (0%) 83 39	62, 101, 142, 189	0
8	CH	129/130 (99%)	0.01	0 100 100	77, 115, 152, 209	0
9	AI	127/130 (97%)	0.50	5 (3%) 37 8	82, 137, 209, 250	0
9	CI	127/130 (97%)	0.70	11 (8%) 10 3	114, 158, 225, 259	0
10	AJ	98/103 (95%)	0.17	2 (2%) 62 19	71, 121, 175, 200	0
10	CJ	98/103 (95%)	0.85	14 (14%) 3 1	117, 166, 211, 238	0
11	AK	117/129 (90%)	0.42	2 (1%) 67 21	54, 123, 177, 206	0
11	CK	117/129 (90%)	-0.03	1 (0%) 81 37	67, 115, 162, 186	0
12	AL	123/124 (99%)	-0.02	1 (0%) 83 39	50, 79, 123, 189	0
12	CL	123/124 (99%)	0.14	2 (1%) 68 22	61, 89, 142, 202	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/118 (96%)	0.11	1 (0%) 81 37	94, 142, 198, 217	0
13	CM	113/118 (95%)	1.59	36 (31%) 1 1	218, 370, 442, 470	0
14	AN	96/101 (95%)	0.23	3 (3%) 47 11	80, 116, 187, 224	0
14	CN	91/101 (90%)	0.98	12 (13%) 4 2	107, 180, 260, 287	0
15	AO	88/89 (98%)	-0.04	0 100 100	64, 102, 139, 188	0
15	CO	88/89 (98%)	-0.17	0 100 100	76, 116, 160, 209	0
16	AP	82/82 (100%)	0.37	5 (6%) 21 5	78, 99, 166, 223	0
16	CP	80/82 (97%)	0.52	3 (3%) 38 9	72, 107, 158, 222	0
17	AQ	80/84 (95%)	0.37	3 (3%) 38 9	62, 96, 136, 164	0
17	CQ	80/84 (95%)	0.69	5 (6%) 19 5	78, 115, 144, 155	0
18	AR	55/75 (73%)	0.20	1 (1%) 65 20	90, 110, 168, 218	0
18	CR	55/75 (73%)	0.06	0 100 100	74, 103, 171, 243	0
19	AS	79/92 (85%)	0.54	3 (3%) 38 9	110, 143, 197, 208	0
19	CS	79/92 (85%)	2.17	38 (48%) 1 0	205, 346, 411, 424	0
20	AT	85/87 (97%)	0.16	0 100 100	74, 103, 147, 179	0
20	CT	85/87 (97%)	0.70	7 (8%) 12 3	91, 134, 190, 216	0
21	AU	51/71 (71%)	0.75	4 (7%) 13 4	96, 139, 187, 225	0
21	CU	51/71 (71%)	0.17	0 100 100	83, 120, 184, 224	0
22	BA	2854/2904 (98%)	-0.53	36 (1%) 74 27	19, 47, 175, 400	0
22	DA	2841/2904 (97%)	0.03	73 (2%) 53 13	64, 141, 260, 408	0
23	BB	118/120 (98%)	-0.66	0 100 100	32, 61, 95, 115	0
23	DB	117/120 (97%)	-0.29	0 100 100	111, 185, 242, 277	0
24	BC	271/273 (99%)	-0.17	5 (1%) 65 20	25, 57, 97, 202	0
24	DC	271/273 (99%)	0.23	6 (2%) 59 16	64, 107, 154, 181	0
25	BD	209/209 (100%)	-0.28	0 100 100	19, 41, 90, 149	0
25	DD	209/209 (100%)	0.44	11 (5%) 25 6	71, 122, 174, 236	0
26	BE	201/201 (100%)	-0.20	0 100 100	23, 58, 116, 177	0
26	DE	201/201 (100%)	1.08	33 (16%) 2 1	91, 214, 335, 378	0
27	BF	177/179 (98%)	0.09	2 (1%) 77 30	52, 93, 166, 225	0
27	DF	178/179 (99%)	1.10	24 (13%) 4 2	154, 229, 270, 299	0
28	BG	176/177 (99%)	-0.07	0 100 100	41, 75, 129, 161	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/177 (99%)	1.03	25 (14%) 3 1	129, 198, 270, 312	0
29	BH	149/149 (100%)	1.29	41 (27%) 1 1	59, 178, 260, 278	0
29	DH	149/149 (100%)	1.29	37 (24%) 1 1	100, 197, 252, 272	0
30	BI	141/142 (99%)	1.83	42 (29%) 1 1	149, 241, 292, 339	0
30	DI	141/142 (99%)	2.30	66 (46%) 1 0	231, 317, 353, 360	0
31	BJ	142/142 (100%)	-0.35	0 100 100	21, 40, 76, 139	0
31	DJ	142/142 (100%)	0.26	4 (2%) 50 12	75, 127, 168, 193	0
32	BK	122/123 (99%)	-0.26	1 (0%) 83 39	23, 45, 94, 191	0
32	DK	122/123 (99%)	0.35	3 (2%) 54 14	66, 107, 155, 228	0
33	BL	143/144 (99%)	-0.31	0 100 100	18, 55, 93, 123	0
33	DL	143/144 (99%)	0.75	10 (6%) 16 4	86, 169, 242, 284	0
34	BM	136/136 (100%)	-0.32	0 100 100	17, 45, 85, 146	0
34	DM	136/136 (100%)	0.56	7 (5%) 27 6	78, 131, 175, 208	0
35	BN	120/127 (94%)	-0.33	0 100 100	18, 41, 63, 132	0
35	DN	120/127 (94%)	0.56	6 (5%) 28 6	88, 136, 190, 237	0
36	BO	116/117 (99%)	-0.17	0 100 100	40, 64, 97, 124	0
36	DO	116/117 (99%)	1.08	19 (16%) 2 1	134, 182, 227, 252	0
37	BP	114/115 (99%)	-0.24	0 100 100	29, 53, 104, 149	0
37	DP	114/115 (99%)	0.32	5 (4%) 33 7	82, 121, 160, 197	0
38	BQ	117/118 (99%)	-0.40	0 100 100	19, 34, 63, 108	0
38	DQ	117/118 (99%)	0.71	9 (7%) 13 4	88, 126, 203, 287	0
39	BR	103/103 (100%)	-0.33	0 100 100	20, 48, 92, 115	0
39	DR	103/103 (100%)	1.06	19 (18%) 2 1	98, 154, 219, 274	0
40	BS	110/110 (100%)	-0.31	0 100 100	20, 38, 83, 143	0
40	DS	110/110 (100%)	0.97	15 (13%) 4 2	86, 141, 208, 266	0
41	BT	93/100 (93%)	0.22	1 (1%) 77 30	35, 69, 134, 207	0
41	DT	93/100 (93%)	1.42	23 (24%) 1 1	133, 215, 282, 315	0
42	BU	102/104 (98%)	-0.02	0 100 100	38, 72, 160, 192	0
42	DU	102/104 (98%)	1.96	44 (43%) 1 0	151, 251, 347, 416	0
43	BV	94/94 (100%)	-0.18	0 100 100	31, 61, 102, 114	0
43	DV	94/94 (100%)	0.57	2 (2%) 60 17	107, 157, 199, 222	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	79/85 (92%)	0.03	1 (1%) 74 27	22, 53, 114, 195	0
44	DW	79/85 (92%)	1.31	20 (25%) 1 1	108, 163, 232, 250	0
45	BX	77/78 (98%)	-0.08	0 100 100	32, 58, 110, 124	0
45	DX	77/78 (98%)	0.57	3 (3%) 37 8	88, 134, 182, 237	0
46	BY	63/63 (100%)	0.13	1 (1%) 68 22	53, 90, 153, 175	0
46	DY	63/63 (100%)	0.85	8 (12%) 4 2	167, 286, 366, 383	0
47	BZ	58/59 (98%)	-0.24	0 100 100	19, 40, 87, 117	0
47	DZ	58/59 (98%)	0.57	3 (5%) 26 6	104, 143, 200, 247	0
48	B0	56/57 (98%)	-0.38	0 100 100	17, 42, 85, 150	0
48	D0	56/57 (98%)	0.74	6 (10%) 6 2	87, 161, 210, 255	0
49	B1	50/55 (90%)	0.08	1 (2%) 62 19	45, 65, 111, 143	0
49	D1	50/55 (90%)	1.06	5 (10%) 8 2	106, 161, 203, 255	0
50	B2	46/46 (100%)	-0.27	1 (2%) 59 16	30, 42, 69, 166	0
50	D2	46/46 (100%)	0.70	2 (4%) 34 8	95, 128, 162, 176	0
51	B3	64/65 (98%)	-0.35	0 100 100	25, 44, 64, 91	0
51	D3	64/65 (98%)	1.15	13 (20%) 1 1	96, 140, 173, 212	0
52	B4	38/38 (100%)	0.02	0 100 100	40, 58, 98, 108	0
52	D4	38/38 (100%)	1.69	13 (34%) 1 0	94, 155, 195, 203	0
All	All	20427/21084 (96%)	0.07	904 (4%) 33 7	17, 111, 252, 470	0

The worst 5 of 904 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	BA	2179	C	13.6
30	BI	52	LEU	11.4
1	CA	209	U	11.0
30	BI	2	LYS	10.8
22	BA	2154	A	10.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
53	MG	DA	3063	1/1	1.62	411.00	273,273,273,273	0
53	MG	DA	3109	1/1	1.52	114.58	227,227,227,227	0
53	MG	DJ	201	1/1	2.46	70.17	319,319,319,319	0
53	MG	DA	3127	1/1	1.27	59.42	248,248,248,248	0
53	MG	DA	3005	1/1	0.70	59.25	282,282,282,282	0
53	MG	BA	3060	1/1	0.53	51.97	236,236,236,236	0
53	MG	AA	1628	1/1	0.22	50.99	142,142,142,142	0
53	MG	BA	3024	1/1	0.49	49.87	210,210,210,210	0
53	MG	DA	3058	1/1	0.38	47.36	249,249,249,249	0
53	MG	BA	3129	1/1	1.02	46.37	285,285,285,285	0
53	MG	BA	3059	1/1	0.41	46.14	207,207,207,207	0
53	MG	CA	1614	1/1	0.86	44.65	236,236,236,236	0
53	MG	DA	3064	1/1	1.07	41.63	256,256,256,256	0
53	MG	DA	3003	1/1	1.50	40.14	238,238,238,238	0
53	MG	BA	3054	1/1	0.34	36.15	198,198,198,198	0
53	MG	AA	1619	1/1	0.58	35.58	230,230,230,230	0
53	MG	BB	201	1/1	0.24	33.25	255,255,255,255	0
53	MG	DA	3060	1/1	0.79	32.28	235,235,235,235	0
53	MG	DA	3079	1/1	0.77	27.74	225,225,225,225	0
53	MG	DA	3108	1/1	0.82	25.82	217,217,217,217	0
53	MG	AA	1636	1/1	0.39	25.10	218,218,218,218	0
53	MG	BA	3055	1/1	0.35	20.04	252,252,252,252	0
53	MG	BA	3096	1/1	0.18	16.67	169,169,169,169	0
53	MG	DA	3132	1/1	0.54	15.32	240,240,240,240	0
53	MG	DA	3074	1/1	0.54	13.53	260,260,260,260	0
53	MG	DA	3002	1/1	0.56	13.29	231,231,231,231	0
53	MG	BA	3120	1/1	0.30	13.04	45,45,45,45	0
53	MG	DA	3019	1/1	0.59	11.76	278,278,278,278	0
53	MG	BA	3018	1/1	0.33	11.04	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
53	MG	DE	301	1/1	0.28	10.57	199,199,199,199	0
53	MG	CA	1626	1/1	0.24	9.92	20,20,20,20	0
53	MG	CA	1608	1/1	0.25	9.53	47,47,47,47	0
53	MG	DA	3075	1/1	0.44	9.37	209,209,209,209	0
53	MG	CA	1624	1/1	0.40	9.32	146,146,146,146	0
53	MG	BA	3122	1/1	0.52	9.27	164,164,164,164	0
53	MG	DC	301	1/1	0.28	9.19	201,201,201,201	0
53	MG	BA	3133	1/1	0.23	8.42	116,116,116,116	0
53	MG	DA	3088	1/1	0.30	8.30	222,222,222,222	0
53	MG	DA	3026	1/1	1.10	8.18	242,242,242,242	0
53	MG	BA	3043	1/1	0.25	8.10	11,11,11,11	0
53	MG	DA	3057	1/1	0.25	7.32	205,205,205,205	0
53	MG	BA	3124	1/1	0.20	7.29	63,63,63,63	0
53	MG	DA	3078	1/1	0.25	6.92	214,214,214,214	0
53	MG	CA	1615	1/1	0.17	6.69	187,187,187,187	0
53	MG	DA	3062	1/1	0.52	6.07	190,190,190,190	0
53	MG	BA	3020	1/1	0.31	5.93	200,200,200,200	0
53	MG	AA	1608	1/1	0.26	5.84	61,61,61,61	0
53	MG	BA	3131	1/1	0.65	5.46	187,187,187,187	0
53	MG	BA	3134	1/1	0.28	5.38	210,210,210,210	0
53	MG	BA	3058	1/1	0.22	5.37	100,100,100,100	0
53	MG	BA	3100	1/1	0.24	5.17	119,119,119,119	0
53	MG	DA	3049	1/1	0.37	5.09	243,243,243,243	0
53	MG	BA	3069	1/1	0.22	4.77	198,198,198,198	0
53	MG	DA	3130	1/1	2.06	4.62	271,271,271,271	0
53	MG	AA	1626	1/1	0.20	4.60	29,29,29,29	0
53	MG	BA	3070	1/1	0.29	4.22	137,137,137,137	0
53	MG	DA	3031	1/1	0.22	4.17	80,80,80,80	0
53	MG	BA	3039	1/1	0.22	4.12	7,7,7,7	0
53	MG	DA	3053	1/1	0.15	4.01	127,127,127,127	0
53	MG	DA	3123	1/1	0.35	3.95	217,217,217,217	0
53	MG	BA	3073	1/1	0.25	3.91	43,43,43,43	0
53	MG	CA	1640	1/1	0.17	3.86	137,137,137,137	0
53	MG	BA	3081	1/1	0.15	3.59	99,99,99,99	0
53	MG	DA	3007	1/1	0.34	3.51	232,232,232,232	0
53	MG	BA	3035	1/1	0.27	3.50	189,189,189,189	0
53	MG	BA	3117	1/1	0.17	3.38	162,162,162,162	0
53	MG	CA	1625	1/1	0.21	3.37	111,111,111,111	0
54	EM1	BA	3135	60/60	0.23	3.32	0,28,50,62	0
53	MG	BA	3114	1/1	0.20	3.13	28,28,28,28	0
53	MG	DA	3033	1/1	0.31	3.07	151,151,151,151	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BA	3036	1/1	0.17	2.87	23,23,23,23	0
53	MG	CA	1628	1/1	0.35	2.82	224,224,224,224	0
53	MG	DA	3008	1/1	0.27	2.75	147,147,147,147	0
53	MG	BA	3089	1/1	0.14	2.72	127,127,127,127	0
53	MG	BA	3105	1/1	0.21	2.72	66,66,66,66	0
53	MG	AA	1631	1/1	0.19	2.72	228,228,228,228	0
53	MG	BA	3085	1/1	0.15	2.68	133,133,133,133	0
53	MG	AA	1614	1/1	0.19	2.55	159,159,159,159	0
53	MG	BA	3099	1/1	0.17	2.52	34,34,34,34	0
53	MG	DA	3021	1/1	0.24	2.49	183,183,183,183	0
53	MG	BA	3107	1/1	0.21	2.49	17,17,17,17	0
53	MG	AA	1639	1/1	0.18	2.28	118,118,118,118	0
53	MG	CA	1627	1/1	0.21	2.24	197,197,197,197	0
53	MG	CA	1616	1/1	0.53	2.15	195,195,195,195	0
53	MG	AA	1641	1/1	0.16	2.12	171,171,171,171	0
53	MG	DA	3022	1/1	0.24	2.07	149,149,149,149	0
53	MG	DA	3105	1/1	0.20	2.04	97,97,97,97	0
53	MG	DA	3120	1/1	0.22	2.04	124,124,124,124	0
53	MG	AA	1621	1/1	0.13	1.99	131,131,131,131	0
53	MG	DA	3128	1/1	0.85	1.86	163,163,163,163	0
53	MG	BA	3106	1/1	0.18	1.86	13,13,13,13	0
53	MG	DA	3115	1/1	0.20	1.85	176,176,176,176	0
53	MG	CA	1610	1/1	0.14	1.83	168,168,168,168	0
53	MG	BA	3102	1/1	0.17	1.83	24,24,24,24	0
53	MG	BA	3003	1/1	0.17	1.77	77,77,77,77	0
53	MG	DA	3129	1/1	0.75	1.76	261,261,261,261	0
53	MG	BA	3028	1/1	0.17	1.75	92,92,92,92	0
53	MG	DA	3076	1/1	0.20	1.74	195,195,195,195	0
53	MG	CA	1605	1/1	0.20	1.73	54,54,54,54	0
53	MG	BA	3004	1/1	0.19	1.61	184,184,184,184	0
53	MG	DA	3013	1/1	0.38	1.58	241,241,241,241	0
53	MG	AA	1627	1/1	0.15	1.41	132,132,132,132	0
53	MG	DA	3093	1/1	0.33	1.40	189,189,189,189	0
53	MG	AA	1605	1/1	0.18	1.37	72,72,72,72	0
53	MG	DA	3020	1/1	0.20	1.33	53,53,53,53	0
53	MG	DA	3133	1/1	0.28	1.26	220,220,220,220	0
53	MG	CA	1631	1/1	0.23	1.24	82,82,82,82	0
53	MG	AA	1634	1/1	0.15	1.18	94,94,94,94	0
53	MG	DA	3125	1/1	0.39	1.17	200,200,200,200	0
53	MG	BA	3053	1/1	0.15	1.13	55,55,55,55	0
53	MG	AA	1610	1/1	0.10	1.12	197,197,197,197	0
53	MG	CA	1620	1/1	0.16	1.06	182,182,182,182	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DA	3009	1/1	0.28	1.06	157,157,157,157	0
53	MG	DA	3028	1/1	0.37	1.04	222,222,222,222	0
53	MG	BA	3090	1/1	0.14	1.04	135,135,135,135	0
53	MG	AA	1622	1/1	0.17	1.01	54,54,54,54	0
53	MG	BA	3065	1/1	0.15	1.01	35,35,35,35	0
53	MG	DA	3046	1/1	0.23	0.99	73,73,73,73	0
53	MG	DA	3101	1/1	0.21	0.87	96,96,96,96	0
53	MG	DA	3104	1/1	0.20	0.86	52,52,52,52	0
53	MG	DA	3071	1/1	0.20	0.81	102,102,102,102	0
53	MG	DA	3047	1/1	0.19	0.78	174,174,174,174	0
53	MG	CA	1636	1/1	0.39	0.75	224,224,224,224	0
53	MG	BA	3005	1/1	0.13	0.69	74,74,74,74	0
53	MG	AA	1623	1/1	0.10	0.68	77,77,77,77	0
53	MG	DA	3059	1/1	0.19	0.65	233,233,233,233	0
53	MG	DA	3069	1/1	0.24	0.64	267,267,267,267	0
53	MG	CA	1641	1/1	0.15	0.61	116,116,116,116	0
53	MG	DA	3027	1/1	0.22	0.59	194,194,194,194	0
53	MG	DA	3107	1/1	0.21	0.57	91,91,91,91	0
53	MG	DA	3097	1/1	0.20	0.56	159,159,159,159	0
53	MG	BA	3029	1/1	0.17	0.52	14,14,14,14	0
53	MG	DA	3011	1/1	0.22	0.52	150,150,150,150	0
53	MG	DA	3004	1/1	0.19	0.48	134,134,134,134	0
53	MG	BA	3050	1/1	0.16	0.46	39,39,39,39	0
53	MG	BA	3048	1/1	0.17	0.39	25,25,25,25	0
53	MG	BA	3095	1/1	0.18	0.37	139,139,139,139	0
53	MG	BA	3006	1/1	0.12	0.32	54,54,54,54	0
53	MG	DA	3091	1/1	0.20	0.29	184,184,184,184	0
53	MG	BA	3109	1/1	0.16	0.29	46,46,46,46	0
53	MG	DA	3082	1/1	0.19	0.23	164,164,164,164	0
53	MG	AA	1633	1/1	0.13	0.23	70,70,70,70	0
53	MG	DA	3029	1/1	0.24	0.21	178,178,178,178	0
53	MG	DA	3089	1/1	0.21	0.14	101,101,101,101	0
53	MG	BA	3062	1/1	0.15	0.14	19,19,19,19	0
53	MG	AA	1616	1/1	0.17	0.12	98,98,98,98	0
53	MG	BA	3041	1/1	0.13	0.09	38,38,38,38	0
53	MG	BA	3091	1/1	0.13	0.05	84,84,84,84	0
53	MG	DA	3126	1/1	0.19	0.03	120,120,120,120	0
53	MG	DA	3122	1/1	0.15	0.00	104,104,104,104	0
53	MG	DA	3066	1/1	0.17	-0.04	105,105,105,105	0
53	MG	BA	3007	1/1	0.10	-0.11	112,112,112,112	0
53	MG	BA	3011	1/1	0.18	-0.11	129,129,129,129	0
53	MG	DA	3050	1/1	0.18	-0.16	154,154,154,154	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BA	3110	1/1	0.15	-0.17	84,84,84,84	0
53	MG	BA	3038	1/1	0.16	-0.28	19,19,19,19	0
53	MG	DA	3036	1/1	0.15	-0.28	205,205,205,205	0
53	MG	CA	1630	1/1	0.15	-0.30	160,160,160,160	0
53	MG	BA	3103	1/1	0.15	-0.31	30,30,30,30	0
53	MG	CA	1613	1/1	0.17	-0.33	147,147,147,147	0
53	MG	BA	3130	1/1	0.24	-0.34	118,118,118,118	0
53	MG	AA	1637	1/1	0.17	-0.39	131,131,131,131	0
53	MG	CA	1633	1/1	0.11	-0.45	79,79,79,79	0
53	MG	BA	3064	1/1	0.13	-0.46	28,28,28,28	0
53	MG	BA	3121	1/1	0.14	-0.46	45,45,45,45	0
53	MG	DA	3043	1/1	0.25	-0.47	155,155,155,155	0
53	MG	BA	3104	1/1	0.16	-0.47	23,23,23,23	0
53	MG	DA	3014	1/1	0.20	-0.48	113,113,113,113	0
53	MG	AA	1617	1/1	0.14	-0.53	129,129,129,129	0
53	MG	BA	3033	1/1	0.15	-0.54	159,159,159,159	0
53	MG	DA	3085	1/1	0.20	-0.60	158,158,158,158	0
53	MG	DA	3080	1/1	0.19	-0.60	154,154,154,154	0
53	MG	BA	3040	1/1	0.12	-0.64	47,47,47,47	0
53	MG	DA	3006	1/1	0.12	-0.64	237,237,237,237	0
53	MG	BA	3014	1/1	0.15	-0.66	38,38,38,38	0
53	MG	DA	3024	1/1	0.17	-0.71	102,102,102,102	0
53	MG	AA	1630	1/1	0.12	-0.73	196,196,196,196	0
53	MG	BA	3118	1/1	0.14	-0.76	48,48,48,48	0
53	MG	DA	3045	1/1	0.20	-0.76	206,206,206,206	0
53	MG	DA	3073	1/1	0.16	-0.80	193,193,193,193	0
53	MG	DA	3084	1/1	0.16	-0.81	168,168,168,168	0
53	MG	BA	3008	1/1	0.13	-0.81	45,45,45,45	0
53	MG	CA	1621	1/1	0.14	-0.83	57,57,57,57	0
53	MG	AA	1612	1/1	0.15	-0.83	113,113,113,113	0
53	MG	BA	3119	1/1	0.08	-0.83	56,56,56,56	0
53	MG	AA	1606	1/1	0.12	-0.84	80,80,80,80	0
53	MG	AA	1642	1/1	0.13	-0.85	79,79,79,79	0
53	MG	BA	3026	1/1	0.14	-0.86	143,143,143,143	0
53	MG	AA	1624	1/1	0.12	-0.86	143,143,143,143	0
53	MG	BB	203	1/1	0.12	-0.88	58,58,58,58	0
53	MG	CA	1638	1/1	0.14	-0.89	204,204,204,204	0
53	MG	BA	3068	1/1	0.12	-0.90	176,176,176,176	0
53	MG	BA	3044	1/1	0.14	-0.92	34,34,34,34	0
53	MG	DA	3017	1/1	0.14	-0.94	185,185,185,185	0
53	MG	CA	1632	1/1	0.10	-0.96	122,122,122,122	0
53	MG	DA	3030	1/1	0.18	-0.97	130,130,130,130	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BA	3063	1/1	0.13	-0.98	26,26,26,26	0
53	MG	DA	3095	1/1	0.14	-1.01	138,138,138,138	0
53	MG	CA	1629	1/1	0.15	-1.04	190,190,190,190	0
53	MG	CA	1617	1/1	0.11	-1.05	202,202,202,202	0
53	MG	DA	3055	1/1	0.16	-1.05	103,103,103,103	0
53	MG	BA	3084	1/1	0.14	-1.05	26,26,26,26	0
53	MG	AA	1602	1/1	0.12	-1.06	177,177,177,177	0
53	MG	AA	1618	1/1	0.14	-1.07	78,78,78,78	0
53	MG	BA	3111	1/1	0.14	-1.07	31,31,31,31	0
53	MG	DA	3083	1/1	0.10	-1.08	214,214,214,214	0
53	MG	DA	3096	1/1	0.14	-1.09	127,127,127,127	0
53	MG	DA	3098	1/1	0.19	-1.14	183,183,183,183	0
53	MG	BB	202	1/1	0.10	-1.16	82,82,82,82	0
53	MG	CA	1609	1/1	0.16	-1.16	98,98,98,98	0
53	MG	DA	3042	1/1	0.16	-1.19	81,81,81,81	0
53	MG	CA	1618	1/1	0.13	-1.20	136,136,136,136	0
53	MG	BA	3013	1/1	0.14	-1.23	18,18,18,18	0
53	MG	BA	3049	1/1	0.12	-1.31	76,76,76,76	0
53	MG	DB	201	1/1	0.09	-1.32	111,111,111,111	0
53	MG	BA	3083	1/1	0.15	-1.34	53,53,53,53	0
53	MG	DA	3070	1/1	0.13	-1.34	91,91,91,91	0
53	MG	DA	3025	1/1	0.14	-1.34	162,162,162,162	0
53	MG	DA	3131	1/1	0.15	-1.37	94,94,94,94	0
53	MG	DA	3018	1/1	0.09	-1.43	185,185,185,185	0
53	MG	DA	3106	1/1	0.15	-1.45	218,218,218,218	0
53	MG	CA	1606	1/1	0.13	-1.48	93,93,93,93	0
53	MG	BA	3126	1/1	0.12	-1.49	40,40,40,40	0
53	MG	CA	1622	1/1	0.07	-1.49	187,187,187,187	0
53	MG	DA	3051	1/1	0.14	-1.51	88,88,88,88	0
53	MG	DA	3110	1/1	0.07	-1.56	120,120,120,120	0
53	MG	AA	1603	1/1	0.09	-1.56	65,65,65,65	0
53	MG	DA	3037	1/1	0.11	-1.57	81,81,81,81	0
53	MG	DA	3116	1/1	0.12	-1.58	84,84,84,84	0
53	MG	BA	3045	1/1	0.14	-1.58	25,25,25,25	0
53	MG	CA	1601	1/1	0.09	-1.59	106,106,106,106	0
53	MG	DA	3001	1/1	0.11	-1.59	141,141,141,141	0
53	MG	AA	1638	1/1	0.13	-1.60	67,67,67,67	0
53	MG	CA	1637	1/1	0.13	-1.63	94,94,94,94	0
53	MG	DA	3067	1/1	0.11	-1.64	72,72,72,72	0
53	MG	BA	3128	1/1	0.14	-1.66	33,33,33,33	0
53	MG	BA	3088	1/1	0.10	-1.70	59,59,59,59	0
53	MG	DA	3111	1/1	0.12	-1.74	202,202,202,202	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
53	MG	BA	3017	1/1	0.08	-1.76	57,57,57,57	0
53	MG	DA	3094	1/1	0.13	-1.77	145,145,145,145	0
55	ZN	D4	101	1/1	0.07	-1.81	169,169,169,169	0
53	MG	CA	1634	1/1	0.12	-1.83	165,165,165,165	0
53	MG	DA	3117	1/1	0.17	-1.85	73,73,73,73	0
53	MG	CA	1619	1/1	0.12	-1.90	212,212,212,212	0
53	MG	BA	3132	1/1	0.10	-1.91	20,20,20,20	0
55	ZN	B4	101	1/1	0.10	-1.94	108,108,108,108	0
53	MG	BA	3113	1/1	0.16	-1.97	190,190,190,190	0
53	MG	DA	3034	1/1	0.13	-1.99	88,88,88,88	0
53	MG	BA	3056	1/1	0.12	-2.00	148,148,148,148	0
53	MG	DA	3099	1/1	0.14	-2.01	188,188,188,188	0
53	MG	DA	3086	1/1	0.15	-2.01	109,109,109,109	0
53	MG	BA	3112	1/1	0.10	-2.03	49,49,49,49	0
53	MG	CA	1642	1/1	0.10	-2.06	139,139,139,139	0
53	MG	BA	3022	1/1	0.12	-2.09	27,27,27,27	0
53	MG	DA	3119	1/1	0.12	-2.09	60,60,60,60	0
53	MG	DA	3121	1/1	0.16	-2.11	168,168,168,168	0
53	MG	AA	1601	1/1	0.05	-2.11	94,94,94,94	0
53	MG	BB	204	1/1	0.12	-2.13	45,45,45,45	0
53	MG	AA	1615	1/1	0.12	-2.14	152,152,152,152	0
53	MG	DA	3072	1/1	0.12	-2.16	183,183,183,183	0
53	MG	DA	3061	1/1	0.11	-2.19	110,110,110,110	0
53	MG	BA	3079	1/1	0.13	-2.21	32,32,32,32	0
53	MG	CA	1612	1/1	0.16	-2.21	125,125,125,125	0
53	MG	BA	3009	1/1	0.13	-2.23	38,38,38,38	0
53	MG	DA	3040	1/1	0.15	-2.25	72,72,72,72	0
53	MG	DA	3054	1/1	0.11	-2.26	86,86,86,86	0
53	MG	BA	3078	1/1	0.13	-2.26	58,58,58,58	0
53	MG	DA	3039	1/1	0.15	-2.26	105,105,105,105	0
53	MG	BA	3098	1/1	0.07	-2.26	49,49,49,49	0
53	MG	DA	3035	1/1	0.11	-2.27	90,90,90,90	0
53	MG	BA	3108	1/1	0.13	-2.27	95,95,95,95	0
53	MG	CA	1623	1/1	0.12	-2.31	108,108,108,108	0
53	MG	DA	3112	1/1	0.09	-2.31	79,79,79,79	0
53	MG	DA	3032	1/1	0.13	-2.32	162,162,162,162	0
53	MG	DA	3065	1/1	0.13	-2.34	88,88,88,88	0
53	MG	AA	1632	1/1	0.13	-2.36	85,85,85,85	0
53	MG	BA	3021	1/1	0.12	-2.41	24,24,24,24	0
53	MG	CA	1602	1/1	0.12	-2.43	139,139,139,139	0
53	MG	AA	1607	1/1	0.12	-2.45	136,136,136,136	0
53	MG	BA	3032	1/1	0.12	-2.50	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	1635	1/1	0.07	-2.52	87,87,87,87	0
53	MG	AA	1620	1/1	0.08	-2.54	116,116,116,116	0
53	MG	BA	3092	1/1	0.09	-2.55	68,68,68,68	0
53	MG	BA	3023	1/1	0.11	-2.57	22,22,22,22	0
53	MG	DA	3092	1/1	0.15	-2.58	169,169,169,169	0
53	MG	DA	3044	1/1	0.15	-2.59	87,87,87,87	0
53	MG	BA	3051	1/1	0.16	-2.62	70,70,70,70	0
53	MG	AA	1640	1/1	0.04	-2.62	79,79,79,79	0
53	MG	DA	3041	1/1	0.12	-2.70	119,119,119,119	0
53	MG	CA	1607	1/1	0.14	-2.70	167,167,167,167	0
53	MG	DA	3068	1/1	0.06	-2.79	98,98,98,98	0
53	MG	DA	3103	1/1	0.12	-2.81	86,86,86,86	0
53	MG	BA	3047	1/1	0.12	-2.84	122,122,122,122	0
53	MG	BA	3010	1/1	0.12	-2.85	31,31,31,31	0
53	MG	DA	3114	1/1	0.11	-3.00	182,182,182,182	0
53	MG	DA	3124	1/1	0.14	-3.25	82,82,82,82	0
53	MG	DA	3100	1/1	0.12	-3.32	124,124,124,124	0
53	MG	BA	3125	1/1	0.13	-3.35	40,40,40,40	0
53	MG	DA	3023	1/1	0.10	-3.43	130,130,130,130	0
53	MG	DA	3048	1/1	0.11	-3.50	103,103,103,103	0
53	MG	CA	1603	1/1	0.08	-3.54	136,136,136,136	0
53	MG	BA	3030	1/1	0.10	-3.62	56,56,56,56	0
53	MG	BA	3037	1/1	0.13	-3.69	30,30,30,30	0
53	MG	BA	3002	1/1	0.10	-3.76	75,75,75,75	0
53	MG	AA	1625	1/1	0.12	-3.76	101,101,101,101	0
53	MG	BA	3067	1/1	0.13	-3.87	28,28,28,28	0
53	MG	BA	3027	1/1	0.11	-3.95	33,33,33,33	0
53	MG	BA	3077	1/1	0.09	-3.96	63,63,63,63	0
53	MG	BA	3123	1/1	0.10	-4.00	24,24,24,24	0
53	MG	BA	3012	1/1	0.11	-4.06	20,20,20,20	0
53	MG	BA	3046	1/1	0.08	-4.10	176,176,176,176	0
53	MG	CA	1604	1/1	0.08	-4.23	96,96,96,96	0
53	MG	DA	3102	1/1	0.12	-4.23	118,118,118,118	0
53	MG	BA	3031	1/1	0.13	-4.29	37,37,37,37	0
53	MG	BA	3066	1/1	0.14	-4.34	32,32,32,32	0
53	MG	BA	3082	1/1	0.12	-4.37	86,86,86,86	0
53	MG	BA	3052	1/1	0.13	-4.44	34,34,34,34	0
53	MG	DA	3052	1/1	0.07	-4.44	72,72,72,72	0
53	MG	AA	1629	1/1	0.06	-4.45	97,97,97,97	0
53	MG	DA	3090	1/1	0.09	-4.50	112,112,112,112	0
53	MG	CA	1639	1/1	0.06	-4.53	159,159,159,159	0
53	MG	AA	1613	1/1	0.08	-4.55	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BA	3061	1/1	0.10	-4.58	18,18,18,18	0
53	MG	BA	3116	1/1	0.08	-4.62	72,72,72,72	0
53	MG	DA	3056	1/1	0.08	-4.77	85,85,85,85	0
53	MG	DA	3012	1/1	0.09	-4.77	72,72,72,72	0
53	MG	DA	3016	1/1	0.09	-4.85	60,60,60,60	0
53	MG	DA	3087	1/1	0.09	-5.00	199,199,199,199	0
53	MG	BA	3076	1/1	0.07	-5.20	107,107,107,107	0
53	MG	DA	3015	1/1	0.17	-5.27	219,219,219,219	0
53	MG	BA	3097	1/1	0.12	-5.45	54,54,54,54	0
53	MG	BA	3057	1/1	0.07	-5.68	71,71,71,71	0
53	MG	DA	3113	1/1	0.05	-5.74	128,128,128,128	0
53	MG	BA	3016	1/1	0.10	-5.79	22,22,22,22	0
53	MG	AA	1611	1/1	0.13	-5.79	57,57,57,57	0
53	MG	CA	1611	1/1	0.11	-5.83	110,110,110,110	0
53	MG	AA	1609	1/1	0.09	-5.92	77,77,77,77	0
53	MG	AA	1643	1/1	0.09	-5.96	67,67,67,67	0
53	MG	BA	3075	1/1	0.05	-6.06	43,43,43,43	0
53	MG	AA	1604	1/1	0.05	-6.09	139,139,139,139	0
53	MG	BA	3086	1/1	0.09	-6.15	151,151,151,151	0
53	MG	BA	3101	1/1	0.10	-6.37	48,48,48,48	0
53	MG	DA	3077	1/1	0.09	-6.41	109,109,109,109	0
53	MG	BA	3094	1/1	0.09	-6.57	32,32,32,32	0
53	MG	BA	3025	1/1	0.06	-6.93	40,40,40,40	0
53	MG	BA	3115	1/1	0.06	-6.97	22,22,22,22	0
53	MG	BA	3080	1/1	0.07	-7.00	60,60,60,60	0
53	MG	DA	3081	1/1	0.09	-7.47	83,83,83,83	0
53	MG	BA	3127	1/1	0.08	-7.54	8,8,8,8	0
53	MG	DA	3118	1/1	0.14	-7.59	100,100,100,100	0
53	MG	BA	3072	1/1	0.06	-7.87	61,61,61,61	0
53	MG	BA	3015	1/1	0.06	-8.04	65,65,65,65	0
53	MG	DA	3038	1/1	0.07	-8.24	234,234,234,234	0
53	MG	BA	3071	1/1	0.10	-8.34	16,16,16,16	0
53	MG	CA	1635	1/1	0.11	-8.60	76,76,76,76	0
53	MG	BA	3093	1/1	0.06	-9.01	45,45,45,45	0
53	MG	BL	201	1/1	0.06	-10.82	61,61,61,61	0
53	MG	BA	3001	1/1	0.09	-14.97	98,98,98,98	0
53	MG	BA	3034	1/1	0.08	-14.99	11,11,11,11	0
53	MG	BA	3087	1/1	0.08	-17.46	47,47,47,47	0
53	MG	BA	3019	1/1	0.06	-18.67	34,34,34,34	0
53	MG	BA	3042	1/1	0.08	-19.64	60,60,60,60	0
53	MG	BA	3074	1/1	0.10	-20.45	93,93,93,93	0
53	MG	DA	3010	1/1	1.08	-	272,272,272,272	0

6.5 Other polymers ⓘ

There are no such residues in this entry.