



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:04 PM BST

PDB ID : 4V85  
Title : Crystal Structure of Release Factor RF3 Trapped in the GTP State on a Rotated Conformation of the Ribosome.  
Authors : Zhou, J.; Lancaster, L.; Trakhanov, S.; Noller, H.F.  
Deposited on : 2011-06-13  
Resolution : 3.20 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

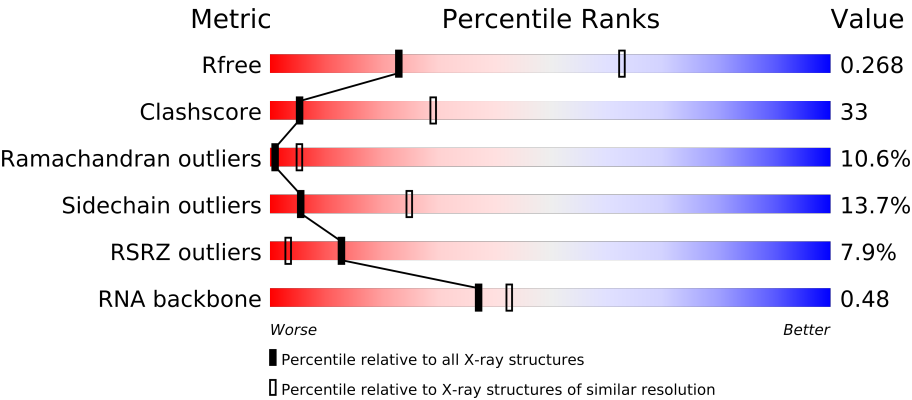
The following versions of software and data (see [references](#)) were used in the production of this report:

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

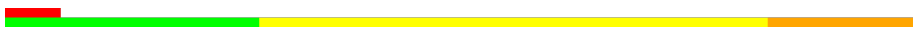
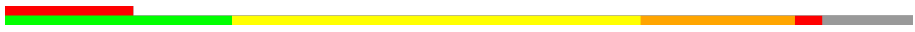


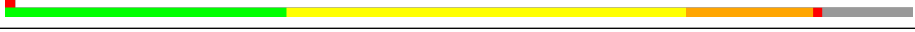

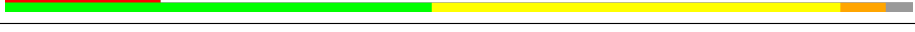





The reported resolution of this entry is 3.20 Å.

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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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  $\geq 3$ , 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	
2	AB	241	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	131	
7	AG	156	
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	

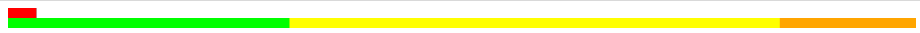
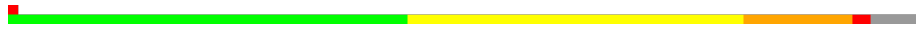



Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	27	
23	AW	529	
24	AY	6	
25	B0	85	
26	B1	78	
27	B2	63	
28	B3	59	
29	B4	57	
30	B5	55	
31	B6	46	
32	B7	65	
33	B8	38	
34	BA	2903	
35	BB	118	
36	BC	273	
37	BD	209	
38	BE	201	
39	BF	179	
40	BG	177	
41	BH	165	
42	BI	142	
43	BJ	121	
43	BK	121	
43	BL	121	
43	BM	121	
44	BN	142	
45	BO	123	
46	BP	144	
47	BQ	136	
48	BR	127	
49	BS	117	
50	BT	115	
51	BU	118	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
52	BV	103	
53	BW	116	
54	BX	100	
55	BY	104	
56	BZ	94	

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

Mol	Type	Chain	Res	Geometry	Electron density
57	MG	AA	1601	-	X
57	MG	AA	1602	-	X
57	MG	AA	1603	-	X
57	MG	AA	1604	-	X
57	MG	AA	1605	-	X
57	MG	AA	1606	-	X
57	MG	AA	1607	-	X
57	MG	AA	1609	-	X
57	MG	AA	1610	-	X
57	MG	AA	1611	-	X
57	MG	AA	1615	-	X
57	MG	AA	1616	-	X
57	MG	AA	1618	-	X
57	MG	AA	1621	-	X
57	MG	AA	1622	-	X
57	MG	AA	1623	-	X
57	MG	AA	1624	-	X
57	MG	AA	1628	-	X
57	MG	AA	1630	-	X
57	MG	AA	1631	-	X
57	MG	AA	1632	-	X
57	MG	AA	1634	-	X
57	MG	AA	1635	-	X
57	MG	AA	1643	-	X
57	MG	AA	1645	-	X
57	MG	AA	1649	-	X
57	MG	AA	1650	-	X
57	MG	AA	1652	-	X
57	MG	AA	1654	-	X
57	MG	AA	1655	-	X
57	MG	AA	1657	-	X
57	MG	AA	1658	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
57	MG	AA	1661	-	X
57	MG	AA	1665	-	X
57	MG	AA	1666	-	X
57	MG	AA	1670	-	X
57	MG	AA	1673	-	X
57	MG	AA	1676	-	X
57	MG	AA	1677	-	X
57	MG	AA	1678	-	X
57	MG	AA	1679	-	X
57	MG	AA	1684	-	X
57	MG	AA	1686	-	X
57	MG	AA	1687	-	X
57	MG	AA	1689	-	X
57	MG	AA	1691	-	X
57	MG	AA	1693	-	X
57	MG	AA	1699	-	X
57	MG	AA	1700	-	X
57	MG	AA	1702	-	X
57	MG	B0	103	-	X
57	MG	B4	101	-	X
57	MG	BA	3001	-	X
57	MG	BA	3003	-	X
57	MG	BA	3005	-	X
57	MG	BA	3006	-	X
57	MG	BA	3007	-	X
57	MG	BA	3008	-	X
57	MG	BA	3009	-	X
57	MG	BA	3010	-	X
57	MG	BA	3011	-	X
57	MG	BA	3012	-	X
57	MG	BA	3013	-	X
57	MG	BA	3014	-	X
57	MG	BA	3015	-	X
57	MG	BA	3016	-	X
57	MG	BA	3017	-	X
57	MG	BA	3018	-	X
57	MG	BA	3020	-	X
57	MG	BA	3021	-	X
57	MG	BA	3022	-	X
57	MG	BA	3023	-	X
57	MG	BA	3024	-	X
57	MG	BA	3025	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
57	MG	BA	3026	-	X
57	MG	BA	3027	-	X
57	MG	BA	3028	-	X
57	MG	BA	3029	-	X
57	MG	BA	3030	-	X
57	MG	BA	3031	-	X
57	MG	BA	3032	-	X
57	MG	BA	3033	-	X
57	MG	BA	3034	-	X
57	MG	BA	3035	-	X
57	MG	BA	3036	-	X
57	MG	BA	3037	-	X
57	MG	BA	3039	-	X
57	MG	BA	3040	-	X
57	MG	BA	3041	-	X
57	MG	BA	3042	-	X
57	MG	BA	3043	-	X
57	MG	BA	3044	-	X
57	MG	BA	3045	-	X
57	MG	BA	3046	-	X
57	MG	BA	3047	-	X
57	MG	BA	3049	-	X
57	MG	BA	3050	-	X
57	MG	BA	3052	-	X
57	MG	BA	3053	-	X
57	MG	BA	3054	-	X
57	MG	BA	3055	-	X
57	MG	BA	3057	-	X
57	MG	BA	3058	-	X
57	MG	BA	3060	-	X
57	MG	BA	3061	-	X
57	MG	BA	3062	-	X
57	MG	BA	3063	-	X
57	MG	BA	3065	-	X
57	MG	BA	3066	-	X
57	MG	BA	3067	-	X
57	MG	BA	3068	-	X
57	MG	BA	3069	-	X
57	MG	BA	3070	-	X
57	MG	BA	3071	-	X
57	MG	BA	3072	-	X
57	MG	BA	3073	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
57	MG	BA	3074	-	X
57	MG	BA	3077	-	X
57	MG	BA	3078	-	X
57	MG	BA	3079	-	X
57	MG	BA	3081	-	X
57	MG	BA	3082	-	X
57	MG	BA	3083	-	X
57	MG	BA	3084	-	X
57	MG	BA	3085	-	X
57	MG	BA	3086	-	X
57	MG	BA	3087	-	X
57	MG	BA	3088	-	X
57	MG	BA	3090	-	X
57	MG	BA	3091	-	X
57	MG	BA	3092	-	X
57	MG	BA	3095	-	X
57	MG	BA	3096	-	X
57	MG	BA	3099	-	X
57	MG	BA	3100	-	X
57	MG	BA	3102	-	X
57	MG	BA	3103	-	X
57	MG	BA	3104	-	X
57	MG	BA	3105	-	X
57	MG	BA	3107	-	X
57	MG	BA	3110	-	X
57	MG	BA	3112	-	X
57	MG	BA	3113	-	X
57	MG	BA	3114	-	X
57	MG	BA	3116	-	X
57	MG	BA	3117	-	X
57	MG	BA	3119	-	X
57	MG	BA	3121	-	X
57	MG	BA	3123	-	X
57	MG	BA	3124	-	X
57	MG	BA	3125	-	X
57	MG	BA	3126	-	X
57	MG	BA	3127	-	X
57	MG	BA	3128	-	X
57	MG	BA	3130	-	X
57	MG	BA	3132	-	X
57	MG	BA	3133	-	X
57	MG	BA	3134	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
57	MG	BA	3136	-	X
57	MG	BA	3137	-	X
57	MG	BA	3138	-	X
57	MG	BA	3139	-	X
57	MG	BA	3145	-	X
57	MG	BA	3146	-	X
57	MG	BA	3148	-	X
57	MG	BA	3149	-	X
57	MG	BA	3150	-	X
57	MG	BA	3151	-	X
57	MG	BA	3153	-	X
57	MG	BA	3154	-	X
57	MG	BA	3155	-	X
57	MG	BA	3157	-	X
57	MG	BA	3158	-	X
57	MG	BA	3159	-	X
57	MG	BA	3161	-	X
57	MG	BA	3163	-	X
57	MG	BA	3167	-	X
57	MG	BA	3170	-	X
57	MG	BA	3171	-	X
57	MG	BA	3174	-	X
57	MG	BA	3177	-	X
57	MG	BA	3178	-	X
57	MG	BA	3181	-	X
57	MG	BA	3182	-	X
57	MG	BA	3183	-	X
57	MG	BA	3185	-	X
57	MG	BA	3186	-	X
57	MG	BA	3188	-	X
57	MG	BA	3190	-	X
57	MG	BA	3192	-	X
57	MG	BA	3193	-	X
57	MG	BA	3194	-	X
57	MG	BA	3196	-	X
57	MG	BA	3197	-	X
57	MG	BA	3200	-	X
57	MG	BA	3202	-	X
57	MG	BA	3203	-	X
57	MG	BA	3204	-	X
57	MG	BA	3205	-	X
57	MG	BA	3206	-	X

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
57	MG	BA	3207	-	X
57	MG	BA	3210	-	X
57	MG	BA	3211	-	X
57	MG	BA	3213	-	X
57	MG	BA	3214	-	X
57	MG	BA	3216	-	X
57	MG	BA	3219	-	X
57	MG	BA	3221	-	X
57	MG	BA	3223	-	X
57	MG	BA	3225	-	X
57	MG	BA	3232	-	X
57	MG	BA	3233	-	X
57	MG	BA	3234	-	X
57	MG	BA	3240	-	X
57	MG	BA	3241	-	X
57	MG	BA	3244	-	X
57	MG	BA	3245	-	X
57	MG	BA	3246	-	X
57	MG	BA	3250	-	X
57	MG	BA	3251	-	X
57	MG	BA	3252	-	X
57	MG	BA	3254	-	X
57	MG	BA	3255	-	X
57	MG	BA	3257	-	X
57	MG	BA	3260	-	X
57	MG	BA	3261	-	X
57	MG	BA	3262	-	X
57	MG	BA	3263	-	X
57	MG	BA	3265	-	X
57	MG	BA	3266	-	X
57	MG	BA	3267	-	X
57	MG	BA	3268	-	X
57	MG	BA	3269	-	X
57	MG	BA	3270	-	X
57	MG	BA	3271	-	X
57	MG	BA	3272	-	X
57	MG	BA	3273	-	X
57	MG	BA	3276	-	X
57	MG	BA	3277	-	X
57	MG	BA	3278	-	X
57	MG	BA	3280	-	X
57	MG	BA	3281	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
57	MG	BA	3282	-	X
57	MG	BA	3283	-	X
57	MG	BA	3284	-	X
57	MG	BA	3291	-	X
57	MG	BA	3292	-	X
57	MG	BA	3293	-	X
57	MG	BA	3294	-	X
57	MG	BA	3295	-	X
57	MG	BA	3296	-	X
57	MG	BA	3297	-	X
57	MG	BA	3298	-	X
57	MG	BA	3300	-	X
57	MG	BA	3302	-	X
57	MG	BA	3304	-	X
57	MG	BA	3305	-	X
57	MG	BA	3306	-	X
57	MG	BA	3308	-	X
57	MG	BA	3311	-	X
57	MG	BA	3313	-	X
57	MG	BA	3314	-	X
57	MG	BA	3316	-	X
57	MG	BA	3317	-	X
57	MG	BA	3318	-	X
57	MG	BA	3320	-	X
57	MG	BA	3323	-	X
57	MG	BA	3324	-	X
57	MG	BA	3325	-	X
57	MG	BA	3329	-	X
57	MG	BA	3330	-	X
57	MG	BA	3331	-	X
57	MG	BA	3333	-	X
57	MG	BA	3337	-	X
57	MG	BA	3340	-	X
57	MG	BA	3341	-	X
57	MG	BA	3345	-	X
57	MG	BA	3349	-	X
57	MG	BA	3350	-	X
57	MG	BA	3352	-	X
57	MG	BA	3353	-	X
57	MG	BA	3356	-	X
57	MG	BA	3357	-	X
57	MG	BB	201	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
57	MG	BB	202	-	X
57	MG	BB	209	-	X
57	MG	BD	302	-	X
57	MG	BD	304	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 147221 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	1532	Total	C	N	O	P	0	0	0
			32873	14661	6031	10649	1532			

- 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			

- 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			

- 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			

- 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			

- Molecule 6 is a protein called 30S ribosomal protein S6 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	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			

- 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			

- 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			

- 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			

- 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			

- Molecule 12 is a protein called 30S ribosomal protein S12 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	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			

- 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			

- Molecule 15 is a protein called 30S ribosomal protein S15 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	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			

- 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			

- 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			

- 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			

- 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			

- 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			

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

- Molecule 23 is a protein called Peptide chain release factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	525	Total	C	N	O	S	0	0	0
			4144	2617	722	783	22			

- Molecule 24 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AY	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	50	Total	C	N	O	S	0	0	0
			409	263	75	71				

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 33 is a protein called 50S ribosomal protein L36 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	2853	Total	C	N	O	P	0	0	0
			61252	27324	11274	19801	2853			

- Molecule 35 is a RNA chain called 5S ribosomal RNA.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 36 is a protein called 50S ribosomal protein L2.

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

- Molecule 37 is a protein called 50S ribosomal protein L3.

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

- Molecule 38 is a protein called 50S ribosomal protein L4.

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

- Molecule 39 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 40 is a protein called 50S ribosomal protein L6.

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

- Molecule 41 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BH	163	Total	C	N	O	S	0	0	0
			1230	775	219	229	7			

- Molecule 42 is a protein called 50S ribosomal protein L11.

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

- Molecule 43 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BJ	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
43	BK	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
43	BL	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
43	BM	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			

- Molecule 44 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BN	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 45 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BO	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 46 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BP	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BP	77	ILE	VAL	SEE REMARK 999	UNP C3SR37

- Molecule 47 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BQ	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 48 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BR	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 49 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BS	116	Total	C	N	O	S	0	0	0
			892	552	178	162				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BT	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 51 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BU	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

- Molecule 52 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BV	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 53 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BW	110	Total	C	N	O	S	0	0	0
			856	532	166	155	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	111	HIS	-	EXPRESSION TAG	UNP C3SQW7
BW	112	HIS	-	EXPRESSION TAG	UNP C3SQW7
BW	113	HIS	-	EXPRESSION TAG	UNP C3SQW7
BW	114	HIS	-	EXPRESSION TAG	UNP C3SQW7
BW	115	HIS	-	EXPRESSION TAG	UNP C3SQW7
BW	116	HIS	-	EXPRESSION TAG	UNP C3SQW7

- Molecule 54 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BX	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 55 is a protein called 50S ribosomal protein L24 1.

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

- Molecule 56 is a protein called 50S ribosomal protein L25 1.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

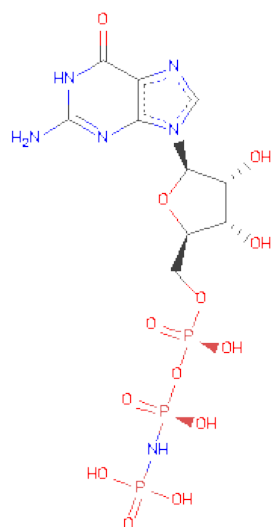
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BT	1	Total	Mg	0	0
			1	1		
57	BB	9	Total	Mg	0	0
			9	9		
57	BO	1	Total	Mg	0	0
			1	1		
57	B4	1	Total	Mg	0	0
			1	1		
57	BA	357	Total	Mg	0	0
			357	357		
57	BN	1	Total	Mg	0	0
			1	1		
57	B2	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AH	1	Total 1	Mg 1	0	0
57	BD	5	Total 5	Mg 5	0	0
57	BE	1	Total 1	Mg 1	0	0
57	AW	1	Total 1	Mg 1	0	0
57	AA	102	Total 102	Mg 102	0	0
57	BQ	1	Total 1	Mg 1	0	0
57	BC	1	Total 1	Mg 1	0	0
57	B0	3	Total 3	Mg 3	0	0
57	BX	1	Total 1	Mg 1	0	0
57	AL	2	Total 2	Mg 2	0	0
57	BR	2	Total 2	Mg 2	0	0
57	AF	1	Total 1	Mg 1	0	0
57	AM	1	Total 1	Mg 1	0	0

- Molecule 58 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	AW	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

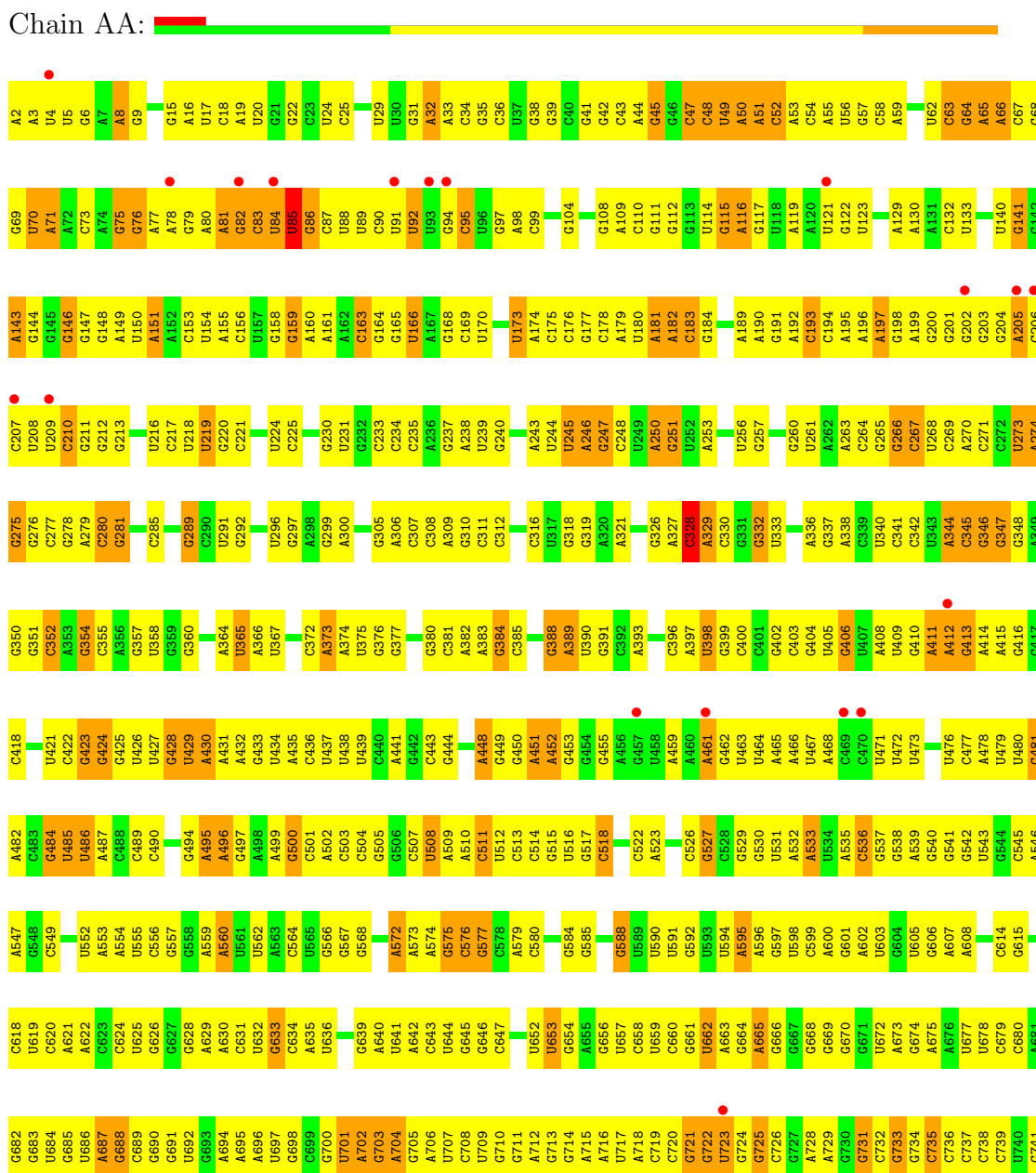
- Molecule 59 is water.

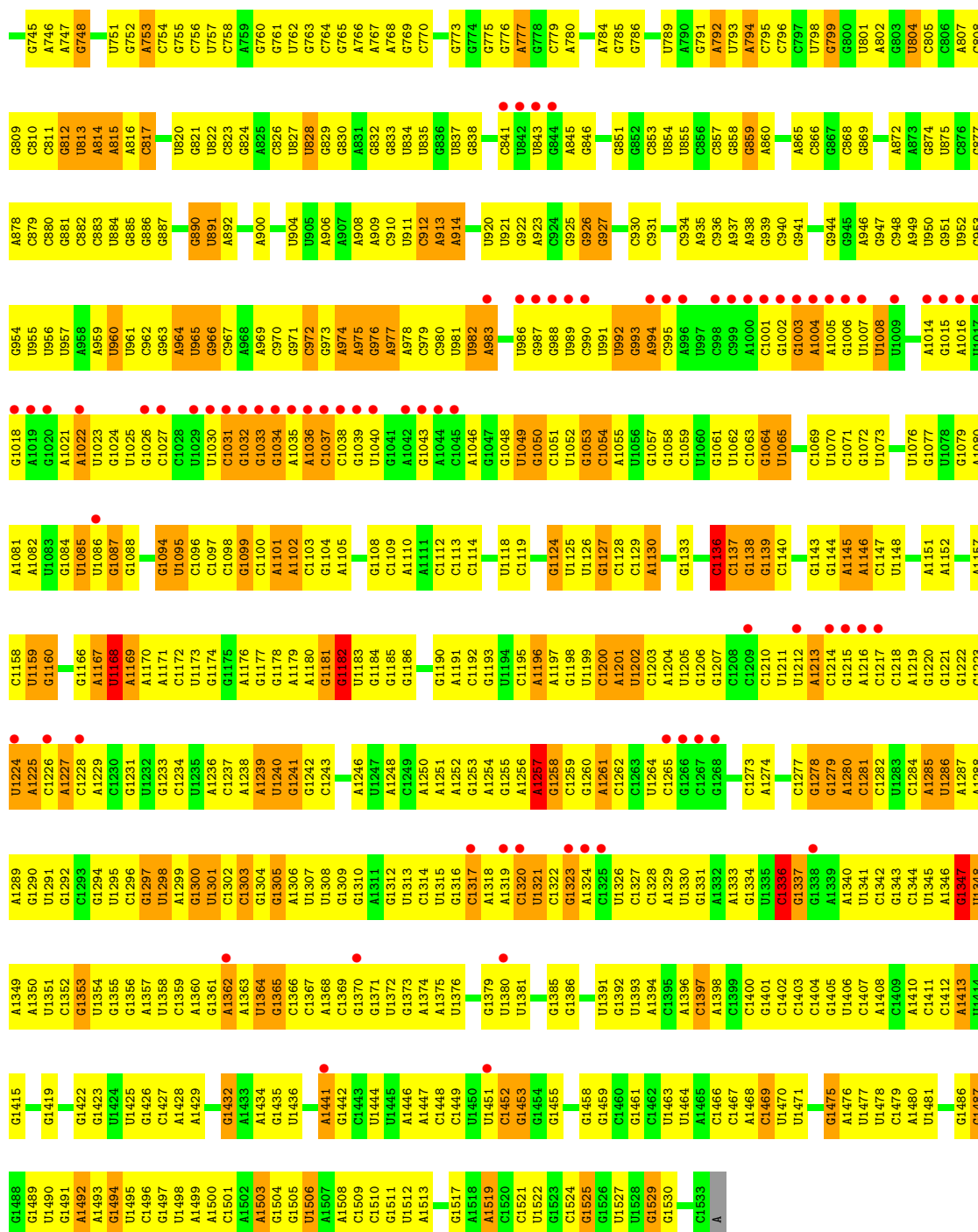
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AW	2	Total	O	0	0
			2	2		
59	B8	1	Total	O	0	0
			1	1		
59	BA	8	Total	O	0	0
			8	8		
59	BC	2	Total	O	0	0
			2	2		
59	BD	1	Total	O	0	0
			1	1		
59	BF	1	Total	O	0	0
			1	1		
59	BG	1	Total	O	0	0
			1	1		
59	BW	1	Total	O	0	0
			1	1		

### 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.

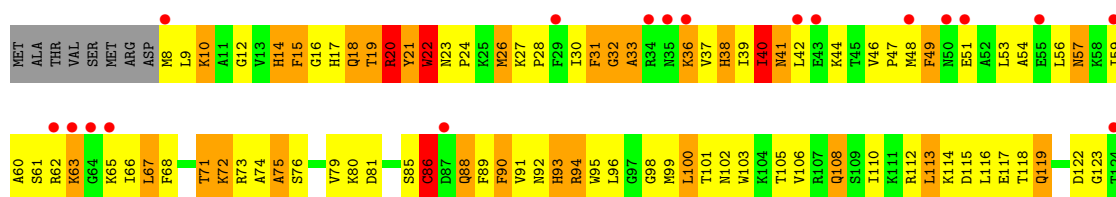
#### • Molecule 1: 16S rRNA





• Molecule 2: 30S ribosomal protein S2

Chain AB:



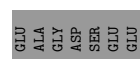
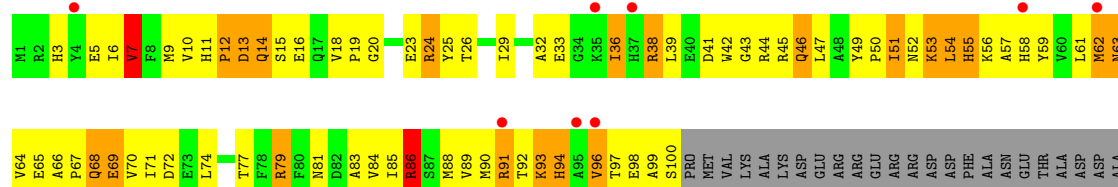






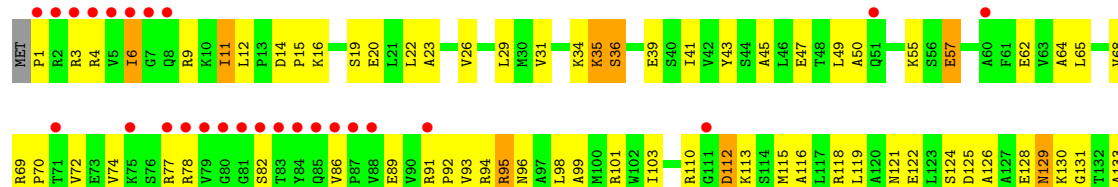
• Molecule 6: 30S ribosomal protein S6 1

Chain AF:



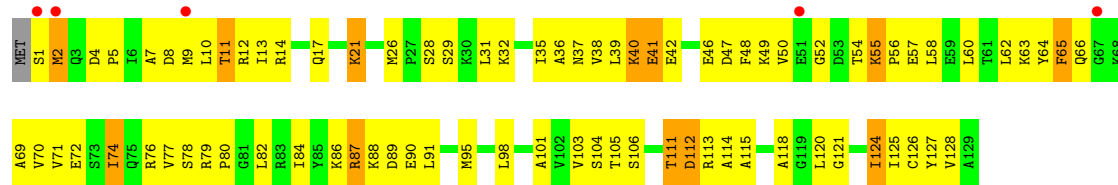
• Molecule 7: 30S ribosomal protein S7

Chain AG:



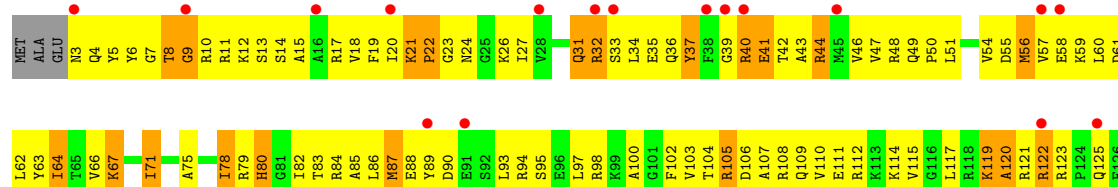
• Molecule 8: 30S ribosomal protein S8

Chain AH:



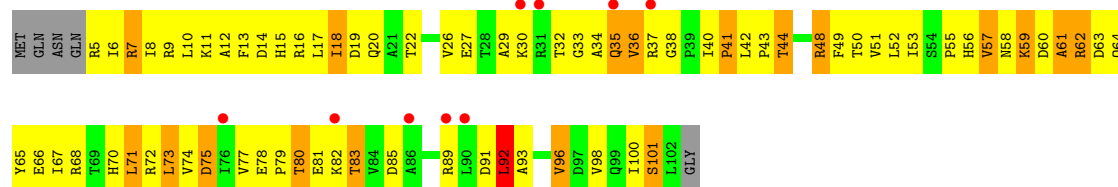
• Molecule 9: 30S ribosomal protein S9

Chain AI:



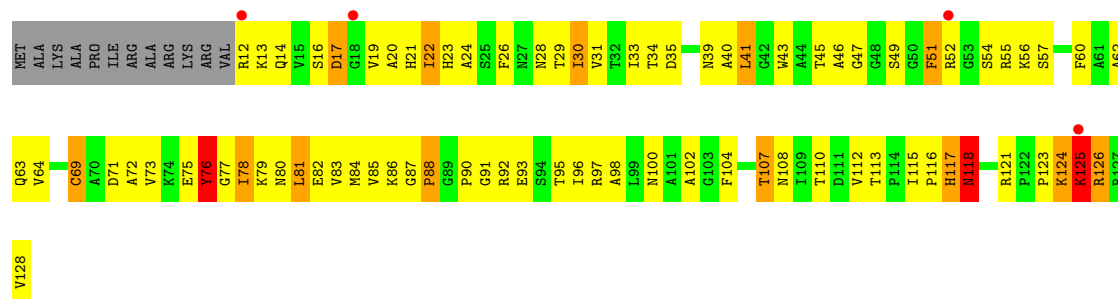
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



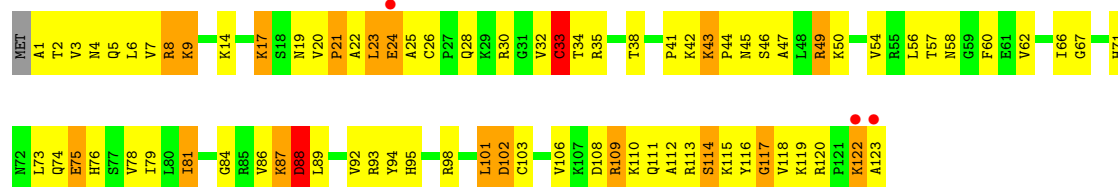
- Molecule 11: 30S ribosomal protein S11

Chain AK:



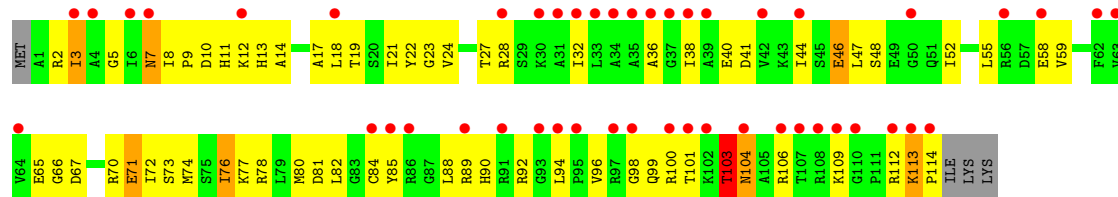
- Molecule 12: 30S ribosomal protein S12 1

Chain AL:



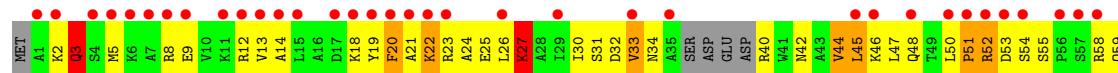
- Molecule 13: 30S ribosomal protein S13

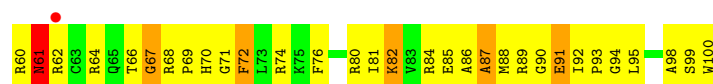
Chain AM:



- Molecule 14: 30S ribosomal protein S14

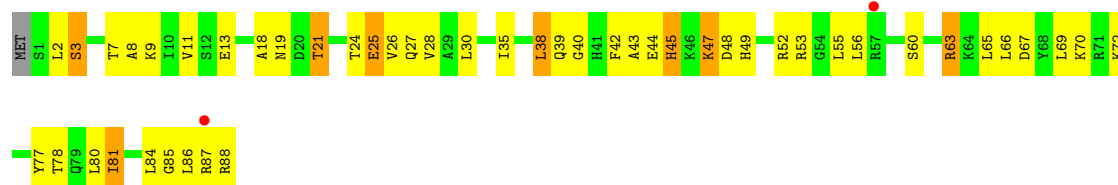
Chain AN:





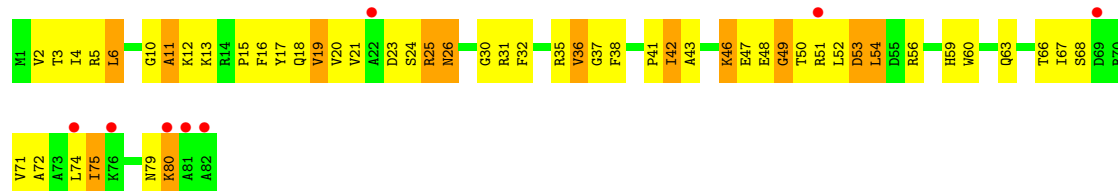
- Molecule 15: 30S ribosomal protein S15 1

Chain AO:



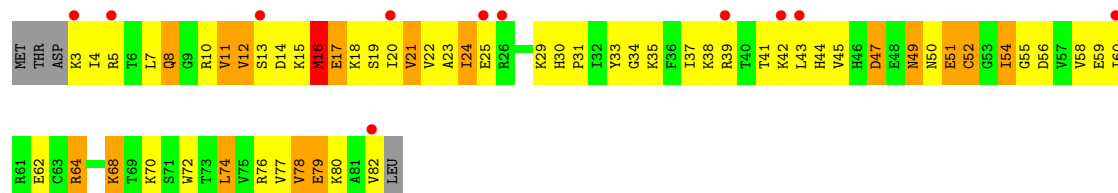
- Molecule 16: 30S ribosomal protein S16

Chain AP:



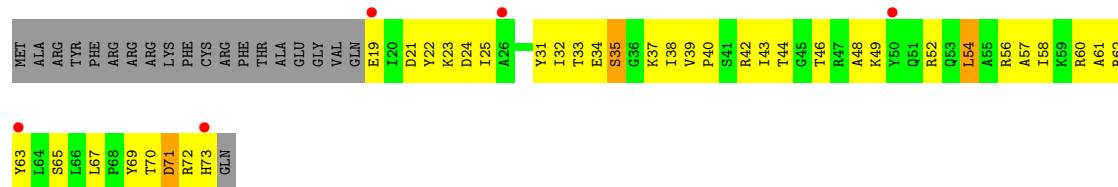
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



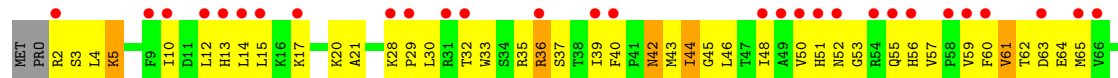
- Molecule 18: 30S ribosomal protein S18

Chain AR:



- Molecule 19: 30S ribosomal protein S19

Chain AS:

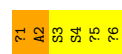






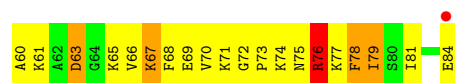
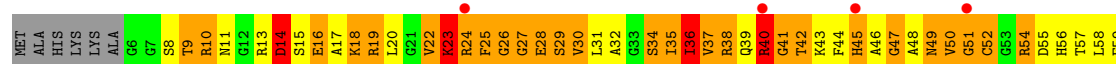
- Molecule 24: Viomycin

Chain AY:



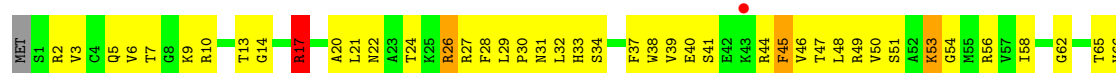
- Molecule 25: 50S ribosomal protein L27

Chain B0:



- Molecule 26: 50S ribosomal protein L28

Chain B1:



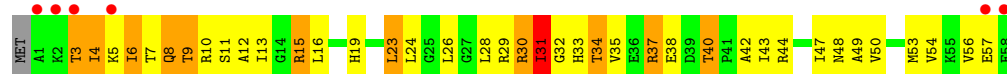
- Molecule 27: 50S ribosomal protein L29

Chain B2:



- Molecule 28: 50S ribosomal protein L30

Chain B3:



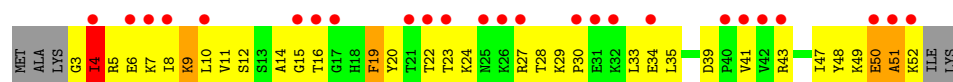
- Molecule 29: 50S ribosomal protein L32

Chain B4:



- Molecule 30: 50S ribosomal protein L33

Chain B5:



- Molecule 31: 50S ribosomal protein L34

Chain B6:



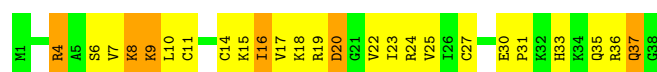
- Molecule 32: 50S ribosomal protein L35

Chain B7:



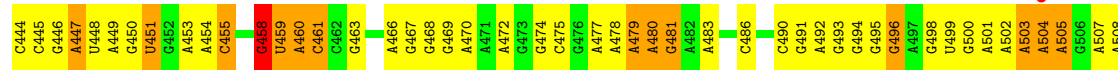
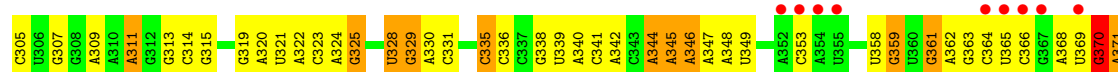
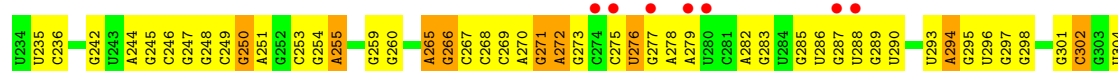
- Molecule 33: 50S ribosomal protein L36 1

Chain B8:



- Molecule 34: 23S rRNA

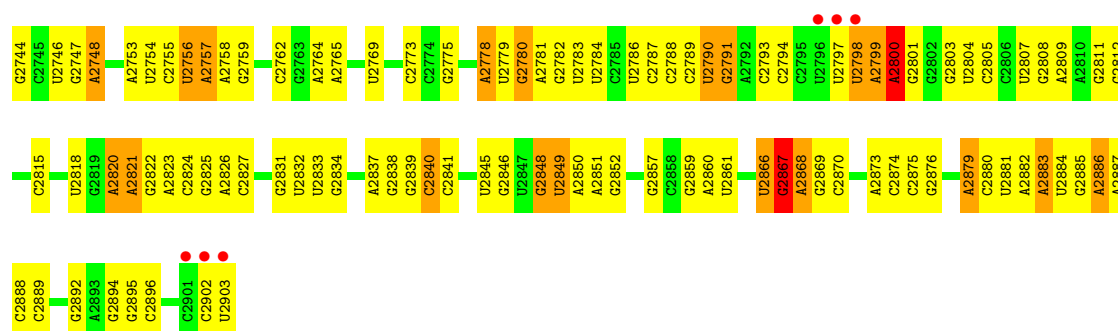
Chain BA:



U1559	C1488	G1415	G1206	A1134	G1063	C992	G862	U724	G651	A582
G1560	C1489	G1416	C1211	C1135	C1064	G993	A863	G725	U652	G583
C1561	G1490	C1417	G1212	G1136	U1065	G994	G864	A928	U653	C584
U1562	G1491	G1418	A1213	G1137	U1066	C995	C865	G726	A654	G585
U1563	G1492	A1419	A1213	G1138	A1067	A996	A866	G728	A655	A586
C1564	G1493	A1420	G1216	G1139	U1068	G997	C867	G729	G656	C587
C1565	A1494	G1421	G1217	C1140	A1069	C998	U868	A730	U657	U588
A1566	A1495	G1422	U1217	U1141	A1070	U999	C869	C731	U658	U589
G1567	A1496	C1297	U1218	A1142	U1071	A1000	U870	C732	G659	A590
G1568	C1497	C1289	U1219	A1143	C1072	C935	U871	G733	C660	U591
A1569	C1498	C1290	U1219	A1143	A1073	A1001	U872	C736	A661	A592
A1570	C1499	G1292	C1293	A1144	C1074	A936	U873	C736	G662	U593
A1571	G1500	C1362	C1293	A1147	C1075	C937	G874	A739	G663	U594
A1572	G1501	G1363	G1225	U1148	G1076	G938	C875	A742	A666	A599
U1576	A1502	A1364	C1229	G1149	U1077	A941	C876	A743	U667	G600
C1577	A1503	A1365	C1230	C1150	U1078	G942	C877	U744	A668	C601
U1578	A1504	G1368	U1231	A1151	C1079	A943	A878	U744	G669	A602
U1581	A1505	G1371	C1232	C1152	A1080	C944	C879	G745	A670	A603
C1582	U1506	G1372	C1233	C1153	U1081	A945	G880	U746	C671	G604
A1583	C1507	G1373	C1233	G1154	U1082	C946	C881	U747	C672	A609
U1584	A1508	G1374	U1234	A1155	U1083	C947	C882	U748	G673	C610
C1585	U1509	U1375	G1235	A1156	A1084	C948	C883	A749	G674	G611
A1586	G1510	C1376	G1236	G1157	A1085	G949	U884	A752	A675	C612
G1587	G1511	C1377	A1237	G1161	U1086	C950	C885	A753	C679	A613
U1588	G1512	A1308	G1238	G1162	G1087	C951	A	U754	C680	U615
G1589	A1513	G1378	G1239	A1165	A1088	C954	U	U755	U683	A616
U1590	G1514	U1379	U1240	C1166	A1089	G955	C	A756	C684	G617
A1591	C1515	C1381	A1244	A1167	U1090	U956	C	G760	A685	G620
C1592	G1516	G1382	A1245	C1167	G1091	G956	C	A761	U686	A621
U1593	G1517	U1316	A1246	G1168	C1092	C957	G	U769	C692	G622
A1594	U1518	U1317	A1247	A1169	G1093	U958	A	G770	A693	C623
U1595	G1519	U1318	G1248	C1170	U1097	C961	C893	C771	U694	A627
C1596	G1520	C1377	U1249	C1171	U1098	G962	U894	C772	G629	G628
A1597	U1521	G1383	G1250	C1172	G1099	U963	U895	G775	A631	G630
U1598	G1522	A1384	A1251	U1173	C1100	C964	U896	G776	A705	A632
A1599	C1523	U1385	A1252	U1174	U1101	U967	U897	G777	A706	C634
G1600	A1524	C1386	A1253	C1175	C1102	C968	C901	G778	G707	C635
U1601	G1525	G1387	A1254	U1176	A1103	G971	C902	U779	G708	A637
A1602	U1530	C1388	U1255	C1177	U1104	A972	C903	A781	U709	G638
U1603	C1531	U1389	U1256	C1178	U1105	G973	G904	U782	U710	U639
C1604	G1532	A1392	G1257	G1179	G1106	A980	U898	A783	G711	C640
U1605	U1533	U1393	C1257	C1180	U1107	A981	C912	G784	G712	U641
A1608	C1534	G1394	U1258	U1181	U1108	A982	C914	C786	U714	A643
C1609	U1535	U1395	G1259	U1182	C1109	A983	C915	A788	A715	A644
A1610	G1536	U1396	A1260	G1183	G1110	A984	C916	A789	A716	C645
U1613	C1537	U1397	C1261	U1184	G1111	G975	A917	A793	U646	G647
A1614	U1538	C1398	A1262	U1185	G1112	G976	A918	A794	G648	C650
C1615	U1539	C1399	C1262	G1186	C1113	A979	A919	A990	A721	G649
U1616	G1540	U1400	C1335	G1187	G1114	A980	C912	A991	C723	
C1617	C1541	G1401	C1336	G1188	C1115	A981	C913	A992		
A1618	U1542	U1402	G1337	G1189	G1116	A982	C914	A993		
G1619	G1543	A1403	C1338	U1188	C1117	A983	C915	A994		
U1620	A1544	U1404	G1339	U1189	G1118	A984	C916	A995		
C1621	U1545	U1405	U1340	G1190	G1119	A985	A917	A996		
A1622	G1546	U1406	C1341	G1191	G1120	A986	A918	A997		
U1623	U1547	U1407	A1342	G1192	G1121	A987	A919	A998		
G1624	C1548	U1408	U1343	G1193	G1122	A988	A920	A999		
A1625	U1549	G1409	U1344	G1194	G1123	A989	A921	A999		
U1626	A1550	U1410	U1345	G1195	G1124	A990	A922	A999		
C1627	C1551	U1411	C1346	G1196	G1125	A991	A923	A999		
A1628	U1552	U1412	U1347	G1197	G1126	A992	A924	A999		
U1629	G1553	U1413	A1348	G1198	G1127	A993	A925	A999		
G1630	A1554	U1414	U1349	G1199	G1128	A994	A926	A999		
C1631	U1555	U1415	U1350	G1200	G1129	A995	A927	A999		
A1632	G1556	U1416	U1351	A1205	G1130	A996	A928	A999		
U1633	U1557	U1417	A1206	G1201	U1131	A997	A929	A999		
G1634	C1558	U1418	A1207	G1202	U1132	A998	A930	A999		
A1635	U1559	U1419	A1208	G1203	U1133	A999	A931	A999		
C1636	G1560	U1420	A1209	G1204	A1134	A999	A932	A999		
U1637	A1561	U1421	U1352	G1205	A1135	A999	A933	A999		
A1638	U1562	U1422	U1353	G1206	A1136	A999	A934	A999		
G1639	C1563	U1423	U1354	G1207	A1137	A999	A935	A999		
U1640	A1564	U1424	U1355	G1208	A1138	A999	A936	A999		
C1641	U1565	U1425	U1356	G1209	A1139	A999	A937	A999		
A1642	G1566	U1426	U1357	G1210	A1140	A999	A938	A999		
U1643	U1567	U1427	U1358	G1211	A1141	A999	A939	A999		
G1644	A1568	U1428	U1359	G1212	A1142	A999	A940	A999		
A1645	C1569	C1429	U1360	G1213	A1143	A999	A941	A999		
U1646	U1570	G1430	C1361	G1214	A1144	A999	A942	A999		
C1647	A1571	U1431	C1362	G1215	A1145	A999	A943	A999		
A1648	G1572	A1432	G1363	G1216	A1146	A999	A944	A999		
U1649	U1573	G1433	A1364	G1217	A1147	A999	A945	A999		
G1650	A1574	A1434	A1365	G1218	A1148	A999	A946	A999		
C1651	U1575	A1435	A1366	G1219	A1149	A999	A947	A999		
U1652	U1576	G1436	G1367	G1220	A1150	A999	A948	A999		
A1653	C1577	G1437	G1368	G1221	A1151	A999	A949	A999		
G1654	U1578	A1438	G1369	G1222	A1152	A999	A950	A999		
U1655	U1579	A1439	G1370	G1223	A1153	A999	A951	A999		
C1656	C1580	G1439	G1371	G1224	A1154	A999	A952	A999		
A1657	A1581	U1440	G1372	G1225	A1155	A999	A953	A999		
U1658	U1582	U1441	G1373	G1226	A1156	A999	A954	A999		
G1659	C1583	U1442	G1374	G1227	A1157	A999	A955	A999		
A1660	A1584	G1443	U1375	G1228	A1158	A999	A956	A999		
C1661	U1585	U1444	C1376	G1229	A1159	A999	A957	A999		
U1662	C1586	G1445	C1377	G1230	A1160	A999	A958	A999		
A1663	U1587	U1446	A1378	G1231	A1161	A999	A959	A999		
G1664	G1588	G1447	U1379	G1232	A1162	A999	A960	A999		
C1665	U1589	U1448	U1380	G1233	A1163	A999	A961	A999		
A1666	C1590	U1449	C1381	G1234	A1164	A999	A962	A999		
U1667	A1591	G1450	G1382	G1235	A1165	A999	A963	A999		
C1668	U1592	U1451	C1383	G1236	A1166	A999	A964	A999		
A1669	G1593	U1452	A1384	G1237	A1167	A999	A965	A999		
U1670	A1594	U1453	U1385	G1238	A1168	A999	A966	A999		
C1671	C1595	G1454	C1386	G1239	A1169	A999	A967	A999		
A1672	U1596	U1455	A1387	G1240	A1170	A999	A968	A999		
G1673	G1597	U1456	G1388	G1241	A1171	A999	A969	A999		
U1674	A1598	C1457	U1389	G1242	A1172	A999	A970	A999		
C1675	U1599	U1458	U1390	G1243	A1173	A999	A971	A999		
A1676	G1600	G1459	U1391	G1244	A1174	A999	A972	A999		
U1677	C1531	U1460	C1392	G1245	A1175	A999	A973	A999		
C1678	U1532	U1461	A1393	G1246	A1176	A999	A974	A999		
A1679	C1533	U1462	U1394	G1247	A1177	A999	A975	A999		
U1680	U1534	U1463	U1395	G1248	A1178	A999	A976	A999		
C1681	A1535	U1464	U1396	G1249	A1179	A999	A977	A999		
A1682	C1536	U1465	U1397	G1250	A1180	A999	A978	A999		
U1683	U1537	U1466	U1398	G1251	A1181	A999	A979	A999		
G1684	G1538	U1467	C1399	G1252	A1182	A999	A980	A999		
C1685	U1539	U1468	U1400	G1253	A1183	A999	A981	A999		
A1686	G1540	U1469	U1401	G1254	A1184	A999	A982	A999		
U1687	U1541	A1470	U1402	G1255	A1185	A999	A983	A999		
C1688	C1542	U1471	U1403	G1256	A1186	A999	A984	A999		
A1689	U1543	G1472	A1404	G1257	A1187	A999	A985	A999		
U1690	G1544	U1473	U1405	G1258	A1188	A999	A986	A999		
C1691	A1545	G1474	U1406	G1259	A1189	A999	A987	A999		
U1692	U1546	U1475	U1407	G1260	A1190	A999	A988	A999		
A1693	G1547	U1476	U1408	G1261	G1191	A999	A989	A999		
C1694	C15									

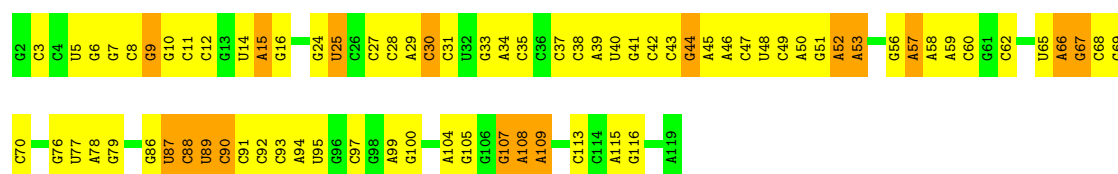


G2674	A2675	G2676	G2677	G2678	G2679	G2680	G2681	G2682	G2683	G2688	G2689	G2690	G2691	G2695	G2696	G2697	G2698	G2699	G2700	G2701	G2702	G2703	G2704	A2705	G2706	G2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2722	G2723	G2724	G2725	G2726	G2727	G2728	G2729	G2730	G2731	G2732	G2733	G2734	G2735	G2740	G2741	G2742	G2743	
G2599	A2600	G2601	A2602	G2603	G2607	G2608	G2609	G2613	G2614	G2615	G2616	G2617	G2618	G2619	G2620	G2623	G2626	G2629	A2632	G2633	A2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	G2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	G2657	G2661	A2662	G2663	G2664	G2667	G2668									
C2512	A2513	G2514	C2515	A2516	C2517	A2518	G2519	C2520	G2529	A2542	G2543	G2544	A2547	G2548	C2551	U2554	G2555	G2556	G2557	C2558	G2559	A2560	U2561	G2562	U2563	A2564	A2565	A2566	G2567	U2568	G2569	G2570	A2571	A2572	C2575	G2576	A2577	G2578	C2579	G2583	U2584	U2585	U2586	A2587	A2590	G2591	G2592	U2593	C2594	A2598									
A2434	A2435	U2441	C2442	C2443	G2444	A2448	U2449	A2450	A2451	C2452	A2453	G2454	G2455	G2456	U2457	G2458	A2459	A2460	A2461	C2467	A2468	A2469	G2470	A2471	G2472	U2473	U2474	C2475	A2476	U2477	A2478	U2479	C2480	G2481	C2486	U2489	G2490	U2491	U2492	G2493	G2494	A2497	C2498	C2499	A2425	A2426	G2427	G2428	G2429	U2430	U2431	A2433							
A2358	C2359	G2360	G2361	C2364	G2365	A2366	G2367	A2368	A2369	G2375	A2376	A2377	A2378	G2379	G2380	A2381	G2382	G2383	G2384	C2385	G2386	U2387	A2388	G2389	U2390	G2391	A2392	G2393	C2394	G2400	U2401	U2402	C2403	A2406	A2407	A2411	A2412	A2418	U2419	C2420	G2421	U2422	U2423	U2424	A2425	A2426	G2427	G2428	G2429	U2430	U2431	A2433							
A2297	A2298	G2299	G2300	C2301	G2302	G2303	G2304	G2305	C2306	G2307	G2308	G2309	C2310	A2311	U2312	A2313	A2314	G2315	G2316	A2317	G2318	U2320	U2321	A2322	G2323	G2324	G2325	C2326	A2327	A2328	U2329	A2330	G2331	C2332	A2333	U2334	A2335	A2336	G2337	A2340	G2341	C2342	U2343	G2344	G2345	G2346	C2347	U2348	G2349	C2350	G2351	G2352	G2353	C2354	U2355	G2356	G2357		
C2296	A2227	G2228	U2229	C2230	U2231	C2232	U2233	G2234	G2237	G2238	G2239	U2243	U2244	U2245	C2248	U2249	U2250	G2255	G2256	U2257	C2258	U2259	G2260	C2261	U2262	C2263	C2264	C2265	C2266	A2268	G2269	A2270	G2271	U2272	A2273	A2274	C2275	G2276	G2277	A2278	G2279	A2280	A2281	G2282	C2283	G2286	A2287	G2288	G2289	G2290	U2291	U2292	G2293	G2294	G2295				
G2156	G2157	A	G	C	C	G	A	C	U	G	A	A	A	U	A	C	C	C	C	C2179	U2180	U2181	U2182	A2183	U2184	U2185	G2186	U2187	U2188	U2189	U2194	U2195	C2196	U2197	A2198	A2199	C2200	G2201	U2202	U2203	G2204	U2210	A2211	A2212	U2213	G2217	G2218	U2219	U2220	C2221	C2222	G2223	G2224	A2225					
G2093	A2094	A2095	G2096	A2097	G2102	C2103	C2104	U2105	U2106	G2107	A2108	U2109	G2110	U	U	U	A	G	C	C2179	U2180	U2181	U2182	A2183	U2184	U2185	G2186	U2187	U2188	U2189	U2194	U2195	C2196	U2197	A2198	A2199	C2200	G2201	U2202	U2203	G2204	U2210	A2211	A2212	U2213	G2217	G2218	U2219	U2220	C2221	C2222	G2223	G2224	A2225					
U2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	U2034	U2035	U2036	G2037	U2038	U2039	G2040	U2041	A2042	C2043	G2046	G2047	G2048	C2049	A2050	A2051	A2052	G2055	G2056	G2057	A2058	A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	G2069	A2070	U2071	C2072	C2073	U2074	U2075	U2076	A2077	C2078	U2079	A2080	U2081	U2082	A2083	A2084	A2085	A2086	A2087	A2090	C2091	U2092	
U1943	U1944	G1945	U1946	C1947	A1952	A1953	G1954	U1955	U1956	C1957	C1961	A1962	G1963	U1964	C1965	A1966	A1967	G1968	A1969	U1970	U1971	G1972	C1973	C1974	G1984	C1985	C1986	C1990	U1991	G1992	U1993	C1996	C1997	A1998	C1999	C2000	G2004	A2005	C2006	A2013	A2014	A2015	U2016	U2017	G2018	A2019	A2020	C2021	U2022	C2023	G2024								
G1867	C1868	G1869	A1870	A1871	C1872	C1873	C1874	A1875	A1876	G1884	U1885	U1886	G1887	G1888	A1889	C1893	C1894	C1895	G1896	A1900	G1901	C1902	G1903	G1904	C1905	G1906	G1907	C1908	C1909	G1910	U1911	A1912	A1913	U1914	U1915	U1916	U1917	G1920	G1921	G1922	U1923	U1924	C1925	U1926	A1927	U1928	G1929	G1930	A1931	C1934	G1935	A1936	A1937	A1938					
U1798	G1799	C1800	A1801	A1805	A1808	A1809	A1810	G1811	U1812	U1813	G1814	A1815	A1816	G1817	U1818	A1819	U1820	A1821	G1822	G1823	U1824	G1825	G1826	U1827	G1828	A1829	G1830	G1831	C1832	G1833	C1838	G1839	G1840	U1841	G1842	C1843	G1846	A1847	A1848	G1849	G1850	A1851	U1852	A1853	U1854	U1855	U1856	G1857	A1858	U1859	G1860	G1863	U1864						
U1725	C1726	C1727	C1728	U1729	U1730	G1731	C1732	G1733	U1734	U1735	U1736	G1737	G1738	A1739	G1740	C1741	U1742	G1743	A1744	A1745	A1746	A1749	G1756	A1757	U1758	A1759	C1760	G1761	C1764	U1765	A1773	C1774	U1775	G1776	U1777	U1778	U1779	U1780	U1781	U1782	A1783	A1784	A1785	A1786	A1787	C1788	A1789	G1790	U1791	G1792	C1793	A1794	C1795	U1796	G1797				
G1628	U1629	C1638	C1639	C1644	U1647	U1648	G1649	A1650	G1651	A1652	G1653	A1654	A1655	C1656	U1657	A1665	G1667	A1668	A1669	G1674	G1675	A1676	A1677	G1682	U1683	G1687	U1688	U1692	U1693	C1694	G1695	A1701	A1705	C1706	G1707	C1708	U1709	G1710	U1714	G1715	U1716	A1717	G1718	A1722	C1723	G1724													



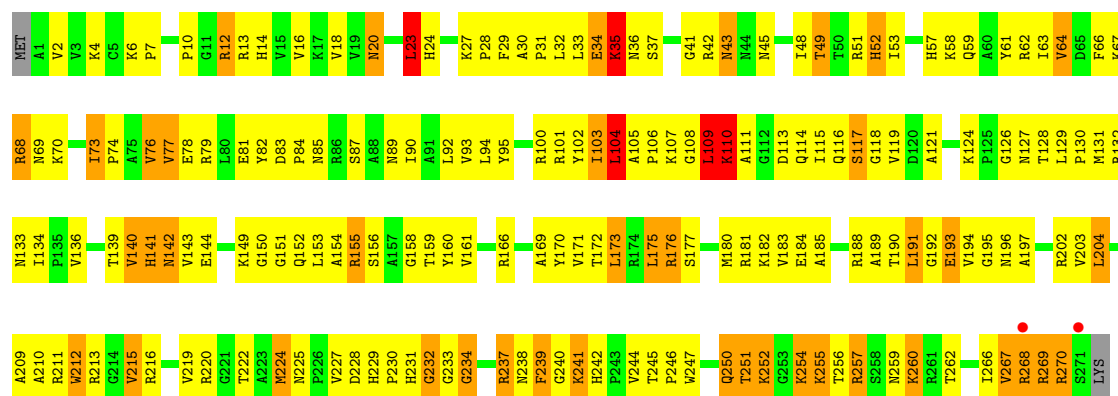
• Molecule 35: 5S ribosomal RNA

Chain BB:



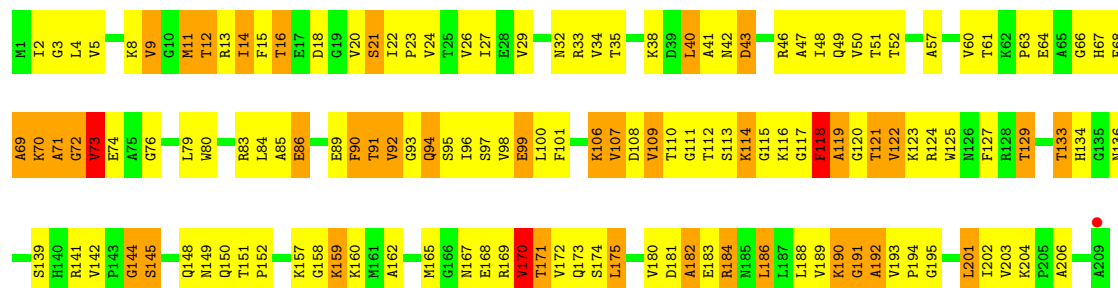
• Molecule 36: 50S ribosomal protein L2

Chain BC:



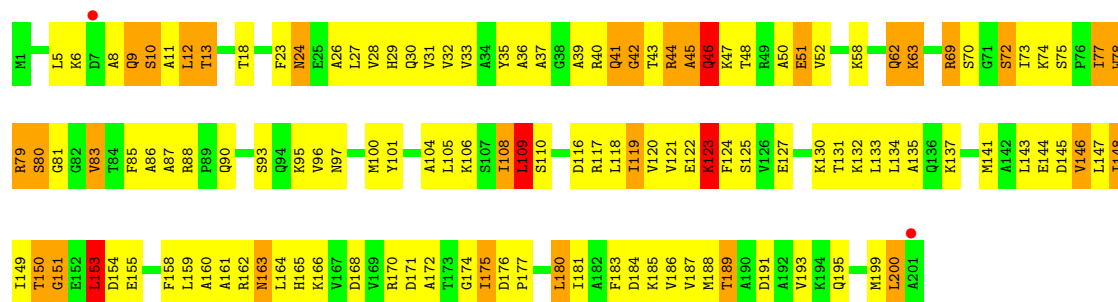
• Molecule 37: 50S ribosomal protein L3

Chain BD:



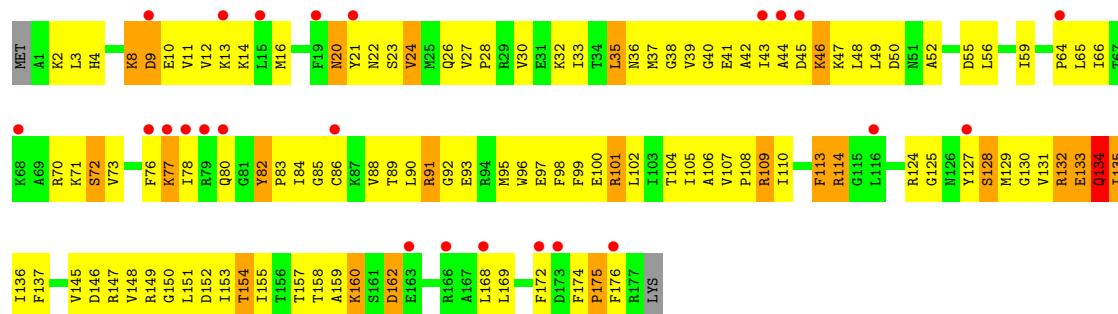
• Molecule 38: 50S ribosomal protein L4

Chain BE:



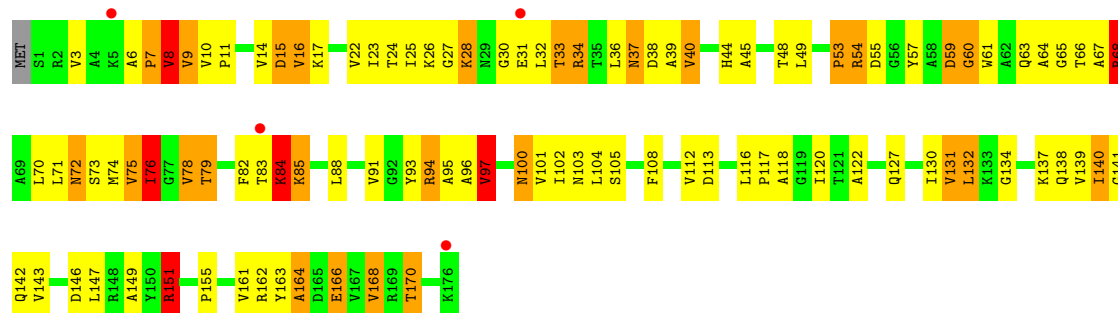
• Molecule 39: 50S ribosomal protein L5

Chain BF:



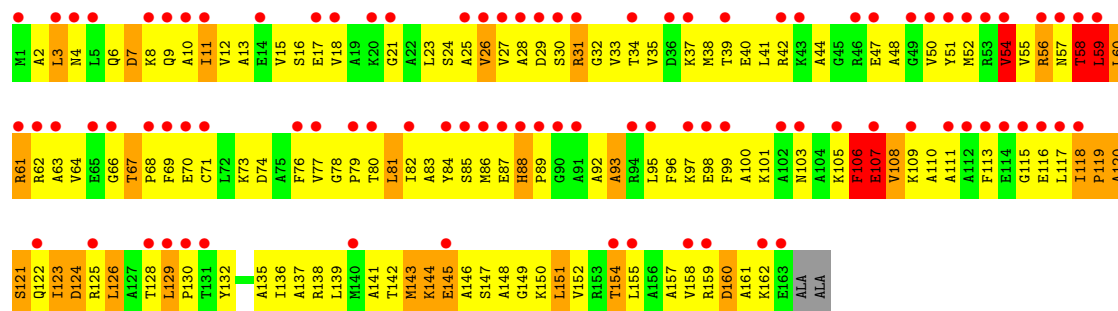
• Molecule 40: 50S ribosomal protein L6

Chain BG:



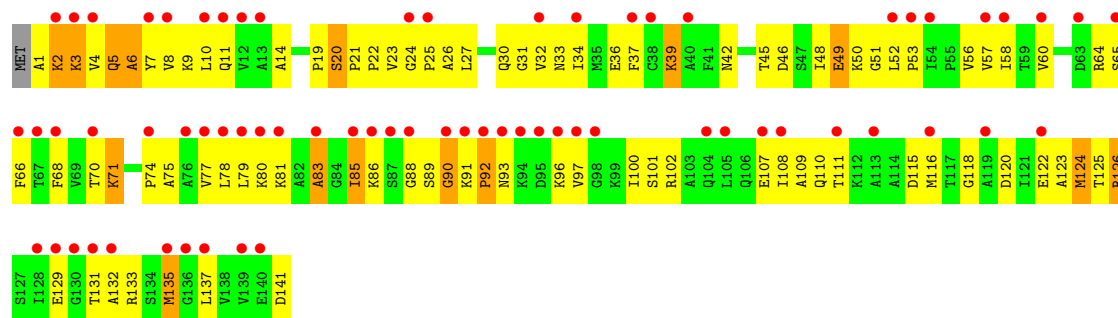
• Molecule 41: 50S ribosomal protein L10

Chain BH:



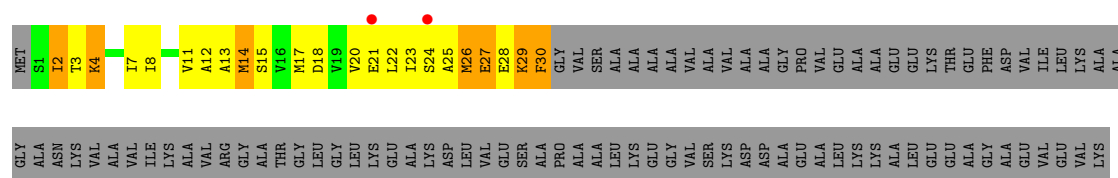
• Molecule 42: 50S ribosomal protein L11

Chain BI:



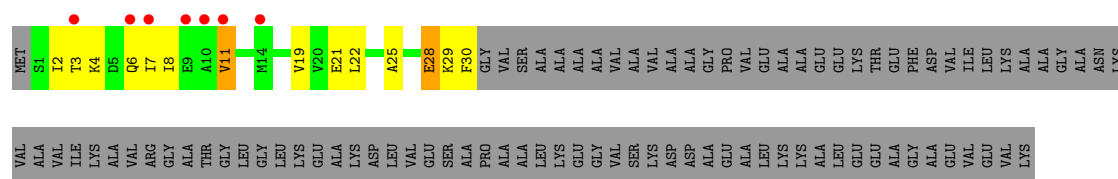
- Molecule 43: 50S ribosomal protein L7/L12

Chain BJ:



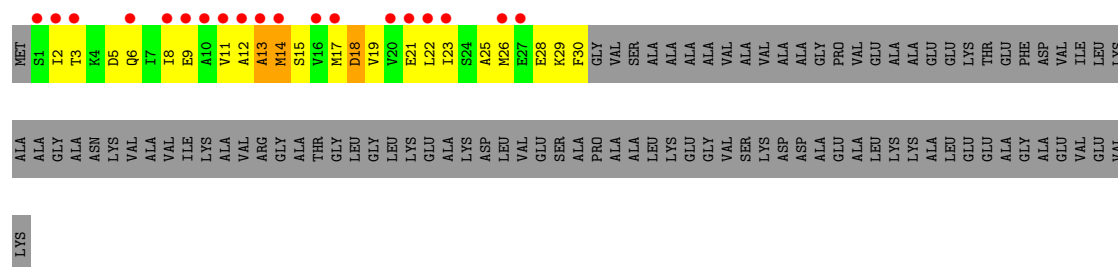
- Molecule 43: 50S ribosomal protein L7/L12

Chain BK:



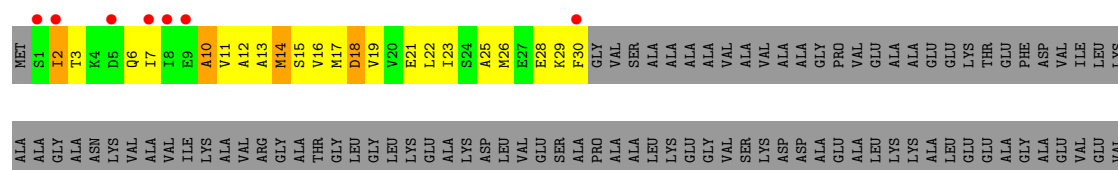
- Molecule 43: 50S ribosomal protein L7/L12

Chain BL:



- Molecule 43: 50S ribosomal protein L7/L12

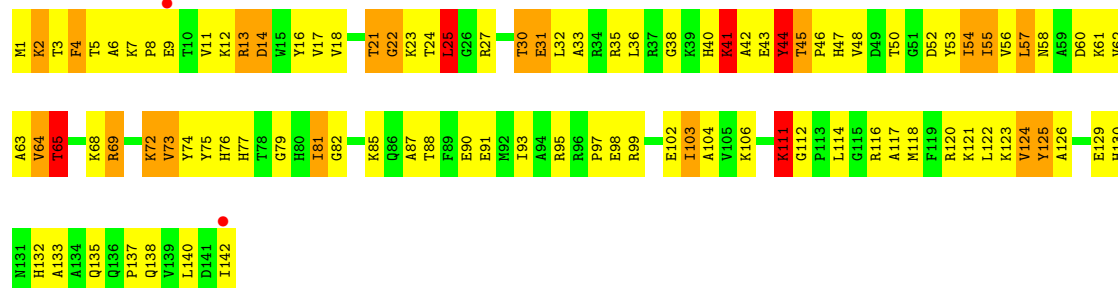
Chain BM:



LYS

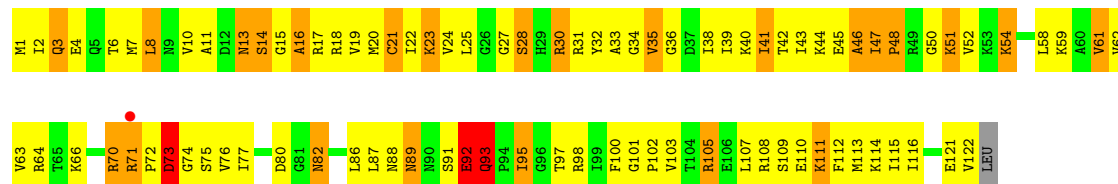
- Molecule 44: 50S ribosomal protein L13

Chain BN:



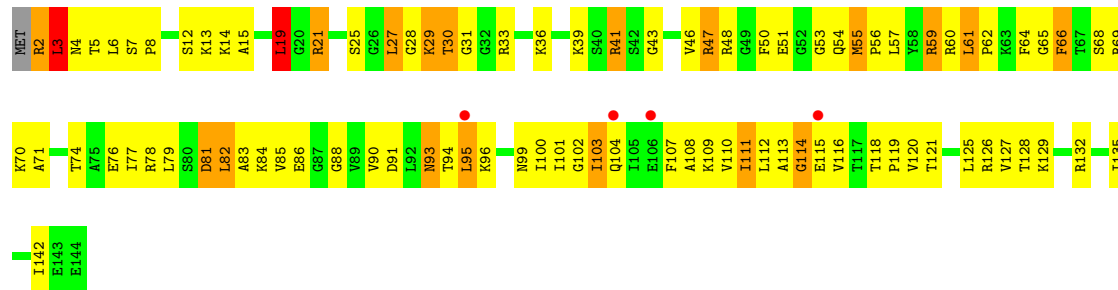
- Molecule 45: 50S ribosomal protein L14

Chain BO:



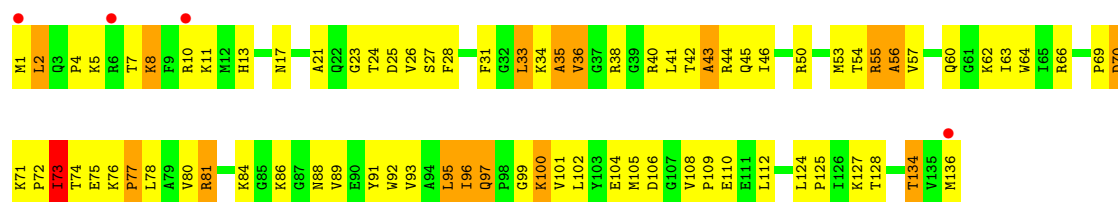
- Molecule 46: 50S ribosomal protein L15

Chain BP:



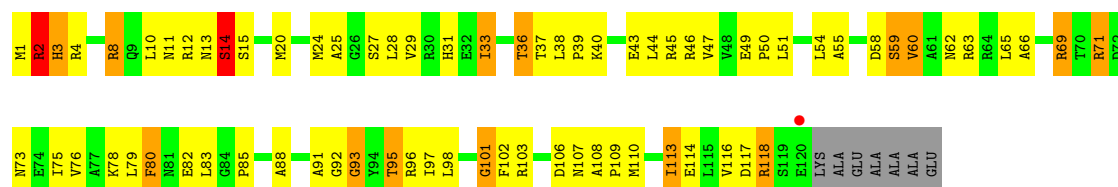
- Molecule 47: 50S ribosomal protein L16

Chain BQ:



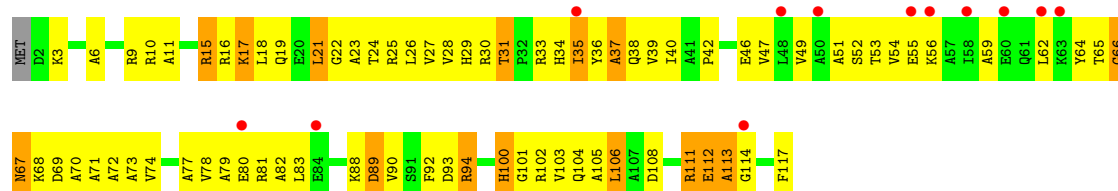
- Molecule 48: 50S ribosomal protein L17

Chain BR:



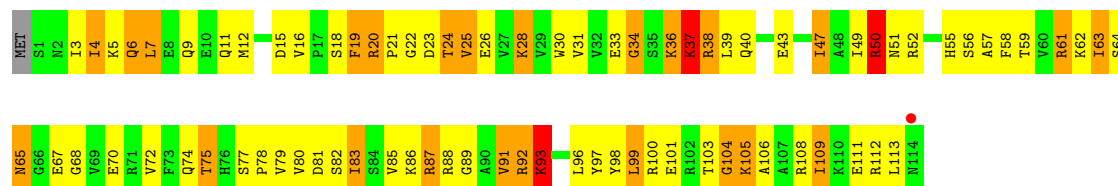
• Molecule 49: 50S ribosomal protein L18

Chain BS:



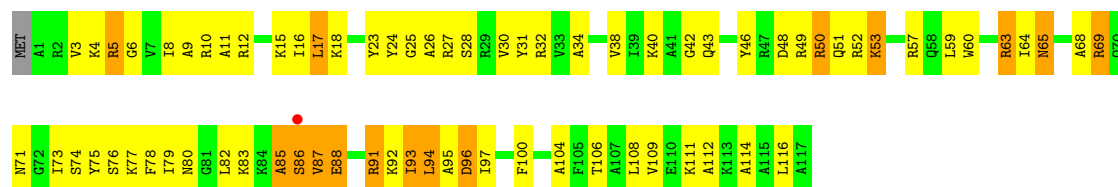
• Molecule 50: 50S ribosomal protein L19

Chain BT:



• Molecule 51: 50S ribosomal protein L20

Chain BU:



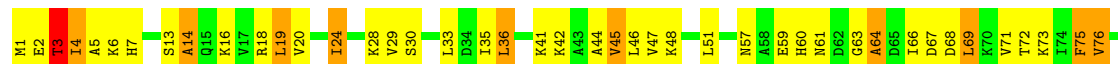
• Molecule 52: 50S ribosomal protein L21

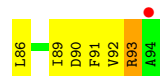
Chain BV:



• Molecule 53: 50S ribosomal protein L22

Chain BW:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	257.60Å 312.90Å 328.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 59.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 99.9 (59.36-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2, phenix	Depositor
R, $R_{free}$	0.210 , 0.250 0.244 , 0.268	Depositor DCC
$R_{free}$ test set	26311 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.7	EDS
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 524622 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	147221	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	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.*

<sup>1</sup>Intensities 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: GNP, DPP, MG, KBE, UAL, 5OH

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	0.44	0/36809	0.81	26/57423 (0.0%)
2	AB	0.29	0/1735	0.48	0/2338
3	AC	0.29	0/1651	0.51	0/2225
4	AD	0.29	0/1665	0.50	0/2227
5	AE	0.34	0/1118	0.58	0/1504
6	AF	0.27	0/835	0.49	0/1128
7	AG	0.23	0/1195	0.41	0/1602
8	AH	0.30	0/989	0.50	0/1326
9	AI	0.26	0/1034	0.49	0/1375
10	AJ	0.30	0/796	0.54	0/1077
11	AK	0.29	0/893	0.51	0/1205
12	AL	0.38	0/969	0.65	0/1300
13	AM	0.21	0/892	0.42	0/1193
14	AN	0.28	0/785	0.47	0/1043
15	AO	0.28	0/722	0.49	0/964
16	AP	0.30	0/659	0.48	0/884
17	AQ	0.30	0/657	0.52	0/881
18	AR	0.30	0/462	0.49	0/621
19	AS	0.23	0/652	0.42	0/877
20	AT	0.31	0/671	0.53	0/888
21	AU	0.31	0/430	0.46	0/570
22	AV	0.53	0/144	0.91	0/222
23	AW	0.47	2/4221 (0.0%)	0.73	5/5702 (0.1%)
24	AY	0.97	0/11	0.62	0/13
25	B0	0.43	0/603	0.64	0/797
26	B1	0.37	0/635	0.66	0/848
27	B2	0.31	0/510	0.55	0/677
28	B3	0.34	0/453	0.59	0/605
29	B4	0.42	0/450	0.64	0/599
30	B5	0.27	0/416	0.46	0/554
31	B6	0.42	0/380	0.64	0/498
32	B7	0.37	0/513	0.57	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	B8	0.42	0/303	0.65	0/397
34	BA	0.61	9/68601 (0.0%)	0.98	142/107017 (0.1%)
35	BB	0.40	0/2828	0.78	1/4410 (0.0%)
36	BC	0.42	0/2121	0.70	0/2852
37	BD	0.46	0/1586	0.70	0/2134
38	BE	0.36	0/1571	0.56	0/2113
39	BF	0.27	0/1434	0.45	0/1926
40	BG	0.34	0/1343	0.60	0/1816
41	BH	0.28	0/1244	0.53	1/1675 (0.1%)
42	BI	0.22	0/1046	0.42	0/1410
43	BJ	0.28	0/227	0.52	0/304
43	BK	0.25	0/227	0.44	0/304
43	BL	0.27	0/227	0.49	0/304
43	BM	0.25	0/227	0.42	0/304
44	BN	0.41	0/1152	0.66	0/1551
45	BO	0.47	0/947	0.70	0/1268
46	BP	0.35	0/1054	0.64	0/1403
47	BQ	0.38	0/1093	0.61	0/1460
48	BR	0.42	0/973	0.64	0/1301
49	BS	0.32	0/902	0.51	0/1209
50	BT	0.43	0/929	0.67	0/1242
51	BU	0.42	0/960	0.58	0/1278
52	BV	0.36	0/829	0.62	0/1107
53	BW	0.45	0/863	0.63	0/1156
54	BX	0.40	0/744	0.65	0/994
55	BY	0.38	0/787	0.60	0/1051
56	BZ	0.32	0/766	0.50	0/1025
All	All	0.50	11/158939 (0.0%)	0.84	175/236853 (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
12	AL	0	1
23	AW	0	2
24	AY	0	2
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BA	2106	U	O3'-P	20.78	1.86	1.61
34	BA	2183	A	O3'-P	15.69	1.79	1.61
34	BA	974	G	O3'-P	-15.38	1.42	1.61
34	BA	973	A	O3'-P	-13.70	1.44	1.61
34	BA	974	G	N7-C5	-6.57	1.35	1.39

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	2183	A	O3'-P-O5'	-12.34	80.55	104.00
34	BA	2183	A	OP2-P-O3'	12.19	132.01	105.20
34	BA	752	A	C5-N7-C8	-8.85	99.48	103.90
34	BA	2106	U	OP2-P-O3'	8.38	123.64	105.20
34	BA	2183	A	P-O3'-C3'	-8.25	109.80	119.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	AL	22	ALA	Peptide
23	AW	410	LYS	Peptide
23	AW	411	GLN	Peptide
24	AY	1	KBE	Mainchain
24	AY	2	DPP	Mainchain

## 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	32873	0	16542	1452	0
2	AB	1704	0	1732	189	0
3	AC	1624	0	1699	162	7
4	AD	1643	0	1710	196	0
5	AE	1105	0	1148	135	0
6	AF	817	0	808	102	0
7	AG	1181	0	1240	70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AH	979	0	1034	91	0
9	AI	1022	0	1070	126	0
10	AJ	786	0	828	97	0
11	AK	877	0	887	104	0
12	AL	955	0	1019	123	0
13	AM	883	0	944	96	0
14	AN	774	0	827	90	0
15	AO	714	0	737	45	0
16	AP	649	0	666	63	0
17	AQ	648	0	691	62	0
18	AR	455	0	478	41	0
19	AS	637	0	665	70	0
20	AT	665	0	714	60	0
21	AU	425	0	449	67	0
22	AV	129	0	65	9	0
23	AW	4144	0	4127	284	0
24	AY	48	0	40	31	0
25	B0	596	0	610	166	0
26	B1	625	0	655	54	0
27	B2	509	0	543	40	0
28	B3	449	0	491	53	0
29	B4	444	0	461	33	0
30	B5	409	0	440	39	0
31	B6	377	0	418	20	0
32	B7	504	0	574	49	0
33	B8	302	0	340	40	0
34	BA	61252	0	30808	2055	7
35	BB	2529	0	1281	94	0
36	BC	2082	0	2157	226	0
37	BD	1565	0	1616	201	0
38	BE	1552	0	1619	151	0
39	BF	1410	0	1447	142	0
40	BG	1323	0	1374	134	0
41	BH	1230	0	1282	253	0
42	BI	1032	0	1088	85	0
43	BJ	227	0	237	48	0
43	BK	227	0	237	23	0
43	BL	227	0	237	38	0
43	BM	227	0	237	47	0
44	BN	1129	0	1162	147	0
45	BO	938	0	1012	117	0
46	BP	1045	0	1117	108	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BQ	1074	0	1157	79	0
48	BR	960	0	1000	87	0
49	BS	892	0	923	77	0
50	BT	917	0	965	123	0
51	BU	947	0	1022	108	0
52	BV	816	0	839	96	0
53	BW	856	0	922	55	0
54	BX	738	0	807	110	0
55	BY	779	0	834	74	0
56	BZ	753	0	780	54	0
57	AA	102	0	0	0	0
57	AF	1	0	0	0	0
57	AH	1	0	0	0	0
57	AL	2	0	0	0	0
57	AM	1	0	0	0	0
57	AW	1	0	0	0	0
57	B0	3	0	0	0	0
57	B2	1	0	0	0	0
57	B4	1	0	0	0	0
57	BA	357	0	0	0	0
57	BB	9	0	0	0	0
57	BC	1	0	0	0	0
57	BD	5	0	0	0	0
57	BE	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BQ	1	0	0	0	0
57	BR	2	0	0	0	0
57	BT	1	0	0	0	0
57	BX	1	0	0	0	0
58	AW	32	0	13	6	0
59	AW	2	0	0	2	0
59	B8	1	0	0	0	0
59	BA	8	0	0	0	0
59	BC	2	0	0	0	0
59	BD	1	0	0	0	0
59	BF	1	0	0	0	0
59	BG	1	0	0	0	0
59	BW	1	0	0	1	0
All	All	147221	0	100825	8116	7

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 33.

The worst 5 of 8116 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:1495:U:O4	24:AY:1:KBE:CE	1.84	1.26
1:AA:1494:G:N7	24:AY:1:KBE:HGA	1.52	1.24
1:AA:1494:G:O6	24:AY:1:KBE:HG	1.35	1.22
1:AA:1495:U:C4	24:AY:1:KBE:HE	1.75	1.20
51:BU:63:ARG:NH1	51:BU:96:ASP:HA	1.58	1.18

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:131:ARG:NH2	34:BA:2157:G:P[4_445]	1.17	1.03
3:AC:131:ARG:CZ	34:BA:2157:G:OP1[4_445]	1.23	0.97
3:AC:131:ARG:NH2	34:BA:2157:G:OP1[4_445]	1.40	0.80
3:AC:131:ARG:NH2	34:BA:2157:G:O5'[4_445]	1.48	0.72
3:AC:131:ARG:NE	34:BA:2157:G:OP1[4_445]	1.68	0.52

## 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%)	130 (60%)	52 (24%)	34 (16%)	0	1
3	AC	204/233 (88%)	156 (76%)	32 (16%)	16 (8%)	1	11
4	AD	203/206 (98%)	134 (66%)	45 (22%)	24 (12%)	1	4
5	AE	148/167 (89%)	97 (66%)	31 (21%)	20 (14%)	0	2
6	AF	98/131 (75%)	66 (67%)	19 (19%)	13 (13%)	0	2
7	AG	149/156 (96%)	112 (75%)	28 (19%)	9 (6%)	2	20
8	AH	127/130 (98%)	96 (76%)	27 (21%)	4 (3%)	7	41
9	AI	125/130 (96%)	83 (66%)	25 (20%)	17 (14%)	0	2
10	AJ	96/103 (93%)	68 (71%)	18 (19%)	10 (10%)	1	5
11	AK	115/129 (89%)	82 (71%)	25 (22%)	8 (7%)	2	13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AL	121/124 (98%)	89 (74%)	22 (18%)	10 (8%)	1	9
13	AM	112/118 (95%)	78 (70%)	27 (24%)	7 (6%)	2	18
14	AN	92/101 (91%)	55 (60%)	24 (26%)	13 (14%)	0	2
15	AO	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	6	37
16	AP	80/82 (98%)	57 (71%)	16 (20%)	7 (9%)	1	8
17	AQ	78/84 (93%)	57 (73%)	10 (13%)	11 (14%)	0	2
18	AR	53/75 (71%)	38 (72%)	12 (23%)	3 (6%)	3	22
19	AS	77/92 (84%)	60 (78%)	14 (18%)	3 (4%)	5	33
20	AT	83/87 (95%)	59 (71%)	20 (24%)	4 (5%)	4	27
21	AU	49/71 (69%)	24 (49%)	19 (39%)	6 (12%)	1	3
23	AW	523/529 (99%)	381 (73%)	82 (16%)	60 (12%)	1	4
24	AY	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
25	B0	77/85 (91%)	35 (46%)	18 (23%)	24 (31%)	0	0
26	B1	75/78 (96%)	56 (75%)	16 (21%)	3 (4%)	5	32
27	B2	61/63 (97%)	41 (67%)	15 (25%)	5 (8%)	1	10
28	B3	56/59 (95%)	46 (82%)	5 (9%)	5 (9%)	1	8
29	B4	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	2	12
30	B5	48/55 (87%)	41 (85%)	3 (6%)	4 (8%)	1	9
31	B6	44/46 (96%)	35 (80%)	7 (16%)	2 (4%)	4	29
32	B7	62/65 (95%)	53 (86%)	6 (10%)	3 (5%)	4	27
33	B8	36/38 (95%)	27 (75%)	5 (14%)	4 (11%)	1	4
36	BC	269/273 (98%)	212 (79%)	31 (12%)	26 (10%)	1	7
37	BD	207/209 (99%)	157 (76%)	23 (11%)	27 (13%)	0	3
38	BE	199/201 (99%)	143 (72%)	33 (17%)	23 (12%)	1	4
39	BF	175/179 (98%)	117 (67%)	41 (23%)	17 (10%)	1	7
40	BG	174/177 (98%)	104 (60%)	44 (25%)	26 (15%)	0	1
41	BH	161/165 (98%)	98 (61%)	38 (24%)	25 (16%)	0	1
42	BI	139/142 (98%)	83 (60%)	38 (27%)	18 (13%)	0	3
43	BJ	28/121 (23%)	17 (61%)	6 (21%)	5 (18%)	0	1
43	BK	28/121 (23%)	21 (75%)	5 (18%)	2 (7%)	2	13
43	BL	28/121 (23%)	22 (79%)	4 (14%)	2 (7%)	2	13

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BM	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	2	13
44	BN	140/142 (99%)	101 (72%)	24 (17%)	15 (11%)	1	5
45	BO	120/123 (98%)	88 (73%)	19 (16%)	13 (11%)	1	5
46	BP	141/144 (98%)	88 (62%)	34 (24%)	19 (14%)	0	2
47	BQ	134/136 (98%)	104 (78%)	18 (13%)	12 (9%)	1	8
48	BR	118/127 (93%)	86 (73%)	20 (17%)	12 (10%)	1	6
49	BS	114/117 (97%)	90 (79%)	14 (12%)	10 (9%)	1	8
50	BT	112/115 (97%)	74 (66%)	21 (19%)	17 (15%)	0	1
51	BU	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	2	19
52	BV	101/103 (98%)	75 (74%)	18 (18%)	8 (8%)	1	11
53	BW	108/116 (93%)	89 (82%)	15 (14%)	4 (4%)	5	34
54	BX	91/100 (91%)	49 (54%)	23 (25%)	19 (21%)	0	0
55	BY	100/104 (96%)	65 (65%)	22 (22%)	13 (13%)	0	3
56	BZ	92/94 (98%)	72 (78%)	14 (15%)	6 (6%)	2	17
All	All	6272/6999 (90%)	4427 (71%)	1181 (19%)	664 (11%)	1	5

5 of 664 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	21	TYR
2	AB	22	TRP
2	AB	33	ALA
2	AB	40	ILE
2	AB	75	ALA

### 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%)	145 (81%)	35 (19%)	2	10
3	AC	170/190 (90%)	146 (86%)	24 (14%)	5	23
4	AD	172/173 (99%)	152 (88%)	20 (12%)	8	34

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	113/126 (90%)	95 (84%)	18 (16%)	4	16
6	AF	87/112 (78%)	73 (84%)	14 (16%)	3	16
7	AG	124/129 (96%)	121 (98%)	3 (2%)	61	91
8	AH	104/105 (99%)	94 (90%)	10 (10%)	12	44
9	AI	105/107 (98%)	92 (88%)	13 (12%)	7	30
10	AJ	86/90 (96%)	70 (81%)	16 (19%)	2	11
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	13
12	AL	103/104 (99%)	89 (86%)	14 (14%)	5	25
13	AM	92/96 (96%)	87 (95%)	5 (5%)	31	75
14	AN	79/84 (94%)	71 (90%)	8 (10%)	11	41
15	AO	76/77 (99%)	66 (87%)	10 (13%)	6	27
16	AP	65/65 (100%)	57 (88%)	8 (12%)	7	31
17	AQ	74/78 (95%)	61 (82%)	13 (18%)	3	13
18	AR	48/65 (74%)	44 (92%)	4 (8%)	16	55
19	AS	70/79 (89%)	64 (91%)	6 (9%)	15	52
20	AT	65/66 (98%)	60 (92%)	5 (8%)	18	59
21	AU	44/61 (72%)	37 (84%)	7 (16%)	4	16
23	AW	447/453 (99%)	381 (85%)	66 (15%)	4	20
24	AY	2/2 (100%)	2 (100%)	0	100	100
25	B0	59/63 (94%)	42 (71%)	17 (29%)	0	1
26	B1	67/68 (98%)	56 (84%)	11 (16%)	3	15
27	B2	55/55 (100%)	46 (84%)	9 (16%)	3	15
28	B3	48/49 (98%)	39 (81%)	9 (19%)	2	11
29	B4	47/48 (98%)	40 (85%)	7 (15%)	4	20
30	B5	45/49 (92%)	42 (93%)	3 (7%)	23	66
31	B6	38/38 (100%)	34 (90%)	4 (10%)	10	39
32	B7	51/52 (98%)	48 (94%)	3 (6%)	28	72
33	B8	34/34 (100%)	32 (94%)	2 (6%)	28	72
36	BC	216/218 (99%)	177 (82%)	39 (18%)	2	12
37	BD	164/164 (100%)	143 (87%)	21 (13%)	6	28
38	BE	165/165 (100%)	138 (84%)	27 (16%)	3	15

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BF	148/150 (99%)	136 (92%)	12 (8%)	17	56
40	BG	137/138 (99%)	116 (85%)	21 (15%)	4	18
41	BH	123/123 (100%)	109 (89%)	14 (11%)	8	35
42	BI	109/110 (99%)	101 (93%)	8 (7%)	20	62
43	BJ	26/85 (31%)	23 (88%)	3 (12%)	8	35
43	BK	26/85 (31%)	26 (100%)	0	100	100
43	BL	26/85 (31%)	25 (96%)	1 (4%)	44	84
43	BM	26/85 (31%)	24 (92%)	2 (8%)	18	59
44	BN	116/116 (100%)	94 (81%)	22 (19%)	2	11
45	BO	103/104 (99%)	80 (78%)	23 (22%)	1	6
46	BP	102/103 (99%)	85 (83%)	17 (17%)	3	14
47	BQ	109/109 (100%)	91 (84%)	18 (16%)	3	14
48	BR	100/103 (97%)	88 (88%)	12 (12%)	7	32
49	BS	86/87 (99%)	76 (88%)	10 (12%)	8	34
50	BT	99/100 (99%)	81 (82%)	18 (18%)	2	12
51	BU	89/90 (99%)	77 (86%)	12 (14%)	6	26
52	BV	84/84 (100%)	74 (88%)	10 (12%)	8	33
53	BW	93/99 (94%)	73 (78%)	20 (22%)	1	7
54	BX	80/84 (95%)	66 (82%)	14 (18%)	3	13
55	BY	83/85 (98%)	74 (89%)	9 (11%)	9	37
56	BZ	78/78 (100%)	74 (95%)	4 (5%)	33	77
All	All	5228/5666 (92%)	4511 (86%)	717 (14%)	5	25

5 of 717 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	B0	42	THR
36	BC	173	LEU
52	BV	37	GLU
26	B1	10	ARG
29	B4	27	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
27	B2	20	ASN
36	BC	43	ASN
54	BX	48	GLN
27	B2	41	HIS
31	B6	13	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1531/1533 (99%)	298 (19%)	45 (2%)
22	AV	5/27 (18%)	3 (60%)	0
34	BA	2849/2903 (98%)	570 (20%)	95 (3%)
35	BB	117/118 (99%)	22 (18%)	3 (2%)
All	All	4502/4581 (98%)	893 (19%)	143 (3%)

5 of 893 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	9	G
1	AA	19	A
1	AA	22	G
1	AA	31	G

5 of 143 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	442	G
34	BA	859	G
34	BA	2726	A
34	BA	479	A
34	BA	627	A

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
24	KBE	AY	1	24	8,8,9	8.19	1 (12%)	6,8,10	0.79	0
24	DPP	AY	2	24	5,5,6	10.89	2 (40%)	3,5,7	2.68	1 (33%)
24	UAL	AY	5	24	7,8,9	2.18	3 (42%)	6,9,11	0.80	0
24	5OH	AY	6	24	12,12,13	5.37	4 (33%)	13,16,18	0.80	0

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
24	KBE	AY	1	24	-	0/6/7/8	0/0/0/0
24	DPP	AY	2	24	-	0/2/4/6	0/0/0/0
24	UAL	AY	5	24	-	0/3/7/9	0/0/0/0
24	5OH	AY	6	24	-	0/2/18/20	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	2	DPP	O-C	24.19	1.28	1.11
24	AY	1	KBE	O-C	23.13	1.27	1.11
24	AY	6	5OH	O-C	17.41	1.23	1.11
24	AY	6	5OH	CQ-NP	4.47	1.40	1.35
24	AY	5	UAL	CB-CA	4.01	1.41	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	2	DPP	C-CA-N	4.34	118.16	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 494 ligands modelled in this entry, 493 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	$\# Z  > 2$
58	GNP	AW	602	-	34,34,34	1.85	6 (17%)	48,54,54	5.85	14 (29%)

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
58	GNP	AW	602	-	-	0/18/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AW	602	GNP	PG-O1G	6.65	1.53	1.46
58	AW	602	GNP	PB-N3B	-4.48	1.60	1.64
58	AW	602	GNP	PA-O3A	-2.81	1.54	1.59
58	AW	602	GNP	PB-O3A	-2.48	1.56	1.59
58	AW	602	GNP	PA-O2A	-2.19	1.45	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AW	602	GNP	C6-C5-N7	-37.38	129.11	134.14
58	AW	602	GNP	C6-N1-C2	8.75	125.14	120.20
58	AW	602	GNP	PA-O3A-PB	-4.66	116.08	132.05
58	AW	602	GNP	C2-N3-C4	-4.55	109.85	115.30
58	AW	602	GNP	C5-C4-N3	4.09	130.78	126.07

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1532/1533 (99%)	0.33	95 (6%) 20 4	51, 102, 197, 245	0
2	AB	218/241 (90%)	0.87	34 (15%) 3 1	91, 120, 142, 158	0
3	AC	206/233 (88%)	0.34	9 (4%) 33 7	75, 114, 132, 139	0
4	AD	205/206 (99%)	0.85	26 (12%) 4 1	86, 110, 132, 147	0
5	AE	150/167 (89%)	0.05	1 (0%) 84 38	73, 94, 129, 143	0
6	AF	100/131 (76%)	0.56	8 (8%) 12 3	98, 122, 135, 145	0
7	AG	151/156 (96%)	1.27	26 (17%) 2 1	107, 144, 159, 163	0
8	AH	129/130 (99%)	0.36	5 (3%) 37 7	77, 97, 121, 139	0
9	AI	127/130 (97%)	1.07	20 (15%) 3 1	77, 122, 148, 159	0
10	AJ	98/103 (95%)	0.81	9 (9%) 9 2	89, 106, 143, 156	0
11	AK	117/129 (90%)	0.36	4 (3%) 43 9	73, 105, 133, 150	0
12	AL	123/124 (99%)	0.38	3 (2%) 56 13	55, 74, 111, 143	0
13	AM	114/118 (96%)	2.03	47 (41%) 1 0	137, 149, 163, 165	0
14	AN	96/101 (95%)	1.79	36 (37%) 1 0	79, 128, 152, 160	0
15	AO	88/89 (98%)	0.33	2 (2%) 57 13	79, 101, 131, 142	0
16	AP	82/82 (100%)	0.91	8 (9%) 8 2	72, 95, 131, 147	0
17	AQ	80/84 (95%)	1.05	11 (13%) 4 1	78, 111, 136, 147	0
18	AR	55/75 (73%)	0.66	5 (9%) 9 2	77, 101, 126, 165	0
19	AS	79/92 (85%)	2.20	36 (45%) 1 0	131, 153, 159, 164	0
20	AT	85/87 (97%)	0.68	2 (2%) 56 13	80, 105, 126, 142	0
21	AU	51/71 (71%)	1.45	14 (27%) 1 1	106, 132, 153, 157	0
22	AV	6/27 (22%)	5.66	6 (100%) 0 0	181, 198, 202, 206	0
23	AW	525/529 (99%)	0.30	17 (3%) 45 9	47, 99, 188, 267	0
24	AY	2/6 (33%)	-0.08	0 100 100	85, 85, 85, 88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	B0	79/85 (92%)	0.64	5 (6%) 19 4	62, 87, 115, 129	0
26	B1	77/78 (98%)	0.33	2 (2%) 53 11	55, 71, 124, 126	0
27	B2	63/63 (100%)	0.03	2 (3%) 45 9	69, 101, 126, 140	0
28	B3	58/59 (98%)	0.67	6 (10%) 7 2	63, 75, 121, 129	0
29	B4	56/57 (98%)	0.07	2 (3%) 41 8	42, 63, 97, 125	0
30	B5	50/55 (90%)	2.21	25 (50%) 0 0	114, 128, 137, 151	0
31	B6	46/46 (100%)	0.32	1 (2%) 59 14	43, 56, 77, 114	0
32	B7	64/65 (98%)	0.24	0 100 100	57, 68, 83, 90	0
33	B8	38/38 (100%)	0.37	0 100 100	61, 78, 90, 105	0
34	BA	2853/2903 (98%)	0.14	121 (4%) 35 7	35, 67, 195, 445	0
35	BB	118/118 (100%)	-0.12	0 100 100	61, 106, 152, 188	0
36	BC	271/273 (99%)	0.17	2 (0%) 84 38	36, 66, 83, 108	0
37	BD	209/209 (100%)	-0.06	1 (0%) 88 46	37, 57, 89, 99	0
38	BE	201/201 (100%)	0.09	2 (0%) 79 29	37, 76, 109, 131	0
39	BF	177/179 (98%)	0.91	24 (13%) 4 1	106, 128, 152, 165	0
40	BG	176/177 (99%)	0.22	4 (2%) 57 13	54, 80, 117, 131	0
41	BH	163/165 (98%)	2.97	92 (56%) 0 0	80, 145, 163, 185	1 (0%)
42	BI	141/142 (99%)	2.13	68 (48%) 1 0	135, 157, 169, 176	0
43	BJ	30/121 (24%)	0.65	2 (6%) 17 4	126, 137, 143, 145	0
43	BK	30/121 (24%)	1.03	7 (23%) 1 1	133, 146, 152, 156	0
43	BL	30/121 (24%)	2.64	19 (63%) 0 0	132, 148, 158, 163	0
43	BM	30/121 (24%)	1.43	7 (23%) 1 1	128, 142, 149, 151	0
44	BN	142/142 (100%)	0.26	2 (1%) 72 22	45, 65, 91, 117	0
45	BO	122/123 (99%)	0.11	1 (0%) 83 35	41, 61, 84, 104	0
46	BP	143/144 (99%)	0.32	4 (2%) 50 11	41, 84, 112, 132	0
47	BQ	136/136 (100%)	0.30	4 (2%) 49 10	47, 70, 100, 126	0
48	BR	120/127 (94%)	0.23	1 (0%) 83 35	40, 56, 72, 138	0
49	BS	116/117 (99%)	0.94	12 (10%) 7 2	81, 100, 121, 128	0
50	BT	114/115 (99%)	0.15	1 (0%) 81 32	48, 71, 112, 121	0
51	BU	117/118 (99%)	0.00	1 (0%) 81 32	37, 59, 94, 108	0
52	BV	103/103 (100%)	0.20	3 (2%) 49 10	43, 86, 111, 119	0

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
53	BW	110/116 (94%)	-0.05	1 (0%) 81 32	41, 54, 82, 127	0
54	BX	93/100 (93%)	0.70	7 (7%) 14 3	50, 81, 134, 144	0
55	BY	102/104 (98%)	0.87	10 (9%) 8 2	63, 84, 126, 141	0
56	BZ	94/94 (100%)	0.33	2 (2%) 60 15	68, 94, 113, 126	0
All	All	10891/11580 (94%)	0.46	865 (7%) 13 3	35, 89, 165, 445	1 (0%)

The worst 5 of 865 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	BA	2903	U	23.1
34	BA	2133	G	15.3
34	BA	2151	U	14.7
34	BA	2152	G	14.6
34	BA	2107	G	14.6

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
24	KBE	AY	1	9/10	0.57	15.44	78,79,82,82	0
24	5OH	AY	6	12/13	0.30	2.60	84,89,92,94	0
24	DPP	AY	2	6/7	0.30	2.49	79,82,82,84	0
24	UAL	AY	5	9/10	0.30	2.25	81,82,83,84	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
57	MG	BA	3137	1/1	0.53	723.00	42,42,42,42	0
57	MG	BA	3271	1/1	0.37	88.41	53,53,53,53	0
57	MG	BA	3077	1/1	0.58	73.93	41,41,41,41	0
57	MG	BA	3291	1/1	0.40	63.86	58,58,58,58	0
57	MG	BA	3223	1/1	1.09	55.59	75,75,75,75	0
57	MG	AA	1687	1/1	0.82	54.32	81,81,81,81	0
57	MG	BA	3356	1/1	0.22	47.00	61,61,61,61	0
57	MG	BA	3284	1/1	0.32	46.87	73,73,73,73	0
57	MG	BA	3260	1/1	0.30	46.48	50,50,50,50	0
57	MG	BA	3232	1/1	0.34	46.11	54,54,54,54	0
57	MG	BA	3063	1/1	0.43	42.36	32,32,32,32	0
57	MG	BA	3134	1/1	0.58	42.06	49,49,49,49	0
57	MG	BA	3079	1/1	0.63	42.00	44,44,44,44	0
57	MG	BA	3353	1/1	0.50	41.04	73,73,73,73	0
57	MG	AA	1700	1/1	0.30	39.00	65,65,65,65	0
57	MG	BA	3155	1/1	0.65	38.34	51,51,51,51	0
57	MG	BA	3333	1/1	0.81	37.54	77,77,77,77	0
57	MG	AA	1603	1/1	0.45	35.96	42,42,42,42	0
57	MG	BA	3313	1/1	0.34	35.06	67,67,67,67	0
57	MG	BA	3314	1/1	0.40	34.99	56,56,56,56	0
57	MG	BA	3027	1/1	0.44	34.46	40,40,40,40	0
57	MG	BB	201	1/1	0.34	32.78	54,54,54,54	0
57	MG	BA	3046	1/1	0.40	32.04	27,27,27,27	0
57	MG	AA	1609	1/1	0.49	32.03	40,40,40,40	0
57	MG	BA	3015	1/1	0.56	31.81	38,38,38,38	0
57	MG	BA	3244	1/1	0.46	31.73	76,76,76,76	0
57	MG	BA	3121	1/1	0.41	31.51	39,39,39,39	0
57	MG	BA	3190	1/1	0.58	31.45	43,43,43,43	0
57	MG	BA	3302	1/1	0.54	31.36	68,68,68,68	0
57	MG	BA	3163	1/1	0.25	30.23	49,49,49,49	0
57	MG	BA	3157	1/1	0.47	29.64	46,46,46,46	0
57	MG	AA	1661	1/1	0.27	28.50	49,49,49,49	0
57	MG	BA	3040	1/1	0.41	27.96	43,43,43,43	0
57	MG	AA	1676	1/1	0.37	27.07	52,52,52,52	0
57	MG	AA	1686	1/1	0.62	26.92	93,93,93,93	0
57	MG	BA	3011	1/1	0.48	26.73	23,23,23,23	0
57	MG	BA	3293	1/1	0.35	26.63	53,53,53,53	0
57	MG	BA	3136	1/1	0.62	25.77	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3325	1/1	0.35	25.47	59,59,59,59	0
57	MG	BA	3087	1/1	0.47	25.44	42,42,42,42	0
57	MG	BA	3012	1/1	0.40	24.86	18,18,18,18	0
57	MG	BA	3154	1/1	0.55	23.99	43,43,43,43	0
57	MG	BA	3210	1/1	0.39	23.72	73,73,73,73	0
57	MG	BA	3100	1/1	0.41	23.17	36,36,36,36	0
57	MG	BA	3185	1/1	0.30	22.75	52,52,52,52	0
57	MG	BA	3240	1/1	0.52	22.32	56,56,56,56	0
57	MG	BA	3250	1/1	0.61	22.26	66,66,66,66	0
57	MG	AA	1634	1/1	0.34	21.92	55,55,55,55	0
57	MG	AA	1649	1/1	0.37	21.89	49,49,49,49	0
57	MG	BA	3245	1/1	0.44	21.72	46,46,46,46	0
57	MG	BA	3182	1/1	0.60	21.65	48,48,48,48	0
57	MG	BA	3053	1/1	0.51	20.66	31,31,31,31	0
57	MG	BA	3204	1/1	0.53	20.54	72,72,72,72	0
57	MG	BA	3345	1/1	0.42	20.39	67,67,67,67	0
57	MG	BA	3099	1/1	0.46	20.30	44,44,44,44	0
57	MG	BA	3233	1/1	0.43	20.14	46,46,46,46	0
57	MG	BA	3050	1/1	0.39	19.89	33,33,33,33	0
57	MG	BA	3273	1/1	0.47	19.53	72,72,72,72	0
57	MG	BA	3043	1/1	0.44	19.50	26,26,26,26	0
57	MG	BA	3021	1/1	0.34	19.44	18,18,18,18	0
57	MG	BA	3311	1/1	0.22	19.00	48,48,48,48	0
57	MG	BA	3013	1/1	0.38	18.65	20,20,20,20	0
57	MG	BA	3261	1/1	0.21	18.34	63,63,63,63	0
57	MG	BA	3177	1/1	0.50	17.99	59,59,59,59	0
57	MG	BA	3082	1/1	0.38	17.71	36,36,36,36	0
57	MG	BA	3057	1/1	0.30	17.50	33,33,33,33	0
57	MG	BA	3073	1/1	0.48	17.36	42,42,42,42	0
57	MG	BA	3207	1/1	0.31	17.32	54,54,54,54	0
57	MG	BA	3074	1/1	0.41	17.25	44,44,44,44	0
57	MG	BA	3054	1/1	0.42	17.22	36,36,36,36	0
57	MG	BA	3340	1/1	0.46	17.19	61,61,61,61	0
57	MG	B4	101	1/1	0.42	17.05	40,40,40,40	0
57	MG	BA	3234	1/1	0.40	16.95	49,49,49,49	0
57	MG	BA	3044	1/1	0.43	16.75	37,37,37,37	0
57	MG	BA	3071	1/1	0.38	16.65	35,35,35,35	0
57	MG	BA	3124	1/1	0.56	16.33	42,42,42,42	0
57	MG	BA	3341	1/1	0.43	15.69	57,57,57,57	0
57	MG	BA	3052	1/1	0.39	15.57	39,39,39,39	0
57	MG	BA	3159	1/1	0.47	15.40	49,49,49,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3300	1/1	0.58	15.39	69,69,69,69	0
57	MG	BA	3047	1/1	0.41	15.20	51,51,51,51	0
57	MG	BA	3003	1/1	0.41	15.20	18,18,18,18	0
57	MG	BA	3039	1/1	0.36	15.12	31,31,31,31	0
57	MG	BA	3033	1/1	0.42	14.95	25,25,25,25	0
57	MG	BA	3096	1/1	0.36	14.90	44,44,44,44	0
57	MG	BA	3170	1/1	0.35	14.89	52,52,52,52	0
57	MG	BA	3192	1/1	0.43	14.79	59,59,59,59	0
57	MG	BA	3304	1/1	0.38	14.61	50,50,50,50	0
57	MG	BA	3066	1/1	0.48	14.33	41,41,41,41	0
57	MG	AA	1678	1/1	0.54	14.30	65,65,65,65	0
57	MG	BD	304	1/1	0.39	14.25	28,28,28,28	0
57	MG	AA	1677	1/1	0.47	13.57	57,57,57,57	0
57	MG	BA	3257	1/1	0.31	13.53	48,48,48,48	0
57	MG	BA	3280	1/1	0.36	13.46	73,73,73,73	0
57	MG	BA	3146	1/1	0.28	13.23	40,40,40,40	0
57	MG	AA	1666	1/1	0.36	13.17	62,62,62,62	0
57	MG	BA	3001	1/1	0.42	13.11	42,42,42,42	0
57	MG	BA	3095	1/1	0.24	12.92	42,42,42,42	0
57	MG	AA	1624	1/1	0.48	12.57	51,51,51,51	0
57	MG	BA	3296	1/1	0.27	12.54	60,60,60,60	0
57	MG	BA	3203	1/1	0.27	12.38	50,50,50,50	0
57	MG	AA	1611	1/1	0.41	12.35	44,44,44,44	0
57	MG	BA	3200	1/1	0.38	12.09	44,44,44,44	0
57	MG	BA	3029	1/1	0.36	12.08	28,28,28,28	0
57	MG	BA	3225	1/1	0.40	11.94	60,60,60,60	0
57	MG	BA	3213	1/1	0.30	11.75	46,46,46,46	0
57	MG	BA	3062	1/1	0.32	11.70	42,42,42,42	0
57	MG	BA	3023	1/1	0.42	11.69	39,39,39,39	0
57	MG	BA	3045	1/1	0.49	11.61	35,35,35,35	0
57	MG	BA	3035	1/1	0.33	11.61	26,26,26,26	0
57	MG	BA	3216	1/1	0.43	11.60	63,63,63,63	0
57	MG	BA	3065	1/1	0.35	11.31	46,46,46,46	0
57	MG	AA	1691	1/1	0.30	11.23	63,63,63,63	0
57	MG	AA	1630	1/1	0.43	11.22	48,48,48,48	0
57	MG	AA	1631	1/1	0.37	11.18	60,60,60,60	0
57	MG	BA	3219	1/1	0.71	11.15	69,69,69,69	0
57	MG	BA	3171	1/1	0.28	11.09	57,57,57,57	0
57	MG	BA	3252	1/1	0.32	11.02	49,49,49,49	0
57	MG	BA	3042	1/1	0.33	11.00	27,27,27,27	0
57	MG	BA	3193	1/1	0.48	10.98	61,61,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	BA	3006	1/1	0.35	10.89	22,22,22,22	0
57	MG	BA	3308	1/1	0.47	10.86	82,82,82,82	0
57	MG	BA	3017	1/1	0.34	10.82	30,30,30,30	0
57	MG	BA	3127	1/1	0.25	10.80	38,38,38,38	0
57	MG	BA	3024	1/1	0.40	10.74	32,32,32,32	0
57	MG	AA	1606	1/1	0.37	10.70	45,45,45,45	0
57	MG	BA	3070	1/1	0.33	10.67	44,44,44,44	0
57	MG	BA	3255	1/1	0.33	10.66	66,66,66,66	0
57	MG	BA	3025	1/1	0.30	10.65	32,32,32,32	0
57	MG	BA	3055	1/1	0.41	10.63	24,24,24,24	0
57	MG	BA	3266	1/1	0.40	10.47	56,56,56,56	0
57	MG	BA	3181	1/1	0.28	10.17	44,44,44,44	0
57	MG	AA	1684	1/1	0.45	10.15	60,60,60,60	0
57	MG	BA	3107	1/1	0.31	10.14	36,36,36,36	0
57	MG	BA	3221	1/1	0.36	10.14	43,43,43,43	0
57	MG	BA	3138	1/1	0.34	10.05	58,58,58,58	0
57	MG	BA	3130	1/1	0.42	10.01	41,41,41,41	0
57	MG	BA	3196	1/1	0.51	10.00	46,46,46,46	0
57	MG	BA	3268	1/1	0.28	9.96	52,52,52,52	0
57	MG	BA	3211	1/1	0.48	9.82	48,48,48,48	0
57	MG	BA	3202	1/1	0.36	9.70	57,57,57,57	0
57	MG	BA	3117	1/1	0.23	9.65	46,46,46,46	0
57	MG	BA	3292	1/1	0.24	9.58	54,54,54,54	0
57	MG	BA	3294	1/1	0.26	9.54	43,43,43,43	0
57	MG	AA	1601	1/1	0.29	9.53	22,22,22,22	0
57	MG	BA	3032	1/1	0.54	9.44	38,38,38,38	0
57	MG	BA	3092	1/1	0.52	9.41	43,43,43,43	0
57	MG	AA	1616	1/1	0.37	9.39	37,37,37,37	0
57	MG	BA	3149	1/1	0.30	9.29	42,42,42,42	0
57	MG	AA	1635	1/1	0.31	9.27	58,58,58,58	0
57	MG	BA	3090	1/1	0.46	9.24	40,40,40,40	0
57	MG	BA	3297	1/1	0.29	9.20	49,49,49,49	0
57	MG	BA	3139	1/1	0.38	9.17	43,43,43,43	0
57	MG	BB	202	1/1	0.24	9.10	43,43,43,43	0
57	MG	BA	3126	1/1	0.26	8.90	31,31,31,31	0
57	MG	BA	3037	1/1	0.44	8.89	36,36,36,36	0
57	MG	BA	3317	1/1	0.32	8.85	88,88,88,88	0
57	MG	BA	3016	1/1	0.36	8.83	39,39,39,39	0
57	MG	BA	3316	1/1	0.34	8.69	61,61,61,61	0
57	MG	BA	3174	1/1	0.27	8.68	49,49,49,49	0
57	MG	BA	3031	1/1	0.39	8.59	25,25,25,25	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3028	1/1	0.36	8.48	26,26,26,26	0
57	MG	BA	3151	1/1	0.32	8.48	47,47,47,47	0
57	MG	BA	3010	1/1	0.30	8.46	33,33,33,33	0
57	MG	BA	3167	1/1	0.36	8.33	48,48,48,48	0
57	MG	BA	3083	1/1	0.35	8.29	47,47,47,47	0
57	MG	BA	3277	1/1	0.30	7.93	42,42,42,42	0
57	MG	BA	3186	1/1	0.25	7.82	47,47,47,47	0
57	MG	BA	3188	1/1	0.28	7.76	51,51,51,51	0
57	MG	AA	1670	1/1	0.38	7.69	62,62,62,62	0
57	MG	AA	1607	1/1	0.36	7.69	33,33,33,33	0
57	MG	BA	3205	1/1	0.22	7.67	50,50,50,50	0
57	MG	BA	3281	1/1	0.60	7.48	73,73,73,73	0
57	MG	BA	3324	1/1	0.24	7.29	59,59,59,59	0
57	MG	AA	1604	1/1	0.45	7.24	42,42,42,42	0
57	MG	BA	3009	1/1	0.34	7.10	14,14,14,14	0
57	MG	BA	3022	1/1	0.29	7.03	28,28,28,28	0
57	MG	BA	3150	1/1	0.37	7.03	53,53,53,53	0
57	MG	BA	3306	1/1	0.32	6.93	67,67,67,67	0
57	MG	BA	3125	1/1	0.52	6.93	53,53,53,53	0
57	MG	BA	3331	1/1	0.35	6.79	64,64,64,64	0
57	MG	BA	3103	1/1	0.31	6.70	28,28,28,28	0
57	MG	BA	3102	1/1	0.32	6.57	36,36,36,36	0
57	MG	BA	3084	1/1	0.31	6.54	21,21,21,21	0
57	MG	BA	3183	1/1	0.28	6.51	48,48,48,48	0
57	MG	BA	3030	1/1	0.27	6.51	38,38,38,38	0
57	MG	BA	3026	1/1	0.31	6.39	24,24,24,24	0
57	MG	BA	3352	1/1	0.26	6.36	61,61,61,61	0
57	MG	BA	3113	1/1	0.28	6.20	34,34,34,34	0
57	MG	AA	1699	1/1	0.33	6.18	49,49,49,49	0
57	MG	AA	1623	1/1	0.27	6.18	42,42,42,42	0
57	MG	BA	3295	1/1	0.20	6.12	57,57,57,57	0
57	MG	AA	1628	1/1	0.26	6.12	44,44,44,44	0
57	MG	AA	1621	1/1	0.39	6.05	57,57,57,57	0
57	MG	BA	3246	1/1	0.26	6.03	48,48,48,48	0
57	MG	BA	3081	1/1	0.39	6.02	35,35,35,35	0
57	MG	BA	3318	1/1	0.32	5.96	57,57,57,57	0
57	MG	BA	3283	1/1	0.32	5.92	25,25,25,25	0
57	MG	BA	3194	1/1	0.22	5.89	49,49,49,49	0
57	MG	AA	1657	1/1	0.38	5.83	83,83,83,83	0
57	MG	BA	3178	1/1	0.23	5.73	49,49,49,49	0
57	MG	BD	302	1/1	0.48	5.69	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3251	1/1	0.25	5.67	49,49,49,49	0
57	MG	AA	1679	1/1	0.29	5.62	62,62,62,62	0
57	MG	BA	3072	1/1	0.25	5.61	36,36,36,36	0
57	MG	BA	3049	1/1	0.23	5.60	31,31,31,31	0
57	MG	BA	3034	1/1	0.30	5.55	36,36,36,36	0
57	MG	BA	3269	1/1	0.28	5.45	51,51,51,51	0
57	MG	BA	3132	1/1	0.24	5.41	52,52,52,52	0
57	MG	AA	1610	1/1	0.31	5.40	45,45,45,45	0
57	MG	AA	1615	1/1	0.29	5.38	40,40,40,40	0
57	MG	BA	3014	1/1	0.23	5.37	27,27,27,27	0
57	MG	BA	3214	1/1	0.21	5.26	43,43,43,43	0
57	MG	BA	3114	1/1	0.31	5.19	32,32,32,32	0
57	MG	BA	3263	1/1	0.23	5.12	53,53,53,53	0
57	MG	AA	1650	1/1	0.28	5.07	67,67,67,67	0
57	MG	BA	3116	1/1	0.24	5.02	41,41,41,41	0
57	MG	AA	1622	1/1	0.30	4.98	42,42,42,42	0
57	MG	AA	1632	1/1	0.49	4.92	40,40,40,40	0
57	MG	BA	3060	1/1	0.38	4.91	27,27,27,27	0
57	MG	BA	3110	1/1	0.32	4.87	38,38,38,38	0
57	MG	BA	3041	1/1	0.28	4.87	27,27,27,27	0
57	MG	B0	103	1/1	0.49	4.75	54,54,54,54	0
57	MG	BA	3330	1/1	0.21	4.73	83,83,83,83	0
57	MG	BA	3091	1/1	0.38	4.73	42,42,42,42	0
57	MG	BA	3298	1/1	0.27	4.71	76,76,76,76	0
57	MG	BA	3272	1/1	0.26	4.67	55,55,55,55	0
57	MG	BA	3104	1/1	0.25	4.52	45,45,45,45	0
57	MG	AA	1665	1/1	0.53	4.50	56,56,56,56	0
57	MG	AA	1645	1/1	0.46	4.49	62,62,62,62	0
57	MG	BA	3265	1/1	0.31	4.49	45,45,45,45	0
57	MG	BA	3282	1/1	0.28	4.40	55,55,55,55	0
57	MG	BA	3206	1/1	0.26	4.19	52,52,52,52	0
57	MG	AA	1618	1/1	0.27	4.18	49,49,49,49	0
57	MG	BA	3323	1/1	0.28	4.18	64,64,64,64	0
57	MG	BA	3270	1/1	0.28	4.16	59,59,59,59	0
57	MG	BA	3305	1/1	0.17	4.12	71,71,71,71	0
57	MG	BA	3254	1/1	0.22	4.08	59,59,59,59	0
57	MG	BA	3337	1/1	0.23	3.87	55,55,55,55	0
57	MG	AA	1652	1/1	0.29	3.87	60,60,60,60	0
57	MG	BA	3133	1/1	0.25	3.86	45,45,45,45	0
57	MG	BA	3123	1/1	0.32	3.82	36,36,36,36	0
57	MG	BA	3105	1/1	0.42	3.79	49,49,49,49	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3112	1/1	0.24	3.75	41,41,41,41	0
57	MG	BA	3153	1/1	0.26	3.73	59,59,59,59	0
57	MG	BA	3007	1/1	0.35	3.61	17,17,17,17	0
57	MG	BA	3008	1/1	0.28	3.61	22,22,22,22	0
57	MG	BA	3069	1/1	0.25	3.60	39,39,39,39	0
57	MG	BA	3061	1/1	0.26	3.53	48,48,48,48	0
57	MG	BA	3241	1/1	0.24	3.51	57,57,57,57	0
57	MG	BA	3078	1/1	0.40	3.46	32,32,32,32	0
57	MG	BA	3086	1/1	0.41	3.44	43,43,43,43	0
57	MG	AA	1602	1/1	0.29	3.40	37,37,37,37	0
57	MG	BA	3005	1/1	0.24	3.33	20,20,20,20	0
57	MG	BA	3276	1/1	0.32	3.31	58,58,58,58	0
57	MG	BA	3119	1/1	0.24	3.30	29,29,29,29	0
57	MG	BA	3350	1/1	0.23	3.29	80,80,80,80	0
57	MG	BA	3020	1/1	0.40	3.26	29,29,29,29	0
57	MG	BA	3036	1/1	0.28	3.26	43,43,43,43	0
57	MG	AA	1654	1/1	0.32	3.25	58,58,58,58	0
57	MG	AA	1689	1/1	0.28	3.24	69,69,69,69	0
57	MG	BA	3262	1/1	0.24	3.22	85,85,85,85	0
57	MG	AA	1673	1/1	0.44	3.10	84,84,84,84	0
57	MG	BA	3018	1/1	0.25	3.08	16,16,16,16	0
57	MG	BA	3068	1/1	0.30	3.07	28,28,28,28	0
57	MG	BA	3085	1/1	0.25	3.06	40,40,40,40	0
57	MG	AA	1655	1/1	0.26	3.04	60,60,60,60	0
57	MG	BA	3058	1/1	0.32	3.00	35,35,35,35	0
57	MG	AA	1702	1/1	0.24	2.96	58,58,58,58	0
57	MG	BA	3148	1/1	0.23	2.90	50,50,50,50	0
57	MG	AA	1643	1/1	0.31	2.86	56,56,56,56	0
57	MG	BA	3158	1/1	0.26	2.85	35,35,35,35	0
57	MG	AA	1605	1/1	0.24	2.85	38,38,38,38	0
57	MG	BA	3067	1/1	0.30	2.80	35,35,35,35	0
57	MG	AA	1693	1/1	0.27	2.67	56,56,56,56	0
57	MG	BA	3128	1/1	0.27	2.61	33,33,33,33	0
57	MG	BA	3197	1/1	0.22	2.57	38,38,38,38	0
57	MG	BA	3349	1/1	0.31	2.55	79,79,79,79	0
57	MG	BA	3357	1/1	0.19	2.48	81,81,81,81	0
57	MG	BA	3145	1/1	0.24	2.45	55,55,55,55	0
57	MG	BA	3088	1/1	0.27	2.43	36,36,36,36	0
57	MG	BA	3278	1/1	0.32	2.37	48,48,48,48	0
57	MG	AA	1658	1/1	0.49	2.33	61,61,61,61	0
57	MG	BB	209	1/1	0.32	2.22	36,36,36,36	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3320	1/1	0.20	2.18	52,52,52,52	0
57	MG	BA	3161	1/1	0.22	2.11	42,42,42,42	0
57	MG	BA	3329	1/1	0.20	2.09	58,58,58,58	0
57	MG	BA	3267	1/1	0.23	2.02	52,52,52,52	0
57	MG	BA	3051	1/1	0.25	1.96	33,33,33,33	0
57	MG	BA	3201	1/1	0.19	1.94	47,47,47,47	0
57	MG	BA	3048	1/1	0.39	1.88	40,40,40,40	0
57	MG	BA	3239	1/1	0.19	1.87	71,71,71,71	0
57	MG	BA	3226	1/1	0.22	1.82	51,51,51,51	0
57	MG	AA	1641	1/1	0.31	1.80	67,67,67,67	0
57	MG	BA	3122	1/1	0.21	1.78	38,38,38,38	0
57	MG	AA	1662	1/1	0.27	1.72	57,57,57,57	0
57	MG	BA	3093	1/1	0.23	1.72	42,42,42,42	0
57	MG	BA	3286	1/1	0.21	1.67	48,48,48,48	0
57	MG	AA	1671	1/1	0.16	1.66	53,53,53,53	0
57	MG	BA	3115	1/1	0.24	1.57	37,37,37,37	0
57	MG	BA	3097	1/1	0.41	1.57	48,48,48,48	0
57	MG	BA	3080	1/1	0.24	1.53	43,43,43,43	0
57	MG	AA	1638	1/1	0.25	1.48	55,55,55,55	0
57	MG	BB	208	1/1	0.30	1.43	59,59,59,59	0
57	MG	BA	3227	1/1	0.29	1.42	63,63,63,63	0
57	MG	AA	1613	1/1	0.20	1.41	58,58,58,58	0
57	MG	BA	3176	1/1	0.22	1.37	50,50,50,50	0
57	MG	BA	3342	1/1	0.24	1.35	54,54,54,54	0
57	MG	AA	1633	1/1	0.29	1.35	53,53,53,53	0
57	MG	AA	1668	1/1	0.21	1.33	51,51,51,51	0
57	MG	AA	1651	1/1	0.27	1.28	51,51,51,51	0
57	MG	BA	3334	1/1	0.20	1.27	56,56,56,56	0
57	MG	BA	3242	1/1	0.24	1.27	72,72,72,72	0
57	MG	AF	201	1/1	0.33	1.27	65,65,65,65	0
57	MG	AA	1690	1/1	0.31	1.25	83,83,83,83	0
57	MG	BA	3228	1/1	0.20	1.24	42,42,42,42	0
57	MG	BA	3118	1/1	0.22	1.20	40,40,40,40	0
57	MG	AA	1647	1/1	0.20	1.14	60,60,60,60	0
57	MG	BA	3315	1/1	0.18	1.05	63,63,63,63	0
57	MG	AA	1663	1/1	0.26	1.05	74,74,74,74	0
57	MG	BA	3172	1/1	0.17	1.00	53,53,53,53	0
57	MG	AA	1660	1/1	0.19	0.94	46,46,46,46	0
57	MG	BA	3064	1/1	0.20	0.90	24,24,24,24	0
57	MG	BA	3106	1/1	0.23	0.87	37,37,37,37	0
57	MG	AA	1625	1/1	0.23	0.86	40,40,40,40	0
57	MG	BA	3056	1/1	0.21	0.75	26,26,26,26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3076	1/1	0.20	0.68	36,36,36,36	0
57	MG	BA	3004	1/1	0.23	0.58	21,21,21,21	0
57	MG	BB	203	1/1	0.21	0.58	51,51,51,51	0
57	MG	AA	1696	1/1	0.24	0.55	89,89,89,89	0
57	MG	BA	3301	1/1	0.22	0.48	64,64,64,64	0
57	MG	BX	201	1/1	0.31	0.45	47,47,47,47	0
57	MG	BA	3351	1/1	0.18	0.44	58,58,58,58	0
57	MG	AA	1619	1/1	0.18	0.39	40,40,40,40	0
57	MG	BA	3238	1/1	0.16	0.38	50,50,50,50	0
57	MG	BA	3236	1/1	0.20	0.38	46,46,46,46	0
57	MG	BA	3235	1/1	0.26	0.37	64,64,64,64	0
57	MG	BA	3129	1/1	0.17	0.36	43,43,43,43	0
57	MG	AA	1683	1/1	0.19	0.31	63,63,63,63	0
57	MG	AA	1620	1/1	0.17	0.29	52,52,52,52	0
57	MG	AA	1629	1/1	0.20	0.23	41,41,41,41	0
57	MG	AA	1672	1/1	0.17	0.13	52,52,52,52	0
57	MG	BA	3355	1/1	0.28	0.09	69,69,69,69	0
57	MG	AL	201	1/1	0.28	0.07	54,54,54,54	0
57	MG	BA	3111	1/1	0.21	0.05	29,29,29,29	0
57	MG	BA	3131	1/1	0.18	0.00	40,40,40,40	0
57	MG	BA	3327	1/1	0.21	-0.01	64,64,64,64	0
57	MG	BD	301	1/1	0.22	-0.11	49,49,49,49	0
57	MG	BA	3264	1/1	0.17	-0.14	67,67,67,67	0
57	MG	AA	1642	1/1	0.28	-0.19	53,53,53,53	0
57	MG	BA	3108	1/1	0.19	-0.21	42,42,42,42	0
57	MG	BA	3143	1/1	0.18	-0.22	32,32,32,32	0
57	MG	AA	1612	1/1	0.21	-0.29	29,29,29,29	0
57	MG	BA	3220	1/1	0.30	-0.30	56,56,56,56	0
57	MG	BA	3094	1/1	0.21	-0.33	47,47,47,47	0
57	MG	BA	3059	1/1	0.20	-0.35	43,43,43,43	0
57	MG	BA	3142	1/1	0.21	-0.36	50,50,50,50	0
57	MG	BR	202	1/1	0.18	-0.37	51,51,51,51	0
57	MG	BB	204	1/1	0.14	-0.38	53,53,53,53	0
57	MG	BA	3285	1/1	0.28	-0.38	75,75,75,75	0
57	MG	BA	3303	1/1	0.39	-0.39	56,56,56,56	0
57	MG	BA	3208	1/1	0.26	-0.40	62,62,62,62	0
57	MG	BA	3212	1/1	0.19	-0.42	45,45,45,45	0
57	MG	B0	102	1/1	0.26	-0.42	33,33,33,33	0
57	MG	BA	3287	1/1	0.22	-0.45	83,83,83,83	0
57	MG	BA	3019	1/1	0.22	-0.49	15,15,15,15	0
57	MG	BA	3256	1/1	0.17	-0.51	56,56,56,56	0
57	MG	BA	3101	1/1	0.21	-0.52	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3289	1/1	0.17	-0.53	62,62,62,62	0
57	MG	BA	3135	1/1	0.15	-0.54	45,45,45,45	0
57	MG	BQ	201	1/1	0.17	-0.55	44,44,44,44	0
57	MG	BA	3338	1/1	0.13	-0.57	61,61,61,61	0
57	MG	AA	1701	1/1	0.16	-0.59	79,79,79,79	0
57	MG	BA	3312	1/1	0.25	-0.61	56,56,56,56	0
57	MG	BD	303	1/1	0.19	-0.61	57,57,57,57	0
57	MG	BA	3336	1/1	0.20	-0.62	86,86,86,86	0
57	MG	AA	1653	1/1	0.16	-0.66	41,41,41,41	0
57	MG	AA	1698	1/1	0.17	-0.66	51,51,51,51	0
57	MG	AA	1685	1/1	0.29	-0.66	64,64,64,64	0
57	MG	BN	201	1/1	0.29	-0.70	51,51,51,51	0
57	MG	BA	3109	1/1	0.14	-0.71	38,38,38,38	0
57	MG	AA	1626	1/1	0.19	-0.71	45,45,45,45	0
57	MG	AH	201	1/1	0.20	-0.72	50,50,50,50	0
57	MG	AA	1675	1/1	0.16	-0.72	57,57,57,57	0
57	MG	AA	1681	1/1	0.16	-0.73	38,38,38,38	0
57	MG	AA	1627	1/1	0.24	-0.75	40,40,40,40	0
57	MG	BA	3198	1/1	0.17	-0.76	60,60,60,60	0
57	MG	BR	201	1/1	0.17	-0.79	69,69,69,69	0
57	MG	BA	3209	1/1	0.11	-0.82	42,42,42,42	0
57	MG	BA	3002	1/1	0.18	-0.84	13,13,13,13	0
57	MG	BO	201	1/1	0.16	-0.84	41,41,41,41	0
57	MG	AA	1608	1/1	0.19	-0.88	59,59,59,59	0
57	MG	BA	3249	1/1	0.10	-0.89	49,49,49,49	0
57	MG	BA	3258	1/1	0.13	-0.93	50,50,50,50	0
57	MG	BA	3247	1/1	0.20	-1.00	61,61,61,61	0
57	MG	BA	3175	1/1	0.15	-1.02	44,44,44,44	0
57	MG	BA	3321	1/1	0.15	-1.03	73,73,73,73	0
57	MG	BD	305	1/1	0.17	-1.04	16,16,16,16	0
57	MG	BA	3215	1/1	0.14	-1.05	53,53,53,53	0
57	MG	BA	3335	1/1	0.16	-1.09	58,58,58,58	0
58	GNP	AW	602	32/32	0.16	-1.11	58,71,81,83	0
57	MG	B2	101	1/1	0.12	-1.17	49,49,49,49	0
57	MG	BA	3339	1/1	0.16	-1.19	76,76,76,76	0
57	MG	BA	3147	1/1	0.21	-1.20	46,46,46,46	0
57	MG	BA	3288	1/1	0.20	-1.20	95,95,95,95	0
57	MG	BA	3354	1/1	0.14	-1.21	62,62,62,62	0
57	MG	AA	1667	1/1	0.15	-1.24	87,87,87,87	0
57	MG	AA	1617	1/1	0.16	-1.26	47,47,47,47	0
57	MG	BA	3038	1/1	0.16	-1.27	21,21,21,21	0
57	MG	BA	3098	1/1	0.13	-1.31	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3075	1/1	0.15	-1.32	43,43,43,43	0
57	MG	AA	1697	1/1	0.10	-1.36	64,64,64,64	0
57	MG	AL	202	1/1	0.15	-1.36	73,73,73,73	0
57	MG	BB	205	1/1	0.15	-1.38	79,79,79,79	0
57	MG	AA	1644	1/1	0.15	-1.38	49,49,49,49	0
57	MG	BA	3332	1/1	0.21	-1.39	96,96,96,96	0
57	MG	BE	301	1/1	0.08	-1.40	67,67,67,67	0
57	MG	B0	101	1/1	0.10	-1.41	23,23,23,23	0
57	MG	BB	207	1/1	0.09	-1.41	47,47,47,47	0
57	MG	AA	1639	1/1	0.17	-1.45	49,49,49,49	0
57	MG	AM	201	1/1	0.12	-1.46	80,80,80,80	0
57	MG	BA	3299	1/1	0.15	-1.51	64,64,64,64	0
57	MG	BA	3248	1/1	0.17	-1.57	52,52,52,52	0
57	MG	BA	3189	1/1	0.15	-1.68	51,51,51,51	0
57	MG	BA	3180	1/1	0.12	-1.70	45,45,45,45	0
57	MG	BA	3275	1/1	0.10	-1.71	59,59,59,59	0
57	MG	BA	3274	1/1	0.12	-1.76	52,52,52,52	0
57	MG	BA	3179	1/1	0.14	-1.83	46,46,46,46	0
57	MG	AW	601	1/1	0.15	-1.83	36,36,36,36	0
57	MG	AA	1646	1/1	0.16	-1.85	50,50,50,50	0
57	MG	BA	3344	1/1	0.16	-1.88	71,71,71,71	0
57	MG	BA	3140	1/1	0.14	-1.90	46,46,46,46	0
57	MG	AA	1656	1/1	0.17	-1.91	73,73,73,73	0
57	MG	BA	3230	1/1	0.14	-1.96	46,46,46,46	0
57	MG	BA	3309	1/1	0.15	-1.99	62,62,62,62	0
57	MG	BA	3089	1/1	0.09	-2.11	52,52,52,52	0
57	MG	AA	1688	1/1	0.09	-2.12	77,77,77,77	0
57	MG	BT	201	1/1	0.12	-2.19	40,40,40,40	0
57	MG	BA	3144	1/1	0.12	-2.20	68,68,68,68	0
57	MG	AA	1648	1/1	0.17	-2.20	54,54,54,54	0
57	MG	BA	3237	1/1	0.12	-2.33	51,51,51,51	0
57	MG	BA	3290	1/1	0.10	-2.38	56,56,56,56	0
57	MG	BA	3156	1/1	0.16	-2.44	41,41,41,41	0
57	MG	BA	3347	1/1	0.14	-2.48	76,76,76,76	0
57	MG	BA	3253	1/1	0.10	-2.52	65,65,65,65	0
57	MG	AA	1682	1/1	0.12	-2.66	76,76,76,76	0
57	MG	AA	1636	1/1	0.15	-2.73	36,36,36,36	0
57	MG	BA	3217	1/1	0.07	-2.80	56,56,56,56	0
57	MG	BA	3307	1/1	0.14	-2.88	52,52,52,52	0
57	MG	BA	3322	1/1	0.17	-2.90	62,62,62,62	0
57	MG	AA	1694	1/1	0.11	-2.93	75,75,75,75	0
57	MG	AA	1674	1/1	0.13	-2.94	55,55,55,55	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3195	1/1	0.14	-3.01	47,47,47,47	0
57	MG	AA	1614	1/1	0.15	-3.11	42,42,42,42	0
57	MG	BA	3229	1/1	0.08	-3.34	46,46,46,46	0
57	MG	AA	1669	1/1	0.10	-3.42	71,71,71,71	0
57	MG	AA	1695	1/1	0.10	-3.45	62,62,62,62	0
57	MG	AA	1664	1/1	0.13	-3.48	41,41,41,41	0
57	MG	BA	3310	1/1	0.16	-3.49	75,75,75,75	0
57	MG	BA	3191	1/1	0.08	-3.54	57,57,57,57	0
57	MG	BA	3141	1/1	0.17	-3.55	54,54,54,54	0
57	MG	BA	3164	1/1	0.10	-3.57	45,45,45,45	0
57	MG	BA	3184	1/1	0.14	-3.60	37,37,37,37	0
57	MG	AA	1692	1/1	0.17	-3.83	67,67,67,67	0
57	MG	BA	3326	1/1	0.14	-4.14	42,42,42,42	0
57	MG	BA	3168	1/1	0.13	-4.38	32,32,32,32	0
57	MG	BA	3243	1/1	0.09	-4.40	62,62,62,62	0
57	MG	BA	3328	1/1	0.14	-4.41	71,71,71,71	0
57	MG	BB	206	1/1	0.09	-4.79	65,65,65,65	0
57	MG	BA	3152	1/1	0.07	-4.88	41,41,41,41	0
57	MG	AA	1637	1/1	0.09	-5.18	54,54,54,54	0
57	MG	BA	3231	1/1	0.09	-5.84	56,56,56,56	0
57	MG	AA	1680	1/1	0.08	-5.91	55,55,55,55	0
57	MG	BA	3222	1/1	0.15	-6.79	50,50,50,50	0
57	MG	BA	3120	1/1	0.10	-7.01	31,31,31,31	0
57	MG	BA	3173	1/1	0.11	-7.50	36,36,36,36	0
57	MG	BA	3224	1/1	0.12	-8.12	41,41,41,41	0
57	MG	BA	3319	1/1	0.18	-8.70	68,68,68,68	0
57	MG	BA	3279	1/1	0.10	-8.91	50,50,50,50	0
57	MG	AA	1659	1/1	0.12	-12.76	55,55,55,55	0
57	MG	AA	1640	1/1	0.06	-17.00	41,41,41,41	0
57	MG	BA	3218	1/1	0.14	-17.40	50,50,50,50	0
57	MG	BA	3187	1/1	0.09	-18.54	56,56,56,56	0
57	MG	BA	3162	1/1	0.10	-18.91	56,56,56,56	0
57	MG	BA	3166	1/1	0.07	-25.67	50,50,50,50	0
57	MG	BA	3259	1/1	0.11	-87.80	69,69,69,69	0
57	MG	BA	3343	1/1	0.07	-	71,71,71,71	0
57	MG	BC	301	1/1	0.30	-	53,53,53,53	0
57	MG	BA	3169	1/1	0.24	-	39,39,39,39	0
57	MG	BA	3199	1/1	0.40	-	42,42,42,42	0
57	MG	BA	3346	1/1	0.56	-	83,83,83,83	0
57	MG	BA	3165	1/1	0.48	-	52,52,52,52	0
57	MG	BA	3160	1/1	0.32	-	49,49,49,49	0
57	MG	BA	3348	1/1	0.27	-	67,67,67,67	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.