



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:04 am GMT

PDB ID : 4V7K
Title : Structure of RelE nuclease bound to the 70S ribosome (postcleavage state)
Authors : Neubauer, C.; Gao, Y.-G.; Andersen, K.R.; Dunham, C.M.; Kelley, A.C.;
Hentschel, J.; Gerdes, K.; Ramakrishnan, V.; Brodersen, D.E.
Deposited on : 2009-11-02
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

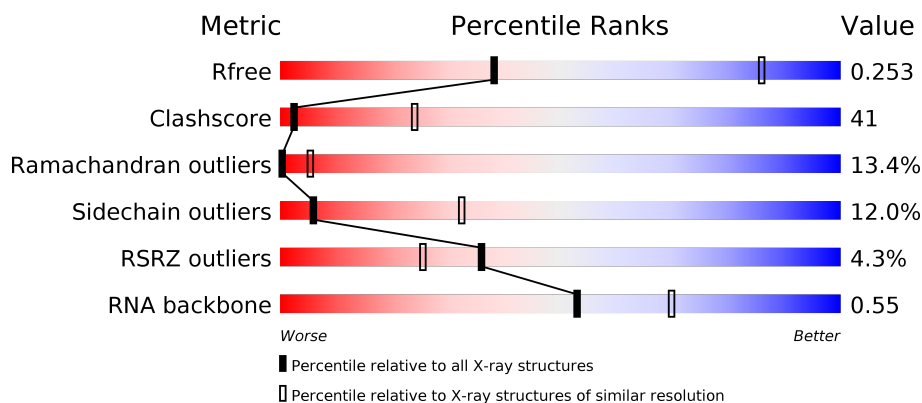
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)
RNA backbone	2435	1002 (4.30-2.90)

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

Mol	Chain	Length	Quality of chain
1	Ab	256	 3% 70% 20% 9%
1	Bb	256	 3% 71% 19% 9%
2	Ac	239	 5% 69% 16% 14%
2	Bc	239	 3% 69% 16% 14%

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Mol	Chain	Length	Quality of chain
3	Ad	209	
3	Bd	209	
4	Ae	162	
4	Be	162	
5	Af	101	
5	Bf	101	
6	Ag	156	
6	Bg	156	
7	Ah	138	
7	Bh	138	
8	Ai	128	
8	Bi	128	
9	Aj	105	
9	Bj	105	
10	Ak	129	
10	Bk	129	
11	Al	132	
11	Bl	132	
12	Am	126	
12	Bm	126	
13	An	61	
13	Bn	61	
14	Ao	89	
14	Bo	89	
15	Ap	88	

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Mol	Chain	Length	Quality of chain
15	Bp	88	
16	Aq	105	
16	Bq	105	
17	Ar	88	
17	Br	88	
18	As	93	
18	Bs	93	
19	At	106	
19	Bt	106	
20	Au	27	
20	Bu	27	
21	Ay	95	
21	By	95	
22	Aa	1504	
22	Ba	1504	
23	Ax	14	
23	Bx	14	
24	Av	77	
24	Bv	77	
25	Aw	77	
25	Bw	77	
26	AC	229	
26	BC	229	
27	AD	276	
27	BD	276	

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Mol	Chain	Length	Quality of chain
28	AE	206	
28	BE	206	
29	AF	210	
29	BF	210	
30	AG	182	
30	BG	182	
31	AH	180	
31	BH	180	
32	AI	148	
32	BI	148	
33	AJ	173	
33	BJ	173	
34	AN	140	
34	BN	140	
35	AO	122	
35	BO	122	
36	AP	150	
36	BP	150	
37	AQ	141	
37	BQ	141	
38	AR	118	
38	BR	118	
39	AS	112	
39	BS	112	
40	AT	146	

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Mol	Chain	Length	Quality of chain
40	BT	146	
41	AU	118	
41	BU	118	
42	AV	101	
42	BV	101	
43	AW	113	
43	BW	113	
44	AX	96	
44	BX	96	
45	AY	110	
45	BY	110	
46	AZ	206	
46	BZ	206	
47	A0	85	
47	B0	85	
48	A1	98	
48	B1	98	
49	A2	72	
49	B2	72	
50	A3	60	
50	B3	60	
51	A4	71	
51	B4	71	
52	A5	60	
52	B5	60	

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Mol	Chain	Length	Quality of chain
53	A6	54	
53	B6	54	
54	A7	49	
54	B7	49	
55	A8	65	
55	B8	65	
56	A9	37	
56	B9	37	
57	AA	2848	
57	BA	2848	
58	AB	119	
58	BB	119	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	A7	101	-	-	-	X
60	MG	AA	2906	-	-	-	X
60	MG	AA	2907	-	-	-	X
60	MG	AA	2909	-	-	-	X
60	MG	AA	2913	-	-	-	X
60	MG	AA	2914	-	-	-	X
60	MG	AA	2915	-	-	-	X
60	MG	AA	2918	-	-	-	X
60	MG	AA	2919	-	-	-	X
60	MG	AA	2920	-	-	-	X
60	MG	AA	2921	-	-	-	X
60	MG	AA	2925	-	-	-	X
60	MG	AA	2928	-	-	-	X
60	MG	AA	2929	-	-	-	X
60	MG	AA	2931	-	-	-	X
60	MG	AA	2932	-	-	-	X
60	MG	AA	2943	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	2949	-	-	-	X
60	MG	AA	2951	-	-	-	X
60	MG	AA	2953	-	-	-	X
60	MG	AA	2960	-	-	-	X
60	MG	AA	2964	-	-	-	X
60	MG	AA	2965	-	-	-	X
60	MG	AA	2968	-	-	-	X
60	MG	AA	2969	-	-	-	X
60	MG	AA	2976	-	-	-	X
60	MG	AA	2980	-	-	-	X
60	MG	AA	2981	-	-	-	X
60	MG	AA	2985	-	-	-	X
60	MG	AA	2987	-	-	-	X
60	MG	AA	2988	-	-	-	X
60	MG	AA	2991	-	-	-	X
60	MG	AA	2996	-	-	-	X
60	MG	AA	2997	-	-	-	X
60	MG	AA	3011	-	-	-	X
60	MG	AA	3012	-	-	-	X
60	MG	AA	3019	-	-	-	X
60	MG	AA	3023	-	-	-	X
60	MG	AA	3025	-	-	-	X
60	MG	AA	3028	-	-	-	X
60	MG	AA	3029	-	-	-	X
60	MG	AA	3035	-	-	-	X
60	MG	AA	3038	-	-	-	X
60	MG	AA	3039	-	-	-	X
60	MG	AA	3044	-	-	-	X
60	MG	AA	3046	-	-	-	X
60	MG	AA	3051	-	-	-	X
60	MG	AA	3054	-	-	-	X
60	MG	AA	3056	-	-	-	X
60	MG	AA	3061	-	-	-	X
60	MG	AA	3069	-	-	-	X
60	MG	AA	3070	-	-	-	X
60	MG	AA	3072	-	-	-	X
60	MG	AA	3083	-	-	-	X
60	MG	AA	3088	-	-	-	X
60	MG	AA	3095	-	-	-	X
60	MG	AA	3096	-	-	-	X
60	MG	AA	3097	-	-	-	X
60	MG	AA	3099	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	3101	-	-	-	X
60	MG	AA	3102	-	-	-	X
60	MG	AA	3121	-	-	-	X
60	MG	AA	3124	-	-	-	X
60	MG	AA	3126	-	-	-	X
60	MG	AA	3128	-	-	-	X
60	MG	AA	3133	-	-	-	X
60	MG	AA	3134	-	-	-	X
60	MG	AA	3138	-	-	-	X
60	MG	AA	3147	-	-	-	X
60	MG	AA	3150	-	-	-	X
60	MG	AA	3158	-	-	-	X
60	MG	AA	3163	-	-	-	X
60	MG	AA	3172	-	-	-	X
60	MG	AA	3175	-	-	-	X
60	MG	AA	3177	-	-	-	X
60	MG	AA	3179	-	-	-	X
60	MG	AA	3190	-	-	-	X
60	MG	AA	3194	-	-	-	X
60	MG	AA	3195	-	-	-	X
60	MG	AA	3197	-	-	-	X
60	MG	AA	3205	-	-	-	X
60	MG	AA	3219	-	-	-	X
60	MG	AA	3221	-	-	-	X
60	MG	AA	3231	-	-	-	X
60	MG	AA	3233	-	-	-	X
60	MG	AA	3236	-	-	-	X
60	MG	AA	3243	-	-	-	X
60	MG	AA	3245	-	-	-	X
60	MG	AA	3247	-	-	-	X
60	MG	AA	3256	-	-	-	X
60	MG	AA	3259	-	-	-	X
60	MG	AA	3261	-	-	-	X
60	MG	AA	3265	-	-	-	X
60	MG	Aa	1611	-	-	-	X
60	MG	Aa	1613	-	-	-	X
60	MG	Aa	1622	-	-	-	X
60	MG	Aa	1624	-	-	-	X
60	MG	Aa	1628	-	-	-	X
60	MG	Aa	1631	-	-	-	X
60	MG	Aa	1633	-	-	-	X
60	MG	Aa	1635	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	Aa	1642	-	-	-	X
60	MG	Aa	1645	-	-	-	X
60	MG	Aa	1662	-	-	-	X
60	MG	Aa	1666	-	-	-	X
60	MG	Aa	1670	-	-	-	X
60	MG	Aa	1674	-	-	-	X
60	MG	Aa	1678	-	-	-	X
60	MG	Aa	1679	-	-	-	X
60	MG	Aa	1685	-	-	-	X
60	MG	Aa	1686	-	-	-	X
60	MG	Aa	1725	-	-	-	X
60	MG	Aa	1727	-	-	-	X
60	MG	Aa	1729	-	-	-	X
60	MG	Aa	1735	-	-	-	X
60	MG	Aa	1738	-	-	-	X
60	MG	Aa	1744	-	-	-	X
60	MG	Ae	202	-	-	-	X
60	MG	Av	102	-	-	-	X
60	MG	B0	101	-	-	-	X
60	MG	B7	101	-	-	-	X
60	MG	BA	2905	-	-	-	X
60	MG	BA	2908	-	-	-	X
60	MG	BA	2912	-	-	-	X
60	MG	BA	2913	-	-	-	X
60	MG	BA	2914	-	-	-	X
60	MG	BA	2917	-	-	-	X
60	MG	BA	2920	-	-	-	X
60	MG	BA	2927	-	-	-	X
60	MG	BA	2928	-	-	-	X
60	MG	BA	2930	-	-	-	X
60	MG	BA	2931	-	-	-	X
60	MG	BA	2951	-	-	-	X
60	MG	BA	2957	-	-	-	X
60	MG	BA	2962	-	-	-	X
60	MG	BA	2965	-	-	-	X
60	MG	BA	2966	-	-	-	X
60	MG	BA	2967	-	-	-	X
60	MG	BA	2968	-	-	-	X
60	MG	BA	2979	-	-	-	X
60	MG	BA	2980	-	-	-	X
60	MG	BA	2982	-	-	-	X
60	MG	BA	2984	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	2987	-	-	-	X
60	MG	BA	2990	-	-	-	X
60	MG	BA	2995	-	-	-	X
60	MG	BA	2996	-	-	-	X
60	MG	BA	3010	-	-	-	X
60	MG	BA	3011	-	-	-	X
60	MG	BA	3013	-	-	-	X
60	MG	BA	3018	-	-	-	X
60	MG	BA	3022	-	-	-	X
60	MG	BA	3024	-	-	-	X
60	MG	BA	3027	-	-	-	X
60	MG	BA	3028	-	-	-	X
60	MG	BA	3029	-	-	-	X
60	MG	BA	3034	-	-	-	X
60	MG	BA	3035	-	-	-	X
60	MG	BA	3037	-	-	-	X
60	MG	BA	3038	-	-	-	X
60	MG	BA	3043	-	-	-	X
60	MG	BA	3045	-	-	-	X
60	MG	BA	3052	-	-	-	X
60	MG	BA	3053	-	-	-	X
60	MG	BA	3055	-	-	-	X
60	MG	BA	3060	-	-	-	X
60	MG	BA	3069	-	-	-	X
60	MG	BA	3070	-	-	-	X
60	MG	BA	3084	-	-	-	X
60	MG	BA	3088	-	-	-	X
60	MG	BA	3091	-	-	-	X
60	MG	BA	3093	-	-	-	X
60	MG	BA	3094	-	-	-	X
60	MG	BA	3095	-	-	-	X
60	MG	BA	3097	-	-	-	X
60	MG	BA	3100	-	-	-	X
60	MG	BA	3101	-	-	-	X
60	MG	BA	3102	-	-	-	X
60	MG	BA	3105	-	-	-	X
60	MG	BA	3120	-	-	-	X
60	MG	BA	3123	-	-	-	X
60	MG	BA	3127	-	-	-	X
60	MG	BA	3131	-	-	-	X
60	MG	BA	3133	-	-	-	X
60	MG	BA	3134	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3138	-	-	-	X
60	MG	BA	3147	-	-	-	X
60	MG	BA	3150	-	-	-	X
60	MG	BA	3156	-	-	-	X
60	MG	BA	3160	-	-	-	X
60	MG	BA	3165	-	-	-	X
60	MG	BA	3171	-	-	-	X
60	MG	BA	3172	-	-	-	X
60	MG	BA	3176	-	-	-	X
60	MG	BA	3183	-	-	-	X
60	MG	BA	3187	-	-	-	X
60	MG	BA	3191	-	-	-	X
60	MG	BA	3194	-	-	-	X
60	MG	BA	3211	-	-	-	X
60	MG	BA	3217	-	-	-	X
60	MG	BA	3231	-	-	-	X
60	MG	BA	3234	-	-	-	X
60	MG	BA	3236	-	-	-	X
60	MG	BA	3241	-	-	-	X
60	MG	BA	3254	-	-	-	X
60	MG	BA	3257	-	-	-	X
60	MG	BD	301	-	-	-	X
60	MG	Ba	1608	-	-	-	X
60	MG	Ba	1609	-	-	-	X
60	MG	Ba	1621	-	-	-	X
60	MG	Ba	1630	-	-	-	X
60	MG	Ba	1634	-	-	-	X
60	MG	Ba	1644	-	-	-	X
60	MG	Ba	1654	-	-	-	X
60	MG	Ba	1668	-	-	-	X
60	MG	Ba	1671	-	-	-	X
60	MG	Ba	1684	-	-	-	X
60	MG	Ba	1685	-	-	-	X
60	MG	Ba	1691	-	-	-	X
60	MG	Ba	1695	-	-	-	X
60	MG	Ba	1724	-	-	-	X
60	MG	Ba	1726	-	-	-	X
60	MG	Ba	1728	-	-	-	X
60	MG	Ba	1731	-	-	-	X
60	MG	Ba	1739	-	-	-	X
60	MG	Ba	1742	-	-	-	X
60	MG	Bv	105	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 297230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ab	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
1	Bb	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Ac	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
2	Bc	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Ad	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
3	Bd	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Ae	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			
4	Be	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Af	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
5	Bf	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	Ag	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
6	Bg	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Ah	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
7	Bh	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	Ai	127	Total	C	N	O	0	0	0
			1010	639	197	174			
8	Bi	127	Total	C	N	O	0	0	0
			1010	639	197	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Aj	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
9	Bj	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	Ak	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	Bk	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	Al	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			
11	Bl	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Am	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			
12	Bm	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	An	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
13	Bn	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Ao	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
14	Bo	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	Ap	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
15	Bp	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Aq	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
16	Bq	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Ar	70	Total	C	N	O	0	0	0
			574	367	112	95			
17	Br	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	As	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			
18	Bs	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	At	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
19	Bt	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	Au	24	Total	C	N	O	0	0	0
			208	128	50	30			
20	Bu	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 21 is a protein called Toxin relE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Ay	94	Total	C	N	O	S	0	0	0
			782	502	139	139	2			
21	By	94	Total	C	N	O	S	0	0	0
			782	502	139	139	2			

- Molecule 22 is a RNA chain called RNA (1504-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Aa	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
22	Ba	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 23 is a RNA chain called RNA (5'-R(*A*AP*GP*UP*AP*AP*AP*AP*AP*UP*GP*UP*A*(CCC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Ax	13	Total	C	N	O	P	0	0	0
			260	117	51	80	12			
23	Bx	13	Total	C	N	O	P	0	0	0
			260	117	51	80	12			

- Molecule 24 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Av	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			
24	Bv	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 25 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Aw	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
25	Bw	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 26 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
26	BC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	AD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			
27	BD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	AE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
28	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			
29	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
30	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AH	164	Total	C	N	O	S	0	0	0
			1259	800	233	225	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	164	Total	C	N	O	S	0	0	0
			1259	800	233	225	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
32	BI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AJ	130	Total	C	N	O	S	0	0	0
			641	381	130	130				
33	BJ	130	Total	C	N	O	S	0	0	0
			641	381	130	130				

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
34	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
35	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
36	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AQ	140	Total	C	N	O	S	0	0	0
			1112	710	210	185	7			
37	BQ	140	Total	C	N	O	S	0	0	0
			1112	710	210	185	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	AR	117	Total	C	N	O	0	0	0
			960	599	202	159			
38	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	AS	98	Total	C	N	O	0	0	0
			770	486	154	130			
39	BS	98	Total	C	N	O	0	0	0
			770	486	154	130			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	AT	135	Total	C	N	O	S	0	0	0
			1123	699	230	193	1			
40	BT	135	Total	C	N	O	S	0	0	0
			1123	699	230	193	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
41	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
42	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
43	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AX	92	Total	C	N	O		0	0	0
			725	471	131	123				
44	BX	92	Total	C	N	O		0	0	0
			725	471	131	123				

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	AY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
45	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	AZ	184	Total	C	N	O	S	0	0	0
			1467	936	261	268	2			
46	BZ	184	Total	C	N	O	S	0	0	0
			1467	936	261	268	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	A0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	A1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			
48	B1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	A2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	A3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			
50	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	A4	57	Total	C	N	O	S	0	0	0
			450	285	77	83	5			
51	B4	57	Total	C	N	O	S	0	0	0
			450	285	77	83	5			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	A5	55	Total	C	N	O	S	0	0	0
			427	267	86	69	5			
52	B5	55	Total	C	N	O	S	0	0	0
			427	267	86	69	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	A6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
53	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	A7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
54	B7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	A8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
55	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	A9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
56	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 57 is a RNA chain called RNA (2848-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	AA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			
57	BA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			

- Molecule 58 is a RNA chain called RNA (119-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	AB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0
58	BB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total 1	Zn 1	0	0
59	Ad	1	Total 1	Zn 1	0	0
59	Bn	1	Total 1	Zn 1	0	0
59	B9	1	Total 1	Zn 1	0	0
59	Bd	1	Total 1	Zn 1	0	0
59	A4	1	Total 1	Zn 1	0	0
59	An	1	Total 1	Zn 1	0	0
59	A9	1	Total 1	Zn 1	0	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	365	Total 365	Mg 365	0	0
60	AB	3	Total 3	Mg 3	0	0
60	Bd	1	Total 1	Mg 1	0	0
60	AX	1	Total 1	Mg 1	0	0
60	Bw	1	Total 1	Mg 1	0	0
60	B5	2	Total 2	Mg 2	0	0
60	BB	3	Total 3	Mg 3	0	0
60	Ba	143	Total 143	Mg 143	0	0

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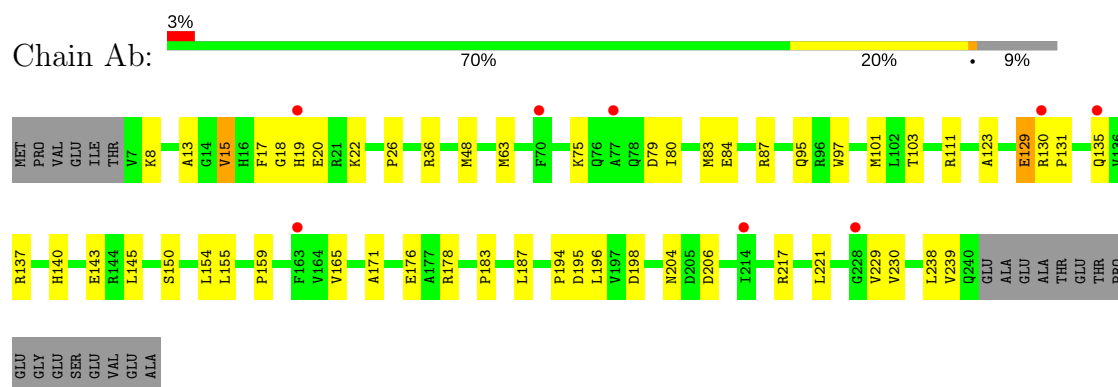
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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60	BF	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0
60	Aw	1	Total 1	Mg 1	0	0
60	AA	367	Total 367	Mg 367	0	0
60	A5	1	Total 1	Mg 1	0	0
60	A1	2	Total 2	Mg 2	0	0
60	AD	2	Total 2	Mg 2	0	0
60	Ae	2	Total 2	Mg 2	0	0
60	Bm	1	Total 1	Mg 1	0	0
60	Av	5	Total 5	Mg 5	0	0
60	Bx	1	Total 1	Mg 1	0	0
60	Aa	145	Total 145	Mg 145	0	0
60	B7	2	Total 2	Mg 2	0	0
60	BO	1	Total 1	Mg 1	0	0
60	AQ	1	Total 1	Mg 1	0	0
60	A7	1	Total 1	Mg 1	0	0
60	BD	2	Total 2	Mg 2	0	0
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60	Bv	5	Total 5	Mg 5	0	0
60	AF	1	Total 1	Mg 1	0	0

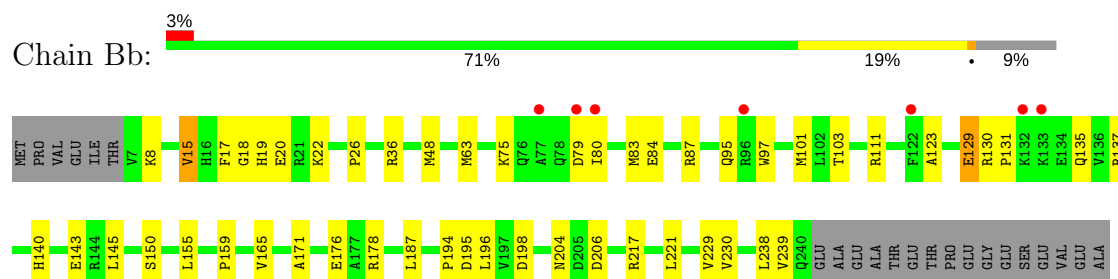
3 Residue-property plots [i](#)

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

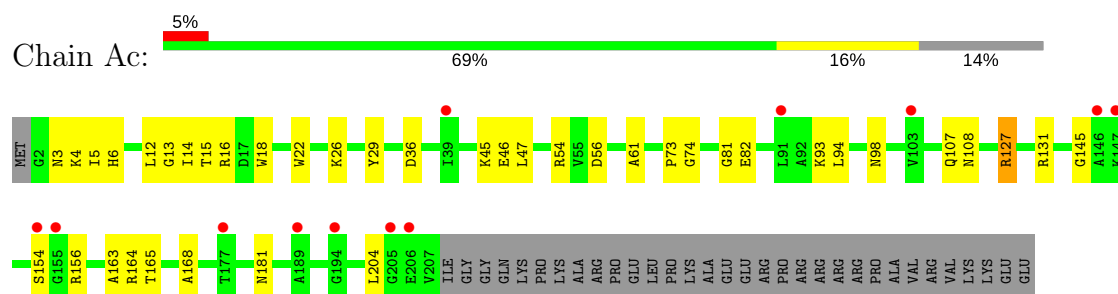
• Molecule 1: 30S ribosomal protein S2



• Molecule 1: 30S ribosomal protein S2

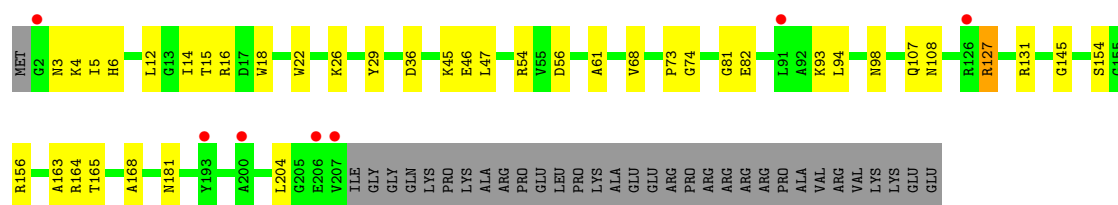


• Molecule 2: 30S ribosomal protein S3



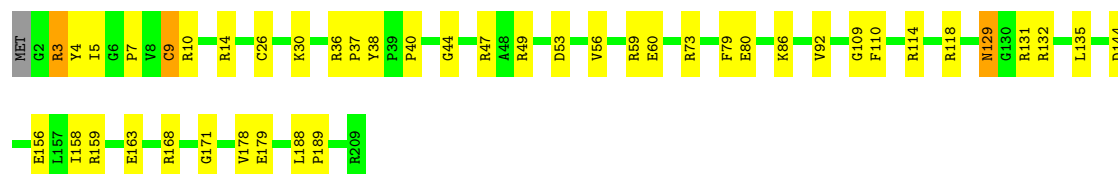
• Molecule 2: 30S ribosomal protein S3





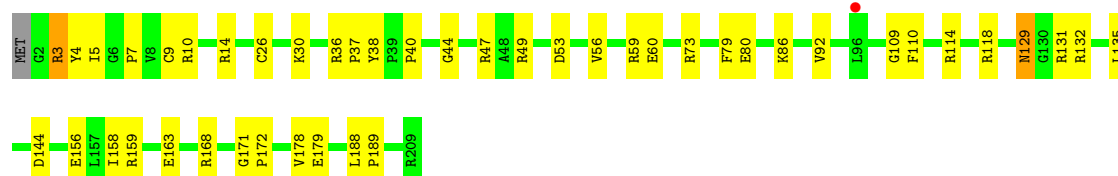
• Molecule 3: 30S ribosomal protein S4

Chain Ad: 78% 20%



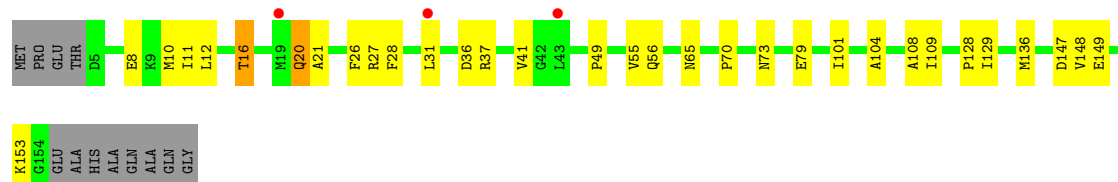
• Molecule 3: 30S ribosomal protein S4

Chain Bd: 78% 21%



• Molecule 4: 30S ribosomal protein S5

Chain Ae: 73% 19% 7%



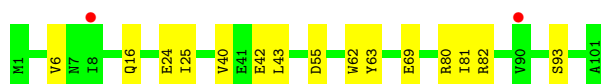
• Molecule 4: 30S ribosomal protein S5

Chain Be: 72% 20% 7%



• Molecule 5: 30S ribosomal protein S6

Chain Af: 85% 15%



- Molecule 5: 30S ribosomal protein S6

Chain Bf: 85% 14%



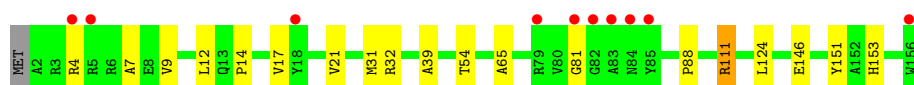
- Molecule 6: 30S ribosomal protein S7

Chain Ag: 6% 87% 13%



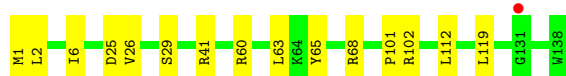
- Molecule 6: 30S ribosomal protein S7

Chain Bg: 6% 87% 12%



- Molecule 7: 30S ribosomal protein S8

Chain Ah: % 89% 11%



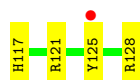
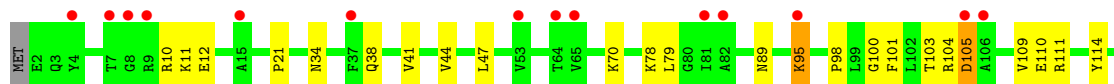
- Molecule 7: 30S ribosomal protein S8

Chain Bh: % 89% 11%

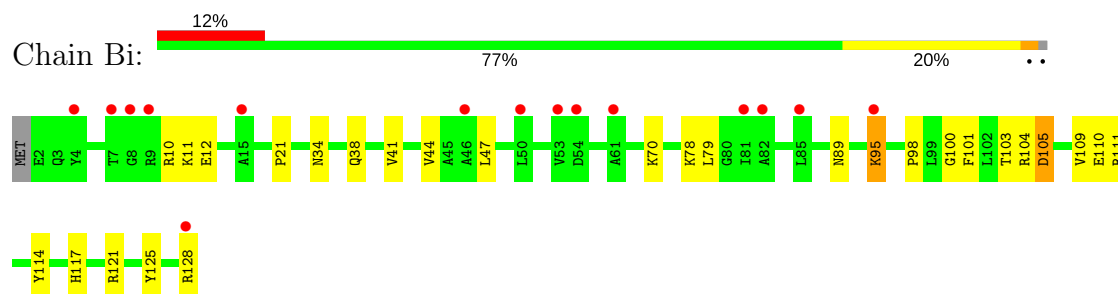


- Molecule 8: 30S ribosomal protein S9

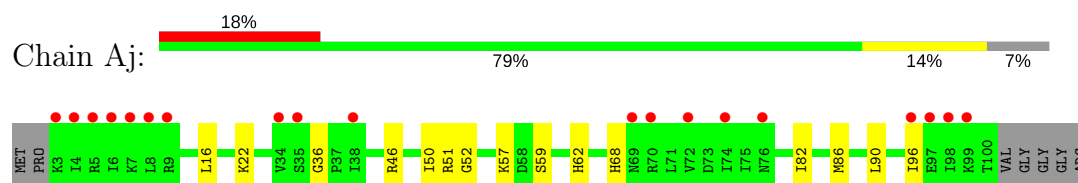
Chain Ai: 12% 77% 20%



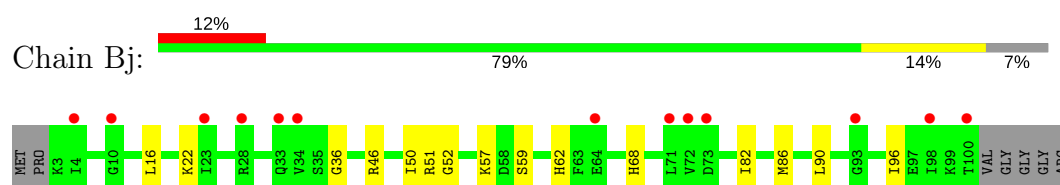
- Molecule 8: 30S ribosomal protein S9



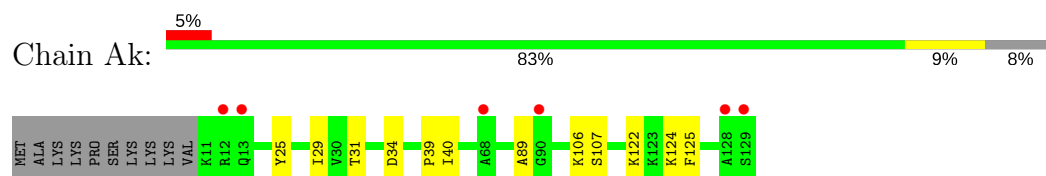
- Molecule 9: 30S ribosomal protein S10



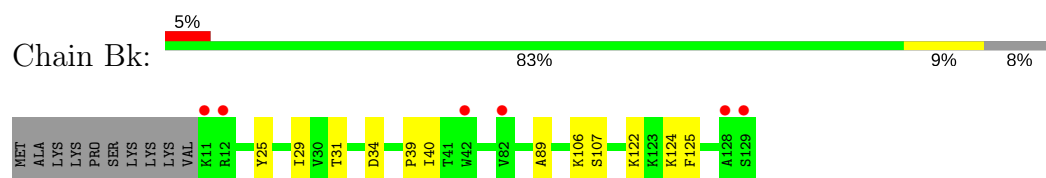
- Molecule 9: 30S ribosomal protein S10



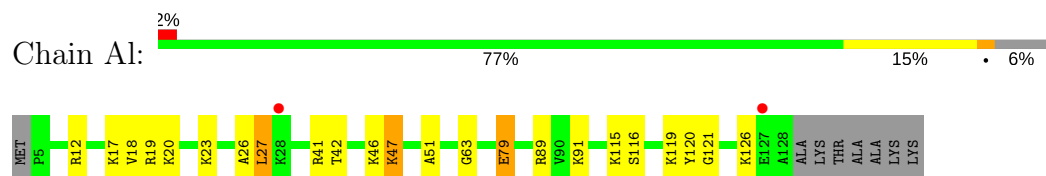
- Molecule 10: 30S ribosomal protein S11



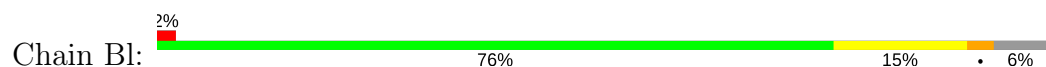
- Molecule 10: 30S ribosomal protein S11

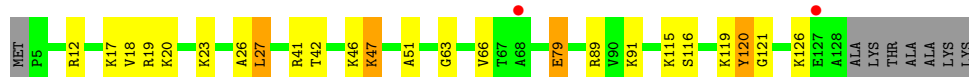


- Molecule 11: 30S ribosomal protein S12



- Molecule 11: 30S ribosomal protein S12

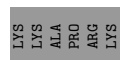




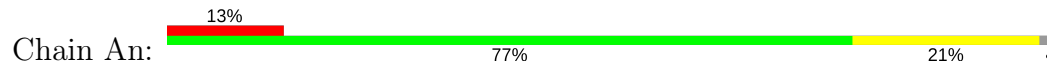
- Molecule 12: 30S ribosomal protein S13



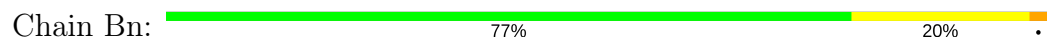
- Molecule 12: 30S ribosomal protein S13



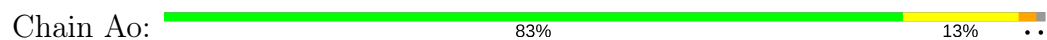
- Molecule 13: 30S ribosomal protein S14 type Z



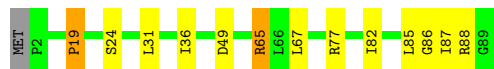
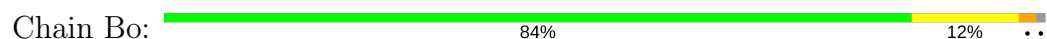
- Molecule 13: 30S ribosomal protein S14 type Z



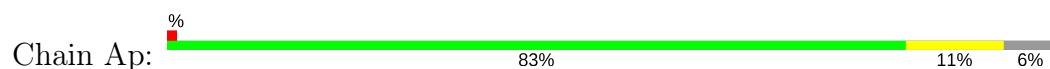
- Molecule 14: 30S ribosomal protein S15



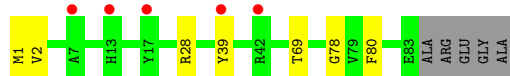
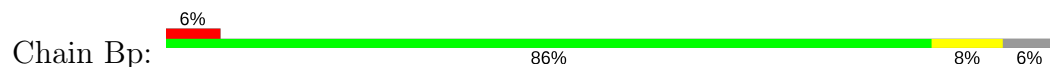
- Molecule 14: 30S ribosomal protein S15



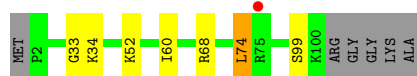
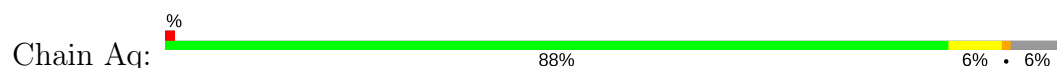
- Molecule 15: 30S ribosomal protein S16



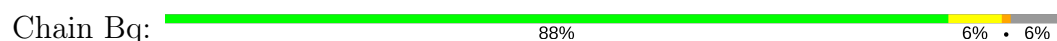
- Molecule 15: 30S ribosomal protein S16



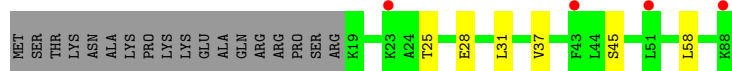
- Molecule 16: 30S ribosomal protein S17



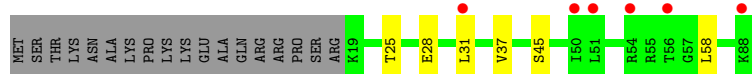
- Molecule 16: 30S ribosomal protein S17



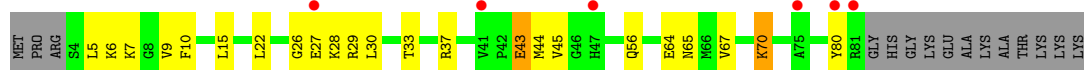
- Molecule 17: 30S ribosomal protein S18



- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19



- Chain By:
-
- | Chain | Category |
|-------|----------|
| MET | Red |
| A2 | Green |
| Y3 | Green |
| F4 | Green |
| L5 | Green |
| E9 | Green |
| R10 | Green |
| A11 | Green |
| E14 | Green |
| R16 | Green |
| K17 | Yellow |
| R23 | Green |
| E24 | Green |
| K29 | Green |
| L30 | Green |
| R38 | Green |
| L44 | Yellow |
| Y51 | Green |
| R56 | Green |
| Y64 | Green |
| V71 | Green |
| F74 | Green |
| S77 | Green |
| K80 | Green |
| R81 | Green |
| E82 | Green |
| R83 | Green |
| S84 | Green |
| E85 | Green |
| V86 | Green |
| Y87 | Green |
| S88 | Green |
| E89 | Green |
| L95 | Green |

Chain Aa:

2% 85% 14%

US
G9
G31
A32
G39
C47
C48
A51
A60
G61
G79
G80
U81
U82
U83
U84
A88
C89
U90
C91
G97
A101
G115
A116
A120
C121
C131
G144
C150
A172
U182
G189H
A195
A196
A197
C201
U202
U203
U204
G216
U244
G247
G251
G266
C267
A279
G289
A321
C328
A329
G332
C345
C352
A353
G354
C366
U367
C372
A373
A397
A412
G413
A414
U421
C422
G428
U429
A430
C435
C436
U437
G438
A439
A441
C442
A452
A453
C454
A461
G484
G485
U494
A496
U498
A509
A510
C511
G518
G527
A532
A533
U534
A547
A559
U560
U561
C562
A572
A573
G575
G576
G577
G588
G631
A632
A653
G658
A665
A687
G688
G724
G731
C749
G755
U793
A794
A816
C817
G818
A1004
U820
G821
A828
C832
U833
U839
C840
U841
C948
A859
U884
G898
G902
A913
A914
G927
C934
A935
U960
U961
G966
C967
A968
A969
C970
G971
A974
A975
G976
A977
A978
C979
C980
U991
U992
G993
A996
C999
A1000
A1001
G1001A
C1003
A1004
A1005
U1020
G1024
U1025
G1026
G1027
C1028
C1029
C1030
G1030B
C1030B
G1033
G1034
A1035
G1036
C1037
G1050
C1054
A1067
G1068
G1077
G1094
U1095
A1101
G1108
C1115
G1116
G1117
G1124
U1125
U1126
G1129
A1130
G1131
U1136
C1137
G1138
G1139
A1146
A1152
U1153
G1182
A1183
G1184
U1196
G1197
G1202
U1212
A1213
A1225
C1226
A1227
A1238
C1249
A1256
U1257
A1280
U1281
C1282
A1286
A1287
A1288
G1294
G1300
U1301
U1302
G1305
C1317
C1320
C1321
C1322
G1323
G1331
C1336
A1346
G1347
C1363
A1363A
U1364
A1398

Chain Ba:

2% 85% 14%

U1: A828, A829, A830, A831, A832, A833, A834, A835, A836, A837

U2: A838, A839, A840, A841, A842, A843, A844, A845, A846, A847

U3: A848, A849, A850, A851, A852, A853, A854, A855, A856, A857

U4: A858, A859, A860, A861, A862, A863, A864, A865, A866, A867

U5: A868, A869, A870, A871, A872, A873, A874, A875, A876, A877

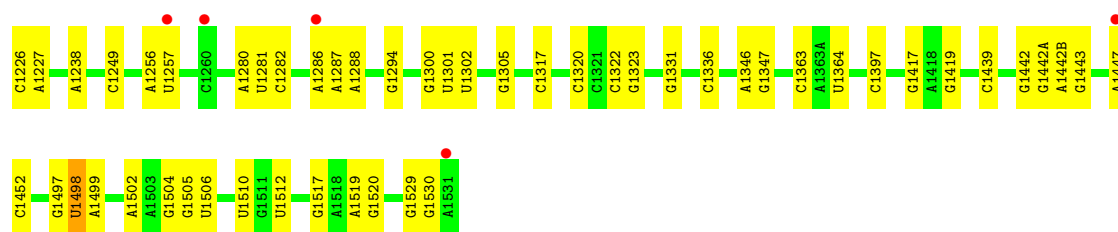
U6: A878, A879, A880, A881, A882, A883, A884, A885, A886, A887

U7: A888, A889, A890, A891, A892, A893, A894, A895, A896, A897

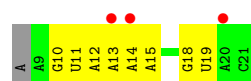
U8: A898, A899, A900, A901, A902, A903, A904, A905, A906, A907

U9: A908, A909, A910, A911, A912, A913, A914, A915, A916, A917

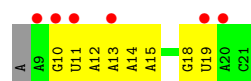
U10: A918, A919, A920, A921, A922, A923, A924, A925, A926, A927



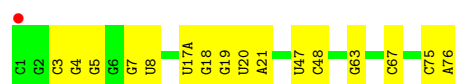
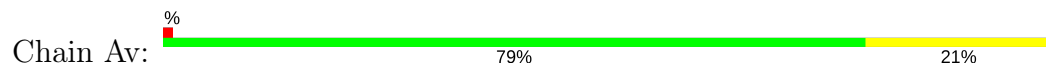
- Molecule 23: RNA (5'-R(*A*AP*GP*UP*AP*AP*AP*AP*AP*UP*GP*UP*A*(CCC))-3')



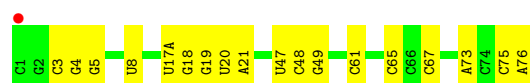
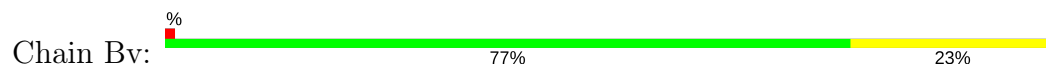
- Molecule 23: RNA (5'-R(*A*AP*GP*UP*AP*AP*AP*AP*AP*UP*GP*UP*A*(CCC))-3')



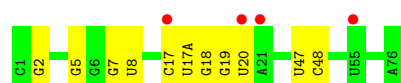
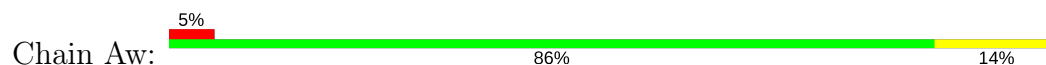
- Molecule 24: RNA (77-MER)



- Molecule 24: RNA (77-MER)

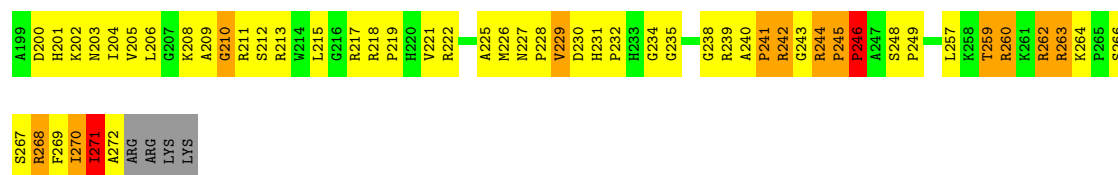


- Molecule 25: RNA (77-MER)



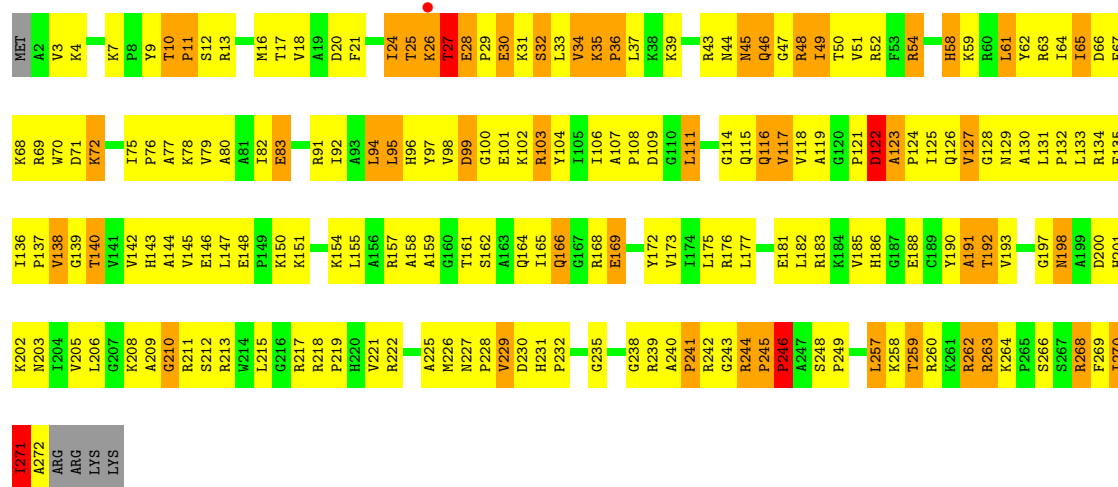
- Molecule 25: RNA (77-MER)





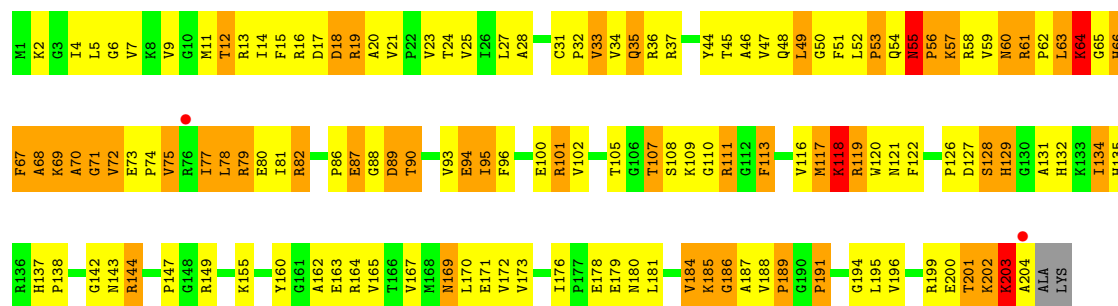
• Molecule 27: 50S ribosomal protein L2

Chain BD: 28% 51% 17%



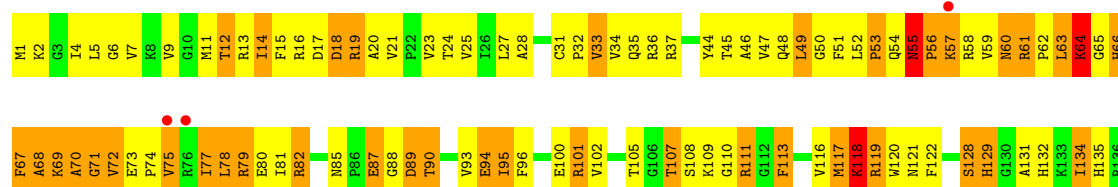
• Molecule 28: 50S ribosomal protein L3

Chain AE: 31% 44% 23%



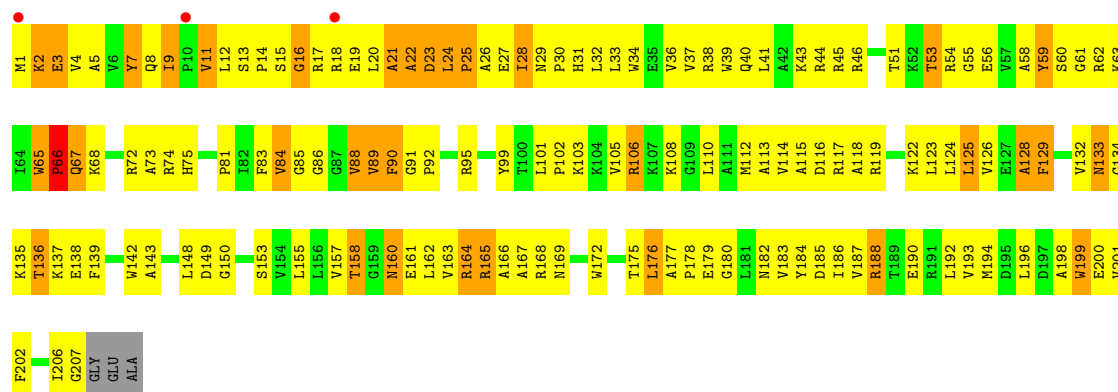
• Molecule 28: 50S ribosomal protein L3

Chain BE: 31% 44% 23%

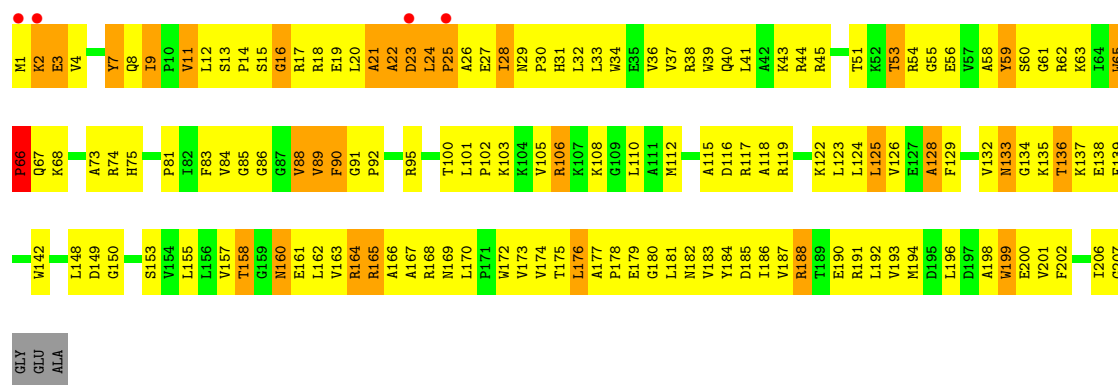




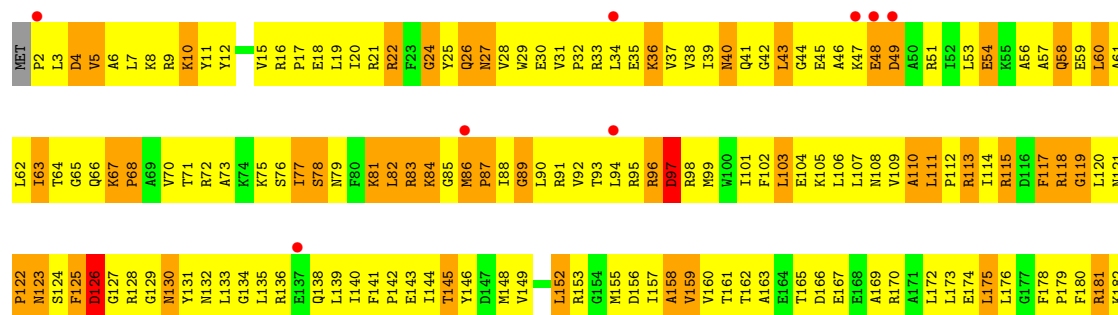
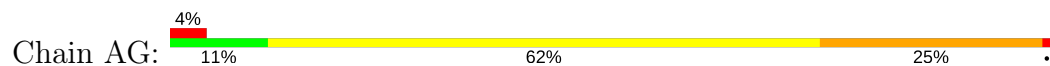
• Molecule 29: 50S ribosomal protein L4



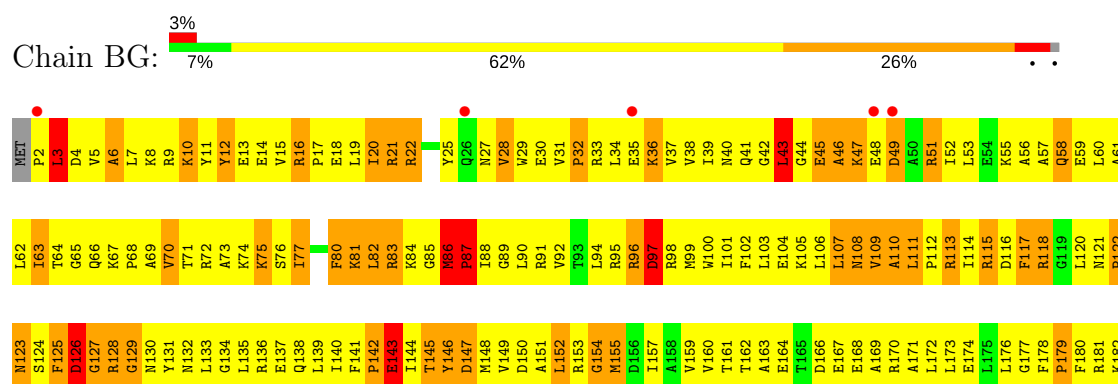
• Molecule 29: 50S ribosomal protein L4



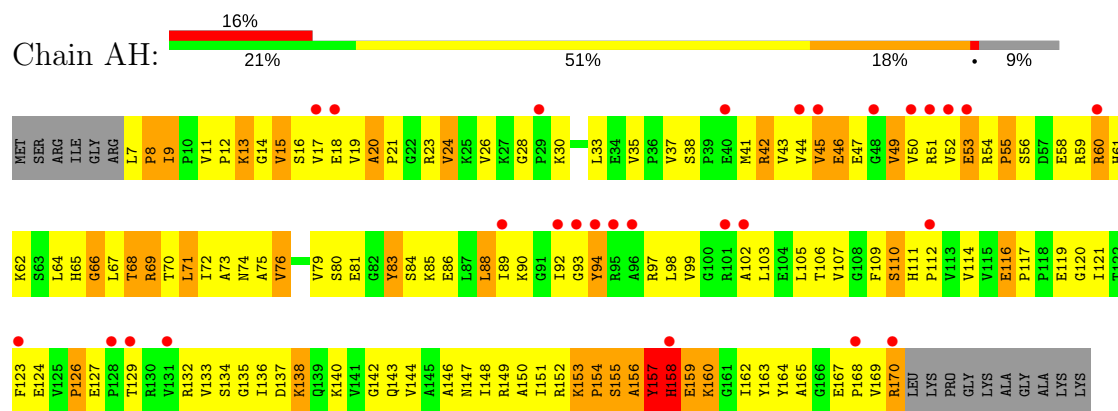
• Molecule 30: 50S ribosomal protein L5



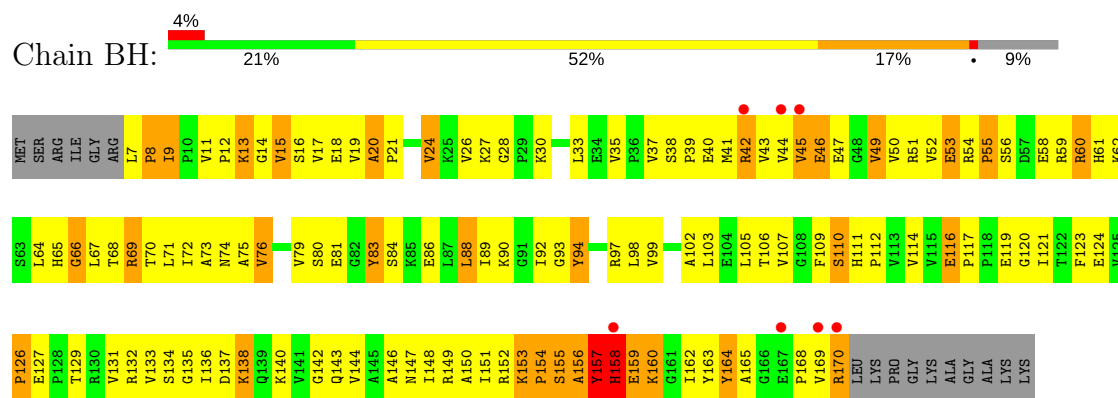
• Molecule 30: 50S ribosomal protein L5



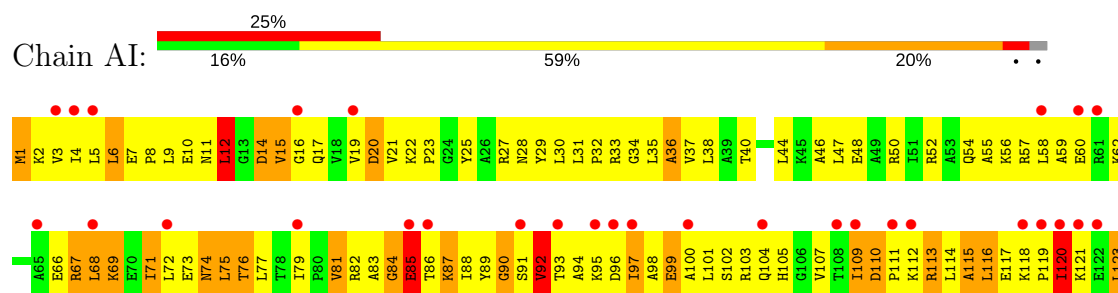
• Molecule 31: 50S ribosomal protein L6

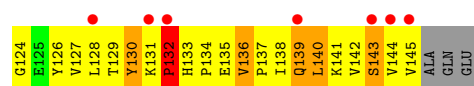


• Molecule 31: 50S ribosomal protein L6

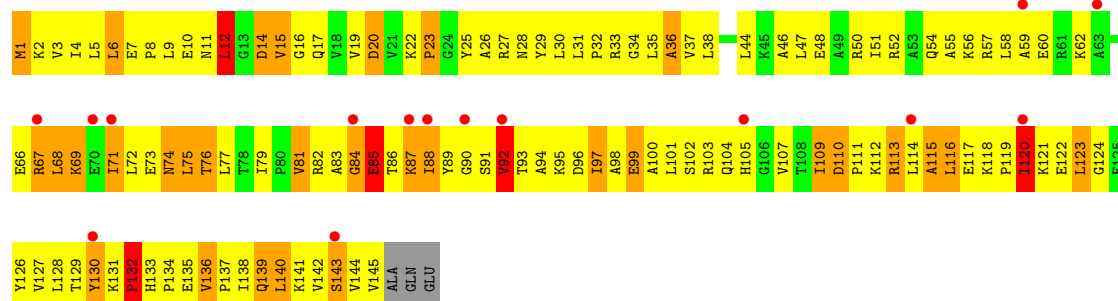
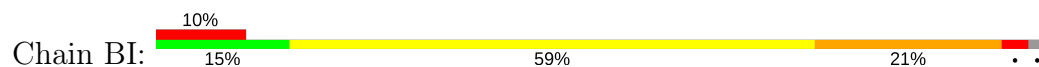


• Molecule 32: 50S ribosomal protein L9

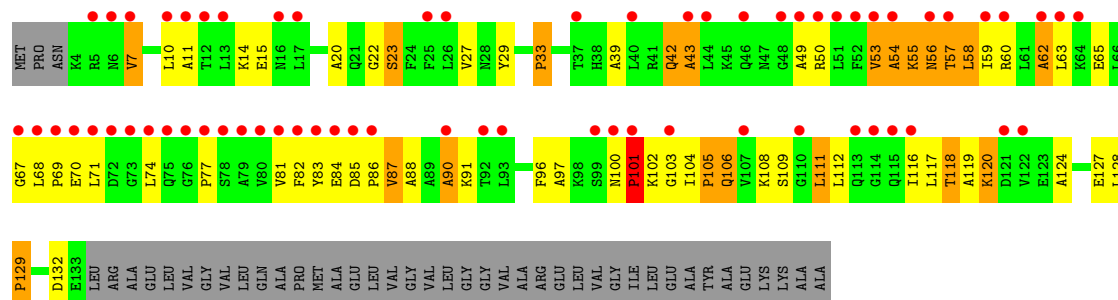




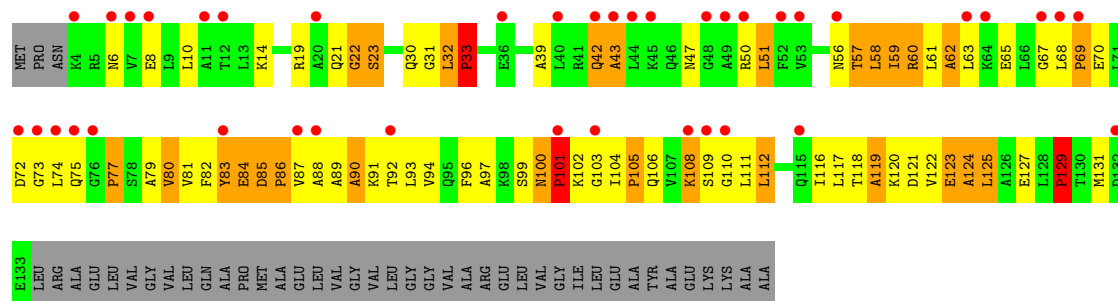
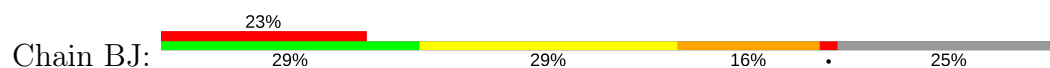
• Molecule 32: 50S ribosomal protein L9



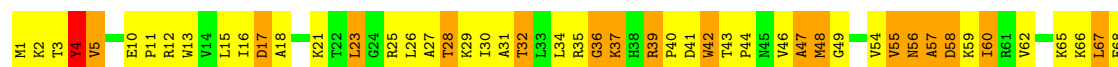
• Molecule 33: 50S ribosomal protein L10



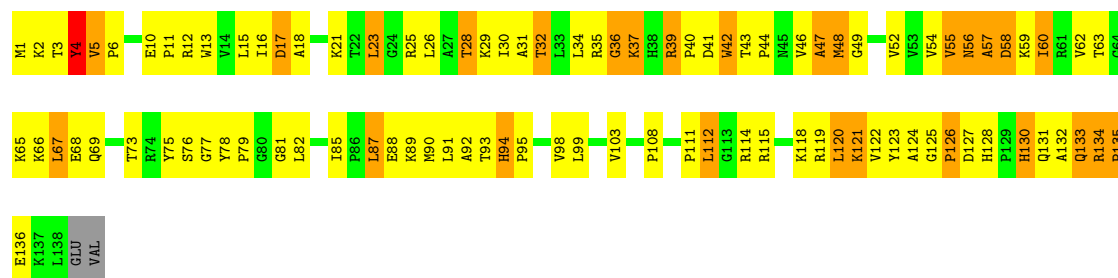
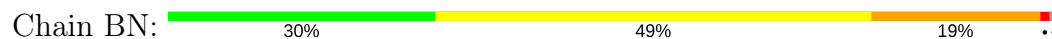
• Molecule 33: 50S ribosomal protein L10



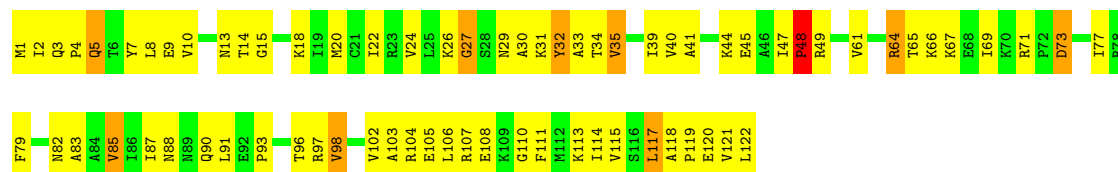
• Molecule 34: 50S ribosomal protein L13



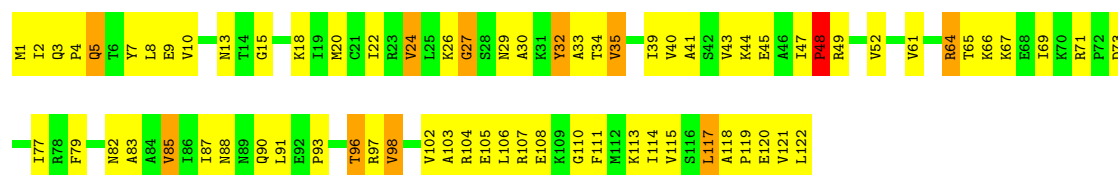
- Molecule 34: 50S ribosomal protein L13



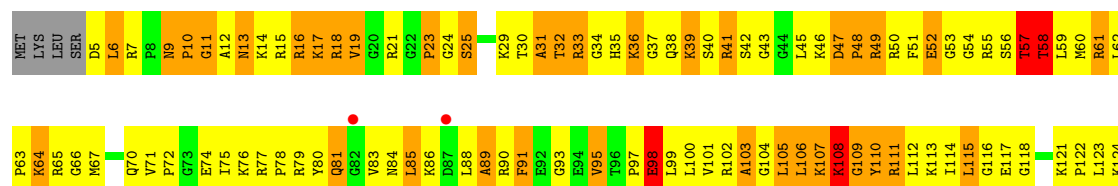
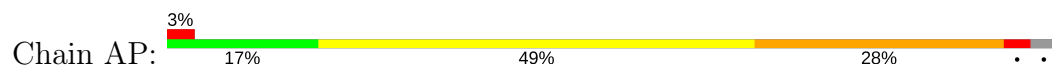
- Molecule 35: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L14



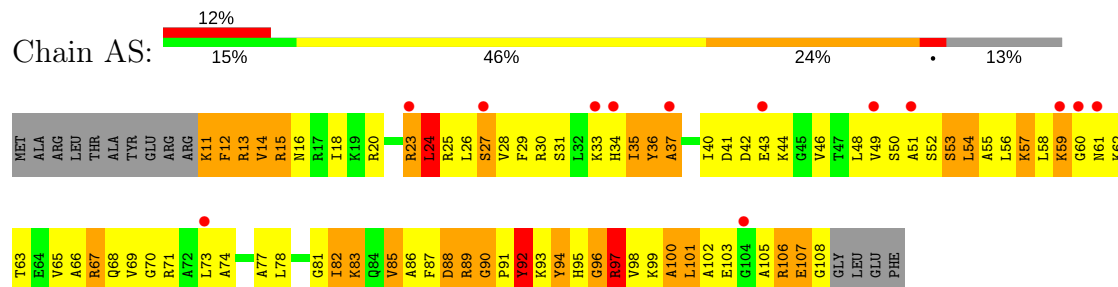
- Molecule 36: 50S ribosomal protein L15



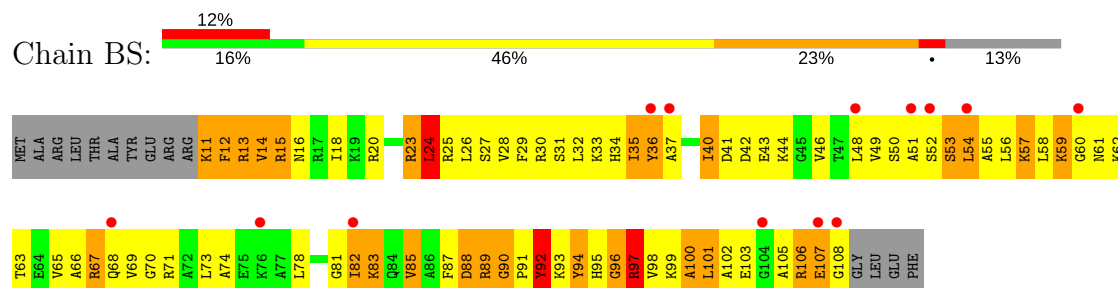
- Molecule 38: 50S ribosomal protein L17



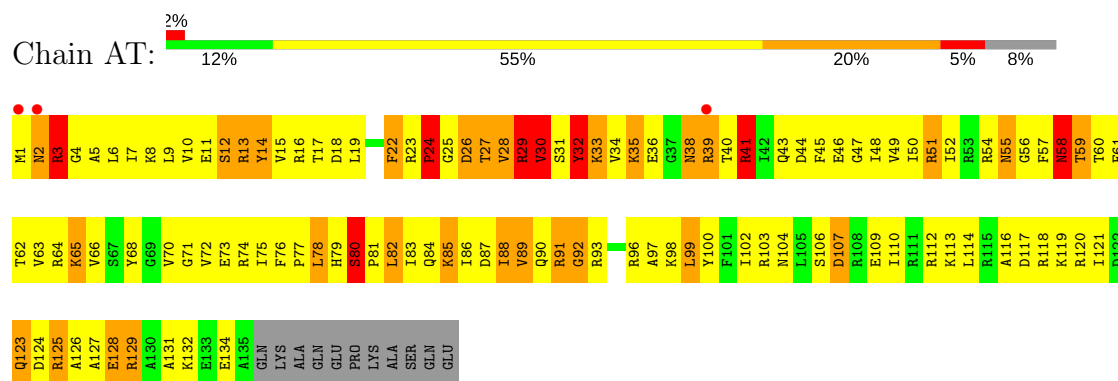
- Molecule 39: 50S ribosomal protein L18



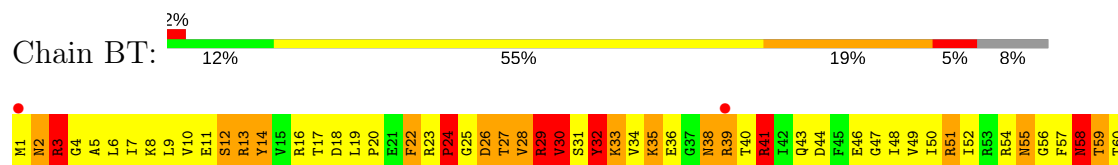
- Molecule 39: 50S ribosomal protein L18

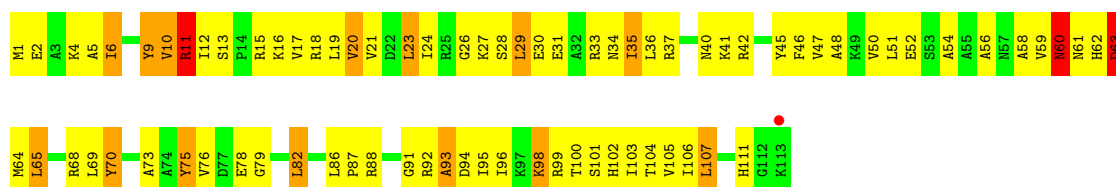


- Molecule 40: 50S ribosomal protein L19

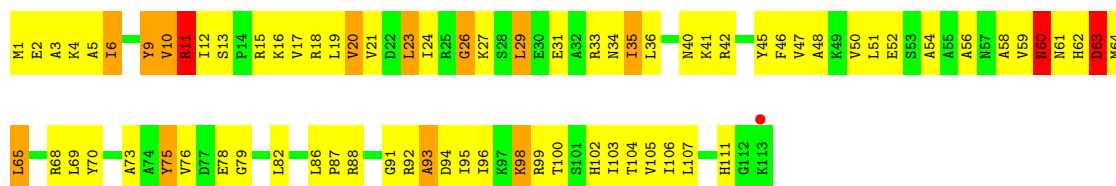


- Molecule 40: 50S ribosomal protein L19

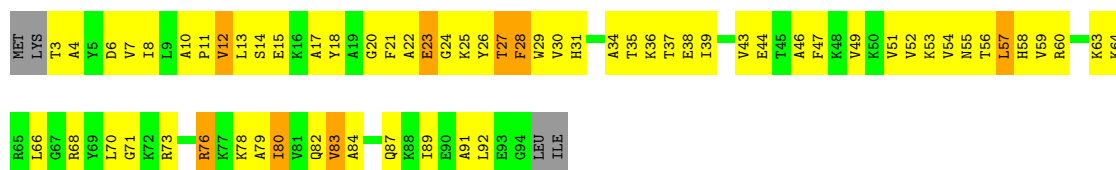




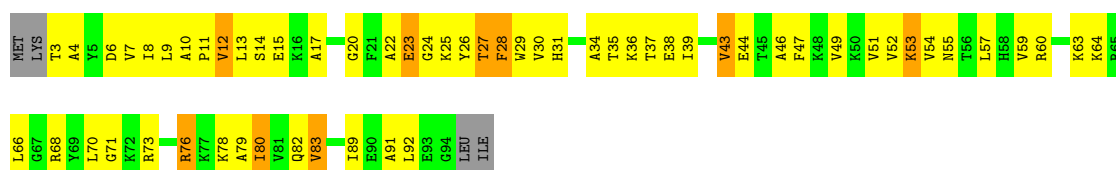
• Molecule 43: 50S ribosomal protein L22



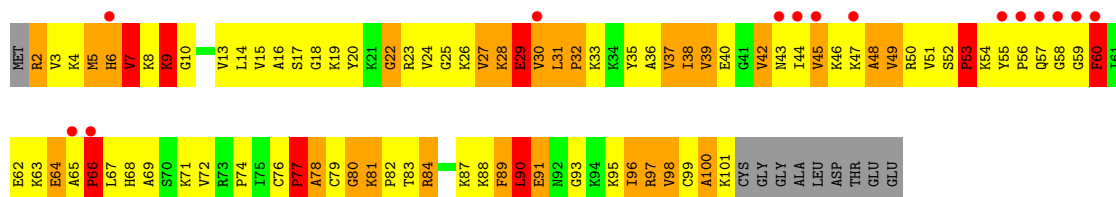
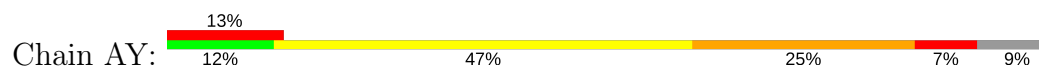
• Molecule 44: 50S ribosomal protein L23



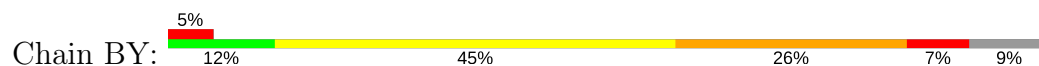
• Molecule 44: 50S ribosomal protein L23

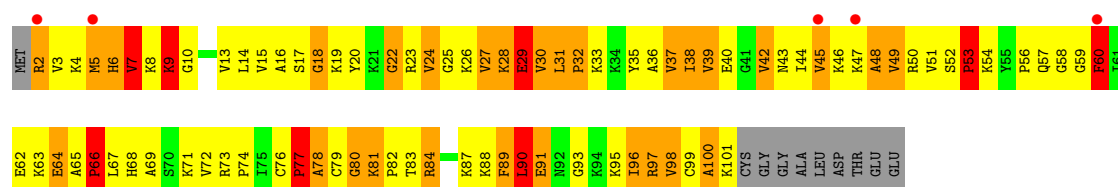


• Molecule 45: 50S ribosomal protein L24

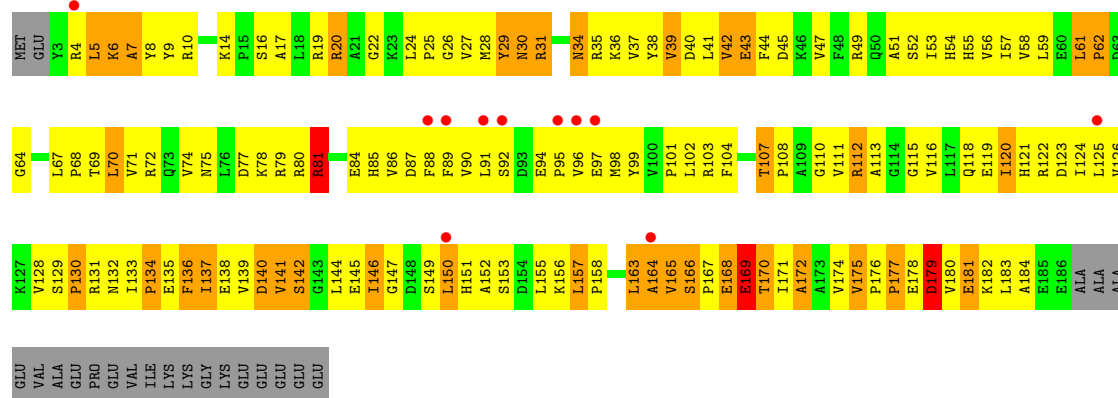
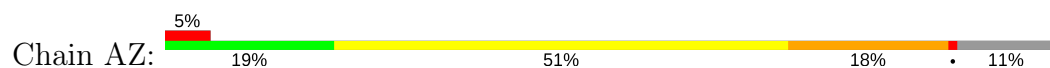


• Molecule 45: 50S ribosomal protein L24

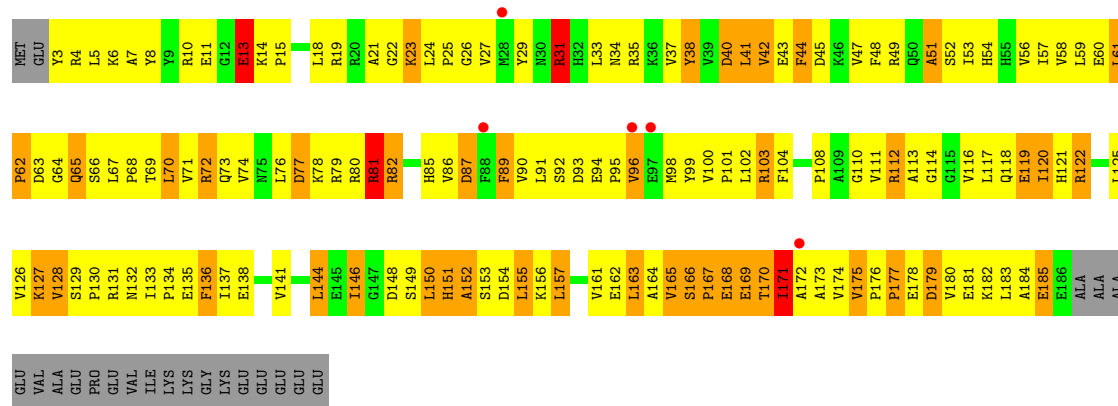
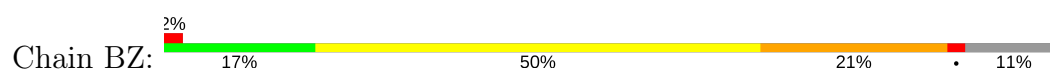




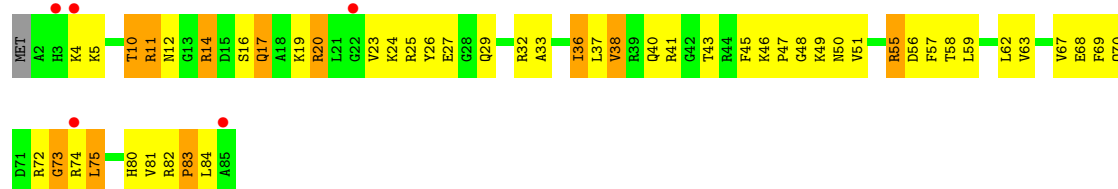
• Molecule 46: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L25

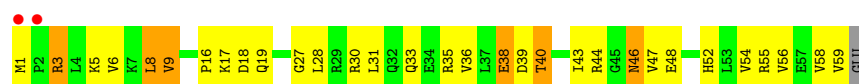


• Molecule 47: 50S ribosomal protein L27

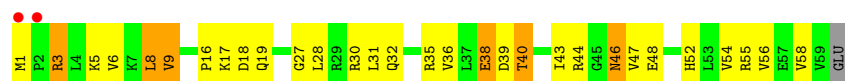


• Molecule 47: 50S ribosomal protein L27

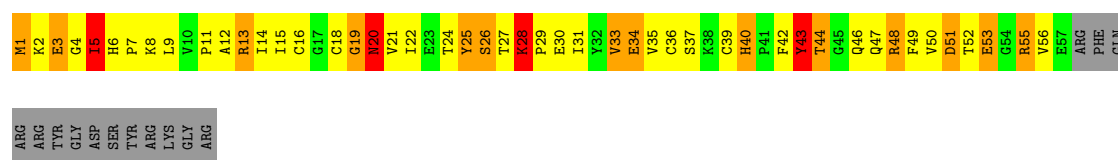




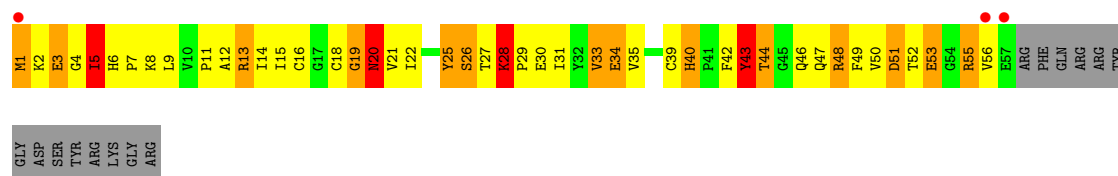
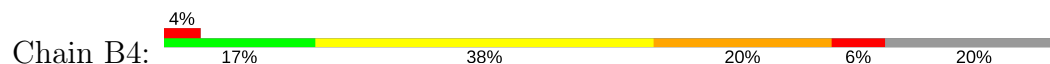
- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L31



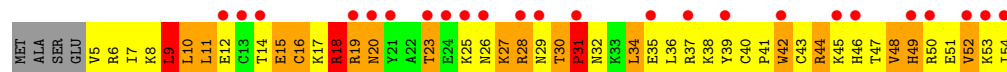
- Molecule 52: 50S ribosomal protein L32



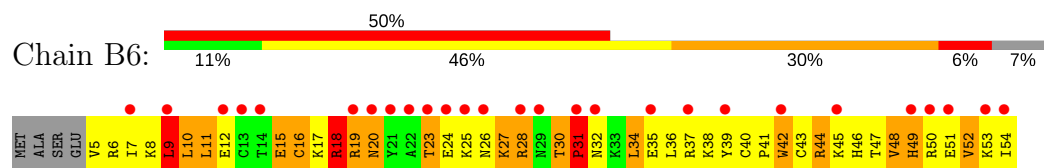
- Molecule 52: 50S ribosomal protein L32



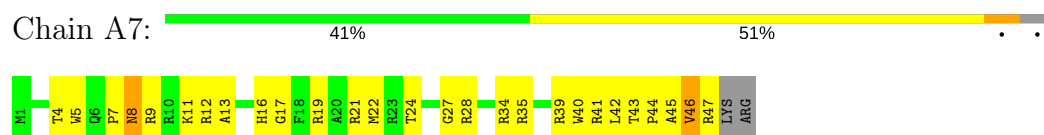
- Molecule 53: 50S ribosomal protein L33



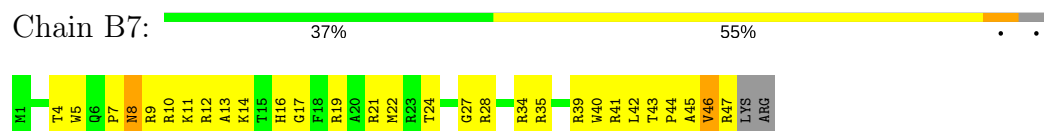
- Molecule 53: 50S ribosomal protein L33



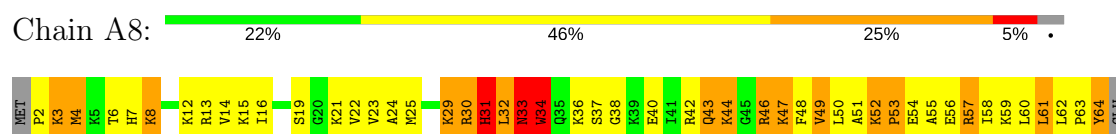
- Molecule 54: 50S ribosomal protein L34



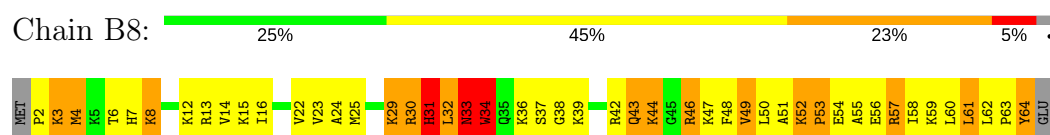
- Molecule 54: 50S ribosomal protein L34



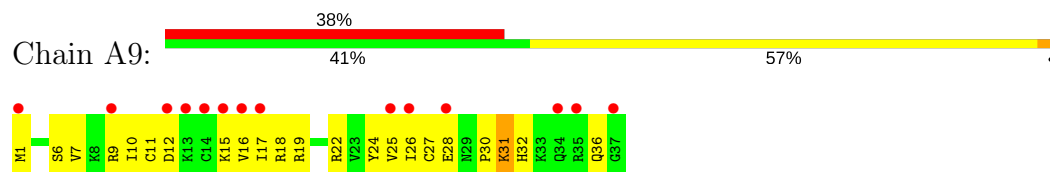
- Molecule 55: 50S ribosomal protein L35



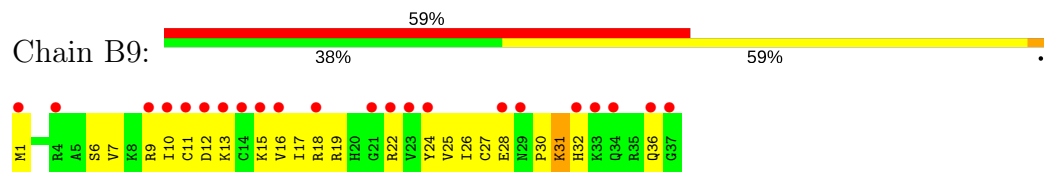
- Molecule 55: 50S ribosomal protein L35



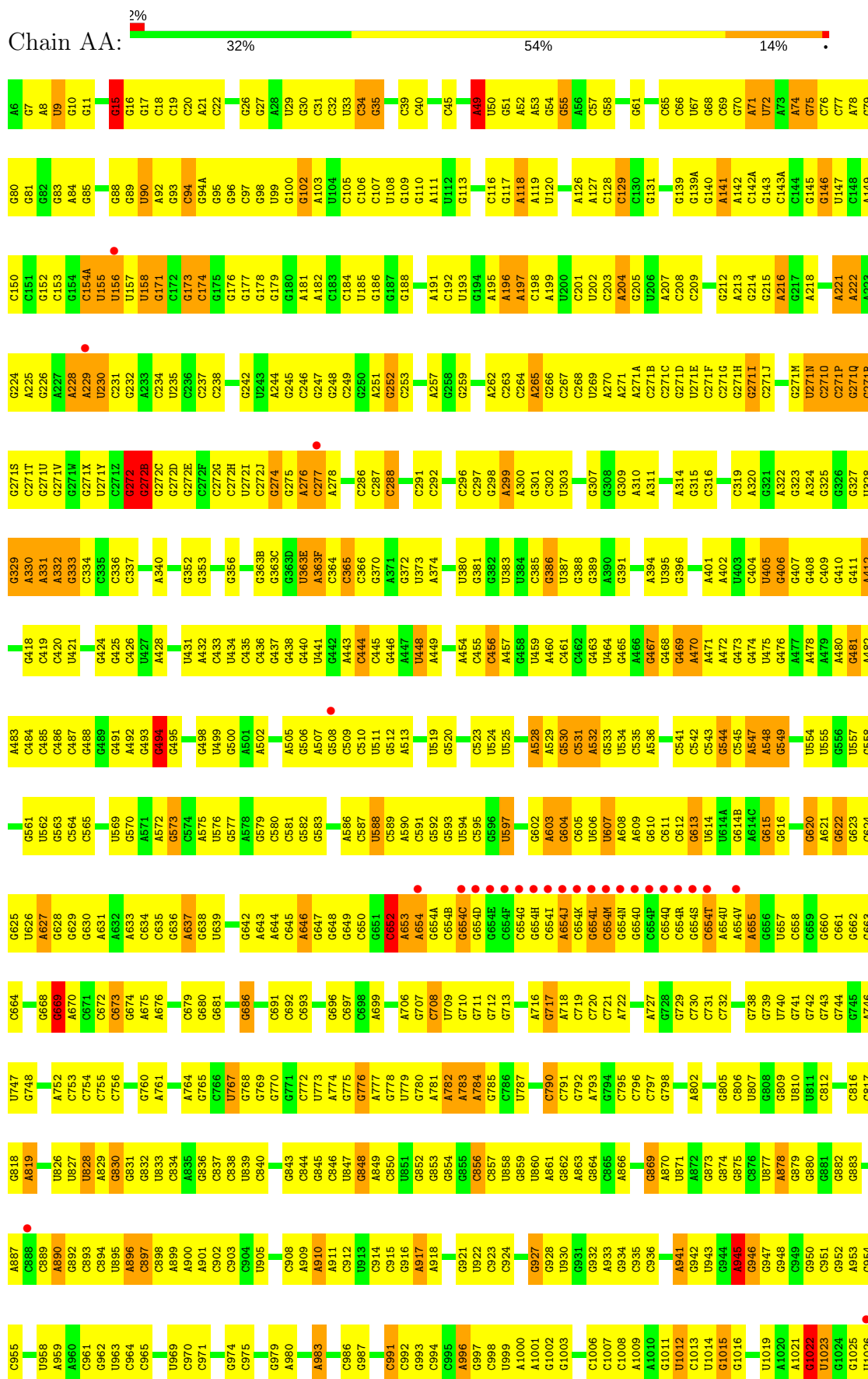
- Molecule 56: 50S ribosomal protein L36



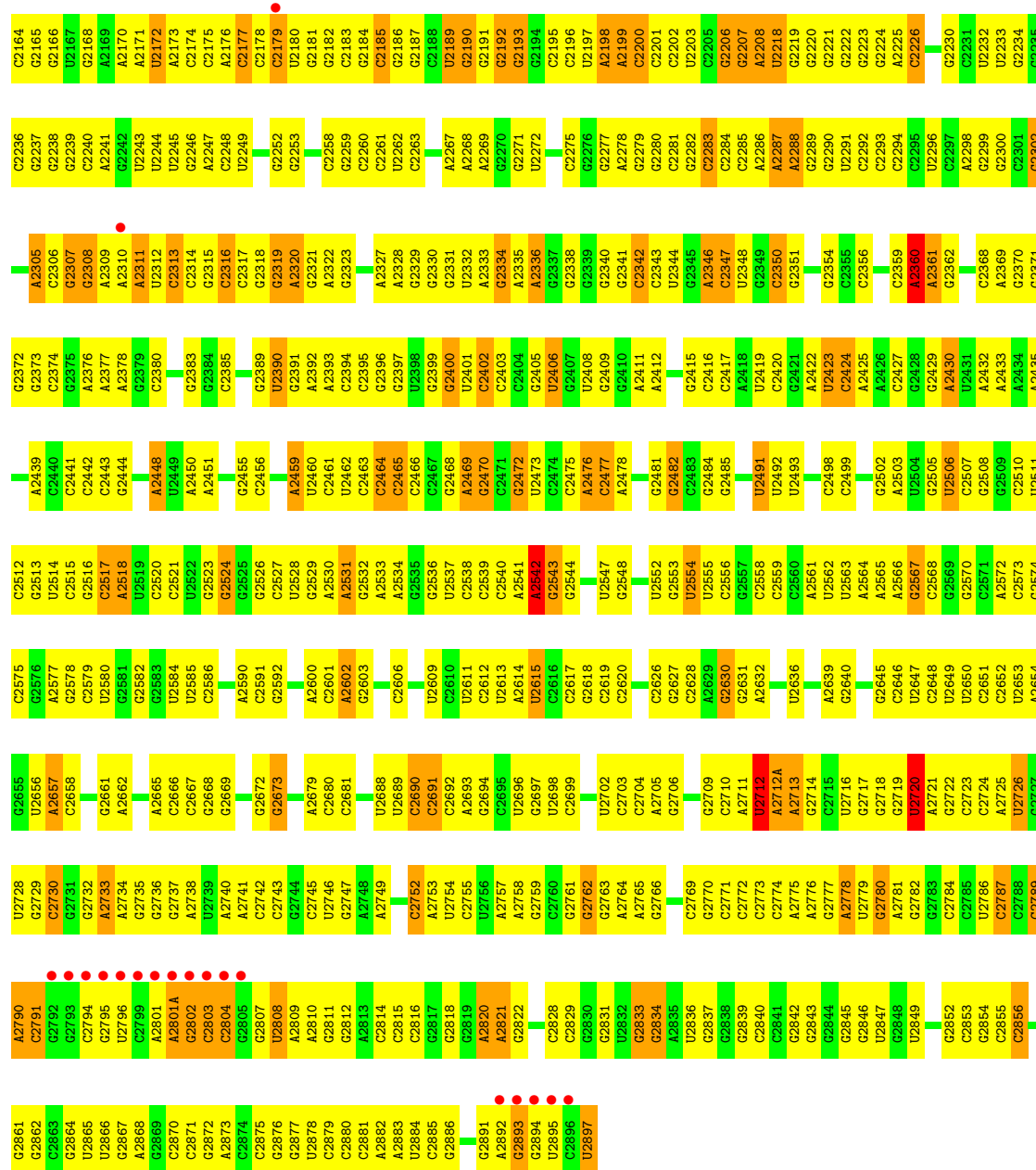
- Molecule 56: 50S ribosomal protein L36



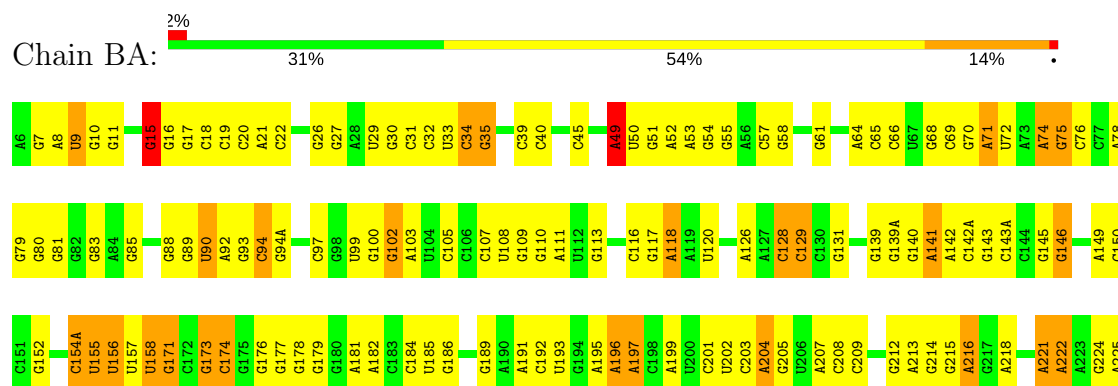
- Molecule 57: RNA (2848-MER)



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U2102	U2034	G1964	A1890	U1720	G1650	G1573	C1501	A1434	G1364	C1293	C1221	G1151	A1028
G2103	G2035	C1985	G1891	G1721	G1651	G1574	C1502	G1435	A1365	U1294	C1221A	C1152	
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G2105	C2039	G1967	C1893	U1739	G1653	U1577	C1504	A1437	A1367			A1155	G1037
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G2107	A1969	A1969	U1898	A1741	A1655	A1579	C1506	A1439	G1369	A1301	G1228	G1157	C1039
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U2109	A2042	A1971	G1899	G1743	C1658	G1582	C1509	G1441	G1374	A1306	G1231	U1159	C1041
G2110	C2043	A1972	A1901			A1583	C1509A	G1442	G1374	C1306	G1232	U1160	
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G2112	G2046		G1903	G1748	A1663	C1584	G1510	G1444	A1378	A1308	U1234	G1162	A1046
U2113		C1979	G1904	A1749	A1664	A1586	G1511	A1445	A1379	G1309		G1163	G1047
A2114	G2052	G1980	C1905	G1750	A1665	A1587		C1446	G1380		U1240	G1164	A1048
G2115	G2053	A1981	G1906	C1751	G1666	C1588	C1516	C1447	A1384	G1310	U1241	U1165	A1049
G2116	A2054	G1982	A1987	A1825	G1667	C1589	U1517	G1448	G1385	G1311	A1242	A1050	A1050
A2117	G2055	C1983	C1908	G1754	A1668	U1590	U1518	A1449	G1386	U1313	G1243	U1167	G1051
G2118	C2056	G1984	A1969	A1755	A1669	G1591	U1519	G1450	C1387	C1314	G1244	G1168	C1052
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G2068	G2068	G1922	G1839		A1603	C1604	C1532	G1465	U1397	G1329	G1256	C1180	G1115
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G2070	G2070	C1924	G1846	A1773	G1683	C1605	U1534	G1467	G1401	A1331	G1260	G1187	G1117
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G2072	G2072	U1926	A1847	U1775	C1685	C1607	C1536	A1469	G1403	C1333		U1187	G1119
A2134	C2073	G2000	A1848	G1776	C1686	A1608	G1537	A1469	C1404		G1264	G1187	G1120
U2074	U2074	A2001			G1687	G1609	G1538	G1470	G1404	U1341		U1194	
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A2077	A2077	A1932	G1855	A1780	A1690	G1613	A1542	C1474	G1408	A1268	G1270	G1192	
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G2083	G2083	A1937	G1862		G1696	A1618	C1547	G1478	G1412	U1274	U1275	C1200	A1132
C2084	C2084	U1938	G1863	C1790	G1697		C1548	G1479	G1346	A1274	A1275	C1201	G1136
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G2095	G2095	U1955	G1883	A1802	C1711	A1641		G1491	C1429	A1287	A1287	G1145	C1145
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A2031	A2031	U1887	C1887	G1647	G1714		A1570	A1495				G1217	
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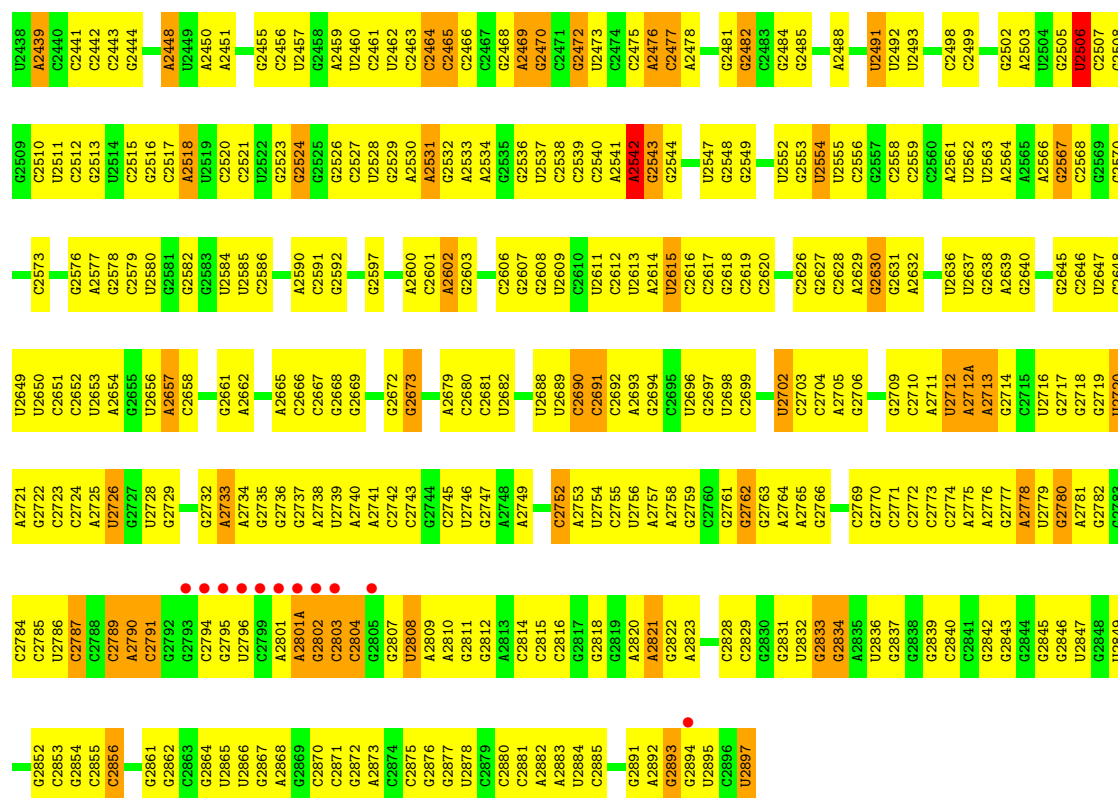


• Molecule 57: RNA (2848-MER)

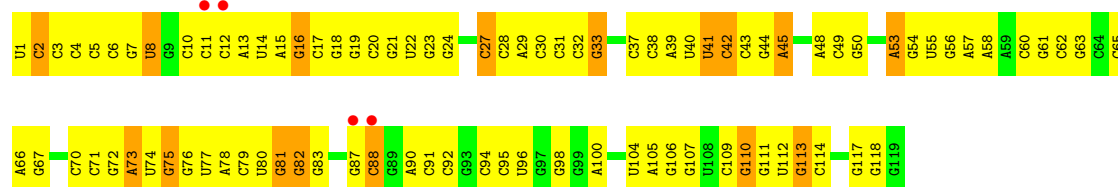


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U1289	U1290	U1291	G1215	C1145	A1021	G950	G879	C817	G748	U667	G628	U562	C484	G419	A331	G271V	A227
C1292	U1292	U1293	G1216	C1146	U1022	G951	G880	G818	A751	G668	G629	C563	A485	C420	G332	G271W	A228
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U1300	A1301	C1305	G1218	C1150	G1024	G953	G882	A820	A753	A670	A631	C565	C487	U421	C334	U271Y	C231
A1301	C1306	C1307	G1219	C1151	U1026	C955	G883	A821	C754	C672	A632	U569	G489	G424	C335	G271Z	G232
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A1315	A1314	C1315	G1226	C1158	C1041	C964	A890	A829	G766	G639	U640	C576	G497	G431	G355	G272G	G242
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U1318	A1317	C1318	G1229	C1161	G1046	C970	C893	G832	G769	G644	A645	C580	A506	U434	G363B	G272J	G245
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G1327	A1324	C1325	G1236	C1168	G1053	G979	U906	C840	G776	G652	C653	C513	A514	U441	C366	G272Q	G252
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A1336	A1329	C1330	G1241	C1173	G1110	C986	C911	G845	G781	G657	A658	C518	A519	U446	G373	G298	G298
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U1341	A1331	C1332	G1243	C1175	G1112	C988	C913	G847	G783	G659	A660	C520	A521	U448	G375	G301	G301
A1344	A1332	C1333	G1244	C1176	G1113	C989	C914	U847	G784	G660	A661	C521	A522	U449	G376	G302	G302
G1345	A1333	C1334	G1245	C1177	G1114	C990	C915	G848	G785	G661	A662	C522	A523	U450	G377	G303	G303
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A1354	A1350	C1351	G1262	C1194	G1131	C1007	C932	G865	C802	G678	A679	C539	A540	U467	G394	G320	G320
G1355	A1351	C1352	G1263	C1195	G1132	C1008	C933	G866	C803	G679	A680	C540	A541	U468	G395	G321	G321
U1352	A1352	C1353	G1264	C1196	G1133	C1009	C934	U866	C804	G680	A681	C541	A542	U469	G396	G322	G322
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G1355	A1354	C1355	G1266	C1198	G1135	C1011	C936	G868	C806	G682	A683	C543	A544	U471	G400	G324	G324
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A1354	A1356	C1357	G1268	C1200	G1137	C1013	C938	G870	C808	G684	A685	C545	A546	U473	G402	G326	G326
G1355	A1357	C1358	G1269	C1201	G1138	C1014	C939	U871	C809	G685	A686	C546	A547	U474	G403	G327	G327
U1352	A1358	C1359	G1270	C1202	G1139	C1015	C940	U872	C810	G686	A687	C547	A548	U475	G404	G328	G328
A1354	A1359	C1360	G1271	C1203	G1140	C1016	C941	U873	C811	G687	A688	C548	A549	U476	G405	G329	G329
U1352	A1360	C1361	G1272	C1204	G1141	C1017	C942	U874	C812	G688	A689	C549	A550	U477	G406	G330	G330
A1354	A1361	C1362	G1273	C1205	G1142	C1018	C943	U875	C813	G689	A690	C550	A551	U478	G407	G331	G331
G1355	A1362	C1363	G1274	C1206	G1143	C1019	C944	U876	C814	G690	A691	C551	A552	U479	G408	G332	G332
U1352	A1363	C1364	G1275	C1207	G1144	C1020	C945	U877	C815	G691	A692	C552	A553	U480	G409	G333	G333
A1354	A1364	C1365	G1276	C1208	G1145	C1021	C946	U878	C816	G692	A693	C553	A554	U481	G410	G334	G334
G1355	A1365	C1366	G1277	C1209	G1146	C1022	C947	U879	C817	G693	A694	C554	A555	U482	G411	G335	G335
U1352	A1366	C1367	G1278	C1210	G1147	C1023	C948	U880	C818	G694	A695	C555	A556	U483	G412	G336	G336
A1354	A1367	C1368	G1279	C1211	G1148	C1024	C949	U881	C819	G695	A696	C556	A557	U484	G413	G337	G337
G1355	A1368	C1369	G1280	C1212	G1149	C1025	C950	U882	C820	G696	A697	C557	A558	U485	G414	G338	G338
U1352	A1369	C1370	G1281	C1213	G1150	C1026	C951	U883	C821	G697	A698	C558	A559	U486	G415	G339	G339
A1354	A1370	C1371	G1282	C1214	G1151	C1027	C952	U884	C822	G698	A699	C559	A560	U487	G416	G340	G340
G1355	A1371	C1372	G1283	C1215	G1152	C1028	C953	U885	C823	G699	A700	C560	A561	U488	G417	G341	G341
U1352	A1372	C1373	G1284	C1216	G1153	C1029	C954	U886	C824	G700	A701	C561	A562	U489	G418	G342	G342
A1354	A1373	C1374	G1285	C1217	G1154	C1030	C955	U887	C825	G701	A702	C562	A563	U490	G419	G343	G343
G1355	A1374	C1375	G1286	C1218	G1155	C1031	C956	U888	C826	G702	A703	C563	A564	U491	G420	G344	G344
U1352	A1375	C1376	G1287	C1219	G1156	C1032	C957	U889	C827	G703	A704	C564	A565	U492	G421	G345	G345
A1354	A1376	C1377	G1288	C1220	G1157	C1033	C958	U890	C828	G704	A705	C565	A566	U493	G422	G346	G346
G1355	A1377	C1378	G1289	C1221	G1158	C1034	C959	U891	C829	G705	A706	C566	A567	U494	G423	G347	G347
U1352	A1378	C1379	G1290	C1222	G1159	C1035	C960	U892	C830	G706	A707	C567	A568	U495	G424	G348	G348
A1354	A1379	C1380	G1291	C1223	G1160	C1036	C961	U893	C831	G707	A708	C568	A569	U496	G425	G349	G349
G1355	A																

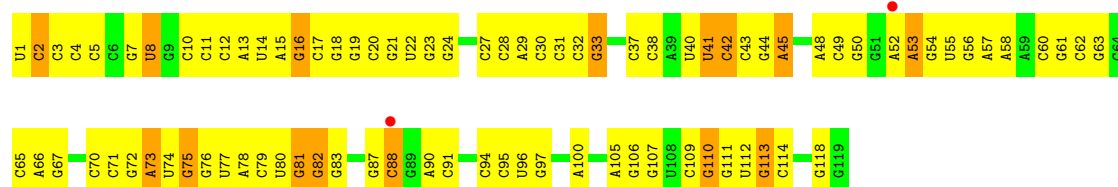
WORLDWIDE
PDB
PROTEIN DATA BANK



• Molecule 58: RNA (119-MER)



• Molecule 58: RNA (119-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.23Å 451.43Å 623.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.60 49.63 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.63-3.60) 99.8 (49.63-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.57Å)	Xtriage
Refinement program	CNS1.2	Depositor
R, R_{free}	0.215 , 0.245 0.221 , 0.253	Depositor DCC
R_{free} test set	30861 reflections (4.75%)	DCC
Wilson B-factor (Å ²)	103.4	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 102.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	297230	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MG, CCC

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	Ab	0.33	0/1935	0.61	0/2609
1	Bb	0.33	0/1935	0.62	0/2609
2	Ac	0.31	0/1636	0.58	0/2205
2	Bc	0.32	0/1636	0.58	0/2205
3	Ad	0.37	0/1733	0.65	1/2318 (0.0%)
3	Bd	0.36	0/1733	0.64	1/2318 (0.0%)
4	Ae	0.35	0/1162	0.64	0/1564
4	Be	0.37	0/1162	0.65	0/1564
5	Af	0.34	0/856	0.64	0/1154
5	Bf	0.37	0/856	0.65	0/1154
6	Ag	0.32	0/1276	0.57	0/1709
6	Bg	0.32	0/1276	0.57	0/1709
7	Ah	0.35	0/1136	0.64	0/1527
7	Bh	0.35	0/1136	0.64	0/1527
8	Ai	0.33	0/1029	0.57	0/1379
8	Bi	0.33	0/1029	0.57	0/1379
9	Aj	0.33	0/807	0.62	0/1085
9	Bj	0.33	0/807	0.62	0/1085
10	Ak	0.36	0/900	0.64	0/1213
10	Bk	0.36	0/900	0.64	0/1213
11	Al	0.40	0/986	0.72	1/1320 (0.1%)
11	Bl	0.41	0/986	0.72	1/1320 (0.1%)
12	Am	0.30	0/947	0.56	0/1270
12	Bm	0.30	0/947	0.61	0/1270
13	An	0.35	0/501	0.56	0/664
13	Bn	0.36	0/501	0.57	0/664
14	Ao	0.33	0/745	0.59	0/992
14	Bo	0.35	0/745	0.60	0/992
15	Ap	0.34	0/716	0.62	0/963
15	Bp	0.32	0/716	0.62	0/963
16	Aq	0.38	0/836	0.67	0/1117
16	Bq	0.36	0/836	0.66	0/1117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Ar	0.36	0/579	0.66	0/768
17	Br	0.36	0/579	0.67	0/768
18	As	0.36	0/642	0.63	0/865
18	Bs	0.35	0/642	0.64	0/865
19	At	0.34	0/765	0.63	0/1007
19	Bt	0.34	0/765	0.63	0/1007
20	Au	0.42	0/212	0.59	0/277
20	Bu	0.40	0/212	0.59	0/277
21	Ay	0.35	0/793	0.59	0/1059
21	By	0.35	0/793	0.68	0/1059
22	Aa	0.41	0/36190	0.69	13/56486 (0.0%)
22	Ba	0.42	0/36190	0.70	11/56486 (0.0%)
23	Ax	0.43	0/289	0.73	0/449
23	Bx	0.43	0/289	0.73	0/449
24	Av	0.43	0/1810	0.70	0/2821
24	Bv	0.46	0/1810	0.72	0/2821
25	Aw	0.36	0/1832	0.70	0/2855
25	Bw	0.36	0/1832	0.71	0/2855
26	AC	0.32	0/956	0.56	0/1288
26	BC	0.30	0/956	0.56	0/1288
27	AD	0.46	0/2154	0.81	1/2905 (0.0%)
27	BD	0.48	0/2154	0.82	1/2905 (0.0%)
28	AE	0.45	0/1596	0.80	1/2153 (0.0%)
28	BE	0.47	0/1596	0.79	1/2153 (0.0%)
29	AF	0.41	0/1658	0.72	0/2244
29	BF	0.43	0/1658	0.73	0/2244
30	AG	0.37	0/1499	0.73	1/2016 (0.0%)
30	BG	0.39	0/1499	0.73	0/2016
31	AH	0.39	0/1284	0.75	1/1739 (0.1%)
31	BH	0.44	0/1284	0.78	1/1739 (0.1%)
32	AI	0.40	0/1146	0.92	4/1551 (0.3%)
32	BI	0.39	0/1146	0.91	4/1551 (0.3%)
33	AJ	0.36	0/640	0.77	7/889 (0.8%)
33	BJ	0.39	0/640	0.88	6/889 (0.7%)
34	AN	0.39	0/1131	0.74	1/1525 (0.1%)
34	BN	0.43	0/1131	0.75	1/1525 (0.1%)
35	AO	0.45	0/943	0.71	0/1269
35	BO	0.45	0/943	0.71	0/1269
36	AP	0.46	0/1131	1.00	6/1504 (0.4%)
36	BP	0.52	0/1131	1.03	6/1504 (0.4%)
37	AQ	0.40	0/1133	0.65	0/1515
37	BQ	0.40	0/1133	0.66	0/1515
38	AR	0.43	0/974	0.79	1/1302 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	BR	0.46	0/974	0.79	1/1302 (0.1%)
39	AS	0.37	0/778	0.71	0/1036
39	BS	0.39	0/778	0.72	0/1036
40	AT	0.47	0/1137	0.89	4/1519 (0.3%)
40	BT	0.47	0/1137	0.89	4/1519 (0.3%)
41	AU	0.45	1/975 (0.1%)	0.71	0/1297
41	BU	0.49	0/975	0.73	0/1297
42	AV	0.40	0/790	0.77	0/1057
42	BV	0.42	0/790	0.78	0/1057
43	AW	0.45	0/907	0.75	1/1216 (0.1%)
43	BW	0.47	0/907	0.76	1/1216 (0.1%)
44	AX	0.43	0/739	0.69	0/993
44	BX	0.47	0/739	0.72	0/993
45	AY	0.43	0/788	0.76	1/1051 (0.1%)
45	BY	0.48	0/788	0.78	1/1051 (0.1%)
46	AZ	0.36	0/1499	0.68	0/2035
46	BZ	0.37	0/1499	0.72	0/2035
47	A0	0.39	0/671	0.65	0/892
47	B0	0.42	0/671	0.67	0/892
48	A1	0.39	0/738	0.76	1/981 (0.1%)
48	B1	0.46	0/738	0.80	1/981 (0.1%)
49	A2	0.34	0/600	0.63	0/793
49	B2	0.44	0/600	0.75	0/793
50	A3	0.36	0/472	0.66	0/634
50	B3	0.41	0/472	0.67	0/634
51	A4	0.36	0/460	0.70	1/621 (0.2%)
51	B4	0.40	0/460	0.70	1/621 (0.2%)
52	A5	0.48	0/441	0.81	0/596
52	B5	0.50	0/441	0.83	0/596
53	A6	0.43	0/440	0.81	0/586
53	B6	0.46	0/440	0.81	0/586
54	A7	0.41	0/417	0.65	0/550
54	B7	0.46	0/417	0.68	0/550
55	A8	0.52	0/515	0.90	0/679
55	B8	0.53	0/515	0.92	0/679
56	A9	0.34	0/310	0.60	0/407
56	B9	0.38	0/310	0.62	0/407
57	AA	0.50	1/68704 (0.0%)	0.74	40/107260 (0.0%)
57	BA	0.55	2/68704 (0.0%)	0.74	48/107260 (0.0%)
58	AB	0.41	0/2853	0.70	0/4451
58	BB	0.44	0/2853	0.71	0/4451
All	All	0.46	4/321584 (0.0%)	0.72	176/480460 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	Ay	0	1
22	Aa	0	8
22	Ba	1	11
24	Av	0	1
24	Bv	0	1
34	AN	0	1
34	BN	0	1
43	AW	0	1
43	BW	0	1
52	A5	0	1
52	B5	0	1
57	AA	3	48
57	BA	3	49
All	All	7	125

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	2506	U	N1-C2	5.94	1.43	1.38
57	BA	783	A	C5-C6	-5.52	1.36	1.41
41	AU	58	ARG	CG-CD	5.12	1.64	1.51
57	AA	783	A	C5-C6	-5.07	1.36	1.41

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	AI	50	ARG	NE-CZ-NH1	-13.91	113.34	120.30
32	BI	50	ARG	NE-CZ-NH1	13.44	127.02	120.30
32	BI	50	ARG	NE-CZ-NH2	-13.41	113.60	120.30
32	AI	50	ARG	NE-CZ-NH2	13.03	126.81	120.30
57	BA	790	C	C2'-C3'-O3'	10.57	132.76	109.50

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	AA	1799	G	C3'
57	AA	1819	A	C3'
57	AA	1820	U	C3'

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Mol	Chain	Res	Type	Atom
22	Ba	1498	U	C3'
57	BA	1799	G	C3'

5 of 125 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	Aa	436	C	Sidechain
22	Aa	484	G	Sidechain
22	Aa	494	U	Sidechain
22	Aa	832	C	Sidechain
21	Ay	56	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ab	1900	0	1951	0	0
1	Bb	1900	0	1951	0	0
2	Ac	1612	0	1677	0	0
2	Bc	1612	0	1677	0	0
3	Ad	1703	0	1763	0	0
3	Bd	1703	0	1764	0	0
4	Ae	1146	0	1207	0	0
4	Be	1146	0	1207	0	0
5	Af	843	0	857	0	0
5	Bf	843	0	857	0	0
6	Ag	1257	0	1296	0	0
6	Bg	1257	0	1296	0	0
7	Ah	1116	0	1177	0	0
7	Bh	1116	0	1177	0	0
8	Ai	1010	0	1037	0	0
8	Bi	1010	0	1037	0	0
9	Aj	794	0	840	0	0
9	Bj	794	0	840	0	0
10	Ak	885	0	904	0	0
10	Bk	885	0	904	0	0
11	Al	970	0	1057	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Bl	970	0	1057	0	0
12	Am	937	0	992	0	0
12	Bm	937	0	990	0	0
13	An	492	0	530	0	0
13	Bn	492	0	530	0	0
14	Ao	734	0	771	0	0
14	Bo	734	0	771	0	0
15	Ap	700	0	720	0	0
15	Bp	700	0	720	0	0
16	Aq	823	0	891	0	0
16	Bq	823	0	891	0	0
17	Ar	574	0	644	0	0
17	Br	574	0	644	0	0
18	As	629	0	652	0	0
18	Bs	629	0	652	0	0
19	At	763	0	861	0	0
19	Bt	763	0	861	0	0
20	Au	208	0	221	0	0
20	Bu	208	0	221	0	0
21	Ay	782	0	827	0	0
21	By	782	0	827	0	0
22	Aa	32329	0	16316	0	0
22	Ba	32329	0	16317	0	0
23	Ax	260	0	129	0	0
23	Bx	260	0	129	0	0
24	Av	1641	0	839	0	0
24	Bv	1641	0	839	0	0
25	Aw	1640	0	837	0	0
25	Bw	1640	0	837	0	0
26	AC	937	0	957	112	0
26	BC	937	0	957	116	0
27	AD	2104	0	2182	327	0
27	BD	2104	0	2182	329	0
28	AE	1563	0	1629	259	0
28	BE	1563	0	1629	252	0
29	AF	1623	0	1677	223	0
29	BF	1623	0	1677	216	0
30	AG	1474	0	1533	341	0
30	BG	1474	0	1532	319	0
31	AH	1259	0	1326	192	0
31	BH	1259	0	1326	187	0
32	AI	1131	0	1218	246	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BI	1131	0	1218	264	0
33	AJ	641	0	309	34	0
33	BJ	641	0	309	47	0
34	AN	1104	0	1180	146	0
34	BN	1104	0	1180	151	0
35	AO	933	0	996	98	0
35	BO	933	0	996	99	0
36	AP	1114	0	1187	304	0
36	BP	1114	0	1187	302	0
37	AQ	1112	0	1171	122	0
37	BQ	1112	0	1171	124	0
38	AR	960	0	1021	128	0
38	BR	960	0	1021	126	0
39	AS	770	0	832	139	0
39	BS	770	0	832	137	0
40	AT	1123	0	1181	229	0
40	BT	1123	0	1181	234	0
41	AU	958	0	1015	148	0
41	BU	958	0	1015	145	0
42	AV	779	0	852	151	0
42	BV	779	0	852	153	0
43	AW	896	0	953	94	0
43	BW	896	0	953	89	0
44	AX	725	0	778	88	0
44	BX	725	0	778	91	0
45	AY	775	0	870	189	0
45	BY	775	0	870	197	0
46	AZ	1467	0	1492	238	0
46	BZ	1467	0	1492	238	0
47	A0	662	0	688	79	0
47	B0	662	0	688	77	0
48	A1	731	0	808	98	0
48	B1	731	0	808	89	0
49	A2	598	0	653	96	0
49	B2	598	0	653	57	0
50	A3	467	0	523	40	0
50	B3	467	0	523	38	0
51	A4	450	0	449	91	0
51	B4	450	0	449	80	0
52	A5	427	0	445	83	0
52	B5	427	0	445	90	0
53	A6	433	0	461	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	B6	433	0	461	117	0
54	A7	409	0	454	38	0
54	B7	409	0	454	38	0
55	A8	507	0	576	112	0
55	B8	507	0	576	120	0
56	A9	307	0	336	19	0
56	B9	307	0	336	25	0
57	AA	61341	0	30925	2266	0
57	BA	61341	0	30926	2267	0
58	AB	2551	0	1295	140	0
58	BB	2551	0	1295	115	0
59	A4	1	0	0	0	0
59	A9	1	0	0	0	0
59	Ad	1	0	0	0	0
59	An	1	0	0	0	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	Bd	1	0	0	0	0
59	Bn	1	0	0	0	0
60	A1	2	0	0	0	0
60	A5	1	0	0	0	0
60	A7	1	0	0	0	0
60	AA	367	0	0	0	0
60	AB	3	0	0	0	0
60	AD	2	0	0	0	0
60	AF	1	0	0	0	0
60	AQ	1	0	0	0	0
60	AX	1	0	0	0	0
60	Aa	145	0	0	0	0
60	Ae	2	0	0	0	0
60	Av	5	0	0	0	0
60	Aw	1	0	0	0	0
60	B0	2	0	0	0	0
60	B5	2	0	0	0	0
60	B7	2	0	0	0	0
60	BA	365	0	0	0	0
60	BB	3	0	0	0	0
60	BD	2	0	0	0	0
60	BF	1	0	0	0	0
60	BO	1	0	0	0	0
60	BX	1	0	0	0	0
60	Ba	143	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	Bd	1	0	0	0	0
60	Bl	1	0	0	0	0
60	Bm	1	0	0	0	0
60	Bv	5	0	0	0	0
60	Bw	1	0	0	0	0
60	Bx	1	0	0	0	0
All	All	297230	0	201936	12630	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

The worst 5 of 12630 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AG:106:LEU:O	30:AG:110:ALA:HB3	1.29	1.28
27:AD:242:ARG:HH21	57:AA:1826:G:H4'	1.06	1.17
32:AI:118:LYS:HG2	32:AI:119:PRO:HD2	1.24	1.17
57:BA:1884:A:H2'	57:BA:1885:A:H5''	1.18	1.16
40:BT:28:VAL:HG13	40:BT:46:GLU:HA	1.28	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ab	232/256 (91%)	149 (64%)	48 (21%)	35 (15%)	0	4
1	Bb	232/256 (91%)	148 (64%)	52 (22%)	32 (14%)	0	5
2	Ac	204/239 (85%)	132 (65%)	43 (21%)	29 (14%)	0	5
2	Bc	204/239 (85%)	134 (66%)	41 (20%)	29 (14%)	0	5
3	Ad	206/209 (99%)	131 (64%)	52 (25%)	23 (11%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Bd	206/209 (99%)	132 (64%)	51 (25%)	23 (11%)	0	8
4	Ae	148/162 (91%)	105 (71%)	24 (16%)	19 (13%)	0	6
4	Be	148/162 (91%)	104 (70%)	23 (16%)	21 (14%)	0	5
5	Af	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	1	18
5	Bf	99/101 (98%)	66 (67%)	26 (26%)	7 (7%)	1	18
6	Ag	153/156 (98%)	108 (71%)	31 (20%)	14 (9%)	1	12
6	Bg	153/156 (98%)	106 (69%)	33 (22%)	14 (9%)	1	12
7	Ah	136/138 (99%)	97 (71%)	32 (24%)	7 (5%)	2	26
7	Bh	136/138 (99%)	97 (71%)	33 (24%)	6 (4%)	3	30
8	Ai	125/128 (98%)	83 (66%)	24 (19%)	18 (14%)	0	5
8	Bi	125/128 (98%)	82 (66%)	25 (20%)	18 (14%)	0	5
9	Aj	96/105 (91%)	76 (79%)	13 (14%)	7 (7%)	1	17
9	Bj	96/105 (91%)	76 (79%)	13 (14%)	7 (7%)	1	17
10	Ak	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	2	22
10	Bk	117/129 (91%)	87 (74%)	23 (20%)	7 (6%)	2	22
11	Al	122/132 (92%)	82 (67%)	25 (20%)	15 (12%)	0	7
11	Bl	122/132 (92%)	82 (67%)	24 (20%)	16 (13%)	0	6
12	Am	116/126 (92%)	58 (50%)	28 (24%)	30 (26%)	0	1
12	Bm	116/126 (92%)	66 (57%)	25 (22%)	25 (22%)	0	1
13	An	58/61 (95%)	38 (66%)	10 (17%)	10 (17%)	0	3
13	Bn	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	3
14	Ao	86/89 (97%)	52 (60%)	24 (28%)	10 (12%)	0	7
14	Bo	86/89 (97%)	52 (60%)	25 (29%)	9 (10%)	0	9
15	Ap	81/88 (92%)	55 (68%)	20 (25%)	6 (7%)	1	16
15	Bp	81/88 (92%)	55 (68%)	23 (28%)	3 (4%)	4	35
16	Aq	97/105 (92%)	74 (76%)	18 (19%)	5 (5%)	2	25
16	Bq	97/105 (92%)	73 (75%)	19 (20%)	5 (5%)	2	25
17	Ar	68/88 (77%)	43 (63%)	20 (29%)	5 (7%)	1	16
17	Br	68/88 (77%)	42 (62%)	21 (31%)	5 (7%)	1	16
18	As	76/93 (82%)	43 (57%)	20 (26%)	13 (17%)	0	3
18	Bs	76/93 (82%)	43 (57%)	20 (26%)	13 (17%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	At	97/106 (92%)	60 (62%)	25 (26%)	12 (12%)	0	7
19	Bt	97/106 (92%)	60 (62%)	25 (26%)	12 (12%)	0	7
20	Au	22/27 (82%)	13 (59%)	6 (27%)	3 (14%)	0	5
20	Bu	22/27 (82%)	12 (54%)	7 (32%)	3 (14%)	0	5
21	Ay	92/95 (97%)	51 (55%)	24 (26%)	17 (18%)	0	2
21	By	92/95 (97%)	58 (63%)	20 (22%)	14 (15%)	0	4
26	AC	116/229 (51%)	87 (75%)	25 (22%)	4 (3%)	4	38
26	BC	116/229 (51%)	86 (74%)	26 (22%)	4 (3%)	4	38
27	AD	269/276 (98%)	187 (70%)	50 (19%)	32 (12%)	0	7
27	BD	269/276 (98%)	190 (71%)	50 (19%)	29 (11%)	0	9
28	AE	202/206 (98%)	138 (68%)	35 (17%)	29 (14%)	0	5
28	BE	202/206 (98%)	140 (69%)	34 (17%)	28 (14%)	0	5
29	AF	205/210 (98%)	148 (72%)	29 (14%)	28 (14%)	0	5
29	BF	205/210 (98%)	148 (72%)	30 (15%)	27 (13%)	0	6
30	AG	179/182 (98%)	98 (55%)	47 (26%)	34 (19%)	0	2
30	BG	179/182 (98%)	99 (55%)	42 (24%)	38 (21%)	0	2
31	AH	162/180 (90%)	97 (60%)	36 (22%)	29 (18%)	0	3
31	BH	162/180 (90%)	97 (60%)	36 (22%)	29 (18%)	0	3
32	AI	143/148 (97%)	75 (52%)	44 (31%)	24 (17%)	0	3
32	BI	143/148 (97%)	76 (53%)	40 (28%)	27 (19%)	0	2
33	AJ	128/173 (74%)	46 (36%)	43 (34%)	39 (30%)	0	0
33	BJ	128/173 (74%)	40 (31%)	36 (28%)	52 (41%)	0	0
34	AN	136/140 (97%)	96 (71%)	23 (17%)	17 (12%)	0	7
34	BN	136/140 (97%)	98 (72%)	21 (15%)	17 (12%)	0	7
35	AO	120/122 (98%)	103 (86%)	11 (9%)	6 (5%)	2	26
35	BO	120/122 (98%)	103 (86%)	12 (10%)	5 (4%)	3	31
36	AP	144/150 (96%)	75 (52%)	37 (26%)	32 (22%)	0	1
36	BP	144/150 (96%)	75 (52%)	38 (26%)	31 (22%)	0	1
37	AQ	138/141 (98%)	105 (76%)	20 (14%)	13 (9%)	1	11
37	BQ	138/141 (98%)	105 (76%)	18 (13%)	15 (11%)	0	8
38	AR	115/118 (98%)	82 (71%)	21 (18%)	12 (10%)	0	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BR	115/118 (98%)	83 (72%)	20 (17%)	12 (10%)	0	10
39	AS	96/112 (86%)	45 (47%)	29 (30%)	22 (23%)	0	1
39	BS	96/112 (86%)	45 (47%)	29 (30%)	22 (23%)	0	1
40	AT	133/146 (91%)	87 (65%)	19 (14%)	27 (20%)	0	2
40	BT	133/146 (91%)	87 (65%)	20 (15%)	26 (20%)	0	2
41	AU	115/118 (98%)	86 (75%)	23 (20%)	6 (5%)	2	25
41	BU	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	2	22
42	AV	99/101 (98%)	66 (67%)	22 (22%)	11 (11%)	0	8
42	BV	99/101 (98%)	67 (68%)	20 (20%)	12 (12%)	0	7
43	AW	111/113 (98%)	85 (77%)	16 (14%)	10 (9%)	1	12
43	BW	111/113 (98%)	86 (78%)	14 (13%)	11 (10%)	1	10
44	AX	90/96 (94%)	65 (72%)	22 (24%)	3 (3%)	4	38
44	BX	90/96 (94%)	64 (71%)	24 (27%)	2 (2%)	8	47
45	AY	98/110 (89%)	45 (46%)	23 (24%)	30 (31%)	0	0
45	BY	98/110 (89%)	46 (47%)	21 (21%)	31 (32%)	0	0
46	AZ	182/206 (88%)	104 (57%)	46 (25%)	32 (18%)	0	3
46	BZ	182/206 (88%)	105 (58%)	46 (25%)	31 (17%)	0	3
47	A0	82/85 (96%)	62 (76%)	15 (18%)	5 (6%)	2	22
47	B0	82/85 (96%)	61 (74%)	16 (20%)	5 (6%)	2	22
48	A1	91/98 (93%)	66 (72%)	15 (16%)	10 (11%)	0	8
48	B1	91/98 (93%)	71 (78%)	11 (12%)	9 (10%)	1	10
49	A2	69/72 (96%)	41 (59%)	18 (26%)	10 (14%)	0	5
49	B2	69/72 (96%)	47 (68%)	16 (23%)	6 (9%)	1	12
50	A3	57/60 (95%)	48 (84%)	7 (12%)	2 (4%)	4	37
50	B3	57/60 (95%)	48 (84%)	7 (12%)	2 (4%)	4	37
51	A4	55/71 (78%)	22 (40%)	20 (36%)	13 (24%)	0	1
51	B4	55/71 (78%)	23 (42%)	19 (34%)	13 (24%)	0	1
52	A5	53/60 (88%)	37 (70%)	8 (15%)	8 (15%)	0	4
52	B5	53/60 (88%)	37 (70%)	8 (15%)	8 (15%)	0	4
53	A6	48/54 (89%)	22 (46%)	13 (27%)	13 (27%)	0	0
53	B6	48/54 (89%)	22 (46%)	13 (27%)	13 (27%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	A7	45/49 (92%)	42 (93%)	2 (4%)	1 (2%)	8	47
54	B7	45/49 (92%)	42 (93%)	2 (4%)	1 (2%)	8	47
55	A8	61/65 (94%)	35 (57%)	15 (25%)	11 (18%)	0	3
55	B8	61/65 (94%)	35 (57%)	15 (25%)	11 (18%)	0	3
56	A9	35/37 (95%)	25 (71%)	9 (26%)	1 (3%)	5	41
56	B9	35/37 (95%)	25 (71%)	9 (26%)	1 (3%)	5	41
All	All	12016/13122 (92%)	7873 (66%)	2533 (21%)	1610 (13%)	0	5

5 of 1610 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ab	15	VAL
1	Ab	18	GLY
1	Ab	75	LYS
1	Ab	123	ALA
1	Ab	143	GLU

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	
1	Ab	202/220 (92%)	181 (90%)	21 (10%)	8	39
1	Bb	202/220 (92%)	181 (90%)	21 (10%)	8	39
2	Ac	160/188 (85%)	148 (92%)	12 (8%)	16	53
2	Bc	160/188 (85%)	148 (92%)	12 (8%)	16	53
3	Ad	180/181 (99%)	157 (87%)	23 (13%)	5	29
3	Bd	180/181 (99%)	157 (87%)	23 (13%)	5	29
4	Ae	115/123 (94%)	100 (87%)	15 (13%)	5	29
4	Be	115/123 (94%)	100 (87%)	15 (13%)	5	29
5	Af	90/90 (100%)	82 (91%)	8 (9%)	11	46
5	Bf	90/90 (100%)	81 (90%)	9 (10%)	9	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Ag	126/127 (99%)	120 (95%)	6 (5%)	30	68
6	Bg	126/127 (99%)	120 (95%)	6 (5%)	30	68
7	Ah	119/119 (100%)	111 (93%)	8 (7%)	19	58
7	Bh	119/119 (100%)	110 (92%)	9 (8%)	15	52
8	Ai	98/99 (99%)	86 (88%)	12 (12%)	6	31
8	Bi	98/99 (99%)	86 (88%)	12 (12%)	6	31
9	Aj	88/92 (96%)	80 (91%)	8 (9%)	11	45
9	Bj	88/92 (96%)	80 (91%)	8 (9%)	11	45
10	Ak	90/99 (91%)	85 (94%)	5 (6%)	25	63
10	Bk	90/99 (91%)	85 (94%)	5 (6%)	25	63
11	Al	104/109 (95%)	94 (90%)	10 (10%)	10	43
11	Bl	104/109 (95%)	93 (89%)	11 (11%)	8	38
12	Am	94/101 (93%)	82 (87%)	12 (13%)	5	29
12	Bm	94/101 (93%)	83 (88%)	11 (12%)	6	34
13	An	49/50 (98%)	46 (94%)	3 (6%)	22	61
13	Bn	49/50 (98%)	45 (92%)	4 (8%)	13	49
14	Ao	79/80 (99%)	73 (92%)	6 (8%)	15	52
14	Bo	79/80 (99%)	73 (92%)	6 (8%)	15	52
15	Ap	72/74 (97%)	68 (94%)	4 (6%)	25	63
15	Bp	72/74 (97%)	68 (94%)	4 (6%)	25	63
16	Aq	94/97 (97%)	91 (97%)	3 (3%)	44	78
16	Bq	94/97 (97%)	91 (97%)	3 (3%)	44	78
17	Ar	61/77 (79%)	60 (98%)	1 (2%)	68	88
17	Br	61/77 (79%)	60 (98%)	1 (2%)	68	88
18	As	69/80 (86%)	57 (83%)	12 (17%)	2	15
18	Bs	69/80 (86%)	57 (83%)	12 (17%)	2	15
19	At	76/82 (93%)	71 (93%)	5 (7%)	19	59
19	Bt	76/82 (93%)	71 (93%)	5 (7%)	19	59
20	Au	19/22 (86%)	18 (95%)	1 (5%)	26	65
20	Bu	19/22 (86%)	18 (95%)	1 (5%)	26	65
21	Ay	86/87 (99%)	75 (87%)	11 (13%)	5	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	By	86/87 (99%)	77 (90%)	9 (10%)	8	39
26	AC	99/181 (55%)	92 (93%)	7 (7%)	17	55
26	BC	99/181 (55%)	92 (93%)	7 (7%)	17	55
27	AD	213/218 (98%)	178 (84%)	35 (16%)	2	18
27	BD	213/218 (98%)	180 (84%)	33 (16%)	3	21
28	AE	165/166 (99%)	135 (82%)	30 (18%)	2	13
28	BE	165/166 (99%)	133 (81%)	32 (19%)	1	11
29	AF	165/166 (99%)	143 (87%)	22 (13%)	4	28
29	BF	165/166 (99%)	145 (88%)	20 (12%)	6	32
30	AG	155/156 (99%)	137 (88%)	18 (12%)	6	34
30	BG	155/156 (99%)	128 (83%)	27 (17%)	2	15
31	AH	137/148 (93%)	123 (90%)	14 (10%)	8	40
31	BH	137/148 (93%)	122 (89%)	15 (11%)	7	37
32	AI	122/124 (98%)	103 (84%)	19 (16%)	3	21
32	BI	122/124 (98%)	103 (84%)	19 (16%)	3	21
34	AN	117/119 (98%)	102 (87%)	15 (13%)	5	29
34	BN	117/119 (98%)	102 (87%)	15 (13%)	5	29
35	AO	100/100 (100%)	90 (90%)	10 (10%)	9	41
35	BO	100/100 (100%)	89 (89%)	11 (11%)	7	37
36	AP	112/116 (97%)	93 (83%)	19 (17%)	2	17
36	BP	112/116 (97%)	92 (82%)	20 (18%)	2	13
37	AQ	110/111 (99%)	100 (91%)	10 (9%)	11	45
37	BQ	110/111 (99%)	100 (91%)	10 (9%)	11	45
38	AR	100/101 (99%)	86 (86%)	14 (14%)	4	26
38	BR	100/101 (99%)	86 (86%)	14 (14%)	4	26
39	AS	77/88 (88%)	63 (82%)	14 (18%)	2	13
39	BS	77/88 (88%)	63 (82%)	14 (18%)	2	13
40	AT	118/127 (93%)	99 (84%)	19 (16%)	3	19
40	BT	118/127 (93%)	99 (84%)	19 (16%)	3	19
41	AU	92/94 (98%)	79 (86%)	13 (14%)	4	26
41	BU	92/94 (98%)	79 (86%)	13 (14%)	4	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	AV	82/82 (100%)	66 (80%)	16 (20%)	1	11
42	BV	82/82 (100%)	65 (79%)	17 (21%)	1	9
43	AW	91/92 (99%)	80 (88%)	11 (12%)	6	32
43	BW	91/92 (99%)	81 (89%)	10 (11%)	7	37
44	AX	74/78 (95%)	64 (86%)	10 (14%)	4	28
44	BX	74/78 (95%)	63 (85%)	11 (15%)	3	23
45	AY	84/91 (92%)	68 (81%)	16 (19%)	2	11
45	BY	84/91 (92%)	68 (81%)	16 (19%)	2	11
46	AZ	162/179 (90%)	141 (87%)	21 (13%)	5	29
46	BZ	162/179 (90%)	134 (83%)	28 (17%)	2	15
47	A0	66/67 (98%)	59 (89%)	7 (11%)	8	38
47	B0	66/67 (98%)	59 (89%)	7 (11%)	8	38
48	A1	78/83 (94%)	66 (85%)	12 (15%)	3	22
48	B1	78/83 (94%)	62 (80%)	16 (20%)	1	10
49	A2	66/67 (98%)	63 (96%)	3 (4%)	32	70
49	B2	66/67 (98%)	56 (85%)	10 (15%)	3	22
50	A3	51/52 (98%)	46 (90%)	5 (10%)	9	42
50	B3	51/52 (98%)	46 (90%)	5 (10%)	9	42
51	A4	51/63 (81%)	41 (80%)	10 (20%)	1	11
51	B4	51/63 (81%)	41 (80%)	10 (20%)	1	11
52	A5	47/52 (90%)	42 (89%)	5 (11%)	8	38
52	B5	47/52 (90%)	42 (89%)	5 (11%)	8	38
53	A6	49/52 (94%)	40 (82%)	9 (18%)	2	12
53	B6	49/52 (94%)	40 (82%)	9 (18%)	2	12
54	A7	40/42 (95%)	37 (92%)	3 (8%)	16	53
54	B7	40/42 (95%)	37 (92%)	3 (8%)	16	53
55	A8	53/55 (96%)	42 (79%)	11 (21%)	1	9
55	B8	53/55 (96%)	42 (79%)	11 (21%)	1	9
56	A9	34/34 (100%)	34 (100%)	0	100	100
56	B9	34/34 (100%)	34 (100%)	0	100	100
All	All	9962/10602 (94%)	8764 (88%)	1198 (12%)	6	32

5 of 1198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	A3	8	LEU
7	Bh	1	MET
46	BZ	103	ARG
52	A5	25	LEU
2	Bc	18	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 327 such sidechains are listed below:

Mol	Chain	Res	Type
48	A1	47	GLN
4	Be	72	GLN
44	BX	41	ASN
50	A3	46	ASN
1	Bb	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	Aa	1503/1504 (99%)	211 (14%)	0
22	Ba	1503/1504 (99%)	210 (13%)	0
23	Ax	11/14 (78%)	8 (72%)	0
23	Bx	11/14 (78%)	8 (72%)	0
24	Av	76/77 (98%)	15 (19%)	0
24	Bv	76/77 (98%)	17 (22%)	0
25	Aw	76/77 (98%)	11 (14%)	0
25	Bw	76/77 (98%)	8 (10%)	0
57	AA	2847/2848 (99%)	521 (18%)	0
57	BA	2847/2848 (99%)	517 (18%)	0
58	AB	118/119 (99%)	21 (17%)	0
58	BB	118/119 (99%)	21 (17%)	0
All	All	9262/9278 (99%)	1568 (16%)	0

5 of 1568 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	Aa	9	G
22	Aa	31	G
22	Aa	32	A
22	Aa	39	G
22	Aa	47	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	5MU	Av	54	24	14,22,23	1.15	2 (14%)	16,32,35	4.28	3 (18%)
23	CCC	Ax	21	-	0,2,26	0.00	-	0,1,41	0.00	-
24	5MU	Bv	54	24	14,22,23	1.11	2 (14%)	16,32,35	4.33	2 (12%)
23	CCC	Bx	21	-	0,2,26	0.00	-	0,1,41	0.00	-

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	5MU	Av	54	24	-	0/3/25/26	0/2/2/2
23	CCC	Ax	21	-	-	0/0/0/36	0/0/0/3
24	5MU	Bv	54	24	-	0/3/25/26	0/2/2/2
23	CCC	Bx	21	-	-	0/0/0/36	0/0/0/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Bv	54	5MU	C6-C5	-2.37	1.33	1.40
24	Av	54	5MU	C6-C5	-2.12	1.34	1.40
24	Bv	54	5MU	C4-N3	3.00	1.38	1.33
24	Av	54	5MU	C4-N3	3.44	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Bv	54	5MU	C5-C4-N3	-9.34	114.94	125.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Av	54	5MU	C5-C4-N3	-9.27	115.02	125.24
24	Av	54	5MU	C5M-C5-C6	2.06	122.77	118.67
24	Av	54	5MU	C4-N3-C2	14.04	127.44	115.16
24	Bv	54	5MU	C4-N3-C2	14.25	127.62	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1072 ligands modelled in this entry, 1072 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Ab	234/256 (91%)	0.11	8 (3%) 46 33	114, 153, 181, 193	0
1	Bb	234/256 (91%)	0.13	7 (2%) 51 37	113, 152, 181, 193	0
2	Ac	206/239 (86%)	0.31	12 (5%) 24 17	123, 150, 166, 178	0
2	Bc	206/239 (86%)	0.21	7 (3%) 46 33	124, 149, 166, 179	0
3	Ad	208/209 (99%)	-0.08	0 100 100	97, 119, 144, 155	0
3	Bd	208/209 (99%)	0.03	1 (0%) 90 84	97, 119, 145, 154	0
4	Ae	150/162 (92%)	0.07	3 (2%) 65 51	88, 114, 138, 159	0
4	Be	150/162 (92%)	0.08	0 100 100	84, 112, 138, 160	0
5	Af	101/101 (100%)	-0.14	2 (1%) 65 51	91, 121, 138, 155	0
5	Bf	101/101 (100%)	-0.31	0 100 100	91, 120, 137, 155	0
6	Ag	155/156 (99%)	0.12	10 (6%) 20 14	118, 137, 171, 188	0
6	Bg	155/156 (99%)	0.24	10 (6%) 20 14	118, 138, 171, 188	0
7	Ah	138/138 (100%)	-0.05	1 (0%) 87 78	96, 117, 132, 157	0
7	Bh	138/138 (100%)	-0.02	1 (0%) 87 78	95, 116, 131, 158	0
8	Ai	127/128 (99%)	0.71	15 (11%) 5 5	120, 160, 178, 186	0
8	Bi	127/128 (99%)	0.82	15 (11%) 5 5	119, 160, 178, 186	0
9	Aj	98/105 (93%)	0.89	19 (19%) 1 1	126, 164, 184, 190	0
9	Bj	98/105 (93%)	0.88	13 (13%) 4 4	124, 164, 184, 190	0
10	Ak	119/129 (92%)	0.04	6 (5%) 30 21	89, 117, 145, 171	0
10	Bk	119/129 (92%)	0.06	6 (5%) 30 21	89, 117, 145, 171	0
11	Al	124/132 (93%)	0.01	2 (1%) 72 59	75, 97, 123, 161	0
11	Bl	124/132 (93%)	0.08	2 (1%) 72 59	77, 97, 125, 162	0
12	Am	118/126 (93%)	0.27	9 (7%) 15 11	115, 143, 157, 166	0
12	Bm	118/126 (93%)	0.32	5 (4%) 37 26	115, 142, 157, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	An	60/61 (98%)	0.84	8 (13%) 4 4	126, 139, 159, 162	0
13	Bn	60/61 (98%)	0.20	0 100 100	127, 138, 159, 162	0
14	Ao	88/89 (98%)	0.05	0 100 100	81, 110, 131, 138	0
14	Bo	88/89 (98%)	-0.08	0 100 100	81, 110, 132, 137	0
15	Ap	83/88 (94%)	0.27	1 (1%) 79 66	93, 110, 128, 148	0
15	Bp	83/88 (94%)	0.47	5 (6%) 23 16	94, 111, 130, 147	0
16	Aq	99/105 (94%)	-0.05	1 (1%) 82 70	80, 107, 124, 132	0
16	Bq	99/105 (94%)	-0.13	0 100 100	80, 107, 123, 132	0
17	Ar	70/88 (79%)	0.35	4 (5%) 24 17	96, 122, 142, 158	0
17	Br	70/88 (79%)	0.53	6 (8%) 11 9	95, 122, 141, 157	0
18	As	78/93 (83%)	0.54	6 (7%) 14 11	131, 153, 173, 181	0
18	Bs	78/93 (83%)	0.48	6 (7%) 14 11	130, 153, 172, 181	0
19	At	99/106 (93%)	0.12	1 (1%) 82 70	86, 114, 145, 149	0
19	Bt	99/106 (93%)	0.04	2 (2%) 65 51	86, 114, 145, 149	0
20	Au	24/27 (88%)	2.28	11 (45%) 0 0	108, 138, 162, 168	0
20	Bu	24/27 (88%)	1.05	3 (12%) 4 5	106, 137, 162, 168	0
21	Ay	94/95 (98%)	0.87	13 (13%) 3 3	118, 154, 186, 189	0
21	By	94/95 (98%)	0.92	11 (11%) 5 5	110, 146, 182, 188	0
22	Aa	1504/1504 (100%)	0.09	36 (2%) 59 45	65, 119, 193, 208	0
22	Ba	1504/1504 (100%)	0.07	29 (1%) 67 53	63, 119, 193, 208	0
23	Ax	12/14 (85%)	1.64	3 (25%) 1 1	108, 191, 198, 199	0
23	Bx	12/14 (85%)	2.10	6 (50%) 0 0	108, 191, 198, 199	0
24	Av	76/77 (98%)	-0.23	1 (1%) 77 64	96, 119, 161, 163	0
24	Bv	76/77 (98%)	-0.22	1 (1%) 77 64	69, 107, 141, 167	0
25	Aw	77/77 (100%)	0.25	4 (5%) 28 20	103, 191, 201, 203	0
25	Bw	77/77 (100%)	0.14	3 (3%) 40 29	93, 188, 200, 202	0
26	AC	120/229 (52%)	1.70	43 (35%) 0 0	147, 177, 190, 193	0
26	BC	120/229 (52%)	1.63	35 (29%) 1 1	145, 177, 189, 194	0
27	AD	271/276 (98%)	-0.19	3 (1%) 80 67	48, 76, 98, 121	0
27	BD	271/276 (98%)	-0.22	1 (0%) 92 87	46, 75, 96, 122	0
28	AE	204/206 (99%)	-0.11	2 (0%) 82 70	49, 81, 127, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	BE	204/206 (99%)	-0.04	4 (1%) 65 51	49, 80, 128, 148	0
29	AF	207/210 (98%)	-0.18	3 (1%) 75 62	48, 89, 153, 181	0
29	BF	207/210 (98%)	-0.13	4 (1%) 67 53	46, 86, 154, 180	0
30	AG	181/182 (99%)	0.18	8 (4%) 35 25	117, 142, 161, 186	0
30	BG	181/182 (99%)	0.06	5 (2%) 53 40	99, 128, 154, 175	0
31	AH	164/180 (91%)	0.89	28 (17%) 2 2	98, 127, 143, 166	0
31	BH	164/180 (91%)	0.22	7 (4%) 36 25	94, 124, 141, 164	0
32	AI	145/148 (97%)	1.29	37 (25%) 1 1	81, 154, 171, 176	0
32	BI	145/148 (97%)	0.53	15 (10%) 7 6	82, 153, 172, 176	0
33	AJ	130/173 (75%)	2.74	65 (50%) 0 0	170, 195, 202, 203	0
33	BJ	130/173 (75%)	1.44	40 (30%) 0 1	147, 180, 194, 196	0
34	AN	138/140 (98%)	-0.02	1 (0%) 87 78	65, 91, 126, 138	0
34	BN	138/140 (98%)	-0.12	0 100 100	63, 88, 126, 136	0
35	AO	122/122 (100%)	-0.31	0 100 100	59, 75, 98, 122	0
35	BO	122/122 (100%)	-0.30	0 100 100	56, 74, 99, 120	0
36	AP	146/150 (97%)	0.19	4 (2%) 55 41	51, 106, 133, 169	0
36	BP	146/150 (97%)	0.18	3 (2%) 64 50	50, 104, 133, 169	0
37	AQ	140/141 (99%)	-0.05	1 (0%) 87 78	75, 96, 124, 147	0
37	BQ	140/141 (99%)	-0.02	1 (0%) 87 78	74, 94, 125, 147	0
38	AR	117/118 (99%)	-0.24	0 100 100	48, 80, 108, 128	0
38	BR	117/118 (99%)	-0.16	0 100 100	47, 79, 107, 127	0
39	AS	98/112 (87%)	0.68	13 (13%) 4 4	111, 137, 154, 161	0
39	BS	98/112 (87%)	0.84	13 (13%) 4 4	110, 136, 153, 162	0
40	AT	135/146 (92%)	-0.19	3 (2%) 62 48	66, 92, 150, 183	0
40	BT	135/146 (92%)	-0.04	3 (2%) 62 48	66, 92, 150, 183	0
41	AU	117/118 (99%)	-0.23	1 (0%) 84 72	58, 81, 117, 156	0
41	BU	117/118 (99%)	-0.28	0 100 100	52, 78, 116, 158	0
42	AV	101/101 (100%)	0.06	1 (0%) 82 70	59, 106, 125, 134	0
42	BV	101/101 (100%)	-0.04	1 (0%) 82 70	54, 103, 125, 134	0
43	AW	113/113 (100%)	-0.19	1 (0%) 84 72	58, 73, 106, 183	0
43	BW	113/113 (100%)	-0.17	1 (0%) 84 72	55, 71, 105, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AX	92/96 (95%)	-0.21	0 100 100	63, 86, 110, 120	0
44	BX	92/96 (95%)	-0.06	0 100 100	56, 84, 110, 120	0
45	AY	100/110 (90%)	0.91	14 (14%) 3 3	78, 117, 153, 160	0
45	BY	100/110 (90%)	0.37	5 (5%) 30 21	74, 115, 152, 158	0
46	AZ	184/206 (89%)	0.16	11 (5%) 23 16	117, 141, 158, 188	0
46	BZ	184/206 (89%)	0.16	5 (2%) 55 41	87, 126, 150, 173	0
47	A0	84/85 (98%)	0.51	5 (5%) 23 16	81, 100, 148, 168	0
47	B0	84/85 (98%)	0.46	7 (8%) 12 10	78, 100, 148, 168	0
48	A1	93/98 (94%)	0.06	2 (2%) 62 48	64, 87, 127, 137	0
48	B1	93/98 (94%)	0.08	0 100 100	55, 82, 119, 133	0
49	A2	71/72 (98%)	-0.29	0 100 100	81, 116, 134, 156	0
49	B2	71/72 (98%)	-0.34	0 100 100	51, 85, 123, 159	0
50	A3	59/60 (98%)	0.53	2 (3%) 46 33	70, 94, 112, 162	0
50	B3	59/60 (98%)	0.18	2 (3%) 46 33	62, 91, 111, 162	0
51	A4	57/71 (80%)	-0.07	0 100 100	150, 164, 175, 177	0
51	B4	57/71 (80%)	0.00	3 (5%) 27 20	150, 164, 174, 177	0
52	A5	55/60 (91%)	-0.30	2 (3%) 43 32	54, 80, 113, 119	0
52	B5	55/60 (91%)	-0.31	1 (1%) 69 55	54, 78, 112, 121	0
53	A6	50/54 (92%)	1.88	24 (48%) 0 0	121, 149, 165, 175	0
53	B6	50/54 (92%)	1.91	27 (54%) 0 0	121, 149, 164, 176	0
54	A7	47/49 (95%)	-0.04	0 100 100	50, 64, 86, 133	0
54	B7	47/49 (95%)	-0.12	0 100 100	47, 60, 84, 131	0
55	A8	63/65 (96%)	0.15	0 100 100	66, 83, 117, 146	0
55	B8	63/65 (96%)	0.01	0 100 100	63, 83, 116, 145	0
56	A9	37/37 (100%)	1.66	14 (37%) 0 0	121, 134, 149, 151	0
56	B9	37/37 (100%)	2.25	22 (59%) 0 0	121, 132, 148, 152	0
57	AA	2848/2848 (100%)	-0.08	60 (2%) 64 50	47, 83, 185, 208	0
57	BA	2848/2848 (100%)	0.03	44 (1%) 74 61	44, 80, 185, 208	0
58	AB	119/119 (100%)	-0.11	4 (3%) 46 33	90, 143, 176, 196	0
58	BB	119/119 (100%)	0.01	2 (1%) 70 57	86, 142, 175, 197	0
All	All	21500/22400 (95%)	0.14	918 (4%) 36 25	44, 108, 181, 208	0

The worst 5 of 918 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	Ba	89	C	14.3
57	BA	277	C	11.4
32	BI	88	ILE	11.3
22	Aa	89	C	11.1
57	AA	654(E)	G	10.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	CCC	Bx	21	3/24	0.95	0.61	-	20,20,20,20	0
23	CCC	Ax	21	3/24	0.88	0.57	-	20,20,20,20	0
24	5MU	Av	54	21/22	0.90	0.19	-	130,133,148,148	0
24	5MU	Bv	54	21/22	0.93	0.16	-	114,116,124,125	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	Aa	1645	1/1	0.54	1.51	134.62	79,79,79,79	0
60	MG	AA	2968	1/1	0.31	1.47	77.90	76,76,76,76	0
60	MG	AA	3243	1/1	0.93	1.21	64.11	79,79,79,79	0
60	MG	BA	3254	1/1	0.57	0.88	62.24	66,66,66,66	0
60	MG	BA	3013	1/1	0.95	0.98	50.84	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3131	1/1	0.89	0.63	48.79	96,96,96,96	0
60	MG	Aa	1631	1/1	0.77	1.14	47.80	72,72,72,72	0
60	MG	Ba	1630	1/1	0.77	0.82	44.69	76,76,76,76	0
60	MG	Ba	1644	1/1	0.49	1.03	37.39	67,67,67,67	0
60	MG	AA	3245	1/1	0.18	0.92	37.18	97,97,97,97	0
60	MG	AA	3097	1/1	0.80	0.42	35.72	43,43,43,43	0
60	MG	AA	3261	1/1	0.54	0.84	35.57	76,76,76,76	0
60	MG	Ba	1724	1/1	0.87	0.68	35.46	68,68,68,68	0
60	MG	AA	3197	1/1	0.96	0.49	35.26	22,22,22,22	0
60	MG	BA	3187	1/1	0.87	0.66	33.42	36,36,36,36	0
60	MG	Aa	1727	1/1	0.17	1.24	33.34	98,98,98,98	1
60	MG	Ba	1621	1/1	0.73	1.12	33.06	82,82,82,82	0
60	MG	AA	3011	1/1	0.95	0.61	30.54	14,14,14,14	0
60	MG	AA	3147	1/1	0.53	0.47	29.68	79,79,79,79	0
60	MG	Ba	1684	1/1	0.93	0.68	28.34	75,75,75,75	0
60	MG	BA	2905	1/1	0.93	0.53	26.77	29,29,29,29	0
60	MG	AA	3023	1/1	0.99	0.54	25.78	13,13,13,13	0
60	MG	BA	2995	1/1	0.94	0.53	25.31	14,14,14,14	0
60	MG	AA	3044	1/1	0.92	0.86	25.05	17,17,17,17	0
60	MG	Ba	1726	1/1	0.93	0.73	23.71	34,34,34,34	1
60	MG	AA	3069	1/1	0.94	0.57	22.62	68,68,68,68	0
60	MG	AA	2931	1/1	0.95	0.60	22.47	35,35,35,35	0
60	MG	Ba	1685	1/1	0.93	0.83	22.18	25,25,25,25	1
60	MG	AA	2980	1/1	0.82	0.64	22.16	69,69,69,69	0
60	MG	Aa	1725	1/1	0.72	0.63	21.85	74,74,74,74	0
60	MG	BA	3084	1/1	0.97	0.41	21.54	34,34,34,34	0
60	MG	BA	2912	1/1	0.97	0.60	21.09	37,37,37,37	0
60	MG	AA	3190	1/1	0.81	0.49	20.66	43,43,43,43	0
60	MG	BA	3010	1/1	0.85	0.50	20.10	13,13,13,13	0
60	MG	BA	3257	1/1	0.48	0.41	20.09	72,72,72,72	0
60	MG	BA	3150	1/1	0.66	0.64	19.55	76,76,76,76	0
60	MG	Ba	1739	1/1	0.93	0.51	18.96	53,53,53,53	0
60	MG	AA	2987	1/1	0.93	0.37	18.79	53,53,53,53	0
60	MG	AA	3099	1/1	0.85	0.66	18.72	57,57,57,57	0
60	MG	BA	2917	1/1	0.84	0.65	18.31	23,23,23,23	0
60	MG	BA	2913	1/1	0.96	0.43	18.24	11,11,11,11	0
60	MG	BA	3038	1/1	0.97	0.43	18.17	26,26,26,26	0
60	MG	BA	3055	1/1	0.98	0.45	17.86	7,7,7,7	0
60	MG	BA	3236	1/1	0.48	0.54	17.75	116,116,116,116	0
60	MG	BA	3231	1/1	0.90	0.66	17.63	64,64,64,64	0
60	MG	AA	3259	1/1	0.74	0.62	17.35	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3052	1/1	0.95	0.48	17.14	10,10,10,10	0
60	MG	BA	3035	1/1	0.94	0.54	16.57	52,52,52,52	0
60	MG	BA	3241	1/1	0.87	0.52	16.53	49,49,49,49	0
60	MG	AA	3179	1/1	0.83	0.67	16.18	56,56,56,56	0
60	MG	AA	3028	1/1	0.88	0.64	16.12	60,60,60,60	0
60	MG	Aa	1633	1/1	0.95	0.68	15.92	62,62,62,62	0
60	MG	AA	3102	1/1	0.70	0.70	15.92	68,68,68,68	0
60	MG	AA	3096	1/1	0.90	0.52	15.38	73,73,73,73	0
60	MG	BA	3211	1/1	0.92	0.33	15.17	24,24,24,24	0
60	MG	BA	3160	1/1	0.81	0.47	14.91	74,74,74,74	0
60	MG	BA	2967	1/1	0.96	0.51	14.63	20,20,20,20	0
60	MG	BA	2962	1/1	0.64	0.50	14.62	54,54,54,54	0
60	MG	Ba	1654	1/1	0.80	0.37	14.44	50,50,50,50	0
60	MG	BA	3120	1/1	0.98	0.44	14.43	16,16,16,16	0
60	MG	AA	2909	1/1	0.85	0.46	14.06	41,41,41,41	0
60	MG	BA	2980	1/1	0.90	0.49	13.89	9,9,9,9	0
60	MG	AA	3072	1/1	0.86	0.47	13.76	122,122,122,122	0
60	MG	Aa	1622	1/1	0.71	0.98	13.69	79,79,79,79	0
60	MG	AA	3177	1/1	0.96	0.45	13.64	57,57,57,57	0
60	MG	AA	2964	1/1	0.28	0.49	13.57	65,65,65,65	0
60	MG	AA	3150	1/1	0.85	0.70	13.56	62,62,62,62	0
60	MG	AA	2996	1/1	0.89	0.51	13.54	40,40,40,40	0
60	MG	Ba	1691	1/1	0.88	0.67	13.40	58,58,58,58	0
60	MG	AA	3056	1/1	0.91	0.45	13.05	19,19,19,19	0
60	MG	BA	3101	1/1	0.67	0.59	12.99	52,52,52,52	0
60	MG	BA	3027	1/1	0.60	0.44	12.86	43,43,43,43	0
60	MG	AA	2928	1/1	0.71	0.50	12.74	110,110,110,110	0
60	MG	BA	3123	1/1	0.97	0.51	12.71	2,2,2,2	0
60	MG	AA	3095	1/1	0.95	0.70	12.68	26,26,26,26	0
60	MG	BA	3053	1/1	0.98	0.35	12.51	12,12,12,12	0
60	MG	AA	2918	1/1	0.94	0.59	12.50	25,25,25,25	0
60	MG	AA	3247	1/1	0.92	0.29	12.50	103,103,103,103	0
60	MG	AA	3124	1/1	0.99	0.40	12.47	15,15,15,15	0
60	MG	BA	2968	1/1	0.95	0.37	12.20	69,69,69,69	0
60	MG	AA	3126	1/1	0.44	0.55	12.09	47,47,47,47	0
60	MG	BA	3034	1/1	0.97	0.39	12.01	11,11,11,11	0
60	MG	BA	2979	1/1	0.89	0.43	11.89	55,55,55,55	0
60	MG	BA	3100	1/1	0.93	0.42	11.86	62,62,62,62	0
60	MG	AA	2969	1/1	0.98	0.28	11.74	22,22,22,22	0
60	MG	BA	2930	1/1	0.98	0.40	11.72	28,28,28,28	0
60	MG	BA	3094	1/1	0.94	0.63	11.64	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3025	1/1	0.84	0.41	11.60	26,26,26,26	0
60	MG	Aa	1662	1/1	0.70	0.48	11.34	73,73,73,73	0
60	MG	BA	3156	1/1	0.94	0.42	11.32	29,29,29,29	0
60	MG	AA	2981	1/1	0.92	0.51	11.29	13,13,13,13	0
60	MG	AA	2932	1/1	0.86	0.68	11.10	57,57,57,57	0
60	MG	BA	3024	1/1	0.78	0.43	10.92	24,24,24,24	0
60	MG	AA	2976	1/1	0.93	0.47	10.73	46,46,46,46	0
60	MG	Aa	1729	1/1	0.93	0.41	10.68	30,30,30,30	0
60	MG	BA	3043	1/1	0.95	0.52	10.61	17,17,17,17	0
60	MG	Aa	1679	1/1	0.28	0.58	10.46	116,116,116,116	0
60	MG	Ba	1728	1/1	0.80	0.43	10.40	30,30,30,30	0
60	MG	Ba	1634	1/1	0.95	0.38	10.35	37,37,37,37	0
60	MG	Aa	1666	1/1	0.87	0.39	10.09	61,61,61,61	0
60	MG	AA	3221	1/1	0.79	0.44	10.06	47,47,47,47	0
60	MG	AA	2949	1/1	0.82	0.44	9.99	41,41,41,41	0
60	MG	BA	2931	1/1	0.76	0.41	9.91	62,62,62,62	0
60	MG	AA	2925	1/1	0.84	0.36	9.80	79,79,79,79	0
60	MG	AA	2906	1/1	0.93	0.53	9.79	25,25,25,25	0
60	MG	AA	3205	1/1	0.50	0.50	9.57	51,51,51,51	0
60	MG	BA	2990	1/1	0.96	0.42	9.45	10,10,10,10	0
60	MG	AA	3051	1/1	0.70	0.34	9.39	81,81,81,81	0
60	MG	BA	3171	1/1	0.76	0.49	9.35	69,69,69,69	0
60	MG	AA	3256	1/1	0.69	0.44	9.27	71,71,71,71	0
60	MG	AA	2920	1/1	0.98	0.43	9.26	22,22,22,22	0
60	MG	BA	2987	1/1	0.95	0.35	8.91	9,9,9,9	0
60	MG	AA	3133	1/1	0.55	0.31	8.90	48,48,48,48	0
60	MG	A7	101	1/1	0.73	0.62	8.88	80,80,80,80	0
60	MG	Ba	1742	1/1	0.94	0.42	8.88	92,92,92,92	0
60	MG	AA	3101	1/1	0.89	0.26	8.86	46,46,46,46	0
60	MG	BA	2996	1/1	0.96	0.42	8.74	18,18,18,18	0
60	MG	BA	2982	1/1	0.97	0.39	8.54	4,4,4,4	0
60	MG	AA	3172	1/1	0.96	0.41	8.45	38,38,38,38	0
60	MG	AA	3134	1/1	0.76	0.32	8.37	98,98,98,98	0
60	MG	AA	3088	1/1	0.53	0.33	8.30	85,85,85,85	0
60	MG	BA	3095	1/1	0.81	0.35	8.23	33,33,33,33	0
60	MG	AA	3138	1/1	0.95	0.31	8.23	56,56,56,56	0
60	MG	BA	3165	1/1	0.42	0.35	8.14	67,67,67,67	0
60	MG	Aa	1686	1/1	0.82	0.30	8.12	37,37,37,37	1
60	MG	BA	3093	1/1	0.58	0.48	8.05	61,61,61,61	0
60	MG	BA	3172	1/1	0.94	0.50	8.05	50,50,50,50	0
60	MG	AA	3054	1/1	0.97	0.40	8.04	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	2927	1/1	0.92	0.39	7.94	83,83,83,83	0
60	MG	BA	3018	1/1	0.99	0.30	7.90	2,2,2,2	0
60	MG	BA	3134	1/1	0.94	0.40	7.87	52,52,52,52	0
60	MG	Ae	202	1/1	0.57	0.96	7.85	89,89,89,89	0
60	MG	AA	3039	1/1	0.96	0.29	7.83	19,19,19,19	0
60	MG	AA	3038	1/1	0.80	0.35	7.75	64,64,64,64	0
60	MG	AA	3265	1/1	0.48	0.41	7.60	70,70,70,70	0
60	MG	AA	2997	1/1	0.93	0.26	7.51	43,43,43,43	0
60	MG	BA	2984	1/1	0.96	0.41	7.48	22,22,22,22	0
60	MG	AA	2991	1/1	0.94	0.48	7.41	19,19,19,19	0
60	MG	Ba	1608	1/1	0.90	0.48	7.31	79,79,79,79	0
60	MG	AA	2921	1/1	0.96	0.31	7.25	50,50,50,50	0
60	MG	BA	2908	1/1	0.94	0.39	7.20	20,20,20,20	0
60	MG	BA	2951	1/1	0.86	0.30	7.11	72,72,72,72	0
60	MG	Aa	1624	1/1	0.99	0.26	7.09	37,37,37,37	0
60	MG	AA	2913	1/1	0.92	0.50	7.07	22,22,22,22	0
60	MG	Bv	105	1/1	0.86	0.33	7.05	81,81,81,81	1
60	MG	BA	3011	1/1	0.98	0.42	7.03	11,11,11,11	0
60	MG	Aa	1744	1/1	0.90	0.34	6.94	87,87,87,87	0
60	MG	BA	3069	1/1	0.84	0.33	6.87	35,35,35,35	0
60	MG	AA	3019	1/1	1.00	0.33	6.78	26,26,26,26	0
60	MG	Av	102	1/1	0.97	0.36	6.54	77,77,77,77	0
60	MG	AA	2915	1/1	0.94	0.34	6.33	21,21,21,21	0
60	MG	AA	2907	1/1	0.97	0.24	6.28	48,48,48,48	0
60	MG	AA	3061	1/1	0.89	0.38	6.20	42,42,42,42	0
60	MG	BA	2914	1/1	0.98	0.27	6.17	11,11,11,11	0
60	MG	BA	3176	1/1	0.75	0.40	6.11	48,48,48,48	0
60	MG	BA	2957	1/1	0.99	0.40	5.85	13,13,13,13	0
60	MG	Ba	1671	1/1	0.91	0.32	5.84	87,87,87,87	0
60	MG	AA	3236	1/1	0.88	0.37	5.83	90,90,90,90	0
60	MG	Aa	1611	1/1	0.88	0.78	5.82	60,60,60,60	0
60	MG	BA	3029	1/1	0.92	0.33	5.82	27,27,27,27	0
60	MG	BA	3194	1/1	0.94	0.37	5.79	12,12,12,12	0
60	MG	BA	3102	1/1	0.92	0.24	5.73	47,47,47,47	0
60	MG	AA	2919	1/1	0.91	0.31	5.73	36,36,36,36	0
60	MG	Aa	1635	1/1	0.92	0.29	5.71	39,39,39,39	0
60	MG	AA	3046	1/1	0.97	0.40	5.69	47,47,47,47	0
60	MG	BA	3091	1/1	0.95	0.37	5.60	32,32,32,32	0
60	MG	B7	101	1/1	0.86	0.31	5.58	36,36,36,36	0
60	MG	AA	2943	1/1	0.82	0.30	5.49	70,70,70,70	0
60	MG	AA	3163	1/1	0.76	0.32	5.46	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3035	1/1	0.94	0.29	5.38	21,21,21,21	0
60	MG	AA	3121	1/1	0.95	0.41	5.31	31,31,31,31	0
60	MG	AA	3233	1/1	0.90	0.35	5.09	44,44,44,44	0
60	MG	BA	3022	1/1	0.98	0.29	5.01	16,16,16,16	0
60	MG	BA	3097	1/1	0.81	0.26	5.01	54,54,54,54	0
60	MG	AA	3175	1/1	0.86	0.48	4.91	40,40,40,40	0
60	MG	AA	2951	1/1	0.75	0.29	4.87	53,53,53,53	0
60	MG	Aa	1735	1/1	0.81	0.26	4.74	68,68,68,68	1
60	MG	Ba	1609	1/1	0.69	0.84	4.60	74,74,74,74	0
60	MG	Aa	1674	1/1	0.62	0.32	4.56	90,90,90,90	0
60	MG	Aa	1738	1/1	0.95	0.28	4.52	55,55,55,55	0
60	MG	BD	301	1/1	0.94	0.32	4.50	14,14,14,14	0
60	MG	BA	2965	1/1	0.79	0.30	4.50	58,58,58,58	0
60	MG	BA	2966	1/1	0.50	0.30	4.49	67,67,67,67	0
60	MG	AA	3158	1/1	0.89	0.30	4.32	46,46,46,46	0
60	MG	AA	3219	1/1	0.96	0.48	4.27	30,30,30,30	0
60	MG	Aa	1628	1/1	0.89	0.30	4.21	92,92,92,92	0
60	MG	AA	3231	1/1	0.92	0.25	4.17	51,51,51,51	0
60	MG	BA	3133	1/1	0.85	0.27	4.13	54,54,54,54	0
60	MG	BA	3183	1/1	0.84	0.23	4.10	44,44,44,44	0
60	MG	BA	3060	1/1	0.97	0.37	4.09	16,16,16,16	0
60	MG	BA	3127	1/1	0.99	0.52	4.08	20,20,20,20	0
60	MG	AA	2960	1/1	0.79	0.33	4.08	17,17,17,17	0
60	MG	BA	3088	1/1	0.62	0.39	4.07	107,107,107,107	0
60	MG	AA	2953	1/1	0.96	0.27	4.04	96,96,96,96	0
60	MG	AA	3128	1/1	0.99	0.49	3.93	23,23,23,23	0
60	MG	AA	3195	1/1	0.97	0.23	3.87	30,30,30,30	0
60	MG	BA	3138	1/1	0.78	0.23	3.85	54,54,54,54	0
60	MG	BA	3147	1/1	0.81	0.27	3.85	56,56,56,56	0
60	MG	AA	2985	1/1	0.94	0.43	3.84	31,31,31,31	0
60	MG	BA	3037	1/1	0.88	0.24	3.84	35,35,35,35	0
60	MG	AA	3083	1/1	0.95	0.26	3.76	76,76,76,76	0
60	MG	BA	3028	1/1	0.96	0.26	3.73	24,24,24,24	0
60	MG	AA	2914	1/1	0.96	0.30	3.73	15,15,15,15	0
60	MG	Ba	1695	1/1	0.33	0.36	3.56	86,86,86,86	0
60	MG	Aa	1678	1/1	0.65	0.29	3.50	93,93,93,93	0
60	MG	Aa	1685	1/1	0.88	0.24	3.48	53,53,53,53	0
60	MG	BA	3217	1/1	0.99	0.37	3.46	26,26,26,26	0
60	MG	AA	3194	1/1	0.97	0.28	3.44	26,26,26,26	0
60	MG	BA	3045	1/1	0.97	0.27	3.20	16,16,16,16	0
60	MG	BA	2920	1/1	0.97	0.24	3.20	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	Ba	1731	1/1	0.96	0.30	3.10	20,20,20,20	0
60	MG	AA	2929	1/1	0.93	0.28	3.09	29,29,29,29	0
60	MG	Ba	1668	1/1	0.92	0.33	3.05	49,49,49,49	0
60	MG	AA	3012	1/1	0.95	0.23	3.00	22,22,22,22	0
60	MG	BA	3191	1/1	0.97	0.23	2.94	23,23,23,23	0
60	MG	Aa	1613	1/1	0.90	0.34	2.91	100,100,100,100	0
60	MG	AA	3070	1/1	0.92	0.23	2.84	54,54,54,54	0
60	MG	BA	2928	1/1	0.90	0.23	2.83	17,17,17,17	0
60	MG	AA	2965	1/1	0.92	0.24	2.71	69,69,69,69	0
60	MG	Aa	1642	1/1	0.90	0.26	2.62	95,95,95,95	0
60	MG	BA	3070	1/1	0.90	0.30	2.58	83,83,83,83	0
60	MG	BA	3105	1/1	0.93	0.32	2.44	40,40,40,40	0
60	MG	Aa	1670	1/1	0.92	0.23	2.35	43,43,43,43	0
60	MG	AA	3029	1/1	0.96	0.22	2.18	37,37,37,37	0
60	MG	BA	3234	1/1	0.68	0.26	2.10	74,74,74,74	0
60	MG	AA	2988	1/1	0.97	0.28	2.00	33,33,33,33	0
60	MG	Aa	1732	1/1	0.85	0.29	1.98	49,49,49,49	0
60	MG	Ba	1718	1/1	0.84	0.31	1.94	107,107,107,107	0
60	MG	BA	3090	1/1	0.96	0.23	1.83	32,32,32,32	0
60	MG	AA	3094	1/1	0.87	0.33	1.79	67,67,67,67	0
60	MG	Aa	1654	1/1	0.90	0.17	1.77	56,56,56,56	0
60	MG	AA	3091	1/1	0.95	0.23	1.70	27,27,27,27	0
60	MG	AA	3085	1/1	0.98	0.23	1.63	47,47,47,47	0
60	MG	AA	3123	1/1	0.97	0.30	1.58	18,18,18,18	0
60	MG	Ba	1736	1/1	0.83	0.32	1.56	59,59,59,59	0
60	MG	BA	2923	1/1	0.99	0.24	1.53	29,29,29,29	0
60	MG	AA	3182	1/1	0.90	0.40	1.30	40,40,40,40	0
60	MG	BA	3179	1/1	0.68	0.37	1.24	24,24,24,24	0
60	MG	BA	2910	1/1	0.93	0.22	1.23	2,2,2,2	0
60	MG	AA	3002	1/1	0.83	0.17	1.23	58,58,58,58	0
60	MG	AA	2922	1/1	0.95	0.22	1.20	48,48,48,48	0
60	MG	Ba	1648	1/1	0.92	0.25	1.15	32,32,32,32	0
60	MG	Aa	1657	1/1	0.92	0.36	1.13	71,71,71,71	0
60	MG	BA	3169	1/1	0.94	0.22	1.10	25,25,25,25	0
60	MG	AD	301	1/1	0.96	0.33	1.06	21,21,21,21	0
60	MG	BA	3063	1/1	0.98	0.21	1.06	26,26,26,26	0
60	MG	Aa	1668	1/1	0.98	0.25	1.06	40,40,40,40	0
60	MG	BA	3020	1/1	0.96	0.21	1.04	84,84,84,84	0
60	MG	Bv	102	1/1	0.97	0.27	1.03	37,37,37,37	0
60	MG	BA	3015	1/1	0.95	0.20	0.88	18,18,18,18	0
60	MG	BA	3086	1/1	0.80	0.19	0.79	48,48,48,48	0
60	MG	Ba	1693	1/1	0.91	0.18	0.75	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AD	302	1/1	0.86	0.34	0.74	21,21,21,21	0
60	MG	BA	2939	1/1	0.98	0.24	0.72	71,71,71,71	0
60	MG	Aa	1740	1/1	0.94	0.24	0.71	42,42,42,42	0
60	MG	AA	3032	1/1	0.98	0.21	0.69	33,33,33,33	0
60	MG	Ba	1672	1/1	0.78	0.29	0.65	95,95,95,95	0
60	MG	AA	3184	1/1	0.94	0.19	0.61	44,44,44,44	0
60	MG	Aa	1616	1/1	0.88	0.25	0.59	64,64,64,64	0
59	ZN	Ad	301	1/1	0.99	0.29	0.57	76,76,76,76	0
60	MG	BA	2950	1/1	0.97	0.20	0.54	37,37,37,37	0
60	MG	BA	2921	1/1	0.98	0.21	0.54	31,31,31,31	0
60	MG	B0	101	1/1	0.70	0.48	0.51	71,71,71,71	0
60	MG	AA	2912	1/1	0.97	0.20	0.50	26,26,26,26	0
60	MG	BA	3230	1/1	0.83	0.21	0.44	45,45,45,45	0
60	MG	BA	2918	1/1	0.87	0.18	0.43	29,29,29,29	0
60	MG	BA	2978	1/1	0.94	0.16	0.40	56,56,56,56	0
59	ZN	Bd	302	1/1	0.99	0.29	0.33	80,80,80,80	0
60	MG	Ba	1623	1/1	0.95	0.18	0.26	34,34,34,34	0
60	MG	AA	3063	1/1	0.93	0.22	0.05	53,53,53,53	0
60	MG	BA	3050	1/1	0.87	0.20	0.02	29,29,29,29	0
60	MG	BD	302	1/1	0.98	0.24	-0.04	18,18,18,18	0
60	MG	AA	3049	1/1	0.97	0.20	-0.05	54,54,54,54	0
60	MG	BA	3122	1/1	0.96	0.24	-0.06	24,24,24,24	0
60	MG	Aa	1721	1/1	0.87	0.23	-0.35	68,68,68,68	0
60	MG	BA	3001	1/1	0.93	0.15	-0.36	37,37,37,37	0
60	MG	Aa	1673	1/1	0.89	0.19	-0.36	60,60,60,60	0
60	MG	Aa	1609	1/1	0.95	0.20	-0.38	64,64,64,64	0
60	MG	Ba	1612	1/1	0.90	0.14	-0.42	82,82,82,82	0
60	MG	AF	301	1/1	0.66	0.22	-0.43	74,74,74,74	0
60	MG	Aa	1649	1/1	0.90	0.23	-0.46	32,32,32,32	0
60	MG	BA	3031	1/1	0.97	0.18	-0.49	14,14,14,14	0
60	MG	Ba	1611	1/1	0.92	0.19	-0.50	97,97,97,97	0
60	MG	AA	3062	1/1	0.97	0.21	-0.53	26,26,26,26	0
60	MG	AA	3030	1/1	0.87	0.17	-0.55	28,28,28,28	0
60	MG	Bm	201	1/1	0.75	0.28	-0.57	118,118,118,118	0
60	MG	BA	2942	1/1	0.72	0.15	-0.59	42,42,42,42	0
60	MG	AA	3050	1/1	0.98	0.17	-0.61	96,96,96,96	0
60	MG	Aa	1688	1/1	0.52	0.23	-0.70	63,63,63,63	1
60	MG	AA	3213	1/1	0.94	0.19	-0.71	33,33,33,33	0
60	MG	BA	2986	1/1	0.95	0.17	-0.74	63,63,63,63	0
60	MG	Ba	1694	1/1	0.89	0.17	-0.84	83,83,83,83	0
60	MG	Ba	1673	1/1	0.95	0.20	-0.85	39,39,39,39	0
60	MG	Ba	1674	1/1	0.84	0.15	-0.85	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Aa	1620	1/1	0.94	0.17	-0.86	73,73,73,73	0
60	MG	Ba	1687	1/1	0.83	0.18	-0.86	50,50,50,50	1
60	MG	BA	2988	1/1	0.98	0.18	-0.89	34,34,34,34	0
60	MG	AA	2971	1/1	0.85	0.12	-0.95	52,52,52,52	0
60	MG	Aa	1694	1/1	0.97	0.16	-0.98	89,89,89,89	0
60	MG	Aa	1614	1/1	0.74	0.11	-1.03	69,69,69,69	0
60	MG	Ba	1670	1/1	0.92	0.18	-1.08	58,58,58,58	0
60	MG	AA	3171	1/1	0.88	0.15	-1.13	57,57,57,57	0
60	MG	AA	3232	1/1	0.92	0.19	-1.15	64,64,64,64	0
60	MG	BA	3195	1/1	0.89	0.17	-1.24	37,37,37,37	0
59	ZN	An	101	1/1	0.98	0.13	-1.25	153,153,153,153	0
59	ZN	Bn	101	1/1	0.97	0.14	-1.30	137,137,137,137	0
60	MG	AA	2979	1/1	0.93	0.12	-1.37	51,51,51,51	0
60	MG	AA	2911	1/1	0.97	0.16	-1.54	20,20,20,20	0
59	ZN	A4	101	1/1	0.83	0.08	-1.54	186,186,186,186	0
60	MG	BA	2911	1/1	0.99	0.16	-1.65	21,21,21,21	0
60	MG	BF	301	1/1	0.90	0.14	-1.67	40,40,40,40	0
60	MG	BA	2919	1/1	0.97	0.19	-1.68	13,13,13,13	0
60	MG	BA	3017	1/1	0.95	0.19	-1.76	38,38,38,38	0
60	MG	BA	3203	1/1	0.95	0.13	-1.79	95,95,95,95	0
60	MG	BA	3132	1/1	0.70	0.15	-1.81	43,43,43,43	0
60	MG	Ba	1680	1/1	0.93	0.12	-1.83	63,63,63,63	0
60	MG	BA	3168	1/1	0.85	0.14	-1.91	53,53,53,53	0
59	ZN	A9	101	1/1	0.97	0.07	-1.95	138,138,138,138	0
60	MG	BA	3181	1/1	0.64	0.14	-2.03	61,61,61,61	0
60	MG	BA	3096	1/1	0.94	0.12	-2.06	49,49,49,49	0
60	MG	AA	3106	1/1	0.96	0.15	-2.12	65,65,65,65	0
60	MG	AA	3103	1/1	0.90	0.09	-2.17	35,35,35,35	0
60	MG	AA	3186	1/1	0.90	0.11	-2.20	77,77,77,77	0
60	MG	Ba	1677	1/1	0.96	0.11	-2.21	138,138,138,138	0
60	MG	Ba	1606	1/1	0.98	0.16	-2.26	50,50,50,50	0
60	MG	Aa	1677	1/1	0.91	0.12	-2.29	69,69,69,69	0
60	MG	BA	2959	1/1	0.85	0.12	-2.32	37,37,37,37	0
60	MG	AA	3016	1/1	0.98	0.13	-2.42	31,31,31,31	0
60	MG	AA	2940	1/1	0.96	0.11	-2.54	34,34,34,34	0
59	ZN	B4	101	1/1	0.87	0.08	-2.64	201,201,201,201	0
60	MG	Aa	1733	1/1	0.97	0.12	-2.71	60,60,60,60	0
60	MG	BA	3192	1/1	0.96	0.14	-2.76	34,34,34,34	0
60	MG	Aa	1653	1/1	0.95	0.12	-2.79	59,59,59,59	0
60	MG	AA	3064	1/1	0.98	0.16	-3.11	29,29,29,29	0
60	MG	AA	2924	1/1	0.99	0.11	-3.30	32,32,32,32	0
60	MG	AA	2962	1/1	0.96	0.07	-3.48	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	2929	1/1	0.89	0.12	-3.61	10,10,10,10	0
60	MG	AA	3174	1/1	0.96	0.13	-3.61	72,72,72,72	0
59	ZN	B9	101	1/1	0.99	0.07	-3.93	116,116,116,116	0
60	MG	AA	2989	1/1	0.98	0.10	-3.96	33,33,33,33	0
60	MG	BA	3210	1/1	0.99	0.14	-3.99	22,22,22,22	0
60	MG	Ba	1619	1/1	0.96	0.07	-4.19	44,44,44,44	0
60	MG	BA	2969	1/1	0.87	0.10	-4.25	35,35,35,35	0
60	MG	Aa	1608	1/1	0.99	0.15	-4.38	39,39,39,39	0
60	MG	Aa	1737	1/1	0.97	0.14	-4.52	119,119,119,119	0
60	MG	Ba	1633	1/1	0.98	0.09	-5.22	39,39,39,39	0
60	MG	Aa	1634	1/1	0.99	0.07	-5.43	47,47,47,47	0
60	MG	Aa	1671	1/1	0.94	0.14	-5.56	49,49,49,49	0
60	MG	Aa	1695	1/1	0.96	0.08	-6.11	78,78,78,78	0
60	MG	Aa	1681	1/1	0.97	0.08	-6.67	76,76,76,76	0
60	MG	Ba	1652	1/1	0.97	0.09	-8.86	69,69,69,69	0
60	MG	Ba	1732	1/1	0.98	0.11	-11.19	70,70,70,70	0
60	MG	BA	3056	1/1	0.92	0.21	-	92,92,92,92	0
60	MG	BA	3200	1/1	0.90	0.26	-	33,33,33,33	0
60	MG	AA	3250	1/1	0.95	0.59	-	40,40,40,40	0
60	MG	Ba	1702	1/1	0.85	1.11	-	97,97,97,97	0
60	MG	BA	2993	1/1	0.96	0.39	-	12,12,12,12	0
60	MG	AA	3013	1/1	0.72	0.96	-	78,78,78,78	0
60	MG	Ba	1717	1/1	0.79	1.16	-	71,71,71,71	0
60	MG	AA	3037	1/1	0.95	0.39	-	27,27,27,27	0
60	MG	Ba	1729	1/1	0.77	1.25	-	66,66,66,66	0
60	MG	Ba	1716	1/1	0.68	0.41	-	63,63,63,63	0
60	MG	AA	3107	1/1	0.93	0.29	-	47,47,47,47	0
60	MG	AA	2916	1/1	0.98	0.41	-	25,25,25,25	0
60	MG	Ba	1605	1/1	0.89	0.73	-	73,73,73,73	0
60	MG	Ba	1676	1/1	0.61	0.28	-	137,137,137,137	1
60	MG	Ba	1699	1/1	0.46	1.12	-	88,88,88,88	0
60	MG	Bl	201	1/1	0.80	0.66	-	5,5,5,5	1
60	MG	Aa	1698	1/1	0.91	1.04	-	98,98,98,98	1
60	MG	Ba	1666	1/1	0.89	0.80	-	73,73,73,73	0
60	MG	AA	2995	1/1	0.95	0.63	-	18,18,18,18	0
60	MG	BA	2935	1/1	0.97	0.58	-	25,25,25,25	0
60	MG	BA	3044	1/1	0.97	0.44	-	21,21,21,21	0
60	MG	AA	3251	1/1	0.89	0.71	-	84,84,84,84	0
60	MG	Aa	1709	1/1	0.92	0.12	-	148,148,148,148	0
60	MG	Ba	1629	1/1	0.97	0.14	-	36,36,36,36	0
60	MG	BA	2926	1/1	0.96	0.50	-	24,24,24,24	0
60	MG	BA	3039	1/1	0.98	0.28	-	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3051	1/1	0.95	0.39	-	16,16,16,16	0
60	MG	Ba	1667	1/1	0.85	0.49	-	50,50,50,50	0
60	MG	AA	3206	1/1	0.47	0.34	-	115,115,115,115	0
60	MG	AA	2958	1/1	0.91	0.22	-	47,47,47,47	0
60	MG	BA	3007	1/1	0.70	0.41	-	90,90,90,90	0
60	MG	Ba	1722	1/1	0.81	0.33	-	63,63,63,63	0
60	MG	AA	3189	1/1	0.97	0.35	-	107,107,107,107	0
60	MG	AQ	201	1/1	0.78	1.97	-	94,94,94,94	0
60	MG	Aa	1615	1/1	0.76	1.01	-	53,53,53,53	0
60	MG	Ba	1686	1/1	0.86	0.30	-	84,84,84,84	0
60	MG	Ba	1641	1/1	0.96	0.67	-	94,94,94,94	0
60	MG	AA	3113	1/1	0.91	0.56	-	76,76,76,76	0
60	MG	Aa	1731	1/1	0.89	0.42	-	64,64,64,64	0
60	MG	BA	3003	1/1	0.99	0.31	-	22,22,22,22	0
60	MG	Ba	1737	1/1	0.74	0.56	-	76,76,76,76	0
60	MG	Aa	1717	1/1	0.73	0.39	-	66,66,66,66	0
60	MG	BA	3216	1/1	0.75	0.56	-	117,117,117,117	0
60	MG	BA	3049	1/1	0.96	0.35	-	62,62,62,62	0
60	MG	BA	2973	1/1	0.77	0.41	-	52,52,52,52	0
60	MG	BA	3174	1/1	0.88	0.25	-	63,63,63,63	0
60	MG	BA	3110	1/1	0.93	0.36	-	23,23,23,23	0
60	MG	BO	201	1/1	0.85	0.53	-	122,122,122,122	0
60	MG	AA	3223	1/1	0.60	0.54	-	78,78,78,78	0
60	MG	AA	2986	1/1	0.87	0.74	-	46,46,46,46	0
60	MG	BA	3214	1/1	0.81	0.63	-	34,34,34,34	0
60	MG	Aa	1625	1/1	0.91	0.80	-	76,76,76,76	0
60	MG	Aa	1713	1/1	0.90	1.27	-	98,98,98,98	0
60	MG	Ba	1616	1/1	0.84	0.29	-	29,29,29,29	1
60	MG	AA	3117	1/1	0.31	0.52	-	148,148,148,148	0
60	MG	Aa	1730	1/1	0.03	1.12	-	77,77,77,77	0
60	MG	BA	3012	1/1	0.60	0.85	-	61,61,61,61	0
60	MG	Aa	1711	1/1	0.83	0.43	-	70,70,70,70	0
60	MG	AA	3191	1/1	0.96	0.19	-	74,74,74,74	0
60	MG	BA	3066	1/1	0.81	0.72	-	32,32,32,32	0
60	MG	AA	3074	1/1	0.89	0.39	-	33,33,33,33	0
60	MG	AA	3162	1/1	0.92	0.35	-	94,94,94,94	0
60	MG	AA	3067	1/1	0.88	0.59	-	34,34,34,34	0
60	MG	BA	3263	1/1	0.51	0.27	-	68,68,68,68	0
60	MG	BA	2903	1/1	0.96	0.10	-	99,99,99,99	0
60	MG	BA	3040	1/1	0.97	0.21	-	17,17,17,17	0
60	MG	BA	3225	1/1	0.88	0.57	-	38,38,38,38	0
60	MG	BA	3092	1/1	0.91	0.27	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	AA	3218	1/1	0.80	0.81	-	98,98,98,98	0
60	MG	Aa	1726	1/1	0.90	0.72	-	36,36,36,36	0
60	MG	BA	3083	1/1	0.86	0.54	-	52,52,52,52	0
60	MG	BA	3113	1/1	0.96	0.43	-	24,24,24,24	1
60	MG	AA	3055	1/1	0.94	0.43	-	67,67,67,67	0
60	MG	AA	3022	1/1	0.98	0.47	-	22,22,22,22	0
60	MG	BA	3114	1/1	0.90	0.27	-	8,8,8,8	0
60	MG	AA	3203	1/1	0.79	0.23	-	66,66,66,66	0
60	MG	BA	3158	1/1	0.81	0.32	-	88,88,88,88	0
60	MG	Ba	1720	1/1	0.77	0.38	-	91,91,91,91	0
60	MG	Ba	1697	1/1	0.74	1.00	-	93,93,93,93	1
60	MG	AA	3266	1/1	0.83	0.30	-	87,87,87,87	0
60	MG	Ba	1721	1/1	0.53	0.77	-	92,92,92,92	0
60	MG	BA	3235	1/1	0.75	0.64	-	51,51,51,51	0
60	MG	BA	2943	1/1	0.85	0.30	-	35,35,35,35	0
60	MG	Aa	1745	1/1	0.96	0.39	-	48,48,48,48	0
60	MG	BA	3185	1/1	0.96	0.44	-	40,40,40,40	0
60	MG	Aa	1693	1/1	0.73	0.56	-	75,75,75,75	0
60	MG	BA	2941	1/1	0.90	0.27	-	62,62,62,62	0
60	MG	BA	3157	1/1	0.99	0.12	-	85,85,85,85	0
60	MG	Ba	1647	1/1	0.80	0.60	-	117,117,117,117	0
60	MG	Ba	1624	1/1	0.75	1.05	-	76,76,76,76	0
60	MG	AA	2933	1/1	0.95	0.59	-	67,67,67,67	0
60	MG	Ba	1657	1/1	0.92	0.43	-	52,52,52,52	0
60	MG	BA	3177	1/1	0.95	0.23	-	70,70,70,70	0
60	MG	BA	2992	1/1	0.96	0.20	-	33,33,33,33	0
60	MG	AA	3090	1/1	0.97	0.46	-	59,59,59,59	0
60	MG	BA	3228	1/1	0.76	1.00	-	94,94,94,94	0
60	MG	Aa	1610	1/1	0.73	0.78	-	115,115,115,115	0
60	MG	AA	3157	1/1	0.87	0.92	-	66,66,66,66	0
60	MG	Bv	101	1/1	0.71	0.58	-	52,52,52,52	1
60	MG	Av	104	1/1	0.86	0.77	-	50,50,50,50	1
60	MG	AA	3119	1/1	0.71	0.91	-	68,68,68,68	0
60	MG	AA	3084	1/1	0.71	0.57	-	54,54,54,54	0
60	MG	AA	2904	1/1	0.95	0.29	-	131,131,131,131	0
60	MG	BA	3106	1/1	0.97	0.40	-	41,41,41,41	0
60	MG	AB	201	1/1	0.85	0.41	-	63,63,63,63	0
60	MG	Ba	1710	1/1	0.84	0.36	-	65,65,65,65	0
60	MG	BA	3116	1/1	0.83	0.45	-	91,91,91,91	0
60	MG	AA	3159	1/1	0.95	0.20	-	114,114,114,114	0
60	MG	AA	3220	1/1	0.50	0.57	-	54,54,54,54	0
60	MG	BA	2909	1/1	0.92	0.48	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3183	1/1	0.92	0.38	-	69,69,69,69	0
60	MG	Ba	1683	1/1	0.67	0.54	-	65,65,65,65	0
60	MG	AA	3115	1/1	0.94	0.31	-	19,19,19,19	0
60	MG	Ba	1639	1/1	0.81	0.52	-	58,58,58,58	0
60	MG	BA	3112	1/1	0.94	0.19	-	69,69,69,69	0
60	MG	AA	2973	1/1	0.76	0.39	-	79,79,79,79	0
60	MG	Aa	1639	1/1	0.68	0.38	-	65,65,65,65	0
60	MG	AA	3066	1/1	0.96	0.48	-	27,27,27,27	0
60	MG	Ba	1679	1/1	0.65	0.73	-	92,92,92,92	0
60	MG	AA	3217	1/1	0.95	0.29	-	85,85,85,85	0
60	MG	AA	3093	1/1	0.96	0.23	-	56,56,56,56	0
60	MG	BA	2946	1/1	0.95	0.20	-	75,75,75,75	0
60	MG	AA	3075	1/1	0.42	0.90	-	84,84,84,84	0
60	MG	Ba	1741	1/1	0.88	0.25	-	73,73,73,73	0
60	MG	AA	2957	1/1	0.48	0.48	-	72,72,72,72	0
60	MG	Aa	1665	1/1	0.78	2.75	-	120,120,120,120	0
60	MG	BA	3042	1/1	0.94	0.19	-	30,30,30,30	0
60	MG	Bw	101	1/1	0.61	0.13	-	132,132,132,132	1
60	MG	AA	3036	1/1	0.96	1.26	-	100,100,100,100	0
60	MG	BA	2960	1/1	0.73	0.13	-	101,101,101,101	0
60	MG	AA	3001	1/1	0.91	0.61	-	26,26,26,26	0
60	MG	AA	3257	1/1	0.95	0.30	-	78,78,78,78	0
60	MG	BA	3206	1/1	0.53	0.52	-	71,71,71,71	0
60	MG	AA	3263	1/1	0.27	0.85	-	75,75,75,75	0
60	MG	BA	3261	1/1	0.54	0.64	-	68,68,68,68	0
60	MG	BA	3207	1/1	0.81	0.36	-	118,118,118,118	0
60	MG	BA	3077	1/1	0.92	0.28	-	46,46,46,46	0
60	MG	Ba	1692	1/1	0.61	0.56	-	83,83,83,83	0
60	MG	AA	3249	1/1	0.97	0.13	-	55,55,55,55	0
60	MG	AA	3089	1/1	0.68	0.16	-	75,75,75,75	0
60	MG	Aa	1680	1/1	0.62	0.56	-	107,107,107,107	0
60	MG	AA	3161	1/1	0.93	0.48	-	61,61,61,61	0
60	MG	AA	3255	1/1	0.78	0.38	-	50,50,50,50	0
60	MG	BA	3170	1/1	0.88	0.25	-	13,13,13,13	0
60	MG	AA	3224	1/1	0.94	0.83	-	73,73,73,73	0
60	MG	Aa	1629	1/1	0.85	0.44	-	59,59,59,59	0
60	MG	AA	3137	1/1	0.68	0.85	-	90,90,90,90	0
60	MG	BA	3229	1/1	0.93	0.21	-	32,32,32,32	0
60	MG	BA	3125	1/1	0.94	0.44	-	40,40,40,40	0
60	MG	Aa	1603	1/1	0.99	0.13	-	68,68,68,68	1
60	MG	BA	3212	1/1	0.94	1.44	-	68,68,68,68	0
60	MG	AA	3237	1/1	0.88	0.33	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Aa	1701	1/1	0.83	0.40	-	71,71,71,71	0
60	MG	AA	2901	1/1	0.80	0.40	-	84,84,84,84	0
60	MG	AA	3185	1/1	0.90	0.37	-	83,83,83,83	0
60	MG	BA	3201	1/1	0.93	0.56	-	43,43,43,43	0
60	MG	BA	3129	1/1	0.68	0.45	-	53,53,53,53	0
60	MG	BA	3008	1/1	0.99	0.43	-	32,32,32,32	0
60	MG	Ba	1688	1/1	0.97	0.19	-	120,120,120,120	1
60	MG	Ba	1622	1/1	0.89	0.23	-	57,57,57,57	0
60	MG	BA	3115	1/1	0.89	0.55	-	21,21,21,21	0
60	MG	BA	3048	1/1	0.85	0.28	-	31,31,31,31	0
60	MG	Aa	1638	1/1	0.82	0.36	-	62,62,62,62	0
60	MG	BA	3202	1/1	0.91	0.19	-	76,76,76,76	0
60	MG	AA	2930	1/1	0.87	0.07	-	15,15,15,15	0
60	MG	AA	3131	1/1	0.87	0.49	-	46,46,46,46	0
60	MG	AA	3033	1/1	0.99	0.32	-	57,57,57,57	0
60	MG	BA	3059	1/1	0.89	0.18	-	52,52,52,52	0
60	MG	Ba	1703	1/1	0.91	0.44	-	25,25,25,25	1
60	MG	AA	3031	1/1	0.94	0.54	-	45,45,45,45	0
60	MG	AA	2947	1/1	0.92	0.32	-	72,72,72,72	0
60	MG	Ba	1618	1/1	0.97	0.37	-	57,57,57,57	0
60	MG	BA	3030	1/1	0.97	0.51	-	26,26,26,26	0
60	MG	Ba	1632	1/1	0.90	0.78	-	41,41,41,41	0
60	MG	BA	3065	1/1	0.97	0.27	-	13,13,13,13	0
60	MG	BA	3218	1/1	0.69	0.82	-	80,80,80,80	0
60	MG	Aa	1655	1/1	0.88	0.96	-	87,87,87,87	0
60	MG	Aa	1650	1/1	0.69	0.78	-	64,64,64,64	0
60	MG	BA	3005	1/1	0.94	0.34	-	21,21,21,21	0
60	MG	BA	3074	1/1	0.65	0.73	-	75,75,75,75	0
60	MG	BA	3109	1/1	0.84	1.22	-	90,90,90,90	0
60	MG	AB	203	1/1	0.71	0.68	-	56,56,56,56	0
60	MG	BA	2976	1/1	0.82	0.37	-	104,104,104,104	0
60	MG	AA	3079	1/1	0.93	0.58	-	55,55,55,55	0
60	MG	AA	3193	1/1	0.95	0.26	-	20,20,20,20	0
60	MG	Ae	201	1/1	0.82	0.92	-	108,108,108,108	0
60	MG	AA	3226	1/1	0.73	0.38	-	95,95,95,95	0
60	MG	AA	3015	1/1	0.94	0.24	-	14,14,14,14	0
60	MG	AA	3252	1/1	0.78	1.27	-	80,80,80,80	0
60	MG	BA	3025	1/1	0.98	0.19	-	12,12,12,12	0
60	MG	Ba	1675	1/1	0.86	0.97	-	58,58,58,58	0
60	MG	BA	3076	1/1	0.95	0.39	-	83,83,83,83	0
60	MG	BA	2944	1/1	0.99	0.14	-	62,62,62,62	0
60	MG	AA	3059	1/1	0.82	0.77	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Aa	1715	1/1	0.88	0.16	-	57,57,57,57	0
60	MG	Ba	1614	1/1	0.94	0.44	-	68,68,68,68	0
60	MG	BA	2989	1/1	0.97	0.60	-	31,31,31,31	0
60	MG	AA	3058	1/1	0.97	0.26	-	44,44,44,44	0
60	MG	AA	3253	1/1	0.93	0.24	-	71,71,71,71	0
60	MG	AA	2982	1/1	0.94	1.17	-	56,56,56,56	0
60	MG	Aa	1669	1/1	0.83	0.68	-	122,122,122,122	0
60	MG	Ba	1704	1/1	0.77	0.47	-	62,62,62,62	0
60	MG	AA	2978	1/1	0.79	0.64	-	124,124,124,124	0
60	MG	Aa	1656	1/1	0.64	0.44	-	88,88,88,88	0
60	MG	BA	3073	1/1	0.93	0.32	-	30,30,30,30	0
60	MG	BA	3188	1/1	0.95	0.07	-	64,64,64,64	0
60	MG	BA	3186	1/1	0.90	0.66	-	70,70,70,70	0
60	MG	AA	3021	1/1	0.92	0.24	-	96,96,96,96	0
60	MG	Aa	1707	1/1	0.91	0.48	-	79,79,79,79	0
60	MG	AA	2938	1/1	0.99	0.12	-	84,84,84,84	0
60	MG	BA	2972	1/1	0.96	0.61	-	30,30,30,30	0
60	MG	BA	3208	1/1	0.91	0.28	-	52,52,52,52	0
60	MG	AA	3122	1/1	0.85	0.42	-	39,39,39,39	0
60	MG	Aa	1676	1/1	0.73	0.82	-	90,90,90,90	1
60	MG	AA	2974	1/1	0.96	0.76	-	43,43,43,43	0
60	MG	AA	3118	1/1	0.91	0.50	-	74,74,74,74	0
60	MG	Ba	1615	1/1	0.83	0.15	-	81,81,81,81	0
60	MG	AA	3042	1/1	0.98	0.47	-	27,27,27,27	0
60	MG	Aa	1623	1/1	0.95	0.32	-	74,74,74,74	0
60	MG	AA	3188	1/1	0.97	0.30	-	36,36,36,36	0
60	MG	AA	3155	1/1	0.72	0.16	-	92,92,92,92	1
60	MG	BA	3223	1/1	0.90	0.18	-	43,43,43,43	0
60	MG	Aa	1640	1/1	0.91	0.36	-	60,60,60,60	0
60	MG	Aa	1667	1/1	0.88	0.69	-	78,78,78,78	0
60	MG	BA	3199	1/1	0.86	0.23	-	34,34,34,34	0
60	MG	Ba	1738	1/1	0.65	0.94	-	106,106,106,106	0
60	MG	Ba	1709	1/1	0.96	0.35	-	52,52,52,52	0
60	MG	AA	3153	1/1	0.69	0.35	-	71,71,71,71	0
60	MG	BA	3021	1/1	0.91	0.32	-	31,31,31,31	0
60	MG	BA	2933	1/1	0.92	0.38	-	18,18,18,18	1
60	MG	AA	3007	1/1	0.98	0.13	-	43,43,43,43	0
60	MG	BA	2953	1/1	0.97	0.21	-	25,25,25,25	0
60	MG	BA	3006	1/1	0.98	0.37	-	21,21,21,21	0
60	MG	AA	2975	1/1	0.96	0.42	-	90,90,90,90	0
60	MG	AA	2934	1/1	0.96	0.25	-	32,32,32,32	1
60	MG	BA	3265	1/1	0.50	0.51	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	2927	1/1	0.93	0.48	-	32,32,32,32	0
60	MG	AA	3200	1/1	0.72	0.75	-	72,72,72,72	1
60	MG	B5	101	1/1	0.91	0.38	-	27,27,27,27	0
60	MG	AA	3240	1/1	0.67	0.77	-	106,106,106,106	0
60	MG	Ba	1640	1/1	0.77	0.84	-	80,80,80,80	0
60	MG	BA	3111	1/1	0.64	0.41	-	74,74,74,74	0
60	MG	Aa	1605	1/1	0.97	0.11	-	43,43,43,43	0
60	MG	AA	3060	1/1	0.94	0.24	-	46,46,46,46	0
60	MG	BA	3232	1/1	0.95	0.22	-	77,77,77,77	0
60	MG	BA	3164	1/1	0.93	0.51	-	31,31,31,31	0
60	MG	BA	2956	1/1	0.72	0.15	-	50,50,50,50	0
60	MG	BA	3082	1/1	0.91	0.17	-	34,34,34,34	0
60	MG	BA	3198	1/1	0.77	1.32	-	91,91,91,91	0
60	MG	AA	3215	1/1	0.98	0.14	-	56,56,56,56	0
60	MG	AA	3160	1/1	0.91	0.51	-	99,99,99,99	0
60	MG	BA	3149	1/1	0.75	0.42	-	76,76,76,76	0
60	MG	AA	3198	1/1	0.95	0.46	-	52,52,52,52	0
60	MG	Ba	1662	1/1	0.81	0.27	-	67,67,67,67	0
60	MG	BA	3117	1/1	0.95	0.62	-	63,63,63,63	0
60	MG	Aa	1691	1/1	0.93	0.33	-	53,53,53,53	0
60	MG	BA	3085	1/1	0.82	0.20	-	60,60,60,60	0
60	MG	BA	3000	1/1	0.93	0.44	-	16,16,16,16	0
60	MG	BA	3209	1/1	0.81	0.43	-	74,74,74,74	0
60	MG	Ba	1740	1/1	0.70	0.28	-	78,78,78,78	0
60	MG	BA	3242	1/1	0.75	0.84	-	52,52,52,52	0
60	MG	AA	3241	1/1	0.70	0.51	-	64,64,64,64	0
60	MG	BA	2916	1/1	0.96	0.68	-	62,62,62,62	0
60	MG	AA	3100	1/1	0.85	0.92	-	97,97,97,97	0
60	MG	AA	3229	1/1	0.78	0.53	-	73,73,73,73	0
60	MG	AA	3145	1/1	0.89	0.65	-	78,78,78,78	0
60	MG	Ba	1637	1/1	0.76	0.60	-	80,80,80,80	0
60	MG	BA	2994	1/1	0.91	0.56	-	14,14,14,14	0
60	MG	BA	3249	1/1	0.83	0.85	-	67,67,67,67	0
60	MG	Ba	1715	1/1	0.52	0.27	-	94,94,94,94	0
60	MG	BA	3153	1/1	0.73	0.63	-	46,46,46,46	0
60	MG	AA	3076	1/1	0.90	0.23	-	78,78,78,78	0
60	MG	BA	3130	1/1	0.74	0.41	-	45,45,45,45	0
60	MG	BA	3252	1/1	0.77	0.18	-	40,40,40,40	0
60	MG	BA	3145	1/1	0.94	0.83	-	63,63,63,63	0
60	MG	BA	3262	1/1	0.75	0.32	-	39,39,39,39	0
60	MG	BA	3081	1/1	0.87	0.16	-	83,83,83,83	0
60	MG	AA	3008	1/1	0.69	0.37	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Ba	1604	1/1	0.67	0.58	-	75,75,75,75	0
60	MG	AA	2917	1/1	0.66	0.49	-	112,112,112,112	0
60	MG	BA	3144	1/1	0.69	1.04	-	59,59,59,59	0
60	MG	AA	3068	1/1	0.97	0.27	-	19,19,19,19	0
60	MG	Ba	1730	1/1	0.93	0.24	-	62,62,62,62	0
60	MG	BA	2936	1/1	0.79	0.22	-	35,35,35,35	0
60	MG	AA	2944	1/1	0.73	0.51	-	56,56,56,56	0
60	MG	Ba	1725	1/1	0.95	0.86	-	45,45,45,45	0
60	MG	Aa	1716	1/1	0.88	0.12	-	70,70,70,70	0
60	MG	AA	3196	1/1	0.87	0.67	-	70,70,70,70	0
60	MG	Aa	1659	1/1	0.80	0.40	-	88,88,88,88	0
60	MG	BA	3009	1/1	0.98	0.32	-	3,3,3,3	0
60	MG	Ba	1698	1/1	0.55	0.85	-	89,89,89,89	1
60	MG	BA	3098	1/1	0.57	0.81	-	52,52,52,52	0
60	MG	BA	3016	1/1	0.93	0.25	-	11,11,11,11	0
60	MG	BA	3036	1/1	0.99	0.41	-	34,34,34,34	0
60	MG	Ba	1663	1/1	0.33	0.80	-	85,85,85,85	0
60	MG	Aa	1699	1/1	0.58	0.60	-	84,84,84,84	1
60	MG	AA	2956	1/1	0.95	0.21	-	61,61,61,61	0
60	MG	AA	3246	1/1	0.68	0.27	-	70,70,70,70	0
60	MG	BA	3250	1/1	0.89	1.26	-	88,88,88,88	0
60	MG	Aa	1697	1/1	0.93	0.66	-	65,65,65,65	0
60	MG	Ba	1664	1/1	0.76	0.77	-	46,46,46,46	0
60	MG	BA	2932	1/1	0.93	0.39	-	67,67,67,67	0
60	MG	AA	3057	1/1	0.98	0.10	-	92,92,92,92	0
60	MG	BA	3046	1/1	0.88	0.35	-	28,28,28,28	0
60	MG	Aa	1607	1/1	0.93	0.65	-	69,69,69,69	0
60	MG	BA	3057	1/1	0.96	0.26	-	45,45,45,45	0
60	MG	BA	3078	1/1	0.94	0.58	-	32,32,32,32	0
60	MG	BA	2970	1/1	0.98	0.42	-	53,53,53,53	0
60	MG	AA	3144	1/1	0.85	1.08	-	50,50,50,50	0
60	MG	A1	101	1/1	0.93	0.28	-	53,53,53,53	0
60	MG	Aa	1687	1/1	0.68	0.15	-	64,64,64,64	0
60	MG	BA	3196	1/1	0.92	0.31	-	68,68,68,68	0
60	MG	BA	3162	1/1	0.85	0.34	-	57,57,57,57	0
60	MG	AA	3214	1/1	0.89	0.79	-	88,88,88,88	0
60	MG	Aa	1661	1/1	0.92	0.22	-	64,64,64,64	0
60	MG	Aa	1658	1/1	0.89	0.57	-	75,75,75,75	0
60	MG	AA	2937	1/1	0.98	0.16	-	67,67,67,67	0
60	MG	Ba	1712	1/1	0.36	0.83	-	79,79,79,79	0
60	MG	AA	3154	1/1	0.46	0.20	-	142,142,142,142	0
60	MG	AA	3077	1/1	0.90	0.47	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3143	1/1	0.96	0.38	-	29,29,29,29	0
60	MG	Aa	1720	1/1	0.84	1.05	-	75,75,75,75	0
60	MG	BA	3224	1/1	0.93	0.41	-	62,62,62,62	0
60	MG	AA	3227	1/1	0.99	0.31	-	39,39,39,39	0
60	MG	BA	3163	1/1	0.90	0.74	-	71,71,71,71	0
60	MG	BA	3220	1/1	0.69	0.79	-	50,50,50,50	0
60	MG	BA	3184	1/1	0.96	0.14	-	57,57,57,57	0
60	MG	Av	103	1/1	0.97	0.06	-	84,84,84,84	0
60	MG	BA	3071	1/1	0.82	0.49	-	39,39,39,39	0
60	MG	Aa	1619	1/1	0.97	0.46	-	65,65,65,65	0
60	MG	Ba	1659	1/1	0.52	0.33	-	79,79,79,79	0
60	MG	Aa	1632	1/1	0.87	0.41	-	72,72,72,72	0
60	MG	Ba	1651	1/1	0.81	1.00	-	62,62,62,62	0
60	MG	AA	3024	1/1	0.93	0.36	-	25,25,25,25	0
60	MG	AA	3151	1/1	0.83	0.48	-	85,85,85,85	0
60	MG	AA	3202	1/1	0.96	0.33	-	57,57,57,57	0
60	MG	AA	3187	1/1	0.96	0.39	-	49,49,49,49	0
60	MG	BA	3237	1/1	0.93	0.25	-	55,55,55,55	0
60	MG	Aa	1723	1/1	0.79	0.40	-	83,83,83,83	0
60	MG	Aa	1612	1/1	0.89	0.19	-	32,32,32,32	0
60	MG	Ba	1669	1/1	0.39	0.60	-	94,94,94,94	0
60	MG	BA	2945	1/1	0.85	0.32	-	112,112,112,112	0
60	MG	AA	3264	1/1	0.92	0.97	-	78,78,78,78	0
60	MG	AA	3027	1/1	0.88	0.21	-	54,54,54,54	0
60	MG	AA	3010	1/1	0.98	0.48	-	10,10,10,10	0
60	MG	BA	3079	1/1	0.89	0.24	-	82,82,82,82	0
60	MG	AA	3140	1/1	0.94	0.49	-	45,45,45,45	0
60	MG	BA	2991	1/1	0.89	0.55	-	32,32,32,32	0
60	MG	AA	3165	1/1	0.88	0.37	-	97,97,97,97	0
60	MG	BA	3253	1/1	0.88	0.67	-	43,43,43,43	0
60	MG	AA	3082	1/1	0.74	0.43	-	72,72,72,72	0
60	MG	Ba	1642	1/1	0.84	0.46	-	78,78,78,78	0
60	MG	B7	102	1/1	0.91	0.66	-	57,57,57,57	0
60	MG	AA	3120	1/1	0.96	0.15	-	76,76,76,76	0
60	MG	AA	3080	1/1	0.93	0.54	-	67,67,67,67	0
60	MG	AA	3207	1/1	0.93	0.50	-	59,59,59,59	0
60	MG	AA	2935	1/1	0.84	0.64	-	69,69,69,69	0
60	MG	BA	3004	1/1	0.96	0.14	-	46,46,46,46	0
60	MG	BA	2961	1/1	0.93	0.28	-	28,28,28,28	0
60	MG	BB	201	1/1	0.84	0.49	-	54,54,54,54	0
60	MG	AA	3199	1/1	0.98	0.43	-	53,53,53,53	0
60	MG	BA	3087	1/1	0.87	0.59	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3235	1/1	0.76	0.58	-	72,72,72,72	0
60	MG	AA	3166	1/1	0.79	0.35	-	48,48,48,48	0
60	MG	AA	3176	1/1	0.74	1.25	-	74,74,74,74	0
60	MG	AA	3267	1/1	0.92	0.88	-	74,74,74,74	0
60	MG	AA	3105	1/1	0.93	0.17	-	47,47,47,47	0
60	MG	AA	2950	1/1	0.94	0.24	-	51,51,51,51	0
60	MG	Aa	1683	1/1	0.94	0.12	-	66,66,66,66	0
60	MG	AA	3173	1/1	0.90	0.32	-	14,14,14,14	0
60	MG	AA	2992	1/1	0.95	0.44	-	45,45,45,45	0
60	MG	BA	3032	1/1	0.89	0.41	-	32,32,32,32	0
60	MG	AA	2926	1/1	0.96	0.36	-	26,26,26,26	0
60	MG	Ba	1650	1/1	0.93	0.52	-	49,49,49,49	0
60	MG	BA	2924	1/1	0.73	0.32	-	93,93,93,93	0
60	MG	AA	2993	1/1	0.86	0.28	-	56,56,56,56	0
60	MG	BA	3155	1/1	0.98	0.33	-	59,59,59,59	0
60	MG	BA	2907	1/1	0.97	0.51	-	49,49,49,49	0
60	MG	BA	3175	1/1	0.84	0.72	-	57,57,57,57	0
60	MG	AA	3238	1/1	0.64	0.75	-	75,75,75,75	0
60	MG	AA	2967	1/1	0.91	1.41	-	69,69,69,69	0
60	MG	BA	3142	1/1	0.93	0.84	-	53,53,53,53	0
60	MG	BA	2952	1/1	0.84	0.41	-	102,102,102,102	0
60	MG	BA	3248	1/1	0.95	0.83	-	47,47,47,47	0
60	MG	Ba	1653	1/1	0.83	0.38	-	74,74,74,74	0
60	MG	BA	3140	1/1	0.95	0.33	-	25,25,25,25	0
60	MG	BA	3061	1/1	0.99	0.14	-	35,35,35,35	0
60	MG	BA	3137	1/1	0.82	0.88	-	80,80,80,80	0
60	MG	BA	2922	1/1	0.97	0.29	-	52,52,52,52	0
60	MG	BA	2902	1/1	0.94	0.32	-	60,60,60,60	0
60	MG	AA	3132	1/1	0.67	0.99	-	78,78,78,78	0
60	MG	BA	3246	1/1	0.79	0.31	-	89,89,89,89	0
60	MG	BA	2983	1/1	0.99	0.16	-	21,21,21,21	0
60	MG	AA	3052	1/1	0.93	0.29	-	18,18,18,18	0
60	MG	Aa	1696	1/1	0.90	0.22	-	67,67,67,67	0
60	MG	AA	3212	1/1	0.88	0.65	-	68,68,68,68	0
60	MG	AA	2939	1/1	0.85	0.87	-	68,68,68,68	0
60	MG	Aa	1602	1/1	0.74	0.28	-	126,126,126,126	0
60	MG	Ba	1620	1/1	0.75	0.21	-	55,55,55,55	0
60	MG	AA	3201	1/1	0.74	1.19	-	88,88,88,88	0
60	MG	AA	3211	1/1	0.98	0.17	-	60,60,60,60	0
60	MG	BA	3245	1/1	0.85	0.27	-	90,90,90,90	0
60	MG	BA	2975	1/1	0.90	0.60	-	105,105,105,105	0
60	MG	BA	3189	1/1	0.72	0.70	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3170	1/1	0.88	0.42	-	47,47,47,47	0
60	MG	AA	3003	1/1	0.95	0.28	-	43,43,43,43	0
60	MG	Ba	1705	1/1	0.60	0.34	-	76,76,76,76	0
60	MG	Ba	1707	1/1	0.45	0.46	-	76,76,76,76	0
60	MG	Aa	1712	1/1	0.44	1.12	-	117,117,117,117	0
60	MG	Ba	1690	1/1	0.86	0.37	-	56,56,56,56	0
60	MG	BA	2998	1/1	0.99	0.23	-	14,14,14,14	0
60	MG	Aa	1618	1/1	0.94	0.35	-	28,28,28,28	0
60	MG	AA	3156	1/1	0.97	0.36	-	73,73,73,73	0
60	MG	BA	3264	1/1	0.77	0.89	-	89,89,89,89	0
60	MG	AA	3204	1/1	0.76	0.67	-	51,51,51,51	0
60	MG	Ba	1708	1/1	0.71	0.20	-	132,132,132,132	0
60	MG	BA	2925	1/1	0.95	0.45	-	31,31,31,31	0
60	MG	AA	3071	1/1	0.85	0.41	-	74,74,74,74	0
60	MG	Ba	1602	1/1	0.85	0.28	-	93,93,93,93	0
60	MG	Ba	1655	1/1	0.98	0.60	-	43,43,43,43	0
60	MG	Aa	1710	1/1	0.96	0.25	-	29,29,29,29	0
60	MG	BA	3107	1/1	0.98	0.38	-	45,45,45,45	0
60	MG	Aa	1689	1/1	0.88	0.25	-	65,65,65,65	1
60	MG	AA	3073	1/1	0.88	0.89	-	78,78,78,78	0
60	MG	BA	3023	1/1	0.97	0.40	-	21,21,21,21	0
60	MG	AA	2999	1/1	0.95	0.29	-	46,46,46,46	0
60	MG	Aa	1637	1/1	0.78	0.36	-	75,75,75,75	0
60	MG	BA	3205	1/1	0.78	0.42	-	92,92,92,92	0
60	MG	BA	3121	1/1	0.86	1.31	-	70,70,70,70	0
60	MG	AA	3169	1/1	0.94	0.07	-	44,44,44,44	0
60	MG	BA	2904	1/1	0.98	0.35	-	1,1,1,1	0
60	MG	AA	3142	1/1	0.84	0.40	-	53,53,53,53	0
60	MG	AA	2902	1/1	0.95	0.18	-	167,167,167,167	0
60	MG	Aa	1641	1/1	0.87	0.35	-	74,74,74,74	0
60	MG	A5	101	1/1	0.92	0.48	-	34,34,34,34	0
60	MG	BA	3128	1/1	0.96	0.39	-	26,26,26,26	0
60	MG	AA	3086	1/1	0.92	0.12	-	74,74,74,74	0
60	MG	Ba	1626	1/1	0.96	0.31	-	56,56,56,56	0
60	MG	BA	2985	1/1	0.84	0.32	-	26,26,26,26	0
60	MG	AA	3014	1/1	0.89	0.85	-	50,50,50,50	0
60	MG	Ba	1646	1/1	0.84	0.26	-	128,128,128,128	0
60	MG	BA	3135	1/1	0.92	1.30	-	96,96,96,96	0
60	MG	BA	3159	1/1	0.98	0.23	-	52,52,52,52	0
60	MG	AA	2955	1/1	0.96	0.41	-	48,48,48,48	0
60	MG	BA	2949	1/1	0.98	0.31	-	42,42,42,42	0
60	MG	Aa	1739	1/1	0.94	0.49	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Aa	1684	1/1	0.82	1.01	-	74,74,74,74	0
60	MG	AA	2941	1/1	0.76	0.76	-	92,92,92,92	0
60	MG	Ba	1735	1/1	0.71	0.21	-	122,122,122,122	0
60	MG	Ba	1714	1/1	0.75	0.10	-	62,62,62,62	0
60	MG	BA	3197	1/1	0.97	0.17	-	103,103,103,103	1
60	MG	Ba	1706	1/1	0.69	0.74	-	104,104,104,104	0
60	MG	Ba	1658	1/1	0.62	0.32	-	50,50,50,50	0
60	MG	BA	3180	1/1	0.95	0.86	-	105,105,105,105	0
60	MG	Ba	1631	1/1	0.79	0.55	-	73,73,73,73	0
60	MG	BA	3238	1/1	0.55	0.95	-	113,113,113,113	0
60	MG	AA	3000	1/1	0.82	0.62	-	63,63,63,63	0
60	MG	BA	2915	1/1	0.95	0.53	-	20,20,20,20	0
60	MG	Aa	1652	1/1	0.80	0.83	-	58,58,58,58	0
60	MG	BA	2974	1/1	0.87	0.42	-	31,31,31,31	0
60	MG	BA	2963	1/1	0.96	0.23	-	55,55,55,55	0
60	MG	AA	2966	1/1	0.98	0.56	-	57,57,57,57	0
60	MG	Ba	1665	1/1	0.74	0.74	-	144,144,144,144	0
60	MG	AA	3254	1/1	0.91	0.49	-	53,53,53,53	0
60	MG	Aa	1714	1/1	0.92	0.17	-	47,47,47,47	0
60	MG	BA	2940	1/1	0.93	0.25	-	82,82,82,82	0
60	MG	Ba	1601	1/1	0.73	0.48	-	90,90,90,90	0
60	MG	AA	3141	1/1	0.81	1.13	-	86,86,86,86	0
60	MG	Aa	1627	1/1	0.96	0.19	-	53,53,53,53	0
60	MG	BA	3148	1/1	0.82	0.44	-	74,74,74,74	0
60	MG	BA	3080	1/1	0.76	0.34	-	58,58,58,58	0
60	MG	AA	3146	1/1	0.62	0.75	-	90,90,90,90	0
60	MG	BA	2947	1/1	0.64	0.33	-	44,44,44,44	0
60	MG	AA	3045	1/1	0.98	0.49	-	22,22,22,22	0
60	MG	BA	3118	1/1	0.65	0.47	-	70,70,70,70	0
60	MG	BA	3041	1/1	0.96	0.42	-	15,15,15,15	0
60	MG	BA	3026	1/1	0.93	0.20	-	40,40,40,40	0
60	MG	Aa	1742	1/1	0.33	0.55	-	106,106,106,106	0
60	MG	BA	3167	1/1	0.93	0.77	-	59,59,59,59	0
60	MG	Aa	1736	1/1	0.88	0.27	-	117,117,117,117	0
60	MG	BA	3068	1/1	0.86	0.52	-	64,64,64,64	0
60	MG	Ba	1689	1/1	0.69	0.42	-	57,57,57,57	0
60	MG	AA	3168	1/1	0.82	0.27	-	82,82,82,82	0
60	MG	BA	2977	1/1	0.74	0.40	-	46,46,46,46	0
60	MG	AA	3164	1/1	0.97	0.64	-	69,69,69,69	0
60	MG	BB	203	1/1	0.72	0.55	-	55,55,55,55	0
60	MG	Av	101	1/1	0.91	0.74	-	90,90,90,90	1
60	MG	Aa	1734	1/1	0.95	0.58	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Av	105	1/1	0.81	0.33	-	92,92,92,92	1
60	MG	Ba	1628	1/1	0.85	0.34	-	46,46,46,46	0
60	MG	BA	3143	1/1	0.89	1.02	-	95,95,95,95	0
60	MG	BA	3067	1/1	0.96	0.29	-	28,28,28,28	0
60	MG	AA	2923	1/1	0.97	0.54	-	36,36,36,36	0
60	MG	AA	3148	1/1	0.68	0.27	-	77,77,77,77	0
60	MG	AA	3178	1/1	0.79	0.33	-	35,35,35,35	0
60	MG	AA	2942	1/1	0.93	0.34	-	40,40,40,40	0
60	MG	BA	3247	1/1	0.83	0.36	-	54,54,54,54	0
60	MG	AA	3110	1/1	0.70	1.25	-	91,91,91,91	0
60	MG	BA	2964	1/1	0.94	0.39	-	49,49,49,49	0
60	MG	BA	2981	1/1	0.73	1.34	-	46,46,46,46	0
60	MG	Ba	1723	1/1	0.98	0.14	-	103,103,103,103	0
60	MG	AA	2994	1/1	0.84	0.58	-	30,30,30,30	0
60	MG	BA	3256	1/1	0.97	0.50	-	39,39,39,39	0
60	MG	Ba	1660	1/1	0.87	0.73	-	60,60,60,60	0
60	MG	Aa	1703	1/1	0.34	0.93	-	94,94,94,94	0
60	MG	AA	3260	1/1	0.19	0.75	-	80,80,80,80	0
60	MG	BA	3119	1/1	0.82	0.33	-	67,67,67,67	0
60	MG	Ba	1713	1/1	0.70	0.61	-	83,83,83,83	0
60	MG	AA	2970	1/1	0.88	0.20	-	53,53,53,53	0
60	MG	AA	3017	1/1	0.91	0.32	-	18,18,18,18	0
60	MG	Bv	103	1/1	0.79	0.30	-	93,93,93,93	0
60	MG	BA	3259	1/1	0.84	0.25	-	86,86,86,86	0
60	MG	BA	2997	1/1	0.97	0.22	-	22,22,22,22	0
60	MG	AA	2908	1/1	0.95	0.40	-	25,25,25,25	0
60	MG	BA	3014	1/1	0.97	0.26	-	1,1,1,1	0
60	MG	Ba	1678	1/1	0.92	0.49	-	51,51,51,51	0
60	MG	Aa	1644	1/1	0.92	0.29	-	56,56,56,56	0
60	MG	BA	3124	1/1	0.96	0.29	-	40,40,40,40	0
60	MG	Ba	1696	1/1	0.72	0.64	-	83,83,83,83	0
60	MG	Ba	1734	1/1	0.94	0.25	-	84,84,84,84	1
60	MG	BB	202	1/1	0.84	0.33	-	46,46,46,46	0
60	MG	Aa	1643	1/1	0.76	1.21	-	90,90,90,90	0
60	MG	AA	2903	1/1	0.83	0.59	-	65,65,65,65	0
60	MG	Aa	1601	1/1	0.38	0.90	-	123,123,123,123	0
60	MG	Aa	1702	1/1	0.90	0.41	-	91,91,91,91	0
60	MG	BA	3152	1/1	0.77	0.34	-	71,71,71,71	0
60	MG	AA	3129	1/1	0.98	0.37	-	29,29,29,29	0
60	MG	BA	3204	1/1	0.59	0.53	-	64,64,64,64	0
60	MG	Aa	1604	1/1	0.96	0.13	-	76,76,76,76	0
60	MG	Aa	1651	1/1	0.83	0.66	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Aa	1617	1/1	0.86	0.36	-	49,49,49,49	1
60	MG	Aa	1660	1/1	0.89	0.47	-	49,49,49,49	0
60	MG	AA	2972	1/1	0.83	0.25	-	43,43,43,43	0
60	MG	Aa	1682	1/1	0.91	0.59	-	59,59,59,59	0
60	MG	AA	2945	1/1	0.97	0.12	-	74,74,74,74	0
60	MG	BA	3072	1/1	0.66	0.90	-	55,55,55,55	0
60	MG	BA	2934	1/1	0.80	0.68	-	72,72,72,72	0
60	MG	Ba	1636	1/1	0.92	0.20	-	60,60,60,60	0
60	MG	BA	3161	1/1	0.88	0.41	-	71,71,71,71	0
60	MG	BA	3033	1/1	0.65	0.58	-	61,61,61,61	0
60	MG	Aa	1708	1/1	0.71	0.55	-	81,81,81,81	0
60	MG	Ba	1682	1/1	0.97	0.10	-	66,66,66,66	0
60	MG	Ba	1627	1/1	0.98	0.56	-	74,74,74,74	0
60	MG	AA	3234	1/1	0.91	0.20	-	79,79,79,79	0
60	MG	BA	3240	1/1	0.86	0.99	-	84,84,84,84	0
60	MG	Bd	301	1/1	0.84	0.86	-	55,55,55,55	0
60	MG	BA	3103	1/1	0.87	0.27	-	50,50,50,50	0
60	MG	Ba	1610	1/1	0.73	0.20	-	50,50,50,50	0
60	MG	BA	3178	1/1	0.49	0.39	-	55,55,55,55	0
60	MG	Ba	1727	1/1	0.92	0.49	-	46,46,46,46	0
60	MG	AX	101	1/1	0.84	0.85	-	55,55,55,55	1
60	MG	AA	3228	1/1	0.82	0.64	-	51,51,51,51	0
60	MG	AA	3239	1/1	0.95	0.34	-	77,77,77,77	0
60	MG	AA	3040	1/1	0.94	0.14	-	21,21,21,21	0
60	MG	BA	2999	1/1	0.93	0.41	-	26,26,26,26	0
60	MG	Aa	1621	1/1	0.74	0.30	-	89,89,89,89	0
60	MG	BA	3104	1/1	0.92	0.20	-	31,31,31,31	0
60	MG	AA	3104	1/1	0.79	0.33	-	56,56,56,56	0
60	MG	BA	3047	1/1	0.93	0.27	-	36,36,36,36	0
60	MG	AA	2952	1/1	0.74	0.44	-	88,88,88,88	0
60	MG	AA	3210	1/1	0.62	0.17	-	115,115,115,115	0
60	MG	AA	3180	1/1	0.95	0.22	-	73,73,73,73	0
60	MG	Aa	1647	1/1	0.87	0.21	-	138,138,138,138	0
60	MG	AA	3081	1/1	0.96	0.34	-	99,99,99,99	0
60	MG	BA	3193	1/1	0.95	0.44	-	44,44,44,44	0
60	MG	Aa	1626	1/1	0.92	0.12	-	63,63,63,63	0
60	MG	AA	3136	1/1	0.82	0.64	-	84,84,84,84	0
60	MG	BA	3151	1/1	0.60	0.99	-	119,119,119,119	0
60	MG	Aa	1692	1/1	0.89	0.63	-	46,46,46,46	0
60	MG	AA	3053	1/1	0.97	0.64	-	42,42,42,42	0
60	MG	AA	3135	1/1	0.90	0.59	-	71,71,71,71	0
60	MG	BA	3227	1/1	0.94	0.64	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3108	1/1	0.98	0.13	-	38,38,38,38	0
60	MG	BA	3243	1/1	0.81	1.07	-	111,111,111,111	0
60	MG	AA	3087	1/1	0.90	0.37	-	60,60,60,60	0
60	MG	BA	3173	1/1	0.70	0.96	-	72,72,72,72	0
60	MG	Aa	1646	1/1	0.62	0.90	-	102,102,102,102	0
60	MG	Aa	1724	1/1	0.93	0.17	-	71,71,71,71	0
60	MG	Aa	1705	1/1	0.69	0.51	-	71,71,71,71	0
60	MG	BA	3213	1/1	0.97	0.17	-	36,36,36,36	0
60	MG	Aa	1728	1/1	0.96	0.55	-	83,83,83,83	0
60	MG	BA	3058	1/1	0.82	0.49	-	34,34,34,34	0
60	MG	Ba	1625	1/1	0.95	0.20	-	72,72,72,72	0
60	MG	Aa	1690	1/1	0.79	0.21	-	49,49,49,49	0
60	MG	BA	3233	1/1	0.72	0.42	-	97,97,97,97	0
60	MG	BA	3222	1/1	0.70	0.52	-	61,61,61,61	0
60	MG	BA	2954	1/1	0.95	0.22	-	57,57,57,57	0
60	MG	AA	3111	1/1	0.93	0.66	-	54,54,54,54	0
60	MG	Ba	1743	1/1	0.92	0.55	-	57,57,57,57	0
60	MG	AA	3262	1/1	0.02	1.11	-	81,81,81,81	0
60	MG	Aa	1719	1/1	0.81	0.39	-	101,101,101,101	0
60	MG	Ba	1635	1/1	0.65	0.61	-	57,57,57,57	0
60	MG	Ba	1656	1/1	0.79	0.51	-	73,73,73,73	0
60	MG	AA	3222	1/1	0.93	0.64	-	45,45,45,45	0
60	MG	BA	3126	1/1	0.82	0.37	-	122,122,122,122	0
60	MG	AA	2963	1/1	0.80	0.81	-	46,46,46,46	0
60	MG	AA	3225	1/1	0.91	0.18	-	57,57,57,57	0
60	MG	BA	3019	1/1	0.96	0.35	-	30,30,30,30	0
60	MG	BA	3182	1/1	0.89	0.32	-	63,63,63,63	0
60	MG	Ba	1607	1/1	0.97	0.18	-	75,75,75,75	0
60	MG	AA	3098	1/1	0.56	0.58	-	75,75,75,75	0
60	MG	AA	3065	1/1	0.51	0.74	-	73,73,73,73	0
60	MG	Ba	1700	1/1	0.69	0.50	-	58,58,58,58	0
60	MG	AA	3248	1/1	0.67	0.70	-	106,106,106,106	0
60	MG	AA	2990	1/1	0.85	0.60	-	34,34,34,34	0
60	MG	AA	3216	1/1	0.70	0.47	-	49,49,49,49	0
60	MG	AA	2954	1/1	0.55	0.53	-	112,112,112,112	0
60	MG	AA	3192	1/1	0.88	1.12	-	101,101,101,101	0
60	MG	AA	3020	1/1	0.88	0.29	-	39,39,39,39	0
60	MG	BA	2948	1/1	0.65	0.50	-	73,73,73,73	0
60	MG	BA	2971	1/1	0.78	0.93	-	66,66,66,66	0
60	MG	AA	3018	1/1	0.94	0.49	-	48,48,48,48	0
60	MG	AA	3181	1/1	0.59	0.46	-	61,61,61,61	0
60	MG	Aa	1718	1/1	0.95	1.02	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	BA	3221	1/1	0.64	0.44	-	106,106,106,106	0
60	MG	Aa	1704	1/1	0.70	0.42	-	29,29,29,29	1
60	MG	Aa	1743	1/1	0.68	0.60	-	67,67,67,67	0
60	MG	BA	3255	1/1	0.96	0.34	-	81,81,81,81	0
60	MG	Aa	1741	1/1	0.59	1.45	-	79,79,79,79	0
60	MG	AA	2910	1/1	0.93	0.54	-	49,49,49,49	0
60	MG	BA	3226	1/1	0.92	0.35	-	75,75,75,75	0
60	MG	AA	3242	1/1	0.86	0.89	-	85,85,85,85	0
60	MG	AA	3009	1/1	0.99	0.45	-	31,31,31,31	0
60	MG	Ba	1733	1/1	0.22	0.39	-	86,86,86,86	0
60	MG	BA	3166	1/1	0.91	0.13	-	50,50,50,50	0
60	MG	AA	2948	1/1	0.93	0.25	-	67,67,67,67	0
60	MG	AA	3152	1/1	0.78	0.83	-	62,62,62,62	0
60	MG	BA	3190	1/1	0.98	0.29	-	13,13,13,13	0
60	MG	BA	3146	1/1	0.59	0.85	-	84,84,84,84	0
60	MG	Aa	1636	1/1	0.45	1.40	-	88,88,88,88	0
60	MG	AA	2946	1/1	0.98	0.10	-	101,101,101,101	0
60	MG	AA	2959	1/1	0.65	0.44	-	73,73,73,73	0
60	MG	AB	202	1/1	0.74	0.40	-	62,62,62,62	0
60	MG	Aa	1672	1/1	0.65	0.33	-	87,87,87,87	0
60	MG	Ba	1649	1/1	0.86	0.36	-	49,49,49,49	0
60	MG	Ba	1638	1/1	0.84	0.24	-	40,40,40,40	0
60	MG	BA	2955	1/1	0.73	0.26	-	49,49,49,49	0
60	MG	Ba	1681	1/1	0.45	0.84	-	122,122,122,122	0
60	MG	Aa	1700	1/1	0.57	2.14	-	114,114,114,114	0
60	MG	A1	102	1/1	0.97	0.42	-	116,116,116,116	0
60	MG	BA	3089	1/1	0.97	0.20	-	56,56,56,56	0
60	MG	BA	3239	1/1	0.67	0.27	-	64,64,64,64	0
60	MG	Bv	104	1/1	0.70	1.01	-	75,75,75,75	1
60	MG	AA	3078	1/1	0.97	0.14	-	83,83,83,83	0
60	MG	AA	3139	1/1	0.89	0.40	-	44,44,44,44	0
60	MG	Ba	1603	1/1	0.94	0.10	-	64,64,64,64	0
60	MG	BA	3244	1/1	0.68	0.23	-	91,91,91,91	0
60	MG	AA	3112	1/1	0.92	0.34	-	60,60,60,60	0
60	MG	Ba	1643	1/1	0.76	0.37	-	108,108,108,108	0
60	MG	AA	3109	1/1	0.88	0.31	-	78,78,78,78	0
60	MG	BA	3215	1/1	0.95	0.39	-	65,65,65,65	0
60	MG	AA	3209	1/1	0.83	0.66	-	84,84,84,84	0
60	MG	AA	2998	1/1	0.97	0.28	-	36,36,36,36	0
60	MG	BA	3141	1/1	0.89	0.55	-	57,57,57,57	0
60	MG	Aa	1606	1/1	0.89	0.82	-	66,66,66,66	0
60	MG	Ba	1661	1/1	0.93	0.29	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3047	1/1	0.95	0.51	-	40,40,40,40	0
60	MG	BA	2901	1/1	0.85	0.21	-	138,138,138,138	0
60	MG	BA	3099	1/1	0.85	0.77	-	90,90,90,90	0
60	MG	AA	3258	1/1	0.87	0.54	-	38,38,38,38	0
60	MG	AA	2977	1/1	0.97	0.84	-	54,54,54,54	0
60	MG	BA	2958	1/1	0.75	1.59	-	88,88,88,88	0
60	MG	Ba	1617	1/1	0.95	0.25	-	36,36,36,36	0
60	MG	AA	3149	1/1	0.90	0.85	-	100,100,100,100	0
60	MG	Aa	1675	1/1	0.47	0.87	-	72,72,72,72	0
60	MG	AA	3041	1/1	0.99	0.18	-	21,21,21,21	0
60	MG	B0	102	1/1	0.92	0.21	-	47,47,47,47	0
60	MG	AA	3125	1/1	0.98	0.66	-	42,42,42,42	0
60	MG	BA	3002	1/1	0.99	0.25	-	41,41,41,41	0
60	MG	AA	3005	1/1	0.96	0.23	-	57,57,57,57	0
60	MG	AA	3034	1/1	0.68	0.60	-	55,55,55,55	0
60	MG	BA	2938	1/1	0.53	1.22	-	84,84,84,84	0
60	MG	BA	3260	1/1	0.91	1.12	-	80,80,80,80	0
60	MG	Ba	1711	1/1	0.68	0.35	-	123,123,123,123	0
60	MG	AA	3004	1/1	0.96	0.23	-	39,39,39,39	0
60	MG	AA	2961	1/1	0.92	0.49	-	76,76,76,76	0
60	MG	BA	3136	1/1	0.60	0.74	-	106,106,106,106	0
60	MG	AA	3043	1/1	0.98	0.19	-	37,37,37,37	0
60	MG	AA	3127	1/1	0.90	0.46	-	89,89,89,89	0
60	MG	Aa	1630	1/1	0.99	0.11	-	36,36,36,36	0
60	MG	AA	3116	1/1	0.69	0.40	-	35,35,35,35	0
60	MG	Aa	1663	1/1	0.31	0.54	-	112,112,112,112	0
60	MG	Ba	1719	1/1	0.72	0.68	-	57,57,57,57	0
60	MG	Bx	101	1/1	0.56	0.28	-	83,83,83,83	0
60	MG	BA	2906	1/1	0.97	0.22	-	26,26,26,26	0
60	MG	AA	2984	1/1	0.98	0.21	-	45,45,45,45	0
60	MG	BA	2937	1/1	0.91	0.26	-	67,67,67,67	0
60	MG	BA	3108	1/1	0.98	0.13	-	50,50,50,50	0
60	MG	Ba	1701	1/1	0.97	0.47	-	60,60,60,60	0
60	MG	AA	2983	1/1	0.90	0.28	-	27,27,27,27	0
60	MG	BA	3075	1/1	0.94	0.29	-	44,44,44,44	0
60	MG	AA	3167	1/1	0.95	0.48	-	73,73,73,73	0
60	MG	AA	3026	1/1	0.86	0.23	-	35,35,35,35	0
60	MG	BA	3054	1/1	0.92	0.40	-	36,36,36,36	0
60	MG	Aa	1664	1/1	0.81	0.58	-	44,44,44,44	0
60	MG	BA	3064	1/1	0.88	0.29	-	44,44,44,44	0
60	MG	AA	3208	1/1	0.87	0.76	-	86,86,86,86	0
60	MG	Aa	1648	1/1	0.12	0.59	-	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3006	1/1	0.91	0.28	-	32,32,32,32	0
60	MG	BA	3251	1/1	0.82	0.29	-	65,65,65,65	0
60	MG	AA	3244	1/1	0.79	0.99	-	67,67,67,67	0
60	MG	Aw	101	1/1	0.78	0.44	-	83,83,83,83	1
60	MG	BA	3219	1/1	0.83	0.46	-	40,40,40,40	0
60	MG	Ba	1613	1/1	0.94	0.85	-	38,38,38,38	0
60	MG	BX	101	1/1	0.94	0.60	-	31,31,31,31	1
60	MG	B5	102	1/1	0.83	0.60	-	76,76,76,76	0
60	MG	AA	3230	1/1	0.85	0.99	-	78,78,78,78	0
60	MG	AA	2936	1/1	0.96	0.53	-	5,5,5,5	0
60	MG	Aa	1706	1/1	0.77	0.58	-	54,54,54,54	0
60	MG	Ba	1645	1/1	0.79	1.00	-	101,101,101,101	0
60	MG	BA	3154	1/1	0.85	0.21	-	73,73,73,73	1
60	MG	BA	3139	1/1	0.98	0.14	-	15,15,15,15	0
60	MG	AA	3130	1/1	0.76	0.63	-	76,76,76,76	0
60	MG	Aa	1722	1/1	0.55	0.36	-	78,78,78,78	0
60	MG	AA	3048	1/1	0.79	0.42	-	68,68,68,68	0
60	MG	BA	3258	1/1	0.49	0.36	-	84,84,84,84	0
60	MG	AA	3092	1/1	0.87	0.23	-	51,51,51,51	0
60	MG	AA	3114	1/1	0.90	0.39	-	18,18,18,18	1
60	MG	AA	2905	1/1	0.93	0.36	-	15,15,15,15	0
60	MG	BA	3062	1/1	0.95	0.25	-	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.