



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2021 – 06:45 AM EDT

PDB ID : 4V7J  
Title : Structure of RelE nuclease bound to the 70S ribosome (precleavage 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 : 3.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

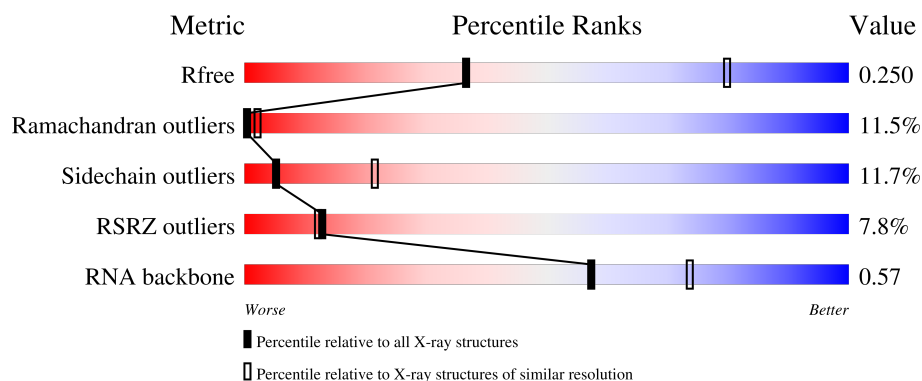
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Ab	256	<div> <div>8%</div> <div>77%</div> <div>14%</div> <div>9%</div> </div>
1	Bb	256	<div> <div>7%</div> <div>77%</div> <div>14%</div> <div>9%</div> </div>
2	Ac	239	<div> <div>7%</div> <div>69%</div> <div>17%</div> <div>14%</div> </div>
2	Bc	239	<div> <div>9%</div> <div>69%</div> <div>16%</div> <div>14%</div> </div>
3	Ad	209	<div> <div>%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
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	
15	Bp	88	

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Mol	Chain	Length	Quality of chain
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	25	
23	Bx	25	
24	Av	77	
24	Bv	77	
25	Aw	77	
25	Bw	77	
26	AC	229	
26	BC	229	
27	AD	276	
27	BD	276	
28	AE	206	

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Mol	Chain	Length	Quality of chain
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	
40	BT	146	

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Mol	Chain	Length	Quality of chain
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	
53	A6	54	

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Mol	Chain	Length	Quality of chain
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	2917	-	-	-	X
60	MG	AA	2925	-	-	-	X
60	MG	AA	2946	-	-	-	X
60	MG	AA	2968	-	-	-	X
60	MG	AA	2975	-	-	-	X
60	MG	AA	3002	-	-	-	X
60	MG	AA	3016	-	-	-	X
60	MG	AA	3030	-	-	-	X
60	MG	AA	3040	-	-	-	X
60	MG	AA	3067	-	-	-	X
60	MG	AA	3069	-	-	-	X
60	MG	AA	3084	-	-	-	X
60	MG	AA	3087	-	-	-	X
60	MG	AA	3102	-	-	-	X
60	MG	AA	3103	-	-	-	X
60	MG	AA	3106	-	-	-	X
60	MG	AA	3112	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	3138	-	-	-	X
60	MG	AA	3139	-	-	-	X
60	MG	AA	3143	-	-	-	X
60	MG	AA	3146	-	-	-	X
60	MG	AA	3149	-	-	-	X
60	MG	AA	3152	-	-	-	X
60	MG	AA	3165	-	-	-	X
60	MG	AA	3168	-	-	-	X
60	MG	AA	3176	-	-	-	X
60	MG	AA	3185	-	-	-	X
60	MG	AA	3194	-	-	-	X
60	MG	AA	3206	-	-	-	X
60	MG	AA	3207	-	-	-	X
60	MG	AA	3209	-	-	-	X
60	MG	AA	3219	-	-	-	X
60	MG	AA	3222	-	-	-	X
60	MG	AA	3224	-	-	-	X
60	MG	AA	3225	-	-	-	X
60	MG	AA	3230	-	-	-	X
60	MG	AA	3236	-	-	-	X
60	MG	AA	3237	-	-	-	X
60	MG	AA	3239	-	-	-	X
60	MG	AA	3241	-	-	-	X
60	MG	AA	3242	-	-	-	X
60	MG	AA	3248	-	-	-	X
60	MG	AA	3249	-	-	-	X
60	MG	AA	3253	-	-	-	X
60	MG	AA	3257	-	-	-	X
60	MG	AA	3260	-	-	-	X
60	MG	AA	3261	-	-	-	X
60	MG	AA	3262	-	-	-	X
60	MG	AA	3264	-	-	-	X
60	MG	AA	3266	-	-	-	X
60	MG	AB	202	-	-	-	X
60	MG	AQ	201	-	-	-	X
60	MG	AX	101	-	-	-	X
60	MG	Aa	1610	-	-	-	X
60	MG	Aa	1611	-	-	-	X
60	MG	Aa	1616	-	-	-	X
60	MG	Aa	1618	-	-	-	X
60	MG	Aa	1623	-	-	-	X
60	MG	Aa	1630	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	Aa	1633	-	-	-	X
60	MG	Aa	1637	-	-	-	X
60	MG	Aa	1641	-	-	-	X
60	MG	Aa	1651	-	-	-	X
60	MG	Aa	1652	-	-	-	X
60	MG	Aa	1658	-	-	-	X
60	MG	Aa	1665	-	-	-	X
60	MG	Aa	1677	-	-	-	X
60	MG	Aa	1681	-	-	-	X
60	MG	Aa	1700	-	-	-	X
60	MG	Aa	1706	-	-	-	X
60	MG	Aa	1713	-	-	-	X
60	MG	Aa	1714	-	-	-	X
60	MG	Aa	1723	-	-	-	X
60	MG	Aa	1727	-	-	-	X
60	MG	Aa	1730	-	-	-	X
60	MG	Am	201	-	-	-	X
60	MG	Aw	101	-	-	-	X
60	MG	B0	101	-	-	-	X
60	MG	BA	2921	-	-	-	X
60	MG	BA	2938	-	-	-	X
60	MG	BA	2945	-	-	-	X
60	MG	BA	2958	-	-	-	X
60	MG	BA	2965	-	-	-	X
60	MG	BA	2976	-	-	-	X
60	MG	BA	2984	-	-	-	X
60	MG	BA	2998	-	-	-	X
60	MG	BA	3011	-	-	-	X
60	MG	BA	3036	-	-	-	X
60	MG	BA	3049	-	-	-	X
60	MG	BA	3065	-	-	-	X
60	MG	BA	3071	-	-	-	X
60	MG	BA	3074	-	-	-	X
60	MG	BA	3086	-	-	-	X
60	MG	BA	3088	-	-	-	X
60	MG	BA	3109	-	-	-	X
60	MG	BA	3126	-	-	-	X
60	MG	BA	3129	-	-	-	X
60	MG	BA	3135	-	-	-	X
60	MG	BA	3136	-	-	-	X
60	MG	BA	3148	-	-	-	X
60	MG	BA	3149	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3150	-	-	-	X
60	MG	BA	3154	-	-	-	X
60	MG	BA	3157	-	-	-	X
60	MG	BA	3162	-	-	-	X
60	MG	BA	3173	-	-	-	X
60	MG	BA	3175	-	-	-	X
60	MG	BA	3180	-	-	-	X
60	MG	BA	3182	-	-	-	X
60	MG	BA	3191	-	-	-	X
60	MG	BA	3204	-	-	-	X
60	MG	BA	3206	-	-	-	X
60	MG	BA	3219	-	-	-	X
60	MG	BA	3229	-	-	-	X
60	MG	BA	3231	-	-	-	X
60	MG	BA	3235	-	-	-	X
60	MG	BA	3237	-	-	-	X
60	MG	BA	3244	-	-	-	X
60	MG	BA	3246	-	-	-	X
60	MG	BA	3253	-	-	-	X
60	MG	BA	3255	-	-	-	X
60	MG	BA	3258	-	-	-	X
60	MG	BA	3261	-	-	-	X
60	MG	BA	3265	-	-	-	X
60	MG	BB	203	-	-	-	X
60	MG	Ba	1610	-	-	-	X
60	MG	Ba	1631	-	-	-	X
60	MG	Ba	1640	-	-	-	X
60	MG	Ba	1643	-	-	-	X
60	MG	Ba	1645	-	-	-	X
60	MG	Ba	1646	-	-	-	X
60	MG	Ba	1647	-	-	-	X
60	MG	Ba	1648	-	-	-	X
60	MG	Ba	1660	-	-	-	X
60	MG	Ba	1664	-	-	-	X
60	MG	Ba	1665	-	-	-	X
60	MG	Ba	1670	-	-	-	X
60	MG	Ba	1676	-	-	-	X
60	MG	Ba	1680	-	-	-	X
60	MG	Ba	1682	-	-	-	X
60	MG	Ba	1695	-	-	-	X
60	MG	Ba	1698	-	-	-	X
60	MG	Ba	1699	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	Ba	1706	-	-	-	X
60	MG	Ba	1712	-	-	-	X
60	MG	Ba	1716	-	-	-	X
60	MG	Ba	1717	-	-	-	X
60	MG	Ba	1728	-	-	-	X
60	MG	Ba	1732	-	-	-	X
60	MG	Ba	1739	-	-	-	X
60	MG	Bm	202	-	-	-	X
60	MG	Bv	104	-	-	-	X

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 297206 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
			770	496	133	139	2			
21	By	94	Total	C	N	O	S	0	0	0
			766	495	130	139	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ay	45	ALA	ARG	engineered mutation	UNP P0C077
Ay	81	ALA	ARG	engineered mutation	UNP P0C077
By	45	ALA	ARG	engineered mutation	UNP P0C077
By	81	ALA	ARG	engineered mutation	UNP P0C077

- 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(\*GP\*GP\*CP\*AP\*AP\*GP\*GP\*AP\*GP\*GP\*UP\*A\*AP\*AP\*AP\*AP\*UP\*GP\*(OMU)P\*(A2M)P\*(OMG)P\*AP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Ax	12	Total	C	N	O	P	0	0	0
			262	121	54	76	11			
23	Bx	12	Total	C	N	O	P	0	0	0
			262	121	54	76	11			

- 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			

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

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

- 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	Ad	1	Total 1	Zn 1	0	0
59	An	1	Total 1	Zn 1	0	0
59	A4	1	Total 1	Zn 1	0	0
59	A9	1	Total 1	Zn 1	0	0
59	Bd	1	Total 1	Zn 1	0	0
59	Bn	1	Total 1	Zn 1	0	0
59	B4	1	Total 1	Zn 1	0	0
59	B9	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	Am	1	Total 1	Mg 1	0	0
60	Aq	1	Total 1	Mg 1	0	0
60	Aa	145	Total 145	Mg 145	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	Av	4	Total 4	Mg 4	0	0
60	Aw	1	Total 1	Mg 1	0	0
60	AD	2	Total 2	Mg 2	0	0
60	AF	1	Total 1	Mg 1	0	0
60	AQ	1	Total 1	Mg 1	0	0
60	AX	1	Total 1	Mg 1	0	0
60	A1	1	Total 1	Mg 1	0	0
60	A5	1	Total 1	Mg 1	0	0
60	A7	2	Total 2	Mg 2	0	0
60	AA	368	Total 368	Mg 368	0	0
60	AB	3	Total 3	Mg 3	0	0
60	Bm	2	Total 2	Mg 2	0	0
60	Bq	1	Total 1	Mg 1	0	0
60	Ba	143	Total 143	Mg 143	0	0
60	Bx	1	Total 1	Mg 1	0	0
60	Bv	5	Total 5	Mg 5	0	0
60	Bw	1	Total 1	Mg 1	0	0
60	BD	2	Total 2	Mg 2	0	0
60	BF	1	Total 1	Mg 1	0	0
60	BQ	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0

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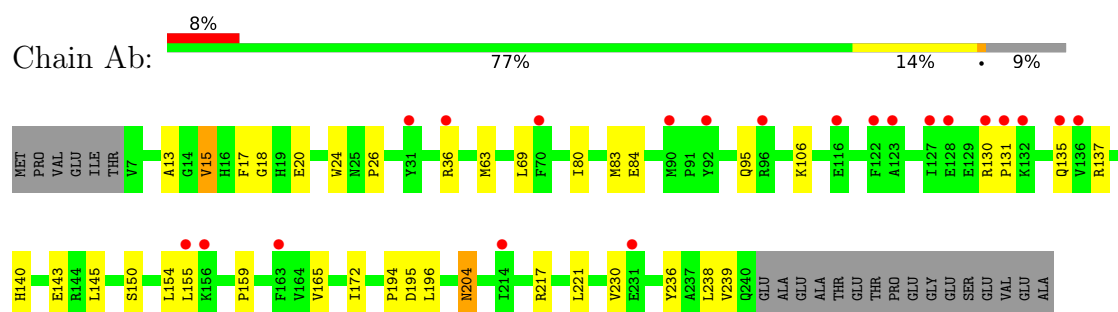
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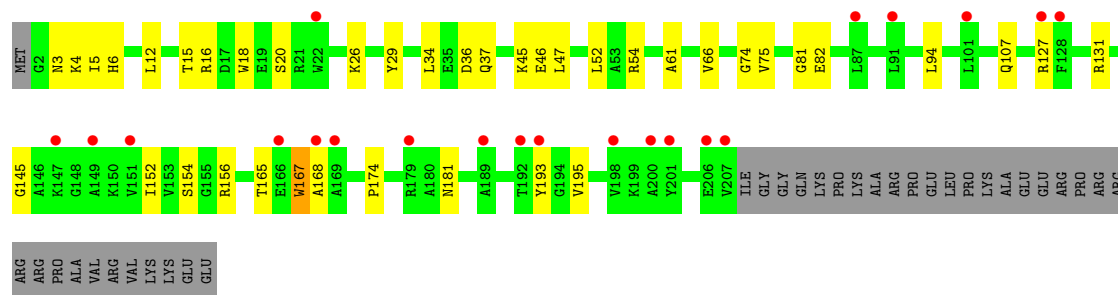
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60	B5	1	Total 1	Mg 1	0	0
60	B7	2	Total 2	Mg 2	0	0
60	BA	366	Total 366	Mg 366	0	0
60	BB	3	Total 3	Mg 3	0	0

### 3 Residue-property plots [i](#)

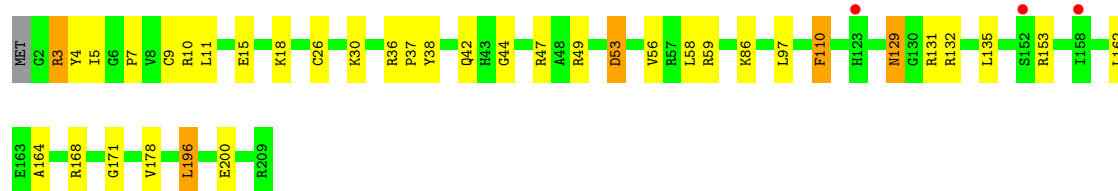
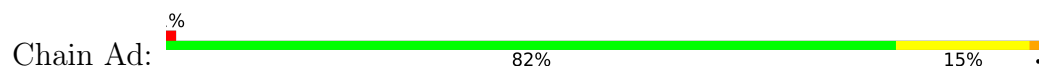
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: 30S ribosomal protein S2

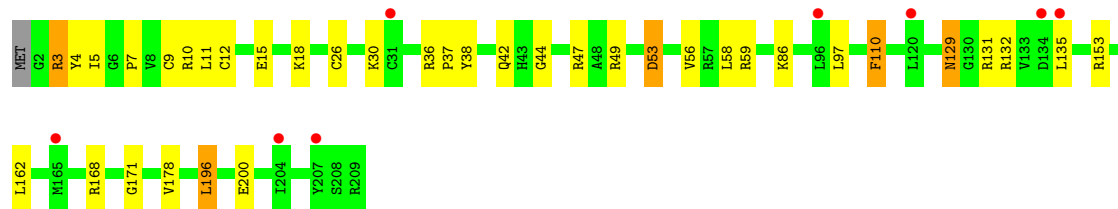
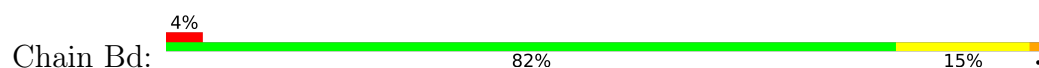




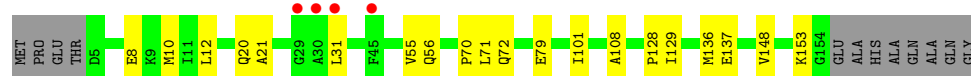
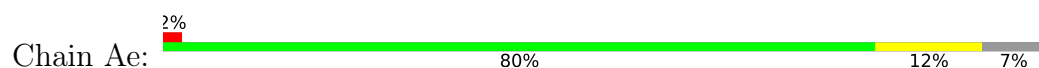
• Molecule 3: 30S ribosomal protein S4



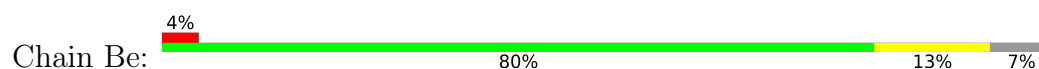
• Molecule 3: 30S ribosomal protein S4



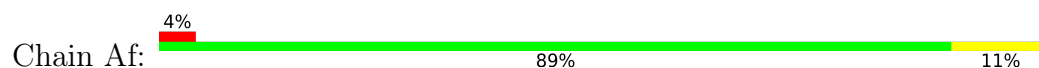
• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5

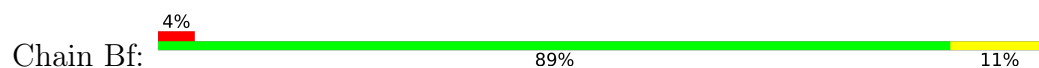


• Molecule 5: 30S ribosomal protein S6

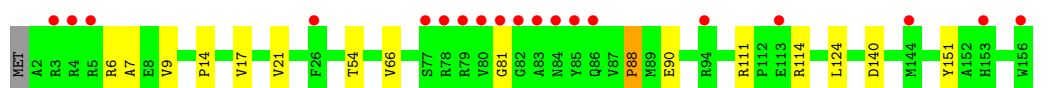
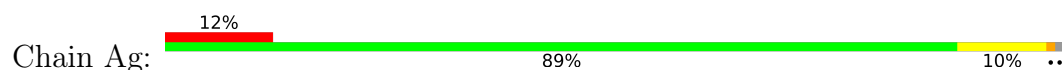




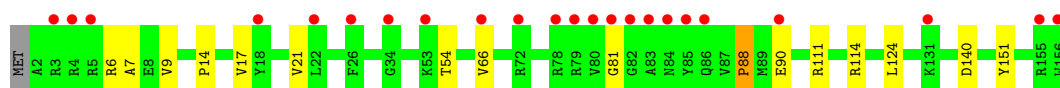
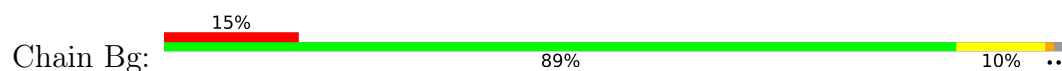
- Molecule 5: 30S ribosomal protein S6



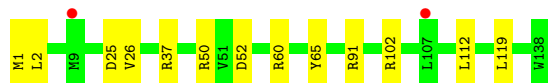
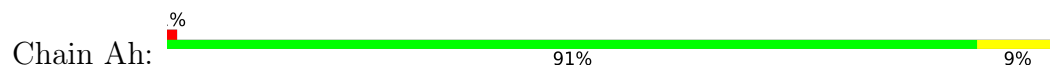
- Molecule 6: 30S ribosomal protein S7



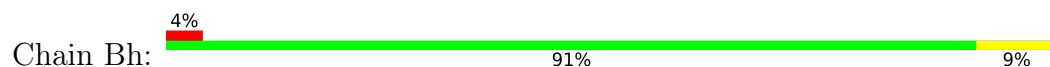
- Molecule 6: 30S ribosomal protein S7



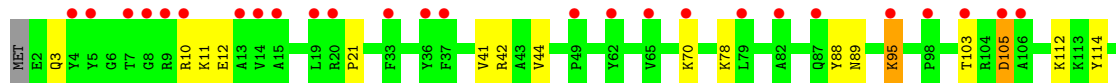
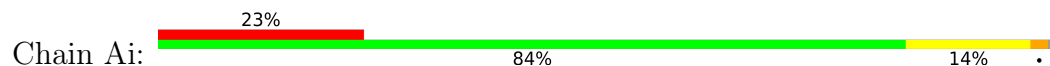
- Molecule 7: 30S ribosomal protein S8

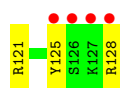


- Molecule 7: 30S ribosomal protein S8

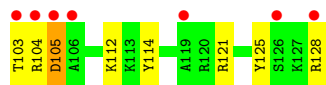
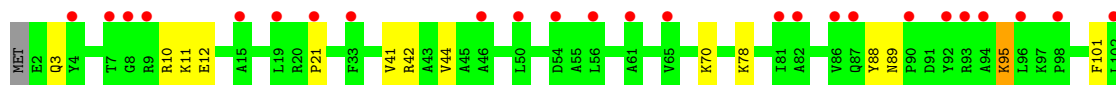
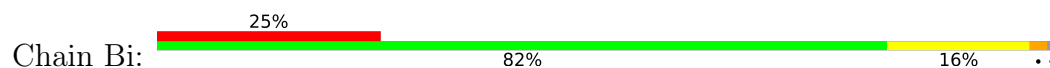


- Molecule 8: 30S ribosomal protein S9

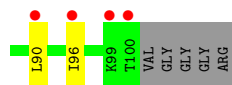
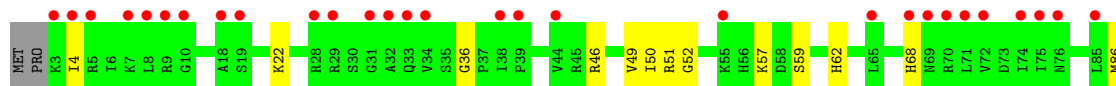
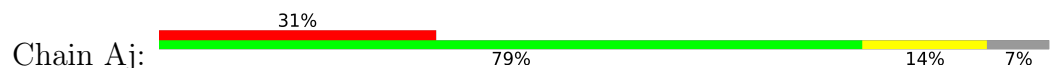




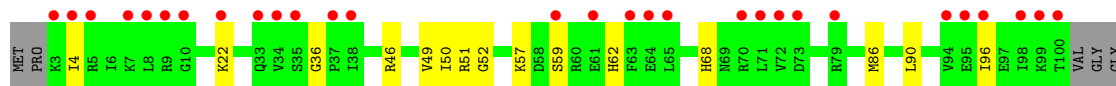
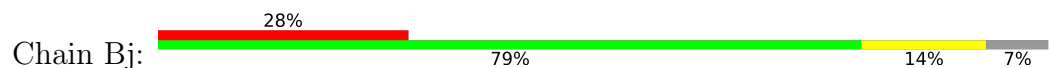
• Molecule 8: 30S ribosomal protein S9



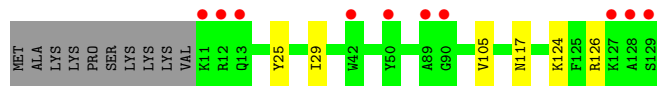
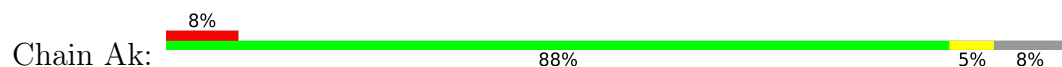
• Molecule 9: 30S ribosomal protein S10



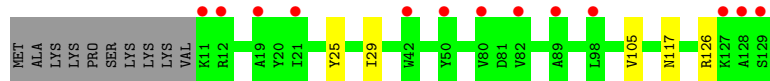
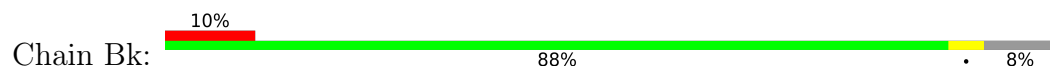
• Molecule 9: 30S ribosomal protein S10



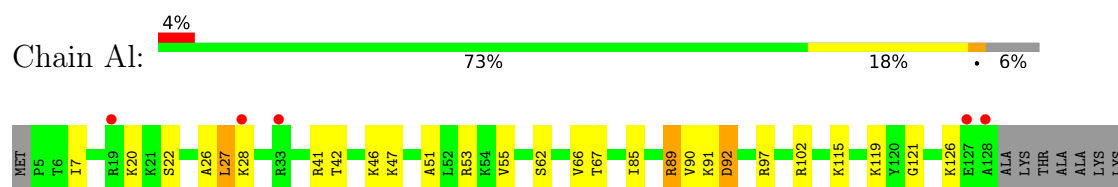
• Molecule 10: 30S ribosomal protein S11



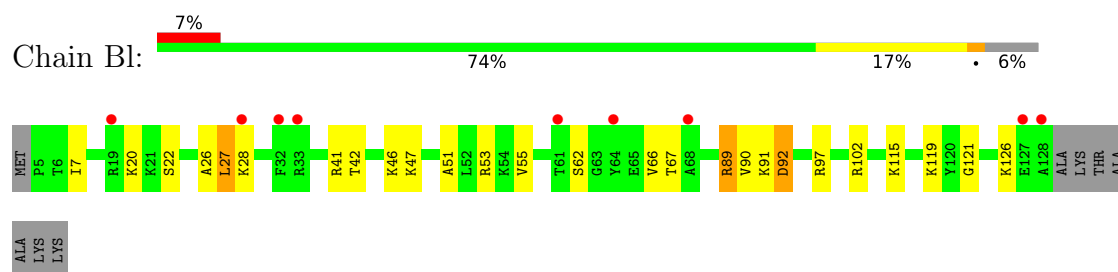
• Molecule 10: 30S ribosomal protein S11



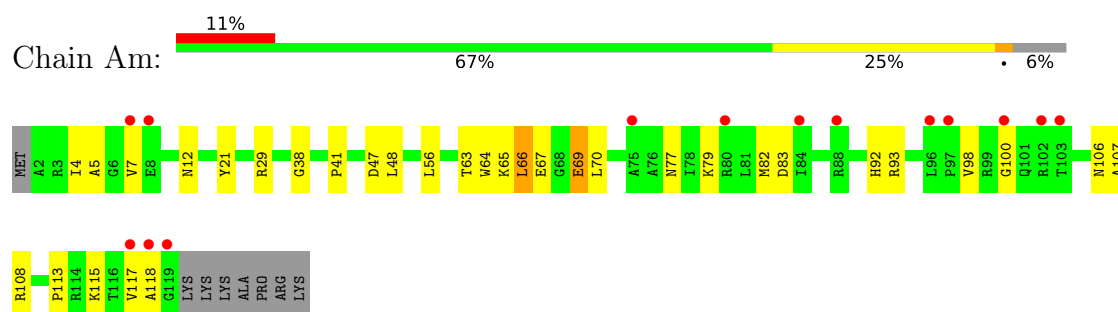
- Molecule 11: 30S ribosomal protein S12



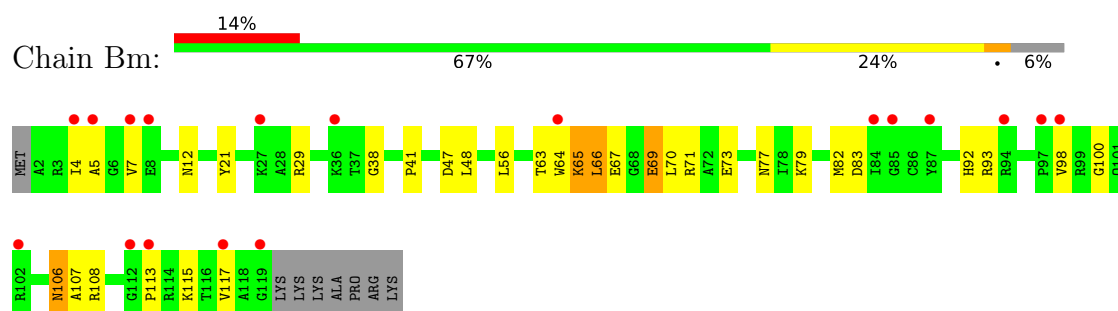
- Molecule 11: 30S ribosomal protein S12



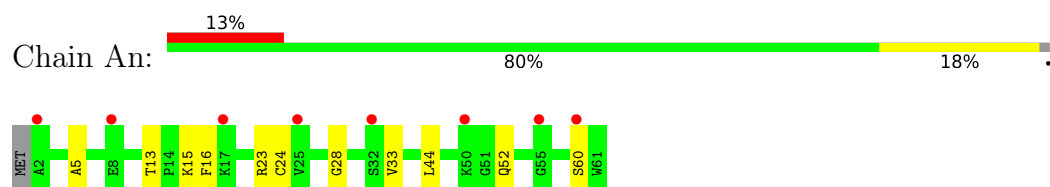
- Molecule 12: 30S ribosomal protein S13



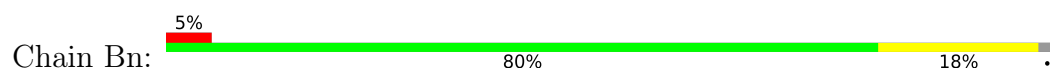
- Molecule 12: 30S ribosomal protein S13

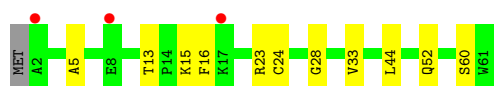


- Molecule 13: 30S ribosomal protein S14 type Z

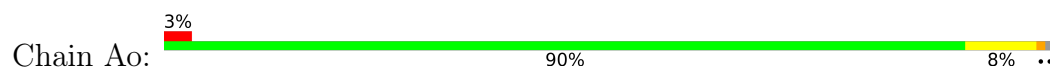


- Molecule 13: 30S ribosomal protein S14 type Z

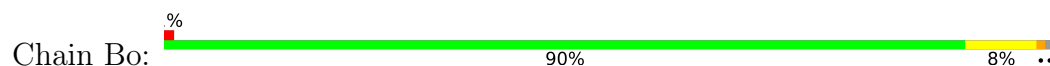




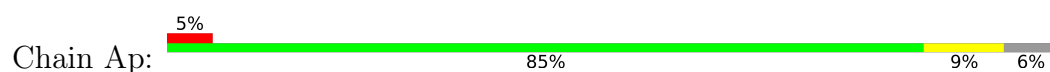
- Molecule 14: 30S ribosomal protein S15



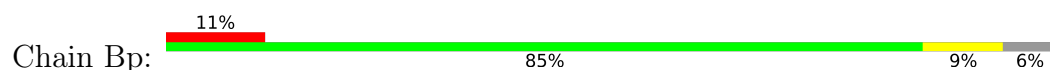
- Molecule 14: 30S ribosomal protein S15



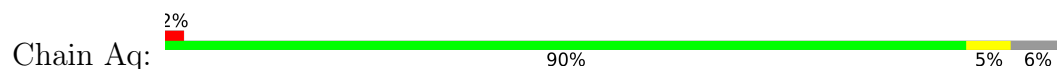
- Molecule 15: 30S ribosomal protein S16



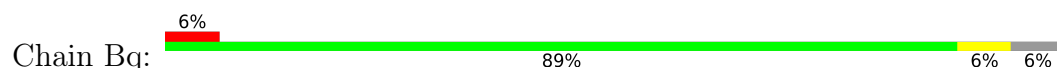
- Molecule 15: 30S ribosomal protein S16



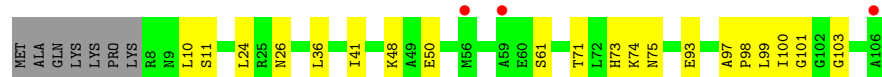
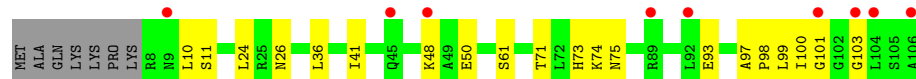
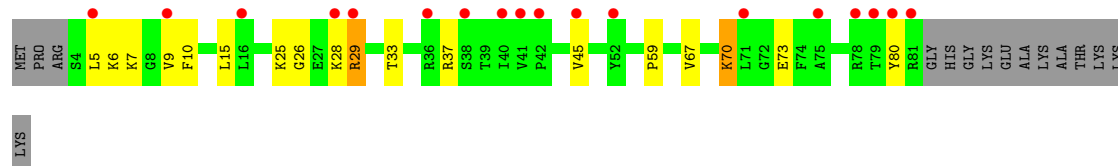
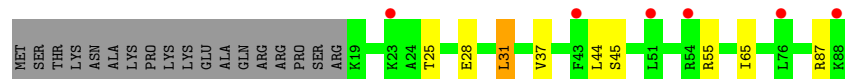
- Molecule 16: 30S ribosomal protein S17



- Molecule 16: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S18

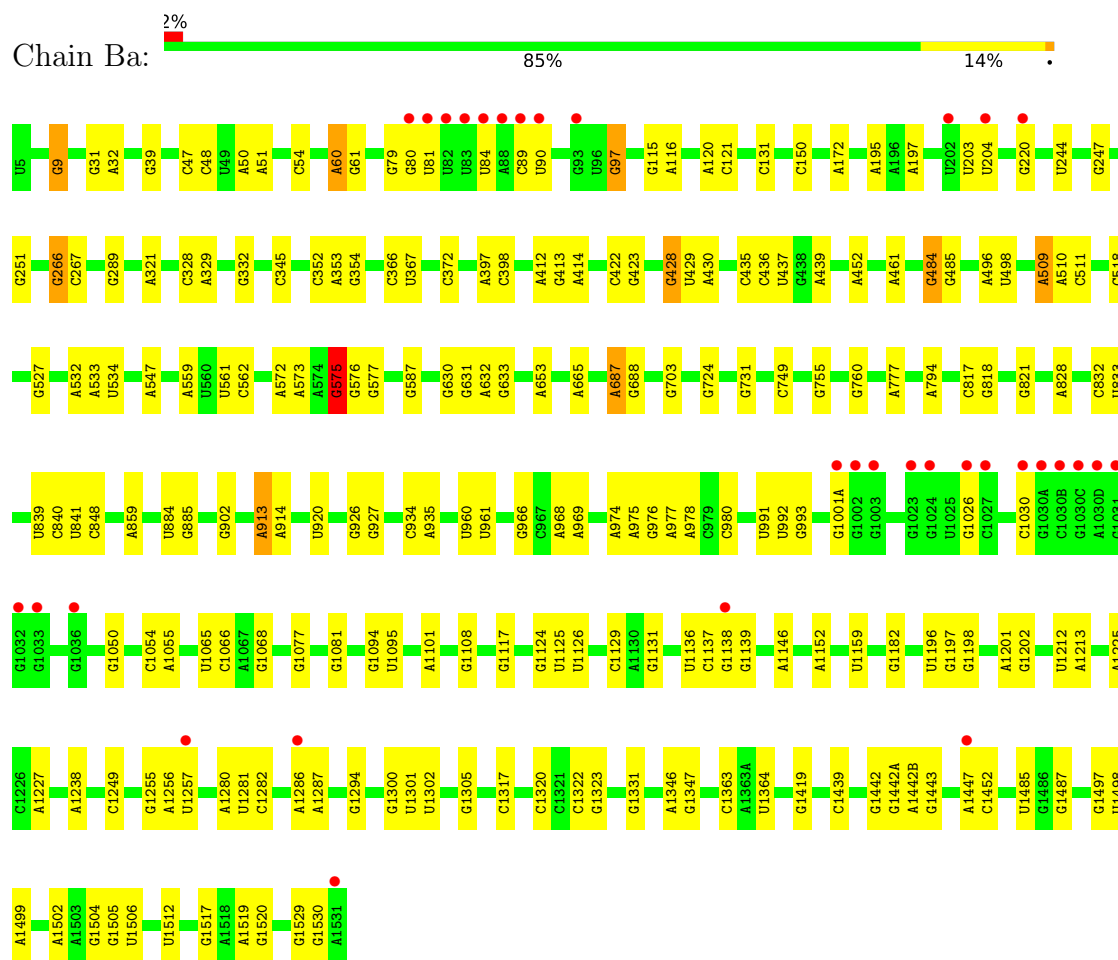




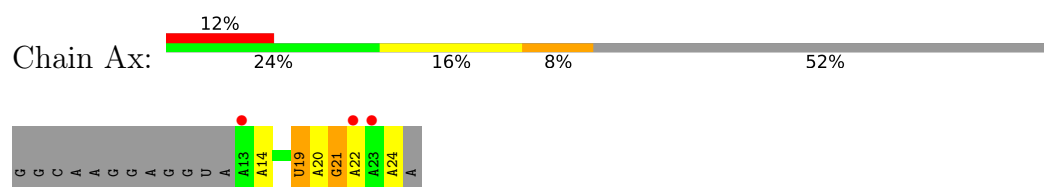




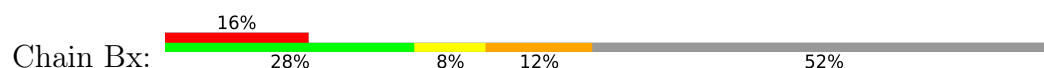
• Molecule 22: RNA (1504-MER)

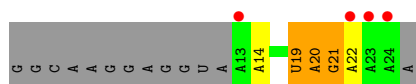


• Molecule 23: RNA (5'-R(\*GP\*GP\*CP\*AP\*AP\*GP\*GP\*AP\*GP\*GP\*UP\*A\*AP\*AP\*AP\*AP\*UP\*GP\*(OMU)P\*(A2M)P\*(OMG)P\*AP\*AP\*AP\*A)-3')

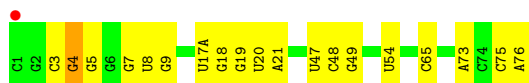
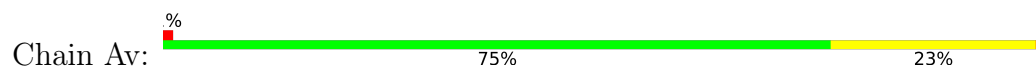


• Molecule 23: RNA (5'-R(\*GP\*GP\*CP\*AP\*AP\*GP\*GP\*AP\*GP\*GP\*UP\*A\*AP\*AP\*AP\*AP\*UP\*GP\*(OMU)P\*(A2M)P\*(OMG)P\*AP\*AP\*AP\*A)-3')

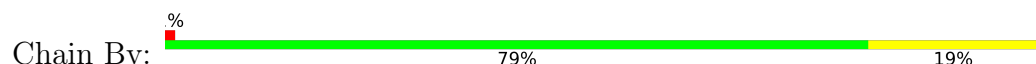




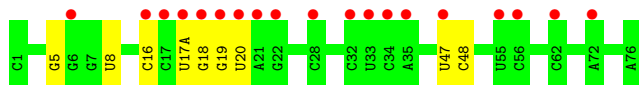
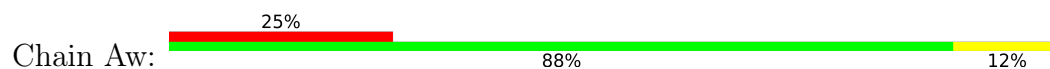
• Molecule 24: RNA (77-MER)



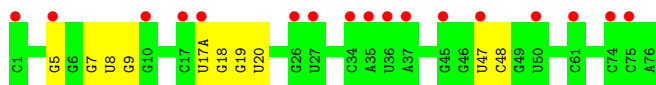
• Molecule 24: RNA (77-MER)



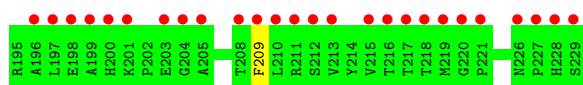
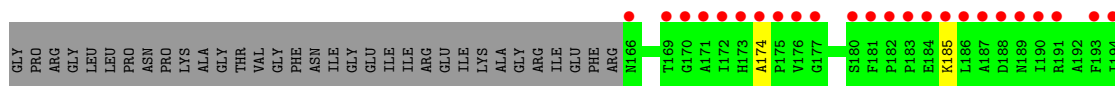
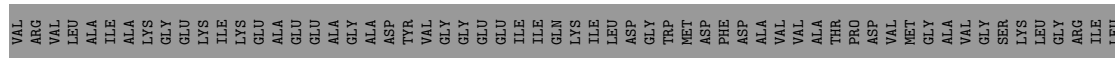
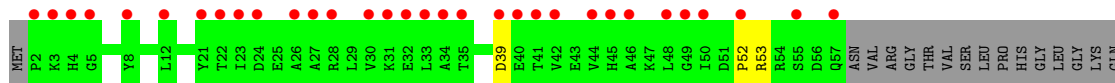
• Molecule 25: RNA (77-MER)



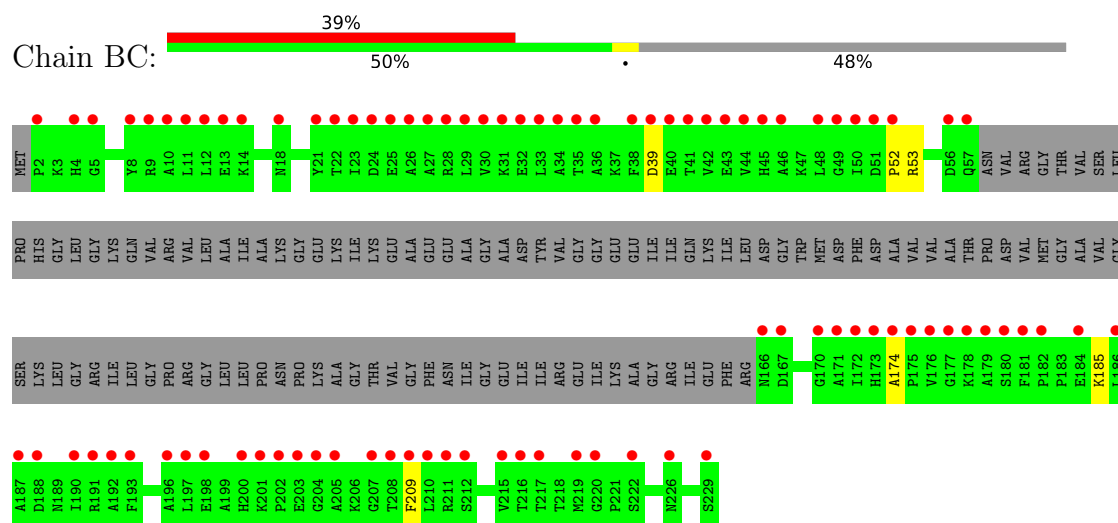
• Molecule 25: RNA (77-MER)



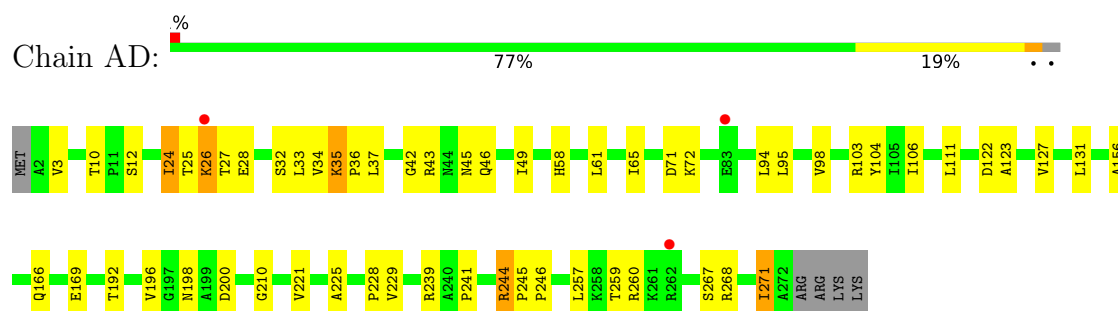
• Molecule 26: 50S ribosomal protein L1



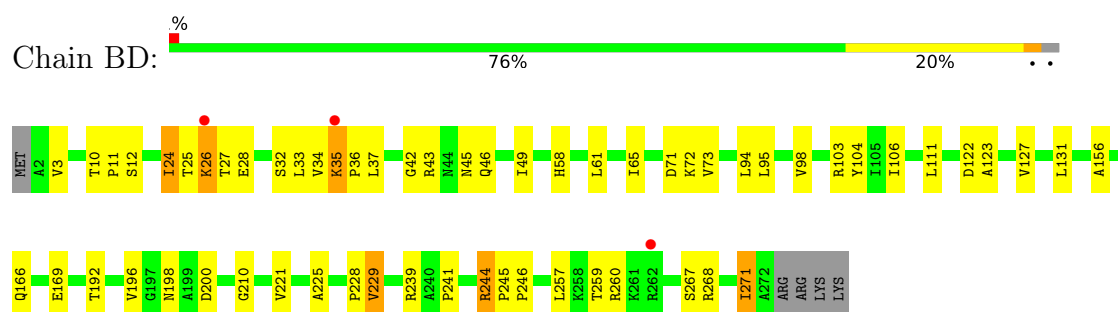
- Molecule 26: 50S ribosomal protein L1



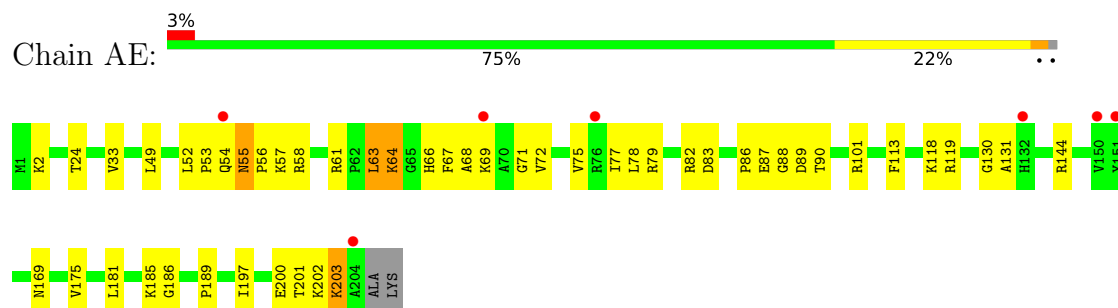
- Molecule 27: 50S ribosomal protein L2



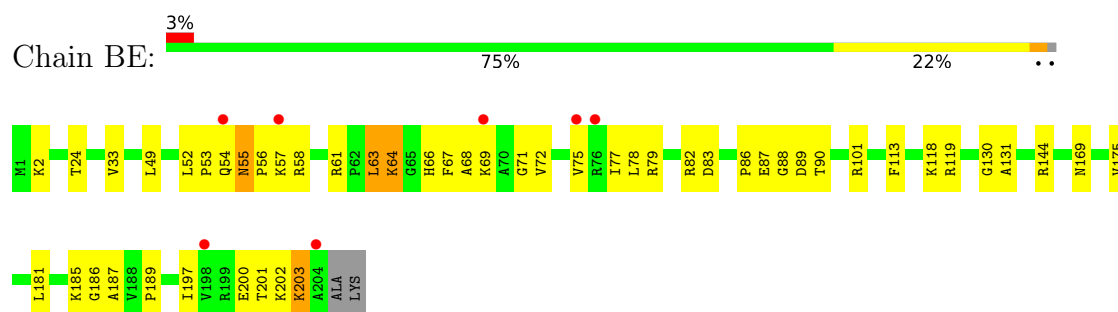
- Molecule 27: 50S ribosomal protein L2



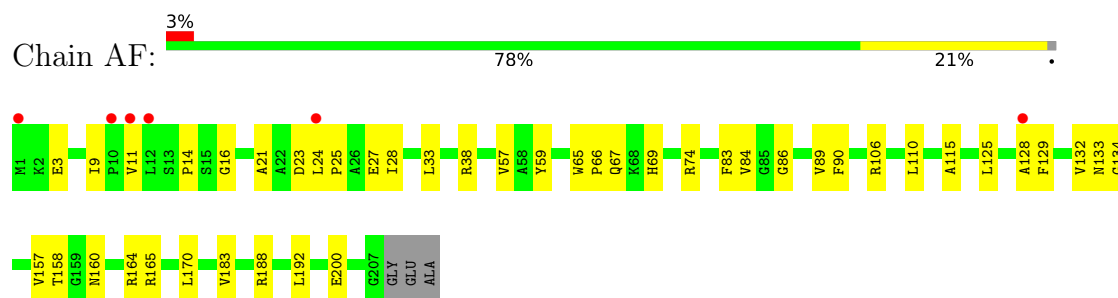
- Molecule 28: 50S ribosomal protein L3



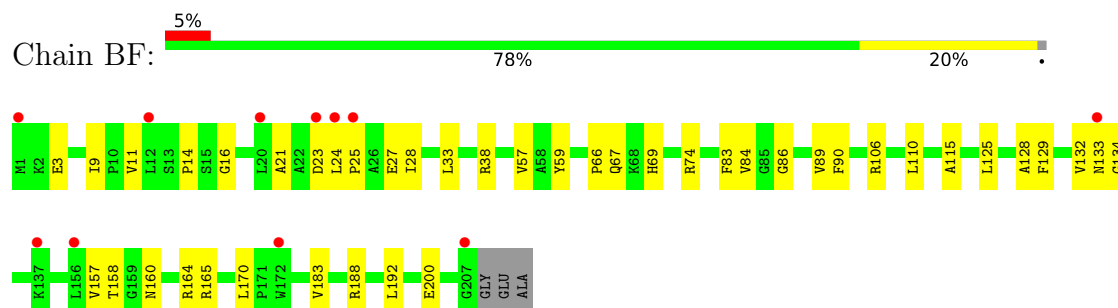
- Molecule 28: 50S ribosomal protein L3



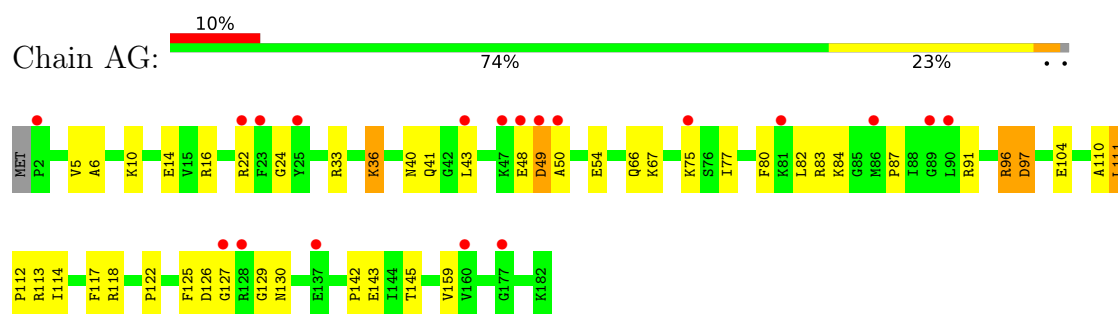
- Molecule 29: 50S ribosomal protein L4



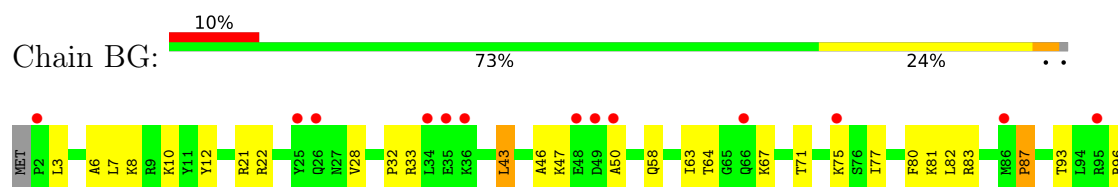
- Molecule 29: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L5

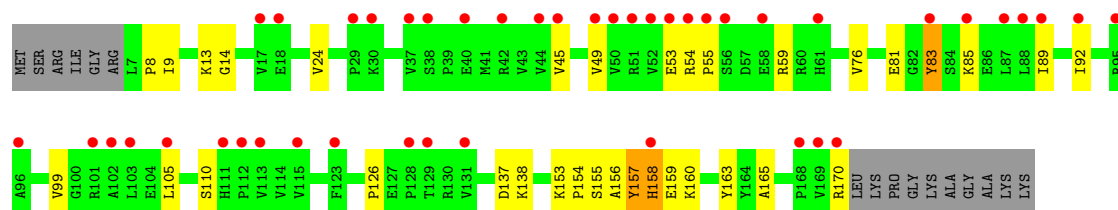
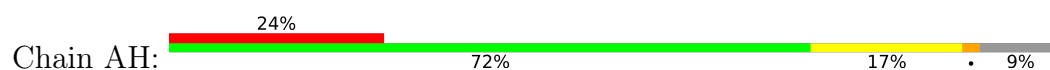


- Molecule 30: 50S ribosomal protein L5

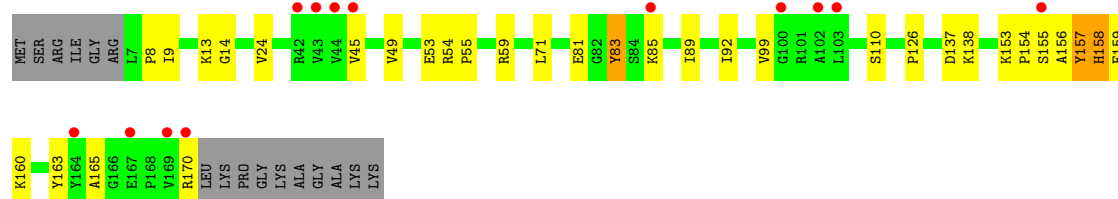
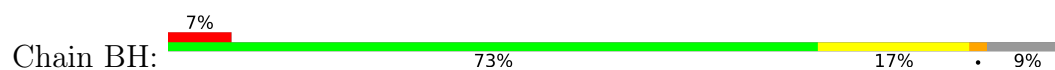




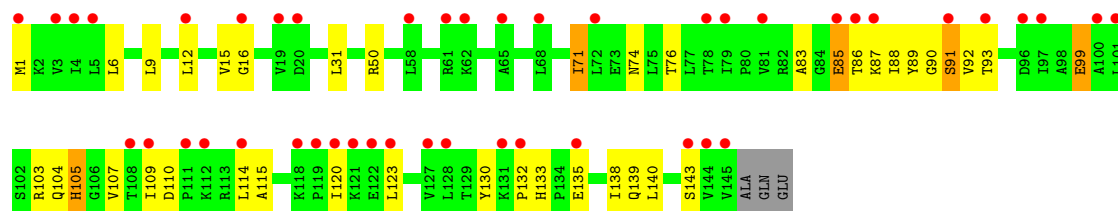
- Molecule 31: 50S ribosomal protein L6



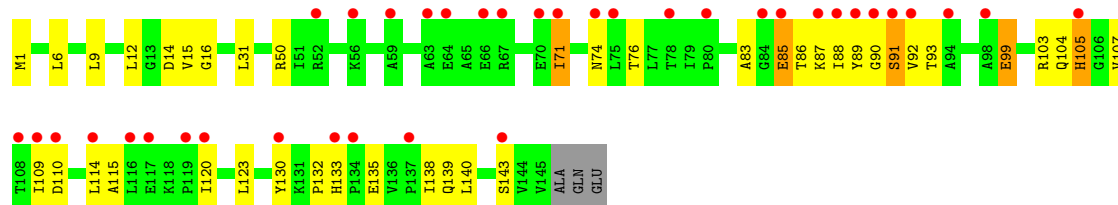
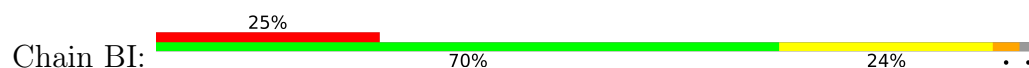
- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9

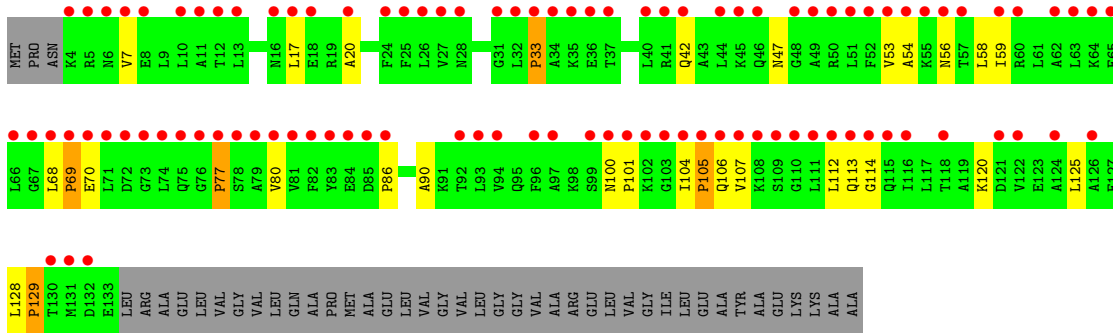


- Molecule 32: 50S ribosomal protein L9

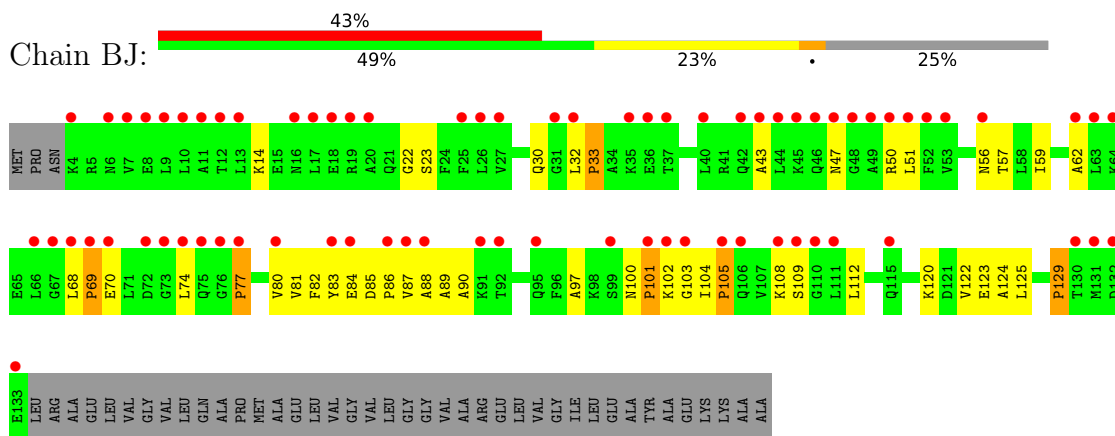


- Molecule 33: 50S ribosomal protein L10

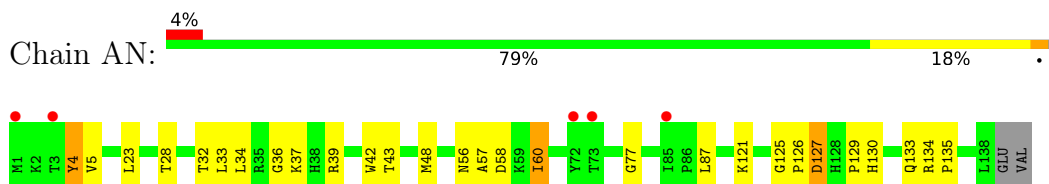




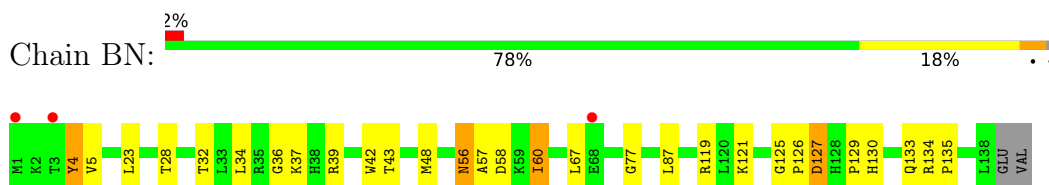
- Molecule 33: 50S ribosomal protein L10



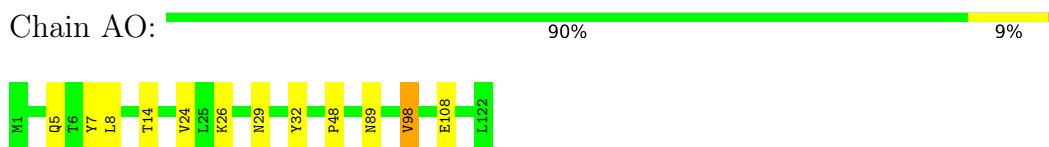
- Molecule 34: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L14

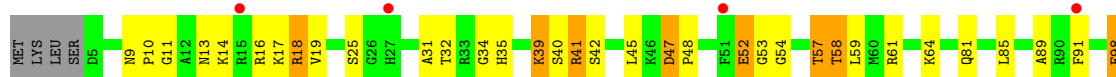


- Molecule 35: 50S ribosomal protein L14





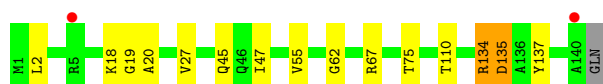
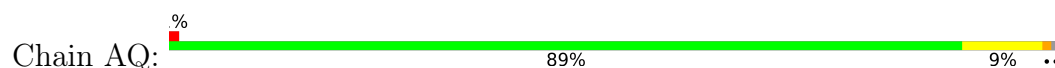
- Molecule 36: 50S ribosomal protein L15



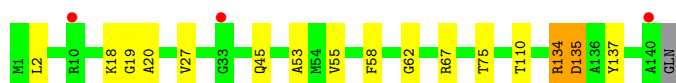
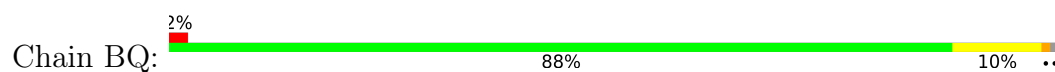
- Molecule 36: 50S ribosomal protein L15



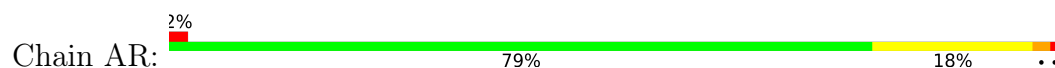
- Molecule 37: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L16

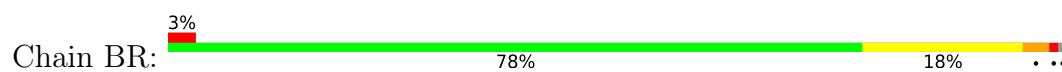


- Molecule 38: 50S ribosomal protein L17

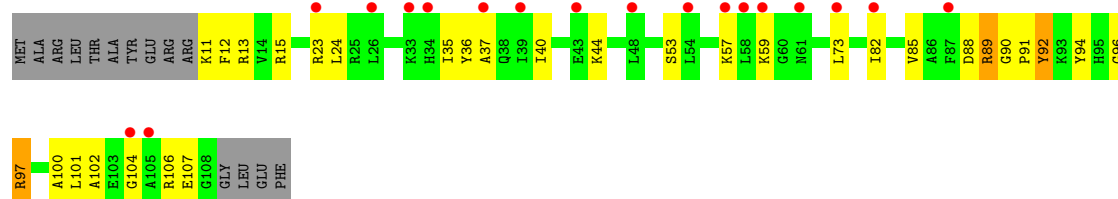


- Molecule 38: 50S ribosomal protein L17

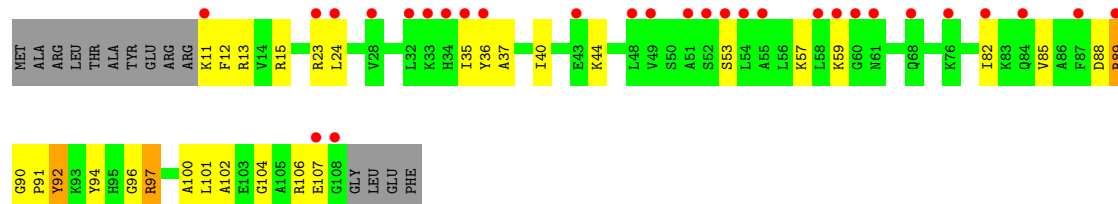




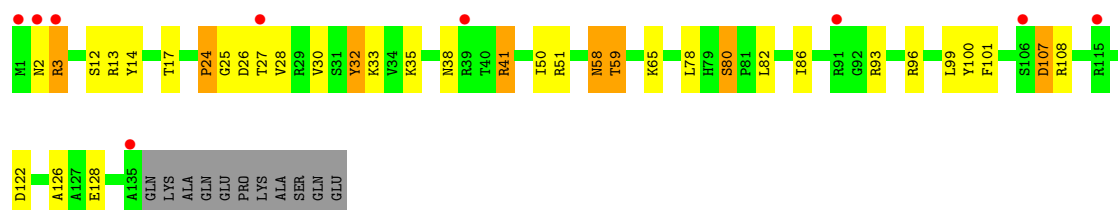
- Molecule 39: 50S ribosomal protein L18



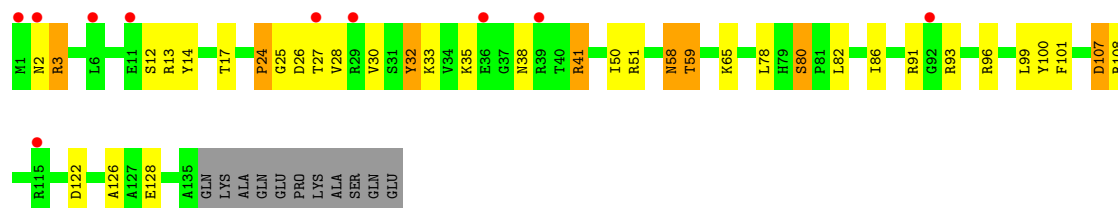
- Molecule 39: 50S ribosomal protein L18



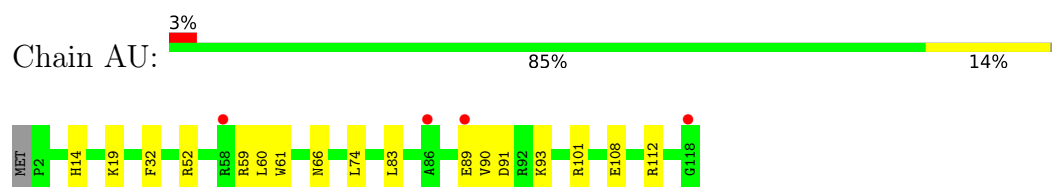
- Molecule 40: 50S ribosomal protein L19



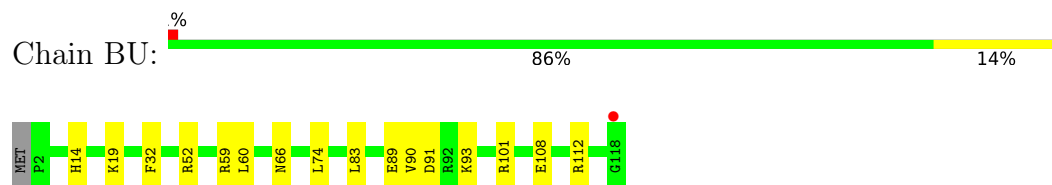
- Molecule 40: 50S ribosomal protein L19



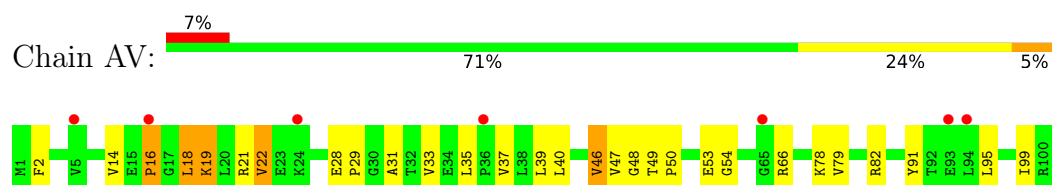
- Molecule 41: 50S ribosomal protein L20



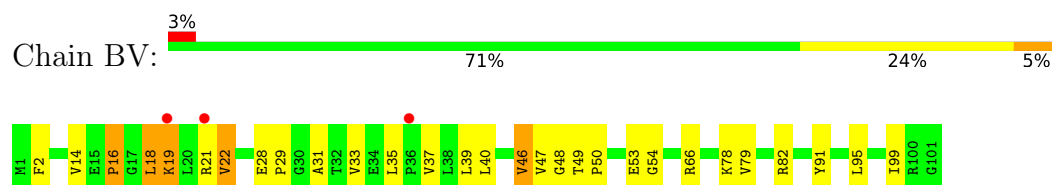
- Molecule 41: 50S ribosomal protein L20



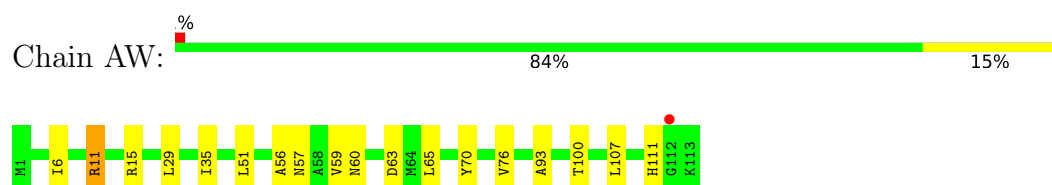
- Molecule 42: 50S ribosomal protein L21



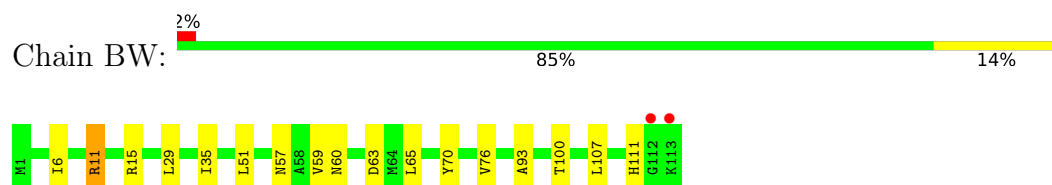
- Molecule 42: 50S ribosomal protein L21



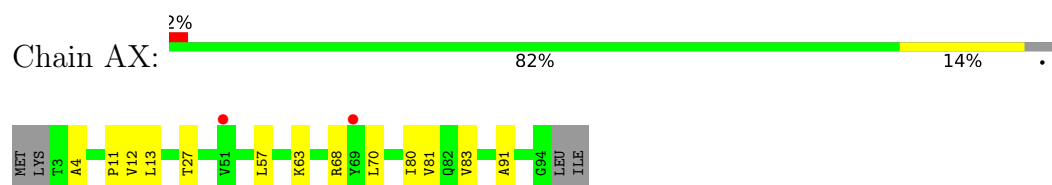
- Molecule 43: 50S ribosomal protein L22




- Molecule 43: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L23



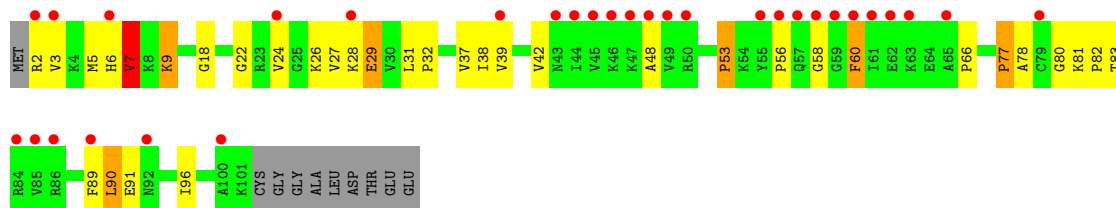
- Molecule 44: 50S ribosomal protein L23

Chain BX:  80% 16% .



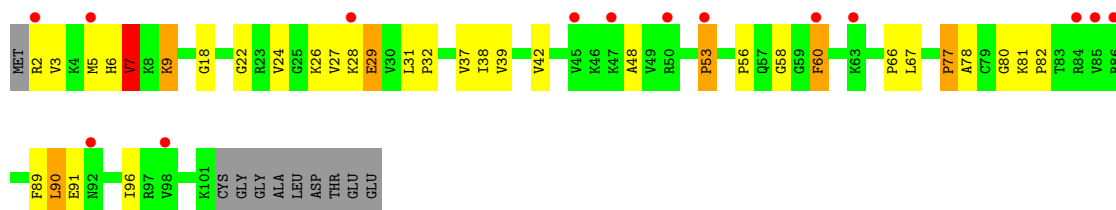
- Molecule 45: 50S ribosomal protein L24

Chain AY:  28% 59% 25% 5% . 9%



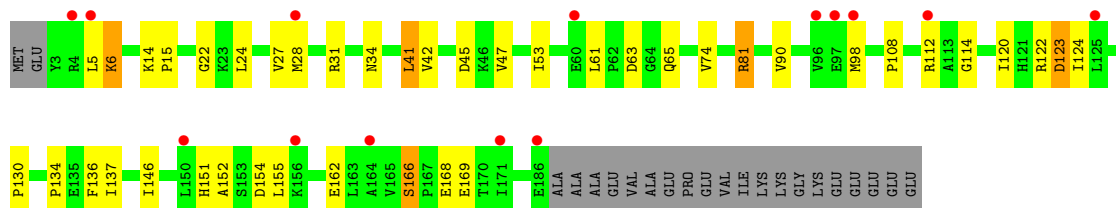
- Molecule 45: 50S ribosomal protein L24

Chain BY:  13% 59% 25% 5% . 9%



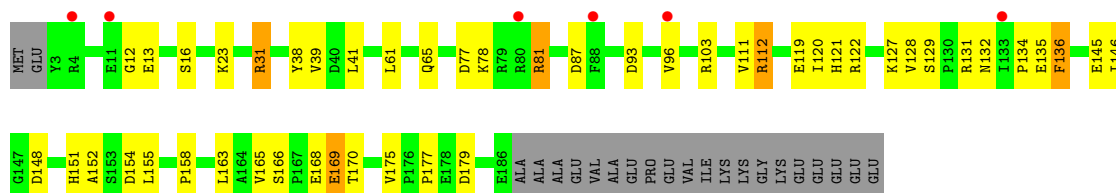
- Molecule 46: 50S ribosomal protein L25

Chain AZ:  7% 69% 18% . 11%

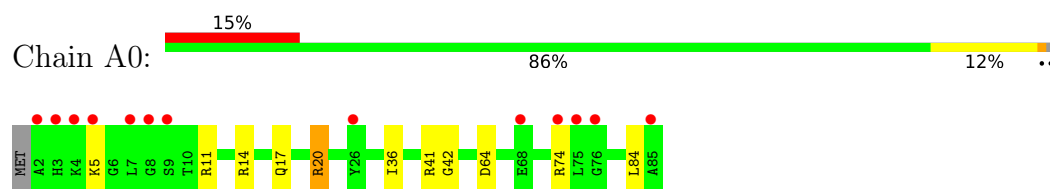


- Molecule 46: 50S ribosomal protein L25

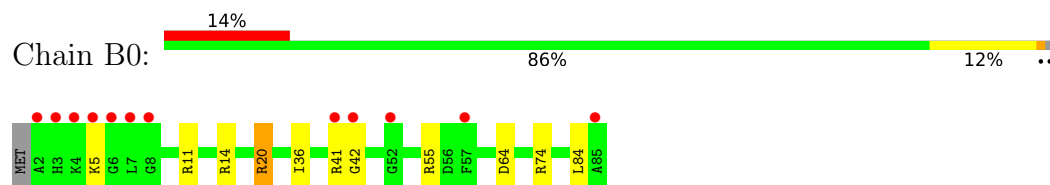
Chain BZ:  3% 66% 21% . 11%



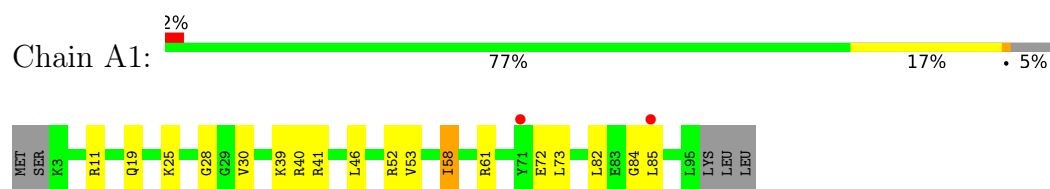
- Molecule 47: 50S ribosomal protein L27



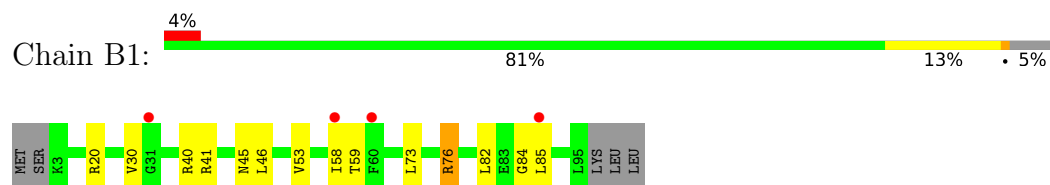
- Molecule 47: 50S ribosomal protein L27



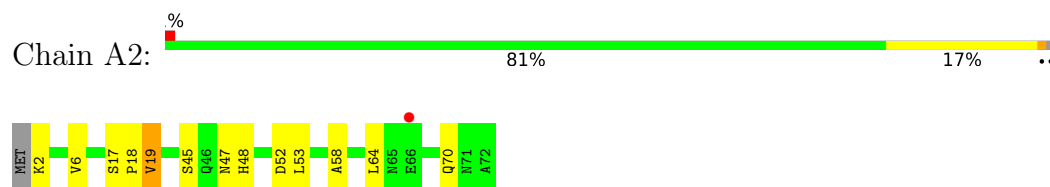
- Molecule 48: 50S ribosomal protein L28



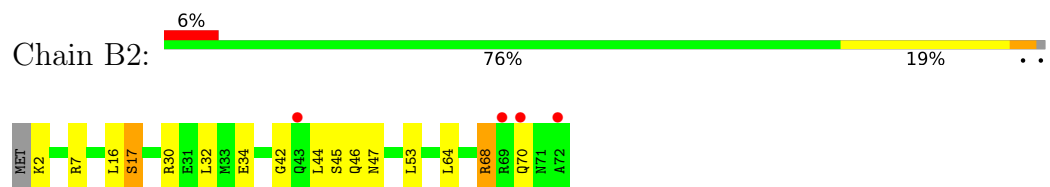
- Molecule 48: 50S ribosomal protein L28



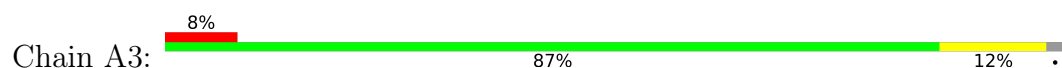
- Molecule 49: 50S ribosomal protein L29

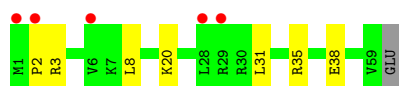


- Molecule 49: 50S ribosomal protein L29

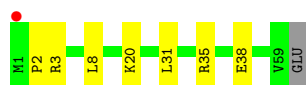
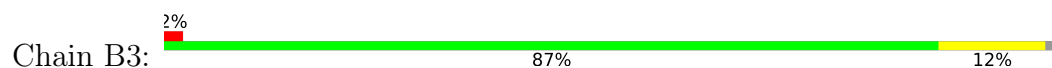


- Molecule 50: 50S ribosomal protein L30

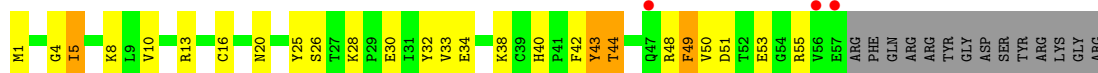
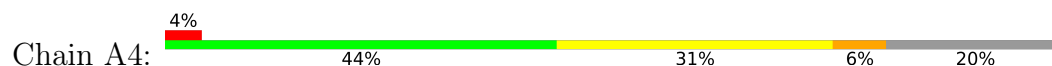




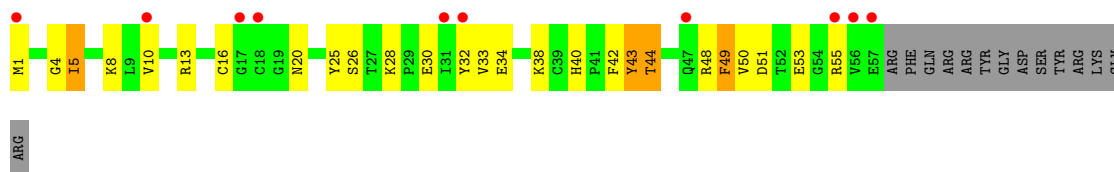
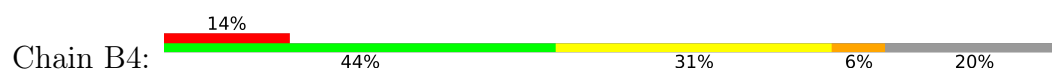
- Molecule 50: 50S ribosomal protein L30



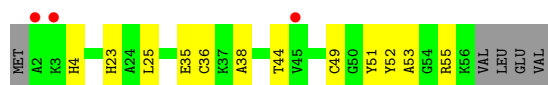
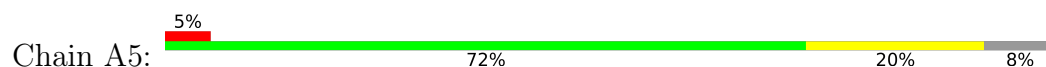
- Molecule 51: 50S ribosomal protein L31



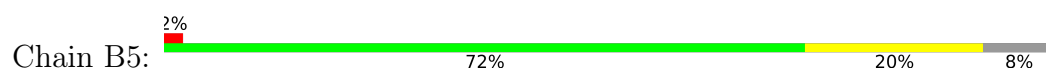
- Molecule 51: 50S ribosomal protein L31



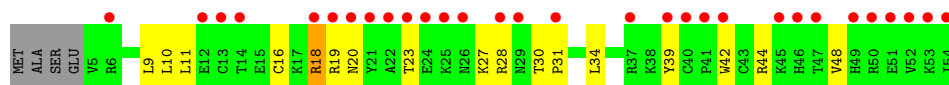
- Molecule 52: 50S ribosomal protein L32



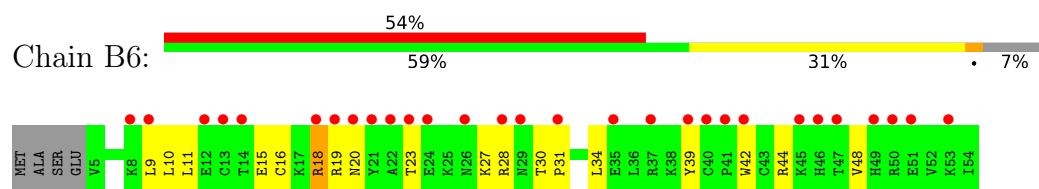
- Molecule 52: 50S ribosomal protein L32



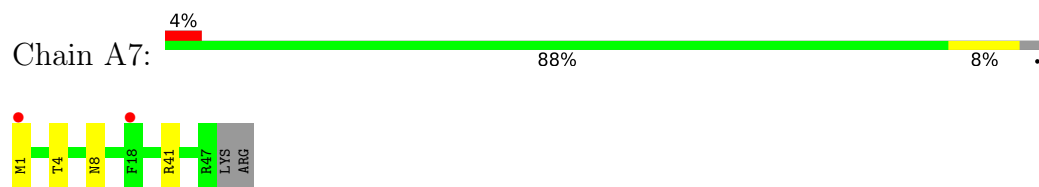
- Molecule 53: 50S ribosomal protein L33



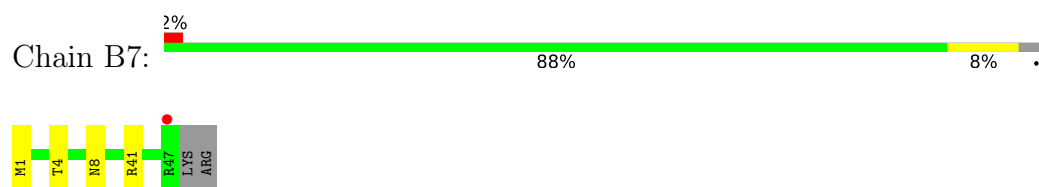
## • Molecule 53: 50S ribosomal protein L33



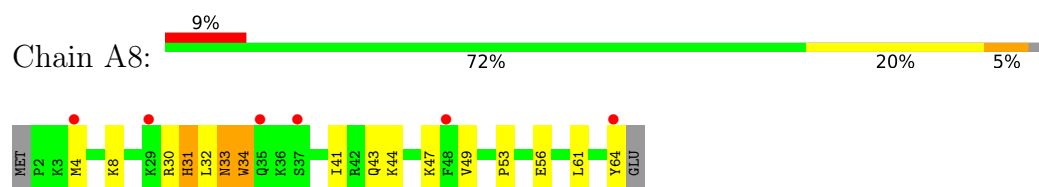
## • Molecule 54: 50S ribosomal protein L34



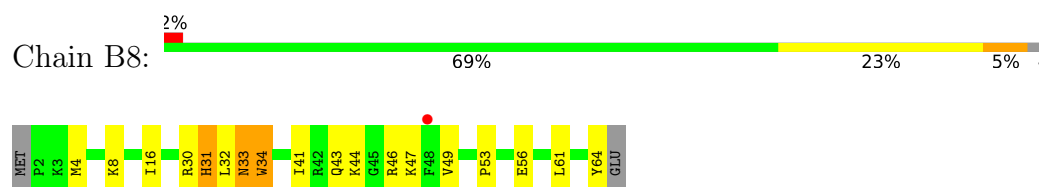
## • Molecule 54: 50S ribosomal protein L34



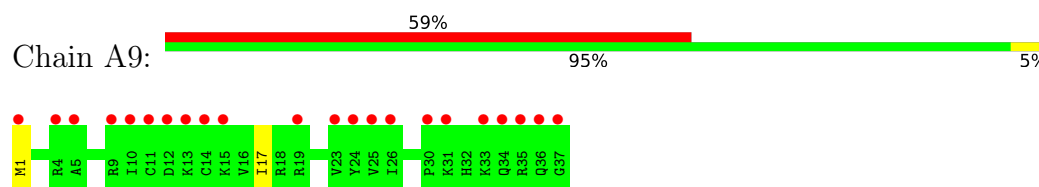
## • Molecule 55: 50S ribosomal protein L35



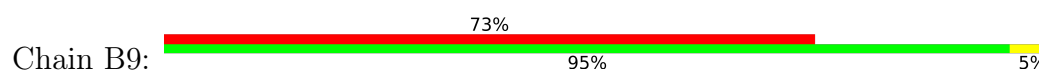
## • Molecule 55: 50S ribosomal protein L35

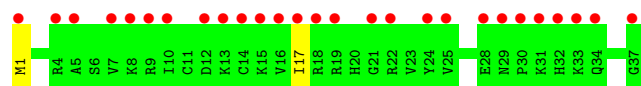


## • Molecule 56: 50S ribosomal protein L36

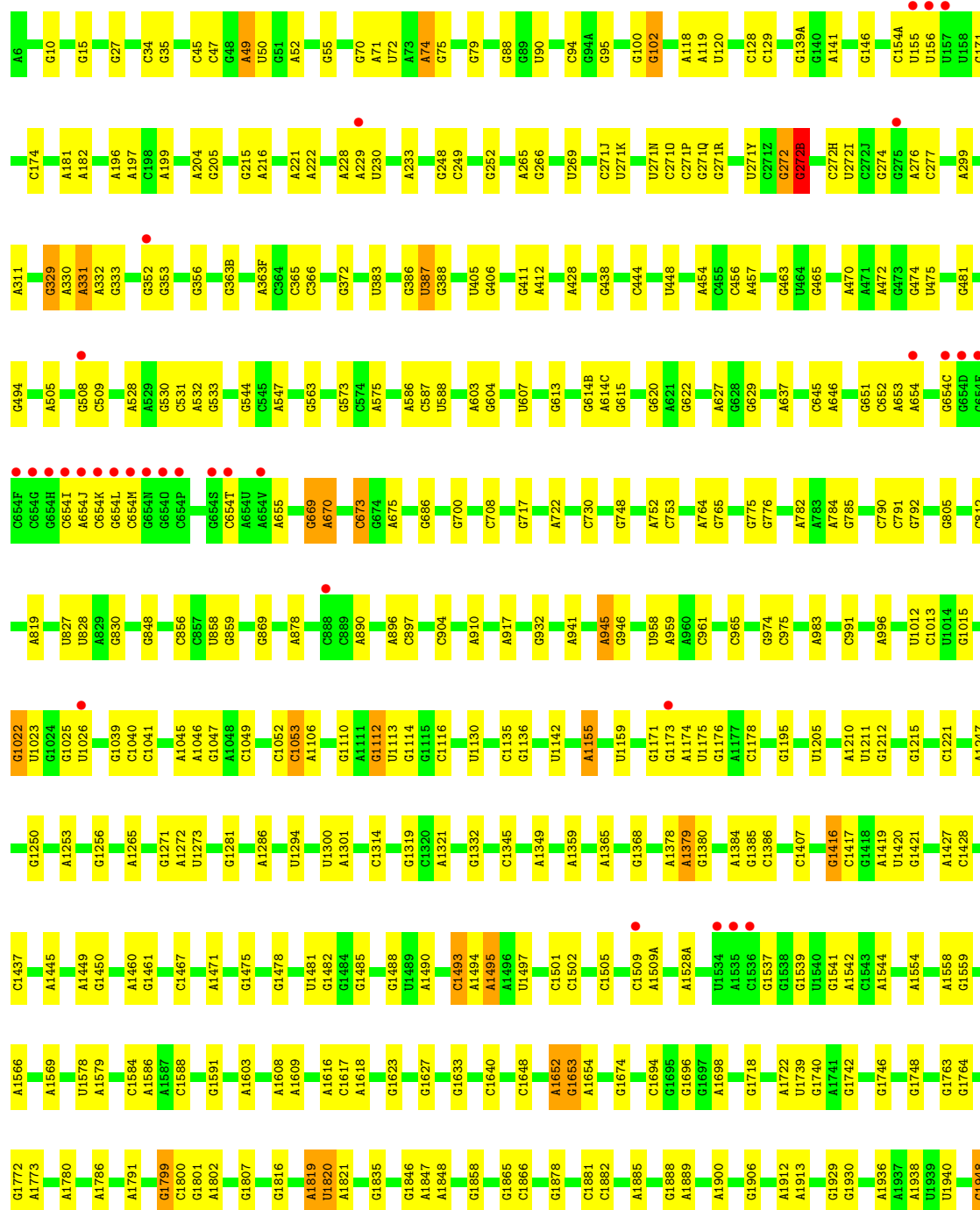
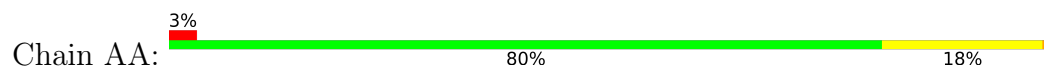


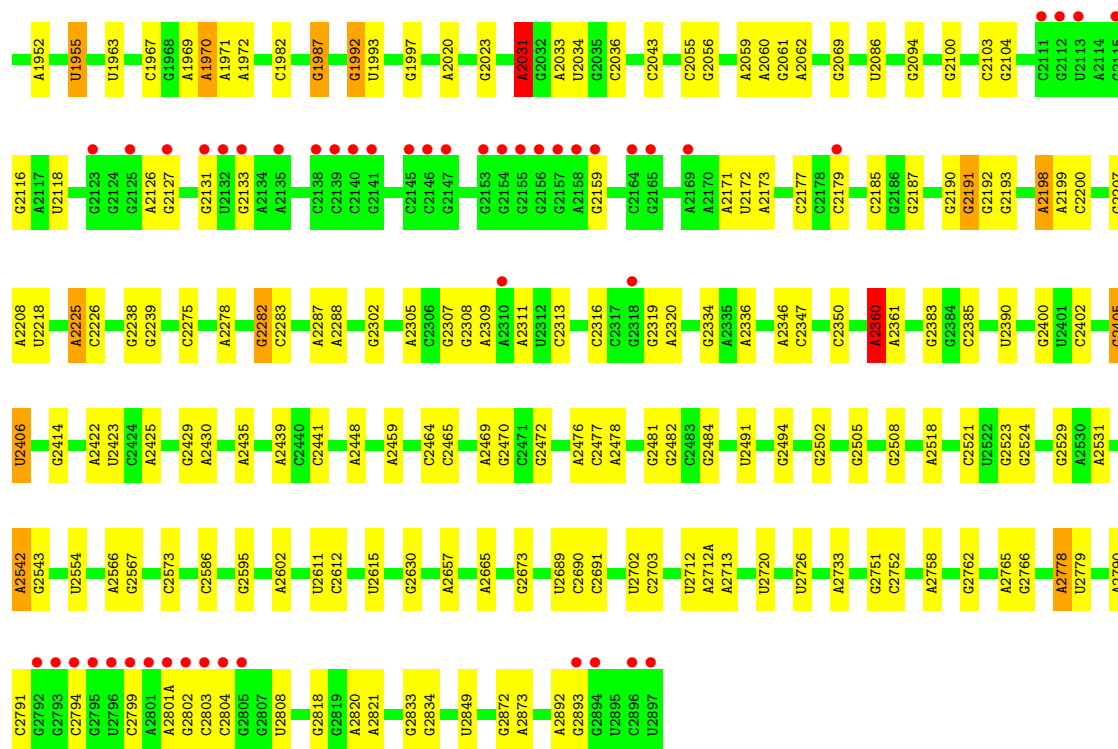
## • Molecule 56: 50S ribosomal protein L36



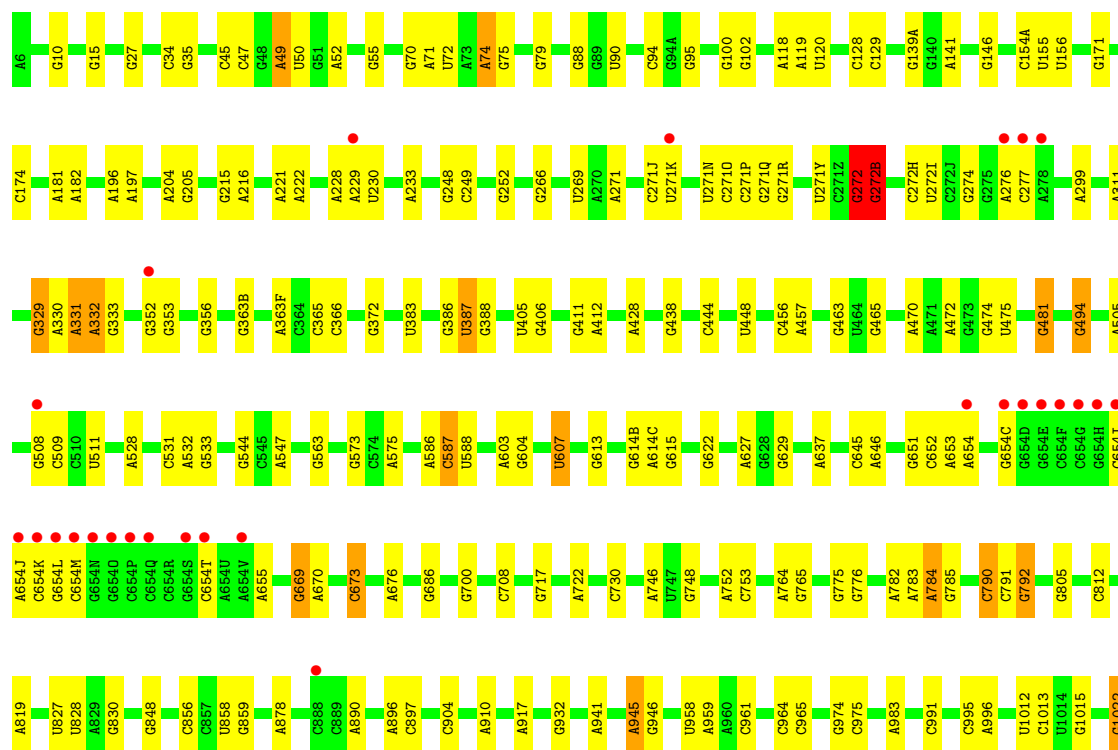
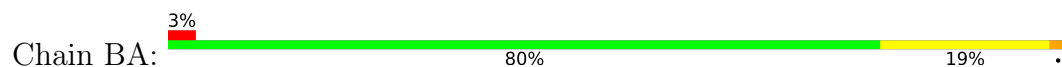


● Molecule 57: RNA (2848-MER)

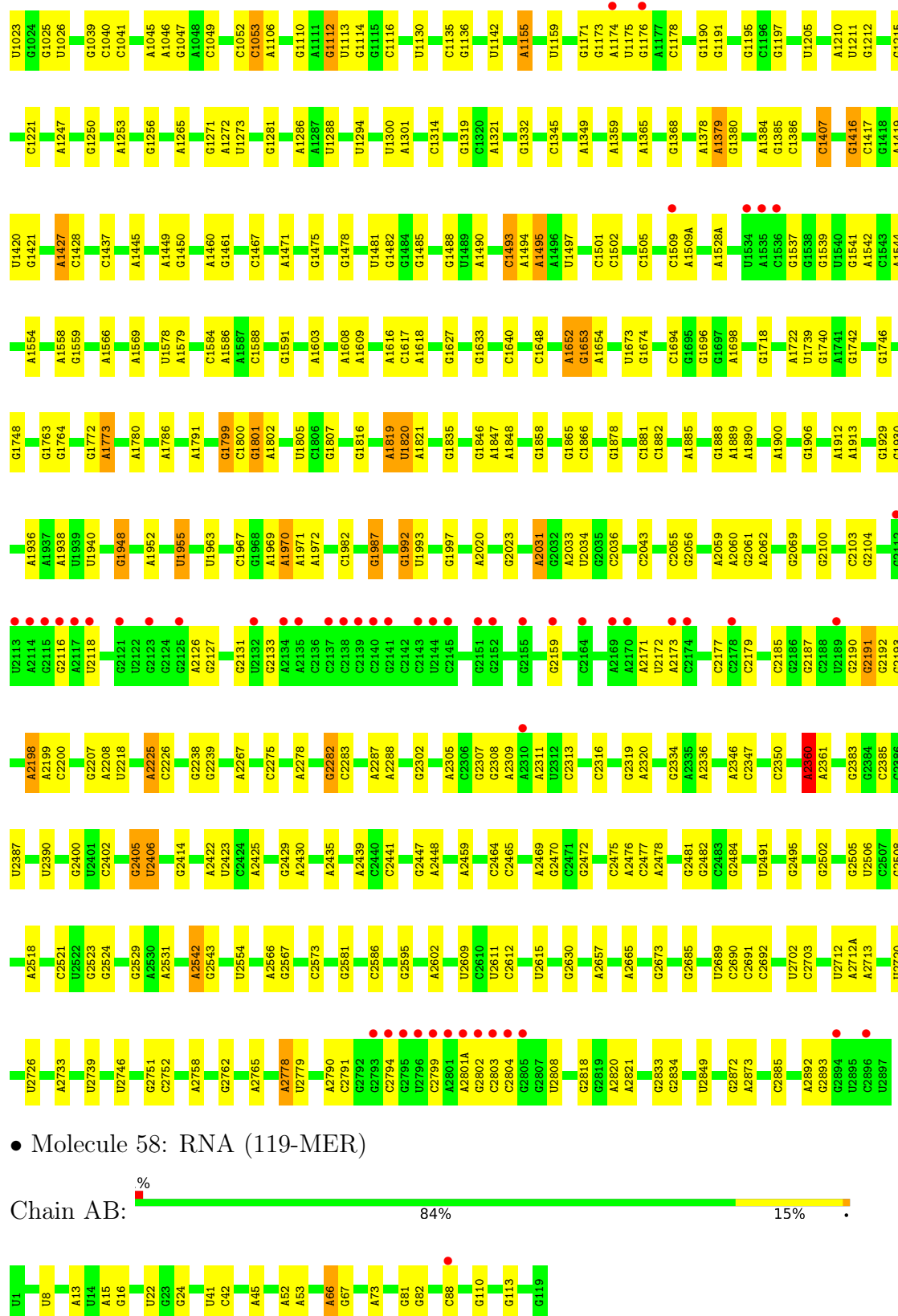


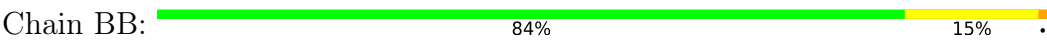


• Molecule 57: RNA (2848-MER)









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.57Å 451.96Å 622.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.99 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.30) 99.9 (49.99-3.30)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	0.02	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.219 , 0.247 0.221 , 0.250	Depositor DCC
$R_{free}$ test set	40918 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 85.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	297206	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, OMG, ZN, A2M, MG, OMU

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	0.34	0/1935	0.61	0/2609
1	Bb	0.34	0/1935	0.61	0/2609
2	Ac	0.33	0/1636	0.57	0/2205
2	Bc	0.33	0/1636	0.57	0/2205
3	Ad	0.38	0/1733	0.64	0/2318
3	Bd	0.38	0/1733	0.64	0/2318
4	Ae	0.35	0/1162	0.63	0/1564
4	Be	0.36	0/1162	0.63	0/1564
5	Af	0.33	0/856	0.65	0/1154
5	Bf	0.35	0/856	0.65	0/1154
6	Ag	0.32	0/1276	0.54	0/1709
6	Bg	0.32	0/1276	0.54	0/1709
7	Ah	0.35	0/1136	0.65	0/1527
7	Bh	0.35	0/1136	0.65	0/1527
8	Ai	0.33	0/1029	0.53	0/1379
8	Bi	0.34	0/1029	0.55	0/1379
9	Aj	0.34	0/807	0.62	0/1085
9	Bj	0.35	0/807	0.62	0/1085
10	Ak	0.34	0/900	0.62	0/1213
10	Bk	0.36	0/900	0.62	0/1213
11	Al	0.41	0/986	0.74	1/1320 (0.1%)
11	Bl	0.41	0/986	0.74	1/1320 (0.1%)
12	Am	0.30	0/947	0.63	0/1270
12	Bm	0.31	0/947	0.61	0/1270
13	An	0.34	0/501	0.57	0/664
13	Bn	0.35	0/501	0.58	0/664
14	Ao	0.33	0/745	0.60	0/992
14	Bo	0.34	0/745	0.61	0/992
15	Ap	0.34	0/716	0.60	0/963
15	Bp	0.34	0/716	0.59	0/963
16	Aq	0.35	0/836	0.64	0/1117
16	Bq	0.36	0/836	0.64	0/1117

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Ar	0.35	0/579	0.65	0/768
17	Br	0.36	0/579	0.65	0/768
18	As	0.34	0/642	0.63	0/865
18	Bs	0.34	0/642	0.63	0/865
19	At	0.34	0/765	0.61	0/1007
19	Bt	0.32	0/765	0.60	0/1007
20	Au	0.40	0/212	0.56	0/277
20	Bu	0.37	0/212	0.56	0/277
21	Ay	0.31	0/781	0.67	1/1045 (0.1%)
21	By	0.38	0/777	0.69	0/1040
22	Aa	0.41	0/36190	0.69	14/56486 (0.0%)
22	Ba	0.41	0/36190	0.69	14/56486 (0.0%)
23	Ax	0.52	0/219	0.74	0/340
23	Bx	0.45	0/219	0.75	0/340
24	Av	0.43	0/1810	0.70	0/2821
24	Bv	0.46	0/1810	0.72	1/2821 (0.0%)
25	Aw	0.42	0/1832	0.70	0/2855
25	Bw	0.44	0/1832	0.69	0/2855
26	AC	0.33	0/956	0.53	0/1288
26	BC	0.34	0/956	0.53	0/1288
27	AD	0.45	0/2154	0.81	3/2905 (0.1%)
27	BD	0.48	0/2154	0.82	4/2905 (0.1%)
28	AE	0.45	0/1596	0.79	0/2153
28	BE	0.47	0/1596	0.80	0/2153
29	AF	0.42	0/1658	0.72	0/2244
29	BF	0.45	0/1658	0.74	0/2244
30	AG	0.37	0/1499	0.69	1/2016 (0.0%)
30	BG	0.39	0/1499	0.71	1/2016 (0.0%)
31	AH	0.38	0/1284	0.74	1/1739 (0.1%)
31	BH	0.42	0/1284	0.76	1/1739 (0.1%)
32	AI	0.42	0/1146	0.92	3/1551 (0.2%)
32	BI	0.41	0/1146	0.93	3/1551 (0.2%)
33	AJ	0.36	0/640	0.78	7/889 (0.8%)
33	BJ	0.39	0/640	0.78	6/889 (0.7%)
34	AN	0.38	0/1131	0.74	0/1525
34	BN	0.42	0/1131	0.75	1/1525 (0.1%)
35	AO	0.44	0/943	0.69	0/1269
35	BO	0.45	0/943	0.70	0/1269
36	AP	0.49	0/1131	1.03	5/1504 (0.3%)
36	BP	0.53	0/1131	1.05	5/1504 (0.3%)
37	AQ	0.39	0/1133	0.65	0/1515
37	BQ	0.42	0/1133	0.66	0/1515
38	AR	0.41	0/974	0.79	2/1302 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	BR	0.42	0/974	0.80	3/1302 (0.2%)
39	AS	0.41	0/778	0.72	0/1036
39	BS	0.44	0/778	0.73	0/1036
40	AT	0.44	0/1137	0.82	2/1519 (0.1%)
40	BT	0.45	0/1137	0.83	2/1519 (0.1%)
41	AU	0.45	0/975	0.70	0/1297
41	BU	0.50	0/975	0.74	0/1297
42	AV	0.40	0/790	0.74	0/1057
42	BV	0.44	0/790	0.76	0/1057
43	AW	0.43	0/907	0.73	0/1216
43	BW	0.44	0/907	0.73	0/1216
44	AX	0.44	0/739	0.71	0/993
44	BX	0.47	0/739	0.73	0/993
45	AY	0.47	0/788	0.75	1/1051 (0.1%)
45	BY	0.51	0/788	0.77	1/1051 (0.1%)
46	AZ	0.36	0/1499	0.66	0/2035
46	BZ	0.39	0/1499	0.71	0/2035
47	A0	0.39	0/671	0.69	0/892
47	B0	0.43	0/671	0.71	0/892
48	A1	0.41	0/738	0.77	0/981
48	B1	0.44	0/738	0.80	0/981
49	A2	0.34	0/600	0.60	0/793
49	B2	0.43	0/600	0.70	0/793
50	A3	0.35	0/472	0.68	0/634
50	B3	0.38	0/472	0.68	0/634
51	A4	0.40	0/460	0.71	1/621 (0.2%)
51	B4	0.42	0/460	0.72	1/621 (0.2%)
52	A5	0.45	0/441	0.76	0/596
52	B5	0.48	0/441	0.79	0/596
53	A6	0.45	0/440	0.77	0/586
53	B6	0.46	0/440	0.77	0/586
54	A7	0.41	0/417	0.67	0/550
54	B7	0.46	0/417	0.67	0/550
55	A8	0.53	0/515	0.87	0/679
55	B8	0.53	0/515	0.88	0/679
56	A9	0.35	0/310	0.59	0/407
56	B9	0.37	0/310	0.60	0/407
57	AA	0.49	0/68704	0.74	49/107260 (0.0%)
57	BA	0.54	2/68704 (0.0%)	0.74	59/107260 (0.1%)
58	AB	0.41	0/2853	0.70	0/4451
58	BB	0.45	0/2853	0.71	0/4451
All	All	0.45	2/321416 (0.0%)	0.72	194/480209 (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	11
22	Ba	1	11
24	Av	0	1
24	Bv	0	1
38	AR	0	1
38	BR	0	1
52	A5	0	1
52	B5	0	1
57	AA	2	50
57	BA	2	68
58	AB	0	1
58	BB	0	1
All	All	5	149

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	2685	G	C6-O6	5.93	1.29	1.24
57	BA	2506	U	N1-C2	5.03	1.43	1.38

The worst 5 of 194 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BI	50	ARG	NE-CZ-NH2	-14.23	113.19	120.30
32	AI	50	ARG	NE-CZ-NH1	-14.08	113.26	120.30
32	BI	50	ARG	NE-CZ-NH1	13.66	127.13	120.30
32	AI	50	ARG	NE-CZ-NH2	13.15	126.88	120.30
57	AA	1992	G	C2'-C3'-O3'	10.34	132.24	109.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	AA	1799	G	C3'
57	AA	1819	A	C3'
22	Ba	1498	U	C3'
57	BA	1799	G	C3'
57	BA	1819	A	C3'

5 of 149 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	Aa	265	G	Sidechain
22	Aa	436	C	Sidechain
22	Aa	484	G	Sidechain
22	Aa	97	G	Sidechain
21	Ay	83	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	160 (69%)	45 (19%)	27 (12%)	0	2
1	Bb	232/256 (91%)	160 (69%)	46 (20%)	26 (11%)	0	2
2	Ac	204/239 (85%)	128 (63%)	51 (25%)	25 (12%)	0	1
2	Bc	204/239 (85%)	131 (64%)	49 (24%)	24 (12%)	0	2
3	Ad	206/209 (99%)	142 (69%)	45 (22%)	19 (9%)	1	4
3	Bd	206/209 (99%)	142 (69%)	46 (22%)	18 (9%)	1	5
4	Ae	148/162 (91%)	112 (76%)	24 (16%)	12 (8%)	1	6
4	Be	148/162 (91%)	111 (75%)	25 (17%)	12 (8%)	1	6
5	Af	99/101 (98%)	72 (73%)	19 (19%)	8 (8%)	1	6
5	Bf	99/101 (98%)	72 (73%)	19 (19%)	8 (8%)	1	6
6	Ag	153/156 (98%)	119 (78%)	24 (16%)	10 (6%)	1	9
6	Bg	153/156 (98%)	121 (79%)	22 (14%)	10 (6%)	1	9
7	Ah	136/138 (99%)	106 (78%)	27 (20%)	3 (2%)	6	30
7	Bh	136/138 (99%)	107 (79%)	26 (19%)	3 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Ai	125/128 (98%)	92 (74%)	22 (18%)	11 (9%)	1	5
8	Bi	125/128 (98%)	90 (72%)	23 (18%)	12 (10%)	0	4
9	Aj	96/105 (91%)	71 (74%)	18 (19%)	7 (7%)	1	7
9	Bj	96/105 (91%)	69 (72%)	20 (21%)	7 (7%)	1	7
10	Ak	117/129 (91%)	98 (84%)	16 (14%)	3 (3%)	5	27
10	Bk	117/129 (91%)	98 (84%)	16 (14%)	3 (3%)	5	27
11	Al	122/132 (92%)	93 (76%)	17 (14%)	12 (10%)	0	3
11	Bl	122/132 (92%)	93 (76%)	17 (14%)	12 (10%)	0	3
12	Am	116/126 (92%)	76 (66%)	21 (18%)	19 (16%)	0	1
12	Bm	116/126 (92%)	74 (64%)	23 (20%)	19 (16%)	0	1
13	An	58/61 (95%)	39 (67%)	10 (17%)	9 (16%)	0	1
13	Bn	58/61 (95%)	39 (67%)	10 (17%)	9 (16%)	0	1
14	Ao	86/89 (97%)	66 (77%)	16 (19%)	4 (5%)	2	14
14	Bo	86/89 (97%)	66 (77%)	16 (19%)	4 (5%)	2	14
15	Ap	81/88 (92%)	55 (68%)	21 (26%)	5 (6%)	1	10
15	Bp	81/88 (92%)	56 (69%)	20 (25%)	5 (6%)	1	10
16	Aq	97/105 (92%)	82 (84%)	13 (13%)	2 (2%)	7	31
16	Bq	97/105 (92%)	83 (86%)	11 (11%)	3 (3%)	4	23
17	Ar	68/88 (77%)	47 (69%)	14 (21%)	7 (10%)	0	3
17	Br	68/88 (77%)	47 (69%)	15 (22%)	6 (9%)	1	5
18	As	76/93 (82%)	50 (66%)	14 (18%)	12 (16%)	0	1
18	Bs	76/93 (82%)	49 (64%)	15 (20%)	12 (16%)	0	1
19	At	97/106 (92%)	70 (72%)	15 (16%)	12 (12%)	0	1
19	Bt	97/106 (92%)	70 (72%)	15 (16%)	12 (12%)	0	1
20	Au	22/27 (82%)	16 (73%)	5 (23%)	1 (4%)	2	15
20	Bu	22/27 (82%)	15 (68%)	6 (27%)	1 (4%)	2	15
21	Ay	92/95 (97%)	55 (60%)	12 (13%)	25 (27%)	0	0
21	By	92/95 (97%)	58 (63%)	21 (23%)	13 (14%)	0	1
26	AC	116/229 (51%)	93 (80%)	20 (17%)	3 (3%)	5	27
26	BC	116/229 (51%)	93 (80%)	20 (17%)	3 (3%)	5	27
27	AD	269/276 (98%)	203 (76%)	37 (14%)	29 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	BD	269/276 (98%)	203 (76%)	36 (13%)	30 (11%)	0	2
28	AE	202/206 (98%)	138 (68%)	32 (16%)	32 (16%)	0	1
28	BE	202/206 (98%)	138 (68%)	31 (15%)	33 (16%)	0	1
29	AF	205/210 (98%)	154 (75%)	31 (15%)	20 (10%)	0	3
29	BF	205/210 (98%)	155 (76%)	30 (15%)	20 (10%)	0	3
30	AG	179/182 (98%)	106 (59%)	44 (25%)	29 (16%)	0	1
30	BG	179/182 (98%)	119 (66%)	31 (17%)	29 (16%)	0	1
31	AH	162/180 (90%)	109 (67%)	27 (17%)	26 (16%)	0	1
31	BH	162/180 (90%)	109 (67%)	27 (17%)	26 (16%)	0	1
32	AI	143/148 (97%)	84 (59%)	38 (27%)	21 (15%)	0	1
32	BI	143/148 (97%)	85 (59%)	36 (25%)	22 (15%)	0	1
33	AJ	128/173 (74%)	56 (44%)	43 (34%)	29 (23%)	0	0
33	BJ	128/173 (74%)	44 (34%)	38 (30%)	46 (36%)	0	0
34	AN	136/140 (97%)	101 (74%)	20 (15%)	15 (11%)	0	2
34	BN	136/140 (97%)	100 (74%)	20 (15%)	16 (12%)	0	2
35	AO	120/122 (98%)	104 (87%)	10 (8%)	6 (5%)	2	14
35	BO	120/122 (98%)	102 (85%)	13 (11%)	5 (4%)	3	17
36	AP	144/150 (96%)	76 (53%)	35 (24%)	33 (23%)	0	0
36	BP	144/150 (96%)	79 (55%)	32 (22%)	33 (23%)	0	0
37	AQ	138/141 (98%)	109 (79%)	21 (15%)	8 (6%)	1	11
37	BQ	138/141 (98%)	109 (79%)	21 (15%)	8 (6%)	1	11
38	AR	115/118 (98%)	85 (74%)	20 (17%)	10 (9%)	1	5
38	BR	115/118 (98%)	84 (73%)	21 (18%)	10 (9%)	1	5
39	AS	96/112 (86%)	60 (62%)	13 (14%)	23 (24%)	0	0
39	BS	96/112 (86%)	60 (62%)	13 (14%)	23 (24%)	0	0
40	AT	133/146 (91%)	90 (68%)	24 (18%)	19 (14%)	0	1
40	BT	133/146 (91%)	90 (68%)	23 (17%)	20 (15%)	0	1
41	AU	115/118 (98%)	88 (76%)	21 (18%)	6 (5%)	2	13
41	BU	115/118 (98%)	90 (78%)	20 (17%)	5 (4%)	2	16
42	AV	99/101 (98%)	65 (66%)	17 (17%)	17 (17%)	0	1
42	BV	99/101 (98%)	64 (65%)	18 (18%)	17 (17%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	AW	111/113 (98%)	89 (80%)	11 (10%)	11 (10%)	0	3
43	BW	111/113 (98%)	90 (81%)	11 (10%)	10 (9%)	1	4
44	AX	90/96 (94%)	72 (80%)	13 (14%)	5 (6%)	2	11
44	BX	90/96 (94%)	72 (80%)	11 (12%)	7 (8%)	1	6
45	AY	98/110 (89%)	51 (52%)	18 (18%)	29 (30%)	0	0
45	BY	98/110 (89%)	52 (53%)	16 (16%)	30 (31%)	0	0
46	AZ	182/206 (88%)	115 (63%)	40 (22%)	27 (15%)	0	1
46	BZ	182/206 (88%)	118 (65%)	37 (20%)	27 (15%)	0	1
47	A0	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	2	14
47	B0	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	2	14
48	A1	91/98 (93%)	74 (81%)	10 (11%)	7 (8%)	1	6
48	B1	91/98 (93%)	71 (78%)	14 (15%)	6 (7%)	1	8
49	A2	69/72 (96%)	44 (64%)	16 (23%)	9 (13%)	0	1
49	B2	69/72 (96%)	50 (72%)	13 (19%)	6 (9%)	1	5
50	A3	57/60 (95%)	47 (82%)	7 (12%)	3 (5%)	2	12
50	B3	57/60 (95%)	47 (82%)	7 (12%)	3 (5%)	2	12
51	A4	55/71 (78%)	23 (42%)	18 (33%)	14 (26%)	0	0
51	B4	55/71 (78%)	23 (42%)	18 (33%)	14 (26%)	0	0
52	A5	53/60 (88%)	40 (76%)	7 (13%)	6 (11%)	0	2
52	B5	53/60 (88%)	40 (76%)	7 (13%)	6 (11%)	0	2
53	A6	48/54 (89%)	24 (50%)	14 (29%)	10 (21%)	0	0
53	B6	48/54 (89%)	24 (50%)	14 (29%)	10 (21%)	0	0
54	A7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
54	B7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
55	A8	61/65 (94%)	41 (67%)	14 (23%)	6 (10%)	0	3
55	B8	61/65 (94%)	41 (67%)	14 (23%)	6 (10%)	0	3
56	A9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
56	B9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	12016/13122 (92%)	8475 (70%)	2157 (18%)	1384 (12%)	0	2

5 of 1384 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ab	15	VAL
1	Ab	18	GLY
1	Ab	26	PRO
1	Ab	63	MET
1	Ab	80	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ab	202/220 (92%)	189 (94%)	13 (6%)	17	46
1	Bb	202/220 (92%)	189 (94%)	13 (6%)	17	46
2	Ac	160/188 (85%)	143 (89%)	17 (11%)	6	25
2	Bc	160/188 (85%)	143 (89%)	17 (11%)	6	25
3	Ad	180/181 (99%)	157 (87%)	23 (13%)	4	18
3	Bd	180/181 (99%)	156 (87%)	24 (13%)	4	17
4	Ae	115/123 (94%)	107 (93%)	8 (7%)	15	43
4	Be	115/123 (94%)	106 (92%)	9 (8%)	12	38
5	Af	90/90 (100%)	87 (97%)	3 (3%)	38	66
5	Bf	90/90 (100%)	87 (97%)	3 (3%)	38	66
6	Ag	126/127 (99%)	119 (94%)	7 (6%)	21	52
6	Bg	126/127 (99%)	119 (94%)	7 (6%)	21	52
7	Ah	119/119 (100%)	109 (92%)	10 (8%)	11	35
7	Bh	119/119 (100%)	109 (92%)	10 (8%)	11	35
8	Ai	98/99 (99%)	87 (89%)	11 (11%)	6	23
8	Bi	98/99 (99%)	86 (88%)	12 (12%)	5	20
9	Aj	88/92 (96%)	80 (91%)	8 (9%)	9	31
9	Bj	88/92 (96%)	80 (91%)	8 (9%)	9	31
10	Ak	90/99 (91%)	87 (97%)	3 (3%)	38	66
10	Bk	90/99 (91%)	88 (98%)	2 (2%)	52	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	Al	104/109 (95%)	87 (84%)	17 (16%)	2	10
11	Bl	104/109 (95%)	88 (85%)	16 (15%)	2	12
12	Am	94/101 (93%)	78 (83%)	16 (17%)	2	9
12	Bm	94/101 (93%)	75 (80%)	19 (20%)	1	5
13	An	49/50 (98%)	47 (96%)	2 (4%)	30	61
13	Bn	49/50 (98%)	47 (96%)	2 (4%)	30	61
14	Ao	79/80 (99%)	74 (94%)	5 (6%)	18	47
14	Bo	79/80 (99%)	74 (94%)	5 (6%)	18	47
15	Ap	72/74 (97%)	69 (96%)	3 (4%)	30	60
15	Bp	72/74 (97%)	69 (96%)	3 (4%)	30	60
16	Aq	94/97 (97%)	91 (97%)	3 (3%)	39	67
16	Bq	94/97 (97%)	91 (97%)	3 (3%)	39	67
17	Ar	61/77 (79%)	58 (95%)	3 (5%)	25	56
17	Br	61/77 (79%)	58 (95%)	3 (5%)	25	56
18	As	69/80 (86%)	61 (88%)	8 (12%)	5	22
18	Bs	69/80 (86%)	61 (88%)	8 (12%)	5	22
19	At	76/82 (93%)	68 (90%)	8 (10%)	7	25
19	Bt	76/82 (93%)	68 (90%)	8 (10%)	7	25
20	Au	19/22 (86%)	19 (100%)	0	100	100
20	Bu	19/22 (86%)	19 (100%)	0	100	100
21	Ay	84/85 (99%)	64 (76%)	20 (24%)	0	2
21	By	83/85 (98%)	72 (87%)	11 (13%)	4	17
26	AC	99/181 (55%)	96 (97%)	3 (3%)	41	68
26	BC	99/181 (55%)	96 (97%)	3 (3%)	41	68
27	AD	213/218 (98%)	182 (85%)	31 (15%)	3	14
27	BD	213/218 (98%)	181 (85%)	32 (15%)	3	13
28	AE	165/166 (99%)	144 (87%)	21 (13%)	4	19
28	BE	165/166 (99%)	144 (87%)	21 (13%)	4	19
29	AF	165/166 (99%)	141 (86%)	24 (14%)	3	14
29	BF	165/166 (99%)	142 (86%)	23 (14%)	3	16
30	AG	155/156 (99%)	134 (86%)	21 (14%)	4	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BG	155/156 (99%)	131 (84%)	24 (16%)	2	12
31	AH	137/148 (93%)	127 (93%)	10 (7%)	14	41
31	BH	137/148 (93%)	128 (93%)	9 (7%)	16	46
32	AI	122/124 (98%)	99 (81%)	23 (19%)	1	6
32	BI	122/124 (98%)	99 (81%)	23 (19%)	1	6
34	AN	117/119 (98%)	101 (86%)	16 (14%)	3	16
34	BN	117/119 (98%)	101 (86%)	16 (14%)	3	16
35	AO	100/100 (100%)	93 (93%)	7 (7%)	15	43
35	BO	100/100 (100%)	93 (93%)	7 (7%)	15	43
36	AP	112/116 (97%)	89 (80%)	23 (20%)	1	4
36	BP	112/116 (97%)	87 (78%)	25 (22%)	1	3
37	AQ	110/111 (99%)	101 (92%)	9 (8%)	11	36
37	BQ	110/111 (99%)	100 (91%)	10 (9%)	9	31
38	AR	100/101 (99%)	85 (85%)	15 (15%)	3	13
38	BR	100/101 (99%)	84 (84%)	16 (16%)	2	11
39	AS	77/88 (88%)	66 (86%)	11 (14%)	3	15
39	BS	77/88 (88%)	67 (87%)	10 (13%)	4	17
40	AT	118/127 (93%)	95 (80%)	23 (20%)	1	5
40	BT	118/127 (93%)	95 (80%)	23 (20%)	1	5
41	AU	92/94 (98%)	81 (88%)	11 (12%)	5	20
41	BU	92/94 (98%)	81 (88%)	11 (12%)	5	20
42	AV	82/82 (100%)	65 (79%)	17 (21%)	1	4
42	BV	82/82 (100%)	65 (79%)	17 (21%)	1	4
43	AW	91/92 (99%)	83 (91%)	8 (9%)	10	33
43	BW	91/92 (99%)	83 (91%)	8 (9%)	10	33
44	AX	74/78 (95%)	66 (89%)	8 (11%)	6	24
44	BX	74/78 (95%)	66 (89%)	8 (11%)	6	24
45	AY	84/91 (92%)	71 (84%)	13 (16%)	2	12
45	BY	84/91 (92%)	72 (86%)	12 (14%)	3	15
46	AZ	162/179 (90%)	142 (88%)	20 (12%)	4	20
46	BZ	162/179 (90%)	136 (84%)	26 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	A0	66/67 (98%)	58 (88%)	8 (12%)	5	20
47	B0	66/67 (98%)	58 (88%)	8 (12%)	5	20
48	A1	78/83 (94%)	66 (85%)	12 (15%)	2	12
48	B1	78/83 (94%)	69 (88%)	9 (12%)	5	22
49	A2	66/67 (98%)	61 (92%)	5 (8%)	13	39
49	B2	66/67 (98%)	54 (82%)	12 (18%)	1	7
50	A3	51/52 (98%)	47 (92%)	4 (8%)	12	38
50	B3	51/52 (98%)	47 (92%)	4 (8%)	12	38
51	A4	51/63 (81%)	36 (71%)	15 (29%)	0	1
51	B4	51/63 (81%)	36 (71%)	15 (29%)	0	1
52	A5	47/52 (90%)	42 (89%)	5 (11%)	6	25
52	B5	47/52 (90%)	42 (89%)	5 (11%)	6	25
53	A6	49/52 (94%)	41 (84%)	8 (16%)	2	10
53	B6	49/52 (94%)	40 (82%)	9 (18%)	1	7
54	A7	40/42 (95%)	36 (90%)	4 (10%)	7	27
54	B7	40/42 (95%)	36 (90%)	4 (10%)	7	27
55	A8	53/55 (96%)	40 (76%)	13 (24%)	0	2
55	B8	53/55 (96%)	38 (72%)	15 (28%)	0	1
56	A9	34/34 (100%)	32 (94%)	2 (6%)	19	49
56	B9	34/34 (100%)	32 (94%)	2 (6%)	19	49
All	All	9957/10598 (94%)	8789 (88%)	1168 (12%)	5	21

5 of 1168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	BP	45	LEU
53	B6	42	TRP
37	BQ	137	TYR
36	BP	42	SER
44	BX	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 314 such sidechains are listed below:

Mol	Chain	Res	Type
28	BE	143	ASN
44	BX	55	ASN
29	BF	169	ASN
36	BP	84	ASN
50	B3	46	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	Aa	1503/1504 (99%)	208 (13%)	0
22	Ba	1503/1504 (99%)	209 (13%)	0
23	Ax	11/25 (44%)	5 (45%)	0
23	Bx	11/25 (44%)	5 (45%)	0
24	Av	76/77 (98%)	18 (23%)	0
24	Bv	76/77 (98%)	14 (18%)	0
25	Aw	76/77 (98%)	9 (11%)	0
25	Bw	76/77 (98%)	10 (13%)	0
57	AA	2847/2848 (99%)	491 (17%)	61 (2%)
57	BA	2847/2848 (99%)	486 (17%)	64 (2%)
58	AB	118/119 (99%)	18 (15%)	1 (0%)
58	BB	118/119 (99%)	18 (15%)	1 (0%)
All	All	9262/9300 (99%)	1491 (16%)	127 (1%)

5 of 1491 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

5 of 127 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	AA	2481	G
57	BA	1992	G
57	BA	266	G
57	BA	1970	A
57	BA	2311	A



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

8 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
23	A2M	Bx	20	23	18,25,26	0.63	0	18,36,39	1.21	3 (16%)
23	A2M	Ax	20	23	18,25,26	0.63	0	18,36,39	1.10	1 (5%)
23	OMG	Ax	21	23	18,26,27	1.17	1 (5%)	20,38,41	2.71	5 (25%)
24	5MU	Bv	54	24	15,22,23	1.15	3 (20%)	16,32,35	3.74	1 (6%)
23	OMU	Ax	19	23	14,22,23	1.14	1 (7%)	14,31,34	1.26	1 (7%)
23	OMG	Bx	21	23	18,26,27	1.11	2 (11%)	20,38,41	2.67	6 (30%)
24	5MU	Av	54	24	15,22,23	1.19	2 (13%)	16,32,35	3.71	1 (6%)
23	OMU	Bx	19	23	14,22,23	1.23	2 (14%)	14,31,34	1.20	1 (7%)

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
23	A2M	Bx	20	23	-	0/5/27/28	0/3/3/3
23	A2M	Ax	20	23	-	1/5/27/28	0/3/3/3
23	OMG	Ax	21	23	-	2/5/27/28	0/3/3/3
24	5MU	Bv	54	24	-	0/5/25/26	0/2/2/2
23	OMU	Ax	19	23	-	2/7/27/28	0/2/2/2
23	OMG	Bx	21	23	-	0/5/27/28	0/3/3/3
24	5MU	Av	54	24	-	0/5/25/26	0/2/2/2
23	OMU	Bx	19	23	-	3/7/27/28	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Ax	21	OMG	C6-N1	3.88	1.39	1.33
23	Bx	21	OMG	C6-N1	3.66	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Av	54	5MU	C4-N3	3.46	1.39	1.33
23	Bx	19	OMU	C4-N3	3.27	1.38	1.33
23	Ax	19	OMU	C4-N3	3.08	1.38	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Bv	54	5MU	C4-N3-C2	14.65	127.51	115.14
24	Av	54	5MU	C4-N3-C2	14.47	127.36	115.14
23	Bx	21	OMG	C5-C6-N1	-8.71	111.52	123.43
23	Ax	21	OMG	C5-C6-N1	-8.67	111.57	123.43
23	Ax	21	OMG	C6-N1-C2	5.86	125.23	115.93

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Ax	19	OMU	C2'-C1'-N1-C6
23	Ax	19	OMU	O4'-C1'-N1-C6
23	Bx	19	OMU	C2'-C1'-N1-C6
23	Bx	19	OMU	O4'-C1'-N1-C6
23	Ax	21	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Ab	234/256 (91%)	0.43	21 (8%) 9 9	119, 151, 187, 193	0
1	Bb	234/256 (91%)	0.50	18 (7%) 13 12	117, 151, 186, 193	0
2	Ac	206/239 (86%)	0.60	17 (8%) 11 11	116, 147, 171, 173	0
2	Bc	206/239 (86%)	0.63	21 (10%) 6 6	115, 147, 171, 174	0
3	Ad	208/209 (99%)	0.16	3 (1%) 75 75	94, 123, 145, 154	0
3	Bd	208/209 (99%)	0.34	8 (3%) 40 37	94, 124, 146, 155	0
4	Ae	150/162 (92%)	0.21	4 (2%) 54 52	90, 114, 142, 160	0
4	Be	150/162 (92%)	0.33	7 (4%) 31 29	91, 114, 143, 161	0
5	Af	101/101 (100%)	0.16	4 (3%) 38 36	103, 127, 143, 167	0
5	Bf	101/101 (100%)	0.16	4 (3%) 38 36	100, 126, 143, 167	0
6	Ag	155/156 (99%)	0.57	19 (12%) 4 3	119, 141, 173, 189	0
6	Bg	155/156 (99%)	0.77	23 (14%) 2 2	120, 141, 173, 189	0
7	Ah	138/138 (100%)	0.17	2 (1%) 75 75	99, 118, 133, 143	0
7	Bh	138/138 (100%)	0.48	6 (4%) 35 34	100, 118, 133, 144	0
8	Ai	127/128 (99%)	1.23	30 (23%) 0 1	121, 162, 182, 190	0
8	Bi	127/128 (99%)	1.17	32 (25%) 0 0	121, 162, 182, 189	0
9	Aj	98/105 (93%)	1.58	33 (33%) 0 0	118, 165, 185, 187	0
9	Bj	98/105 (93%)	1.50	29 (29%) 0 0	116, 164, 184, 188	0
10	Ak	119/129 (92%)	0.42	10 (8%) 11 10	89, 121, 156, 176	0
10	Bk	119/129 (92%)	0.50	13 (10%) 5 5	91, 120, 155, 175	0
11	Al	124/132 (93%)	0.30	5 (4%) 38 36	81, 101, 133, 169	0
11	Bl	124/132 (93%)	0.43	9 (7%) 15 15	83, 102, 134, 169	0
12	Am	118/126 (93%)	0.56	14 (11%) 4 4	115, 147, 161, 169	0
12	Bm	118/126 (93%)	0.77	18 (15%) 2 2	115, 146, 161, 168	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9	
13	An	60/61 (98%)	0.93	8 (13%)	3	3	127, 140, 158, 161	0
13	Bn	60/61 (98%)	0.69	3 (5%)	28	27	125, 140, 157, 160	0
14	Ao	88/89 (98%)	0.28	3 (3%)	45	43	87, 114, 138, 146	0
14	Bo	88/89 (98%)	0.17	1 (1%)	80	81	88, 114, 138, 146	0
15	Ap	83/88 (94%)	0.51	4 (4%)	30	28	96, 114, 135, 162	0
15	Bp	83/88 (94%)	0.73	10 (12%)	4	3	97, 116, 136, 163	0
16	Aq	99/105 (94%)	0.24	2 (2%)	65	64	89, 112, 125, 133	0
16	Bq	99/105 (94%)	0.34	6 (6%)	21	20	92, 112, 125, 133	0
17	Ar	70/88 (79%)	0.69	6 (8%)	10	10	98, 125, 147, 153	0
17	Br	70/88 (79%)	0.54	5 (7%)	16	16	98, 123, 147, 153	0
18	As	78/93 (83%)	1.10	18 (23%)	0	1	135, 151, 180, 185	0
18	Bs	78/93 (83%)	1.15	17 (21%)	0	1	135, 151, 180, 185	0
19	At	99/106 (93%)	0.60	9 (9%)	9	9	105, 123, 157, 161	0
19	Bt	99/106 (93%)	0.50	3 (3%)	50	49	107, 124, 158, 162	0
20	Au	24/27 (88%)	3.00	15 (62%)	0	0	113, 141, 162, 175	0
20	Bu	24/27 (88%)	2.50	12 (50%)	0	0	113, 141, 162, 174	0
21	Ay	94/95 (98%)	0.80	15 (15%)	1	2	67, 133, 155, 159	0
21	By	94/95 (98%)	0.89	9 (9%)	8	8	112, 136, 154, 169	0
22	Aa	1504/1504 (100%)	0.07	28 (1%)	66	65	70, 123, 196, 208	0
22	Ba	1504/1504 (100%)	0.05	33 (2%)	62	60	70, 124, 196, 208	0
23	Ax	9/25 (36%)	1.25	3 (33%)	0	0	102, 161, 194, 201	0
23	Bx	9/25 (36%)	1.29	4 (44%)	0	0	100, 159, 202, 204	0
24	Av	76/77 (98%)	-0.33	1 (1%)	77	77	93, 120, 159, 176	0
24	Bv	76/77 (98%)	-0.27	1 (1%)	77	77	82, 113, 154, 168	0
25	Aw	77/77 (100%)	1.36	19 (24%)	0	0	135, 202, 204, 205	0
25	Bw	77/77 (100%)	1.54	17 (22%)	0	1	134, 203, 205, 207	0
26	AC	120/229 (52%)	3.11	82 (68%)	0	0	167, 186, 194, 195	0
26	BC	120/229 (52%)	3.73	89 (74%)	0	0	166, 186, 194, 195	0
27	AD	271/276 (98%)	0.08	3 (1%)	80	81	58, 81, 109, 137	0
27	BD	271/276 (98%)	0.02	3 (1%)	80	81	55, 79, 108, 137	0
28	AE	204/206 (99%)	0.21	7 (3%)	45	43	62, 88, 143, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
28	BE	204/206 (99%)	0.27	7 (3%)	45	43	59, 87, 143, 160	0
29	AF	207/210 (98%)	0.15	6 (2%)	51	50	61, 93, 150, 182	0
29	BF	207/210 (98%)	0.16	11 (5%)	26	24	55, 90, 150, 182	0
30	AG	181/182 (99%)	0.48	19 (10%)	6	6	113, 140, 165, 181	0
30	BG	181/182 (99%)	0.49	18 (9%)	7	7	102, 133, 164, 183	0
31	AH	164/180 (91%)	1.20	44 (26%)	0	0	103, 134, 154, 175	0
31	BH	164/180 (91%)	0.46	13 (7%)	12	12	96, 131, 151, 176	0
32	AI	145/148 (97%)	1.91	45 (31%)	0	0	91, 163, 180, 185	0
32	BI	145/148 (97%)	1.44	37 (25%)	0	0	90, 163, 181, 186	0
33	AJ	130/173 (75%)	4.47	99 (76%)	0	0	180, 195, 199, 201	0
33	BJ	130/173 (75%)	2.72	74 (56%)	0	0	167, 185, 194, 197	0
34	AN	138/140 (98%)	0.27	5 (3%)	42	40	76, 98, 133, 153	0
34	BN	138/140 (98%)	0.13	3 (2%)	62	60	73, 95, 132, 152	0
35	AO	122/122 (100%)	-0.07	0	100	100	65, 84, 106, 133	0
35	BO	122/122 (100%)	-0.04	0	100	100	64, 83, 106, 131	0
36	AP	146/150 (97%)	0.64	10 (6%)	17	17	63, 112, 139, 175	0
36	BP	146/150 (97%)	0.52	9 (6%)	20	20	62, 111, 139, 173	0
37	AQ	140/141 (99%)	0.10	2 (1%)	75	75	76, 99, 132, 153	0
37	BQ	140/141 (99%)	0.23	3 (2%)	63	62	74, 99, 131, 153	0
38	AR	117/118 (99%)	0.15	2 (1%)	70	68	70, 90, 119, 144	0
38	BR	117/118 (99%)	0.31	3 (2%)	56	53	67, 89, 119, 143	0
39	AS	98/112 (87%)	0.97	18 (18%)	1	1	115, 139, 161, 162	0
39	BS	98/112 (87%)	1.42	29 (29%)	0	0	112, 138, 161, 163	0
40	AT	135/146 (92%)	0.14	9 (6%)	17	17	78, 103, 154, 185	0
40	BT	135/146 (92%)	0.22	10 (7%)	14	14	78, 103, 154, 185	0
41	AU	117/118 (99%)	0.12	4 (3%)	45	43	67, 88, 124, 155	0
41	BU	117/118 (99%)	0.03	1 (0%)	84	84	63, 84, 123, 156	0
42	AV	101/101 (100%)	0.33	7 (6%)	16	16	62, 114, 136, 151	0
42	BV	101/101 (100%)	0.27	3 (2%)	50	49	59, 110, 135, 151	0
43	AW	113/113 (100%)	0.15	1 (0%)	84	84	67, 83, 110, 183	0
43	BW	113/113 (100%)	0.18	2 (1%)	68	67	65, 81, 108, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	AX	92/96 (95%)	0.13	2 (2%) 62 60	74, 93, 115, 124	0
44	BX	92/96 (95%)	0.12	0 100 100	66, 90, 113, 125	0
45	AY	100/110 (90%)	1.61	31 (31%) 0 0	85, 122, 162, 169	0
45	BY	100/110 (90%)	0.72	14 (14%) 2 2	84, 120, 162, 168	0
46	AZ	184/206 (89%)	0.38	14 (7%) 13 13	109, 138, 158, 192	0
46	BZ	184/206 (89%)	0.17	6 (3%) 46 44	96, 128, 152, 187	0
47	A0	84/85 (98%)	0.82	13 (15%) 2 2	87, 104, 152, 185	0
47	B0	84/85 (98%)	1.06	12 (14%) 2 2	86, 102, 153, 185	0
48	A1	93/98 (94%)	0.17	2 (2%) 62 60	68, 93, 132, 144	0
48	B1	93/98 (94%)	0.35	4 (4%) 35 34	60, 87, 133, 146	0
49	A2	71/72 (98%)	0.13	1 (1%) 75 75	89, 124, 144, 163	0
49	B2	71/72 (98%)	0.06	4 (5%) 24 23	60, 90, 134, 169	0
50	A3	59/60 (98%)	0.86	5 (8%) 10 10	79, 100, 124, 169	0
50	B3	59/60 (98%)	0.39	1 (1%) 70 68	75, 98, 121, 169	0
51	A4	57/71 (80%)	0.21	3 (5%) 26 24	153, 167, 183, 186	0
51	B4	57/71 (80%)	1.06	10 (17%) 1 1	154, 167, 182, 187	0
52	A5	55/60 (91%)	-0.04	3 (5%) 25 23	55, 91, 137, 144	0
52	B5	55/60 (91%)	-0.06	1 (1%) 68 67	54, 89, 137, 145	0
53	A6	50/54 (92%)	2.86	30 (60%) 0 0	128, 155, 169, 182	0
53	B6	50/54 (92%)	2.73	29 (58%) 0 0	128, 154, 169, 182	0
54	A7	47/49 (95%)	0.38	2 (4%) 35 34	58, 70, 95, 144	0
54	B7	47/49 (95%)	0.17	1 (2%) 63 62	53, 66, 91, 144	0
55	A8	63/65 (96%)	0.61	6 (9%) 8 8	70, 91, 118, 155	0
55	B8	63/65 (96%)	0.47	1 (1%) 72 70	70, 89, 117, 155	0
56	A9	37/37 (100%)	2.59	22 (59%) 0 0	109, 121, 141, 144	0
56	B9	37/37 (100%)	2.93	27 (72%) 0 0	105, 120, 141, 144	0
57	AA	2848/2848 (100%)	-0.05	79 (2%) 53 51	56, 90, 194, 209	0
57	BA	2848/2848 (100%)	0.09	79 (2%) 53 51	53, 87, 195, 208	0
58	AB	119/119 (100%)	-0.17	1 (0%) 86 86	96, 140, 176, 197	0
58	BB	119/119 (100%)	-0.03	0 100 100	94, 139, 175, 197	0
All	All	21494/22422 (95%)	0.38	1683 (7%) 13 12	53, 114, 186, 209	0

The worst 5 of 1683 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	AJ	63	LEU	17.7
33	AJ	85	ASP	17.5
26	BC	177	GLY	15.2
33	AJ	84	GLU	14.8
32	BI	88	ILE	14.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	OMG	Ax	21	24/25	0.78	0.33	174,180,182,184	0
23	A2M	Ax	20	23/24	0.85	0.28	160,168,169,173	0
23	OMU	Bx	19	21/22	0.86	0.29	129,157,162,162	0
23	OMU	Ax	19	21/22	0.89	0.23	133,158,162,164	0
23	OMG	Bx	21	24/25	0.89	0.27	177,182,184,186	0
23	A2M	Bx	20	23/24	0.91	0.22	161,170,172,175	0
24	5MU	Av	54	21/22	0.93	0.15	139,140,144,145	0
24	5MU	Bv	54	21/22	0.93	0.15	121,125,138,138	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	MG	AA	3239	1/1	0.17	1.07	113,113,113,113	0
60	MG	Aa	1665	1/1	0.20	0.72	88,88,88,88	0
60	MG	Ba	1712	1/1	0.29	0.59	96,96,96,96	0
60	MG	BA	2945	1/1	0.29	0.69	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	Ba	1647	1/1	0.33	0.91	148,148,148,148	0
60	MG	BA	3206	1/1	0.33	0.58	78,78,78,78	0
60	MG	BA	3258	1/1	0.34	0.99	110,110,110,110	0
60	MG	Ba	1645	1/1	0.37	1.25	89,89,89,89	0
60	MG	Aa	1674	1/1	0.37	0.27	108,108,108,108	0
60	MG	Aa	1706	1/1	0.40	0.50	91,91,91,91	0
60	MG	Ba	1698	1/1	0.40	0.62	123,123,123,123	1
60	MG	AA	2968	1/1	0.41	0.67	73,73,73,73	0
60	MG	AA	3261	1/1	0.41	0.71	110,110,110,110	0
60	MG	BA	2902	1/1	0.41	0.36	129,129,129,129	0
60	MG	AA	3134	1/1	0.42	0.40	98,98,98,98	0
60	MG	AA	3187	1/1	0.42	0.32	98,98,98,98	0
60	MG	Ba	1713	1/1	0.42	0.37	105,105,105,105	0
60	MG	Bw	101	1/1	0.42	0.31	140,140,140,140	1
60	MG	Aw	101	1/1	0.43	0.85	95,95,95,95	1
60	MG	Aa	1699	1/1	0.43	0.35	125,125,125,125	1
60	MG	Ba	1728	1/1	0.45	1.09	113,113,113,113	0
60	MG	BA	3191	1/1	0.45	0.70	116,116,116,116	0
60	MG	Aa	1689	1/1	0.47	0.20	57,57,57,57	1
60	MG	Aa	1727	1/1	0.47	0.61	90,90,90,90	1
60	MG	Am	201	1/1	0.48	0.86	88,88,88,88	0
60	MG	Ba	1664	1/1	0.48	0.55	88,88,88,88	0
60	MG	Aa	1641	1/1	0.49	0.84	87,87,87,87	0
60	MG	BA	3135	1/1	0.51	0.46	146,146,146,146	0
60	MG	AA	2954	1/1	0.51	0.26	103,103,103,103	0
60	MG	AA	3249	1/1	0.52	1.15	109,109,109,109	0
60	MG	AA	3165	1/1	0.52	0.48	83,83,83,83	0
60	MG	AA	3069	1/1	0.52	0.93	87,87,87,87	0
60	MG	Aa	1614	1/1	0.52	0.29	88,88,88,88	0
60	MG	BA	3265	1/1	0.52	0.83	104,104,104,104	0
60	MG	Ba	1737	1/1	0.54	0.34	101,101,101,101	0
60	MG	BA	3148	1/1	0.54	0.49	82,82,82,82	0
60	MG	AA	3146	1/1	0.54	1.05	87,87,87,87	0
60	MG	Ba	1643	1/1	0.56	0.86	95,95,95,95	0
60	MG	Ba	1699	1/1	0.56	1.55	113,113,113,113	0
60	MG	BA	3261	1/1	0.56	0.69	95,95,95,95	0
60	MG	A7	101	1/1	0.56	0.65	73,73,73,73	0
60	MG	Aa	1610	1/1	0.57	0.91	117,117,117,117	0
60	MG	Ba	1646	1/1	0.57	1.35	122,122,122,122	0
60	MG	AA	3262	1/1	0.57	0.57	94,94,94,94	0
60	MG	Bm	202	1/1	0.57	0.99	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	Aa	1616	1/1	0.57	0.72	123,123,123,123	0
60	MG	AA	3208	1/1	0.58	0.33	72,72,72,72	0
60	MG	Ba	1676	1/1	0.59	0.75	113,113,113,113	0
60	MG	Ba	1631	1/1	0.60	1.27	101,101,101,101	0
60	MG	AA	3253	1/1	0.60	1.36	87,87,87,87	0
60	MG	Ba	1660	1/1	0.60	0.54	127,127,127,127	0
60	MG	Aa	1658	1/1	0.60	0.52	105,105,105,105	0
60	MG	BA	3180	1/1	0.60	0.56	92,92,92,92	0
60	MG	BA	3182	1/1	0.61	0.48	140,140,140,140	0
60	MG	BA	3149	1/1	0.61	1.31	126,126,126,126	0
60	MG	AA	3144	1/1	0.61	0.39	85,85,85,85	0
60	MG	BA	2938	1/1	0.62	1.11	104,104,104,104	0
60	MG	AA	3211	1/1	0.62	0.14	97,97,97,97	0
60	MG	AA	3176	1/1	0.62	0.45	84,84,84,84	0
60	MG	AA	3149	1/1	0.62	1.36	109,109,109,109	0
60	MG	Ba	1601	1/1	0.62	0.22	77,77,77,77	0
60	MG	AA	3092	1/1	0.62	0.32	112,112,112,112	0
60	MG	AA	2959	1/1	0.63	0.31	77,77,77,77	0
60	MG	Aa	1715	1/1	0.63	0.22	84,84,84,84	0
60	MG	BA	3147	1/1	0.64	0.38	67,67,67,67	0
60	MG	Ba	1695	1/1	0.64	0.91	148,148,148,148	0
60	MG	Aa	1630	1/1	0.64	0.76	89,89,89,89	0
60	MG	AA	3002	1/1	0.64	0.71	84,84,84,84	0
60	MG	BA	2937	1/1	0.64	0.25	70,70,70,70	0
60	MG	AA	3225	1/1	0.64	0.58	71,71,71,71	0
60	MG	AA	3150	1/1	0.64	0.39	81,81,81,81	0
60	MG	BA	3071	1/1	0.64	1.32	113,113,113,113	0
60	MG	BA	3080	1/1	0.64	0.28	79,79,79,79	0
60	MG	AB	202	1/1	0.64	0.61	103,103,103,103	0
60	MG	BA	3154	1/1	0.65	0.54	164,164,164,164	0
60	MG	AQ	201	1/1	0.65	1.07	105,105,105,105	0
60	MG	BA	3074	1/1	0.65	0.65	97,97,97,97	0
60	MG	B0	101	1/1	0.65	0.66	104,104,104,104	0
60	MG	AA	3241	1/1	0.65	0.91	100,100,100,100	0
60	MG	AA	3247	1/1	0.65	0.31	92,92,92,92	0
60	MG	AA	3194	1/1	0.65	0.82	108,108,108,108	0
60	MG	AA	3207	1/1	0.65	0.71	122,122,122,122	0
60	MG	BA	3162	1/1	0.66	0.45	86,86,86,86	0
60	MG	AA	3103	1/1	0.66	0.54	103,103,103,103	0
60	MG	AA	3204	1/1	0.66	0.24	84,84,84,84	0
60	MG	Aa	1651	1/1	0.66	0.70	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3257	1/1	0.66	0.46	75,75,75,75	0
60	MG	Ba	1740	1/1	0.66	0.25	93,93,93,93	0
60	MG	BA	2965	1/1	0.66	0.61	74,74,74,74	0
60	MG	Aa	1601	1/1	0.66	0.34	93,93,93,93	0
60	MG	BA	3011	1/1	0.67	1.35	81,81,81,81	0
60	MG	Aa	1713	1/1	0.67	1.62	149,149,149,149	0
60	MG	Ba	1718	1/1	0.67	0.34	75,75,75,75	0
60	MG	BA	3237	1/1	0.67	1.20	98,98,98,98	0
60	MG	Ba	1688	1/1	0.67	0.24	90,90,90,90	1
60	MG	BA	3119	1/1	0.67	0.25	79,79,79,79	0
60	MG	Aa	1730	1/1	0.67	0.77	104,104,104,104	0
60	MG	Ba	1670	1/1	0.68	0.59	132,132,132,132	0
60	MG	Ba	1717	1/1	0.68	1.03	99,99,99,99	0
60	MG	Aa	1681	1/1	0.68	0.51	86,86,86,86	0
60	MG	AA	3237	1/1	0.68	0.81	88,88,88,88	0
60	MG	Aa	1700	1/1	0.68	0.48	84,84,84,84	1
60	MG	BA	3253	1/1	0.68	0.46	72,72,72,72	0
60	MG	Ba	1648	1/1	0.68	0.71	145,145,145,145	0
60	MG	AA	3112	1/1	0.68	1.15	114,114,114,114	0
60	MG	Aa	1633	1/1	0.68	0.46	71,71,71,71	0
60	MG	AA	2946	1/1	0.69	0.41	116,116,116,116	0
60	MG	Aa	1618	1/1	0.69	0.55	73,73,73,73	1
60	MG	AA	3264	1/1	0.69	0.77	101,101,101,101	0
60	MG	BA	3246	1/1	0.69	0.43	107,107,107,107	0
60	MG	BA	3088	1/1	0.69	0.52	113,113,113,113	0
60	MG	AA	3067	1/1	0.69	0.47	66,66,66,66	0
60	MG	BA	3126	1/1	0.69	0.77	154,154,154,154	0
60	MG	AA	2925	1/1	0.69	0.50	92,92,92,92	0
60	MG	AA	3157	1/1	0.70	0.11	123,123,123,123	0
60	MG	AA	3209	1/1	0.70	1.10	108,108,108,108	0
60	MG	AA	3267	1/1	0.70	0.37	89,89,89,89	0
60	MG	BA	3150	1/1	0.70	1.22	104,104,104,104	0
60	MG	AA	3260	1/1	0.71	0.72	104,104,104,104	0
60	MG	BA	3173	1/1	0.71	0.45	91,91,91,91	0
60	MG	AA	3114	1/1	0.71	0.34	84,84,84,84	0
60	MG	Ba	1734	1/1	0.71	0.12	138,138,138,138	0
60	MG	BA	2947	1/1	0.71	0.35	68,68,68,68	0
60	MG	BA	3136	1/1	0.71	1.06	109,109,109,109	0
60	MG	BA	3219	1/1	0.71	0.53	88,88,88,88	0
60	MG	BA	3138	1/1	0.71	0.24	61,61,61,61	0
60	MG	Ba	1612	1/1	0.71	0.38	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	Ba	1706	1/1	0.71	0.53	131,131,131,131	0
60	MG	Ba	1673	1/1	0.71	0.16	83,83,83,83	0
60	MG	Ba	1616	1/1	0.71	0.23	99,99,99,99	0
60	MG	Bm	201	1/1	0.71	0.18	103,103,103,103	0
60	MG	BA	3049	1/1	0.72	0.97	82,82,82,82	0
60	MG	AA	3016	1/1	0.72	1.19	82,82,82,82	0
60	MG	BA	3239	1/1	0.72	0.40	88,88,88,88	0
60	MG	AA	3224	1/1	0.72	0.53	86,86,86,86	0
60	MG	AA	3138	1/1	0.72	1.37	115,115,115,115	0
60	MG	Aa	1652	1/1	0.72	1.01	91,91,91,91	0
60	MG	BA	3259	1/1	0.72	0.34	99,99,99,99	0
59	ZN	B4	101	1/1	0.72	0.10	203,203,203,203	0
60	MG	AA	3086	1/1	0.72	0.29	94,94,94,94	0
60	MG	BA	3065	1/1	0.73	0.77	66,66,66,66	0
60	MG	AA	3143	1/1	0.73	0.98	72,72,72,72	0
60	MG	AA	2917	1/1	0.73	0.67	99,99,99,99	0
60	MG	BA	3146	1/1	0.73	0.36	112,112,112,112	0
60	MG	Aa	1637	1/1	0.73	1.21	99,99,99,99	0
60	MG	AA	3168	1/1	0.73	0.42	84,84,84,84	0
60	MG	AA	3040	1/1	0.73	0.49	82,82,82,82	0
60	MG	Ba	1602	1/1	0.73	0.39	73,73,73,73	0
60	MG	Aa	1611	1/1	0.74	1.01	82,82,82,82	0
60	MG	BA	3109	1/1	0.74	0.84	83,83,83,83	0
60	MG	AA	3219	1/1	0.74	0.66	94,94,94,94	0
60	MG	AA	3087	1/1	0.74	0.63	81,81,81,81	0
60	MG	AA	3053	1/1	0.74	0.32	79,79,79,79	0
60	MG	Aa	1723	1/1	0.74	0.78	98,98,98,98	0
60	MG	BA	3175	1/1	0.74	0.78	91,91,91,91	0
60	MG	AA	3106	1/1	0.74	0.41	75,75,75,75	0
60	MG	Aa	1714	1/1	0.74	0.54	111,111,111,111	0
60	MG	Ba	1610	1/1	0.74	0.62	87,87,87,87	0
60	MG	Ba	1716	1/1	0.75	0.67	102,102,102,102	0
60	MG	BA	3172	1/1	0.75	0.35	45,45,45,45	0
60	MG	AA	3236	1/1	0.75	1.19	90,90,90,90	0
60	MG	AX	101	1/1	0.75	1.11	96,96,96,96	1
60	MG	BA	2976	1/1	0.75	1.30	93,93,93,93	0
60	MG	BA	3255	1/1	0.75	0.64	74,74,74,74	0
60	MG	BA	3129	1/1	0.75	0.61	75,75,75,75	0
60	MG	BA	3075	1/1	0.75	0.33	56,56,56,56	0
60	MG	AA	2970	1/1	0.75	0.20	67,67,67,67	0
60	MG	BA	3209	1/1	0.75	0.22	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	3244	1/1	0.76	1.20	89,89,89,89	0
60	MG	BA	3204	1/1	0.76	0.57	92,92,92,92	0
60	MG	BA	2955	1/1	0.76	0.22	67,67,67,67	0
60	MG	AF	301	1/1	0.76	0.24	87,87,87,87	0
60	MG	Aa	1677	1/1	0.76	1.32	82,82,82,82	0
60	MG	BA	3229	1/1	0.76	0.60	101,101,101,101	0
60	MG	BA	2984	1/1	0.76	0.77	69,69,69,69	0
60	MG	BA	3264	1/1	0.76	0.31	68,68,68,68	0
60	MG	BA	3102	1/1	0.76	0.16	81,81,81,81	0
60	MG	Aa	1697	1/1	0.77	0.27	129,129,129,129	0
60	MG	AA	3248	1/1	0.77	0.47	141,141,141,141	0
60	MG	BA	2946	1/1	0.77	0.24	74,74,74,74	0
60	MG	Ba	1665	1/1	0.77	1.00	80,80,80,80	0
60	MG	AA	3266	1/1	0.77	0.44	73,73,73,73	0
60	MG	Ba	1621	1/1	0.77	0.33	84,84,84,84	0
60	MG	AA	2951	1/1	0.77	0.30	61,61,61,61	0
60	MG	Ba	1680	1/1	0.77	0.86	134,134,134,134	0
60	MG	BA	3231	1/1	0.77	0.48	105,105,105,105	0
60	MG	Ba	1682	1/1	0.77	0.69	113,113,113,113	0
60	MG	BA	3036	1/1	0.77	0.63	73,73,73,73	0
60	MG	Ba	1739	1/1	0.77	0.80	82,82,82,82	0
60	MG	AA	3136	1/1	0.77	0.31	88,88,88,88	0
60	MG	AA	3255	1/1	0.77	0.32	70,70,70,70	0
60	MG	BF	301	1/1	0.77	0.18	87,87,87,87	0
60	MG	BA	3157	1/1	0.77	0.76	78,78,78,78	0
60	MG	AA	2937	1/1	0.77	0.24	63,63,63,63	0
60	MG	AA	3171	1/1	0.77	0.26	68,68,68,68	0
60	MG	BA	3086	1/1	0.77	0.43	65,65,65,65	0
60	MG	AA	3242	1/1	0.77	0.46	78,78,78,78	0
60	MG	AA	3222	1/1	0.78	0.47	67,67,67,67	0
60	MG	AA	3102	1/1	0.78	0.82	92,92,92,92	0
60	MG	AA	2975	1/1	0.78	1.60	97,97,97,97	0
60	MG	BA	2958	1/1	0.78	1.17	100,100,100,100	0
60	MG	AA	3142	1/1	0.78	0.25	65,65,65,65	0
60	MG	Av	102	1/1	0.78	0.12	107,107,107,107	0
60	MG	AA	3206	1/1	0.78	0.60	75,75,75,75	0
60	MG	Ba	1640	1/1	0.78	1.20	105,105,105,105	0
60	MG	BB	203	1/1	0.78	0.70	79,79,79,79	0
60	MG	AA	3186	1/1	0.79	0.14	74,74,74,74	0
60	MG	AA	3156	1/1	0.79	0.38	83,83,83,83	0
60	MG	Ba	1613	1/1	0.79	0.35	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	2921	1/1	0.79	0.77	77,77,77,77	0
60	MG	BA	2998	1/1	0.79	0.60	59,59,59,59	0
60	MG	Aa	1623	1/1	0.79	1.12	107,107,107,107	0
60	MG	AA	3030	1/1	0.79	0.85	94,94,94,94	0
60	MG	Aa	1604	1/1	0.79	0.31	82,82,82,82	0
60	MG	Bq	201	1/1	0.79	0.36	116,116,116,116	0
60	MG	AA	3139	1/1	0.79	0.68	90,90,90,90	0
60	MG	AA	3084	1/1	0.79	0.41	84,84,84,84	0
60	MG	AA	3185	1/1	0.80	0.47	95,95,95,95	0
60	MG	BA	3222	1/1	0.80	0.34	109,109,109,109	0
60	MG	BA	3226	1/1	0.80	0.35	50,50,50,50	0
60	MG	AA	3268	1/1	0.80	0.71	102,102,102,102	0
60	MG	Bv	104	1/1	0.80	1.58	118,118,118,118	1
60	MG	BA	3235	1/1	0.80	0.52	90,90,90,90	0
60	MG	AB	201	1/1	0.80	0.38	69,69,69,69	0
60	MG	AA	3075	1/1	0.80	0.48	104,104,104,104	0
60	MG	AA	3050	1/1	0.80	0.52	87,87,87,87	0
60	MG	Aa	1735	1/1	0.80	0.33	80,80,80,80	1
60	MG	BA	3032	1/1	0.80	0.81	88,88,88,88	0
60	MG	Aa	1646	1/1	0.80	1.32	81,81,81,81	0
60	MG	Ba	1644	1/1	0.80	0.46	109,109,109,109	0
60	MG	AA	3015	1/1	0.80	1.00	103,103,103,103	0
60	MG	Ba	1732	1/1	0.80	0.65	135,135,135,135	0
60	MG	BA	3263	1/1	0.80	0.57	66,66,66,66	0
60	MG	AA	3152	1/1	0.80	1.01	113,113,113,113	0
60	MG	BA	3208	1/1	0.80	0.79	97,97,97,97	0
60	MG	AA	3230	1/1	0.80	1.16	94,94,94,94	0
60	MG	Ba	1657	1/1	0.81	0.69	109,109,109,109	0
60	MG	Ba	1617	1/1	0.81	0.56	69,69,69,69	1
60	MG	BA	2925	1/1	0.81	0.26	82,82,82,82	0
60	MG	BA	2932	1/1	0.81	0.53	87,87,87,87	0
60	MG	Ba	1661	1/1	0.81	0.88	98,98,98,98	0
60	MG	BA	3234	1/1	0.81	0.62	116,116,116,116	0
60	MG	AA	3212	1/1	0.81	0.42	79,79,79,79	0
60	MG	Ba	1625	1/1	0.81	1.38	113,113,113,113	0
60	MG	AA	2980	1/1	0.81	1.01	97,97,97,97	0
60	MG	Ba	1636	1/1	0.81	1.17	91,91,91,91	0
60	MG	BA	3245	1/1	0.81	0.31	80,80,80,80	0
60	MG	AA	2988	1/1	0.81	1.15	89,89,89,89	0
60	MG	AA	3179	1/1	0.81	0.50	76,76,76,76	0
60	MG	Aa	1671	1/1	0.81	0.40	113,113,113,113	0
60	MG	AA	3167	1/1	0.81	0.22	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	Aa	1736	1/1	0.81	0.14	126,126,126,126	0
60	MG	BA	3200	1/1	0.81	1.37	98,98,98,98	0
60	MG	BA	3130	1/1	0.81	0.55	63,63,63,63	0
60	MG	AA	3192	1/1	0.81	0.65	59,59,59,59	0
60	MG	AA	3238	1/1	0.81	0.70	74,74,74,74	0
60	MG	Ba	1655	1/1	0.81	0.39	66,66,66,66	0
60	MG	BA	2951	1/1	0.82	0.56	90,90,90,90	0
60	MG	Aa	1717	1/1	0.82	0.17	90,90,90,90	0
60	MG	Aa	1719	1/1	0.82	0.79	92,92,92,92	0
60	MG	BA	2961	1/1	0.82	0.36	60,60,60,60	0
60	MG	BA	3210	1/1	0.82	0.78	93,93,93,93	0
60	MG	Aa	1622	1/1	0.82	0.26	101,101,101,101	0
60	MG	BA	2973	1/1	0.82	0.57	61,61,61,61	0
60	MG	Ba	1637	1/1	0.82	0.53	103,103,103,103	0
60	MG	Ba	1605	1/1	0.82	0.61	99,99,99,99	0
60	MG	Ba	1707	1/1	0.82	0.47	100,100,100,100	0
60	MG	AA	3099	1/1	0.82	0.63	78,78,78,78	0
60	MG	Ba	1667	1/1	0.82	0.63	91,91,91,91	0
60	MG	BA	3236	1/1	0.82	0.29	64,64,64,64	0
60	MG	Ba	1715	1/1	0.82	0.17	121,121,121,121	0
60	MG	Ba	1668	1/1	0.82	0.65	80,80,80,80	0
60	MG	BA	3153	1/1	0.82	0.82	73,73,73,73	0
60	MG	BA	3053	1/1	0.82	1.04	70,70,70,70	0
60	MG	AA	3170	1/1	0.82	0.25	82,82,82,82	0
60	MG	BA	2935	1/1	0.82	0.75	124,124,124,124	0
60	MG	Aa	1725	1/1	0.82	0.81	88,88,88,88	0
60	MG	Ba	1720	1/1	0.82	0.98	123,123,123,123	0
60	MG	BA	2943	1/1	0.82	0.54	79,79,79,79	0
60	MG	BA	3082	1/1	0.82	0.22	71,71,71,71	0
60	MG	AB	203	1/1	0.82	0.57	71,71,71,71	0
60	MG	AA	2978	1/1	0.82	0.39	100,100,100,100	0
60	MG	Aa	1682	1/1	0.82	0.34	97,97,97,97	0
60	MG	BA	3202	1/1	0.82	0.31	65,65,65,65	0
60	MG	AA	3163	1/1	0.83	0.62	89,89,89,89	0
60	MG	BA	3228	1/1	0.83	0.87	82,82,82,82	0
60	MG	AA	2940	1/1	0.83	0.61	102,102,102,102	0
60	MG	BA	3167	1/1	0.83	0.48	74,74,74,74	0
60	MG	BA	3118	1/1	0.83	0.53	82,82,82,82	0
60	MG	AA	2964	1/1	0.83	0.55	76,76,76,76	0
60	MG	AA	3246	1/1	0.83	0.95	103,103,103,103	0
60	MG	BA	3179	1/1	0.83	0.52	90,90,90,90	0
60	MG	Ba	1702	1/1	0.83	0.57	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
60	MG	Ba	1704	1/1	0.83	1.21	108,108,108,108	0
60	MG	BA	3184	1/1	0.83	0.36	83,83,83,83	0
60	MG	Ba	1705	1/1	0.83	0.20	80,80,80,80	0
60	MG	BA	3248	1/1	0.83	0.22	64,64,64,64	0
60	MG	AA	3226	1/1	0.83	0.27	91,91,91,91	0
60	MG	Ba	1743	1/1	0.83	0.82	90,90,90,90	0
60	MG	Ba	1622	1/1	0.83	0.98	88,88,88,88	0
60	MG	Ba	1672	1/1	0.83	0.59	106,106,106,106	0
60	MG	AA	3151	1/1	0.83	0.28	88,88,88,88	0
60	MG	AA	3108	1/1	0.83	0.39	69,69,69,69	0
60	MG	AA	3137	1/1	0.83	0.71	95,95,95,95	0
60	MG	Aa	1695	1/1	0.83	0.55	97,97,97,97	0
60	MG	BA	2975	1/1	0.83	0.71	93,93,93,93	0
60	MG	Ba	1686	1/1	0.84	0.11	79,79,79,79	0
60	MG	BA	3207	1/1	0.84	0.26	90,90,90,90	0
60	MG	Aa	1707	1/1	0.84	0.64	79,79,79,79	0
60	MG	Ba	1690	1/1	0.84	0.46	67,67,67,67	0
60	MG	Ba	1692	1/1	0.84	0.63	99,99,99,99	0
60	MG	BA	3140	1/1	0.84	0.88	60,60,60,60	0
60	MG	BA	3143	1/1	0.84	2.37	90,90,90,90	0
60	MG	BA	3225	1/1	0.84	0.41	99,99,99,99	0
60	MG	AA	3223	1/1	0.84	0.81	75,75,75,75	0
60	MG	Aa	1626	1/1	0.84	0.77	85,85,85,85	0
60	MG	BX	101	1/1	0.84	0.65	59,59,59,59	1
60	MG	AA	2973	1/1	0.84	0.38	82,82,82,82	0
60	MG	AA	3188	1/1	0.84	0.24	91,91,91,91	0
60	MG	Aa	1656	1/1	0.84	0.12	67,67,67,67	0
60	MG	AA	3231	1/1	0.84	1.03	107,107,107,107	0
60	MG	BA	3069	1/1	0.84	0.40	72,72,72,72	0
60	MG	AA	3162	1/1	0.84	0.45	126,126,126,126	0
60	MG	Aa	1644	1/1	0.84	1.01	100,100,100,100	0
60	MG	AA	3141	1/1	0.84	0.18	54,54,54,54	0
60	MG	Aa	1701	1/1	0.84	1.09	96,96,96,96	0
60	MG	AA	3105	1/1	0.84	1.44	92,92,92,92	0
60	MG	Aa	1662	1/1	0.84	0.56	76,76,76,76	0
60	MG	AA	3245	1/1	0.84	0.55	71,71,71,71	0
60	MG	A7	102	1/1	0.84	0.47	98,98,98,98	0
60	MG	BA	3183	1/1	0.84	0.28	67,67,67,67	0
60	MG	Ba	1641	1/1	0.84	0.68	92,92,92,92	0
60	MG	Ba	1677	1/1	0.84	0.45	152,152,152,152	1
60	MG	AA	3081	1/1	0.84	0.28	89,89,89,89	0
60	MG	Aa	1741	1/1	0.84	1.01	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	Ba	1684	1/1	0.84	0.51	76,76,76,76	0
60	MG	AA	2971	1/1	0.85	0.17	77,77,77,77	0
60	MG	Ba	1650	1/1	0.85	0.81	82,82,82,82	0
60	MG	BA	3061	1/1	0.85	0.32	64,64,64,64	0
60	MG	BA	3233	1/1	0.85	0.60	109,109,109,109	0
60	MG	BA	3131	1/1	0.85	0.71	89,89,89,89	0
60	MG	AA	3227	1/1	0.85	0.47	110,110,110,110	0
60	MG	Ba	1656	1/1	0.85	1.15	80,80,80,80	0
60	MG	AA	2942	1/1	0.85	0.20	65,65,65,65	0
60	MG	B7	102	1/1	0.85	0.34	80,80,80,80	0
60	MG	Ba	1721	1/1	0.85	0.63	108,108,108,108	0
60	MG	Ba	1725	1/1	0.85	0.76	72,72,72,72	1
60	MG	BA	3081	1/1	0.85	0.36	106,106,106,106	0
60	MG	BA	3247	1/1	0.85	0.32	99,99,99,99	0
60	MG	Aa	1676	1/1	0.85	0.13	120,120,120,120	0
60	MG	AA	3091	1/1	0.85	0.61	104,104,104,104	0
60	MG	AA	2977	1/1	0.85	0.60	69,69,69,69	0
60	MG	BA	3096	1/1	0.85	0.16	49,49,49,49	0
60	MG	BA	3101	1/1	0.85	0.86	64,64,64,64	0
60	MG	BA	3217	1/1	0.85	0.67	76,76,76,76	0
60	MG	AA	2902	1/1	0.85	0.31	131,131,131,131	0
60	MG	Ba	1711	1/1	0.85	0.71	117,117,117,117	0
60	MG	Aa	1709	1/1	0.85	0.21	92,92,92,92	0
60	MG	AA	3254	1/1	0.85	0.34	84,84,84,84	0
60	MG	AA	2944	1/1	0.86	0.68	82,82,82,82	0
60	MG	BA	3121	1/1	0.86	1.26	82,82,82,82	0
60	MG	AA	2979	1/1	0.86	0.72	71,71,71,71	0
60	MG	BA	3177	1/1	0.86	0.67	66,66,66,66	0
60	MG	AA	2935	1/1	0.86	0.50	90,90,90,90	0
60	MG	AA	3183	1/1	0.86	0.37	79,79,79,79	0
60	MG	Ba	1741	1/1	0.86	0.52	81,81,81,81	0
60	MG	AA	2985	1/1	0.86	0.39	44,44,44,44	0
60	MG	AA	3101	1/1	0.86	0.28	92,92,92,92	0
60	MG	AA	2948	1/1	0.86	0.16	80,80,80,80	0
60	MG	Ba	1694	1/1	0.86	0.35	112,112,112,112	0
60	MG	AA	3140	1/1	0.86	0.53	107,107,107,107	0
60	MG	AA	3074	1/1	0.86	0.39	87,87,87,87	0
60	MG	Aa	1642	1/1	0.86	0.65	102,102,102,102	0
60	MG	Ba	1723	1/1	0.86	0.64	89,89,89,89	0
60	MG	AA	2919	1/1	0.86	0.31	49,49,49,49	0
60	MG	Aa	1743	1/1	0.86	0.63	80,80,80,80	0
60	MG	BA	2985	1/1	0.86	0.44	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	3260	1/1	0.86	0.24	93,93,93,93	0
60	MG	Ba	1731	1/1	0.86	0.25	103,103,103,103	0
60	MG	BA	3262	1/1	0.86	0.58	100,100,100,100	0
60	MG	BA	3006	1/1	0.86	0.56	107,107,107,107	0
60	MG	AA	2961	1/1	0.86	1.12	99,99,99,99	0
60	MG	BA	3164	1/1	0.86	0.46	78,78,78,78	0
60	MG	BA	3023	1/1	0.86	0.63	54,54,54,54	0
60	MG	BA	3211	1/1	0.87	0.43	81,81,81,81	0
60	MG	BA	3213	1/1	0.87	1.01	81,81,81,81	0
60	MG	AA	3059	1/1	0.87	0.27	90,90,90,90	0
60	MG	AA	3062	1/1	0.87	0.17	62,62,62,62	0
60	MG	Aa	1686	1/1	0.87	0.55	74,74,74,74	0
60	MG	BA	3151	1/1	0.87	1.49	105,105,105,105	0
60	MG	Ba	1652	1/1	0.87	0.80	80,80,80,80	0
60	MG	BA	2980	1/1	0.87	1.08	80,80,80,80	0
60	MG	BA	3097	1/1	0.87	0.18	65,65,65,65	0
60	MG	BA	3158	1/1	0.87	0.50	61,61,61,61	0
60	MG	BA	2901	1/1	0.87	0.42	122,122,122,122	0
60	MG	Aa	1648	1/1	0.87	0.44	118,118,118,118	0
60	MG	BA	2919	1/1	0.87	0.18	40,40,40,40	0
60	MG	BA	3111	1/1	0.87	0.53	99,99,99,99	0
60	MG	BA	3116	1/1	0.87	0.72	99,99,99,99	0
60	MG	Aa	1649	1/1	0.87	0.14	88,88,88,88	0
60	MG	BA	3240	1/1	0.87	0.28	73,73,73,73	0
60	MG	AA	2932	1/1	0.87	0.39	79,79,79,79	0
60	MG	AA	3078	1/1	0.87	0.87	94,94,94,94	0
60	MG	BA	3125	1/1	0.87	0.42	68,68,68,68	0
60	MG	AA	2952	1/1	0.87	0.27	81,81,81,81	0
60	MG	Ba	1633	1/1	0.87	0.77	71,71,71,71	0
60	MG	BA	3250	1/1	0.87	0.94	97,97,97,97	0
60	MG	AA	3120	1/1	0.87	0.59	90,90,90,90	0
60	MG	BA	3190	1/1	0.87	0.21	98,98,98,98	0
60	MG	AA	3028	1/1	0.87	0.26	53,53,53,53	0
60	MG	BA	3132	1/1	0.87	0.49	73,73,73,73	0
60	MG	Aa	1722	1/1	0.87	0.71	110,110,110,110	0
60	MG	Aa	1731	1/1	0.87	0.46	82,82,82,82	0
60	MG	Aa	1734	1/1	0.87	0.65	125,125,125,125	0
60	MG	AA	2903	1/1	0.87	0.22	98,98,98,98	0
60	MG	Ba	1675	1/1	0.87	0.08	69,69,69,69	0
60	MG	Ba	1606	1/1	0.87	0.52	101,101,101,101	0
60	MG	AA	3057	1/1	0.87	1.26	73,73,73,73	0
60	MG	Aa	1602	1/1	0.88	0.19	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3164	1/1	0.88	0.20	81,81,81,81	0
60	MG	Ba	1708	1/1	0.88	0.08	139,139,139,139	0
60	MG	AA	3083	1/1	0.88	0.45	74,74,74,74	0
60	MG	BA	3178	1/1	0.88	0.98	71,71,71,71	0
60	MG	AA	3135	1/1	0.88	0.49	89,89,89,89	0
60	MG	Ba	1628	1/1	0.88	0.32	79,79,79,79	0
60	MG	BA	2959	1/1	0.88	0.17	62,62,62,62	0
60	MG	AA	2938	1/1	0.88	1.08	95,95,95,95	0
60	MG	Ba	1687	1/1	0.88	0.19	69,69,69,69	1
60	MG	BA	3185	1/1	0.88	0.14	66,66,66,66	0
60	MG	BA	3189	1/1	0.88	0.89	62,62,62,62	0
60	MG	AA	3036	1/1	0.88	0.78	99,99,99,99	0
60	MG	Ba	1689	1/1	0.88	0.43	82,82,82,82	0
60	MG	Aa	1693	1/1	0.88	0.71	65,65,65,65	0
60	MG	AA	3175	1/1	0.88	0.63	54,54,54,54	0
60	MG	AA	3259	1/1	0.88	0.51	65,65,65,65	0
60	MG	BA	3251	1/1	0.88	1.00	78,78,78,78	0
60	MG	AA	3010	1/1	0.88	0.26	94,94,94,94	0
60	MG	BA	3099	1/1	0.88	0.88	97,97,97,97	0
60	MG	AA	3155	1/1	0.88	0.83	72,72,72,72	0
60	MG	Aa	1710	1/1	0.88	0.08	128,128,128,128	0
60	MG	BA	3103	1/1	0.88	0.28	63,63,63,63	0
60	MG	AA	2962	1/1	0.88	0.16	53,53,53,53	0
60	MG	AA	3221	1/1	0.88	0.26	59,59,59,59	0
60	MG	BA	3029	1/1	0.88	0.60	49,49,49,49	0
60	MG	BA	3117	1/1	0.88	0.82	106,106,106,106	0
60	MG	AA	3118	1/1	0.88	0.60	59,59,59,59	0
60	MG	Ba	1738	1/1	0.88	0.38	77,77,77,77	0
60	MG	Aa	1738	1/1	0.89	0.49	78,78,78,78	0
60	MG	BA	3221	1/1	0.89	0.65	66,66,66,66	0
60	MG	AA	3182	1/1	0.89	0.32	82,82,82,82	0
60	MG	AA	3076	1/1	0.89	0.56	92,92,92,92	0
60	MG	BA	2963	1/1	0.89	0.90	91,91,91,91	0
60	MG	AA	2930	1/1	0.89	0.18	38,38,38,38	0
60	MG	Aa	1690	1/1	0.89	0.23	96,96,96,96	1
60	MG	Bv	101	1/1	0.89	0.56	71,71,71,71	1
60	MG	BA	3232	1/1	0.89	0.35	82,82,82,82	0
60	MG	AA	3119	1/1	0.89	0.25	143,143,143,143	0
60	MG	AA	3033	1/1	0.89	0.77	68,68,68,68	0
60	MG	Ba	1710	1/1	0.89	0.44	81,81,81,81	0
60	MG	AA	3129	1/1	0.89	0.35	112,112,112,112	0
60	MG	Aa	1659	1/1	0.89	0.25	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	2956	1/1	0.89	0.77	111,111,111,111	0
60	MG	AA	2957	1/1	0.89	0.31	83,83,83,83	0
60	MG	BA	3243	1/1	0.89	0.75	75,75,75,75	0
60	MG	BA	3018	1/1	0.89	0.39	51,51,51,51	0
60	MG	Aa	1745	1/1	0.89	0.45	70,70,70,70	0
60	MG	Aa	1678	1/1	0.89	1.24	111,111,111,111	1
60	MG	Av	104	1/1	0.89	0.49	88,88,88,88	1
60	MG	AA	3001	1/1	0.89	0.42	68,68,68,68	0
60	MG	AA	3063	1/1	0.89	0.33	47,47,47,47	0
60	MG	AA	3252	1/1	0.89	0.64	85,85,85,85	0
60	MG	BA	3252	1/1	0.89	0.26	72,72,72,72	0
60	MG	AA	2909	1/1	0.89	0.38	46,46,46,46	0
60	MG	Ba	1654	1/1	0.89	1.19	97,97,97,97	0
60	MG	Ba	1730	1/1	0.89	0.40	64,64,64,64	0
60	MG	AA	3173	1/1	0.89	0.13	72,72,72,72	0
60	MG	Aa	1687	1/1	0.89	0.55	51,51,51,51	1
60	MG	Ba	1733	1/1	0.89	0.18	100,100,100,100	1
60	MG	BA	3079	1/1	0.89	0.36	79,79,79,79	0
60	MG	Aa	1663	1/1	0.89	0.23	68,68,68,68	0
60	MG	BA	2952	1/1	0.89	0.23	87,87,87,87	0
60	MG	AA	3178	1/1	0.89	1.09	86,86,86,86	0
60	MG	BA	3083	1/1	0.89	0.57	73,73,73,73	0
60	MG	BA	2970	1/1	0.90	1.14	104,104,104,104	0
60	MG	AA	3115	1/1	0.90	0.59	108,108,108,108	0
60	MG	BA	3087	1/1	0.90	0.49	74,74,74,74	0
60	MG	AA	2939	1/1	0.90	0.16	53,53,53,53	0
60	MG	BA	3155	1/1	0.90	0.23	77,77,77,77	1
60	MG	BA	3093	1/1	0.90	0.18	71,71,71,71	0
60	MG	Aa	1653	1/1	0.90	0.94	71,71,71,71	0
60	MG	AA	3235	1/1	0.90	0.21	102,102,102,102	0
60	MG	BA	2981	1/1	0.90	0.51	45,45,45,45	0
60	MG	AA	3205	1/1	0.90	0.52	58,58,58,58	0
60	MG	BA	3170	1/1	0.90	0.17	58,58,58,58	0
60	MG	Ba	1618	1/1	0.90	0.36	56,56,56,56	0
60	MG	AA	2972	1/1	0.90	0.37	75,75,75,75	0
60	MG	BA	3000	1/1	0.90	0.15	61,61,61,61	0
60	MG	AA	3147	1/1	0.90	0.84	66,66,66,66	0
60	MG	AA	3121	1/1	0.90	0.45	83,83,83,83	0
60	MG	AA	3100	1/1	0.90	0.29	64,64,64,64	0
60	MG	BA	3241	1/1	0.90	0.55	106,106,106,106	0
60	MG	Ba	1662	1/1	0.90	0.20	68,68,68,68	0
60	MG	AA	3210	1/1	0.90	1.01	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	Ba	1632	1/1	0.90	0.21	81,81,81,81	0
60	MG	BA	3034	1/1	0.90	0.58	78,78,78,78	0
60	MG	Aa	1679	1/1	0.90	0.24	131,131,131,131	0
60	MG	BA	3186	1/1	0.90	0.18	70,70,70,70	0
60	MG	AA	3004	1/1	0.90	0.07	84,84,84,84	0
60	MG	AA	3153	1/1	0.90	0.70	92,92,92,92	0
60	MG	BA	2949	1/1	0.90	0.21	63,63,63,63	0
60	MG	BA	3197	1/1	0.90	0.23	58,58,58,58	0
60	MG	Aa	1655	1/1	0.90	1.01	88,88,88,88	0
60	MG	Aa	1603	1/1	0.90	0.24	112,112,112,112	1
60	MG	Aa	1705	1/1	0.90	1.08	50,50,50,50	1
60	MG	BA	3072	1/1	0.90	0.69	75,75,75,75	0
60	MG	AA	3085	1/1	0.90	0.25	86,86,86,86	0
60	MG	Bv	102	1/1	0.90	0.25	54,54,54,54	0
60	MG	Aa	1615	1/1	0.90	0.65	58,58,58,58	0
60	MG	Aa	1729	1/1	0.90	0.43	60,60,60,60	0
60	MG	BA	2964	1/1	0.90	1.34	84,84,84,84	0
60	MG	Ba	1681	1/1	0.90	0.14	71,71,71,71	0
60	MG	AA	3090	1/1	0.91	0.49	86,86,86,86	0
60	MG	BA	3142	1/1	0.91	0.70	61,61,61,61	0
60	MG	BA	2944	1/1	0.91	0.14	86,86,86,86	0
60	MG	AA	3122	1/1	0.91	0.13	101,101,101,101	0
60	MG	Ba	1615	1/1	0.91	0.81	86,86,86,86	0
60	MG	Ba	1693	1/1	0.91	0.18	108,108,108,108	0
60	MG	BA	2948	1/1	0.91	0.58	93,93,93,93	0
60	MG	AA	3154	1/1	0.91	0.68	86,86,86,86	0
60	MG	BA	3223	1/1	0.91	0.26	74,74,74,74	0
60	MG	Ba	1736	1/1	0.91	0.37	88,88,88,88	0
60	MG	BA	3152	1/1	0.91	1.00	92,92,92,92	0
60	MG	Aa	1702	1/1	0.91	0.54	65,65,65,65	0
59	ZN	A4	101	1/1	0.91	0.06	195,195,195,195	0
60	MG	BA	2956	1/1	0.91	0.25	89,89,89,89	0
60	MG	Ba	1619	1/1	0.91	0.31	70,70,70,70	0
60	MG	Aa	1624	1/1	0.91	0.53	86,86,86,86	0
60	MG	BA	3161	1/1	0.91	0.20	51,51,51,51	0
60	MG	AA	3263	1/1	0.91	0.54	94,94,94,94	0
60	MG	AA	3005	1/1	0.91	0.35	64,64,64,64	0
60	MG	AD	301	1/1	0.91	0.29	38,38,38,38	0
60	MG	Aa	1645	1/1	0.91	0.39	83,83,83,83	0
60	MG	Aa	1683	1/1	0.91	0.08	59,59,59,59	0
60	MG	Aa	1640	1/1	0.91	0.52	82,82,82,82	0
60	MG	Ba	1634	1/1	0.91	0.16	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	A5	101	1/1	0.91	0.59	62,62,62,62	0
60	MG	Aa	1632	1/1	0.91	0.98	86,86,86,86	0
60	MG	B0	102	1/1	0.91	0.24	77,77,77,77	0
60	MG	Ba	1639	1/1	0.91	0.41	68,68,68,68	0
60	MG	Aa	1742	1/1	0.91	0.32	91,91,91,91	0
60	MG	Aa	1728	1/1	0.91	0.38	81,81,81,81	0
60	MG	BA	2909	1/1	0.91	0.27	36,36,36,36	0
60	MG	BA	2917	1/1	0.91	0.50	75,75,75,75	0
60	MG	AA	3048	1/1	0.91	0.37	69,69,69,69	0
60	MG	AA	3217	1/1	0.91	0.56	70,70,70,70	0
60	MG	AA	3116	1/1	0.91	0.62	39,39,39,39	1
60	MG	Ba	1722	1/1	0.91	0.18	106,106,106,106	0
60	MG	AA	3049	1/1	0.91	0.52	64,64,64,64	0
60	MG	Aa	1664	1/1	0.91	0.70	114,114,114,114	0
60	MG	AA	2989	1/1	0.91	0.30	50,50,50,50	0
60	MG	BA	3133	1/1	0.91	0.28	83,83,83,83	0
60	MG	BA	2941	1/1	0.91	0.40	98,98,98,98	0
60	MG	BA	2942	1/1	0.91	0.20	78,78,78,78	0
60	MG	BB	202	1/1	0.91	0.36	55,55,55,55	0
60	MG	BA	3056	1/1	0.91	0.22	53,53,53,53	0
60	MG	AA	3124	1/1	0.92	0.66	63,63,63,63	0
60	MG	BA	3091	1/1	0.92	0.39	66,66,66,66	0
60	MG	BA	2957	1/1	0.92	0.45	38,38,38,38	0
60	MG	BA	3188	1/1	0.92	0.85	90,90,90,90	0
60	MG	BA	3095	1/1	0.92	0.44	61,61,61,61	0
60	MG	AA	2974	1/1	0.92	1.26	85,85,85,85	0
60	MG	AA	3166	1/1	0.92	0.49	94,94,94,94	0
60	MG	Ba	1638	1/1	0.92	0.52	79,79,79,79	0
60	MG	BA	2962	1/1	0.92	0.32	71,71,71,71	0
60	MG	AA	3133	1/1	0.92	0.97	78,78,78,78	0
60	MG	Ba	1742	1/1	0.92	0.41	105,105,105,105	0
60	MG	BA	3205	1/1	0.92	0.39	113,113,113,113	0
60	MG	AA	3029	1/1	0.92	0.40	74,74,74,74	0
60	MG	BA	2967	1/1	0.92	0.14	58,58,58,58	0
60	MG	Aa	1657	1/1	0.92	1.05	93,93,93,93	0
60	MG	BA	2971	1/1	0.92	0.78	63,63,63,63	0
60	MG	AA	2920	1/1	0.92	0.34	45,45,45,45	0
60	MG	AD	302	1/1	0.92	0.49	64,64,64,64	0
60	MG	Aa	1654	1/1	0.92	0.21	93,93,93,93	0
60	MG	BA	3215	1/1	0.92	0.48	61,61,61,61	0
60	MG	Aa	1606	1/1	0.92	1.07	105,105,105,105	0
60	MG	Aa	1692	1/1	0.92	0.30	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3233	1/1	0.92	0.19	90,90,90,90	0
60	MG	Aa	1667	1/1	0.92	0.54	100,100,100,100	0
60	MG	B7	101	1/1	0.92	0.37	57,57,57,57	0
60	MG	Aa	1694	1/1	0.92	0.70	107,107,107,107	0
60	MG	BA	3004	1/1	0.92	0.29	45,45,45,45	0
60	MG	AA	2998	1/1	0.92	0.67	51,51,51,51	0
60	MG	Aa	1660	1/1	0.92	0.47	88,88,88,88	0
60	MG	AA	3061	1/1	0.92	0.73	89,89,89,89	0
60	MG	Aa	1696	1/1	0.92	0.15	93,93,93,93	0
60	MG	BA	3026	1/1	0.92	0.55	59,59,59,59	0
60	MG	AA	3148	1/1	0.92	0.73	72,72,72,72	0
60	MG	BA	3144	1/1	0.92	0.67	59,59,59,59	0
60	MG	Aa	1711	1/1	0.92	0.30	61,61,61,61	0
60	MG	Aa	1661	1/1	0.92	0.29	91,91,91,91	0
60	MG	AA	3007	1/1	0.92	0.21	83,83,83,83	0
60	MG	BA	3046	1/1	0.92	0.55	76,76,76,76	0
60	MG	BA	3048	1/1	0.92	0.58	95,95,95,95	0
60	MG	AA	3073	1/1	0.92	0.52	84,84,84,84	0
60	MG	AA	2945	1/1	0.92	0.11	73,73,73,73	0
60	MG	AA	3250	1/1	0.92	0.23	65,65,65,65	0
60	MG	BA	2940	1/1	0.92	0.28	76,76,76,76	0
60	MG	BA	3063	1/1	0.92	0.30	59,59,59,59	0
60	MG	Ba	1620	1/1	0.92	0.13	102,102,102,102	0
60	MG	BA	3066	1/1	0.92	0.24	28,28,28,28	0
60	MG	BA	3067	1/1	0.92	0.41	78,78,78,78	0
60	MG	AA	3013	1/1	0.92	0.85	49,49,49,49	0
60	MG	Aa	1617	1/1	0.92	0.31	66,66,66,66	0
60	MG	Ba	1674	1/1	0.92	0.13	57,57,57,57	0
60	MG	BA	3073	1/1	0.92	0.44	54,54,54,54	0
60	MG	AA	2947	1/1	0.92	0.24	103,103,103,103	0
60	MG	Ba	1729	1/1	0.92	0.31	84,84,84,84	0
60	MG	Ba	1626	1/1	0.92	0.30	92,92,92,92	0
60	MG	Ba	1627	1/1	0.92	0.38	71,71,71,71	0
60	MG	AA	3079	1/1	0.92	0.33	95,95,95,95	0
60	MG	AA	3017	1/1	0.92	0.22	59,59,59,59	0
60	MG	AA	3082	1/1	0.92	0.52	69,69,69,69	0
60	MG	BB	201	1/1	0.92	0.29	50,50,50,50	0
60	MG	BA	2953	1/1	0.92	0.43	100,100,100,100	0
60	MG	AA	3215	1/1	0.92	1.14	89,89,89,89	0
60	MG	BA	3199	1/1	0.93	0.29	89,89,89,89	1
60	MG	AA	3214	1/1	0.93	0.27	57,57,57,57	0
60	MG	AA	2967	1/1	0.93	1.80	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	2923	1/1	0.93	0.77	75,75,75,75	0
60	MG	Ba	1683	1/1	0.93	0.10	93,93,93,93	0
60	MG	Aq	201	1/1	0.93	0.31	91,91,91,91	0
60	MG	AA	2984	1/1	0.93	0.70	79,79,79,79	0
60	MG	BA	3047	1/1	0.93	0.31	57,57,57,57	0
60	MG	Ba	1611	1/1	0.93	0.25	81,81,81,81	0
60	MG	BA	3134	1/1	0.93	0.84	98,98,98,98	0
60	MG	AA	3107	1/1	0.93	0.16	58,58,58,58	0
60	MG	Aa	1638	1/1	0.93	0.31	84,84,84,84	0
60	MG	AA	3159	1/1	0.93	0.23	75,75,75,75	0
60	MG	AA	3054	1/1	0.93	0.43	43,43,43,43	0
60	MG	AA	3258	1/1	0.93	0.68	103,103,103,103	0
60	MG	Aa	1732	1/1	0.93	0.37	58,58,58,58	0
60	MG	AA	3193	1/1	0.93	0.16	85,85,85,85	0
60	MG	BA	3145	1/1	0.93	0.65	62,62,62,62	0
60	MG	Ba	1696	1/1	0.93	0.87	99,99,99,99	0
60	MG	Aa	1716	1/1	0.93	0.10	79,79,79,79	0
60	MG	AA	3200	1/1	0.93	0.39	82,82,82,82	0
60	MG	Ba	1658	1/1	0.93	0.34	84,84,84,84	0
60	MG	AA	3232	1/1	0.93	0.40	70,70,70,70	0
60	MG	Ba	1623	1/1	0.93	0.40	75,75,75,75	0
60	MG	Ba	1624	1/1	0.93	0.24	73,73,73,73	0
60	MG	BQ	201	1/1	0.93	1.22	79,79,79,79	0
60	MG	Ba	1663	1/1	0.93	0.21	86,86,86,86	0
60	MG	AA	2994	1/1	0.93	0.41	69,69,69,69	0
60	MG	Ba	1709	1/1	0.93	0.39	63,63,63,63	0
60	MG	BA	3238	1/1	0.93	0.33	89,89,89,89	0
60	MG	BA	2969	1/1	0.93	0.35	58,58,58,58	0
60	MG	B5	101	1/1	0.93	0.42	43,43,43,43	0
60	MG	AA	3265	1/1	0.93	0.82	83,83,83,83	0
60	MG	BA	3242	1/1	0.93	0.46	73,73,73,73	0
60	MG	AA	3027	1/1	0.93	0.51	57,57,57,57	0
60	MG	BA	3165	1/1	0.93	0.60	73,73,73,73	0
60	MG	BA	3166	1/1	0.93	0.62	54,54,54,54	0
60	MG	AA	2995	1/1	0.93	0.38	82,82,82,82	0
60	MG	AA	2997	1/1	0.93	0.69	44,44,44,44	0
60	MG	BA	2903	1/1	0.93	0.93	91,91,91,91	0
60	MG	Ba	1671	1/1	0.93	0.19	75,75,75,75	0
60	MG	Aa	1672	1/1	0.93	0.30	77,77,77,77	0
60	MG	BA	3098	1/1	0.93	0.56	77,77,77,77	0
60	MG	AA	3031	1/1	0.93	0.23	56,56,56,56	0
60	MG	BA	3100	1/1	0.93	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	3256	1/1	0.93	0.51	84,84,84,84	0
60	MG	Aa	1650	1/1	0.93	0.30	53,53,53,53	0
60	MG	BA	2923	1/1	0.93	0.41	60,60,60,60	0
60	MG	BA	3001	1/1	0.93	0.29	45,45,45,45	0
60	MG	Aa	1720	1/1	0.93	0.58	90,90,90,90	0
60	MG	BA	2929	1/1	0.93	0.23	43,43,43,43	0
60	MG	BA	3112	1/1	0.93	0.32	81,81,81,81	0
60	MG	BA	3113	1/1	0.93	1.18	55,55,55,55	1
60	MG	AA	3132	1/1	0.93	0.62	93,93,93,93	0
60	MG	AA	3213	1/1	0.93	0.83	98,98,98,98	0
60	MG	BA	3019	1/1	0.93	0.42	72,72,72,72	0
60	MG	Ba	1679	1/1	0.93	0.54	67,67,67,67	0
60	MG	Ba	1678	1/1	0.94	0.44	131,131,131,131	0
60	MG	Ba	1635	1/1	0.94	0.65	86,86,86,86	0
60	MG	BA	2939	1/1	0.94	0.15	44,44,44,44	0
60	MG	AA	3097	1/1	0.94	0.48	69,69,69,69	0
60	MG	BA	3038	1/1	0.94	0.37	52,52,52,52	0
60	MG	BA	3045	1/1	0.94	0.49	47,47,47,47	0
60	MG	AA	3234	1/1	0.94	0.14	59,59,59,59	0
60	MG	AA	3130	1/1	0.94	0.46	42,42,42,42	0
60	MG	Aa	1675	1/1	0.94	0.12	58,58,58,58	0
60	MG	Aa	1612	1/1	0.94	0.25	58,58,58,58	0
60	MG	AA	3160	1/1	0.94	0.74	65,65,65,65	0
60	MG	BA	3055	1/1	0.94	0.24	64,64,64,64	0
60	MG	AA	3035	1/1	0.94	0.47	74,74,74,74	0
60	MG	BA	3141	1/1	0.94	0.53	82,82,82,82	0
60	MG	AA	3240	1/1	0.94	0.69	104,104,104,104	0
60	MG	BA	3220	1/1	0.94	0.49	59,59,59,59	0
60	MG	Aa	1609	1/1	0.94	0.13	82,82,82,82	0
60	MG	Aa	1620	1/1	0.94	0.39	79,79,79,79	0
60	MG	AA	3244	1/1	0.94	0.80	98,98,98,98	0
60	MG	Ba	1609	1/1	0.94	0.42	104,104,104,104	0
60	MG	Av	101	1/1	0.94	0.51	65,65,65,65	1
60	MG	Aa	1698	1/1	0.94	0.67	86,86,86,86	0
60	MG	AA	2958	1/1	0.94	0.23	77,77,77,77	0
60	MG	Av	103	1/1	0.94	0.78	69,69,69,69	1
60	MG	Bv	103	1/1	0.94	0.24	110,110,110,110	0
60	MG	AA	3109	1/1	0.94	0.54	73,73,73,73	0
60	MG	Bv	105	1/1	0.94	0.26	95,95,95,95	1
60	MG	Aa	1605	1/1	0.94	0.18	70,70,70,70	0
60	MG	BD	302	1/1	0.94	0.33	53,53,53,53	0
60	MG	Ba	1703	1/1	0.94	0.77	69,69,69,69	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3113	1/1	0.94	0.49	55,55,55,55	0
60	MG	AA	2910	1/1	0.94	0.70	71,71,71,71	0
60	MG	AA	3058	1/1	0.94	0.70	54,54,54,54	0
60	MG	AA	2943	1/1	0.94	0.37	77,77,77,77	0
60	MG	BA	3090	1/1	0.94	0.32	47,47,47,47	0
60	MG	AA	3256	1/1	0.94	0.48	74,74,74,74	0
60	MG	BA	3092	1/1	0.94	0.44	83,83,83,83	0
60	MG	BA	3168	1/1	0.94	0.11	87,87,87,87	0
60	MG	Aa	1721	1/1	0.94	1.07	97,97,97,97	0
60	MG	AA	3180	1/1	0.94	0.46	58,58,58,58	0
60	MG	Ba	1666	1/1	0.94	1.17	84,84,84,84	0
60	MG	BA	3249	1/1	0.94	0.60	55,55,55,55	0
60	MG	AA	3181	1/1	0.94	0.30	65,65,65,65	0
60	MG	AA	3089	1/1	0.94	0.24	74,74,74,74	0
60	MG	Ba	1714	1/1	0.94	0.13	90,90,90,90	0
60	MG	BA	2914	1/1	0.94	0.35	32,32,32,32	0
60	MG	BA	3254	1/1	0.94	0.58	56,56,56,56	0
59	ZN	An	101	1/1	0.94	0.20	171,171,171,171	0
60	MG	BA	3181	1/1	0.94	0.37	51,51,51,51	0
60	MG	Aa	1712	1/1	0.94	0.43	86,86,86,86	0
60	MG	Aa	1635	1/1	0.94	0.09	61,61,61,61	0
60	MG	Ba	1629	1/1	0.94	0.29	69,69,69,69	0
60	MG	AA	3228	1/1	0.94	0.22	57,57,57,57	0
60	MG	AA	3095	1/1	0.94	0.28	67,67,67,67	0
60	MG	BA	3013	1/1	0.94	0.28	41,41,41,41	0
60	MG	BA	2930	1/1	0.94	0.11	34,34,34,34	0
60	MG	AA	3128	1/1	0.94	0.37	71,71,71,71	0
60	MG	BA	2934	1/1	0.94	0.52	65,65,65,65	1
60	MG	BA	3194	1/1	0.94	0.19	28,28,28,28	0
60	MG	AA	3190	1/1	0.94	0.39	52,52,52,52	0
60	MG	AA	3077	1/1	0.95	0.58	60,60,60,60	0
60	MG	AA	3243	1/1	0.95	1.47	117,117,117,117	0
60	MG	AA	2924	1/1	0.95	0.23	54,54,54,54	0
60	MG	AA	3009	1/1	0.95	0.25	61,61,61,61	0
60	MG	AA	2960	1/1	0.95	0.43	37,37,37,37	0
60	MG	BA	2966	1/1	0.95	0.59	39,39,39,39	0
60	MG	AA	3012	1/1	0.95	0.57	46,46,46,46	0
60	MG	Aa	1668	1/1	0.95	0.62	84,84,84,84	0
60	MG	AA	3191	1/1	0.95	0.59	102,102,102,102	0
60	MG	AA	2926	1/1	0.95	0.57	62,62,62,62	0
60	MG	AA	3251	1/1	0.95	0.61	68,68,68,68	0
60	MG	AA	2963	1/1	0.95	0.85	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	Ba	1691	1/1	0.95	0.59	61,61,61,61	0
60	MG	BA	3201	1/1	0.95	0.29	62,62,62,62	0
60	MG	BA	2978	1/1	0.95	0.51	72,72,72,72	0
60	MG	BA	3104	1/1	0.95	0.19	36,36,36,36	0
60	MG	BA	3107	1/1	0.95	0.36	58,58,58,58	0
60	MG	BA	2979	1/1	0.95	0.47	36,36,36,36	0
60	MG	AA	2928	1/1	0.95	0.29	89,89,89,89	0
60	MG	AA	3199	1/1	0.95	0.44	44,44,44,44	0
60	MG	AA	3022	1/1	0.95	0.36	43,43,43,43	0
60	MG	AA	3202	1/1	0.95	0.44	85,85,85,85	1
60	MG	BA	2986	1/1	0.95	0.45	42,42,42,42	0
60	MG	BA	2988	1/1	0.95	0.56	45,45,45,45	0
60	MG	BA	2995	1/1	0.95	0.52	45,45,45,45	0
60	MG	AA	3024	1/1	0.95	0.45	51,51,51,51	0
60	MG	AA	3145	1/1	0.95	0.64	68,68,68,68	0
60	MG	AA	2965	1/1	0.95	0.22	80,80,80,80	0
60	MG	Ba	1700	1/1	0.95	0.63	113,113,113,113	0
60	MG	Aa	1669	1/1	0.95	0.68	71,71,71,71	0
60	MG	BA	3009	1/1	0.95	0.65	38,38,38,38	0
60	MG	BA	3224	1/1	0.95	0.16	89,89,89,89	0
60	MG	AA	2931	1/1	0.95	0.51	63,63,63,63	0
60	MG	BA	3012	1/1	0.95	1.12	69,69,69,69	0
60	MG	BA	2911	1/1	0.95	0.27	36,36,36,36	0
60	MG	Aa	1703	1/1	0.95	0.32	70,70,70,70	0
60	MG	BA	3230	1/1	0.95	0.16	61,61,61,61	0
60	MG	AA	2933	1/1	0.95	0.82	84,84,84,84	0
60	MG	AA	3032	1/1	0.95	0.21	64,64,64,64	0
60	MG	AA	2934	1/1	0.95	0.34	53,53,53,53	1
60	MG	AA	3034	1/1	0.95	0.23	49,49,49,49	0
60	MG	BA	3031	1/1	0.95	0.53	46,46,46,46	0
60	MG	Ba	1649	1/1	0.95	0.21	52,52,52,52	0
60	MG	BA	2926	1/1	0.95	0.42	58,58,58,58	0
60	MG	Aa	1733	1/1	0.95	0.26	79,79,79,79	0
60	MG	BA	3037	1/1	0.95	0.29	41,41,41,41	0
60	MG	Ba	1651	1/1	0.95	0.47	51,51,51,51	0
60	MG	Aa	1704	1/1	0.95	0.55	86,86,86,86	0
60	MG	BA	2933	1/1	0.95	0.57	84,84,84,84	0
60	MG	AA	3038	1/1	0.95	0.82	95,95,95,95	0
60	MG	Aa	1680	1/1	0.95	0.33	115,115,115,115	0
60	MG	A1	101	1/1	0.95	0.33	70,70,70,70	0
60	MG	Aa	1613	1/1	0.95	0.40	85,85,85,85	0
60	MG	AA	3161	1/1	0.95	0.49	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	Aa	1643	1/1	0.95	0.17	117,117,117,117	0
60	MG	Aa	1739	1/1	0.95	0.86	100,100,100,100	0
60	MG	AA	2901	1/1	0.95	0.15	77,77,77,77	0
60	MG	Ba	1604	1/1	0.95	0.09	78,78,78,78	0
60	MG	AA	3055	1/1	0.95	0.70	59,59,59,59	0
60	MG	Aa	1708	1/1	0.95	0.36	89,89,89,89	0
60	MG	Aa	1627	1/1	0.95	0.23	84,84,84,84	0
60	MG	AA	2905	1/1	0.95	0.66	45,45,45,45	0
60	MG	AA	2992	1/1	0.95	0.63	61,61,61,61	0
60	MG	BA	3257	1/1	0.95	0.58	63,63,63,63	0
60	MG	Aa	1724	1/1	0.95	0.26	100,100,100,100	0
60	MG	BA	2950	1/1	0.95	0.30	69,69,69,69	0
60	MG	AA	2950	1/1	0.95	0.48	59,59,59,59	0
60	MG	Aa	1684	1/1	0.95	0.55	71,71,71,71	0
60	MG	AA	2911	1/1	0.95	0.30	39,39,39,39	0
60	MG	BA	3176	1/1	0.95	0.54	66,66,66,66	0
60	MG	AA	3072	1/1	0.95	0.26	79,79,79,79	0
60	MG	Aa	1726	1/1	0.95	0.34	57,57,57,57	0
60	MG	BA	3266	1/1	0.95	0.18	80,80,80,80	0
60	MG	Aa	1639	1/1	0.95	0.59	83,83,83,83	0
60	MG	Aa	1619	1/1	0.95	0.47	62,62,62,62	0
60	MG	Aa	1636	1/1	0.95	0.45	62,62,62,62	0
60	MG	AA	2941	1/1	0.96	0.48	68,68,68,68	0
60	MG	AA	2996	1/1	0.96	0.61	62,62,62,62	0
60	MG	AA	3220	1/1	0.96	0.50	47,47,47,47	0
60	MG	BA	3010	1/1	0.96	0.38	28,28,28,28	0
60	MG	BA	3195	1/1	0.96	0.51	57,57,57,57	0
60	MG	AA	2921	1/1	0.96	0.41	59,59,59,59	0
60	MG	AA	3172	1/1	0.96	0.46	58,58,58,58	0
60	MG	Aa	1688	1/1	0.96	0.51	72,72,72,72	0
60	MG	BA	3015	1/1	0.96	0.36	39,39,39,39	0
60	MG	BA	3016	1/1	0.96	0.30	50,50,50,50	0
60	MG	AA	3041	1/1	0.96	0.35	49,49,49,49	0
60	MG	AA	2999	1/1	0.96	0.46	61,61,61,61	0
60	MG	Aa	1647	1/1	0.96	1.12	105,105,105,105	0
60	MG	Ba	1642	1/1	0.96	0.38	83,83,83,83	0
60	MG	BA	3028	1/1	0.96	0.31	44,44,44,44	0
60	MG	Aa	1629	1/1	0.96	0.20	76,76,76,76	0
60	MG	AA	3093	1/1	0.96	0.32	73,73,73,73	0
60	MG	BA	3127	1/1	0.96	0.63	38,38,38,38	0
60	MG	AA	3229	1/1	0.96	0.34	87,87,87,87	0
60	MG	BA	3214	1/1	0.96	0.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3052	1/1	0.96	0.56	98,98,98,98	0
60	MG	Bx	101	1/1	0.96	0.42	92,92,92,92	0
60	MG	AA	3096	1/1	0.96	0.64	109,109,109,109	0
60	MG	Aa	1718	1/1	0.96	0.56	78,78,78,78	0
60	MG	BA	3044	1/1	0.96	0.48	52,52,52,52	0
60	MG	AA	3184	1/1	0.96	0.56	69,69,69,69	0
60	MG	Ba	1697	1/1	0.96	0.32	98,98,98,98	1
60	MG	AA	2927	1/1	0.96	0.47	50,50,50,50	0
60	MG	BA	3139	1/1	0.96	0.11	67,67,67,67	0
60	MG	Aa	1691	1/1	0.96	0.55	73,73,73,73	0
60	MG	BA	3227	1/1	0.96	0.23	73,73,73,73	0
60	MG	BD	301	1/1	0.96	0.44	39,39,39,39	0
60	MG	AA	3056	1/1	0.96	0.39	48,48,48,48	0
60	MG	AA	2929	1/1	0.96	0.40	68,68,68,68	0
60	MG	AA	3189	1/1	0.96	0.40	73,73,73,73	0
60	MG	BA	3058	1/1	0.96	0.20	60,60,60,60	0
60	MG	BA	3060	1/1	0.96	0.27	51,51,51,51	0
60	MG	AA	2906	1/1	0.96	0.40	38,38,38,38	0
60	MG	AA	2976	1/1	0.96	0.26	85,85,85,85	0
60	MG	BA	3064	1/1	0.96	0.50	44,44,44,44	0
60	MG	Aa	1621	1/1	0.96	0.17	91,91,91,91	0
60	MG	Aa	1666	1/1	0.96	0.80	66,66,66,66	0
60	MG	Aa	1744	1/1	0.96	0.39	114,114,114,114	0
60	MG	BA	3068	1/1	0.96	0.20	91,91,91,91	0
60	MG	AA	2912	1/1	0.96	0.22	56,56,56,56	0
60	MG	BA	2968	1/1	0.96	0.12	63,63,63,63	0
60	MG	AA	2981	1/1	0.96	0.07	54,54,54,54	0
60	MG	AA	3201	1/1	0.96	0.31	70,70,70,70	0
60	MG	BA	3160	1/1	0.96	0.32	73,73,73,73	0
60	MG	AA	3071	1/1	0.96	0.39	87,87,87,87	0
60	MG	BA	2905	1/1	0.96	0.55	31,31,31,31	0
60	MG	BA	3163	1/1	0.96	0.14	87,87,87,87	0
60	MG	BA	2974	1/1	0.96	0.20	118,118,118,118	0
60	MG	AA	3023	1/1	0.96	0.29	96,96,96,96	0
60	MG	BA	2910	1/1	0.96	0.47	70,70,70,70	0
60	MG	AA	2982	1/1	0.96	0.84	83,83,83,83	0
60	MG	AA	3025	1/1	0.96	0.46	39,39,39,39	0
60	MG	BA	3085	1/1	0.96	0.12	72,72,72,72	0
60	MG	AA	2914	1/1	0.96	0.30	37,37,37,37	0
60	MG	AA	2936	1/1	0.96	0.56	33,33,33,33	0
60	MG	AA	2986	1/1	0.96	0.33	86,86,86,86	0
60	MG	BA	3089	1/1	0.96	0.34	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	2916	1/1	0.96	0.43	35,35,35,35	0
60	MG	Aa	1685	1/1	0.96	0.08	85,85,85,85	0
60	MG	AA	2991	1/1	0.96	0.29	62,62,62,62	0
60	MG	BA	2990	1/1	0.96	0.56	56,56,56,56	0
60	MG	BA	3094	1/1	0.96	0.53	39,39,39,39	0
60	MG	AA	3126	1/1	0.96	0.70	49,49,49,49	0
60	MG	BA	2997	1/1	0.96	0.38	49,49,49,49	0
60	MG	Ba	1724	1/1	0.96	0.79	74,74,74,74	0
60	MG	BA	2999	1/1	0.96	0.49	41,41,41,41	0
60	MG	Aa	1673	1/1	0.96	0.17	91,91,91,91	0
60	MG	Aa	1634	1/1	0.96	0.66	56,56,56,56	0
60	MG	AA	3018	1/1	0.97	0.21	46,46,46,46	0
60	MG	BA	2936	1/1	0.97	0.48	40,40,40,40	0
60	MG	BA	3003	1/1	0.97	0.17	73,73,73,73	0
60	MG	AA	3196	1/1	0.97	0.40	59,59,59,59	0
60	MG	BA	3005	1/1	0.97	0.50	57,57,57,57	0
60	MG	AA	3197	1/1	0.97	0.19	34,34,34,34	0
60	MG	BA	3187	1/1	0.97	0.61	68,68,68,68	0
60	MG	BA	3007	1/1	0.97	0.41	56,56,56,56	0
60	MG	AA	3198	1/1	0.97	0.35	73,73,73,73	0
60	MG	AA	3019	1/1	0.97	0.32	48,48,48,48	0
60	MG	AA	3020	1/1	0.97	0.46	63,63,63,63	0
60	MG	BA	3192	1/1	0.97	0.39	43,43,43,43	0
60	MG	BA	3193	1/1	0.97	0.25	44,44,44,44	0
60	MG	Ba	1608	1/1	0.97	0.28	91,91,91,91	0
60	MG	AA	2913	1/1	0.97	0.47	44,44,44,44	0
60	MG	BA	3196	1/1	0.97	0.55	45,45,45,45	0
60	MG	BA	3014	1/1	0.97	0.30	38,38,38,38	0
60	MG	AA	2953	1/1	0.97	0.21	81,81,81,81	0
60	MG	BA	3105	1/1	0.97	0.22	55,55,55,55	0
60	MG	BA	3106	1/1	0.97	0.55	58,58,58,58	0
60	MG	AA	2966	1/1	0.97	0.63	74,74,74,74	0
60	MG	BA	3203	1/1	0.97	0.56	67,67,67,67	0
60	MG	BA	3108	1/1	0.97	0.15	71,71,71,71	0
60	MG	Ba	1653	1/1	0.97	0.13	91,91,91,91	0
60	MG	Aa	1670	1/1	0.97	0.38	70,70,70,70	0
60	MG	BA	3022	1/1	0.97	0.39	33,33,33,33	0
60	MG	AA	3131	1/1	0.97	0.36	75,75,75,75	0
60	MG	BA	3115	1/1	0.97	0.57	50,50,50,50	0
60	MG	AA	3026	1/1	0.97	0.50	43,43,43,43	0
60	MG	AA	2955	1/1	0.97	0.41	60,60,60,60	0
60	MG	BA	3212	1/1	0.97	0.21	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	2969	1/1	0.97	0.40	36,36,36,36	0
60	MG	Ba	1659	1/1	0.97	0.50	77,77,77,77	0
60	MG	BA	3120	1/1	0.97	0.46	39,39,39,39	0
60	MG	BA	3216	1/1	0.97	0.45	89,89,89,89	0
60	MG	AA	3169	1/1	0.97	0.72	78,78,78,78	0
60	MG	BA	3033	1/1	0.97	0.43	42,42,42,42	0
60	MG	AA	3003	1/1	0.97	0.54	43,43,43,43	0
60	MG	AA	2915	1/1	0.97	0.45	50,50,50,50	0
60	MG	AA	2907	1/1	0.97	0.38	58,58,58,58	0
60	MG	AA	3065	1/1	0.97	0.54	82,82,82,82	0
60	MG	BA	3040	1/1	0.97	0.46	41,41,41,41	0
60	MG	BA	3043	1/1	0.97	0.51	49,49,49,49	0
60	MG	AA	2987	1/1	0.97	0.57	41,41,41,41	0
60	MG	BA	2960	1/1	0.97	0.54	45,45,45,45	0
60	MG	AA	3068	1/1	0.97	0.51	50,50,50,50	0
60	MG	AA	3177	1/1	0.97	0.45	54,54,54,54	0
60	MG	AA	2908	1/1	0.97	0.28	53,53,53,53	0
60	MG	Ba	1669	1/1	0.97	0.41	55,55,55,55	0
60	MG	BA	3050	1/1	0.97	0.51	34,34,34,34	0
60	MG	BA	3051	1/1	0.97	0.59	38,38,38,38	0
60	MG	AA	3104	1/1	0.97	0.15	64,64,64,64	0
60	MG	Aa	1740	1/1	0.97	0.52	65,65,65,65	0
60	MG	AA	3011	1/1	0.97	0.52	55,55,55,55	0
60	MG	BA	3057	1/1	0.97	0.40	58,58,58,58	0
60	MG	Aa	1607	1/1	0.97	0.29	95,95,95,95	0
60	MG	AA	3037	1/1	0.97	0.45	52,52,52,52	0
60	MG	Ba	1719	1/1	0.97	0.86	85,85,85,85	0
60	MG	AA	2949	1/1	0.97	0.48	63,63,63,63	0
60	MG	BA	2972	1/1	0.97	0.48	79,79,79,79	0
60	MG	BA	2913	1/1	0.97	0.58	47,47,47,47	0
60	MG	AA	3111	1/1	0.97	0.26	91,91,91,91	0
60	MG	BA	2916	1/1	0.97	0.50	28,28,28,28	0
60	MG	AA	2993	1/1	0.97	0.51	57,57,57,57	0
60	MG	BA	2977	1/1	0.97	0.15	74,74,74,74	0
60	MG	BA	3156	1/1	0.97	0.29	64,64,64,64	0
60	MG	BA	3070	1/1	0.97	0.54	96,96,96,96	0
60	MG	Aa	1608	1/1	0.97	0.20	48,48,48,48	0
60	MG	BA	2920	1/1	0.97	0.19	31,31,31,31	0
60	MG	AA	3044	1/1	0.97	0.42	46,46,46,46	0
60	MG	AA	3045	1/1	0.97	0.23	55,55,55,55	0
60	MG	Ba	1726	1/1	0.97	0.54	65,65,65,65	0
60	MG	BA	3076	1/1	0.97	0.53	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	3078	1/1	0.97	0.60	61,61,61,61	0
60	MG	Ba	1727	1/1	0.97	0.49	44,44,44,44	0
60	MG	BA	2928	1/1	0.97	0.48	77,77,77,77	0
60	MG	AA	3080	1/1	0.97	0.57	120,120,120,120	0
60	MG	BA	2989	1/1	0.97	0.34	49,49,49,49	0
60	MG	AA	3046	1/1	0.97	0.87	59,59,59,59	0
60	MG	BA	3084	1/1	0.97	0.47	64,64,64,64	0
60	MG	BA	3174	1/1	0.97	0.59	63,63,63,63	0
60	MG	BA	2993	1/1	0.97	0.62	40,40,40,40	0
60	MG	BA	2994	1/1	0.97	0.57	44,44,44,44	0
60	MG	BA	2931	1/1	0.97	0.55	52,52,52,52	0
60	MG	AA	3047	1/1	0.97	0.44	62,62,62,62	0
59	ZN	A9	101	1/1	0.97	0.07	143,143,143,143	0
60	MG	Ba	1685	1/1	0.97	0.74	42,42,42,42	1
60	MG	AA	3039	1/1	0.98	0.41	50,50,50,50	0
60	MG	AA	2983	1/1	0.98	0.61	43,43,43,43	0
60	MG	BA	3035	1/1	0.98	0.36	43,43,43,43	0
60	MG	BA	2982	1/1	0.98	0.31	53,53,53,53	0
60	MG	BA	2983	1/1	0.98	0.53	37,37,37,37	0
60	MG	AA	3203	1/1	0.98	0.32	79,79,79,79	0
60	MG	AA	3110	1/1	0.98	0.19	59,59,59,59	0
60	MG	BA	3041	1/1	0.98	0.25	42,42,42,42	0
59	ZN	Bn	101	1/1	0.98	0.14	142,142,142,142	0
60	MG	BA	2987	1/1	0.98	0.22	43,43,43,43	0
60	MG	BA	3218	1/1	0.98	0.35	38,38,38,38	0
60	MG	BA	2907	1/1	0.98	0.44	51,51,51,51	0
60	MG	BA	2908	1/1	0.98	0.48	49,49,49,49	0
60	MG	BA	3159	1/1	0.98	0.18	110,110,110,110	0
60	MG	AA	3042	1/1	0.98	0.18	49,49,49,49	0
60	MG	BA	2991	1/1	0.98	0.33	48,48,48,48	0
60	MG	Ba	1735	1/1	0.98	0.15	79,79,79,79	0
60	MG	Ba	1614	1/1	0.98	0.82	60,60,60,60	0
60	MG	BA	2912	1/1	0.98	0.24	39,39,39,39	0
60	MG	AA	3158	1/1	0.98	0.13	104,104,104,104	1
60	MG	AA	3043	1/1	0.98	0.23	63,63,63,63	0
60	MG	BA	2915	1/1	0.98	0.37	32,32,32,32	0
60	MG	AA	3021	1/1	0.98	0.30	42,42,42,42	0
60	MG	BA	3169	1/1	0.98	0.58	58,58,58,58	0
60	MG	BA	3110	1/1	0.98	0.47	46,46,46,46	0
60	MG	BA	3171	1/1	0.98	0.29	38,38,38,38	0
60	MG	AA	2918	1/1	0.98	0.59	42,42,42,42	0
60	MG	BA	3002	1/1	0.98	0.23	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	2918	1/1	0.98	0.53	32,32,32,32	0
60	MG	BA	3114	1/1	0.98	0.43	36,36,36,36	0
60	MG	BA	3062	1/1	0.98	0.25	45,45,45,45	0
60	MG	AA	3060	1/1	0.98	0.38	55,55,55,55	0
60	MG	AA	3098	1/1	0.98	0.49	47,47,47,47	0
59	ZN	Bd	301	1/1	0.98	0.33	103,103,103,103	0
60	MG	AA	3014	1/1	0.98	0.53	51,51,51,51	0
60	MG	BA	3008	1/1	0.98	0.49	34,34,34,34	0
60	MG	BA	2924	1/1	0.98	0.32	43,43,43,43	0
60	MG	BA	3122	1/1	0.98	0.39	51,51,51,51	0
60	MG	BA	3124	1/1	0.98	0.45	45,45,45,45	0
60	MG	Aa	1737	1/1	0.98	0.32	107,107,107,107	0
60	MG	AA	3216	1/1	0.98	0.30	74,74,74,74	0
60	MG	BA	2927	1/1	0.98	0.64	45,45,45,45	0
60	MG	BA	3128	1/1	0.98	0.34	40,40,40,40	0
60	MG	AA	3064	1/1	0.98	0.32	59,59,59,59	0
60	MG	AA	3123	1/1	0.98	0.48	54,54,54,54	0
60	MG	Aa	1628	1/1	0.98	0.32	72,72,72,72	0
60	MG	AA	3125	1/1	0.98	0.44	49,49,49,49	0
60	MG	AA	3195	1/1	0.98	0.33	41,41,41,41	0
60	MG	BA	3077	1/1	0.98	0.36	69,69,69,69	0
60	MG	Ba	1630	1/1	0.98	0.11	53,53,53,53	0
60	MG	BA	3020	1/1	0.98	0.37	47,47,47,47	0
60	MG	BA	3137	1/1	0.98	0.13	94,94,94,94	0
60	MG	BA	3198	1/1	0.98	0.21	70,70,70,70	0
60	MG	AA	3066	1/1	0.98	0.24	55,55,55,55	0
60	MG	AA	3127	1/1	0.98	0.66	44,44,44,44	0
60	MG	BA	3025	1/1	0.98	0.33	69,69,69,69	0
60	MG	Ba	1603	1/1	0.98	0.17	73,73,73,73	1
60	MG	BA	3027	1/1	0.98	0.32	53,53,53,53	0
60	MG	AA	2922	1/1	0.98	0.26	52,52,52,52	0
60	MG	AA	3051	1/1	0.98	0.36	66,66,66,66	0
60	MG	AA	2990	1/1	0.98	0.43	51,51,51,51	0
60	MG	Ba	1607	1/1	0.98	0.12	67,67,67,67	0
60	MG	AA	3070	1/1	0.99	0.33	47,47,47,47	0
60	MG	AA	3006	1/1	0.99	0.28	39,39,39,39	0
60	MG	AA	3000	1/1	0.99	0.17	49,49,49,49	0
60	MG	AA	3174	1/1	0.99	0.42	50,50,50,50	0
60	MG	BA	3059	1/1	0.99	0.51	52,52,52,52	0
60	MG	BA	3030	1/1	0.99	0.27	37,37,37,37	0
60	MG	AA	3008	1/1	0.99	0.33	44,44,44,44	0
60	MG	Aa	1631	1/1	0.99	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	3123	1/1	0.99	0.56	37,37,37,37	0
60	MG	AA	3094	1/1	0.99	0.42	65,65,65,65	0
60	MG	AA	3117	1/1	0.99	0.32	43,43,43,43	0
60	MG	AA	3218	1/1	0.99	0.34	104,104,104,104	0
60	MG	Aa	1625	1/1	0.99	0.38	61,61,61,61	0
59	ZN	Ad	301	1/1	0.99	0.34	94,94,94,94	0
60	MG	BA	2992	1/1	0.99	0.47	40,40,40,40	0
60	MG	BA	3039	1/1	0.99	0.31	44,44,44,44	0
60	MG	BA	2954	1/1	0.99	0.33	37,37,37,37	0
60	MG	Ba	1701	1/1	0.99	0.32	71,71,71,71	0
60	MG	BA	3042	1/1	0.99	0.60	48,48,48,48	0
59	ZN	B9	101	1/1	0.99	0.06	124,124,124,124	0
60	MG	BA	3017	1/1	0.99	0.38	40,40,40,40	0
60	MG	BA	2996	1/1	0.99	0.24	35,35,35,35	0
60	MG	AA	2904	1/1	0.99	0.14	142,142,142,142	0
60	MG	BA	2904	1/1	0.99	0.12	138,138,138,138	0
60	MG	BA	3021	1/1	0.99	0.68	45,45,45,45	0
60	MG	BA	2922	1/1	0.99	0.20	45,45,45,45	0
60	MG	AA	3088	1/1	0.99	0.31	64,64,64,64	0
60	MG	BA	3024	1/1	0.99	0.28	46,46,46,46	0
60	MG	BA	3052	1/1	0.99	0.52	30,30,30,30	0
60	MG	BA	2906	1/1	0.99	0.41	35,35,35,35	0
60	MG	BA	3054	1/1	0.99	0.52	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.