



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 08:20 AM UTC

PDB ID : 4V7K / pdb_00004v7k
Title : Structure of RelE nuclease bound to the 70S ribosome (postcleavage state)
Authors : Neubauer, C.; Gao, Y.-G.; Andersen, K.R.; Dunham, C.M.; Kelley, A.C.;
Hentschel, J.; Gerdes, K.; Ramakrishnan, V.; Brodersen, D.E.
Deposited on : 2009-11-02
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

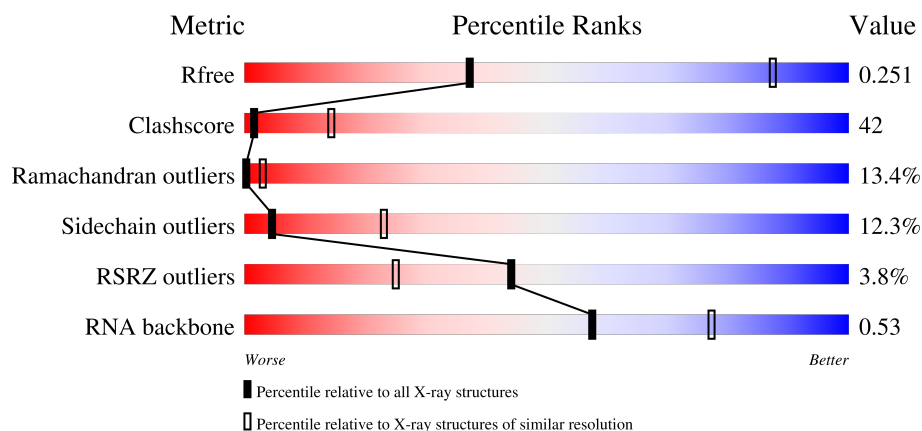
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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 ≥ 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	3% 12% 58% 20% 9%
1	Bb	256	3% 14% 56% 20% 9%
2	Ac	239	% 18% 53% 15% 14%
2	Bc	239	2% 19% 52% 15% 14%

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

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

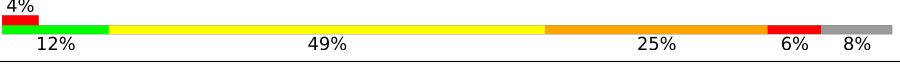
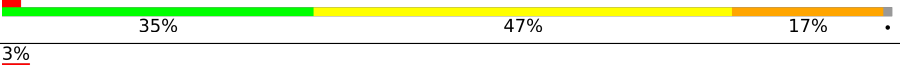
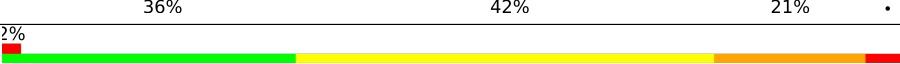
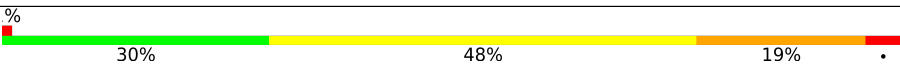
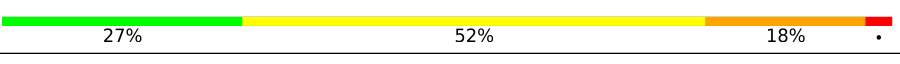
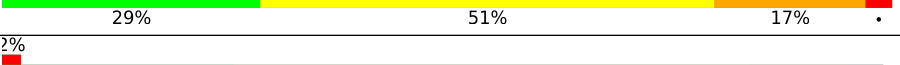
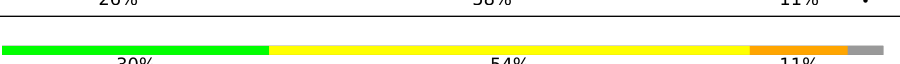
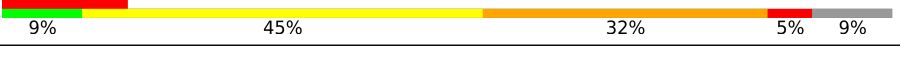
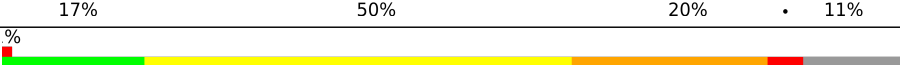
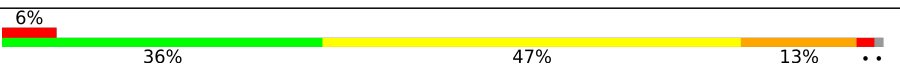
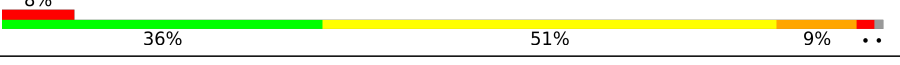
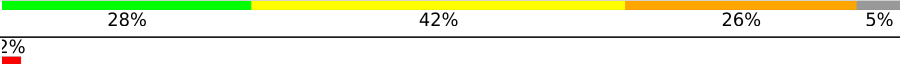
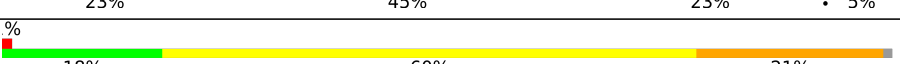
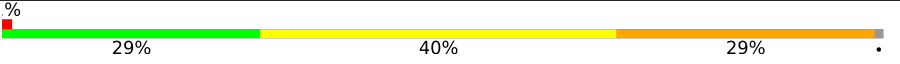
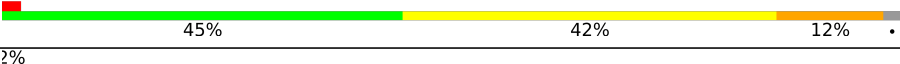
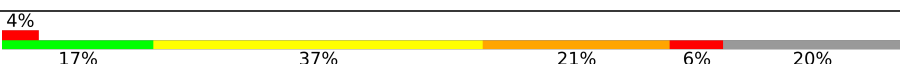
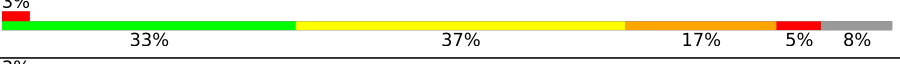
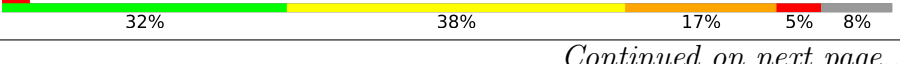
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Mol	Chain	Length	Quality of chain
28	AE	206	
28	BE	206	
29	AF	210	
29	BF	210	
30	AG	182	
30	BG	182	
31	AH	180	
31	BH	180	
32	AI	148	
32	BI	148	
33	AJ	173	
33	BJ	173	
34	AN	140	
34	BN	140	
35	AO	122	
35	BO	122	
36	AP	150	
36	BP	150	
37	AQ	141	
37	BQ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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	2928	-	-	-	X
60	MG	AA	3117	-	-	-	X
60	MG	AA	3214	-	-	-	X
60	MG	AA	3218	-	-	-	X
60	MG	AA	3248	-	-	-	X
60	MG	AQ	201	-	-	-	X
60	MG	Aa	1602	-	-	-	X
60	MG	Aa	1615	-	-	-	X
60	MG	Aa	1636	-	-	-	X
60	MG	Aa	1669	-	-	-	X
60	MG	Aa	1700	-	-	-	X
60	MG	Aa	1703	-	-	-	X
60	MG	Aa	1713	-	-	-	X
60	MG	Aa	1727	-	-	-	X
60	MG	Ae	201	-	-	-	X
60	MG	BA	2958	-	-	-	X
60	MG	BA	3099	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3160	-	-	-	X
60	MG	BA	3180	-	-	-	X
60	MG	BA	3198	-	-	-	X
60	MG	BA	3243	-	-	-	X
60	MG	BA	3254	-	-	-	X
60	MG	BA	3264	-	-	-	X
60	MG	Ba	1665	-	-	-	X
60	MG	Ba	1676	-	-	-	X
60	MG	Ba	1681	-	-	-	X
60	MG	Ba	1702	-	-	-	X
60	MG	Ba	1706	-	-	-	X

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is a protein called Toxin relE.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AJ	130	Total	C	N	O		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			
46	BZ	184	Total	C	N	O	S	0	0	0
			1467	936	261	268	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	Ae	2	Total	Mg	0	0
			2	2		
60	Aa	145	Total	Mg	0	0
			145	145		
60	Av	5	Total	Mg	0	0
			5	5		
60	Aw	1	Total	Mg	0	0
			1	1		
60	AD	2	Total	Mg	0	0
			2	2		
60	AF	1	Total	Mg	0	0
			1	1		
60	AQ	1	Total	Mg	0	0
			1	1		
60	AX	1	Total	Mg	0	0
			1	1		

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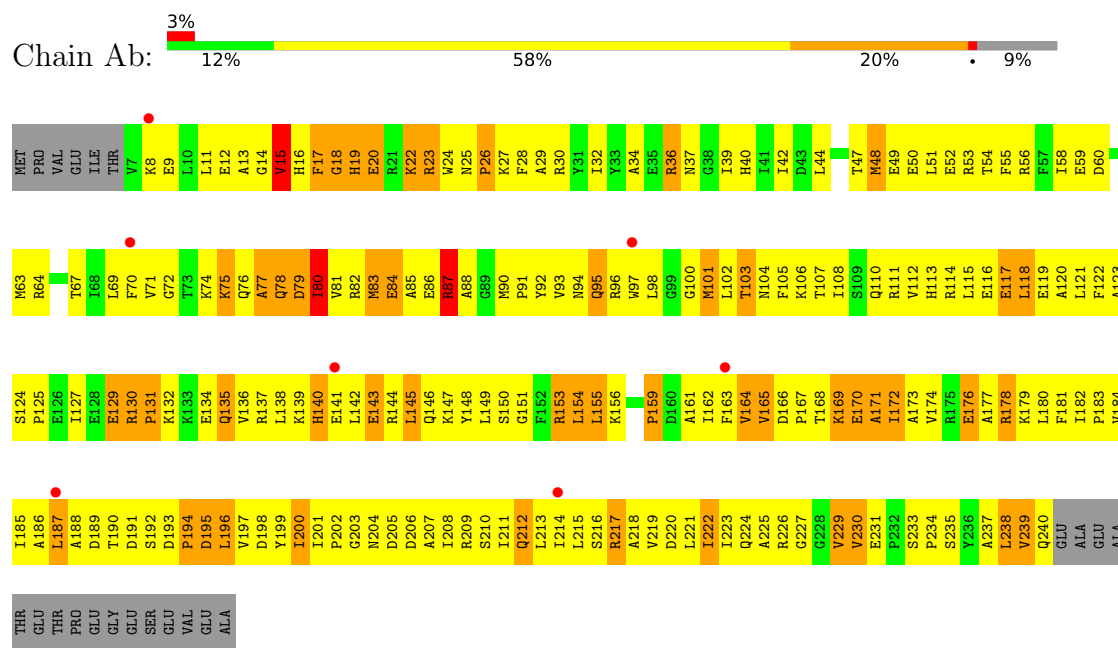
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	A1	2	Total 2	Mg 2	0	0
60	A5	1	Total 1	Mg 1	0	0
60	A7	1	Total 1	Mg 1	0	0
60	AA	367	Total 367	Mg 367	0	0
60	AB	3	Total 3	Mg 3	0	0
60	Bd	1	Total 1	Mg 1	0	0
60	Bl	1	Total 1	Mg 1	0	0
60	Bm	1	Total 1	Mg 1	0	0
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	BO	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0
60	B0	2	Total 2	Mg 2	0	0
60	B5	2	Total 2	Mg 2	0	0
60	B7	2	Total 2	Mg 2	0	0
60	BA	365	Total 365	Mg 365	0	0
60	BB	3	Total 3	Mg 3	0	0

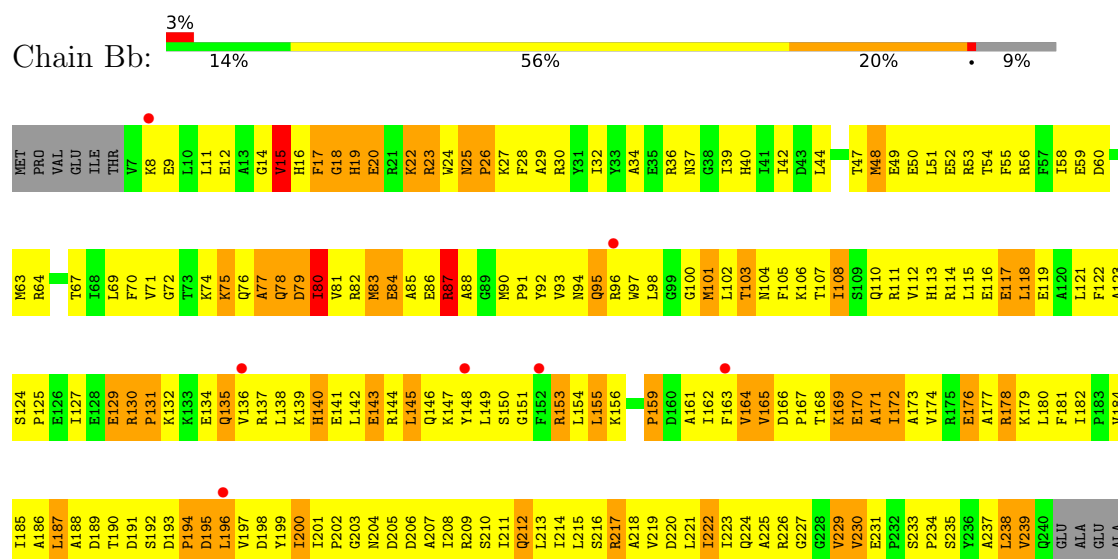
3 Residue-property plots [i](#)

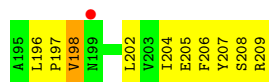
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

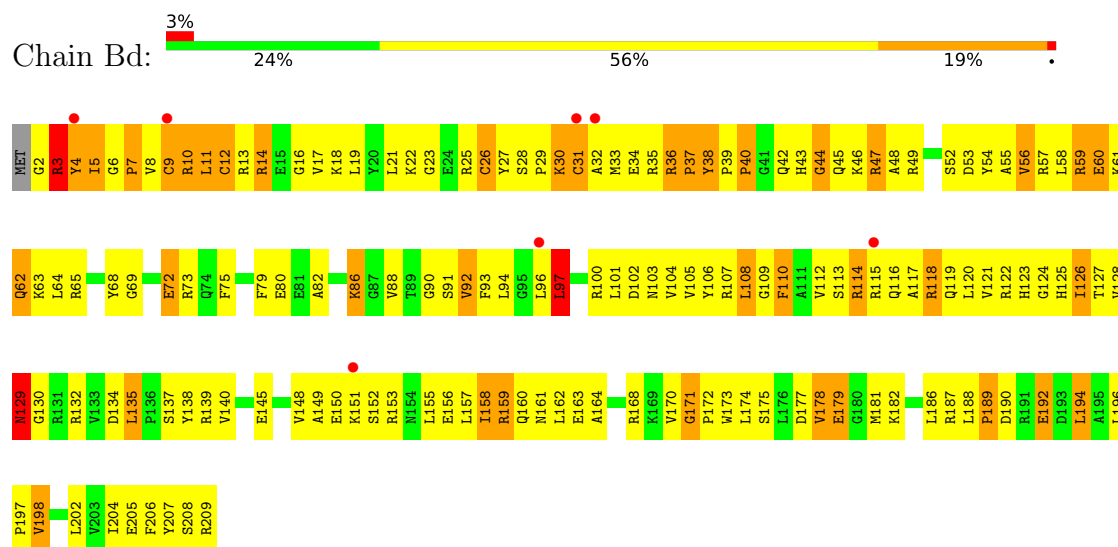


• Molecule 1: 30S ribosomal protein S2

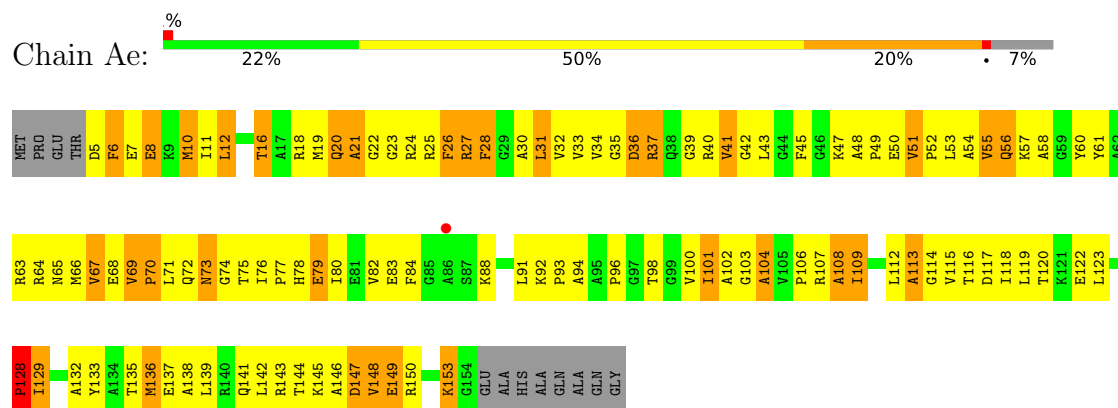




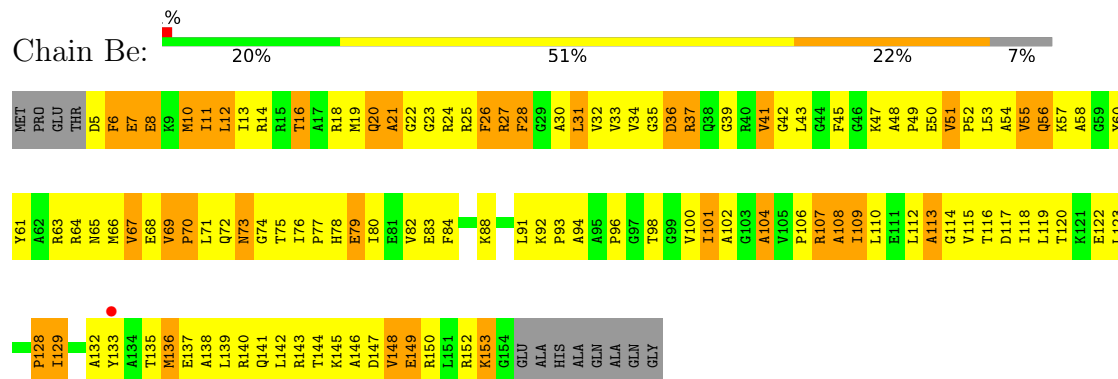
• Molecule 3: 30S ribosomal protein S4



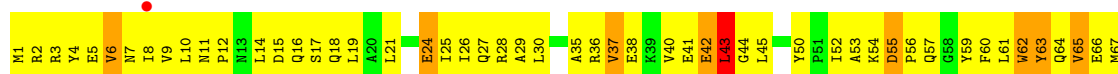
• Molecule 4: 30S ribosomal protein S5



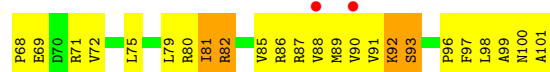
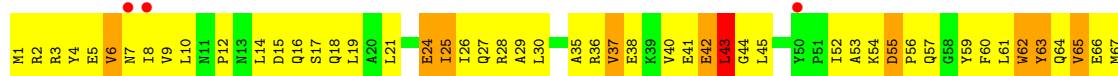
• Molecule 4: 30S ribosomal protein S5



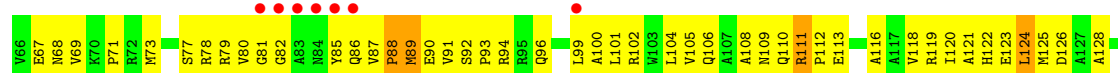
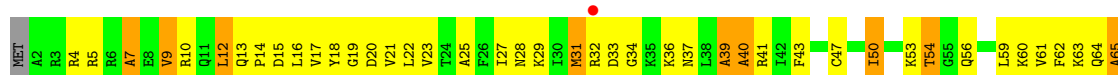
• Molecule 5: 30S ribosomal protein S6



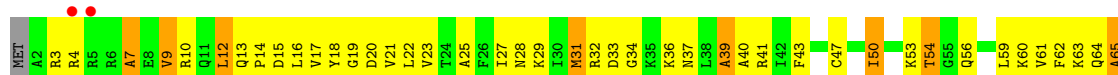
• Molecule 5: 30S ribosomal protein S6



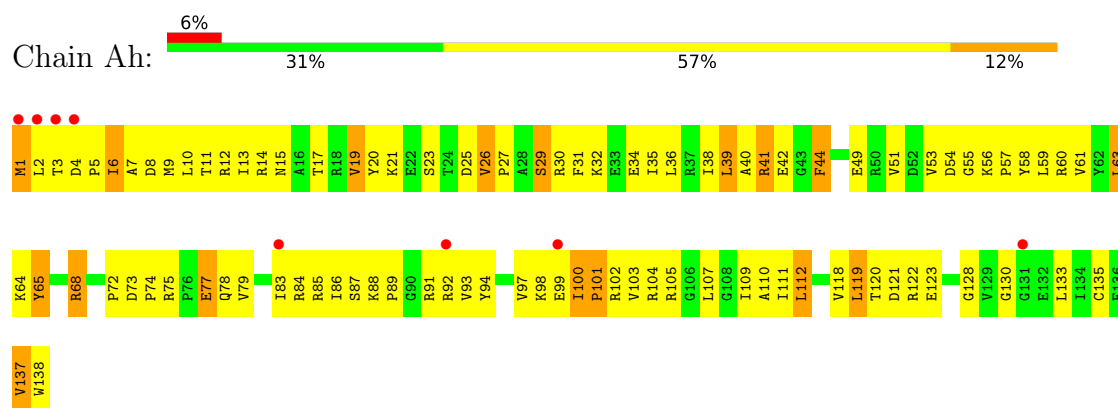
• Molecule 6: 30S ribosomal protein S7



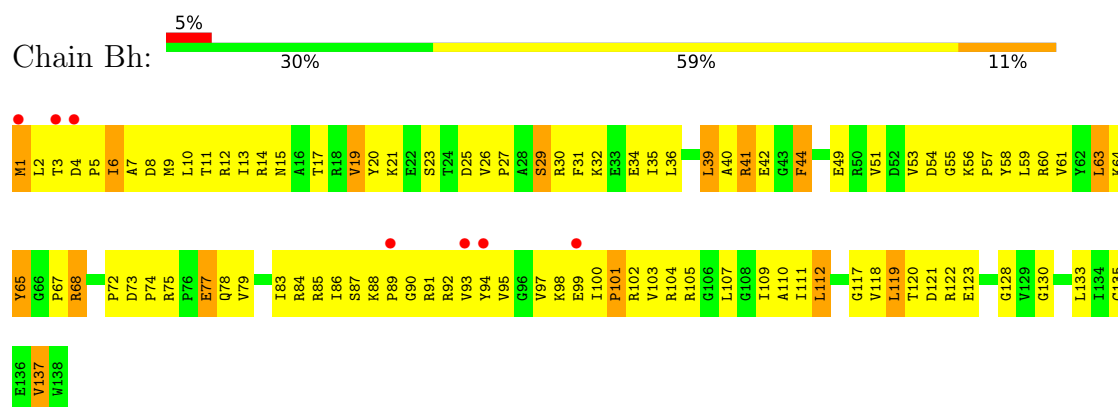
• Molecule 6: 30S ribosomal protein S7



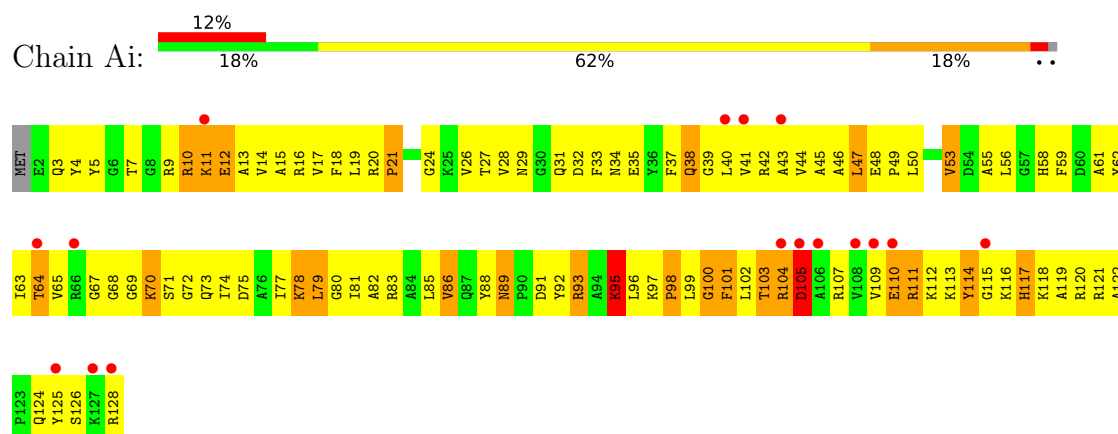
• Molecule 7: 30S ribosomal protein S8



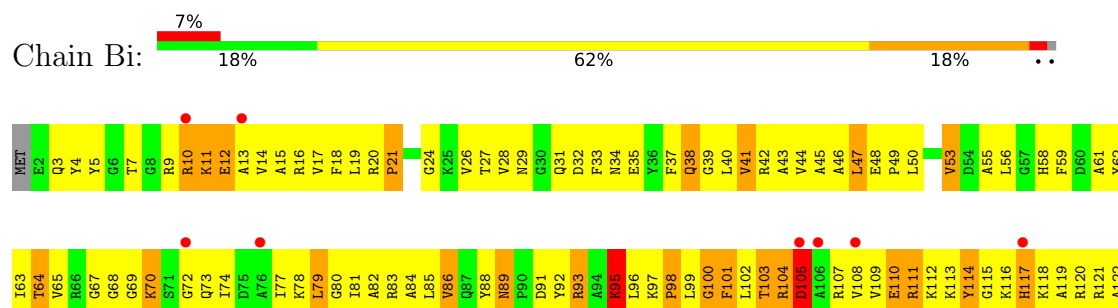
- Molecule 7: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S9

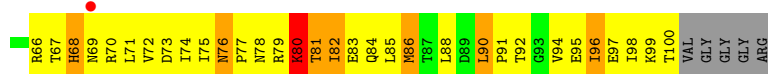
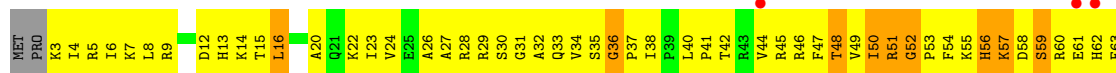
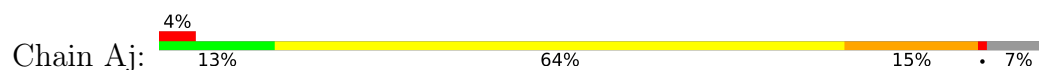


- Molecule 8: 30S ribosomal protein S9

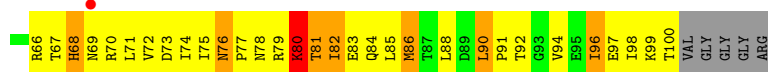
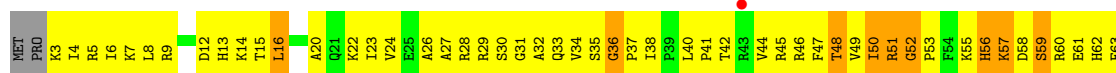
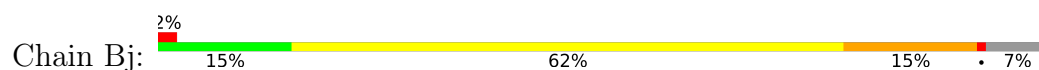




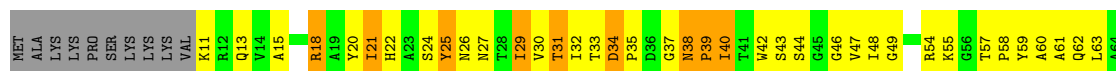
• Molecule 9: 30S ribosomal protein S10



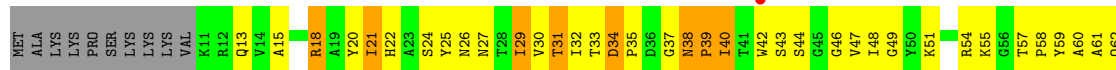
• Molecule 9: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S11

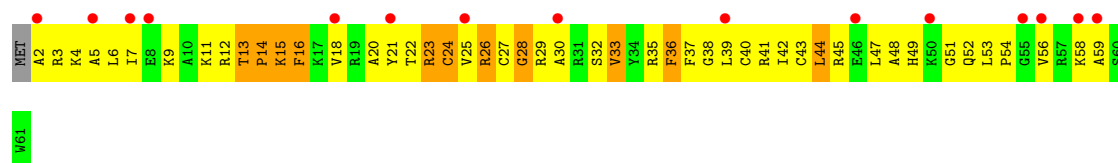


• Molecule 10: 30S ribosomal protein S11

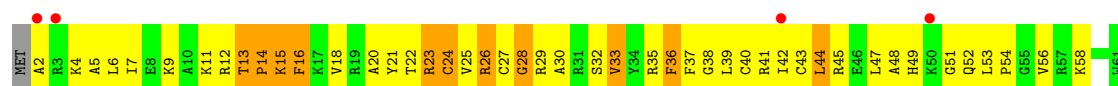


• Molecule 11: 30S ribosomal protein S12

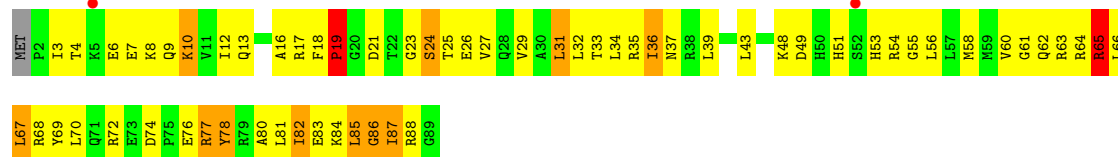




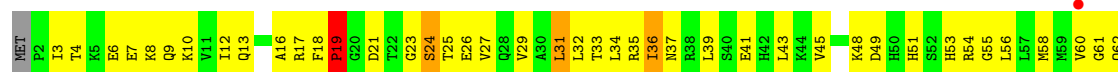
- Molecule 13: 30S ribosomal protein S14 type Z



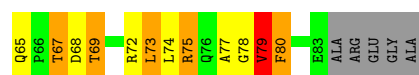
- Molecule 14: 30S ribosomal protein S15



- Molecule 14: 30S ribosomal protein S15



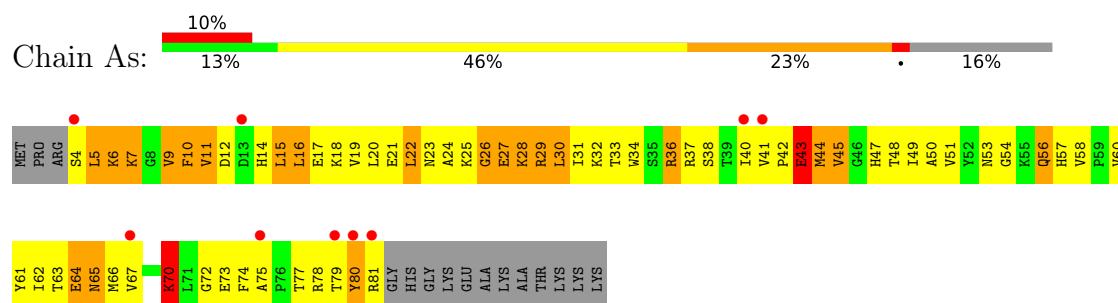
- Molecule 15: 30S ribosomal protein S16



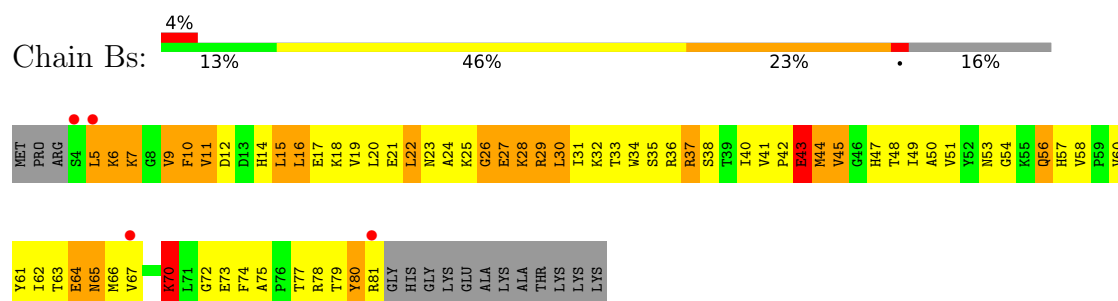
- Molecule 15: 30S ribosomal protein S16



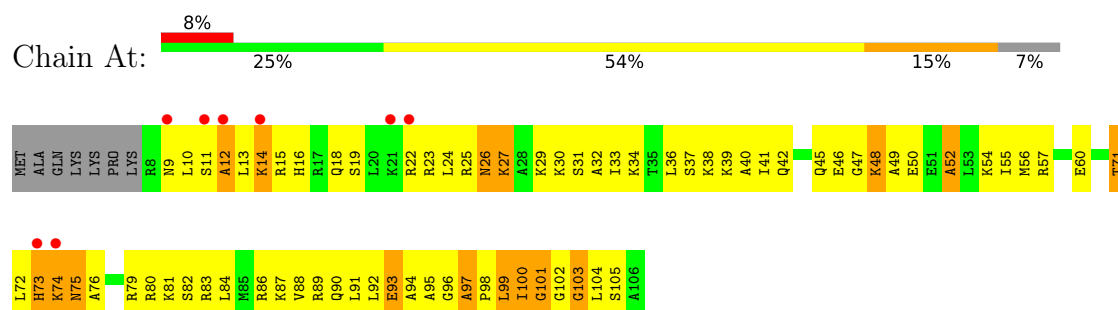
- Molecule 18: 30S ribosomal protein S19



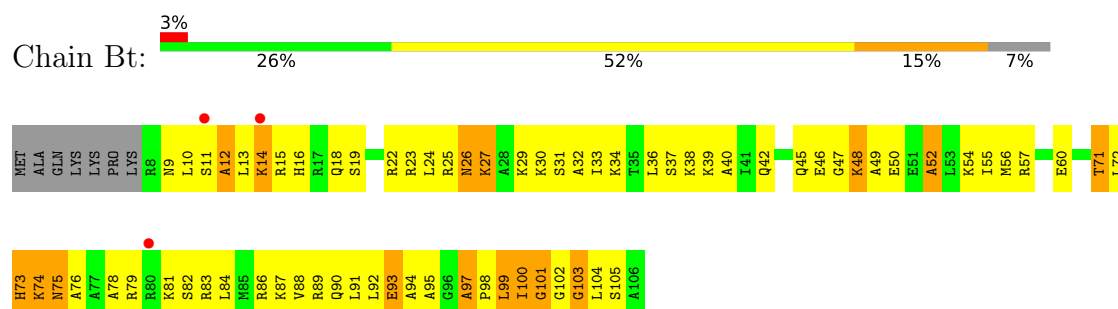
- Molecule 18: 30S ribosomal protein S19



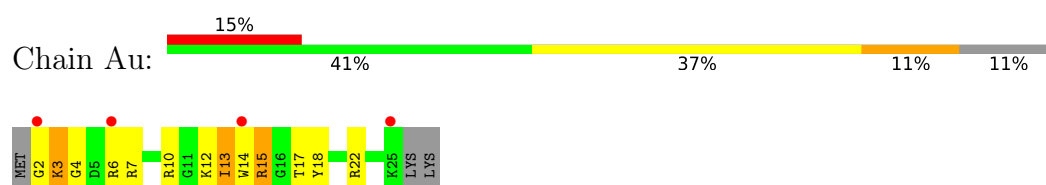
- Molecule 19: 30S ribosomal protein S20



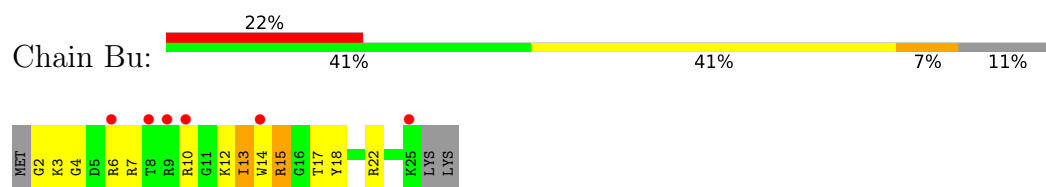
- Molecule 19: 30S ribosomal protein S20



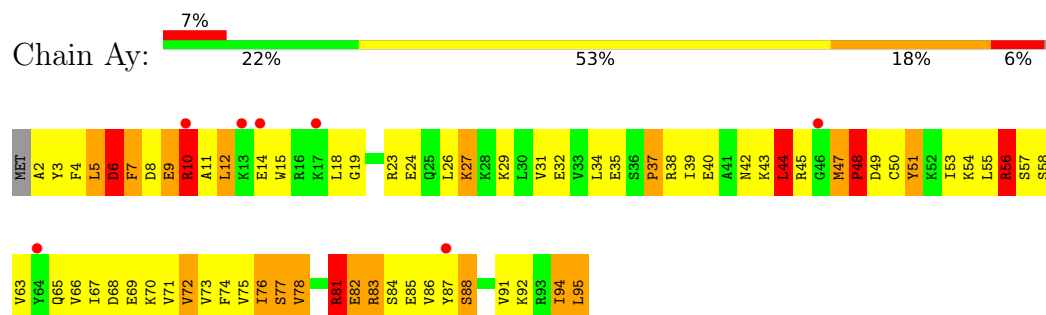
- Molecule 20: 30S ribosomal protein Thx



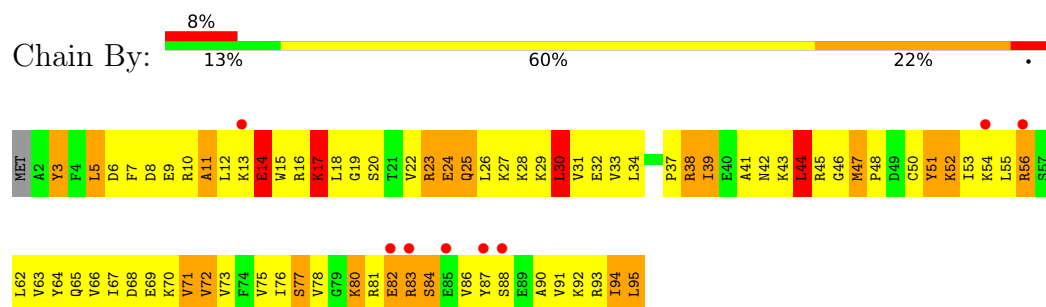
- Molecule 20: 30S ribosomal protein Thx



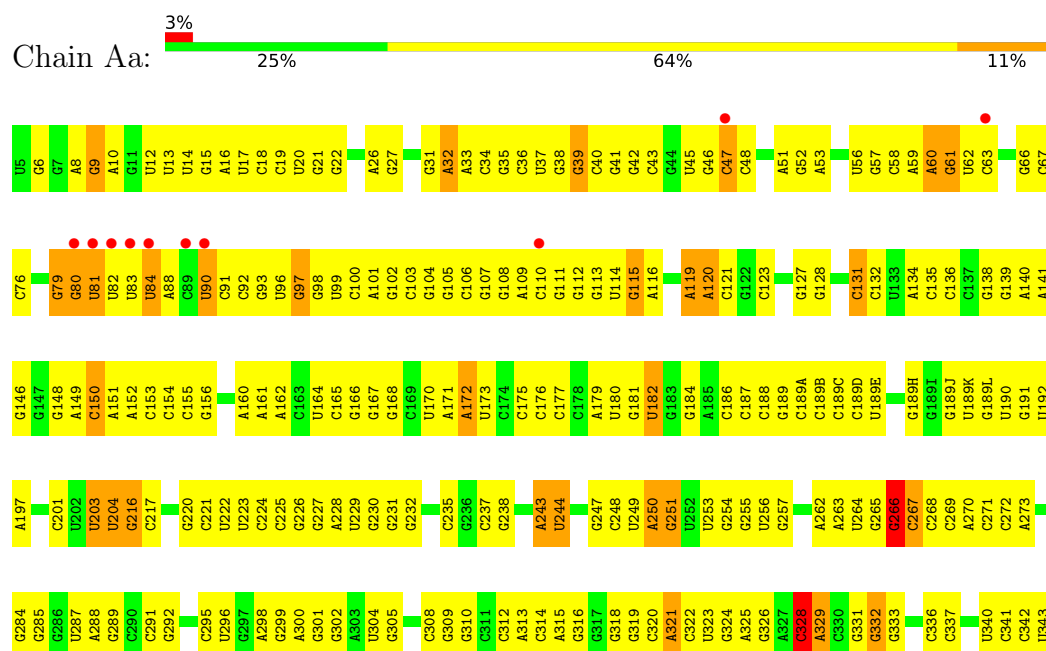
- Molecule 21: Toxin relE



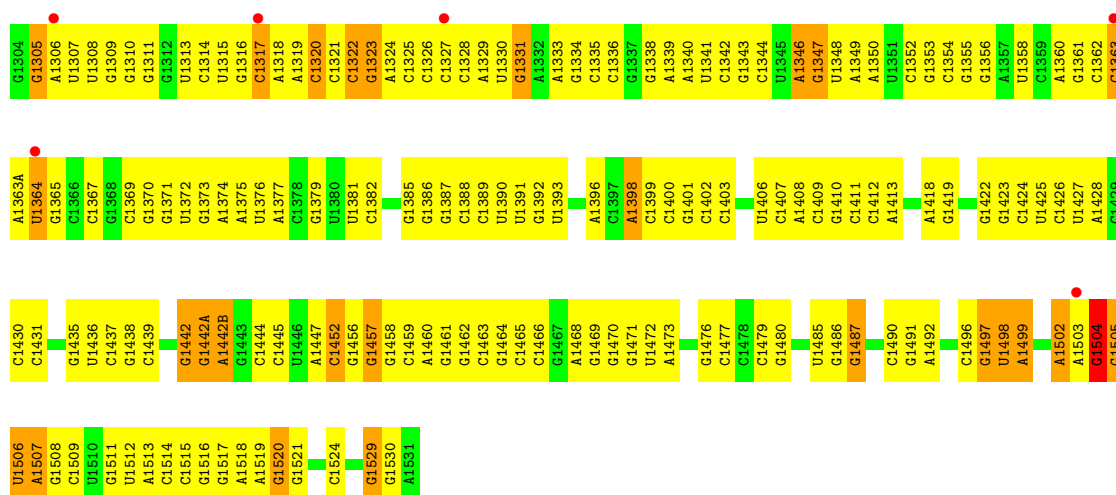
- Molecule 21: Toxin relE



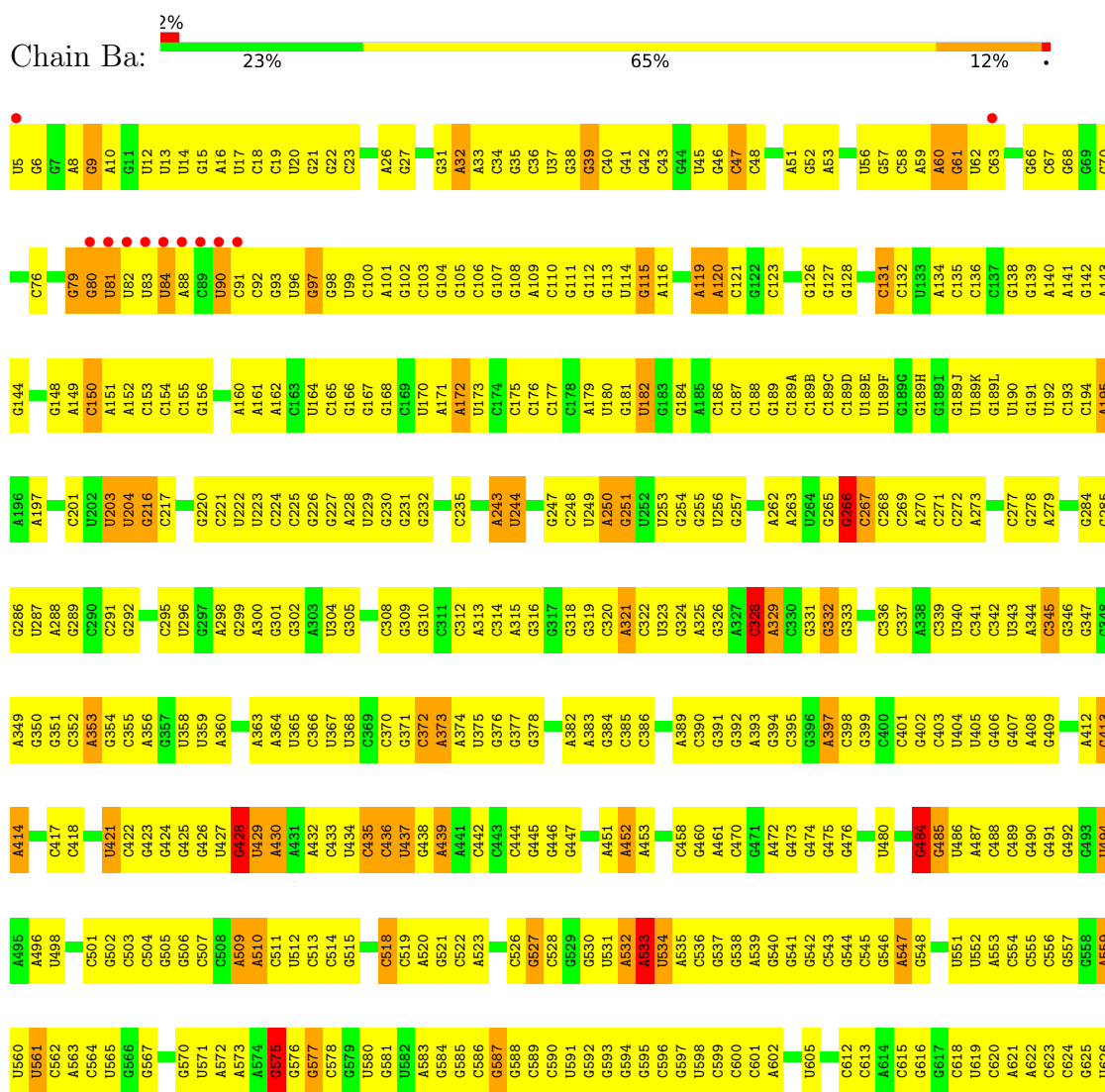
- Molecule 22: RNA (1504-MER)



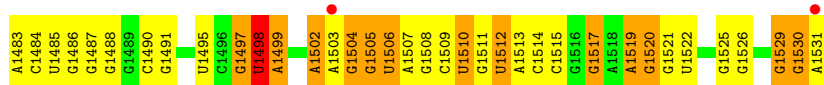
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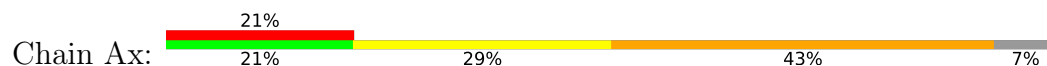
• Molecule 22: RNA (1504-MER)







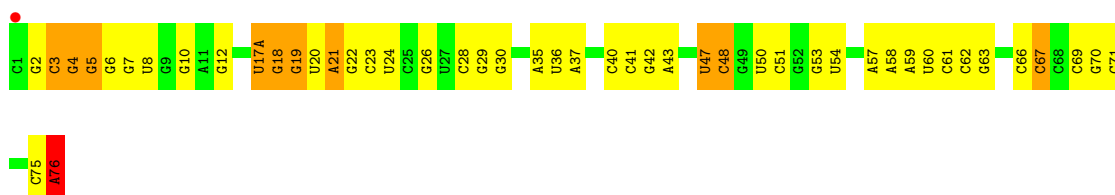
- Molecule 23: RNA (5'-R(*A*AP*GP*UP*AP*AP*AP*AP*AP*UP*GP*UP*A*(CCC))-3')



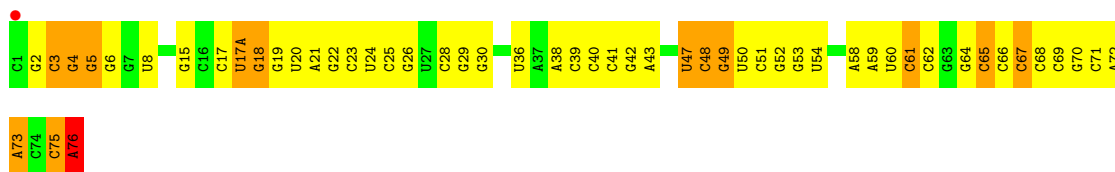
- Molecule 23: RNA (5'-R(*A*AP*GP*UP*AP*AP*AP*AP*AP*UP*GP*UP*A*(CCC))-3')



- Molecule 24: RNA (77-MER)

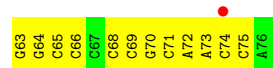


- Molecule 24: RNA (77-MER)

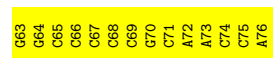
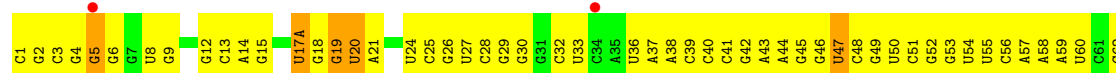


- Molecule 25: RNA (77-MER)

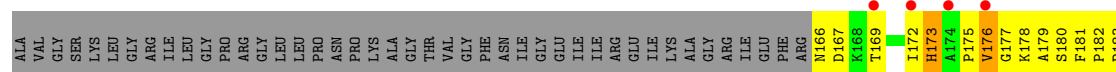
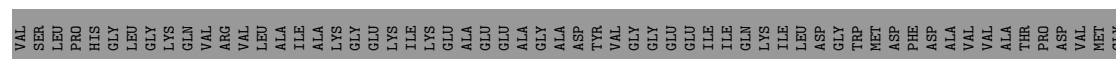
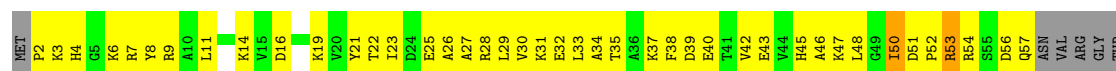




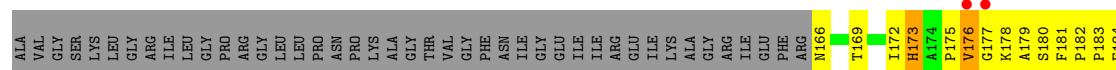
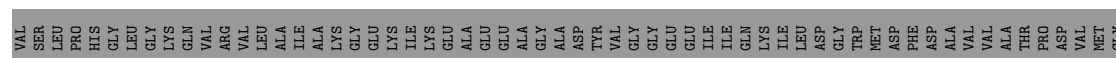
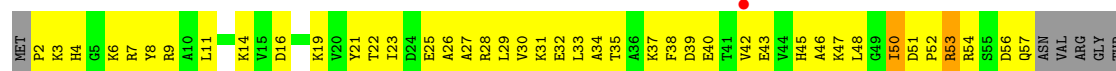
• Molecule 25: RNA (77-MER)



• Molecule 26: 50S ribosomal protein L1

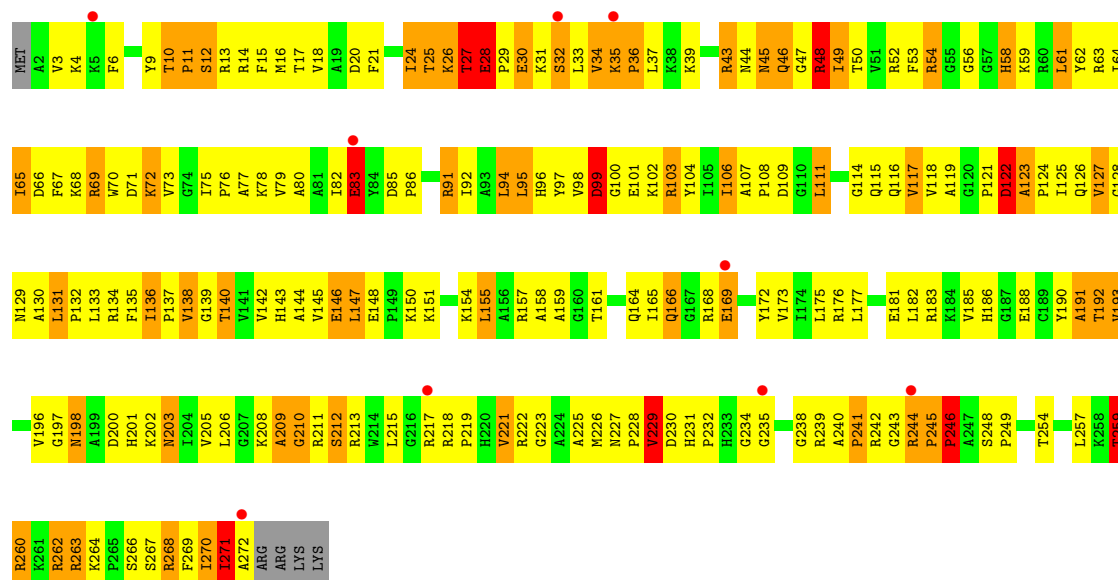


• Molecule 26: 50S ribosomal protein L1

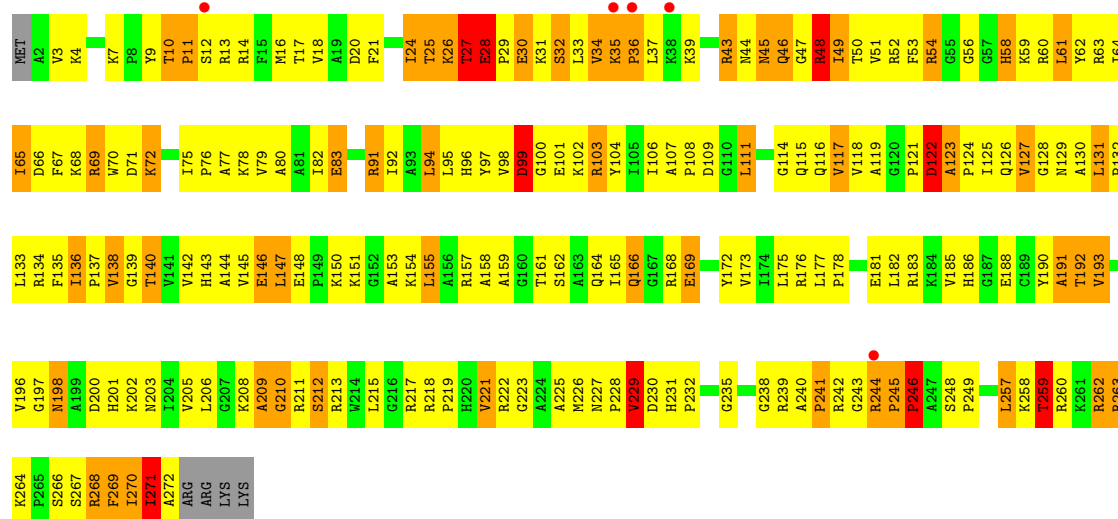


• Molecule 27: 50S ribosomal protein L2

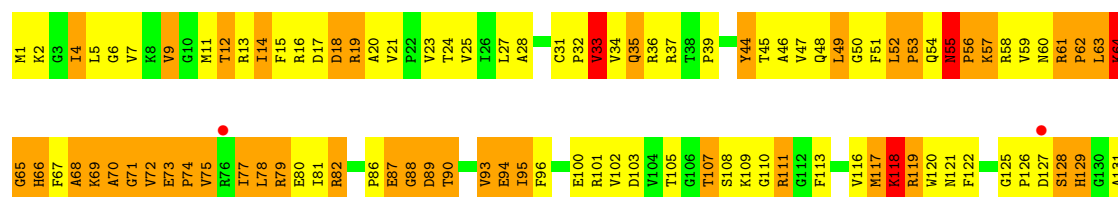




• Molecule 27: 50S ribosomal protein L2

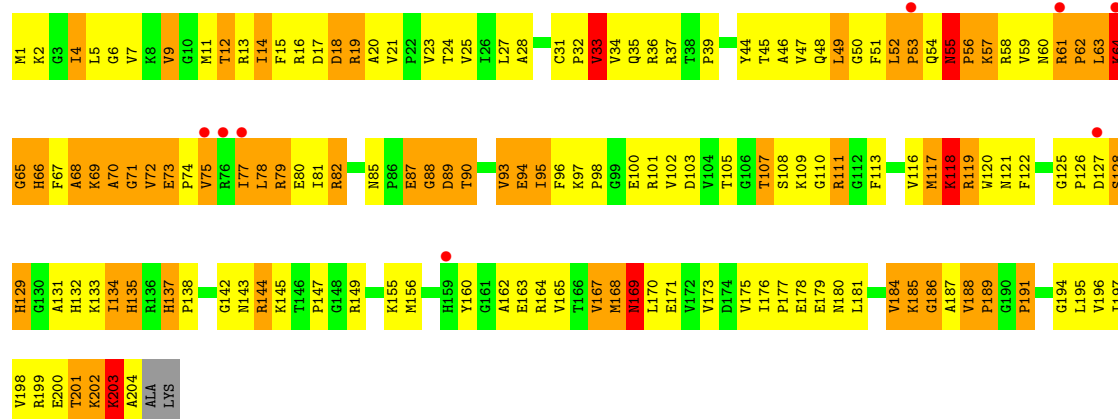


• Molecule 28: 50S ribosomal protein L3

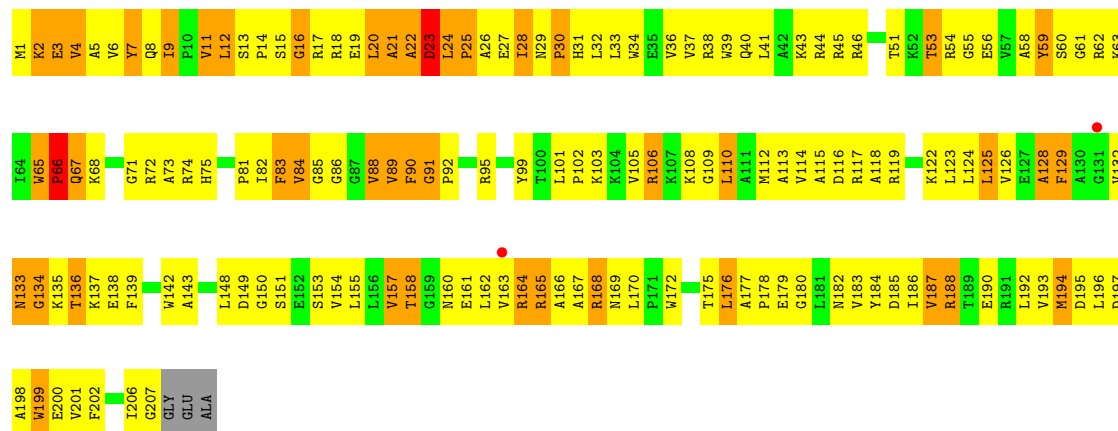




• Molecule 28: 50S ribosomal protein L3

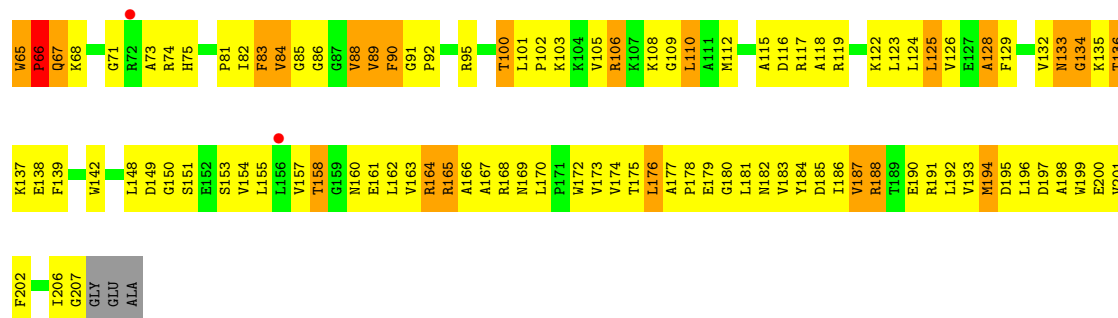


• Molecule 29: 50S ribosomal protein L4

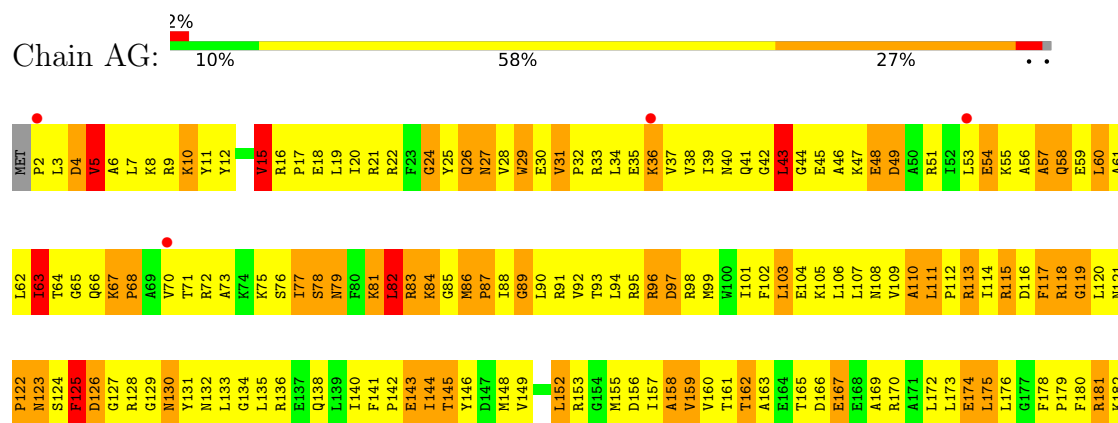


• Molecule 29: 50S ribosomal protein L4

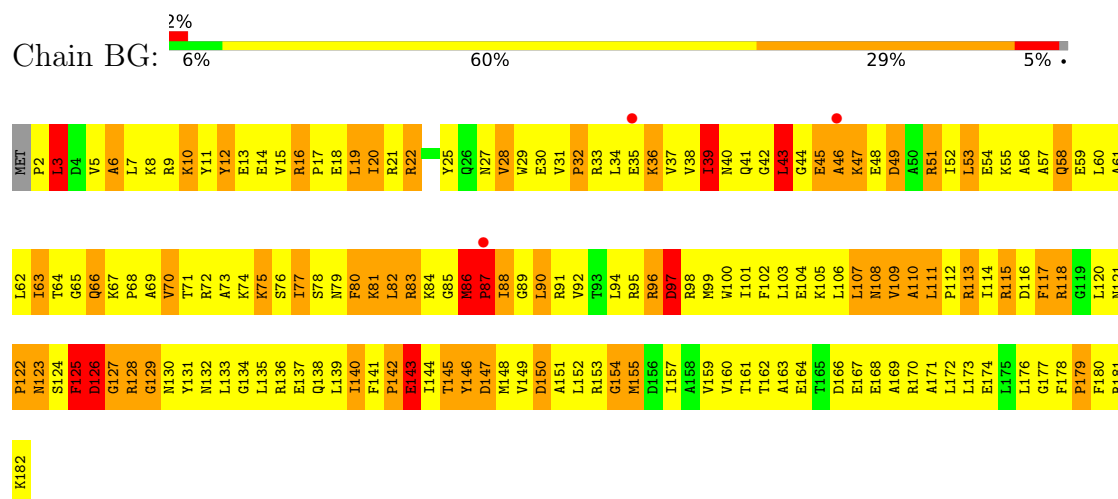




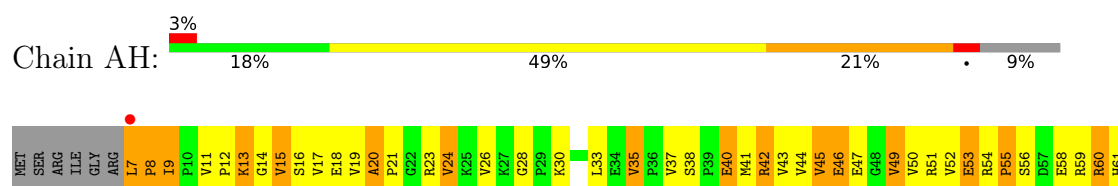
- Molecule 30: 50S ribosomal protein L5

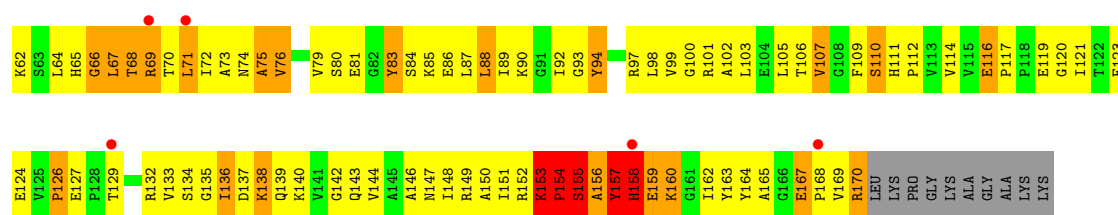


- Molecule 30: 50S ribosomal protein L5

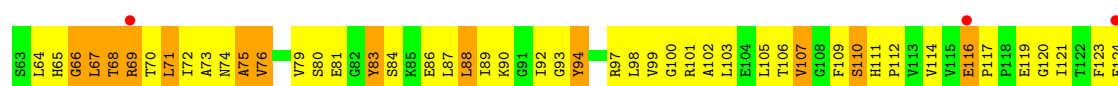
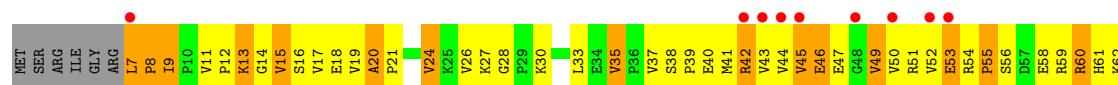
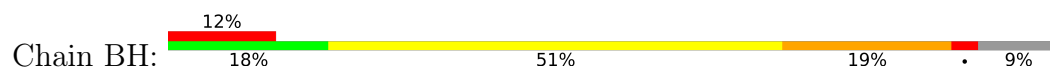


- Molecule 31: 50S ribosomal protein L6

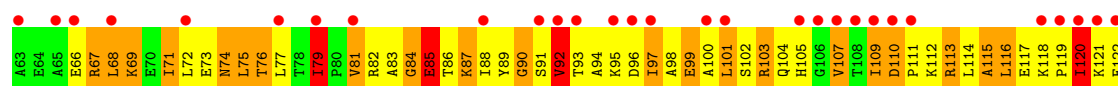
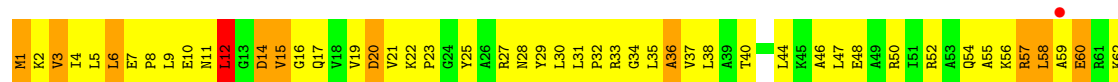
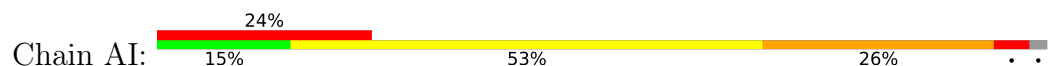




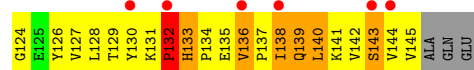
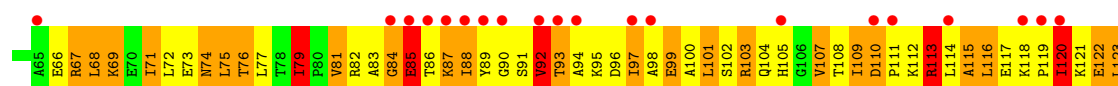
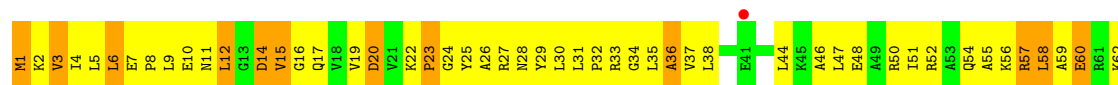
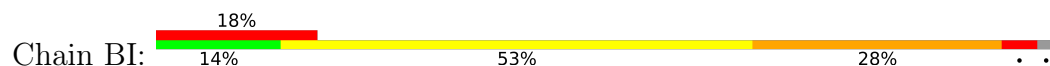
● Molecule 31: 50S ribosomal protein L6



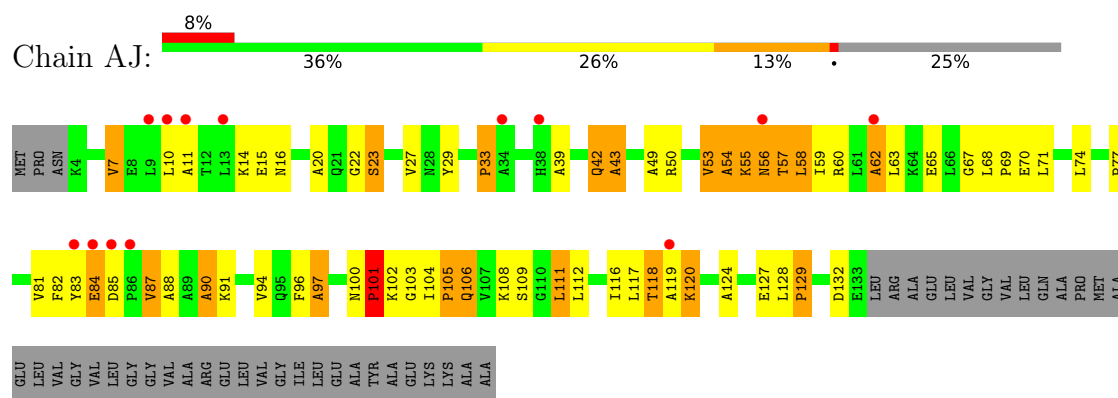
● Molecule 32: 50S ribosomal protein L9



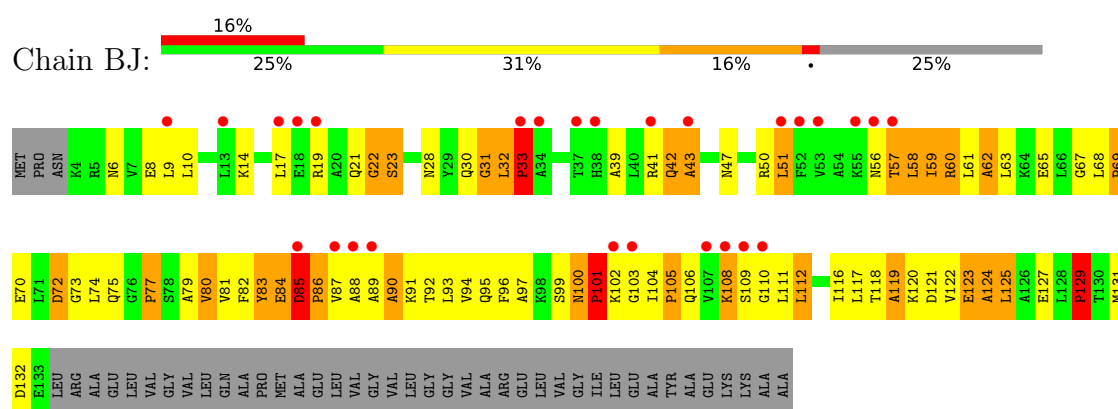
● Molecule 32: 50S ribosomal protein L9



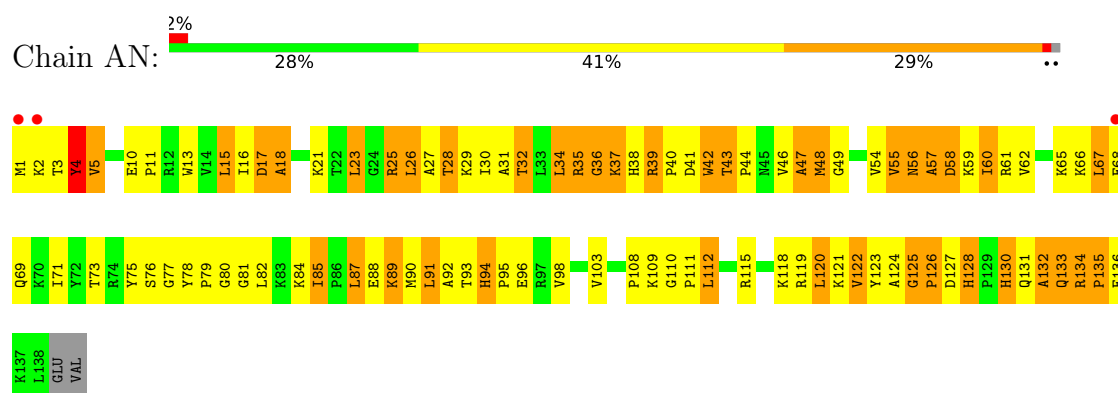
- Molecule 33: 50S ribosomal protein L10



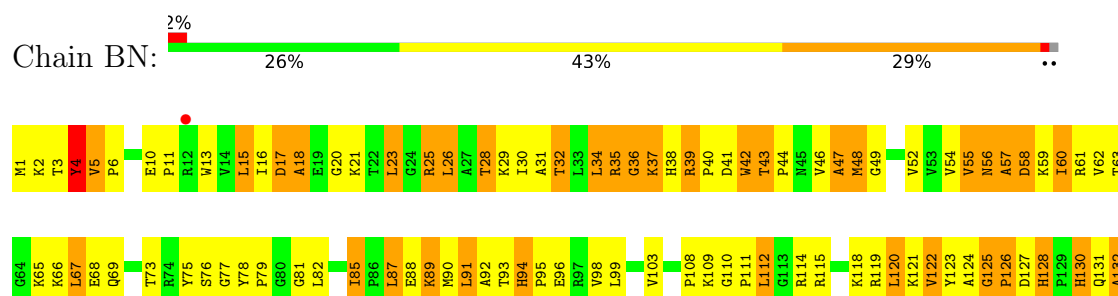
- Molecule 33: 50S ribosomal protein L10

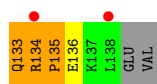


- Molecule 34: 50S ribosomal protein L13



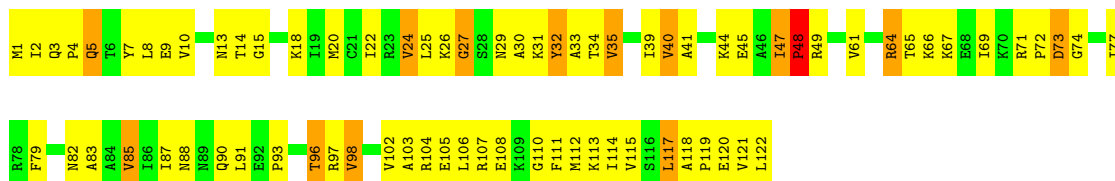
- Molecule 34: 50S ribosomal protein L13





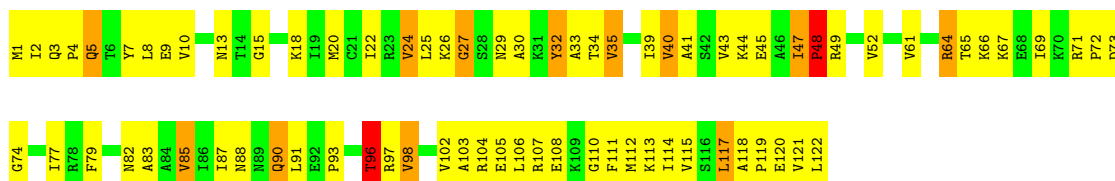
• Molecule 35: 50S ribosomal protein L14

Chain AO: 38% 51% 11%



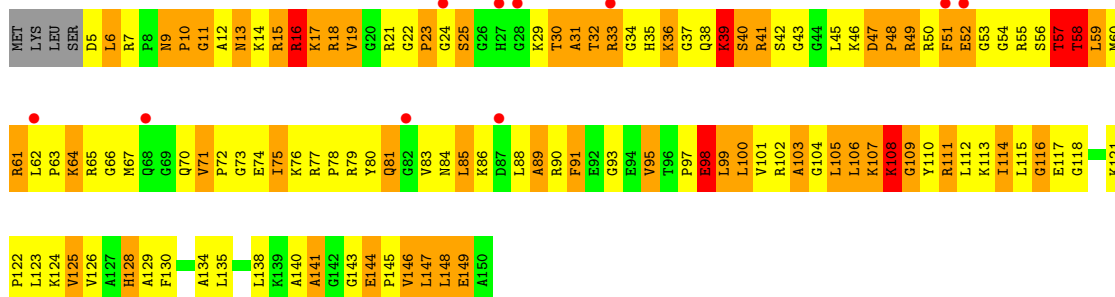
• Molecule 35: 50S ribosomal protein L14

Chain BO: 38% 51% 10%



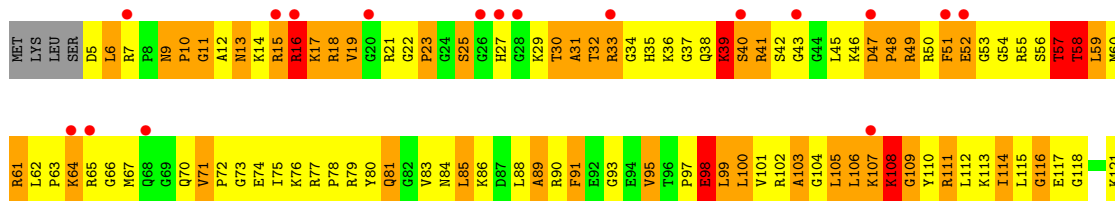
• Molecule 36: 50S ribosomal protein L15

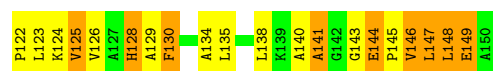
Chain AP: 7% 16% 43% 34%



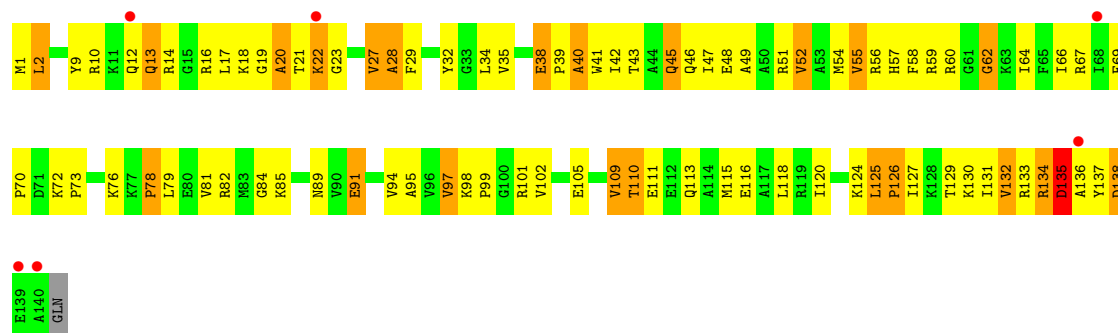
• Molecule 36: 50S ribosomal protein L15

Chain BP: 11% 16% 44% 33%

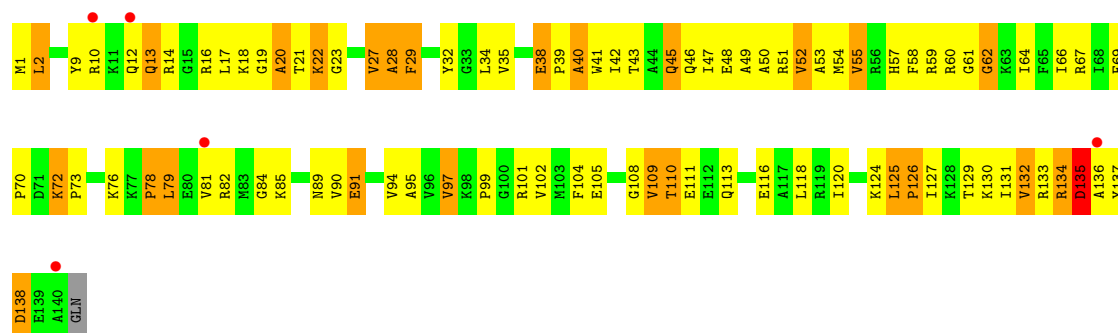




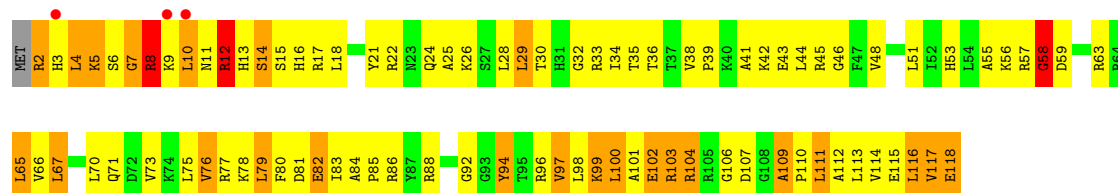
• Molecule 37: 50S ribosomal protein L16



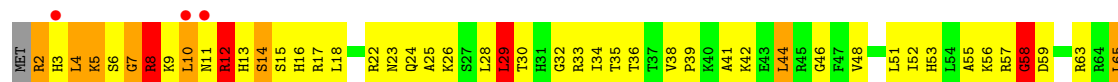
• Molecule 37: 50S ribosomal protein L16

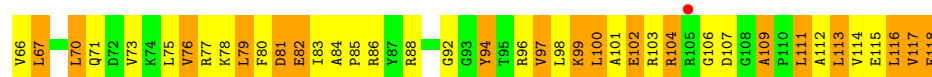


• Molecule 38: 50S ribosomal protein L17

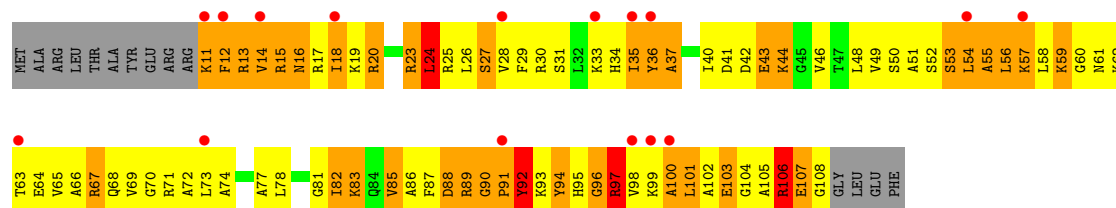


• Molecule 38: 50S ribosomal protein L17

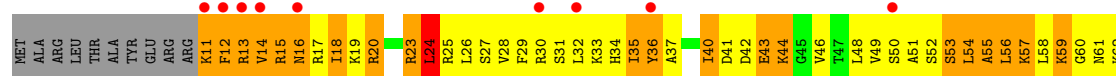




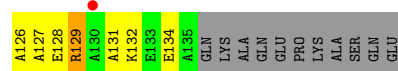
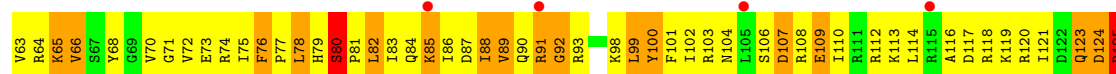
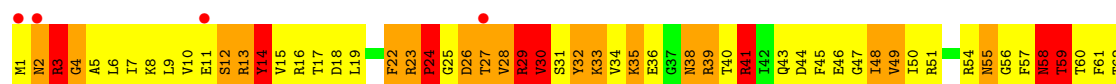
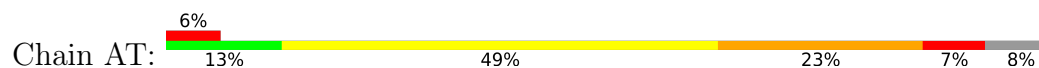
• Molecule 39: 50S ribosomal protein L18



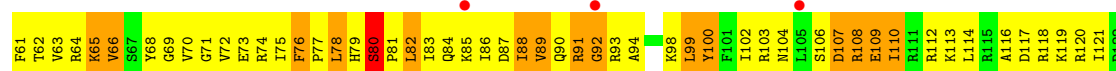
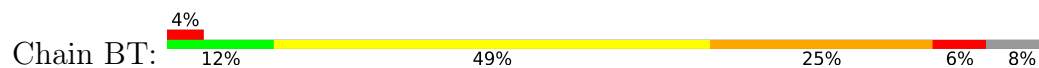
• Molecule 39: 50S ribosomal protein L18



• Molecule 40: 50S ribosomal protein L19

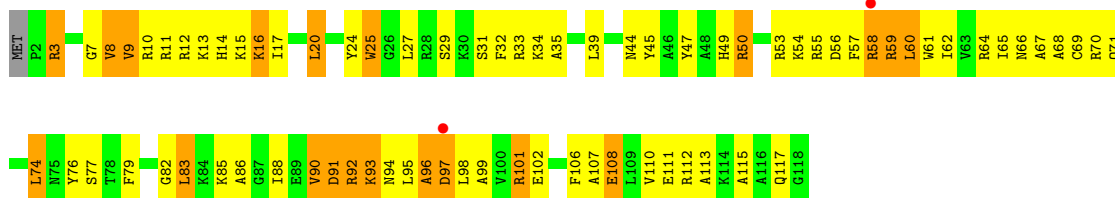


• Molecule 40: 50S ribosomal protein L19

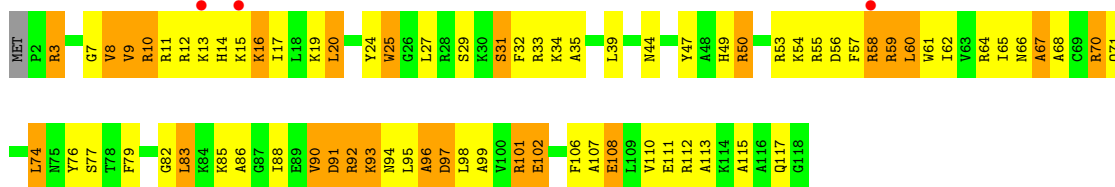




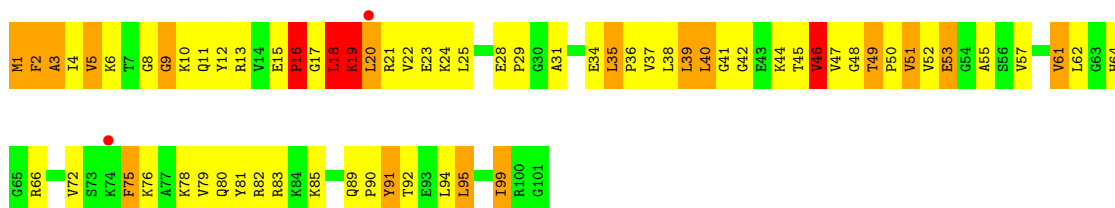
- Molecule 41: 50S ribosomal protein L20



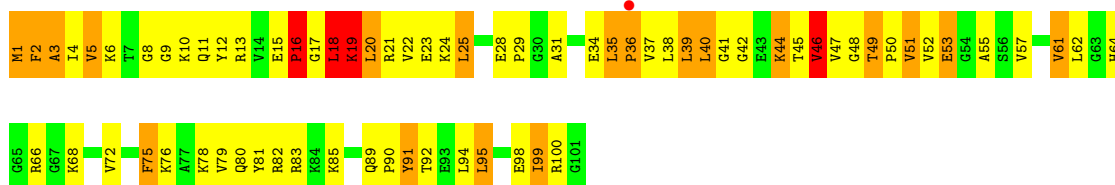
- Molecule 41: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L21

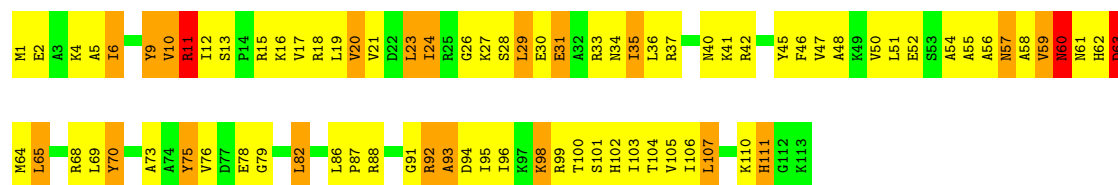


- Molecule 42: 50S ribosomal protein L21

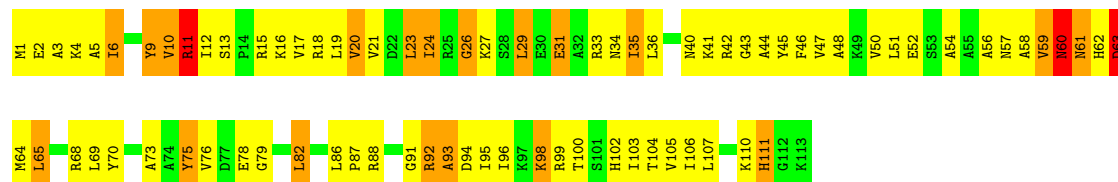


- Molecule 43: 50S ribosomal protein L22

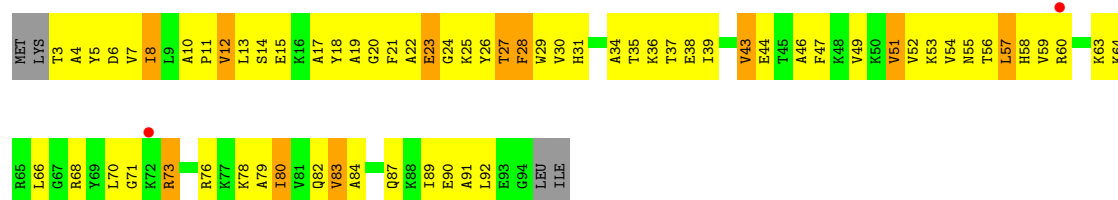




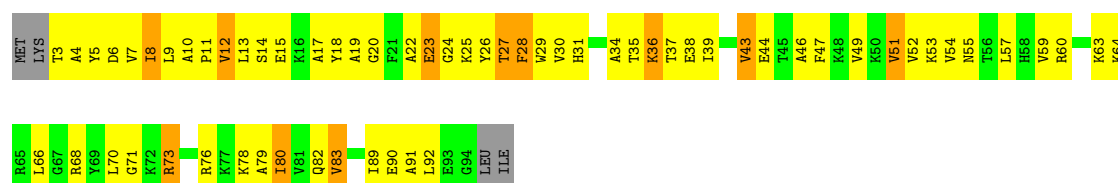
• Molecule 43: 50S ribosomal protein L22



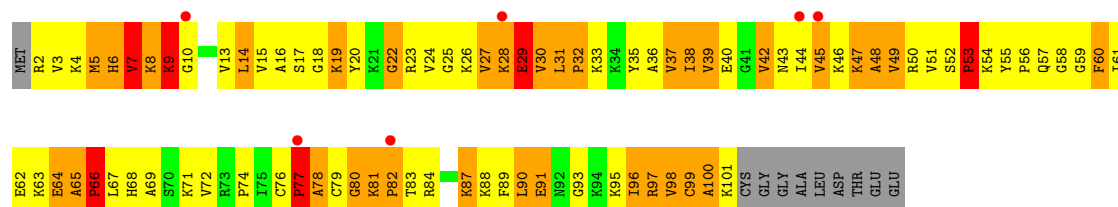
• Molecule 44: 50S ribosomal protein L23



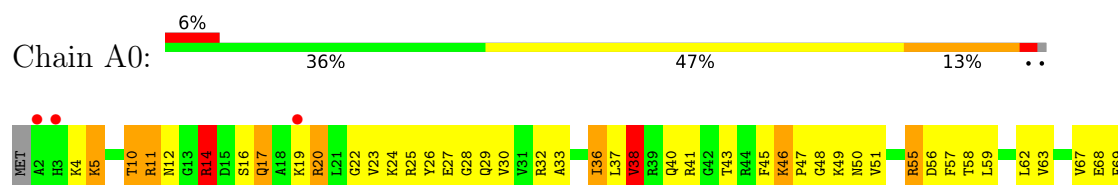
• Molecule 44: 50S ribosomal protein L23

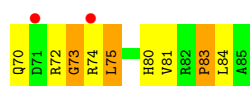


• Molecule 45: 50S ribosomal protein L24



• Molecule 45: 50S ribosomal protein L24

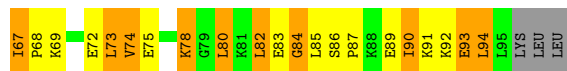
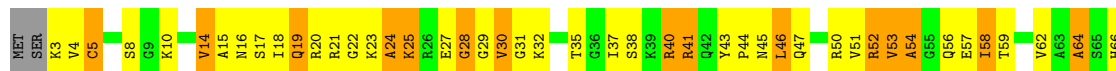
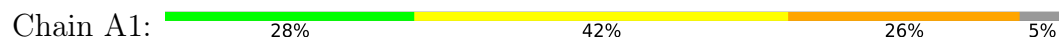




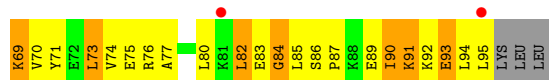
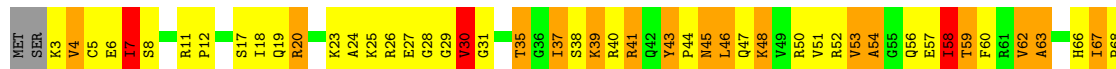
- Molecule 47: 50S ribosomal protein L27



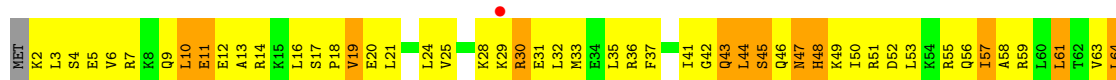
- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28

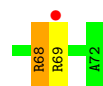


- Molecule 49: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L29

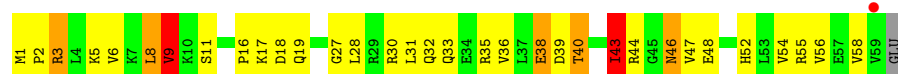
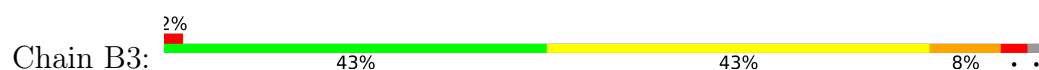




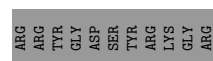
- Molecule 50: 50S ribosomal protein L30



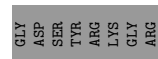
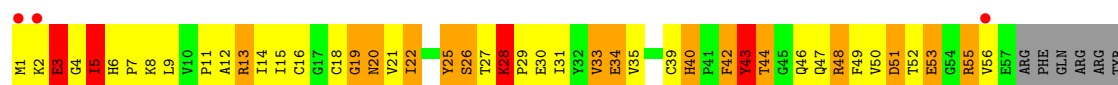
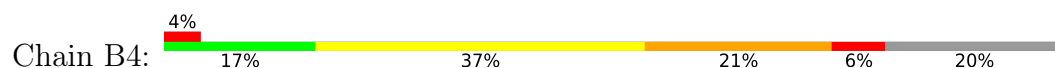
- Molecule 50: 50S ribosomal protein L30



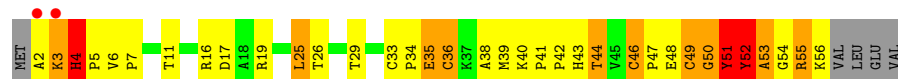
- Molecule 51: 50S ribosomal protein L31



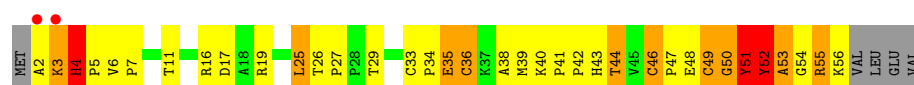
- Molecule 51: 50S ribosomal protein L31



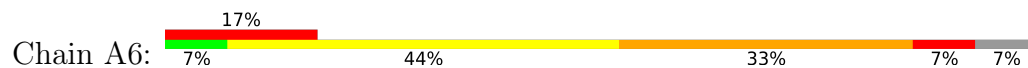
- Molecule 52: 50S ribosomal protein L32



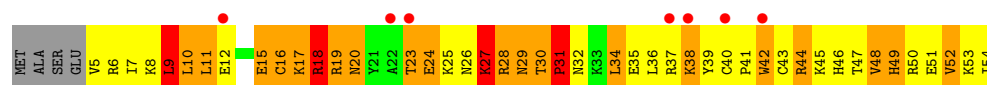
- Molecule 52: 50S ribosomal protein L32



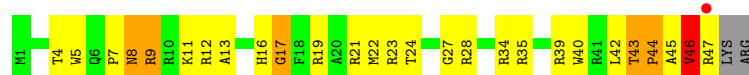
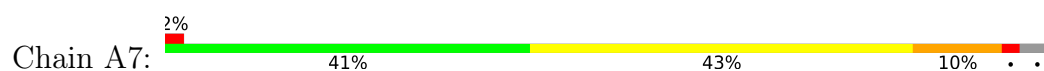
- Molecule 53: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L33



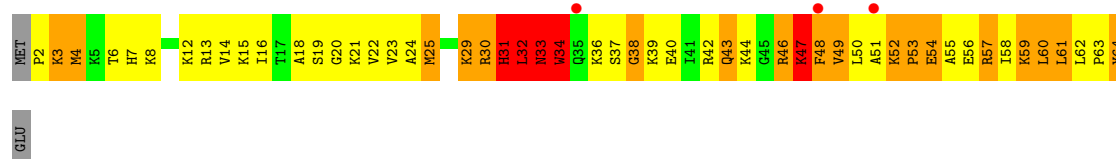
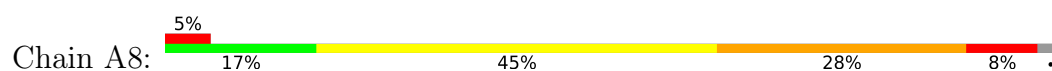
- Molecule 54: 50S ribosomal protein L34



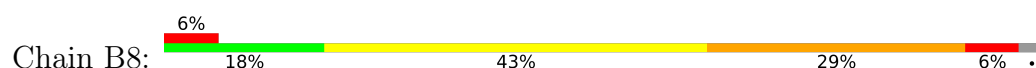
- Molecule 54: 50S ribosomal protein L34

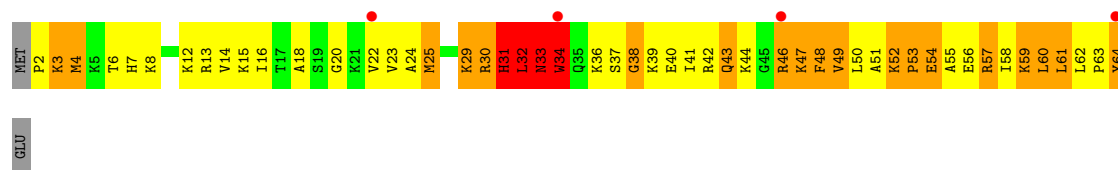


- Molecule 55: 50S ribosomal protein L35

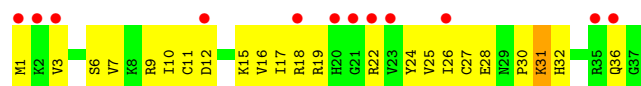


- Molecule 55: 50S ribosomal protein L35

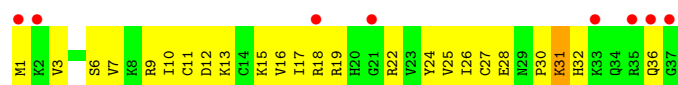




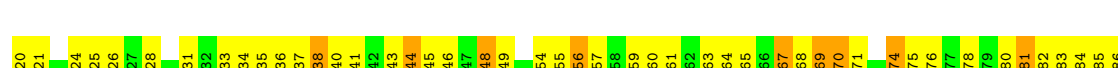
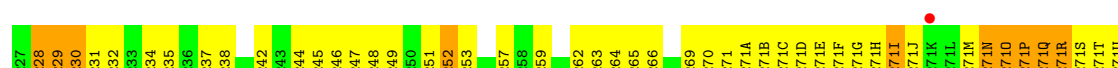
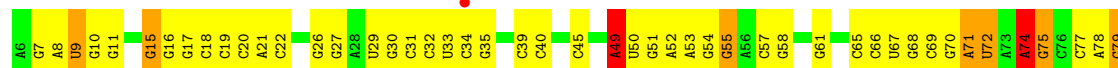
- Molecule 56: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L36

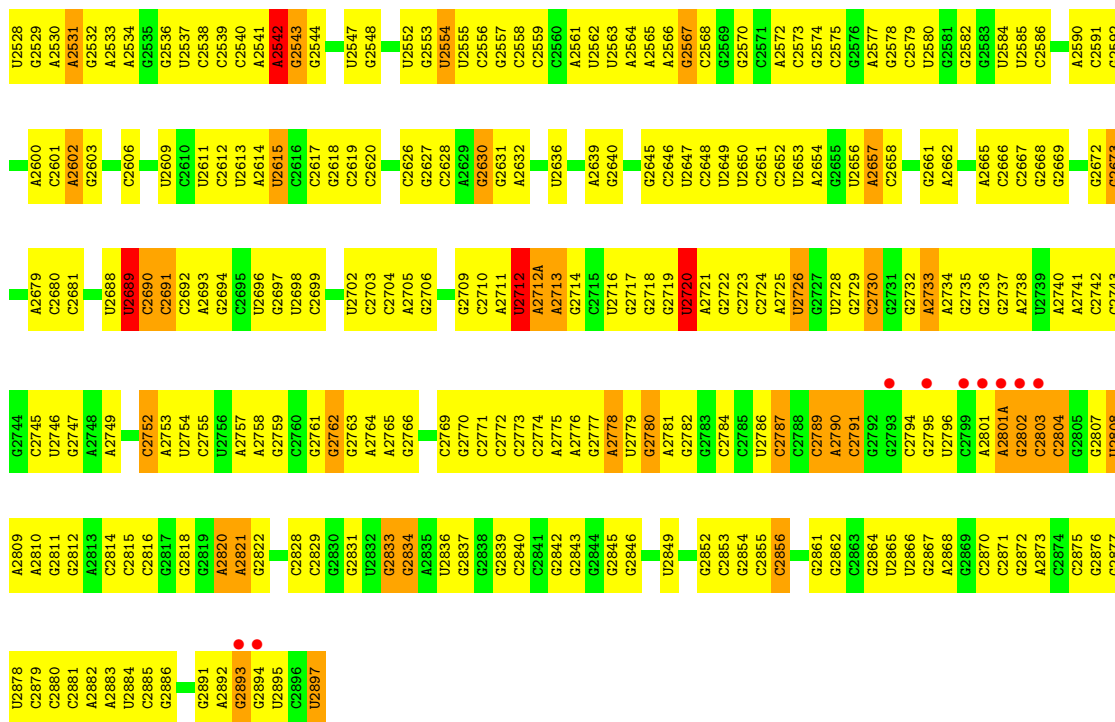


- Molecule 57: RNA (2848-MER)

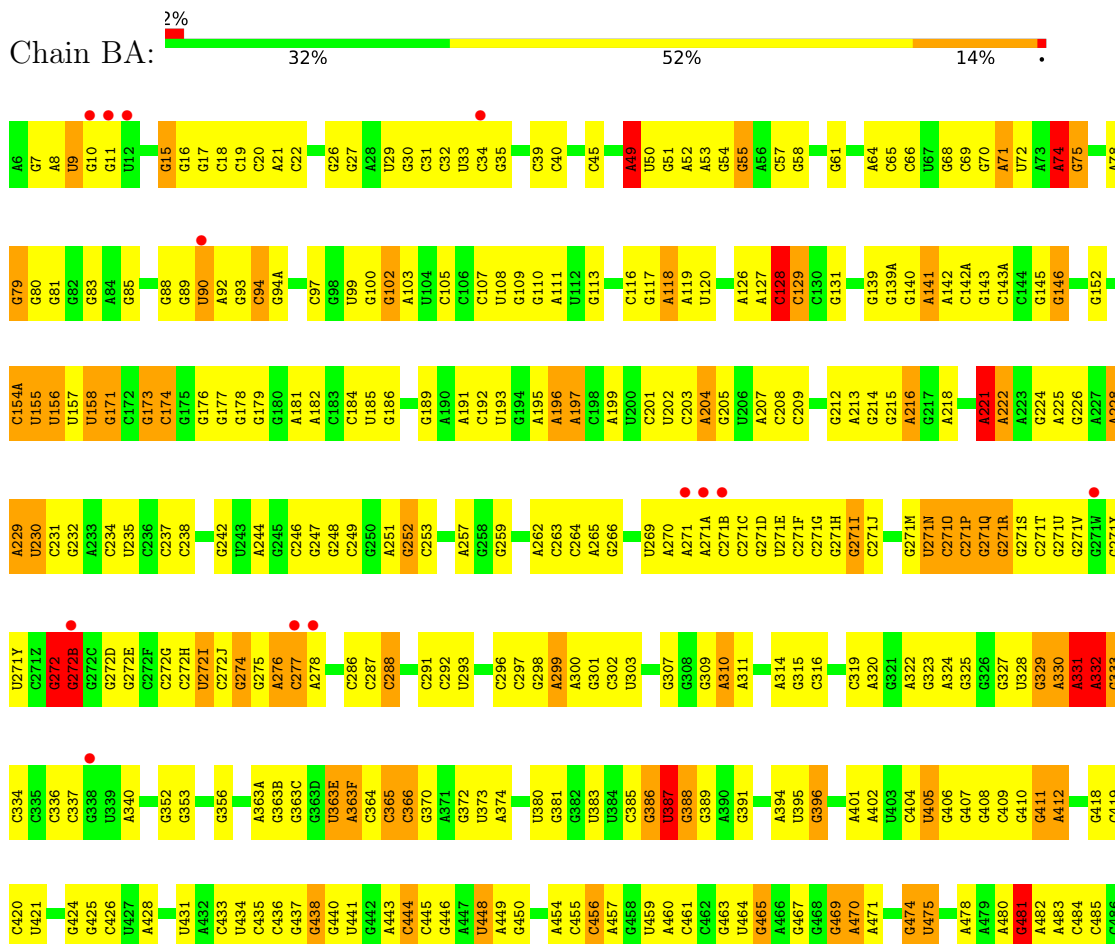


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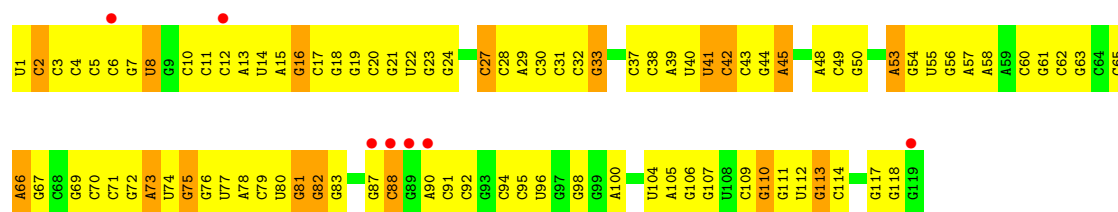
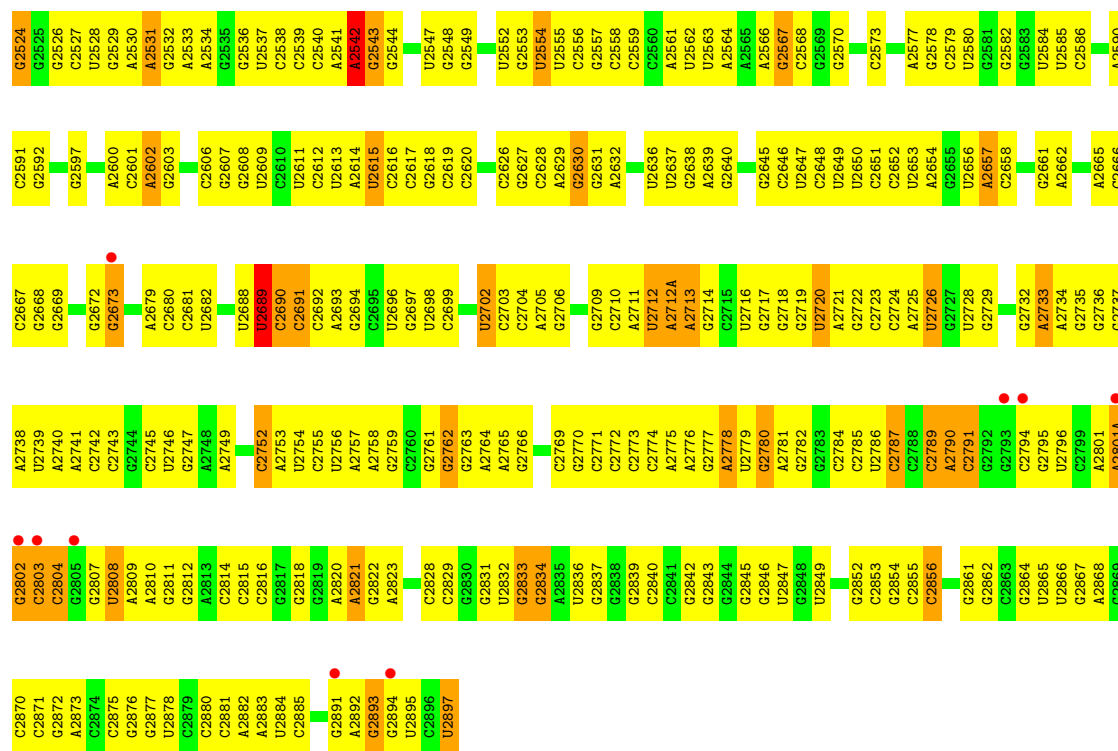


• Molecule 57: RNA (2848-MER)

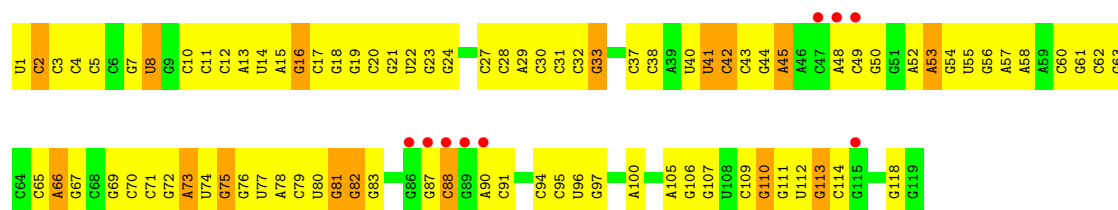




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U2519	G2519	U2449	U2249	U2113	U2249	U2113	U2113	U1973	A1911	A1831	C1759	A1674	G1596
U2520	G2520	A2451	G2257	G2119	A2451	G2119	G2119	U1974	A1912	A1832	C1760	A1675	U1591
U2521	G2521	C2385	G2258	G2120	G2258	G2120	G2120	U1975	A1913	A1833	C1761	A1676	G1592
U2522	G2522	A2386	G2259	G2121	A2386	G2121	G2121	U1976	A1914	A1834	C1762	A1677	G1593
U2523	G2523	C2387	G2260	G2122	G2260	G2122	G2122	U1977	A1915	A1835	C1763	A1678	G1594
U2524	G2524	U2452	U2250	U2123	U2250	U2123	U2123	U1978	A1916	A1836	C1764	A1679	G1595
U2525	G2525	A2453	G2261	G2124	A2453	G2124	G2124	U1979	A1917	A1837	C1765	A1680	G1596
U2526	G2526	C2388	G2262	G2125	G2262	G2125	G2125	U1980	A1918	A1838	C1766	A1681	G1597
U2527	G2527	U2454	U2251	U2124	U2251	U2124	U2124	U1981	A1919	A1839	C1767	A1682	G1598
U2528	G2528	A2455	G2263	G2126	A2455	G2126	G2126	U1982	A1920	A1840	C1768	A1683	G1599
U2529	G2529	C2389	G2264	G2127	G2264	G2127	G2127	U1983	A1921	A1841	C1769	A1684	G1600
U2530	G2530	U2456	U2252	U2125	U2252	U2125	U2125	U1984	A1922	A1842	C1770	A1685	G1601
U2531	G2531	A2457	G2265	G2128	A2457	G2128	G2128	U1985	A1923	A1843	C1771	A1686	G1602
U2532	G2532	C2390	G2266	G2129	G2266	G2129	G2129	U1986	A1924	A1844	C1772	A1687	G1603
U2533	G2533	U2458	U2253	U2126	U2253	U2126	U2126	U1987	A1925	A1845	C1773	A1688	G1604
U2534	G2534	A2459	G2267	G2130	A2459	G2130	G2130	U1988	A1926	A1846	C1774	A1689	G1605
U2535	G2535	C2391	G2268	G2131	G2268	G2131	G2131	U1989	A1927	A1847	C1775	A1690	G1606
U2536	G2536	U2460	U2254	U2132	U2254	U2132	U2132	U1990	A1928	A1848	C1776	A1691	G1607
U2537	G2537	A2461	G2269	G2133	A2461	G2133	G2133	U1991	A1929	A1849	C1777	A1692	G1608
U2538	G2538	C2392	G2270	G2134	G2270	G2134	G2134	U1992	A1930	A1850	C1778	A1693	G1609
U2539	G2539	U2462	U2255	U2135	U2255	U2135	U2135	U1993	A1931	A1851	C1779	A1694	G1610
U2540	G2540	G2393	G2271	G2136	G2271	G2136	G2136	U1994	A1932	A1852	C1780	A1695	G1611
U2541	G2541	C2394	C2280	C2281	C2137	C2138	C2073	U1995	A1933	A1853	C1781	A1696	G1612
U2542	G2542	U2344	U2203	G2282	C2139	U2075	U2075	U1996	A1934	A1854	C1782	A1697	G1613
U2543	G2543	G2345	C2205	C2283	U2076	U2076	A2077	U1997	A1935	A1855	C1783	A1698	G1614
U2544	G2544	A2346	G2206	C2284	U2077	C2078	C2078	U1998	A1936	A1856	C1784	A1699	G1615
U2545	G2545	C2347	A2207	A2285	U2144	C2078	C2078	U1999	A1937	A1857	C1785	A1700	G1616
U2546	G2546	U2348	A2208	U2218	G2145	A2082	A2082	U2000	A1938	A1858	C1786	A1701	G1617
U2547	G2547	C2349	G2219	G2219	G2146	G2083	G2083	U2001	A1939	A1859	C1787	A1702	G1618
U2548	G2548	C2350	G2220	G2220	G2147	A2084	A2084	U2002	A1940	A1860	C1788	A1703	G1619
U2549	G2549	G2351	G2221	C2084	G2148	C2085	C2085	U2003	A1941	A1861	C1789	A17	



• Molecule 58: RNA (119-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.23Å 451.43Å 623.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.60 49.63 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.63-3.60) 99.8 (49.63-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.245 0.219 , 0.251	Depositor DCC
R_{free} test set	30861 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	103.4	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 99.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	297230	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	Ab	0.39	0/1935	1.01	15/2609 (0.6%)
1	Bb	0.39	0/1935	1.02	17/2609 (0.7%)
2	Ac	0.40	0/1636	0.89	6/2205 (0.3%)
2	Bc	0.39	0/1636	0.89	6/2205 (0.3%)
3	Ad	0.43	0/1733	0.97	11/2318 (0.5%)
3	Bd	0.42	0/1733	0.98	9/2318 (0.4%)
4	Ae	0.42	0/1162	1.00	4/1564 (0.3%)
4	Be	0.45	0/1162	1.01	4/1564 (0.3%)
5	Af	0.40	0/856	0.91	0/1154
5	Bf	0.43	0/856	0.92	0/1154
6	Ag	0.39	0/1276	0.92	6/1709 (0.4%)
6	Bg	0.38	0/1276	0.92	6/1709 (0.4%)
7	Ah	0.42	0/1136	1.03	6/1527 (0.4%)
7	Bh	0.41	0/1136	1.02	8/1527 (0.5%)
8	Ai	0.38	0/1029	0.92	4/1379 (0.3%)
8	Bi	0.38	0/1029	0.91	4/1379 (0.3%)
9	Aj	0.42	0/807	0.99	5/1085 (0.5%)
9	Bj	0.43	0/807	0.99	5/1085 (0.5%)
10	Ak	0.41	0/900	0.96	4/1213 (0.3%)
10	Bk	0.42	0/900	0.97	4/1213 (0.3%)
11	Al	0.49	0/986	1.08	9/1320 (0.7%)
11	Bl	0.47	0/986	1.08	7/1320 (0.5%)
12	Am	0.36	0/947	0.87	1/1270 (0.1%)
12	Bm	0.37	0/947	0.95	4/1270 (0.3%)
13	An	0.39	0/501	0.79	0/664
13	Bn	0.40	0/501	0.80	0/664
14	Ao	0.41	0/745	0.89	2/992 (0.2%)
14	Bo	0.42	0/745	0.89	2/992 (0.2%)
15	Ap	0.43	0/716	0.98	3/963 (0.3%)
15	Bp	0.39	0/716	0.97	3/963 (0.3%)
16	Aq	0.42	0/836	1.02	5/1117 (0.4%)
16	Bq	0.42	0/836	1.01	5/1117 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Ar	0.40	0/579	1.12	12/768 (1.6%)
17	Br	0.41	0/579	1.12	11/768 (1.4%)
18	As	0.44	0/642	0.94	1/865 (0.1%)
18	Bs	0.44	0/642	0.94	0/865
19	At	0.43	0/765	1.02	5/1007 (0.5%)
19	Bt	0.42	0/765	1.01	5/1007 (0.5%)
20	Au	0.46	0/212	0.78	0/277
20	Bu	0.44	0/212	0.78	0/277
21	Ay	0.42	0/793	0.86	3/1059 (0.3%)
21	By	0.41	0/793	1.12	14/1059 (1.3%)
22	Aa	0.42	0/36190	0.63	34/56486 (0.1%)
22	Ba	0.42	0/36190	0.64	29/56486 (0.1%)
23	Ax	0.46	0/289	0.80	0/449
23	Bx	0.46	0/289	0.80	0/449
24	Av	0.42	0/1810	0.67	1/2821 (0.0%)
24	Bv	0.42	0/1810	0.71	1/2821 (0.0%)
25	Aw	0.43	0/1832	0.59	1/2855 (0.0%)
25	Bw	0.43	0/1832	0.57	0/2855
26	AC	0.41	0/956	0.93	2/1288 (0.2%)
26	BC	0.39	0/956	0.93	2/1288 (0.2%)
27	AD	0.58	0/2154	1.20	25/2905 (0.9%)
27	BD	0.62	0/2154	1.22	25/2905 (0.9%)
28	AE	0.58	0/1596	1.25	18/2153 (0.8%)
28	BE	0.61	0/1596	1.24	18/2153 (0.8%)
29	AF	0.52	0/1658	1.15	19/2244 (0.8%)
29	BF	0.54	0/1658	1.17	17/2244 (0.8%)
30	AG	0.44	0/1499	1.12	14/2016 (0.7%)
30	BG	0.47	0/1499	1.11	10/2016 (0.5%)
31	AH	0.46	0/1284	1.22	17/1739 (1.0%)
31	BH	0.54	0/1284	1.26	17/1739 (1.0%)
32	AI	0.54	0/1146	1.19	10/1551 (0.6%)
32	BI	0.54	0/1146	1.17	12/1551 (0.8%)
33	AJ	0.59	0/640	1.23	10/889 (1.1%)
33	BJ	0.59	0/640	1.37	13/889 (1.5%)
34	AN	0.48	0/1131	1.19	15/1525 (1.0%)
34	BN	0.55	0/1131	1.21	15/1525 (1.0%)
35	AO	0.56	0/943	1.01	5/1269 (0.4%)
35	BO	0.57	0/943	1.02	6/1269 (0.5%)
36	AP	0.57	0/1131	1.43	24/1504 (1.6%)
36	BP	0.65	0/1131	1.46	23/1504 (1.5%)
37	AQ	0.47	0/1133	1.03	8/1515 (0.5%)
37	BQ	0.49	0/1133	1.05	10/1515 (0.7%)
38	AR	0.57	0/974	1.15	9/1302 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	BR	0.62	0/974	1.16	9/1302 (0.7%)
39	AS	0.45	0/778	1.14	11/1036 (1.1%)
39	BS	0.47	0/778	1.13	12/1036 (1.2%)
40	AT	0.58	0/1137	1.34	16/1519 (1.1%)
40	BT	0.60	0/1137	1.35	18/1519 (1.2%)
41	AU	0.54	0/975	1.13	7/1297 (0.5%)
41	BU	0.63	0/975	1.15	9/1297 (0.7%)
42	AV	0.49	0/790	1.03	2/1057 (0.2%)
42	BV	0.53	0/790	1.05	3/1057 (0.3%)
43	AW	0.55	0/907	1.07	5/1216 (0.4%)
43	BW	0.57	0/907	1.09	6/1216 (0.5%)
44	AX	0.50	0/739	0.98	2/993 (0.2%)
44	BX	0.56	0/739	1.02	3/993 (0.3%)
45	AY	0.57	0/788	1.26	8/1051 (0.8%)
45	BY	0.63	0/788	1.29	9/1051 (0.9%)
46	AZ	0.42	0/1499	1.04	8/2035 (0.4%)
46	BZ	0.46	0/1499	1.12	15/2035 (0.7%)
47	A0	0.48	0/671	0.99	6/892 (0.7%)
47	B0	0.50	0/671	0.99	6/892 (0.7%)
48	A1	0.51	1/738 (0.1%)	1.18	8/981 (0.8%)
48	B1	0.59	0/738	1.19	8/981 (0.8%)
49	A2	0.41	0/600	0.87	1/793 (0.1%)
49	B2	0.58	0/600	1.06	2/793 (0.3%)
50	A3	0.47	0/472	1.03	2/634 (0.3%)
50	B3	0.52	0/472	1.03	4/634 (0.6%)
51	A4	0.51	0/460	1.07	3/621 (0.5%)
51	B4	0.52	0/460	1.06	2/621 (0.3%)
52	A5	0.58	0/441	1.28	6/596 (1.0%)
52	B5	0.61	0/441	1.29	6/596 (1.0%)
53	A6	0.55	0/440	1.22	4/586 (0.7%)
53	B6	0.56	0/440	1.21	4/586 (0.7%)
54	A7	0.53	0/417	1.08	2/550 (0.4%)
54	B7	0.62	0/417	1.14	3/550 (0.5%)
55	A8	0.67	0/515	1.29	7/679 (1.0%)
55	B8	0.70	0/515	1.32	7/679 (1.0%)
56	A9	0.43	0/310	0.99	1/407 (0.2%)
56	B9	0.48	0/310	1.00	1/407 (0.2%)
57	AA	0.44	0/68704	0.70	67/107260 (0.1%)
57	BA	0.46	0/68704	0.72	69/107260 (0.1%)
58	AB	0.41	0/2853	0.66	0/4451
58	BB	0.43	0/2853	0.67	0/4451
All	All	0.46	1/321584 (0.0%)	0.81	988/480460 (0.2%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A1	67	ILE	CA-CB	-5.46	1.51	1.54

The worst 5 of 988 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	790	C	C2'-C3'-O3'	15.51	132.76	109.50
22	Ba	1498	U	C2'-C3'-O3'	15.41	132.61	109.50
57	AA	790	C	C2'-C3'-O3'	14.65	131.47	109.50
57	AA	1992	G	C2'-C3'-O3'	14.60	131.40	109.50
57	BA	1992	G	C2'-C3'-O3'	14.49	131.24	109.50

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
57	AA	1799	G	C3'
57	AA	1819	A	C3'
57	AA	1820	U	C3'
22	Ba	1498	U	C3'
57	BA	1799	G	C3'

5 of 125 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ab	1900	0	1951	303	0
1	Bb	1900	0	1951	305	0
2	Ac	1612	0	1677	231	0
2	Bc	1612	0	1677	225	0
3	Ad	1703	0	1763	243	0
3	Bd	1703	0	1764	239	0
4	Ae	1146	0	1207	156	0
4	Be	1146	0	1207	162	0
5	Af	843	0	857	89	0
5	Bf	843	0	857	94	0
6	Ag	1257	0	1296	146	0
6	Bg	1257	0	1296	149	0
7	Ah	1116	0	1177	149	0
7	Bh	1116	0	1177	149	0
8	Ai	1010	0	1037	180	0
8	Bi	1010	0	1037	187	0
9	Aj	794	0	840	197	0
9	Bj	794	0	840	187	0
10	Ak	885	0	904	121	0
10	Bk	885	0	904	125	0
11	Al	970	0	1057	125	0
11	Bl	970	0	1057	126	0
12	Am	937	0	992	223	0
12	Bm	937	0	990	225	0
13	An	492	0	530	74	0
13	Bn	492	0	530	70	0
14	Ao	734	0	771	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	Bo	734	0	771	81	0
15	Ap	700	0	720	78	0
15	Bp	700	0	720	81	0
16	Aq	823	0	891	65	0
16	Bq	823	0	891	65	0
17	Ar	574	0	644	77	0
17	Br	574	0	644	78	0
18	As	629	0	652	108	0
18	Bs	629	0	652	106	0
19	At	763	0	861	94	0
19	Bt	763	0	861	91	0
20	Au	208	0	221	20	0
20	Bu	208	0	221	21	0
21	Ay	782	0	827	128	0
21	By	782	0	827	146	0
22	Aa	32329	0	16316	1406	0
22	Ba	32329	0	16317	1421	0
23	Ax	260	0	129	15	0
23	Bx	260	0	129	25	0
24	Av	1641	0	839	46	0
24	Bv	1641	0	839	59	0
25	Aw	1640	0	837	76	0
25	Bw	1640	0	837	78	0
26	AC	937	0	957	122	0
26	BC	937	0	957	126	0
27	AD	2104	0	2182	333	0
27	BD	2104	0	2182	338	0
28	AE	1563	0	1629	274	0
28	BE	1563	0	1629	272	0
29	AF	1623	0	1677	230	0
29	BF	1623	0	1677	224	0
30	AG	1474	0	1533	354	0
30	BG	1474	0	1532	340	0
31	AH	1259	0	1326	201	0
31	BH	1259	0	1326	195	0
32	AI	1131	0	1218	254	0
32	BI	1131	0	1218	261	0
33	AJ	641	0	309	36	0
33	BJ	641	0	309	53	0
34	AN	1104	0	1180	158	0
34	BN	1104	0	1180	167	0
35	AO	933	0	996	103	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	BO	933	0	996	106	0
36	AP	1114	0	1187	308	0
36	BP	1114	0	1187	310	0
37	AQ	1112	0	1171	125	0
37	BQ	1112	0	1171	127	0
38	AR	960	0	1021	135	0
38	BR	960	0	1021	132	0
39	AS	770	0	832	148	0
39	BS	770	0	832	145	0
40	AT	1123	0	1181	249	0
40	BT	1123	0	1181	252	0
41	AU	958	0	1015	155	0
41	BU	958	0	1015	151	0
42	AV	779	0	852	152	0
42	BV	779	0	852	157	0
43	AW	896	0	953	97	0
43	BW	896	0	953	92	0
44	AX	725	0	778	94	0
44	BX	725	0	778	92	0
45	AY	775	0	870	198	0
45	BY	775	0	870	206	0
46	AZ	1467	0	1492	251	0
46	BZ	1467	0	1492	252	0
47	A0	662	0	688	78	0
47	B0	662	0	688	77	0
48	A1	731	0	808	105	0
48	B1	731	0	808	95	0
49	A2	598	0	653	102	0
49	B2	598	0	653	62	0
50	A3	467	0	523	39	0
50	B3	467	0	523	39	0
51	A4	450	0	449	92	0
51	B4	450	0	449	87	0
52	A5	427	0	445	85	0
52	B5	427	0	445	91	0
53	A6	433	0	461	118	0
53	B6	433	0	461	121	0
54	A7	409	0	454	40	0
54	B7	409	0	454	39	0
55	A8	507	0	576	115	0
55	B8	507	0	576	126	0
56	A9	307	0	336	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B9	307	0	336	25	0
57	AA	61341	0	30925	2164	0
57	BA	61341	0	30926	2165	0
58	AB	2551	0	1295	140	0
58	BB	2551	0	1295	116	0
59	A4	1	0	0	0	0
59	A9	1	0	0	0	0
59	Ad	1	0	0	0	0
59	An	1	0	0	0	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	Bd	1	0	0	1	0
59	Bn	1	0	0	0	0
60	A1	2	0	0	0	0
60	A5	1	0	0	0	0
60	A7	1	0	0	0	0
60	AA	367	0	0	0	0
60	AB	3	0	0	0	0
60	AD	2	0	0	0	0
60	AF	1	0	0	0	0
60	AQ	1	0	0	0	0
60	AX	1	0	0	0	0
60	Aa	145	0	0	0	0
60	Ae	2	0	0	0	0
60	Av	5	0	0	0	0
60	Aw	1	0	0	0	0
60	B0	2	0	0	0	0
60	B5	2	0	0	0	0
60	B7	2	0	0	0	0
60	BA	365	0	0	0	0
60	BB	3	0	0	0	0
60	BD	2	0	0	0	0
60	BF	1	0	0	0	0
60	BO	1	0	0	0	0
60	BX	1	0	0	0	0
60	Ba	143	0	0	0	0
60	Bd	1	0	0	0	0
60	Bl	1	0	0	0	0
60	Bm	1	0	0	0	0
60	Bv	5	0	0	0	0
60	Bw	1	0	0	0	0
60	Bx	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	297230	0	201936	20960	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

The worst 5 of 20960 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Bm:65:LYS:CB	12:Bm:66:LEU:HB2	1.40	1.52
12:Am:3:ARG:NH2	30:AG:113:ARG:HG2	1.26	1.43
12:Bm:108:ARG:CZ	12:Bm:114:ARG:HG2	1.48	1.42
12:Am:69:GLU:HA	12:Am:70:LEU:C	1.41	1.39
12:Am:3:ARG:CD	30:AG:113:ARG:HH12	1.36	1.36

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ab	232/256 (91%)	149 (64%)	48 (21%)	35 (15%)	0	2
1	Bb	232/256 (91%)	148 (64%)	52 (22%)	32 (14%)	0	3
2	Ac	204/239 (85%)	132 (65%)	43 (21%)	29 (14%)	0	3
2	Bc	204/239 (85%)	134 (66%)	41 (20%)	29 (14%)	0	3
3	Ad	206/209 (99%)	131 (64%)	52 (25%)	23 (11%)	0	4
3	Bd	206/209 (99%)	132 (64%)	51 (25%)	23 (11%)	0	4
4	Ae	148/162 (91%)	105 (71%)	24 (16%)	19 (13%)	0	3
4	Be	148/162 (91%)	104 (70%)	23 (16%)	21 (14%)	0	3
5	Af	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Bf	99/101 (98%)	66 (67%)	26 (26%)	7 (7%)	1	10
6	Ag	153/156 (98%)	108 (71%)	31 (20%)	14 (9%)	0	6
6	Bg	153/156 (98%)	106 (69%)	33 (22%)	14 (9%)	0	6
7	Ah	136/138 (99%)	97 (71%)	32 (24%)	7 (5%)	1	15
7	Bh	136/138 (99%)	97 (71%)	33 (24%)	6 (4%)	2	18
8	Ai	125/128 (98%)	83 (66%)	24 (19%)	18 (14%)	0	3
8	Bi	125/128 (98%)	82 (66%)	25 (20%)	18 (14%)	0	3
9	Aj	96/105 (91%)	76 (79%)	13 (14%)	7 (7%)	1	10
9	Bj	96/105 (91%)	76 (79%)	13 (14%)	7 (7%)	1	10
10	Ak	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	1	13
10	Bk	117/129 (91%)	87 (74%)	23 (20%)	7 (6%)	1	13
11	Al	122/132 (92%)	82 (67%)	25 (20%)	15 (12%)	0	4
11	Bl	122/132 (92%)	82 (67%)	24 (20%)	16 (13%)	0	3
12	Am	116/126 (92%)	58 (50%)	28 (24%)	30 (26%)	0	0
12	Bm	116/126 (92%)	66 (57%)	25 (22%)	25 (22%)	0	1
13	An	58/61 (95%)	38 (66%)	10 (17%)	10 (17%)	0	2
13	Bn	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	2
14	Ao	86/89 (97%)	52 (60%)	24 (28%)	10 (12%)	0	4
14	Bo	86/89 (97%)	52 (60%)	25 (29%)	9 (10%)	0	5
15	Ap	81/88 (92%)	55 (68%)	20 (25%)	6 (7%)	1	9
15	Bp	81/88 (92%)	55 (68%)	23 (28%)	3 (4%)	2	21
16	Aq	97/105 (92%)	74 (76%)	18 (19%)	5 (5%)	1	15
16	Bq	97/105 (92%)	73 (75%)	19 (20%)	5 (5%)	1	15
17	Ar	68/88 (77%)	43 (63%)	20 (29%)	5 (7%)	1	9
17	Br	68/88 (77%)	42 (62%)	21 (31%)	5 (7%)	1	9
18	As	76/93 (82%)	43 (57%)	20 (26%)	13 (17%)	0	2
18	Bs	76/93 (82%)	43 (57%)	20 (26%)	13 (17%)	0	2
19	At	97/106 (92%)	60 (62%)	25 (26%)	12 (12%)	0	4
19	Bt	97/106 (92%)	60 (62%)	25 (26%)	12 (12%)	0	4
20	Au	22/27 (82%)	13 (59%)	6 (27%)	3 (14%)	0	3
20	Bu	22/27 (82%)	12 (54%)	7 (32%)	3 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Ay	92/95 (97%)	51 (55%)	24 (26%)	17 (18%)	0	1
21	By	92/95 (97%)	58 (63%)	20 (22%)	14 (15%)	0	2
26	AC	116/229 (51%)	87 (75%)	25 (22%)	4 (3%)	3	23
26	BC	116/229 (51%)	86 (74%)	26 (22%)	4 (3%)	3	23
27	AD	269/276 (98%)	187 (70%)	50 (19%)	32 (12%)	0	4
27	BD	269/276 (98%)	190 (71%)	50 (19%)	29 (11%)	0	5
28	AE	202/206 (98%)	138 (68%)	35 (17%)	29 (14%)	0	3
28	BE	202/206 (98%)	140 (69%)	34 (17%)	28 (14%)	0	3
29	AF	205/210 (98%)	148 (72%)	29 (14%)	28 (14%)	0	3
29	BF	205/210 (98%)	148 (72%)	30 (15%)	27 (13%)	0	3
30	AG	179/182 (98%)	98 (55%)	47 (26%)	34 (19%)	0	1
30	BG	179/182 (98%)	99 (55%)	42 (24%)	38 (21%)	0	1
31	AH	162/180 (90%)	97 (60%)	36 (22%)	29 (18%)	0	1
31	BH	162/180 (90%)	97 (60%)	36 (22%)	29 (18%)	0	1
32	AI	143/148 (97%)	75 (52%)	44 (31%)	24 (17%)	0	2
32	BI	143/148 (97%)	76 (53%)	40 (28%)	27 (19%)	0	1
33	AJ	128/173 (74%)	46 (36%)	43 (34%)	39 (30%)	0	0
33	BJ	128/173 (74%)	40 (31%)	36 (28%)	52 (41%)	0	0
34	AN	136/140 (97%)	96 (71%)	23 (17%)	17 (12%)	0	4
34	BN	136/140 (97%)	98 (72%)	21 (15%)	17 (12%)	0	4
35	AO	120/122 (98%)	103 (86%)	11 (9%)	6 (5%)	1	16
35	BO	120/122 (98%)	103 (86%)	12 (10%)	5 (4%)	2	19
36	AP	144/150 (96%)	75 (52%)	37 (26%)	32 (22%)	0	0
36	BP	144/150 (96%)	75 (52%)	38 (26%)	31 (22%)	0	1
37	AQ	138/141 (98%)	105 (76%)	20 (14%)	13 (9%)	0	6
37	BQ	138/141 (98%)	105 (76%)	18 (13%)	15 (11%)	0	5
38	AR	115/118 (98%)	82 (71%)	21 (18%)	12 (10%)	0	5
38	BR	115/118 (98%)	83 (72%)	20 (17%)	12 (10%)	0	5
39	AS	96/112 (86%)	45 (47%)	29 (30%)	22 (23%)	0	0
39	BS	96/112 (86%)	45 (47%)	29 (30%)	22 (23%)	0	0
40	AT	133/146 (91%)	87 (65%)	19 (14%)	27 (20%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BT	133/146 (91%)	87 (65%)	20 (15%)	26 (20%)	0	1
41	AU	115/118 (98%)	86 (75%)	23 (20%)	6 (5%)	1	15
41	BU	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	1	13
42	AV	99/101 (98%)	66 (67%)	22 (22%)	11 (11%)	0	4
42	BV	99/101 (98%)	67 (68%)	20 (20%)	12 (12%)	0	4
43	AW	111/113 (98%)	85 (77%)	16 (14%)	10 (9%)	0	6
43	BW	111/113 (98%)	86 (78%)	14 (13%)	11 (10%)	0	6
44	AX	90/96 (94%)	65 (72%)	22 (24%)	3 (3%)	3	24
44	BX	90/96 (94%)	64 (71%)	24 (27%)	2 (2%)	5	30
45	AY	98/110 (89%)	45 (46%)	23 (24%)	30 (31%)	0	0
45	BY	98/110 (89%)	46 (47%)	21 (21%)	31 (32%)	0	0
46	AZ	182/206 (88%)	104 (57%)	46 (25%)	32 (18%)	0	1
46	BZ	182/206 (88%)	105 (58%)	46 (25%)	31 (17%)	0	2
47	A0	82/85 (96%)	62 (76%)	15 (18%)	5 (6%)	1	13
47	B0	82/85 (96%)	61 (74%)	16 (20%)	5 (6%)	1	13
48	A1	91/98 (93%)	66 (72%)	15 (16%)	10 (11%)	0	5
48	B1	91/98 (93%)	71 (78%)	11 (12%)	9 (10%)	0	6
49	A2	69/72 (96%)	41 (59%)	18 (26%)	10 (14%)	0	3
49	B2	69/72 (96%)	47 (68%)	16 (23%)	6 (9%)	0	7
50	A3	57/60 (95%)	48 (84%)	7 (12%)	2 (4%)	3	23
50	B3	57/60 (95%)	48 (84%)	7 (12%)	2 (4%)	3	23
51	A4	55/71 (78%)	22 (40%)	20 (36%)	13 (24%)	0	0
51	B4	55/71 (78%)	23 (42%)	19 (34%)	13 (24%)	0	0
52	A5	53/60 (88%)	37 (70%)	8 (15%)	8 (15%)	0	2
52	B5	53/60 (88%)	37 (70%)	8 (15%)	8 (15%)	0	2
53	A6	48/54 (89%)	22 (46%)	13 (27%)	13 (27%)	0	0
53	B6	48/54 (89%)	22 (46%)	13 (27%)	13 (27%)	0	0
54	A7	45/49 (92%)	42 (93%)	2 (4%)	1 (2%)	5	30
54	B7	45/49 (92%)	42 (93%)	2 (4%)	1 (2%)	5	30
55	A8	61/65 (94%)	35 (57%)	15 (25%)	11 (18%)	0	1
55	B8	61/65 (94%)	35 (57%)	15 (25%)	11 (18%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	A9	35/37 (95%)	25 (71%)	9 (26%)	1 (3%)	3	26
56	B9	35/37 (95%)	25 (71%)	9 (26%)	1 (3%)	3	26
All	All	12016/13122 (92%)	7873 (66%)	2533 (21%)	1610 (13%)	0	3

5 of 1610 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ab	202/220 (92%)	181 (90%)	21 (10%)	7	29
1	Bb	202/220 (92%)	181 (90%)	21 (10%)	7	29
2	Ac	160/188 (85%)	150 (94%)	10 (6%)	16	44
2	Bc	160/188 (85%)	150 (94%)	10 (6%)	16	44
3	Ad	180/181 (99%)	159 (88%)	21 (12%)	5	25
3	Bd	180/181 (99%)	160 (89%)	20 (11%)	6	27
4	Ae	115/123 (94%)	98 (85%)	17 (15%)	3	17
4	Be	115/123 (94%)	100 (87%)	15 (13%)	4	21
5	Af	90/90 (100%)	80 (89%)	10 (11%)	6	27
5	Bf	90/90 (100%)	80 (89%)	10 (11%)	6	27
6	Ag	126/127 (99%)	119 (94%)	7 (6%)	19	47
6	Bg	126/127 (99%)	119 (94%)	7 (6%)	19	47
7	Ah	119/119 (100%)	113 (95%)	6 (5%)	22	49
7	Bh	119/119 (100%)	113 (95%)	6 (5%)	22	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Ai	98/99 (99%)	87 (89%)	11 (11%)	6	27
8	Bi	98/99 (99%)	87 (89%)	11 (11%)	6	27
9	Aj	88/92 (96%)	81 (92%)	7 (8%)	11	37
9	Bj	88/92 (96%)	81 (92%)	7 (8%)	11	37
10	Ak	90/99 (91%)	84 (93%)	6 (7%)	15	42
10	Bk	90/99 (91%)	84 (93%)	6 (7%)	15	42
11	Al	104/109 (95%)	92 (88%)	12 (12%)	5	25
11	Bl	104/109 (95%)	90 (86%)	14 (14%)	4	21
12	Am	94/101 (93%)	84 (89%)	10 (11%)	6	28
12	Bm	94/101 (93%)	82 (87%)	12 (13%)	4	22
13	An	49/50 (98%)	47 (96%)	2 (4%)	27	53
13	Bn	49/50 (98%)	47 (96%)	2 (4%)	27	53
14	Ao	79/80 (99%)	74 (94%)	5 (6%)	16	44
14	Bo	79/80 (99%)	74 (94%)	5 (6%)	16	44
15	Ap	72/74 (97%)	68 (94%)	4 (6%)	19	47
15	Bp	72/74 (97%)	67 (93%)	5 (7%)	14	41
16	Aq	94/97 (97%)	90 (96%)	4 (4%)	26	52
16	Bq	94/97 (97%)	90 (96%)	4 (4%)	26	52
17	Ar	61/77 (79%)	60 (98%)	1 (2%)	55	69
17	Br	61/77 (79%)	59 (97%)	2 (3%)	33	58
18	As	69/80 (86%)	55 (80%)	14 (20%)	1	8
18	Bs	69/80 (86%)	55 (80%)	14 (20%)	1	8
19	At	76/82 (93%)	70 (92%)	6 (8%)	11	37
19	Bt	76/82 (93%)	70 (92%)	6 (8%)	11	37
20	Au	19/22 (86%)	19 (100%)	0	100	100
20	Bu	19/22 (86%)	19 (100%)	0	100	100
21	Ay	86/87 (99%)	77 (90%)	9 (10%)	6	29
21	By	86/87 (99%)	78 (91%)	8 (9%)	8	32
26	AC	99/181 (55%)	94 (95%)	5 (5%)	21	49
26	BC	99/181 (55%)	94 (95%)	5 (5%)	21	49
27	AD	213/218 (98%)	180 (84%)	33 (16%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BD	213/218 (98%)	180 (84%)	33 (16%)	2	16
28	AE	165/166 (99%)	132 (80%)	33 (20%)	1	8
28	BE	165/166 (99%)	131 (79%)	34 (21%)	1	8
29	AF	165/166 (99%)	144 (87%)	21 (13%)	4	22
29	BF	165/166 (99%)	145 (88%)	20 (12%)	5	23
30	AG	155/156 (99%)	138 (89%)	17 (11%)	6	27
30	BG	155/156 (99%)	129 (83%)	26 (17%)	2	13
31	AH	137/148 (93%)	121 (88%)	16 (12%)	5	25
31	BH	137/148 (93%)	121 (88%)	16 (12%)	5	25
32	AI	122/124 (98%)	99 (81%)	23 (19%)	1	9
32	BI	122/124 (98%)	100 (82%)	22 (18%)	2	11
34	AN	117/119 (98%)	100 (86%)	17 (14%)	3	18
34	BN	117/119 (98%)	100 (86%)	17 (14%)	3	18
35	AO	100/100 (100%)	89 (89%)	11 (11%)	6	27
35	BO	100/100 (100%)	89 (89%)	11 (11%)	6	27
36	AP	112/116 (97%)	90 (80%)	22 (20%)	1	8
36	BP	112/116 (97%)	90 (80%)	22 (20%)	1	8
37	AQ	110/111 (99%)	100 (91%)	10 (9%)	9	33
37	BQ	110/111 (99%)	99 (90%)	11 (10%)	7	30
38	AR	100/101 (99%)	85 (85%)	15 (15%)	3	17
38	BR	100/101 (99%)	84 (84%)	16 (16%)	2	15
39	AS	77/88 (88%)	63 (82%)	14 (18%)	2	11
39	BS	77/88 (88%)	62 (80%)	15 (20%)	1	9
40	AT	118/127 (93%)	97 (82%)	21 (18%)	2	11
40	BT	118/127 (93%)	97 (82%)	21 (18%)	2	11
41	AU	92/94 (98%)	81 (88%)	11 (12%)	5	24
41	BU	92/94 (98%)	80 (87%)	12 (13%)	4	21
42	AV	82/82 (100%)	68 (83%)	14 (17%)	2	13
42	BV	82/82 (100%)	68 (83%)	14 (17%)	2	13
43	AW	91/92 (99%)	79 (87%)	12 (13%)	4	21
43	BW	91/92 (99%)	79 (87%)	12 (13%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	AX	74/78 (95%)	63 (85%)	11 (15%)	3	17
44	BX	74/78 (95%)	63 (85%)	11 (15%)	3	17
45	AY	84/91 (92%)	71 (84%)	13 (16%)	2	16
45	BY	84/91 (92%)	71 (84%)	13 (16%)	2	16
46	AZ	162/179 (90%)	138 (85%)	24 (15%)	3	17
46	BZ	162/179 (90%)	134 (83%)	28 (17%)	2	12
47	A0	66/67 (98%)	57 (86%)	9 (14%)	3	20
47	B0	66/67 (98%)	58 (88%)	8 (12%)	5	23
48	A1	78/83 (94%)	66 (85%)	12 (15%)	2	16
48	B1	78/83 (94%)	61 (78%)	17 (22%)	1	7
49	A2	66/67 (98%)	62 (94%)	4 (6%)	17	45
49	B2	66/67 (98%)	50 (76%)	16 (24%)	1	5
50	A3	51/52 (98%)	45 (88%)	6 (12%)	5	24
50	B3	51/52 (98%)	45 (88%)	6 (12%)	5	24
51	A4	51/63 (81%)	40 (78%)	11 (22%)	1	7
51	B4	51/63 (81%)	41 (80%)	10 (20%)	1	8
52	A5	47/52 (90%)	41 (87%)	6 (13%)	4	22
52	B5	47/52 (90%)	42 (89%)	5 (11%)	6	28
53	A6	49/52 (94%)	39 (80%)	10 (20%)	1	8
53	B6	49/52 (94%)	39 (80%)	10 (20%)	1	8
54	A7	40/42 (95%)	35 (88%)	5 (12%)	4	22
54	B7	40/42 (95%)	35 (88%)	5 (12%)	4	22
55	A8	53/55 (96%)	43 (81%)	10 (19%)	1	9
55	B8	53/55 (96%)	43 (81%)	10 (19%)	1	9
56	A9	34/34 (100%)	34 (100%)	0	100	100
56	B9	34/34 (100%)	34 (100%)	0	100	100
All	All	9962/10602 (94%)	8732 (88%)	1230 (12%)	4	23

5 of 1230 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	BI	85	GLU
47	B0	14	ARG

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Mol	Chain	Res	Type
34	BN	108	PRO
32	BI	81	VAL
40	BT	49	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 356 such sidechains are listed below:

Mol	Chain	Res	Type
10	Bk	104	GLN
30	BG	130	ASN
12	Bm	92	HIS
27	BD	58	HIS
36	BP	68	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	Aa	1503/1504 (99%)	211 (14%)	0
22	Ba	1503/1504 (99%)	210 (13%)	0
23	Ax	11/14 (78%)	8 (72%)	0
23	Bx	11/14 (78%)	8 (72%)	0
24	Av	76/77 (98%)	15 (19%)	0
24	Bv	76/77 (98%)	17 (22%)	0
25	Aw	76/77 (98%)	11 (14%)	0
25	Bw	76/77 (98%)	8 (10%)	0
57	AA	2847/2848 (99%)	523 (18%)	55 (1%)
57	BA	2847/2848 (99%)	520 (18%)	56 (1%)
58	AB	118/119 (99%)	21 (17%)	1 (0%)
58	BB	118/119 (99%)	21 (17%)	1 (0%)
All	All	9262/9278 (99%)	1573 (16%)	113 (1%)

5 of 1573 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 113 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	BA	71	A
57	BA	2611	U
57	BA	587	C
57	BA	2481	G
57	BA	2126	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	5MU	Av	54	24	19,22,23	0.27	0	27,32,35	0.39	0
23	CCC	Bx	21	-	0,2,26	-	-	0,1,41	-	-
23	CCC	Ax	21	-	0,2,26	-	-	0,1,41	-	-
24	5MU	Bv	54	24	19,22,23	0.33	0	27,32,35	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	5MU	Av	54	24	-	0/7/25/26	0/2/2/2
24	5MU	Bv	54	24	-	0/7/25/26	0/2/2/2

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.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Av	54	5MU	1	0
23	Bx	21	CCC	5	0
24	Bv	54	5MU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Ab	234/256 (91%)	0.28	7 (2%) 52 30	114, 153, 181, 193	0
1	Bb	234/256 (91%)	0.30	7 (2%) 52 30	113, 152, 181, 193	0
2	Ac	206/239 (86%)	0.30	2 (0%) 79 54	123, 150, 166, 178	0
2	Bc	206/239 (86%)	0.25	5 (2%) 59 34	124, 149, 166, 179	0
3	Ad	208/209 (99%)	0.42	9 (4%) 40 22	96, 119, 144, 155	0
3	Bd	208/209 (99%)	0.41	7 (3%) 48 27	97, 119, 145, 154	0
4	Ae	150/162 (92%)	0.13	1 (0%) 84 61	88, 114, 138, 159	0
4	Be	150/162 (92%)	0.15	1 (0%) 84 61	84, 112, 138, 160	0
5	Af	101/101 (100%)	0.03	2 (1%) 65 38	91, 121, 138, 155	0
5	Bf	101/101 (100%)	0.24	5 (4%) 34 19	91, 120, 137, 155	0
6	Ag	155/156 (99%)	0.32	8 (5%) 33 19	118, 137, 171, 188	0
6	Bg	155/156 (99%)	0.32	6 (3%) 43 24	118, 138, 171, 188	0
7	Ah	138/138 (100%)	0.27	8 (5%) 29 17	96, 117, 132, 157	0
7	Bh	138/138 (100%)	0.19	7 (5%) 33 19	95, 116, 131, 158	0
8	Ai	127/128 (99%)	0.88	16 (12%) 8 7	120, 160, 178, 186	0
8	Bi	127/128 (99%)	0.74	9 (7%) 22 14	119, 160, 178, 186	0
9	Aj	98/105 (93%)	0.70	4 (4%) 41 23	126, 164, 184, 190	0
9	Bj	98/105 (93%)	0.58	2 (2%) 65 38	124, 164, 184, 190	0
10	Ak	119/129 (92%)	0.16	3 (2%) 58 34	89, 117, 145, 171	0
10	Bk	119/129 (92%)	0.21	4 (3%) 48 27	89, 117, 144, 171	0
11	Al	124/132 (93%)	0.31	6 (4%) 35 20	75, 97, 123, 161	0
11	Bl	124/132 (93%)	0.33	6 (4%) 35 20	77, 97, 125, 162	0
12	Am	118/126 (93%)	0.80	14 (11%) 9 8	115, 143, 157, 166	0
12	Bm	118/126 (93%)	0.59	8 (6%) 23 15	115, 142, 157, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	An	60/61 (98%)	1.42	15 (25%) 2 2	126, 139, 159, 162	0
13	Bn	60/61 (98%)	0.69	4 (6%) 24 15	127, 138, 159, 162	0
14	Ao	88/89 (98%)	0.05	2 (2%) 61 35	81, 110, 131, 138	0
14	Bo	88/89 (98%)	0.14	2 (2%) 61 35	81, 110, 132, 137	0
15	Ap	83/88 (94%)	0.60	2 (2%) 59 34	93, 110, 128, 148	0
15	Bp	83/88 (94%)	0.39	3 (3%) 46 26	94, 111, 130, 147	0
16	Aq	99/105 (94%)	0.24	4 (4%) 42 24	80, 107, 124, 132	0
16	Bq	99/105 (94%)	0.20	4 (4%) 42 24	80, 107, 123, 132	0
17	Ar	70/88 (79%)	0.27	3 (4%) 40 22	96, 122, 142, 158	0
17	Br	70/88 (79%)	0.20	0 100 100	95, 122, 141, 157	0
18	As	78/93 (83%)	0.62	9 (11%) 9 8	131, 153, 173, 181	0
18	Bs	78/93 (83%)	0.58	4 (5%) 33 19	130, 153, 172, 181	0
19	At	99/106 (93%)	0.49	8 (8%) 18 12	86, 114, 145, 149	0
19	Bt	99/106 (93%)	0.29	3 (3%) 52 30	86, 114, 145, 149	0
20	Au	24/27 (88%)	1.37	4 (16%) 4 5	108, 138, 162, 168	0
20	Bu	24/27 (88%)	1.69	6 (25%) 2 2	106, 137, 162, 168	0
21	Ay	94/95 (98%)	0.51	7 (7%) 20 14	118, 154, 186, 189	0
21	By	94/95 (98%)	0.45	8 (8%) 16 12	110, 146, 182, 188	0
22	Aa	1504/1504 (100%)	0.31	41 (2%) 56 32	65, 119, 193, 208	0
22	Ba	1504/1504 (100%)	0.29	36 (2%) 59 34	63, 119, 193, 208	0
23	Ax	12/14 (85%)	1.32	3 (25%) 2 2	108, 191, 198, 199	0
23	Bx	12/14 (85%)	2.62	8 (66%) 0 0	108, 191, 198, 199	0
24	Av	76/77 (98%)	0.15	1 (1%) 75 48	96, 119, 160, 163	0
24	Bv	76/77 (98%)	-0.07	1 (1%) 75 48	69, 107, 141, 167	0
25	Aw	77/77 (100%)	0.32	2 (2%) 57 33	103, 191, 201, 203	0
25	Bw	77/77 (100%)	0.12	2 (2%) 57 33	93, 188, 200, 202	0
26	AC	120/229 (52%)	0.45	6 (5%) 34 19	147, 177, 190, 193	0
26	BC	120/229 (52%)	0.46	4 (3%) 49 28	145, 177, 189, 194	0
27	AD	271/276 (98%)	0.11	9 (3%) 49 28	48, 76, 98, 121	0
27	BD	271/276 (98%)	0.07	5 (1%) 67 40	46, 75, 96, 122	0
28	AE	204/206 (99%)	0.11	4 (1%) 65 38	49, 81, 127, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	BE	204/206 (99%)	0.16	8 (3%) 43 24	49, 80, 128, 148	0
29	AF	207/210 (98%)	0.04	2 (0%) 79 54	48, 89, 153, 181	0
29	BF	207/210 (98%)	0.17	4 (1%) 66 39	46, 86, 154, 180	0
30	AG	181/182 (99%)	0.39	4 (2%) 62 36	117, 142, 161, 186	0
30	BG	181/182 (99%)	0.30	3 (1%) 69 41	99, 128, 154, 175	0
31	AH	164/180 (91%)	0.39	6 (3%) 45 25	98, 127, 143, 166	0
31	BH	164/180 (91%)	0.90	21 (12%) 7 7	94, 124, 141, 164	0
32	AI	145/148 (97%)	1.30	36 (24%) 2 2	81, 154, 171, 176	0
32	BI	145/148 (97%)	1.12	27 (18%) 3 4	82, 153, 172, 176	0
33	AJ	130/173 (75%)	0.71	13 (10%) 12 10	170, 195, 202, 203	0
33	BJ	130/173 (75%)	1.13	27 (20%) 2 3	147, 180, 194, 196	0
34	AN	138/140 (98%)	0.14	3 (2%) 62 36	65, 91, 126, 138	0
34	BN	138/140 (98%)	0.34	3 (2%) 62 36	63, 88, 126, 136	0
35	AO	122/122 (100%)	-0.20	0 100 100	59, 75, 98, 122	0
35	BO	122/122 (100%)	-0.21	0 100 100	56, 74, 99, 120	0
36	AP	146/150 (97%)	0.66	10 (6%) 23 15	51, 106, 133, 169	0
36	BP	146/150 (97%)	0.82	17 (11%) 9 8	50, 104, 133, 169	0
37	AQ	140/141 (99%)	0.33	6 (4%) 40 22	75, 96, 124, 147	0
37	BQ	140/141 (99%)	0.38	5 (3%) 46 26	74, 94, 125, 147	0
38	AR	117/118 (99%)	0.14	3 (2%) 57 33	48, 80, 108, 128	0
38	BR	117/118 (99%)	0.19	4 (3%) 48 27	47, 79, 107, 127	0
39	AS	98/112 (87%)	0.94	16 (16%) 4 5	111, 137, 154, 161	0
39	BS	98/112 (87%)	1.00	14 (14%) 6 6	110, 136, 153, 162	0
40	AT	135/146 (92%)	0.34	9 (6%) 24 15	66, 92, 150, 183	0
40	BT	135/146 (92%)	0.37	6 (4%) 39 22	66, 92, 150, 183	0
41	AU	117/118 (99%)	0.09	2 (1%) 69 41	58, 81, 117, 156	0
41	BU	117/118 (99%)	0.30	3 (2%) 57 33	52, 78, 116, 158	0
42	AV	101/101 (100%)	0.15	2 (1%) 65 38	59, 106, 125, 134	0
42	BV	101/101 (100%)	0.24	1 (0%) 79 54	54, 103, 125, 134	0
43	AW	113/113 (100%)	-0.12	0 100 100	58, 73, 106, 183	0
43	BW	113/113 (100%)	-0.01	0 100 100	55, 71, 105, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AX	92/96 (95%)	0.18	2 (2%) 62 36	63, 86, 110, 120	0
44	BX	92/96 (95%)	0.36	0 100 100	56, 84, 110, 120	0
45	AY	100/110 (90%)	0.71	6 (6%) 27 17	78, 117, 153, 160	0
45	BY	100/110 (90%)	1.05	15 (15%) 5 5	74, 115, 152, 158	0
46	AZ	184/206 (89%)	0.17	1 (0%) 87 66	117, 141, 158, 188	0
46	BZ	184/206 (89%)	0.23	3 (1%) 70 43	87, 126, 150, 173	0
47	A0	84/85 (98%)	0.46	5 (5%) 27 17	81, 100, 148, 168	0
47	B0	84/85 (98%)	0.64	7 (8%) 17 12	78, 100, 148, 168	0
48	A1	93/98 (94%)	0.15	0 100 100	64, 87, 127, 137	0
48	B1	93/98 (94%)	0.22	2 (2%) 62 36	55, 82, 119, 133	0
49	A2	71/72 (98%)	0.13	1 (1%) 73 46	81, 116, 134, 156	0
49	B2	71/72 (98%)	0.06	1 (1%) 73 46	51, 85, 123, 159	0
50	A3	59/60 (98%)	0.24	1 (1%) 69 41	70, 94, 112, 162	0
50	B3	59/60 (98%)	0.29	1 (1%) 69 41	62, 91, 111, 162	0
51	A4	57/71 (80%)	0.27	1 (1%) 67 40	150, 164, 175, 177	0
51	B4	57/71 (80%)	0.55	3 (5%) 32 19	150, 164, 174, 177	0
52	A5	55/60 (91%)	0.35	2 (3%) 46 26	54, 80, 113, 119	0
52	B5	55/60 (91%)	0.24	2 (3%) 46 26	54, 78, 112, 121	0
53	A6	50/54 (92%)	1.05	9 (18%) 3 4	121, 149, 165, 175	0
53	B6	50/54 (92%)	0.97	7 (14%) 6 6	121, 149, 164, 176	0
54	A7	47/49 (95%)	0.12	1 (2%) 63 37	50, 64, 86, 133	0
54	B7	47/49 (95%)	0.04	1 (2%) 63 37	47, 60, 84, 131	0
55	A8	63/65 (96%)	0.70	3 (4%) 35 20	66, 83, 117, 146	0
55	B8	63/65 (96%)	0.76	4 (6%) 26 16	63, 83, 116, 145	0
56	A9	37/37 (100%)	1.60	12 (32%) 1 1	121, 134, 149, 151	0
56	B9	37/37 (100%)	1.30	8 (21%) 2 3	121, 132, 148, 152	0
57	AA	2848/2848 (100%)	-0.06	39 (1%) 73 46	47, 83, 185, 208	0
57	BA	2848/2848 (100%)	0.04	57 (2%) 65 38	44, 80, 185, 208	0
58	AB	119/119 (100%)	0.50	7 (5%) 28 17	90, 143, 176, 196	0
58	BB	119/119 (100%)	0.79	9 (7%) 20 13	86, 142, 175, 197	0
All	All	21500/22400 (95%)	0.27	822 (3%) 44 25	44, 108, 181, 208	0

The worst 5 of 822 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	BI	88	ILE	10.5
8	Ai	106	ALA	9.2
10	Bk	129	SER	8.8
32	AI	72	LEU	8.6
32	BI	92	VAL	8.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	5MU	Av	54	21/22	0.83	0.10	130,133,148,148	0
24	5MU	Bv	54	21/22	0.87	0.11	114,116,124,125	0
23	CCC	Bx	21	3/24	0.96	0.46	20,20,20,20	0
23	CCC	Ax	21	3/24	0.96	0.44	20,20,20,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	AA	3262	1/1	-0.07	0.26	81,81,81,81	0
60	MG	Aa	1727	1/1	0.05	0.46	98,98,98,98	1
60	MG	Aa	1601	1/1	0.05	0.35	123,123,123,123	0
60	MG	Aa	1742	1/1	0.19	0.31	106,106,106,106	0
60	MG	Aa	1648	1/1	0.27	0.22	121,121,121,121	0
60	MG	Ba	1665	1/1	0.31	0.48	144,144,144,144	0
60	MG	Ba	1708	1/1	0.32	0.13	132,132,132,132	0
60	MG	Aa	1663	1/1	0.34	0.22	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Aa	1713	1/1	0.35	0.41	98,98,98,98	0
60	MG	BA	3258	1/1	0.35	0.31	84,84,84,84	0
60	MG	Aa	1669	1/1	0.36	0.41	122,122,122,122	0
60	MG	Ba	1715	1/1	0.36	0.16	94,94,94,94	0
60	MG	AA	3210	1/1	0.36	0.21	115,115,115,115	0
60	MG	AA	3263	1/1	0.37	0.16	75,75,75,75	0
60	MG	Aa	1704	1/1	0.39	0.27	29,29,29,29	1
60	MG	Ba	1713	1/1	0.39	0.32	83,83,83,83	0
60	MG	AA	3154	1/1	0.40	0.11	142,142,142,142	0
60	MG	Ba	1681	1/1	0.40	0.47	122,122,122,122	0
60	MG	Ba	1712	1/1	0.42	0.22	79,79,79,79	0
60	MG	Bw	101	1/1	0.43	0.19	132,132,132,132	1
60	MG	Aa	1700	1/1	0.44	0.46	114,114,114,114	0
60	MG	Ba	1729	1/1	0.44	0.36	66,66,66,66	0
60	MG	AA	3132	1/1	0.48	0.27	78,78,78,78	0
60	MG	Aa	1679	1/1	0.48	0.18	116,116,116,116	0
60	MG	Ba	1663	1/1	0.48	0.22	85,85,85,85	0
60	MG	Aa	1703	1/1	0.48	0.40	94,94,94,94	0
60	MG	Ba	1692	1/1	0.49	0.31	83,83,83,83	0
60	MG	AA	3240	1/1	0.49	0.33	106,106,106,106	0
60	MG	Ba	1724	1/1	0.50	0.27	68,68,68,68	0
60	MG	Ba	1737	1/1	0.50	0.37	76,76,76,76	0
60	MG	Ba	1707	1/1	0.51	0.28	76,76,76,76	0
60	MG	Bv	104	1/1	0.51	0.33	75,75,75,75	1
60	MG	AA	3192	1/1	0.52	0.30	101,101,101,101	0
60	MG	AA	3117	1/1	0.52	0.52	148,148,148,148	0
60	MG	Ba	1644	1/1	0.53	0.27	67,67,67,67	0
60	MG	AA	3134	1/1	0.53	0.23	98,98,98,98	0
60	MG	BA	3207	1/1	0.54	0.18	118,118,118,118	0
60	MG	AA	3088	1/1	0.54	0.27	85,85,85,85	0
60	MG	Ba	1721	1/1	0.55	0.22	92,92,92,92	0
60	MG	BA	3198	1/1	0.55	0.41	91,91,91,91	0
60	MG	Ba	1695	1/1	0.56	0.14	86,86,86,86	0
60	MG	Aa	1675	1/1	0.56	0.32	72,72,72,72	0
60	MG	BA	3151	1/1	0.56	0.30	119,119,119,119	0
60	MG	Ba	1677	1/1	0.56	0.13	138,138,138,138	0
60	MG	AA	3168	1/1	0.56	0.12	82,82,82,82	0
60	MG	BA	3233	1/1	0.56	0.39	97,97,97,97	0
60	MG	Aa	1725	1/1	0.56	0.25	74,74,74,74	0
60	MG	BA	3131	1/1	0.57	0.27	96,96,96,96	0
60	MG	Ba	1653	1/1	0.57	0.19	74,74,74,74	0
60	MG	AA	2943	1/1	0.58	0.29	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	1602	1/1	0.58	0.44	126,126,126,126	0
60	MG	AA	3245	1/1	0.58	0.17	97,97,97,97	0
60	MG	AA	3256	1/1	0.58	0.27	71,71,71,71	0
60	MG	BA	3180	1/1	0.58	0.41	105,105,105,105	0
60	MG	AA	3260	1/1	0.58	0.37	80,80,80,80	0
60	MG	AA	3155	1/1	0.58	0.17	92,92,92,92	1
60	MG	Aa	1698	1/1	0.58	0.36	98,98,98,98	1
60	MG	Aa	1676	1/1	0.58	0.34	90,90,90,90	1
60	MG	BA	3261	1/1	0.58	0.26	68,68,68,68	0
60	MG	AA	3100	1/1	0.59	0.38	97,97,97,97	0
60	MG	Aa	1646	1/1	0.59	0.28	102,102,102,102	0
60	MG	BA	2958	1/1	0.60	0.40	88,88,88,88	0
60	MG	BA	3126	1/1	0.60	0.22	122,122,122,122	0
60	MG	AA	3162	1/1	0.60	0.36	94,94,94,94	0
60	MG	AA	3248	1/1	0.60	0.42	106,106,106,106	0
60	MG	Ba	1733	1/1	0.60	0.19	86,86,86,86	0
60	MG	AA	3153	1/1	0.61	0.27	71,71,71,71	0
60	MG	Ae	201	1/1	0.61	0.41	108,108,108,108	0
60	MG	Aa	1688	1/1	0.62	0.13	63,63,63,63	1
60	MG	BA	2945	1/1	0.62	0.21	112,112,112,112	0
60	MG	Ba	1601	1/1	0.62	0.34	90,90,90,90	0
60	MG	AA	3073	1/1	0.62	0.36	78,78,78,78	0
60	MG	BA	3257	1/1	0.63	0.19	72,72,72,72	0
60	MG	BA	3225	1/1	0.63	0.27	38,38,38,38	0
60	MG	AA	3231	1/1	0.63	0.28	51,51,51,51	0
60	MG	AA	3061	1/1	0.64	0.33	42,42,42,42	0
60	MG	Aa	1647	1/1	0.64	0.19	138,138,138,138	0
60	MG	AA	3109	1/1	0.65	0.30	78,78,78,78	0
60	MG	Ba	1656	1/1	0.65	0.16	73,73,73,73	0
60	MG	Aa	1723	1/1	0.65	0.23	83,83,83,83	0
60	MG	AA	3238	1/1	0.65	0.22	75,75,75,75	0
60	MG	BA	3209	1/1	0.65	0.25	74,74,74,74	0
60	MG	AA	3220	1/1	0.66	0.10	54,54,54,54	0
60	MG	BA	2952	1/1	0.66	0.21	102,102,102,102	0
60	MG	Aa	1718	1/1	0.66	0.40	84,84,84,84	0
60	MG	AA	3206	1/1	0.66	0.23	115,115,115,115	0
60	MG	AA	3191	1/1	0.66	0.30	74,74,74,74	0
60	MG	Ba	1703	1/1	0.66	0.31	25,25,25,25	1
60	MG	BA	3154	1/1	0.66	0.11	73,73,73,73	1
60	MG	Ba	1706	1/1	0.66	0.46	104,104,104,104	0
60	MG	AQ	201	1/1	0.67	0.41	94,94,94,94	0
60	MG	BA	3074	1/1	0.67	0.36	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	BA	3240	1/1	0.67	0.27	84,84,84,84	0
60	MG	Aa	1665	1/1	0.67	0.39	120,120,120,120	0
60	MG	Ba	1735	1/1	0.67	0.08	122,122,122,122	0
60	MG	Ba	1604	1/1	0.67	0.26	75,75,75,75	0
60	MG	Ba	1643	1/1	0.68	0.22	108,108,108,108	0
60	MG	AA	3261	1/1	0.68	0.31	76,76,76,76	0
60	MG	BA	3098	1/1	0.68	0.28	52,52,52,52	0
60	MG	BA	3099	1/1	0.68	0.41	90,90,90,90	0
60	MG	Ba	1646	1/1	0.68	0.19	128,128,128,128	0
60	MG	Aa	1674	1/1	0.68	0.12	90,90,90,90	0
60	MG	AA	2954	1/1	0.68	0.26	112,112,112,112	0
60	MG	Ae	202	1/1	0.68	0.38	89,89,89,89	0
60	MG	AA	3072	1/1	0.68	0.32	122,122,122,122	0
60	MG	Aa	1622	1/1	0.69	0.32	79,79,79,79	0
60	MG	BA	3205	1/1	0.69	0.23	92,92,92,92	0
60	MG	Ba	1669	1/1	0.69	0.17	94,94,94,94	0
60	MG	AA	3264	1/1	0.69	0.40	78,78,78,78	0
60	MG	AA	3265	1/1	0.69	0.26	70,70,70,70	0
60	MG	AA	3077	1/1	0.69	0.16	99,99,99,99	0
60	MG	AA	2917	1/1	0.69	0.18	112,112,112,112	0
60	MG	BA	3252	1/1	0.69	0.12	40,40,40,40	0
60	MG	Ba	1696	1/1	0.69	0.23	83,83,83,83	0
60	MG	BA	2947	1/1	0.69	0.23	44,44,44,44	0
60	MG	Ba	1630	1/1	0.69	0.33	76,76,76,76	0
60	MG	Aa	1686	1/1	0.70	0.09	37,37,37,37	1
60	MG	Aa	1631	1/1	0.70	0.30	72,72,72,72	0
60	MG	Aa	1632	1/1	0.70	0.29	72,72,72,72	0
60	MG	BA	3247	1/1	0.70	0.17	54,54,54,54	0
60	MG	Ba	1699	1/1	0.70	0.31	88,88,88,88	0
60	MG	Aa	1614	1/1	0.70	0.14	69,69,69,69	0
60	MG	AA	3130	1/1	0.70	0.28	76,76,76,76	0
60	MG	AA	3081	1/1	0.70	0.23	99,99,99,99	0
60	MG	Bm	201	1/1	0.71	0.21	118,118,118,118	0
60	MG	AA	3204	1/1	0.71	0.17	51,51,51,51	0
60	MG	Ba	1702	1/1	0.71	0.50	97,97,97,97	0
60	MG	AA	3141	1/1	0.71	0.28	86,86,86,86	0
60	MG	Aa	1662	1/1	0.71	0.28	73,73,73,73	0
60	MG	AA	3247	1/1	0.71	0.15	103,103,103,103	0
60	MG	Ba	1738	1/1	0.71	0.24	106,106,106,106	0
60	MG	Aa	1734	1/1	0.71	0.28	84,84,84,84	0
60	MG	Ba	1688	1/1	0.71	0.22	120,120,120,120	1
60	MG	AX	101	1/1	0.71	0.19	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Bl	201	1/1	0.71	0.17	5,5,5,5	1
60	MG	Ba	1679	1/1	0.72	0.25	92,92,92,92	0
60	MG	AB	201	1/1	0.72	0.20	63,63,63,63	0
60	MG	BA	3222	1/1	0.72	0.24	61,61,61,61	0
60	MG	AA	3148	1/1	0.72	0.08	77,77,77,77	0
60	MG	Ba	1711	1/1	0.72	0.13	123,123,123,123	0
60	MG	Aa	1736	1/1	0.72	0.15	117,117,117,117	0
60	MG	AA	3097	1/1	0.72	0.10	43,43,43,43	0
60	MG	AA	3214	1/1	0.72	0.42	88,88,88,88	0
60	MG	Ba	1621	1/1	0.72	0.29	82,82,82,82	0
60	MG	Aw	101	1/1	0.72	0.08	83,83,83,83	1
60	MG	AA	3196	1/1	0.72	0.33	70,70,70,70	0
60	MG	BA	3012	1/1	0.73	0.28	61,61,61,61	0
60	MG	AA	3203	1/1	0.73	0.16	66,66,66,66	0
60	MG	BA	3236	1/1	0.73	0.31	116,116,116,116	0
60	MG	BO	201	1/1	0.73	0.37	122,122,122,122	0
60	MG	BA	3202	1/1	0.73	0.10	76,76,76,76	0
60	MG	Ba	1697	1/1	0.73	0.29	93,93,93,93	1
60	MG	Aa	1621	1/1	0.73	0.09	89,89,89,89	0
60	MG	AA	3149	1/1	0.73	0.35	100,100,100,100	0
60	MG	Ba	1605	1/1	0.73	0.34	73,73,73,73	0
60	MG	AA	3036	1/1	0.74	0.34	100,100,100,100	0
60	MG	BA	3188	1/1	0.74	0.21	64,64,64,64	0
60	MG	BA	3234	1/1	0.74	0.27	74,74,74,74	0
60	MG	BA	3189	1/1	0.74	0.26	75,75,75,75	0
60	MG	Ba	1676	1/1	0.74	0.71	137,137,137,137	1
60	MG	AA	3167	1/1	0.74	0.14	73,73,73,73	0
60	MG	Aa	1615	1/1	0.74	0.42	53,53,53,53	0
60	MG	BA	3254	1/1	0.74	0.49	66,66,66,66	0
60	MG	AA	3205	1/1	0.74	0.19	51,51,51,51	0
60	MG	Aa	1667	1/1	0.74	0.25	78,78,78,78	0
60	MG	Aa	1655	1/1	0.74	0.18	87,87,87,87	0
60	MG	BA	3264	1/1	0.74	0.45	89,89,89,89	0
60	MG	AA	3111	1/1	0.75	0.38	54,54,54,54	0
60	MG	Aa	1744	1/1	0.75	0.30	87,87,87,87	0
60	MG	AA	3120	1/1	0.75	0.15	76,76,76,76	0
60	MG	AA	3189	1/1	0.75	0.27	107,107,107,107	0
60	MG	Aa	1692	1/1	0.75	0.32	46,46,46,46	0
60	MG	Aa	1645	1/1	0.75	0.35	79,79,79,79	0
60	MG	Aa	1610	1/1	0.75	0.17	115,115,115,115	0
60	MG	Aa	1719	1/1	0.75	0.38	101,101,101,101	0
60	MG	Ba	1684	1/1	0.75	0.26	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	Ba	1720	1/1	0.75	0.24	91,91,91,91	0
60	MG	Ba	1687	1/1	0.75	0.14	50,50,50,50	1
60	MG	BA	3238	1/1	0.75	0.38	113,113,113,113	0
60	MG	BA	3118	1/1	0.75	0.15	70,70,70,70	0
60	MG	BA	3243	1/1	0.75	0.43	111,111,111,111	0
60	MG	BA	3244	1/1	0.75	0.23	91,91,91,91	0
60	MG	AA	2928	1/1	0.75	0.49	110,110,110,110	0
60	MG	Aa	1741	1/1	0.75	0.37	79,79,79,79	0
60	MG	BA	3132	1/1	0.75	0.18	43,43,43,43	0
60	MG	Aa	1690	1/1	0.75	0.18	49,49,49,49	0
60	MG	AA	2957	1/1	0.75	0.16	72,72,72,72	0
60	MG	Ba	1647	1/1	0.75	0.31	117,117,117,117	0
60	MG	AA	2968	1/1	0.75	0.37	76,76,76,76	0
60	MG	AA	3218	1/1	0.76	0.40	98,98,98,98	0
60	MG	BA	3216	1/1	0.76	0.33	117,117,117,117	0
60	MG	AA	3028	1/1	0.76	0.27	60,60,60,60	0
60	MG	Ba	1612	1/1	0.76	0.10	82,82,82,82	0
60	MG	Ba	1615	1/1	0.76	0.14	81,81,81,81	0
60	MG	Aa	1706	1/1	0.76	0.31	54,54,54,54	0
60	MG	AA	2941	1/1	0.76	0.36	92,92,92,92	0
60	MG	Ba	1739	1/1	0.76	0.25	53,53,53,53	0
60	MG	Ba	1641	1/1	0.76	0.36	94,94,94,94	0
60	MG	AA	3165	1/1	0.76	0.17	97,97,97,97	0
60	MG	Aa	1611	1/1	0.76	0.31	60,60,60,60	0
60	MG	BA	3186	1/1	0.76	0.29	70,70,70,70	0
60	MG	Aa	1722	1/1	0.76	0.21	78,78,78,78	0
60	MG	Aa	1730	1/1	0.76	0.26	77,77,77,77	0
60	MG	Ba	1718	1/1	0.76	0.18	107,107,107,107	0
60	MG	Aa	1743	1/1	0.76	0.29	67,67,67,67	0
60	MG	BA	2966	1/1	0.76	0.18	67,67,67,67	0
60	MG	AA	3259	1/1	0.76	0.31	78,78,78,78	0
60	MG	BB	201	1/1	0.76	0.28	54,54,54,54	0
60	MG	BA	3204	1/1	0.77	0.33	64,64,64,64	0
60	MG	BA	2960	1/1	0.77	0.09	101,101,101,101	0
60	MG	Ba	1683	1/1	0.77	0.12	65,65,65,65	0
60	MG	AA	3114	1/1	0.77	0.21	18,18,18,18	1
60	MG	BA	3035	1/1	0.77	0.31	52,52,52,52	0
60	MG	Aa	1643	1/1	0.77	0.33	90,90,90,90	0
60	MG	Aa	1606	1/1	0.77	0.22	66,66,66,66	0
60	MG	AA	2959	1/1	0.77	0.19	73,73,73,73	0
60	MG	AA	3110	1/1	0.77	0.33	91,91,91,91	0
60	MG	BA	3119	1/1	0.77	0.17	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Aa	1636	1/1	0.77	0.43	88,88,88,88	0
60	MG	Ba	1740	1/1	0.78	0.28	78,78,78,78	0
60	MG	BA	3160	1/1	0.78	0.44	74,74,74,74	0
60	MG	Bv	103	1/1	0.78	0.33	93,93,93,93	0
60	MG	BA	3181	1/1	0.78	0.12	61,61,61,61	0
60	MG	BA	3067	1/1	0.78	0.24	28,28,28,28	0
60	MG	BA	3072	1/1	0.78	0.25	55,55,55,55	0
60	MG	BA	3241	1/1	0.78	0.31	49,49,49,49	0
60	MG	Ba	1659	1/1	0.78	0.20	79,79,79,79	0
60	MG	Aa	1689	1/1	0.78	0.14	65,65,65,65	1
60	MG	AA	3236	1/1	0.78	0.24	90,90,90,90	0
60	MG	BA	3203	1/1	0.78	0.14	95,95,95,95	0
60	MG	AA	2961	1/1	0.78	0.28	76,76,76,76	0
60	MG	AA	3209	1/1	0.78	0.27	84,84,84,84	0
60	MG	AA	3089	1/1	0.78	0.24	75,75,75,75	0
60	MG	Aa	1656	1/1	0.78	0.15	88,88,88,88	0
60	MG	AA	2978	1/1	0.78	0.40	124,124,124,124	0
60	MG	Av	105	1/1	0.78	0.18	92,92,92,92	1
60	MG	Ba	1689	1/1	0.79	0.30	57,57,57,57	0
60	MG	BA	2968	1/1	0.79	0.27	69,69,69,69	0
60	MG	Ba	1690	1/1	0.79	0.22	56,56,56,56	0
60	MG	Ba	1726	1/1	0.79	0.22	34,34,34,34	1
60	MG	AA	3098	1/1	0.79	0.10	75,75,75,75	0
60	MG	Ba	1730	1/1	0.79	0.21	62,62,62,62	0
60	MG	Aa	1652	1/1	0.79	0.21	58,58,58,58	0
60	MG	BA	3088	1/1	0.79	0.24	107,107,107,107	0
60	MG	BA	3220	1/1	0.79	0.23	50,50,50,50	0
60	MG	Ba	1654	1/1	0.79	0.23	50,50,50,50	0
60	MG	Ba	1736	1/1	0.79	0.13	59,59,59,59	0
60	MG	AA	3008	1/1	0.79	0.12	75,75,75,75	0
60	MG	AA	3257	1/1	0.79	0.19	78,78,78,78	0
60	MG	Aa	1728	1/1	0.79	0.20	83,83,83,83	0
60	MG	AA	2952	1/1	0.79	0.21	88,88,88,88	0
60	MG	AA	3224	1/1	0.79	0.19	73,73,73,73	0
60	MG	BA	3138	1/1	0.79	0.16	54,54,54,54	0
60	MG	AA	2965	1/1	0.79	0.20	69,69,69,69	0
60	MG	Ba	1624	1/1	0.79	0.33	76,76,76,76	0
60	MG	BA	3158	1/1	0.79	0.15	88,88,88,88	0
60	MG	AA	3092	1/1	0.79	0.18	51,51,51,51	0
60	MG	BA	3172	1/1	0.79	0.37	50,50,50,50	0
60	MG	Ba	1635	1/1	0.79	0.25	57,57,57,57	0
60	MG	AA	3094	1/1	0.79	0.35	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3127	1/1	0.79	0.18	89,89,89,89	0
60	MG	Aa	1712	1/1	0.79	0.09	117,117,117,117	0
60	MG	AB	203	1/1	0.79	0.33	56,56,56,56	0
60	MG	BA	3116	1/1	0.80	0.28	91,91,91,91	0
60	MG	BA	3182	1/1	0.80	0.20	63,63,63,63	0
60	MG	BA	2963	1/1	0.80	0.16	55,55,55,55	0
60	MG	AA	3075	1/1	0.80	0.40	84,84,84,84	0
60	MG	AA	3246	1/1	0.80	0.12	70,70,70,70	0
60	MG	Ba	1675	1/1	0.80	0.30	58,58,58,58	0
60	MG	Aa	1702	1/1	0.80	0.33	91,91,91,91	0
60	MG	AA	3221	1/1	0.80	0.19	47,47,47,47	0
60	MG	AA	3099	1/1	0.80	0.29	57,57,57,57	0
60	MG	AA	2909	1/1	0.80	0.29	41,41,41,41	0
60	MG	AA	3083	1/1	0.80	0.30	76,76,76,76	0
60	MG	AA	3145	1/1	0.80	0.35	78,78,78,78	0
60	MG	BA	3163	1/1	0.80	0.23	71,71,71,71	0
60	MG	BA	3165	1/1	0.80	0.24	67,67,67,67	0
60	MG	AA	3163	1/1	0.80	0.21	54,54,54,54	0
60	MG	BA	3111	1/1	0.80	0.32	74,74,74,74	0
60	MG	AA	2944	1/1	0.81	0.17	56,56,56,56	0
60	MG	BA	3080	1/1	0.81	0.20	58,58,58,58	0
60	MG	BA	3221	1/1	0.81	0.40	106,106,106,106	0
60	MG	BA	2938	1/1	0.81	0.51	84,84,84,84	0
60	MG	Ba	1705	1/1	0.81	0.32	76,76,76,76	0
60	MG	BA	3170	1/1	0.81	0.11	13,13,13,13	0
60	MG	AA	3226	1/1	0.81	0.28	95,95,95,95	0
60	MG	BA	3178	1/1	0.81	0.11	55,55,55,55	0
60	MG	AA	3118	1/1	0.81	0.26	74,74,74,74	0
60	MG	AA	2963	1/1	0.81	0.32	46,46,46,46	0
60	MG	Ba	1671	1/1	0.81	0.27	87,87,87,87	0
60	MG	AA	3175	1/1	0.81	0.31	40,40,40,40	0
60	MG	BA	3121	1/1	0.81	0.39	70,70,70,70	0
60	MG	Ba	1694	1/1	0.81	0.19	83,83,83,83	0
60	MG	Aa	1691	1/1	0.81	0.19	53,53,53,53	0
60	MG	Aa	1705	1/1	0.81	0.10	71,71,71,71	0
60	MG	Aa	1677	1/1	0.81	0.08	69,69,69,69	0
60	MG	BA	3149	1/1	0.81	0.15	76,76,76,76	0
60	MG	BA	3150	1/1	0.81	0.16	76,76,76,76	0
60	MG	AA	3005	1/1	0.81	0.15	57,57,57,57	0
60	MG	Aa	1641	1/1	0.81	0.17	74,74,74,74	0
60	MG	Aa	1659	1/1	0.82	0.19	88,88,88,88	0
60	MG	AA	3013	1/1	0.82	0.31	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3162	1/1	0.82	0.16	57,57,57,57	0
60	MG	Aa	1739	1/1	0.82	0.16	78,78,78,78	0
60	MG	AA	2953	1/1	0.82	0.13	96,96,96,96	0
60	MG	AB	202	1/1	0.82	0.23	62,62,62,62	0
60	MG	AA	3223	1/1	0.82	0.60	78,78,78,78	0
60	MG	BA	2965	1/1	0.82	0.14	58,58,58,58	0
60	MG	AA	3059	1/1	0.82	0.37	68,68,68,68	0
60	MG	AA	2967	1/1	0.82	0.34	69,69,69,69	0
60	MG	BA	3129	1/1	0.82	0.23	53,53,53,53	0
60	MG	AA	3229	1/1	0.82	0.17	73,73,73,73	0
60	MG	Aa	1678	1/1	0.82	0.18	93,93,93,93	0
60	MG	BA	3135	1/1	0.82	0.30	96,96,96,96	0
60	MG	BA	3250	1/1	0.82	0.34	88,88,88,88	0
60	MG	Ba	1650	1/1	0.82	0.28	49,49,49,49	0
60	MG	BA	3141	1/1	0.82	0.22	57,57,57,57	0
60	MG	BA	3147	1/1	0.82	0.21	56,56,56,56	0
60	MG	Aa	1661	1/1	0.82	0.28	64,64,64,64	0
60	MG	BA	2922	1/1	0.82	0.16	52,52,52,52	0
60	MG	BA	3076	1/1	0.82	0.14	83,83,83,83	0
60	MG	Aa	1680	1/1	0.82	0.37	107,107,107,107	0
60	MG	BB	203	1/1	0.82	0.32	55,55,55,55	0
60	MG	Ba	1658	1/1	0.83	0.18	50,50,50,50	0
60	MG	AA	3048	1/1	0.83	0.16	68,68,68,68	0
60	MG	Aa	1639	1/1	0.83	0.26	65,65,65,65	0
60	MG	AA	3230	1/1	0.83	0.16	78,78,78,78	0
60	MG	BA	3206	1/1	0.83	0.25	71,71,71,71	0
60	MG	AA	2980	1/1	0.83	0.40	69,69,69,69	0
60	MG	AA	3065	1/1	0.83	0.30	73,73,73,73	0
60	MG	BA	3212	1/1	0.83	0.33	68,68,68,68	0
60	MG	BA	2981	1/1	0.83	0.18	46,46,46,46	0
60	MG	BA	3007	1/1	0.83	0.23	90,90,90,90	0
60	MG	AA	3208	1/1	0.83	0.30	86,86,86,86	0
60	MG	AA	2945	1/1	0.83	0.10	74,74,74,74	0
60	MG	Aa	1720	1/1	0.83	0.31	75,75,75,75	0
60	MG	AA	3179	1/1	0.83	0.11	56,56,56,56	0
60	MG	Bx	101	1/1	0.83	0.16	83,83,83,83	0
60	MG	BA	3161	1/1	0.83	0.31	71,71,71,71	0
60	MG	Ba	1645	1/1	0.83	0.35	101,101,101,101	0
60	MG	Aa	1617	1/1	0.83	0.09	49,49,49,49	1
60	MG	BA	3081	1/1	0.83	0.27	83,83,83,83	0
60	MG	BA	3087	1/1	0.83	0.33	51,51,51,51	0
60	MG	AA	2971	1/1	0.83	0.12	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	3175	1/1	0.83	0.31	57,57,57,57	0
60	MG	AA	2975	1/1	0.83	0.29	90,90,90,90	0
60	MG	BA	2901	1/1	0.83	0.33	138,138,138,138	0
60	MG	Ba	1651	1/1	0.83	0.35	62,62,62,62	0
60	MG	AA	3160	1/1	0.83	0.28	99,99,99,99	0
60	MG	AA	3201	1/1	0.83	0.50	88,88,88,88	0
60	MG	Ba	1691	1/1	0.83	0.29	58,58,58,58	0
60	MG	BA	2948	1/1	0.83	0.39	73,73,73,73	0
60	MG	BA	3196	1/1	0.83	0.08	68,68,68,68	0
60	MG	Ba	1608	1/1	0.83	0.18	79,79,79,79	0
60	MG	BA	3167	1/1	0.84	0.29	59,59,59,59	0
60	MG	BA	3168	1/1	0.84	0.11	53,53,53,53	0
60	MG	Ba	1701	1/1	0.84	0.21	60,60,60,60	0
60	MG	Aa	1628	1/1	0.84	0.14	92,92,92,92	0
60	MG	Aa	1619	1/1	0.84	0.28	65,65,65,65	0
60	MG	BA	3176	1/1	0.84	0.14	48,48,48,48	0
60	MG	Aa	1717	1/1	0.84	0.21	66,66,66,66	0
60	MG	BA	3179	1/1	0.84	0.10	24,24,24,24	0
60	MG	Ba	1628	1/1	0.84	0.18	46,46,46,46	0
60	MG	AA	3112	1/1	0.84	0.27	60,60,60,60	0
60	MG	BA	3239	1/1	0.84	0.13	64,64,64,64	0
60	MG	Ba	1631	1/1	0.84	0.18	73,73,73,73	0
60	MG	Aa	1735	1/1	0.84	0.20	68,68,68,68	1
60	MG	BA	3086	1/1	0.84	0.16	48,48,48,48	0
60	MG	AA	2925	1/1	0.84	0.29	79,79,79,79	0
60	MG	Aa	1658	1/1	0.84	0.32	75,75,75,75	0
60	MG	BA	3097	1/1	0.84	0.14	54,54,54,54	0
60	MG	AA	3151	1/1	0.84	0.15	85,85,85,85	0
60	MG	AA	3207	1/1	0.84	0.30	59,59,59,59	0
60	MG	BA	3255	1/1	0.84	0.18	81,81,81,81	0
60	MG	BA	3107	1/1	0.84	0.22	45,45,45,45	0
60	MG	AA	2932	1/1	0.84	0.21	57,57,57,57	0
60	MG	BA	2977	1/1	0.84	0.20	46,46,46,46	0
60	MG	AA	3183	1/1	0.84	0.11	69,69,69,69	0
60	MG	BA	3208	1/1	0.84	0.26	52,52,52,52	0
60	MG	Aa	1687	1/1	0.84	0.19	64,64,64,64	0
60	MG	AA	3126	1/1	0.85	0.12	47,47,47,47	0
60	MG	Ba	1666	1/1	0.85	0.23	73,73,73,73	0
60	MG	AA	2992	1/1	0.85	0.21	45,45,45,45	0
60	MG	AA	3185	1/1	0.85	0.39	83,83,83,83	0
60	MG	AA	2997	1/1	0.85	0.13	43,43,43,43	0
60	MG	AA	2999	1/1	0.85	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3243	1/1	0.85	0.72	79,79,79,79	0
60	MG	BA	2959	1/1	0.85	0.16	37,37,37,37	0
60	MG	AA	3000	1/1	0.85	0.30	63,63,63,63	0
60	MG	AA	3001	1/1	0.85	0.22	26,26,26,26	0
60	MG	Aa	1738	1/1	0.85	0.17	55,55,55,55	0
60	MG	AA	3146	1/1	0.85	0.51	90,90,90,90	0
60	MG	BA	3146	1/1	0.85	0.29	84,84,84,84	0
60	MG	Ba	1725	1/1	0.85	0.30	45,45,45,45	0
60	MG	AA	3147	1/1	0.85	0.24	79,79,79,79	0
60	MG	Aa	1672	1/1	0.85	0.06	87,87,87,87	0
60	MG	BA	3000	1/1	0.85	0.20	16,16,16,16	0
60	MG	BA	3232	1/1	0.85	0.18	77,77,77,77	0
60	MG	Aa	1654	1/1	0.85	0.12	56,56,56,56	0
60	MG	AA	3021	1/1	0.85	0.24	96,96,96,96	0
60	MG	BA	3019	1/1	0.85	0.16	30,30,30,30	0
60	MG	BA	3020	1/1	0.85	0.18	84,84,84,84	0
60	MG	BA	3027	1/1	0.85	0.20	43,43,43,43	0
60	MG	AA	2901	1/1	0.85	0.14	84,84,84,84	0
60	MG	AA	3034	1/1	0.85	0.23	55,55,55,55	0
60	MG	AA	2904	1/1	0.85	0.15	131,131,131,131	0
60	MG	AA	3158	1/1	0.85	0.22	46,46,46,46	0
60	MG	AA	2947	1/1	0.85	0.20	72,72,72,72	0
60	MG	BA	3249	1/1	0.85	0.45	67,67,67,67	0
60	MG	Aa	1732	1/1	0.85	0.16	49,49,49,49	0
60	MG	Ba	1742	1/1	0.85	0.25	92,92,92,92	0
60	MG	AA	2973	1/1	0.85	0.12	79,79,79,79	0
60	MG	Ba	1700	1/1	0.85	0.16	58,58,58,58	0
60	MG	Aa	1699	1/1	0.85	0.12	84,84,84,84	1
60	MG	Aa	1684	1/1	0.85	0.24	74,74,74,74	0
60	MG	Aa	1701	1/1	0.85	0.19	71,71,71,71	0
60	MG	AA	2985	1/1	0.85	0.30	31,31,31,31	0
60	MG	BA	2908	1/1	0.85	0.22	20,20,20,20	0
60	MG	BA	3109	1/1	0.85	0.44	90,90,90,90	0
60	MG	AA	3051	1/1	0.86	0.13	81,81,81,81	0
60	MG	AA	3157	1/1	0.86	0.21	66,66,66,66	0
60	MG	Ba	1698	1/1	0.86	0.22	89,89,89,89	1
60	MG	AA	3056	1/1	0.86	0.29	19,19,19,19	0
60	MG	BA	3029	1/1	0.86	0.17	27,27,27,27	0
60	MG	Ba	1662	1/1	0.86	0.14	67,67,67,67	0
60	MG	BA	3153	1/1	0.86	0.25	46,46,46,46	0
60	MG	Aa	1714	1/1	0.86	0.08	47,47,47,47	0
60	MG	Ba	1664	1/1	0.86	0.27	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3073	1/1	0.86	0.21	30,30,30,30	0
60	MG	Ba	1609	1/1	0.86	0.25	74,74,74,74	0
60	MG	A7	101	1/1	0.86	0.42	80,80,80,80	0
60	MG	AA	3128	1/1	0.86	0.29	23,23,23,23	0
60	MG	AA	3252	1/1	0.86	0.30	80,80,80,80	0
60	MG	Aa	1625	1/1	0.86	0.25	76,76,76,76	0
60	MG	AA	2993	1/1	0.86	0.14	56,56,56,56	0
60	MG	AA	3217	1/1	0.86	0.27	85,85,85,85	0
60	MG	Aa	1637	1/1	0.86	0.15	75,75,75,75	0
60	MG	AA	3074	1/1	0.86	0.24	33,33,33,33	0
60	MG	AA	3107	1/1	0.86	0.21	47,47,47,47	0
60	MG	Ba	1719	1/1	0.86	0.27	57,57,57,57	0
60	MG	BA	3245	1/1	0.86	0.13	90,90,90,90	0
60	MG	Aa	1682	1/1	0.86	0.17	59,59,59,59	0
60	MG	Ba	1686	1/1	0.86	0.13	84,84,84,84	0
60	MG	Aa	1696	1/1	0.86	0.13	67,67,67,67	0
60	MG	AA	3079	1/1	0.86	0.29	55,55,55,55	0
60	MG	AA	3267	1/1	0.86	0.47	74,74,74,74	0
60	MG	Ba	1728	1/1	0.86	0.23	30,30,30,30	0
60	MG	Aa	1607	1/1	0.86	0.22	69,69,69,69	0
60	MG	BA	2971	1/1	0.86	0.34	66,66,66,66	0
60	MG	AA	3050	1/1	0.86	0.17	96,96,96,96	0
60	MG	AA	3152	1/1	0.86	0.25	62,62,62,62	0
60	MG	BA	3265	1/1	0.86	0.20	74,74,74,74	0
60	MG	AA	3116	1/1	0.86	0.22	35,35,35,35	0
60	MG	BB	202	1/1	0.86	0.15	46,46,46,46	0
60	MG	AA	3087	1/1	0.86	0.25	60,60,60,60	0
60	MG	AA	3253	1/1	0.87	0.19	71,71,71,71	0
60	MG	AA	3159	1/1	0.87	0.20	114,114,114,114	0
60	MG	Ba	1611	1/1	0.87	0.14	97,97,97,97	0
60	MG	Ba	1722	1/1	0.87	0.13	63,63,63,63	0
60	MG	Aa	1651	1/1	0.87	0.32	58,58,58,58	0
60	MG	AA	3038	1/1	0.87	0.18	64,64,64,64	0
60	MG	BA	3156	1/1	0.87	0.21	29,29,29,29	0
60	MG	BA	3084	1/1	0.87	0.23	34,34,34,34	0
60	MG	AA	3046	1/1	0.87	0.15	47,47,47,47	0
60	MG	AA	3164	1/1	0.87	0.34	69,69,69,69	0
60	MG	BA	3228	1/1	0.87	0.26	94,94,94,94	0
60	MG	BA	3229	1/1	0.87	0.18	32,32,32,32	0
60	MG	AA	2923	1/1	0.87	0.18	36,36,36,36	0
60	MG	BA	3094	1/1	0.87	0.26	11,11,11,11	0
60	MG	AA	3166	1/1	0.87	0.20	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Ba	1667	1/1	0.87	0.16	50,50,50,50	0
60	MG	Aa	1697	1/1	0.87	0.25	65,65,65,65	0
60	MG	BA	3106	1/1	0.87	0.23	41,41,41,41	0
60	MG	Av	101	1/1	0.87	0.37	90,90,90,90	1
60	MG	Ba	1674	1/1	0.87	0.10	66,66,66,66	0
60	MG	BA	3242	1/1	0.87	0.34	52,52,52,52	0
60	MG	BA	2976	1/1	0.87	0.37	104,104,104,104	0
60	MG	Ba	1640	1/1	0.87	0.32	80,80,80,80	0
60	MG	Ba	1704	1/1	0.87	0.23	62,62,62,62	0
60	MG	AA	3009	1/1	0.87	0.17	31,31,31,31	0
60	MG	AA	3241	1/1	0.87	0.29	64,64,64,64	0
60	MG	AA	3242	1/1	0.87	0.32	85,85,85,85	0
60	MG	BA	3183	1/1	0.87	0.17	44,44,44,44	0
60	MG	Av	104	1/1	0.87	0.23	50,50,50,50	1
60	MG	Aa	1627	1/1	0.87	0.08	53,53,53,53	0
60	MG	BA	3024	1/1	0.87	0.26	24,24,24,24	0
60	MG	BA	3193	1/1	0.87	0.16	44,44,44,44	0
60	MG	AA	3216	1/1	0.87	0.32	49,49,49,49	0
60	MG	BA	3136	1/1	0.87	0.23	106,106,106,106	0
60	MG	BA	3137	1/1	0.87	0.27	80,80,80,80	0
60	MG	AA	2955	1/1	0.87	0.13	48,48,48,48	0
60	MG	AA	3139	1/1	0.87	0.10	44,44,44,44	0
60	MG	Aa	1695	1/1	0.87	0.16	78,78,78,78	0
60	MG	Aa	1683	1/1	0.88	0.10	66,66,66,66	0
60	MG	Ba	1638	1/1	0.88	0.18	40,40,40,40	0
60	MG	Aa	1694	1/1	0.88	0.12	89,89,89,89	0
60	MG	AA	3002	1/1	0.88	0.14	58,58,58,58	0
60	MG	AA	2915	1/1	0.88	0.15	21,21,21,21	0
60	MG	AA	3113	1/1	0.88	0.20	76,76,76,76	0
60	MG	BA	3101	1/1	0.88	0.28	52,52,52,52	0
60	MG	AA	2970	1/1	0.88	0.11	53,53,53,53	0
60	MG	BA	3230	1/1	0.88	0.10	45,45,45,45	0
60	MG	AA	3250	1/1	0.88	0.22	40,40,40,40	0
60	MG	AA	3200	1/1	0.88	0.38	72,72,72,72	1
60	MG	BA	3110	1/1	0.88	0.21	23,23,23,23	0
60	MG	AA	2948	1/1	0.88	0.15	67,67,67,67	0
60	MG	BA	3237	1/1	0.88	0.09	55,55,55,55	0
60	MG	Aa	1629	1/1	0.88	0.22	59,59,59,59	0
60	MG	AA	3020	1/1	0.88	0.12	39,39,39,39	0
60	MG	Ba	1714	1/1	0.88	0.10	62,62,62,62	0
60	MG	Aa	1740	1/1	0.88	0.15	42,42,42,42	0
60	MG	Ba	1716	1/1	0.88	0.23	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	3128	1/1	0.88	0.18	26,26,26,26	0
60	MG	AA	3125	1/1	0.88	0.21	42,42,42,42	0
60	MG	Ba	1657	1/1	0.88	0.14	52,52,52,52	0
60	MG	BA	3036	1/1	0.88	0.18	34,34,34,34	0
60	MG	BA	3046	1/1	0.88	0.13	28,28,28,28	0
60	MG	BA	3059	1/1	0.88	0.18	52,52,52,52	0
60	MG	BA	3251	1/1	0.88	0.17	65,65,65,65	0
60	MG	AA	3080	1/1	0.88	0.31	67,67,67,67	0
60	MG	Ba	1620	1/1	0.88	0.10	55,55,55,55	0
60	MG	AA	3104	1/1	0.88	0.29	56,56,56,56	0
60	MG	BA	3143	1/1	0.88	0.34	95,95,95,95	0
60	MG	BA	3145	1/1	0.88	0.38	63,63,63,63	0
60	MG	AA	3239	1/1	0.88	0.27	77,77,77,77	0
60	MG	AA	3177	1/1	0.88	0.15	57,57,57,57	0
60	MG	AA	3058	1/1	0.88	0.29	44,44,44,44	0
60	MG	AA	3266	1/1	0.88	0.33	87,87,87,87	0
60	MG	Ba	1634	1/1	0.88	0.21	37,37,37,37	0
60	MG	BA	2962	1/1	0.88	0.14	54,54,54,54	0
60	MG	AA	2990	1/1	0.89	0.24	34,34,34,34	0
60	MG	AA	3035	1/1	0.89	0.15	21,21,21,21	0
60	MG	Aa	1620	1/1	0.89	0.11	73,73,73,73	0
60	MG	BA	3034	1/1	0.89	0.16	11,11,11,11	0
60	MG	Aa	1640	1/1	0.89	0.12	60,60,60,60	0
60	MG	AA	2964	1/1	0.89	0.20	65,65,65,65	0
60	MG	Av	102	1/1	0.89	0.17	77,77,77,77	0
60	MG	BA	3215	1/1	0.89	0.29	65,65,65,65	0
60	MG	BA	3058	1/1	0.89	0.30	34,34,34,34	0
60	MG	Aa	1609	1/1	0.89	0.12	64,64,64,64	0
60	MG	BA	3060	1/1	0.89	0.26	16,16,16,16	0
60	MG	Aa	1670	1/1	0.89	0.12	43,43,43,43	0
60	MG	Ba	1622	1/1	0.89	0.09	57,57,57,57	0
60	MG	AA	3090	1/1	0.89	0.23	59,59,59,59	0
60	MG	BA	2924	1/1	0.89	0.17	93,93,93,93	0
60	MG	AA	2949	1/1	0.89	0.24	41,41,41,41	0
60	MG	BA	2939	1/1	0.89	0.20	71,71,71,71	0
60	MG	AA	2921	1/1	0.89	0.21	50,50,50,50	0
60	MG	AA	3096	1/1	0.89	0.58	73,73,73,73	0
60	MG	Ba	1632	1/1	0.89	0.18	41,41,41,41	0
60	MG	Aa	1633	1/1	0.89	0.27	62,62,62,62	0
60	MG	BA	2955	1/1	0.89	0.11	49,49,49,49	0
60	MG	BA	3093	1/1	0.89	0.21	61,61,61,61	0
60	MG	AA	3133	1/1	0.89	0.27	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AF	301	1/1	0.89	0.14	74,74,74,74	0
60	MG	AA	3172	1/1	0.89	0.18	38,38,38,38	0
60	MG	AA	3138	1/1	0.89	0.12	56,56,56,56	0
60	MG	AA	3064	1/1	0.89	0.09	29,29,29,29	0
60	MG	Aa	1616	1/1	0.89	0.06	64,64,64,64	0
60	MG	AA	3181	1/1	0.89	0.09	61,61,61,61	0
60	MG	Ba	1727	1/1	0.89	0.14	46,46,46,46	0
60	MG	AA	3103	1/1	0.89	0.08	35,35,35,35	0
60	MG	AA	3066	1/1	0.89	0.21	27,27,27,27	0
60	MG	Aa	1623	1/1	0.89	0.08	74,74,74,74	0
60	MG	BA	3117	1/1	0.89	0.25	63,63,63,63	0
60	MG	Bd	301	1/1	0.89	0.19	55,55,55,55	0
60	MG	BA	3187	1/1	0.89	0.26	36,36,36,36	0
60	MG	BA	2996	1/1	0.89	0.19	18,18,18,18	0
60	MG	BA	3260	1/1	0.89	0.29	80,80,80,80	0
60	MG	AA	2983	1/1	0.89	0.18	27,27,27,27	0
60	MG	Aa	1721	1/1	0.89	0.08	68,68,68,68	0
60	MG	AA	3031	1/1	0.89	0.19	45,45,45,45	0
60	MG	Ba	1602	1/1	0.89	0.23	93,93,93,93	0
60	MG	BA	3130	1/1	0.89	0.21	45,45,45,45	0
60	MG	AA	3198	1/1	0.89	0.20	52,52,52,52	0
60	MG	AA	2933	1/1	0.90	0.31	67,67,67,67	0
60	MG	AA	3180	1/1	0.90	0.10	73,73,73,73	0
60	MG	AA	3067	1/1	0.90	0.20	34,34,34,34	0
60	MG	AA	3069	1/1	0.90	0.26	68,68,68,68	0
60	MG	Ba	1672	1/1	0.90	0.08	95,95,95,95	0
60	MG	Aa	1673	1/1	0.90	0.12	60,60,60,60	0
60	MG	AA	3055	1/1	0.90	0.34	67,67,67,67	0
60	MG	BA	3124	1/1	0.90	0.10	40,40,40,40	0
60	MG	BA	3125	1/1	0.90	0.16	40,40,40,40	0
60	MG	BA	3010	1/1	0.90	0.18	13,13,13,13	0
60	MG	AA	3244	1/1	0.90	0.43	67,67,67,67	0
60	MG	AA	3190	1/1	0.90	0.18	43,43,43,43	0
60	MG	Aa	1685	1/1	0.90	0.11	53,53,53,53	0
60	MG	B0	101	1/1	0.90	0.15	71,71,71,71	0
60	MG	B0	102	1/1	0.90	0.16	47,47,47,47	0
60	MG	AA	3219	1/1	0.90	0.24	30,30,30,30	0
60	MG	BA	3218	1/1	0.90	0.45	80,80,80,80	0
60	MG	BA	2903	1/1	0.90	0.05	99,99,99,99	0
60	MG	BA	2905	1/1	0.90	0.17	29,29,29,29	0
60	MG	BA	2907	1/1	0.90	0.22	49,49,49,49	0
60	MG	BA	3044	1/1	0.90	0.17	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Aa	1635	1/1	0.90	0.21	39,39,39,39	0
60	MG	BA	3048	1/1	0.90	0.13	31,31,31,31	0
60	MG	BA	2917	1/1	0.90	0.30	23,23,23,23	0
60	MG	AA	3249	1/1	0.90	0.21	55,55,55,55	0
60	MG	AA	3076	1/1	0.90	0.07	78,78,78,78	0
60	MG	BA	2925	1/1	0.90	0.23	31,31,31,31	0
60	MG	BA	3235	1/1	0.90	0.10	51,51,51,51	0
60	MG	BA	2931	1/1	0.90	0.18	62,62,62,62	0
60	MG	BA	2932	1/1	0.90	0.15	67,67,67,67	0
60	MG	BA	2933	1/1	0.90	0.17	18,18,18,18	1
60	MG	BA	3075	1/1	0.90	0.12	44,44,44,44	0
60	MG	Aa	1613	1/1	0.90	0.17	100,100,100,100	0
60	MG	BA	3077	1/1	0.90	0.07	46,46,46,46	0
60	MG	AA	3170	1/1	0.90	0.20	47,47,47,47	0
60	MG	AA	3254	1/1	0.90	0.23	53,53,53,53	0
60	MG	BA	3082	1/1	0.90	0.16	34,34,34,34	0
60	MG	Ba	1610	1/1	0.90	0.09	50,50,50,50	0
60	MG	AA	3171	1/1	0.90	0.09	57,57,57,57	0
60	MG	BA	2951	1/1	0.90	0.29	72,72,72,72	0
60	MG	AA	3228	1/1	0.90	0.15	51,51,51,51	0
60	MG	BA	3091	1/1	0.90	0.21	32,32,32,32	0
60	MG	BA	3173	1/1	0.90	0.21	72,72,72,72	0
60	MG	BA	3174	1/1	0.90	0.10	63,63,63,63	0
60	MG	Aa	1657	1/1	0.90	0.09	71,71,71,71	0
60	MG	Ba	1616	1/1	0.90	0.05	29,29,29,29	1
60	MG	Aa	1666	1/1	0.90	0.23	61,61,61,61	0
60	MG	Ba	1660	1/1	0.90	0.20	60,60,60,60	0
60	MG	AA	3025	1/1	0.90	0.18	26,26,26,26	0
60	MG	BA	3263	1/1	0.90	0.11	68,68,68,68	0
60	MG	AA	3235	1/1	0.90	0.33	72,72,72,72	0
60	MG	BA	3103	1/1	0.90	0.28	50,50,50,50	0
60	MG	Ba	1734	1/1	0.90	0.11	84,84,84,84	1
60	MG	AA	3178	1/1	0.90	0.12	35,35,35,35	0
60	MG	Ba	1627	1/1	0.90	0.19	74,74,74,74	0
60	MG	BA	3021	1/1	0.91	0.15	31,31,31,31	0
60	MG	AA	2977	1/1	0.91	0.32	54,54,54,54	0
60	MG	AA	3037	1/1	0.91	0.14	27,27,27,27	0
60	MG	Ba	1613	1/1	0.91	0.32	38,38,38,38	0
60	MG	AA	3135	1/1	0.91	0.18	71,71,71,71	0
60	MG	AA	3251	1/1	0.91	0.33	84,84,84,84	0
60	MG	BA	2912	1/1	0.91	0.27	37,37,37,37	0
60	MG	Ba	1617	1/1	0.91	0.19	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	BA	2918	1/1	0.91	0.07	29,29,29,29	0
60	MG	Ba	1618	1/1	0.91	0.17	57,57,57,57	0
60	MG	AA	3212	1/1	0.91	0.22	68,68,68,68	0
60	MG	AA	3136	1/1	0.91	0.21	84,84,84,84	0
60	MG	AA	2929	1/1	0.91	0.12	29,29,29,29	0
60	MG	BA	3066	1/1	0.91	0.29	32,32,32,32	0
60	MG	AA	3255	1/1	0.91	0.18	50,50,50,50	0
60	MG	BA	3224	1/1	0.91	0.23	62,62,62,62	0
60	MG	AA	3003	1/1	0.91	0.15	43,43,43,43	0
60	MG	BA	3148	1/1	0.91	0.12	74,74,74,74	0
60	MG	Aa	1650	1/1	0.91	0.39	64,64,64,64	0
60	MG	Ba	1678	1/1	0.91	0.19	51,51,51,51	0
60	MG	BA	3231	1/1	0.91	0.09	64,64,64,64	0
60	MG	BA	2940	1/1	0.91	0.18	82,82,82,82	0
60	MG	AA	3144	1/1	0.91	0.35	50,50,50,50	0
60	MG	AA	2951	1/1	0.91	0.09	53,53,53,53	0
60	MG	BA	3078	1/1	0.91	0.22	32,32,32,32	0
60	MG	AA	3078	1/1	0.91	0.10	83,83,83,83	0
60	MG	Aa	1715	1/1	0.91	0.06	57,57,57,57	0
60	MG	AA	2986	1/1	0.91	0.24	46,46,46,46	0
60	MG	BA	2953	1/1	0.91	0.14	25,25,25,25	0
60	MG	Aa	1716	1/1	0.91	0.12	70,70,70,70	0
60	MG	BA	2956	1/1	0.91	0.13	50,50,50,50	0
60	MG	AA	3150	1/1	0.91	0.19	62,62,62,62	0
60	MG	AA	3186	1/1	0.91	0.13	77,77,77,77	0
60	MG	AA	2991	1/1	0.91	0.20	19,19,19,19	0
60	MG	AA	3085	1/1	0.91	0.11	47,47,47,47	0
60	MG	AA	3023	1/1	0.91	0.23	13,13,13,13	0
60	MG	AA	3060	1/1	0.91	0.10	46,46,46,46	0
60	MG	AA	3119	1/1	0.91	0.31	68,68,68,68	0
60	MG	Ba	1648	1/1	0.91	0.17	32,32,32,32	0
60	MG	BA	2969	1/1	0.91	0.10	35,35,35,35	0
60	MG	Aa	1707	1/1	0.91	0.17	79,79,79,79	0
60	MG	AA	3122	1/1	0.91	0.23	39,39,39,39	0
60	MG	Ba	1743	1/1	0.91	0.32	57,57,57,57	0
60	MG	Aa	1653	1/1	0.91	0.08	59,59,59,59	0
60	MG	AA	3202	1/1	0.91	0.22	57,57,57,57	0
60	MG	BA	3115	1/1	0.91	0.20	21,21,21,21	0
60	MG	Aa	1693	1/1	0.91	0.25	75,75,75,75	0
60	MG	AA	3033	1/1	0.91	0.15	57,57,57,57	0
60	MG	AA	2907	1/1	0.91	0.13	48,48,48,48	0
60	MG	AA	3068	1/1	0.91	0.16	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	2960	1/1	0.91	0.22	17,17,17,17	0
60	MG	B5	102	1/1	0.91	0.32	76,76,76,76	0
60	MG	AA	3258	1/1	0.92	0.34	38,38,38,38	0
60	MG	AA	3084	1/1	0.92	0.22	54,54,54,54	0
60	MG	AA	3047	1/1	0.92	0.14	40,40,40,40	0
60	MG	BA	2973	1/1	0.92	0.14	52,52,52,52	0
60	MG	Ba	1637	1/1	0.92	0.26	80,80,80,80	0
60	MG	AA	3086	1/1	0.92	0.14	74,74,74,74	0
60	MG	Aa	1644	1/1	0.92	0.18	56,56,56,56	0
60	MG	BA	3201	1/1	0.92	0.20	43,43,43,43	0
60	MG	AA	3049	1/1	0.92	0.15	54,54,54,54	0
60	MG	Ba	1642	1/1	0.92	0.21	78,78,78,78	0
60	MG	Bv	105	1/1	0.92	0.11	81,81,81,81	1
60	MG	AA	3222	1/1	0.92	0.22	45,45,45,45	0
60	MG	Aa	1612	1/1	0.92	0.09	32,32,32,32	0
60	MG	BA	3123	1/1	0.92	0.24	2,2,2,2	0
60	MG	BA	3013	1/1	0.92	0.50	50,50,50,50	0
60	MG	AA	2939	1/1	0.92	0.37	68,68,68,68	0
60	MG	BA	3211	1/1	0.92	0.14	24,24,24,24	0
60	MG	AA	2940	1/1	0.92	0.12	34,34,34,34	0
60	MG	AA	3227	1/1	0.92	0.15	39,39,39,39	0
60	MG	B7	101	1/1	0.92	0.11	36,36,36,36	0
60	MG	AA	2903	1/1	0.92	0.26	65,65,65,65	0
60	MG	BA	3219	1/1	0.92	0.23	40,40,40,40	0
60	MG	Aa	1729	1/1	0.92	0.21	30,30,30,30	0
60	MG	BA	3032	1/1	0.92	0.18	32,32,32,32	0
60	MG	BA	3134	1/1	0.92	0.11	52,52,52,52	0
60	MG	BA	3033	1/1	0.92	0.30	61,61,61,61	0
60	MG	AA	2905	1/1	0.92	0.15	15,15,15,15	0
60	MG	BA	3226	1/1	0.92	0.27	75,75,75,75	0
59	ZN	B4	101	1/1	0.92	0.07	201,201,201,201	0
60	MG	AA	3232	1/1	0.92	0.07	64,64,64,64	0
60	MG	Ba	1655	1/1	0.92	0.13	43,43,43,43	0
60	MG	AA	2972	1/1	0.92	0.16	43,43,43,43	0
60	MG	AA	3063	1/1	0.92	0.08	53,53,53,53	0
60	MG	BA	3049	1/1	0.92	0.20	62,62,62,62	0
60	MG	Aa	1604	1/1	0.92	0.07	76,76,76,76	0
60	MG	AA	3018	1/1	0.92	0.18	48,48,48,48	0
60	MG	Ba	1606	1/1	0.92	0.14	50,50,50,50	0
60	MG	BA	2927	1/1	0.92	0.36	83,83,83,83	0
60	MG	Aa	1733	1/1	0.92	0.09	60,60,60,60	0
60	MG	AA	2976	1/1	0.92	0.22	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Aa	1605	1/1	0.92	0.07	43,43,43,43	0
60	MG	AA	3024	1/1	0.92	0.19	25,25,25,25	0
60	MG	Aa	1708	1/1	0.92	0.12	81,81,81,81	0
60	MG	AA	2922	1/1	0.92	0.12	48,48,48,48	0
60	MG	BA	2942	1/1	0.92	0.12	42,42,42,42	0
60	MG	Ba	1668	1/1	0.92	0.19	49,49,49,49	0
60	MG	AA	3030	1/1	0.92	0.10	28,28,28,28	0
60	MG	Aa	1711	1/1	0.92	0.11	70,70,70,70	0
60	MG	Aa	1642	1/1	0.92	0.15	95,95,95,95	0
60	MG	AA	2926	1/1	0.92	0.16	26,26,26,26	0
60	MG	AA	2987	1/1	0.92	0.17	53,53,53,53	0
60	MG	BA	3253	1/1	0.92	0.20	43,43,43,43	0
59	ZN	A4	101	1/1	0.92	0.06	186,186,186,186	0
60	MG	AA	3121	1/1	0.92	0.35	31,31,31,31	0
60	MG	AA	2958	1/1	0.92	0.19	47,47,47,47	0
60	MG	BA	3092	1/1	0.92	0.14	79,79,79,79	0
60	MG	Ba	1731	1/1	0.92	0.16	20,20,20,20	0
60	MG	BA	3177	1/1	0.92	0.16	70,70,70,70	0
60	MG	Ba	1626	1/1	0.92	0.18	56,56,56,56	0
60	MG	AA	3211	1/1	0.92	0.19	60,60,60,60	0
60	MG	AA	3124	1/1	0.92	0.22	15,15,15,15	0
60	MG	Aa	1668	1/1	0.92	0.13	40,40,40,40	0
60	MG	AA	2931	1/1	0.92	0.24	35,35,35,35	0
60	MG	BA	3102	1/1	0.92	0.13	47,47,47,47	0
60	MG	BA	2972	1/1	0.93	0.24	30,30,30,30	0
60	MG	BA	2926	1/1	0.93	0.21	24,24,24,24	0
60	MG	AA	3188	1/1	0.93	0.20	36,36,36,36	0
60	MG	BA	2930	1/1	0.93	0.21	28,28,28,28	0
60	MG	BA	2979	1/1	0.93	0.20	55,55,55,55	0
60	MG	BA	3144	1/1	0.93	0.26	59,59,59,59	0
60	MG	AA	3006	1/1	0.93	0.11	32,32,32,32	0
60	MG	BA	2986	1/1	0.93	0.12	63,63,63,63	0
60	MG	BA	2987	1/1	0.93	0.20	9,9,9,9	0
60	MG	AA	3026	1/1	0.93	0.18	35,35,35,35	0
60	MG	AA	3027	1/1	0.93	0.11	54,54,54,54	0
60	MG	AA	2994	1/1	0.93	0.27	30,30,30,30	0
60	MG	BA	3008	1/1	0.93	0.16	32,32,32,32	0
60	MG	Ba	1717	1/1	0.93	0.41	71,71,71,71	0
60	MG	Aa	1709	1/1	0.93	0.06	148,148,148,148	0
60	MG	BA	2941	1/1	0.93	0.13	62,62,62,62	0
60	MG	BA	3015	1/1	0.93	0.14	18,18,18,18	0
60	MG	BA	3227	1/1	0.93	0.49	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3159	1/1	0.93	0.19	52,52,52,52	0
60	MG	BA	3016	1/1	0.93	0.17	11,11,11,11	0
60	MG	AD	302	1/1	0.93	0.12	21,21,21,21	0
60	MG	BA	2943	1/1	0.93	0.16	35,35,35,35	0
60	MG	BA	2944	1/1	0.93	0.09	62,62,62,62	0
60	MG	BA	3164	1/1	0.93	0.14	31,31,31,31	0
60	MG	BA	3023	1/1	0.93	0.21	21,21,21,21	0
60	MG	AA	3053	1/1	0.93	0.17	42,42,42,42	0
60	MG	Ba	1614	1/1	0.93	0.28	68,68,68,68	0
60	MG	AA	3137	1/1	0.93	0.23	90,90,90,90	0
60	MG	AA	3173	1/1	0.93	0.13	14,14,14,14	0
60	MG	Ba	1670	1/1	0.93	0.12	58,58,58,58	0
60	MG	BA	3112	1/1	0.93	0.07	69,69,69,69	0
60	MG	BA	3113	1/1	0.93	0.15	24,24,24,24	1
60	MG	AA	3014	1/1	0.93	0.37	50,50,50,50	0
60	MG	AA	3225	1/1	0.93	0.16	57,57,57,57	0
60	MG	Ba	1619	1/1	0.93	0.05	44,44,44,44	0
60	MG	AA	3156	1/1	0.93	0.10	73,73,73,73	0
60	MG	AA	2950	1/1	0.93	0.14	51,51,51,51	0
60	MG	BA	3047	1/1	0.93	0.16	36,36,36,36	0
60	MG	AA	2956	1/1	0.93	0.11	61,61,61,61	0
60	MG	AA	3142	1/1	0.93	0.19	53,53,53,53	0
60	MG	BA	3057	1/1	0.93	0.19	45,45,45,45	0
60	MG	BA	2913	1/1	0.93	0.18	11,11,11,11	0
60	MG	BA	3127	1/1	0.93	0.26	20,20,20,20	0
60	MG	AA	2920	1/1	0.93	0.20	22,22,22,22	0
60	MG	BA	3191	1/1	0.93	0.12	23,23,23,23	0
60	MG	AA	3161	1/1	0.93	0.27	61,61,61,61	0
60	MG	BA	2967	1/1	0.93	0.21	20,20,20,20	0
60	MG	BA	3197	1/1	0.93	0.17	103,103,103,103	1
60	MG	AA	2911	1/1	0.93	0.28	20,20,20,20	0
60	MG	BA	3199	1/1	0.93	0.13	34,34,34,34	0
60	MG	Ba	1709	1/1	0.93	0.13	52,52,52,52	0
60	MG	BA	3133	1/1	0.93	0.08	54,54,54,54	0
60	MG	BA	2970	1/1	0.93	0.27	53,53,53,53	0
60	MG	AA	2984	1/1	0.93	0.09	45,45,45,45	0
60	MG	BA	3089	1/1	0.94	0.14	56,56,56,56	0
60	MG	AA	3054	1/1	0.94	0.12	24,24,24,24	0
60	MG	AA	3029	1/1	0.94	0.14	37,37,37,37	0
60	MG	AA	2982	1/1	0.94	0.27	56,56,56,56	0
60	MG	AA	3010	1/1	0.94	0.17	10,10,10,10	0
60	MG	BA	3096	1/1	0.94	0.06	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3102	1/1	0.94	0.35	68,68,68,68	0
60	MG	BA	2957	1/1	0.94	0.24	13,13,13,13	0
60	MG	AA	3011	1/1	0.94	0.17	14,14,14,14	0
60	MG	Ba	1639	1/1	0.94	0.15	58,58,58,58	0
60	MG	AA	3176	1/1	0.94	0.31	74,74,74,74	0
60	MG	BA	2909	1/1	0.94	0.22	45,45,45,45	0
60	MG	AA	2996	1/1	0.94	0.28	40,40,40,40	0
60	MG	AA	3233	1/1	0.94	0.09	44,44,44,44	0
60	MG	BA	3108	1/1	0.94	0.14	50,50,50,50	0
60	MG	AA	2919	1/1	0.94	0.14	36,36,36,36	0
60	MG	AA	3082	1/1	0.94	0.09	72,72,72,72	0
60	MG	AA	2998	1/1	0.94	0.07	36,36,36,36	0
60	MG	BA	2923	1/1	0.94	0.12	29,29,29,29	0
60	MG	BA	3169	1/1	0.94	0.08	25,25,25,25	0
60	MG	AA	2906	1/1	0.94	0.18	25,25,25,25	0
60	MG	BA	3171	1/1	0.94	0.23	69,69,69,69	0
60	MG	BA	3114	1/1	0.94	0.15	8,8,8,8	0
60	MG	BA	3052	1/1	0.94	0.12	10,10,10,10	0
60	MG	BA	3054	1/1	0.94	0.19	36,36,36,36	0
60	MG	BA	3055	1/1	0.94	0.19	7,7,7,7	0
60	MG	Aa	1737	1/1	0.94	0.13	119,119,119,119	0
60	MG	AA	3022	1/1	0.94	0.14	22,22,22,22	0
60	MG	BA	3120	1/1	0.94	0.21	16,16,16,16	0
60	MG	Ba	1649	1/1	0.94	0.24	49,49,49,49	0
60	MG	BA	3122	1/1	0.94	0.13	24,24,24,24	0
60	MG	BA	2974	1/1	0.94	0.21	31,31,31,31	0
60	MG	BA	3064	1/1	0.94	0.09	44,44,44,44	0
60	MG	AA	2902	1/1	0.94	0.24	167,167,167,167	0
60	MG	Ba	1710	1/1	0.94	0.07	65,65,65,65	0
60	MG	BA	3071	1/1	0.94	0.19	39,39,39,39	0
60	MG	Ba	1741	1/1	0.94	0.17	73,73,73,73	0
60	MG	AA	3187	1/1	0.94	0.24	49,49,49,49	0
60	MG	BA	2936	1/1	0.94	0.06	35,35,35,35	0
60	MG	Aa	1649	1/1	0.94	0.11	32,32,32,32	0
60	MG	AA	3140	1/1	0.94	0.24	45,45,45,45	0
60	MG	Bv	101	1/1	0.94	0.21	52,52,52,52	1
60	MG	Ba	1685	1/1	0.94	0.13	25,25,25,25	1
60	MG	BA	3259	1/1	0.94	0.14	86,86,86,86	0
60	MG	A1	101	1/1	0.94	0.18	53,53,53,53	0
60	MG	AA	3071	1/1	0.94	0.21	74,74,74,74	0
60	MG	BA	3262	1/1	0.94	0.15	39,39,39,39	0
60	MG	BA	3011	1/1	0.94	0.15	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Aa	1664	1/1	0.94	0.24	44,44,44,44	0
60	MG	BA	3085	1/1	0.94	0.08	60,60,60,60	0
60	MG	BD	301	1/1	0.94	0.19	14,14,14,14	0
60	MG	AA	2927	1/1	0.94	0.24	32,32,32,32	0
60	MG	AA	2981	1/1	0.94	0.23	13,13,13,13	0
60	MG	BA	2915	1/1	0.95	0.20	20,20,20,20	0
60	MG	BA	3022	1/1	0.95	0.13	16,16,16,16	0
60	MG	BA	2916	1/1	0.95	0.18	62,62,62,62	0
60	MG	BA	3090	1/1	0.95	0.11	32,32,32,32	0
60	MG	Aa	1608	1/1	0.95	0.13	39,39,39,39	0
60	MG	AA	2913	1/1	0.95	0.17	22,22,22,22	0
60	MG	BA	3028	1/1	0.95	0.15	24,24,24,24	0
60	MG	BA	3213	1/1	0.95	0.11	36,36,36,36	0
60	MG	BA	3214	1/1	0.95	0.25	34,34,34,34	0
60	MG	AA	3237	1/1	0.95	0.17	37,37,37,37	0
60	MG	BA	3152	1/1	0.95	0.18	71,71,71,71	0
60	MG	BA	3217	1/1	0.95	0.18	26,26,26,26	0
60	MG	AA	3015	1/1	0.95	0.18	14,14,14,14	0
60	MG	AA	3213	1/1	0.95	0.17	33,33,33,33	0
60	MG	AA	3123	1/1	0.95	0.18	18,18,18,18	0
60	MG	AA	3215	1/1	0.95	0.10	56,56,56,56	0
60	MG	AA	2935	1/1	0.95	0.28	69,69,69,69	0
60	MG	BA	3223	1/1	0.95	0.10	43,43,43,43	0
60	MG	BA	3040	1/1	0.95	0.11	17,17,17,17	0
60	MG	BA	3041	1/1	0.95	0.20	15,15,15,15	0
60	MG	AA	3052	1/1	0.95	0.13	18,18,18,18	0
60	MG	BA	3045	1/1	0.95	0.11	16,16,16,16	0
60	MG	AA	3106	1/1	0.95	0.19	65,65,65,65	0
60	MG	AA	2937	1/1	0.95	0.10	67,67,67,67	0
60	MG	AA	2914	1/1	0.95	0.14	15,15,15,15	0
60	MG	BA	2934	1/1	0.95	0.35	72,72,72,72	0
60	MG	BA	3051	1/1	0.95	0.14	16,16,16,16	0
60	MG	AA	3194	1/1	0.95	0.10	26,26,26,26	0
60	MG	Aa	1731	1/1	0.95	0.43	64,64,64,64	0
60	MG	Av	103	1/1	0.95	0.06	84,84,84,84	0
60	MG	BX	101	1/1	0.95	0.13	31,31,31,31	1
60	MG	BA	2982	1/1	0.95	0.21	4,4,4,4	0
60	MG	Ba	1603	1/1	0.95	0.05	64,64,64,64	0
60	MG	Aa	1618	1/1	0.95	0.12	28,28,28,28	0
60	MG	BA	3061	1/1	0.95	0.09	35,35,35,35	0
60	MG	AA	3174	1/1	0.95	0.08	72,72,72,72	0
60	MG	BA	2999	1/1	0.95	0.19	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Aa	1745	1/1	0.95	0.19	48,48,48,48	0
60	MG	BA	3070	1/1	0.95	0.09	83,83,83,83	0
60	MG	BA	3004	1/1	0.95	0.07	46,46,46,46	0
60	MG	BA	3005	1/1	0.95	0.17	21,21,21,21	0
60	MG	BA	3184	1/1	0.95	0.10	57,57,57,57	0
60	MG	AA	3093	1/1	0.95	0.11	56,56,56,56	0
60	MG	BA	2946	1/1	0.95	0.06	75,75,75,75	0
60	MG	AA	3115	1/1	0.95	0.15	19,19,19,19	0
60	MG	AA	3043	1/1	0.95	0.10	37,37,37,37	0
60	MG	BA	3190	1/1	0.95	0.13	13,13,13,13	0
60	MG	AA	3044	1/1	0.95	0.35	17,17,17,17	0
60	MG	AA	2910	1/1	0.95	0.33	49,49,49,49	0
60	MG	BA	3194	1/1	0.95	0.13	12,12,12,12	0
60	MG	BA	3195	1/1	0.95	0.09	37,37,37,37	0
60	MG	BA	3079	1/1	0.95	0.15	82,82,82,82	0
60	MG	BA	3014	1/1	0.95	0.18	1,1,1,1	0
60	MG	AA	2946	1/1	0.95	0.06	101,101,101,101	0
60	MG	BA	2910	1/1	0.95	0.20	2,2,2,2	0
60	MG	BA	3200	1/1	0.95	0.10	33,33,33,33	0
60	MG	BA	3083	1/1	0.95	0.30	52,52,52,52	0
60	MG	BA	3017	1/1	0.95	0.11	38,38,38,38	0
60	MG	AA	3182	1/1	0.95	0.14	40,40,40,40	0
60	MG	AA	3234	1/1	0.95	0.17	79,79,79,79	0
60	MG	AA	2979	1/1	0.96	0.10	51,51,51,51	0
60	MG	BA	2964	1/1	0.96	0.23	49,49,49,49	0
60	MG	BA	3026	1/1	0.96	0.07	40,40,40,40	0
60	MG	A5	101	1/1	0.96	0.19	34,34,34,34	0
60	MG	AA	3045	1/1	0.96	0.12	22,22,22,22	0
60	MG	Ba	1693	1/1	0.96	0.07	78,78,78,78	0
60	MG	BA	3030	1/1	0.96	0.18	26,26,26,26	0
60	MG	Aa	1660	1/1	0.96	0.14	49,49,49,49	0
60	MG	BA	2928	1/1	0.96	0.09	17,17,17,17	0
60	MG	AA	3101	1/1	0.96	0.16	46,46,46,46	0
60	MG	AA	2969	1/1	0.96	0.08	22,22,22,22	0
60	MG	BD	302	1/1	0.96	0.10	18,18,18,18	0
60	MG	BA	3037	1/1	0.96	0.12	35,35,35,35	0
60	MG	BA	3038	1/1	0.96	0.12	26,26,26,26	0
60	MG	Ba	1723	1/1	0.96	0.05	103,103,103,103	0
60	MG	AA	3193	1/1	0.96	0.10	20,20,20,20	0
60	MG	Aa	1724	1/1	0.96	0.05	71,71,71,71	0
60	MG	BA	3166	1/1	0.96	0.08	50,50,50,50	0
60	MG	BA	2937	1/1	0.96	0.19	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Aa	1638	1/1	0.96	0.18	62,62,62,62	0
60	MG	B5	101	1/1	0.96	0.15	27,27,27,27	0
60	MG	AA	2942	1/1	0.96	0.20	40,40,40,40	0
60	MG	BA	2984	1/1	0.96	0.18	22,22,22,22	0
60	MG	BA	3050	1/1	0.96	0.05	29,29,29,29	0
60	MG	AA	3016	1/1	0.96	0.10	31,31,31,31	0
60	MG	B7	102	1/1	0.96	0.25	57,57,57,57	0
60	MG	BA	2988	1/1	0.96	0.11	34,34,34,34	0
60	MG	BA	2989	1/1	0.96	0.28	31,31,31,31	0
60	MG	BA	2991	1/1	0.96	0.25	32,32,32,32	0
60	MG	BA	2995	1/1	0.96	0.17	14,14,14,14	0
60	MG	AA	3108	1/1	0.96	0.04	38,38,38,38	0
60	MG	BA	2998	1/1	0.96	0.11	14,14,14,14	0
60	MG	BA	2902	1/1	0.96	0.19	60,60,60,60	0
60	MG	BA	3063	1/1	0.96	0.12	26,26,26,26	0
60	MG	AA	3129	1/1	0.96	0.10	29,29,29,29	0
60	MG	BA	3001	1/1	0.96	0.05	37,37,37,37	0
60	MG	BA	3002	1/1	0.96	0.15	41,41,41,41	0
60	MG	BA	3246	1/1	0.96	0.10	89,89,89,89	0
60	MG	BA	3068	1/1	0.96	0.22	64,64,64,64	0
60	MG	BA	3069	1/1	0.96	0.09	35,35,35,35	0
60	MG	AA	3070	1/1	0.96	0.10	54,54,54,54	0
60	MG	BA	2906	1/1	0.96	0.13	26,26,26,26	0
60	MG	Ba	1652	1/1	0.96	0.04	69,69,69,69	0
60	MG	BA	2950	1/1	0.96	0.08	37,37,37,37	0
60	MG	AA	3131	1/1	0.96	0.26	46,46,46,46	0
60	MG	AA	3017	1/1	0.96	0.14	18,18,18,18	0
60	MG	Ba	1682	1/1	0.96	0.05	66,66,66,66	0
60	MG	BA	2954	1/1	0.96	0.09	57,57,57,57	0
60	MG	Aa	1626	1/1	0.96	0.06	63,63,63,63	0
60	MG	AA	2934	1/1	0.96	0.20	32,32,32,32	1
60	MG	AD	301	1/1	0.96	0.14	21,21,21,21	0
60	MG	BA	3139	1/1	0.96	0.04	15,15,15,15	0
60	MG	AA	2936	1/1	0.96	0.23	5,5,5,5	0
60	MG	BA	3142	1/1	0.96	0.27	53,53,53,53	0
60	MG	AA	2966	1/1	0.96	0.23	57,57,57,57	0
60	MG	AA	3095	1/1	0.96	0.24	26,26,26,26	0
60	MG	BA	2961	1/1	0.96	0.08	28,28,28,28	0
60	MG	AA	3042	1/1	0.96	0.20	27,27,27,27	0
60	MG	A1	102	1/1	0.97	0.16	116,116,116,116	0
60	MG	BF	301	1/1	0.97	0.04	40,40,40,40	0
60	MG	BA	3039	1/1	0.97	0.11	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	3169	1/1	0.97	0.07	44,44,44,44	0
60	MG	BA	3192	1/1	0.97	0.04	34,34,34,34	0
60	MG	BA	3006	1/1	0.97	0.13	21,21,21,21	0
60	MG	AA	3184	1/1	0.97	0.07	44,44,44,44	0
60	MG	BA	2920	1/1	0.97	0.11	24,24,24,24	0
60	MG	BA	3155	1/1	0.97	0.07	59,59,59,59	0
60	MG	AA	3062	1/1	0.97	0.10	26,26,26,26	0
60	MG	AA	2918	1/1	0.97	0.34	25,25,25,25	0
60	MG	BA	2949	1/1	0.97	0.07	42,42,42,42	0
60	MG	AA	2962	1/1	0.97	0.05	19,19,19,19	0
60	MG	AA	2938	1/1	0.97	0.11	84,84,84,84	0
60	MG	Ba	1636	1/1	0.97	0.15	60,60,60,60	0
60	MG	BA	2980	1/1	0.97	0.22	9,9,9,9	0
60	MG	AA	3039	1/1	0.97	0.12	19,19,19,19	0
60	MG	AA	3040	1/1	0.97	0.05	21,21,21,21	0
60	MG	BA	3056	1/1	0.97	0.17	92,92,92,92	0
60	MG	Aa	1624	1/1	0.97	0.09	37,37,37,37	0
60	MG	BA	3248	1/1	0.97	0.29	47,47,47,47	0
60	MG	BA	2985	1/1	0.97	0.09	26,26,26,26	0
60	MG	AA	2988	1/1	0.97	0.17	33,33,33,33	0
60	MG	BA	2904	1/1	0.97	0.15	1,1,1,1	0
60	MG	BA	3095	1/1	0.97	0.10	33,33,33,33	0
60	MG	AA	2916	1/1	0.97	0.18	25,25,25,25	0
60	MG	Ba	1661	1/1	0.97	0.12	41,41,41,41	0
60	MG	BA	2990	1/1	0.97	0.09	10,10,10,10	0
60	MG	BA	3256	1/1	0.97	0.26	39,39,39,39	0
60	MG	BA	3065	1/1	0.97	0.12	13,13,13,13	0
60	MG	BA	2935	1/1	0.97	0.26	25,25,25,25	0
60	MG	BA	2994	1/1	0.97	0.20	14,14,14,14	0
60	MG	AA	3032	1/1	0.97	0.07	33,33,33,33	0
60	MG	BA	3140	1/1	0.97	0.17	25,25,25,25	0
60	MG	BA	3104	1/1	0.97	0.06	31,31,31,31	0
60	MG	BA	3105	1/1	0.97	0.12	40,40,40,40	0
60	MG	AA	2930	1/1	0.97	0.05	15,15,15,15	0
60	MG	AA	2974	1/1	0.97	0.33	43,43,43,43	0
60	MG	AA	3199	1/1	0.97	0.12	53,53,53,53	0
60	MG	Ba	1625	1/1	0.97	0.10	72,72,72,72	0
60	MG	Ba	1607	1/1	0.97	0.06	75,75,75,75	0
60	MG	AA	3197	1/1	0.98	0.25	22,22,22,22	0
60	MG	Aa	1710	1/1	0.98	0.09	29,29,29,29	0
60	MG	AA	2924	1/1	0.98	0.04	32,32,32,32	0
60	MG	AA	2908	1/1	0.98	0.11	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	Ba	1623	1/1	0.98	0.05	34,34,34,34	0
60	MG	AA	3012	1/1	0.98	0.07	22,22,22,22	0
60	MG	Aa	1726	1/1	0.98	0.21	36,36,36,36	0
59	ZN	Bn	101	1/1	0.98	0.04	137,137,137,137	0
60	MG	BA	3157	1/1	0.98	0.08	85,85,85,85	0
60	MG	BA	3042	1/1	0.98	0.09	30,30,30,30	0
60	MG	BA	3043	1/1	0.98	0.28	17,17,17,17	0
59	ZN	An	101	1/1	0.98	0.03	153,153,153,153	0
60	MG	AA	2912	1/1	0.98	0.07	26,26,26,26	0
60	MG	Bv	102	1/1	0.98	0.08	37,37,37,37	0
60	MG	Ba	1673	1/1	0.98	0.06	39,39,39,39	0
60	MG	BA	3009	1/1	0.98	0.11	3,3,3,3	0
60	MG	BA	2914	1/1	0.98	0.08	11,11,11,11	0
60	MG	Ba	1629	1/1	0.98	0.06	36,36,36,36	0
60	MG	BA	2975	1/1	0.98	0.20	105,105,105,105	0
60	MG	AA	3004	1/1	0.98	0.10	39,39,39,39	0
60	MG	AA	3105	1/1	0.98	0.09	47,47,47,47	0
60	MG	BA	3210	1/1	0.98	0.11	22,22,22,22	0
60	MG	BA	2978	1/1	0.98	0.05	56,56,56,56	0
60	MG	Aa	1634	1/1	0.98	0.05	47,47,47,47	0
60	MG	Ba	1633	1/1	0.98	0.07	39,39,39,39	0
60	MG	BA	2921	1/1	0.98	0.06	31,31,31,31	0
60	MG	AA	3091	1/1	0.98	0.11	27,27,27,27	0
60	MG	Ba	1680	1/1	0.98	0.02	63,63,63,63	0
60	MG	AA	3019	1/1	0.98	0.10	26,26,26,26	0
60	MG	BA	3100	1/1	0.98	0.10	62,62,62,62	0
60	MG	AA	2995	1/1	0.98	0.20	18,18,18,18	0
60	MG	AA	3007	1/1	0.98	0.06	43,43,43,43	0
60	MG	BA	3025	1/1	0.98	0.09	12,12,12,12	0
60	MG	Ba	1732	1/1	0.98	0.08	70,70,70,70	0
60	MG	AA	3143	1/1	0.98	0.05	29,29,29,29	0
60	MG	BA	2929	1/1	0.98	0.04	10,10,10,10	0
60	MG	AA	3195	1/1	0.98	0.07	30,30,30,30	0
60	MG	BA	2992	1/1	0.98	0.12	33,33,33,33	0
60	MG	BA	2993	1/1	0.98	0.20	12,12,12,12	0
60	MG	Aa	1603	1/1	0.98	0.05	68,68,68,68	1
60	MG	BA	2911	1/1	0.99	0.05	21,21,21,21	0
60	MG	BA	3003	1/1	0.99	0.07	22,22,22,22	0
60	MG	BA	3018	1/1	0.99	0.09	2,2,2,2	0
60	MG	AA	3041	1/1	0.99	0.06	21,21,21,21	0
59	ZN	Bd	302	1/1	0.99	0.17	80,80,80,80	0
60	MG	BA	3053	1/1	0.99	0.08	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	ZN	B9	101	1/1	0.99	0.04	116,116,116,116	0
59	ZN	A9	101	1/1	0.99	0.04	138,138,138,138	0
60	MG	Aa	1630	1/1	0.99	0.03	36,36,36,36	0
60	MG	BA	2983	1/1	0.99	0.03	21,21,21,21	0
60	MG	AA	2989	1/1	0.99	0.04	33,33,33,33	0
60	MG	BA	3185	1/1	0.99	0.27	40,40,40,40	0
60	MG	BA	2997	1/1	0.99	0.07	22,22,22,22	0
60	MG	Aa	1681	1/1	0.99	0.02	76,76,76,76	0
60	MG	BA	2919	1/1	0.99	0.05	13,13,13,13	0
60	MG	BA	3062	1/1	0.99	0.07	36,36,36,36	0
60	MG	Aa	1671	1/1	0.99	0.05	49,49,49,49	0
60	MG	AA	3057	1/1	0.99	0.05	92,92,92,92	0
60	MG	BA	3031	1/1	0.99	0.06	14,14,14,14	0
59	ZN	Ad	301	1/1	1.00	0.18	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.