



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:53 PM BST

PDB ID : 4V7K
Title : Structure of RelE nuclease bound to the 70S ribosome (postcleavage state)
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Deposited on : 2009-11-02
Resolution : 3.60 Å(reported)

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

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

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

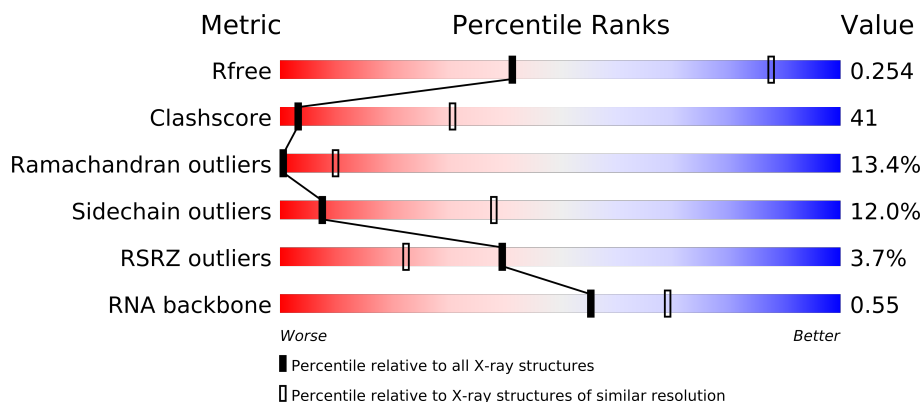
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

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}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)
RNA backbone	1838	1012 (4.40-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	Ab	256	
1	Bb	256	
2	Ac	239	
2	Bc	239	
3	Ad	209	
3	Bd	209	
4	Ae	162	
4	Be	162	
5	Af	101	
5	Bf	101	
6	Ag	156	
6	Bg	156	

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Mol	Chain	Length	Quality of chain
7	Ah	138	
7	Bh	138	
8	Ai	128	
8	Bi	128	
9	Aj	105	
9	Bj	105	
10	Ak	129	
10	Bk	129	
11	Al	132	
11	Bl	132	
12	Am	126	
12	Bm	126	
13	An	61	
13	Bn	61	
14	Ao	89	
14	Bo	89	
15	Ap	88	
15	Bp	88	
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	
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	

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Mol	Chain	Length	Quality of chain
49	A2	72	
49	B2	72	
50	A3	60	
50	B3	60	
51	A4	71	
51	B4	71	
52	A5	60	
52	B5	60	
53	A6	54	
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	

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is a protein called Toxin relE.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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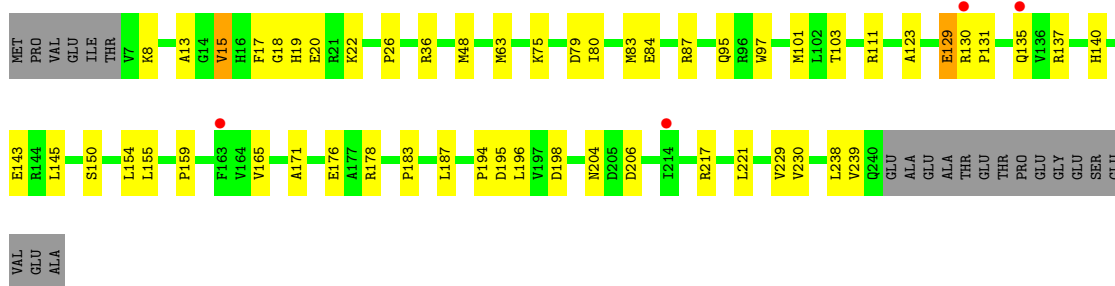
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	Bl	1	Total 1	Mg 1	0	0
60	BF	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0
60	Aw	1	Total 1	Mg 1	0	0
60	AA	367	Total 367	Mg 367	0	0
60	A5	1	Total 1	Mg 1	0	0
60	A1	2	Total 2	Mg 2	0	0
60	AD	2	Total 2	Mg 2	0	0
60	Ae	2	Total 2	Mg 2	0	0
60	Bm	1	Total 1	Mg 1	0	0
60	Av	5	Total 5	Mg 5	0	0
60	Bx	1	Total 1	Mg 1	0	0
60	Aa	145	Total 145	Mg 145	0	0
60	B7	2	Total 2	Mg 2	0	0
60	BO	1	Total 1	Mg 1	0	0
60	AQ	1	Total 1	Mg 1	0	0
60	A7	1	Total 1	Mg 1	0	0
60	BD	2	Total 2	Mg 2	0	0
60	B0	2	Total 2	Mg 2	0	0
60	Bv	5	Total 5	Mg 5	0	0
60	AF	1	Total 1	Mg 1	0	0

3 Residue-property plots


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

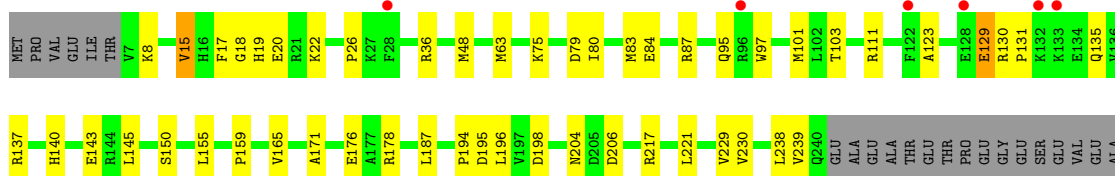
- Molecule 1: 30S ribosomal protein S2

Chain Ab: 



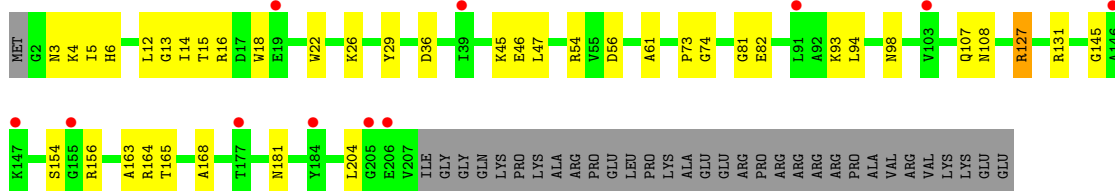
- Molecule 1: 30S ribosomal protein S2

Chain Bb: 



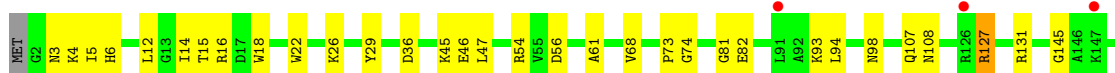
- Molecule 2: 30S ribosomal protein S3

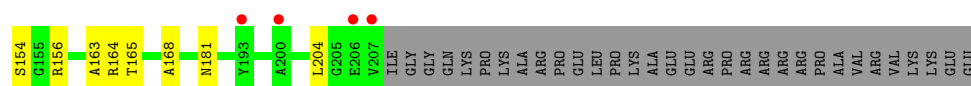
Chain Ac: 



- Molecule 2: 30S ribosomal protein S3

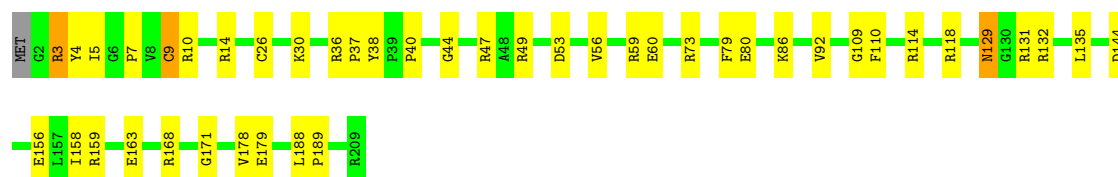
Chain Bc: 





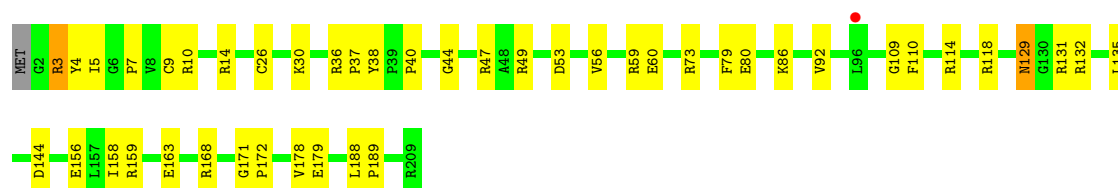
- Molecule 3: 30S ribosomal protein S4

Chain Ad:



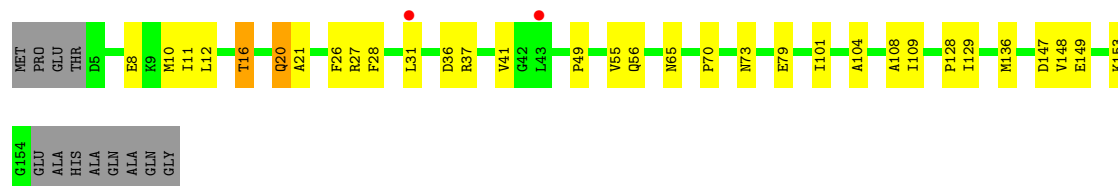
- Molecule 3: 30S ribosomal protein S4

Chain Bd:



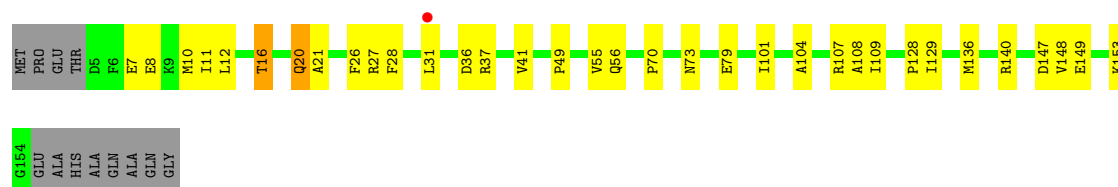
- Molecule 4: 30S ribosomal protein S5

Chain Ae:



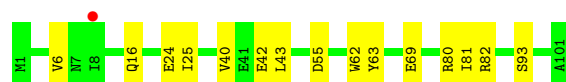
- Molecule 4: 30S ribosomal protein S5

Chain Be:



- Molecule 5: 30S ribosomal protein S6

Chain Af:



- Molecule 5: 30S ribosomal protein S6

Chain Bf:



- Molecule 6: 30S ribosomal protein S7

Chain Ag:



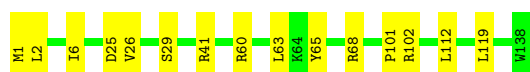
- Molecule 6: 30S ribosomal protein S7

Chain Bg:



- Molecule 7: 30S ribosomal protein S8

Chain Ah:



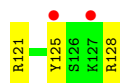
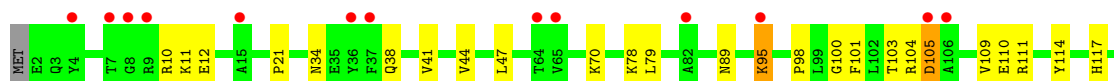
- Molecule 7: 30S ribosomal protein S8

Chain Bh:



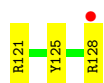
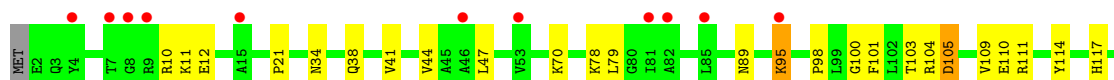
- Molecule 8: 30S ribosomal protein S9

Chain Ai:



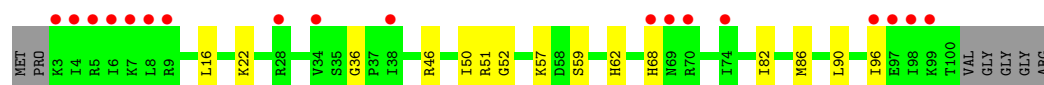
- Molecule 8: 30S ribosomal protein S9

Chain Bi:



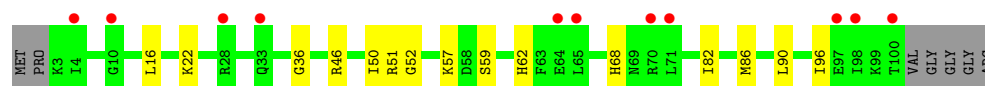
- Molecule 9: 30S ribosomal protein S10

Chain Aj:



- Molecule 9: 30S ribosomal protein S10

Chain Bj:



- Molecule 10: 30S ribosomal protein S11

Chain Ak:



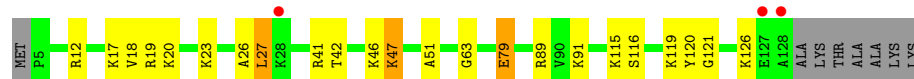
- Molecule 10: 30S ribosomal protein S11

Chain Bk:



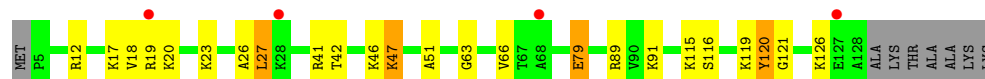
- Molecule 11: 30S ribosomal protein S12

Chain Al:



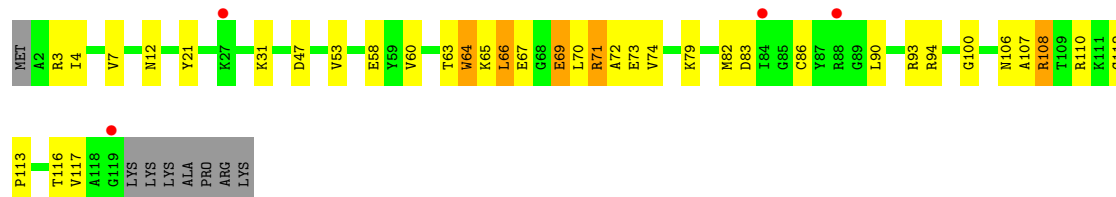
- Molecule 11: 30S ribosomal protein S12

Chain Bl:



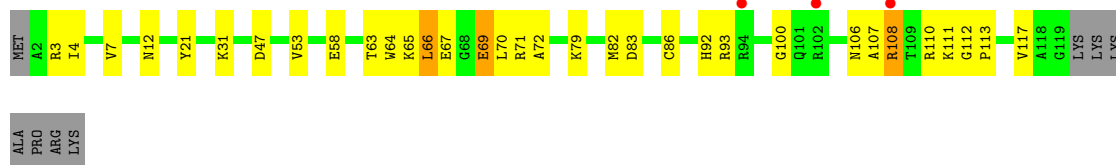
- Molecule 12: 30S ribosomal protein S13

Chain Am:



- Molecule 12: 30S ribosomal protein S13

Chain Bm:



- Molecule 13: 30S ribosomal protein S14 type Z

Chain An:



- Molecule 13: 30S ribosomal protein S14 type Z

Chain Bn:



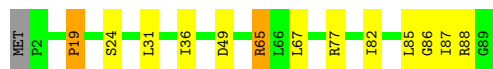
- Molecule 14: 30S ribosomal protein S15

Chain Ao:



- Molecule 14: 30S ribosomal protein S15

Chain Bo:



- Molecule 15: 30S ribosomal protein S16

Chain Ap:



- Molecule 15: 30S ribosomal protein S16

Chain Bp:



- Molecule 16: 30S ribosomal protein S17

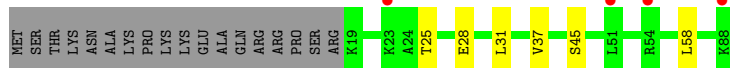
Chain Aq:



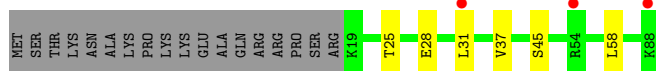
- Chain Bq:



- Chain Ar:



- Chain Br:



- Chain As:



- Chain Bs:



- Chain At:



- Chain Bt: 

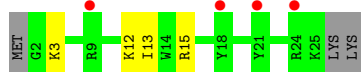


- Chain Au:



- Molecule 20: 30S ribosomal protein Thx

Chain Bu:



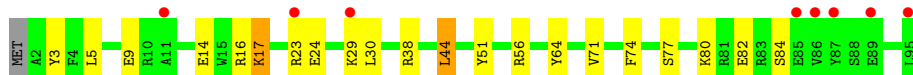
- Molecule 21: Toxin relE

Chain Ay:



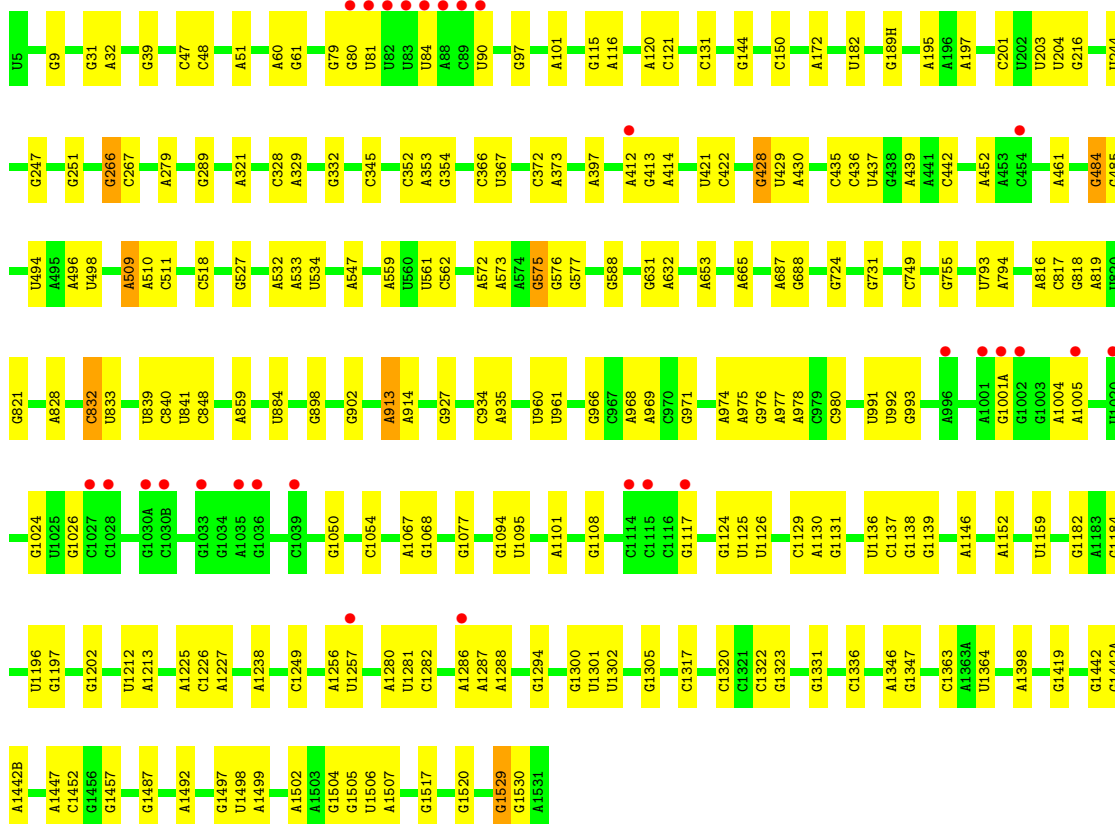
- Molecule 21: Toxin relE

Chain By:



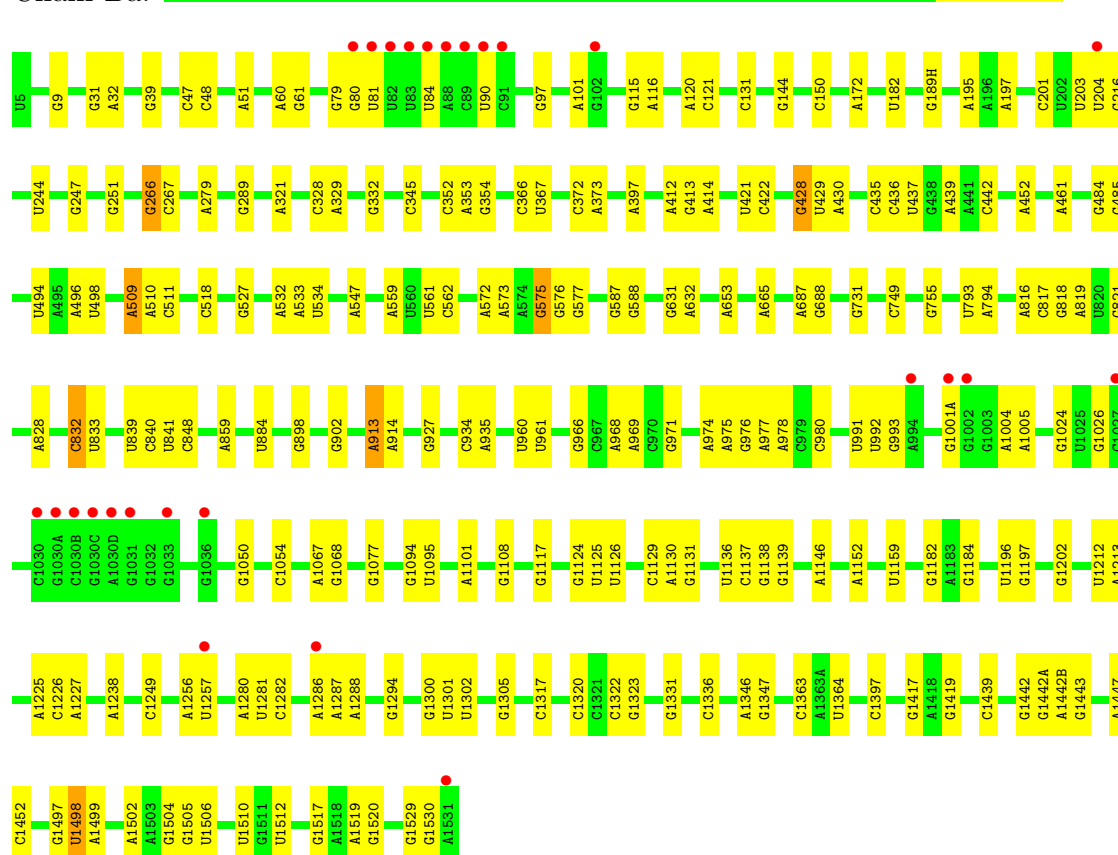
- Molecule 22: RNA (1504-MER)

Chain Aa:



- Molecule 22: RNA (1504-MER)

Chain Ba:



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

Chain Ax:



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

Chain Bx:



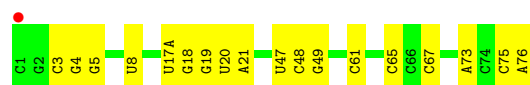
- Molecule 24: RNA (77-MER)

Chain Av:



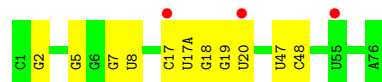
- Molecule 24: RNA (77-MER)

Chain Bv: 



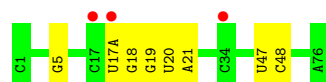
- Molecule 25: RNA (77-MER)

Chain Aw: 



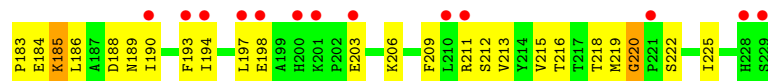
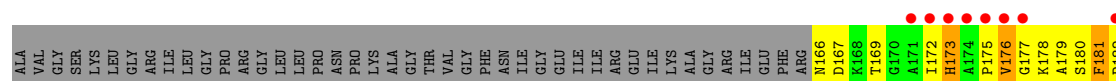
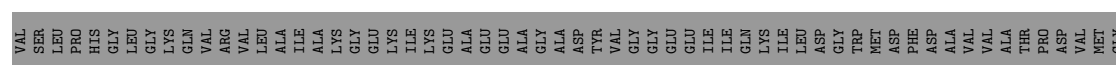
- Molecule 25: RNA (77-MER)

Chain Bw: 



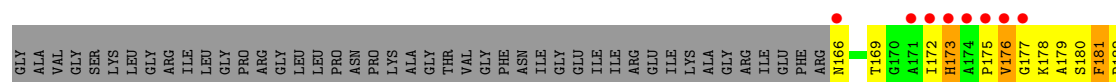
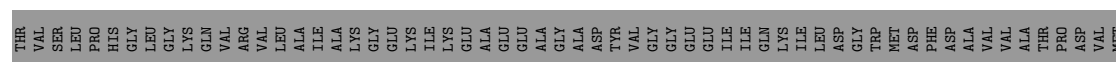
- Molecule 26: 50S ribosomal protein L1

Chain AC: 



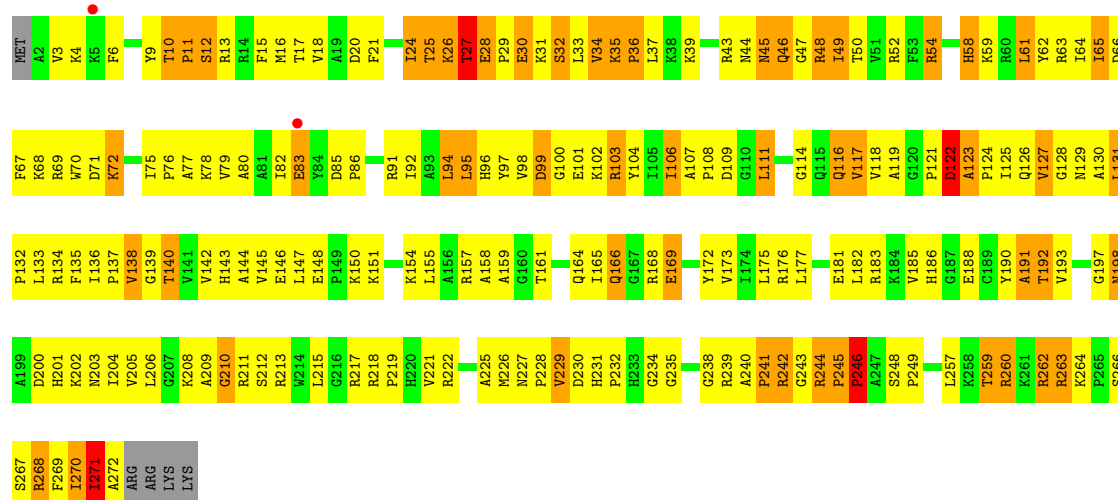
- Molecule 26: 50S ribosomal protein L1

Chain BC: 



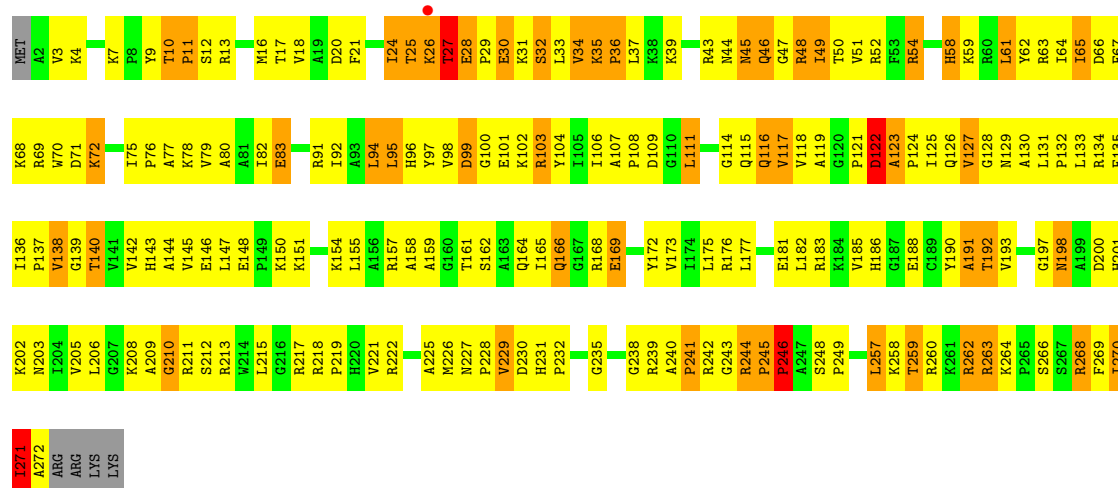
- Molecule 27: 50S ribosomal protein L2

Chain AD:



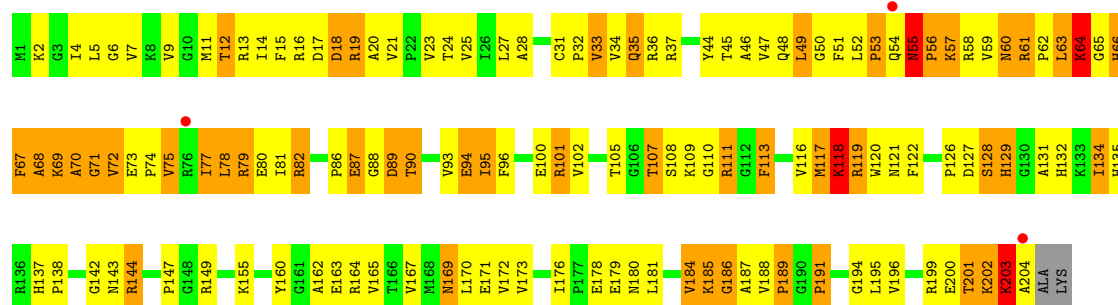
- Molecule 27: 50S ribosomal protein L2

Chain BD:



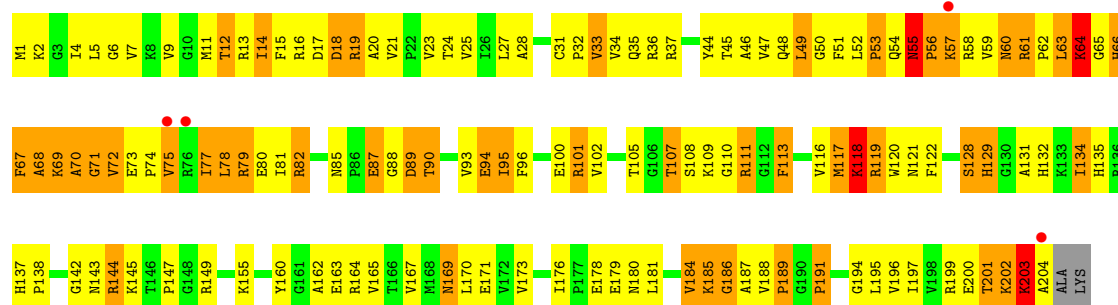
- Molecule 28: 50S ribosomal protein L3

Chain AE:



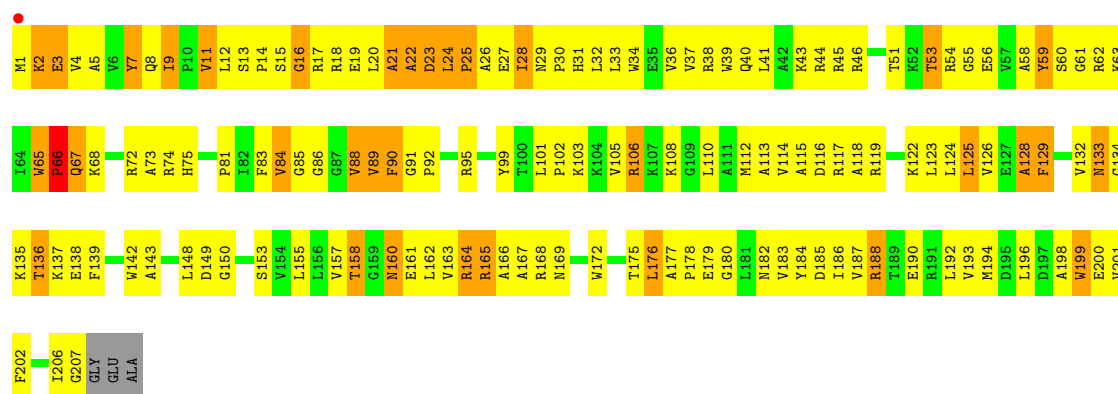
- Molecule 28: 50S ribosomal protein L3

Chain BE:



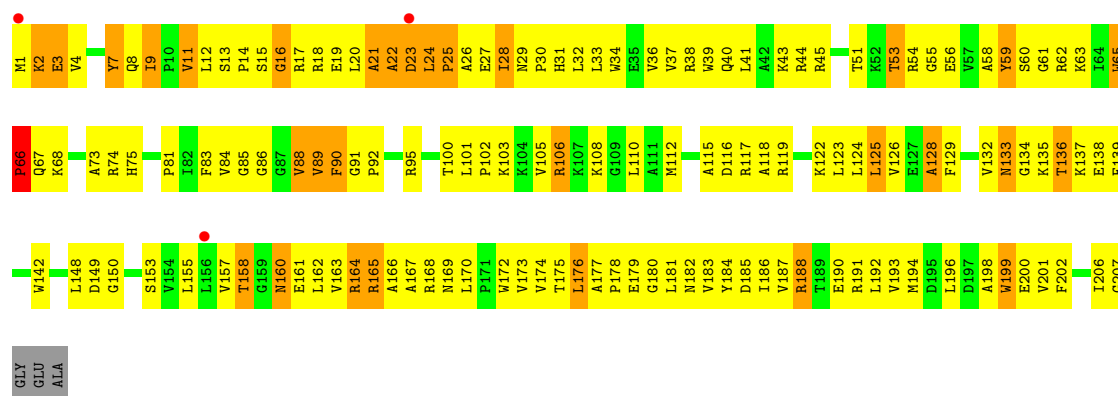
- Molecule 29: 50S ribosomal protein L4

Chain AF:



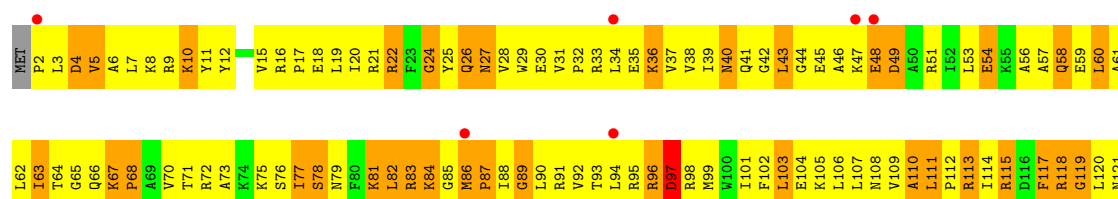
- Molecule 29: 50S ribosomal protein L4

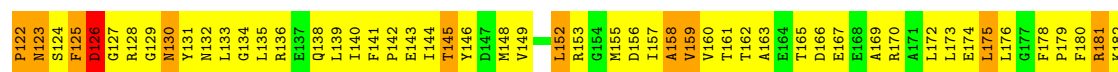
Chain BF:



- Molecule 30: 50S ribosomal protein L5

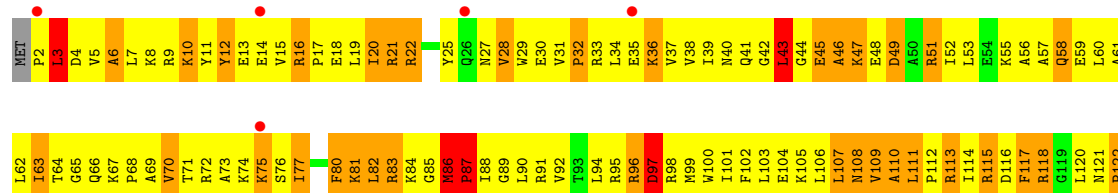
Chain AG:





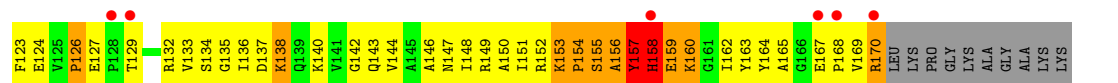
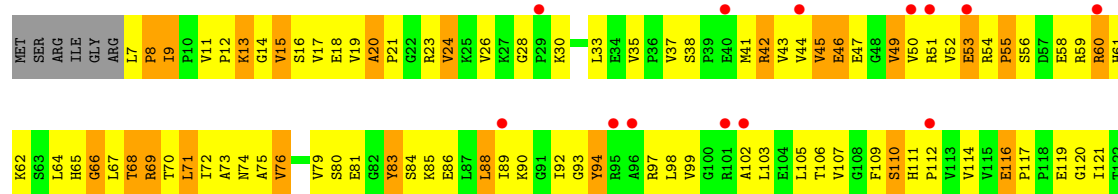
• Molecule 30: 50S ribosomal protein L5

Chain BG:



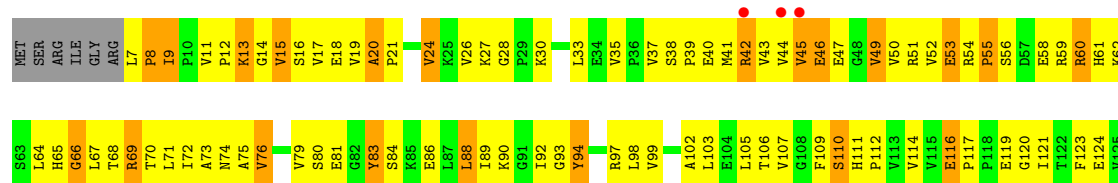
• Molecule 31: 50S ribosomal protein L6

Chain AH:



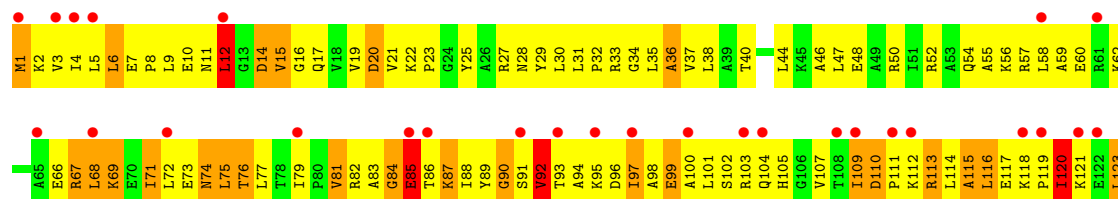
• Molecule 31: 50S ribosomal protein L6

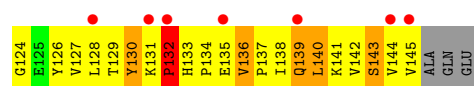
Chain BH:



• Molecule 32: 50S ribosomal protein L9

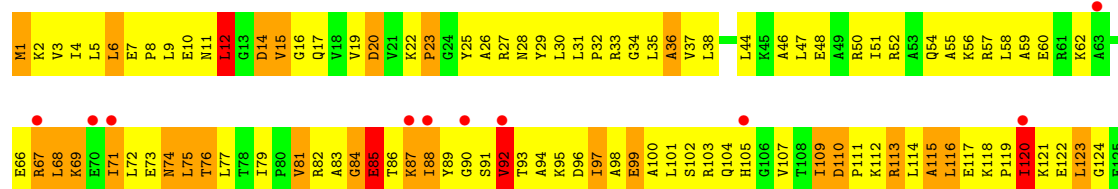
Chain AI:





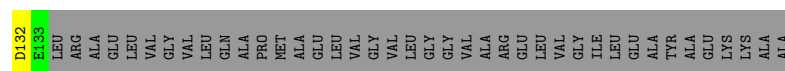
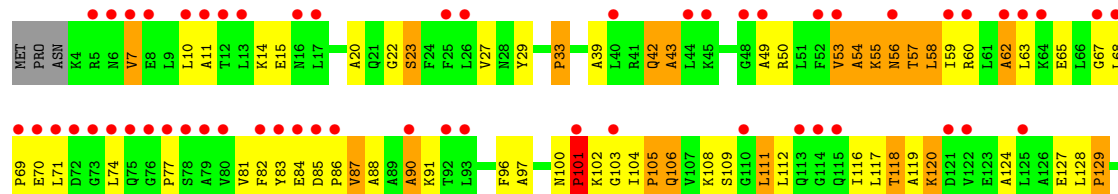
- Molecule 32: 50S ribosomal protein L9

Chain BI:



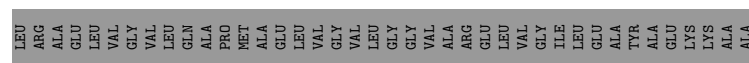
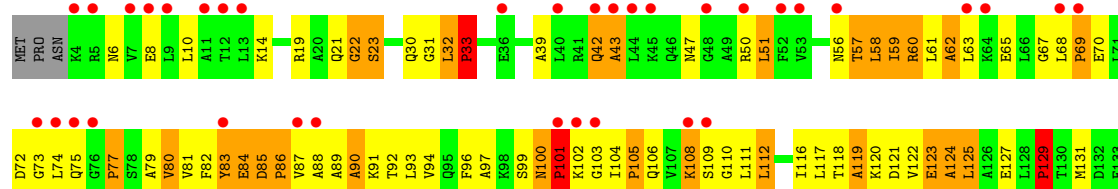
- Molecule 33: 50S ribosomal protein L10

Chain AJ:



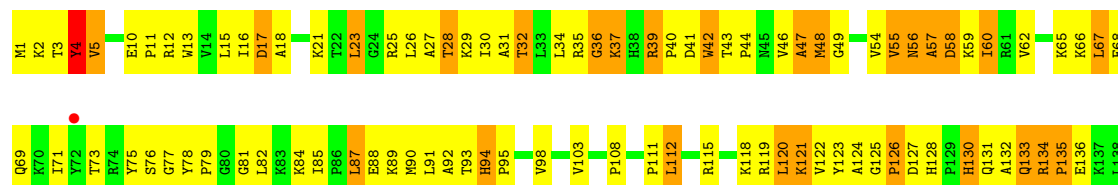
- Molecule 33: 50S ribosomal protein L10

Chain BJ:



- Molecule 34: 50S ribosomal protein L13

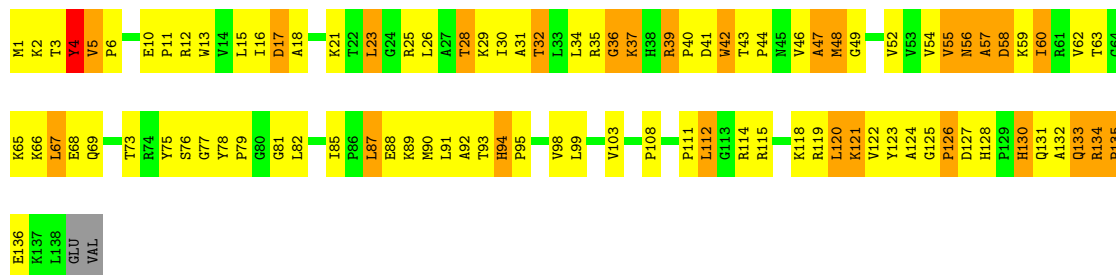
Chain AN:



GLU
VAL

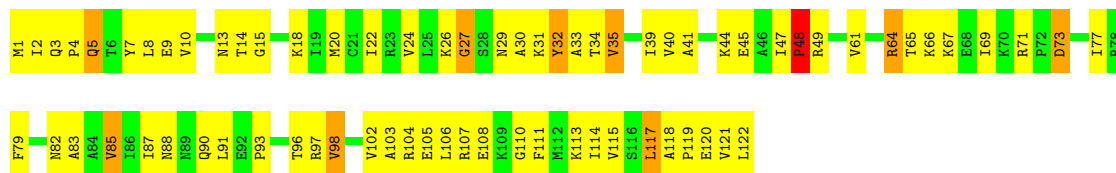
- Molecule 34: 50S ribosomal protein L13

Chain BN:



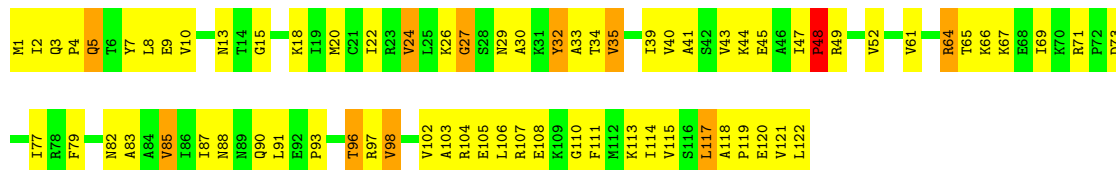
- Molecule 35: 50S ribosomal protein L14

Chain AO:



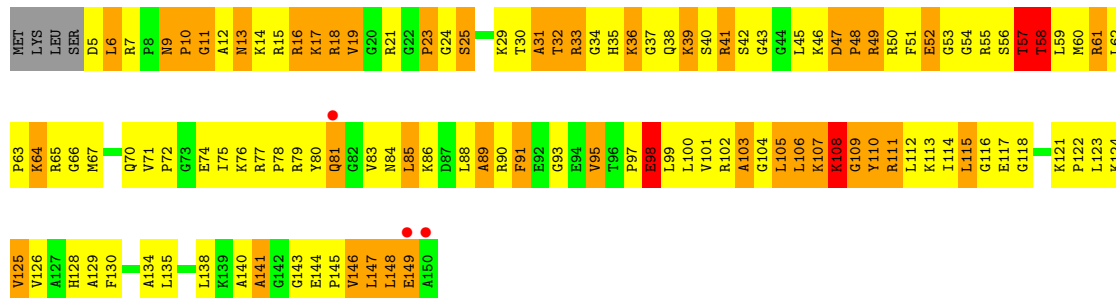
- Molecule 35: 50S ribosomal protein L14

Chain BO:



- Molecule 36: 50S ribosomal protein L15

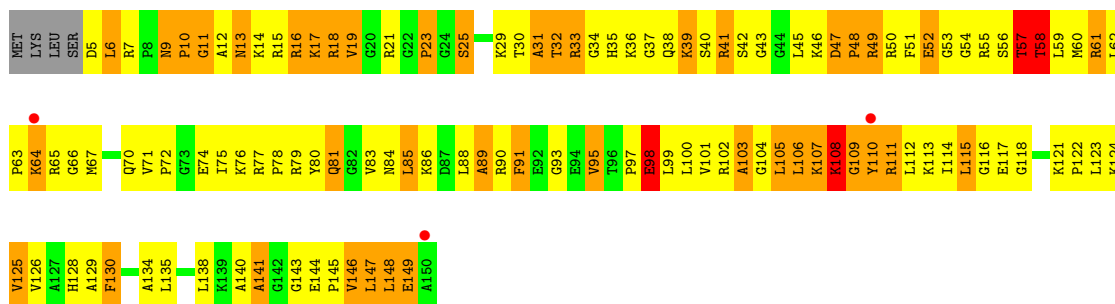
Chain AP:



- Molecule 36: 50S ribosomal protein L15

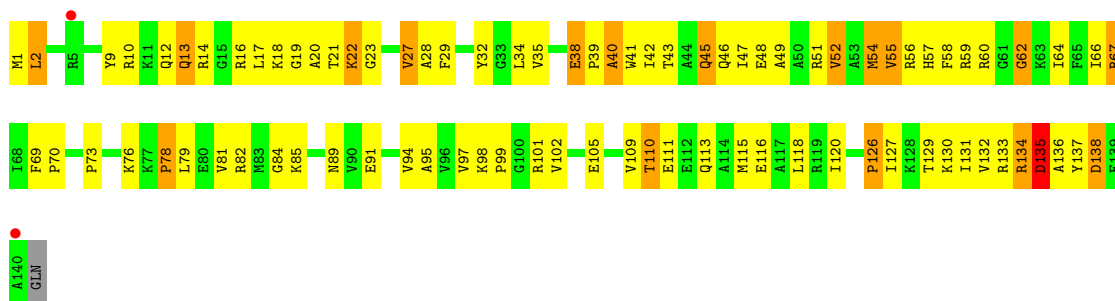
Chain BP:





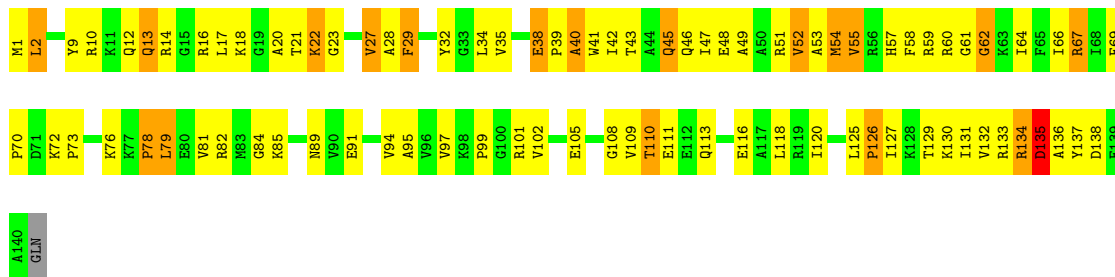
- Molecule 37: 50S ribosomal protein L16

Chain AQ:



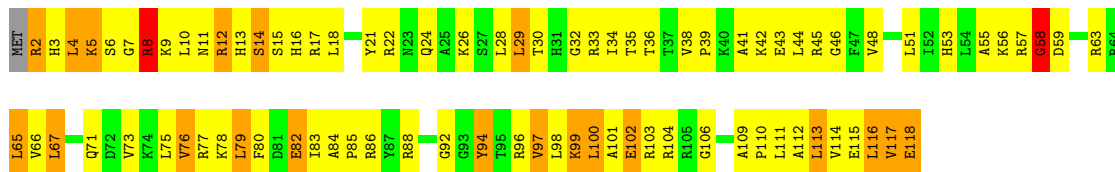
- Molecule 37: 50S ribosomal protein L16

Chain BQ:



- Molecule 38: 50S ribosomal protein L17

Chain AR:



- Molecule 38: 50S ribosomal protein L17

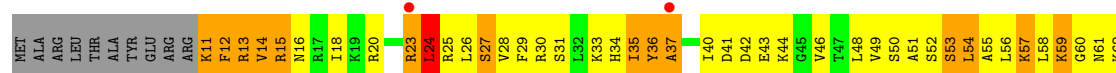
Chain BR:





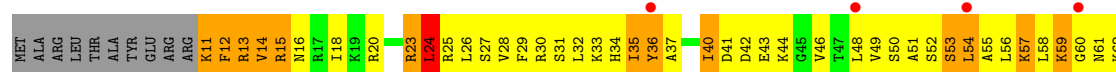
• Molecule 39: 50S ribosomal protein L18

Chain AS:



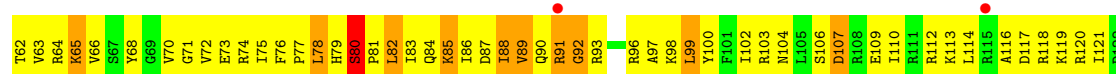
• Molecule 39: 50S ribosomal protein L18

Chain BS:



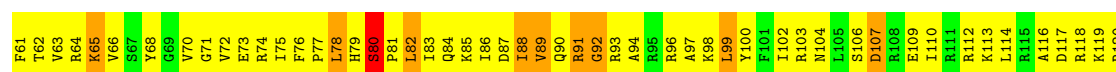
• Molecule 40: 50S ribosomal protein L19

Chain AT:



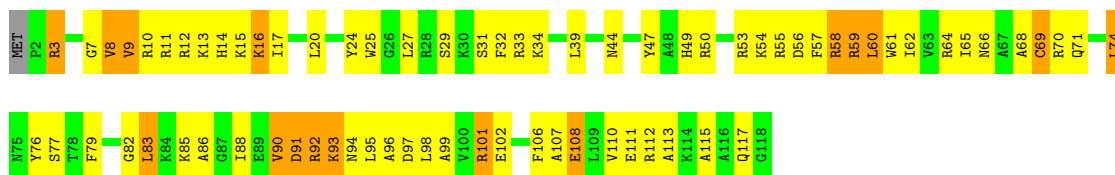
• Molecule 40: 50S ribosomal protein L19

Chain BT:



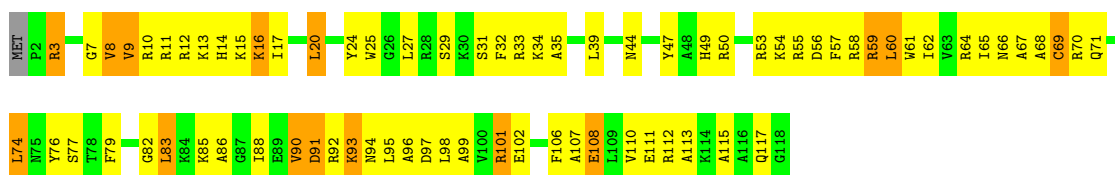
• Molecule 41: 50S ribosomal protein L20

Chain AU:



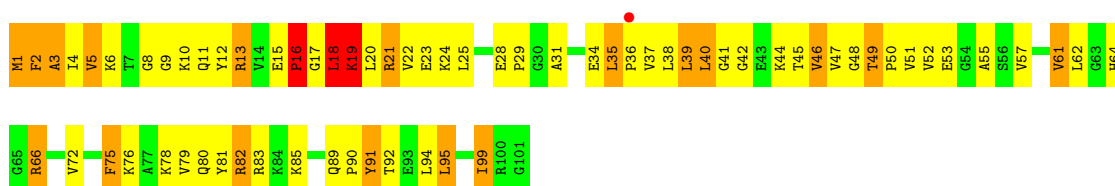
- Molecule 41: 50S ribosomal protein L20

Chain BU:



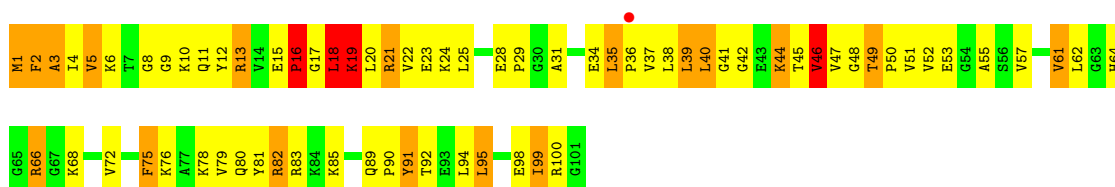
- Molecule 42: 50S ribosomal protein L21

Chain AV:



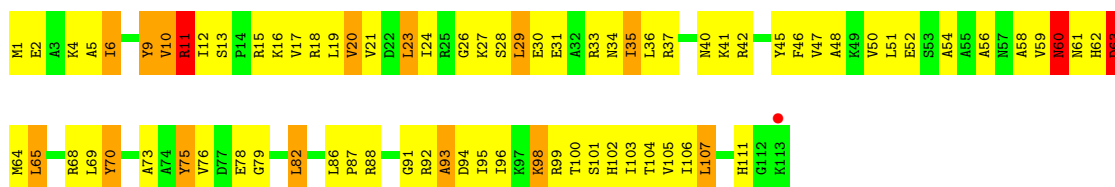
- Molecule 42: 50S ribosomal protein L21

Chain BV:



- Molecule 43: 50S ribosomal protein L22

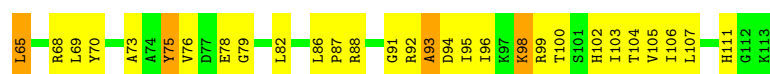
Chain AW:



- Molecule 43: 50S ribosomal protein L22

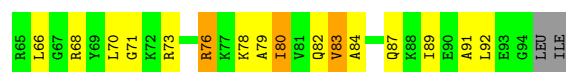
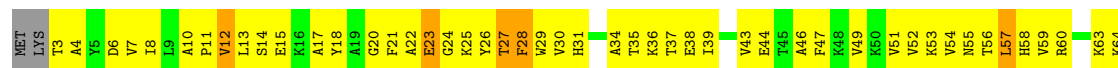
Chain BW:





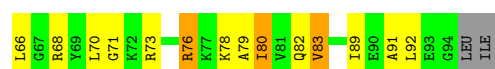
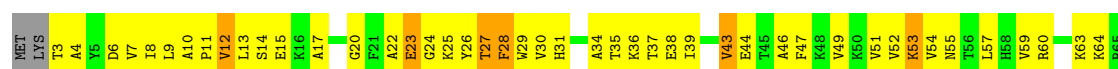
• Molecule 44: 50S ribosomal protein L23

Chain AX:



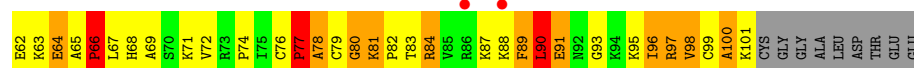
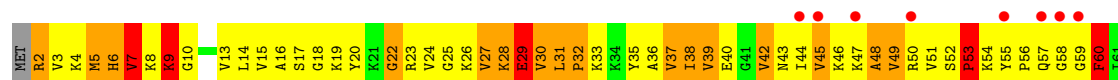
• Molecule 44: 50S ribosomal protein L23

Chain BX:



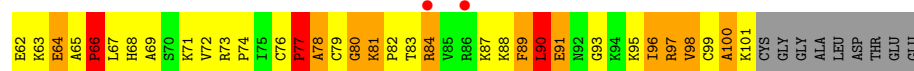
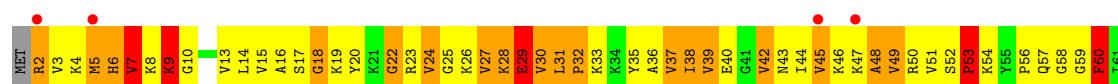
• Molecule 45: 50S ribosomal protein L24

Chain AY:



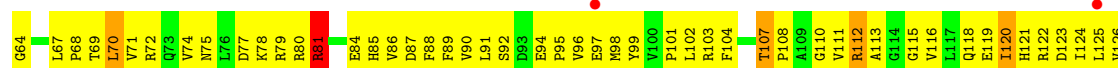
• Molecule 45: 50S ribosomal protein L24

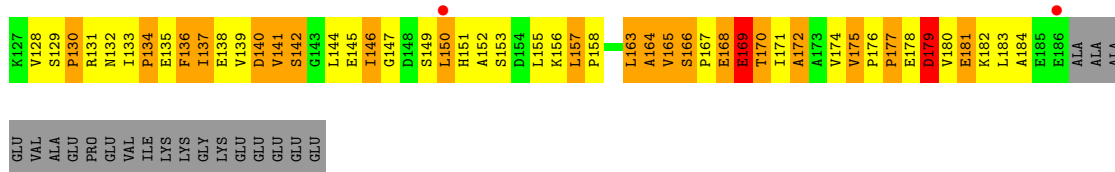
Chain BY:



• Molecule 46: 50S ribosomal protein L25

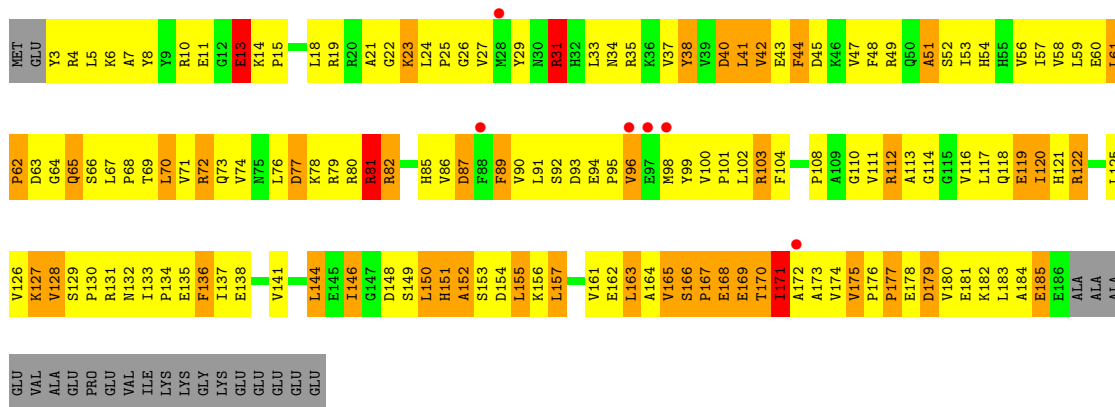
Chain AZ:





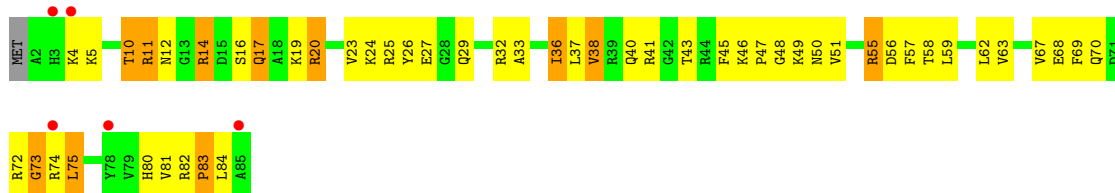
• Molecule 46: 50S ribosomal protein L25

Chain BZ:



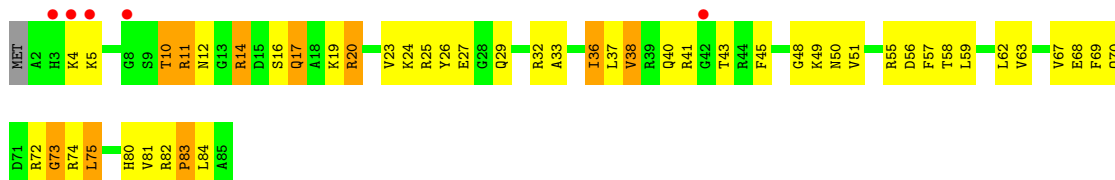
• Molecule 47: 50S ribosomal protein L27

Chain A0:



• Molecule 47: 50S ribosomal protein L27

Chain B0:



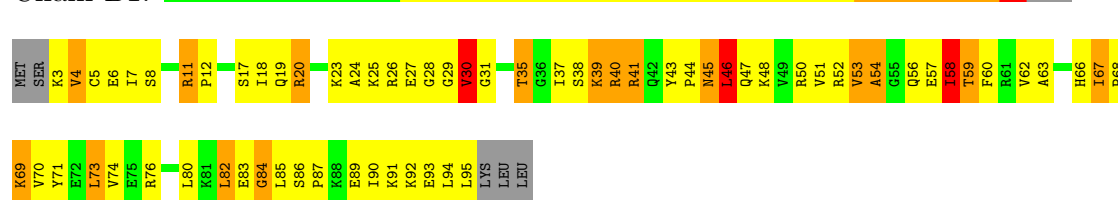
• Molecule 48: 50S ribosomal protein L28

Chain A1:



- Molecule 48: 50S ribosomal protein L28

Chain B1:



- Molecule 49: 50S ribosomal protein L29

Chain A2:



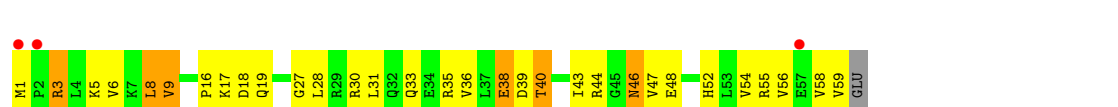
- Molecule 49: 50S ribosomal protein L29

Chain B2:



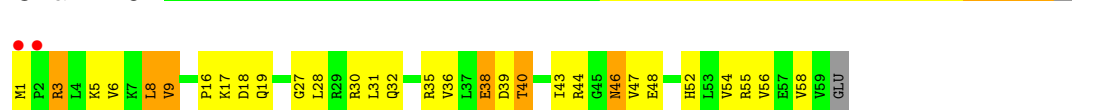
- Molecule 50: 50S ribosomal protein L30

Chain A3:



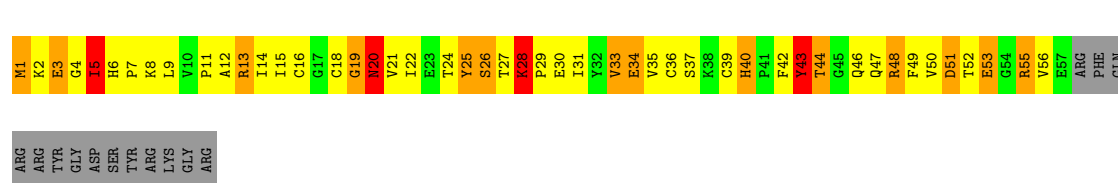
- Molecule 50: 50S ribosomal protein L30

Chain B3:



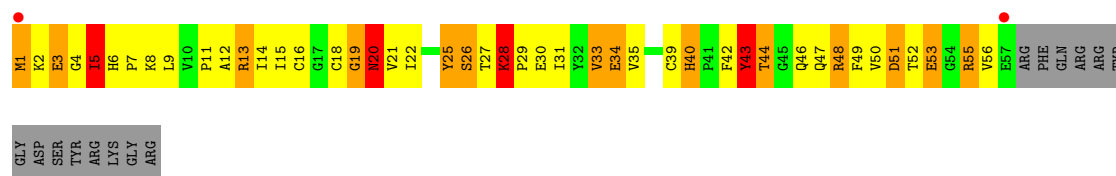
- Molecule 51: 50S ribosomal protein L31

Chain A4:



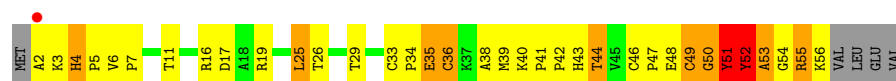
- Molecule 51: 50S ribosomal protein L31

Chain B4:



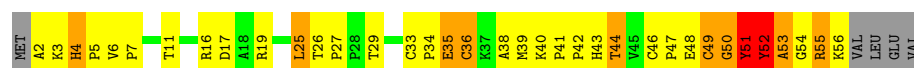
- Molecule 52: 50S ribosomal protein L32

Chain A5:



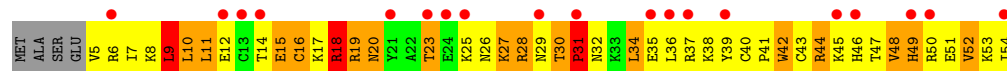
- Molecule 52: 50S ribosomal protein L32

Chain B5:



- Molecule 53: 50S ribosomal protein L33

Chain A6:



- Molecule 53: 50S ribosomal protein L33

Chain B6:



- Molecule 54: 50S ribosomal protein L34

Chain A7:



- Molecule 54: 50S ribosomal protein L34

Chain B7:



- Molecule 55: 50S ribosomal protein L35

Chain A8:



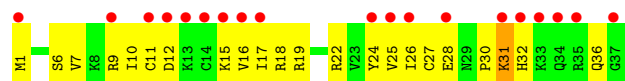
- Molecule 55: 50S ribosomal protein L35

Chain B8:



- Molecule 56: 50S ribosomal protein L36

Chain A9:



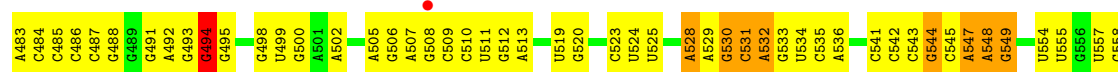
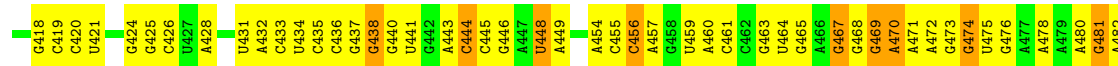
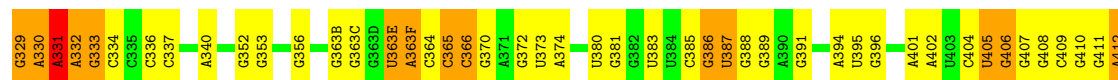
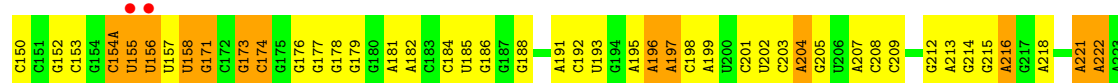
- Molecule 56: 50S ribosomal protein L36

Chain B9:

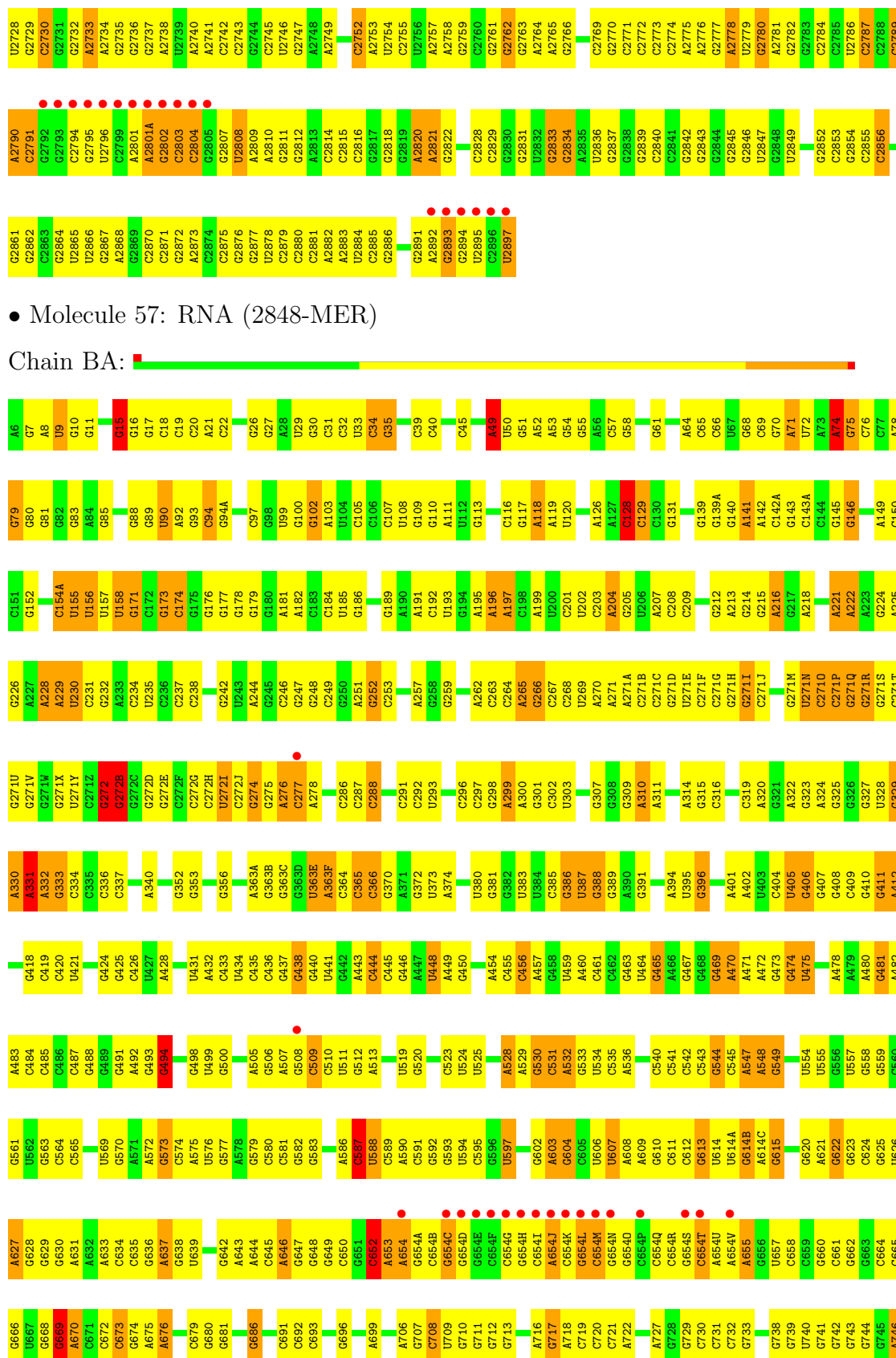


- Molecule 57: RNA (2848-MER)

Chain AA:



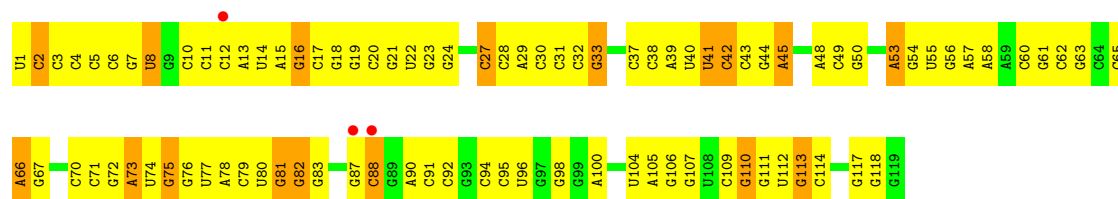
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A2721	A2722	A2723	A2724	A2725	A2726	A2727	A2728	A2729	A2730	A2731	A2732	A2733	A2734	A2735	A2736	A2737	A2738	A2739	A2740	A2741	A2742	A2743	A2744	A2745	A2746	A2747	A2748	A2749	A2750	A2751	A2752	A2753	A2754	A2755	A2756	A2757	A2758	A2759	A2760	A2761	A2762	A2763	A2764	A2765	A2766	A2767	A2768	A2769	A2770	A2771	A2772	A2773	A2774	A2775	A2776	A2777	A2778	A2779	A2780	A2781	A2782	A2783	A2784	A2785	A2786	A2787	A2788	A2789																	
U2649	U2650	U2651	U2652	U2653	U2654	U2655	U2656	U2657	U2658	U2659	U2660	U2661	U2662	U2663	U2664	U2665	U2666	U2667	U2668	U2669	U2670	U2671	U2672	U2673	U2674	U2675	U2676	U2677	U2678	U2679	U2680	U2681	U2682	U2683	U2684	U2685	U2686	U2687	U2688	U2689	U2690	U2691	U2692	U2693	U2694	U2695	U2696	U2697	U2698	U2699	U2700	U2701	U2702	U2703	U2704	U2705	U2706	U2707	U2708	U2709	U2710	U2711	U2712	U2713	U2714	U2715	U2716	U2717	U2718	U2719	U2720														
C2573	C2574	C2575	C2576	C2577	C2578	C2579	C2580	C2581	C2582	C2583	C2584	C2585	C2586	C2587	C2588	C2589	C2590	C2591	C2592	C2593	C2594	C2595	C2596	C2597	C2598	C2599	C2600	C2601	C2602	C2603	C2604	C2605	C2606	C2607	C2608	C2609	C2610	C2611	C2612	C2613	C2614	C2615	C2616	C2617	C2618	C2619	C2620	C2621	C2622	C2623	C2624	C2625	C2626	C2627	C2628	C2629	C2630	C2631	C2632	C2633	C2634	C2635	C2636	C2637	C2638	C2639	C2640	C2641	C2642	C2643	C2644	C2645	C2646	C2647	C2648	C2649									
U2438	U2439	U2440	U2441	U2442	U2443	U2444	U2445	U2446	U2447	U2448	U2449	U2450	U2451	U2452	U2453	U2454	U2455	U2456	U2457	U2458	U2459	U2460	U2461	U2462	U2463	U2464	U2465	U2466	U2467	U2468	U2469	U2470	U2471	U2472	U2473	U2474	U2475	U2476	U2477	U2478	U2479	U2480	U2481	U2482	U2483	U2484	U2485	U2486	U2487	U2488	U2489	U2490	U2491	U2492	U2493	U2494	U2495	U2496	U2497	U2498	U2499	U2500	U2501	U2502	U2503	U2504	U2505	U2506	U2507	U2508															
C2371	C2372	C2373	C2374	C2375	C2376	C2377	C2378	C2379	C2380	C2381	C2382	C2383	C2384	C2385	C2386	C2387	C2388	C2389	C2390	C2391	C2392	C2393	C2394	C2395	C2396	C2397	C2398	C2399	C2400	C2401	C2402	C2403	C2404	C2405	C2406	C2407	C2408	C2409	C2410	C2411	C2412	C2413	C2414	C2415	C2416	C2417	C2418	C2419	C2420	C2421	C2422	C2423	C2424	C2425	C2426	C2427	C2428	C2429	C2430	C2431	C2432	C2433	C2434	C2435	C2436	C2437																			
G2307	G2308	G2309	G2310	G2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	G2319	G2320	G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	G2344	G2345	G2346	G2347	G2348	G2349	G2350	G2351	G2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370																						
C2240	C2241	C2242	C2243	C2244	C2245	C2246	C2247	C2248	C2249	C2250	C2251	C2252	C2253	C2254	C2255	C2256	C2257	C2258	C2259	C2260	C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281	C2282	C2283	C2284	C2285	C2286	C2287	C2288	C2289	C2290	C2291	C2292	C2293	C2294	C2295	C2296	C2297	C2298	C2299	C2300	C2301	C2302	C2303	C2304	C2305	C2306																			
A2168	A2169	A2170	A2171	A2172	A2173	A2174	A2175	A2176	A2177	A2178	A2179	A2180	A2181	A2182	A2183	A2184	A2185	A2186	A2187	A2188	A2189	A2190	A2191	A2192	A2193	A2194	A2195	A2196	A2197	A2198	A2199	A2200	A2201	A2202	A2203	A2204	A2205	A2206	A2207	A2208	A2209	A2210	A2211	A2212	A2213	A2214	A2215	A2216	A2217	A2218	A2219	A2220	A2221	A2222	A2223	A2224	A2225	A2226	A2227	A2228	A2229	A2230	A2231	A2232	A2233	A2234	A2235	A2236	A2237	A2238	A2239														
G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	G2113	G2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167																					
U2033	U2034	U2035	U2036	U2037	U2038	U2039	U2040	U2041	U2042	U2043	U2044	U2045	U2046	U2047	U2048	U2049	U2050	U2051	U2052	U2053	U2054	U2055	U2056	U2057	U2058	U2059	U2060	U2061	U2062	U2063	U2064	U2065	U2066	U2067	U2068	U2069	U2070	U2071	U2072	U2073	U2074	U2075	U2076	U2077	U2078	U2079	U2080	U2081	U2082	U2083	U2084	U2085	U2086	U2087	U2088	U2089	U2090	U2091	U2092	U2093	U2094	U2095	U2096	U2097	U2098	U2099	U2100	U2101	U2102																
A1889	A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1903	A1904	A1905	A1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1923	A1924	A1925	A1926	A1927	A1928	A1929	A1930	A1931	A1932	A1933	A1934	A1935	A1936	A1937	A1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958																

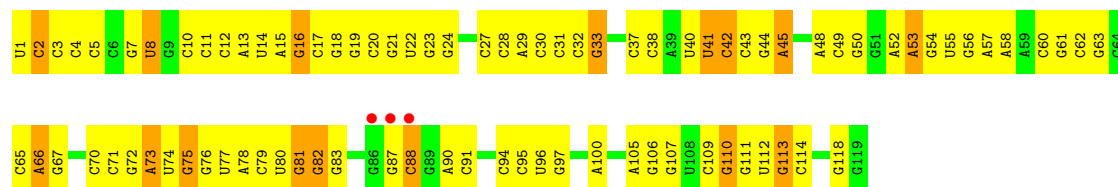
- Molecule 58: RNA (119-MER)

Chain AB:



- Molecule 58: RNA (119-MER)

Chain BB:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.23Å 451.43Å 623.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.60 49.63 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.63-3.60) 99.8 (49.63-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.57Å)	Xtriage
Refinement program	CNS1.2	Depositor
R, R_{free}	0.215 , 0.245 0.222 , 0.254	Depositor DCC
R_{free} test set	30861 reflections (4.75%)	DCC
Wilson B-factor (Å ²)	103.4	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 55.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 680802 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	297230	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

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

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

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

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

All (4) bond length outliers are listed below:

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

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

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

5 of 7 chirality outliers are listed below:

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

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

5 of 125 planarity outliers are listed below:

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

5.2 Close contacts ⓘ

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

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	AI	1131	0	1218	246	0
32	BI	1131	0	1218	264	0
33	AJ	641	0	309	34	0
33	BJ	641	0	309	47	0
34	AN	1104	0	1180	146	0
34	BN	1104	0	1180	151	0
35	AO	933	0	996	98	0
35	BO	933	0	996	99	0
36	AP	1114	0	1187	304	0
36	BP	1114	0	1187	302	0
37	AQ	1112	0	1171	122	0
37	BQ	1112	0	1171	124	0
38	AR	960	0	1021	128	0
38	BR	960	0	1021	126	0
39	AS	770	0	832	139	0
39	BS	770	0	832	137	0
40	AT	1123	0	1181	229	0
40	BT	1123	0	1181	234	0
41	AU	958	0	1015	148	0
41	BU	958	0	1015	145	0
42	AV	779	0	852	151	0
42	BV	779	0	852	153	0
43	AW	896	0	953	94	0
43	BW	896	0	953	89	0
44	AX	725	0	778	88	0
44	BX	725	0	778	91	0
45	AY	775	0	870	189	0
45	BY	775	0	870	197	0
46	AZ	1467	0	1492	238	0
46	BZ	1467	0	1492	238	0
47	A0	662	0	688	79	0
47	B0	662	0	688	77	0
48	A1	731	0	808	98	0
48	B1	731	0	808	89	0
49	A2	598	0	653	96	0
49	B2	598	0	653	57	0
50	A3	467	0	523	40	0
50	B3	467	0	523	38	0
51	A4	450	0	449	91	0
51	B4	450	0	449	80	0
52	A5	427	0	445	83	0
52	B5	427	0	445	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	A6	433	0	461	115	0
53	B6	433	0	461	117	0
54	A7	409	0	454	38	0
54	B7	409	0	454	38	0
55	A8	507	0	576	112	0
55	B8	507	0	576	120	0
56	A9	307	0	336	19	0
56	B9	307	0	336	25	0
57	AA	61341	0	30925	2266	0
57	BA	61341	0	30926	2267	0
58	AB	2551	0	1295	140	0
58	BB	2551	0	1295	115	0
59	A4	1	0	0	0	0
59	A9	1	0	0	0	0
59	Ad	1	0	0	0	0
59	An	1	0	0	0	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	Bd	1	0	0	0	0
59	Bn	1	0	0	0	0
60	A1	2	0	0	0	0
60	A5	1	0	0	0	0
60	A7	1	0	0	0	0
60	AA	367	0	0	0	0
60	AB	3	0	0	0	0
60	AD	2	0	0	0	0
60	AF	1	0	0	0	0
60	AQ	1	0	0	0	0
60	AX	1	0	0	0	0
60	Aa	145	0	0	0	0
60	Ae	2	0	0	0	0
60	Av	5	0	0	0	0
60	Aw	1	0	0	0	0
60	B0	2	0	0	0	0
60	B5	2	0	0	0	0
60	B7	2	0	0	0	0
60	BA	365	0	0	0	0
60	BB	3	0	0	0	0
60	BD	2	0	0	0	0
60	BF	1	0	0	0	0
60	BO	1	0	0	0	0
60	BX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	297230	0	201936	12630	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

The worst 5 of 12630 close contacts within the same asymmetric unit are listed below.

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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ab	232/256 (91%)	149 (64%)	48 (21%)	35 (15%)	0	7
1	Bb	232/256 (91%)	148 (64%)	52 (22%)	32 (14%)	0	9
2	Ac	204/239 (85%)	132 (65%)	43 (21%)	29 (14%)	0	9
2	Bc	204/239 (85%)	134 (66%)	41 (20%)	29 (14%)	0	9
3	Ad	206/209 (99%)	131 (64%)	52 (25%)	23 (11%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Bd	206/209 (99%)	132 (64%)	51 (25%)	23 (11%)	1	14
4	Ae	148/162 (91%)	105 (71%)	24 (16%)	19 (13%)	0	11
4	Be	148/162 (91%)	104 (70%)	23 (16%)	21 (14%)	0	9
5	Af	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	2	29
5	Bf	99/101 (98%)	66 (67%)	26 (26%)	7 (7%)	2	29
6	Ag	153/156 (98%)	108 (71%)	31 (20%)	14 (9%)	1	20
6	Bg	153/156 (98%)	106 (69%)	33 (22%)	14 (9%)	1	20
7	Ah	136/138 (99%)	97 (71%)	32 (24%)	7 (5%)	3	40
7	Bh	136/138 (99%)	97 (71%)	33 (24%)	6 (4%)	4	45
8	Ai	125/128 (98%)	83 (66%)	24 (19%)	18 (14%)	0	8
8	Bi	125/128 (98%)	82 (66%)	25 (20%)	18 (14%)	0	8
9	Aj	96/105 (91%)	76 (79%)	13 (14%)	7 (7%)	2	28
9	Bj	96/105 (91%)	76 (79%)	13 (14%)	7 (7%)	2	28
10	Ak	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	2	34
10	Bk	117/129 (91%)	87 (74%)	23 (20%)	7 (6%)	2	34
11	Al	122/132 (92%)	82 (67%)	25 (20%)	15 (12%)	1	12
11	Bl	122/132 (92%)	82 (67%)	24 (20%)	16 (13%)	0	11
12	Am	116/126 (92%)	58 (50%)	28 (24%)	30 (26%)	0	1
12	Bm	116/126 (92%)	66 (57%)	25 (22%)	25 (22%)	0	2
13	An	58/61 (95%)	38 (66%)	10 (17%)	10 (17%)	0	5
13	Bn	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	5
14	Ao	86/89 (97%)	52 (60%)	24 (28%)	10 (12%)	1	13
14	Bo	86/89 (97%)	52 (60%)	25 (29%)	9 (10%)	1	15
15	Ap	81/88 (92%)	55 (68%)	20 (25%)	6 (7%)	2	28
15	Bp	81/88 (92%)	55 (68%)	23 (28%)	3 (4%)	5	51
16	Aq	97/105 (92%)	74 (76%)	18 (19%)	5 (5%)	3	39
16	Bq	97/105 (92%)	73 (75%)	19 (20%)	5 (5%)	3	39
17	Ar	68/88 (77%)	43 (63%)	20 (29%)	5 (7%)	2	28
17	Br	68/88 (77%)	42 (62%)	21 (31%)	5 (7%)	2	28
18	As	76/93 (82%)	43 (57%)	20 (26%)	13 (17%)	0	5
18	Bs	76/93 (82%)	43 (57%)	20 (26%)	13 (17%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	At	97/106 (92%)	60 (62%)	25 (26%)	12 (12%)	1	12
19	Bt	97/106 (92%)	60 (62%)	25 (26%)	12 (12%)	1	12
20	Au	22/27 (82%)	13 (59%)	6 (27%)	3 (14%)	0	9
20	Bu	22/27 (82%)	12 (54%)	7 (32%)	3 (14%)	0	9
21	Ay	92/95 (97%)	51 (55%)	24 (26%)	17 (18%)	0	4
21	By	92/95 (97%)	58 (63%)	20 (22%)	14 (15%)	0	7
26	AC	116/229 (51%)	87 (75%)	25 (22%)	4 (3%)	6	54
26	BC	116/229 (51%)	86 (74%)	26 (22%)	4 (3%)	6	54
27	AD	269/276 (98%)	187 (70%)	50 (19%)	32 (12%)	1	12
27	BD	269/276 (98%)	190 (71%)	50 (19%)	29 (11%)	1	15
28	AE	202/206 (98%)	138 (68%)	35 (17%)	29 (14%)	0	8
28	BE	202/206 (98%)	140 (69%)	34 (17%)	28 (14%)	0	9
29	AF	205/210 (98%)	148 (72%)	29 (14%)	28 (14%)	0	9
29	BF	205/210 (98%)	148 (72%)	30 (15%)	27 (13%)	0	10
30	AG	179/182 (98%)	98 (55%)	47 (26%)	34 (19%)	0	3
30	BG	179/182 (98%)	99 (55%)	42 (24%)	38 (21%)	0	3
31	AH	162/180 (90%)	97 (60%)	36 (22%)	29 (18%)	0	4
31	BH	162/180 (90%)	97 (60%)	36 (22%)	29 (18%)	0	4
32	AI	143/148 (97%)	75 (52%)	44 (31%)	24 (17%)	0	5
32	BI	143/148 (97%)	76 (53%)	40 (28%)	27 (19%)	0	3
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%)	1	12
34	BN	136/140 (97%)	98 (72%)	21 (15%)	17 (12%)	1	12
35	AO	120/122 (98%)	103 (86%)	11 (9%)	6 (5%)	3	40
35	BO	120/122 (98%)	103 (86%)	12 (10%)	5 (4%)	4	46
36	AP	144/150 (96%)	75 (52%)	37 (26%)	32 (22%)	0	2
36	BP	144/150 (96%)	75 (52%)	38 (26%)	31 (22%)	0	2
37	AQ	138/141 (98%)	105 (76%)	20 (14%)	13 (9%)	1	20
37	BQ	138/141 (98%)	105 (76%)	18 (13%)	15 (11%)	1	14
38	AR	115/118 (98%)	82 (71%)	21 (18%)	12 (10%)	1	16

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	A7	45/49 (92%)	42 (93%)	2 (4%)	1 (2%)	10	64
54	B7	45/49 (92%)	42 (93%)	2 (4%)	1 (2%)	10	64
55	A8	61/65 (94%)	35 (57%)	15 (25%)	11 (18%)	0	4
55	B8	61/65 (94%)	35 (57%)	15 (25%)	11 (18%)	0	4
56	A9	35/37 (95%)	25 (71%)	9 (26%)	1 (3%)	7	58
56	B9	35/37 (95%)	25 (71%)	9 (26%)	1 (3%)	7	58
All	All	12016/13122 (92%)	7873 (66%)	2533 (21%)	1610 (13%)	0	10

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%)	10	48
1	Bb	202/220 (92%)	181 (90%)	21 (10%)	10	48
2	Ac	160/188 (85%)	148 (92%)	12 (8%)	19	67
2	Bc	160/188 (85%)	148 (92%)	12 (8%)	19	67
3	Ad	180/181 (99%)	157 (87%)	23 (13%)	6	35
3	Bd	180/181 (99%)	157 (87%)	23 (13%)	6	35
4	Ae	115/123 (94%)	100 (87%)	15 (13%)	6	34
4	Be	115/123 (94%)	100 (87%)	15 (13%)	6	34
5	Af	90/90 (100%)	82 (91%)	8 (9%)	14	58
5	Bf	90/90 (100%)	81 (90%)	9 (10%)	11	50
6	Ag	126/127 (99%)	120 (95%)	6 (5%)	35	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Bg	126/127 (99%)	120 (95%)	6 (5%)	35	82
7	Ah	119/119 (100%)	111 (93%)	8 (7%)	23	72
7	Bh	119/119 (100%)	110 (92%)	9 (8%)	19	66
8	Ai	98/99 (99%)	86 (88%)	12 (12%)	7	37
8	Bi	98/99 (99%)	86 (88%)	12 (12%)	7	37
9	Aj	88/92 (96%)	80 (91%)	8 (9%)	14	55
9	Bj	88/92 (96%)	80 (91%)	8 (9%)	14	55
10	Ak	90/99 (91%)	85 (94%)	5 (6%)	30	78
10	Bk	90/99 (91%)	85 (94%)	5 (6%)	30	78
11	Al	104/109 (95%)	94 (90%)	10 (10%)	12	52
11	Bl	104/109 (95%)	93 (89%)	11 (11%)	10	46
12	Am	94/101 (93%)	82 (87%)	12 (13%)	6	35
12	Bm	94/101 (93%)	83 (88%)	11 (12%)	8	40
13	An	49/50 (98%)	46 (94%)	3 (6%)	26	75
13	Bn	49/50 (98%)	45 (92%)	4 (8%)	17	62
14	Ao	79/80 (99%)	73 (92%)	6 (8%)	19	66
14	Bo	79/80 (99%)	73 (92%)	6 (8%)	19	66
15	Ap	72/74 (97%)	68 (94%)	4 (6%)	30	78
15	Bp	72/74 (97%)	68 (94%)	4 (6%)	30	78
16	Aq	94/97 (97%)	91 (97%)	3 (3%)	51	89
16	Bq	94/97 (97%)	91 (97%)	3 (3%)	51	89
17	Ar	61/77 (79%)	60 (98%)	1 (2%)	75	95
17	Br	61/77 (79%)	60 (98%)	1 (2%)	75	95
18	As	69/80 (86%)	57 (83%)	12 (17%)	3	18
18	Bs	69/80 (86%)	57 (83%)	12 (17%)	3	18
19	At	76/82 (93%)	71 (93%)	5 (7%)	24	73
19	Bt	76/82 (93%)	71 (93%)	5 (7%)	24	73
20	Au	19/22 (86%)	18 (95%)	1 (5%)	32	79
20	Bu	19/22 (86%)	18 (95%)	1 (5%)	32	79
21	Ay	86/87 (99%)	75 (87%)	11 (13%)	6	35
21	By	86/87 (99%)	77 (90%)	9 (10%)	10	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	AC	99/181 (55%)	92 (93%)	7 (7%)	21	69
26	BC	99/181 (55%)	92 (93%)	7 (7%)	21	69
27	AD	213/218 (98%)	178 (84%)	35 (16%)	3	22
27	BD	213/218 (98%)	180 (84%)	33 (16%)	4	25
28	AE	165/166 (99%)	135 (82%)	30 (18%)	2	16
28	BE	165/166 (99%)	133 (81%)	32 (19%)	2	13
29	AF	165/166 (99%)	143 (87%)	22 (13%)	6	33
29	BF	165/166 (99%)	145 (88%)	20 (12%)	7	38
30	AG	155/156 (99%)	137 (88%)	18 (12%)	8	40
30	BG	155/156 (99%)	128 (83%)	27 (17%)	3	18
31	AH	137/148 (93%)	123 (90%)	14 (10%)	11	49
31	BH	137/148 (93%)	122 (89%)	15 (11%)	9	45
32	AI	122/124 (98%)	103 (84%)	19 (16%)	4	25
32	BI	122/124 (98%)	103 (84%)	19 (16%)	4	25
34	AN	117/119 (98%)	102 (87%)	15 (13%)	6	35
34	BN	117/119 (98%)	102 (87%)	15 (13%)	6	35
35	AO	100/100 (100%)	90 (90%)	10 (10%)	11	50
35	BO	100/100 (100%)	89 (89%)	11 (11%)	9	44
36	AP	112/116 (97%)	93 (83%)	19 (17%)	3	20
36	BP	112/116 (97%)	92 (82%)	20 (18%)	2	17
37	AQ	110/111 (99%)	100 (91%)	10 (9%)	14	55
37	BQ	110/111 (99%)	100 (91%)	10 (9%)	14	55
38	AR	100/101 (99%)	86 (86%)	14 (14%)	5	30
38	BR	100/101 (99%)	86 (86%)	14 (14%)	5	30
39	AS	77/88 (88%)	63 (82%)	14 (18%)	2	16
39	BS	77/88 (88%)	63 (82%)	14 (18%)	2	16
40	AT	118/127 (93%)	99 (84%)	19 (16%)	3	23
40	BT	118/127 (93%)	99 (84%)	19 (16%)	3	23
41	AU	92/94 (98%)	79 (86%)	13 (14%)	5	30
41	BU	92/94 (98%)	79 (86%)	13 (14%)	5	30
42	AV	82/82 (100%)	66 (80%)	16 (20%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BV	82/82 (100%)	65 (79%)	17 (21%)	2	11
43	AW	91/92 (99%)	80 (88%)	11 (12%)	7	38
43	BW	91/92 (99%)	81 (89%)	10 (11%)	9	44
44	AX	74/78 (95%)	64 (86%)	10 (14%)	6	32
44	BX	74/78 (95%)	63 (85%)	11 (15%)	4	27
45	AY	84/91 (92%)	68 (81%)	16 (19%)	2	14
45	BY	84/91 (92%)	68 (81%)	16 (19%)	2	14
46	AZ	162/179 (90%)	141 (87%)	21 (13%)	6	34
46	BZ	162/179 (90%)	134 (83%)	28 (17%)	3	19
47	A0	66/67 (98%)	59 (89%)	7 (11%)	10	46
47	B0	66/67 (98%)	59 (89%)	7 (11%)	10	46
48	A1	78/83 (94%)	66 (85%)	12 (15%)	4	25
48	B1	78/83 (94%)	62 (80%)	16 (20%)	2	11
49	A2	66/67 (98%)	63 (96%)	3 (4%)	38	83
49	B2	66/67 (98%)	56 (85%)	10 (15%)	4	26
50	A3	51/52 (98%)	46 (90%)	5 (10%)	12	51
50	B3	51/52 (98%)	46 (90%)	5 (10%)	12	51
51	A4	51/63 (81%)	41 (80%)	10 (20%)	2	13
51	B4	51/63 (81%)	41 (80%)	10 (20%)	2	13
52	A5	47/52 (90%)	42 (89%)	5 (11%)	10	46
52	B5	47/52 (90%)	42 (89%)	5 (11%)	10	46
53	A6	49/52 (94%)	40 (82%)	9 (18%)	2	15
53	B6	49/52 (94%)	40 (82%)	9 (18%)	2	15
54	A7	40/42 (95%)	37 (92%)	3 (8%)	19	67
54	B7	40/42 (95%)	37 (92%)	3 (8%)	19	67
55	A8	53/55 (96%)	42 (79%)	11 (21%)	2	11
55	B8	53/55 (96%)	42 (79%)	11 (21%)	2	11
56	A9	34/34 (100%)	34 (100%)	0	100	100
56	B9	34/34 (100%)	34 (100%)	0	100	100
All	All	9962/10602 (94%)	8764 (88%)	1198 (12%)	7	38

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

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

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

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	Aa	1503/1504 (99%)	211 (14%)	0
22	Ba	1503/1504 (99%)	210 (13%)	0
23	Ax	11/14 (78%)	8 (72%)	0
23	Bx	11/14 (78%)	8 (72%)	0
24	Av	76/77 (98%)	15 (19%)	0
24	Bv	76/77 (98%)	17 (22%)	0
25	Aw	76/77 (98%)	11 (14%)	0
25	Bw	76/77 (98%)	8 (10%)	0
57	AA	2847/2848 (99%)	521 (18%)	55 (1%)
57	BA	2847/2848 (99%)	517 (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%)	1568 (16%)	113 (1%)

5 of 1568 RNA backbone outliers are listed below:

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

5 of 113 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	AA	2439	A
57	BA	266	G
57	BA	2311	A
57	AA	2481	G
57	BA	71	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	20,22,23	1.13	3 (15%)	25,32,35	1.28	3 (12%)
23	CCC	Ax	21	-	0,2,26	0.00	-	0,1,41	0.00	-
24	5MU	Bv	54	24	20,22,23	1.05	3 (15%)	25,32,35	1.27	2 (8%)
23	CCC	Bx	21	-	0,2,26	0.00	-	0,1,41	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	5MU	Av	54	24	-	0/6/25/26	0/2/2/2
23	CCC	Ax	21	-	-	0/0/0/36	0/0/0/3
24	5MU	Bv	54	24	-	0/6/25/26	0/2/2/2
23	CCC	Bx	21	-	-	0/0/0/36	0/0/0/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Av	54	5MU	C6-N1	2.56	1.38	1.34
24	Bv	54	5MU	C6-C5	-2.36	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Bv	54	5MU	C4-C5	2.27	1.45	1.40
24	Bv	54	5MU	C6-N1	2.22	1.38	1.34
24	Av	54	5MU	C6-C5	-2.11	1.34	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Av	54	5MU	C6-N1-C2	-4.44	121.14	122.41
24	Bv	54	5MU	C6-N1-C2	-4.33	121.18	122.41
24	Bv	54	5MU	C5-C6-N1	2.13	123.93	122.02
24	Av	54	5MU	C5-C6-N1	2.11	123.91	122.02
24	Av	54	5MU	C5M-C5-C6	2.00	122.77	118.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Ab	234/256 (91%)	0.29	4 (1%) 67 40	114, 153, 181, 193	0
1	Bb	234/256 (91%)	0.30	6 (2%) 53 30	113, 152, 181, 193	0
2	Ac	206/239 (86%)	0.52	11 (5%) 25 14	123, 150, 166, 178	0
2	Bc	206/239 (86%)	0.41	7 (3%) 43 24	124, 149, 166, 179	0
3	Ad	208/209 (99%)	0.20	0 100 100	97, 119, 144, 155	0
3	Bd	208/209 (99%)	0.25	1 (0%) 88 71	97, 119, 145, 154	0
4	Ae	150/162 (92%)	0.27	2 (1%) 74 47	88, 114, 138, 159	0
4	Be	150/162 (92%)	0.30	1 (0%) 84 63	84, 112, 138, 160	0
5	Af	101/101 (100%)	0.14	1 (0%) 79 53	91, 121, 138, 155	0
5	Bf	101/101 (100%)	0.02	0 100 100	91, 120, 137, 155	0
6	Ag	155/156 (99%)	0.40	14 (9%) 10 7	118, 137, 171, 188	0
6	Bg	155/156 (99%)	0.47	12 (7%) 13 8	118, 138, 171, 188	0
7	Ah	138/138 (100%)	0.20	0 100 100	96, 117, 132, 157	0
7	Bh	138/138 (100%)	0.19	0 100 100	95, 116, 131, 158	0
8	Ai	127/128 (99%)	0.88	15 (11%) 5 5	120, 160, 178, 186	0
8	Bi	127/128 (99%)	0.77	12 (9%) 9 7	119, 160, 178, 186	0
9	Aj	98/105 (93%)	1.02	18 (18%) 2 2	126, 164, 184, 190	0
9	Bj	98/105 (93%)	0.91	11 (11%) 6 5	124, 164, 184, 190	0
10	Ak	119/129 (92%)	0.25	4 (3%) 43 24	89, 117, 145, 171	0
10	Bk	119/129 (92%)	0.22	4 (3%) 43 24	89, 117, 145, 171	0
11	Al	124/132 (93%)	0.25	3 (2%) 56 32	75, 97, 123, 161	0
11	Bl	124/132 (93%)	0.32	4 (3%) 45 25	77, 97, 125, 162	0
12	Am	118/126 (93%)	0.47	4 (3%) 43 24	115, 143, 157, 166	0
12	Bm	118/126 (93%)	0.50	3 (2%) 54 31	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%)	1.02	9 (15%) 3 3	126, 139, 159, 162	0
13	Bn	60/61 (98%)	0.37	0 100 100	127, 138, 159, 162	0
14	Ao	88/89 (98%)	0.28	0 100 100	81, 110, 131, 138	0
14	Bo	88/89 (98%)	0.14	0 100 100	81, 110, 132, 137	0
15	Ap	83/88 (94%)	0.49	0 100 100	93, 110, 128, 148	0
15	Bp	83/88 (94%)	0.59	2 (2%) 56 32	94, 111, 130, 147	0
16	Aq	99/105 (94%)	0.24	2 (2%) 62 36	80, 107, 124, 132	0
16	Bq	99/105 (94%)	0.25	2 (2%) 62 36	80, 107, 123, 132	0
17	Ar	70/88 (79%)	0.59	4 (5%) 23 12	96, 122, 142, 158	0
17	Br	70/88 (79%)	0.64	3 (4%) 34 19	95, 122, 141, 157	0
18	As	78/93 (83%)	0.64	5 (6%) 19 11	131, 153, 173, 181	0
18	Bs	78/93 (83%)	0.56	5 (6%) 19 11	130, 153, 172, 181	0
19	At	99/106 (93%)	0.42	2 (2%) 62 36	86, 114, 145, 149	0
19	Bt	99/106 (93%)	0.23	1 (1%) 79 53	86, 114, 145, 149	0
20	Au	24/27 (88%)	2.26	12 (50%) 0 1	108, 138, 162, 168	0
20	Bu	24/27 (88%)	1.42	4 (16%) 2 3	106, 137, 162, 168	0
21	Ay	94/95 (98%)	0.90	12 (12%) 4 4	118, 154, 186, 189	0
21	By	94/95 (98%)	0.93	8 (8%) 11 7	110, 146, 182, 188	0
22	Aa	1504/1504 (100%)	0.04	29 (1%) 64 37	65, 119, 193, 208	0
22	Ba	1504/1504 (100%)	0.03	26 (1%) 67 40	63, 119, 193, 208	0
23	Ax	13/14 (92%)	2.16	5 (38%) 1 1	20, 174, 198, 199	0
23	Bx	13/14 (92%)	3.03	7 (53%) 0 1	20, 174, 198, 199	0
24	Av	77/77 (100%)	-0.24	1 (1%) 74 47	96, 119, 161, 163	0
24	Bv	77/77 (100%)	-0.25	1 (1%) 74 47	69, 107, 141, 167	0
25	Aw	77/77 (100%)	0.17	3 (3%) 37 21	103, 191, 201, 203	0
25	Bw	77/77 (100%)	0.08	3 (3%) 37 21	93, 188, 200, 202	0
26	AC	120/229 (52%)	1.49	35 (29%) 1 1	147, 177, 190, 193	0
26	BC	120/229 (52%)	1.44	30 (25%) 1 2	145, 177, 189, 194	0
27	AD	271/276 (98%)	0.07	2 (0%) 84 63	48, 76, 98, 121	0
27	BD	271/276 (98%)	0.05	1 (0%) 90 76	46, 75, 96, 122	0
28	AE	204/206 (99%)	0.12	3 (1%) 70 43	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%)	0.13	4 (1%) 62 36	49, 80, 128, 148	0
29	AF	207/210 (98%)	0.07	1 (0%) 88 71	48, 89, 153, 181	0
29	BF	207/210 (98%)	0.12	3 (1%) 72 45	46, 86, 154, 180	0
30	AG	181/182 (99%)	0.38	6 (3%) 44 25	117, 142, 161, 186	0
30	BG	181/182 (99%)	0.29	5 (2%) 50 29	99, 128, 154, 175	0
31	AH	164/180 (91%)	0.93	19 (11%) 5 5	98, 127, 143, 166	0
31	BH	164/180 (91%)	0.42	7 (4%) 34 19	94, 124, 141, 164	0
32	AI	145/148 (97%)	1.26	35 (24%) 1 2	81, 154, 171, 176	0
32	BI	145/148 (97%)	0.68	11 (7%) 14 8	82, 153, 172, 176	0
33	AJ	130/173 (75%)	2.15	56 (43%) 1 1	170, 195, 202, 203	0
33	BJ	130/173 (75%)	1.29	35 (26%) 1 2	147, 180, 194, 196	0
34	AN	138/140 (98%)	0.22	1 (0%) 84 63	65, 91, 126, 138	0
34	BN	138/140 (98%)	0.07	0 100 100	63, 88, 126, 136	0
35	AO	122/122 (100%)	-0.02	0 100 100	59, 75, 98, 122	0
35	BO	122/122 (100%)	0.00	0 100 100	56, 74, 99, 120	0
36	AP	146/150 (97%)	0.43	3 (2%) 60 35	51, 106, 133, 169	0
36	BP	146/150 (97%)	0.38	3 (2%) 60 35	50, 104, 133, 169	0
37	AQ	140/141 (99%)	0.21	2 (1%) 72 45	75, 96, 124, 147	0
37	BQ	140/141 (99%)	0.22	0 100 100	74, 94, 125, 147	0
38	AR	117/118 (99%)	0.06	0 100 100	48, 80, 108, 128	0
38	BR	117/118 (99%)	0.12	0 100 100	47, 79, 107, 127	0
39	AS	98/112 (87%)	0.61	4 (4%) 35 20	111, 137, 154, 161	0
39	BS	98/112 (87%)	0.79	8 (8%) 12 8	110, 136, 153, 162	0
40	AT	135/146 (92%)	0.14	5 (3%) 39 22	66, 92, 150, 183	0
40	BT	135/146 (92%)	0.15	2 (1%) 70 43	66, 92, 150, 183	0
41	AU	117/118 (99%)	0.07	0 100 100	58, 81, 117, 156	0
41	BU	117/118 (99%)	0.00	0 100 100	52, 78, 116, 158	0
42	AV	101/101 (100%)	0.25	1 (0%) 79 53	59, 106, 125, 134	0
42	BV	101/101 (100%)	0.17	1 (0%) 79 53	54, 103, 125, 134	0
43	AW	113/113 (100%)	0.10	1 (0%) 81 57	58, 73, 106, 183	0
43	BW	113/113 (100%)	0.03	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%)	0.13	0 100 100	63, 86, 110, 120	0
44	BX	92/96 (95%)	0.14	0 100 100	56, 84, 110, 120	0
45	AY	100/110 (90%)	0.93	10 (10%) 8 6	78, 117, 153, 160	0
45	BY	100/110 (90%)	0.52	6 (6%) 21 12	74, 115, 152, 158	0
46	AZ	184/206 (89%)	0.33	4 (2%) 59 34	117, 141, 158, 188	0
46	BZ	184/206 (89%)	0.37	6 (3%) 44 25	87, 126, 150, 173	0
47	A0	84/85 (98%)	0.63	5 (5%) 21 12	81, 100, 148, 168	0
47	B0	84/85 (98%)	0.51	5 (5%) 21 12	78, 100, 148, 168	0
48	A1	93/98 (94%)	0.24	2 (2%) 59 34	64, 87, 127, 137	0
48	B1	93/98 (94%)	0.26	0 100 100	55, 82, 119, 133	0
49	A2	71/72 (98%)	-0.03	0 100 100	81, 116, 134, 156	0
49	B2	71/72 (98%)	-0.01	0 100 100	51, 85, 123, 159	0
50	A3	59/60 (98%)	0.66	3 (5%) 27 15	70, 94, 112, 162	0
50	B3	59/60 (98%)	0.40	2 (3%) 43 24	62, 91, 111, 162	0
51	A4	57/71 (80%)	0.12	0 100 100	150, 164, 175, 177	0
51	B4	57/71 (80%)	0.32	2 (3%) 42 23	150, 164, 174, 177	0
52	A5	55/60 (91%)	-0.01	1 (1%) 65 39	54, 80, 113, 119	0
52	B5	55/60 (91%)	-0.05	0 100 100	54, 78, 112, 121	0
53	A6	50/54 (92%)	1.68	19 (38%) 1 1	121, 149, 165, 175	0
53	B6	50/54 (92%)	1.42	14 (28%) 1 2	121, 149, 164, 176	0
54	A7	47/49 (95%)	0.17	1 (2%) 60 35	50, 64, 86, 133	0
54	B7	47/49 (95%)	0.17	0 100 100	47, 60, 84, 131	0
55	A8	63/65 (96%)	0.44	0 100 100	66, 83, 117, 146	0
55	B8	63/65 (96%)	0.31	0 100 100	63, 83, 116, 145	0
56	A9	37/37 (100%)	2.19	19 (51%) 0 1	121, 134, 149, 151	0
56	B9	37/37 (100%)	2.34	23 (62%) 0 1	121, 132, 148, 152	0
57	AA	2848/2848 (100%)	-0.13	66 (2%) 57 33	47, 83, 185, 208	0
57	BA	2848/2848 (100%)	-0.03	42 (1%) 70 43	44, 80, 185, 208	0
58	AB	119/119 (100%)	-0.07	3 (2%) 54 31	90, 143, 176, 196	0
58	BB	119/119 (100%)	0.05	3 (2%) 54 31	86, 142, 175, 197	0
All	All	21504/22400 (96%)	0.22	803 (3%) 39 22	20, 108, 181, 208	0

The worst 5 of 803 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	Ba	89	C	14.3
22	Aa	83	U	10.8
57	BA	277	C	10.6
57	BA	654(K)	C	10.2
22	Aa	82	U	10.1

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	CCC	Bx	21	3/24	0.62	-	20,20,20,20	0
23	CCC	Ax	21	3/24	0.56	-	20,20,20,20	0
24	5MU	Av	54	21/22	0.20	-	130,133,148,148	0
24	5MU	Bv	54	21/22	0.17	-	114,116,124,125	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	Aa	1632	1/1	0.43	-	72,72,72,72	0
60	MG	A1	102	1/1	0.37	-	116,116,116,116	0
60	MG	AA	3203	1/1	0.24	-	66,66,66,66	0
60	MG	Ba	1632	1/1	0.78	-	41,41,41,41	0
60	MG	BA	3037	1/1	0.24	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Av	105	1/1	0.31	-	92,92,92,92	1
60	MG	Aa	1677	1/1	0.11	-	69,69,69,69	0
60	MG	BA	3147	1/1	0.25	-	56,56,56,56	0
60	MG	Aa	1639	1/1	0.37	-	65,65,65,65	0
60	MG	Ba	1692	1/1	0.60	-	83,83,83,83	0
60	MG	BA	3132	1/1	0.15	-	43,43,43,43	0
60	MG	AA	3060	1/1	0.21	-	46,46,46,46	0
60	MG	Aa	1607	1/1	0.61	-	69,69,69,69	0
60	MG	AA	3144	1/1	1.03	-	50,50,50,50	0
60	MG	AA	3103	1/1	0.10	-	35,35,35,35	0
60	MG	AA	3010	1/1	0.46	-	10,10,10,10	0
60	MG	AA	3140	1/1	0.51	-	45,45,45,45	0
60	MG	BA	2907	1/1	0.48	-	49,49,49,49	0
60	MG	Ba	1655	1/1	0.61	-	43,43,43,43	0
60	MG	Aa	1710	1/1	0.27	-	29,29,29,29	0
60	MG	Ba	1646	1/1	0.28	-	128,128,128,128	0
60	MG	BA	2947	1/1	0.36	-	44,44,44,44	0
60	MG	BA	3118	1/1	0.47	-	70,70,70,70	0
60	MG	BA	3068	1/1	0.56	-	64,64,64,64	0
60	MG	BA	2967	1/1	0.46	-	20,20,20,20	0
60	MG	Ba	1678	1/1	0.51	-	51,51,51,51	0
60	MG	BA	2999	1/1	0.39	-	26,26,26,26	0
60	MG	BA	3151	1/1	0.91	-	119,119,119,119	0
60	MG	Ba	1635	1/1	0.58	-	57,57,57,57	0
60	MG	Ba	1607	1/1	0.18	-	75,75,75,75	0
60	MG	Aa	1741	1/1	1.50	-	79,79,79,79	0
60	MG	AA	3121	1/1	0.44	-	31,31,31,31	0
60	MG	AA	3149	1/1	0.91	-	100,100,100,100	0
60	MG	B0	102	1/1	0.19	-	47,47,47,47	0
60	MG	BX	101	1/1	0.58	-	31,31,31,31	1
60	MG	AA	3130	1/1	0.62	-	76,76,76,76	0
60	MG	AA	3250	1/1	0.62	-	40,40,40,40	0
60	MG	Ba	1605	1/1	0.74	-	73,73,73,73	0
60	MG	BA	2973	1/1	0.42	-	52,52,52,52	0
60	MG	Ba	1616	1/1	0.30	-	29,29,29,29	1
60	MG	Aa	1730	1/1	1.16	-	77,77,77,77	0
60	MG	AA	3195	1/1	0.22	-	30,30,30,30	0
60	MG	BA	2943	1/1	0.28	-	35,35,35,35	0
60	MG	BA	3105	1/1	0.32	-	40,40,40,40	0
60	MG	BA	3207	1/1	0.42	-	118,118,118,118	0
60	MG	BA	3077	1/1	0.31	-	46,46,46,46	0
60	MG	AA	3261	1/1	0.79	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3237	1/1	0.37	-	37,37,37,37	0
60	MG	BA	3048	1/1	0.32	-	31,31,31,31	0
60	MG	AA	2918	1/1	0.55	-	25,25,25,25	0
60	MG	Ae	201	1/1	1.00	-	108,108,108,108	0
60	MG	BA	3025	1/1	0.16	-	12,12,12,12	0
60	MG	Aa	1715	1/1	0.16	-	57,57,57,57	0
60	MG	BA	2989	1/1	0.61	-	31,31,31,31	0
60	MG	AA	3058	1/1	0.25	-	44,44,44,44	0
60	MG	AA	2982	1/1	1.16	-	56,56,56,56	0
60	MG	Aa	1656	1/1	0.49	-	88,88,88,88	0
60	MG	BA	2972	1/1	0.58	-	30,30,30,30	0
60	MG	BA	3021	1/1	0.33	-	31,31,31,31	0
60	MG	AA	2934	1/1	0.24	-	32,32,32,32	1
60	MG	AA	2927	1/1	0.46	-	32,32,32,32	0
60	MG	AA	3200	1/1	0.71	-	72,72,72,72	1
60	MG	AA	3030	1/1	0.17	-	28,28,28,28	0
60	MG	AA	3145	1/1	0.72	-	78,78,78,78	0
60	MG	AA	3196	1/1	0.61	-	70,70,70,70	0
60	MG	BA	3250	1/1	1.56	-	88,88,88,88	0
60	MG	BA	3095	1/1	0.33	-	33,33,33,33	0
60	MG	BA	2980	1/1	0.55	-	9,9,9,9	0
60	MG	AA	3214	1/1	0.96	-	88,88,88,88	0
60	MG	Ba	1712	1/1	0.87	-	79,79,79,79	0
60	MG	AA	3077	1/1	0.47	-	99,99,99,99	0
60	MG	BA	3163	1/1	0.71	-	71,71,71,71	0
60	MG	Ba	1691	1/1	0.68	-	58,58,58,58	0
60	MG	BA	3237	1/1	0.27	-	55,55,55,55	0
60	MG	BA	3179	1/1	0.34	-	24,24,24,24	0
60	MG	AA	3175	1/1	0.47	-	40,40,40,40	0
60	MG	BA	2991	1/1	0.56	-	32,32,32,32	0
60	MG	AA	2992	1/1	0.45	-	45,45,45,45	0
60	MG	AA	3177	1/1	0.47	-	57,57,57,57	0
60	MG	BA	3246	1/1	0.31	-	89,89,89,89	0
60	MG	Aa	1725	1/1	0.61	-	74,74,74,74	0
60	MG	BA	3017	1/1	0.20	-	38,38,38,38	0
60	MG	Aa	1637	1/1	0.37	-	75,75,75,75	0
60	MG	Ba	1673	1/1	0.22	-	39,39,39,39	0
60	MG	BA	3096	1/1	0.13	-	49,49,49,49	0
60	MG	AA	3083	1/1	0.31	-	76,76,76,76	0
60	MG	BA	2966	1/1	0.30	-	67,67,67,67	0
60	MG	Ba	1689	1/1	0.43	-	57,57,57,57	0
60	MG	AA	3164	1/1	0.66	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3219	1/1	0.47	-	30,30,30,30	0
60	MG	AA	3178	1/1	0.32	-	35,35,35,35	0
60	MG	AA	2943	1/1	0.35	-	70,70,70,70	0
60	MG	BA	3124	1/1	0.24	-	40,40,40,40	0
60	MG	AA	3228	1/1	0.59	-	51,51,51,51	0
60	MG	AA	2985	1/1	0.45	-	31,31,31,31	0
60	MG	AA	3180	1/1	0.21	-	73,73,73,73	0
60	MG	Aa	1611	1/1	0.76	-	60,60,60,60	0
60	MG	Aa	1724	1/1	0.17	-	71,71,71,71	0
60	MG	BA	3058	1/1	0.50	-	34,34,34,34	0
60	MG	BA	3038	1/1	0.42	-	26,26,26,26	0
60	MG	BA	3126	1/1	0.42	-	122,122,122,122	0
60	MG	Aa	1608	1/1	0.16	-	39,39,39,39	0
60	MG	AA	3248	1/1	0.66	-	106,106,106,106	0
60	MG	BA	3217	1/1	0.37	-	26,26,26,26	0
60	MG	BA	2955	1/1	0.25	-	49,49,49,49	0
60	MG	Aa	1613	1/1	0.39	-	100,100,100,100	0
60	MG	AA	2998	1/1	0.28	-	36,36,36,36	0
60	MG	Aa	1606	1/1	0.78	-	66,66,66,66	0
60	MG	BA	3099	1/1	0.78	-	90,90,90,90	0
60	MG	Aa	1668	1/1	0.25	-	40,40,40,40	0
60	MG	AA	3041	1/1	0.19	-	21,21,21,21	0
60	MG	AA	2913	1/1	0.51	-	22,22,22,22	0
60	MG	Bx	101	1/1	0.32	-	83,83,83,83	0
60	MG	Ba	1701	1/1	0.45	-	60,60,60,60	0
60	MG	AA	3208	1/1	0.71	-	86,86,86,86	0
60	MG	AA	2981	1/1	0.54	-	13,13,13,13	0
60	MG	Ba	1645	1/1	1.01	-	101,101,101,101	0
60	MG	BA	3010	1/1	0.50	-	13,13,13,13	0
60	MG	Aa	1722	1/1	0.36	-	78,78,78,78	0
60	MG	BA	3062	1/1	0.20	-	36,36,36,36	0
60	MG	BA	3181	1/1	0.18	-	61,61,61,61	0
60	MG	AA	3037	1/1	0.39	-	27,27,27,27	0
60	MG	AA	2953	1/1	0.24	-	96,96,96,96	0
60	MG	AA	2995	1/1	0.64	-	18,18,18,18	0
60	MG	AA	3251	1/1	0.79	-	84,84,84,84	0
60	MG	Ba	1629	1/1	0.15	-	36,36,36,36	0
60	MG	Ba	1667	1/1	0.51	-	50,50,50,50	0
60	MG	Ba	1737	1/1	0.56	-	76,76,76,76	0
60	MG	Aa	1622	1/1	1.06	-	79,79,79,79	0
60	MG	BA	3174	1/1	0.28	-	63,63,63,63	0
60	MG	BA	3214	1/1	0.66	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3197	1/1	0.48	-	22,22,22,22	0
60	MG	BA	2908	1/1	0.35	-	20,20,20,20	0
60	MG	Aa	1711	1/1	0.41	-	70,70,70,70	0
60	MG	BA	3066	1/1	0.75	-	32,32,32,32	0
60	MG	AA	3074	1/1	0.39	-	33,33,33,33	0
60	MG	BA	3040	1/1	0.19	-	17,17,17,17	0
60	MG	BA	3225	1/1	0.65	-	38,38,38,38	0
60	MG	BA	3092	1/1	0.27	-	79,79,79,79	0
60	MG	AA	3055	1/1	0.47	-	67,67,67,67	0
60	MG	Ba	1718	1/1	0.35	-	107,107,107,107	0
60	MG	AA	3266	1/1	0.30	-	87,87,87,87	0
60	MG	Ba	1721	1/1	0.89	-	92,92,92,92	0
60	MG	BA	3211	1/1	0.32	-	24,24,24,24	0
60	MG	BA	3177	1/1	0.26	-	70,70,70,70	0
60	MG	Av	104	1/1	0.78	-	50,50,50,50	1
60	MG	BA	3116	1/1	0.50	-	91,91,91,91	0
60	MG	AA	3115	1/1	0.32	-	19,19,19,19	0
60	MG	BA	3112	1/1	0.20	-	69,69,69,69	0
60	MG	BA	3127	1/1	0.52	-	20,20,20,20	0
60	MG	Aa	1665	1/1	2.87	-	120,120,120,120	0
60	MG	BA	3042	1/1	0.18	-	30,30,30,30	0
60	MG	Bw	101	1/1	0.16	-	132,132,132,132	1
60	MG	BA	2960	1/1	0.10	-	101,101,101,101	0
60	MG	BA	3206	1/1	0.52	-	71,71,71,71	0
60	MG	AA	3263	1/1	0.86	-	75,75,75,75	0
60	MG	Ba	1674	1/1	0.14	-	66,66,66,66	0
60	MG	BA	2930	1/1	0.40	-	28,28,28,28	0
60	MG	AA	3124	1/1	0.41	-	15,15,15,15	0
60	MG	AA	3089	1/1	0.18	-	75,75,75,75	0
60	MG	Aa	1629	1/1	0.47	-	59,59,59,59	0
60	MG	BA	3229	1/1	0.21	-	32,32,32,32	0
60	MG	BA	3212	1/1	1.39	-	68,68,68,68	0
60	MG	BA	2988	1/1	0.17	-	34,34,34,34	0
60	MG	AA	3185	1/1	0.40	-	83,83,83,83	0
60	MG	Ba	1688	1/1	0.25	-	120,120,120,120	1
60	MG	BA	2942	1/1	0.16	-	42,42,42,42	0
60	MG	Aa	1638	1/1	0.39	-	62,62,62,62	0
60	MG	AA	2947	1/1	0.32	-	72,72,72,72	0
60	MG	AA	2979	1/1	0.14	-	51,51,51,51	0
60	MG	BA	2976	1/1	0.34	-	104,104,104,104	0
60	MG	Aa	1678	1/1	0.34	-	93,93,93,93	0
60	MG	AA	3015	1/1	0.23	-	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3252	1/1	1.11	-	80,80,80,80	0
60	MG	BA	3120	1/1	0.43	-	16,16,16,16	0
60	MG	BA	2944	1/1	0.14	-	62,62,62,62	0
60	MG	AA	3134	1/1	0.34	-	98,98,98,98	0
60	MG	AA	3128	1/1	0.48	-	23,23,23,23	0
60	MG	AA	3097	1/1	0.45	-	43,43,43,43	0
60	MG	AA	3253	1/1	0.26	-	71,71,71,71	0
60	MG	AA	2914	1/1	0.28	-	15,15,15,15	0
60	MG	Ba	1680	1/1	0.08	-	63,63,63,63	0
60	MG	AA	2915	1/1	0.37	-	21,21,21,21	0
60	MG	Aa	1676	1/1	0.76	-	90,90,90,90	1
60	MG	Aa	1623	1/1	0.30	-	74,74,74,74	0
60	MG	AA	3155	1/1	0.17	-	92,92,92,92	1
60	MG	Ba	1709	1/1	0.38	-	52,52,52,52	0
60	MG	Ba	1724	1/1	0.70	-	68,68,68,68	0
60	MG	AA	3007	1/1	0.12	-	43,43,43,43	0
60	MG	BA	3006	1/1	0.34	-	21,21,21,21	0
60	MG	AA	2928	1/1	0.49	-	110,110,110,110	0
60	MG	BA	3183	1/1	0.25	-	44,44,44,44	0
60	MG	Aa	1671	1/1	0.13	-	49,49,49,49	0
60	MG	AA	3240	1/1	0.89	-	106,106,106,106	0
60	MG	Aa	1645	1/1	1.50	-	79,79,79,79	0
60	MG	AA	3215	1/1	0.17	-	56,56,56,56	0
60	MG	BA	3117	1/1	0.66	-	63,63,63,63	0
60	MG	BA	3000	1/1	0.42	-	16,16,16,16	0
60	MG	BA	2916	1/1	0.75	-	62,62,62,62	0
60	MG	AA	3229	1/1	0.47	-	73,73,73,73	0
60	MG	BA	3122	1/1	0.26	-	24,24,24,24	0
60	MG	Ba	1637	1/1	0.65	-	80,80,80,80	0
60	MG	AA	3076	1/1	0.27	-	78,78,78,78	0
60	MG	BA	3130	1/1	0.41	-	45,45,45,45	0
60	MG	BA	3252	1/1	0.19	-	40,40,40,40	0
60	MG	Aa	1716	1/1	0.14	-	70,70,70,70	0
60	MG	Aa	1674	1/1	0.29	-	90,90,90,90	0
60	MG	Ba	1698	1/1	0.89	-	89,89,89,89	1
60	MG	Ba	1663	1/1	0.74	-	85,85,85,85	0
60	MG	AA	3050	1/1	0.16	-	96,96,96,96	0
60	MG	Ba	1664	1/1	0.71	-	46,46,46,46	0
60	MG	BA	2932	1/1	0.30	-	67,67,67,67	0
60	MG	BA	3046	1/1	0.39	-	28,28,28,28	0
59	ZN	A9	101	1/1	0.13	-	138,138,138,138	0
60	MG	BA	3057	1/1	0.23	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3078	1/1	0.60	-	32,32,32,32	0
60	MG	AA	3099	1/1	0.55	-	57,57,57,57	0
60	MG	Aa	1687	1/1	0.15	-	64,64,64,64	0
60	MG	AA	3190	1/1	0.46	-	43,43,43,43	0
60	MG	Aa	1658	1/1	0.58	-	75,75,75,75	0
60	MG	BA	3131	1/1	0.75	-	96,96,96,96	0
60	MG	AA	3102	1/1	0.75	-	68,68,68,68	0
60	MG	BA	3015	1/1	0.22	-	18,18,18,18	0
60	MG	BA	3184	1/1	0.17	-	57,57,57,57	0
60	MG	Ba	1659	1/1	0.35	-	79,79,79,79	0
60	MG	AA	3184	1/1	0.21	-	44,44,44,44	0
60	MG	AA	3024	1/1	0.34	-	25,25,25,25	0
60	MG	BA	3203	1/1	0.12	-	95,95,95,95	0
60	MG	Aa	1612	1/1	0.19	-	32,32,32,32	0
60	MG	BA	2945	1/1	0.33	-	112,112,112,112	0
60	MG	AA	3264	1/1	0.99	-	78,78,78,78	0
60	MG	AA	3027	1/1	0.21	-	54,54,54,54	0
60	MG	Ba	1672	1/1	0.21	-	95,95,95,95	0
60	MG	Aa	1654	1/1	0.20	-	56,56,56,56	0
60	MG	AA	3096	1/1	0.63	-	73,73,73,73	0
60	MG	AA	3082	1/1	0.41	-	72,72,72,72	0
60	MG	Ba	1642	1/1	0.62	-	78,78,78,78	0
60	MG	AA	3207	1/1	0.52	-	59,59,59,59	0
60	MG	BB	201	1/1	0.50	-	54,54,54,54	0
60	MG	BA	3087	1/1	0.60	-	51,51,51,51	0
60	MG	AA	3166	1/1	0.35	-	48,48,48,48	0
60	MG	Aa	1695	1/1	0.10	-	78,78,78,78	0
60	MG	AA	3174	1/1	0.12	-	72,72,72,72	0
60	MG	AA	3238	1/1	0.90	-	75,75,75,75	0
60	MG	BA	2913	1/1	0.44	-	11,11,11,11	0
60	MG	Aa	1696	1/1	0.24	-	67,67,67,67	0
60	MG	AA	3201	1/1	1.12	-	88,88,88,88	0
60	MG	BA	2975	1/1	0.56	-	105,105,105,105	0
60	MG	Ba	1690	1/1	0.38	-	56,56,56,56	0
60	MG	BA	2925	1/1	0.41	-	31,31,31,31	0
60	MG	AA	3071	1/1	0.40	-	74,74,74,74	0
60	MG	AA	2987	1/1	0.41	-	53,53,53,53	0
60	MG	AA	2960	1/1	0.32	-	17,17,17,17	0
60	MG	AA	2929	1/1	0.26	-	29,29,29,29	0
60	MG	BA	3205	1/1	0.41	-	92,92,92,92	0
60	MG	BA	3121	1/1	1.33	-	70,70,70,70	0
60	MG	BA	2904	1/1	0.32	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3142	1/1	0.42	-	53,53,53,53	0
60	MG	AA	2902	1/1	0.18	-	167,167,167,167	0
60	MG	A5	101	1/1	0.49	-	34,34,34,34	0
60	MG	Aa	1657	1/1	0.32	-	71,71,71,71	0
60	MG	BA	3159	1/1	0.21	-	52,52,52,52	0
60	MG	AA	2955	1/1	0.45	-	48,48,48,48	0
60	MG	Ba	1706	1/1	0.72	-	104,104,104,104	0
60	MG	AA	3000	1/1	0.62	-	63,63,63,63	0
60	MG	AA	3012	1/1	0.28	-	22,22,22,22	0
60	MG	AA	2988	1/1	0.28	-	33,33,33,33	0
60	MG	Aa	1742	1/1	0.54	-	106,106,106,106	0
60	MG	BA	3167	1/1	0.77	-	59,59,59,59	0
60	MG	BA	3034	1/1	0.40	-	11,11,11,11	0
60	MG	BA	2911	1/1	0.17	-	21,21,21,21	0
60	MG	AA	3168	1/1	0.30	-	82,82,82,82	0
60	MG	BA	2977	1/1	0.40	-	46,46,46,46	0
60	MG	AA	3158	1/1	0.30	-	46,46,46,46	0
60	MG	AA	3094	1/1	0.36	-	67,67,67,67	0
60	MG	BA	3143	1/1	1.30	-	95,95,95,95	0
60	MG	BA	3067	1/1	0.33	-	28,28,28,28	0
60	MG	Aa	1635	1/1	0.28	-	39,39,39,39	0
60	MG	BA	2964	1/1	0.40	-	49,49,49,49	0
60	MG	BA	3256	1/1	0.51	-	39,39,39,39	0
60	MG	Ba	1713	1/1	0.64	-	83,83,83,83	0
60	MG	AA	2908	1/1	0.35	-	25,25,25,25	0
60	MG	BA	2905	1/1	0.49	-	29,29,29,29	0
60	MG	AA	3126	1/1	0.53	-	47,47,47,47	0
60	MG	BB	202	1/1	0.33	-	46,46,46,46	0
60	MG	Aa	1601	1/1	0.91	-	123,123,123,123	0
60	MG	BA	3152	1/1	0.38	-	71,71,71,71	0
60	MG	Aa	1660	1/1	0.45	-	49,49,49,49	0
60	MG	AA	2945	1/1	0.14	-	74,74,74,74	0
60	MG	Ba	1636	1/1	0.20	-	60,60,60,60	0
60	MG	Ba	1627	1/1	0.59	-	74,74,74,74	0
60	MG	BA	3103	1/1	0.33	-	50,50,50,50	0
60	MG	Ba	1619	1/1	0.08	-	44,44,44,44	0
60	MG	AA	3171	1/1	0.15	-	57,57,57,57	0
59	ZN	Bn	101	1/1	0.14	-	137,137,137,137	0
60	MG	Aa	1647	1/1	0.22	-	138,138,138,138	0
60	MG	BA	3176	1/1	0.39	-	48,48,48,48	0
60	MG	AA	3108	1/1	0.12	-	38,38,38,38	0
60	MG	BA	3243	1/1	1.52	-	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3087	1/1	0.38	-	60,60,60,60	0
60	MG	BA	3173	1/1	0.97	-	72,72,72,72	0
60	MG	Ba	1644	1/1	1.09	-	67,67,67,67	0
60	MG	Aa	1686	1/1	0.32	-	37,37,37,37	1
60	MG	Ba	1743	1/1	0.56	-	57,57,57,57	0
60	MG	AA	3262	1/1	1.12	-	81,81,81,81	0
60	MG	BA	3052	1/1	0.48	-	10,10,10,10	0
60	MG	Ba	1656	1/1	0.55	-	73,73,73,73	0
60	MG	AA	3222	1/1	0.67	-	45,45,45,45	0
60	MG	Ba	1668	1/1	0.32	-	49,49,49,49	0
60	MG	BA	3182	1/1	0.30	-	63,63,63,63	0
60	MG	AA	3247	1/1	0.32	-	103,103,103,103	0
60	MG	Aa	1624	1/1	0.30	-	37,37,37,37	0
60	MG	AA	3216	1/1	0.49	-	49,49,49,49	0
60	MG	AA	3192	1/1	1.04	-	101,101,101,101	0
60	MG	AA	2980	1/1	0.64	-	69,69,69,69	0
60	MG	AA	3152	1/1	0.74	-	62,62,62,62	0
60	MG	BA	3146	1/1	0.69	-	84,84,84,84	0
60	MG	BA	3086	1/1	0.21	-	48,48,48,48	0
60	MG	Aa	1700	1/1	1.94	-	114,114,114,114	0
60	MG	AA	3051	1/1	0.37	-	81,81,81,81	0
60	MG	BA	3239	1/1	0.26	-	64,64,64,64	0
60	MG	AA	3078	1/1	0.14	-	83,83,83,83	0
60	MG	AA	3139	1/1	0.38	-	44,44,44,44	0
60	MG	Ba	1603	1/1	0.10	-	64,64,64,64	0
60	MG	BA	3244	1/1	0.24	-	91,91,91,91	0
60	MG	AA	3109	1/1	0.37	-	78,78,78,78	0
60	MG	AA	3091	1/1	0.23	-	27,27,27,27	0
60	MG	AA	3245	1/1	1.43	-	97,97,97,97	0
60	MG	Aa	1721	1/1	0.25	-	68,68,68,68	0
60	MG	AA	2977	1/1	0.91	-	54,54,54,54	0
60	MG	BA	3029	1/1	0.35	-	27,27,27,27	0
60	MG	Aa	1675	1/1	0.74	-	72,72,72,72	0
60	MG	AA	2969	1/1	0.28	-	22,22,22,22	0
60	MG	AA	3213	1/1	0.17	-	33,33,33,33	0
60	MG	AA	3034	1/1	0.57	-	55,55,55,55	0
60	MG	BA	2938	1/1	1.16	-	84,84,84,84	0
60	MG	Ba	1711	1/1	0.38	-	123,123,123,123	0
60	MG	BA	2951	1/1	0.31	-	72,72,72,72	0
60	MG	AA	2984	1/1	0.22	-	45,45,45,45	0
60	MG	Ba	1732	1/1	0.10	-	70,70,70,70	0
60	MG	AA	2983	1/1	0.28	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3026	1/1	0.23	-	35,35,35,35	0
60	MG	BA	3064	1/1	0.36	-	44,44,44,44	0
60	MG	BA	3027	1/1	0.44	-	43,43,43,43	0
60	MG	AA	3006	1/1	0.29	-	32,32,32,32	0
60	MG	BA	2929	1/1	0.11	-	10,10,10,10	0
60	MG	AA	3049	1/1	0.21	-	54,54,54,54	0
60	MG	BA	3154	1/1	0.24	-	73,73,73,73	1
60	MG	BA	2986	1/1	0.23	-	63,63,63,63	0
60	MG	Aa	1633	1/1	0.69	-	62,62,62,62	0
60	MG	AA	3048	1/1	0.47	-	68,68,68,68	0
60	MG	BA	2910	1/1	0.19	-	2,2,2,2	0
60	MG	BA	3056	1/1	0.22	-	92,92,92,92	0
60	MG	BA	3200	1/1	0.26	-	33,33,33,33	0
60	MG	BA	3055	1/1	0.42	-	7,7,7,7	0
60	MG	Ba	1702	1/1	1.19	-	97,97,97,97	0
60	MG	BA	2993	1/1	0.42	-	12,12,12,12	0
60	MG	AA	3013	1/1	1.00	-	78,78,78,78	0
60	MG	Ba	1717	1/1	1.09	-	71,71,71,71	0
60	MG	AA	3072	1/1	0.47	-	122,122,122,122	0
60	MG	Ba	1729	1/1	1.24	-	66,66,66,66	0
60	MG	Ba	1716	1/1	0.40	-	63,63,63,63	0
60	MG	AA	3107	1/1	0.29	-	47,47,47,47	0
60	MG	AA	2916	1/1	0.44	-	25,25,25,25	0
60	MG	BA	3088	1/1	0.37	-	107,107,107,107	0
60	MG	Ba	1676	1/1	0.18	-	137,137,137,137	1
60	MG	Ba	1699	1/1	1.16	-	88,88,88,88	0
60	MG	Bl	201	1/1	0.75	-	5,5,5,5	1
60	MG	Aa	1698	1/1	1.07	-	98,98,98,98	1
60	MG	Ba	1666	1/1	0.83	-	73,73,73,73	0
60	MG	Ba	1621	1/1	1.24	-	82,82,82,82	0
60	MG	BA	2935	1/1	0.55	-	25,25,25,25	0
60	MG	BA	3044	1/1	0.42	-	21,21,21,21	0
60	MG	BF	301	1/1	0.15	-	40,40,40,40	0
60	MG	Aa	1709	1/1	0.12	-	148,148,148,148	0
60	MG	AA	3147	1/1	0.45	-	79,79,79,79	0
60	MG	BA	2926	1/1	0.51	-	24,24,24,24	0
60	MG	BA	3039	1/1	0.27	-	15,15,15,15	0
60	MG	BA	3051	1/1	0.36	-	16,16,16,16	0
60	MG	Aa	1737	1/1	0.14	-	119,119,119,119	0
60	MG	AA	3206	1/1	0.29	-	115,115,115,115	0
60	MG	AA	2958	1/1	0.22	-	47,47,47,47	0
60	MG	BA	3007	1/1	0.44	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Ba	1722	1/1	0.32	-	63,63,63,63	0
60	MG	AA	3189	1/1	0.39	-	107,107,107,107	0
60	MG	AQ	201	1/1	1.97	-	94,94,94,94	0
60	MG	Aa	1615	1/1	1.01	-	53,53,53,53	0
60	MG	Ba	1686	1/1	0.20	-	84,84,84,84	0
60	MG	Ba	1641	1/1	0.77	-	94,94,94,94	0
60	MG	AA	3113	1/1	0.57	-	76,76,76,76	0
60	MG	Aa	1731	1/1	0.40	-	64,64,64,64	0
60	MG	BA	3003	1/1	0.30	-	22,22,22,22	0
60	MG	AA	2907	1/1	0.24	-	48,48,48,48	0
60	MG	Aa	1717	1/1	0.38	-	66,66,66,66	0
60	MG	BA	3216	1/1	0.51	-	117,117,117,117	0
60	MG	BA	3049	1/1	0.37	-	62,62,62,62	0
60	MG	AA	2965	1/1	0.24	-	69,69,69,69	0
59	ZN	A4	101	1/1	0.07	-	186,186,186,186	0
60	MG	BA	3110	1/1	0.39	-	23,23,23,23	0
60	MG	BO	201	1/1	0.48	-	122,122,122,122	0
60	MG	AA	3223	1/1	0.52	-	78,78,78,78	0
60	MG	AA	2986	1/1	0.77	-	46,46,46,46	0
60	MG	Ba	1612	1/1	0.14	-	82,82,82,82	0
60	MG	Aa	1625	1/1	0.78	-	76,76,76,76	0
60	MG	Aa	1713	1/1	1.15	-	98,98,98,98	0
60	MG	BA	2990	1/1	0.38	-	10,10,10,10	0
60	MG	AA	3117	1/1	0.72	-	148,148,148,148	0
60	MG	AA	3231	1/1	0.26	-	51,51,51,51	0
60	MG	BA	3012	1/1	0.88	-	61,61,61,61	0
60	MG	BA	3234	1/1	0.27	-	74,74,74,74	0
60	MG	AA	3191	1/1	0.26	-	74,74,74,74	0
60	MG	AA	2991	1/1	0.46	-	19,19,19,19	0
60	MG	AA	3186	1/1	0.10	-	77,77,77,77	0
60	MG	AA	3162	1/1	0.40	-	94,94,94,94	0
60	MG	AA	3067	1/1	0.61	-	34,34,34,34	0
60	MG	BA	3263	1/1	0.26	-	68,68,68,68	0
60	MG	BA	2903	1/1	0.10	-	99,99,99,99	0
60	MG	AA	3063	1/1	0.25	-	53,53,53,53	0
60	MG	BA	3191	1/1	0.21	-	23,23,23,23	0
60	MG	AA	3179	1/1	0.66	-	56,56,56,56	0
60	MG	AA	3218	1/1	1.01	-	98,98,98,98	0
60	MG	Aa	1726	1/1	0.68	-	36,36,36,36	0
60	MG	BA	3083	1/1	0.54	-	52,52,52,52	0
60	MG	BA	3113	1/1	0.47	-	24,24,24,24	1
60	MG	AA	2940	1/1	0.10	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3022	1/1	0.48	-	22,22,22,22	0
60	MG	BA	3114	1/1	0.28	-	8,8,8,8	0
60	MG	AA	3035	1/1	0.28	-	21,21,21,21	0
60	MG	BA	3158	1/1	0.36	-	88,88,88,88	0
60	MG	Ba	1720	1/1	0.38	-	91,91,91,91	0
60	MG	Ba	1697	1/1	1.05	-	93,93,93,93	1
60	MG	AA	2931	1/1	0.61	-	35,35,35,35	0
60	MG	BD	302	1/1	0.21	-	18,18,18,18	0
60	MG	BA	3235	1/1	0.70	-	51,51,51,51	0
60	MG	AA	2962	1/1	0.09	-	19,19,19,19	0
60	MG	Aa	1745	1/1	0.40	-	48,48,48,48	0
60	MG	BA	3185	1/1	0.46	-	40,40,40,40	0
60	MG	Aa	1693	1/1	0.62	-	75,75,75,75	0
60	MG	BA	2941	1/1	0.29	-	62,62,62,62	0
60	MG	BA	3157	1/1	0.12	-	85,85,85,85	0
60	MG	Ba	1647	1/1	0.57	-	117,117,117,117	0
60	MG	Ba	1624	1/1	1.04	-	76,76,76,76	0
60	MG	AA	2933	1/1	0.43	-	67,67,67,67	0
60	MG	Ba	1657	1/1	0.41	-	52,52,52,52	0
60	MG	Ba	1608	1/1	0.41	-	79,79,79,79	0
60	MG	BA	2992	1/1	0.19	-	33,33,33,33	0
60	MG	AA	3090	1/1	0.48	-	59,59,59,59	0
60	MG	BA	3228	1/1	1.11	-	94,94,94,94	0
60	MG	Aa	1610	1/1	0.82	-	115,115,115,115	0
60	MG	AA	3157	1/1	0.96	-	66,66,66,66	0
60	MG	Bv	101	1/1	0.59	-	52,52,52,52	1
59	ZN	B4	101	1/1	0.10	-	201,201,201,201	0
60	MG	AA	3119	1/1	0.89	-	68,68,68,68	0
60	MG	AA	3084	1/1	0.59	-	54,54,54,54	0
60	MG	AA	2904	1/1	0.31	-	131,131,131,131	0
60	MG	BA	3106	1/1	0.41	-	41,41,41,41	0
60	MG	AB	201	1/1	0.40	-	63,63,63,63	0
60	MG	Ba	1710	1/1	0.36	-	65,65,65,65	0
60	MG	BA	3084	1/1	0.41	-	34,34,34,34	0
60	MG	AA	3159	1/1	0.22	-	114,114,114,114	0
60	MG	AA	3220	1/1	0.54	-	54,54,54,54	0
60	MG	BA	2909	1/1	0.58	-	45,45,45,45	0
60	MG	AA	3183	1/1	0.39	-	69,69,69,69	0
60	MG	Ba	1683	1/1	0.48	-	65,65,65,65	0
60	MG	AA	3194	1/1	0.26	-	26,26,26,26	0
60	MG	Ba	1639	1/1	0.60	-	58,58,58,58	0
60	MG	Aa	1733	1/1	0.12	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	2973	1/1	0.39	-	79,79,79,79	0
60	MG	AA	3259	1/1	0.73	-	78,78,78,78	0
60	MG	AA	3066	1/1	0.45	-	27,27,27,27	0
60	MG	Ba	1679	1/1	0.76	-	92,92,92,92	0
60	MG	AA	3217	1/1	0.27	-	85,85,85,85	0
60	MG	AA	3093	1/1	0.30	-	56,56,56,56	0
60	MG	BA	2946	1/1	0.22	-	75,75,75,75	0
60	MG	AA	3075	1/1	0.89	-	84,84,84,84	0
60	MG	Ba	1741	1/1	0.28	-	73,73,73,73	0
60	MG	AA	2957	1/1	0.51	-	72,72,72,72	0
60	MG	BA	2959	1/1	0.12	-	37,37,37,37	0
60	MG	BA	3168	1/1	0.15	-	53,53,53,53	0
60	MG	BA	3020	1/1	0.19	-	84,84,84,84	0
60	MG	AA	3036	1/1	1.28	-	100,100,100,100	0
60	MG	BA	2996	1/1	0.43	-	18,18,18,18	0
60	MG	AA	3001	1/1	0.62	-	26,26,26,26	0
60	MG	AA	3257	1/1	0.41	-	78,78,78,78	0
60	MG	Ba	1630	1/1	0.95	-	76,76,76,76	0
60	MG	Aa	1681	1/1	0.05	-	76,76,76,76	0
60	MG	BA	3261	1/1	0.67	-	68,68,68,68	0
60	MG	BA	3031	1/1	0.19	-	14,14,14,14	0
60	MG	AA	3023	1/1	0.53	-	13,13,13,13	0
60	MG	Ae	202	1/1	0.94	-	89,89,89,89	0
60	MG	AA	3249	1/1	0.13	-	55,55,55,55	0
60	MG	AA	3088	1/1	0.33	-	85,85,85,85	0
60	MG	Aa	1680	1/1	0.59	-	107,107,107,107	0
60	MG	AA	3161	1/1	0.46	-	61,61,61,61	0
60	MG	AA	3255	1/1	0.39	-	50,50,50,50	0
60	MG	BA	3170	1/1	0.25	-	13,13,13,13	0
60	MG	AA	3224	1/1	0.76	-	73,73,73,73	0
60	MG	AD	302	1/1	0.33	-	21,21,21,21	0
60	MG	AA	3137	1/1	0.86	-	90,90,90,90	0
60	MG	BA	2917	1/1	0.61	-	23,23,23,23	0
60	MG	BA	3125	1/1	0.41	-	40,40,40,40	0
60	MG	Aa	1603	1/1	0.12	-	68,68,68,68	1
60	MG	AA	3044	1/1	0.85	-	17,17,17,17	0
60	MG	Aa	1688	1/1	0.19	-	63,63,63,63	1
60	MG	Aa	1701	1/1	0.39	-	71,71,71,71	0
60	MG	AA	2901	1/1	0.35	-	84,84,84,84	0
60	MG	Aa	1679	1/1	0.57	-	116,116,116,116	0
60	MG	BA	3201	1/1	0.52	-	43,43,43,43	0
60	MG	BA	3129	1/1	0.44	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3008	1/1	0.43	-	32,32,32,32	0
60	MG	BD	301	1/1	0.30	-	14,14,14,14	0
60	MG	Ba	1622	1/1	0.21	-	57,57,57,57	0
60	MG	BA	3115	1/1	0.57	-	21,21,21,21	0
60	MG	Ba	1736	1/1	0.31	-	59,59,59,59	0
60	MG	AA	2906	1/1	0.50	-	25,25,25,25	0
60	MG	BA	3202	1/1	0.21	-	76,76,76,76	0
60	MG	AA	2930	1/1	0.07	-	15,15,15,15	0
60	MG	AA	3131	1/1	0.48	-	46,46,46,46	0
60	MG	AA	3033	1/1	0.34	-	57,57,57,57	0
60	MG	BA	3059	1/1	0.21	-	52,52,52,52	0
60	MG	Ba	1703	1/1	0.46	-	25,25,25,25	1
60	MG	AA	3031	1/1	0.58	-	45,45,45,45	0
60	MG	BA	3165	1/1	0.34	-	67,67,67,67	0
60	MG	Ba	1618	1/1	0.33	-	57,57,57,57	0
60	MG	BA	3030	1/1	0.55	-	26,26,26,26	0
60	MG	Ba	1611	1/1	0.17	-	97,97,97,97	0
60	MG	BA	3065	1/1	0.24	-	13,13,13,13	0
60	MG	BA	3218	1/1	0.94	-	80,80,80,80	0
60	MG	Aa	1655	1/1	1.01	-	87,87,87,87	0
60	MG	Aa	1650	1/1	0.76	-	64,64,64,64	0
60	MG	BA	3005	1/1	0.36	-	21,21,21,21	0
60	MG	BA	3074	1/1	0.73	-	75,75,75,75	0
60	MG	BA	3109	1/1	1.09	-	90,90,90,90	0
60	MG	AB	203	1/1	0.71	-	56,56,56,56	0
60	MG	Aa	1670	1/1	0.24	-	43,43,43,43	0
60	MG	AA	3079	1/1	0.60	-	55,55,55,55	0
60	MG	AA	3193	1/1	0.25	-	20,20,20,20	0
60	MG	AA	3138	1/1	0.30	-	56,56,56,56	0
60	MG	AA	3226	1/1	0.37	-	95,95,95,95	0
60	MG	BA	3210	1/1	0.12	-	22,22,22,22	0
60	MG	BA	3093	1/1	0.47	-	61,61,61,61	0
60	MG	BA	2982	1/1	0.39	-	4,4,4,4	0
60	MG	Ba	1675	1/1	0.91	-	58,58,58,58	0
60	MG	BA	3076	1/1	0.38	-	83,83,83,83	0
60	MG	Ba	1693	1/1	0.18	-	78,78,78,78	0
60	MG	AA	3059	1/1	0.75	-	68,68,68,68	0
60	MG	Bm	201	1/1	0.33	-	118,118,118,118	0
60	MG	Ba	1614	1/1	0.47	-	68,68,68,68	0
60	MG	AA	3029	1/1	0.21	-	37,37,37,37	0
60	MG	BA	2969	1/1	0.10	-	35,35,35,35	0
60	MG	BA	3018	1/1	0.31	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3101	1/1	0.33	-	46,46,46,46	0
60	MG	Aa	1669	1/1	0.61	-	122,122,122,122	0
60	MG	Ba	1704	1/1	0.44	-	62,62,62,62	0
60	MG	AA	2978	1/1	0.69	-	124,124,124,124	0
60	MG	AA	3039	1/1	0.28	-	19,19,19,19	0
60	MG	BA	3073	1/1	0.32	-	30,30,30,30	0
60	MG	BA	3188	1/1	0.10	-	64,64,64,64	0
60	MG	BA	3186	1/1	0.77	-	70,70,70,70	0
60	MG	AA	3021	1/1	0.25	-	96,96,96,96	0
60	MG	Aa	1707	1/1	0.42	-	79,79,79,79	0
60	MG	AA	2938	1/1	0.12	-	84,84,84,84	0
60	MG	BA	3053	1/1	0.35	-	12,12,12,12	0
60	MG	BA	3208	1/1	0.27	-	52,52,52,52	0
60	MG	AA	3122	1/1	0.41	-	39,39,39,39	0
60	MG	AA	3019	1/1	0.33	-	26,26,26,26	0
60	MG	AA	2974	1/1	0.76	-	43,43,43,43	0
60	MG	AA	3118	1/1	0.55	-	74,74,74,74	0
60	MG	Ba	1615	1/1	0.20	-	81,81,81,81	0
60	MG	AA	3042	1/1	0.44	-	27,27,27,27	0
60	MG	AA	2920	1/1	0.43	-	22,22,22,22	0
60	MG	AA	3188	1/1	0.32	-	36,36,36,36	0
60	MG	Ba	1685	1/1	0.94	-	25,25,25,25	1
60	MG	BA	3223	1/1	0.18	-	43,43,43,43	0
60	MG	Aa	1640	1/1	0.33	-	60,60,60,60	0
60	MG	Aa	1667	1/1	0.71	-	78,78,78,78	0
60	MG	BA	3199	1/1	0.24	-	34,34,34,34	0
60	MG	Ba	1738	1/1	1.00	-	106,106,106,106	0
60	MG	AA	3163	1/1	0.33	-	54,54,54,54	0
60	MG	AA	3153	1/1	0.36	-	71,71,71,71	0
60	MG	Aa	1732	1/1	0.31	-	49,49,49,49	0
60	MG	BA	2933	1/1	0.40	-	18,18,18,18	1
60	MG	BA	3035	1/1	0.51	-	52,52,52,52	0
60	MG	BA	2953	1/1	0.23	-	25,25,25,25	0
60	MG	BA	2931	1/1	0.40	-	62,62,62,62	0
60	MG	AA	2975	1/1	0.38	-	90,90,90,90	0
60	MG	Bv	105	1/1	0.36	-	81,81,81,81	1
60	MG	BA	3265	1/1	0.52	-	74,74,74,74	0
60	MG	BA	3069	1/1	0.33	-	35,35,35,35	0
60	MG	BA	2962	1/1	0.51	-	54,54,54,54	0
60	MG	B5	101	1/1	0.39	-	27,27,27,27	0
60	MG	BA	3028	1/1	0.26	-	24,24,24,24	0
60	MG	Ba	1640	1/1	0.82	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3111	1/1	0.44	-	74,74,74,74	0
60	MG	Aa	1605	1/1	0.11	-	43,43,43,43	0
60	MG	BA	3022	1/1	0.30	-	16,16,16,16	0
60	MG	BA	3232	1/1	0.23	-	77,77,77,77	0
60	MG	BA	3164	1/1	0.47	-	31,31,31,31	0
60	MG	BA	2956	1/1	0.14	-	50,50,50,50	0
60	MG	BA	3082	1/1	0.16	-	34,34,34,34	0
60	MG	BA	3198	1/1	1.23	-	91,91,91,91	0
60	MG	Ba	1728	1/1	0.44	-	30,30,30,30	0
60	MG	AA	3160	1/1	0.59	-	99,99,99,99	0
60	MG	BA	3149	1/1	0.41	-	76,76,76,76	0
60	MG	AA	3198	1/1	0.50	-	52,52,52,52	0
60	MG	Ba	1662	1/1	0.25	-	67,67,67,67	0
60	MG	BA	2978	1/1	0.14	-	56,56,56,56	0
60	MG	Aa	1691	1/1	0.36	-	53,53,53,53	0
60	MG	BA	3085	1/1	0.17	-	60,60,60,60	0
60	MG	BA	2912	1/1	0.62	-	37,37,37,37	0
60	MG	BA	3209	1/1	0.44	-	74,74,74,74	0
60	MG	Ba	1740	1/1	0.27	-	78,78,78,78	0
60	MG	BA	3242	1/1	0.79	-	52,52,52,52	0
60	MG	AA	3241	1/1	0.51	-	64,64,64,64	0
60	MG	BA	2995	1/1	0.52	-	14,14,14,14	0
60	MG	AA	3100	1/1	0.88	-	97,97,97,97	0
60	MG	AA	3205	1/1	0.53	-	51,51,51,51	0
60	MG	BA	2918	1/1	0.18	-	29,29,29,29	0
60	MG	BA	3094	1/1	0.60	-	11,11,11,11	0
60	MG	BA	2994	1/1	0.57	-	14,14,14,14	0
60	MG	BA	3249	1/1	0.87	-	67,67,67,67	0
60	MG	Ba	1715	1/1	0.25	-	94,94,94,94	0
60	MG	BA	3153	1/1	0.63	-	46,46,46,46	0
60	MG	Aa	1740	1/1	0.26	-	42,42,42,42	0
60	MG	AA	3095	1/1	0.68	-	26,26,26,26	0
60	MG	Ba	1652	1/1	0.08	-	69,69,69,69	0
60	MG	BA	3145	1/1	0.83	-	63,63,63,63	0
60	MG	BA	3262	1/1	0.33	-	39,39,39,39	0
60	MG	BA	3081	1/1	0.19	-	83,83,83,83	0
60	MG	AA	3008	1/1	0.31	-	75,75,75,75	0
60	MG	Ba	1604	1/1	0.59	-	75,75,75,75	0
60	MG	AA	2917	1/1	0.49	-	112,112,112,112	0
60	MG	BA	3144	1/1	1.05	-	59,59,59,59	0
60	MG	AA	3068	1/1	0.27	-	19,19,19,19	0
60	MG	Ba	1730	1/1	0.23	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	2936	1/1	0.22	-	35,35,35,35	0
60	MG	AA	2944	1/1	0.46	-	56,56,56,56	0
60	MG	Ba	1725	1/1	0.81	-	45,45,45,45	0
60	MG	AA	2921	1/1	0.30	-	50,50,50,50	0
60	MG	BA	2965	1/1	0.30	-	58,58,58,58	0
60	MG	Aa	1659	1/1	0.44	-	88,88,88,88	0
60	MG	BA	3009	1/1	0.31	-	3,3,3,3	0
60	MG	BA	3013	1/1	1.06	-	50,50,50,50	0
60	MG	BA	3098	1/1	0.77	-	52,52,52,52	0
60	MG	BA	3016	1/1	0.27	-	11,11,11,11	0
60	MG	BA	3036	1/1	0.39	-	34,34,34,34	0
60	MG	Ba	1633	1/1	0.08	-	39,39,39,39	0
60	MG	Aa	1699	1/1	0.60	-	84,84,84,84	1
60	MG	AA	2956	1/1	0.19	-	61,61,61,61	0
60	MG	AA	3246	1/1	0.32	-	70,70,70,70	0
60	MG	B7	101	1/1	0.26	-	36,36,36,36	0
60	MG	Aa	1697	1/1	0.72	-	65,65,65,65	0
60	MG	AA	3123	1/1	0.28	-	18,18,18,18	0
60	MG	AA	2976	1/1	0.44	-	46,46,46,46	0
60	MG	AA	3057	1/1	0.09	-	92,92,92,92	0
60	MG	AA	3061	1/1	0.35	-	42,42,42,42	0
60	MG	AA	3069	1/1	0.57	-	68,68,68,68	0
60	MG	AA	3085	1/1	0.25	-	47,47,47,47	0
60	MG	BA	3060	1/1	0.34	-	16,16,16,16	0
60	MG	BA	2970	1/1	0.45	-	53,53,53,53	0
60	MG	BA	3187	1/1	0.61	-	36,36,36,36	0
60	MG	A1	101	1/1	0.26	-	53,53,53,53	0
60	MG	Aa	1653	1/1	0.14	-	59,59,59,59	0
60	MG	BA	3196	1/1	0.31	-	68,68,68,68	0
60	MG	BA	3162	1/1	0.34	-	57,57,57,57	0
60	MG	Ba	1731	1/1	0.32	-	20,20,20,20	0
60	MG	Aa	1661	1/1	0.23	-	64,64,64,64	0
60	MG	BA	3011	1/1	0.41	-	11,11,11,11	0
60	MG	AA	2937	1/1	0.15	-	67,67,67,67	0
60	MG	BA	2928	1/1	0.23	-	17,17,17,17	0
60	MG	AA	3154	1/1	0.19	-	142,142,142,142	0
60	MG	AA	3025	1/1	0.47	-	26,26,26,26	0
60	MG	AA	3143	1/1	0.41	-	29,29,29,29	0
60	MG	Aa	1720	1/1	1.05	-	75,75,75,75	0
60	MG	BA	3224	1/1	0.51	-	62,62,62,62	0
60	MG	AA	3227	1/1	0.29	-	39,39,39,39	0
60	MG	A7	101	1/1	0.58	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3220	1/1	0.78	-	50,50,50,50	0
60	MG	Aa	1628	1/1	0.36	-	92,92,92,92	0
60	MG	Av	103	1/1	0.06	-	84,84,84,84	0
60	MG	BA	3071	1/1	0.46	-	39,39,39,39	0
60	MG	Aa	1619	1/1	0.45	-	65,65,65,65	0
60	MG	Ba	1726	1/1	0.79	-	34,34,34,34	1
60	MG	AA	3062	1/1	0.25	-	26,26,26,26	0
60	MG	Ba	1651	1/1	0.98	-	62,62,62,62	0
60	MG	AA	2949	1/1	0.46	-	41,41,41,41	0
60	MG	AA	3151	1/1	0.43	-	85,85,85,85	0
60	MG	AA	3202	1/1	0.31	-	57,57,57,57	0
60	MG	AA	3187	1/1	0.38	-	49,49,49,49	0
60	MG	AA	3256	1/1	0.44	-	71,71,71,71	0
60	MG	Aa	1723	1/1	0.39	-	83,83,83,83	0
60	MG	Ba	1694	1/1	0.23	-	83,83,83,83	0
60	MG	Ba	1669	1/1	0.56	-	94,94,94,94	0
60	MG	AF	301	1/1	0.22	-	74,74,74,74	0
60	MG	Ba	1687	1/1	0.17	-	50,50,50,50	1
60	MG	Aa	1735	1/1	0.24	-	68,68,68,68	1
60	MG	Aa	1738	1/1	0.25	-	55,55,55,55	0
60	MG	BA	3079	1/1	0.26	-	82,82,82,82	0
60	MG	AA	3172	1/1	0.39	-	38,38,38,38	0
60	MG	BA	2968	1/1	0.43	-	69,69,69,69	0
60	MG	AA	3165	1/1	0.51	-	97,97,97,97	0
60	MG	BA	3253	1/1	0.65	-	43,43,43,43	0
60	MG	AA	2911	1/1	0.14	-	20,20,20,20	0
60	MG	Aa	1744	1/1	0.40	-	87,87,87,87	0
60	MG	B7	102	1/1	0.66	-	57,57,57,57	0
60	MG	AA	3120	1/1	0.18	-	76,76,76,76	0
60	MG	AA	3080	1/1	0.54	-	67,67,67,67	0
60	MG	BA	3101	1/1	0.61	-	52,52,52,52	0
60	MG	AA	2935	1/1	0.70	-	69,69,69,69	0
60	MG	BA	3004	1/1	0.14	-	46,46,46,46	0
60	MG	BA	2961	1/1	0.28	-	28,28,28,28	0
60	MG	Aa	1620	1/1	0.17	-	73,73,73,73	0
60	MG	AA	3199	1/1	0.41	-	53,53,53,53	0
60	MG	Aa	1634	1/1	0.07	-	47,47,47,47	0
60	MG	AA	3235	1/1	0.56	-	72,72,72,72	0
60	MG	BA	3063	1/1	0.19	-	26,26,26,26	0
60	MG	AA	3176	1/1	1.29	-	74,74,74,74	0
60	MG	AA	3267	1/1	0.89	-	74,74,74,74	0
60	MG	AA	3105	1/1	0.25	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	2950	1/1	0.25	-	51,51,51,51	0
60	MG	Aa	1683	1/1	0.13	-	66,66,66,66	0
60	MG	AA	3173	1/1	0.28	-	14,14,14,14	0
60	MG	AA	3232	1/1	0.20	-	64,64,64,64	0
60	MG	BA	3032	1/1	0.41	-	32,32,32,32	0
60	MG	AA	2926	1/1	0.33	-	26,26,26,26	0
60	MG	Ba	1650	1/1	0.48	-	49,49,49,49	0
60	MG	BA	2924	1/1	0.34	-	93,93,93,93	0
60	MG	AA	2993	1/1	0.27	-	56,56,56,56	0
60	MG	BA	3155	1/1	0.34	-	59,59,59,59	0
60	MG	AA	2925	1/1	0.32	-	79,79,79,79	0
60	MG	BA	3175	1/1	0.68	-	57,57,57,57	0
60	MG	AA	2912	1/1	0.19	-	26,26,26,26	0
60	MG	AA	2967	1/1	1.46	-	69,69,69,69	0
60	MG	BA	3142	1/1	0.85	-	53,53,53,53	0
60	MG	BA	2952	1/1	0.40	-	102,102,102,102	0
60	MG	BA	3248	1/1	0.85	-	47,47,47,47	0
60	MG	Ba	1653	1/1	0.36	-	74,74,74,74	0
60	MG	BA	3140	1/1	0.34	-	25,25,25,25	0
60	MG	BA	3061	1/1	0.17	-	35,35,35,35	0
60	MG	BA	3137	1/1	0.85	-	80,80,80,80	0
60	MG	BA	2922	1/1	0.28	-	52,52,52,52	0
60	MG	BA	2902	1/1	0.34	-	60,60,60,60	0
60	MG	AA	3132	1/1	1.04	-	78,78,78,78	0
60	MG	BA	3169	1/1	0.21	-	25,25,25,25	0
60	MG	BA	2983	1/1	0.17	-	21,21,21,21	0
60	MG	AA	3052	1/1	0.29	-	18,18,18,18	0
60	MG	Ba	1739	1/1	0.52	-	53,53,53,53	0
60	MG	AA	3212	1/1	0.63	-	68,68,68,68	0
60	MG	AA	2939	1/1	0.82	-	68,68,68,68	0
60	MG	Aa	1602	1/1	0.27	-	126,126,126,126	0
60	MG	Ba	1620	1/1	0.24	-	55,55,55,55	0
60	MG	AA	3236	1/1	0.43	-	90,90,90,90	0
60	MG	AA	3211	1/1	0.23	-	60,60,60,60	0
60	MG	BA	3245	1/1	0.30	-	90,90,90,90	0
60	MG	BA	3172	1/1	0.49	-	50,50,50,50	0
60	MG	BA	3189	1/1	0.66	-	75,75,75,75	0
60	MG	AA	3170	1/1	0.47	-	47,47,47,47	0
60	MG	AA	3003	1/1	0.26	-	43,43,43,43	0
60	MG	Ba	1705	1/1	0.39	-	76,76,76,76	0
60	MG	Ba	1707	1/1	0.53	-	76,76,76,76	0
60	MG	Aa	1712	1/1	1.25	-	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3090	1/1	0.27	-	32,32,32,32	0
60	MG	BA	2998	1/1	0.22	-	14,14,14,14	0
60	MG	Aa	1618	1/1	0.37	-	28,28,28,28	0
60	MG	AA	3156	1/1	0.32	-	73,73,73,73	0
60	MG	BA	3264	1/1	0.98	-	89,89,89,89	0
60	MG	AA	3204	1/1	0.60	-	51,51,51,51	0
60	MG	Ba	1708	1/1	0.19	-	132,132,132,132	0
60	MG	Ba	1671	1/1	0.32	-	87,87,87,87	0
60	MG	BA	3195	1/1	0.16	-	37,37,37,37	0
60	MG	Ba	1602	1/1	0.21	-	93,93,93,93	0
60	MG	AA	3064	1/1	0.16	-	29,29,29,29	0
60	MG	Ba	1684	1/1	0.67	-	75,75,75,75	0
60	MG	BA	3107	1/1	0.38	-	45,45,45,45	0
60	MG	Aa	1689	1/1	0.27	-	65,65,65,65	1
60	MG	AA	3073	1/1	0.87	-	78,78,78,78	0
60	MG	BA	3023	1/1	0.41	-	21,21,21,21	0
60	MG	AA	2999	1/1	0.28	-	46,46,46,46	0
60	MG	AA	3106	1/1	0.15	-	65,65,65,65	0
60	MG	Ba	1609	1/1	0.90	-	74,74,74,74	0
60	MG	AA	3070	1/1	0.23	-	54,54,54,54	0
60	MG	AA	3169	1/1	0.07	-	44,44,44,44	0
60	MG	Ba	1677	1/1	0.14	-	138,138,138,138	0
60	MG	AA	3016	1/1	0.15	-	31,31,31,31	0
60	MG	Aa	1729	1/1	0.41	-	30,30,30,30	0
60	MG	Aa	1641	1/1	0.38	-	74,74,74,74	0
60	MG	Aa	1609	1/1	0.19	-	64,64,64,64	0
60	MG	BA	3128	1/1	0.38	-	26,26,26,26	0
60	MG	AA	3086	1/1	0.12	-	74,74,74,74	0
60	MG	Ba	1626	1/1	0.33	-	56,56,56,56	0
60	MG	BA	2985	1/1	0.34	-	26,26,26,26	0
60	MG	AA	3014	1/1	0.89	-	50,50,50,50	0
60	MG	AD	301	1/1	0.32	-	21,21,21,21	0
60	MG	BA	3135	1/1	1.37	-	96,96,96,96	0
60	MG	Aa	1614	1/1	0.12	-	69,69,69,69	0
60	MG	BA	3024	1/1	0.45	-	24,24,24,24	0
60	MG	BA	2949	1/1	0.32	-	42,42,42,42	0
60	MG	Aa	1739	1/1	0.55	-	78,78,78,78	0
60	MG	Aa	1684	1/1	0.83	-	74,74,74,74	0
60	MG	AA	2941	1/1	0.82	-	92,92,92,92	0
60	MG	Ba	1735	1/1	0.23	-	122,122,122,122	0
60	MG	Ba	1714	1/1	0.10	-	62,62,62,62	0
60	MG	BA	3197	1/1	0.16	-	103,103,103,103	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Aa	1642	1/1	0.24	-	95,95,95,95	0
60	MG	Ba	1658	1/1	0.33	-	50,50,50,50	0
60	MG	BA	3180	1/1	0.97	-	105,105,105,105	0
60	MG	Ba	1631	1/1	0.55	-	73,73,73,73	0
60	MG	BA	3238	1/1	1.19	-	113,113,113,113	0
60	MG	Ba	1606	1/1	0.17	-	50,50,50,50	0
60	MG	BA	2915	1/1	0.54	-	20,20,20,20	0
60	MG	Aa	1652	1/1	0.84	-	58,58,58,58	0
60	MG	BA	2974	1/1	0.39	-	31,31,31,31	0
60	MG	BA	2963	1/1	0.23	-	55,55,55,55	0
60	MG	AA	2966	1/1	0.54	-	57,57,57,57	0
60	MG	Ba	1665	1/1	0.80	-	144,144,144,144	0
60	MG	AA	3254	1/1	0.47	-	53,53,53,53	0
60	MG	Aa	1714	1/1	0.16	-	47,47,47,47	0
60	MG	BA	2940	1/1	0.24	-	82,82,82,82	0
60	MG	Ba	1601	1/1	0.53	-	90,90,90,90	0
60	MG	AA	3141	1/1	1.09	-	86,86,86,86	0
60	MG	Aa	1627	1/1	0.21	-	53,53,53,53	0
60	MG	BA	3148	1/1	0.48	-	74,74,74,74	0
60	MG	BA	3080	1/1	0.39	-	58,58,58,58	0
60	MG	AA	3146	1/1	0.70	-	90,90,90,90	0
60	MG	BA	3001	1/1	0.15	-	37,37,37,37	0
60	MG	AA	3045	1/1	0.43	-	22,22,22,22	0
60	MG	BA	2923	1/1	0.24	-	29,29,29,29	0
60	MG	BA	3041	1/1	0.42	-	15,15,15,15	0
60	MG	BA	3026	1/1	0.21	-	40,40,40,40	0
60	MG	Aa	1631	1/1	1.19	-	72,72,72,72	0
60	MG	BA	2919	1/1	0.18	-	13,13,13,13	0
60	MG	Aa	1736	1/1	0.30	-	117,117,117,117	0
60	MG	AA	2909	1/1	0.46	-	41,41,41,41	0
60	MG	Aa	1666	1/1	0.44	-	61,61,61,61	0
60	MG	AA	2932	1/1	0.68	-	57,57,57,57	0
60	MG	AA	2971	1/1	0.13	-	52,52,52,52	0
60	MG	BA	3231	1/1	0.60	-	64,64,64,64	0
60	MG	BB	203	1/1	0.59	-	55,55,55,55	0
60	MG	Av	101	1/1	0.82	-	90,90,90,90	1
60	MG	Aa	1734	1/1	0.57	-	84,84,84,84	0
60	MG	BA	3236	1/1	0.70	-	116,116,116,116	0
60	MG	Ba	1628	1/1	0.34	-	46,46,46,46	0
60	MG	Ba	1695	1/1	0.37	-	86,86,86,86	0
60	MG	AA	3002	1/1	0.18	-	58,58,58,58	0
60	MG	AA	2923	1/1	0.55	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	3148	1/1	0.25	-	77,77,77,77	0
60	MG	AA	3150	1/1	0.54	-	62,62,62,62	0
60	MG	AA	2942	1/1	0.45	-	40,40,40,40	0
60	MG	BA	3247	1/1	0.38	-	54,54,54,54	0
60	MG	AA	3110	1/1	1.22	-	91,91,91,91	0
60	MG	Ba	1623	1/1	0.19	-	34,34,34,34	0
60	MG	BA	2981	1/1	1.36	-	46,46,46,46	0
60	MG	Ba	1723	1/1	0.14	-	103,103,103,103	0
60	MG	AA	2994	1/1	0.60	-	30,30,30,30	0
60	MG	BA	2987	1/1	0.36	-	9,9,9,9	0
60	MG	Ba	1660	1/1	0.74	-	60,60,60,60	0
60	MG	Aa	1703	1/1	0.91	-	94,94,94,94	0
60	MG	AA	3260	1/1	0.73	-	80,80,80,80	0
60	MG	BA	3119	1/1	0.30	-	67,67,67,67	0
60	MG	BA	3230	1/1	0.21	-	45,45,45,45	0
60	MG	AA	2970	1/1	0.20	-	53,53,53,53	0
60	MG	AA	3017	1/1	0.32	-	18,18,18,18	0
60	MG	Bv	103	1/1	0.32	-	93,93,93,93	0
60	MG	BA	3259	1/1	0.25	-	86,86,86,86	0
60	MG	BA	2997	1/1	0.23	-	22,22,22,22	0
60	MG	AA	3054	1/1	0.41	-	24,24,24,24	0
60	MG	BA	3014	1/1	0.28	-	1,1,1,1	0
60	MG	AA	2996	1/1	0.55	-	40,40,40,40	0
60	MG	Aa	1644	1/1	0.30	-	56,56,56,56	0
60	MG	BA	2920	1/1	0.23	-	24,24,24,24	0
60	MG	Ba	1696	1/1	0.68	-	83,83,83,83	0
60	MG	Ba	1734	1/1	0.29	-	84,84,84,84	1
60	MG	BA	3043	1/1	0.53	-	17,17,17,17	0
60	MG	Aa	1643	1/1	1.25	-	90,90,90,90	0
60	MG	AA	2903	1/1	0.69	-	65,65,65,65	0
60	MG	AA	3233	1/1	0.35	-	44,44,44,44	0
60	MG	Aa	1702	1/1	0.42	-	91,91,91,91	0
60	MG	AA	3243	1/1	1.19	-	79,79,79,79	0
60	MG	AA	3129	1/1	0.34	-	29,29,29,29	0
60	MG	BA	3204	1/1	0.54	-	64,64,64,64	0
60	MG	Aa	1604	1/1	0.17	-	76,76,76,76	0
60	MG	Aa	1651	1/1	0.68	-	58,58,58,58	0
60	MG	Aa	1617	1/1	0.39	-	49,49,49,49	1
60	MG	BA	3156	1/1	0.42	-	29,29,29,29	0
60	MG	AA	2972	1/1	0.28	-	43,43,43,43	0
60	MG	Aa	1682	1/1	0.59	-	59,59,59,59	0
60	MG	BA	3091	1/1	0.40	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3072	1/1	0.84	-	55,55,55,55	0
60	MG	BA	2934	1/1	0.70	-	72,72,72,72	0
60	MG	Ba	1634	1/1	0.35	-	37,37,37,37	0
60	MG	BA	3161	1/1	0.46	-	71,71,71,71	0
60	MG	BA	3033	1/1	0.55	-	61,61,61,61	0
60	MG	Aa	1708	1/1	0.56	-	81,81,81,81	0
60	MG	Ba	1682	1/1	0.10	-	66,66,66,66	0
60	MG	AA	3046	1/1	0.40	-	47,47,47,47	0
60	MG	AA	3234	1/1	0.21	-	79,79,79,79	0
60	MG	BA	3240	1/1	0.91	-	84,84,84,84	0
60	MG	Bd	301	1/1	0.83	-	55,55,55,55	0
60	MG	Aa	1694	1/1	0.14	-	89,89,89,89	0
60	MG	Ba	1610	1/1	0.22	-	50,50,50,50	0
60	MG	BA	3178	1/1	0.36	-	55,55,55,55	0
60	MG	Ba	1727	1/1	0.49	-	46,46,46,46	0
60	MG	AX	101	1/1	0.81	-	55,55,55,55	1
60	MG	AA	3032	1/1	0.23	-	33,33,33,33	0
60	MG	AA	3239	1/1	0.36	-	77,77,77,77	0
60	MG	AA	3040	1/1	0.12	-	21,21,21,21	0
60	MG	AA	2964	1/1	0.47	-	65,65,65,65	0
60	MG	Aa	1621	1/1	0.23	-	89,89,89,89	0
60	MG	BA	3104	1/1	0.20	-	31,31,31,31	0
60	MG	AA	3104	1/1	0.31	-	56,56,56,56	0
60	MG	BA	3047	1/1	0.26	-	36,36,36,36	0
60	MG	AA	2952	1/1	0.44	-	88,88,88,88	0
60	MG	AA	3210	1/1	0.15	-	115,115,115,115	0
60	MG	BA	2939	1/1	0.22	-	71,71,71,71	0
60	MG	AA	3182	1/1	0.36	-	40,40,40,40	0
60	MG	AA	3081	1/1	0.38	-	99,99,99,99	0
60	MG	BA	3193	1/1	0.40	-	44,44,44,44	0
60	MG	Aa	1626	1/1	0.13	-	63,63,63,63	0
60	MG	AA	3136	1/1	0.57	-	84,84,84,84	0
60	MG	Ba	1670	1/1	0.19	-	58,58,58,58	0
60	MG	Aa	1692	1/1	0.66	-	46,46,46,46	0
60	MG	AA	3053	1/1	0.66	-	42,42,42,42	0
60	MG	AA	3135	1/1	0.53	-	71,71,71,71	0
60	MG	BA	3227	1/1	0.61	-	82,82,82,82	0
60	MG	Bv	102	1/1	0.25	-	37,37,37,37	0
60	MG	AA	3221	1/1	0.43	-	47,47,47,47	0
60	MG	AA	2989	1/1	0.09	-	33,33,33,33	0
60	MG	BA	2921	1/1	0.21	-	31,31,31,31	0
60	MG	Aa	1646	1/1	0.77	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3254	1/1	0.86	-	66,66,66,66	0
60	MG	Aa	1705	1/1	0.41	-	71,71,71,71	0
60	MG	BA	3213	1/1	0.20	-	36,36,36,36	0
60	MG	Aa	1728	1/1	0.60	-	83,83,83,83	0
60	MG	BA	3133	1/1	0.31	-	54,54,54,54	0
60	MG	Ba	1625	1/1	0.18	-	72,72,72,72	0
60	MG	Aa	1690	1/1	0.24	-	49,49,49,49	0
60	MG	BA	3233	1/1	0.42	-	97,97,97,97	0
60	MG	BA	3222	1/1	0.39	-	61,61,61,61	0
60	MG	BA	2954	1/1	0.21	-	57,57,57,57	0
60	MG	AA	3111	1/1	0.70	-	54,54,54,54	0
60	MG	Aa	1649	1/1	0.21	-	32,32,32,32	0
59	ZN	Ad	301	1/1	0.29	-	76,76,76,76	0
60	MG	Aa	1719	1/1	0.50	-	101,101,101,101	0
60	MG	AA	2951	1/1	0.28	-	53,53,53,53	0
60	MG	BA	3150	1/1	0.66	-	76,76,76,76	0
60	MG	AA	3011	1/1	0.56	-	14,14,14,14	0
60	MG	AA	3028	1/1	0.66	-	60,60,60,60	0
60	MG	AA	2963	1/1	0.77	-	46,46,46,46	0
60	MG	AA	3225	1/1	0.18	-	57,57,57,57	0
60	MG	BA	3019	1/1	0.35	-	30,30,30,30	0
60	MG	BA	3123	1/1	0.50	-	2,2,2,2	0
60	MG	AA	3038	1/1	0.33	-	64,64,64,64	0
60	MG	AA	3098	1/1	0.49	-	75,75,75,75	0
60	MG	AA	3065	1/1	0.74	-	73,73,73,73	0
60	MG	Ba	1700	1/1	0.48	-	58,58,58,58	0
60	MG	AA	2997	1/1	0.26	-	43,43,43,43	0
60	MG	AA	2990	1/1	0.61	-	34,34,34,34	0
60	MG	BA	2984	1/1	0.39	-	22,22,22,22	0
60	MG	AA	2954	1/1	0.61	-	112,112,112,112	0
60	MG	Ba	1742	1/1	0.42	-	92,92,92,92	0
60	MG	AA	3020	1/1	0.28	-	39,39,39,39	0
60	MG	BA	2948	1/1	0.53	-	73,73,73,73	0
60	MG	BA	2971	1/1	0.91	-	66,66,66,66	0
60	MG	AA	3018	1/1	0.50	-	48,48,48,48	0
60	MG	AA	3181	1/1	0.44	-	61,61,61,61	0
60	MG	Aa	1718	1/1	0.95	-	84,84,84,84	0
60	MG	BA	3221	1/1	0.42	-	106,106,106,106	0
60	MG	Aa	1704	1/1	0.40	-	29,29,29,29	1
60	MG	Aa	1743	1/1	0.62	-	67,67,67,67	0
60	MG	BA	3255	1/1	0.37	-	81,81,81,81	0
60	MG	BA	3070	1/1	0.33	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	2910	1/1	0.61	-	49,49,49,49	0
60	MG	BA	3226	1/1	0.35	-	75,75,75,75	0
60	MG	AA	3242	1/1	0.87	-	85,85,85,85	0
60	MG	AA	3009	1/1	0.43	-	31,31,31,31	0
60	MG	Ba	1733	1/1	0.38	-	86,86,86,86	0
60	MG	BA	3166	1/1	0.12	-	50,50,50,50	0
60	MG	AA	2948	1/1	0.25	-	67,67,67,67	0
60	MG	AA	2924	1/1	0.11	-	32,32,32,32	0
60	MG	BA	3190	1/1	0.27	-	13,13,13,13	0
60	MG	Aa	1662	1/1	0.52	-	73,73,73,73	0
60	MG	Aa	1636	1/1	1.44	-	88,88,88,88	0
60	MG	AA	2946	1/1	0.09	-	101,101,101,101	0
60	MG	AA	2959	1/1	0.44	-	73,73,73,73	0
60	MG	AB	202	1/1	0.40	-	62,62,62,62	0
60	MG	Aa	1672	1/1	0.26	-	87,87,87,87	0
60	MG	Ba	1649	1/1	0.34	-	49,49,49,49	0
60	MG	Ba	1638	1/1	0.26	-	40,40,40,40	0
60	MG	BA	3050	1/1	0.21	-	29,29,29,29	0
60	MG	Ba	1681	1/1	0.93	-	122,122,122,122	0
60	MG	B0	101	1/1	0.51	-	71,71,71,71	0
60	MG	BA	3138	1/1	0.23	-	54,54,54,54	0
60	MG	BA	3089	1/1	0.20	-	56,56,56,56	0
60	MG	BA	3102	1/1	0.28	-	47,47,47,47	0
60	MG	Bv	104	1/1	1.11	-	75,75,75,75	1
60	MG	AA	3265	1/1	0.43	-	70,70,70,70	0
60	MG	Aa	1616	1/1	0.25	-	64,64,64,64	0
60	MG	BA	3100	1/1	0.40	-	62,62,62,62	0
60	MG	Aa	1673	1/1	0.16	-	60,60,60,60	0
60	MG	AA	3112	1/1	0.35	-	60,60,60,60	0
60	MG	Ba	1643	1/1	0.47	-	108,108,108,108	0
60	MG	AA	3056	1/1	0.44	-	19,19,19,19	0
60	MG	BA	3215	1/1	0.41	-	65,65,65,65	0
60	MG	AA	3209	1/1	0.69	-	84,84,84,84	0
60	MG	BA	3134	1/1	0.40	-	52,52,52,52	0
60	MG	BA	3141	1/1	0.56	-	57,57,57,57	0
60	MG	BA	3171	1/1	0.50	-	69,69,69,69	0
60	MG	Ba	1661	1/1	0.30	-	41,41,41,41	0
60	MG	AA	3047	1/1	0.55	-	40,40,40,40	0
60	MG	BA	2901	1/1	0.18	-	138,138,138,138	0
60	MG	AA	2968	1/1	1.50	-	76,76,76,76	0
60	MG	AA	3258	1/1	0.54	-	38,38,38,38	0
60	MG	AA	2919	1/1	0.28	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	2958	1/1	1.73	-	88,88,88,88	0
60	MG	Ba	1617	1/1	0.24	-	36,36,36,36	0
60	MG	Ba	1654	1/1	0.39	-	50,50,50,50	0
60	MG	BA	3194	1/1	0.32	-	12,12,12,12	0
60	MG	BA	2950	1/1	0.21	-	37,37,37,37	0
60	MG	Aa	1685	1/1	0.25	-	53,53,53,53	0
60	MG	AA	3125	1/1	0.67	-	42,42,42,42	0
60	MG	BA	3002	1/1	0.27	-	41,41,41,41	0
60	MG	AA	3005	1/1	0.21	-	57,57,57,57	0
60	MG	AA	2922	1/1	0.21	-	48,48,48,48	0
60	MG	BA	2957	1/1	0.40	-	13,13,13,13	0
60	MG	BA	3260	1/1	1.13	-	80,80,80,80	0
60	MG	BA	3192	1/1	0.12	-	34,34,34,34	0
60	MG	AA	3004	1/1	0.22	-	39,39,39,39	0
60	MG	AA	2961	1/1	0.48	-	76,76,76,76	0
60	MG	BA	3136	1/1	0.75	-	106,106,106,106	0
60	MG	AA	3043	1/1	0.19	-	37,37,37,37	0
60	MG	AA	3127	1/1	0.50	-	89,89,89,89	0
60	MG	Aa	1630	1/1	0.12	-	36,36,36,36	0
60	MG	AA	3116	1/1	0.43	-	35,35,35,35	0
60	MG	Aa	1663	1/1	0.55	-	112,112,112,112	0
60	MG	Ba	1719	1/1	0.64	-	57,57,57,57	0
60	MG	BA	3257	1/1	0.40	-	72,72,72,72	0
60	MG	BA	2906	1/1	0.24	-	26,26,26,26	0
60	MG	BA	2979	1/1	0.43	-	55,55,55,55	0
60	MG	BA	2937	1/1	0.26	-	67,67,67,67	0
60	MG	BA	3108	1/1	0.13	-	50,50,50,50	0
59	ZN	Bd	302	1/1	0.29	-	80,80,80,80	0
60	MG	Ba	1648	1/1	0.23	-	32,32,32,32	0
60	MG	BA	3075	1/1	0.28	-	44,44,44,44	0
60	MG	AA	3167	1/1	0.43	-	73,73,73,73	0
60	MG	BA	3160	1/1	0.48	-	74,74,74,74	0
60	MG	BA	3054	1/1	0.40	-	36,36,36,36	0
60	MG	Aa	1664	1/1	0.52	-	44,44,44,44	0
60	MG	BA	3097	1/1	0.26	-	54,54,54,54	0
60	MG	Aa	1727	1/1	1.31	-	98,98,98,98	1
60	MG	Aa	1648	1/1	0.57	-	121,121,121,121	0
60	MG	BA	3045	1/1	0.26	-	16,16,16,16	0
60	MG	BA	3251	1/1	0.29	-	65,65,65,65	0
60	MG	AA	3244	1/1	0.90	-	67,67,67,67	0
60	MG	Aw	101	1/1	0.39	-	83,83,83,83	1
60	MG	BA	3219	1/1	0.46	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Ba	1613	1/1	0.84	-	38,38,38,38	0
59	ZN	An	101	1/1	0.12	-	153,153,153,153	0
60	MG	B5	102	1/1	0.62	-	76,76,76,76	0
60	MG	AA	3230	1/1	1.31	-	78,78,78,78	0
60	MG	AA	2936	1/1	0.50	-	5,5,5,5	0
60	MG	Aa	1706	1/1	0.61	-	54,54,54,54	0
60	MG	AA	3133	1/1	0.29	-	48,48,48,48	0
60	MG	BA	3241	1/1	0.51	-	49,49,49,49	0
60	MG	BA	3139	1/1	0.14	-	15,15,15,15	0
60	MG	BA	2927	1/1	0.50	-	83,83,83,83	0
59	ZN	B9	101	1/1	0.09	-	116,116,116,116	0
60	MG	BA	2914	1/1	0.29	-	11,11,11,11	0
60	MG	BA	3258	1/1	0.35	-	84,84,84,84	0
60	MG	AA	3092	1/1	0.21	-	51,51,51,51	0
60	MG	AA	3114	1/1	0.39	-	18,18,18,18	1
60	MG	AA	2905	1/1	0.36	-	15,15,15,15	0
60	MG	Av	102	1/1	0.35	-	77,77,77,77	0

6.5 Other polymers ⓘ

There are no such residues in this entry.