



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 09:22 PM BST

PDB ID : 4V9A  
Title : Crystal Structure of the 70S ribosome with tetracycline. This entry contains the 30S subunit of molecule A.  
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.  
Deposited on : 2012-07-18  
Resolution : 3.30 Å(reported)

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

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

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

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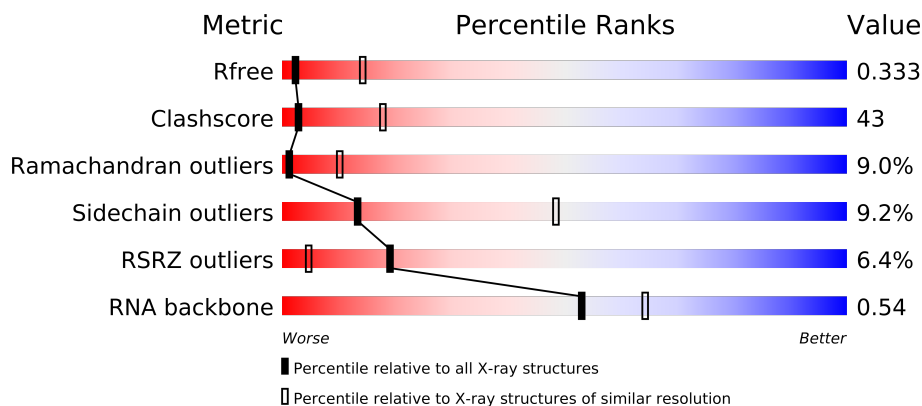
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 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 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

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

Mol	Chain	Length	Quality of chain
1	AA	1506	
1	CA	1506	
2	AE	256	
2	CE	256	
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
5	AH	162	
5	CH	162	
6	AI	101	

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Mol	Chain	Length	Quality of chain
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	128	
12	CO	128	
13	AP	126	
13	CP	126	
14	AQ	61	
14	CQ	61	
15	AR	89	
15	CR	89	
16	AS	88	
16	CS	88	
17	AT	105	
17	CT	105	
18	AU	88	
18	CU	88	
19	AV	93	
19	CV	93	
20	AW	106	
20	CW	106	
21	AX	27	
21	CX	27	
22	AC	77	
22	CC	77	
23	A1	4	
23	C1	4	
24	BA	2912	
24	DA	2912	
25	BB	122	
25	DB	122	
26	BD	276	
26	DD	276	
27	BE	206	

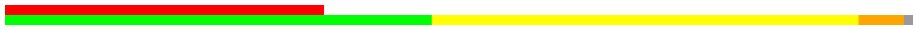
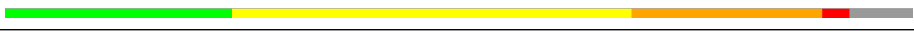


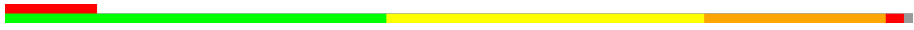



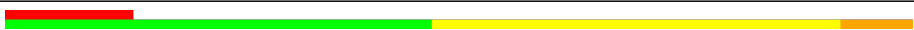
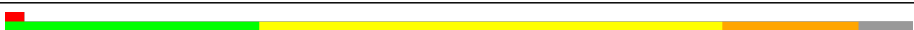
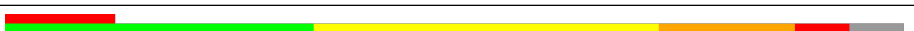
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Mol	Chain	Length	Quality of chain
27	DE	206	
28	BF	210	
28	DF	210	
29	BG	182	
29	DG	182	
30	BH	180	
30	DH	180	
31	BK	148	
31	DK	148	
32	BM	140	
32	DM	140	
33	BN	122	
33	DN	122	
34	BO	150	
34	DO	150	
35	BP	141	
35	DP	141	
36	B0	118	
36	D0	118	
37	BQ	112	
37	DQ	112	
38	BR	146	
38	DR	146	
39	B1	118	
39	D1	118	
40	B2	101	
40	D2	101	
41	BS	113	
41	DS	113	
42	BT	96	
42	DT	96	
43	BU	110	
43	DU	110	
44	BV	206	
44	DV	206	
45	B3	85	
45	D3	85	
46	BZ	98	
46	DZ	98	
47	BW	72	
47	DW	72	
48	BX	60	

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Mol	Chain	Length	Quality of chain
48	DX	60	
49	B4	71	
49	D4	71	
50	B5	60	
50	D5	60	
51	B6	54	
51	D6	54	
52	B7	49	
52	D7	49	
53	B8	65	
53	D8	65	

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 292440 atoms, of which 1 is hydrogen and 0 are deuterium.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1506	Total	C	N	O	P	0	0	0
			32369	14408	5997	10459	1505			
1	CA	1506	Total	C	N	O	P	0	0	0
			32372	14408	5997	10461	1506			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	CE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	CF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	CH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AL	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	CL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	CO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	CP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			



- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	CS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	CT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AU	72	Total	C	N	O	0	0	0
			591	376	117	98			
18	CU	72	Total	C	N	O	0	0	0
			591	376	117	98			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AX	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	CX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AC	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			
22	CC	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	17A	C	U	CONFLICT	GB AP008226.1
AC	50	U	C	CONFLICT	GB AP008226.1
AC	51	C	G	CONFLICT	GB AP008226.1
AC	63	G	C	CONFLICT	GB AP008226.1
CC	17A	C	U	CONFLICT	GB AP008226.1
CC	50	U	C	CONFLICT	GB AP008226.1
CC	51	C	G	CONFLICT	GB AP008226.1
CC	63	G	C	CONFLICT	GB AP008226.1

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	A1	4	Total	C	N	O	P	0	0	0
			85	38	14	29	4			
23	C1	4	Total	C	N	O	P	0	0	0
			85	38	14	29	4			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
24	DA	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	U	-	INSERTION	GB AP008226.1
BA	654A	A	G	CONFLICT	GB AP008226.1
BA	654E	C	G	CONFLICT	GB AP008226.1
BA	654P	G	C	CONFLICT	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1
DA	158	U	-	INSERTION	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

- Molecule 25 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
25	DB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
26	DD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
27	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
28	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
30	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
31	DK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
32	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	DN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
34	DO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
35	DP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	B0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
36	D0	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BQ	111	Total	C	N	O	0	0	0
			882	556	176	150			
37	DQ	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
38	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
39	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
40	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
41	DS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BT	92	Total	C	N	O	0	0	0
			725	471	131	123			
42	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
43	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
44	DV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
45	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
46	DZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
47	DW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BX	59	Total	C	N	O	0	0	0
			469	298	90	81			
48	DX	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
50	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
51	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
52	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
53	D8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	627	Total	Mg	0	0
			627	627		
54	CA	204	Total	Mg	0	0
			204	204		

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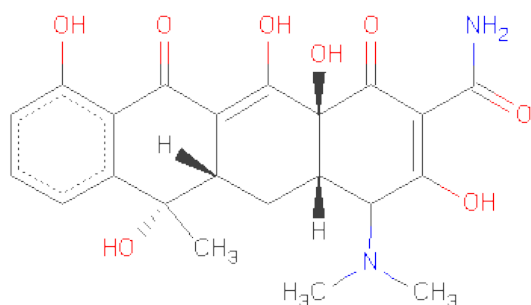
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CH	1	Total 1	Mg 1	0	0
54	DZ	2	Total 2	Mg 2	0	0
54	B8	1	Total 1	Mg 1	0	0
54	BE	5	Total 5	Mg 5	0	0
54	DU	1	Total 1	Mg 1	0	0
54	B1	2	Total 2	Mg 2	0	0
54	BP	1	Total 1	Mg 1	0	0
54	AS	1	Total 1	Mg 1	0	0
54	B5	2	Total 2	Mg 2	0	0
54	BB	17	Total 17	Mg 17	0	0
54	AJ	1	Total 1	Mg 1	0	0
54	BF	2	Total 2	Mg 2	0	0
54	DR	1	Total 1	Mg 1	0	0
54	B2	1	Total 1	Mg 1	0	0
54	AA	232	Total 232	Mg 232	0	0
54	AR	1	Total 1	Mg 1	0	0
54	B6	1	Total 1	Mg 1	0	0
54	CG	2	Total 2	Mg 2	0	0
54	BU	2	Total 2	Mg 2	0	0
54	A1	1	Total 1	Mg 1	0	0
54	DD	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CC	8	Total 8	Mg 8	0	0
54	DE	3	Total 3	Mg 3	0	0
54	B3	2	Total 2	Mg 2	0	0
54	DA	525	Total 525	Mg 525	0	0
54	B7	3	Total 3	Mg 3	0	0
54	AG	2	Total 2	Mg 2	0	0
54	BO	3	Total 3	Mg 3	0	0
54	AQ	2	Total 2	Mg 2	0	0
54	D1	1	Total 1	Mg 1	0	0
54	AH	2	Total 2	Mg 2	0	0
54	BZ	1	Total 1	Mg 1	0	0
54	AC	9	Total 9	Mg 9	0	0
54	D5	1	Total 1	Mg 1	0	0
54	DP	1	Total 1	Mg 1	0	0
54	CS	1	Total 1	Mg 1	0	0
54	DB	14	Total 14	Mg 14	0	0

- Molecule 55 is TETRACYCLINE (three-letter code: TAC) (formula:  $C_{22}H_{24}N_2O_8$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	AA	1	Total	C	H	N	O	0	0
			33	22	1	2	8		
55	CA	1	Total	C	N	O		0	0
			32	22	2	8			

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

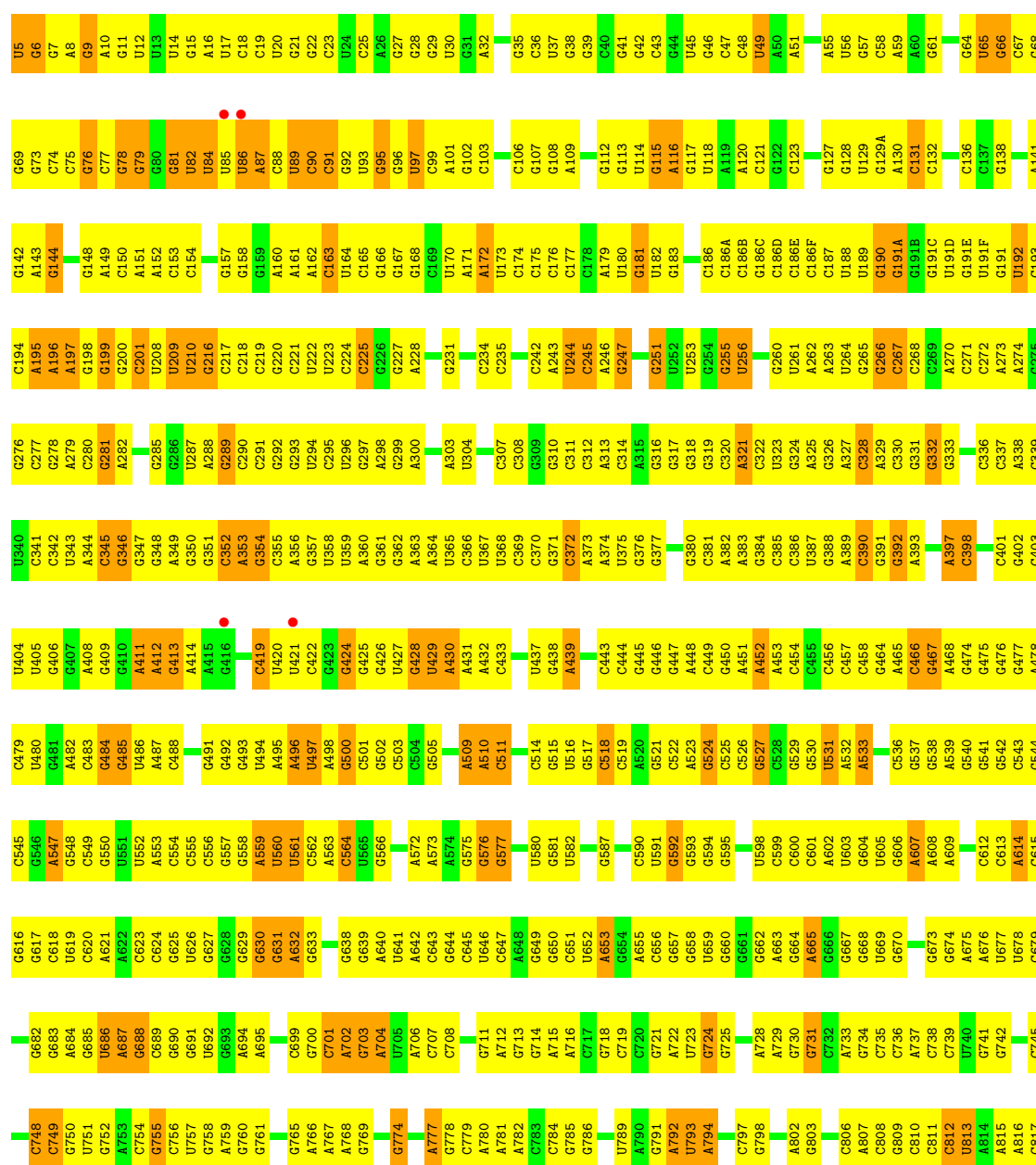
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total	Zn	0	0
			1	1		
56	AQ	1	Total	Zn	0	0
			1	1		
56	CQ	1	Total	Zn	0	0
			1	1		
56	CG	1	Total	Zn	0	0
			1	1		

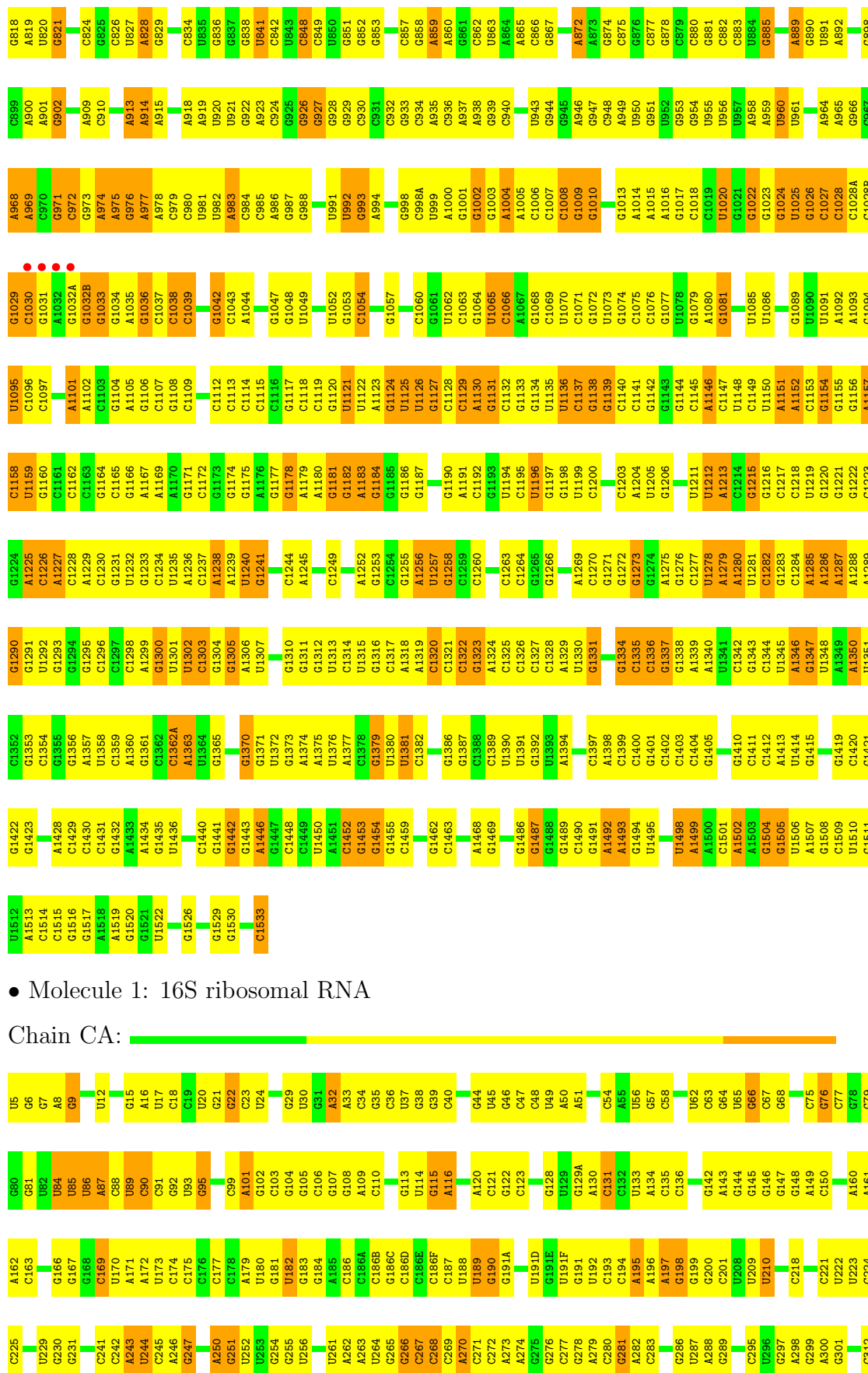
### 3 Residue-property plots

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

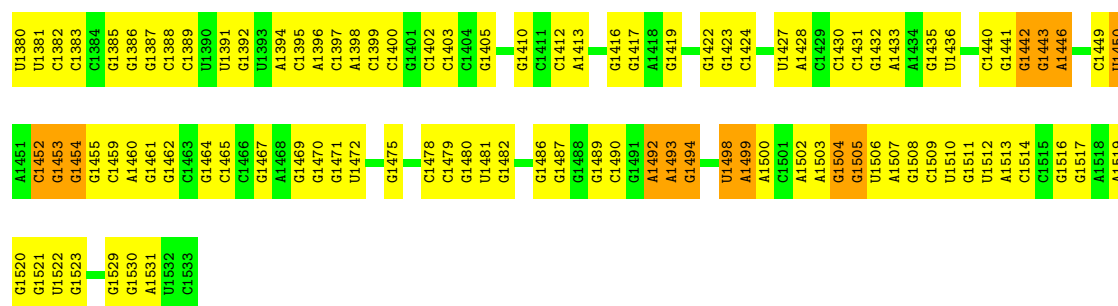
- Molecule 1: 16S ribosomal RNA

Chain AA: 



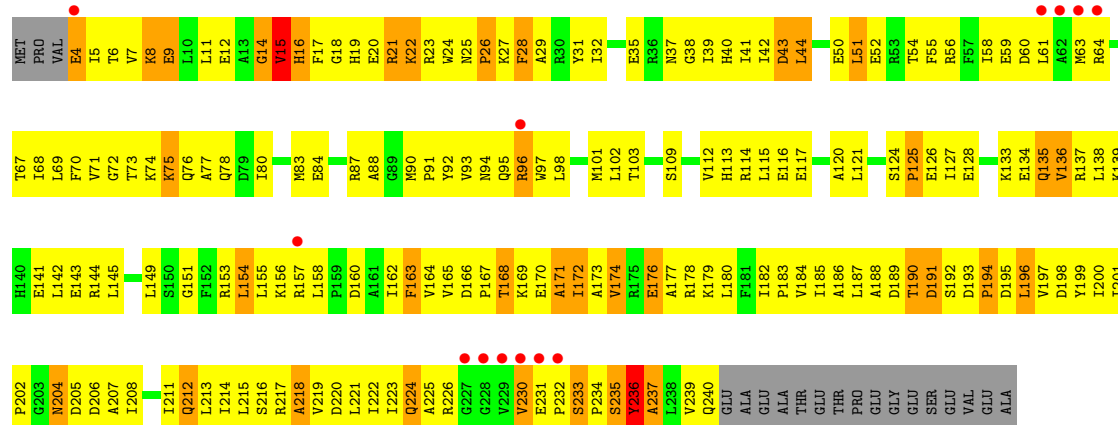


A1319	G1255	C1195	C1128	A1067	G1009	U950	C880	U801	G730	G661	C528	A452	C386	A1319
C1320	A1256	U1196	C1129	G1068	G1010	G951	C881	A802	G731	G662	C529	A453	U387	C1320
C1321	U1257	G1197	A1130	C1069	G1011	U952	C882	A803	G732	G663	C530	A454	C388	C1321
C1322	G1258	C1198	G1131	U1070	U1012	G953	C883	C811	G734	G664	U531	C457	A389	C1322
C1323	C1259	U1199	C1132	G1071	G1013	G954	U884	C812	C735	A665	A532	C457	C390	C1323
A1324	C1260	C1200	G1133	G1072	A1014	U955	C885	U813	C736	G666	A533	C458	C391	A1324
C1325	A1201	C1325	G1134	U1073	A1015	U956	A889	U814	A737	C600	U534	C464	G392	C1325
C1326	C1263	G1202	U1135	G1074	A1016	U957	G890	A815	C738	G671	A535	C465	A393	C1326
C1327	C1264	C1203	U1136	C1075	U1070	A958	G891	A816	C739	U672	C536	C466	A394	C1327
C1328	G1265	A1204	C1137	G1076	U891	A959	A892	A817	U740	G673	G537	C467	C395	C1328
A1329	U1205	G1138	G1138	U1077	U1020	U960	C893	C817	G741	G674	G538	A468	G396	A1329
C1330	C1266	G1206	G1139	U1078	G1021	U961	C894	C818	G742	A675	A539	G474	A397	C1330
C1331	A1268	G1207	C1140	G1079	G1022	C962	C894	A819	C743	G676	G540	G475	C398	C1331
A1332	C1269	C1208	G1141	G1080	G1023	G963	C895	U820	C738	U677	G541	G476	C399	A1332
C1333	C1270	C1209	G1142	G1081	G1024	A964	C896	C821	C745	U678	G542	G477	G332	C1333
C1334	C1271	G1143	G1143	U1082	U1025	A965	C897	C826	C748	G682	G544	A478	G333	C1334
C1335	U1211	U1211	G1144	U1083	G1026	G966	C987	U827	C749	G683	G545	C479	C337	C1335
C1336	U1212	U1212	C1145	G1084	C1027	C967	A900	U828	G750	G684	C546	U480	U404	C1336
C1337	C1277	A1213	A1146	U1085	C1028	A968	A901	A829	U751	G685	C547	G481	U405	C1337
C1338	U1278	C1214	C1147	U1086	G1028A	A969	G902	C829	G752	U686	A547	A482	G406	C1338
A1339	A1279	G1215	U1148	G1087	C1028B	C970	G903	U833	C753	U687	G550	C483	A408	C1339
C1340	A1280	G1216	C1149	G1088	G1029	C971	G906	U834	C754	A687	U551	G484	G409	C1340
C1341	U1281	C1217	U1150	U1089	G1030	C972	A907	U835	G755	G688	U552	G485	G410	C1341
C1342	C1282	C1218	A1151	U1090	G1031	C973	C974	U836	C756	C689	U553	U486	A411	C1342
C1343	G1283	U1219	A1152	U1091	A1032	A974	C912	C837	U757	G690	A554	C490	A412	C1343
C1344	C1284	G1220	C1153	A1092	G1032A	A975	C913	U838	G763	G691	C554	G490	G413	C1344
C1345	G1221	G1154	A1154	A1093	G1032B	G976	A913	U841	C764	U692	C554	G491	A414	C1345
A1346	A1285	C1222	G1155	G1094	G1033	A977	A914	C842	C765	G693	C555	C491	C347	C1346
C1347	A1287	G1223	G1156	U1095	G1034	A978	A915	U843	A766	A694	G558	A495	A349	C1347
C1348	A1288	G1224	A1157	C1096	A1035	C979	G916	U843	C766	A695	A559	A496	C351	C1348
C1349	A1289	A1225	C1158	C1097	G1036	C980	G917	C848	A767	A696	U560	U497	C352	C1349
C1350	G1290	C1226	U1159	C1098	C1037	U981	A918	C849	G768	U697	U561	A498	C353	C1350
C1351	A1291	A1227	G1160	C1099	C1038	U982	A919	U850	C769	G698	C562	G500	C354	C1351
C1352	U1292	C1228	C1161	C1100	C1039	A983	U920	G851	C770	C708	A563	C501	C355	C1352
C1353	G1293	A1229	C1162	A1101	U1040	C984	U921	G852	G771	A702	U565	G502	C356	C1353
C1356	G1294	C1230	C1162	A1102	A1041	C985	C922	C853	U772	G703	U565	C503	C357	C1356
A1357	U1295	G1231	A1167	C1103	G1042	A986	A923	G854	G773	A704	C504	G426	U358	C1357
C1358	C1296	U1232	A1169	C1104	C1043	A987	G926	C855	A777	U705	G505	U427	U359	C1358
C1359	C1297	G1233	A1170	A1105	A1044	G988	G927	C856	G778	C707	A572	G428	A360	C1359
A1360	C1298	G1234	C1172	C1106	A1045	C989	C927	C857	C778	C708	A573	U429	C361	C1360
C1361	A1301	U1235	G1173	C1107	C1046	C990	C980	C858	C779	C709	A574	A430	U365	C1361
C1362	G1300	A1236	C1173	C1108	G1047	U991	C930	A859	A782	G709	A574	A431	U366	C1362
C1362A	U1301	C1237	A1176	C1109	G1048	U992	C931	A860	C783	G710	A574	A431	U366	C1362A
A1363	A1302	A1238	G1177	C1110	U1049	G993	C932	A861	C784	G711	A574	A432	C366	A1363
C1364	C1303	A1239	G1178	A1111	G1050	A994	G933	C862	C785	A712	A574	A433	C367	C1364
G1365	G1304	U1240	A1179	C1112	C1051	C995	C934	U863	G786	G713	C435	C435	C370	C1365
C1366	G1305	G1241	A1180	C1113	U1052	A996	A935	A864	A787	A714	C436	C436	C371	C1366
C1367	A1306	C1242	G1181	C1114	G1053	U997	C936	A865	U788	G715	C437	C437	C372	C1367
C1368	U1307	C1243	G1182	C1115	C1054	G998	A937	C866	U789	A716	C438	C438	A373	C1368
C1369	C1308	A1244	A1183	G1117	U1049	C998A	A938	C867	C784	G717	A583	A439	A374	C1369
C1370	G1309	C1245	G1184	C1118	G1057	U999	G939	C868	C791	G718	A584	C440	U375	C1370
C1371	C1310	C1246	G1185	C1119	U1058	U999	C940	C869	A792	C719	C585	C442	G376	C1371
C1372	G1311	U1247	G1186	C1120	C1059	G1001	G941	U870	U793	C720	C586	C443	G377	C1372
C1373	C1312	A1248	G1187	U1121	C1060	G1002	G944	U871	A794	G721	C587	C444	C378	C1373
A1374	U1313	C1249	A1188	U1122	G1061	G1003	G944	A872	C795	A722	C588	C444	C379	A1374
A1375	C1314	A1250	C1189	A1123	U1062	G945	A873	C796	C796	U723	C589	A523	A382	A1375
C1376	U1315	A1251	G1190	G1124	C1063	A1005	G946	C874	C797	G724	C590	G524	A383	C1376
A1377	C1316	A1252	A1191	U1125	G1064	C1006	A947	C875	G798	G725	C591	C526	A383	C1377
C1378	C1317	G1253	C1317	U1126	U1065	C1007	C948	C878	G799	C726	C592	C527	G384	C1378
C1379	A1318	C1254	U1126	C1127	U1065	C1008	A949	C879	C800	C593	C593	C528	G385	C1379



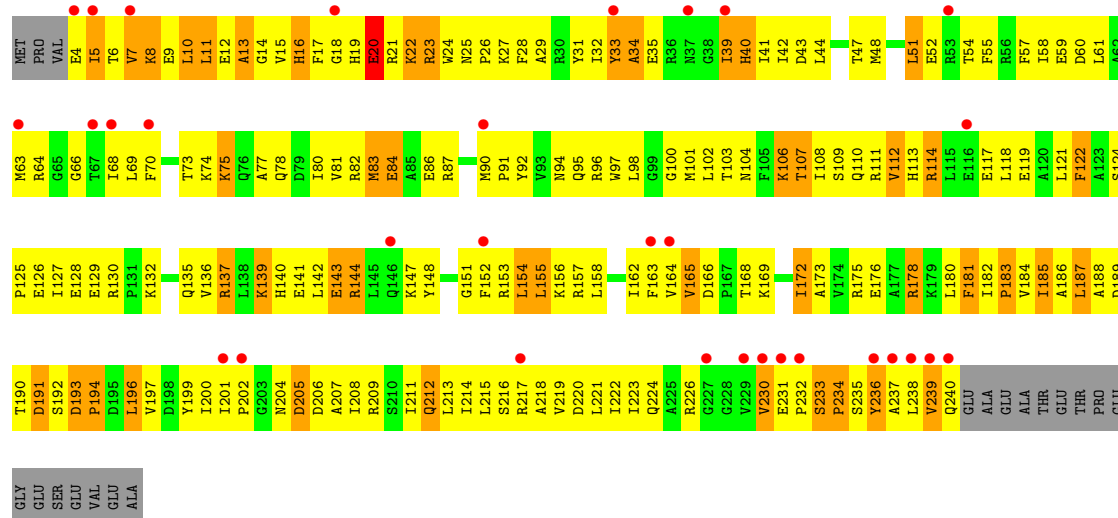
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AE:



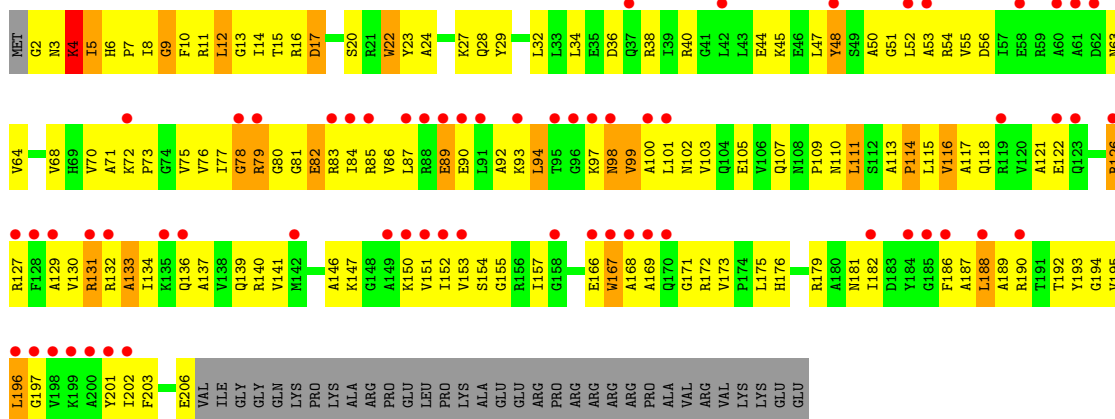
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CE:



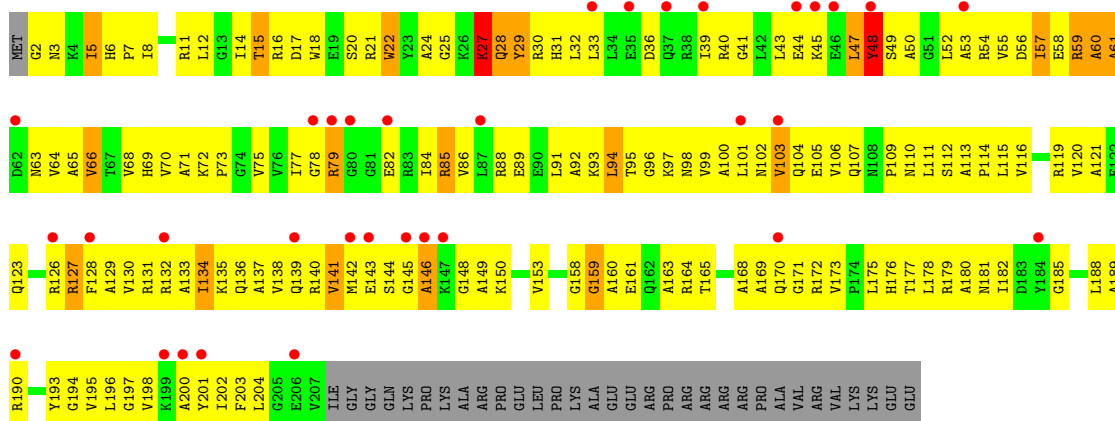
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AF:



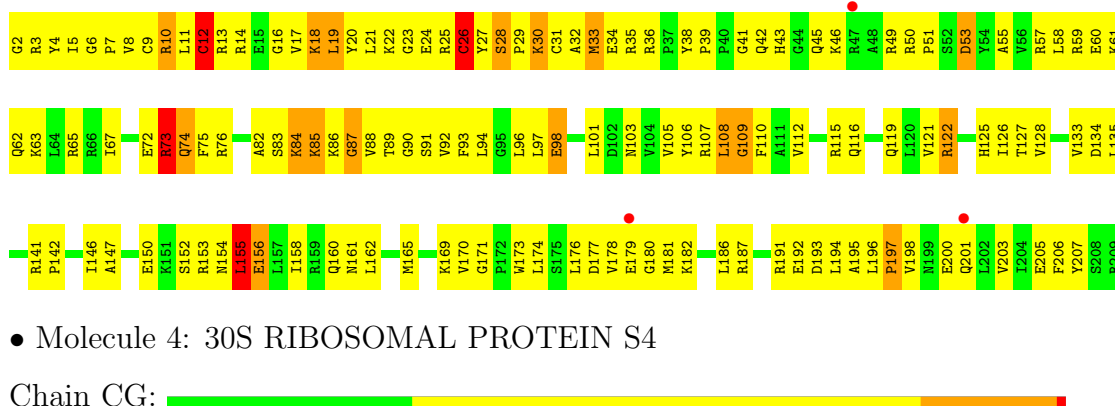
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CF:



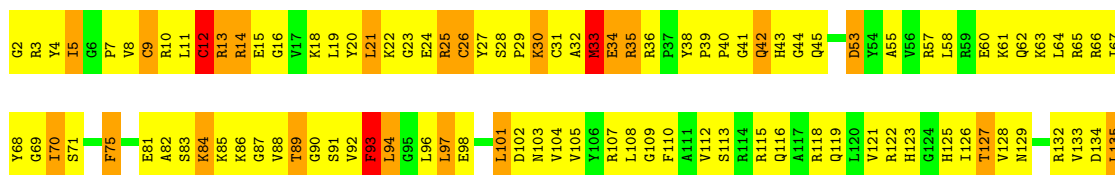
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AG:

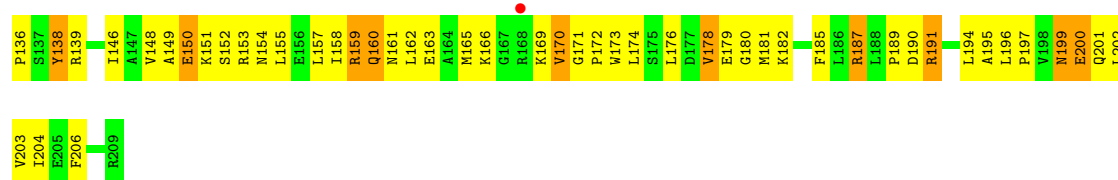


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CG:

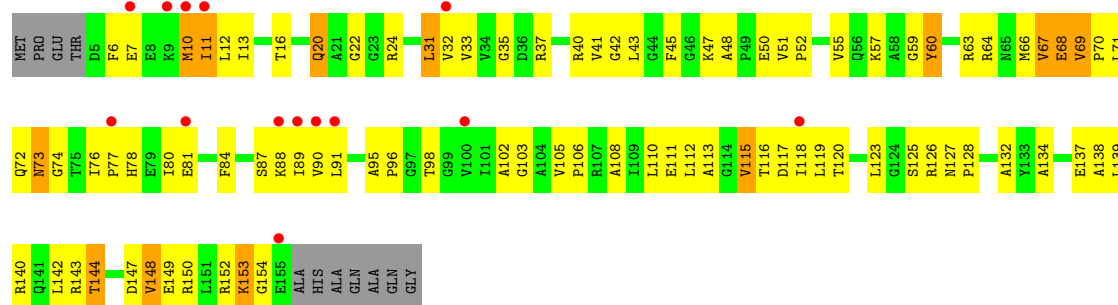






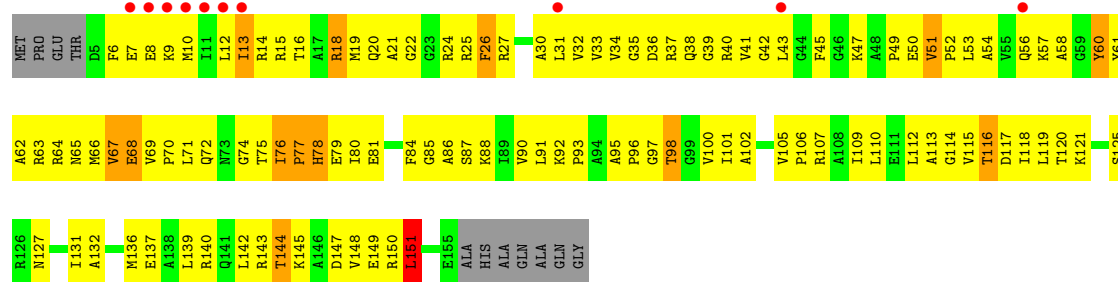
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AH:



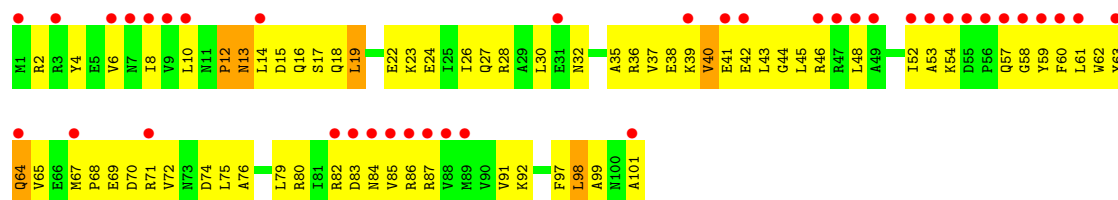
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CH:



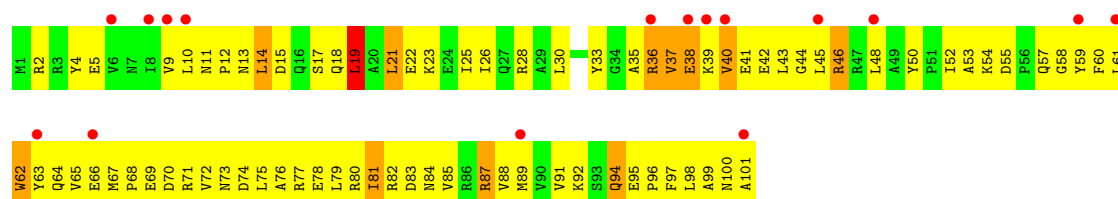
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AI:



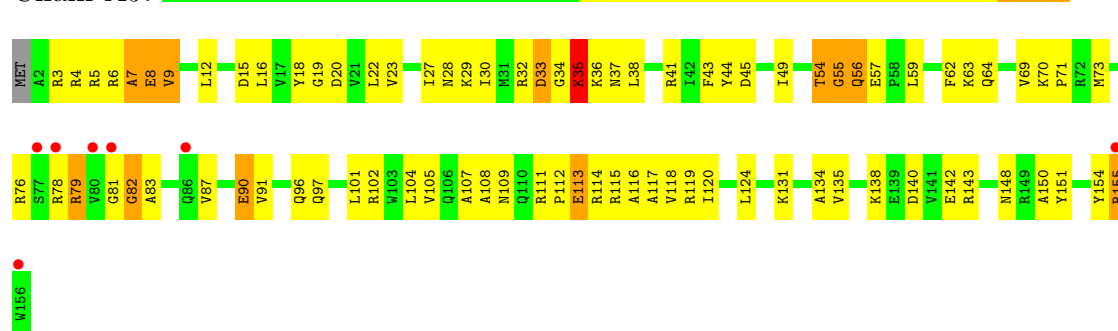
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CI:



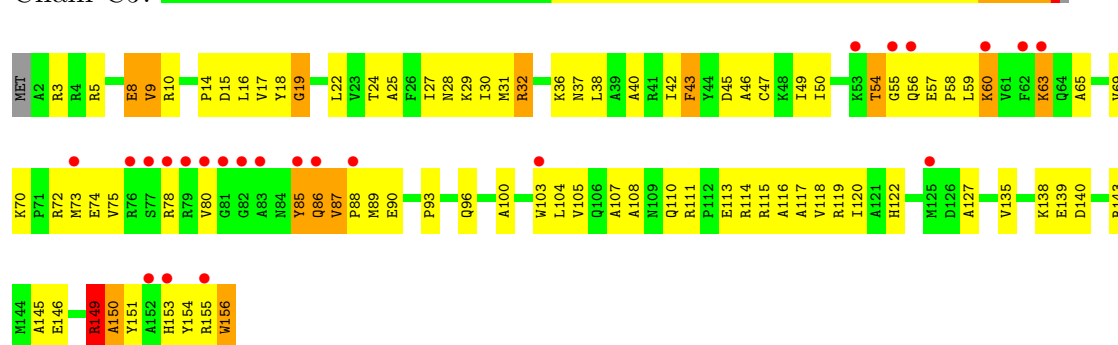
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AJ:



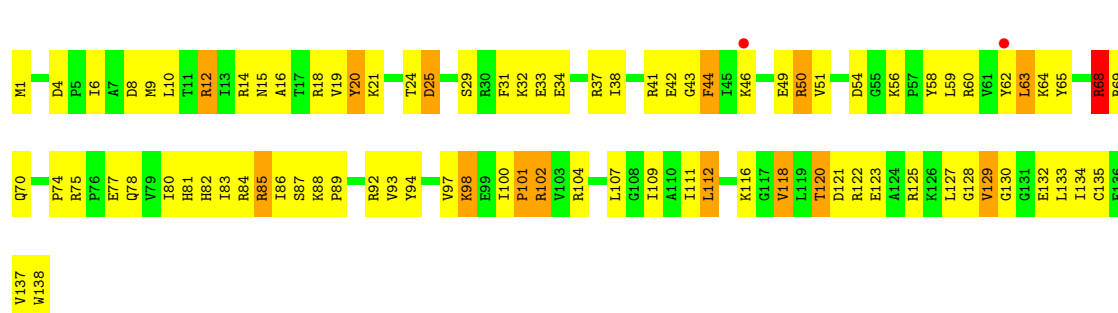
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CJ:



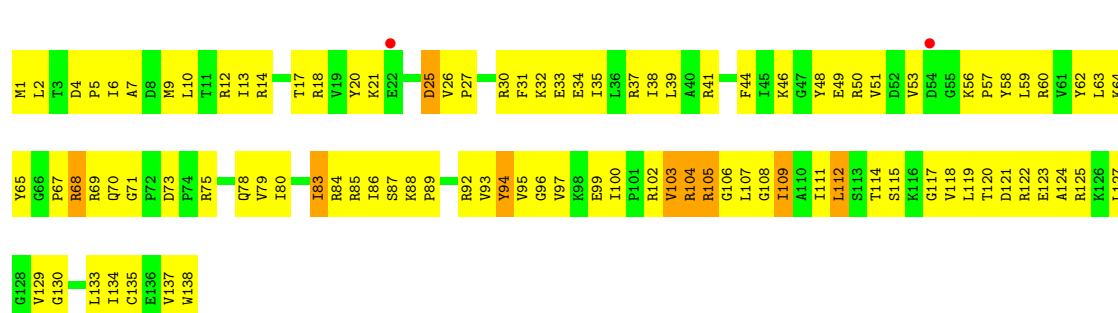
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AK:



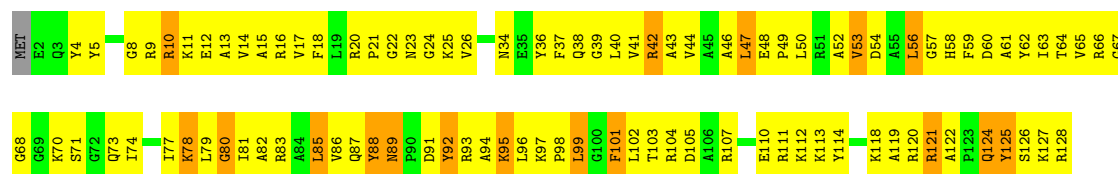
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CK:



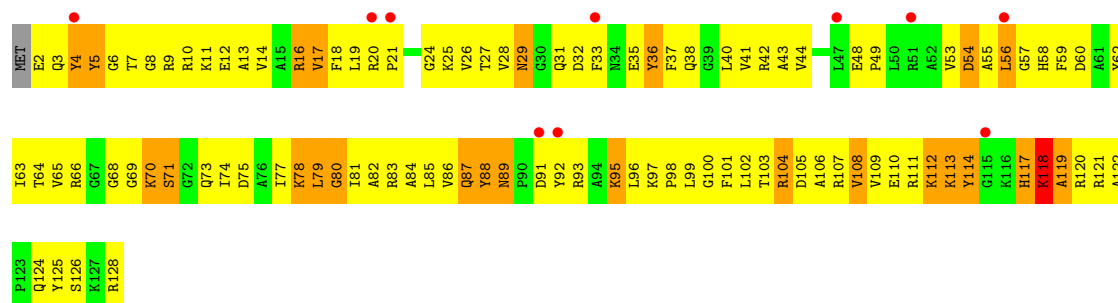
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AL:



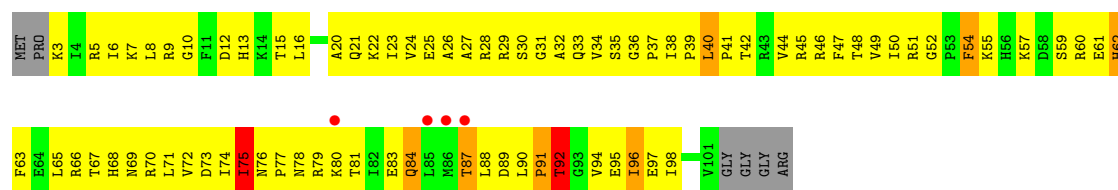
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL:



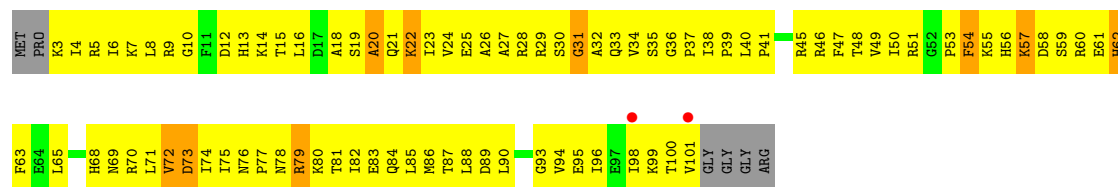
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AM:



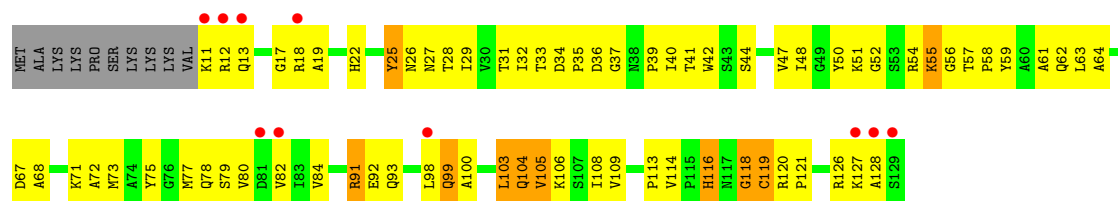
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CM:



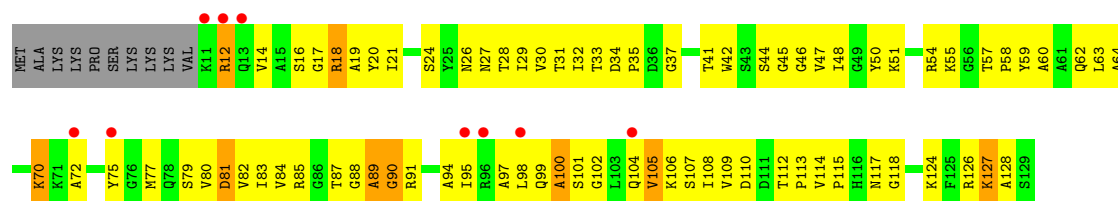
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AN:



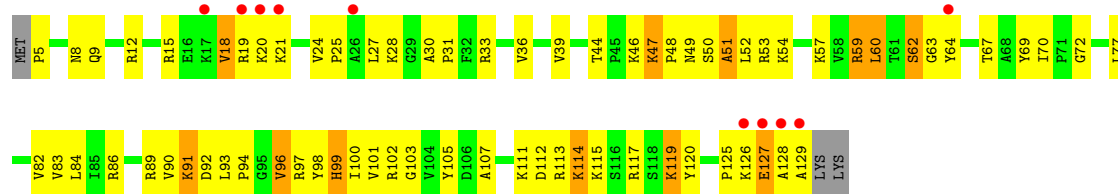
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CN:



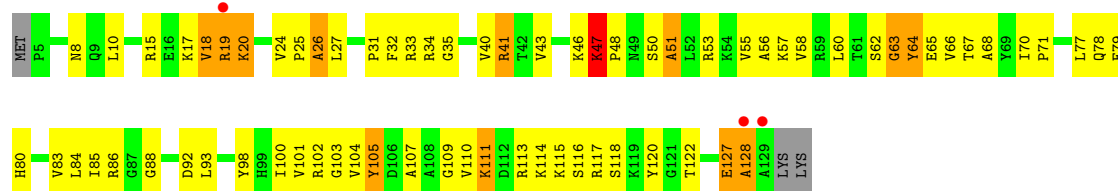
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AO:



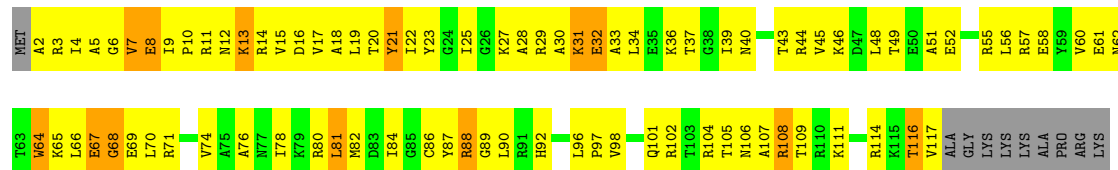
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CO:



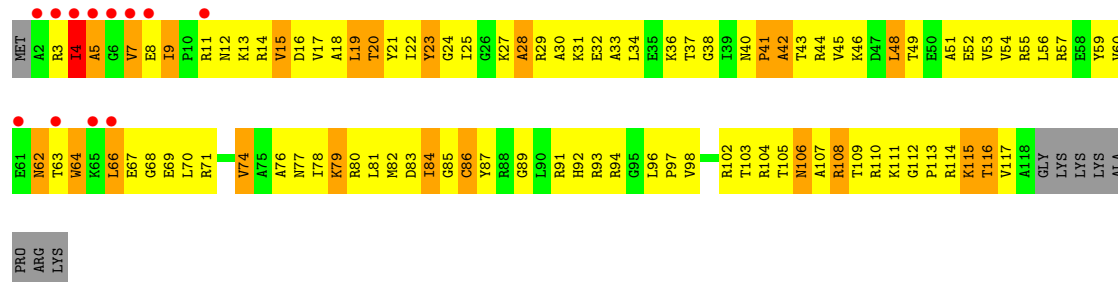
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AP:



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CP:



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AQ: 



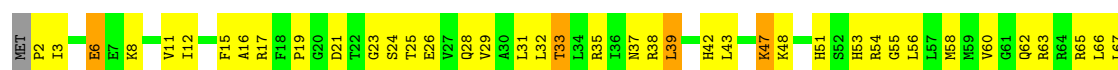
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CQ: 



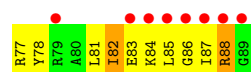
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AR: 



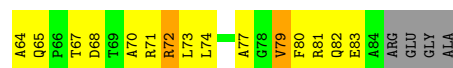
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CR: 



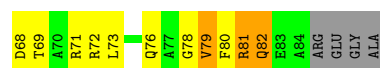
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AS: 



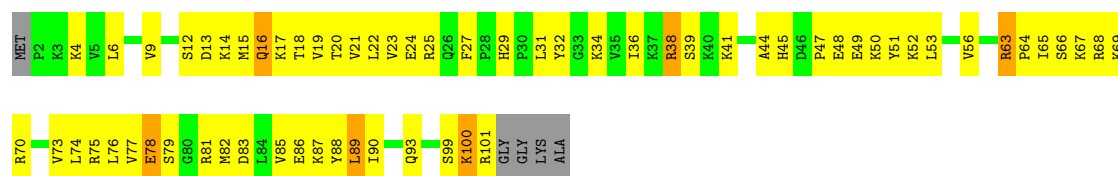
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS: 



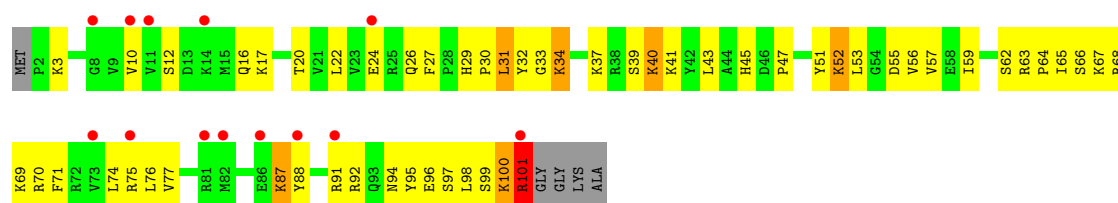
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AT:



- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CT:



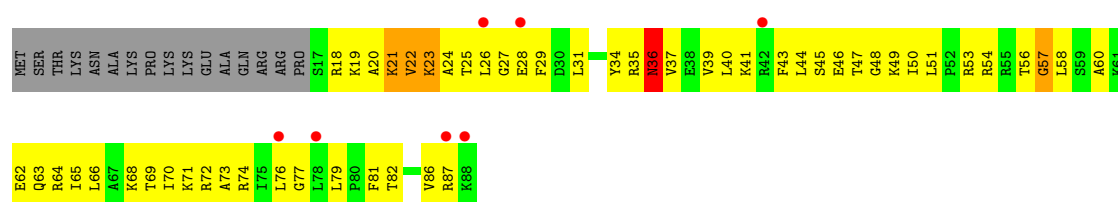
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AU:



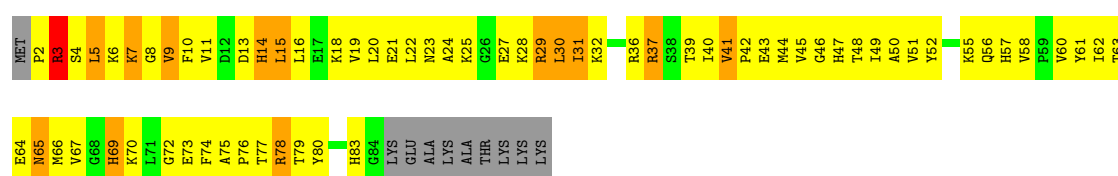
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CU:



- Molecule 19: 30S RIBOSOMAL PROTEIN S19

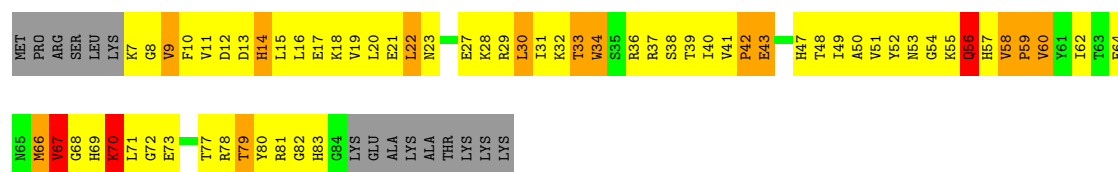
Chain AV:



- Molecule 19: 30S RIBOSOMAL PROTEIN S19

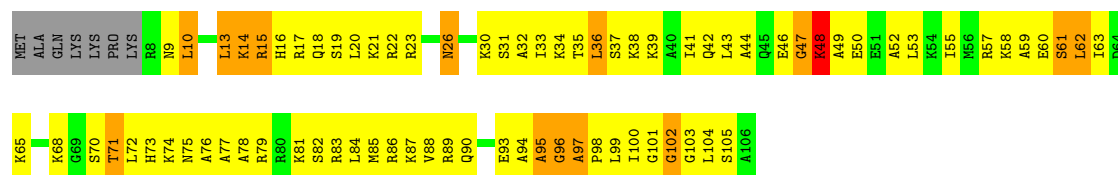
Chain CV:





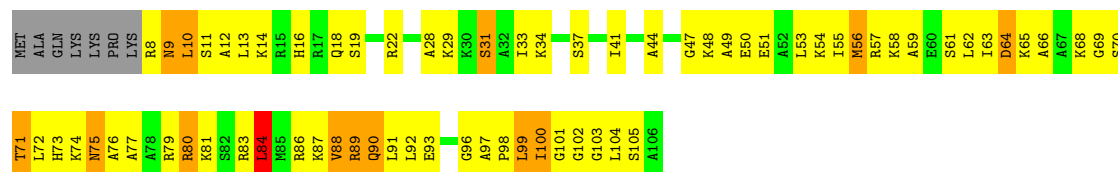
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AW:



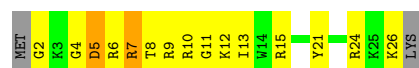
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CW:



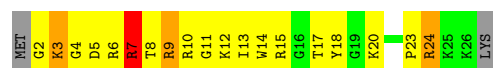
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AX:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX:



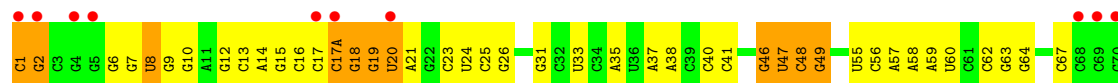
• Molecule 22: TRNA-FMET

Chain AC:



• Molecule 22: TRNA-FMET

Chain CC:





- Molecule 23: MRNA

Chain A1:



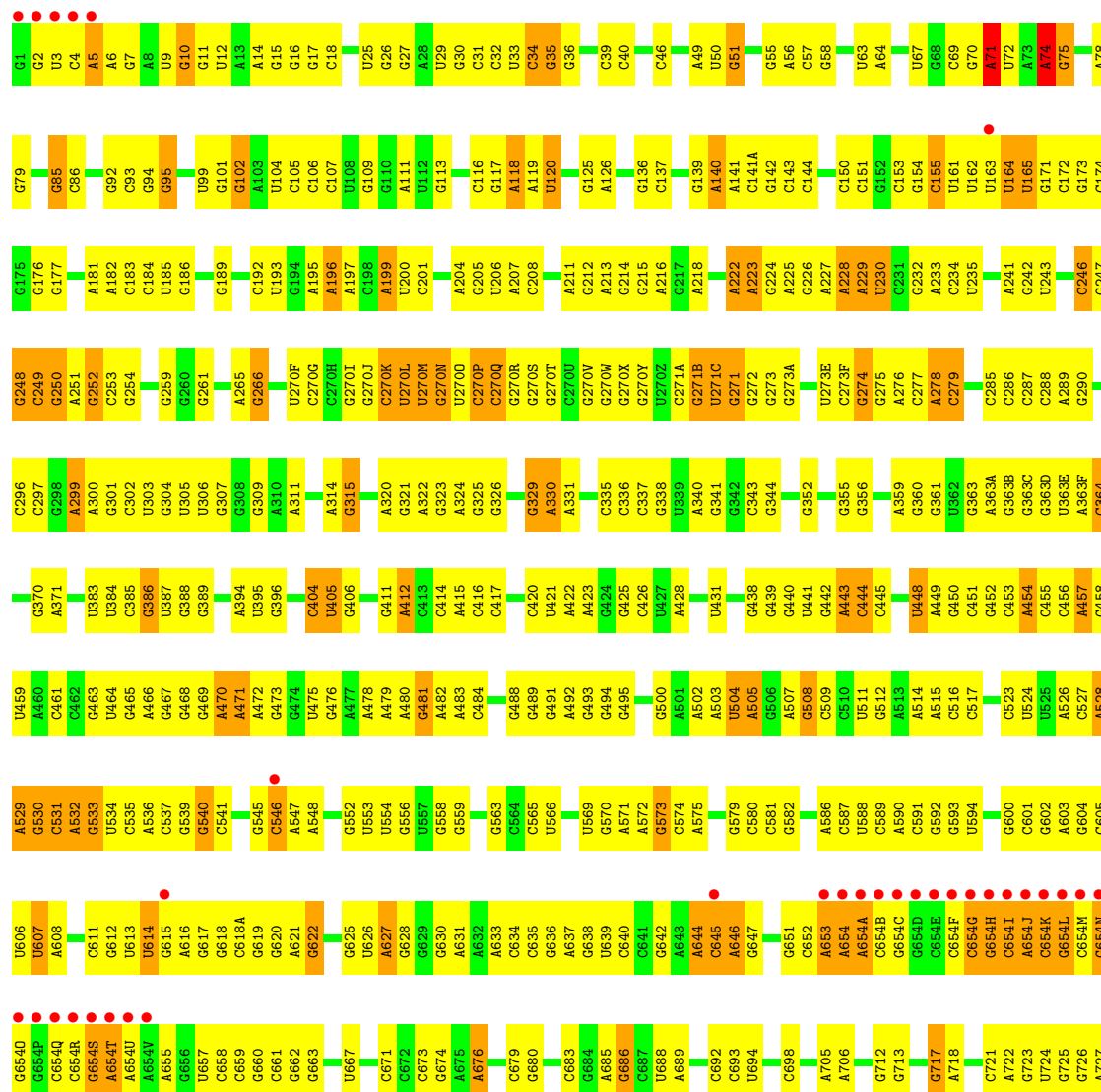
- Molecule 23: MRNA

Chain C1:



- Molecule 24: 23S ribosomal RNA

Chain BA:



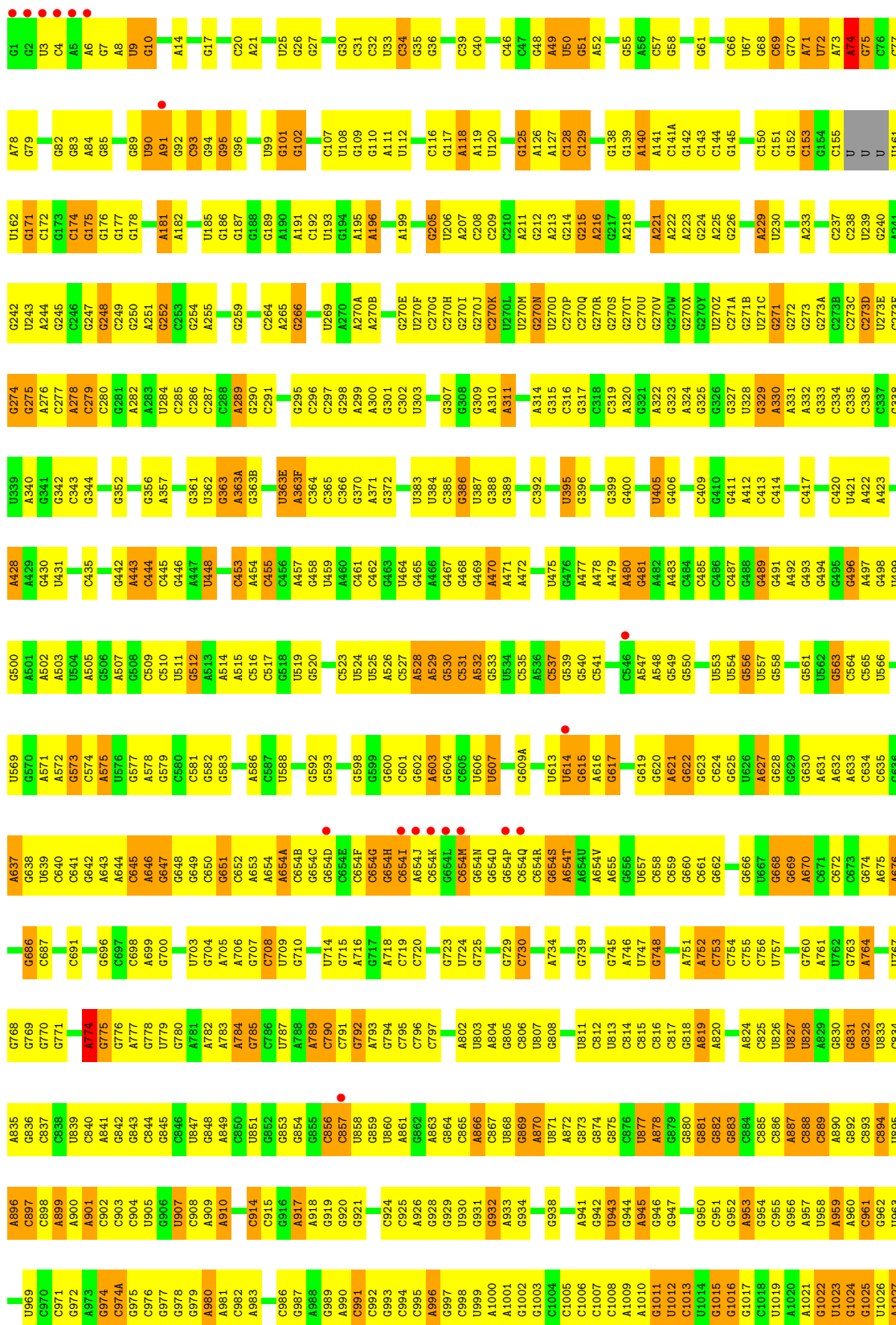


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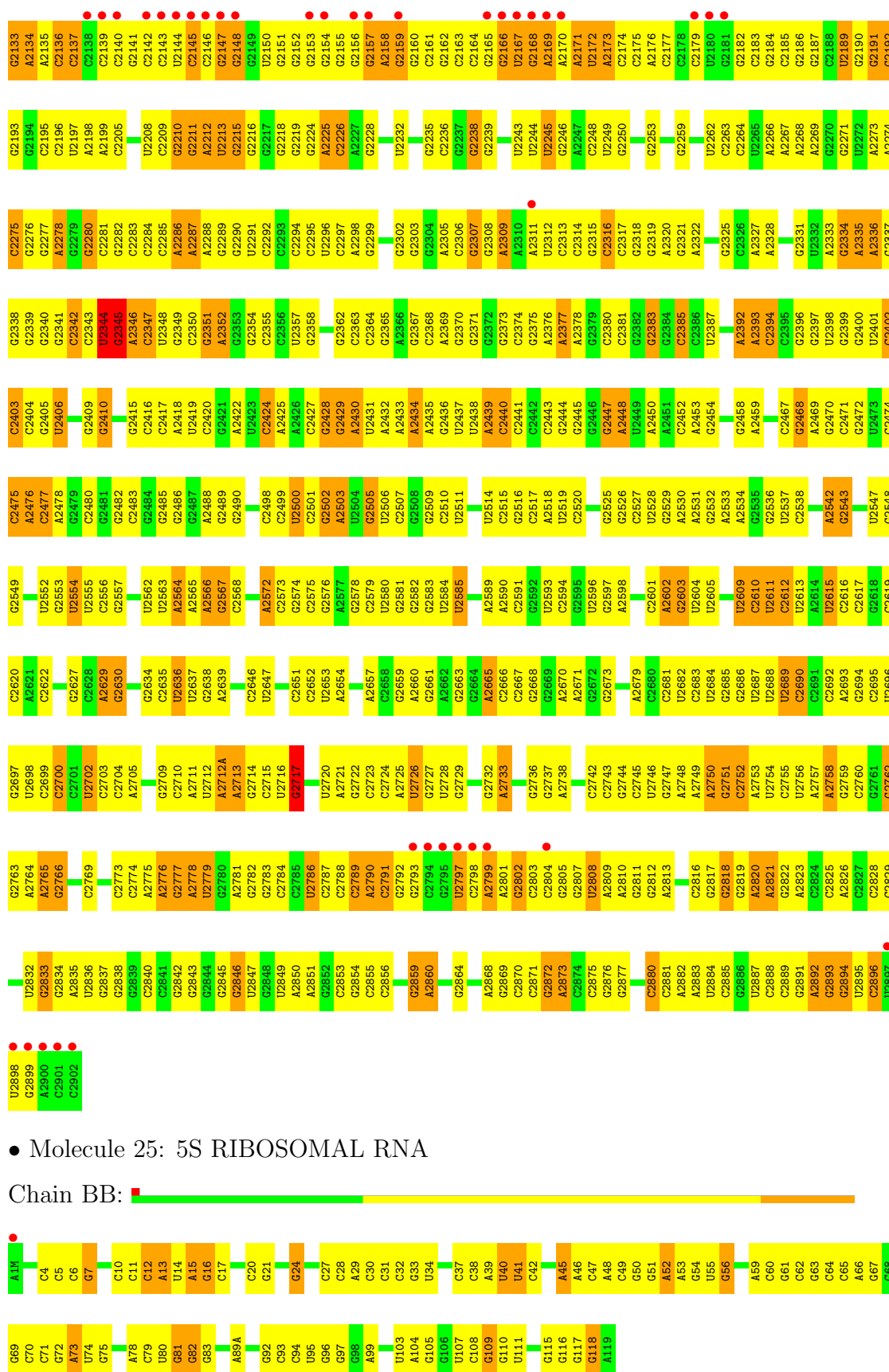
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A1936	A1937	A1938	U1939	G1947	G1948	G1949	G1950	U1951	A1952	A1953	U1955	U1956	G1957	C1958	U1963	G1964	G1967	G1968	A1969	A1970	A1971	A1972	G1973	C1974	G1975	U1976	G1980	A1981	G1982	G1985	A1986	G1989	C1990	C1991	G1992	U1993	G1996	G1997	G1998	G1999	G2000	G2001	G2002	G2007	G2008	G2009	G2010	G2011	G2012	C1934	G1935										
G1889	A1900	A1901	C1902	G1903	G1904	C1905	G1906	G1907	C1908	C1909	G1910	U1911	A1912	C1913	C1914	U1915	A1916	U1917	A1918	A1919	C1920	G1921	G1922	U1923	G1924	U1926	G1929	G1930	U1931	C1934	G1935																														

## ● Molecule 24: 23S ribosomal RNA

Chain DA:

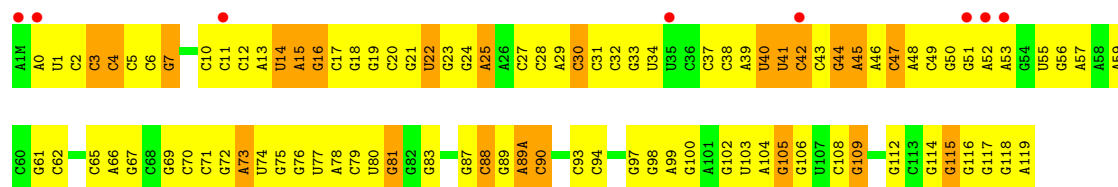


C2065	U1993	A1821	G1748	C1656	A1583	C1513	G1448	A1373	C1297	A1227	G1160	C1092	A1028
C2066	C1994	G1826	A1749	C1657	C1585	U1514	A1448	G1374	C1298	G1228	G1160	G1093	A1029
C2067	U1995	A1913	G1753	C1658	A1586	C1515	A1449	C1375	U1300	G1229	G1161	U1094	A1030
U2068	C1996	G1827	G1763	U1659	A1587		C1376	C1376	A1301	C1230	A1095	A1096	G1036
C2069	G1997	A1828	G1766	G1660	C1588	U1519	C1451	A1377	A1302	G1231	U1165	U1097	G1037
G2070	G1998	A1829	U1767	G1661	U1590	G1520	U1453	A1379	G1303	G1232	C1166	U1098	C1038
A2071	C1999	U1767	U1767	G1665	U1591	G1521	U1454	G1380	C1304	C1233	U1167	G1099	C1039
U2074	G2000	C1832	G1768	G1666	C1592	G1522	U1455	A1384	C1306	G1235	G1168	U1101	C1040
G2080	A2001	U1833		G1666	G1592			U1384	A1307		G1170	U1101	C1041
C2081	G2002	U1834	G1761	G1667	G1526	G1525	G1459	A1384	A1308	U1240	G1171	C1102	C1042
A2082	G1921	G1835	A1762	G1668	G1594	G1527	A1460	C1386	G1309	A1241	G1173	A1103	G1043
G2083	G1922	C1836	G1763	A1669	G1595	A1528	G1461	C1387	A1241	U1240	G1173	C1104	C1044
C2084	C1923	G1837	G1764	C1670	A1596	A1529	C1462	G1388	G1310	A1242	A1174	U1105	G1045
C2085	C1924	G1837	G1765	U1671	A1597	A1530	C1463	G1389	G1311		G1175	G1106	A1046
U2086	C1925	C1672	C1672	C1672	C1598	G1530	C1464	U1390	G1312	G1245	G1176		A1047
C2087	U1926	G1673	C1673	G1674	C1599	C1531	G1465	U1390	U1313		G1177	G1109	A1048
U2088	G1929	C1674	C1675	G1675	G1600	C1532	G1466	U1394	U1314	A1247	A1177	C1110	G1049
C2089	U1930	A1676	A1676	U1602	G1601	C1533	G1467	A1395	G1317	U1249	C1180	G1112	A1050
A2090	G1931	A1677	A1677		U1602	G1534	C1468	U1397	A1318	U1249	C1181	G1113	G1051
U2092	A1932	G1678	G1678	G1678	C1607	U1535	C1468	U1397	G1325	G1250	C1182	G1114	A1054
G2093	G1933	C1678	C1686	C1686	A1608	C1537	A1470	C1401	G1326	C1251	A1182	G1115	G1055
C2094	C1934	U1687	U1687	U1688	A1609	G1538	A1471	G1401	C1327	G1252	G1183	G1116	G1056
C2095	G1935	U1688	G1688	A1689	A1610	G1539	A1472	C1402	G1328	G1259	G1190	G1117	A1057
A2096	A1936	U1689	U1689		C1611	G1540	G1473	U1405	G1329	G1260	G1191	G1118	U1058
C2097	U1938	A1689	A1689		C1612	U1541	C1474	U1406	C1330	C1265	G1192	G1119	G1062
U2098	G1939	G1696	G1696	G1697	G1613	G1542	G1475	C1407	A1331	U1266	G1193	A1129	C1064
C2099	U1940	G1697	G1697	G1698	G1614	A1543	C1476	C1417	G1332	G1267	G1194	U1130	C1065
G2100	G1941	C1698	C1698	U1700	C1615	A1544	A1477	C1408	C1333	G1264	A1194	G1131	U1066
C2101	A1942	G1700	G1700	A1701	G1630	C1548	A1486	G1418	G1334	A1265	U1199	U1133	A1067
U2102	U1943	A1701	G1705	G1705	U1632	G1552	G1487	A1419	U1335	G1266	G1200	U1133	G1068
C2105	U1944	G1706	U1706	U1706	G1633	G1555	G1488	U1420	A1336	G1267	C1201	G1135	A1069
G2106	C1945	G1707	G1707	G1707	A1634	C1556	U1489	G1421	G1337	A1268	G1202	G1137	A1070
C2107	U1946	C1708	C1708	C1708	G1635	C1557	A1490	G1422	G1338	G1270	G1203	G1138	C1072
C2108	C1947	U1709	U1709	U1709	G1637	A1568	G1491	G1423	G1339	G1271	G1204	G1139	A1073
U2109	A1948	C1710	C1710	C1710	G1638	G1569	G1492	G1424	U1341	A1272	U1205	C1140	C1074
C2110	G1949	G1711	G1711	G1711	U1639	G1580	A1494	G1425	A1342	U1273	G1206	U1141	G1075
G2111	U1950	C1712	C1712	C1712	G1640	A1566	A1495	G1426	G1343	A1274	U1142	C1076	C1076
C2112	A1951	U1716	U1716	U1716	A1641	A1567	A1496	A1427	G1344	A1275	A1210	A1142A	U1077
U2113	C1952	G1717	G1717	G1717	G1642	A1567	U1497	C1428		A1276	U1211	A1143	U1078
C2114	G1953	G1718	G1718	G1718	G1643	G1568	C1498		G1348	G1277	G1212	G1144	C1079
G2115	U1954	G1725	G1725	G1725	G1644	A1569	C1499	A1434	A1349	A1278	G1145	C1145	A1080
C2116	C1955	G1728	G1728	G1728	G1645	A1570	G1500	G1435	C1350	G1279	G1215	C1146	U1081
A2117	G1956	U1730	U1730	U1730	G1646	A1571	C1504	C1437	C1351		G1216	C1147	U1082
U2118	U1957	G1731	G1731	G1731	G1647	A1572	C1505	U1438	A1359	U1288	G1217	A1148	U1083
C2119	C1958	U1732	U1732	U1732	G1648	G1573	C1506	A1439	A1360		A1220	G1149	A1084
G2120	A1959	A1732	A1732	A1732	G1649		A1507	G1440	G1291	G1291	G1221	C1151	A1085
C2121	G1960	G1742	G1742	G1742	G1650	U1577	A1508	G1441	U1292	C1222	G1152	G1151	A1086
U2122	U1961	C1742	C1742	C1742	A1652	U1578	C1509	G1442	C1293	C1223	C1153	G1154	G1087
G2123	C1962	G1743	G1743	G1743	G1653	A1580	A1510	A1444	U1294	G1224	G1155	G1154	A1088
C2124	U1963	U1747	U1747	U1747	A1655	C1582	G1512	C1445	C1295	G1296	G1225	A1155	U1089
A2125	G1964								G1368		G1226	A1156	G1091
C2126	C1965												
G2127	U1966												
A2128	A1967												
C2129	C1968												
U2130	U1969												
G2131	C1970												
U2132	A1971												



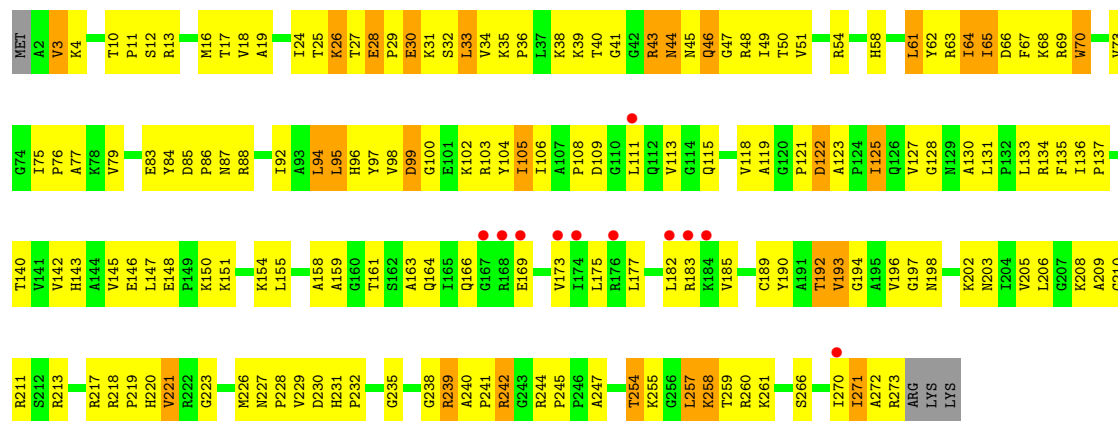
• Molecule 25: 5S RIBOSOMAL RNA

Chain DB:



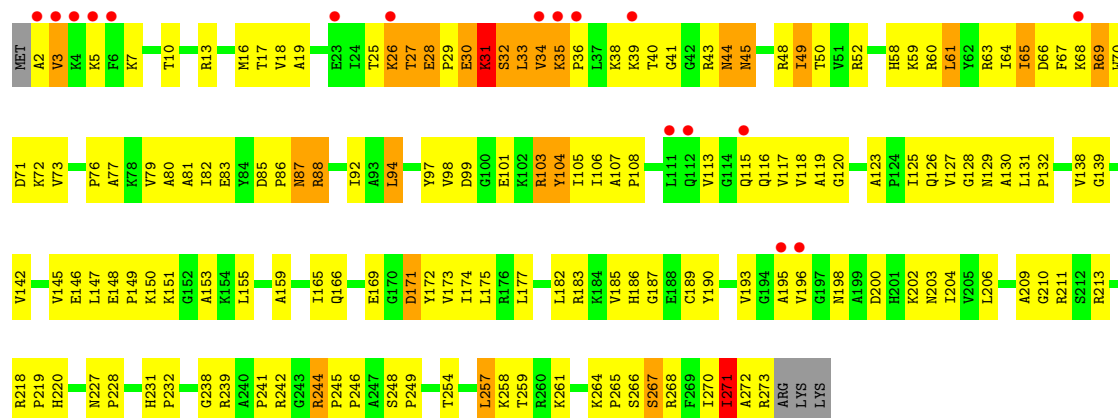
- Molecule 26: 50S ribosomal protein L2

Chain BD:



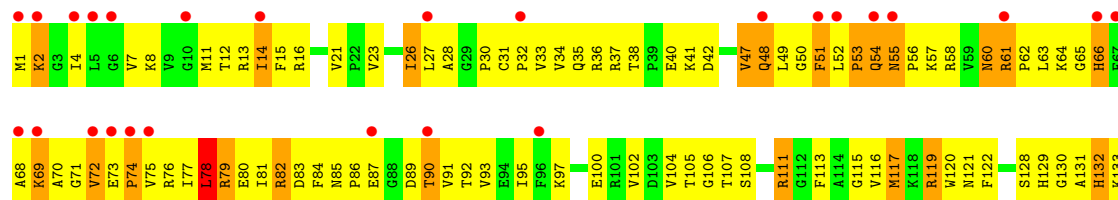
- Molecule 26: 50S ribosomal protein L2

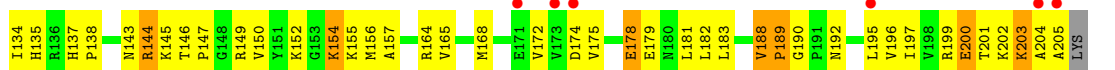
Chain DD:



- Molecule 27: 50S ribosomal protein L3

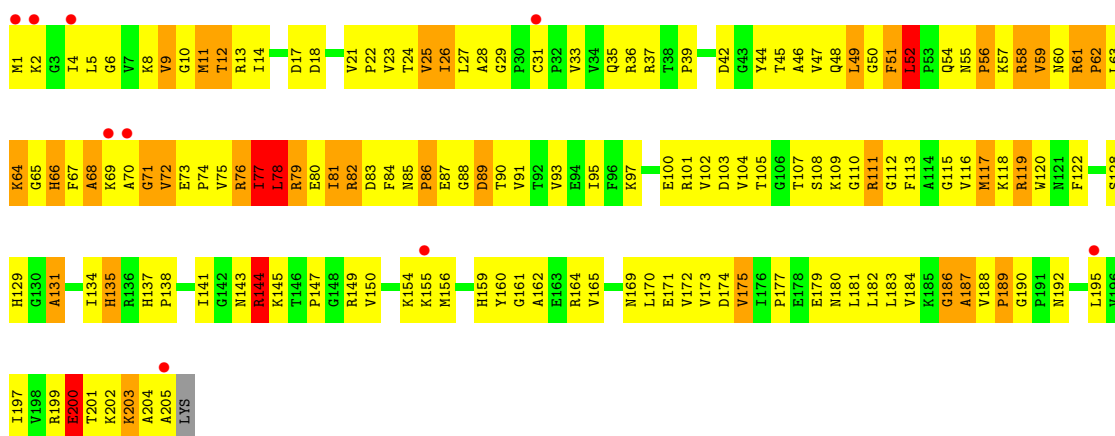
Chain BE:





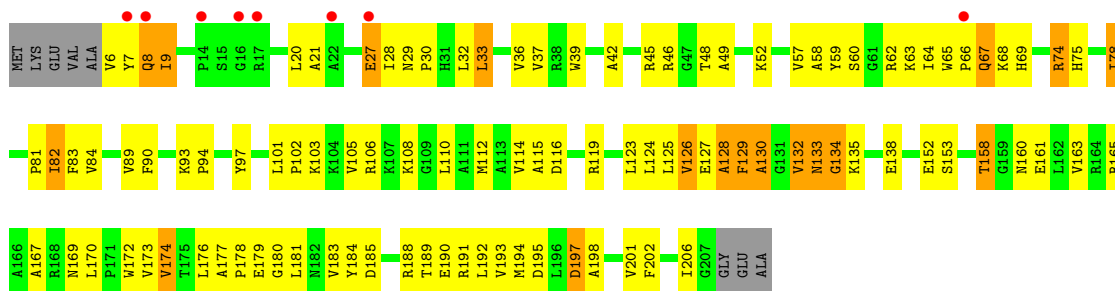
• Molecule 27: 50S ribosomal protein L3

Chain DE:



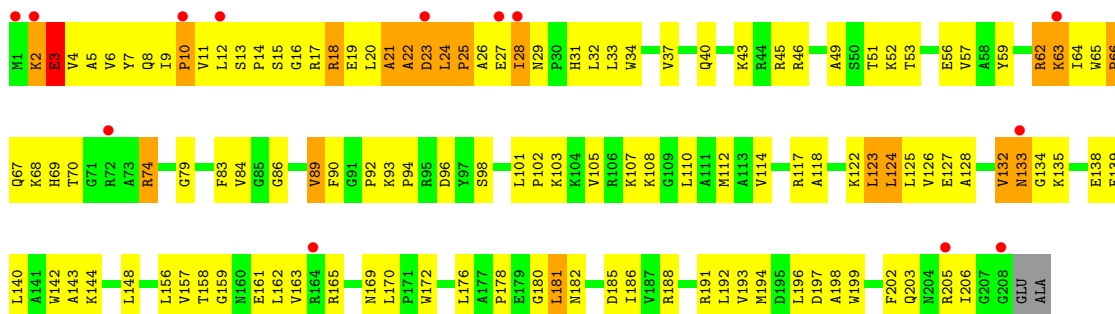
• Molecule 28: 50S ribosomal protein L4

Chain BF:



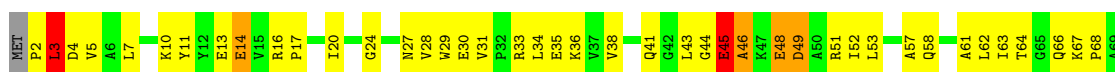
• Molecule 28: 50S ribosomal protein L4

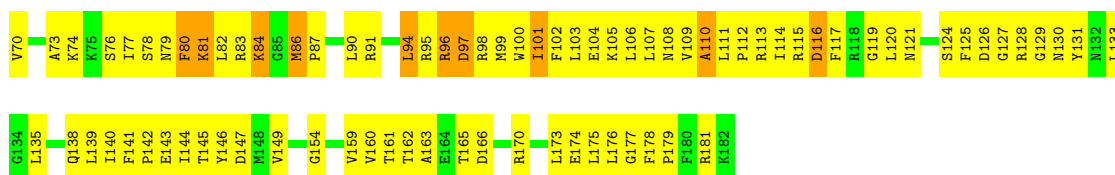
Chain DF:



• Molecule 29: 50S ribosomal protein L5

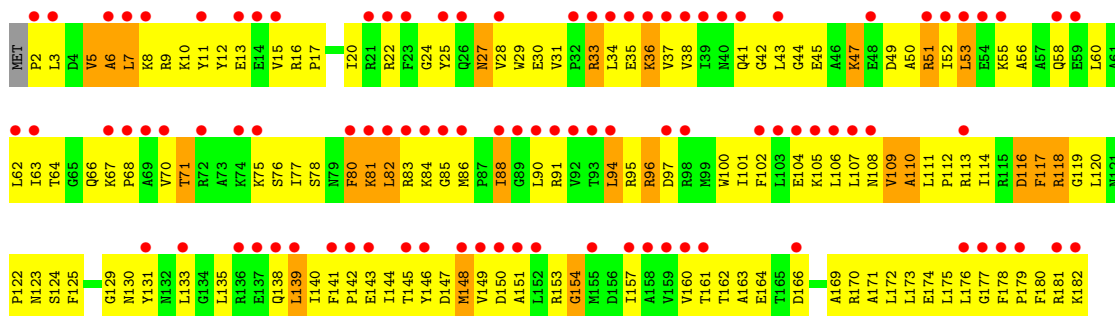
Chain BG:





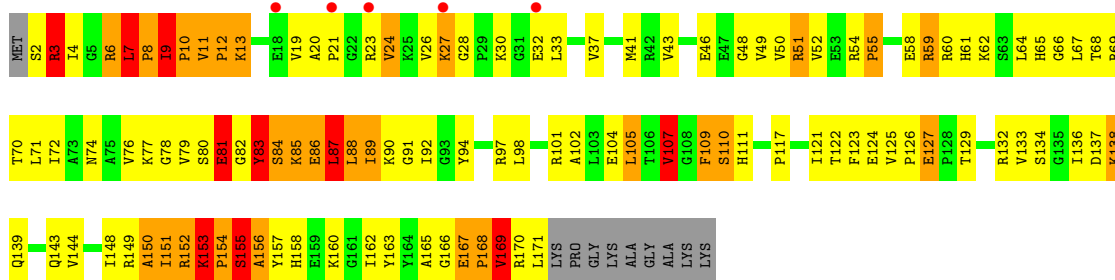
• Molecule 29: 50S ribosomal protein L5

Chain DG:



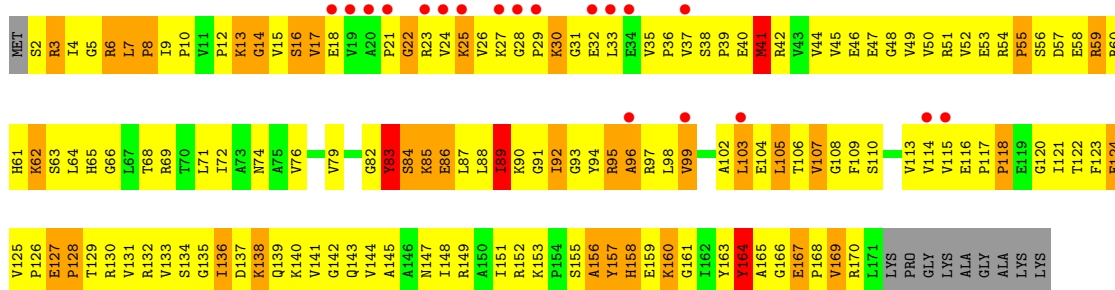
• Molecule 30: 50S ribosomal protein L6

Chain BH:



• Molecule 30: 50S ribosomal protein L6

Chain DH:

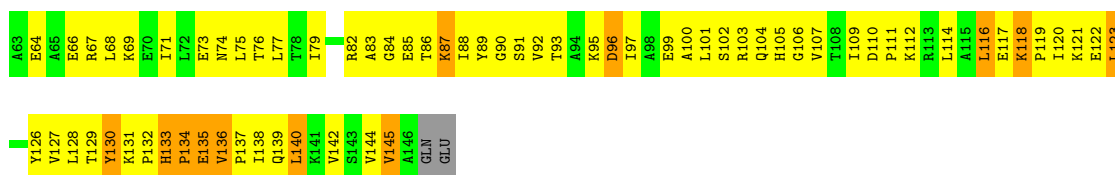


• Molecule 31: 50S ribosomal protein L9

Chain BK:

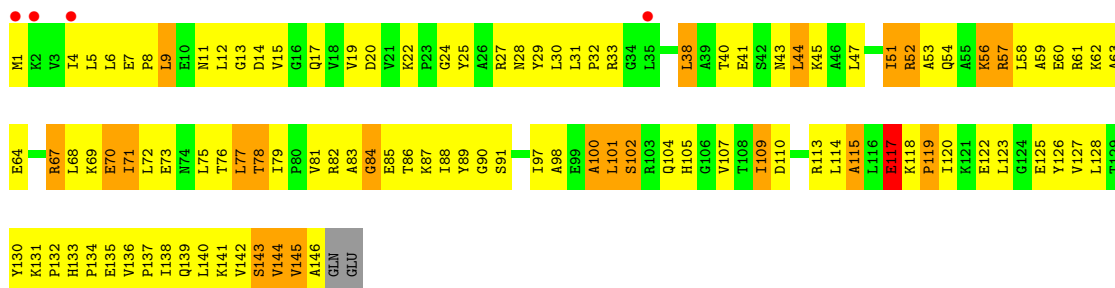






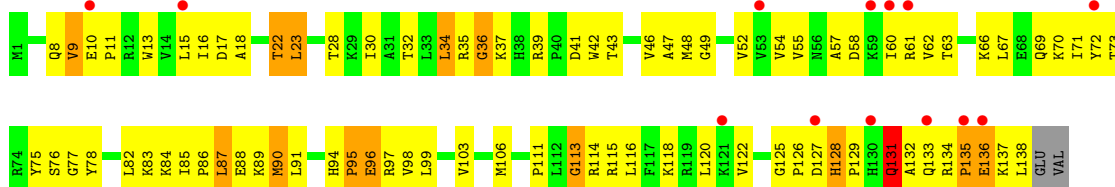
- Molecule 31: 50S ribosomal protein L9

Chain DK:



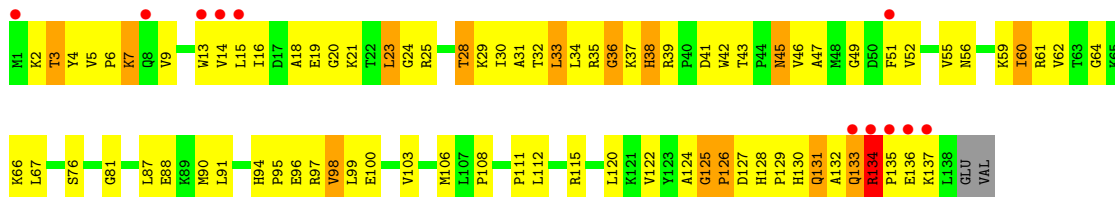
- Molecule 32: 50S ribosomal protein L13

Chain BM:



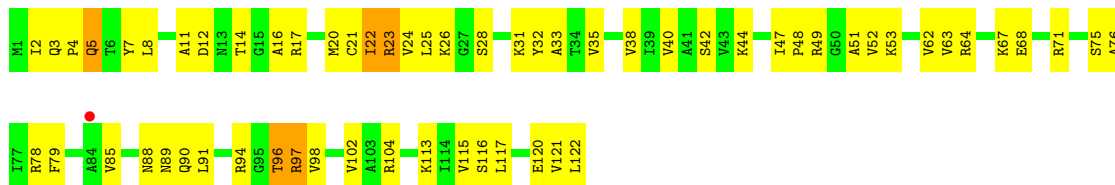
- Molecule 32: 50S ribosomal protein L13

Chain DM:



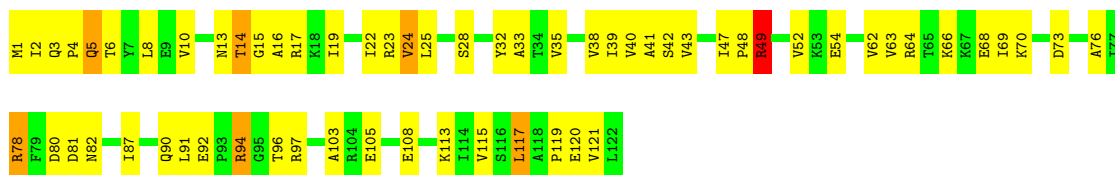
- Molecule 33: 50S ribosomal protein L14

Chain BN:



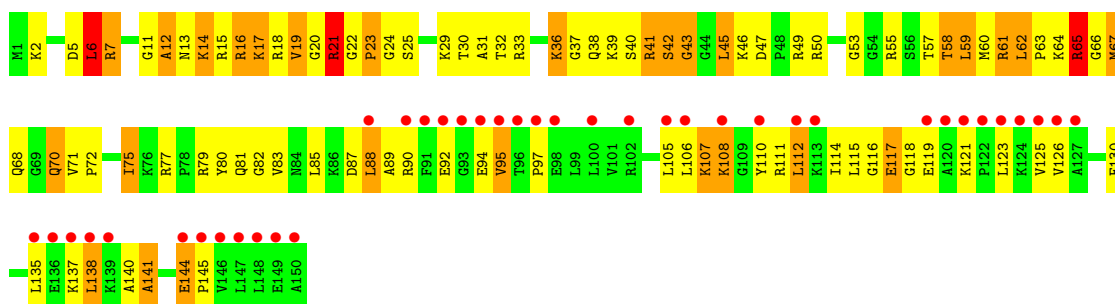
- Molecule 33: 50S ribosomal protein L14

Chain DN:



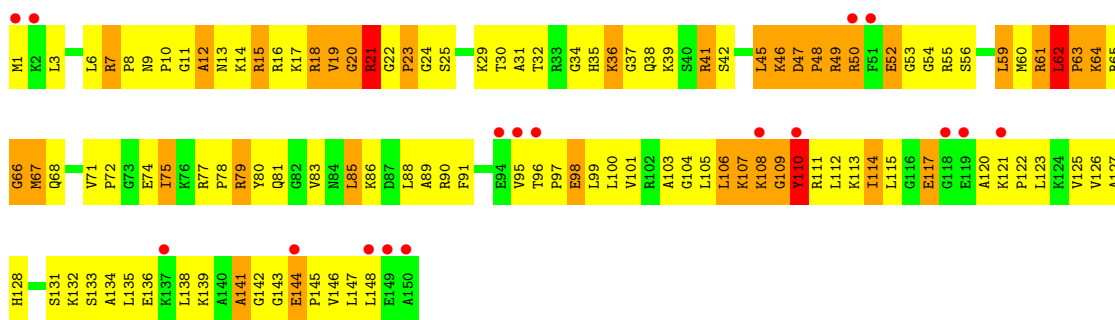
- Molecule 34: 50S ribosomal protein L15

Chain BO:



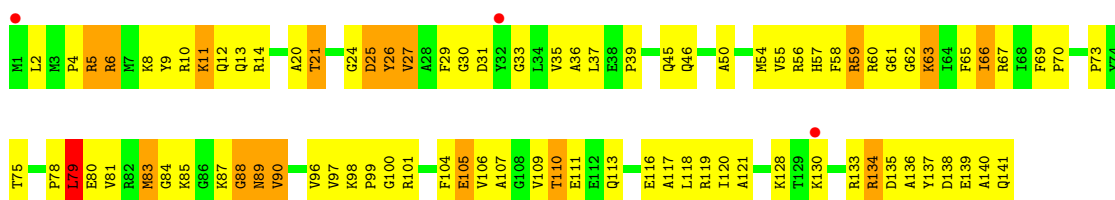
- Molecule 34: 50S ribosomal protein L15

Chain DO:



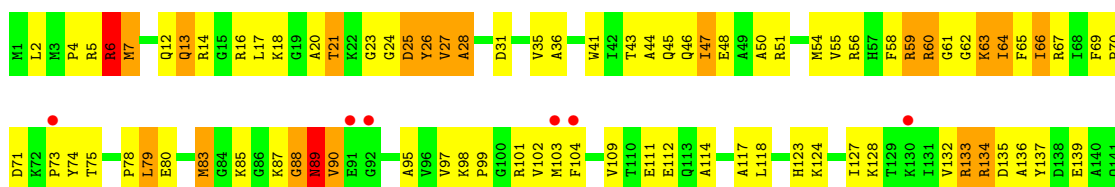
- Molecule 35: 50S ribosomal protein L16

Chain BP:



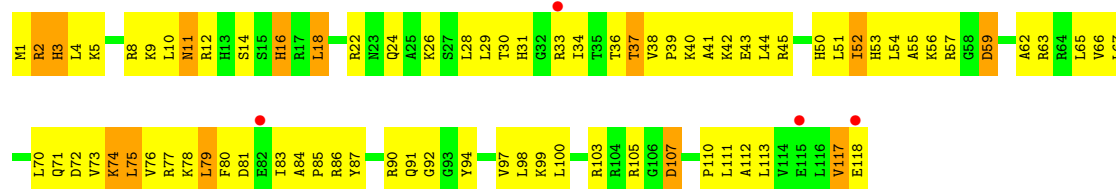
- Molecule 35: 50S ribosomal protein L16

Chain DP:



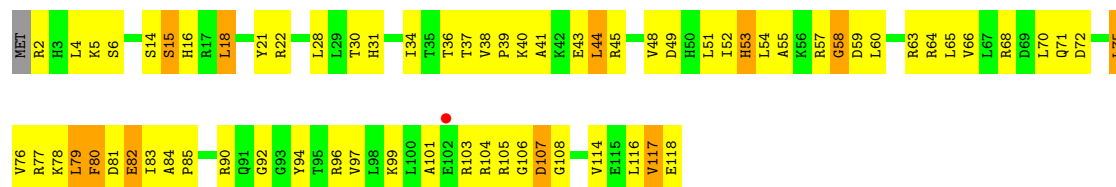
- Molecule 36: 50S ribosomal protein L17

Chain B0:



- Molecule 36: 50S ribosomal protein L17

Chain D0:



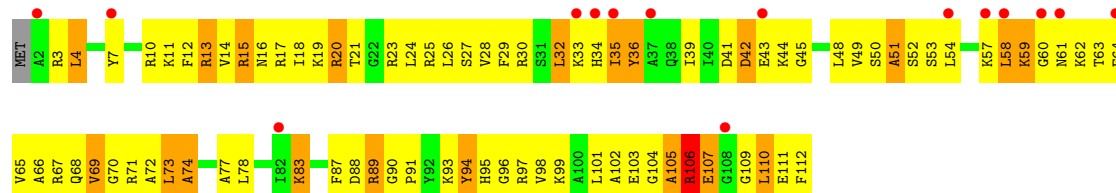
- Molecule 37: 50S ribosomal protein L18

Chain BQ:



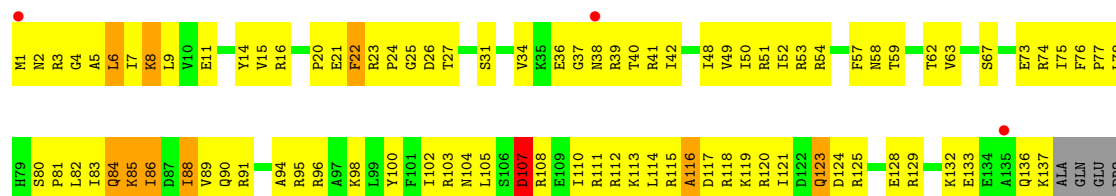
- Molecule 37: 50S ribosomal protein L18

Chain DQ:



- Molecule 38: 50S ribosomal protein L19

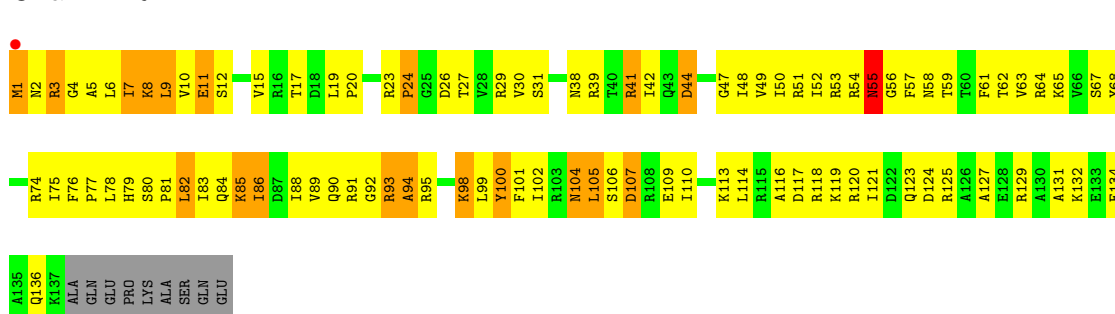
Chain BR:



LYS  
ALA  
SER  
GLN  
GLU

• Molecule 38: 50S ribosomal protein L19

Chain DR:



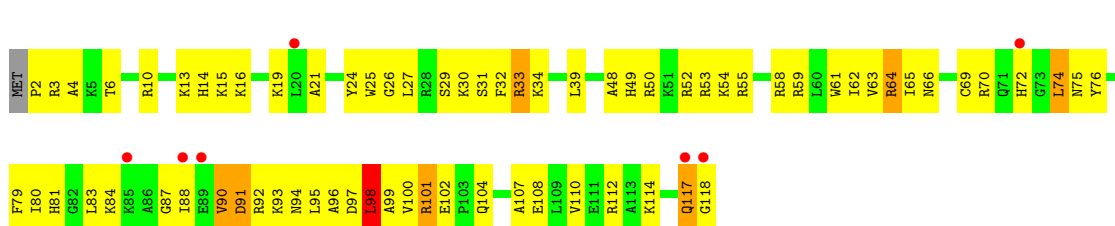
• Molecule 39: 50S ribosomal protein L20

Chain B1:



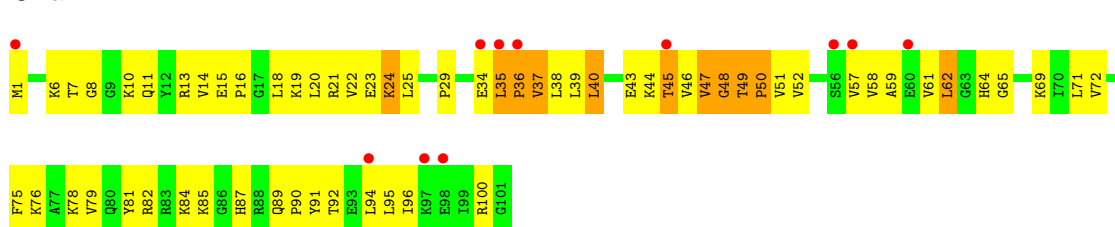
• Molecule 39: 50S ribosomal protein L20

Chain D1:



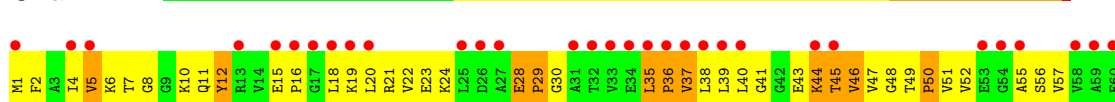
• Molecule 40: 50S ribosomal protein L21

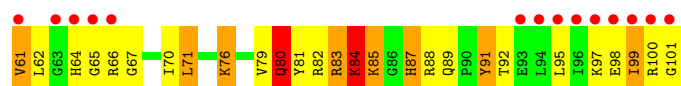
Chain B2:



• Molecule 40: 50S ribosomal protein L21

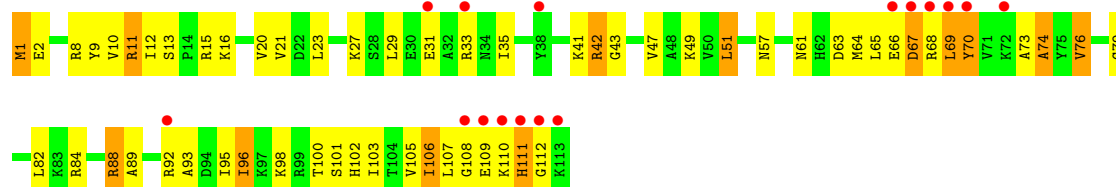
Chain D2:





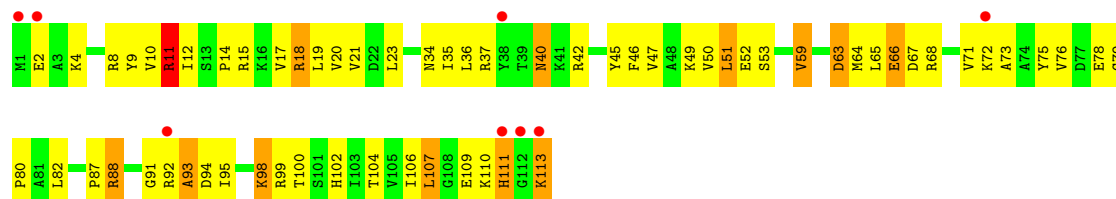
- Molecule 41: 50S ribosomal protein L22

Chain BS:



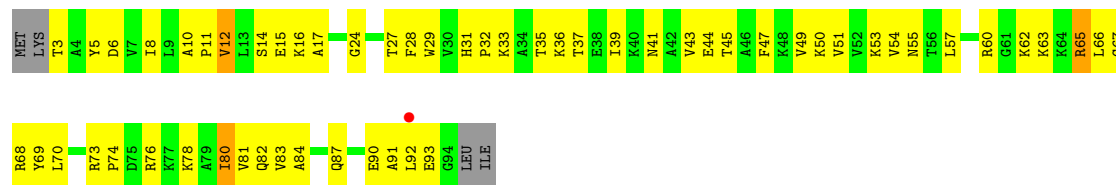
- Molecule 41: 50S ribosomal protein L22

Chain DS:



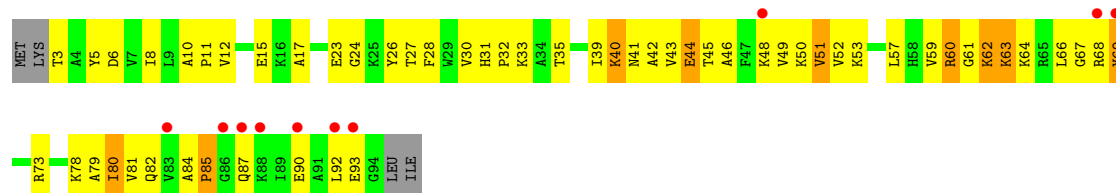
- Molecule 42: 50S ribosomal protein L23

Chain BT:



- Molecule 42: 50S ribosomal protein L23

Chain DT:

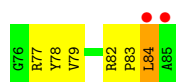


- Molecule 43: 50S ribosomal protein L24

Chain BU:

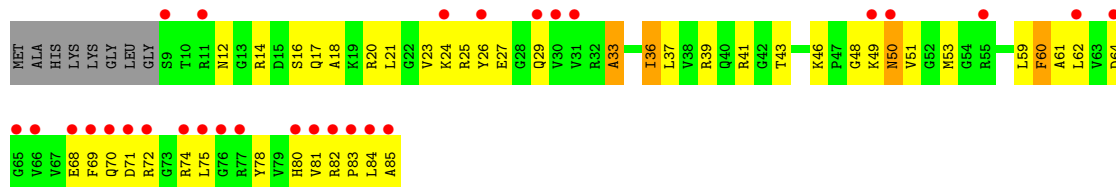






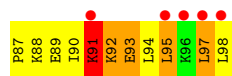
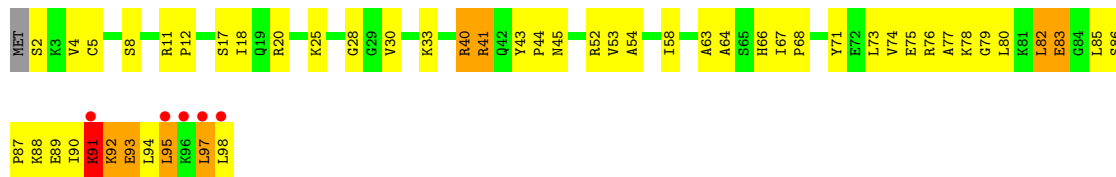
- Molecule 45: 50S ribosomal protein L27

Chain D3:



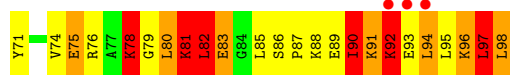
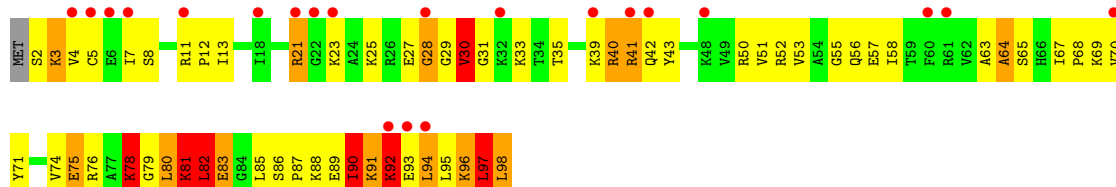
- Molecule 46: 50S ribosomal protein L28

Chain BZ:



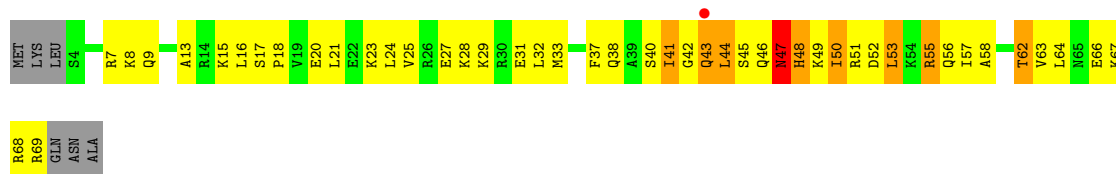
- Molecule 46: 50S ribosomal protein L28

Chain DZ:



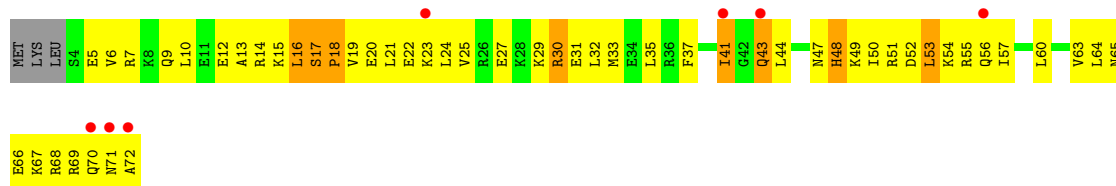
- Molecule 47: 50S ribosomal protein L29

Chain BW:



- Molecule 47: 50S ribosomal protein L29

Chain DW:



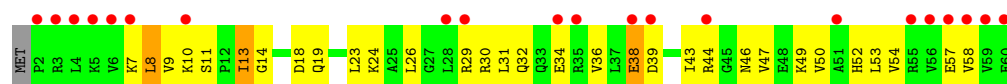
- Molecule 48: 50S ribosomal protein L30

Chain BX: 



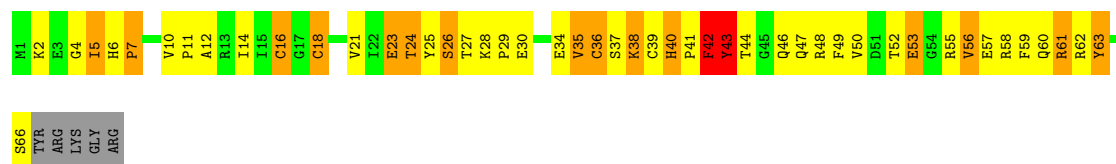
- Molecule 48: 50S ribosomal protein L30

Chain DX: 



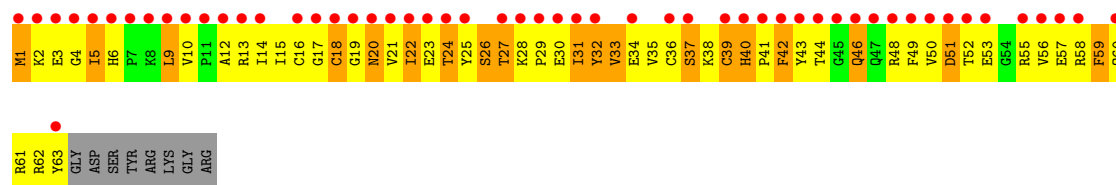
- Molecule 49: 50S ribosomal protein L31

Chain B4: 



- Molecule 49: 50S ribosomal protein L31

Chain D4: 



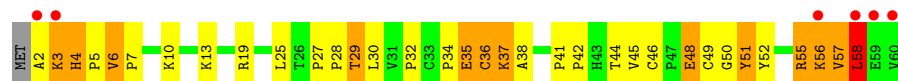
- Molecule 50: 50S ribosomal protein L32

Chain B5: 



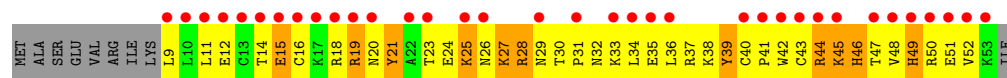
- Molecule 50: 50S ribosomal protein L32

Chain D5: 



- Molecule 51: 50S ribosomal protein L33

Chain B6: 





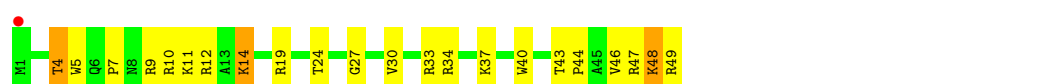
- Molecule 51: 50S ribosomal protein L33

Chain D6:



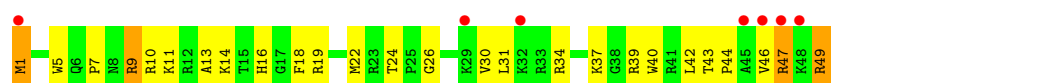
- Molecule 52: 50S ribosomal protein L34

Chain B7:



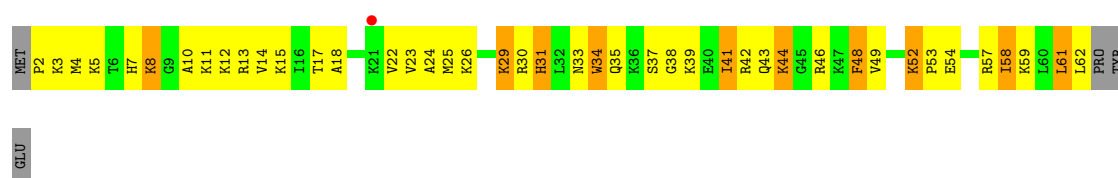
- Molecule 52: 50S ribosomal protein L34

Chain D7:



- Molecule 53: 50S ribosomal protein L35

Chain B8:



- Molecule 53: 50S ribosomal protein L35

Chain D8:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.27Å 448.54Å 615.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.07 – 3.30 224.27 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (173.07-3.30) 93.5 (224.27-3.30)	Depositor EDS
$R_{merge}$	0.42	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_987)	Depositor
R, $R_{free}$	0.202 , 0.254 0.298 , 0.333	Depositor DCC
$R_{free}$ test set	892 reflections (0.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	101.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 67.5	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 859965 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	292440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AA	0.31	2/36234 (0.0%)	0.62	7/56554 (0.0%)
1	CA	0.30	0/36237	0.60	4/56558 (0.0%)
2	AE	0.28	0/1959	0.47	0/2642
2	CE	0.25	0/1959	0.43	0/2642
3	AF	0.25	0/1629	0.41	0/2195
3	CF	0.26	0/1636	0.42	0/2205
4	AG	0.40	2/1733 (0.1%)	0.49	0/2318
4	CG	0.36	1/1733 (0.1%)	0.50	1/2318 (0.0%)
5	AH	0.29	0/1171	0.46	0/1576
5	CH	0.28	0/1171	0.47	0/1576
6	AI	0.28	0/856	0.43	0/1154
6	CI	0.27	0/856	0.43	0/1154
7	AJ	0.28	0/1276	0.42	0/1709
7	CJ	0.32	0/1276	0.45	0/1709
8	AK	0.28	0/1136	0.46	0/1527
8	CK	0.68	4/1136 (0.4%)	0.57	1/1527 (0.1%)
9	AL	0.39	1/1029 (0.1%)	0.49	0/1379
9	CL	0.31	0/1029	0.46	0/1379
10	AM	0.25	0/814	0.44	0/1095
10	CM	0.28	0/814	0.47	0/1095
11	AN	0.27	0/900	0.46	0/1213
11	CN	0.25	0/900	0.43	0/1213
12	AO	0.29	0/991	0.47	0/1327
12	CO	0.31	0/991	0.47	0/1327
13	AP	0.30	0/938	0.47	0/1258
13	CP	0.26	0/943	0.44	0/1265
14	AQ	0.31	0/501	0.45	0/664
14	CQ	0.31	0/501	0.54	1/664 (0.2%)
15	AR	0.27	0/745	0.42	0/992
15	CR	0.26	0/745	0.38	0/992
16	AS	0.32	0/721	0.47	0/970
16	CS	0.27	0/721	0.44	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AT	0.30	0/847	0.44	0/1131
17	CT	0.33	0/847	0.53	1/1131 (0.1%)
18	AU	0.26	0/596	0.44	0/790
18	CU	0.28	0/596	0.45	0/790
19	AV	0.34	0/680	0.58	0/915
19	CV	0.35	0/638	0.58	0/860
20	AW	0.41	0/765	0.54	0/1007
20	CW	0.27	0/765	0.44	0/1007
21	AX	0.28	0/221	0.43	0/288
21	CX	0.41	0/221	0.61	0/288
22	AC	0.47	2/1832 (0.1%)	0.82	5/2855 (0.2%)
22	CC	0.45	2/1832 (0.1%)	0.80	5/2855 (0.2%)
23	A1	0.33	0/94	0.62	0/144
23	C1	0.40	0/94	0.67	0/144
24	BA	0.43	1/70233 (0.0%)	0.77	36/109643 (0.0%)
24	DA	0.39	4/70167 (0.0%)	0.73	38/109541 (0.0%)
25	BB	0.37	0/2928	0.73	1/4568 (0.0%)
25	DB	0.34	0/2928	0.62	0/4568
26	BD	0.39	0/2165	0.57	0/2919
26	DD	0.59	5/2165 (0.2%)	0.55	0/2919
27	BE	0.32	0/1601	0.52	0/2160
27	DE	0.32	0/1601	0.55	0/2160
28	BF	0.32	0/1620	0.49	0/2194
28	DF	0.29	0/1662	0.49	0/2249
29	BG	0.30	0/1499	0.48	0/2016
29	DG	0.27	0/1499	0.46	0/2016
30	BH	0.38	0/1332	0.63	2/1802 (0.1%)
30	DH	0.25	0/1332	0.52	2/1802 (0.1%)
31	BK	0.28	0/1151	0.47	0/1558
31	DK	0.27	0/1151	0.48	0/1558
32	BM	0.28	0/1131	0.50	0/1525
32	DM	0.28	0/1131	0.46	0/1525
33	BN	0.30	0/943	0.48	0/1269
33	DN	0.30	0/943	0.47	0/1269
34	BO	0.39	0/1162	0.64	0/1544
34	DO	0.38	0/1162	0.57	0/1544
35	BP	0.35	0/1143	0.53	0/1527
35	DP	0.41	2/1143 (0.2%)	0.82	3/1527 (0.2%)
36	B0	0.35	0/982	0.53	1/1312 (0.1%)
36	D0	0.30	0/974	0.50	0/1302
37	BQ	0.32	0/892	0.54	0/1187
37	DQ	0.39	0/892	0.51	0/1187
38	BR	0.31	0/1155	0.47	0/1542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DR	0.34	0/1155	0.51	0/1542
39	B1	0.36	0/982	0.52	0/1306
39	D1	0.31	0/982	0.46	0/1306
40	B2	0.32	0/790	0.52	0/1057
40	D2	0.35	0/790	0.53	0/1057
41	BS	0.31	0/911	0.50	0/1220
41	DS	0.30	0/911	0.50	0/1220
42	BT	0.42	0/739	0.52	0/993
42	DT	0.36	0/739	0.50	0/993
43	BU	0.37	0/798	0.51	0/1064
43	DU	0.33	0/798	0.50	0/1064
44	BV	0.32	0/1427	0.50	0/1935
44	DV	0.27	0/1460	0.45	0/1982
45	B3	0.33	0/615	0.50	0/819
45	D3	0.32	0/621	0.48	0/827
46	BZ	0.37	0/770	0.56	0/1022
46	DZ	0.33	0/770	0.55	0/1022
47	BW	0.39	0/560	0.55	0/741
47	DW	0.29	0/583	0.48	0/771
48	BX	0.31	0/474	0.48	0/635
48	DX	0.26	0/474	0.45	0/635
49	B4	0.81	3/545 (0.6%)	0.65	2/733 (0.3%)
49	D4	0.44	1/527 (0.2%)	0.55	0/709
50	B5	0.33	0/473	0.54	0/639
50	D5	0.29	0/473	0.47	0/639
51	B6	0.44	0/396	0.70	2/529 (0.4%)
51	D6	0.44	0/396	0.62	0/529
52	B7	0.43	0/438	0.68	0/575
52	D7	0.31	0/438	0.53	0/575
53	B8	0.40	0/494	0.58	0/649
53	D8	0.49	0/494	0.84	3/649 (0.5%)
All	All	0.37	30/316019 (0.0%)	0.66	115/472742 (0.0%)

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	DA	2377	A	N9-C4	20.50	1.50	1.37
26	DD	104	TYR	CD1-CE1	13.75	1.59	1.39
8	CK	94	TYR	CD2-CE2	-13.18	1.19	1.39
49	B4	16	CYS	CB-SG	-12.84	1.60	1.82
26	DD	104	TYR	CD2-CE2	12.77	1.58	1.39

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	DA	2377	A	C2-N3-C4	28.76	124.98	110.60
24	BA	2751	G	N1-C6-O6	20.94	132.47	119.90
24	DA	2377	A	C8-N9-C4	-20.26	97.69	105.80
35	DP	6	ARG	NE-CZ-NH1	19.44	130.02	120.30
22	CC	17(A)	C	N3-C4-C5	-18.15	114.64	121.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32369	0	16335	1780	1
1	CA	32372	0	16338	2038	3
2	AE	1924	0	1975	321	0
2	CE	1924	0	1975	349	0
3	AF	1605	0	1668	210	0
3	CF	1612	0	1677	235	0
4	AG	1703	0	1764	273	0
4	CG	1703	0	1763	334	0
5	AH	1155	0	1213	125	0
5	CH	1155	0	1212	196	0
6	AI	843	0	857	100	0
6	CI	843	0	857	107	0
7	AJ	1257	0	1296	153	0
7	CJ	1257	0	1296	176	0
8	AK	1116	0	1177	120	0
8	CK	1116	0	1176	177	0
9	AL	1010	0	1037	267	0
9	CL	1010	0	1037	291	0
10	AM	801	0	849	149	0
10	CM	801	0	849	238	1
11	AN	885	0	904	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CN	885	0	904	87	0
12	AO	975	0	1062	108	0
12	CO	975	0	1062	91	0
13	AP	928	0	987	157	0
13	CP	933	0	992	195	0
14	AQ	492	0	529	74	0
14	CQ	492	0	530	133	0
15	AR	734	0	771	54	0
15	CR	734	0	771	76	0
16	AS	705	0	725	116	0
16	CS	705	0	725	94	0
17	AT	834	0	904	96	0
17	CT	834	0	904	88	0
18	AU	591	0	662	60	0
18	CU	591	0	662	69	0
19	AV	665	0	686	181	0
19	CV	624	0	636	250	0
20	AW	763	0	861	140	0
20	CW	763	0	861	87	0
21	AX	217	0	234	26	0
21	CX	217	0	234	60	0
22	AC	1640	0	836	47	0
22	CC	1640	0	836	67	0
23	A1	85	0	43	1	0
23	C1	85	0	43	5	0
24	BA	62707	0	31611	2736	0
24	DA	62647	0	31583	2861	2
25	BB	2617	0	1328	127	0
25	DB	2617	0	1328	167	0
26	BD	2115	0	2195	286	0
26	DD	2115	0	2192	237	0
27	BE	1568	0	1634	180	0
27	DE	1568	0	1634	297	0
28	BF	1585	0	1632	147	0
28	DF	1627	0	1680	173	0
29	BG	1474	0	1535	213	0
29	DG	1474	0	1535	220	0
30	BH	1307	0	1382	220	0
30	DH	1307	0	1382	277	0
31	BK	1136	0	1223	174	1
31	DK	1136	0	1223	158	0
32	BM	1104	0	1180	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	DM	1104	0	1180	132	0
33	BN	933	0	996	66	0
33	DN	933	0	996	84	0
34	BO	1145	0	1228	187	0
34	DO	1145	0	1228	239	0
35	BP	1122	0	1179	127	0
35	DP	1122	0	1178	151	0
36	B0	968	0	1033	102	0
36	D0	960	0	1021	95	0
37	BQ	882	0	943	149	0
37	DQ	882	0	943	207	0
38	BR	1141	0	1202	135	0
38	DR	1141	0	1202	123	0
39	B1	964	0	1022	114	0
39	D1	964	0	1021	140	0
40	B2	779	0	852	103	0
40	D2	779	0	851	175	0
41	BS	900	0	964	66	0
41	DS	900	0	964	75	0
42	BT	725	0	778	72	0
42	DT	725	0	778	86	0
43	BU	785	0	878	136	0
43	DU	785	0	878	153	0
44	BV	1397	0	1430	209	0
44	DV	1428	0	1454	255	0
45	B3	607	0	628	43	0
45	D3	613	0	633	59	0
46	BZ	763	0	848	91	0
46	DZ	763	0	848	93	0
47	BW	558	0	610	62	0
47	DW	581	0	629	71	0
48	BX	469	0	518	31	0
48	DX	469	0	518	39	0
49	B4	533	0	522	132	0
49	D4	515	0	510	157	0
50	B5	459	0	480	67	0
50	D5	459	0	476	46	0
51	B6	389	0	404	142	0
51	D6	389	0	404	166	0
52	B7	430	0	480	55	0
52	D7	430	0	479	73	0
53	B8	488	0	560	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	D8	488	0	559	138	0
54	A1	1	0	0	0	0
54	AA	232	0	0	0	0
54	AC	9	0	0	0	0
54	AG	2	0	0	0	0
54	AH	2	0	0	0	0
54	AJ	1	0	0	0	0
54	AQ	2	0	0	0	0
54	AR	1	0	0	0	0
54	AS	1	0	0	0	0
54	B1	2	0	0	0	0
54	B2	1	0	0	0	0
54	B3	2	0	0	0	0
54	B5	2	0	0	0	0
54	B6	1	0	0	0	0
54	B7	3	0	0	0	0
54	B8	1	0	0	0	0
54	BA	627	0	0	0	0
54	BB	17	0	0	0	0
54	BE	5	0	0	0	0
54	BF	2	0	0	0	0
54	BO	3	0	0	0	0
54	BP	1	0	0	0	0
54	BU	2	0	0	0	0
54	BZ	1	0	0	0	0
54	CA	204	0	0	0	0
54	CC	8	0	0	0	0
54	CG	2	0	0	0	0
54	CH	1	0	0	0	0
54	CS	1	0	0	0	0
54	D1	1	0	0	0	0
54	D5	1	0	0	0	0
54	DA	525	0	0	0	0
54	DB	14	0	0	0	0
54	DD	1	0	0	0	0
54	DE	3	0	0	0	0
54	DP	1	0	0	0	0
54	DR	1	0	0	0	0
54	DU	1	0	0	0	0
54	DZ	2	0	0	0	0
55	AA	32	1	20	4	0
55	CA	32	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0
56	CG	1	0	0	2	0
56	CQ	1	0	0	0	0
All	All	292439	1	197339	20528	4

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 43.

The worst 5 of 20528 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:DA:1600:C:C2'	52:D7:49:ARG:HE	0.98	1.56
4:CG:31:CYS:SG	4:CG:33:MET:HE2	1.43	1.53
1:CA:598:U:O3'	8:CK:94:TYR:CE2	1.65	1.48
19:CV:70:LYS:CE	19:CV:73:GLU:HG3	1.44	1.48
24:DA:1600:C:H2'	52:D7:49:ARG:NE	1.12	1.43

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:BK:89:TYR:O	1:CA:357:G:O2'[4.555]	2.01	0.19
1:CA:86:U:O2'	24:DA:276:A:OP2[3.545]	2.09	0.11
1:AA:1175:G:O2'	10:CM:80:LYS:NZ[4.555]	2.18	0.02
1:CA:84:U:O2'	24:DA:273:G:OP1[3.545]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AE	235/256 (92%)	162 (69%)	47 (20%)	26 (11%)	<b>1</b> <b>5</b>
2	CE	235/256 (92%)	166 (71%)	44 (19%)	25 (11%)	<b>1</b> <b>6</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AF	203/239 (85%)	150 (74%)	36 (18%)	17 (8%)	1	12
3	CF	204/239 (85%)	138 (68%)	51 (25%)	15 (7%)	2	15
4	AG	206/208 (99%)	157 (76%)	35 (17%)	14 (7%)	2	18
4	CG	206/208 (99%)	140 (68%)	44 (21%)	22 (11%)	1	6
5	AH	149/162 (92%)	127 (85%)	17 (11%)	5 (3%)	6	42
5	CH	149/162 (92%)	112 (75%)	31 (21%)	6 (4%)	5	36
6	AI	99/101 (98%)	81 (82%)	14 (14%)	4 (4%)	5	36
6	CI	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	2	22
7	AJ	153/156 (98%)	126 (82%)	17 (11%)	10 (6%)	2	19
7	CJ	153/156 (98%)	112 (73%)	33 (22%)	8 (5%)	3	27
8	AK	136/138 (99%)	103 (76%)	27 (20%)	6 (4%)	4	32
8	CK	136/138 (99%)	114 (84%)	15 (11%)	7 (5%)	3	28
9	AL	125/128 (98%)	93 (74%)	26 (21%)	6 (5%)	4	30
9	CL	125/128 (98%)	93 (74%)	21 (17%)	11 (9%)	1	11
10	AM	97/105 (92%)	75 (77%)	17 (18%)	5 (5%)	3	27
10	CM	97/105 (92%)	69 (71%)	23 (24%)	5 (5%)	3	27
11	AN	117/129 (91%)	88 (75%)	20 (17%)	9 (8%)	1	14
11	CN	117/129 (91%)	94 (80%)	17 (14%)	6 (5%)	3	28
12	AO	123/128 (96%)	96 (78%)	17 (14%)	10 (8%)	1	13
12	CO	123/128 (96%)	91 (74%)	23 (19%)	9 (7%)	2	16
13	AP	114/126 (90%)	87 (76%)	15 (13%)	12 (10%)	1	6
13	CP	115/126 (91%)	82 (71%)	19 (16%)	14 (12%)	1	4
14	AQ	58/61 (95%)	43 (74%)	11 (19%)	4 (7%)	2	17
14	CQ	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	1	7
15	AR	86/89 (97%)	71 (83%)	9 (10%)	6 (7%)	2	17
15	CR	86/89 (97%)	72 (84%)	13 (15%)	1 (1%)	19	71
16	AS	82/88 (93%)	61 (74%)	18 (22%)	3 (4%)	5	39
16	CS	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	2	16
17	AT	98/105 (93%)	78 (80%)	16 (16%)	4 (4%)	4	35
17	CT	98/105 (93%)	76 (78%)	15 (15%)	7 (7%)	2	17
18	AU	70/88 (80%)	58 (83%)	7 (10%)	5 (7%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CU	70/88 (80%)	53 (76%)	13 (19%)	4 (6%)	3	24
19	AV	81/93 (87%)	53 (65%)	19 (24%)	9 (11%)	1	5
19	CV	76/93 (82%)	48 (63%)	19 (25%)	9 (12%)	1	4
20	AW	97/106 (92%)	67 (69%)	17 (18%)	13 (13%)	0	3
20	CW	97/106 (92%)	64 (66%)	22 (23%)	11 (11%)	1	5
21	AX	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1	11
21	CX	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	1
26	BD	270/276 (98%)	227 (84%)	31 (12%)	12 (4%)	4	32
26	DD	270/276 (98%)	223 (83%)	35 (13%)	12 (4%)	4	32
27	BE	203/206 (98%)	151 (74%)	35 (17%)	17 (8%)	1	12
27	DE	203/206 (98%)	133 (66%)	40 (20%)	30 (15%)	0	2
28	BF	200/210 (95%)	171 (86%)	21 (10%)	8 (4%)	5	36
28	DF	206/210 (98%)	155 (75%)	33 (16%)	18 (9%)	1	11
29	BG	179/182 (98%)	132 (74%)	32 (18%)	15 (8%)	1	12
29	DG	179/182 (98%)	128 (72%)	35 (20%)	16 (9%)	1	10
30	BH	168/180 (93%)	107 (64%)	30 (18%)	31 (18%)	0	1
30	DH	168/180 (93%)	103 (61%)	30 (18%)	35 (21%)	0	1
31	BK	144/148 (97%)	102 (71%)	28 (19%)	14 (10%)	1	8
31	DK	144/148 (97%)	98 (68%)	31 (22%)	15 (10%)	1	7
32	BM	136/140 (97%)	101 (74%)	24 (18%)	11 (8%)	1	13
32	DM	136/140 (97%)	103 (76%)	22 (16%)	11 (8%)	1	13
33	BN	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	14	62
33	DN	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	9	51
34	BO	148/150 (99%)	99 (67%)	27 (18%)	22 (15%)	0	2
34	DO	148/150 (99%)	85 (57%)	31 (21%)	32 (22%)	0	1
35	BP	139/141 (99%)	104 (75%)	21 (15%)	14 (10%)	1	8
35	DP	139/141 (99%)	100 (72%)	24 (17%)	15 (11%)	1	6
36	B0	116/118 (98%)	91 (78%)	14 (12%)	11 (10%)	1	9
36	D0	115/118 (98%)	85 (74%)	21 (18%)	9 (8%)	1	14
37	BQ	109/112 (97%)	82 (75%)	15 (14%)	12 (11%)	1	6
37	DQ	109/112 (97%)	74 (68%)	22 (20%)	13 (12%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BR	135/146 (92%)	101 (75%)	25 (18%)	9 (7%)	2	18
38	DR	135/146 (92%)	105 (78%)	19 (14%)	11 (8%)	1	13
39	B1	115/118 (98%)	92 (80%)	17 (15%)	6 (5%)	3	27
39	D1	115/118 (98%)	89 (77%)	20 (17%)	6 (5%)	3	27
40	B2	99/101 (98%)	74 (75%)	17 (17%)	8 (8%)	1	13
40	D2	99/101 (98%)	68 (69%)	16 (16%)	15 (15%)	0	1
41	BS	111/113 (98%)	91 (82%)	14 (13%)	6 (5%)	3	26
41	DS	111/113 (98%)	86 (78%)	17 (15%)	8 (7%)	2	16
42	BT	90/96 (94%)	75 (83%)	13 (14%)	2 (2%)	10	55
42	DT	90/96 (94%)	67 (74%)	13 (14%)	10 (11%)	1	5
43	BU	100/110 (91%)	64 (64%)	18 (18%)	18 (18%)	0	1
43	DU	100/110 (91%)	57 (57%)	18 (18%)	25 (25%)	0	0
44	BV	173/206 (84%)	105 (61%)	47 (27%)	21 (12%)	1	4
44	DV	177/206 (86%)	110 (62%)	37 (21%)	30 (17%)	0	1
45	B3	74/85 (87%)	57 (77%)	15 (20%)	2 (3%)	8	49
45	D3	75/85 (88%)	63 (84%)	9 (12%)	3 (4%)	5	36
46	BZ	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	2	20
46	DZ	95/98 (97%)	69 (73%)	12 (13%)	14 (15%)	0	2
47	BW	64/72 (89%)	54 (84%)	5 (8%)	5 (8%)	1	14
47	DW	67/72 (93%)	51 (76%)	9 (13%)	7 (10%)	1	7
48	BX	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	13	61
48	DX	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	6	41
49	B4	64/71 (90%)	33 (52%)	21 (33%)	10 (16%)	0	1
49	D4	61/71 (86%)	22 (36%)	23 (38%)	16 (26%)	0	0
50	B5	57/60 (95%)	42 (74%)	10 (18%)	5 (9%)	1	11
50	D5	57/60 (95%)	41 (72%)	6 (10%)	10 (18%)	0	1
51	B6	43/54 (80%)	24 (56%)	12 (28%)	7 (16%)	0	1
51	D6	43/54 (80%)	24 (56%)	13 (30%)	6 (14%)	0	2
52	B7	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	11	56
52	D7	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
53	B8	59/65 (91%)	44 (75%)	10 (17%)	5 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	D8	59/65 (91%)	38 (64%)	8 (14%)	13 (22%)	0	0
All	All	11341/12044 (94%)	8378 (74%)	1945 (17%)	1018 (9%)	1	10

5 of 1018 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AE	135	GLN
2	AE	136	VAL
2	AE	194	PRO
2	AE	195	ASP
2	AE	214	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AE	205/220 (93%)	182 (89%)	23 (11%)	9	37
2	CE	205/220 (93%)	176 (86%)	29 (14%)	5	24
3	AF	159/188 (85%)	147 (92%)	12 (8%)	19	62
3	CF	160/188 (85%)	146 (91%)	14 (9%)	14	52
4	AG	180/180 (100%)	166 (92%)	14 (8%)	18	60
4	CG	180/180 (100%)	161 (89%)	19 (11%)	10	40
5	AH	116/123 (94%)	105 (90%)	11 (10%)	12	46
5	CH	116/123 (94%)	104 (90%)	12 (10%)	10	41
6	AI	90/90 (100%)	85 (94%)	5 (6%)	30	75
6	CI	90/90 (100%)	81 (90%)	9 (10%)	11	43
7	AJ	126/127 (99%)	118 (94%)	8 (6%)	25	70
7	CJ	126/127 (99%)	116 (92%)	10 (8%)	18	59
8	AK	119/119 (100%)	108 (91%)	11 (9%)	13	48
8	CK	119/119 (100%)	108 (91%)	11 (9%)	13	48
9	AL	98/99 (99%)	86 (88%)	12 (12%)	7	32
9	CL	98/99 (99%)	79 (81%)	19 (19%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AM	89/92 (97%)	82 (92%)	7 (8%)	18	59
10	CM	89/92 (97%)	82 (92%)	7 (8%)	18	59
11	AN	90/99 (91%)	86 (96%)	4 (4%)	39	81
11	CN	90/99 (91%)	85 (94%)	5 (6%)	30	75
12	AO	104/107 (97%)	97 (93%)	7 (7%)	23	67
12	CO	104/107 (97%)	97 (93%)	7 (7%)	23	67
13	AP	94/101 (93%)	89 (95%)	5 (5%)	32	76
13	CP	94/101 (93%)	78 (83%)	16 (17%)	3	15
14	AQ	49/50 (98%)	44 (90%)	5 (10%)	11	42
14	CQ	49/50 (98%)	45 (92%)	4 (8%)	17	57
15	AR	79/80 (99%)	73 (92%)	6 (8%)	19	61
15	CR	79/80 (99%)	76 (96%)	3 (4%)	44	84
16	AS	72/74 (97%)	62 (86%)	10 (14%)	5	25
16	CS	72/74 (97%)	68 (94%)	4 (6%)	30	75
17	AT	95/97 (98%)	90 (95%)	5 (5%)	32	76
17	CT	95/97 (98%)	92 (97%)	3 (3%)	51	88
18	AU	63/77 (82%)	60 (95%)	3 (5%)	35	79
18	CU	63/77 (82%)	59 (94%)	4 (6%)	25	70
19	AV	72/80 (90%)	63 (88%)	9 (12%)	7	31
19	CV	67/80 (84%)	56 (84%)	11 (16%)	3	16
20	AW	76/82 (93%)	70 (92%)	6 (8%)	18	59
20	CW	76/82 (93%)	69 (91%)	7 (9%)	13	48
21	AX	20/22 (91%)	20 (100%)	0	100	100
21	CX	20/22 (91%)	18 (90%)	2 (10%)	11	43
26	BD	214/218 (98%)	192 (90%)	22 (10%)	10	41
26	DD	214/218 (98%)	197 (92%)	17 (8%)	18	59
27	BE	165/166 (99%)	149 (90%)	16 (10%)	12	45
27	DE	165/166 (99%)	150 (91%)	15 (9%)	14	49
28	BF	161/166 (97%)	150 (93%)	11 (7%)	22	67
28	DF	165/166 (99%)	156 (94%)	9 (6%)	30	75
29	BG	155/156 (99%)	145 (94%)	10 (6%)	24	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	DG	155/156 (99%)	141 (91%)	14 (9%)	14	50
30	BH	142/148 (96%)	119 (84%)	23 (16%)	3	17
30	DH	142/148 (96%)	128 (90%)	14 (10%)	11	44
31	BK	122/124 (98%)	110 (90%)	12 (10%)	12	45
31	DK	122/124 (98%)	109 (89%)	13 (11%)	10	39
32	BM	117/119 (98%)	113 (97%)	4 (3%)	49	87
32	DM	117/119 (98%)	109 (93%)	8 (7%)	22	67
33	BN	100/100 (100%)	95 (95%)	5 (5%)	34	78
33	DN	100/100 (100%)	95 (95%)	5 (5%)	34	78
34	BO	116/116 (100%)	101 (87%)	15 (13%)	6	29
34	DO	116/116 (100%)	102 (88%)	14 (12%)	7	33
35	BP	111/111 (100%)	102 (92%)	9 (8%)	17	58
35	DP	111/111 (100%)	102 (92%)	9 (8%)	17	58
36	B0	101/101 (100%)	94 (93%)	7 (7%)	22	67
36	D0	100/101 (99%)	95 (95%)	5 (5%)	34	78
37	BQ	87/88 (99%)	82 (94%)	5 (6%)	29	74
37	DQ	87/88 (99%)	78 (90%)	9 (10%)	10	41
38	BR	120/127 (94%)	111 (92%)	9 (8%)	19	62
38	DR	120/127 (94%)	107 (89%)	13 (11%)	9	39
39	B1	93/94 (99%)	87 (94%)	6 (6%)	24	69
39	D1	93/94 (99%)	88 (95%)	5 (5%)	31	76
40	B2	82/82 (100%)	75 (92%)	7 (8%)	15	54
40	D2	82/82 (100%)	71 (87%)	11 (13%)	6	27
41	BS	92/92 (100%)	82 (89%)	10 (11%)	9	38
41	DS	92/92 (100%)	82 (89%)	10 (11%)	9	38
42	BT	74/78 (95%)	69 (93%)	5 (7%)	22	67
42	DT	74/78 (95%)	69 (93%)	5 (7%)	22	67
43	BU	85/91 (93%)	70 (82%)	15 (18%)	3	13
43	DU	85/91 (93%)	73 (86%)	12 (14%)	5	24
44	BV	154/179 (86%)	135 (88%)	19 (12%)	7	32
44	DV	158/179 (88%)	144 (91%)	14 (9%)	14	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	B3	61/67 (91%)	58 (95%)	3 (5%)	35	78
45	D3	62/67 (92%)	57 (92%)	5 (8%)	17	58
46	BZ	82/83 (99%)	77 (94%)	5 (6%)	26	71
46	DZ	82/83 (99%)	65 (79%)	17 (21%)	2	8
47	BW	62/67 (92%)	55 (89%)	7 (11%)	9	36
47	DW	64/67 (96%)	62 (97%)	2 (3%)	52	88
48	BX	51/52 (98%)	47 (92%)	4 (8%)	18	60
48	DX	51/52 (98%)	48 (94%)	3 (6%)	28	73
49	B4	59/63 (94%)	51 (86%)	8 (14%)	5	26
49	D4	57/63 (90%)	51 (90%)	6 (10%)	10	40
50	B5	51/52 (98%)	44 (86%)	7 (14%)	5	26
50	D5	51/52 (98%)	44 (86%)	7 (14%)	5	26
51	B6	44/52 (85%)	40 (91%)	4 (9%)	14	49
51	D6	44/52 (85%)	38 (86%)	6 (14%)	5	26
52	B7	42/42 (100%)	38 (90%)	4 (10%)	12	46
52	D7	42/42 (100%)	36 (86%)	6 (14%)	5	23
53	B8	51/55 (93%)	43 (84%)	8 (16%)	4	19
53	D8	51/55 (93%)	45 (88%)	6 (12%)	8	34
All	All	9584/9992 (96%)	8705 (91%)	879 (9%)	13	48

5 of 879 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	B4	53	GLU
5	CH	78	HIS
44	DV	72	ARG
51	B6	44	ARG
2	CE	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
2	CE	25	ASN
8	CK	82	HIS
43	DU	6	HIS

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Mol	Chain	Res	Type
2	CE	94	ASN
4	CG	43	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1506/1506 (100%)	279 (18%)	29 (1%)
1	CA	1505/1506 (99%)	284 (18%)	32 (2%)
22	AC	76/77 (98%)	5 (6%)	1 (1%)
22	CC	77/77 (100%)	9 (11%)	2 (2%)
23	A1	3/4 (75%)	1 (33%)	0
23	C1	3/4 (75%)	0	0
24	BA	2911/2912 (99%)	552 (18%)	37 (1%)
24	DA	2908/2912 (99%)	571 (19%)	43 (1%)
25	BB	121/122 (99%)	21 (17%)	0
25	DB	121/122 (99%)	25 (20%)	0
All	All	9231/9242 (99%)	1747 (18%)	144 (1%)

5 of 1747 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 144 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2689	U
1	CA	560	U
24	DA	2439	A
1	CA	89	U
1	CA	328	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 1693 ligands modelled in this entry, 1691 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
55	TAC	AA	1833	54	35,35,35	1.36	5 (14%)	58,58,58	1.69	9 (15%)
55	TAC	CA	1805	54	35,35,35	1.33	5 (14%)	58,58,58	1.58	8 (13%)

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
55	TAC	AA	1833	54	-	0/8/74/74	0/4/4/4
55	TAC	CA	1805	54	-	0/8/74/74	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	AA	1833	TAC	C1A-C10	4.39	1.49	1.41
55	CA	1805	TAC	C1A-C10	4.10	1.48	1.41
55	AA	1833	TAC	C1A-C61	3.49	1.49	1.41
55	CA	1805	TAC	C6-C61	-3.42	1.50	1.53
55	CA	1805	TAC	C1A-C61	3.28	1.48	1.41

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AA	1833	TAC	O12-C12-C1B	-5.96	118.37	123.88
55	CA	1805	TAC	O12-C12-C1B	-5.65	118.66	123.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AA	1833	TAC	C41-C1C-C1	-5.03	105.24	111.12
55	CA	1805	TAC	C41-C1C-C1	-4.82	105.49	111.12
55	AA	1833	TAC	O12-C12-C1C	4.11	120.03	113.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1506/1506 (100%)	-0.68	8 (0%) 88 51	89, 141, 216, 277	0
1	CA	1506/1506 (100%)	-0.73	5 (0%) 91 63	103, 152, 218, 275	0
2	AE	237/256 (92%)	0.42	13 (5%) 24 6	139, 172, 204, 216	0
2	CE	237/256 (92%)	0.98	31 (13%) 4 2	160, 191, 219, 228	0
3	AF	205/239 (85%)	1.52	63 (30%) 1 1	116, 151, 183, 201	0
3	CF	206/239 (86%)	0.95	33 (16%) 3 1	148, 179, 201, 211	0
4	AG	208/208 (100%)	0.24	3 (1%) 72 25	112, 149, 172, 183	0
4	CG	208/208 (100%)	-0.02	1 (0%) 88 51	128, 153, 171, 180	0
5	AH	151/162 (93%)	0.70	14 (9%) 9 3	111, 139, 161, 195	0
5	CH	151/162 (93%)	0.29	10 (6%) 18 4	129, 154, 177, 196	0
6	AI	101/101 (100%)	1.69	39 (38%) 1 0	116, 141, 162, 167	0
6	CI	101/101 (100%)	0.92	16 (15%) 3 1	128, 149, 163, 178	0
7	AJ	155/156 (99%)	-0.02	7 (4%) 32 7	129, 151, 187, 211	0
7	CJ	155/156 (99%)	1.09	23 (14%) 3 1	146, 167, 195, 204	0
8	AK	138/138 (100%)	0.17	2 (1%) 72 25	118, 148, 162, 170	0
8	CK	138/138 (100%)	0.14	2 (1%) 72 25	131, 159, 174, 180	0
9	AL	127/128 (99%)	-0.49	0 100 100	119, 169, 186, 192	0
9	CL	127/128 (99%)	0.39	10 (7%) 13 4	133, 185, 199, 208	0
10	AM	99/105 (94%)	0.48	4 (4%) 36 8	119, 170, 197, 210	0
10	CM	99/105 (94%)	0.14	2 (2%) 62 19	149, 191, 204, 209	0
11	AN	119/129 (92%)	0.55	10 (8%) 11 3	115, 137, 170, 198	0
11	CN	119/129 (92%)	0.74	9 (7%) 14 4	124, 149, 178, 196	0
12	AO	125/128 (97%)	0.64	10 (8%) 12 4	106, 128, 150, 192	0
12	CO	125/128 (97%)	0.09	3 (2%) 56 15	111, 134, 159, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AP	116/126 (92%)	-0.56	0 100 100	103, 153, 174, 184	0
13	CP	117/126 (92%)	0.24	12 (10%) 7 2	143, 179, 196, 205	0
14	AQ	60/61 (98%)	-0.00	2 (3%) 44 10	123, 143, 159, 161	0
14	CQ	60/61 (98%)	0.14	2 (3%) 44 10	148, 176, 188, 191	0
15	AR	88/89 (98%)	-0.11	0 100 100	109, 136, 155, 162	0
15	CR	88/89 (98%)	0.72	11 (12%) 5 2	121, 151, 168, 172	0
16	AS	84/88 (95%)	-0.40	0 100 100	135, 156, 179, 198	0
16	CS	84/88 (95%)	-0.50	0 100 100	121, 143, 167, 203	0
17	AT	100/105 (95%)	0.12	0 100 100	123, 147, 162, 173	0
17	CT	100/105 (95%)	0.83	13 (13%) 4 2	122, 145, 159, 182	0
18	AU	72/88 (81%)	0.66	6 (8%) 11 3	118, 142, 168, 195	0
18	CU	72/88 (81%)	0.50	7 (9%) 8 2	134, 157, 181, 199	0
19	AV	83/93 (89%)	-0.37	0 100 100	133, 158, 180, 191	0
19	CV	78/93 (83%)	-0.14	0 100 100	169, 195, 210, 221	0
20	AW	99/106 (93%)	-0.32	0 100 100	137, 159, 187, 196	0
20	CW	99/106 (93%)	-0.31	0 100 100	112, 142, 177, 194	0
21	AX	25/27 (92%)	-0.56	0 100 100	120, 150, 170, 187	0
21	CX	25/27 (92%)	-0.54	0 100 100	144, 171, 192, 209	0
22	AC	77/77 (100%)	-0.60	0 100 100	102, 125, 153, 175	0
22	CC	77/77 (100%)	0.13	10 (12%) 4 2	106, 145, 175, 205	0
23	A1	4/4 (100%)	-0.50	0 100 100	106, 109, 114, 165	0
23	C1	4/4 (100%)	-0.14	0 100 100	127, 131, 143, 184	0
24	BA	2912/2912 (100%)	-0.33	69 (2%) 56 15	68, 102, 240, 278	0
24	DA	2909/2912 (99%)	-0.42	76 (2%) 53 13	79, 114, 258, 279	0
25	BB	122/122 (100%)	-0.60	1 (0%) 83 39	92, 122, 145, 211	0
25	DB	122/122 (100%)	-0.05	8 (6%) 18 4	115, 152, 178, 226	0
26	BD	272/276 (98%)	0.39	11 (4%) 36 8	69, 96, 117, 140	0
26	DD	272/276 (98%)	0.71	17 (6%) 19 5	72, 106, 130, 155	0
27	BE	205/206 (99%)	0.91	32 (15%) 3 1	73, 117, 163, 177	0
27	DE	205/206 (99%)	0.38	9 (4%) 33 7	79, 122, 168, 196	0
28	BF	202/210 (96%)	0.27	8 (3%) 36 8	74, 108, 149, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DF	208/210 (99%)	0.74	13 (6%) 19 5	82, 125, 187, 213	0
29	BG	181/182 (99%)	-0.15	0 100 100	105, 127, 167, 186	0
29	DG	181/182 (99%)	2.13	96 (53%) 0 0	136, 166, 194, 204	0
30	BH	170/180 (94%)	0.22	5 (2%) 49 12	103, 135, 159, 175	0
30	DH	170/180 (94%)	0.58	19 (11%) 6 2	154, 222, 249, 262	0
31	BK	146/148 (98%)	-0.19	0 100 100	103, 151, 170, 179	0
31	DK	146/148 (98%)	-0.02	4 (2%) 52 13	111, 159, 178, 185	0
32	BM	138/140 (98%)	0.77	13 (9%) 9 3	90, 115, 153, 183	0
32	DM	138/140 (98%)	0.52	11 (7%) 12 4	93, 129, 168, 189	0
33	BN	122/122 (100%)	0.14	1 (0%) 83 39	83, 111, 132, 139	0
33	DN	122/122 (100%)	0.32	0 100 100	86, 116, 130, 140	0
34	BO	150/150 (100%)	1.02	39 (26%) 1 1	70, 113, 143, 207	0
34	DO	150/150 (100%)	0.85	17 (11%) 6 2	85, 129, 167, 206	0
35	BP	141/141 (100%)	0.24	3 (2%) 60 17	85, 107, 132, 163	0
35	DP	141/141 (100%)	0.57	6 (4%) 34 8	95, 126, 152, 177	0
36	B0	118/118 (100%)	0.47	4 (3%) 43 10	90, 110, 131, 148	0
36	D0	117/118 (99%)	-0.01	1 (0%) 81 37	88, 111, 135, 146	0
37	BQ	111/112 (99%)	0.43	8 (7%) 15 4	90, 119, 148, 164	0
37	DQ	111/112 (99%)	0.98	15 (13%) 4 2	114, 146, 168, 190	0
38	BR	137/146 (93%)	-0.04	3 (2%) 59 16	104, 125, 173, 202	0
38	DR	137/146 (93%)	0.09	1 (0%) 84 42	103, 121, 177, 212	0
39	B1	117/118 (99%)	0.13	3 (2%) 53 13	77, 106, 141, 168	0
39	D1	117/118 (99%)	0.41	7 (5%) 21 5	90, 122, 155, 178	0
40	B2	101/101 (100%)	0.81	11 (10%) 6 2	79, 122, 154, 181	0
40	D2	101/101 (100%)	1.79	45 (44%) 1 0	95, 149, 165, 181	0
41	BS	113/113 (100%)	1.07	16 (14%) 3 1	81, 102, 141, 191	0
41	DS	113/113 (100%)	0.96	8 (7%) 16 4	83, 107, 140, 194	0
42	BT	92/96 (95%)	0.18	1 (1%) 77 30	81, 98, 126, 145	0
42	DT	92/96 (95%)	0.84	10 (10%) 6 2	96, 117, 140, 159	0
43	BU	102/110 (92%)	0.56	9 (8%) 10 3	95, 123, 171, 190	0
43	DU	102/110 (92%)	1.43	23 (22%) 1 1	104, 142, 195, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BV	175/206 (84%)	0.92	32 (18%) 2 1	104, 142, 218, 229	0
44	DV	179/206 (86%)	1.01	31 (17%) 2 1	132, 174, 237, 251	0
45	B3	76/85 (89%)	0.34	2 (2%) 53 13	85, 101, 121, 163	0
45	D3	77/85 (90%)	1.79	29 (37%) 1 0	98, 117, 141, 175	0
46	BZ	97/98 (98%)	0.54	5 (5%) 26 6	83, 106, 149, 195	0
46	DZ	97/98 (98%)	1.38	21 (21%) 1 1	87, 116, 159, 191	0
47	BW	66/72 (91%)	0.17	1 (1%) 70 24	80, 108, 133, 171	0
47	DW	69/72 (95%)	0.73	7 (10%) 7 2	106, 138, 163, 196	0
48	BX	59/60 (98%)	1.01	13 (22%) 1 1	85, 106, 148, 160	0
48	DX	59/60 (98%)	1.69	21 (35%) 1 0	97, 126, 159, 194	0
49	B4	66/71 (92%)	-0.01	0 100 100	127, 176, 209, 219	0
49	D4	63/71 (88%)	4.06	54 (85%) 0 0	181, 212, 226, 235	0
50	B5	59/60 (98%)	1.43	15 (25%) 1 1	78, 115, 194, 210	0
50	D5	59/60 (98%)	0.81	6 (10%) 7 2	87, 114, 191, 218	0
51	B6	45/54 (83%)	3.97	35 (77%) 0 0	149, 184, 197, 201	0
51	D6	45/54 (83%)	8.77	43 (95%) 0 0	158, 195, 212, 215	0
52	B7	49/49 (100%)	0.29	1 (2%) 62 19	73, 83, 124, 154	0
52	D7	49/49 (100%)	1.12	7 (14%) 3 1	78, 91, 134, 156	0
53	B8	61/65 (93%)	0.22	1 (1%) 68 22	81, 96, 116, 145	0
53	D8	61/65 (93%)	1.06	8 (13%) 4 2	94, 109, 131, 161	0
All	All	20772/21286 (97%)	0.11	1336 (6%) 19 5	68, 133, 207, 279	0

The worst 5 of 1336 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	BA	1	G	23.1
51	D6	13	CYS	21.9
24	DA	2901	C	21.9
24	DA	2902	C	17.8
24	BA	654(K)	C	17.6

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

There are no non-standard protein/DNA/RNA residues in this entry.



## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	BA	3151	1/1	0.30	-	103,103,103,103	0
54	MG	BA	3287	1/1	0.22	-	95,95,95,95	0
54	MG	DA	3295	1/1	0.14	-	105,105,105,105	0
54	MG	AC	107	1/1	0.27	-	111,111,111,111	0
54	MG	BA	3523	1/1	0.17	-	64,64,64,64	0
54	MG	BA	3371	1/1	0.38	-	81,81,81,81	0
54	MG	CA	1779	1/1	0.28	-	112,112,112,112	0
54	MG	BA	3556	1/1	0.13	-	91,91,91,91	0
54	MG	AA	1718	1/1	0.33	-	124,124,124,124	0
54	MG	AA	1794	1/1	0.18	-	116,116,116,116	0
54	MG	BA	3399	1/1	0.43	-	90,90,90,90	0
54	MG	BA	3291	1/1	0.45	-	99,99,99,99	0
54	MG	BA	3349	1/1	0.46	-	69,69,69,69	0
54	MG	AA	1617	1/1	0.41	-	91,91,91,91	0
54	MG	BB	204	1/1	0.40	-	86,86,86,86	0
54	MG	BA	3459	1/1	0.34	-	91,91,91,91	0
54	MG	CA	1737	1/1	0.37	-	97,97,97,97	0
54	MG	DA	3264	1/1	0.30	-	80,80,80,80	0
54	MG	DA	3227	1/1	0.28	-	83,83,83,83	0
54	MG	BB	202	1/1	0.32	-	92,92,92,92	0
54	MG	DA	3313	1/1	0.36	-	122,122,122,122	0
54	MG	BA	3426	1/1	0.29	-	77,77,77,77	0
54	MG	CS	101	1/1	0.38	-	115,115,115,115	0
54	MG	BA	3364	1/1	0.30	-	137,137,137,137	0
54	MG	BA	3547	1/1	0.49	-	108,108,108,108	0
54	MG	BA	3363	1/1	0.32	-	73,73,73,73	0
54	MG	DA	3468	1/1	0.36	-	126,126,126,126	0
54	MG	DA	3233	1/1	0.33	-	79,79,79,79	0
54	MG	BA	3599	1/1	0.42	-	115,115,115,115	0
54	MG	BA	3155	1/1	0.20	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1799	1/1	0.42	-	79,79,79,79	0
54	MG	DA	3340	1/1	0.14	-	89,89,89,89	0
54	MG	BA	3093	1/1	0.34	-	154,154,154,154	0
54	MG	BA	3600	1/1	0.54	-	97,97,97,97	0
54	MG	AA	1769	1/1	0.26	-	124,124,124,124	0
54	MG	BA	3411	1/1	0.49	-	110,110,110,110	0
54	MG	AA	1770	1/1	0.50	-	98,98,98,98	0
54	MG	BA	3152	1/1	0.39	-	90,90,90,90	0
54	MG	DA	3344	1/1	0.07	-	124,124,124,124	0
54	MG	DA	3199	1/1	0.17	-	77,77,77,77	0
54	MG	DA	3402	1/1	0.38	-	105,105,105,105	0
54	MG	DA	3382	1/1	0.43	-	80,80,80,80	0
54	MG	AA	1667	1/1	0.47	-	88,88,88,88	0
54	MG	BA	3493	1/1	0.35	-	116,116,116,116	0
54	MG	BA	3168	1/1	0.30	-	52,52,52,52	0
54	MG	AA	1745	1/1	0.17	-	128,128,128,128	0
54	MG	AA	1611	1/1	0.21	-	138,138,138,138	0
54	MG	AA	1657	1/1	0.44	-	63,63,63,63	0
54	MG	DA	3365	1/1	0.14	-	100,100,100,100	0
54	MG	BA	3460	1/1	0.21	-	90,90,90,90	0
54	MG	BA	3249	1/1	0.28	-	84,84,84,84	0
54	MG	BA	3140	1/1	0.31	-	84,84,84,84	0
54	MG	DA	3510	1/1	0.19	-	77,77,77,77	0
54	MG	DA	3269	1/1	0.21	-	78,78,78,78	0
54	MG	CA	1800	1/1	0.09	-	145,145,145,145	0
54	MG	B7	102	1/1	0.28	-	75,75,75,75	0
54	MG	CA	1725	1/1	0.36	-	106,106,106,106	0
54	MG	BA	3321	1/1	0.23	-	71,71,71,71	0
54	MG	DA	3026	1/1	0.21	-	122,122,122,122	0
54	MG	DA	3448	1/1	0.25	-	89,89,89,89	0
54	MG	BA	3383	1/1	0.35	-	95,95,95,95	0
54	MG	BA	3236	1/1	0.51	-	97,97,97,97	0
54	MG	CA	1674	1/1	0.67	-	117,117,117,117	0
54	MG	BA	3427	1/1	0.39	-	91,91,91,91	0
54	MG	DA	3281	1/1	0.25	-	74,74,74,74	0
54	MG	BA	3583	1/1	0.27	-	59,59,59,59	0
54	MG	AA	1810	1/1	0.61	-	126,126,126,126	0
54	MG	CA	1708	1/1	0.26	-	143,143,143,143	0
54	MG	BA	3302	1/1	0.25	-	101,101,101,101	0
54	MG	BA	3568	1/1	0.72	-	105,105,105,105	0
54	MG	BA	3331	1/1	0.49	-	74,74,74,74	0
54	MG	DA	3272	1/1	0.24	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1718	1/1	0.58	-	114,114,114,114	0
54	MG	BA	3585	1/1	0.23	-	62,62,62,62	0
54	MG	DA	3506	1/1	0.25	-	61,61,61,61	0
54	MG	DA	3369	1/1	0.38	-	76,76,76,76	0
54	MG	DA	3035	1/1	0.10	-	93,93,93,93	0
54	MG	BA	3565	1/1	0.36	-	86,86,86,86	0
54	MG	DA	3326	1/1	0.30	-	82,82,82,82	0
54	MG	BA	3612	1/1	0.48	-	99,99,99,99	0
54	MG	DA	3008	1/1	0.48	-	93,93,93,93	0
54	MG	DA	3213	1/1	0.26	-	67,67,67,67	0
54	MG	AC	106	1/1	0.23	-	119,119,119,119	0
54	MG	DA	3287	1/1	0.24	-	67,67,67,67	0
54	MG	AA	1647	1/1	0.39	-	96,96,96,96	0
54	MG	BA	3464	1/1	0.43	-	80,80,80,80	0
54	MG	BA	3368	1/1	0.39	-	93,93,93,93	0
54	MG	DA	3025	1/1	0.35	-	88,88,88,88	0
54	MG	CA	1695	1/1	0.47	-	111,111,111,111	0
54	MG	BA	3333	1/1	0.49	-	99,99,99,99	0
54	MG	BA	3111	1/1	0.20	-	68,68,68,68	0
54	MG	CA	1612	1/1	0.12	-	122,122,122,122	0
54	MG	DA	3058	1/1	0.25	-	109,109,109,109	0
54	MG	BA	3421	1/1	0.76	-	106,106,106,106	0
54	MG	BA	3013	1/1	0.27	-	63,63,63,63	0
54	MG	DA	3192	1/1	0.28	-	64,64,64,64	0
54	MG	BA	3201	1/1	0.12	-	122,122,122,122	0
54	MG	DA	3525	1/1	0.40	-	103,103,103,103	0
54	MG	AA	1744	1/1	0.20	-	180,180,180,180	0
54	MG	DA	3404	1/1	0.18	-	66,66,66,66	0
54	MG	CA	1683	1/1	0.21	-	113,113,113,113	0
54	MG	CA	1754	1/1	0.44	-	97,97,97,97	0
54	MG	AA	1626	1/1	0.25	-	80,80,80,80	0
54	MG	DA	3235	1/1	0.31	-	89,89,89,89	0
54	MG	BA	3322	1/1	0.28	-	78,78,78,78	0
54	MG	AA	1757	1/1	0.10	-	118,118,118,118	0
54	MG	CA	1676	1/1	0.31	-	102,102,102,102	0
54	MG	DA	3244	1/1	0.19	-	84,84,84,84	0
54	MG	BA	3011	1/1	0.41	-	72,72,72,72	0
54	MG	AA	1614	1/1	0.38	-	114,114,114,114	0
54	MG	BA	3484	1/1	0.30	-	116,116,116,116	0
54	MG	BA	3391	1/1	0.27	-	103,103,103,103	0
54	MG	CA	1634	1/1	0.13	-	110,110,110,110	0
54	MG	DA	3001	1/1	0.29	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3407	1/1	0.31	-	114,114,114,114	0
54	MG	BA	3271	1/1	0.37	-	96,96,96,96	0
54	MG	CA	1791	1/1	0.33	-	78,78,78,78	0
54	MG	DA	3306	1/1	0.23	-	92,92,92,92	0
54	MG	BA	3088	1/1	0.45	-	97,97,97,97	0
54	MG	CA	1787	1/1	0.28	-	129,129,129,129	0
54	MG	CA	1789	1/1	0.44	-	121,121,121,121	0
54	MG	BA	3539	1/1	0.53	-	99,99,99,99	0
54	MG	BA	3415	1/1	0.54	-	90,90,90,90	0
54	MG	BA	3557	1/1	0.15	-	92,92,92,92	0
54	MG	BA	3312	1/1	0.39	-	98,98,98,98	0
54	MG	BA	3588	1/1	0.38	-	109,109,109,109	0
54	MG	BA	3626	1/1	0.35	-	103,103,103,103	0
54	MG	AA	1785	1/1	0.18	-	131,131,131,131	0
54	MG	BA	3220	1/1	0.24	-	76,76,76,76	0
54	MG	BA	3061	1/1	0.43	-	64,64,64,64	0
54	MG	CA	1624	1/1	0.26	-	129,129,129,129	0
54	MG	DA	3505	1/1	0.13	-	72,72,72,72	0
54	MG	BA	3569	1/1	0.50	-	79,79,79,79	0
54	MG	D5	101	1/1	0.09	-	63,63,63,63	0
54	MG	BA	3264	1/1	0.41	-	75,75,75,75	0
54	MG	BA	3297	1/1	0.38	-	78,78,78,78	0
54	MG	DA	3091	1/1	0.14	-	87,87,87,87	0
54	MG	DA	3131	1/1	0.20	-	94,94,94,94	0
54	MG	DA	3368	1/1	0.85	-	95,95,95,95	0
54	MG	BA	3009	1/1	0.25	-	53,53,53,53	0
54	MG	DA	3090	1/1	0.32	-	90,90,90,90	0
54	MG	BA	3422	1/1	0.25	-	120,120,120,120	0
54	MG	BB	206	1/1	0.38	-	97,97,97,97	0
56	ZN	CG	303	1/1	0.17	-	161,161,161,161	0
54	MG	CA	1623	1/1	0.04	-	180,180,180,180	0
54	MG	CA	1742	1/1	0.37	-	98,98,98,98	0
54	MG	CA	1705	1/1	0.56	-	114,114,114,114	0
54	MG	BA	3208	1/1	0.48	-	91,91,91,91	0
54	MG	DA	3393	1/1	0.28	-	76,76,76,76	0
54	MG	AA	1690	1/1	0.34	-	128,128,128,128	0
54	MG	DA	3189	1/1	0.27	-	65,65,65,65	0
54	MG	CA	1724	1/1	0.12	-	98,98,98,98	0
54	MG	BA	3272	1/1	0.27	-	52,52,52,52	0
54	MG	CA	1616	1/1	0.26	-	108,108,108,108	0
54	MG	AA	1791	1/1	0.23	-	104,104,104,104	0
54	MG	AA	1705	1/1	0.28	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AS	101	1/1	0.27	-	106,106,106,106	0
54	MG	AA	1621	1/1	0.46	-	147,147,147,147	0
54	MG	CC	103	1/1	0.10	-	150,150,150,150	0
54	MG	DA	3055	1/1	0.25	-	59,59,59,59	0
54	MG	BA	3285	1/1	0.49	-	114,114,114,114	0
54	MG	DA	3507	1/1	0.18	-	79,79,79,79	0
54	MG	BA	3310	1/1	0.28	-	103,103,103,103	0
54	MG	BE	303	1/1	0.26	-	72,72,72,72	0
54	MG	DA	3208	1/1	0.28	-	94,94,94,94	0
54	MG	AA	1808	1/1	0.14	-	139,139,139,139	0
54	MG	DA	3252	1/1	0.21	-	108,108,108,108	0
54	MG	BA	3130	1/1	0.15	-	92,92,92,92	0
54	MG	CA	1604	1/1	0.49	-	105,105,105,105	0
54	MG	DA	3047	1/1	0.12	-	124,124,124,124	0
54	MG	BA	3245	1/1	0.49	-	120,120,120,120	0
54	MG	DA	3162	1/1	0.23	-	108,108,108,108	0
54	MG	BA	3400	1/1	0.22	-	101,101,101,101	0
54	MG	BA	3385	1/1	0.38	-	72,72,72,72	0
54	MG	DA	3182	1/1	0.28	-	62,62,62,62	0
54	MG	CA	1629	1/1	0.09	-	164,164,164,164	0
54	MG	BA	3229	1/1	0.35	-	89,89,89,89	0
54	MG	BA	3589	1/1	0.28	-	77,77,77,77	0
54	MG	DA	3321	1/1	0.22	-	89,89,89,89	0
54	MG	DA	3427	1/1	0.29	-	114,114,114,114	0
54	MG	AA	1764	1/1	0.19	-	118,118,118,118	0
54	MG	BB	213	1/1	0.35	-	72,72,72,72	0
54	MG	DA	3475	1/1	0.54	-	121,121,121,121	0
54	MG	BA	3619	1/1	0.20	-	88,88,88,88	0
54	MG	BA	3350	1/1	0.55	-	115,115,115,115	0
54	MG	BA	3373	1/1	0.10	-	131,131,131,131	0
54	MG	AA	1722	1/1	0.22	-	109,109,109,109	0
54	MG	BA	3381	1/1	0.52	-	65,65,65,65	0
54	MG	DA	3300	1/1	0.40	-	107,107,107,107	0
54	MG	DA	3194	1/1	0.35	-	91,91,91,91	0
54	MG	DA	3486	1/1	1.14	-	112,112,112,112	0
54	MG	BA	3002	1/1	0.39	-	63,63,63,63	0
54	MG	AA	1635	1/1	0.32	-	122,122,122,122	0
54	MG	CA	1804	1/1	0.15	-	119,119,119,119	0
54	MG	DA	3217	1/1	0.22	-	89,89,89,89	0
54	MG	BA	3625	1/1	0.25	-	99,99,99,99	0
54	MG	BA	3445	1/1	0.18	-	156,156,156,156	0
54	MG	AA	1664	1/1	0.29	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1626	1/1	0.27	-	117,117,117,117	0
54	MG	AA	1734	1/1	0.41	-	146,146,146,146	0
54	MG	DA	3286	1/1	0.36	-	115,115,115,115	0
54	MG	CA	1744	1/1	0.36	-	97,97,97,97	0
54	MG	BA	3386	1/1	0.12	-	117,117,117,117	0
54	MG	AA	1817	1/1	0.19	-	101,101,101,101	0
54	MG	AA	1700	1/1	0.13	-	123,123,123,123	0
54	MG	BA	3486	1/1	0.27	-	108,108,108,108	0
54	MG	DA	3339	1/1	0.47	-	152,152,152,152	0
54	MG	BA	3406	1/1	0.55	-	86,86,86,86	0
54	MG	AA	1658	1/1	0.22	-	79,79,79,79	0
54	MG	BA	3004	1/1	0.27	-	79,79,79,79	0
54	MG	BA	3342	1/1	0.57	-	95,95,95,95	0
54	MG	AA	1709	1/1	0.09	-	155,155,155,155	0
54	MG	CA	1636	1/1	0.31	-	91,91,91,91	0
54	MG	BA	3078	1/1	0.35	-	106,106,106,106	0
54	MG	BA	3075	1/1	0.54	-	97,97,97,97	0
54	MG	CA	1740	1/1	0.13	-	109,109,109,109	0
54	MG	BA	3016	1/1	0.06	-	143,143,143,143	0
54	MG	AA	1821	1/1	0.27	-	110,110,110,110	0
54	MG	DA	3034	1/1	0.17	-	91,91,91,91	0
54	MG	BA	3309	1/1	0.30	-	84,84,84,84	0
54	MG	BA	3479	1/1	0.34	-	72,72,72,72	0
54	MG	BA	3242	1/1	0.54	-	115,115,115,115	0
54	MG	BA	3524	1/1	0.40	-	90,90,90,90	0
54	MG	DA	3165	1/1	0.18	-	59,59,59,59	0
54	MG	BA	3416	1/1	0.13	-	70,70,70,70	0
54	MG	BA	3499	1/1	0.12	-	103,103,103,103	0
54	MG	DA	3450	1/1	0.30	-	130,130,130,130	0
54	MG	BA	3163	1/1	0.21	-	104,104,104,104	0
54	MG	BA	3461	1/1	0.29	-	79,79,79,79	0
54	MG	BA	3222	1/1	0.32	-	57,57,57,57	0
54	MG	BA	3611	1/1	0.30	-	101,101,101,101	0
54	MG	BA	3623	1/1	0.18	-	86,86,86,86	0
54	MG	BA	3463	1/1	0.28	-	77,77,77,77	0
54	MG	CA	1762	1/1	0.42	-	116,116,116,116	0
54	MG	BA	3273	1/1	0.36	-	70,70,70,70	0
54	MG	BA	3158	1/1	0.51	-	67,67,67,67	0
54	MG	CA	1682	1/1	0.24	-	101,101,101,101	0
54	MG	AA	1641	1/1	0.17	-	90,90,90,90	0
54	MG	CA	1731	1/1	0.51	-	110,110,110,110	0
54	MG	AA	1679	1/1	0.30	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3170	1/1	0.22	-	90,90,90,90	0
54	MG	BA	3188	1/1	0.61	-	120,120,120,120	0
54	MG	DA	3290	1/1	0.21	-	107,107,107,107	0
54	MG	DA	3425	1/1	0.28	-	122,122,122,122	0
54	MG	BA	3529	1/1	0.31	-	89,89,89,89	0
54	MG	AA	1775	1/1	0.34	-	80,80,80,80	0
54	MG	BA	3179	1/1	0.64	-	108,108,108,108	0
54	MG	DA	3210	1/1	0.21	-	63,63,63,63	0
54	MG	BA	3010	1/1	0.15	-	128,128,128,128	0
54	MG	BA	3327	1/1	0.17	-	117,117,117,117	0
54	MG	BA	3255	1/1	0.76	-	110,110,110,110	0
54	MG	CA	1646	1/1	0.21	-	101,101,101,101	0
54	MG	AA	1616	1/1	0.27	-	158,158,158,158	0
54	MG	DA	3297	1/1	0.18	-	71,71,71,71	0
54	MG	DA	3077	1/1	0.11	-	96,96,96,96	0
54	MG	AA	1783	1/1	0.10	-	125,125,125,125	0
54	MG	CA	1667	1/1	0.28	-	139,139,139,139	0
54	MG	BA	3438	1/1	0.44	-	62,62,62,62	0
54	MG	BA	3478	1/1	0.14	-	155,155,155,155	0
54	MG	DA	3174	1/1	0.16	-	81,81,81,81	0
54	MG	DA	3285	1/1	0.14	-	67,67,67,67	0
54	MG	BA	3458	1/1	0.39	-	96,96,96,96	0
54	MG	DA	3303	1/1	0.23	-	140,140,140,140	0
54	MG	BA	3372	1/1	0.65	-	99,99,99,99	0
54	MG	BA	3365	1/1	0.54	-	104,104,104,104	0
54	MG	CA	1684	1/1	0.26	-	115,115,115,115	0
54	MG	AA	1601	1/1	0.28	-	80,80,80,80	0
54	MG	AA	1693	1/1	0.41	-	123,123,123,123	0
54	MG	DA	3442	1/1	0.15	-	112,112,112,112	0
54	MG	BA	3108	1/1	0.46	-	82,82,82,82	0
54	MG	BA	3316	1/1	0.28	-	82,82,82,82	0
54	MG	BA	3444	1/1	0.11	-	186,186,186,186	0
54	MG	AA	1797	1/1	0.38	-	82,82,82,82	0
54	MG	DA	3173	1/1	0.17	-	92,92,92,92	0
54	MG	AA	1643	1/1	0.15	-	112,112,112,112	0
54	MG	BA	3069	1/1	0.65	-	115,115,115,115	0
54	MG	BA	3423	1/1	0.54	-	89,89,89,89	0
54	MG	BA	3044	1/1	0.15	-	58,58,58,58	0
54	MG	DA	3126	1/1	0.12	-	58,58,58,58	0
54	MG	AA	1751	1/1	0.38	-	102,102,102,102	0
54	MG	BA	3180	1/1	0.51	-	73,73,73,73	0
54	MG	CA	1640	1/1	0.27	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1762	1/1	0.12	-	124,124,124,124	0
54	MG	CA	1778	1/1	0.51	-	118,118,118,118	0
54	MG	BA	3148	1/1	0.22	-	59,59,59,59	0
54	MG	DA	3268	1/1	0.16	-	63,63,63,63	0
54	MG	DA	3124	1/1	0.18	-	69,69,69,69	0
54	MG	BA	3254	1/1	0.29	-	70,70,70,70	0
54	MG	BA	3621	1/1	0.31	-	66,66,66,66	0
54	MG	DA	3410	1/1	0.47	-	118,118,118,118	0
54	MG	BA	3563	1/1	0.41	-	96,96,96,96	0
54	MG	CA	1795	1/1	0.23	-	112,112,112,112	0
54	MG	BA	3198	1/1	0.39	-	70,70,70,70	0
54	MG	BA	3392	1/1	0.36	-	110,110,110,110	0
54	MG	BA	3092	1/1	0.22	-	111,111,111,111	0
54	MG	AA	1675	1/1	0.16	-	93,93,93,93	0
54	MG	DA	3046	1/1	0.12	-	82,82,82,82	0
54	MG	AA	1755	1/1	0.15	-	143,143,143,143	0
54	MG	BA	3522	1/1	0.17	-	106,106,106,106	0
54	MG	BA	3555	1/1	0.10	-	67,67,67,67	0
54	MG	DA	3314	1/1	0.23	-	83,83,83,83	0
54	MG	BA	3516	1/1	0.18	-	80,80,80,80	0
54	MG	DA	3518	1/1	0.61	-	94,94,94,94	0
54	MG	BA	3181	1/1	0.22	-	79,79,79,79	0
54	MG	BA	3129	1/1	0.16	-	92,92,92,92	0
54	MG	BA	3341	1/1	0.33	-	71,71,71,71	0
54	MG	AH	202	1/1	0.12	-	108,108,108,108	0
54	MG	DA	3374	1/1	0.27	-	106,106,106,106	0
54	MG	BA	3284	1/1	0.13	-	121,121,121,121	0
54	MG	AA	1627	1/1	0.31	-	87,87,87,87	0
54	MG	DA	3027	1/1	0.15	-	115,115,115,115	0
54	MG	BA	3531	1/1	0.33	-	101,101,101,101	0
54	MG	BA	3283	1/1	0.13	-	108,108,108,108	0
54	MG	DA	3186	1/1	0.13	-	60,60,60,60	0
54	MG	DA	3397	1/1	0.35	-	96,96,96,96	0
54	MG	CA	1729	1/1	0.33	-	115,115,115,115	0
54	MG	AA	1726	1/1	0.34	-	132,132,132,132	0
54	MG	AA	1715	1/1	0.31	-	115,115,115,115	0
54	MG	DA	3312	1/1	0.22	-	87,87,87,87	0
54	MG	DA	3063	1/1	0.19	-	76,76,76,76	0
54	MG	BA	3104	1/1	0.34	-	70,70,70,70	0
54	MG	BA	3314	1/1	0.23	-	104,104,104,104	0
54	MG	AA	1651	1/1	0.16	-	108,108,108,108	0
54	MG	AA	1742	1/1	0.26	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3057	1/1	0.38	-	93,93,93,93	0
54	MG	BA	3437	1/1	0.23	-	81,81,81,81	0
54	MG	DA	3453	1/1	0.25	-	104,104,104,104	0
54	MG	AA	1790	1/1	0.50	-	115,115,115,115	0
54	MG	CA	1678	1/1	0.06	-	140,140,140,140	0
54	MG	BA	3579	1/1	0.48	-	85,85,85,85	0
54	MG	BA	3586	1/1	0.35	-	62,62,62,62	0
54	MG	DA	3458	1/1	0.09	-	115,115,115,115	0
54	MG	AA	1804	1/1	0.12	-	130,130,130,130	0
54	MG	DA	3212	1/1	0.29	-	59,59,59,59	0
54	MG	DA	3426	1/1	0.18	-	159,159,159,159	0
54	MG	BB	201	1/1	0.41	-	99,99,99,99	0
54	MG	AH	201	1/1	0.28	-	118,118,118,118	0
54	MG	DA	3226	1/1	0.28	-	81,81,81,81	0
54	MG	BA	3147	1/1	0.35	-	64,64,64,64	0
54	MG	AA	1801	1/1	0.27	-	97,97,97,97	0
54	MG	CA	1690	1/1	0.25	-	102,102,102,102	0
54	MG	CA	1645	1/1	0.09	-	103,103,103,103	0
54	MG	B7	101	1/1	0.37	-	67,67,67,67	0
54	MG	B7	103	1/1	0.18	-	88,88,88,88	0
54	MG	BA	3360	1/1	0.34	-	110,110,110,110	0
54	MG	BA	3378	1/1	0.27	-	129,129,129,129	0
54	MG	CA	1774	1/1	0.26	-	110,110,110,110	0
54	MG	BA	3606	1/1	0.41	-	84,84,84,84	0
54	MG	AA	1695	1/1	0.06	-	152,152,152,152	0
54	MG	DA	3168	1/1	0.16	-	95,95,95,95	0
54	MG	DA	3405	1/1	0.32	-	121,121,121,121	0
54	MG	DA	3345	1/1	0.35	-	107,107,107,107	0
54	MG	CA	1650	1/1	0.57	-	151,151,151,151	0
54	MG	CA	1727	1/1	0.21	-	113,113,113,113	0
54	MG	CA	1673	1/1	0.14	-	89,89,89,89	0
54	MG	CA	1733	1/1	0.34	-	124,124,124,124	0
54	MG	CA	1697	1/1	0.11	-	185,185,185,185	0
54	MG	DA	3111	1/1	0.20	-	64,64,64,64	0
54	MG	CC	106	1/1	0.16	-	112,112,112,112	0
54	MG	AA	1741	1/1	0.38	-	130,130,130,130	0
54	MG	DA	3161	1/1	0.27	-	77,77,77,77	0
54	MG	CA	1771	1/1	0.30	-	92,92,92,92	0
54	MG	AA	1637	1/1	0.54	-	115,115,115,115	0
54	MG	BA	3235	1/1	0.34	-	128,128,128,128	0
54	MG	BA	3519	1/1	0.37	-	75,75,75,75	0
54	MG	DA	3304	1/1	0.30	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3456	1/1	0.32	-	138,138,138,138	0
54	MG	AA	1789	1/1	0.20	-	79,79,79,79	0
54	MG	DA	3129	1/1	0.29	-	115,115,115,115	0
54	MG	DA	3185	1/1	0.19	-	66,66,66,66	0
54	MG	BA	3451	1/1	0.17	-	102,102,102,102	0
54	MG	BA	3538	1/1	0.66	-	111,111,111,111	0
54	MG	BA	3202	1/1	0.24	-	65,65,65,65	0
54	MG	CA	1706	1/1	0.27	-	126,126,126,126	0
54	MG	BA	3566	1/1	0.38	-	100,100,100,100	0
54	MG	DA	3503	1/1	0.72	-	105,105,105,105	0
54	MG	BA	3413	1/1	0.43	-	120,120,120,120	0
54	MG	BA	3338	1/1	0.25	-	103,103,103,103	0
54	MG	BA	3256	1/1	0.25	-	68,68,68,68	0
54	MG	BA	3288	1/1	0.61	-	100,100,100,100	0
54	MG	CA	1763	1/1	0.34	-	94,94,94,94	0
54	MG	DA	3040	1/1	0.13	-	98,98,98,98	0
54	MG	BB	209	1/1	0.45	-	116,116,116,116	0
54	MG	BA	3384	1/1	0.23	-	107,107,107,107	0
54	MG	BA	3319	1/1	0.58	-	129,129,129,129	0
54	MG	BA	3032	1/1	0.32	-	69,69,69,69	0
54	MG	DA	3232	1/1	0.24	-	78,78,78,78	0
54	MG	BA	3187	1/1	0.36	-	56,56,56,56	0
54	MG	BA	3485	1/1	0.32	-	90,90,90,90	0
54	MG	BA	3332	1/1	0.33	-	83,83,83,83	0
54	MG	BA	3225	1/1	0.57	-	92,92,92,92	0
54	MG	DA	3352	1/1	0.32	-	81,81,81,81	0
54	MG	BA	3119	1/1	0.44	-	78,78,78,78	0
54	MG	AA	1768	1/1	0.16	-	126,126,126,126	0
54	MG	BA	3394	1/1	0.45	-	85,85,85,85	0
54	MG	AC	102	1/1	0.35	-	123,123,123,123	0
54	MG	CA	1660	1/1	0.05	-	118,118,118,118	0
54	MG	BA	3308	1/1	0.44	-	110,110,110,110	0
54	MG	DA	3119	1/1	0.31	-	65,65,65,65	0
54	MG	BA	3156	1/1	0.89	-	108,108,108,108	0
54	MG	BA	3052	1/1	0.34	-	107,107,107,107	0
54	MG	BA	3025	1/1	0.35	-	65,65,65,65	0
54	MG	BA	3574	1/1	0.33	-	60,60,60,60	0
54	MG	DA	3429	1/1	0.18	-	97,97,97,97	0
54	MG	AA	1669	1/1	0.29	-	79,79,79,79	0
54	MG	CA	1723	1/1	0.46	-	111,111,111,111	0
54	MG	CA	1692	1/1	0.18	-	104,104,104,104	0
54	MG	BA	3196	1/1	0.29	-	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3440	1/1	0.47	-	83,83,83,83	0
54	MG	AA	1630	1/1	0.22	-	105,105,105,105	0
54	MG	BA	3608	1/1	0.21	-	108,108,108,108	0
54	MG	AA	1782	1/1	0.24	-	168,168,168,168	0
54	MG	BA	3219	1/1	0.22	-	123,123,123,123	0
54	MG	BA	3357	1/1	0.90	-	119,119,119,119	0
54	MG	BA	3377	1/1	0.13	-	109,109,109,109	0
54	MG	CA	1661	1/1	0.28	-	98,98,98,98	0
54	MG	BA	3567	1/1	0.48	-	114,114,114,114	0
54	MG	DA	3359	1/1	0.34	-	102,102,102,102	0
54	MG	DA	3021	1/1	0.14	-	77,77,77,77	0
54	MG	CA	1611	1/1	0.45	-	114,114,114,114	0
54	MG	BA	3545	1/1	0.25	-	108,108,108,108	0
54	MG	BA	3334	1/1	0.12	-	115,115,115,115	0
54	MG	BP	201	1/1	1.49	-	115,115,115,115	0
54	MG	CA	1657	1/1	0.20	-	142,142,142,142	0
54	MG	CA	1739	1/1	0.24	-	112,112,112,112	0
54	MG	BA	3237	1/1	0.56	-	117,117,117,117	0
54	MG	DA	3274	1/1	0.23	-	83,83,83,83	0
54	MG	BA	3262	1/1	0.31	-	63,63,63,63	0
54	MG	BA	3051	1/1	0.20	-	72,72,72,72	0
54	MG	AA	1767	1/1	0.41	-	100,100,100,100	0
54	MG	DA	3112	1/1	0.26	-	71,71,71,71	0
54	MG	CA	1701	1/1	0.52	-	92,92,92,92	0
54	MG	BA	3157	1/1	0.34	-	74,74,74,74	0
54	MG	DA	3364	1/1	0.20	-	112,112,112,112	0
54	MG	BA	3022	1/1	0.43	-	65,65,65,65	0
54	MG	BA	3182	1/1	0.21	-	101,101,101,101	0
54	MG	BA	3072	1/1	0.42	-	87,87,87,87	0
54	MG	CA	1714	1/1	0.27	-	94,94,94,94	0
54	MG	BA	3150	1/1	0.20	-	90,90,90,90	0
54	MG	DA	3305	1/1	0.42	-	91,91,91,91	0
54	MG	DA	3266	1/1	0.10	-	110,110,110,110	0
54	MG	CA	1798	1/1	0.42	-	84,84,84,84	0
54	MG	BA	3110	1/1	0.36	-	92,92,92,92	0
54	MG	DA	3466	1/1	0.31	-	94,94,94,94	0
54	MG	CA	1801	1/1	0.25	-	139,139,139,139	0
54	MG	DA	3331	1/1	0.09	-	116,116,116,116	0
54	MG	BA	3154	1/1	0.32	-	104,104,104,104	0
54	MG	BA	3573	1/1	0.37	-	96,96,96,96	0
54	MG	CC	104	1/1	0.39	-	95,95,95,95	0
54	MG	DA	3134	1/1	0.16	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3091	1/1	0.36	-	103,103,103,103	0
54	MG	CA	1633	1/1	0.40	-	107,107,107,107	0
54	MG	BA	3431	1/1	0.45	-	96,96,96,96	0
54	MG	DA	3409	1/1	0.45	-	132,132,132,132	0
54	MG	CA	1745	1/1	0.35	-	132,132,132,132	0
54	MG	AA	1677	1/1	0.31	-	125,125,125,125	0
54	MG	DA	3083	1/1	0.51	-	117,117,117,117	0
54	MG	CC	101	1/1	0.14	-	130,130,130,130	0
54	MG	BA	3269	1/1	0.21	-	85,85,85,85	0
54	MG	BA	3330	1/1	0.17	-	102,102,102,102	0
54	MG	AA	1620	1/1	0.21	-	105,105,105,105	0
54	MG	BA	3131	1/1	0.22	-	101,101,101,101	0
54	MG	BA	3216	1/1	0.18	-	95,95,95,95	0
54	MG	BA	3127	1/1	0.35	-	109,109,109,109	0
54	MG	BA	3164	1/1	0.43	-	80,80,80,80	0
54	MG	DA	3521	1/1	0.07	-	111,111,111,111	0
54	MG	AA	1639	1/1	0.44	-	91,91,91,91	0
54	MG	BA	3442	1/1	0.46	-	112,112,112,112	0
54	MG	DA	3020	1/1	0.12	-	62,62,62,62	0
54	MG	AA	1608	1/1	0.17	-	111,111,111,111	0
54	MG	BA	3166	1/1	0.33	-	86,86,86,86	0
54	MG	DA	3102	1/1	0.12	-	150,150,150,150	0
54	MG	DA	3241	1/1	0.23	-	69,69,69,69	0
54	MG	DA	3062	1/1	0.36	-	112,112,112,112	0
54	MG	DA	3370	1/1	0.13	-	96,96,96,96	0
54	MG	DA	3099	1/1	0.29	-	74,74,74,74	0
54	MG	DA	3516	1/1	0.21	-	92,92,92,92	0
54	MG	BA	3509	1/1	0.50	-	104,104,104,104	0
54	MG	AA	1628	1/1	0.43	-	142,142,142,142	0
54	MG	BA	3607	1/1	0.17	-	94,94,94,94	0
54	MG	DA	3464	1/1	0.21	-	101,101,101,101	0
54	MG	AA	1618	1/1	0.22	-	98,98,98,98	0
54	MG	BE	304	1/1	0.88	-	112,112,112,112	0
54	MG	CA	1635	1/1	0.27	-	78,78,78,78	0
54	MG	BA	3409	1/1	0.43	-	86,86,86,86	0
54	MG	CA	1614	1/1	0.19	-	121,121,121,121	0
54	MG	DB	202	1/1	0.10	-	113,113,113,113	0
54	MG	CA	1663	1/1	0.19	-	105,105,105,105	0
54	MG	CA	1622	1/1	0.51	-	122,122,122,122	0
54	MG	AA	1750	1/1	0.37	-	110,110,110,110	0
54	MG	BA	3153	1/1	0.38	-	89,89,89,89	0
54	MG	DA	3438	1/1	0.24	-	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3528	1/1	0.56	-	104,104,104,104	0
54	MG	BA	3134	1/1	0.45	-	130,130,130,130	0
54	MG	DA	3179	1/1	0.09	-	85,85,85,85	0
54	MG	DA	3254	1/1	0.45	-	74,74,74,74	0
54	MG	BA	3295	1/1	0.47	-	70,70,70,70	0
54	MG	AG	301	1/1	0.11	-	114,114,114,114	0
54	MG	B5	101	1/1	0.14	-	61,61,61,61	0
54	MG	BA	3627	1/1	0.27	-	89,89,89,89	0
54	MG	CA	1728	1/1	0.37	-	144,144,144,144	0
54	MG	DA	3524	1/1	0.42	-	86,86,86,86	0
54	MG	BA	3214	1/1	0.65	-	93,93,93,93	0
54	MG	DA	3096	1/1	0.33	-	125,125,125,125	0
54	MG	DA	3435	1/1	0.23	-	99,99,99,99	0
54	MG	CA	1803	1/1	0.39	-	123,123,123,123	0
54	MG	DA	3341	1/1	0.52	-	107,107,107,107	0
54	MG	AA	1758	1/1	0.38	-	111,111,111,111	0
54	MG	BE	305	1/1	0.35	-	111,111,111,111	0
54	MG	BA	3274	1/1	0.45	-	93,93,93,93	0
54	MG	CA	1671	1/1	0.39	-	75,75,75,75	0
54	MG	DA	3512	1/1	0.39	-	81,81,81,81	0
54	MG	DA	3228	1/1	0.09	-	80,80,80,80	0
54	MG	BB	214	1/1	0.58	-	108,108,108,108	0
54	MG	CA	1608	1/1	0.25	-	103,103,103,103	0
54	MG	BO	203	1/1	0.14	-	70,70,70,70	0
54	MG	B3	102	1/1	0.28	-	93,93,93,93	0
54	MG	BA	3128	1/1	0.58	-	99,99,99,99	0
54	MG	DA	3258	1/1	0.34	-	98,98,98,98	0
54	MG	BU	202	1/1	0.18	-	80,80,80,80	0
54	MG	DA	3041	1/1	0.22	-	142,142,142,142	0
54	MG	AA	1632	1/1	0.27	-	116,116,116,116	0
54	MG	DA	3140	1/1	0.18	-	74,74,74,74	0
54	MG	BA	3587	1/1	0.33	-	102,102,102,102	0
54	MG	DA	3237	1/1	0.14	-	63,63,63,63	0
54	MG	DA	3103	1/1	0.13	-	117,117,117,117	0
54	MG	DA	3482	1/1	0.12	-	120,120,120,120	0
54	MG	BA	3041	1/1	0.06	-	142,142,142,142	0
54	MG	BA	3161	1/1	0.16	-	101,101,101,101	0
54	MG	BA	3172	1/1	0.43	-	93,93,93,93	0
54	MG	BA	3434	1/1	0.64	-	107,107,107,107	0
54	MG	DA	3184	1/1	0.21	-	68,68,68,68	0
54	MG	AA	1826	1/1	0.13	-	94,94,94,94	0
54	MG	AA	1823	1/1	0.09	-	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1602	1/1	0.58	-	115,115,115,115	0
54	MG	DA	3030	1/1	0.17	-	89,89,89,89	0
54	MG	BA	3345	1/1	0.16	-	95,95,95,95	0
54	MG	BA	3289	1/1	0.23	-	83,83,83,83	0
54	MG	BA	3382	1/1	0.49	-	78,78,78,78	0
54	MG	DA	3325	1/1	0.45	-	74,74,74,74	0
54	MG	DA	3400	1/1	0.25	-	105,105,105,105	0
54	MG	BA	3230	1/1	0.32	-	97,97,97,97	0
54	MG	BA	3615	1/1	0.30	-	92,92,92,92	0
54	MG	BA	3375	1/1	0.48	-	80,80,80,80	0
54	MG	AA	1716	1/1	0.42	-	107,107,107,107	0
54	MG	DA	3200	1/1	0.13	-	112,112,112,112	0
54	MG	BA	3527	1/1	0.39	-	109,109,109,109	0
54	MG	DA	3216	1/1	0.16	-	77,77,77,77	0
54	MG	DA	3218	1/1	0.33	-	77,77,77,77	0
54	MG	BA	3591	1/1	0.44	-	57,57,57,57	0
54	MG	BA	3424	1/1	0.60	-	111,111,111,111	0
54	MG	DA	3421	1/1	0.26	-	141,141,141,141	0
54	MG	DA	3193	1/1	0.20	-	69,69,69,69	0
54	MG	DA	3461	1/1	0.12	-	102,102,102,102	0
54	MG	BA	3185	1/1	0.69	-	112,112,112,112	0
54	MG	DA	3479	1/1	0.30	-	106,106,106,106	0
54	MG	AA	1609	1/1	0.37	-	87,87,87,87	0
54	MG	BA	3465	1/1	0.65	-	107,107,107,107	0
54	MG	BA	3352	1/1	0.38	-	87,87,87,87	0
54	MG	DA	3081	1/1	0.40	-	116,116,116,116	0
54	MG	CA	1749	1/1	0.23	-	120,120,120,120	0
54	MG	B8	101	1/1	0.19	-	101,101,101,101	0
54	MG	CA	1716	1/1	0.47	-	126,126,126,126	0
54	MG	BA	3211	1/1	0.43	-	77,77,77,77	0
54	MG	DA	3439	1/1	0.06	-	84,84,84,84	0
54	MG	BA	3602	1/1	0.49	-	66,66,66,66	0
54	MG	DA	3223	1/1	0.23	-	54,54,54,54	0
54	MG	DA	3260	1/1	0.49	-	128,128,128,128	0
54	MG	BA	3247	1/1	0.48	-	80,80,80,80	0
54	MG	CA	1659	1/1	0.12	-	158,158,158,158	0
54	MG	DA	3012	1/1	0.64	-	129,129,129,129	0
54	MG	DA	3377	1/1	0.38	-	102,102,102,102	0
54	MG	DA	3346	1/1	0.30	-	93,93,93,93	0
54	MG	DA	3398	1/1	0.40	-	130,130,130,130	0
54	MG	BA	3138	1/1	0.20	-	81,81,81,81	0
54	MG	DA	3408	1/1	0.19	-	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3038	1/1	0.29	-	67,67,67,67	0
54	MG	DA	3075	1/1	0.32	-	105,105,105,105	0
54	MG	BA	3232	1/1	0.30	-	93,93,93,93	0
54	MG	BA	3325	1/1	0.22	-	89,89,89,89	0
54	MG	CA	1790	1/1	0.39	-	118,118,118,118	0
54	MG	AA	1623	1/1	0.33	-	81,81,81,81	0
54	MG	AA	1743	1/1	0.26	-	136,136,136,136	0
54	MG	CA	1668	1/1	0.34	-	145,145,145,145	0
54	MG	BA	3124	1/1	0.43	-	110,110,110,110	0
54	MG	BA	3077	1/1	0.36	-	77,77,77,77	0
54	MG	BO	202	1/1	0.24	-	98,98,98,98	0
54	MG	BA	3292	1/1	0.49	-	113,113,113,113	0
54	MG	DA	3276	1/1	0.24	-	97,97,97,97	0
54	MG	BA	3581	1/1	0.35	-	82,82,82,82	0
54	MG	DA	3299	1/1	1.50	-	105,105,105,105	0
54	MG	BA	3548	1/1	0.28	-	96,96,96,96	0
54	MG	AA	1676	1/1	0.45	-	132,132,132,132	0
54	MG	DA	3445	1/1	0.24	-	89,89,89,89	0
54	MG	DA	3487	1/1	0.25	-	108,108,108,108	0
54	MG	BA	3603	1/1	1.14	-	113,113,113,113	0
54	MG	AA	1731	1/1	0.52	-	90,90,90,90	0
54	MG	BA	3117	1/1	0.28	-	102,102,102,102	0
54	MG	DE	303	1/1	0.16	-	70,70,70,70	0
54	MG	CA	1639	1/1	0.27	-	129,129,129,129	0
54	MG	DA	3310	1/1	0.44	-	111,111,111,111	0
54	MG	DA	3010	1/1	0.14	-	103,103,103,103	0
54	MG	BA	3098	1/1	0.47	-	75,75,75,75	0
54	MG	CA	1631	1/1	0.21	-	134,134,134,134	0
54	MG	BA	3429	1/1	0.51	-	129,129,129,129	0
54	MG	B1	201	1/1	0.24	-	61,61,61,61	0
54	MG	AA	1802	1/1	0.32	-	136,136,136,136	0
54	MG	AA	1720	1/1	0.19	-	101,101,101,101	0
54	MG	BA	3026	1/1	0.25	-	66,66,66,66	0
54	MG	BA	3278	1/1	0.33	-	101,101,101,101	0
54	MG	DA	3363	1/1	0.06	-	125,125,125,125	0
54	MG	AA	1727	1/1	0.17	-	110,110,110,110	0
54	MG	DA	3060	1/1	0.14	-	101,101,101,101	0
54	MG	BA	3257	1/1	0.30	-	70,70,70,70	0
54	MG	BA	3552	1/1	0.16	-	98,98,98,98	0
54	MG	DA	3322	1/1	0.35	-	110,110,110,110	0
54	MG	BB	207	1/1	0.54	-	131,131,131,131	0
54	MG	AA	1634	1/1	0.29	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3387	1/1	0.10	-	135,135,135,135	0
54	MG	CA	1681	1/1	0.30	-	96,96,96,96	0
54	MG	AA	1796	1/1	0.29	-	109,109,109,109	0
54	MG	AA	1706	1/1	0.09	-	134,134,134,134	0
54	MG	DA	3476	1/1	0.45	-	99,99,99,99	0
54	MG	DA	3023	1/1	0.27	-	86,86,86,86	0
54	MG	DA	3116	1/1	0.21	-	77,77,77,77	0
54	MG	DB	213	1/1	0.17	-	91,91,91,91	0
54	MG	BA	3244	1/1	0.06	-	112,112,112,112	0
54	MG	BA	3039	1/1	0.39	-	98,98,98,98	0
54	MG	CA	1617	1/1	0.24	-	140,140,140,140	0
54	MG	AC	109	1/1	0.12	-	105,105,105,105	0
54	MG	BA	3275	1/1	0.50	-	111,111,111,111	0
54	MG	BA	3480	1/1	0.14	-	187,187,187,187	0
54	MG	DA	3316	1/1	0.56	-	124,124,124,124	0
54	MG	BA	3543	1/1	0.29	-	90,90,90,90	0
54	MG	BA	3605	1/1	0.17	-	82,82,82,82	0
54	MG	BA	3067	1/1	0.98	-	108,108,108,108	0
54	MG	BA	3205	1/1	0.28	-	88,88,88,88	0
54	MG	DA	3463	1/1	0.40	-	109,109,109,109	0
54	MG	BA	3252	1/1	0.27	-	70,70,70,70	0
54	MG	DA	3056	1/1	0.15	-	86,86,86,86	0
54	MG	CA	1687	1/1	0.43	-	106,106,106,106	0
54	MG	BA	3561	1/1	0.20	-	86,86,86,86	0
54	MG	BF	302	1/1	0.53	-	127,127,127,127	0
54	MG	CA	1784	1/1	0.15	-	94,94,94,94	0
54	MG	CA	1699	1/1	0.33	-	81,81,81,81	0
54	MG	AA	1756	1/1	0.17	-	86,86,86,86	0
54	MG	CA	1694	1/1	0.25	-	108,108,108,108	0
54	MG	AA	1619	1/1	0.22	-	96,96,96,96	0
54	MG	DA	3220	1/1	0.23	-	70,70,70,70	0
54	MG	AA	1713	1/1	0.13	-	107,107,107,107	0
54	MG	DA	3292	1/1	0.18	-	129,129,129,129	0
54	MG	AA	1717	1/1	0.05	-	137,137,137,137	0
54	MG	BA	3443	1/1	0.46	-	124,124,124,124	0
54	MG	DA	3133	1/1	0.18	-	74,74,74,74	0
54	MG	DA	3067	1/1	0.14	-	97,97,97,97	0
54	MG	CA	1760	1/1	0.26	-	135,135,135,135	0
54	MG	DA	3517	1/1	0.25	-	106,106,106,106	0
54	MG	AA	1654	1/1	0.40	-	113,113,113,113	0
54	MG	DB	207	1/1	0.17	-	114,114,114,114	0
54	MG	DA	3515	1/1	0.10	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3115	1/1	0.18	-	75,75,75,75	0
54	MG	DA	3366	1/1	0.43	-	103,103,103,103	0
54	MG	BA	3218	1/1	0.35	-	75,75,75,75	0
54	MG	BA	3200	1/1	0.11	-	149,149,149,149	0
54	MG	BA	3021	1/1	0.42	-	72,72,72,72	0
54	MG	BA	3495	1/1	0.30	-	73,73,73,73	0
54	MG	DA	3044	1/1	0.14	-	96,96,96,96	0
54	MG	DA	3383	1/1	0.36	-	84,84,84,84	0
54	MG	BA	3343	1/1	0.32	-	86,86,86,86	0
54	MG	DA	3064	1/1	0.29	-	79,79,79,79	0
54	MG	CA	1776	1/1	0.34	-	125,125,125,125	0
54	MG	BA	3096	1/1	0.62	-	129,129,129,129	0
54	MG	CA	1751	1/1	0.67	-	118,118,118,118	0
54	MG	AA	1723	1/1	0.27	-	92,92,92,92	0
54	MG	BA	3369	1/1	0.52	-	94,94,94,94	0
54	MG	DA	3007	1/1	0.18	-	116,116,116,116	0
54	MG	DA	3499	1/1	0.15	-	103,103,103,103	0
54	MG	BA	3267	1/1	0.11	-	126,126,126,126	0
54	MG	AA	1822	1/1	0.11	-	144,144,144,144	0
54	MG	BA	3562	1/1	0.32	-	97,97,97,97	0
54	MG	DA	3180	1/1	0.30	-	82,82,82,82	0
54	MG	DA	3086	1/1	0.12	-	84,84,84,84	0
54	MG	CA	1758	1/1	0.50	-	110,110,110,110	0
54	MG	BA	3224	1/1	0.25	-	101,101,101,101	0
54	MG	CA	1679	1/1	0.16	-	94,94,94,94	0
54	MG	BA	3260	1/1	0.12	-	126,126,126,126	0
54	MG	AA	1749	1/1	0.21	-	112,112,112,112	0
54	MG	DA	3330	1/1	0.25	-	82,82,82,82	0
54	MG	BA	3060	1/1	0.23	-	105,105,105,105	0
54	MG	DA	3051	1/1	0.28	-	81,81,81,81	0
54	MG	CA	1712	1/1	0.25	-	105,105,105,105	0
54	MG	BA	3276	1/1	0.32	-	90,90,90,90	0
54	MG	DA	3467	1/1	0.09	-	159,159,159,159	0
54	MG	BA	3417	1/1	0.15	-	78,78,78,78	0
54	MG	BA	3358	1/1	0.33	-	108,108,108,108	0
54	MG	BA	3380	1/1	0.32	-	91,91,91,91	0
54	MG	BA	3020	1/1	0.40	-	109,109,109,109	0
54	MG	BA	3471	1/1	0.46	-	91,91,91,91	0
54	MG	BA	3544	1/1	0.43	-	77,77,77,77	0
54	MG	CA	1658	1/1	0.49	-	120,120,120,120	0
54	MG	BA	3305	1/1	0.35	-	80,80,80,80	0
54	MG	DA	3296	1/1	0.37	-	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	DA	3011	1/1	0.27	-	128,128,128,128	0
54	MG	DA	3477	1/1	0.25	-	93,93,93,93	0
54	MG	BA	3403	1/1	0.39	-	114,114,114,114	0
54	MG	BA	3167	1/1	0.40	-	95,95,95,95	0
54	MG	BA	3507	1/1	0.55	-	127,127,127,127	0
54	MG	AA	1819	1/1	0.16	-	81,81,81,81	0
54	MG	BA	3139	1/1	0.30	-	66,66,66,66	0
54	MG	B6	101	1/1	0.43	-	128,128,128,128	0
54	MG	DA	3367	1/1	0.92	-	125,125,125,125	0
54	MG	BA	3344	1/1	0.24	-	93,93,93,93	0
54	MG	DA	3433	1/1	0.23	-	66,66,66,66	0
54	MG	DA	3204	1/1	0.16	-	126,126,126,126	0
54	MG	DA	3078	1/1	0.08	-	97,97,97,97	0
54	MG	BA	3300	1/1	0.38	-	102,102,102,102	0
54	MG	DA	3338	1/1	0.39	-	95,95,95,95	0
54	MG	BA	3313	1/1	0.23	-	61,61,61,61	0
54	MG	BA	3282	1/1	0.53	-	107,107,107,107	0
54	MG	CA	1654	1/1	0.18	-	128,128,128,128	0
54	MG	BA	3601	1/1	0.47	-	52,52,52,52	0
54	MG	DA	3110	1/1	0.29	-	75,75,75,75	0
54	MG	BA	3353	1/1	0.23	-	93,93,93,93	0
54	MG	BA	3456	1/1	0.22	-	108,108,108,108	0
54	MG	CA	1652	1/1	0.49	-	120,120,120,120	0
54	MG	DA	3394	1/1	0.65	-	106,106,106,106	0
54	MG	DA	3423	1/1	0.23	-	123,123,123,123	0
54	MG	CA	1621	1/1	0.36	-	84,84,84,84	0
54	MG	BA	3223	1/1	0.49	-	84,84,84,84	0
54	MG	AA	1753	1/1	0.10	-	143,143,143,143	0
54	MG	BA	3501	1/1	0.43	-	99,99,99,99	0
54	MG	DA	3139	1/1	0.27	-	67,67,67,67	0
54	MG	B1	202	1/1	0.28	-	100,100,100,100	0
54	MG	BA	3149	1/1	0.27	-	110,110,110,110	0
54	MG	DA	3373	1/1	0.17	-	112,112,112,112	0
54	MG	DA	3336	1/1	0.19	-	115,115,115,115	0
54	MG	AA	1780	1/1	0.07	-	154,154,154,154	0
54	MG	DA	3277	1/1	0.34	-	77,77,77,77	0
54	MG	BA	3346	1/1	0.31	-	112,112,112,112	0
54	MG	AA	1735	1/1	0.50	-	91,91,91,91	0
54	MG	DA	3127	1/1	0.19	-	66,66,66,66	0
54	MG	CA	1704	1/1	0.62	-	95,95,95,95	0
54	MG	DA	3270	1/1	0.19	-	63,63,63,63	0
54	MG	DA	3247	1/1	0.25	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3105	1/1	0.09	-	110,110,110,110	0
54	MG	BB	208	1/1	0.48	-	90,90,90,90	0
54	MG	AA	1738	1/1	0.33	-	117,117,117,117	0
54	MG	BA	3076	1/1	0.08	-	74,74,74,74	0
54	MG	DA	3443	1/1	0.20	-	103,103,103,103	0
54	MG	DA	3413	1/1	0.41	-	115,115,115,115	0
54	MG	BA	3467	1/1	0.10	-	102,102,102,102	0
54	MG	DA	3335	1/1	0.20	-	78,78,78,78	0
54	MG	AA	1610	1/1	0.32	-	71,71,71,71	0
54	MG	BA	3178	1/1	0.50	-	78,78,78,78	0
54	MG	BA	3040	1/1	0.20	-	88,88,88,88	0
54	MG	BA	3541	1/1	0.53	-	120,120,120,120	0
54	MG	DA	3384	1/1	0.15	-	77,77,77,77	0
54	MG	CA	1734	1/1	0.09	-	93,93,93,93	0
54	MG	BA	3095	1/1	0.38	-	92,92,92,92	0
54	MG	BA	3537	1/1	0.35	-	124,124,124,124	0
54	MG	AA	1763	1/1	0.17	-	110,110,110,110	0
54	MG	CA	1670	1/1	0.23	-	91,91,91,91	0
54	MG	AA	1642	1/1	0.18	-	103,103,103,103	0
54	MG	AA	1665	1/1	0.27	-	84,84,84,84	0
54	MG	BA	3393	1/1	0.21	-	108,108,108,108	0
54	MG	BA	3005	1/1	0.20	-	61,61,61,61	0
54	MG	CA	1649	1/1	0.24	-	113,113,113,113	0
54	MG	BA	3094	1/1	0.39	-	97,97,97,97	0
54	MG	AA	1825	1/1	0.17	-	93,93,93,93	0
54	MG	DA	3416	1/1	0.25	-	100,100,100,100	0
54	MG	BA	3428	1/1	0.44	-	80,80,80,80	0
54	MG	DA	3106	1/1	1.27	-	122,122,122,122	0
54	MG	B2	201	1/1	0.13	-	90,90,90,90	0
54	MG	DB	201	1/1	0.13	-	88,88,88,88	0
54	MG	DA	3095	1/1	0.10	-	121,121,121,121	0
54	MG	BA	3337	1/1	0.15	-	75,75,75,75	0
54	MG	AA	1673	1/1	0.22	-	133,133,133,133	0
54	MG	CA	1601	1/1	0.21	-	108,108,108,108	0
54	MG	BA	3469	1/1	0.56	-	125,125,125,125	0
54	MG	BA	3290	1/1	0.24	-	78,78,78,78	0
54	MG	DA	3053	1/1	0.38	-	100,100,100,100	0
54	MG	DA	3118	1/1	0.24	-	61,61,61,61	0
54	MG	DB	211	1/1	0.25	-	107,107,107,107	0
54	MG	DA	3294	1/1	0.29	-	64,64,64,64	0
54	MG	DA	3172	1/1	0.82	-	110,110,110,110	0
54	MG	BA	3034	1/1	0.37	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1665	1/1	0.51	-	103,103,103,103	0
54	MG	AA	1629	1/1	0.08	-	186,186,186,186	0
54	MG	DA	3436	1/1	0.18	-	120,120,120,120	0
54	MG	DA	3183	1/1	0.33	-	92,92,92,92	0
54	MG	DB	204	1/1	0.25	-	111,111,111,111	0
54	MG	AA	1754	1/1	0.14	-	85,85,85,85	0
54	MG	CA	1672	1/1	0.25	-	101,101,101,101	0
54	MG	DA	3496	1/1	0.11	-	72,72,72,72	0
54	MG	CA	1793	1/1	0.38	-	115,115,115,115	0
54	MG	DA	3120	1/1	0.14	-	75,75,75,75	0
54	MG	DA	3071	1/1	0.91	-	123,123,123,123	0
54	MG	BA	3177	1/1	1.52	-	101,101,101,101	0
54	MG	BA	3622	1/1	0.23	-	120,120,120,120	0
54	MG	DA	3520	1/1	0.13	-	100,100,100,100	0
54	MG	DA	3395	1/1	0.31	-	87,87,87,87	0
54	MG	AA	1622	1/1	0.35	-	96,96,96,96	0
54	MG	AA	1671	1/1	0.36	-	110,110,110,110	0
54	MG	AA	1776	1/1	0.26	-	116,116,116,116	0
54	MG	AA	1818	1/1	0.23	-	156,156,156,156	0
54	MG	CA	1736	1/1	0.54	-	85,85,85,85	0
54	MG	DA	3122	1/1	0.24	-	67,67,67,67	0
54	MG	BA	3049	1/1	0.31	-	88,88,88,88	0
54	MG	AA	1740	1/1	0.40	-	75,75,75,75	0
54	MG	AC	103	1/1	0.41	-	75,75,75,75	0
54	MG	BA	3194	1/1	0.13	-	113,113,113,113	0
54	MG	CA	1628	1/1	0.07	-	149,149,149,149	0
54	MG	BA	3530	1/1	0.38	-	110,110,110,110	0
54	MG	DA	3005	1/1	0.21	-	86,86,86,86	0
54	MG	BA	3250	1/1	0.35	-	87,87,87,87	0
54	MG	DA	3428	1/1	0.19	-	89,89,89,89	0
54	MG	DB	210	1/1	0.20	-	73,73,73,73	0
54	MG	DA	3045	1/1	0.17	-	67,67,67,67	0
54	MG	DA	3149	1/1	0.19	-	112,112,112,112	0
54	MG	BA	3210	1/1	0.52	-	78,78,78,78	0
54	MG	BA	3207	1/1	0.81	-	116,116,116,116	0
54	MG	BA	3441	1/1	0.28	-	95,95,95,95	0
54	MG	AA	1772	1/1	0.38	-	155,155,155,155	0
54	MG	BA	3473	1/1	0.44	-	82,82,82,82	0
54	MG	BA	3496	1/1	0.41	-	108,108,108,108	0
54	MG	BA	3045	1/1	0.41	-	66,66,66,66	0
54	MG	DA	3446	1/1	0.19	-	92,92,92,92	0
54	MG	BA	3115	1/1	0.33	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3614	1/1	1.68	-	109,109,109,109	0
54	MG	AA	1685	1/1	0.37	-	95,95,95,95	0
54	MG	DA	3283	1/1	0.25	-	114,114,114,114	0
54	MG	CA	1675	1/1	0.12	-	111,111,111,111	0
54	MG	BA	3033	1/1	0.39	-	75,75,75,75	0
54	MG	DA	3437	1/1	0.21	-	96,96,96,96	0
54	MG	AA	1827	1/1	0.14	-	82,82,82,82	0
54	MG	BA	3162	1/1	0.26	-	72,72,72,72	0
54	MG	DA	3170	1/1	0.28	-	80,80,80,80	0
54	MG	CA	1632	1/1	0.48	-	111,111,111,111	0
54	MG	BA	3120	1/1	0.52	-	97,97,97,97	0
54	MG	BA	3031	1/1	0.34	-	63,63,63,63	0
54	MG	BA	3251	1/1	0.40	-	109,109,109,109	0
54	MG	BA	3047	1/1	0.22	-	64,64,64,64	0
54	MG	BA	3430	1/1	0.16	-	87,87,87,87	0
54	MG	DA	3169	1/1	0.39	-	76,76,76,76	0
54	MG	BF	301	1/1	0.76	-	100,100,100,100	0
54	MG	CA	1770	1/1	0.11	-	106,106,106,106	0
54	MG	BA	3109	1/1	0.45	-	94,94,94,94	0
54	MG	AA	1687	1/1	0.43	-	99,99,99,99	0
54	MG	BA	3504	1/1	0.58	-	88,88,88,88	0
54	MG	AA	1655	1/1	0.47	-	106,106,106,106	0
54	MG	BA	3259	1/1	0.30	-	53,53,53,53	0
54	MG	DA	3375	1/1	0.29	-	127,127,127,127	0
54	MG	CA	1693	1/1	0.41	-	117,117,117,117	0
54	MG	CC	108	1/1	0.26	-	129,129,129,129	0
54	MG	BA	3012	1/1	0.25	-	70,70,70,70	0
54	MG	DA	3356	1/1	0.24	-	64,64,64,64	0
54	MG	DA	3038	1/1	0.33	-	122,122,122,122	0
54	MG	BA	3510	1/1	0.28	-	118,118,118,118	0
54	MG	AA	1701	1/1	0.44	-	115,115,115,115	0
54	MG	AA	1781	1/1	0.49	-	120,120,120,120	0
54	MG	DA	3449	1/1	0.41	-	106,106,106,106	0
54	MG	CA	1677	1/1	0.14	-	114,114,114,114	0
54	MG	BA	3206	1/1	0.36	-	99,99,99,99	0
54	MG	DA	3248	1/1	0.38	-	112,112,112,112	0
54	MG	BA	3086	1/1	0.22	-	88,88,88,88	0
54	MG	BA	3054	1/1	0.43	-	91,91,91,91	0
54	MG	DA	3018	1/1	0.32	-	83,83,83,83	0
54	MG	BA	3454	1/1	0.40	-	103,103,103,103	0
54	MG	BA	3286	1/1	0.26	-	98,98,98,98	0
54	MG	BA	3197	1/1	0.21	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1674	1/1	0.52	-	119,119,119,119	0
54	MG	CA	1797	1/1	0.19	-	127,127,127,127	0
54	MG	BA	3142	1/1	0.42	-	48,48,48,48	0
54	MG	DA	3009	1/1	0.34	-	74,74,74,74	0
54	MG	DA	3318	1/1	0.18	-	91,91,91,91	0
54	MG	DA	3234	1/1	0.17	-	92,92,92,92	0
54	MG	CA	1644	1/1	0.46	-	133,133,133,133	0
54	MG	CA	1773	1/1	0.19	-	114,114,114,114	0
54	MG	BA	3526	1/1	0.56	-	115,115,115,115	0
54	MG	AA	1682	1/1	0.07	-	113,113,113,113	0
54	MG	BA	3502	1/1	0.48	-	90,90,90,90	0
54	MG	BA	3116	1/1	0.34	-	137,137,137,137	0
54	MG	CA	1767	1/1	0.37	-	90,90,90,90	0
54	MG	AA	1747	1/1	0.23	-	159,159,159,159	0
54	MG	DA	3471	1/1	0.11	-	102,102,102,102	0
54	MG	BA	3487	1/1	0.06	-	116,116,116,116	0
54	MG	CA	1765	1/1	0.20	-	126,126,126,126	0
54	MG	BA	3003	1/1	0.34	-	78,78,78,78	0
54	MG	DA	3420	1/1	0.10	-	108,108,108,108	0
54	MG	BA	3560	1/1	0.35	-	91,91,91,91	0
54	MG	DA	3459	1/1	0.29	-	108,108,108,108	0
54	MG	BA	3440	1/1	0.30	-	79,79,79,79	0
54	MG	BA	3512	1/1	0.27	-	97,97,97,97	0
54	MG	AA	1787	1/1	0.20	-	115,115,115,115	0
54	MG	BA	3048	1/1	0.14	-	70,70,70,70	0
54	MG	DA	3441	1/1	0.20	-	116,116,116,116	0
54	MG	DA	3349	1/1	0.23	-	88,88,88,88	0
54	MG	BA	3114	1/1	0.44	-	83,83,83,83	0
54	MG	AA	1606	1/1	0.08	-	155,155,155,155	0
54	MG	BA	3336	1/1	0.25	-	109,109,109,109	0
54	MG	BA	3351	1/1	0.55	-	84,84,84,84	0
54	MG	DA	3236	1/1	0.34	-	60,60,60,60	0
54	MG	CA	1735	1/1	0.09	-	103,103,103,103	0
54	MG	AA	1670	1/1	0.17	-	83,83,83,83	0
54	MG	BA	3241	1/1	0.37	-	91,91,91,91	0
54	MG	DU	201	1/1	0.21	-	103,103,103,103	0
54	MG	BA	3617	1/1	0.38	-	134,134,134,134	0
54	MG	DA	3262	1/1	0.13	-	112,112,112,112	0
54	MG	BA	3015	1/1	0.27	-	61,61,61,61	0
54	MG	AA	1724	1/1	0.42	-	115,115,115,115	0
54	MG	BA	3006	1/1	0.19	-	50,50,50,50	0
54	MG	BB	203	1/1	0.39	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3360	1/1	0.27	-	85,85,85,85	0
54	MG	BA	3046	1/1	0.42	-	86,86,86,86	0
54	MG	AC	108	1/1	1.38	-	112,112,112,112	0
54	MG	BA	3324	1/1	0.29	-	101,101,101,101	0
54	MG	AA	1803	1/1	0.27	-	133,133,133,133	0
54	MG	BB	205	1/1	0.50	-	93,93,93,93	0
54	MG	DA	3207	1/1	0.21	-	86,86,86,86	0
54	MG	DA	3163	1/1	0.17	-	120,120,120,120	0
54	MG	DB	208	1/1	0.10	-	105,105,105,105	0
54	MG	DA	3147	1/1	0.35	-	82,82,82,82	0
54	MG	DA	3087	1/1	0.16	-	111,111,111,111	0
54	MG	DA	3222	1/1	0.27	-	62,62,62,62	0
54	MG	AA	1815	1/1	0.26	-	88,88,88,88	0
54	MG	BA	3056	1/1	0.55	-	101,101,101,101	0
54	MG	DA	3014	1/1	0.36	-	69,69,69,69	0
54	MG	AC	104	1/1	0.32	-	107,107,107,107	0
54	MG	DA	3092	1/1	0.32	-	80,80,80,80	0
54	MG	CA	1721	1/1	0.13	-	128,128,128,128	0
54	MG	BA	3595	1/1	0.45	-	105,105,105,105	0
54	MG	CA	1717	1/1	0.29	-	135,135,135,135	0
54	MG	AA	1792	1/1	0.46	-	93,93,93,93	0
54	MG	DA	3353	1/1	0.41	-	108,108,108,108	0
54	MG	CG	301	1/1	0.35	-	115,115,115,115	0
54	MG	BA	3597	1/1	0.30	-	69,69,69,69	0
54	MG	BA	3398	1/1	0.60	-	105,105,105,105	0
54	MG	CA	1700	1/1	0.28	-	92,92,92,92	0
54	MG	DA	3362	1/1	0.21	-	120,120,120,120	0
54	MG	BA	3554	1/1	0.33	-	99,99,99,99	0
54	MG	DA	3481	1/1	0.44	-	101,101,101,101	0
54	MG	BA	3433	1/1	0.17	-	107,107,107,107	0
54	MG	BA	3410	1/1	0.32	-	120,120,120,120	0
54	MG	DZ	101	1/1	0.31	-	113,113,113,113	0
54	MG	CA	1768	1/1	0.14	-	106,106,106,106	0
54	MG	CA	1753	1/1	0.18	-	95,95,95,95	0
54	MG	DA	3255	1/1	0.19	-	87,87,87,87	0
54	MG	DA	3176	1/1	0.14	-	112,112,112,112	0
54	MG	DA	3351	1/1	0.38	-	90,90,90,90	0
54	MG	AA	1721	1/1	0.29	-	115,115,115,115	0
54	MG	DA	3089	1/1	0.13	-	117,117,117,117	0
54	MG	AA	1680	1/1	0.38	-	104,104,104,104	0
54	MG	DA	3114	1/1	0.19	-	82,82,82,82	0
54	MG	AA	1668	1/1	0.33	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1696	1/1	0.24	-	104,104,104,104	0
54	MG	DA	3231	1/1	0.24	-	74,74,74,74	0
54	MG	BA	3065	1/1	0.16	-	135,135,135,135	0
54	MG	BA	3258	1/1	0.43	-	74,74,74,74	0
54	MG	AA	1633	1/1	0.36	-	80,80,80,80	0
54	MG	BA	3517	1/1	0.16	-	121,121,121,121	0
54	MG	CA	1641	1/1	0.16	-	135,135,135,135	0
54	MG	DA	3513	1/1	0.25	-	95,95,95,95	0
54	MG	AA	1663	1/1	0.15	-	76,76,76,76	0
54	MG	BA	3106	1/1	0.24	-	52,52,52,52	0
54	MG	BA	3549	1/1	0.12	-	140,140,140,140	0
54	MG	AA	1805	1/1	0.32	-	108,108,108,108	0
54	MG	DA	3337	1/1	0.16	-	88,88,88,88	0
54	MG	AA	1773	1/1	0.55	-	137,137,137,137	0
54	MG	BA	3141	1/1	0.22	-	63,63,63,63	0
54	MG	BA	3212	1/1	0.52	-	124,124,124,124	0
54	MG	DA	3123	1/1	0.20	-	106,106,106,106	0
54	MG	BA	3240	1/1	0.38	-	93,93,93,93	0
54	MG	BA	3136	1/1	0.28	-	62,62,62,62	0
54	MG	DA	3238	1/1	0.11	-	117,117,117,117	0
54	MG	BA	3080	1/1	0.22	-	125,125,125,125	0
54	MG	BA	3014	1/1	0.34	-	68,68,68,68	0
54	MG	DA	3155	1/1	0.13	-	80,80,80,80	0
54	MG	AA	1625	1/1	0.13	-	110,110,110,110	0
54	MG	DA	3319	1/1	0.24	-	77,77,77,77	0
54	MG	BA	3303	1/1	0.13	-	119,119,119,119	0
54	MG	AA	1759	1/1	0.28	-	87,87,87,87	0
54	MG	AA	1806	1/1	0.42	-	100,100,100,100	0
54	MG	CA	1610	1/1	0.16	-	147,147,147,147	0
54	MG	DA	3504	1/1	0.44	-	67,67,67,67	0
54	MG	CA	1656	1/1	0.25	-	129,129,129,129	0
54	MG	DA	3201	1/1	0.26	-	73,73,73,73	0
54	MG	DA	3104	1/1	0.34	-	107,107,107,107	0
54	MG	AA	1766	1/1	0.19	-	94,94,94,94	0
54	MG	CA	1696	1/1	0.40	-	98,98,98,98	0
54	MG	CH	201	1/1	0.36	-	114,114,114,114	0
54	MG	DA	3082	1/1	0.14	-	99,99,99,99	0
54	MG	DA	3265	1/1	0.42	-	115,115,115,115	0
54	MG	BA	3027	1/1	0.25	-	69,69,69,69	0
54	MG	AA	1820	1/1	1.41	-	130,130,130,130	0
54	MG	BA	3420	1/1	0.38	-	70,70,70,70	0
54	MG	AA	1719	1/1	0.22	-	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3090	1/1	0.18	-	78,78,78,78	0
56	ZN	CQ	101	1/1	0.04	-	188,188,188,188	0
54	MG	BA	3455	1/1	0.72	-	107,107,107,107	0
54	MG	BA	3476	1/1	0.48	-	59,59,59,59	0
54	MG	BA	3215	1/1	0.33	-	119,119,119,119	0
54	MG	A1	101	1/1	0.33	-	72,72,72,72	0
54	MG	BA	3137	1/1	0.27	-	105,105,105,105	0
54	MG	AA	1816	1/1	0.11	-	115,115,115,115	0
54	MG	DA	3198	1/1	0.36	-	95,95,95,95	0
54	MG	CA	1662	1/1	0.28	-	120,120,120,120	0
54	MG	BA	3594	1/1	0.67	-	94,94,94,94	0
54	MG	BA	3542	1/1	0.56	-	100,100,100,100	0
54	MG	CA	1609	1/1	0.38	-	119,119,119,119	0
54	MG	CA	1780	1/1	0.11	-	137,137,137,137	0
54	MG	AA	1613	1/1	0.18	-	144,144,144,144	0
54	MG	BA	3462	1/1	0.17	-	113,113,113,113	0
54	MG	BA	3176	1/1	0.09	-	89,89,89,89	0
54	MG	AA	1831	1/1	0.16	-	124,124,124,124	0
54	MG	DA	3048	1/1	0.16	-	84,84,84,84	0
54	MG	DA	3376	1/1	0.23	-	87,87,87,87	0
54	MG	AA	1746	1/1	0.22	-	92,92,92,92	0
54	MG	DA	3250	1/1	0.91	-	105,105,105,105	0
54	MG	BA	3598	1/1	0.34	-	84,84,84,84	0
54	MG	BA	3577	1/1	0.28	-	61,61,61,61	0
54	MG	BA	3505	1/1	0.49	-	108,108,108,108	0
54	MG	DA	3522	1/1	0.19	-	113,113,113,113	0
54	MG	CG	302	1/1	0.47	-	180,180,180,180	0
54	MG	BA	3062	1/1	0.23	-	70,70,70,70	0
54	MG	BA	3122	1/1	0.27	-	114,114,114,114	0
54	MG	DA	3424	1/1	0.45	-	115,115,115,115	0
54	MG	DA	3029	1/1	0.24	-	87,87,87,87	0
54	MG	AA	1649	1/1	0.13	-	90,90,90,90	0
54	MG	BA	3028	1/1	0.39	-	57,57,57,57	0
54	MG	DA	3225	1/1	0.11	-	89,89,89,89	0
54	MG	DA	3069	1/1	0.21	-	101,101,101,101	0
54	MG	BA	3425	1/1	0.07	-	137,137,137,137	0
54	MG	BA	3169	1/1	0.40	-	104,104,104,104	0
54	MG	BA	3317	1/1	0.45	-	99,99,99,99	0
54	MG	DA	3498	1/1	0.11	-	106,106,106,106	0
54	MG	BA	3540	1/1	0.52	-	122,122,122,122	0
54	MG	BA	3239	1/1	0.38	-	82,82,82,82	0
54	MG	CA	1625	1/1	0.14	-	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	210	1/1	0.41	-	78,78,78,78	0
54	MG	BA	3449	1/1	0.58	-	118,118,118,118	0
54	MG	DA	3452	1/1	0.45	-	91,91,91,91	0
54	MG	BA	3515	1/1	0.58	-	112,112,112,112	0
54	MG	DA	3308	1/1	0.24	-	94,94,94,94	0
54	MG	BA	3123	1/1	0.35	-	73,73,73,73	0
54	MG	DA	3158	1/1	0.59	-	113,113,113,113	0
54	MG	DA	3431	1/1	0.58	-	101,101,101,101	0
54	MG	BA	3103	1/1	0.31	-	93,93,93,93	0
54	MG	DA	3215	1/1	0.18	-	80,80,80,80	0
54	MG	BA	3171	1/1	0.25	-	87,87,87,87	0
54	MG	DA	3209	1/1	0.21	-	100,100,100,100	0
54	MG	AQ	102	1/1	0.14	-	118,118,118,118	0
54	MG	BA	3189	1/1	0.28	-	88,88,88,88	0
54	MG	BA	3265	1/1	0.33	-	96,96,96,96	0
54	MG	DA	3470	1/1	0.31	-	124,124,124,124	0
54	MG	CA	1747	1/1	0.50	-	122,122,122,122	0
54	MG	BA	3570	1/1	0.23	-	82,82,82,82	0
54	MG	CA	1703	1/1	0.24	-	93,93,93,93	0
54	MG	DA	3153	1/1	0.16	-	145,145,145,145	0
54	MG	BZ	101	1/1	0.21	-	69,69,69,69	0
54	MG	BA	3008	1/1	0.45	-	58,58,58,58	0
54	MG	DA	3242	1/1	0.33	-	64,64,64,64	0
54	MG	CA	1802	1/1	0.47	-	136,136,136,136	0
54	MG	BA	3367	1/1	0.39	-	124,124,124,124	0
54	MG	CA	1605	1/1	0.45	-	131,131,131,131	0
54	MG	AA	1603	1/1	0.25	-	109,109,109,109	0
54	MG	CA	1689	1/1	0.38	-	122,122,122,122	0
54	MG	DA	3004	1/1	0.40	-	120,120,120,120	0
54	MG	CA	1769	1/1	0.27	-	136,136,136,136	0
54	MG	CA	1638	1/1	0.24	-	128,128,128,128	0
54	MG	BA	3315	1/1	0.33	-	91,91,91,91	0
54	MG	BA	3432	1/1	0.18	-	126,126,126,126	0
54	MG	BA	3174	1/1	0.19	-	61,61,61,61	0
54	MG	DB	206	1/1	0.37	-	142,142,142,142	0
54	MG	DA	3084	1/1	0.11	-	98,98,98,98	0
54	MG	CA	1669	1/1	0.16	-	130,130,130,130	0
54	MG	DA	3465	1/1	0.39	-	111,111,111,111	0
54	MG	DA	3016	1/1	0.36	-	123,123,123,123	0
54	MG	BA	3079	1/1	0.55	-	99,99,99,99	0
54	MG	DA	3462	1/1	0.10	-	102,102,102,102	0
54	MG	BA	3402	1/1	0.24	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3280	1/1	0.31	-	106,106,106,106	0
54	MG	DA	3432	1/1	0.28	-	91,91,91,91	0
54	MG	AA	1650	1/1	0.26	-	85,85,85,85	0
54	MG	BA	3070	1/1	0.40	-	119,119,119,119	0
54	MG	DA	3151	1/1	0.27	-	113,113,113,113	0
54	MG	BA	3439	1/1	0.43	-	109,109,109,109	0
54	MG	AA	1737	1/1	0.35	-	132,132,132,132	0
54	MG	DA	3324	1/1	0.33	-	109,109,109,109	0
54	MG	BA	3296	1/1	0.52	-	93,93,93,93	0
54	MG	BA	3209	1/1	0.34	-	79,79,79,79	0
54	MG	BA	3448	1/1	0.34	-	95,95,95,95	0
54	MG	BA	3576	1/1	0.26	-	120,120,120,120	0
54	MG	BA	3609	1/1	0.24	-	102,102,102,102	0
54	MG	BA	3294	1/1	0.52	-	79,79,79,79	0
54	MG	CA	1748	1/1	0.22	-	81,81,81,81	0
54	MG	DA	3036	1/1	0.32	-	108,108,108,108	0
54	MG	BA	3571	1/1	0.45	-	85,85,85,85	0
54	MG	BA	3396	1/1	0.50	-	101,101,101,101	0
54	MG	BA	3481	1/1	0.38	-	99,99,99,99	0
54	MG	DA	3342	1/1	0.30	-	114,114,114,114	0
54	MG	BA	3511	1/1	0.23	-	80,80,80,80	0
54	MG	DA	3028	1/1	0.43	-	122,122,122,122	0
54	MG	DA	3379	1/1	0.47	-	64,64,64,64	0
54	MG	DA	3019	1/1	0.25	-	84,84,84,84	0
54	MG	CA	1794	1/1	0.46	-	109,109,109,109	0
54	MG	AA	1646	1/1	0.08	-	150,150,150,150	0
54	MG	BA	3213	1/1	0.24	-	69,69,69,69	0
54	MG	BA	3261	1/1	0.18	-	90,90,90,90	0
54	MG	BA	3036	1/1	0.28	-	63,63,63,63	0
54	MG	BA	3435	1/1	0.11	-	109,109,109,109	0
54	MG	CA	1620	1/1	0.27	-	73,73,73,73	0
54	MG	CA	1619	1/1	0.15	-	111,111,111,111	0
54	MG	AA	1728	1/1	0.12	-	85,85,85,85	0
54	MG	AA	1698	1/1	0.20	-	132,132,132,132	0
54	MG	CA	1764	1/1	0.34	-	110,110,110,110	0
54	MG	DA	3457	1/1	0.15	-	102,102,102,102	0
54	MG	AA	1689	1/1	0.32	-	153,153,153,153	0
54	MG	BA	3190	1/1	0.32	-	93,93,93,93	0
54	MG	DA	3072	1/1	0.32	-	94,94,94,94	0
54	MG	BA	3270	1/1	0.19	-	87,87,87,87	0
54	MG	AA	1786	1/1	0.31	-	131,131,131,131	0
54	MG	BA	3534	1/1	0.45	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1612	1/1	0.23	-	135,135,135,135	0
54	MG	DA	3391	1/1	0.11	-	94,94,94,94	0
54	MG	DA	3347	1/1	0.40	-	116,116,116,116	0
54	MG	BA	3613	1/1	0.20	-	111,111,111,111	0
54	MG	AJ	201	1/1	0.68	-	108,108,108,108	0
54	MG	DA	3291	1/1	0.43	-	85,85,85,85	0
54	MG	DA	3380	1/1	0.35	-	94,94,94,94	0
54	MG	AA	1692	1/1	0.22	-	108,108,108,108	0
54	MG	CA	1707	1/1	0.50	-	109,109,109,109	0
54	MG	DA	3196	1/1	0.29	-	101,101,101,101	0
54	MG	DA	3271	1/1	0.26	-	62,62,62,62	0
54	MG	DA	3113	1/1	0.30	-	105,105,105,105	0
54	MG	BA	3019	1/1	0.30	-	49,49,49,49	0
54	MG	DA	3372	1/1	0.26	-	101,101,101,101	0
54	MG	DA	3469	1/1	0.25	-	107,107,107,107	0
54	MG	AA	1703	1/1	0.24	-	87,87,87,87	0
54	MG	BA	3087	1/1	0.07	-	142,142,142,142	0
54	MG	DD	301	1/1	0.59	-	119,119,119,119	0
54	MG	DA	3451	1/1	0.19	-	90,90,90,90	0
54	MG	BA	3135	1/1	0.17	-	90,90,90,90	0
54	MG	CA	1732	1/1	0.22	-	144,144,144,144	0
54	MG	DA	3132	1/1	0.21	-	78,78,78,78	0
54	MG	DA	3109	1/1	0.26	-	63,63,63,63	0
54	MG	AA	1644	1/1	0.26	-	72,72,72,72	0
54	MG	BA	3326	1/1	0.29	-	89,89,89,89	0
54	MG	BA	3203	1/1	0.37	-	86,86,86,86	0
54	MG	BA	3186	1/1	0.35	-	62,62,62,62	0
54	MG	AA	1752	1/1	0.26	-	121,121,121,121	0
54	MG	BA	3299	1/1	0.49	-	78,78,78,78	0
54	MG	AA	1624	1/1	0.12	-	98,98,98,98	0
54	MG	CA	1642	1/1	0.17	-	105,105,105,105	0
54	MG	BB	211	1/1	0.40	-	102,102,102,102	0
54	MG	DA	3191	1/1	0.36	-	103,103,103,103	0
54	MG	DA	3160	1/1	0.47	-	84,84,84,84	0
54	MG	BA	3470	1/1	0.50	-	117,117,117,117	0
54	MG	BA	3195	1/1	0.14	-	82,82,82,82	0
54	MG	DA	3511	1/1	0.74	-	111,111,111,111	0
54	MG	DA	3332	1/1	0.25	-	120,120,120,120	0
54	MG	BA	3355	1/1	0.52	-	90,90,90,90	0
54	MG	BA	3447	1/1	0.30	-	116,116,116,116	0
54	MG	BE	301	1/1	0.28	-	61,61,61,61	0
54	MG	AA	1748	1/1	0.27	-	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	DB	212	1/1	0.46	-	102,102,102,102	0
54	MG	BA	3099	1/1	0.44	-	74,74,74,74	0
54	MG	CA	1759	1/1	0.08	-	157,157,157,157	0
54	MG	DA	3135	1/1	0.46	-	99,99,99,99	0
54	MG	AA	1684	1/1	0.40	-	123,123,123,123	0
54	MG	AA	1761	1/1	0.12	-	152,152,152,152	0
54	MG	BA	3231	1/1	0.44	-	93,93,93,93	0
54	MG	BA	3592	1/1	0.28	-	112,112,112,112	0
54	MG	DA	3137	1/1	0.27	-	74,74,74,74	0
54	MG	BA	3323	1/1	0.52	-	116,116,116,116	0
54	MG	BA	3620	1/1	0.17	-	72,72,72,72	0
54	MG	DZ	102	1/1	0.11	-	88,88,88,88	0
54	MG	DA	3022	1/1	0.21	-	86,86,86,86	0
54	MG	DA	3317	1/1	0.45	-	131,131,131,131	0
54	MG	CA	1686	1/1	0.42	-	79,79,79,79	0
54	MG	CA	1792	1/1	0.15	-	160,160,160,160	0
54	MG	DA	3003	1/1	0.27	-	130,130,130,130	0
54	MG	BA	3112	1/1	0.35	-	97,97,97,97	0
54	MG	DB	203	1/1	0.22	-	95,95,95,95	0
54	MG	DA	3490	1/1	0.14	-	120,120,120,120	0
54	MG	DA	3284	1/1	0.33	-	100,100,100,100	0
54	MG	BA	3604	1/1	0.22	-	97,97,97,97	0
54	MG	DA	3251	1/1	0.14	-	91,91,91,91	0
54	MG	BA	3037	1/1	0.46	-	71,71,71,71	0
54	MG	BA	3165	1/1	0.17	-	119,119,119,119	0
54	MG	AA	1605	1/1	0.32	-	108,108,108,108	0
54	MG	BA	3084	1/1	0.82	-	110,110,110,110	0
54	MG	BA	3450	1/1	0.25	-	99,99,99,99	0
54	MG	BA	3482	1/1	0.46	-	88,88,88,88	0
54	MG	DA	3267	1/1	0.15	-	79,79,79,79	0
54	MG	CA	1785	1/1	0.32	-	83,83,83,83	0
54	MG	BA	3085	1/1	0.45	-	95,95,95,95	0
54	MG	BA	3263	1/1	0.30	-	50,50,50,50	0
54	MG	AA	1777	1/1	0.04	-	141,141,141,141	0
54	MG	DA	3164	1/1	0.49	-	136,136,136,136	0
54	MG	BA	3318	1/1	0.34	-	88,88,88,88	0
54	MG	BA	3564	1/1	0.29	-	116,116,116,116	0
54	MG	BA	3518	1/1	0.20	-	86,86,86,86	0
54	MG	CA	1613	1/1	0.38	-	94,94,94,94	0
54	MG	BA	3279	1/1	0.48	-	74,74,74,74	0
54	MG	AA	1710	1/1	0.33	-	116,116,116,116	0
54	MG	CA	1788	1/1	0.32	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3177	1/1	0.30	-	99,99,99,99	0
54	MG	AA	1704	1/1	0.42	-	112,112,112,112	0
54	MG	BA	3559	1/1	0.37	-	105,105,105,105	0
54	MG	DA	3488	1/1	0.55	-	105,105,105,105	0
54	MG	BA	3521	1/1	0.25	-	123,123,123,123	0
54	MG	AA	1828	1/1	0.38	-	94,94,94,94	0
54	MG	DA	3181	1/1	0.15	-	74,74,74,74	0
54	MG	BA	3593	1/1	0.35	-	57,57,57,57	0
54	MG	BA	3097	1/1	0.40	-	83,83,83,83	0
54	MG	CA	1688	1/1	0.41	-	101,101,101,101	0
54	MG	BA	3492	1/1	0.49	-	76,76,76,76	0
54	MG	BA	3173	1/1	0.32	-	62,62,62,62	0
54	MG	CA	1775	1/1	0.12	-	90,90,90,90	0
54	MG	DA	3327	1/1	0.23	-	70,70,70,70	0
54	MG	DA	3202	1/1	0.27	-	88,88,88,88	0
54	MG	DA	3385	1/1	0.19	-	95,95,95,95	0
54	MG	DA	3061	1/1	0.25	-	64,64,64,64	0
54	MG	BA	3407	1/1	0.42	-	105,105,105,105	0
54	MG	DA	3329	1/1	0.08	-	110,110,110,110	0
54	MG	AA	1653	1/1	0.24	-	91,91,91,91	0
54	MG	DA	3017	1/1	0.24	-	111,111,111,111	0
54	MG	DA	3418	1/1	0.35	-	61,61,61,61	0
54	MG	DA	3068	1/1	0.36	-	122,122,122,122	0
54	MG	BA	3304	1/1	0.23	-	90,90,90,90	0
54	MG	DA	3059	1/1	0.18	-	68,68,68,68	0
54	MG	DA	3444	1/1	0.18	-	100,100,100,100	0
54	MG	AA	1683	1/1	0.39	-	116,116,116,116	0
54	MG	BA	3253	1/1	0.10	-	89,89,89,89	0
54	MG	BA	3452	1/1	0.25	-	131,131,131,131	0
54	MG	DA	3417	1/1	0.16	-	110,110,110,110	0
54	MG	DB	209	1/1	0.19	-	131,131,131,131	0
54	MG	BA	3359	1/1	0.16	-	92,92,92,92	0
54	MG	DA	3107	1/1	0.25	-	100,100,100,100	0
54	MG	BA	3017	1/1	0.25	-	67,67,67,67	0
54	MG	BA	3584	1/1	0.39	-	100,100,100,100	0
54	MG	CA	1648	1/1	0.14	-	96,96,96,96	0
54	MG	AA	1795	1/1	0.24	-	102,102,102,102	0
54	MG	DA	3472	1/1	0.53	-	102,102,102,102	0
54	MG	AA	1739	1/1	0.54	-	99,99,99,99	0
54	MG	BA	3491	1/1	0.41	-	84,84,84,84	0
54	MG	BA	3475	1/1	0.07	-	270,270,270,270	0
54	MG	DA	3500	1/1	0.10	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1732	1/1	0.39	-	112,112,112,112	0
54	MG	DB	214	1/1	0.13	-	118,118,118,118	0
54	MG	DA	3175	1/1	0.20	-	101,101,101,101	0
54	MG	DA	3334	1/1	0.10	-	136,136,136,136	0
54	MG	BA	3089	1/1	0.52	-	77,77,77,77	0
54	MG	BA	3107	1/1	0.54	-	76,76,76,76	0
54	MG	BA	3483	1/1	0.15	-	89,89,89,89	0
54	MG	CA	1603	1/1	0.56	-	93,93,93,93	0
54	MG	DA	3052	1/1	0.22	-	120,120,120,120	0
54	MG	DA	3388	1/1	0.07	-	152,152,152,152	0
54	MG	DA	3447	1/1	0.12	-	87,87,87,87	0
54	MG	BA	3535	1/1	0.46	-	116,116,116,116	0
54	MG	BA	3362	1/1	0.61	-	70,70,70,70	0
54	MG	AA	1702	1/1	0.44	-	77,77,77,77	0
54	MG	AA	1784	1/1	0.34	-	91,91,91,91	0
54	MG	CA	1630	1/1	0.47	-	120,120,120,120	0
54	MG	DA	3249	1/1	0.30	-	65,65,65,65	0
54	MG	AA	1824	1/1	0.18	-	120,120,120,120	0
54	MG	DA	3323	1/1	0.14	-	79,79,79,79	0
54	MG	DA	3302	1/1	0.37	-	79,79,79,79	0
54	MG	DA	3279	1/1	0.31	-	125,125,125,125	0
54	MG	DA	3454	1/1	0.14	-	94,94,94,94	0
54	MG	DA	3497	1/1	0.17	-	50,50,50,50	0
54	MG	DA	3243	1/1	0.17	-	86,86,86,86	0
54	MG	DA	3043	1/1	0.19	-	106,106,106,106	0
54	MG	DA	3142	1/1	0.15	-	99,99,99,99	0
54	MG	DA	3378	1/1	0.20	-	100,100,100,100	0
54	MG	BA	3035	1/1	0.27	-	70,70,70,70	0
54	MG	DA	3148	1/1	0.24	-	70,70,70,70	0
54	MG	DA	3333	1/1	0.28	-	128,128,128,128	0
54	MG	AA	1788	1/1	0.30	-	124,124,124,124	0
54	MG	BA	3397	1/1	0.35	-	92,92,92,92	0
54	MG	BA	3436	1/1	0.22	-	118,118,118,118	0
54	MG	DA	3125	1/1	0.18	-	105,105,105,105	0
54	MG	DA	3348	1/1	0.24	-	108,108,108,108	0
54	MG	DA	3509	1/1	0.19	-	93,93,93,93	0
54	MG	DA	3057	1/1	0.15	-	104,104,104,104	0
54	MG	BA	3395	1/1	0.54	-	105,105,105,105	0
54	MG	BA	3293	1/1	0.37	-	77,77,77,77	0
54	MG	BA	3145	1/1	0.38	-	83,83,83,83	0
54	MG	DA	3501	1/1	0.23	-	73,73,73,73	0
54	MG	CA	1796	1/1	0.24	-	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3298	1/1	0.35	-	73,73,73,73	0
54	MG	BA	3340	1/1	0.59	-	95,95,95,95	0
54	MG	AA	1809	1/1	0.43	-	108,108,108,108	0
54	MG	DA	3483	1/1	0.21	-	88,88,88,88	0
54	MG	DA	3275	1/1	0.19	-	93,93,93,93	0
54	MG	BA	3457	1/1	0.34	-	112,112,112,112	0
54	MG	AA	1733	1/1	0.25	-	120,120,120,120	0
54	MG	DA	3145	1/1	0.15	-	110,110,110,110	0
54	MG	DA	3031	1/1	0.29	-	70,70,70,70	0
54	MG	AA	1832	1/1	0.28	-	102,102,102,102	0
54	MG	AA	1771	1/1	0.24	-	117,117,117,117	0
54	MG	DA	3037	1/1	0.29	-	117,117,117,117	0
54	MG	BA	3348	1/1	0.38	-	90,90,90,90	0
54	MG	DA	3097	1/1	0.37	-	74,74,74,74	0
54	MG	DA	3412	1/1	0.20	-	110,110,110,110	0
54	MG	DA	3484	1/1	0.20	-	81,81,81,81	0
54	MG	DA	3230	1/1	0.33	-	65,65,65,65	0
54	MG	DA	3288	1/1	0.16	-	95,95,95,95	0
54	MG	DA	3100	1/1	0.40	-	100,100,100,100	0
54	MG	BA	3217	1/1	0.25	-	92,92,92,92	0
54	MG	AA	1730	1/1	0.81	-	116,116,116,116	0
54	MG	DA	3389	1/1	0.27	-	94,94,94,94	0
54	MG	BA	3024	1/1	0.23	-	81,81,81,81	0
54	MG	CA	1680	1/1	0.25	-	94,94,94,94	0
54	MG	BA	3532	1/1	0.36	-	100,100,100,100	0
54	MG	BA	3301	1/1	0.28	-	85,85,85,85	0
54	MG	BA	3023	1/1	0.21	-	66,66,66,66	0
54	MG	DE	301	1/1	0.16	-	73,73,73,73	0
54	MG	DA	3480	1/1	0.16	-	84,84,84,84	0
54	MG	DA	3430	1/1	0.18	-	105,105,105,105	0
54	MG	BA	3466	1/1	0.24	-	92,92,92,92	0
54	MG	BA	3366	1/1	0.38	-	95,95,95,95	0
54	MG	DA	3473	1/1	0.11	-	157,157,157,157	0
54	MG	AA	1678	1/1	0.44	-	108,108,108,108	0
54	MG	BA	3472	1/1	0.34	-	114,114,114,114	0
54	MG	AA	1661	1/1	0.35	-	94,94,94,94	0
54	MG	BA	3268	1/1	0.41	-	87,87,87,87	0
54	MG	BA	3572	1/1	0.26	-	113,113,113,113	0
54	MG	DA	3094	1/1	0.12	-	85,85,85,85	0
54	MG	CA	1655	1/1	0.43	-	125,125,125,125	0
54	MG	BA	3199	1/1	0.10	-	78,78,78,78	0
54	MG	AA	1714	1/1	0.21	-	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1814	1/1	0.06	-	152,152,152,152	0
54	MG	AA	1699	1/1	0.26	-	122,122,122,122	0
54	MG	BA	3453	1/1	0.40	-	85,85,85,85	0
54	MG	BA	3347	1/1	0.24	-	72,72,72,72	0
54	MG	BA	3376	1/1	0.49	-	96,96,96,96	0
54	MG	BA	3281	1/1	0.65	-	106,106,106,106	0
54	MG	DA	3070	1/1	0.27	-	76,76,76,76	0
54	MG	DA	3128	1/1	0.25	-	65,65,65,65	0
54	MG	DA	3150	1/1	0.42	-	96,96,96,96	0
54	MG	DA	3519	1/1	0.23	-	94,94,94,94	0
54	MG	CA	1643	1/1	0.08	-	148,148,148,148	0
54	MG	DA	3154	1/1	0.21	-	111,111,111,111	0
54	MG	BA	3146	1/1	0.47	-	82,82,82,82	0
54	MG	CA	1685	1/1	0.12	-	121,121,121,121	0
54	MG	DA	3256	1/1	1.20	-	103,103,103,103	0
54	MG	AA	1736	1/1	0.15	-	122,122,122,122	0
54	MG	BA	3066	1/1	0.28	-	97,97,97,97	0
54	MG	BA	3055	1/1	0.49	-	69,69,69,69	0
54	MG	BA	3126	1/1	0.20	-	89,89,89,89	0
54	MG	DA	3492	1/1	0.19	-	111,111,111,111	0
54	MG	DA	3054	1/1	0.31	-	88,88,88,88	0
54	MG	AA	1659	1/1	0.15	-	71,71,71,71	0
54	MG	AA	1691	1/1	0.36	-	105,105,105,105	0
54	MG	CA	1782	1/1	0.42	-	98,98,98,98	0
54	MG	AA	1725	1/1	0.23	-	111,111,111,111	0
54	MG	CA	1666	1/1	0.35	-	120,120,120,120	0
54	MG	CA	1755	1/1	0.15	-	97,97,97,97	0
54	MG	DA	3221	1/1	0.26	-	61,61,61,61	0
54	MG	AC	101	1/1	0.17	-	78,78,78,78	0
54	MG	DA	3390	1/1	0.18	-	144,144,144,144	0
54	MG	BA	3488	1/1	0.51	-	109,109,109,109	0
54	MG	CC	105	1/1	0.08	-	125,125,125,125	0
54	MG	DA	3307	1/1	0.48	-	102,102,102,102	0
54	MG	AA	1662	1/1	0.95	-	111,111,111,111	0
54	MG	DA	3419	1/1	0.22	-	100,100,100,100	0
54	MG	BA	3074	1/1	0.12	-	142,142,142,142	0
54	MG	BA	3160	1/1	0.55	-	109,109,109,109	0
54	MG	CA	1726	1/1	0.28	-	111,111,111,111	0
54	MG	BA	3361	1/1	0.48	-	123,123,123,123	0
54	MG	DA	3328	1/1	0.04	-	138,138,138,138	0
54	MG	DA	3298	1/1	0.11	-	96,96,96,96	0
54	MG	BA	3043	1/1	0.35	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3422	1/1	0.28	-	93,93,93,93	0
54	MG	BA	3328	1/1	0.25	-	119,119,119,119	0
54	MG	DA	3187	1/1	0.18	-	70,70,70,70	0
54	MG	BA	3063	1/1	0.23	-	121,121,121,121	0
54	MG	DA	3146	1/1	0.63	-	87,87,87,87	0
54	MG	DA	3121	1/1	0.26	-	68,68,68,68	0
54	MG	BA	3132	1/1	0.42	-	127,127,127,127	0
54	MG	DA	3396	1/1	0.20	-	95,95,95,95	0
54	MG	BA	3192	1/1	0.30	-	67,67,67,67	0
54	MG	AA	1652	1/1	0.34	-	91,91,91,91	0
54	MG	DA	3495	1/1	0.30	-	78,78,78,78	0
54	MG	DA	3489	1/1	0.22	-	98,98,98,98	0
54	MG	BA	3520	1/1	0.48	-	129,129,129,129	0
54	MG	DA	3282	1/1	0.15	-	88,88,88,88	0
54	MG	AA	1711	1/1	0.26	-	118,118,118,118	0
54	MG	DA	3080	1/1	0.25	-	114,114,114,114	0
54	MG	BU	201	1/1	0.14	-	105,105,105,105	0
54	MG	BE	302	1/1	1.17	-	104,104,104,104	0
54	MG	DA	3024	1/1	0.11	-	112,112,112,112	0
54	MG	BA	3059	1/1	0.13	-	144,144,144,144	0
54	MG	AA	1640	1/1	0.18	-	82,82,82,82	0
54	MG	AA	1708	1/1	0.41	-	104,104,104,104	0
54	MG	DA	3320	1/1	0.34	-	110,110,110,110	0
54	MG	AC	105	1/1	0.12	-	107,107,107,107	0
54	MG	BA	3311	1/1	0.37	-	100,100,100,100	0
54	MG	BA	3497	1/1	0.36	-	78,78,78,78	0
54	MG	DA	3293	1/1	2.00	-	112,112,112,112	0
54	MG	BB	215	1/1	0.08	-	129,129,129,129	0
54	MG	BA	3405	1/1	0.19	-	73,73,73,73	0
54	MG	B3	101	1/1	0.29	-	77,77,77,77	0
54	MG	DA	3399	1/1	0.16	-	126,126,126,126	0
54	MG	BB	212	1/1	0.28	-	103,103,103,103	0
54	MG	CA	1761	1/1	0.20	-	170,170,170,170	0
54	MG	AA	1686	1/1	0.24	-	120,120,120,120	0
54	MG	DA	3166	1/1	0.26	-	65,65,65,65	0
54	MG	AA	1830	1/1	0.09	-	135,135,135,135	0
54	MG	DA	3494	1/1	0.31	-	45,45,45,45	0
54	MG	BA	3050	1/1	0.47	-	75,75,75,75	0
54	MG	BA	3243	1/1	0.29	-	122,122,122,122	0
54	MG	DA	3013	1/1	0.23	-	69,69,69,69	0
54	MG	DA	3136	1/1	0.24	-	64,64,64,64	0
55	TAC	CA	1805	32/32	0.12	-	126,153,170,174	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3206	1/1	0.35	-	58,58,58,58	0
54	MG	DA	3315	1/1	0.25	-	125,125,125,125	0
54	MG	AA	1697	1/1	0.31	-	143,143,143,143	0
54	MG	AA	1760	1/1	0.30	-	122,122,122,122	0
54	MG	CA	1627	1/1	0.53	-	112,112,112,112	0
54	MG	BA	3064	1/1	0.28	-	113,113,113,113	0
54	MG	AA	1829	1/1	0.15	-	112,112,112,112	0
54	MG	DA	3143	1/1	0.11	-	117,117,117,117	0
54	MG	CA	1777	1/1	0.28	-	133,133,133,133	0
54	MG	DA	3141	1/1	0.20	-	85,85,85,85	0
54	MG	AA	1812	1/1	0.30	-	124,124,124,124	0
54	MG	DA	3411	1/1	0.16	-	68,68,68,68	0
54	MG	CA	1799	1/1	0.28	-	150,150,150,150	0
54	MG	DA	3259	1/1	0.46	-	76,76,76,76	0
54	MG	BA	3183	1/1	0.27	-	110,110,110,110	0
54	MG	BA	3335	1/1	0.25	-	96,96,96,96	0
54	MG	DA	3032	1/1	0.47	-	127,127,127,127	0
54	MG	BA	3221	1/1	0.33	-	89,89,89,89	0
54	MG	DA	3076	1/1	0.32	-	75,75,75,75	0
54	MG	BA	3536	1/1	0.40	-	96,96,96,96	0
54	MG	AA	1811	1/1	0.16	-	154,154,154,154	0
54	MG	BA	3101	1/1	0.39	-	58,58,58,58	0
54	MG	AA	1638	1/1	0.38	-	104,104,104,104	0
54	MG	DA	3211	1/1	0.18	-	71,71,71,71	0
54	MG	DA	3514	1/1	0.12	-	71,71,71,71	0
54	MG	CA	1730	1/1	0.39	-	121,121,121,121	0
54	MG	BA	3121	1/1	0.30	-	87,87,87,87	0
54	MG	BA	3306	1/1	0.35	-	81,81,81,81	0
54	MG	BA	3175	1/1	0.10	-	80,80,80,80	0
54	MG	DA	3350	1/1	0.30	-	82,82,82,82	0
54	MG	AA	1800	1/1	0.40	-	92,92,92,92	0
54	MG	DA	3101	1/1	0.43	-	94,94,94,94	0
54	MG	AA	1645	1/1	0.36	-	93,93,93,93	0
54	MG	CA	1738	1/1	0.33	-	114,114,114,114	0
54	MG	DA	3050	1/1	0.13	-	108,108,108,108	0
54	MG	DA	3239	1/1	0.45	-	105,105,105,105	0
54	MG	DA	3455	1/1	0.31	-	147,147,147,147	0
54	MG	CA	1713	1/1	0.14	-	137,137,137,137	0
54	MG	DA	3309	1/1	0.09	-	145,145,145,145	0
54	MG	BA	3551	1/1	0.37	-	105,105,105,105	0
54	MG	BA	3558	1/1	0.38	-	118,118,118,118	0
54	MG	AA	1604	1/1	0.08	-	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3446	1/1	0.49	-	127,127,127,127	0
54	MG	CA	1715	1/1	0.39	-	128,128,128,128	0
54	MG	BA	3525	1/1	0.26	-	96,96,96,96	0
54	MG	DA	3066	1/1	0.18	-	79,79,79,79	0
54	MG	BA	3042	1/1	0.17	-	94,94,94,94	0
54	MG	CC	107	1/1	0.52	-	120,120,120,120	0
54	MG	BA	3227	1/1	0.32	-	82,82,82,82	0
54	MG	DA	3195	1/1	0.37	-	104,104,104,104	0
54	MG	CA	1786	1/1	0.07	-	192,192,192,192	0
54	MG	DA	3355	1/1	0.15	-	89,89,89,89	0
54	MG	DA	3406	1/1	0.16	-	103,103,103,103	0
54	MG	BA	3379	1/1	0.43	-	106,106,106,106	0
54	MG	BA	3307	1/1	0.29	-	90,90,90,90	0
54	MG	DA	3357	1/1	0.23	-	105,105,105,105	0
54	MG	DA	3130	1/1	0.34	-	92,92,92,92	0
54	MG	AA	1656	1/1	0.23	-	71,71,71,71	0
54	MG	DA	3502	1/1	0.24	-	64,64,64,64	0
54	MG	BA	3246	1/1	0.38	-	78,78,78,78	0
54	MG	DA	3039	1/1	0.38	-	116,116,116,116	0
54	MG	BA	3418	1/1	0.26	-	98,98,98,98	0
54	MG	BA	3339	1/1	0.35	-	115,115,115,115	0
54	MG	BA	3248	1/1	0.43	-	74,74,74,74	0
54	MG	DA	3415	1/1	0.12	-	84,84,84,84	0
54	MG	CA	1709	1/1	0.34	-	110,110,110,110	0
54	MG	CA	1750	1/1	0.45	-	122,122,122,122	0
54	MG	CA	1719	1/1	0.08	-	116,116,116,116	0
54	MG	DA	3167	1/1	0.08	-	75,75,75,75	0
56	ZN	AG	303	1/1	0.25	-	153,153,153,153	0
54	MG	AA	1793	1/1	0.43	-	103,103,103,103	0
54	MG	BA	3068	1/1	0.20	-	71,71,71,71	0
54	MG	B5	102	1/1	0.10	-	92,92,92,92	0
54	MG	BA	3596	1/1	0.19	-	88,88,88,88	0
54	MG	DA	3401	1/1	0.22	-	103,103,103,103	0
54	MG	BA	3500	1/1	0.14	-	129,129,129,129	0
54	MG	DA	3371	1/1	0.24	-	111,111,111,111	0
54	MG	BA	3184	1/1	0.20	-	70,70,70,70	0
54	MG	DA	3257	1/1	0.35	-	88,88,88,88	0
54	MG	DA	3403	1/1	0.17	-	84,84,84,84	0
54	MG	DE	302	1/1	0.14	-	97,97,97,97	0
54	MG	DA	3156	1/1	0.55	-	113,113,113,113	0
54	MG	DA	3280	1/1	0.24	-	94,94,94,94	0
54	MG	AA	1807	1/1	0.24	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3001	1/1	0.40	-	53,53,53,53	0
54	MG	AA	1765	1/1	0.23	-	137,137,137,137	0
54	MG	BA	3388	1/1	0.45	-	100,100,100,100	0
54	MG	AA	1602	1/1	0.23	-	95,95,95,95	0
54	MG	DA	3093	1/1	0.23	-	106,106,106,106	0
54	MG	BA	3513	1/1	0.24	-	112,112,112,112	0
54	MG	CA	1698	1/1	0.30	-	96,96,96,96	0
54	MG	BA	3514	1/1	0.55	-	90,90,90,90	0
54	MG	AA	1648	1/1	0.29	-	123,123,123,123	0
54	MG	DA	3015	1/1	0.12	-	98,98,98,98	0
54	MG	BA	3490	1/1	0.38	-	100,100,100,100	0
54	MG	AA	1712	1/1	0.42	-	97,97,97,97	0
54	MG	CA	1618	1/1	0.55	-	123,123,123,123	0
54	MG	BB	217	1/1	0.25	-	132,132,132,132	0
54	MG	BA	3624	1/1	0.42	-	92,92,92,92	0
54	MG	BA	3553	1/1	0.23	-	99,99,99,99	0
54	MG	CA	1720	1/1	0.31	-	98,98,98,98	0
54	MG	DA	3273	1/1	0.28	-	83,83,83,83	0
54	MG	DA	3246	1/1	0.09	-	103,103,103,103	0
54	MG	BA	3618	1/1	0.56	-	107,107,107,107	0
54	MG	CA	1691	1/1	0.34	-	95,95,95,95	0
54	MG	CA	1702	1/1	0.21	-	156,156,156,156	0
54	MG	CA	1781	1/1	0.23	-	126,126,126,126	0
54	MG	DA	3240	1/1	0.19	-	89,89,89,89	0
54	MG	BA	3082	1/1	0.40	-	109,109,109,109	0
54	MG	CA	1637	1/1	0.19	-	121,121,121,121	0
54	MG	DA	3261	1/1	0.21	-	78,78,78,78	0
54	MG	BA	3370	1/1	0.50	-	111,111,111,111	0
54	MG	AA	1778	1/1	0.20	-	136,136,136,136	0
54	MG	DA	3263	1/1	0.14	-	129,129,129,129	0
54	MG	CC	102	1/1	0.14	-	83,83,83,83	0
54	MG	DA	3386	1/1	0.42	-	102,102,102,102	0
54	MG	DA	3229	1/1	0.40	-	94,94,94,94	0
54	MG	DA	3065	1/1	0.24	-	103,103,103,103	0
54	MG	BA	3390	1/1	0.27	-	81,81,81,81	0
54	MG	DA	3508	1/1	0.22	-	68,68,68,68	0
54	MG	DA	3188	1/1	0.34	-	69,69,69,69	0
54	MG	BA	3007	1/1	0.19	-	63,63,63,63	0
54	MG	BA	3610	1/1	0.23	-	85,85,85,85	0
54	MG	DB	205	1/1	0.21	-	85,85,85,85	0
54	MG	DA	3205	1/1	0.17	-	106,106,106,106	0
54	MG	BA	3053	1/1	0.62	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3029	1/1	0.31	-	74,74,74,74	0
54	MG	DA	3361	1/1	0.12	-	93,93,93,93	0
54	MG	DA	3006	1/1	0.40	-	69,69,69,69	0
54	MG	BA	3389	1/1	0.22	-	102,102,102,102	0
54	MG	BA	3578	1/1	0.19	-	88,88,88,88	0
54	MG	BA	3226	1/1	0.44	-	87,87,87,87	0
54	MG	BA	3081	1/1	0.31	-	88,88,88,88	0
54	MG	DA	3387	1/1	0.41	-	106,106,106,106	0
54	MG	BA	3133	1/1	0.37	-	92,92,92,92	0
54	MG	BA	3356	1/1	0.17	-	128,128,128,128	0
54	MG	BA	3404	1/1	0.30	-	93,93,93,93	0
54	MG	DA	3108	1/1	0.23	-	67,67,67,67	0
54	MG	CA	1664	1/1	0.27	-	110,110,110,110	0
54	MG	DA	3144	1/1	0.44	-	85,85,85,85	0
56	ZN	AQ	103	1/1	0.10	-	186,186,186,186	0
54	MG	BA	3468	1/1	0.21	-	84,84,84,84	0
54	MG	AG	302	1/1	0.22	-	162,162,162,162	0
54	MG	BA	3419	1/1	0.22	-	129,129,129,129	0
54	MG	BA	3083	1/1	0.32	-	108,108,108,108	0
54	MG	BA	3412	1/1	0.23	-	94,94,94,94	0
54	MG	BA	3546	1/1	0.28	-	97,97,97,97	0
54	MG	DR	201	1/1	0.20	-	86,86,86,86	0
54	MG	BA	3266	1/1	0.35	-	77,77,77,77	0
54	MG	DA	3381	1/1	0.33	-	97,97,97,97	0
54	MG	AA	1681	1/1	0.10	-	146,146,146,146	0
54	MG	BA	3191	1/1	0.62	-	111,111,111,111	0
54	MG	DA	3171	1/1	0.37	-	87,87,87,87	0
54	MG	AA	1636	1/1	0.39	-	92,92,92,92	0
54	MG	CA	1757	1/1	0.11	-	149,149,149,149	0
54	MG	BA	3408	1/1	0.12	-	109,109,109,109	0
54	MG	DA	3392	1/1	1.38	-	97,97,97,97	0
54	MG	BA	3494	1/1	0.22	-	97,97,97,97	0
54	MG	BA	3058	1/1	0.25	-	103,103,103,103	0
54	MG	CA	1607	1/1	0.41	-	83,83,83,83	0
54	MG	DA	3354	1/1	0.66	-	105,105,105,105	0
54	MG	DA	3278	1/1	0.10	-	80,80,80,80	0
54	MG	BA	3401	1/1	0.36	-	91,91,91,91	0
54	MG	DA	3460	1/1	0.19	-	96,96,96,96	0
54	MG	AA	1798	1/1	0.45	-	100,100,100,100	0
54	MG	BA	3354	1/1	0.41	-	113,113,113,113	0
54	MG	CA	1746	1/1	0.33	-	92,92,92,92	0
54	MG	DA	3073	1/1	0.10	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	TAC	AA	1833	32/32	0.19	-	99,129,142,143	0
54	MG	AA	1660	1/1	0.15	-	126,126,126,126	0
54	MG	DA	3491	1/1	0.30	-	65,65,65,65	0
54	MG	DA	3253	1/1	0.27	-	103,103,103,103	0
54	MG	CA	1710	1/1	0.38	-	104,104,104,104	0
54	MG	BA	3414	1/1	0.23	-	98,98,98,98	0
54	MG	D1	201	1/1	0.21	-	87,87,87,87	0
54	MG	DA	3493	1/1	0.14	-	64,64,64,64	0
54	MG	DA	3033	1/1	0.22	-	89,89,89,89	0
54	MG	BA	3503	1/1	0.20	-	105,105,105,105	0
54	MG	AA	1631	1/1	0.42	-	96,96,96,96	0
54	MG	AQ	101	1/1	0.39	-	84,84,84,84	0
54	MG	BA	3508	1/1	0.40	-	85,85,85,85	0
54	MG	DA	3301	1/1	0.59	-	124,124,124,124	0
54	MG	BA	3580	1/1	0.33	-	64,64,64,64	0
54	MG	CA	1783	1/1	0.48	-	97,97,97,97	0
54	MG	AA	1813	1/1	0.17	-	131,131,131,131	0
54	MG	BA	3550	1/1	0.21	-	99,99,99,99	0
54	MG	BO	201	1/1	0.15	-	90,90,90,90	0
54	MG	DA	3474	1/1	0.32	-	107,107,107,107	0
54	MG	BA	3489	1/1	0.34	-	104,104,104,104	0
54	MG	CA	1653	1/1	0.24	-	122,122,122,122	0
54	MG	CA	1615	1/1	0.34	-	106,106,106,106	0
54	MG	BA	3071	1/1	0.31	-	103,103,103,103	0
54	MG	CA	1741	1/1	0.22	-	136,136,136,136	0
54	MG	BA	3329	1/1	0.46	-	106,106,106,106	0
54	MG	BA	3228	1/1	0.53	-	85,85,85,85	0
54	MG	CA	1743	1/1	0.47	-	117,117,117,117	0
54	MG	AA	1688	1/1	0.10	-	146,146,146,146	0
54	MG	AA	1729	1/1	0.42	-	108,108,108,108	0
54	MG	BA	3018	1/1	0.28	-	53,53,53,53	0
54	MG	DA	3159	1/1	0.16	-	128,128,128,128	0
54	MG	DA	3203	1/1	0.23	-	90,90,90,90	0
54	MG	CA	1722	1/1	0.15	-	109,109,109,109	0
54	MG	BA	3238	1/1	0.27	-	112,112,112,112	0
54	MG	AA	1607	1/1	0.38	-	99,99,99,99	0
54	MG	BA	3105	1/1	0.28	-	68,68,68,68	0
54	MG	BA	3533	1/1	0.59	-	106,106,106,106	0
54	MG	DA	3088	1/1	0.17	-	99,99,99,99	0
54	MG	BA	3277	1/1	0.30	-	97,97,97,97	0
54	MG	CA	1766	1/1	0.26	-	107,107,107,107	0
54	MG	BA	3030	1/1	0.30	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3197	1/1	0.33	-	103,103,103,103	0
54	MG	CA	1606	1/1	0.41	-	100,100,100,100	0
54	MG	BA	3498	1/1	0.53	-	107,107,107,107	0
54	MG	BA	3506	1/1	0.24	-	92,92,92,92	0
54	MG	BA	3233	1/1	0.26	-	106,106,106,106	0
54	MG	DA	3214	1/1	0.16	-	63,63,63,63	0
54	MG	DA	3358	1/1	0.33	-	73,73,73,73	0
54	MG	BA	3143	1/1	0.39	-	52,52,52,52	0
54	MG	DA	3049	1/1	0.17	-	105,105,105,105	0
54	MG	DA	3434	1/1	0.39	-	110,110,110,110	0
54	MG	AA	1672	1/1	0.35	-	112,112,112,112	0
54	MG	DA	3098	1/1	0.12	-	139,139,139,139	0
54	MG	DA	3523	1/1	0.30	-	100,100,100,100	0
54	MG	AA	1779	1/1	0.48	-	88,88,88,88	0
54	MG	AA	1707	1/1	0.12	-	94,94,94,94	0
54	MG	DA	3219	1/1	0.29	-	71,71,71,71	0
54	MG	AR	101	1/1	0.42	-	98,98,98,98	0
54	MG	CA	1651	1/1	0.27	-	116,116,116,116	0
54	MG	DP	201	1/1	0.20	-	102,102,102,102	0
54	MG	DA	3311	1/1	0.16	-	92,92,92,92	0
54	MG	DA	3157	1/1	0.17	-	90,90,90,90	0
54	MG	CA	1752	1/1	0.40	-	106,106,106,106	0
54	MG	BA	3575	1/1	0.26	-	109,109,109,109	0
54	MG	BA	3204	1/1	0.48	-	98,98,98,98	0
54	MG	AA	1694	1/1	0.59	-	105,105,105,105	0
54	MG	AA	1774	1/1	0.31	-	72,72,72,72	0
54	MG	DA	3245	1/1	0.45	-	83,83,83,83	0
54	MG	DA	3085	1/1	0.25	-	113,113,113,113	0
54	MG	DA	3178	1/1	0.23	-	100,100,100,100	0
54	MG	BA	3113	1/1	0.14	-	72,72,72,72	0
54	MG	DA	3485	1/1	0.14	-	104,104,104,104	0
54	MG	CA	1756	1/1	0.28	-	111,111,111,111	0
54	MG	CA	1647	1/1	0.32	-	83,83,83,83	0
54	MG	DA	3289	1/1	0.19	-	83,83,83,83	0
54	MG	DA	3138	1/1	0.26	-	79,79,79,79	0
54	MG	AA	1615	1/1	0.25	-	95,95,95,95	0
54	MG	BA	3144	1/1	0.36	-	73,73,73,73	0
54	MG	BA	3477	1/1	0.42	-	93,93,93,93	0
54	MG	BA	3590	1/1	0.52	-	116,116,116,116	0
54	MG	BA	3320	1/1	0.29	-	104,104,104,104	0
54	MG	CA	1711	1/1	0.20	-	119,119,119,119	0
54	MG	BA	3102	1/1	0.19	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	216	1/1	0.38	-	111,111,111,111	0
54	MG	DA	3074	1/1	0.26	-	109,109,109,109	0
54	MG	BA	3159	1/1	0.24	-	101,101,101,101	0
54	MG	BA	3193	1/1	0.53	-	76,76,76,76	0
54	MG	BA	3125	1/1	0.32	-	88,88,88,88	0
54	MG	BA	3374	1/1	0.15	-	104,104,104,104	0
54	MG	DA	3414	1/1	0.10	-	95,95,95,95	0
54	MG	BA	3073	1/1	0.91	-	108,108,108,108	0
54	MG	DA	3190	1/1	0.38	-	80,80,80,80	0
54	MG	BA	3616	1/1	0.40	-	92,92,92,92	0
54	MG	DA	3152	1/1	0.18	-	112,112,112,112	0
54	MG	DA	3117	1/1	0.30	-	72,72,72,72	0
54	MG	CA	1772	1/1	0.32	-	109,109,109,109	0
54	MG	DA	3042	1/1	0.35	-	111,111,111,111	0
54	MG	DA	3478	1/1	0.41	-	114,114,114,114	0
54	MG	DA	3224	1/1	0.18	-	61,61,61,61	0
54	MG	DA	3079	1/1	0.22	-	97,97,97,97	0
54	MG	AA	1666	1/1	0.20	-	123,123,123,123	0
54	MG	BA	3234	1/1	0.47	-	84,84,84,84	0
54	MG	BA	3474	1/1	0.25	-	102,102,102,102	0
54	MG	BA	3100	1/1	0.46	-	100,100,100,100	0
54	MG	BA	3118	1/1	0.43	-	90,90,90,90	0
54	MG	BA	3582	1/1	0.25	-	68,68,68,68	0
54	MG	DA	3002	1/1	0.42	-	109,109,109,109	0
54	MG	DA	3343	1/1	0.34	-	95,95,95,95	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.