



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:22 PM BST

PDB ID : 4V7X
Title : Structure of the *Thermus thermophilus* ribosome complexed with erythromycin.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-17
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

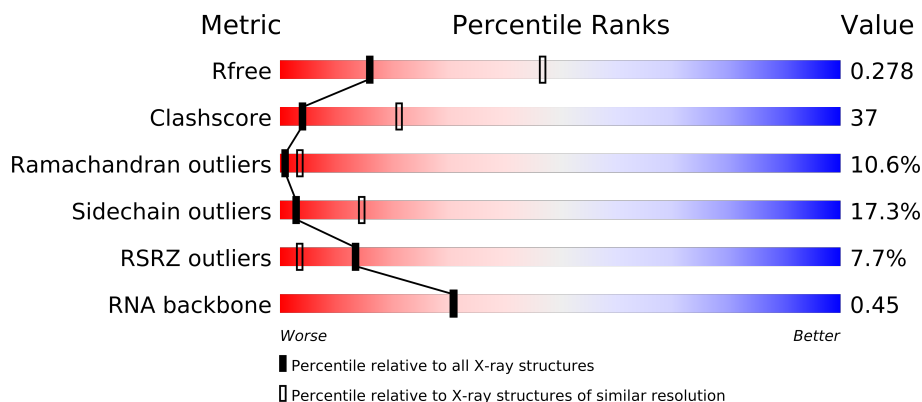
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	160	
5	CE	160	
6	AF	101	
6	CF	101	

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Mol	Chain	Length	Quality of chain
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	B0	85	
22	D0	85	
23	B1	98	
23	D1	98	
24	B2	72	
24	D2	72	
25	B3	60	
25	D3	60	
26	B4	71	
26	D4	71	
27	B5	60	
27	D5	60	

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Mol	Chain	Length	Quality of chain
28	B6	54	
28	D6	54	
29	B7	49	
29	D7	49	
30	B8	65	
30	D8	65	
31	BA	2787	
31	DA	2787	
32	BB	122	
32	DB	122	
33	BD	276	
33	DD	276	
34	BE	206	
34	DE	206	
35	BF	210	
35	DF	210	
36	BG	182	
36	DG	182	
37	BH	180	
37	DH	180	
38	BI	148	
38	DI	148	
39	BN	140	
39	DN	140	
40	BO	122	
40	DO	122	
41	BP	150	
41	DP	150	
42	BQ	141	
42	DQ	141	
43	BR	118	
43	DR	118	
44	BS	112	
44	DS	112	
45	BT	146	
45	DT	146	
46	BU	118	
46	DU	118	
47	BV	101	
47	DV	101	
48	BW	113	
48	DW	113	

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Mol	Chain	Length	Quality of chain
49	BX	96	
49	DX	96	
50	BY	110	
50	DY	110	
51	BZ	206	
51	DZ	206	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 278034 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	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	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	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	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	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	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	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	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374
CI	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	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	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	2	VAL	-	INSERTION	UNP Q5SHN3
AL	3	ALA	-	INSERTION	UNP Q5SHN3
AL	4	LEU	-	INSERTION	UNP Q5SHN3
CL	2	VAL	-	INSERTION	UNP Q5SHN3
CL	3	ALA	-	INSERTION	UNP Q5SHN3
CL	4	LEU	-	INSERTION	UNP Q5SHN3

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			
13	CM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	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	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	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	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	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	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	B0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			
22	D0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	B1	89	Total	C	N	O	0	0	1
			693	435	140	118			
23	D1	89	Total	C	N	O	0	0	1
			693	435	140	118			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	B2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			
24	D2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
25	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B4	32	Total	C	N	O		0	0	0
			157	93	32	32				
26	D4	32	Total	C	N	O		0	0	0
			157	93	32	32				

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B5	59	Total	C	N	O	S	9	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	9	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
28	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
29	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
30	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			
31	DA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 33 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
33	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 34 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
34	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 35 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
37	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 38 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
38	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 39 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
39	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			
42	DQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BS	99	Total	C	N	O	0	0	1
			771	486	155	130			
44	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 45 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			
45	DT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BX	93	Total	C	N	O		0	0	1
			726	471	132	123				
49	DX	93	Total	C	N	O		0	0	1
			726	471	132	123				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
50	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 51 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	BA	362	Total	Mg	0	0
			362	362		
52	CA	50	Total	Mg	0	0
			50	50		
52	DQ	1	Total	Mg	0	0
			1	1		
52	DF	1	Total	Mg	0	0
			1	1		
52	BE	1	Total	Mg	0	0
			1	1		
52	DU	1	Total	Mg	0	0
			1	1		
52	B1	1	Total	Mg	0	0
			1	1		
52	BP	3	Total	Mg	0	0
			3	3		
52	DR	1	Total	Mg	0	0
			1	1		
52	B5	2	Total	Mg	0	0
			2	2		
52	BB	7	Total	Mg	0	0
			7	7		
52	D3	1	Total	Mg	0	0
			1	1		
52	BF	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	AA	54	Total	Mg	0	0
			54	54		
52	BQ	2	Total	Mg	0	0
			2	2		
52	D7	1	Total	Mg	0	0
			1	1		
52	BU	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	D0	1	Total 1	Mg 1	0	0
52	BR	1	Total 1	Mg 1	0	0
52	DA	328	Total 328	Mg 328	0	0
52	DE	1	Total 1	Mg 1	0	0
52	DX	1	Total 1	Mg 1	0	0
52	DP	1	Total 1	Mg 1	0	0
52	D5	1	Total 1	Mg 1	0	0
52	BD	1	Total 1	Mg 1	0	0
52	B0	1	Total 1	Mg 1	0	0
52	DB	3	Total 3	Mg 3	0	0

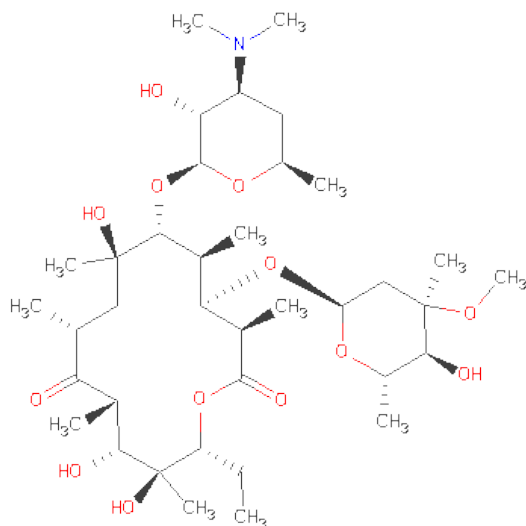
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	CN	1	Total 1	Zn 1	0	0
53	AD	1	Total 1	Zn 1	0	0
53	CD	1	Total 1	Zn 1	0	0
53	AN	1	Total 1	Zn 1	0	0

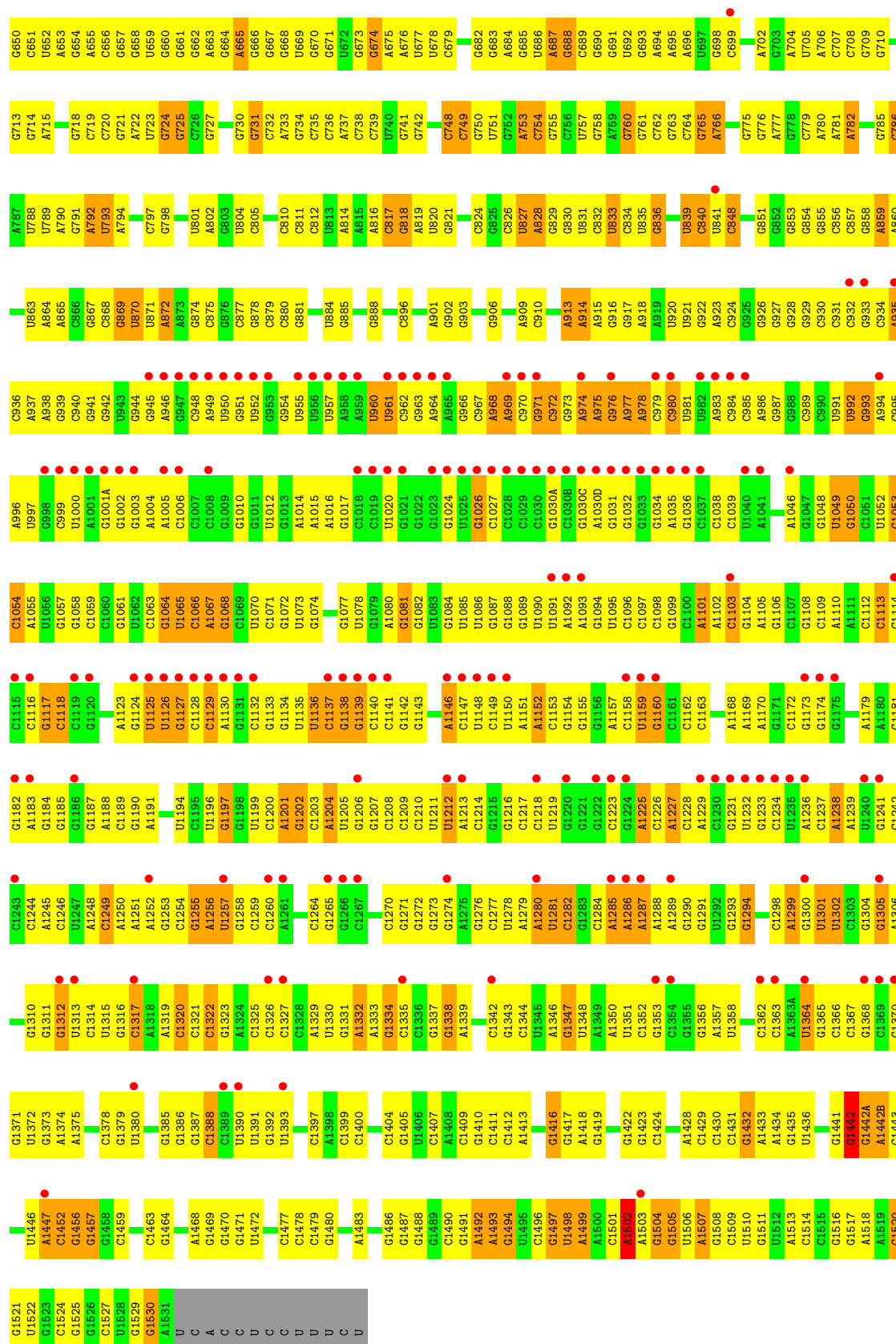
- Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	1	Total 1	K 1	0	0
54	DA	1	Total 1	K 1	0	0

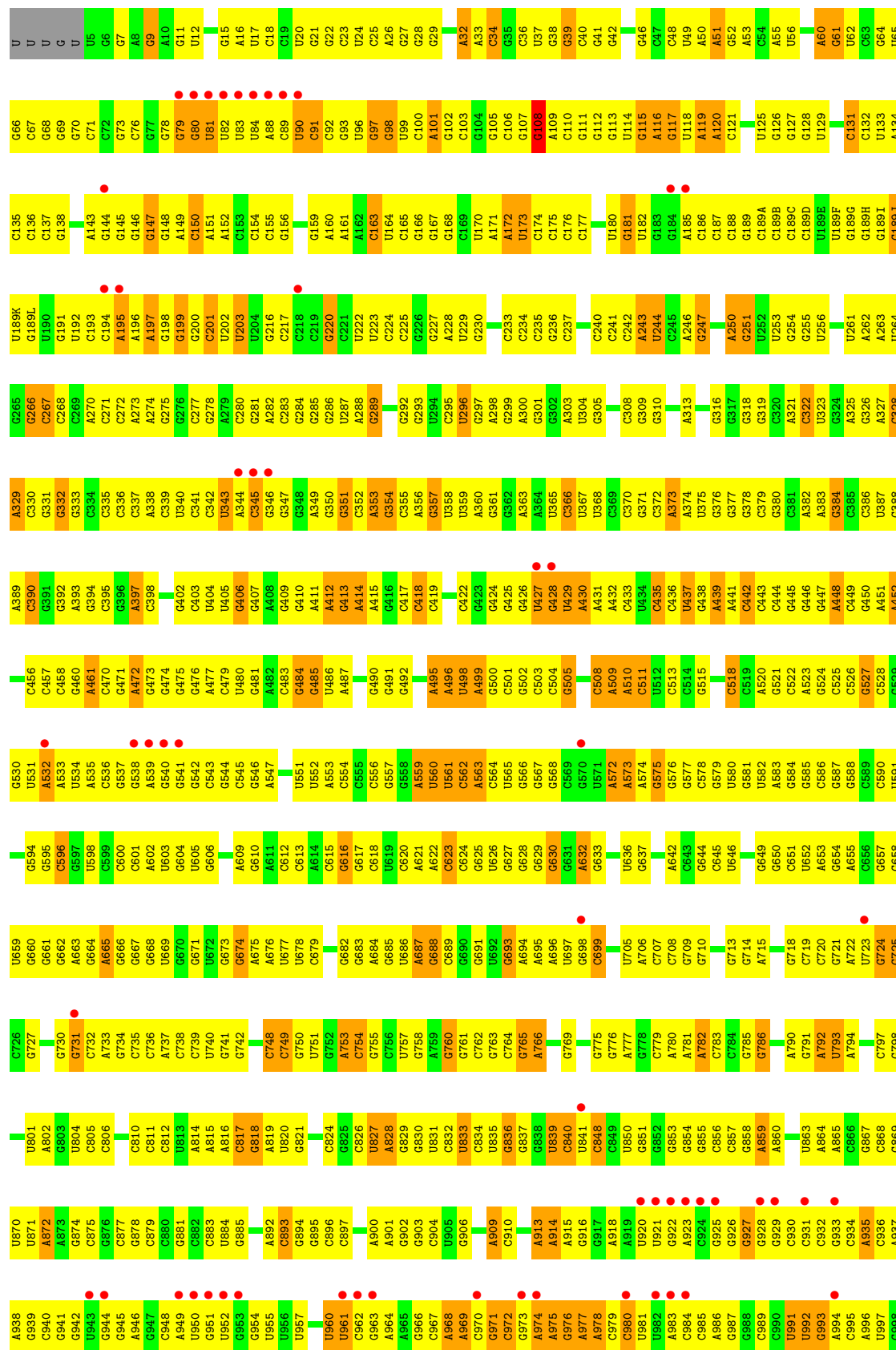
- Molecule 55 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C₃₇H₆₇NO₁₃).

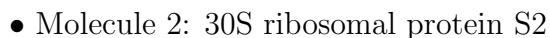


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BA	1	Total	C	N	O	0	0
			51	37	1	13		
55	DA	1	Total	C	N	O	0	0
			51	37	1	13		

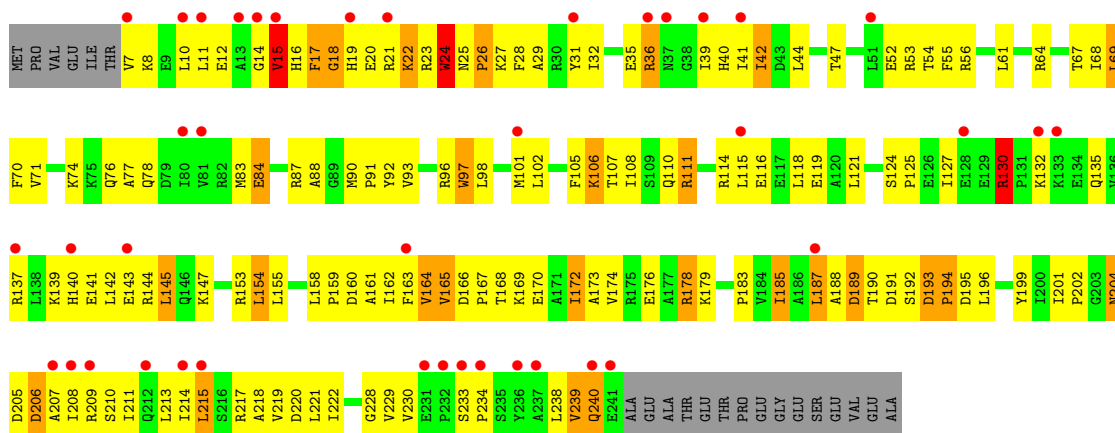


Chain CA:



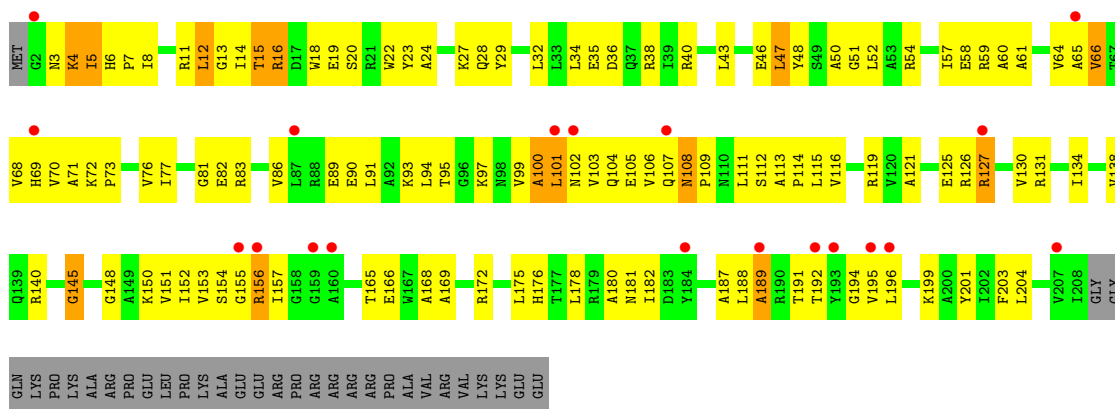


Chain CB:



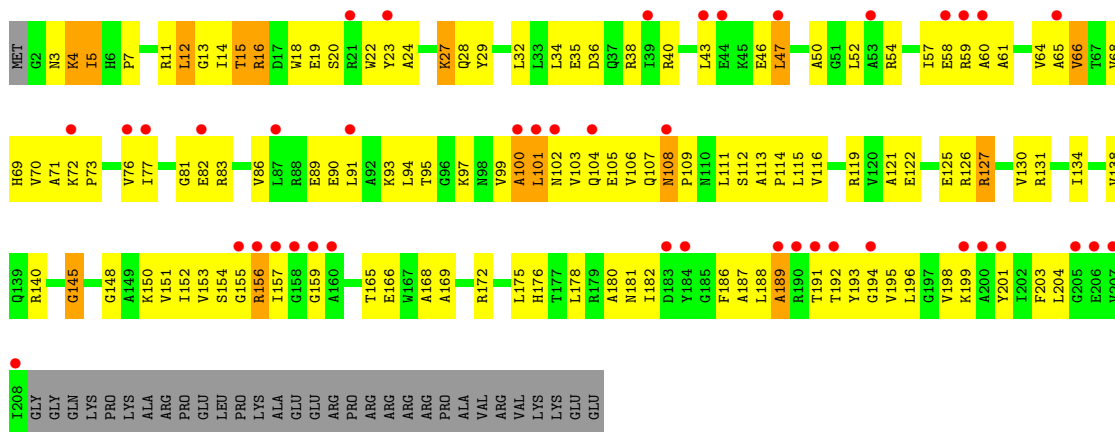
- Molecule 3: 30S ribosomal protein S3

Chain AC:



- Molecule 3: 30S ribosomal protein S3

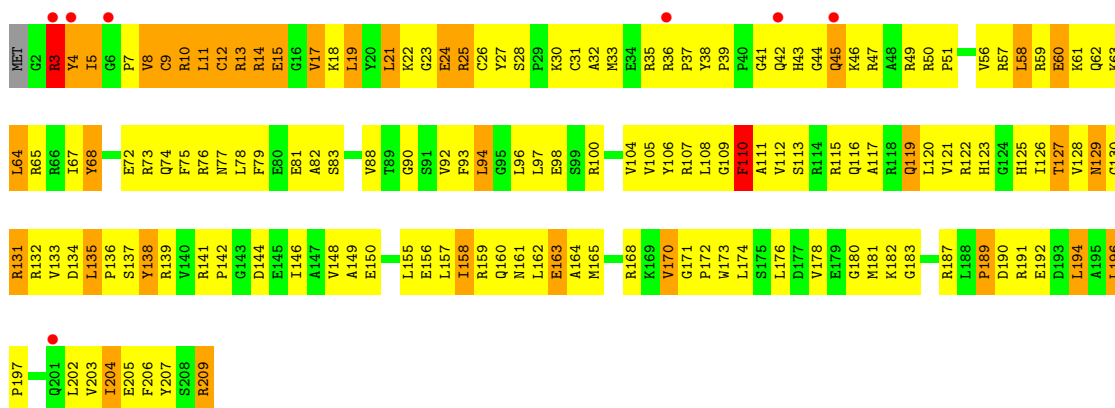
Chain CC:



- Molecule 4: 30S ribosomal protein S4

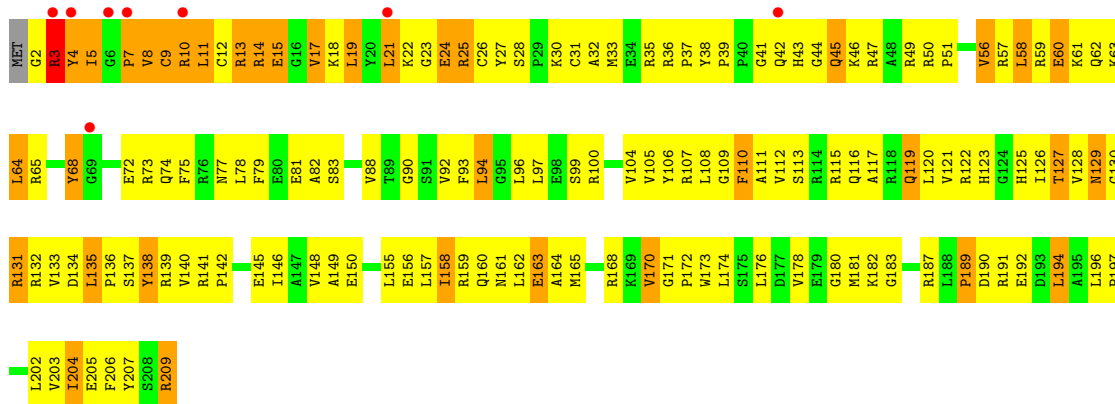
Chain AD:





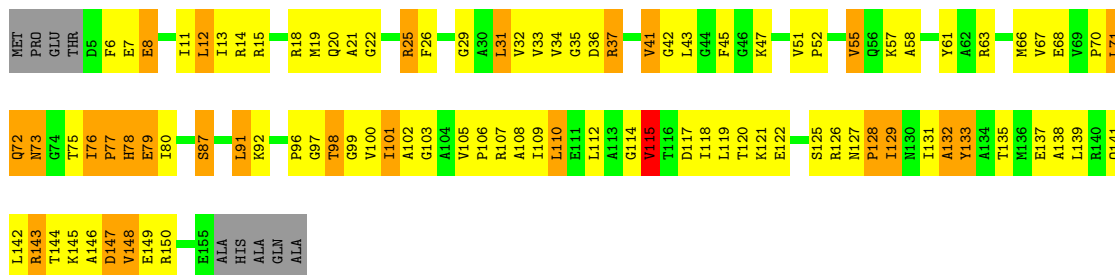
• Molecule 4: 30S ribosomal protein S4

Chain CD:



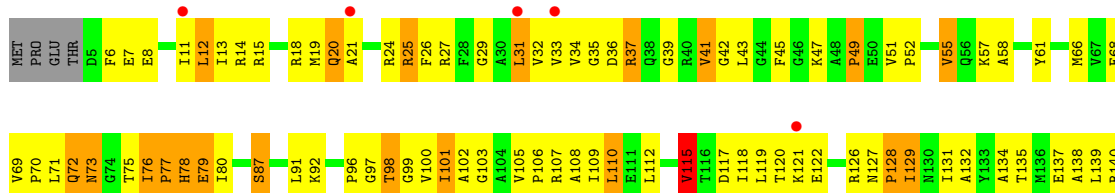
• Molecule 5: 30S ribosomal protein S5

Chain AE:



• Molecule 5: 30S ribosomal protein S5

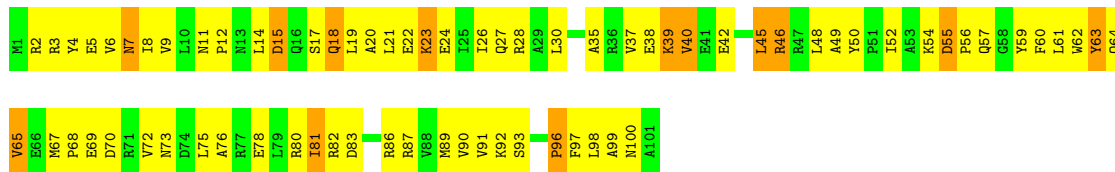
Chain CE:





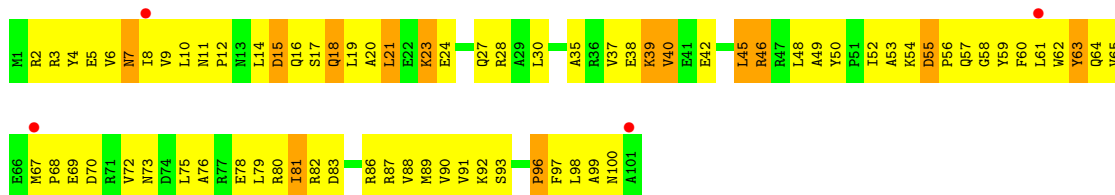
• Molecule 6: 30S ribosomal protein S6

Chain AF:



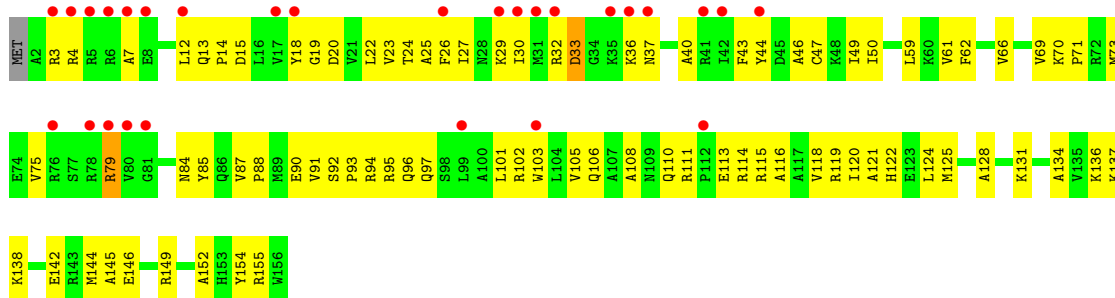
• Molecule 6: 30S ribosomal protein S6

Chain CF:



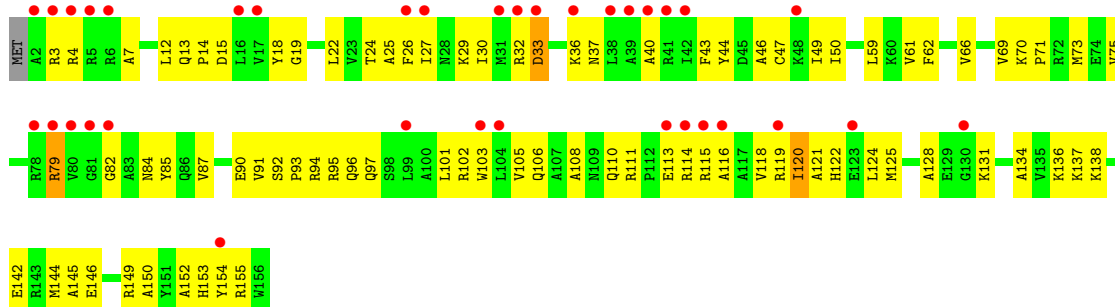
• Molecule 7: 30S ribosomal protein S7

Chain AG:



• Molecule 7: 30S ribosomal protein S7

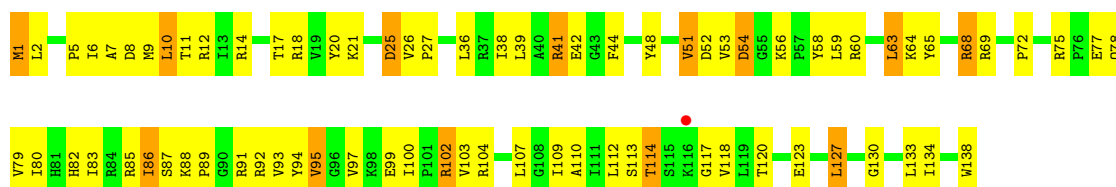
Chain CG:



• Molecule 8: 30S ribosomal protein S8

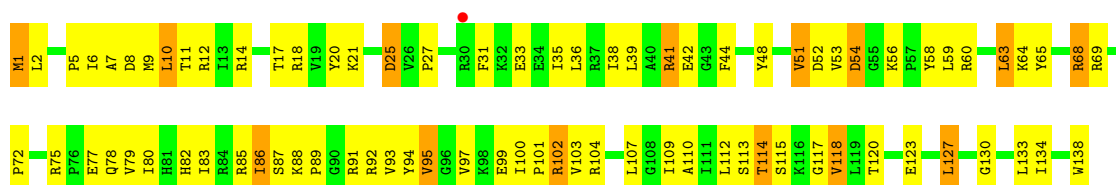
Chain AH:





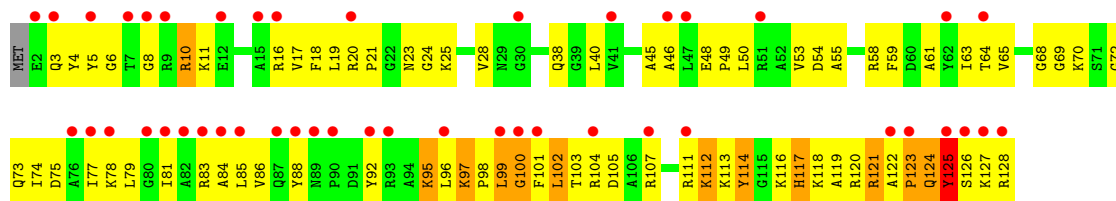
• Molecule 8: 30S ribosomal protein S8

Chain CH:



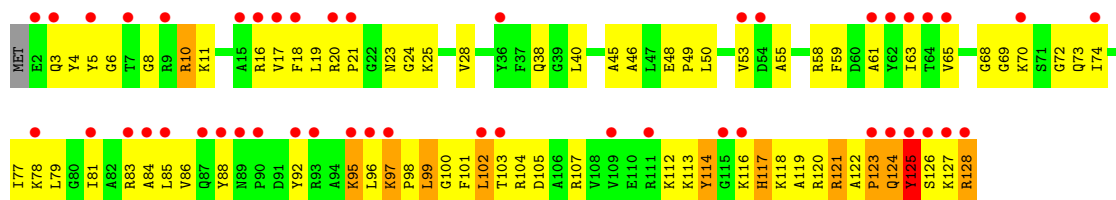
• Molecule 9: 30S ribosomal protein S9

Chain AI:



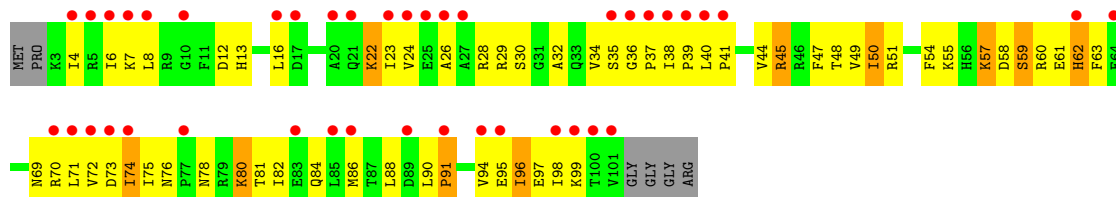
• Molecule 9: 30S ribosomal protein S9

Chain CI:



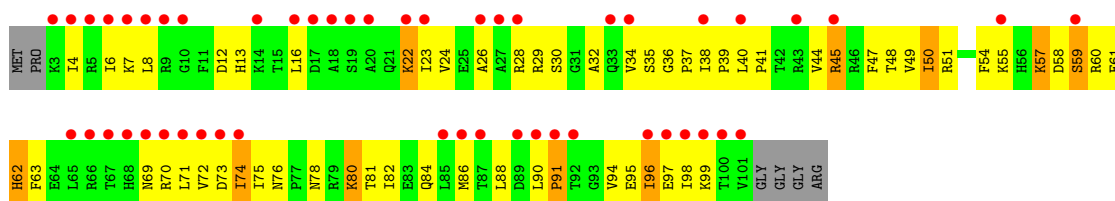
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



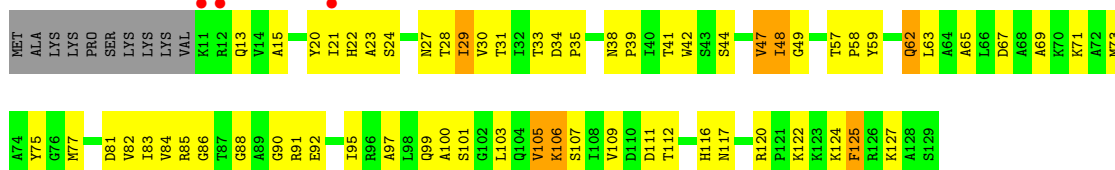
• Molecule 10: 30S ribosomal protein S10

Chain CJ:



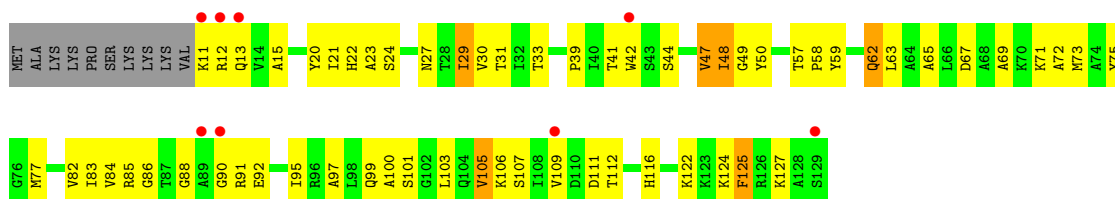
- Molecule 11: 30S ribosomal protein S11

Chain AK:



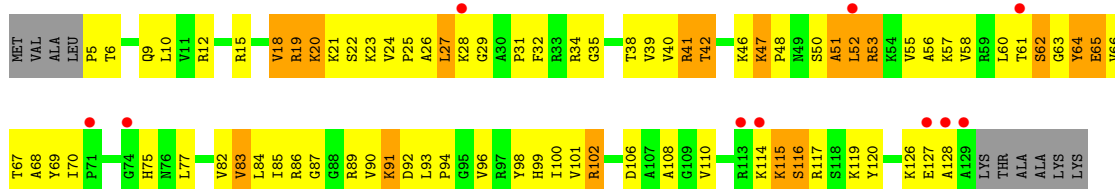
- Molecule 11: 30S ribosomal protein S11

Chain CK:



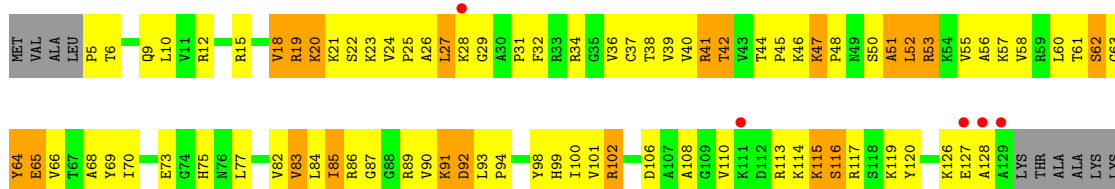
- Molecule 12: 30S ribosomal protein S12

Chain AL:



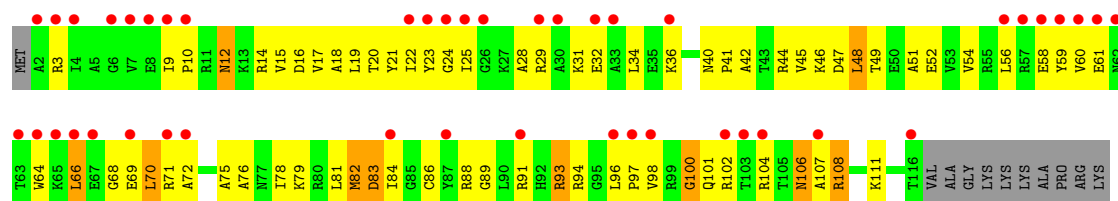
- Molecule 12: 30S ribosomal protein S12

Chain CL:



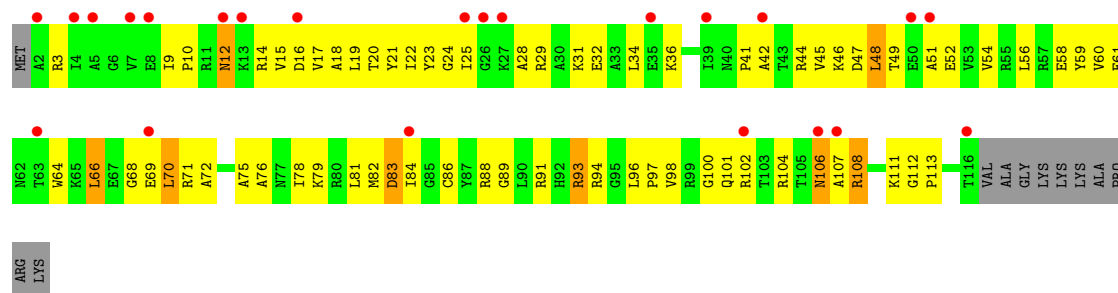
- Molecule 13: 30S ribosomal protein S13

Chain AM:



• Molecule 13: 30S ribosomal protein S13

Chain CM:



• Molecule 14: 30S ribosomal protein S14

Chain AN:



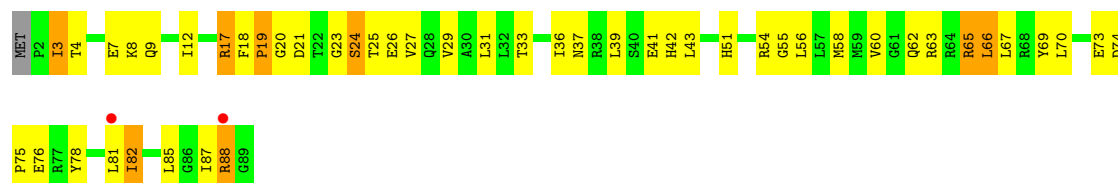
• Molecule 14: 30S ribosomal protein S14

Chain CN:



• Molecule 15: 30S ribosomal protein S15

Chain AO:



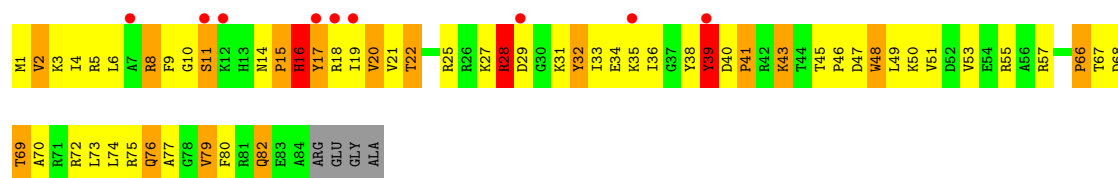
• Molecule 15: 30S ribosomal protein S15

Chain CO:



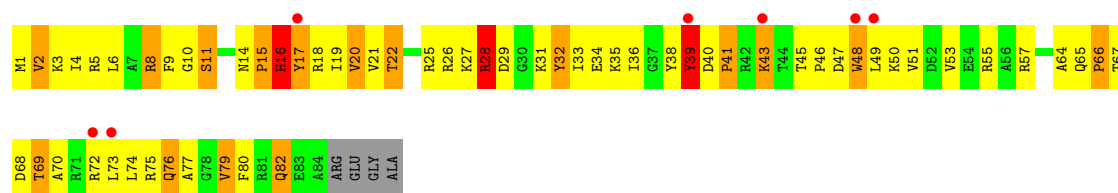
- Molecule 16: 30S ribosomal protein S16

Chain AP:



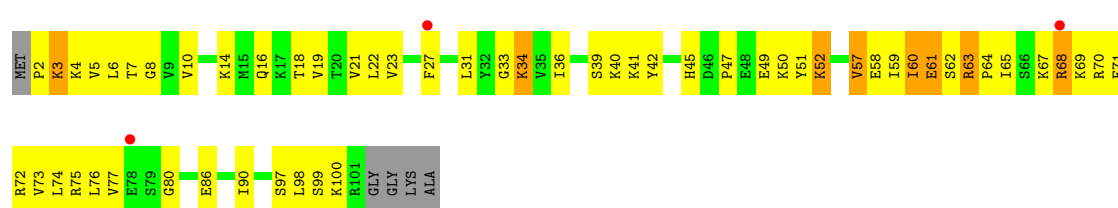
- Molecule 16: 30S ribosomal protein S16

Chain CP:



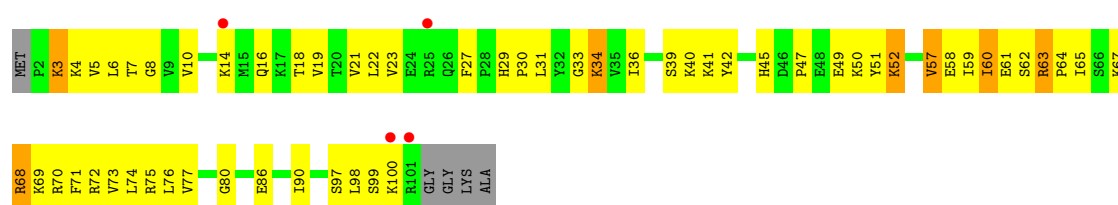
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



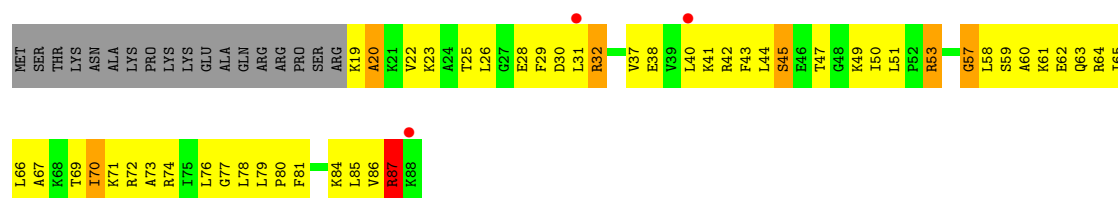
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



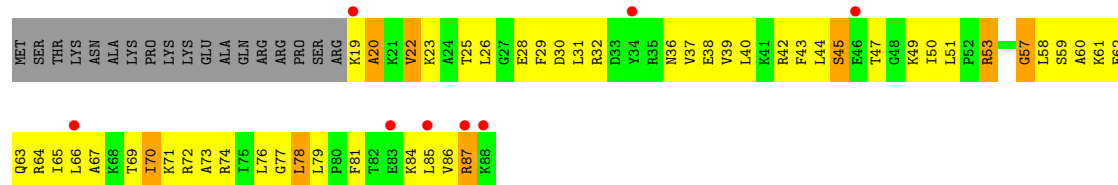
- Molecule 18: 30S ribosomal protein S18

Chain AR:



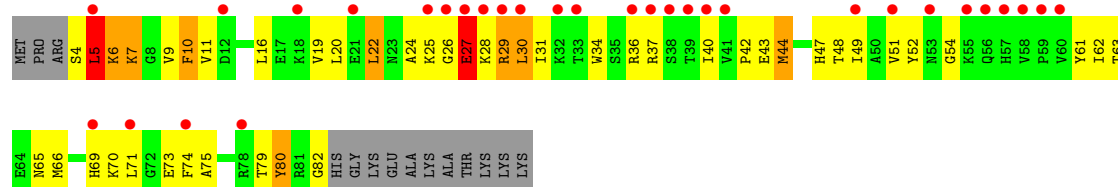
- Molecule 18: 30S ribosomal protein S18

Chain CR:



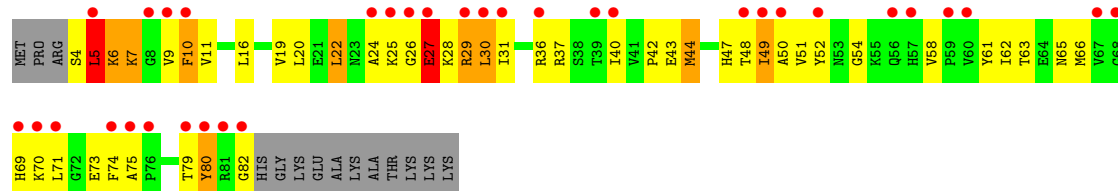
- Molecule 19: 30S ribosomal protein S19

Chain AS:



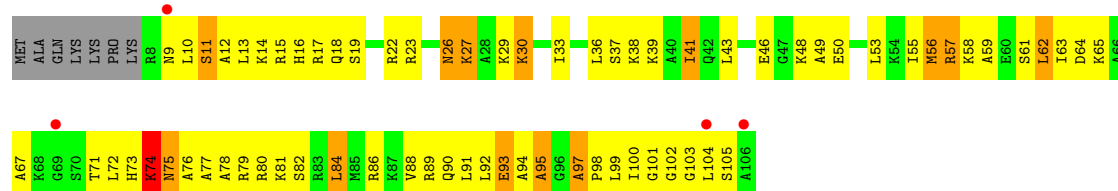
- Molecule 19: 30S ribosomal protein S19

Chain CS:



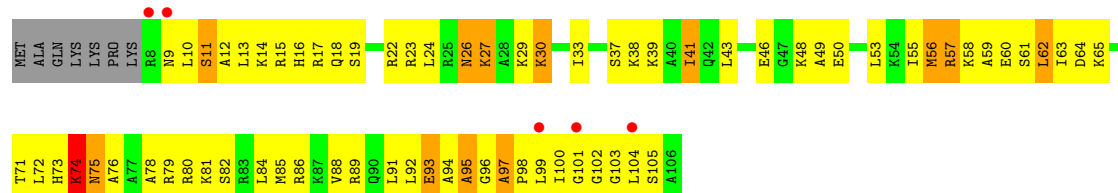
- Molecule 20: 30S ribosomal protein S20

Chain AT:



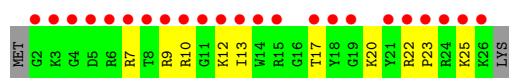
- Molecule 20: 30S ribosomal protein S20

Chain CT:



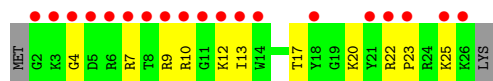
- Molecule 21: 30S ribosomal protein Thx

Chain AU:



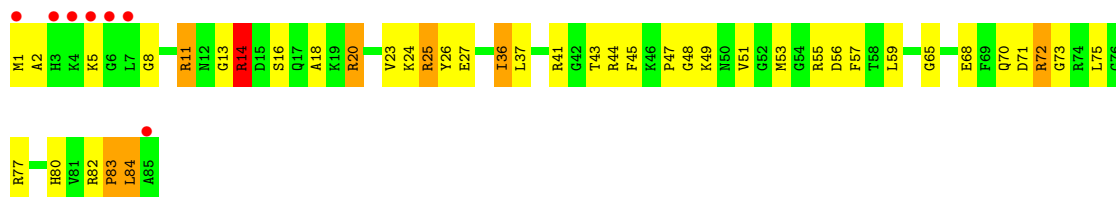
- Molecule 21: 30S ribosomal protein Thx

Chain CU:



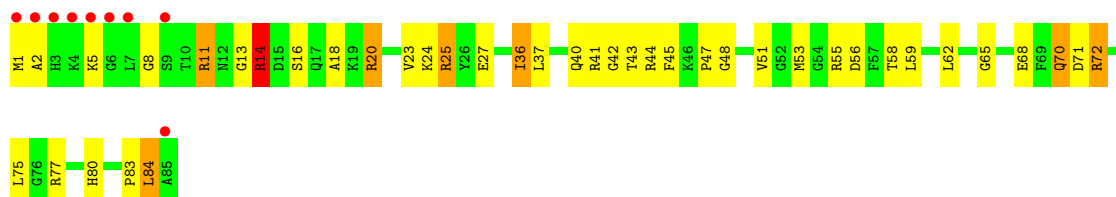
- Molecule 22: 50S ribosomal protein L27

Chain B0:



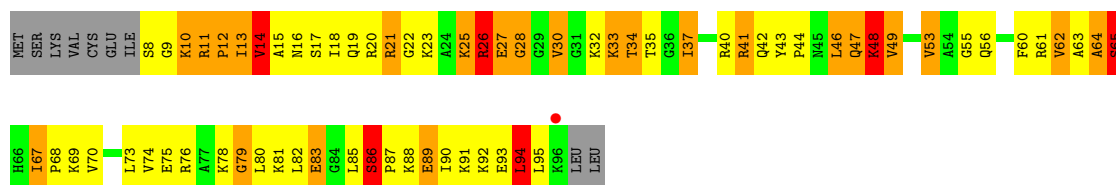
- Molecule 22: 50S ribosomal protein L27

Chain D0:



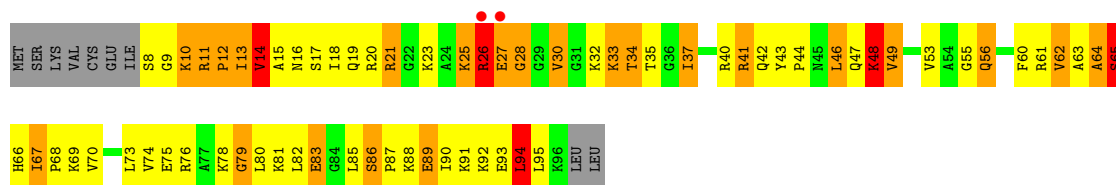
- Molecule 23: 50S ribosomal protein L28

Chain B1:



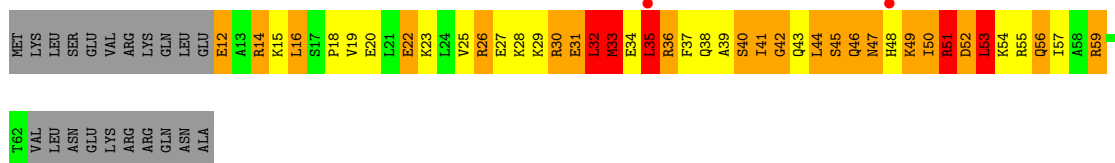
- Molecule 23: 50S ribosomal protein L28

Chain D1:



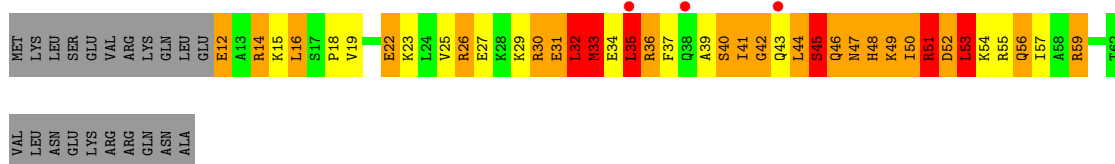
- Molecule 24: 50S ribosomal protein L29

Chain B2:



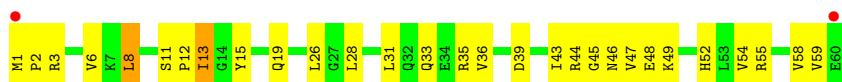
- Molecule 24: 50S ribosomal protein L29

Chain D2:



- Molecule 25: 50S ribosomal protein L30

Chain B3:



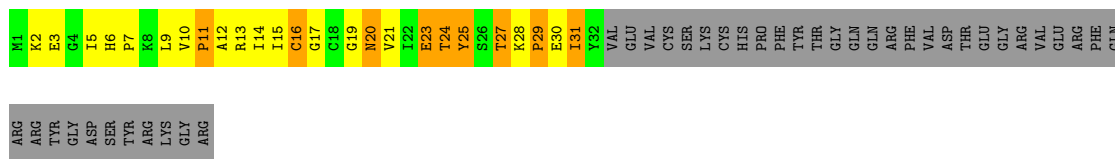
- Molecule 26: 50S ribosomal protein L31

Chain D3:



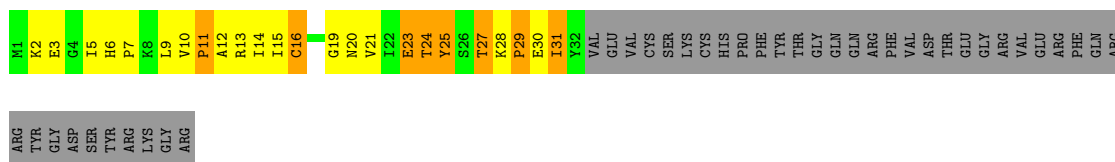
- Molecule 27: 50S ribosomal protein L32

Chain B4:



- Molecule 28: 50S ribosomal protein L33

Chain D4:



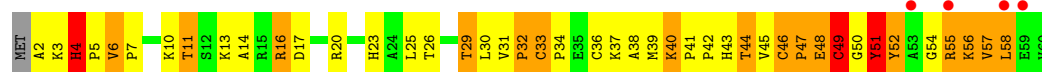
- Molecule 29: 50S ribosomal protein L34

Chain B5:



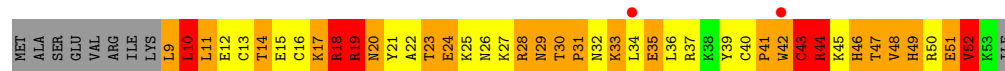
- Molecule 27: 50S ribosomal protein L32

Chain D5:



- Molecule 28: 50S ribosomal protein L33

Chain B6:



- Molecule 28: 50S ribosomal protein L33

Chain D6:



- Molecule 29: 50S ribosomal protein L34

Chain B7:



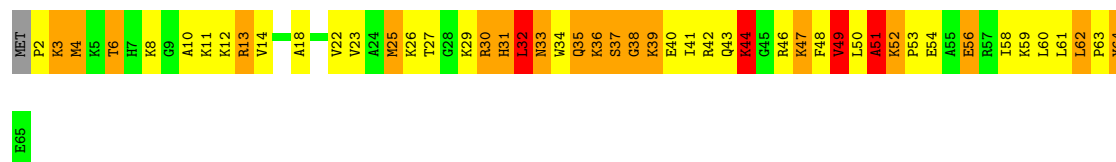
- Molecule 29: 50S ribosomal protein L34

Chain D7:



- Molecule 30: 50S ribosomal protein L35

Chain B8:



- Molecule 30: 50S ribosomal protein L35

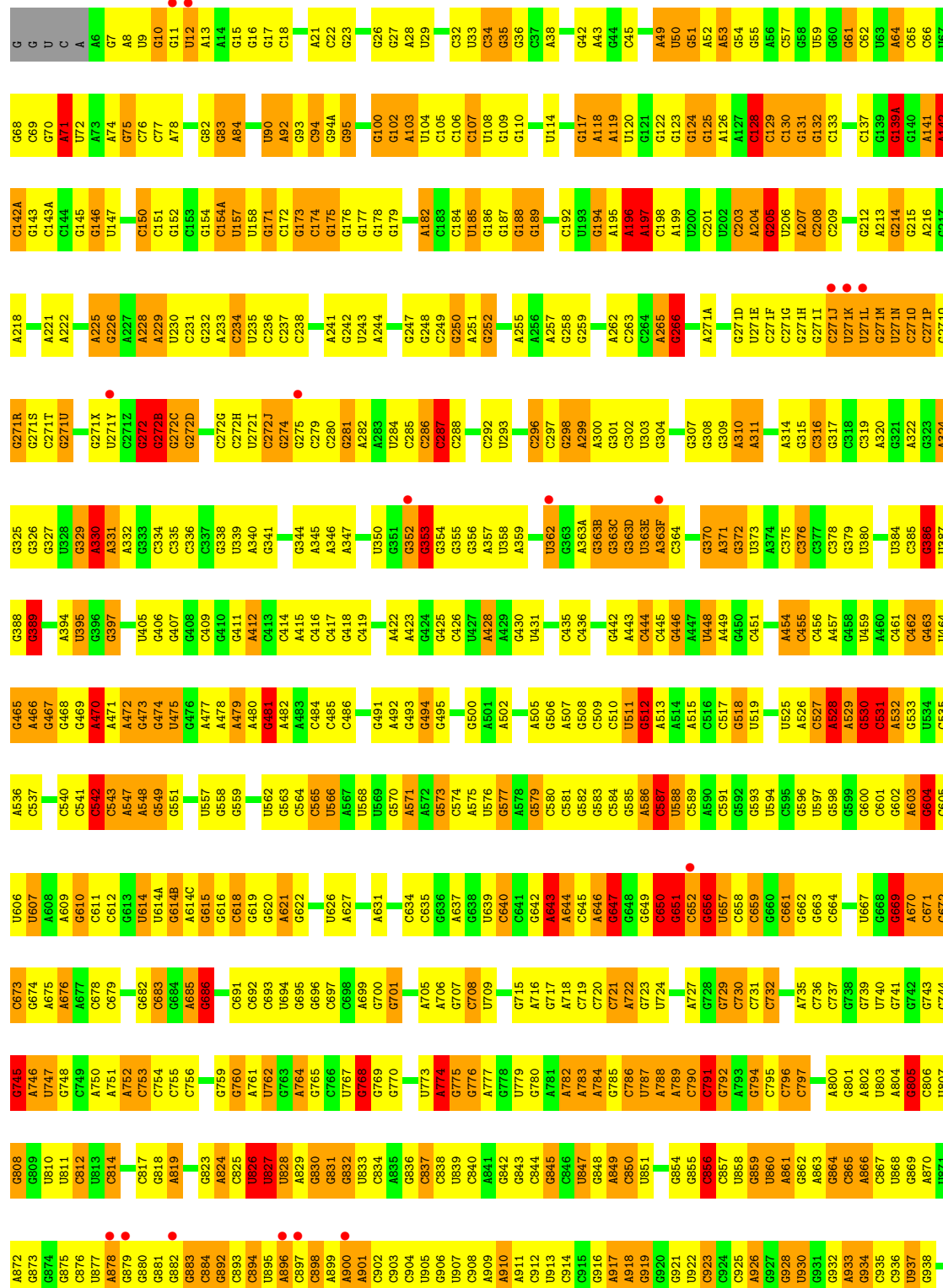
Chain D8:





• Molecule 31: 23S ribosomal RNA

Chain BA:



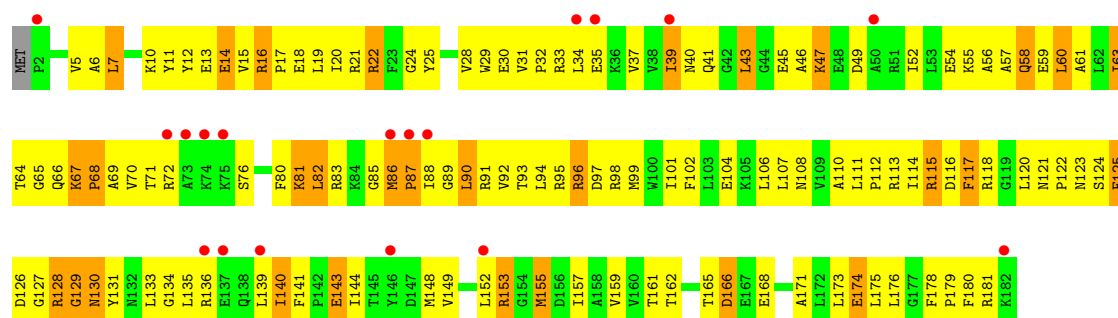
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G2018	U1946	G1878	G1697	G1627	A1553	G1484	G1418	U1341	A1272	U1198	A1127	C1006	G942
A2019	C1947	C1879	A1698	G1628	C1557	G1485	A1419	A1342	U1273	C1201	A1128	A1010	U943
A2020	G1948	G1880	G1699	U1629	C1557	A1486	U1420	G1343	G1343	G1208	A1129	G1011	G944
C2021	G1949	C1881	A1700	A1632	A1558	G1487	G1421	G1344	A1276	A1204	U1130	U1012	A945
U2022	G1950	G1882	A1701	A1632	G1559	G1488	C1425	C1345	A1276	U1205	G1131	C1013	G946
G2023	U1951	G1883	G1702	G1635	G1563	U1489	G1426	G1348	G1277	U1206	C1135	U1014	C949
G2024	A1952	A1884	G1703	C1635	C1564	A1490	A1426	A1348	G1278	C1207	C1136	G1015	G950
C2025	A1953	C1797	G1704	C1637	C1565	G1491	A1427	A1349	G1279	C1207	C1136	G1016	G951
G2026	G1954	G1886	A1637	C1638	A1566	G1492	G1429	C1350	G1208	G1209	G1137	C1019	G952
C2027	U1955	G1887	U1706	C1638	A1566	C1493	G1429	A1353	U1282	G1208	G1138	U1019	A953
U2028	G1956	G1888	U1707	C1639	A1567	A1494	C1430	A1354	G1283	A1210	C1139	A1020	G954
G2029	C1957	A1889	U1709	U1640	G1568	A1495	U1431	G1355	A1284	U1211	C1140	A1021	C955
A2030	C1958	A1890	U1710	A1641	A1569	A1496	U1431	A1356	U1287	A1213	G1141	G1022	G956
G2031	G1959	G1891	U1713	G1642	A1570	U1497	A1434	G1356	U1288	A1213	C1142	U1023	A957
G2032	C1960	C1892	G1714	G1643	A1571	G1498	G1435	A1357	U1289	G1216	A1142A	G1024	U958
A2033	C1962	C1893	G1717	C1644	A1572	C1499	G1436	G1358	G1290	G1216	A1143	U1026	A959
C2034	U1963	C1894	G1718	C1644	A1573	G1500	C1437	A1359	C1291	C1221	G1144	U1027	A960
G2035	G1964	G1895	G1719	G1647	C1574	C1501	U1438	A1360	U1292	C1221	C1153	A1028	G961
C2036	A1810	G1896	U1720	C1648	C1577	G1502	A1439	G1364	U1293	C1221A	G1154	G1030	G962
C2039	A1811	C1897	G1721	G1649	C1577	C1503	G1440	A1365	C1298	C1224	A1155	U1033	G966
C2040	G1899	G1968	U1722	C1649	U1578	C1504	G1441	A1366	G1299	G1225	A1156	G1034	C967
U2041	G1813	G1814	U1723	A1652	A1579	C1505	G1442	G1368	U1300	A1226	C1157	U1035	C971
A2042	G1815	G1816	G1740	G1653	A1580	C1506	G1443	G1369	A1301	G1227	C1158	C1038	G972
C2043	G1816	C1741	A1741	A1654	G1581	A1507	G1444	G1370	G1302	C1235	G1160	G1040	G973
C2044	G1816	G1742	G1742	A1655	C1582	A1508	A1445	G1371	A1303	C1235	C1161	G1041	G975
G1973	A1819	C1743	C1743	C1656	A1583	C1509	C1445A	G1381	G1303	U1234	G1162	G1042	G976
C1974	A1820	G1744	C1744	C1657	A1584	A1509A	C1446	G1382	G1303	U1234	G1163	G1043	G979
G1975	A1821	C1745	C1745	C1658	A1586	A1509B	G1447	G1383	G1303	G1235	G1164	G1044	A980
G2048	G1822	C1746	G1746	U1659	A1587	G1510	G1448	A1384	U1312	A1242	G1169	A1045	A981
G2049	A1977	G1910	G1747	C1660	C1588	C1511	A1449	A1385	U1313	G1245	G1170	A1046	C982
C2053	G1826	C1912	G1747	G1661	C1589	U1512	G1450	A1386	G1314	G1246	G1171	A1048	C983
A2054	C1827	A1912	G1747A	C1662	U1590	U1512	G1450A	C1387	A1317	A1247	G1173	C1049	A984
C2056	G1828	A1913	G1748	C1663	C1591	U1514	C1450A	G1388	C1318	C1250	G1174	A1050	C985
A2057	A1829	C1914	A1749	C1663	C1592	U1514	C1451	G1388	C1319	G1250	A1175	G1051	C986
A2058	C1830	G1750	G1750	G1667	C1593	C1516	C1455	G1389	C1320	G1251	C1176	C1052	G987
A2059	U1833	C1751	C1751	A1668	G1594	C1517	G1455	A1395	A1321	G1252	A1177	C1053	A988
C1988	U1834	C1754	C1754	A1669	G1595	U1518	C1458	U1396	A1322	A1253	C1178	A1106	C989
G1989	C1836	A1755	G1756	C1670	A1596	G1519	A1459	G1397	U1323	A1254	C1179	G1107	A990
U1991	C1837	G1756	G1756	C1670	A1597	G1520	A1460	C1398	G1324	U1255	C1180	U1108	C991
G1992	C1837	A1762	A1762	U1674	C1598	G1525	G1461	C1403	G1325	G1256	C1181	G1110	C992
C1993	G1838	G1763	G1763	C1675	U1602	G1526	C1463	U1404	U1326	C1257	G1182	G1111	G993
C1994	G1839	G1764	G1764	A1677	C1604	G1527	C1464	U1405	C1327	C1258	G1183	A1111	C994
U1995	G1840	C1764	C1764	G1678	C1605	A1528	G1465	U1406	U1329	C1261	C1185	U1113	A996
C1996	C1843	C1771	C1771	G1678	G1606	A1528A	C1467	C1407	G1328	C1262	G1186	G1114	C997
G2069	G1844	G1772	G1772	G1681	C1607	C1530	G1470	U1408	U1329	U1263	C1187	G1115	C998
G2070	G1845	A1773	A1773	G1682	A1608	C1531	A1471	C1409	A1331	G1264	U1188	C1116	U999
A2071	G1846	C1774	C1774	C1685	A1609	C1532	A1472	G1410	C1332	A1265	A1189	G1117	A1000
C2072	A1847	U1777	U1777	C1686	A1610	G1533	A1472	C1411	C1333	A1266	G1190	A1001	A1001
G2073	G1856	U1778	U1778	C1687	A1614	C1543	A1473	A1412	A1336	U1267	G1191	G1122	G1002
U2074	G1857	U1779	U1779	U1688	C1615	A1544	C1474	G1413	G1337	A1268	C1195	C1123	G1003
U2075	G1858	A1780	A1780	A1689	C1616	A1545	G1475	G1413	A1269	G1269	G1195	C1124	G1004
C2076	A1859	C1781	C1781	A1691	C1617	C1546	C1476	A1412	G1339	A1270	G1196	G1125	C1005
G2080	G1865	C1782	C1782	U1692	A1618	C1548	G1478	G1413	G1339	A1270	G1196	G1125	C1005
C2081	A1866	A1783	A1783	C1693	A1624	C1549	G1480	G1413	G1339	A1270	G1196	G1125	C1005
A2082	A1876	C1694	C1694	C1695	G1695	C1551	U1481	G1416	G1339	A1270	G1196	G1125	C1005
G2083	A1876	C1695	C1695	G1695	C1695	C1551	U1481	G1416	G1339	A1270	G1196	G1125	C1005
U2016	C1942	C1942	C1942	C1942	C1942	C1942	C1942	C1942	C1942	C1942	C1942	C1942	C1942





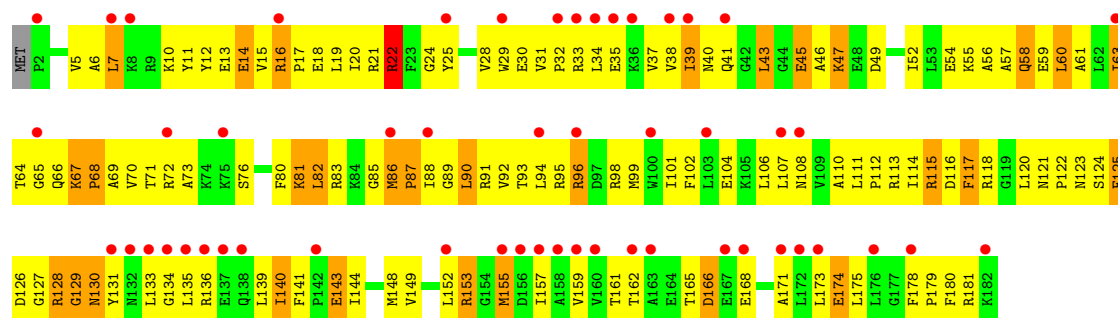
U2096	G2029	G1959	C1800	G1717	A1641	G1577	C1505	G1441	C1370	A1308	G1243	U1175	A1106
C2097	A2030	A1960	G1801	G1718	G1642	U1578	C1506	G1442	G1371	G1309	G1244	G1176	G1107
U2098	C1961	C1981	A1802	U1720	G1643	A1579	A1507	G1443	U1372	G1310	G1245	U1177	U1108
U2099	C1962	A1889	A1803	G1719		A1580	A1508	G1444	G1373	G1311	A1246	C1178	C1109
G2100	U1963	G1890	U1804	G1721	G1643	G1581	C1509	A1445A	G1374	U1313	A1247	C1179	G1110
G2101	G1964	G1891	U1805	A1722	G1649	C1582	A1509A	C1445A	C1375	U1314	G1250	C1180	A1111
U2102		C1892		U1739		A1583	A1509B	C1446		C1315	G1251	C1181	G1112
C2103	C1967	C1893	A1809	G1740	A1632	C1584	G1510	G1447	A1376	C1316	C1252	A1182	U1113
G2104	G1968	C1894	A1810	G1741	G1653	A1586	C1511	G1448	A1379	U1316	G1253	A1183	G1114
C2105	A1969	A1889	A1811	G1742	A1654	A1587	U1512	A1449	G1380	C1317	A1253	G1184	C1115
G2106	C2039	C1895	A1812	C1743	A1655	C1588	C1513	G1450	G1381	C1318	A1254	C1185	C1116
C	C2040	G1896	G1813	G1744	C1656	C1589	U1514	C1450A	G1382	C1319	U1255	G1186	G1117
C	U2041	U1897	G1814	C1745	C1657	U1590	G1515	C1451	C1383	C1320	G1256	C1187	
C	A1972	U1898	G1815	C1745A	C1658	G1591	C1516		A1384	A1321	C1257	U1188	
C	G1973	G1899	A1816	G1746	U1659	C1592	U1517	G1455	G1385	A1322	C1258	U1189	
U	C1974	A1900	G1816	G1747	C1660	G1593	U1518		G1386	U1323	G1259	A1189	
C		A1901		G1748	G1661	G1594	G1519		C1387	G1324	G1260	G1191	
G	G1980	C1902	A1819	G1747A	G1662	G1595	G1520	G1458	G1388	U1326	C1261	G1192	A1126
U	A1981	G1903	U1820	G1748	G1663	A1596		A1460		C1327	U1262	G1193	A1127
A	G1982	G1904	A1821	G1749	C1664	A1597		G1461	A1395	G1328	U1263	A1194	U1128
G	C1983	C1905	G1822	G1750	A1665	C1598		G1462	U1396	C1329	G1264	G1195	A1129
G	U1984	G1906		C1751	G1666	C1599		C1463	U1397	C1330	A1265	G1196	U1130
A	G1985		G1826		G1667	C1600		C1464	C1398	G1331	G1266	G1197	G1131
U		C1909	C1827	C1754	G1668	U1601		G1465		A1331	U1267	U1198	A1132
A		G1910	G1828	A1755	A1669	G1602	G1529	G1466	G1403	G1332	U1268	U1199	U1133
A	G1989		A1829	U1756	A1670	A1803		C1467	C1404	C1333	A1269	G1200	G1135
G	C1990		C1830	G1758	C1604	C1531			U1405		C1270	C1201	U1136
U	U1991			A1759	C1605	C1532		A1471	A1406	A1336	G1271		G1137
G	G1992		U1833	G1760	C1606	G1533		A1472	A1407	G1337	A1272	A1204	G1138
G	A2059		G1834		C1607	C1543		G1473	C1408	G1338	U1273	U1205	G1139
G	C1994		G1835	A1762	C1676	A1608		C1474	C1409	G1339	A1274	G1206	C1140
G	U1917		C1836	G1763	A1677	A1609		G1475	G1410	G1340	A1275	C1207	U1141
A	C1996		G1837	G1764	G1678	A1609		C1476	G1411	U1341	A1276	G1208	U1142
C	G1997		C1838			A1610		A1477	A1412	A1342	G1277	U1209	A1142A
C	U1998		G1839	C1771	G1681	C1611		G1478	G1413	G1343	A1278	U1210	A1143
U	C2065		G1840	G1772	G1682	C1612		G1479	G1414	G1344	G1279	U1211	G1144
C	G2000			A1773	C1683	C1613		G1480	U1415	G1345	G1280	G1212	C1145
G	A2001		G1844	G1774	C1685	A1614		U1481	G1416	G1346	G1281	A1213	
C	G2002			U1775	C1686	G1615		G1482	C1417	G1347	U1282	A1214	
C			A1847	G1776	G1687	A1616		G1484	G1418	G1348	G1283	G1215	C1152
C				U1777	U1688	A1617		G1485	A1349	C1349	A1284	G1216	C1153
C			G1850	U1778	A1689	A1618		A1486	U1419	C1350	G1285	G1216	G1154
C			A1851	U1779		G1619		A1487	A1420	C1351	A1286	A1155	A1156
U				A1780	U1692			G1488	G1421	G1352	A1287	C1221	A1157
G			G1856	C1781	U1693	G1622		U1489	G1422	A1353	U1288	C1221A	C1158
G			G1857	C1782	C1694	G1623		U1490	G1425	A1354	U1289		U1159
A			G1858	A1783	G1695	C1624		G1491	G1426	G1355	C1290	G1224	G1160
A			A1859	A1784	G1696	C1625		C1492	A1427	G1356	C1291	G1225	C1161
A				A1785	G1697	G1626		C1493	C1428	U1357	U1292	A1226	G1162
A			G1865	A1786	G1698	G1627		A1494	G1429	G1358	C1293	G1227	G1163
C			C1866		G1699	G1628		A1495	C1430	A1359	C1297	G1228	U1164
C			A1876	C1790	A1700	U1629		A1496	G1431	A1360	C1298	G1229	G1165
A			A1877	A1791	A1701	U1629		U1497	U1434	C1363	C1299	G1230	U1167
C			G1878	G1792	G1702	A1569		C1498	G1435	G1364	U1300	U1234	G1168
C			C1880	C1793	G1703	A1571		G1499	G1436	A1365	A1301	G1235	G1169
C				U1794	C1708	A1572		C1500	C1437	A1366	A1302		G1170
U	G2023		C1881	C1795	U1709	G1573		C1501	U1438	A1367	G1303	U1240	G1171
C	G2024		G1882	U1796	U1709	C1574		C1502	A1439	A1368	G1304	A1241	G1172
C	G2025		G1883	U1797	U1713	U1503		C1503	U1503	A1369	C1304	A1242	
C	G2026		A1884	U1798	G1714	U1576		C1504	G1440	G1369			A1174
G	U2027												
G	C2183												
G	G2184												





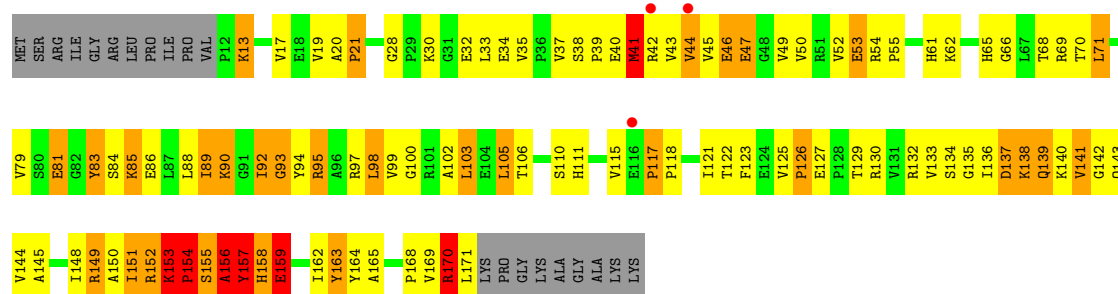
- Molecule 36: 50S ribosomal protein L5

Chain DG:



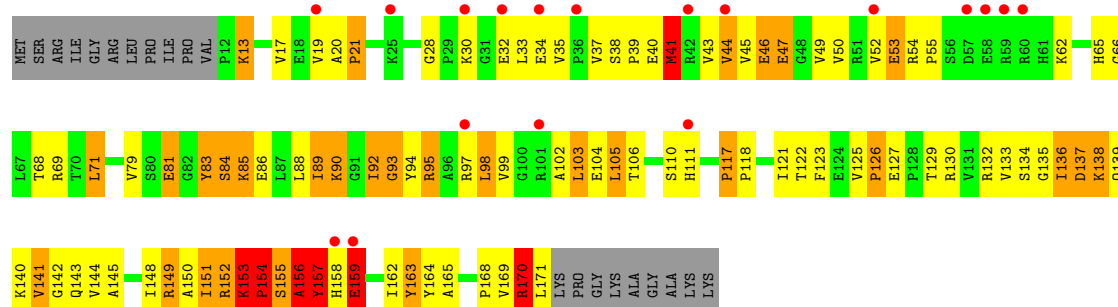
- Molecule 37: 50S ribosomal protein L6

Chain BH:

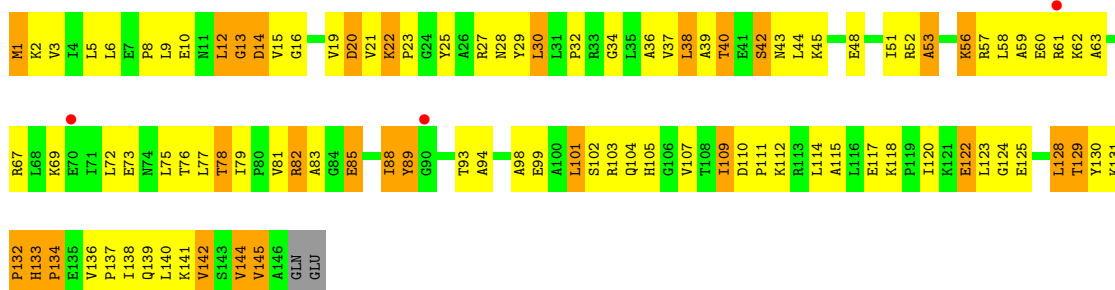


- Molecule 37: 50S ribosomal protein L6

Chain DH:

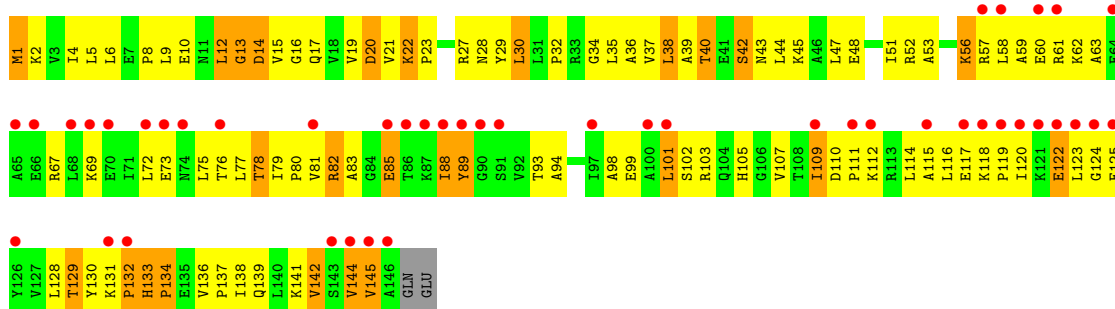


- Molecule 38: 50S ribosomal protein L9



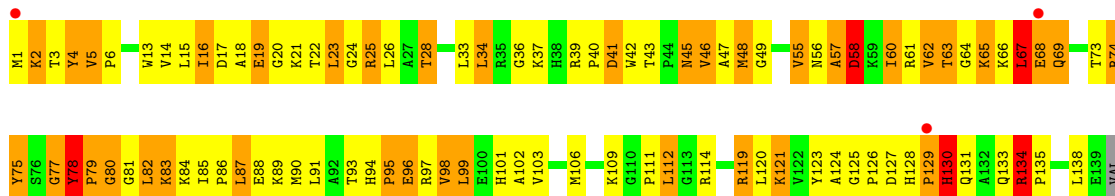
- Molecule 38: 50S ribosomal protein L9

Government	Percentage
Current government	85%
Previous government	15%

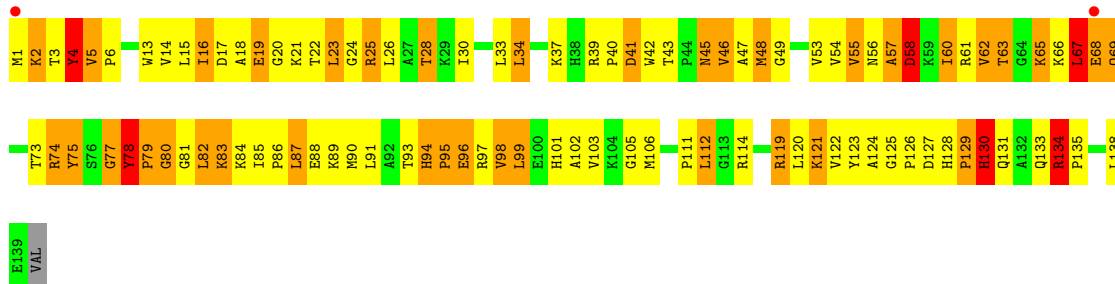


- Molecule 39: 50S ribosomal protein L13

Age Group	Percentage
18-24	~2%
25-34	~35%
35-44	~35%
45-54	~20%
55-64	~5%
65-74	~10%
75-84	~10%
85+	~10%

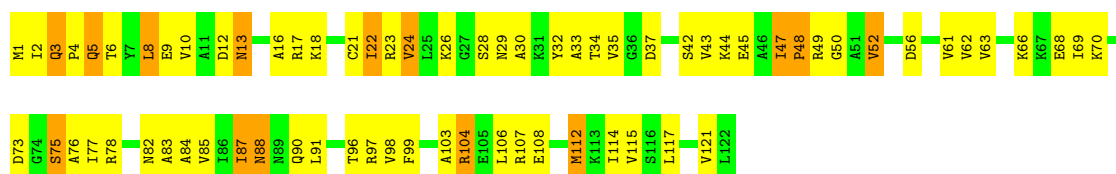


- Molecule 39: 50S ribosomal protein L13



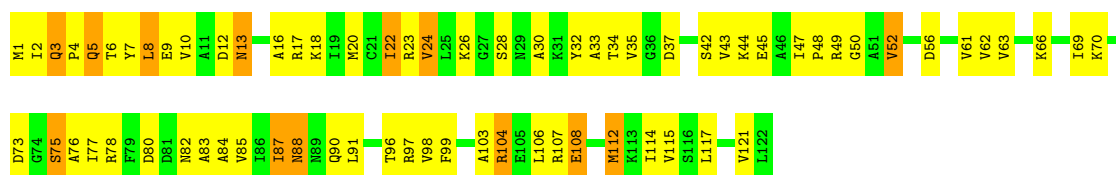
- Molecule 40: 50S ribosomal protein L14

Age Group	Percentage
18-24	15%
25-34	25%
35-44	20%
45-54	15%
55-64	10%
65-74	5%
75-84	2%
85+	1%



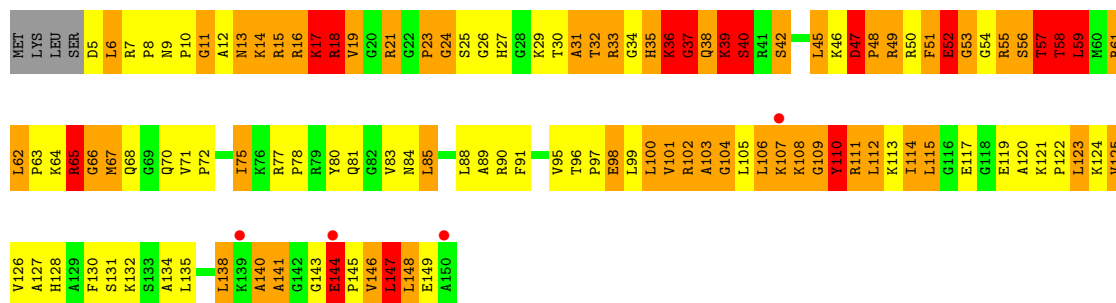
- Molecule 40: 50S ribosomal protein L14

Chain DO:



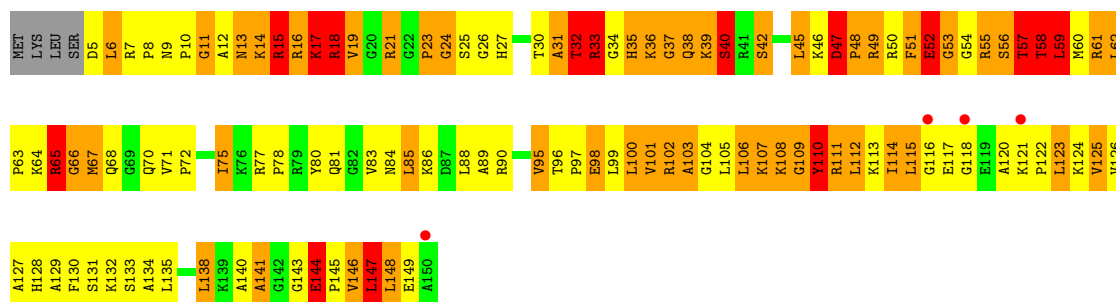
- Molecule 41: 50S ribosomal protein L15

Chain BP:



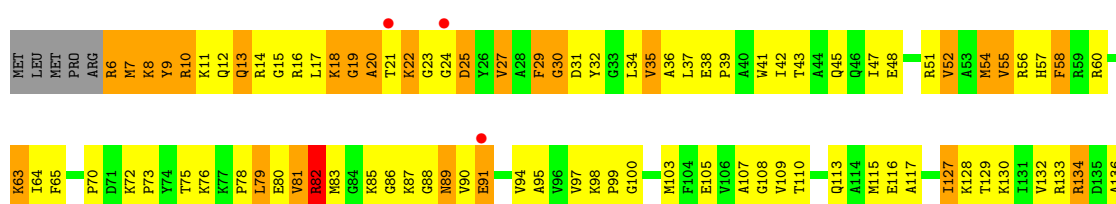
- Molecule 41: 50S ribosomal protein L15

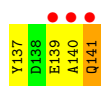
Chain DP:



- Molecule 42: 50S ribosomal protein L16

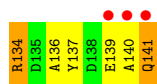
Chain BQ:





- Molecule 42: 50S ribosomal protein L16

Chain DQ:



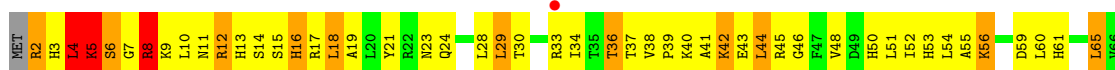
- Molecule 43: 50S ribosomal protein L17

Chain BR:



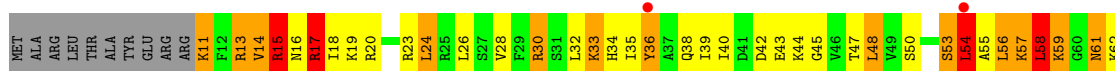
- Molecule 43: 50S ribosomal protein L17

Chain DR:



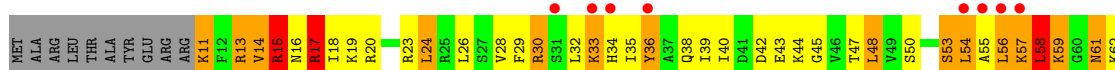
- Molecule 44: 50S ribosomal protein L18

Chain BS:



- Molecule 44: 50S ribosomal protein L18

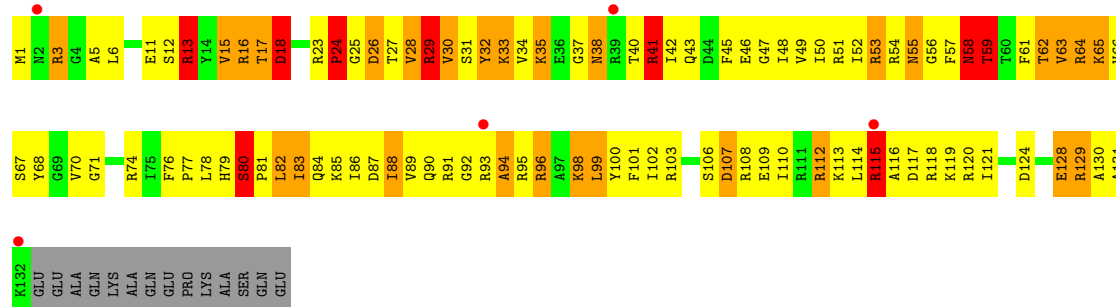
Chain DS:





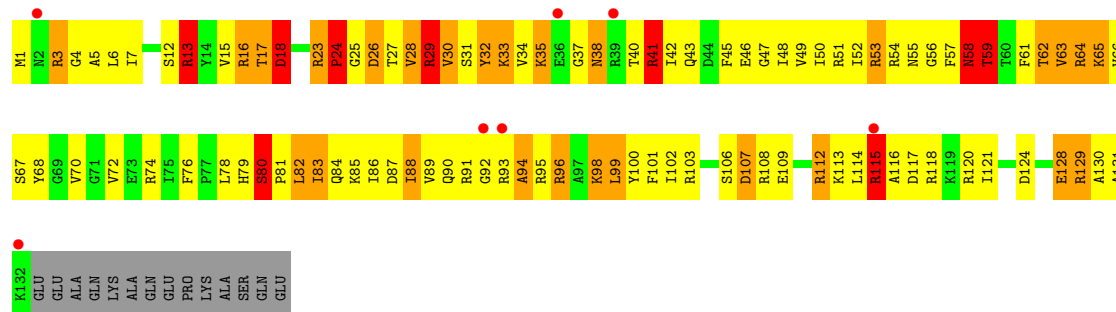
• Molecule 45: 50S ribosomal protein L19

Chain BT:



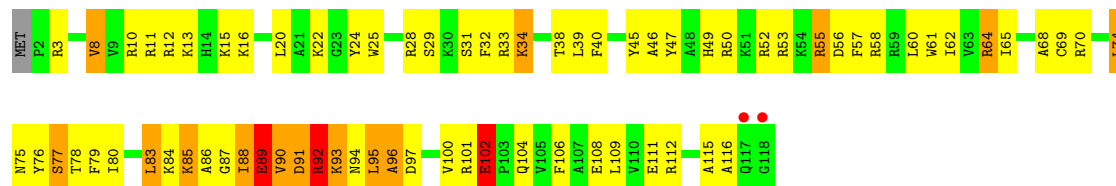
• Molecule 45: 50S ribosomal protein L19

Chain DT:



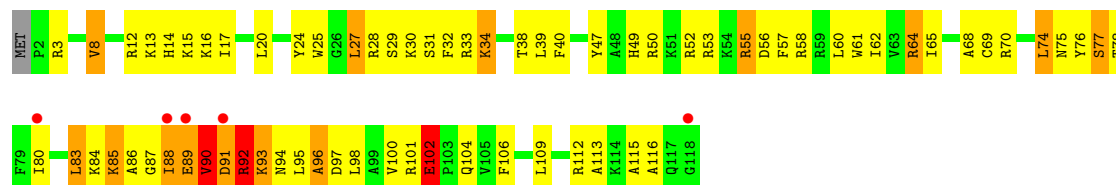
• Molecule 46: 50S ribosomal protein L20

Chain BU:



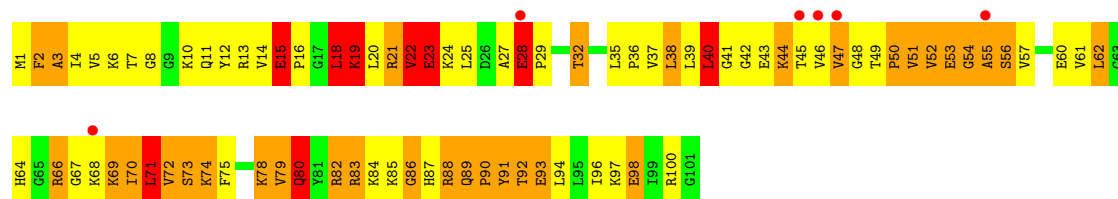
• Molecule 46: 50S ribosomal protein L20

Chain DU:



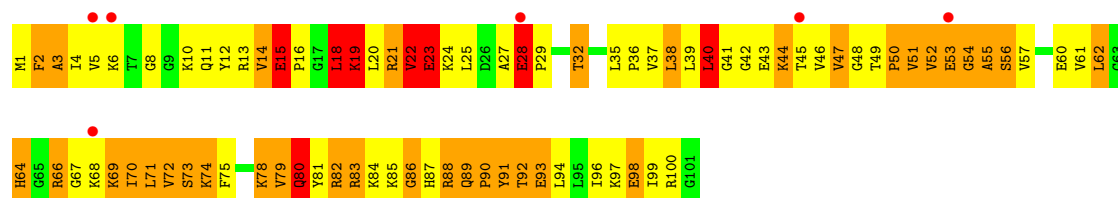
• Molecule 47: 50S ribosomal protein L21

Chain BV:



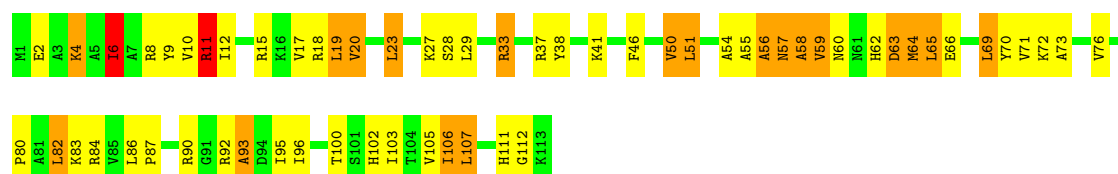
• Molecule 47: 50S ribosomal protein L21

Chain DV:



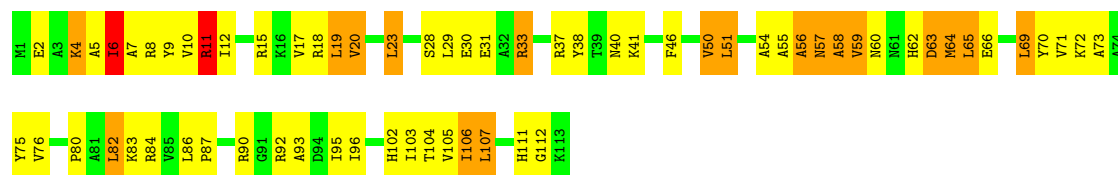
• Molecule 48: 50S ribosomal protein L22

Chain BW:



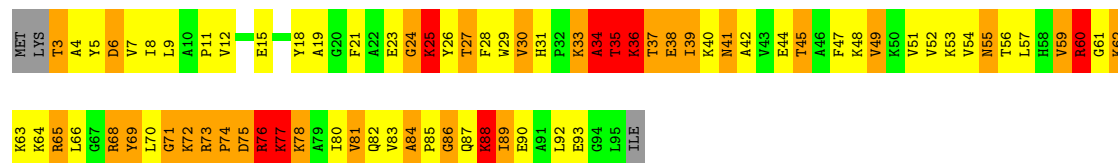
• Molecule 48: 50S ribosomal protein L22

Chain DW:



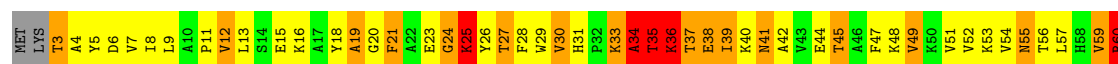
• Molecule 49: 50S ribosomal protein L23

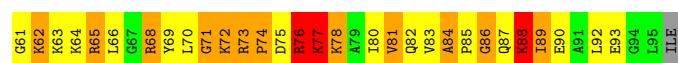
Chain BX:



• Molecule 49: 50S ribosomal protein L23

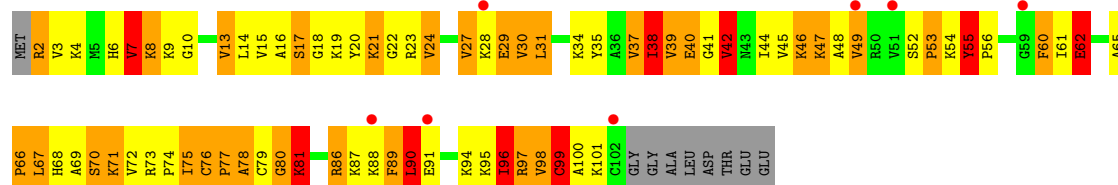
Chain DX:





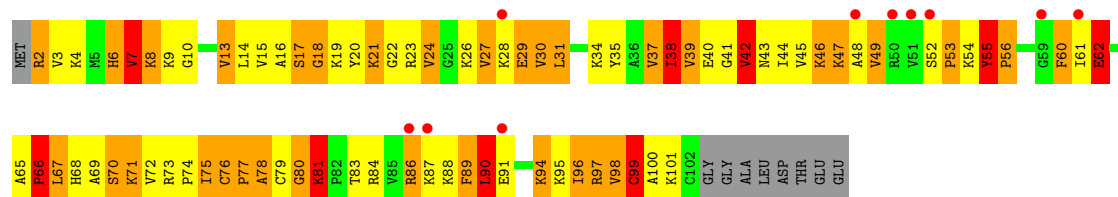
- Molecule 50: 50S ribosomal protein L24

Chain BY:



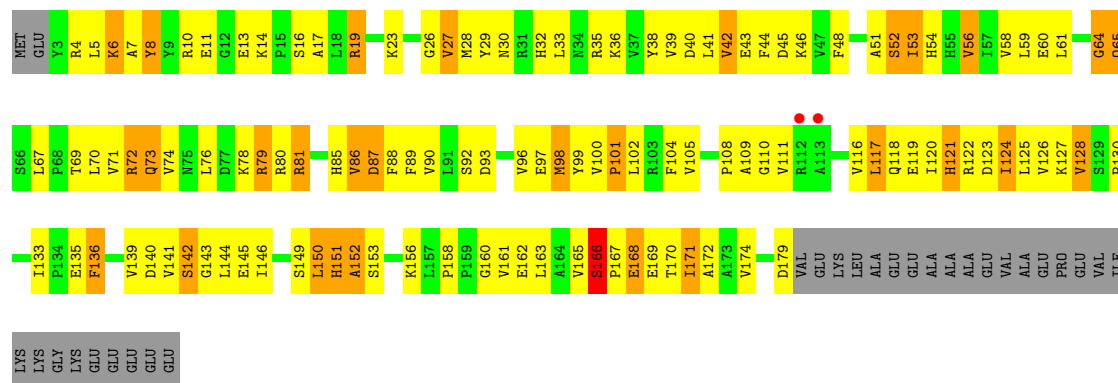
- Molecule 50: 50S ribosomal protein L24

Chain DY:



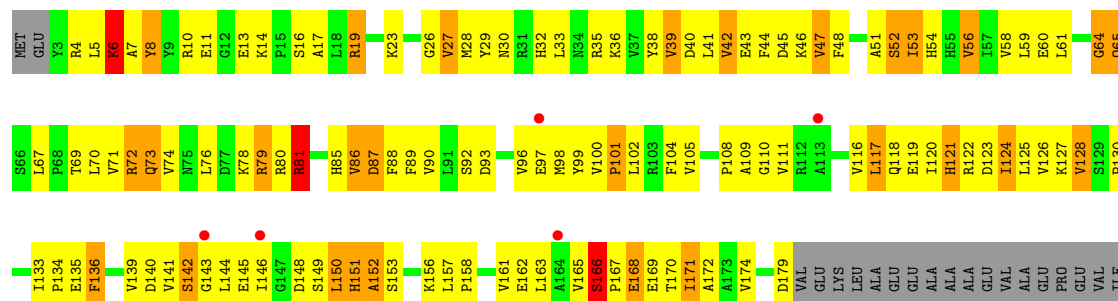
- Molecule 51: 50S ribosomal protein L25

Chain BZ:



- Molecule 51: 50S ribosomal protein L25

Chain DZ:



LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.47Å 447.96Å 620.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 3.00 49.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.61-3.00) 99.8 (49.88-3.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.01Å)	Xtriage
Refinement program	Phenix	Depositor
R, R_{free}	0.243 , 0.278 0.247 , 0.278	Depositor DCC
R_{free} test set	57768 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1152759 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	278034	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.49	0/36190	0.86	24/56486 (0.0%)
1	CA	0.49	0/36190	0.87	35/56486 (0.1%)
2	AB	0.28	0/1936	0.49	0/2611
2	CB	0.28	0/1936	0.49	0/2611
3	AC	0.26	0/1637	0.46	0/2207
3	CC	0.26	0/1637	0.45	0/2207
4	AD	0.34	0/1733	0.52	0/2318
4	CD	0.35	0/1733	0.53	0/2318
5	AE	0.32	0/1163	0.52	0/1566
5	CE	0.33	0/1163	0.54	0/1566
6	AF	0.33	0/856	0.53	0/1154
6	CF	0.33	0/856	0.53	0/1154
7	AG	0.24	0/1276	0.43	0/1709
7	CG	0.24	0/1276	0.43	0/1709
8	AH	0.33	0/1136	0.54	0/1527
8	CH	0.31	0/1136	0.53	0/1527
9	AI	0.26	0/1028	0.42	0/1375
9	CI	0.26	0/1028	0.42	0/1375
10	AJ	0.27	0/808	0.46	0/1087
10	CJ	0.27	0/808	0.47	0/1087
11	AK	0.31	0/900	0.52	0/1213
11	CK	0.32	0/900	0.53	0/1213
12	AL	0.39	0/987	0.61	0/1322
12	CL	0.41	0/987	0.61	0/1322
13	AM	0.24	0/928	0.45	0/1238
13	CM	0.25	0/928	0.45	0/1238
14	AN	0.28	0/501	0.43	0/664
14	CN	0.27	0/501	0.43	0/664
15	AO	0.34	0/745	0.53	0/992
15	CO	0.33	0/745	0.52	0/992
16	AP	0.32	0/717	0.54	0/965
16	CP	0.31	0/717	0.55	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.34	0/837	0.53	0/1119
17	CQ	0.33	0/837	0.53	0/1119
18	AR	0.33	0/579	0.57	0/768
18	CR	0.32	0/579	0.56	0/768
19	AS	0.25	0/643	0.42	0/867
19	CS	0.25	0/643	0.42	0/867
20	AT	0.35	0/765	0.55	0/1007
20	CT	0.34	0/765	0.55	0/1007
21	AU	0.26	0/213	0.42	0/279
21	CU	0.26	0/213	0.42	0/279
22	B0	0.52	0/658	0.70	0/878
22	D0	0.52	0/658	0.70	0/878
23	B1	0.76	0/700	1.02	2/931 (0.2%)
23	D1	0.73	0/700	0.99	2/931 (0.2%)
24	B2	0.65	0/423	0.99	1/560 (0.2%)
24	D2	0.57	0/423	0.92	1/560 (0.2%)
25	B3	0.61	0/473	0.71	0/636
25	D3	0.48	0/473	0.68	0/636
26	B4	0.28	0/156	0.57	0/215
26	D4	0.27	0/156	0.55	0/215
27	B5	0.85	0/473	1.06	3/639 (0.5%)
27	D5	0.78	0/473	1.01	3/639 (0.5%)
28	B6	0.80	0/387	1.04	2/517 (0.4%)
28	D6	0.67	0/387	0.94	0/517
29	B7	0.63	0/427	0.84	0/563
29	D7	0.64	0/427	0.83	1/563 (0.2%)
30	B8	0.73	0/516	1.07	3/681 (0.4%)
30	D8	0.65	0/516	1.03	3/681 (0.4%)
31	BA	1.06	67/65745 (0.1%)	1.40	967/102639 (0.9%)
31	DA	0.87	39/65745 (0.1%)	1.40	970/102639 (0.9%)
32	BB	0.80	0/2853	1.13	12/4451 (0.3%)
32	DB	0.69	0/2853	1.13	20/4451 (0.4%)
33	BD	0.63	0/2155	0.84	1/2907 (0.0%)
33	DD	0.60	0/2155	0.83	0/2907
34	BE	0.62	0/1597	0.83	2/2155 (0.1%)
34	DE	0.55	0/1597	0.81	0/2155
35	BF	0.61	1/1659 (0.1%)	0.76	1/2246 (0.0%)
35	DF	0.52	0/1659	0.76	2/2246 (0.1%)
36	BG	0.31	0/1498	0.53	0/2013
36	DG	0.29	0/1498	0.52	0/2013
37	BH	0.60	0/1246	0.73	0/1684
37	DH	0.42	0/1246	0.68	0/1684
38	BI	0.35	0/1147	0.59	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.38	0/1147	0.59	0/1553
39	BN	0.72	0/1132	0.90	1/1527 (0.1%)
39	DN	0.57	0/1132	0.86	1/1527 (0.1%)
40	BO	0.59	1/943 (0.1%)	0.70	0/1269
40	DO	0.51	0/943	0.69	0/1269
41	BP	0.73	0/1131	1.07	9/1504 (0.6%)
41	DP	0.64	0/1131	1.00	5/1504 (0.3%)
42	BQ	0.69	0/1100	0.85	2/1470 (0.1%)
42	DQ	0.61	0/1100	0.85	2/1470 (0.1%)
43	BR	0.63	0/974	0.85	2/1302 (0.2%)
43	DR	0.57	0/974	0.84	2/1302 (0.2%)
44	BS	0.51	0/779	0.79	0/1038
44	DS	0.45	0/779	0.76	0/1038
45	BT	0.58	0/1114	0.86	1/1488 (0.1%)
45	DT	0.55	0/1114	0.85	2/1488 (0.1%)
46	BU	0.69	0/975	0.79	0/1297
46	DU	0.55	0/975	0.79	0/1297
47	BV	0.75	0/790	0.97	1/1057 (0.1%)
47	DV	0.60	0/790	0.92	1/1057 (0.1%)
48	BW	0.69	0/907	0.85	2/1216 (0.2%)
48	DW	0.60	0/907	0.82	2/1216 (0.2%)
49	BX	0.74	0/740	0.97	2/995 (0.2%)
49	DX	0.65	0/740	0.96	1/995 (0.1%)
50	BY	0.67	0/789	0.86	0/1053
50	DY	0.56	0/789	0.81	0/1053
51	BZ	0.45	0/1436	0.64	1/1951 (0.1%)
51	DZ	0.40	0/1436	0.63	1/1951 (0.1%)
All	All	0.74	108/301002 (0.0%)	1.11	2093/449818 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	B1	0	1
23	D1	0	1
27	B5	0	1
27	D5	0	1
30	B8	0	1
30	D8	0	1
31	BA	21	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	DA	21	0
33	BD	0	2
33	DD	0	2
34	BE	0	2
34	DE	0	2
37	BH	0	2
37	DH	0	2
41	BP	0	5
41	DP	0	3
42	BQ	0	1
42	DQ	0	1
43	BR	0	2
43	DR	0	2
44	BS	0	1
44	DS	0	1
45	BT	0	1
45	DT	0	1
46	BU	0	1
46	DU	0	1
47	BV	0	1
47	DV	0	1
49	BX	0	5
49	DX	0	5
All	All	42	50

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	783	A	N9-C4	-14.89	1.28	1.37
31	BA	783	A	N3-C4	-11.41	1.28	1.34
31	BA	669	G	C4'-C3'	-11.35	1.40	1.53
31	BA	1300	U	C4'-C3'	-10.54	1.41	1.53
31	DA	783	A	N9-C4	-10.54	1.31	1.37

The worst 5 of 2093 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BA	1332	G	N3-C4-C5	21.05	139.12	128.60
31	BA	1332	G	N3-C4-N9	-19.19	114.49	126.00
31	DA	1779	U	C5-C6-N1	-16.63	114.39	122.70
31	BA	1332	G	C2-N3-C4	-16.06	103.87	111.90
31	BA	1779	U	C5-C6-N1	-15.89	114.75	122.70

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	BA	100	G	C1'
31	BA	472	A	C3'
31	BA	669	G	C4',C3',C1'
31	BA	945	A	C1'
31	BA	1300	U	C4',C3',C1'

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	B1	30	VAL	Peptide
27	B5	51	TYR	Peptide
30	B8	51	ALA	Peptide
33	BD	197	GLY	Peptide
33	BD	47	GLY	Peptide

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	32329	0	16318	1467	0
1	CA	32329	0	16318	1441	0
2	AB	1901	0	1951	186	0
2	CB	1901	0	1951	185	0
3	AC	1613	0	1677	120	0
3	CC	1613	0	1677	126	0
4	AD	1703	0	1763	184	0
4	CD	1703	0	1764	184	0
5	AE	1147	0	1207	99	0
5	CE	1147	0	1207	103	0
6	AF	843	0	857	92	0
6	CF	843	0	857	92	0
7	AG	1257	0	1296	72	0
7	CG	1257	0	1296	77	0
8	AH	1116	0	1177	91	0
8	CH	1116	0	1177	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AI	1011	0	1042	99	0
9	CI	1011	0	1042	96	0
10	AJ	795	0	840	88	0
10	CJ	795	0	840	85	0
11	AK	885	0	904	59	0
11	CK	885	0	904	65	0
12	AL	971	0	1057	102	0
12	CL	971	0	1057	103	0
13	AM	921	0	976	81	0
13	CM	921	0	976	81	0
14	AN	492	0	530	44	0
14	CN	492	0	530	43	0
15	AO	734	0	771	49	0
15	CO	734	0	771	47	0
16	AP	701	0	720	78	0
16	CP	701	0	720	81	0
17	AQ	824	0	891	60	0
17	CQ	824	0	891	55	0
18	AR	574	0	644	61	0
18	CR	574	0	644	60	0
19	AS	630	0	652	38	0
19	CS	630	0	652	39	0
20	AT	763	0	861	84	0
20	CT	763	0	861	87	0
21	AU	209	0	221	9	0
21	CU	209	0	221	10	0
22	B0	650	0	654	55	0
22	D0	650	0	654	57	0
23	B1	693	0	764	139	0
23	D1	693	0	764	140	0
24	B2	421	0	461	118	0
24	D2	421	0	461	123	0
25	B3	468	0	523	30	0
25	D3	468	0	523	51	0
26	B4	157	0	69	17	0
26	D4	157	0	69	14	0
27	B5	459	0	480	83	0
27	D5	459	0	480	82	0
28	B6	381	0	390	85	0
28	D6	381	0	390	87	0
29	B7	419	0	467	28	0
29	D7	419	0	467	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B8	508	0	576	137	0
30	D8	508	0	576	134	0
31	BA	58698	0	29591	2319	0
31	DA	58698	0	29590	2541	0
32	BB	2551	0	1295	128	0
32	DB	2551	0	1295	142	0
33	BD	2105	0	2182	298	0
33	DD	2105	0	2182	308	0
34	BE	1564	0	1629	206	0
34	DE	1564	0	1629	213	0
35	BF	1624	0	1677	165	0
35	DF	1624	0	1677	173	0
36	BG	1474	0	1534	150	0
36	DG	1474	0	1534	149	0
37	BH	1223	0	1282	149	0
37	DH	1223	0	1282	141	0
38	BI	1132	0	1218	121	0
38	DI	1132	0	1218	118	0
39	BN	1105	0	1180	181	0
39	DN	1105	0	1180	188	0
40	BO	933	0	996	74	0
40	DO	933	0	996	69	0
41	BP	1114	0	1187	259	0
41	DP	1114	0	1187	245	0
42	BQ	1080	0	1127	142	0
42	DQ	1080	0	1127	151	0
43	BR	960	0	1021	106	0
43	DR	960	0	1021	116	0
44	BS	771	0	832	138	0
44	DS	771	0	832	143	0
45	BT	1100	0	1164	188	0
45	DT	1100	0	1164	182	0
46	BU	958	0	1015	128	0
46	DU	958	0	1015	123	0
47	BV	779	0	852	219	0
47	DV	779	0	852	215	0
48	BW	896	0	953	60	0
48	DW	896	0	953	69	0
49	BX	726	0	778	173	0
49	DX	726	0	778	176	0
50	BY	776	0	870	195	0
50	DY	776	0	870	194	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	BZ	1404	0	1432	152	0
51	DZ	1404	0	1432	154	0
52	AA	54	0	0	0	0
52	B0	1	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	BA	362	0	0	0	0
52	BB	7	0	0	0	0
52	BD	1	0	0	0	0
52	BE	1	0	0	0	0
52	BF	1	0	0	0	0
52	BP	3	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	1	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	50	0	0	0	0
52	D0	1	0	0	0	0
52	D3	1	0	0	0	0
52	D5	1	0	0	0	0
52	D7	1	0	0	0	0
52	DA	328	0	0	0	0
52	DB	3	0	0	0	0
52	DE	1	0	0	0	0
52	DF	1	0	0	0	0
52	DP	1	0	0	0	0
52	DQ	1	0	0	0	0
52	DR	1	0	0	0	0
52	DU	1	0	0	0	0
52	DX	1	0	0	0	0
53	AD	1	0	0	0	0
53	AN	1	0	0	0	0
53	CD	1	0	0	0	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	51	0	67	1	0
55	DA	51	0	67	2	0
All	All	278034	0	189242	17303	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

The worst 5 of 17303 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
42:BQ:81:VAL:O	42:BQ:82:ARG:HD2	1.36	1.26
42:DQ:81:VAL:O	42:DQ:82:ARG:HD2	1.37	1.22
33:BD:35:LYS:HD2	33:BD:104:TYR:CD1	1.78	1.19
50:BY:95:LYS:HD3	50:BY:100:ALA:HB1	1.21	1.19
16:AP:28:ARG:HG2	16:AP:28:ARG:HH11	1.06	1.18

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	165 (71%)	51 (22%)	17 (7%)	2	8
2	CB	233/256 (91%)	165 (71%)	51 (22%)	17 (7%)	2	8
3	AC	205/239 (86%)	156 (76%)	35 (17%)	14 (7%)	2	10
3	CC	205/239 (86%)	156 (76%)	35 (17%)	14 (7%)	2	10
4	AD	206/209 (99%)	128 (62%)	59 (29%)	19 (9%)	1	5
4	CD	206/209 (99%)	128 (62%)	59 (29%)	19 (9%)	1	5
5	AE	149/160 (93%)	106 (71%)	31 (21%)	12 (8%)	1	7
5	CE	149/160 (93%)	104 (70%)	33 (22%)	12 (8%)	1	7
6	AF	99/101 (98%)	76 (77%)	18 (18%)	5 (5%)	3	18
6	CF	99/101 (98%)	77 (78%)	17 (17%)	5 (5%)	3	18
7	AG	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	8	39
7	CG	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	8	39
8	AH	136/138 (99%)	105 (77%)	24 (18%)	7 (5%)	3	18
8	CH	136/138 (99%)	106 (78%)	23 (17%)	7 (5%)	3	18
9	AI	123/128 (96%)	93 (76%)	21 (17%)	9 (7%)	2	8
9	CI	123/128 (96%)	93 (76%)	21 (17%)	9 (7%)	2	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	97/105 (92%)	80 (82%)	13 (13%)	4 (4%)	4	24
10	CJ	97/105 (92%)	80 (82%)	13 (13%)	4 (4%)	4	24
11	AK	117/129 (91%)	92 (79%)	20 (17%)	5 (4%)	4	23
11	CK	117/129 (91%)	94 (80%)	18 (15%)	5 (4%)	4	23
12	AL	123/135 (91%)	85 (69%)	24 (20%)	14 (11%)	1	3
12	CL	123/135 (91%)	86 (70%)	23 (19%)	14 (11%)	1	3
13	AM	107/126 (85%)	85 (79%)	17 (16%)	5 (5%)	4	21
13	CM	107/126 (85%)	84 (78%)	18 (17%)	5 (5%)	4	21
14	AN	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	6	31
14	CN	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	6	31
15	AO	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	6	30
15	CO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	6	30
16	AP	82/88 (93%)	49 (60%)	23 (28%)	10 (12%)	1	2
16	CP	82/88 (93%)	48 (58%)	24 (29%)	10 (12%)	1	2
17	AQ	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	2	14
17	CQ	98/105 (93%)	76 (78%)	16 (16%)	6 (6%)	2	14
18	AR	68/88 (77%)	43 (63%)	21 (31%)	4 (6%)	2	14
18	CR	68/88 (77%)	40 (59%)	22 (32%)	6 (9%)	1	5
19	AS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	1	5
19	CS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	1	5
20	AT	97/106 (92%)	64 (66%)	25 (26%)	8 (8%)	1	6
20	CT	97/106 (92%)	61 (63%)	29 (30%)	7 (7%)	2	8
21	AU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	4	23
21	CU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	4	23
22	B0	83/85 (98%)	68 (82%)	11 (13%)	4 (5%)	4	20
22	D0	83/85 (98%)	70 (84%)	9 (11%)	4 (5%)	4	20
23	B1	87/98 (89%)	52 (60%)	17 (20%)	18 (21%)	0	0
23	D1	87/98 (89%)	52 (60%)	18 (21%)	17 (20%)	0	0
24	B2	49/72 (68%)	22 (45%)	17 (35%)	10 (20%)	0	0
24	D2	49/72 (68%)	24 (49%)	13 (26%)	12 (24%)	0	0
25	B3	58/60 (97%)	50 (86%)	6 (10%)	2 (3%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	D3	58/60 (97%)	51 (88%)	4 (7%)	3 (5%)	3	18
26	B4	30/71 (42%)	4 (13%)	11 (37%)	15 (50%)	0	0
26	D4	30/71 (42%)	4 (13%)	11 (37%)	15 (50%)	0	0
27	B5	57/60 (95%)	41 (72%)	7 (12%)	9 (16%)	0	1
27	D5	57/60 (95%)	42 (74%)	6 (10%)	9 (16%)	0	1
28	B6	41/54 (76%)	21 (51%)	7 (17%)	13 (32%)	0	0
28	D6	41/54 (76%)	21 (51%)	7 (17%)	13 (32%)	0	0
29	B7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
29	D7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
30	B8	62/65 (95%)	42 (68%)	8 (13%)	12 (19%)	0	0
30	D8	62/65 (95%)	44 (71%)	6 (10%)	12 (19%)	0	0
33	BD	270/276 (98%)	217 (80%)	40 (15%)	13 (5%)	4	20
33	DD	270/276 (98%)	214 (79%)	42 (16%)	14 (5%)	3	18
34	BE	203/206 (98%)	153 (75%)	28 (14%)	22 (11%)	1	3
34	DE	203/206 (98%)	151 (74%)	29 (14%)	23 (11%)	1	3
35	BF	206/210 (98%)	155 (75%)	37 (18%)	14 (7%)	2	10
35	DF	206/210 (98%)	151 (73%)	42 (20%)	13 (6%)	2	12
36	BG	177/182 (97%)	123 (70%)	35 (20%)	19 (11%)	1	3
36	DG	177/182 (97%)	125 (71%)	32 (18%)	20 (11%)	1	3
37	BH	158/180 (88%)	103 (65%)	28 (18%)	27 (17%)	0	1
37	DH	158/180 (88%)	103 (65%)	30 (19%)	25 (16%)	0	1
38	BI	144/148 (97%)	89 (62%)	38 (26%)	17 (12%)	1	2
38	DI	144/148 (97%)	89 (62%)	39 (27%)	16 (11%)	1	3
39	BN	137/140 (98%)	96 (70%)	25 (18%)	16 (12%)	1	3
39	DN	137/140 (98%)	94 (69%)	26 (19%)	17 (12%)	1	2
40	BO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	9	40
40	DO	120/122 (98%)	103 (86%)	15 (12%)	2 (2%)	14	54
41	BP	144/150 (96%)	80 (56%)	23 (16%)	41 (28%)	0	0
41	DP	144/150 (96%)	80 (56%)	24 (17%)	40 (28%)	0	0
42	BQ	134/141 (95%)	95 (71%)	23 (17%)	16 (12%)	1	2
42	DQ	134/141 (95%)	94 (70%)	25 (19%)	15 (11%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BR	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	7
43	DR	115/118 (98%)	84 (73%)	21 (18%)	10 (9%)	1	5
44	BS	97/112 (87%)	54 (56%)	19 (20%)	24 (25%)	0	0
44	DS	97/112 (87%)	53 (55%)	21 (22%)	23 (24%)	0	0
45	BT	130/146 (89%)	93 (72%)	20 (15%)	17 (13%)	0	2
45	DT	130/146 (89%)	92 (71%)	22 (17%)	16 (12%)	1	2
46	BU	115/118 (98%)	90 (78%)	17 (15%)	8 (7%)	2	9
46	DU	115/118 (98%)	85 (74%)	22 (19%)	8 (7%)	2	9
47	BV	99/101 (98%)	57 (58%)	15 (15%)	27 (27%)	0	0
47	DV	99/101 (98%)	56 (57%)	15 (15%)	28 (28%)	0	0
48	BW	111/113 (98%)	88 (79%)	14 (13%)	9 (8%)	1	7
48	DW	111/113 (98%)	85 (77%)	18 (16%)	8 (7%)	2	8
49	BX	91/96 (95%)	52 (57%)	16 (18%)	23 (25%)	0	0
49	DX	91/96 (95%)	50 (55%)	18 (20%)	23 (25%)	0	0
50	BY	99/110 (90%)	49 (50%)	21 (21%)	29 (29%)	0	0
50	DY	99/110 (90%)	47 (48%)	23 (23%)	29 (29%)	0	0
51	BZ	175/206 (85%)	115 (66%)	44 (25%)	16 (9%)	1	5
51	DZ	175/206 (85%)	115 (66%)	41 (23%)	19 (11%)	1	3
All	All	11152/12056 (92%)	7925 (71%)	2047 (18%)	1180 (11%)	1	3

5 of 1180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	154	LEU
2	AB	165	VAL
2	AB	194	PRO
2	AB	195	ASP

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	AB	202/220 (92%)	178 (88%)	24 (12%)	8	30
2	CB	202/220 (92%)	178 (88%)	24 (12%)	8	30
3	AC	160/188 (85%)	153 (96%)	7 (4%)	39	82
3	CC	160/188 (85%)	153 (96%)	7 (4%)	39	82
4	AD	180/181 (99%)	150 (83%)	30 (17%)	3	16
4	CD	180/181 (99%)	153 (85%)	27 (15%)	4	20
5	AE	115/122 (94%)	97 (84%)	18 (16%)	4	18
5	CE	115/122 (94%)	97 (84%)	18 (16%)	4	18
6	AF	90/90 (100%)	80 (89%)	10 (11%)	9	34
6	CF	90/90 (100%)	79 (88%)	11 (12%)	7	29
7	AG	126/127 (99%)	123 (98%)	3 (2%)	61	92
7	CG	126/127 (99%)	122 (97%)	4 (3%)	51	89
8	AH	119/119 (100%)	110 (92%)	9 (8%)	19	57
8	CH	119/119 (100%)	110 (92%)	9 (8%)	19	57
9	AI	98/99 (99%)	88 (90%)	10 (10%)	11	38
9	CI	98/99 (99%)	89 (91%)	9 (9%)	13	46
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	8	33
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	8	33
11	AK	90/99 (91%)	84 (93%)	6 (7%)	23	64
11	CK	90/99 (91%)	84 (93%)	6 (7%)	23	64
12	AL	104/111 (94%)	93 (89%)	11 (11%)	10	36
12	CL	104/111 (94%)	92 (88%)	12 (12%)	8	32
13	AM	93/101 (92%)	87 (94%)	6 (6%)	24	65
13	CM	93/101 (92%)	88 (95%)	5 (5%)	31	74
14	AN	49/50 (98%)	46 (94%)	3 (6%)	26	68
14	CN	49/50 (98%)	46 (94%)	3 (6%)	26	68
15	AO	79/80 (99%)	71 (90%)	8 (10%)	11	39
15	CO	79/80 (99%)	71 (90%)	8 (10%)	11	39
16	AP	72/74 (97%)	57 (79%)	15 (21%)	2	8
16	CP	72/74 (97%)	57 (79%)	15 (21%)	2	8
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	32	74
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	32	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	56 (92%)	5 (8%)	17	52
18	CR	61/77 (79%)	57 (93%)	4 (7%)	24	64
19	AS	69/80 (86%)	62 (90%)	7 (10%)	11	39
19	CS	69/80 (86%)	62 (90%)	7 (10%)	11	39
20	AT	76/82 (93%)	65 (86%)	11 (14%)	5	22
20	CT	76/82 (93%)	65 (86%)	11 (14%)	5	22
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
22	B0	61/67 (91%)	53 (87%)	8 (13%)	6	25
22	D0	61/67 (91%)	53 (87%)	8 (13%)	6	25
23	B1	73/83 (88%)	53 (73%)	20 (27%)	0	3
23	D1	73/83 (88%)	55 (75%)	18 (25%)	1	4
24	B2	46/67 (69%)	26 (56%)	20 (44%)	0	0
24	D2	46/67 (69%)	27 (59%)	19 (41%)	0	0
25	B3	51/52 (98%)	48 (94%)	3 (6%)	28	70
25	D3	51/52 (98%)	48 (94%)	3 (6%)	28	70
27	B5	51/52 (98%)	38 (74%)	13 (26%)	1	4
27	D5	51/52 (98%)	38 (74%)	13 (26%)	1	4
28	B6	43/52 (83%)	25 (58%)	18 (42%)	0	0
28	D6	43/52 (83%)	26 (60%)	17 (40%)	0	0
29	B7	41/42 (98%)	33 (80%)	8 (20%)	2	11
29	D7	41/42 (98%)	33 (80%)	8 (20%)	2	11
30	B8	53/55 (96%)	42 (79%)	11 (21%)	2	8
30	D8	53/55 (96%)	43 (81%)	10 (19%)	2	12
33	BD	213/218 (98%)	168 (79%)	45 (21%)	1	8
33	DD	213/218 (98%)	169 (79%)	44 (21%)	2	8
34	BE	165/166 (99%)	125 (76%)	40 (24%)	1	5
34	DE	165/166 (99%)	126 (76%)	39 (24%)	1	5
35	BF	165/166 (99%)	127 (77%)	38 (23%)	1	6
35	DF	165/166 (99%)	129 (78%)	36 (22%)	1	8
36	BG	155/156 (99%)	136 (88%)	19 (12%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DG	155/156 (99%)	135 (87%)	20 (13%)	6	26
37	BH	132/148 (89%)	107 (81%)	25 (19%)	2	12
37	DH	132/148 (89%)	108 (82%)	24 (18%)	2	13
38	BI	122/124 (98%)	105 (86%)	17 (14%)	5	23
38	DI	122/124 (98%)	105 (86%)	17 (14%)	5	23
39	BN	117/119 (98%)	78 (67%)	39 (33%)	0	2
39	DN	117/119 (98%)	78 (67%)	39 (33%)	0	2
40	BO	100/100 (100%)	85 (85%)	15 (15%)	4	20
40	DO	100/100 (100%)	85 (85%)	15 (15%)	4	20
41	BP	112/116 (97%)	73 (65%)	39 (35%)	0	1
41	DP	112/116 (97%)	71 (63%)	41 (37%)	0	1
42	BQ	106/111 (96%)	80 (76%)	26 (24%)	1	5
42	DQ	106/111 (96%)	81 (76%)	25 (24%)	1	5
43	BR	100/101 (99%)	72 (72%)	28 (28%)	0	3
43	DR	100/101 (99%)	73 (73%)	27 (27%)	1	3
44	BS	77/88 (88%)	52 (68%)	25 (32%)	0	2
44	DS	77/88 (88%)	52 (68%)	25 (32%)	0	2
45	BT	116/127 (91%)	86 (74%)	30 (26%)	1	4
45	DT	116/127 (91%)	88 (76%)	28 (24%)	1	5
46	BU	92/94 (98%)	76 (83%)	16 (17%)	3	14
46	DU	92/94 (98%)	75 (82%)	17 (18%)	2	13
47	BV	82/82 (100%)	53 (65%)	29 (35%)	0	1
47	DV	82/82 (100%)	54 (66%)	28 (34%)	0	1
48	BW	91/92 (99%)	76 (84%)	15 (16%)	3	16
48	DW	91/92 (99%)	76 (84%)	15 (16%)	3	16
49	BX	74/78 (95%)	55 (74%)	19 (26%)	1	4
49	DX	74/78 (95%)	54 (73%)	20 (27%)	1	3
50	BY	84/91 (92%)	58 (69%)	26 (31%)	0	2
50	DY	84/91 (92%)	58 (69%)	26 (31%)	0	2
51	BZ	155/179 (87%)	131 (84%)	24 (16%)	4	19
51	DZ	155/179 (87%)	131 (84%)	24 (16%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9322/9874 (94%)	7707 (83%)	1615 (17%)	3 14

5 of 1615 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BW	4	LYS
7	CG	137	LYS
46	DU	74	LEU
49	BX	35	THR
2	CB	42	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 291 such sidechains are listed below:

Mol	Chain	Res	Type
48	BW	57	ASN
5	CE	78	HIS
45	DT	58	ASN
48	BW	111	HIS
2	CB	146	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	283 (18%)	29 (1%)
1	CA	1503/1522 (98%)	280 (18%)	29 (1%)
31	BA	2723/2787 (97%)	723 (26%)	73 (2%)
31	DA	2723/2787 (97%)	726 (26%)	70 (2%)
32	BB	118/122 (96%)	35 (29%)	1 (0%)
32	DB	118/122 (96%)	34 (28%)	1 (0%)
All	All	8688/8862 (98%)	2081 (23%)	203 (2%)

5 of 2081 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C

5 of 203 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	BA	2660	A
1	CA	428	G
31	DA	2225	A
31	BA	2689	U
1	CA	60	A

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 838 ligands modelled in this entry, 836 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	ERY	BA	3364	-	53,53,53	1.14	3 (5%)	82,82,82	0.98	4 (4%)
55	ERY	DA	3330	-	53,53,53	1.14	3 (5%)	82,82,82	0.98	4 (4%)

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	ERY	BA	3364	-	-	0/72/107/107	0/3/3/3
55	ERY	DA	3330	-	-	0/72/107/107	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BA	3364	ERY	C6-C5	2.66	1.61	1.55
55	DA	3330	ERY	C6-C5	2.64	1.61	1.55
55	BA	3364	ERY	C7-C6	2.26	1.58	1.54
55	DA	3330	ERY	C7-C6	2.24	1.58	1.54
55	DA	3330	ERY	C2-C3	2.03	1.60	1.55

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	3330	ERY	C3-C2-C1	-2.60	104.69	110.04
55	BA	3364	ERY	C3-C2-C1	-2.60	104.70	110.04
55	DA	3330	ERY	C25-C24-C23	-2.50	106.45	110.06
55	BA	3364	ERY	C25-C24-C23	-2.49	106.46	110.06
55	DA	3330	ERY	C6-C5-C4	-2.19	111.00	114.09

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	3
13	AM	3
36	DG	1
36	BG	1
9	AI	1
9	CI	1
28	D6	1
28	B6	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CM	69:GLU	C	70:LEU	N	5.58
1	AM	69:GLU	C	70:LEU	N	5.57
1	DG	112:PRO	C	113:ARG	N	4.82
1	BG	112:PRO	C	113:ARG	N	4.80
1	CM	97:PRO	C	98:VAL	N	4.38

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.68	205 (13%) 4 1	46, 116, 201, 202	0
1	CA	1504/1522 (98%)	0.64	189 (12%) 4 1	50, 115, 201, 203	0
2	AB	235/256 (91%)	0.64	28 (11%) 5 1	99, 157, 195, 200	0
2	CB	235/256 (91%)	0.81	40 (17%) 2 1	99, 162, 195, 201	0
3	AC	207/239 (86%)	0.61	19 (9%) 9 2	108, 163, 190, 198	0
3	CC	207/239 (86%)	1.02	42 (20%) 1 1	110, 168, 192, 198	0
4	AD	208/209 (99%)	0.29	7 (3%) 43 8	65, 126, 175, 189	0
4	CD	208/209 (99%)	0.25	8 (3%) 38 7	66, 124, 173, 191	0
5	AE	151/160 (94%)	0.10	0 100 100	65, 111, 162, 199	0
5	CE	151/160 (94%)	0.44	5 (3%) 44 8	72, 115, 172, 198	0
6	AF	101/101 (100%)	0.09	0 100 100	82, 123, 173, 192	0
6	CF	101/101 (100%)	0.25	4 (3%) 36 7	84, 130, 177, 196	0
7	AG	155/156 (99%)	0.97	28 (18%) 2 1	126, 177, 196, 201	0
7	CG	155/156 (99%)	1.26	35 (22%) 1 1	122, 177, 196, 200	0
8	AH	138/138 (100%)	-0.05	1 (0%) 84 28	78, 113, 157, 171	0
8	CH	138/138 (100%)	0.01	1 (0%) 84 28	79, 115, 162, 171	0
9	AI	127/128 (99%)	1.64	45 (35%) 1 0	132, 189, 200, 201	0
9	CI	127/128 (99%)	1.87	47 (37%) 1 0	131, 190, 200, 202	0
10	AJ	99/105 (94%)	1.98	41 (41%) 1 0	119, 178, 199, 200	0
10	CJ	99/105 (94%)	2.45	50 (50%) 0 0	116, 182, 200, 201	0
11	AK	119/129 (92%)	0.34	3 (2%) 54 11	63, 113, 163, 199	0
11	CK	119/129 (92%)	0.48	8 (6%) 17 4	64, 116, 165, 199	0
12	AL	125/135 (92%)	0.39	10 (8%) 12 3	59, 98, 164, 201	0
12	CL	125/135 (92%)	0.41	5 (4%) 36 7	58, 99, 167, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	AM	115/126 (91%)	1.81	44 (38%)	1 0	157, 191, 200, 201	0
13	CM	115/126 (91%)	1.30	23 (20%)	2 1	152, 189, 199, 201	0
14	AN	60/61 (98%)	1.15	15 (25%)	1 1	112, 172, 197, 199	0
14	CN	60/61 (98%)	1.09	9 (15%)	3 1	112, 171, 197, 199	0
15	AO	88/89 (98%)	0.13	2 (2%)	57 12	70, 105, 160, 169	0
15	CO	88/89 (98%)	0.22	0	100 100	71, 107, 162, 171	0
16	AP	84/88 (95%)	0.69	9 (10%)	6 2	82, 109, 170, 187	0
16	CP	84/88 (95%)	0.70	7 (8%)	11 3	80, 107, 165, 183	0
17	AQ	100/105 (95%)	0.29	3 (3%)	48 9	71, 104, 154, 185	0
17	CQ	100/105 (95%)	0.17	4 (4%)	36 7	74, 103, 154, 190	0
18	AR	70/88 (79%)	0.62	3 (4%)	34 7	80, 116, 173, 182	0
18	CR	70/88 (79%)	0.99	8 (11%)	6 2	83, 124, 175, 185	0
19	AS	79/93 (84%)	1.86	31 (39%)	1 0	127, 192, 200, 200	0
19	CS	79/93 (84%)	2.06	34 (43%)	1 0	131, 190, 200, 201	0
20	AT	99/106 (93%)	0.39	4 (4%)	36 7	75, 115, 162, 186	0
20	CT	99/106 (93%)	0.29	5 (5%)	27 6	74, 115, 160, 189	0
21	AU	25/27 (92%)	4.19	23 (92%)	0 0	144, 182, 197, 199	0
21	CU	25/27 (92%)	3.07	19 (76%)	0 0	139, 173, 194, 197	0
22	B0	85/85 (100%)	0.32	7 (8%)	12 3	39, 60, 177, 193	0
22	D0	85/85 (100%)	0.43	9 (10%)	7 2	44, 65, 177, 193	0
23	B1	89/98 (90%)	0.04	1 (1%)	77 21	39, 64, 143, 170	0
23	D1	89/98 (90%)	0.12	2 (2%)	59 12	41, 66, 144, 183	0
24	B2	51/72 (70%)	0.41	2 (3%)	37 7	47, 85, 185, 196	0
24	D2	51/72 (70%)	0.26	3 (5%)	22 5	53, 92, 191, 198	0
25	B3	60/60 (100%)	-0.05	2 (3%)	44 8	36, 59, 135, 186	0
25	D3	60/60 (100%)	0.15	4 (6%)	17 4	42, 66, 141, 182	0
26	B4	32/71 (45%)	-0.16	0	100 100	133, 155, 186, 193	0
26	D4	32/71 (45%)	0.11	0	100 100	143, 169, 187, 197	0
27	B5	58/60 (96%)	0.11	3 (5%)	26 6	20, 47, 177, 199	0
27	D5	58/60 (96%)	0.01	4 (6%)	17 4	23, 50, 176, 199	0
28	B6	45/54 (83%)	0.48	2 (4%)	33 7	41, 74, 129, 184	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	0.49	4 (8%)	10	3	44, 77, 143, 178	0
29	B7	49/49 (100%)	0.16	3 (6%)	21	5	26, 33, 119, 175	0
29	D7	49/49 (100%)	0.27	3 (6%)	21	5	26, 35, 126, 174	0
30	B8	64/65 (98%)	0.16	0	100	100	33, 54, 148, 179	0
30	D8	64/65 (98%)	-0.02	0	100	100	36, 58, 148, 180	0
31	BA	2725/2787 (97%)	-0.10	58 (2%)	60	12	25, 47, 144, 203	0
31	DA	2725/2787 (97%)	-0.17	102 (3%)	39	8	25, 52, 155, 202	0
32	BB	119/122 (97%)	0.22	4 (3%)	43	8	44, 92, 137, 191	0
32	DB	119/122 (97%)	0.63	20 (16%)	2	1	51, 101, 165, 190	0
33	BD	272/276 (98%)	-0.19	2 (0%)	84	28	25, 49, 105, 183	0
33	DD	272/276 (98%)	-0.19	1 (0%)	90	41	23, 53, 109, 172	0
34	BE	205/206 (99%)	-0.07	3 (1%)	70	16	26, 54, 140, 193	0
34	DE	205/206 (99%)	-0.11	4 (1%)	62	12	30, 58, 146, 193	0
35	BF	208/210 (99%)	0.08	7 (3%)	43	8	21, 65, 175, 198	0
35	DF	208/210 (99%)	0.10	7 (3%)	43	8	27, 68, 175, 199	0
36	BG	181/182 (99%)	0.59	18 (9%)	8	2	95, 145, 191, 201	0
36	DG	181/182 (99%)	1.50	52 (28%)	1	0	104, 162, 195, 202	0
37	BH	160/180 (88%)	0.20	3 (1%)	64	13	62, 103, 161, 193	0
37	DH	160/180 (88%)	0.71	18 (11%)	6	2	68, 117, 171, 193	0
38	BI	146/148 (98%)	0.17	3 (2%)	60	12	56, 144, 191, 200	0
38	DI	146/148 (98%)	1.56	45 (30%)	1	0	52, 164, 194, 201	0
39	BN	139/140 (99%)	-0.05	3 (2%)	59	12	35, 63, 136, 190	0
39	DN	139/140 (99%)	-0.15	2 (1%)	72	18	41, 69, 144, 191	0
40	BO	122/122 (100%)	-0.23	0	100	100	34, 57, 109, 141	0
40	DO	122/122 (100%)	-0.37	0	100	100	37, 59, 116, 146	0
41	BP	146/150 (97%)	0.25	4 (2%)	52	10	23, 83, 151, 201	0
41	DP	146/150 (97%)	0.25	4 (2%)	52	10	25, 88, 155, 201	0
42	BQ	136/141 (96%)	0.21	6 (4%)	33	7	38, 68, 149, 195	0
42	DQ	136/141 (96%)	0.19	8 (5%)	22	5	43, 74, 146, 195	0
43	BR	117/118 (99%)	-0.22	0	100	100	29, 45, 120, 144	0
43	DR	117/118 (99%)	-0.25	1 (0%)	81	24	31, 51, 125, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	0.25	2 (2%) 62 12	49, 98, 144, 184	0
44	DS	99/112 (88%)	0.53	8 (8%) 12 3	59, 105, 160, 188	0
45	BT	132/146 (90%)	0.10	5 (3%) 38 7	43, 76, 154, 194	0
45	DT	132/146 (90%)	0.11	7 (5%) 25 5	47, 79, 162, 197	0
46	BU	117/118 (99%)	-0.02	2 (1%) 67 15	29, 51, 121, 190	0
46	DU	117/118 (99%)	0.11	5 (4%) 34 7	35, 58, 130, 192	0
47	BV	101/101 (100%)	0.37	6 (5%) 22 5	32, 98, 188, 199	0
47	DV	101/101 (100%)	0.35	6 (5%) 22 5	39, 105, 189, 199	0
48	BW	113/113 (100%)	-0.30	0 100 100	27, 39, 106, 171	0
48	DW	113/113 (100%)	-0.31	0 100 100	28, 43, 109, 180	0
49	BX	93/96 (96%)	0.09	0 100 100	37, 63, 144, 187	0
49	DX	93/96 (96%)	-0.01	0 100 100	40, 66, 144, 186	0
50	BY	101/110 (91%)	0.44	7 (6%) 17 4	44, 92, 194, 201	0
50	DY	101/110 (91%)	0.38	10 (9%) 8 2	53, 99, 192, 201	0
51	BZ	177/206 (85%)	0.01	2 (1%) 77 21	58, 103, 152, 180	0
51	DZ	177/206 (85%)	0.39	5 (2%) 50 10	63, 110, 156, 188	0
All	All	20062/20918 (95%)	0.31	1553 (7%) 13 3	20, 90, 194, 203	0

The worst 5 of 1553 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	89	C	16.6
31	DA	2802	G	16.2
1	AA	88	A	16.1
31	DA	652	C	14.5
1	CA	1149	C	14.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
52	MG	DA	3264	1/1	0.49	-	58,58,58,58	0
52	MG	AA	1639	1/1	0.28	-	49,49,49,49	0
52	MG	DA	3066	1/1	0.42	-	40,40,40,40	0
52	MG	BA	3292	1/1	0.54	-	56,56,56,56	0
52	MG	DA	3115	1/1	0.34	-	44,44,44,44	0
52	MG	DA	3303	1/1	0.15	-	47,47,47,47	0
52	MG	BB	207	1/1	0.23	-	62,62,62,62	0
52	MG	AA	1638	1/1	0.28	-	67,67,67,67	0
52	MG	BA	3006	1/1	0.47	-	30,30,30,30	0
52	MG	AA	1629	1/1	0.21	-	41,41,41,41	0
52	MG	BA	3241	1/1	0.27	-	26,26,26,26	0
52	MG	DA	3060	1/1	0.26	-	38,38,38,38	0
52	MG	BA	3315	1/1	0.83	-	52,52,52,52	0
52	MG	DA	3112	1/1	0.29	-	30,30,30,30	0
52	MG	DA	3315	1/1	0.26	-	48,48,48,48	0
52	MG	BA	3128	1/1	0.25	-	39,39,39,39	0
52	MG	BA	3167	1/1	0.39	-	31,31,31,31	0
52	MG	AA	1602	1/1	0.52	-	41,41,41,41	0
52	MG	BA	3022	1/1	0.20	-	37,37,37,37	0
52	MG	BA	3137	1/1	0.37	-	10,10,10,10	0
52	MG	BA	3236	1/1	0.34	-	25,25,25,25	0
52	MG	DA	3250	1/1	0.39	-	41,41,41,41	0
52	MG	BA	3344	1/1	0.45	-	60,60,60,60	0
52	MG	DA	3258	1/1	0.25	-	52,52,52,52	0
52	MG	BA	3020	1/1	0.22	-	18,18,18,18	0
52	MG	DA	3327	1/1	0.12	-	60,60,60,60	0
52	MG	DA	3049	1/1	0.45	-	42,42,42,42	0
52	MG	DA	3141	1/1	0.71	-	70,70,70,70	0
52	MG	BA	3276	1/1	0.26	-	17,17,17,17	0
52	MG	BA	3200	1/1	0.52	-	36,36,36,36	0
52	MG	BA	3218	1/1	0.42	-	27,27,27,27	0
52	MG	DA	3210	1/1	0.22	-	43,43,43,43	0
52	MG	DA	3259	1/1	0.19	-	49,49,49,49	0
52	MG	BA	3280	1/1	0.20	-	33,33,33,33	0
52	MG	BA	3186	1/1	0.38	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3275	1/1	0.38	-	60,60,60,60	0
52	MG	DA	3225	1/1	0.13	-	51,51,51,51	0
52	MG	BA	3309	1/1	0.14	-	55,55,55,55	0
52	MG	DA	3005	1/1	0.15	-	63,63,63,63	0
52	MG	CA	1627	1/1	0.63	-	75,75,75,75	0
52	MG	DA	3181	1/1	0.39	-	44,44,44,44	0
52	MG	BA	3083	1/1	0.35	-	35,35,35,35	0
52	MG	BA	3350	1/1	0.19	-	65,65,65,65	0
52	MG	BA	3062	1/1	0.10	-	19,19,19,19	0
52	MG	BA	3104	1/1	0.42	-	31,31,31,31	0
52	MG	BA	3312	1/1	0.10	-	40,40,40,40	0
52	MG	BA	3275	1/1	0.31	-	40,40,40,40	0
52	MG	DA	3322	1/1	0.42	-	48,48,48,48	0
52	MG	DA	3128	1/1	0.25	-	47,47,47,47	0
52	MG	BA	3033	1/1	0.15	-	27,27,27,27	0
52	MG	BA	3001	1/1	0.37	-	46,46,46,46	0
52	MG	BA	3121	1/1	0.44	-	38,38,38,38	0
52	MG	BA	3300	1/1	0.43	-	48,48,48,48	0
52	MG	DA	3310	1/1	0.55	-	56,56,56,56	0
52	MG	DF	301	1/1	0.31	-	57,57,57,57	0
52	MG	DA	3290	1/1	0.23	-	46,46,46,46	0
52	MG	BA	3297	1/1	0.34	-	37,37,37,37	0
52	MG	DA	3292	1/1	0.15	-	54,54,54,54	0
52	MG	DA	3030	1/1	0.28	-	32,32,32,32	0
52	MG	BA	3230	1/1	0.08	-	21,21,21,21	0
52	MG	CA	1642	1/1	0.35	-	55,55,55,55	0
52	MG	BA	3178	1/1	0.36	-	30,30,30,30	0
52	MG	DU	201	1/1	0.17	-	60,60,60,60	0
52	MG	BA	3267	1/1	0.43	-	37,37,37,37	0
52	MG	BE	301	1/1	0.32	-	25,25,25,25	0
52	MG	BA	3362	1/1	0.08	-	70,70,70,70	0
52	MG	AA	1652	1/1	0.39	-	66,66,66,66	0
52	MG	DA	3313	1/1	0.23	-	66,66,66,66	0
52	MG	DA	3092	1/1	0.51	-	40,40,40,40	0
52	MG	BA	3073	1/1	0.30	-	20,20,20,20	0
52	MG	BA	3174	1/1	0.40	-	40,40,40,40	0
52	MG	AA	1626	1/1	0.28	-	46,46,46,46	0
52	MG	DA	3085	1/1	0.11	-	22,22,22,22	0
52	MG	AA	1646	1/1	0.22	-	51,51,51,51	0
52	MG	CA	1632	1/1	0.19	-	63,63,63,63	0
52	MG	DA	3314	1/1	0.11	-	58,58,58,58	0
52	MG	CA	1613	1/1	0.55	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3165	1/1	0.38	-	35,35,35,35	0
52	MG	DA	3308	1/1	0.20	-	36,36,36,36	0
52	MG	CA	1644	1/1	0.40	-	62,62,62,62	0
52	MG	BA	3316	1/1	0.22	-	31,31,31,31	0
52	MG	BA	3251	1/1	0.08	-	40,40,40,40	0
52	MG	DA	3083	1/1	0.48	-	38,38,38,38	0
52	MG	BA	3158	1/1	0.34	-	30,30,30,30	0
52	MG	BA	3320	1/1	0.43	-	50,50,50,50	0
52	MG	DA	3088	1/1	0.23	-	32,32,32,32	0
52	MG	BA	3286	1/1	0.33	-	30,30,30,30	0
52	MG	CA	1646	1/1	0.32	-	59,59,59,59	0
52	MG	DA	3034	1/1	0.38	-	51,51,51,51	0
52	MG	DA	3201	1/1	0.36	-	30,30,30,30	0
52	MG	DA	3268	1/1	0.37	-	52,52,52,52	0
52	MG	BA	3352	1/1	0.56	-	62,62,62,62	0
52	MG	BA	3274	1/1	0.39	-	36,36,36,36	0
52	MG	DA	3187	1/1	0.09	-	54,54,54,54	0
52	MG	DA	3328	1/1	0.26	-	81,81,81,81	0
52	MG	BA	3014	1/1	0.38	-	29,29,29,29	0
52	MG	BA	3232	1/1	0.13	-	4,4,4,4	0
52	MG	DA	3296	1/1	0.37	-	55,55,55,55	0
52	MG	BA	3295	1/1	0.37	-	34,34,34,34	0
52	MG	DA	3018	1/1	0.20	-	23,23,23,23	0
52	MG	BA	3323	1/1	0.18	-	32,32,32,32	0
52	MG	DA	3230	1/1	0.22	-	57,57,57,57	0
52	MG	BA	3110	1/1	0.41	-	36,36,36,36	0
52	MG	BA	3239	1/1	0.24	-	50,50,50,50	0
52	MG	BA	3181	1/1	0.39	-	35,35,35,35	0
52	MG	BA	3319	1/1	0.30	-	64,64,64,64	0
52	MG	BA	3196	1/1	0.22	-	30,30,30,30	0
52	MG	B5	102	1/1	0.31	-	56,56,56,56	0
52	MG	BA	3094	1/1	0.56	-	31,31,31,31	0
52	MG	AA	1632	1/1	0.56	-	68,68,68,68	0
52	MG	BA	3090	1/1	0.36	-	18,18,18,18	0
52	MG	DA	3150	1/1	0.65	-	72,72,72,72	0
52	MG	DA	3103	1/1	0.60	-	32,32,32,32	0
52	MG	DA	3105	1/1	0.18	-	43,43,43,43	0
52	MG	BA	3259	1/1	0.24	-	23,23,23,23	0
52	MG	DA	3192	1/1	0.19	-	29,29,29,29	0
52	MG	DA	3129	1/1	0.12	-	54,54,54,54	0
52	MG	BA	3299	1/1	0.40	-	38,38,38,38	0
52	MG	BA	3184	1/1	0.17	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3152	1/1	0.12	-	55,55,55,55	0
52	MG	BA	3349	1/1	0.30	-	33,33,33,33	0
52	MG	BA	3335	1/1	0.12	-	44,44,44,44	0
52	MG	DA	3263	1/1	0.12	-	45,45,45,45	0
52	MG	AA	1606	1/1	0.38	-	89,89,89,89	0
52	MG	DA	3272	1/1	0.30	-	42,42,42,42	0
52	MG	BA	3262	1/1	0.20	-	25,25,25,25	0
52	MG	DA	3321	1/1	0.15	-	34,34,34,34	0
52	MG	DA	3127	1/1	0.25	-	38,38,38,38	0
52	MG	BA	3078	1/1	0.39	-	30,30,30,30	0
52	MG	DA	3256	1/1	0.38	-	82,82,82,82	0
52	MG	DA	3309	1/1	0.64	-	62,62,62,62	0
52	MG	DA	3245	1/1	0.21	-	38,38,38,38	0
52	MG	BA	3050	1/1	0.28	-	27,27,27,27	0
52	MG	BA	3063	1/1	0.26	-	36,36,36,36	0
52	MG	DA	3172	1/1	0.35	-	56,56,56,56	0
52	MG	BA	3254	1/1	0.27	-	55,55,55,55	0
52	MG	CA	1622	1/1	0.35	-	51,51,51,51	0
52	MG	BA	3009	1/1	0.34	-	27,27,27,27	0
52	MG	DA	3319	1/1	0.15	-	40,40,40,40	0
52	MG	BA	3120	1/1	0.20	-	45,45,45,45	0
52	MG	DA	3158	1/1	0.11	-	53,53,53,53	0
52	MG	DA	3162	1/1	0.34	-	51,51,51,51	0
52	MG	DA	3163	1/1	0.54	-	59,59,59,59	0
52	MG	DA	3213	1/1	0.35	-	30,30,30,30	0
52	MG	DA	3269	1/1	0.43	-	39,39,39,39	0
52	MG	BA	3268	1/1	0.33	-	39,39,39,39	0
52	MG	DA	3015	1/1	0.28	-	39,39,39,39	0
52	MG	DP	201	1/1	0.20	-	27,27,27,27	0
52	MG	BA	3003	1/1	0.78	-	52,52,52,52	0
52	MG	DA	3132	1/1	0.42	-	25,25,25,25	0
52	MG	DA	3122	1/1	0.26	-	48,48,48,48	0
52	MG	DA	3078	1/1	0.34	-	37,37,37,37	0
52	MG	DA	3131	1/1	0.19	-	82,82,82,82	0
52	MG	BA	3214	1/1	0.10	-	12,12,12,12	0
52	MG	BA	3095	1/1	0.34	-	33,33,33,33	0
52	MG	BA	3060	1/1	0.31	-	27,27,27,27	0
52	MG	DA	3235	1/1	0.28	-	40,40,40,40	0
52	MG	DA	3124	1/1	0.16	-	42,42,42,42	0
52	MG	AA	1648	1/1	0.21	-	82,82,82,82	0
52	MG	DA	3008	1/1	0.34	-	36,36,36,36	0
52	MG	DA	3119	1/1	0.17	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	CA	1618	1/1	0.47	-	65,65,65,65	0
52	MG	DA	3267	1/1	0.32	-	49,49,49,49	0
52	MG	DA	3211	1/1	0.25	-	35,35,35,35	0
52	MG	BA	3161	1/1	0.32	-	43,43,43,43	0
52	MG	BA	3035	1/1	0.32	-	26,26,26,26	0
52	MG	DA	3193	1/1	0.23	-	46,46,46,46	0
52	MG	BA	3237	1/1	0.54	-	40,40,40,40	0
52	MG	BA	3132	1/1	0.22	-	18,18,18,18	0
52	MG	DA	3261	1/1	0.20	-	63,63,63,63	0
52	MG	DA	3020	1/1	0.41	-	35,35,35,35	0
52	MG	DA	3324	1/1	0.46	-	69,69,69,69	0
52	MG	BA	3273	1/1	0.41	-	42,42,42,42	0
52	MG	DA	3232	1/1	0.16	-	50,50,50,50	0
52	MG	BA	3004	1/1	0.40	-	28,28,28,28	0
52	MG	BB	206	1/1	0.51	-	50,50,50,50	0
52	MG	BA	3217	1/1	0.14	-	38,38,38,38	0
52	MG	AA	1628	1/1	0.48	-	70,70,70,70	0
52	MG	DA	3002	1/1	0.42	-	29,29,29,29	0
52	MG	BA	3243	1/1	0.25	-	57,57,57,57	0
52	MG	BA	3263	1/1	0.21	-	26,26,26,26	0
52	MG	DA	3082	1/1	0.28	-	47,47,47,47	0
52	MG	BA	3183	1/1	0.21	-	54,54,54,54	0
52	MG	BA	3081	1/1	0.38	-	23,23,23,23	0
52	MG	DA	3242	1/1	0.22	-	53,53,53,53	0
52	MG	BA	3311	1/1	0.92	-	62,62,62,62	0
52	MG	DA	3209	1/1	0.86	-	58,58,58,58	0
52	MG	CA	1602	1/1	0.56	-	55,55,55,55	0
52	MG	DA	3260	1/1	0.22	-	65,65,65,65	0
52	MG	BA	3177	1/1	0.27	-	38,38,38,38	0
52	MG	DA	3134	1/1	0.18	-	67,67,67,67	0
52	MG	BA	3005	1/1	0.23	-	24,24,24,24	0
52	MG	DA	3223	1/1	0.15	-	41,41,41,41	0
52	MG	CA	1608	1/1	0.38	-	74,74,74,74	0
52	MG	DA	3255	1/1	0.14	-	50,50,50,50	0
52	MG	BA	3055	1/1	0.27	-	16,16,16,16	0
52	MG	BA	3202	1/1	0.10	-	54,54,54,54	0
52	MG	AA	1614	1/1	0.40	-	49,49,49,49	0
52	MG	BA	3340	1/1	0.33	-	45,45,45,45	0
52	MG	DA	3113	1/1	0.35	-	52,52,52,52	0
55	ERY	DA	3330	51/51	0.33	-	94,94,94,94	0
52	MG	DA	3248	1/1	0.33	-	82,82,82,82	0
52	MG	BA	3130	1/1	0.41	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3308	1/1	0.15	-	41,41,41,41	0
52	MG	BA	3082	1/1	0.35	-	33,33,33,33	0
52	MG	AA	1651	1/1	0.67	-	57,57,57,57	0
52	MG	BA	3291	1/1	0.15	-	38,38,38,38	0
52	MG	BA	3015	1/1	0.26	-	33,33,33,33	0
52	MG	DA	3174	1/1	0.13	-	67,67,67,67	0
52	MG	BA	3024	1/1	0.30	-	28,28,28,28	0
52	MG	DA	3170	1/1	0.28	-	61,61,61,61	0
52	MG	BA	3030	1/1	0.18	-	15,15,15,15	0
52	MG	D3	101	1/1	0.64	-	52,52,52,52	0
52	MG	DA	3095	1/1	0.17	-	39,39,39,39	0
52	MG	DA	3186	1/1	0.61	-	45,45,45,45	0
52	MG	BA	3301	1/1	0.22	-	41,41,41,41	0
52	MG	BA	3116	1/1	0.21	-	55,55,55,55	0
52	MG	DA	3199	1/1	0.16	-	37,37,37,37	0
52	MG	DA	3233	1/1	0.55	-	52,52,52,52	0
52	MG	DA	3206	1/1	0.47	-	38,38,38,38	0
52	MG	BA	3211	1/1	0.32	-	34,34,34,34	0
52	MG	DA	3221	1/1	0.54	-	40,40,40,40	0
52	MG	BA	3194	1/1	0.53	-	47,47,47,47	0
52	MG	BA	3193	1/1	0.51	-	33,33,33,33	0
52	MG	AA	1637	1/1	0.43	-	53,53,53,53	0
52	MG	DA	3125	1/1	0.14	-	45,45,45,45	0
52	MG	BA	3296	1/1	0.19	-	43,43,43,43	0
52	MG	DA	3037	1/1	0.62	-	35,35,35,35	0
52	MG	DA	3212	1/1	0.32	-	38,38,38,38	0
52	MG	DA	3271	1/1	0.46	-	61,61,61,61	0
52	MG	BA	3225	1/1	0.11	-	20,20,20,20	0
52	MG	BA	3331	1/1	0.32	-	49,49,49,49	0
53	ZN	CN	101	1/1	0.17	-	139,139,139,139	0
52	MG	DA	3253	1/1	0.24	-	58,58,58,58	0
52	MG	DA	3285	1/1	0.12	-	49,49,49,49	0
52	MG	BA	3353	1/1	0.27	-	26,26,26,26	0
52	MG	BA	3053	1/1	0.43	-	27,27,27,27	0
52	MG	DA	3273	1/1	0.74	-	52,52,52,52	0
52	MG	DA	3169	1/1	0.17	-	35,35,35,35	0
52	MG	BA	3240	1/1	0.11	-	42,42,42,42	0
52	MG	BA	3317	1/1	0.27	-	45,45,45,45	0
52	MG	DA	3025	1/1	0.31	-	44,44,44,44	0
52	MG	BA	3185	1/1	0.20	-	46,46,46,46	0
52	MG	DB	203	1/1	0.35	-	46,46,46,46	0
52	MG	CA	1626	1/1	0.38	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3284	1/1	0.16	-	25,25,25,25	0
52	MG	BA	3271	1/1	0.40	-	38,38,38,38	0
52	MG	DA	3055	1/1	0.20	-	30,30,30,30	0
52	MG	AA	1631	1/1	0.66	-	70,70,70,70	0
52	MG	BA	3057	1/1	0.20	-	24,24,24,24	0
52	MG	BA	3159	1/1	0.53	-	43,43,43,43	0
52	MG	DA	3318	1/1	0.09	-	45,45,45,45	0
52	MG	BA	3204	1/1	0.51	-	43,43,43,43	0
52	MG	DA	3126	1/1	0.34	-	42,42,42,42	0
52	MG	DA	3283	1/1	0.51	-	67,67,67,67	0
52	MG	BA	3342	1/1	0.26	-	38,38,38,38	0
52	MG	BA	3203	1/1	0.27	-	46,46,46,46	0
52	MG	BA	3258	1/1	0.30	-	30,30,30,30	0
52	MG	DA	3026	1/1	0.37	-	66,66,66,66	0
52	MG	BA	3303	1/1	0.27	-	65,65,65,65	0
52	MG	DA	3130	1/1	0.28	-	59,59,59,59	0
52	MG	BA	3278	1/1	0.18	-	39,39,39,39	0
52	MG	AA	1604	1/1	0.37	-	73,73,73,73	0
52	MG	DA	3044	1/1	0.37	-	32,32,32,32	0
52	MG	BA	3221	1/1	0.47	-	29,29,29,29	0
52	MG	BA	3046	1/1	0.26	-	28,28,28,28	0
52	MG	DA	3222	1/1	0.41	-	44,44,44,44	0
52	MG	DA	3035	1/1	0.31	-	32,32,32,32	0
52	MG	BA	3077	1/1	0.15	-	21,21,21,21	0
52	MG	BA	3227	1/1	0.50	-	37,37,37,37	0
52	MG	AA	1644	1/1	0.35	-	87,87,87,87	0
52	MG	DA	3139	1/1	0.45	-	44,44,44,44	0
52	MG	BA	3149	1/1	0.27	-	19,19,19,19	0
52	MG	BA	3066	1/1	0.37	-	29,29,29,29	0
52	MG	DA	3215	1/1	0.13	-	37,37,37,37	0
52	MG	D0	101	1/1	0.15	-	46,46,46,46	0
52	MG	BA	3304	1/1	0.52	-	55,55,55,55	0
52	MG	DA	3107	1/1	0.31	-	30,30,30,30	0
52	MG	DA	3040	1/1	0.76	-	50,50,50,50	0
52	MG	BA	3127	1/1	0.48	-	39,39,39,39	0
52	MG	BA	3357	1/1	0.27	-	71,71,71,71	0
52	MG	BB	203	1/1	0.08	-	41,41,41,41	0
52	MG	DA	3160	1/1	0.49	-	33,33,33,33	0
52	MG	DA	3298	1/1	0.16	-	46,46,46,46	0
52	MG	DA	3159	1/1	0.46	-	48,48,48,48	0
53	ZN	CD	301	1/1	0.25	-	116,116,116,116	0
52	MG	BA	3125	1/1	0.16	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3157	1/1	0.40	-	22,22,22,22	0
52	MG	BA	3114	1/1	0.36	-	37,37,37,37	0
52	MG	DA	3152	1/1	0.18	-	30,30,30,30	0
52	MG	BA	3049	1/1	0.39	-	33,33,33,33	0
52	MG	DA	3061	1/1	0.27	-	36,36,36,36	0
52	MG	DA	3146	1/1	0.36	-	52,52,52,52	0
52	MG	DA	3203	1/1	0.47	-	39,39,39,39	0
52	MG	BA	3359	1/1	0.20	-	52,52,52,52	0
52	MG	AA	1611	1/1	0.15	-	82,82,82,82	0
52	MG	BA	3039	1/1	0.44	-	32,32,32,32	0
52	MG	AA	1613	1/1	0.23	-	76,76,76,76	0
52	MG	DA	3140	1/1	0.36	-	52,52,52,52	0
52	MG	BA	3206	1/1	0.88	-	57,57,57,57	0
52	MG	BA	3162	1/1	0.44	-	60,60,60,60	0
52	MG	DA	3009	1/1	0.35	-	49,49,49,49	0
52	MG	DA	3287	1/1	0.20	-	40,40,40,40	0
52	MG	AA	1601	1/1	0.14	-	59,59,59,59	0
52	MG	BA	3092	1/1	0.27	-	9,9,9,9	0
52	MG	BA	3019	1/1	0.46	-	19,19,19,19	0
52	MG	DA	3266	1/1	0.16	-	74,74,74,74	0
52	MG	DA	3027	1/1	0.46	-	34,34,34,34	0
52	MG	DA	3226	1/1	0.20	-	40,40,40,40	0
52	MG	DA	3294	1/1	0.43	-	65,65,65,65	0
52	MG	DA	3157	1/1	0.52	-	52,52,52,52	0
52	MG	DA	3168	1/1	0.33	-	35,35,35,35	0
52	MG	DA	3145	1/1	0.18	-	59,59,59,59	0
52	MG	BA	3272	1/1	0.25	-	28,28,28,28	0
52	MG	CA	1621	1/1	0.33	-	54,54,54,54	0
52	MG	BA	3261	1/1	0.09	-	27,27,27,27	0
52	MG	CA	1636	1/1	1.00	-	76,76,76,76	0
52	MG	DA	3011	1/1	0.48	-	30,30,30,30	0
52	MG	BA	3305	1/1	0.20	-	43,43,43,43	0
52	MG	DA	3046	1/1	0.35	-	48,48,48,48	0
52	MG	BA	3154	1/1	0.35	-	79,79,79,79	0
52	MG	DQ	201	1/1	0.17	-	46,46,46,46	0
52	MG	AA	1622	1/1	0.59	-	63,63,63,63	0
52	MG	BA	3091	1/1	0.13	-	20,20,20,20	0
52	MG	DA	3052	1/1	0.42	-	40,40,40,40	0
53	ZN	AN	101	1/1	0.14	-	157,157,157,157	0
52	MG	BA	3216	1/1	0.29	-	26,26,26,26	0
52	MG	BA	3096	1/1	0.41	-	19,19,19,19	0
52	MG	B1	101	1/1	0.35	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	CA	1624	1/1	0.25	-	55,55,55,55	0
52	MG	BA	3328	1/1	0.37	-	56,56,56,56	0
52	MG	BA	3043	1/1	0.20	-	31,31,31,31	0
52	MG	BA	3318	1/1	0.45	-	40,40,40,40	0
52	MG	BA	3231	1/1	0.22	-	35,35,35,35	0
52	MG	BA	3101	1/1	0.44	-	43,43,43,43	0
52	MG	BA	3012	1/1	0.34	-	23,23,23,23	0
52	MG	DA	3176	1/1	0.41	-	44,44,44,44	0
52	MG	DA	3278	1/1	0.95	-	74,74,74,74	0
52	MG	BP	202	1/1	0.14	-	0,0,0,0	0
52	MG	BA	3169	1/1	0.53	-	38,38,38,38	0
52	MG	AA	1617	1/1	0.31	-	57,57,57,57	0
52	MG	DB	202	1/1	0.35	-	51,51,51,51	0
52	MG	DA	3064	1/1	0.45	-	47,47,47,47	0
52	MG	BA	3131	1/1	0.27	-	21,21,21,21	0
52	MG	DA	3048	1/1	0.33	-	35,35,35,35	0
52	MG	DA	3138	1/1	0.51	-	47,47,47,47	0
52	MG	DA	3183	1/1	0.53	-	56,56,56,56	0
52	MG	BA	3338	1/1	0.47	-	50,50,50,50	0
52	MG	BA	3302	1/1	0.36	-	46,46,46,46	0
52	MG	BQ	202	1/1	0.22	-	38,38,38,38	0
52	MG	DA	3302	1/1	0.34	-	64,64,64,64	0
52	MG	BA	3018	1/1	0.24	-	20,20,20,20	0
52	MG	DA	3102	1/1	0.54	-	36,36,36,36	0
52	MG	BA	3264	1/1	0.10	-	48,48,48,48	0
54	K	BA	3363	1/1	0.13	-	43,43,43,43	0
52	MG	BA	3054	1/1	0.20	-	47,47,47,47	0
52	MG	BA	3277	1/1	0.22	-	41,41,41,41	0
52	MG	BA	3246	1/1	0.52	-	46,46,46,46	0
52	MG	DA	3142	1/1	0.45	-	37,37,37,37	0
52	MG	BA	3245	1/1	0.38	-	56,56,56,56	0
52	MG	BA	3294	1/1	0.13	-	38,38,38,38	0
52	MG	BA	3208	1/1	0.33	-	41,41,41,41	0
52	MG	AA	1633	1/1	0.07	-	39,39,39,39	0
52	MG	BA	3088	1/1	0.43	-	34,34,34,34	0
52	MG	DA	3241	1/1	0.26	-	36,36,36,36	0
52	MG	BA	3016	1/1	0.40	-	21,21,21,21	0
52	MG	DA	3136	1/1	0.36	-	33,33,33,33	0
52	MG	BD	301	1/1	0.21	-	25,25,25,25	0
52	MG	BA	3334	1/1	0.23	-	24,24,24,24	0
52	MG	BA	3010	1/1	0.41	-	33,33,33,33	0
52	MG	DA	3068	1/1	0.54	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3175	1/1	0.37	-	62,62,62,62	0
52	MG	BA	3168	1/1	0.23	-	28,28,28,28	0
52	MG	BA	3201	1/1	0.72	-	51,51,51,51	0
52	MG	BA	3314	1/1	0.28	-	49,49,49,49	0
52	MG	BA	3165	1/1	0.16	-	44,44,44,44	0
52	MG	BA	3134	1/1	0.18	-	36,36,36,36	0
52	MG	DA	3094	1/1	0.47	-	34,34,34,34	0
52	MG	BA	3103	1/1	0.26	-	24,24,24,24	0
52	MG	CA	1616	1/1	0.46	-	67,67,67,67	0
52	MG	DA	3047	1/1	0.38	-	36,36,36,36	0
52	MG	BA	3124	1/1	0.35	-	10,10,10,10	0
52	MG	CA	1623	1/1	0.28	-	62,62,62,62	0
52	MG	BA	3136	1/1	0.22	-	28,28,28,28	0
52	MG	AA	1645	1/1	0.47	-	75,75,75,75	0
52	MG	BA	3269	1/1	0.26	-	43,43,43,43	0
52	MG	BA	3351	1/1	0.25	-	39,39,39,39	0
52	MG	BA	3011	1/1	0.42	-	19,19,19,19	0
52	MG	BA	3097	1/1	0.40	-	54,54,54,54	0
52	MG	BA	3118	1/1	0.43	-	40,40,40,40	0
52	MG	CA	1643	1/1	0.51	-	57,57,57,57	0
52	MG	BA	3100	1/1	0.34	-	28,28,28,28	0
52	MG	CA	1601	1/1	0.16	-	72,72,72,72	0
52	MG	BA	3051	1/1	0.30	-	17,17,17,17	0
52	MG	CA	1640	1/1	0.22	-	42,42,42,42	0
52	MG	DA	3006	1/1	0.48	-	30,30,30,30	0
52	MG	AA	1653	1/1	0.10	-	61,61,61,61	0
52	MG	DA	3104	1/1	0.36	-	36,36,36,36	0
52	MG	BA	3238	1/1	0.22	-	40,40,40,40	0
52	MG	BA	3045	1/1	0.32	-	21,21,21,21	0
52	MG	DA	3045	1/1	0.34	-	29,29,29,29	0
52	MG	BA	3080	1/1	0.52	-	17,17,17,17	0
52	MG	BA	3085	1/1	0.15	-	8,8,8,8	0
52	MG	BA	3336	1/1	0.75	-	69,69,69,69	0
52	MG	BA	3173	1/1	0.33	-	31,31,31,31	0
52	MG	DA	3121	1/1	0.66	-	44,44,44,44	0
52	MG	BA	3270	1/1	0.10	-	66,66,66,66	0
52	MG	BA	3220	1/1	0.30	-	46,46,46,46	0
52	MG	BA	3250	1/1	0.17	-	37,37,37,37	0
52	MG	BA	3229	1/1	0.64	-	45,45,45,45	0
52	MG	BA	3111	1/1	0.17	-	17,17,17,17	0
52	MG	DA	3184	1/1	0.32	-	57,57,57,57	0
52	MG	BA	3307	1/1	0.37	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	AA	1610	1/1	0.17	-	41,41,41,41	0
52	MG	BA	3148	1/1	0.39	-	26,26,26,26	0
52	MG	DA	3156	1/1	0.11	-	39,39,39,39	0
52	MG	DA	3277	1/1	0.39	-	76,76,76,76	0
52	MG	BA	3160	1/1	0.65	-	62,62,62,62	0
52	MG	BA	3355	1/1	0.21	-	64,64,64,64	0
52	MG	BA	3028	1/1	0.32	-	22,22,22,22	0
52	MG	DA	3133	1/1	0.65	-	42,42,42,42	0
52	MG	BA	3191	1/1	0.27	-	21,21,21,21	0
52	MG	BA	3279	1/1	0.29	-	37,37,37,37	0
52	MG	BA	3195	1/1	0.34	-	31,31,31,31	0
52	MG	CA	1641	1/1	0.18	-	52,52,52,52	0
52	MG	DA	3299	1/1	0.31	-	57,57,57,57	0
52	MG	BA	3059	1/1	0.28	-	26,26,26,26	0
52	MG	BA	3036	1/1	0.43	-	19,19,19,19	0
52	MG	BA	3215	1/1	0.53	-	41,41,41,41	0
52	MG	CA	1634	1/1	0.15	-	63,63,63,63	0
52	MG	BB	205	1/1	0.08	-	64,64,64,64	0
52	MG	DA	3041	1/1	0.30	-	31,31,31,31	0
52	MG	BA	3163	1/1	0.35	-	31,31,31,31	0
52	MG	CA	1633	1/1	0.45	-	48,48,48,48	0
52	MG	DA	3295	1/1	0.19	-	46,46,46,46	0
52	MG	DA	3080	1/1	0.71	-	46,46,46,46	0
52	MG	BA	3071	1/1	0.39	-	33,33,33,33	0
52	MG	DA	3307	1/1	0.25	-	41,41,41,41	0
52	MG	BA	3076	1/1	0.22	-	21,21,21,21	0
52	MG	DA	3204	1/1	0.36	-	53,53,53,53	0
52	MG	DA	3051	1/1	0.40	-	36,36,36,36	0
52	MG	BA	3108	1/1	0.40	-	42,42,42,42	0
52	MG	DA	3208	1/1	0.30	-	57,57,57,57	0
52	MG	DA	3100	1/1	0.32	-	37,37,37,37	0
52	MG	DA	3220	1/1	0.43	-	40,40,40,40	0
52	MG	BA	3064	1/1	0.37	-	52,52,52,52	0
52	MG	AA	1640	1/1	0.26	-	67,67,67,67	0
52	MG	CA	1610	1/1	0.17	-	90,90,90,90	0
52	MG	BA	3074	1/1	0.62	-	60,60,60,60	0
52	MG	BA	3140	1/1	0.18	-	46,46,46,46	0
52	MG	DA	3282	1/1	0.10	-	48,48,48,48	0
52	MG	CA	1625	1/1	0.18	-	54,54,54,54	0
52	MG	DA	3003	1/1	0.63	-	41,41,41,41	0
52	MG	BA	3176	1/1	0.27	-	45,45,45,45	0
52	MG	DA	3143	1/1	0.26	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3316	1/1	0.55	-	60,60,60,60	0
52	MG	DA	3022	1/1	0.31	-	39,39,39,39	0
52	MG	CA	1604	1/1	0.33	-	88,88,88,88	0
52	MG	DA	3110	1/1	0.42	-	45,45,45,45	0
52	MG	CA	1619	1/1	0.44	-	47,47,47,47	0
52	MG	DA	3179	1/1	0.67	-	39,39,39,39	0
52	MG	BA	3313	1/1	0.27	-	38,38,38,38	0
52	MG	DA	3239	1/1	0.20	-	29,29,29,29	0
52	MG	BA	3007	1/1	0.45	-	28,28,28,28	0
52	MG	DA	3311	1/1	0.19	-	45,45,45,45	0
52	MG	BA	3190	1/1	0.36	-	23,23,23,23	0
52	MG	DA	3019	1/1	0.50	-	21,21,21,21	0
52	MG	BA	3143	1/1	0.45	-	28,28,28,28	0
52	MG	BA	3041	1/1	0.29	-	24,24,24,24	0
52	MG	BA	3244	1/1	0.19	-	60,60,60,60	0
52	MG	BA	3298	1/1	0.37	-	59,59,59,59	0
52	MG	BA	3253	1/1	0.62	-	42,42,42,42	0
52	MG	DA	3073	1/1	0.34	-	31,31,31,31	0
52	MG	AA	1618	1/1	0.10	-	59,59,59,59	0
52	MG	BB	204	1/1	0.36	-	43,43,43,43	0
52	MG	DA	3279	1/1	0.35	-	59,59,59,59	0
52	MG	DA	3305	1/1	0.27	-	83,83,83,83	0
52	MG	BA	3282	1/1	0.34	-	55,55,55,55	0
52	MG	CA	1603	1/1	0.30	-	44,44,44,44	0
52	MG	DA	3185	1/1	0.54	-	53,53,53,53	0
52	MG	DA	3010	1/1	0.41	-	51,51,51,51	0
52	MG	BA	3068	1/1	0.47	-	35,35,35,35	0
52	MG	AA	1605	1/1	0.33	-	69,69,69,69	0
52	MG	BA	3155	1/1	0.17	-	55,55,55,55	0
52	MG	DA	3072	1/1	0.65	-	58,58,58,58	0
52	MG	DA	3091	1/1	0.42	-	31,31,31,31	0
52	MG	DA	3086	1/1	0.17	-	25,25,25,25	0
52	MG	AA	1607	1/1	0.40	-	58,58,58,58	0
52	MG	AA	1609	1/1	0.38	-	50,50,50,50	0
52	MG	BA	3056	1/1	0.13	-	24,24,24,24	0
52	MG	DA	3014	1/1	0.36	-	56,56,56,56	0
55	ERY	BA	3364	51/51	0.36	-	94,94,94,94	0
52	MG	BA	3023	1/1	0.45	-	35,35,35,35	0
52	MG	AA	1654	1/1	0.20	-	69,69,69,69	0
52	MG	BA	3123	1/1	0.39	-	39,39,39,39	0
52	MG	DA	3252	1/1	0.46	-	54,54,54,54	0
52	MG	BA	3025	1/1	0.15	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3251	1/1	0.14	-	57,57,57,57	0
52	MG	BF	301	1/1	0.22	-	51,51,51,51	0
52	MG	DA	3099	1/1	0.48	-	42,42,42,42	0
52	MG	DA	3171	1/1	0.47	-	39,39,39,39	0
52	MG	BA	3079	1/1	0.11	-	17,17,17,17	0
54	K	DA	3329	1/1	0.20	-	55,55,55,55	0
52	MG	DA	3217	1/1	0.23	-	23,23,23,23	0
52	MG	BA	3339	1/1	0.14	-	53,53,53,53	0
52	MG	BA	3065	1/1	0.28	-	26,26,26,26	0
52	MG	BA	3017	1/1	0.39	-	32,32,32,32	0
52	MG	DA	3293	1/1	0.48	-	62,62,62,62	0
52	MG	BA	3142	1/1	0.53	-	33,33,33,33	0
52	MG	DA	3317	1/1	0.29	-	42,42,42,42	0
52	MG	BA	3086	1/1	0.27	-	24,24,24,24	0
52	MG	DA	3198	1/1	0.20	-	38,38,38,38	0
52	MG	DA	3069	1/1	0.22	-	65,65,65,65	0
52	MG	DA	3297	1/1	0.18	-	21,21,21,21	0
52	MG	DA	3123	1/1	0.18	-	57,57,57,57	0
52	MG	AA	1635	1/1	0.18	-	69,69,69,69	0
52	MG	BA	3222	1/1	0.34	-	32,32,32,32	0
52	MG	BU	201	1/1	0.29	-	31,31,31,31	0
52	MG	BA	3107	1/1	0.17	-	28,28,28,28	0
52	MG	BA	3047	1/1	0.52	-	28,28,28,28	0
52	MG	CA	1648	1/1	0.71	-	70,70,70,70	0
52	MG	DA	3289	1/1	0.58	-	65,65,65,65	0
52	MG	DA	3190	1/1	0.49	-	43,43,43,43	0
52	MG	DA	3237	1/1	0.13	-	46,46,46,46	0
52	MG	DA	3257	1/1	0.38	-	38,38,38,38	0
52	MG	DA	3017	1/1	0.36	-	34,34,34,34	0
52	MG	DA	3323	1/1	0.13	-	57,57,57,57	0
52	MG	BA	3040	1/1	0.51	-	37,37,37,37	0
52	MG	BA	3164	1/1	0.18	-	30,30,30,30	0
52	MG	AA	1616	1/1	0.25	-	76,76,76,76	0
52	MG	DA	3216	1/1	0.36	-	31,31,31,31	0
52	MG	BA	3260	1/1	0.26	-	37,37,37,37	0
52	MG	DA	3247	1/1	0.39	-	76,76,76,76	0
52	MG	B5	101	1/1	0.38	-	40,40,40,40	0
52	MG	DA	3151	1/1	0.53	-	47,47,47,47	0
52	MG	BA	3198	1/1	0.38	-	36,36,36,36	0
52	MG	BA	3072	1/1	0.49	-	39,39,39,39	0
52	MG	DA	3300	1/1	0.83	-	64,64,64,64	0
52	MG	BA	3099	1/1	0.19	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3144	1/1	0.33	-	48,48,48,48	0
52	MG	CA	1645	1/1	0.83	-	64,64,64,64	0
52	MG	DB	201	1/1	0.44	-	58,58,58,58	0
52	MG	BA	3188	1/1	0.15	-	57,57,57,57	0
52	MG	BA	3150	1/1	0.33	-	40,40,40,40	0
52	MG	BA	3287	1/1	0.22	-	44,44,44,44	0
52	MG	BA	3345	1/1	0.27	-	48,48,48,48	0
52	MG	BA	3337	1/1	0.64	-	47,47,47,47	0
52	MG	DA	3071	1/1	0.33	-	35,35,35,35	0
52	MG	AA	1620	1/1	0.58	-	51,51,51,51	0
52	MG	DA	3238	1/1	0.09	-	59,59,59,59	0
52	MG	DX	101	1/1	0.34	-	63,63,63,63	0
52	MG	BA	3126	1/1	0.27	-	33,33,33,33	0
52	MG	DA	3108	1/1	0.29	-	30,30,30,30	0
52	MG	DA	3039	1/1	0.59	-	53,53,53,53	0
52	MG	BA	3105	1/1	0.53	-	34,34,34,34	0
52	MG	AA	1643	1/1	0.66	-	59,59,59,59	0
52	MG	DA	3101	1/1	0.10	-	28,28,28,28	0
52	MG	DA	3036	1/1	0.52	-	29,29,29,29	0
52	MG	BA	3252	1/1	0.30	-	30,30,30,30	0
52	MG	BA	3189	1/1	0.48	-	36,36,36,36	0
52	MG	BA	3180	1/1	0.10	-	48,48,48,48	0
52	MG	BB	201	1/1	0.45	-	35,35,35,35	0
52	MG	DA	3024	1/1	0.31	-	35,35,35,35	0
52	MG	DA	3067	1/1	0.31	-	49,49,49,49	0
52	MG	DA	3218	1/1	0.23	-	41,41,41,41	0
52	MG	CA	1650	1/1	0.21	-	58,58,58,58	0
52	MG	BA	3027	1/1	0.34	-	19,19,19,19	0
52	MG	BA	3322	1/1	0.23	-	50,50,50,50	0
52	MG	DA	3164	1/1	0.22	-	49,49,49,49	0
52	MG	DA	3173	1/1	0.35	-	41,41,41,41	0
52	MG	BA	3170	1/1	0.63	-	31,31,31,31	0
52	MG	AA	1630	1/1	0.50	-	51,51,51,51	0
52	MG	BA	3324	1/1	0.31	-	40,40,40,40	0
52	MG	BA	3135	1/1	0.41	-	28,28,28,28	0
52	MG	BA	3213	1/1	0.15	-	20,20,20,20	0
52	MG	DA	3155	1/1	0.35	-	30,30,30,30	0
52	MG	BA	3293	1/1	0.32	-	36,36,36,36	0
52	MG	BA	3242	1/1	0.57	-	44,44,44,44	0
52	MG	BA	3042	1/1	0.30	-	14,14,14,14	0
52	MG	BA	3109	1/1	0.30	-	31,31,31,31	0
52	MG	DA	3153	1/1	0.44	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	ZN	AD	301	1/1	0.27	-	120,120,120,120	0
52	MG	DA	3200	1/1	0.40	-	46,46,46,46	0
52	MG	DA	3306	1/1	0.26	-	69,69,69,69	0
52	MG	BA	3358	1/1	0.53	-	80,80,80,80	0
52	MG	BA	3321	1/1	0.22	-	48,48,48,48	0
52	MG	BA	3199	1/1	0.26	-	20,20,20,20	0
52	MG	BA	3145	1/1	0.41	-	33,33,33,33	0
52	MG	DA	3189	1/1	0.49	-	42,42,42,42	0
52	MG	BA	3069	1/1	0.33	-	45,45,45,45	0
52	MG	BA	3332	1/1	0.37	-	40,40,40,40	0
52	MG	DA	3167	1/1	0.10	-	44,44,44,44	0
52	MG	BA	3058	1/1	0.28	-	35,35,35,35	0
52	MG	BA	3219	1/1	0.45	-	25,25,25,25	0
52	MG	BA	3034	1/1	0.25	-	61,61,61,61	0
52	MG	BA	3151	1/1	0.45	-	54,54,54,54	0
52	MG	BA	3330	1/1	0.28	-	72,72,72,72	0
52	MG	DA	3031	1/1	0.13	-	62,62,62,62	0
52	MG	BX	101	1/1	0.20	-	38,38,38,38	0
52	MG	BA	3281	1/1	0.82	-	61,61,61,61	0
52	MG	BA	3346	1/1	0.21	-	60,60,60,60	0
52	MG	DA	3084	1/1	0.33	-	38,38,38,38	0
52	MG	BB	202	1/1	0.31	-	26,26,26,26	0
52	MG	AA	1608	1/1	0.28	-	80,80,80,80	0
52	MG	AA	1625	1/1	0.35	-	41,41,41,41	0
52	MG	DA	3280	1/1	0.58	-	64,64,64,64	0
52	MG	DA	3098	1/1	0.31	-	28,28,28,28	0
52	MG	DA	3219	1/1	0.60	-	57,57,57,57	0
52	MG	DA	3175	1/1	0.26	-	44,44,44,44	0
52	MG	BA	3089	1/1	0.20	-	12,12,12,12	0
52	MG	CA	1605	1/1	0.26	-	84,84,84,84	0
52	MG	BA	3197	1/1	0.48	-	47,47,47,47	0
52	MG	BA	3002	1/1	0.42	-	28,28,28,28	0
52	MG	DA	3057	1/1	0.26	-	35,35,35,35	0
52	MG	DA	3023	1/1	0.47	-	38,38,38,38	0
52	MG	BA	3061	1/1	0.29	-	27,27,27,27	0
52	MG	DA	3304	1/1	0.15	-	65,65,65,65	0
52	MG	DA	3231	1/1	0.42	-	58,58,58,58	0
52	MG	BA	3008	1/1	0.35	-	24,24,24,24	0
52	MG	BA	3306	1/1	0.30	-	52,52,52,52	0
52	MG	BA	3087	1/1	0.23	-	18,18,18,18	0
52	MG	BA	3093	1/1	0.41	-	37,37,37,37	0
52	MG	BA	3247	1/1	0.28	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	CA	1631	1/1	0.14	-	73,73,73,73	0
52	MG	CA	1635	1/1	0.42	-	77,77,77,77	0
52	MG	BA	3224	1/1	0.39	-	30,30,30,30	0
52	MG	DA	3224	1/1	0.27	-	54,54,54,54	0
52	MG	AA	1636	1/1	0.22	-	44,44,44,44	0
52	MG	DA	3161	1/1	0.62	-	57,57,57,57	0
52	MG	DA	3135	1/1	0.36	-	29,29,29,29	0
52	MG	DA	3097	1/1	0.18	-	33,33,33,33	0
52	MG	DA	3291	1/1	0.41	-	62,62,62,62	0
52	MG	CA	1617	1/1	0.49	-	54,54,54,54	0
52	MG	BA	3325	1/1	0.52	-	58,58,58,58	0
52	MG	BQ	201	1/1	0.13	-	19,19,19,19	0
52	MG	AA	1619	1/1	0.28	-	49,49,49,49	0
52	MG	BA	3354	1/1	0.26	-	34,34,34,34	0
52	MG	DA	3149	1/1	0.31	-	29,29,29,29	0
52	MG	DA	3147	1/1	0.36	-	30,30,30,30	0
52	MG	BA	3117	1/1	0.10	-	42,42,42,42	0
52	MG	DA	3075	1/1	0.34	-	36,36,36,36	0
52	MG	DA	3243	1/1	0.10	-	41,41,41,41	0
52	MG	BA	3102	1/1	0.31	-	23,23,23,23	0
52	MG	BA	3207	1/1	0.29	-	27,27,27,27	0
52	MG	CA	1609	1/1	0.08	-	34,34,34,34	0
52	MG	BA	3356	1/1	0.34	-	60,60,60,60	0
52	MG	AA	1623	1/1	0.28	-	37,37,37,37	0
52	MG	DA	3249	1/1	0.25	-	51,51,51,51	0
52	MG	DA	3021	1/1	0.25	-	48,48,48,48	0
52	MG	BA	3361	1/1	0.12	-	60,60,60,60	0
52	MG	BA	3037	1/1	0.46	-	22,22,22,22	0
52	MG	DA	3062	1/1	0.08	-	24,24,24,24	0
52	MG	BA	3360	1/1	0.09	-	64,64,64,64	0
52	MG	BA	3026	1/1	0.23	-	48,48,48,48	0
52	MG	BA	3172	1/1	0.21	-	52,52,52,52	0
52	MG	DA	3089	1/1	0.38	-	29,29,29,29	0
52	MG	BA	3147	1/1	0.52	-	37,37,37,37	0
52	MG	DA	3205	1/1	0.50	-	62,62,62,62	0
52	MG	DA	3234	1/1	0.14	-	46,46,46,46	0
52	MG	BA	3187	1/1	0.42	-	48,48,48,48	0
52	MG	BA	3234	1/1	0.51	-	53,53,53,53	0
52	MG	DA	3056	1/1	0.21	-	14,14,14,14	0
52	MG	AA	1627	1/1	0.19	-	51,51,51,51	0
52	MG	DA	3196	1/1	0.44	-	45,45,45,45	0
52	MG	DA	3286	1/1	0.33	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3326	1/1	0.52	-	37,37,37,37	0
52	MG	DA	3077	1/1	0.15	-	33,33,33,33	0
52	MG	DA	3076	1/1	0.26	-	29,29,29,29	0
52	MG	DA	3281	1/1	0.58	-	51,51,51,51	0
52	MG	BR	201	1/1	0.40	-	24,24,24,24	0
52	MG	BA	3209	1/1	0.44	-	31,31,31,31	0
52	MG	CA	1630	1/1	0.50	-	73,73,73,73	0
52	MG	DA	3188	1/1	0.20	-	44,44,44,44	0
52	MG	DA	3028	1/1	0.31	-	36,36,36,36	0
52	MG	BA	3084	1/1	0.34	-	21,21,21,21	0
52	MG	DA	3240	1/1	0.35	-	42,42,42,42	0
52	MG	CA	1647	1/1	0.37	-	66,66,66,66	0
52	MG	BA	3179	1/1	0.44	-	41,41,41,41	0
52	MG	DA	3114	1/1	0.28	-	47,47,47,47	0
52	MG	DR	201	1/1	0.34	-	37,37,37,37	0
52	MG	BA	3113	1/1	0.41	-	33,33,33,33	0
52	MG	DA	3109	1/1	0.27	-	42,42,42,42	0
52	MG	DA	3096	1/1	0.23	-	45,45,45,45	0
52	MG	DA	3301	1/1	0.66	-	54,54,54,54	0
52	MG	AA	1603	1/1	0.23	-	45,45,45,45	0
52	MG	BA	3115	1/1	0.07	-	49,49,49,49	0
52	MG	DA	3262	1/1	0.22	-	57,57,57,57	0
52	MG	BA	3139	1/1	0.41	-	60,60,60,60	0
52	MG	CA	1614	1/1	0.10	-	71,71,71,71	0
52	MG	BA	3348	1/1	0.28	-	38,38,38,38	0
52	MG	DA	3191	1/1	0.47	-	45,45,45,45	0
52	MG	BA	3129	1/1	0.09	-	35,35,35,35	0
52	MG	DA	3016	1/1	0.56	-	31,31,31,31	0
52	MG	BA	3255	1/1	0.14	-	24,24,24,24	0
52	MG	DA	3117	1/1	0.23	-	45,45,45,45	0
52	MG	BA	3210	1/1	0.25	-	33,33,33,33	0
52	MG	CA	1612	1/1	0.28	-	68,68,68,68	0
52	MG	DA	3001	1/1	0.26	-	56,56,56,56	0
52	MG	DA	3079	1/1	0.19	-	41,41,41,41	0
52	MG	DA	3254	1/1	0.21	-	68,68,68,68	0
52	MG	DA	3227	1/1	0.57	-	42,42,42,42	0
52	MG	DE	301	1/1	0.21	-	23,23,23,23	0
52	MG	BA	3257	1/1	0.20	-	23,23,23,23	0
52	MG	DA	3118	1/1	0.41	-	35,35,35,35	0
52	MG	DA	3288	1/1	0.28	-	51,51,51,51	0
52	MG	BA	3265	1/1	0.24	-	41,41,41,41	0
52	MG	BA	3226	1/1	0.35	-	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3038	1/1	0.46	-	26,26,26,26	0
52	MG	BA	3192	1/1	0.16	-	37,37,37,37	0
52	MG	DA	3120	1/1	0.30	-	55,55,55,55	0
52	MG	DA	3042	1/1	0.35	-	37,37,37,37	0
52	MG	DA	3270	1/1	0.29	-	44,44,44,44	0
52	MG	DA	3195	1/1	0.35	-	42,42,42,42	0
52	MG	BA	3327	1/1	0.48	-	48,48,48,48	0
52	MG	DA	3276	1/1	0.44	-	65,65,65,65	0
52	MG	DA	3284	1/1	0.70	-	51,51,51,51	0
52	MG	BA	3290	1/1	0.13	-	46,46,46,46	0
52	MG	BA	3212	1/1	0.45	-	26,26,26,26	0
52	MG	DA	3177	1/1	0.26	-	34,34,34,34	0
52	MG	BA	3205	1/1	0.53	-	43,43,43,43	0
52	MG	DA	3320	1/1	0.64	-	68,68,68,68	0
52	MG	BA	3075	1/1	0.38	-	44,44,44,44	0
52	MG	AA	1642	1/1	0.48	-	73,73,73,73	0
52	MG	AA	1612	1/1	0.55	-	70,70,70,70	0
52	MG	DA	3074	1/1	0.52	-	55,55,55,55	0
52	MG	DA	3154	1/1	0.15	-	49,49,49,49	0
52	MG	DA	3007	1/1	0.27	-	53,53,53,53	0
52	MG	DA	3065	1/1	0.21	-	39,39,39,39	0
52	MG	DA	3265	1/1	0.36	-	47,47,47,47	0
52	MG	DA	3043	1/1	0.21	-	42,42,42,42	0
52	MG	BA	3329	1/1	0.25	-	32,32,32,32	0
52	MG	DA	3081	1/1	0.70	-	48,48,48,48	0
52	MG	BA	3044	1/1	0.33	-	14,14,14,14	0
52	MG	DA	3325	1/1	0.37	-	67,67,67,67	0
52	MG	BA	3144	1/1	0.56	-	37,37,37,37	0
52	MG	BA	3341	1/1	0.13	-	70,70,70,70	0
52	MG	BA	3153	1/1	0.30	-	47,47,47,47	0
52	MG	BA	3235	1/1	0.42	-	34,34,34,34	0
52	MG	DA	3228	1/1	0.17	-	52,52,52,52	0
52	MG	BA	3288	1/1	0.22	-	65,65,65,65	0
52	MG	BA	3013	1/1	0.39	-	24,24,24,24	0
52	MG	BA	3266	1/1	0.24	-	48,48,48,48	0
52	MG	DA	3070	1/1	0.22	-	28,28,28,28	0
52	MG	BA	3052	1/1	0.40	-	24,24,24,24	0
52	MG	BA	3119	1/1	0.28	-	32,32,32,32	0
52	MG	DA	3166	1/1	0.39	-	54,54,54,54	0
52	MG	DA	3116	1/1	0.31	-	62,62,62,62	0
52	MG	AA	1650	1/1	0.37	-	60,60,60,60	0
52	MG	BA	3133	1/1	0.22	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	CA	1638	1/1	0.23	-	61,61,61,61	0
52	MG	BP	201	1/1	0.43	-	39,39,39,39	0
52	MG	BA	3021	1/1	0.35	-	22,22,22,22	0
52	MG	CA	1607	1/1	0.44	-	58,58,58,58	0
52	MG	CA	1628	1/1	0.41	-	73,73,73,73	0
52	MG	DA	3013	1/1	0.46	-	18,18,18,18	0
52	MG	BA	3347	1/1	0.18	-	43,43,43,43	0
52	MG	DA	3063	1/1	0.32	-	44,44,44,44	0
52	MG	BA	3098	1/1	0.20	-	39,39,39,39	0
52	MG	BA	3182	1/1	0.31	-	43,43,43,43	0
52	MG	AA	1647	1/1	0.28	-	62,62,62,62	0
52	MG	BA	3343	1/1	0.20	-	44,44,44,44	0
52	MG	BA	3228	1/1	0.28	-	21,21,21,21	0
52	MG	DA	3214	1/1	0.29	-	48,48,48,48	0
52	MG	BA	3070	1/1	0.23	-	9,9,9,9	0
52	MG	DA	3312	1/1	0.16	-	55,55,55,55	0
52	MG	DA	3029	1/1	0.32	-	45,45,45,45	0
52	MG	BA	3029	1/1	0.19	-	16,16,16,16	0
52	MG	CA	1629	1/1	0.14	-	67,67,67,67	0
52	MG	BA	3310	1/1	0.47	-	59,59,59,59	0
52	MG	CA	1620	1/1	0.28	-	58,58,58,58	0
52	MG	DA	3093	1/1	0.51	-	48,48,48,48	0
52	MG	BA	3067	1/1	0.48	-	28,28,28,28	0
52	MG	BA	3156	1/1	0.45	-	26,26,26,26	0
52	MG	CA	1606	1/1	0.42	-	44,44,44,44	0
52	MG	AA	1624	1/1	0.39	-	58,58,58,58	0
52	MG	BA	3141	1/1	0.45	-	32,32,32,32	0
52	MG	BA	3248	1/1	0.39	-	46,46,46,46	0
52	MG	BA	3031	1/1	0.32	-	50,50,50,50	0
52	MG	DA	3274	1/1	0.10	-	36,36,36,36	0
52	MG	DA	3058	1/1	0.32	-	48,48,48,48	0
52	MG	DA	3202	1/1	0.26	-	64,64,64,64	0
52	MG	BA	3038	1/1	0.37	-	14,14,14,14	0
52	MG	BA	3032	1/1	0.38	-	28,28,28,28	0
52	MG	CA	1615	1/1	0.30	-	69,69,69,69	0
52	MG	BA	3166	1/1	0.26	-	47,47,47,47	0
52	MG	DA	3004	1/1	0.32	-	29,29,29,29	0
52	MG	DA	3236	1/1	0.48	-	43,43,43,43	0
52	MG	D5	101	1/1	0.37	-	35,35,35,35	0
52	MG	BA	3333	1/1	0.18	-	51,51,51,51	0
52	MG	D7	101	1/1	0.29	-	38,38,38,38	0
52	MG	DA	3033	1/1	0.15	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3087	1/1	0.17	-	34,34,34,34	0
52	MG	DA	3246	1/1	0.14	-	67,67,67,67	0
52	MG	BA	3233	1/1	0.18	-	21,21,21,21	0
52	MG	BA	3283	1/1	0.22	-	33,33,33,33	0
52	MG	BA	3289	1/1	0.21	-	37,37,37,37	0
52	MG	CA	1611	1/1	0.40	-	65,65,65,65	0
52	MG	DA	3148	1/1	0.36	-	41,41,41,41	0
52	MG	AA	1634	1/1	0.51	-	55,55,55,55	0
52	MG	DA	3207	1/1	0.26	-	56,56,56,56	0
52	MG	CA	1639	1/1	0.92	-	70,70,70,70	0
52	MG	BA	3171	1/1	0.54	-	32,32,32,32	0
52	MG	AA	1649	1/1	0.62	-	62,62,62,62	0
52	MG	DA	3137	1/1	0.40	-	31,31,31,31	0
52	MG	DA	3012	1/1	0.33	-	25,25,25,25	0
52	MG	DA	3194	1/1	0.31	-	47,47,47,47	0
52	MG	BA	3256	1/1	0.09	-	39,39,39,39	0
52	MG	DA	3054	1/1	0.29	-	43,43,43,43	0
52	MG	DA	3197	1/1	0.49	-	46,46,46,46	0
52	MG	BA	3138	1/1	0.50	-	34,34,34,34	0
52	MG	DA	3032	1/1	0.39	-	25,25,25,25	0
52	MG	DA	3059	1/1	0.39	-	26,26,26,26	0
52	MG	DA	3111	1/1	0.40	-	31,31,31,31	0
52	MG	DA	3178	1/1	0.23	-	58,58,58,58	0
52	MG	DA	3053	1/1	0.31	-	27,27,27,27	0
52	MG	DA	3229	1/1	0.34	-	52,52,52,52	0
52	MG	DA	3090	1/1	0.26	-	34,34,34,34	0
52	MG	AA	1621	1/1	0.47	-	50,50,50,50	0
52	MG	B0	101	1/1	0.13	-	37,37,37,37	0
52	MG	DA	3180	1/1	0.50	-	45,45,45,45	0
52	MG	DA	3106	1/1	0.64	-	63,63,63,63	0
52	MG	BA	3106	1/1	0.23	-	18,18,18,18	0
52	MG	AA	1615	1/1	0.28	-	49,49,49,49	0
52	MG	DA	3050	1/1	0.28	-	39,39,39,39	0
52	MG	BA	3249	1/1	0.43	-	63,63,63,63	0
52	MG	AA	1641	1/1	0.25	-	57,57,57,57	0
52	MG	BP	203	1/1	0.60	-	55,55,55,55	0
52	MG	DA	3244	1/1	0.21	-	32,32,32,32	0
52	MG	CA	1637	1/1	0.37	-	61,61,61,61	0
52	MG	BA	3285	1/1	0.33	-	59,59,59,59	0
52	MG	BA	3048	1/1	0.41	-	23,23,23,23	0
52	MG	DA	3182	1/1	0.10	-	39,39,39,39	0
52	MG	BA	3146	1/1	0.30	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3112	1/1	0.20	-	38,38,38,38	0
52	MG	BA	3122	1/1	0.30	-	35,35,35,35	0
52	MG	DA	3326	1/1	0.26	-	52,52,52,52	0
52	MG	CA	1649	1/1	0.15	-	63,63,63,63	0
52	MG	BA	3223	1/1	0.26	-	41,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.