



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:49 PM BST

PDB ID : 4V7Y  
Title : Structure of the *Thermus thermophilus* 70S ribosome complexed with azithromycin.  
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.  
Deposited on : 2010-08-18  
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](mailto:validation@mail.wwpdb.org)

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

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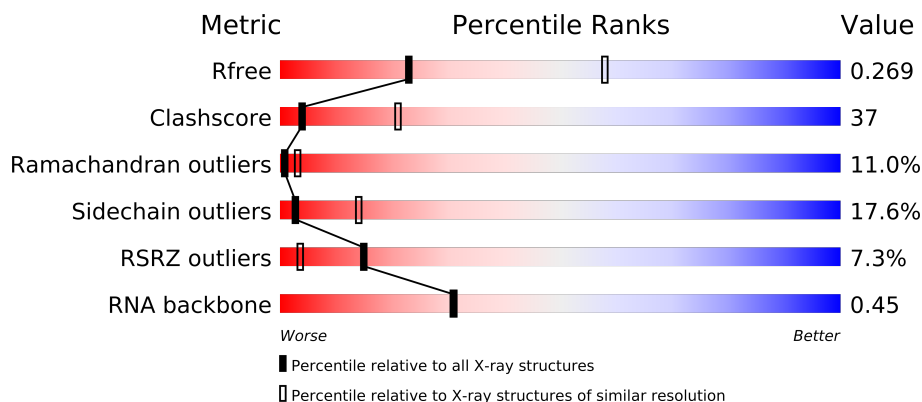
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
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 278000 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	349	Total	Mg	0	0
			349	349		
52	CA	48	Total	Mg	0	0
			48	48		
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	5	Total	Mg	0	0
			5	5		
52	BF	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	AA	51	Total	Mg	0	0
			51	51		
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		
52	DD	1	Total	Mg	0	0
			1	1		

*Continued on next page...*



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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	309	Total 309	Mg 309	0	0
52	B7	1	Total 1	Mg 1	0	0
52	DE	1	Total 1	Mg 1	0	0
52	D1	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	2	Total 2	Mg 2	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).

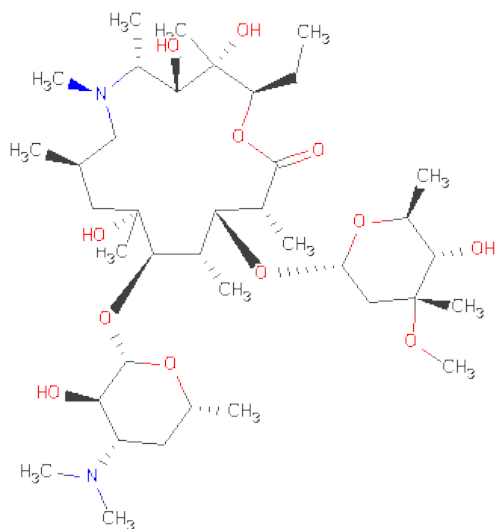
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	1	Total 1	K 1	0	0

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

- Molecule 55 is AZITHROMYCIN (three-letter code: ZIT) (formula:  $C_{38}H_{72}N_2O_{12}$ ).



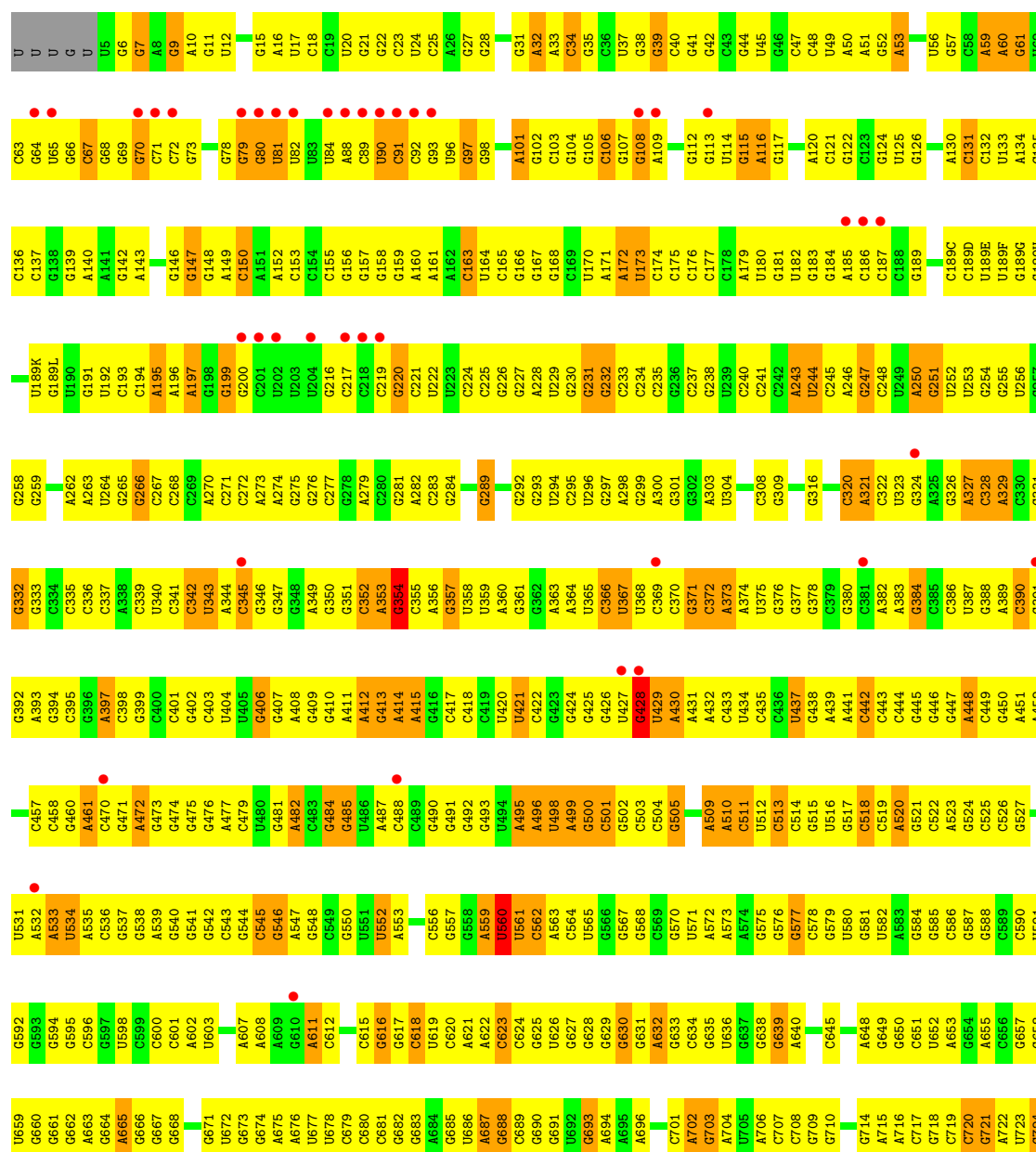
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BA	1	Total	C	N	O	0	0
			52	38	2	12		
55	DA	1	Total	C	N	O	0	0
			52	38	2	12		

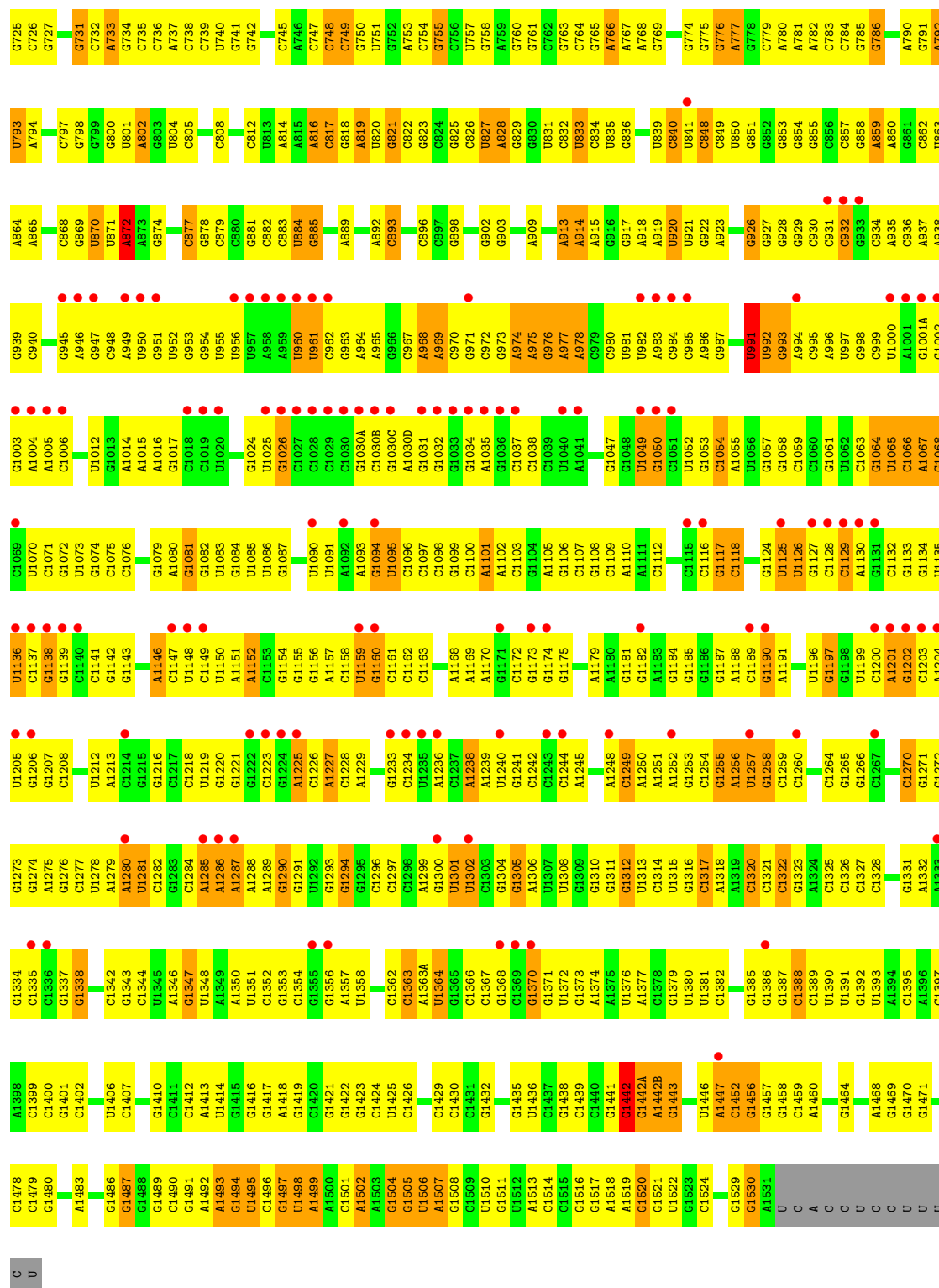
### 3 Residue-property plots

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

#### • Molecule 1: 16S rRNA

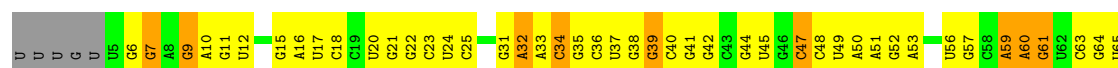
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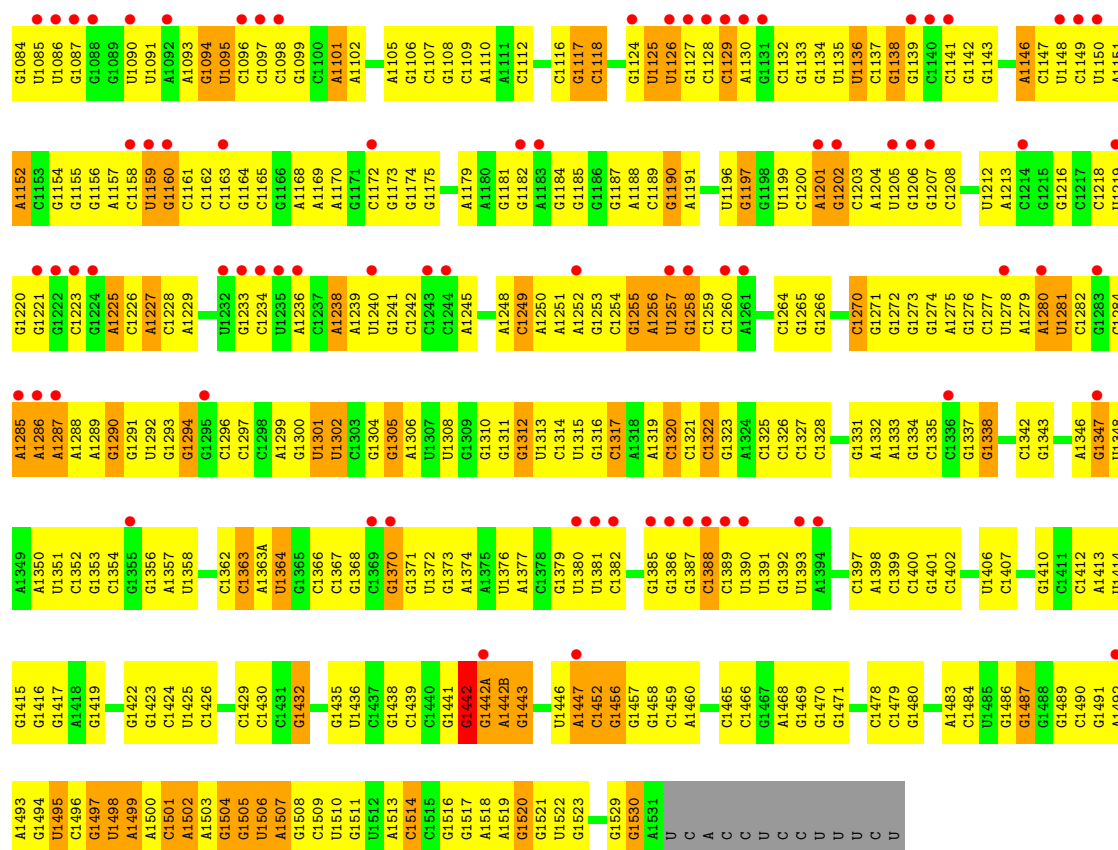


• Molecule 1: 16S rRNA

Chain CA:

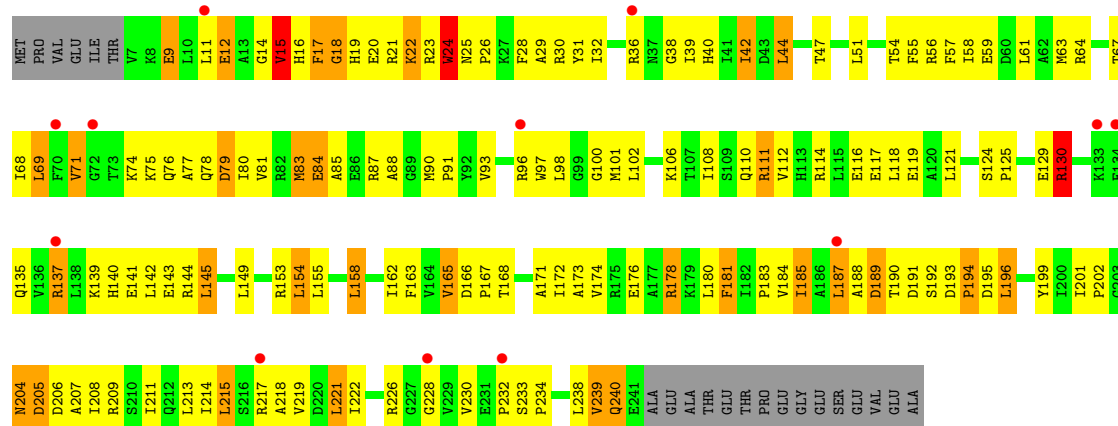


G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1030A	G1030B	G1030C	G1030D	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139																																																																																																																																																																																																																																																																																																																													
U957	A958	A959	U960	U961	C962	C963	A964	A965	C966	C967	A968	A969	C970	C971	C972	C973	A974	A975	C976	A977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139																																																																																																																																																																																																																																																														
A814	A815	A816	C817	C818	A819	U820	C821	C822	C823	C824	C825	C826	U827	A828	C829	U830	C831	C832	C833	C834	U835	C836	U837	U838	C839	C840	U841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139																																																																																																															
C749	G750	U751	G752	A753	C754	G755	C756	U757	G758	A759	G760	G761	C762	G763	G764	G765	A766	A767	A768	G769	C770	G771	U772	G773	G774	G775	G776	A777	G778	G779	A780	A781	A782	G783	C784	G785	G786	G787	G788	G789	G790	G791	A792	U793	A794	C795	C796	C797	C798	C799	C800	U801	A802	G803	U804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139																																														
C345	G346	A347	A348	A349	G350	G351	C352	A353	C354	C355	A356	G357	U358	U359	A360	G361	C362	A363	C364	U365	C366	U367	U368	C369	C370	G371	C372	A373	A374	U375	G376	G377	C378	C379	G380	C381	C382	A383	C384	C385	C386	U387	G388	A389	C390	C391	C392	A393	G394	C395	C396	A397	G398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545	C546	C547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781



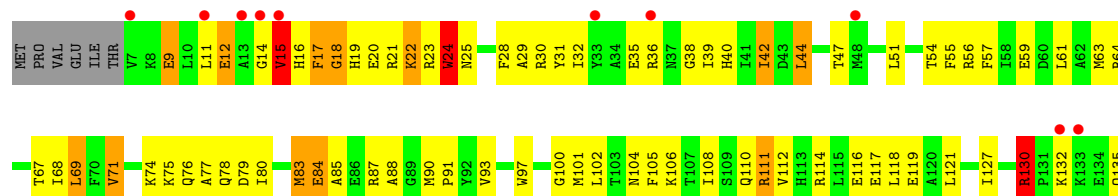
### • Molecule 2: 30S ribosomal protein S2

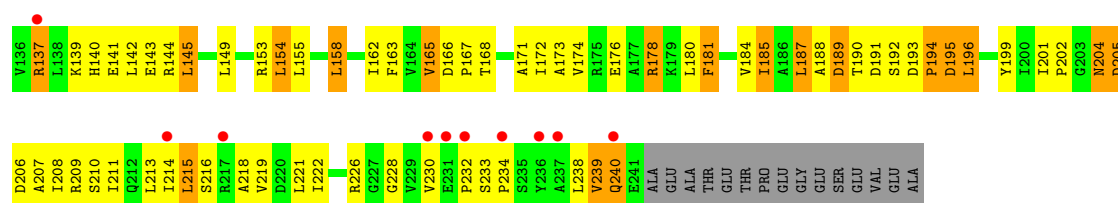
Chain AB:



### • Molecule 2: 30S ribosomal protein S2

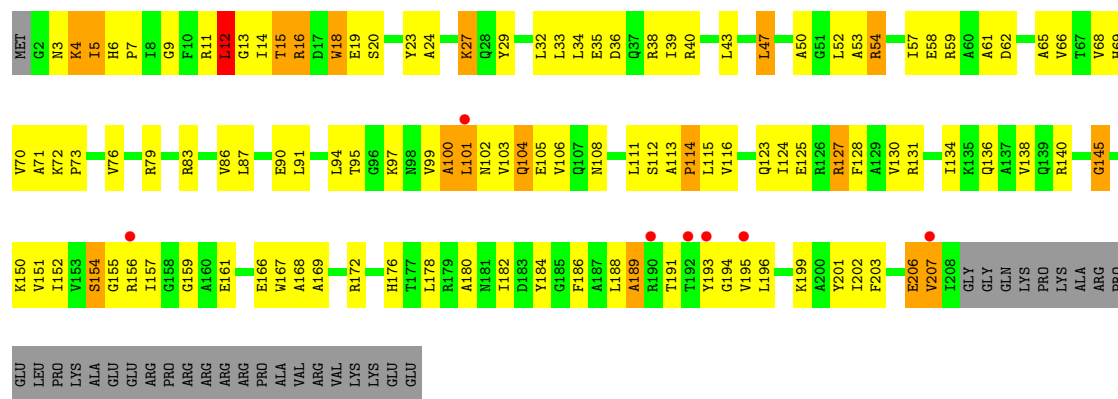
Chain CB:





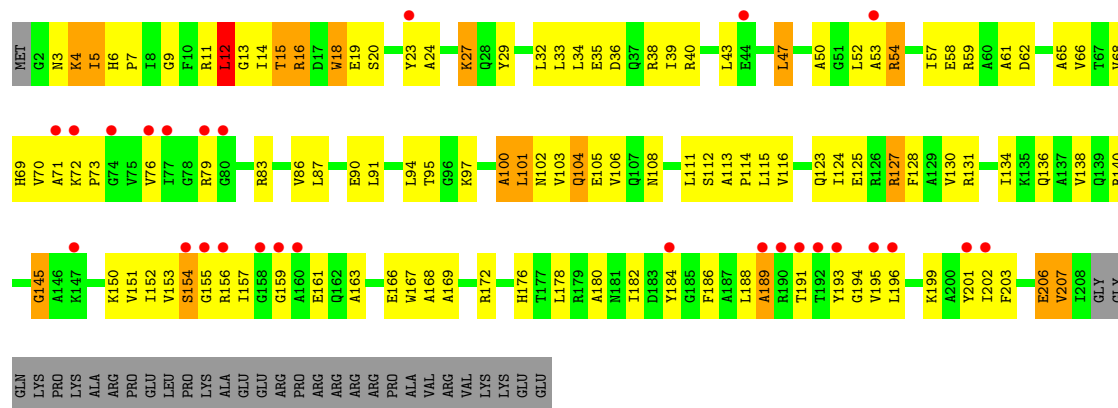
### • Molecule 3: 30S ribosomal protein S3

Chain AC:



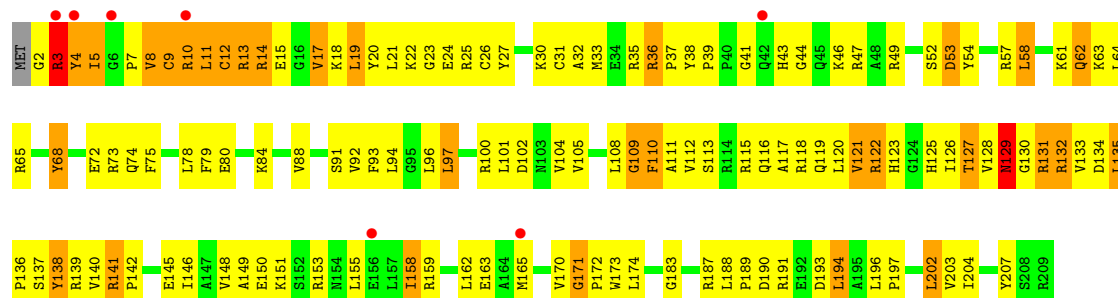
### • Molecule 3: 30S ribosomal protein S3

Chain CC:



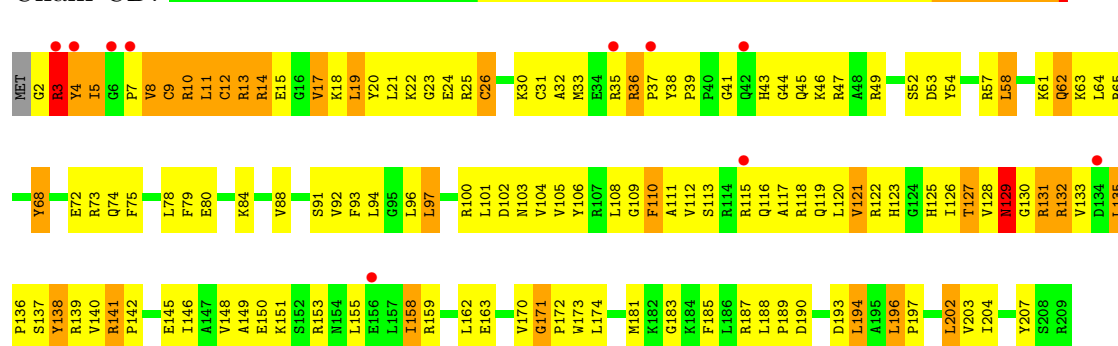
### • Molecule 4: 30S ribosomal protein S4

Chain AD:



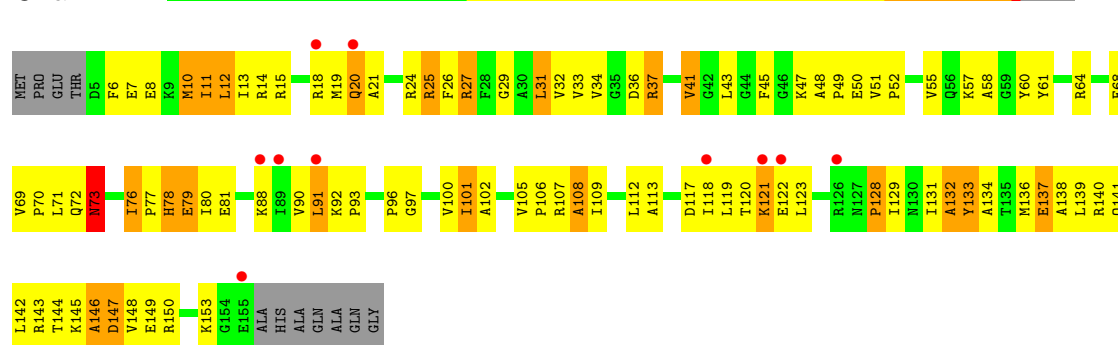
- Molecule 4: 30S ribosomal protein S4

Chain CD:



- Molecule 5: 30S ribosomal protein S5

Chain AE:



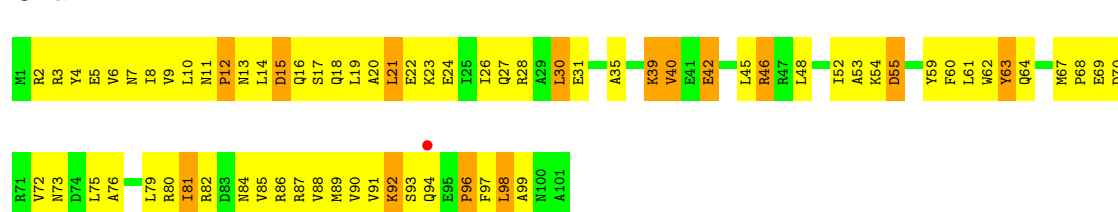
- Molecule 5: 30S ribosomal protein S5

Chain CE:



- Molecule 6: 30S ribosomal protein S6

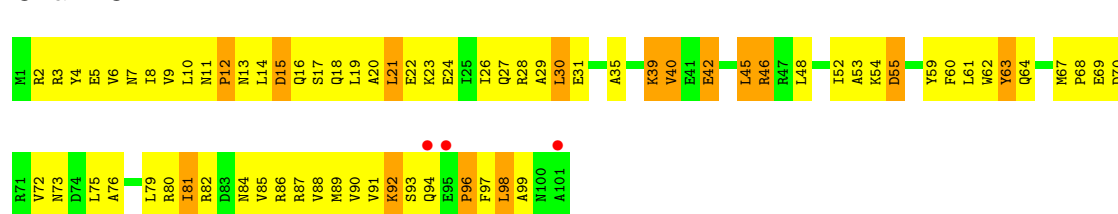
Chain AF:



- Molecule 6: 30S ribosomal protein S6

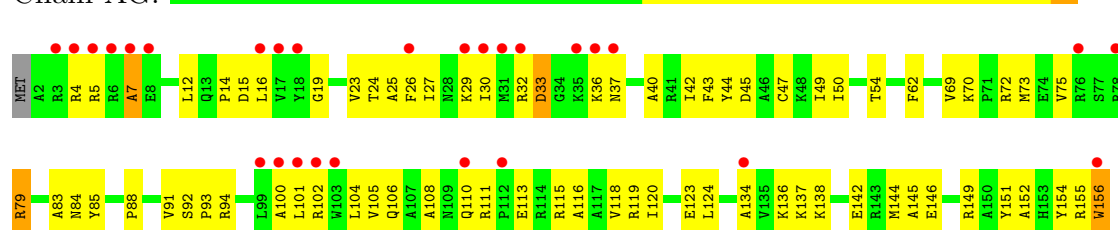


Chain CF:



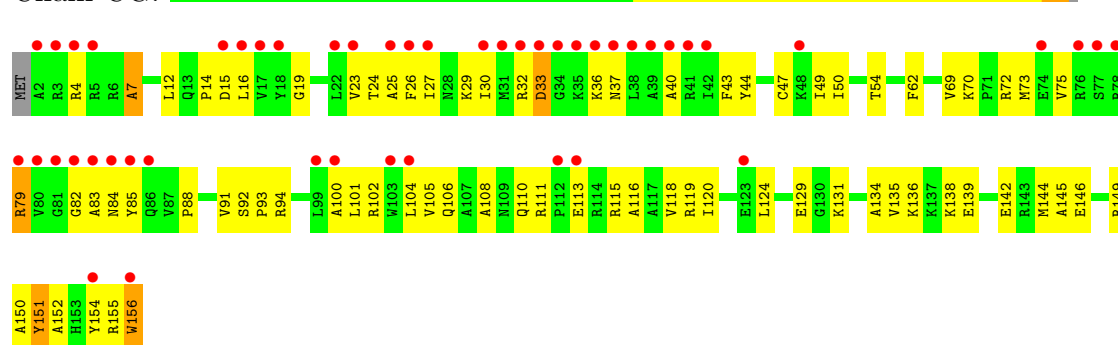
- Molecule 7: 30S ribosomal protein S7

Chain AG:



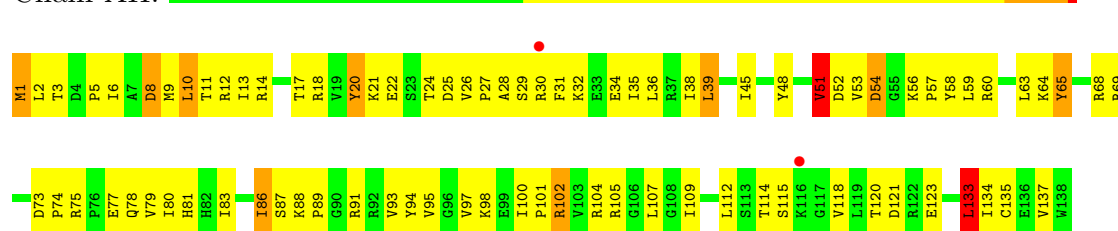
- Molecule 7: 30S ribosomal protein S7

Chain CG:



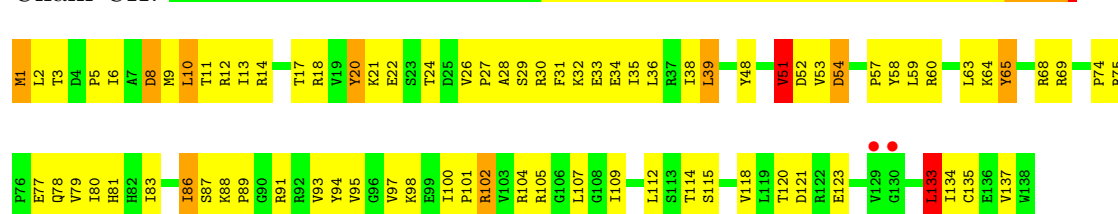
- Molecule 8: 30S ribosomal protein S8

Chain AH:



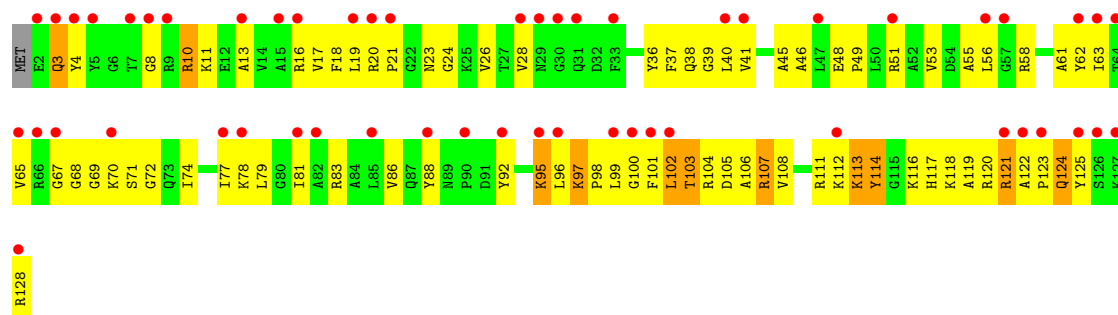
- Molecule 8: 30S ribosomal protein S8

Chain CH:



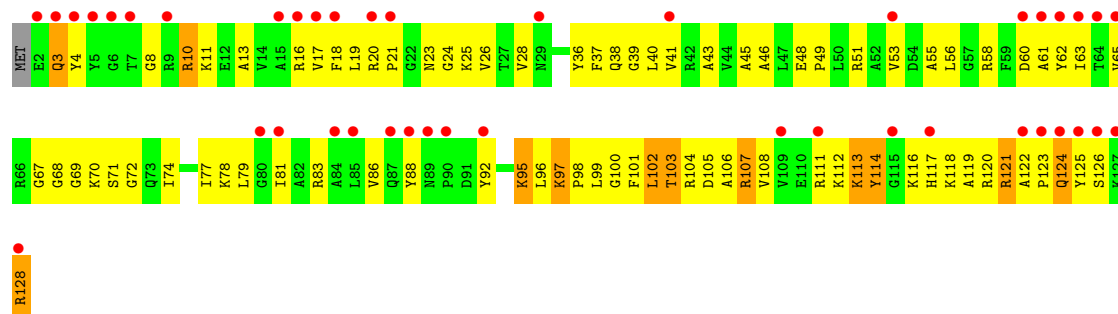
- Molecule 9: 30S ribosomal protein S9

Chain AI:



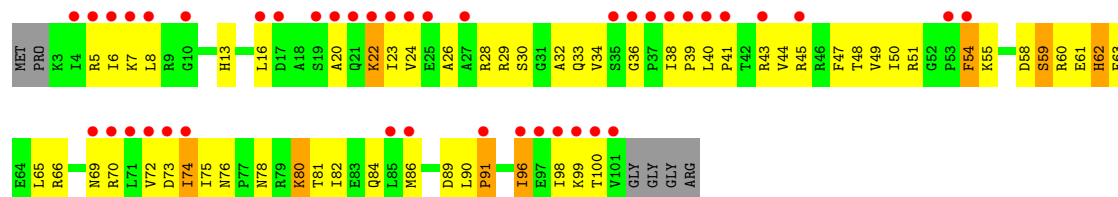
- Molecule 9: 30S ribosomal protein S9

Chain CI:



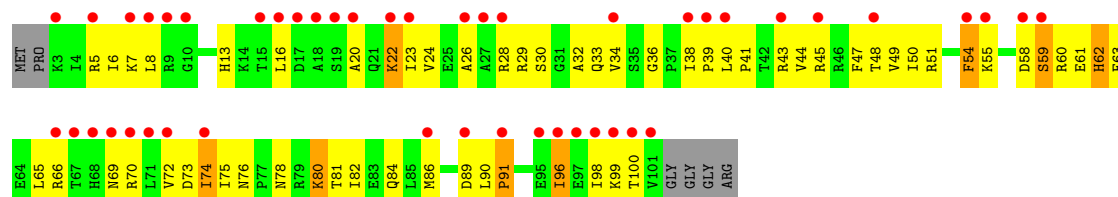
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



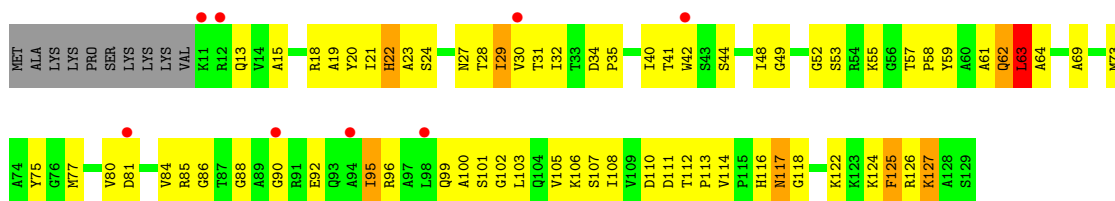
- Molecule 10: 30S ribosomal protein S10

Chain CJ:



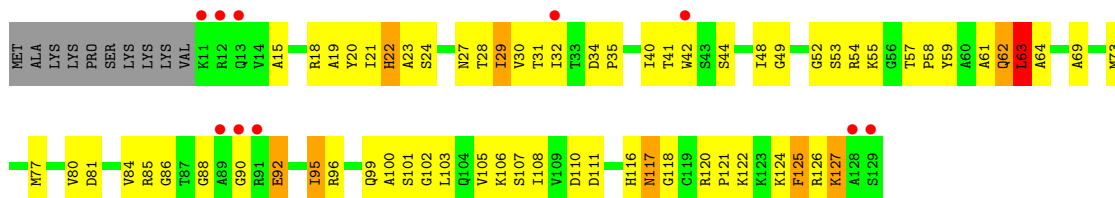
- Molecule 11: 30S ribosomal protein S11

Chain AK:



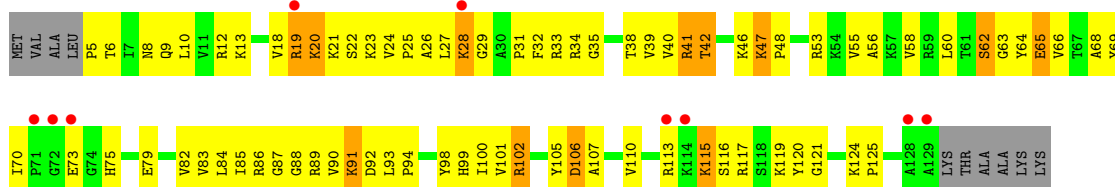
- Molecule 11: 30S ribosomal protein S11

Chain CK:



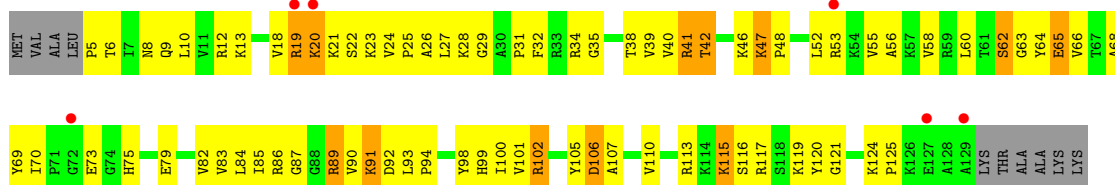
- Molecule 12: 30S ribosomal protein S12

Chain AL:



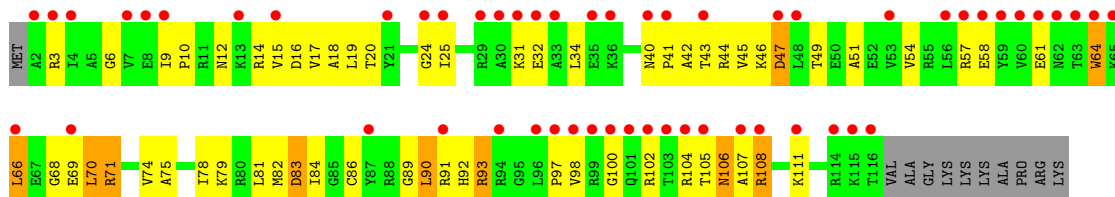
- Molecule 12: 30S ribosomal protein S12

Chain CL:



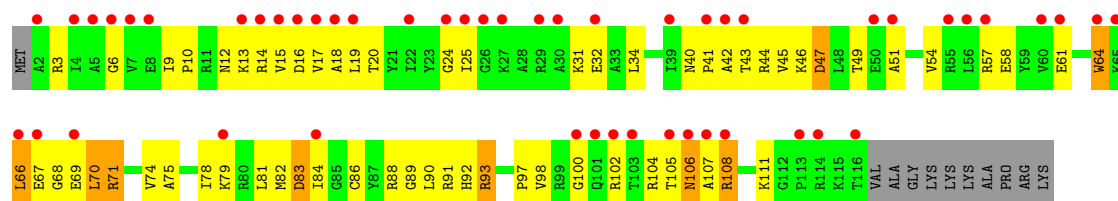
- Molecule 13: 30S ribosomal protein S13

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:



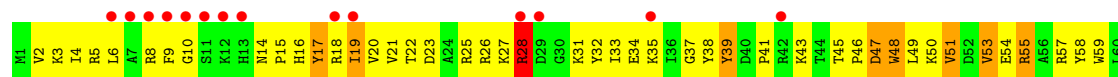
- Molecule 15: 30S ribosomal protein S15

Chain CO:



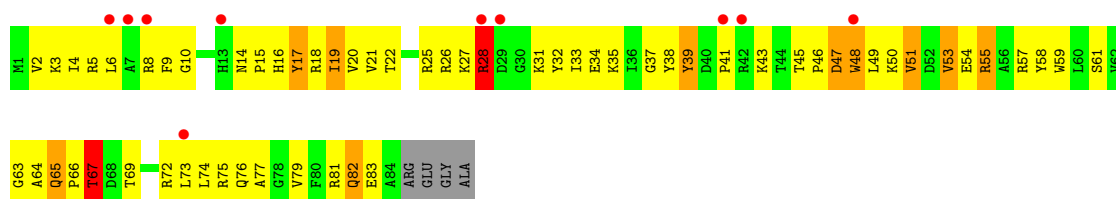
- Molecule 16: 30S ribosomal protein S16

Chain AP:



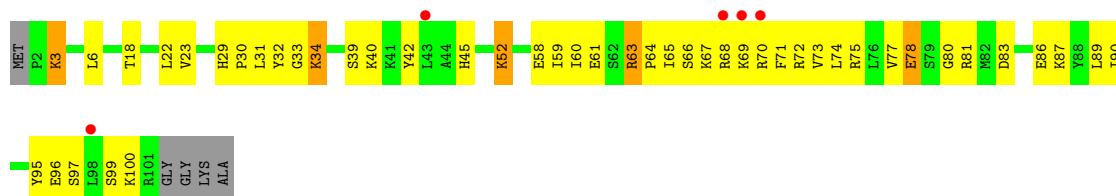
- Molecule 16: 30S ribosomal protein S16

Chain CP:



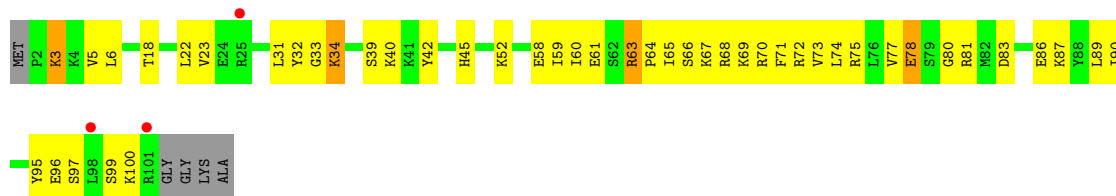
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



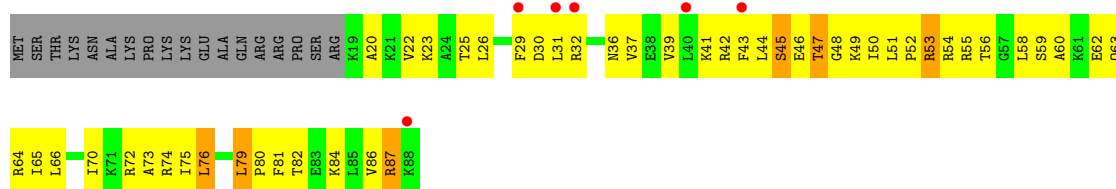
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



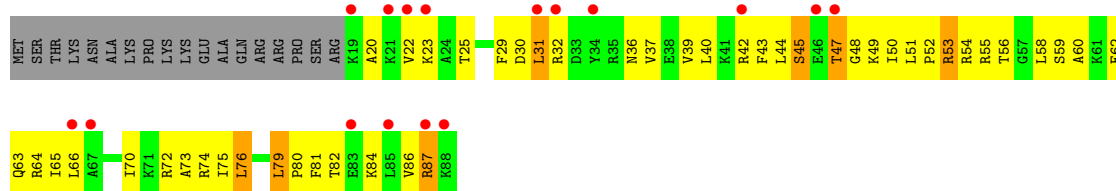
- Molecule 18: 30S ribosomal protein S18

Chain AR:



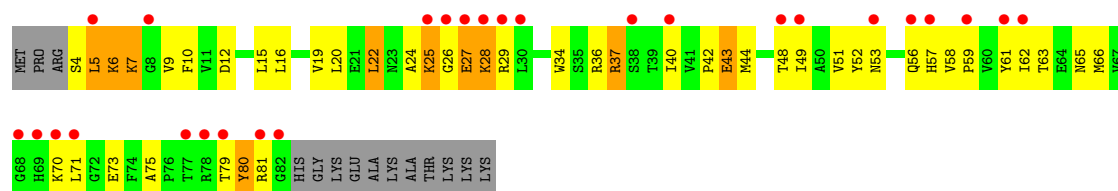
- Molecule 18: 30S ribosomal protein S18

Chain CR:



- Molecule 19: 30S ribosomal protein S19

Chain AS:



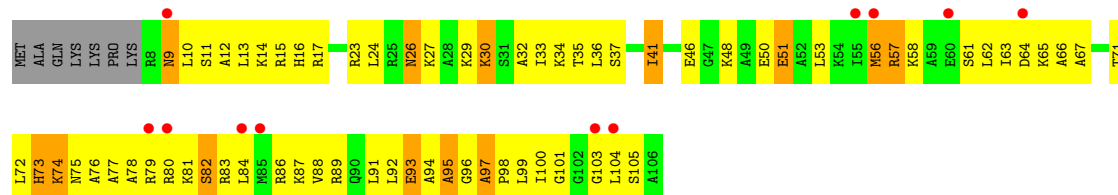
- Molecule 19: 30S ribosomal protein S19

Chain CS:



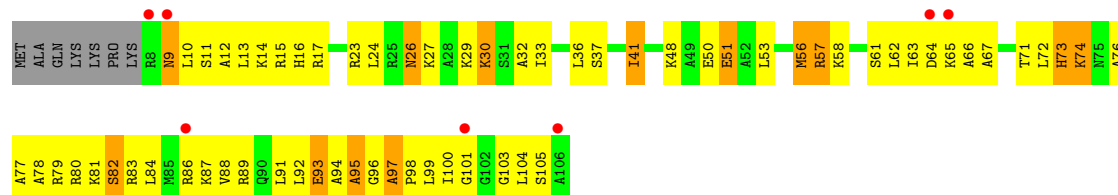
- Molecule 20: 30S ribosomal protein S20

Chain AT:



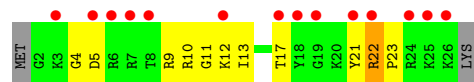
- Molecule 20: 30S ribosomal protein S20

Chain CT:



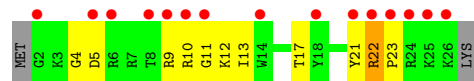
- Molecule 21: 30S ribosomal protein Thx

Chain AU:



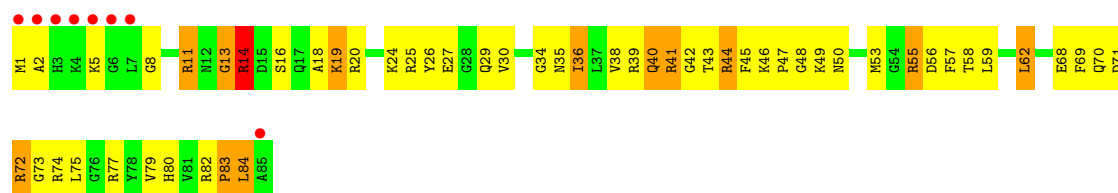
- Molecule 21: 30S ribosomal protein Thx

Chain CU:



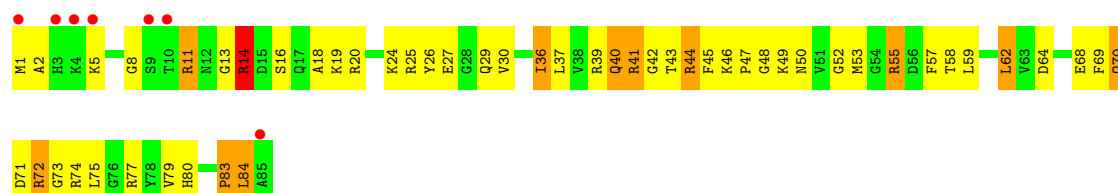
- Molecule 22: 50S ribosomal protein L27

Chain B0:



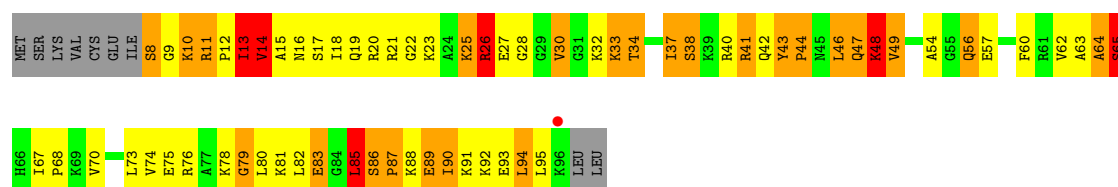
- Molecule 22: 50S ribosomal protein L27

Chain D0:



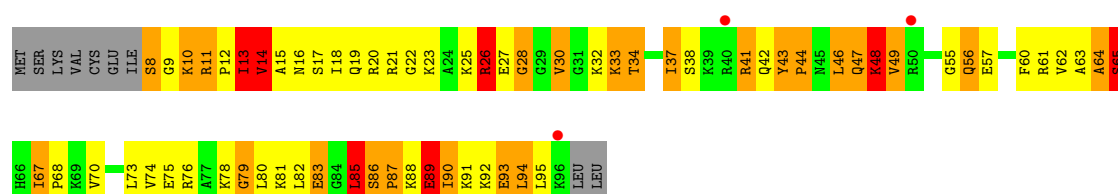
- Molecule 23: 50S ribosomal protein L28

Chain B1:



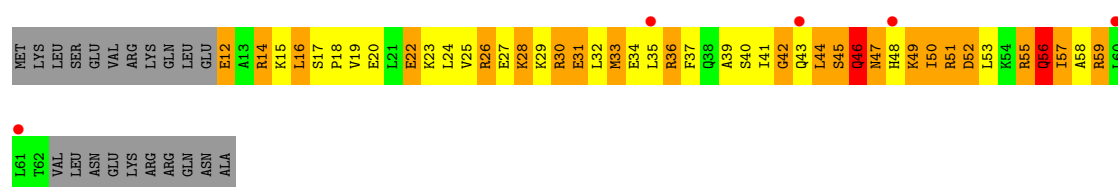
- Molecule 23: 50S ribosomal protein L28

Chain D1:



- Molecule 24: 50S ribosomal protein L29

Chain B2:



- Molecule 24: 50S ribosomal protein L29

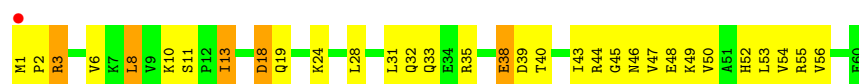
Chain D2:





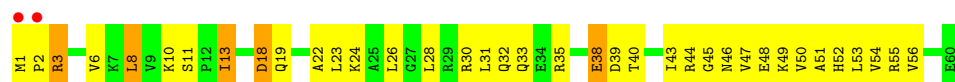
- Molecule 25: 50S ribosomal protein L30

Chain B3:



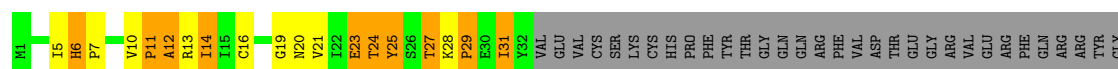
- Molecule 25: 50S ribosomal protein L30

Chain D3:



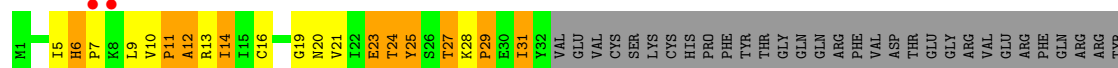
- Molecule 26: 50S ribosomal protein L31

Chain B4:



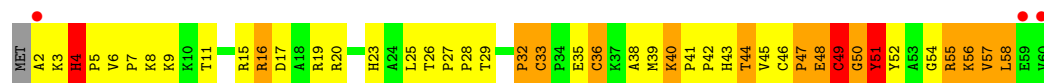
- Molecule 26: 50S ribosomal protein L31

Chain D4:



- Molecule 27: 50S ribosomal protein L32

Chain B5:



- Molecule 27: 50S ribosomal protein L32

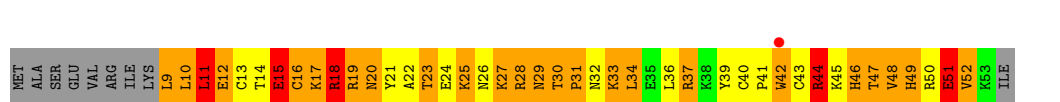
Chain D5:





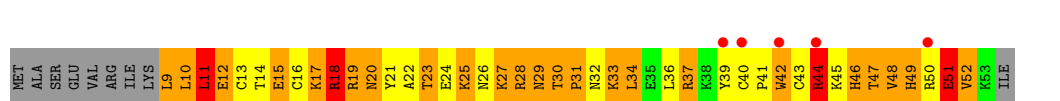
- Molecule 28: 50S ribosomal protein L33

Chain B6:



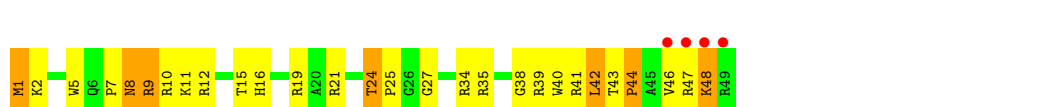
- Molecule 28: 50S ribosomal protein L33

Chain D6:



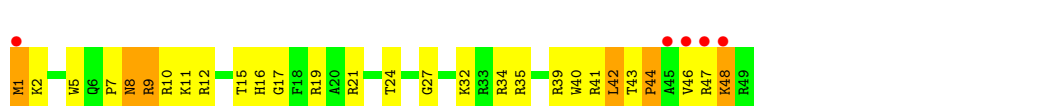
- Molecule 29: 50S ribosomal protein L34

Chain B7:



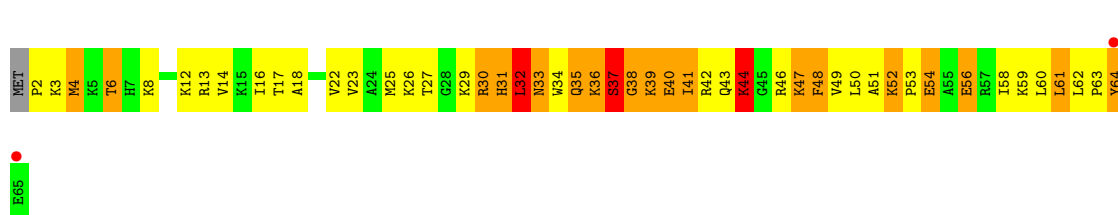
- Molecule 29: 50S ribosomal protein L34

Chain D7:



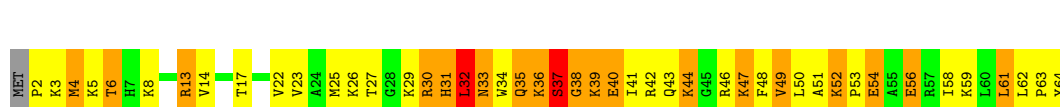
- Molecule 30: 50S ribosomal protein L35

Chain B8:



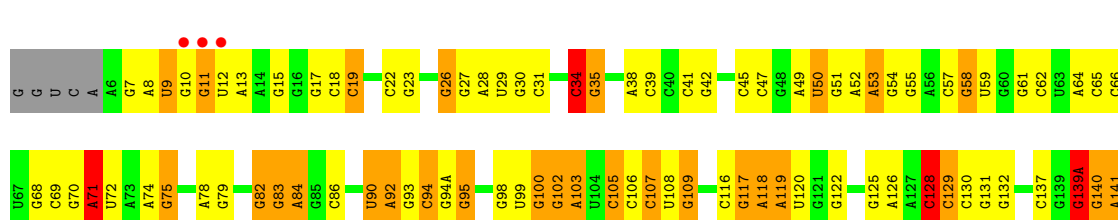
- Molecule 30: 50S ribosomal protein L35

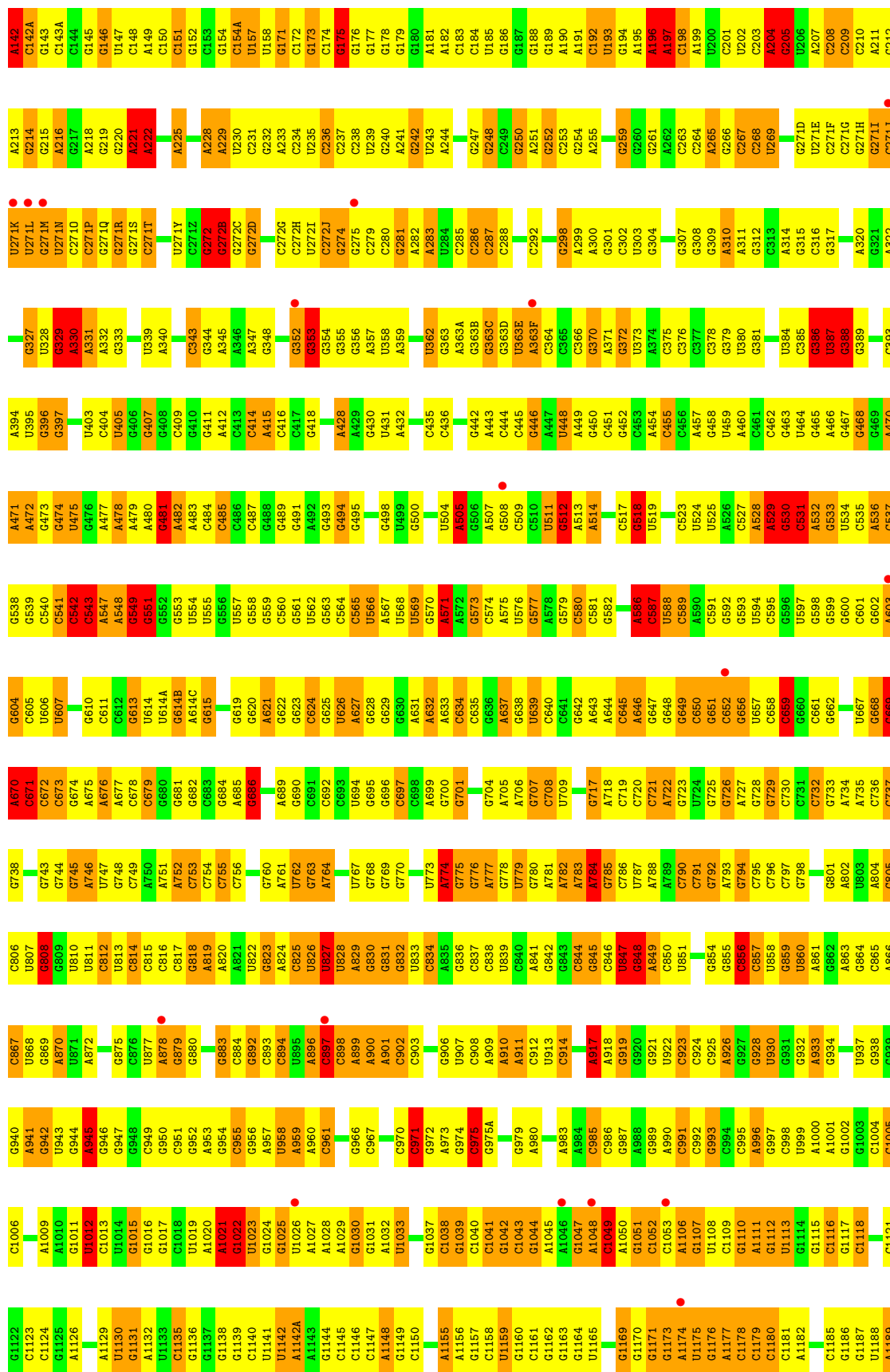
Chain D8:



- Molecule 31: 23S ribosomal RNA

Chain BA:



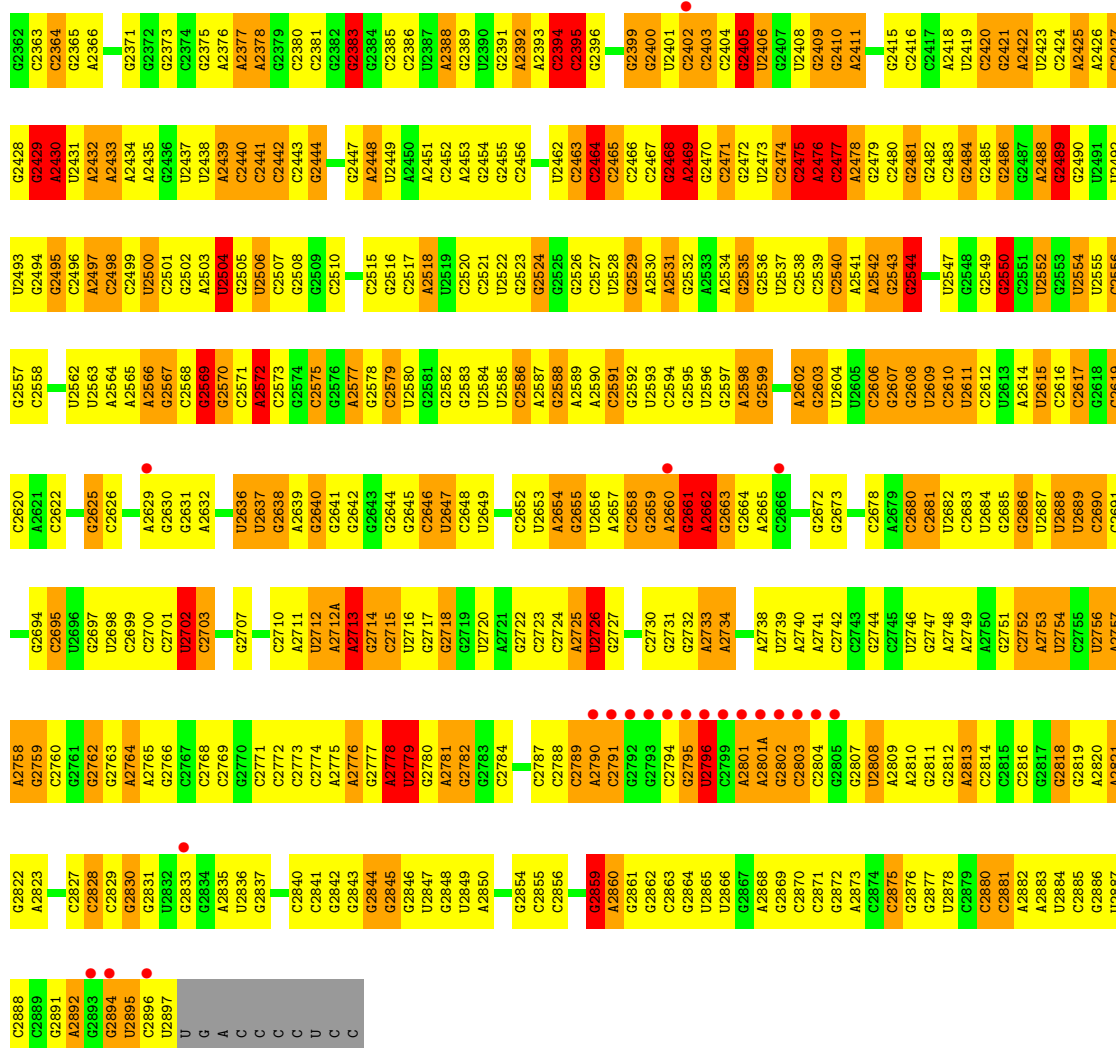






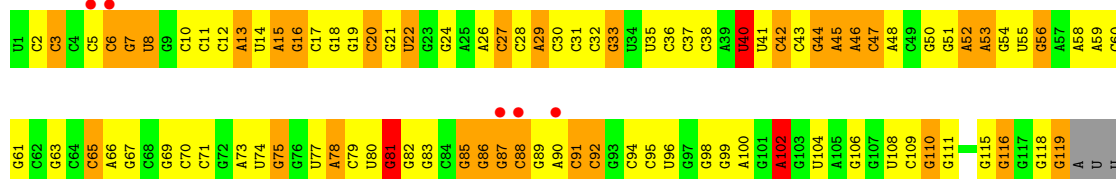
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G1252	C1181	G1115	A1000	G934	G864	A803	C737	U668	A603	C535	U465	U387		U271K
A1253	A1182	G1116	A1001	C935	C865	U804	G738	G669	A604	A536	A466	G388	A320	U271L
A1254	C1185	G1117	G1002	G938	A866	G805	U740	A670	C605	C537	G467	G389	A322	U271M
U1255	G1186	G1118	G1003	G939	U868	G806	G741	C671	U606	C540	G468	G391		U271N
G1256	G1187	C1121	C1005	G940	G869	U807	G742	C672	U607	C541	G469	C392		C271O
C1257	U1188	G1122	C1006	A941	A870	G808	G743	C673		C542	A470	C393	G327	C271P
C1258	A1189	G1123	U871	G942	U871	G809	G744	G674	G610	C543	A471	C394	U328	G271Q
G1259	G1190	C1124	U943	U943	A872	U810	G745	A675	C611	C544	A472	C395	G329	G271R
G1260	G1191	G1125	G944	G944	G873	U811	G746	A676	G612	A547	A473	U396	A330	G271S
C1261	G1192	A1126	A945	A945	G874	C812	U747	A677	G613	G548	G474	G396	A331	G271T
A1262	G1193		G946	G947	G875	U813	G748		U614	G551	U475	G397	A332	G271U
U1263	A1194	U1130	U1014	G947	G876	U814	G749	C679	U614A		G476	C404		G271V
U1264	G1015	G1131	G1015	G948	U877	C815	A750	G680	G614B	U554	A477	U405	C395	G271W
A1265	G1016	A1132	G1016	C949	A878	C816	A751	G681	A614C	U555	A478	G406	U339	G271X
U1266	U1019	U1133	U1019	G950	G879	C817	A752	G682	G615	U556	A479	G407	A340	U271Y
C1267	U1199	G1135	U1020	C951	G880	G818	C753	C683	G616	U557	A480	G408		C271Z
A1268	C1200	G1136	A1021	G952	G883	A819	C754	G684	C618	G558	A481	C409	C343	G272B
A1269	C1201	G1137	A1022	A953	C884	A820	C755	G685	G619	C560	A482	G410	G344	G272C
C1270	U1023	G1138	G1022	C954	C885	A821	C756	G686	A621	G561	C484	A412	A346	G272D
G1271	U1024	C1140	G1024	G956	C893	G823			G622	U562	C485	C413	A347	
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U1273	U1026	U1142	U1026	U958	U895	C825	U762	C691	G624	C564		A415		U272I
C1208	U1027	A1143	A1027	A959	A896	U826	G763	C692	G625	U565	G489	C416		C272J
G1209	U1028	A1144	U1028	A960	C897	U827	A764	C693	U626	C566	G490	C353	G352	G272K
U1211	A1029	G1144	A1029	C961	C898	U828	G765	G695	A627	U567	A492	G418	G354	G274
G1277	G1030	C1145	G1030	G962	A899	A829	C766	G696	G628	U568	C493	C355	C355	C275
A1213	U1031	C1146	U1031	U963	A900	G830	U767	C697	G629	U569	G494	C356	C280	C279
G1280	A1032	C1147	A1032	A966	A901	G831	G768		G630	G570	G495	A428	A357	C281
G1281	U1033	A1148	U1033	G966	C902	G832	G769	G700	A631	A571		G429	A357	A282
	G1034	G1149	G1034	C967	C903	U833	G770	G701	A632	U504	U504	U431	U358	C283
A1284	U1035	C1150	U1035		C904	C834			A633	G572	A505	A432	A359	U284
G1285	G1036	G1151	G1036	C970	A835	A835	U773	A705	C634	C574	G506	C433	U362	C285
C1221	G1037	G1152	G1037	C971	G906	G836	A774	A706	C635	A575	A507	U434	G363	C286
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	G1039	G1154	G1039	A973	C908	C838	G776	C708	A637	G577	C509	C436	G363B	C288
C1224	C1040	A1155	C1040	G974	A909	U839	A777		G638	A578	C510		G363C	
G1225	G1041	G1156	G1041	C975	A910	C940	G778	G715	U639	G579	U511	U441	U363D	C292
G1227	U1042	G1157	G1042	G975A	A911	C941	U779	A716	C640	C580	G512	G442	U363E	
G1228	C1043	U1158	C1043	G979	C912		G780	A717	C641	G581	A513	C443	A363F	G298
G1229	U1044	G1159	G1044	G979	U913	C844	A781	C719	G642	G582	A514	C444	C364	A299
	A1045	G1160	A1045	A980	C914	G845	A782	G725	A643	G583	A515	C445	C365	A300
U1234	A1046	G1161	A1046	A983	A917	G854	A783	G726	G644	C584	C516	C446	C366	G301
G1235	G1047	G1162	G1047	A984	U922	G855	A784	A727	A645	G585	G517	G447	G370	C302
G1236	A1048	G1163	A1048	C985	A918	C856	G785	A722	A646	A586	G518	U448	G371	U303
A1237	G1049	G1164	G1049	C986	G919	G857	G786	G723	G647	C587	U519	G372	G304	G303
A1301	A1050	U1165	A1050	C987	G921	C850	U787	U724	G648	U588		U373	G372	U305
A1302	G1051		G1051	G987	U921	U851	A788	G725	G649	C589	C523	C451	U374	U306
A1303	C1052	G1169	C1052	G987	U922		A789	G726	C650	A590	U524	C452	G375	G307
C1304	U1053	G1170	C1053	A990	C923	G854	C790	A727	G651	C591	U525	C453	G376	G308
C1305	A1106	G1171	A1106	C991	C924	G855	C791	G728	C652	G592	A526	C377	G377	G309
G1306	G1107	C1173	G1107	C992	C925	C856	G792	G729	G656	G593	C527	C455	C378	A310
A1307	U1108	A1174	U1108	G993	A926	G857	A793	C730	U657	U594	A528	C456	G379	A311
G1244	C1109	U1175	C1109	G994	G927	U858	G794	C731	C658	C595	A529	A457	U380	G312
G1309	G1110	G1176	G1110	A995	U928	G859	C795	G732	C659	G596	G530	G458	G381	C313
A1246	A1111	A1177	A1111	A996	U930	U860	C796	G733	G660	U597	C531	U459	A314	A314
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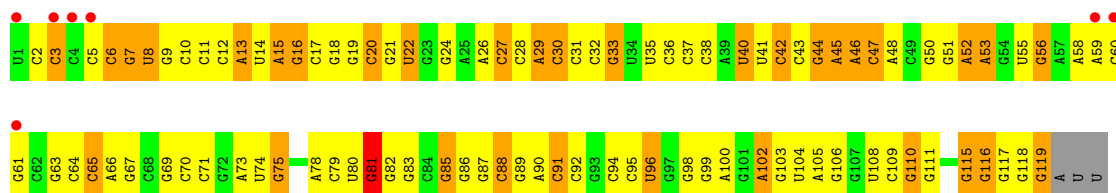
• Molecule 32: 5S ribosomal RNA

Chain BB:



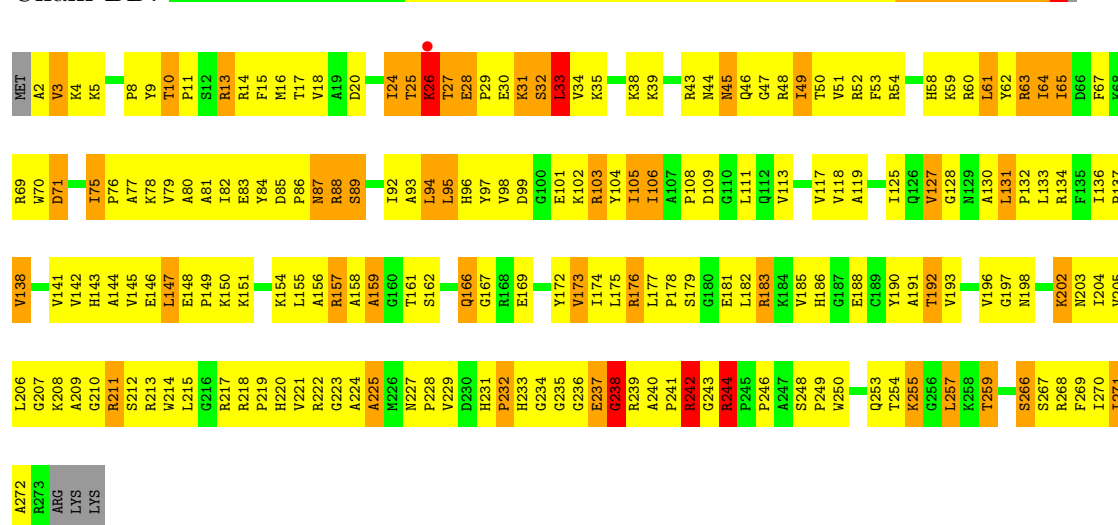
• Molecule 32: 5S ribosomal RNA

Chain DB:



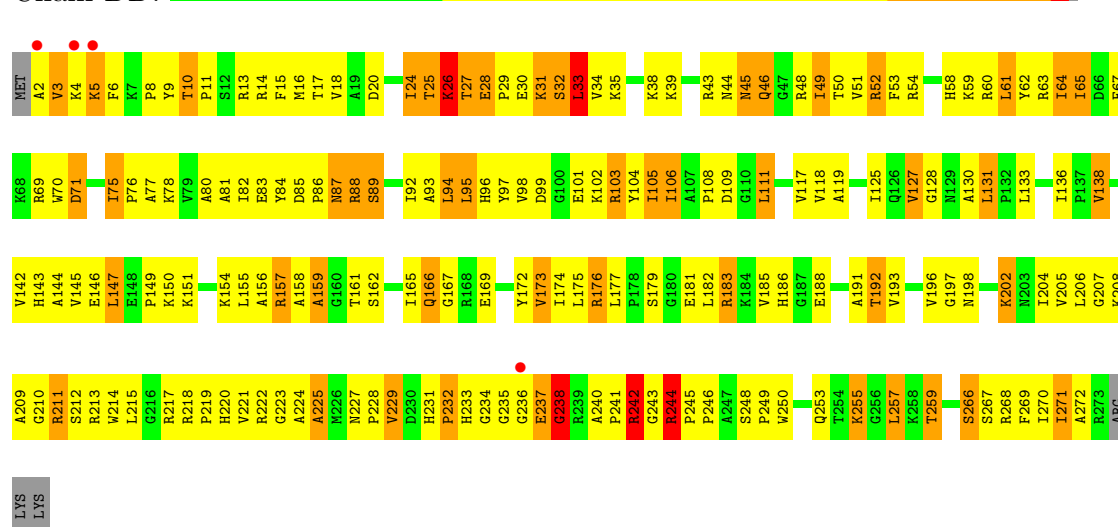
- Molecule 33: 50S ribosomal protein L2

Chain BD:



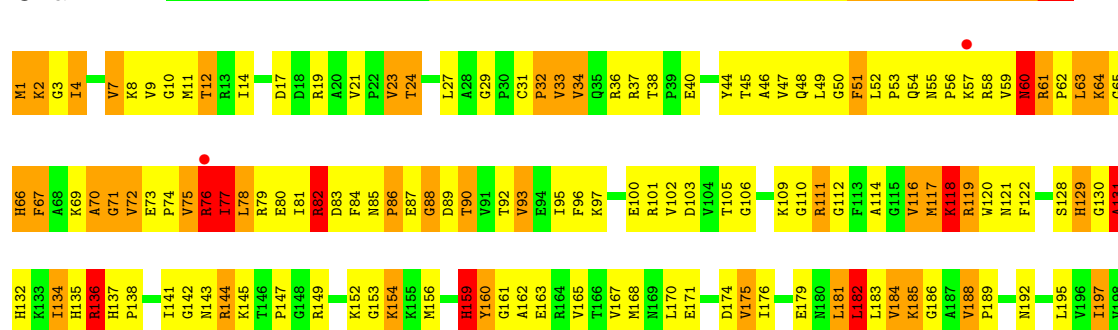
- Molecule 33: 50S ribosomal protein L2

Chain DD:

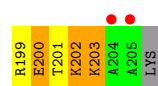


- Molecule 34: 50S ribosomal protein L3

Chain BE:

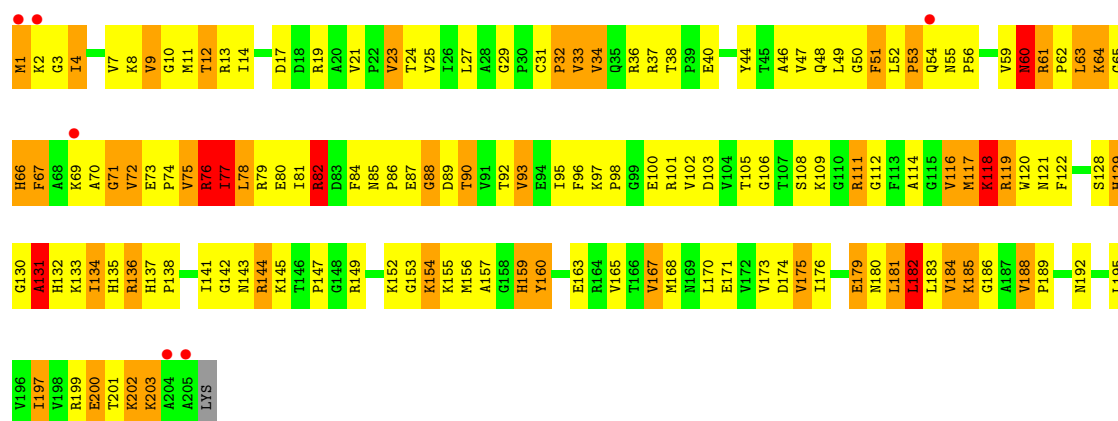






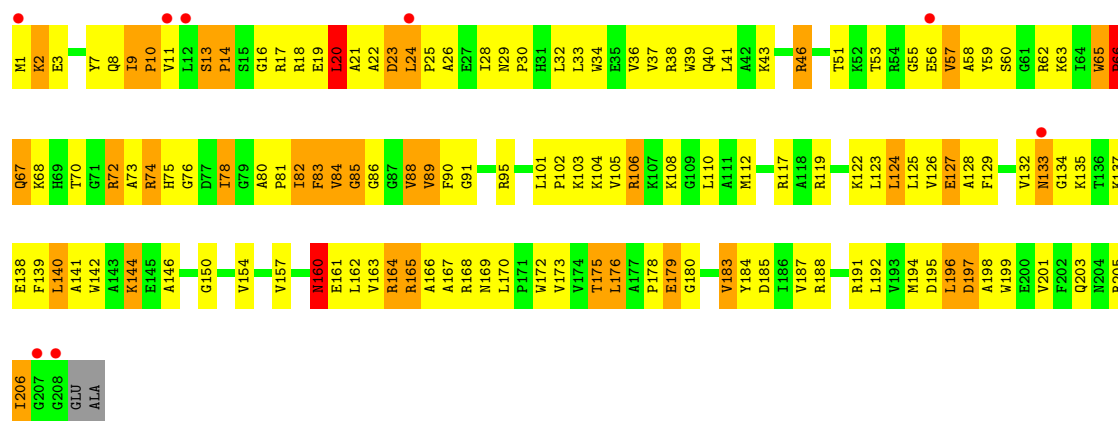
• Molecule 34: 50S ribosomal protein L3

Chain DE:



• Molecule 35: 50S ribosomal protein L4

Chain BF:



• Molecule 35: 50S ribosomal protein L4

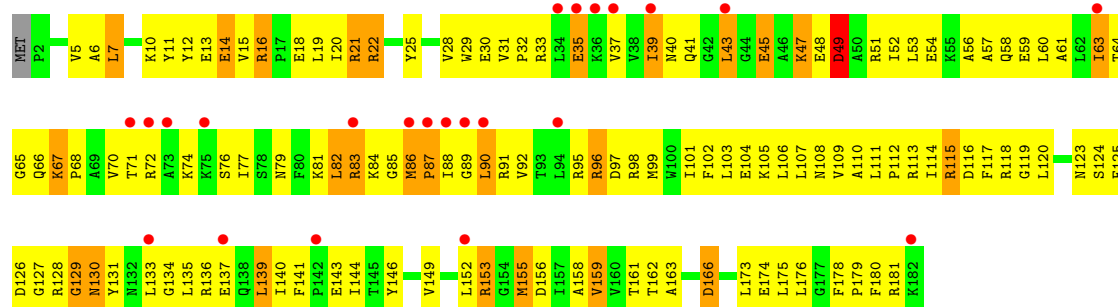
Chain DF:





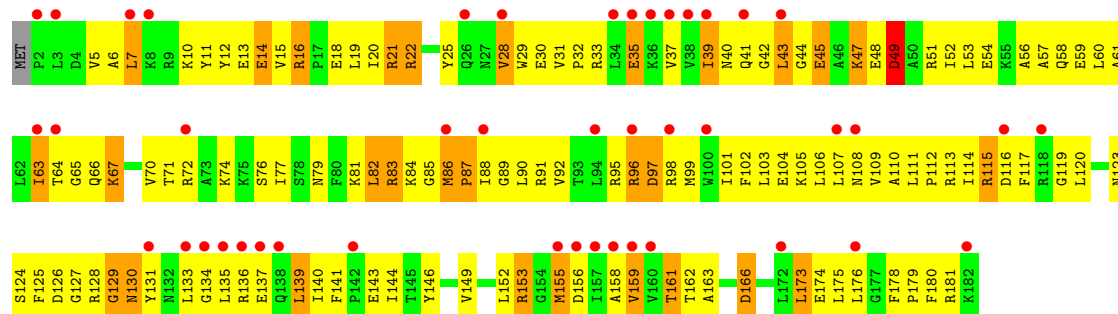
- Molecule 36: 50S ribosomal protein L5

Chain BG:



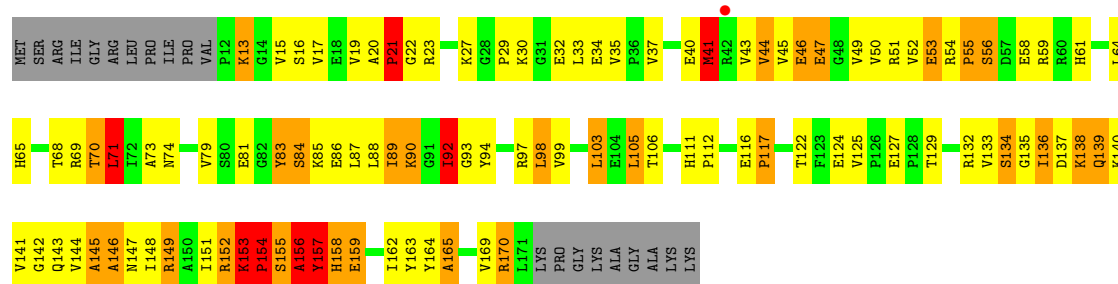
- Molecule 36: 50S ribosomal protein L5

Chain DG:



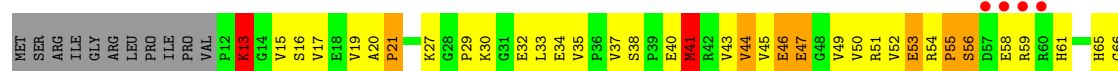
- Molecule 37: 50S ribosomal protein L6

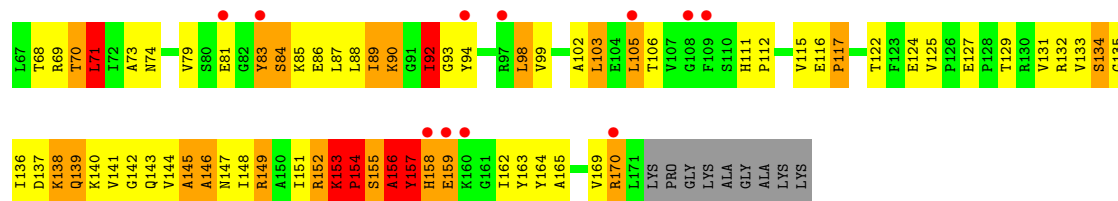
Chain BH:



- Molecule 37: 50S ribosomal protein L6

Chain DH:





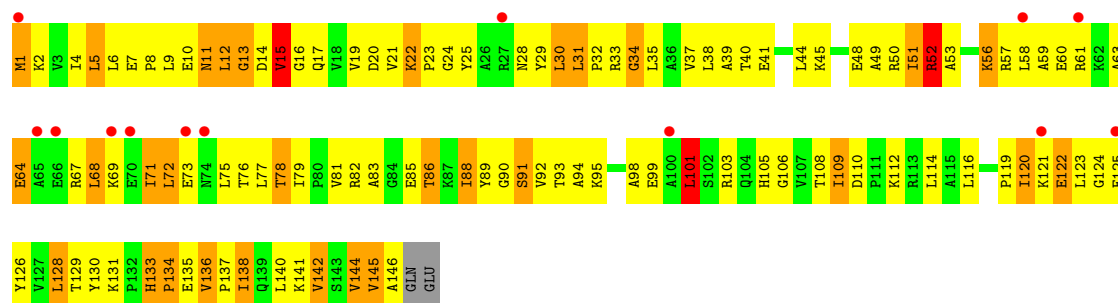
• Molecule 38: 50S ribosomal protein L9

Chain BI:



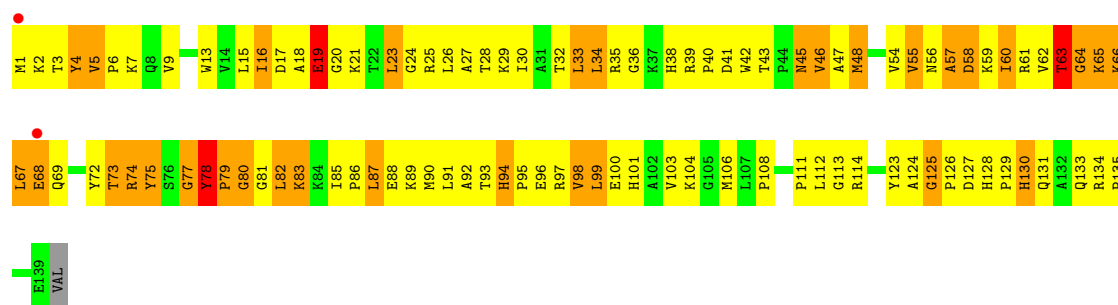
• Molecule 38: 50S ribosomal protein L9

Chain DI:



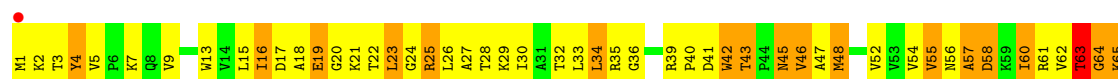
• Molecule 39: 50S ribosomal protein L13

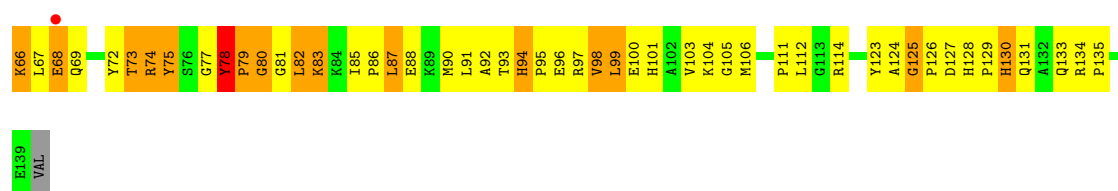
Chain BN:



• Molecule 39: 50S ribosomal protein L13

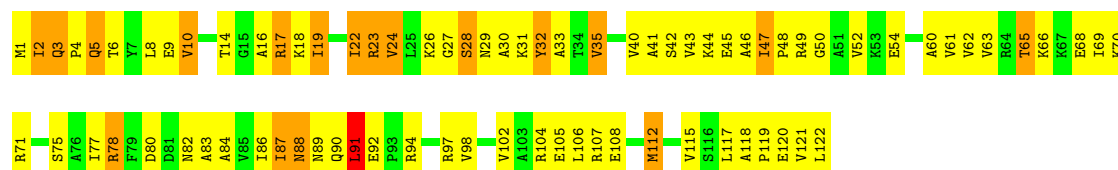
Chain DN:





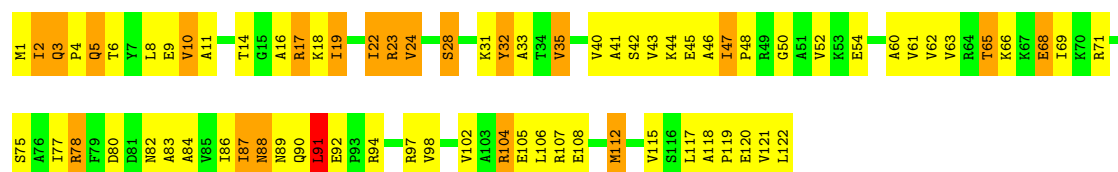
- Molecule 40: 50S ribosomal protein L14

Chain BO:



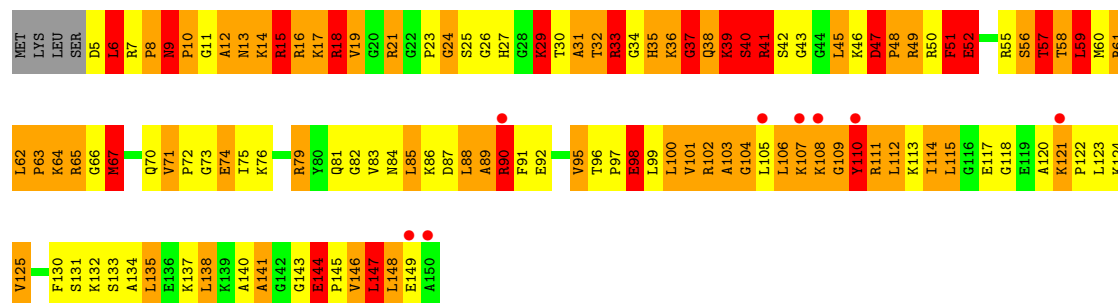
- Molecule 40: 50S ribosomal protein L14

Chain DO:



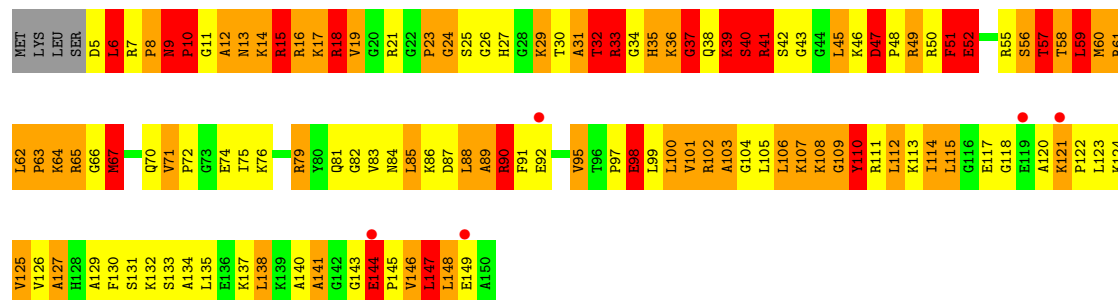
- Molecule 41: 50S ribosomal protein L15

Chain BP:



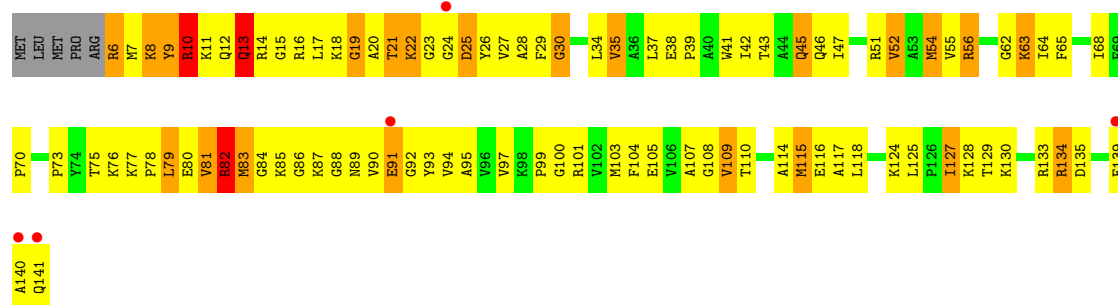
- Molecule 41: 50S ribosomal protein L15

Chain DP:



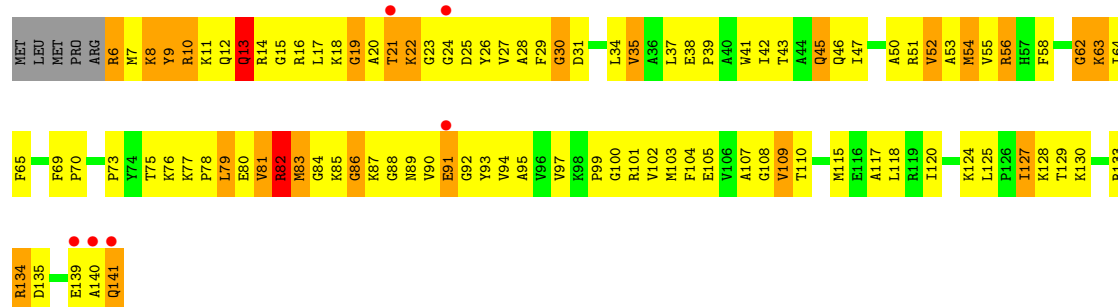
- Molecule 42: 50S ribosomal protein L16

Chain BQ: 



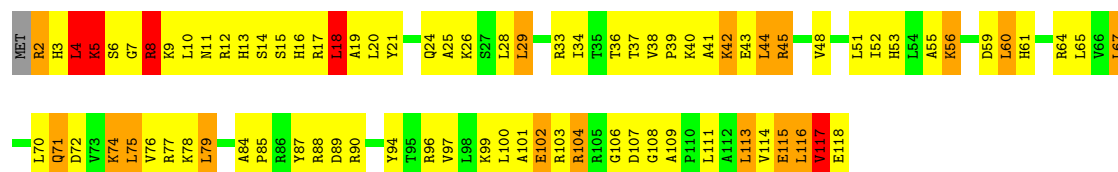
- Molecule 42: 50S ribosomal protein L16

Chain DQ: 



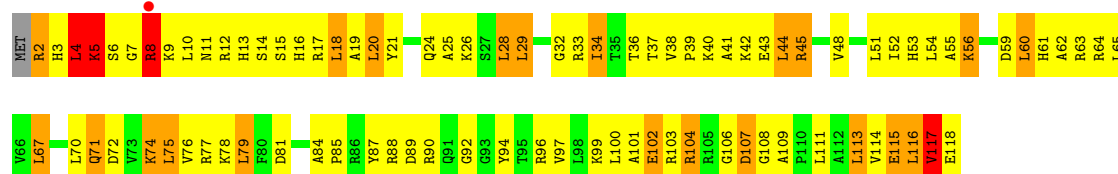
- Molecule 43: 50S ribosomal protein L17

Chain BR: 



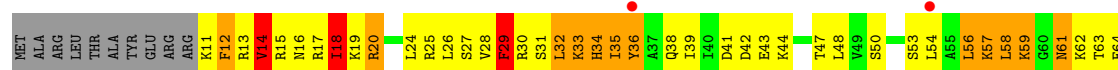
- Molecule 43: 50S ribosomal protein L17

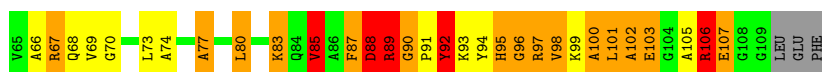
Chain DR: 



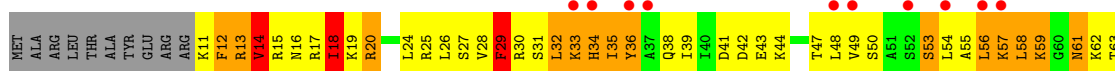
- Molecule 44: 50S ribosomal protein L18

Chain BS: 

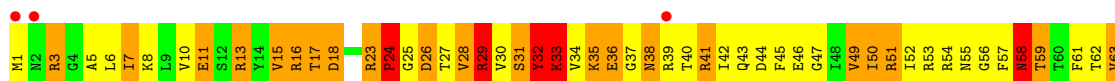




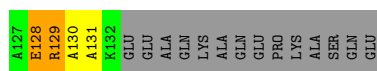
• Molecule 44: 50S ribosomal protein L18



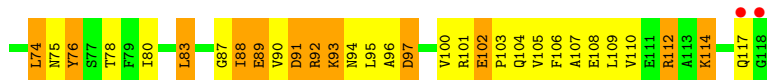
• Molecule 45: 50S ribosomal protein L19



• Molecule 45: 50S ribosomal protein L19



• Molecule 46: 50S ribosomal protein L20



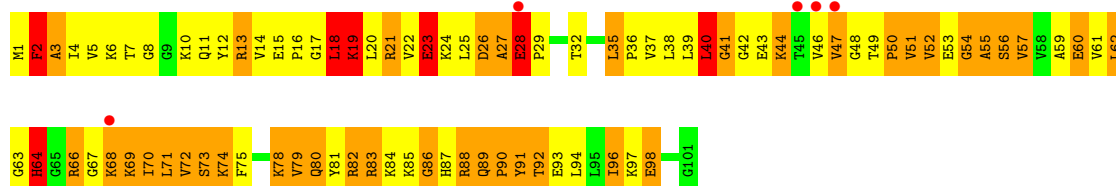
• Molecule 46: 50S ribosomal protein L20





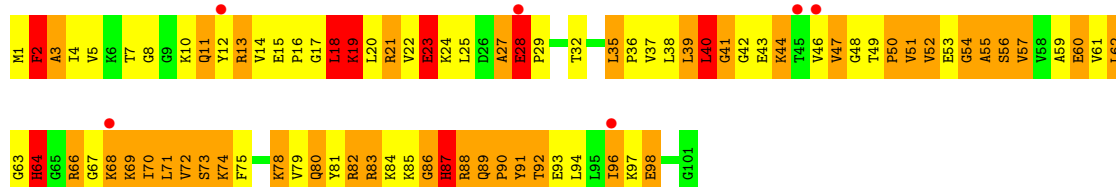
• Molecule 47: 50S ribosomal protein L21

Chain BV:



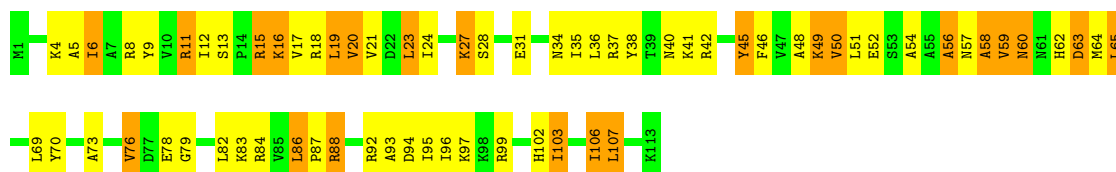
• Molecule 47: 50S ribosomal protein L21

Chain DV:



• Molecule 48: 50S ribosomal protein L22

Chain BW:



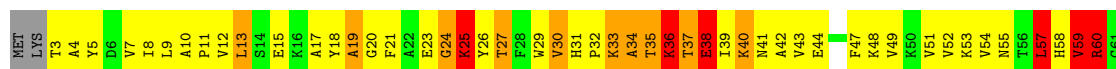
• Molecule 48: 50S ribosomal protein L22

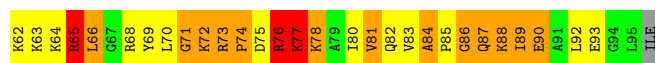
Chain DW:



• Molecule 49: 50S ribosomal protein L23

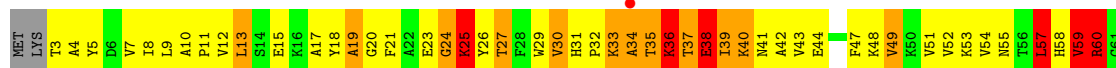
Chain BX:





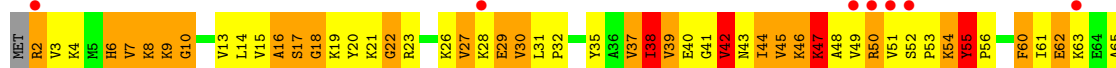
- Molecule 49: 50S ribosomal protein L23

Chain DX:



- Molecule 50: 50S ribosomal protein L24

Chain BY:



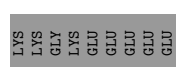
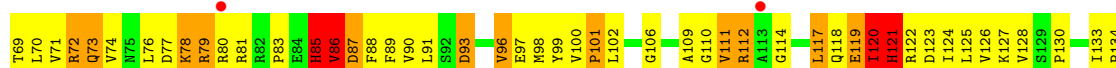
- Molecule 50: 50S ribosomal protein L24

Chain DY:



- Molecule 51: 50S ribosomal protein L25

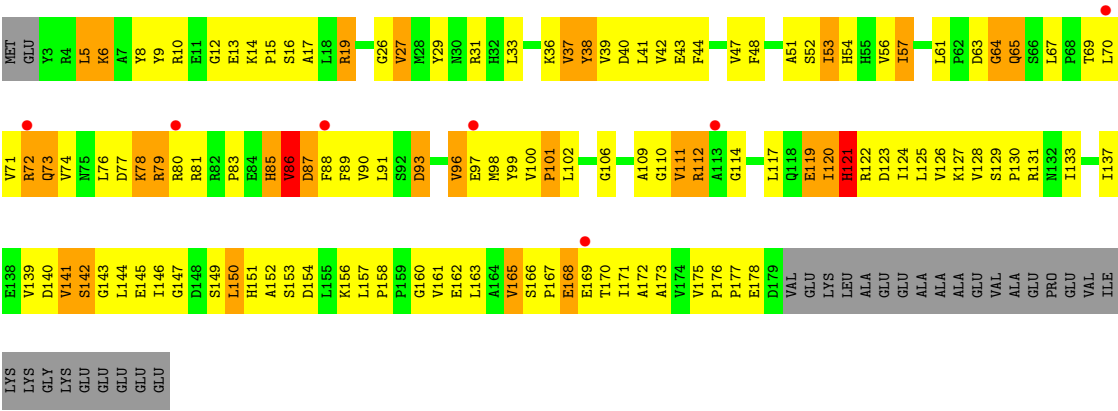
Chain BZ:



- Molecule 51: 50S ribosomal protein L25

Chain DZ:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.22Å 450.25Å 623.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 3.00 49.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.80-3.00) 88.7 (49.80-3.00)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 3.01Å)	Xtriage
Refinement program	Phenix	Depositor
R, $R_{free}$	0.235 , 0.269 0.235 , 0.269	Depositor DCC
$R_{free}$ test set	51892 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.9	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1035238 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	278000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	0.51	0/36190	0.87	34/56486 (0.1%)
1	CA	0.50	0/36190	0.88	40/56486 (0.1%)
2	AB	0.29	0/1936	0.51	0/2611
2	CB	0.29	0/1936	0.50	0/2611
3	AC	0.27	0/1637	0.45	0/2207
3	CC	0.27	0/1637	0.45	0/2207
4	AD	0.34	0/1733	0.52	0/2318
4	CD	0.34	0/1733	0.53	0/2318
5	AE	0.34	0/1163	0.55	0/1566
5	CE	0.34	0/1163	0.55	0/1566
6	AF	0.35	0/856	0.54	0/1154
6	CF	0.36	0/856	0.54	0/1154
7	AG	0.25	0/1276	0.44	0/1709
7	CG	0.26	0/1276	0.44	0/1709
8	AH	0.34	0/1136	0.55	0/1527
8	CH	0.33	0/1136	0.54	0/1527
9	AI	0.27	0/1028	0.44	0/1375
9	CI	0.27	0/1028	0.44	0/1375
10	AJ	0.29	0/808	0.48	0/1087
10	CJ	0.29	0/808	0.48	0/1087
11	AK	0.32	0/900	0.52	0/1213
11	CK	0.32	0/900	0.52	0/1213
12	AL	0.38	0/987	0.61	1/1322 (0.1%)
12	CL	0.39	0/987	0.62	0/1322
13	AM	0.26	0/928	0.47	0/1238
13	CM	0.27	0/928	0.47	0/1238
14	AN	0.27	0/501	0.45	0/664
14	CN	0.28	0/501	0.44	0/664
15	AO	0.35	0/745	0.56	0/992
15	CO	0.33	0/745	0.56	0/992
16	AP	0.33	0/717	0.55	0/965
16	CP	0.33	0/717	0.55	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.33	0/837	0.57	0/1119
17	CQ	0.34	0/837	0.56	0/1119
18	AR	0.35	0/579	0.57	0/768
18	CR	0.37	0/579	0.57	0/768
19	AS	0.28	0/643	0.46	0/867
19	CS	0.28	0/643	0.46	0/867
20	AT	0.34	0/765	0.56	0/1007
20	CT	0.34	0/765	0.55	0/1007
21	AU	0.27	0/213	0.43	0/279
21	CU	0.28	0/213	0.43	0/279
22	B0	0.58	0/658	0.76	1/878 (0.1%)
22	D0	0.52	0/658	0.74	0/878
23	B1	0.74	0/700	0.98	0/931
23	D1	0.65	0/700	0.95	1/931 (0.1%)
24	B2	0.68	0/423	0.92	0/560
24	D2	0.59	0/423	0.89	0/560
25	B3	0.62	0/473	0.71	0/636
25	D3	0.47	0/473	0.69	0/636
26	B4	0.31	0/156	0.59	0/215
26	D4	0.33	0/156	0.57	0/215
27	B5	0.86	1/473 (0.2%)	1.17	2/639 (0.3%)
27	D5	0.74	0/473	1.07	2/639 (0.3%)
28	B6	0.86	1/387 (0.3%)	1.05	2/517 (0.4%)
28	D6	0.70	0/387	0.97	1/517 (0.2%)
29	B7	0.65	0/427	0.79	0/563
29	D7	0.59	0/427	0.78	0/563
30	B8	0.76	0/516	1.08	3/681 (0.4%)
30	D8	0.64	0/516	1.02	3/681 (0.4%)
31	BA	1.11	98/65745 (0.1%)	1.45	1072/102639 (1.0%)
31	DA	0.84	36/65745 (0.1%)	1.38	904/102639 (0.9%)
32	BB	0.87	0/2853	1.26	29/4451 (0.7%)
32	DB	0.69	0/2853	1.18	27/4451 (0.6%)
33	BD	0.61	0/2155	0.82	1/2907 (0.0%)
33	DD	0.56	0/2155	0.80	1/2907 (0.0%)
34	BE	0.64	0/1597	0.82	2/2155 (0.1%)
34	DE	0.57	0/1597	0.80	0/2155
35	BF	0.63	1/1659 (0.1%)	0.77	0/2246
35	DF	0.53	0/1659	0.75	2/2246 (0.1%)
36	BG	0.33	0/1498	0.55	0/2013
36	DG	0.31	0/1498	0.53	0/2013
37	BH	0.64	0/1246	0.77	0/1684
37	DH	0.47	0/1246	0.70	0/1684
38	BI	0.39	0/1147	0.64	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DI	0.38	0/1147	0.63	0/1553
39	BN	0.70	0/1132	0.88	1/1527 (0.1%)
39	DN	0.54	0/1132	0.79	0/1527
40	BO	0.57	0/943	0.71	0/1269
40	DO	0.50	0/943	0.69	0/1269
41	BP	0.72	1/1131 (0.1%)	1.03	4/1504 (0.3%)
41	DP	0.63	0/1131	0.95	4/1504 (0.3%)
42	BQ	0.65	0/1100	0.84	1/1470 (0.1%)
42	DQ	0.58	0/1100	0.80	0/1470
43	BR	0.63	0/974	0.91	4/1302 (0.3%)
43	DR	0.56	0/974	0.87	3/1302 (0.2%)
44	BS	0.56	0/779	0.83	0/1038
44	DS	0.49	0/779	0.78	0/1038
45	BT	0.58	0/1114	0.83	1/1488 (0.1%)
45	DT	0.53	0/1114	0.80	0/1488
46	BU	0.71	0/975	0.77	0/1297
46	DU	0.59	0/975	0.71	0/1297
47	BV	0.76	0/789	0.96	1/1054 (0.1%)
47	DV	0.58	0/789	0.89	1/1054 (0.1%)
48	BW	0.67	0/907	0.84	0/1216
48	DW	0.58	0/907	0.79	0/1216
49	BX	0.74	0/740	0.99	3/995 (0.3%)
49	DX	0.64	0/740	0.90	2/995 (0.2%)
50	BY	0.67	1/789 (0.1%)	0.88	1/1053 (0.1%)
50	DY	0.56	0/789	0.82	1/1053 (0.1%)
51	BZ	0.46	0/1436	0.64	2/1951 (0.1%)
51	DZ	0.40	0/1436	0.62	2/1951 (0.1%)
All	All	0.75	139/301000 (0.0%)	1.13	2159/449812 (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
24	B2	0	3
24	D2	0	1
27	B5	0	1
27	D5	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
35	BF	0	1
37	BH	0	2
37	DH	0	2
41	BP	0	5
41	DP	0	4
42	BQ	0	1
42	DQ	0	1
43	BR	0	1
43	DR	0	1
44	BS	0	1
44	DS	0	1
45	BT	0	1
45	DT	0	1
47	BV	0	1
47	DV	0	2
49	BX	0	3
49	DX	0	3
All	All	42	47

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	783	A	N9-C4	-12.00	1.30	1.37
31	BA	669	G	C4'-C3'	-11.54	1.40	1.53
31	DA	528	A	N9-C4	-11.40	1.31	1.37
31	BA	2346	A	N3-C4	-10.07	1.28	1.34
31	DA	669	G	C4'-C3'	-9.54	1.42	1.53

The worst 5 of 2159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	DA	1779	U	C5-C6-N1	-19.83	112.78	122.70
31	DA	2447	G	N1-C6-O6	16.89	130.03	119.90
31	BA	1779	U	C5-C6-N1	-16.70	114.35	122.70
31	DA	2447	G	C5-C6-O6	-16.69	118.58	128.60
31	BA	676	A	C5-N7-C8	-15.75	96.03	103.90

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 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	B1	30	VAL	Peptide
24	B2	55	ARG	Peptide
24	B2	56	GLN	Peptide
24	B2	57	ILE	Peptide
27	B5	51	TYR	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	1409	0
1	CA	32329	0	16318	1381	0
2	AB	1901	0	1951	169	0
2	CB	1901	0	1951	167	0
3	AC	1613	0	1677	116	0
3	CC	1613	0	1677	117	0
4	AD	1703	0	1763	158	0
4	CD	1703	0	1763	160	0
5	AE	1147	0	1207	103	0
5	CE	1147	0	1207	107	0
6	AF	843	0	857	80	0
6	CF	843	0	857	86	0
7	AG	1257	0	1296	60	0
7	CG	1257	0	1296	62	0
8	AH	1116	0	1177	83	0
8	CH	1116	0	1177	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AI	1011	0	1042	84	0
9	CI	1011	0	1042	85	0
10	AJ	795	0	840	80	0
10	CJ	795	0	840	82	0
11	AK	885	0	904	64	0
11	CK	885	0	904	69	0
12	AL	971	0	1057	104	0
12	CL	971	0	1057	106	0
13	AM	921	0	976	60	0
13	CM	921	0	976	63	0
14	AN	492	0	530	35	0
14	CN	492	0	529	33	0
15	AO	734	0	771	54	0
15	CO	734	0	771	56	0
16	AP	701	0	720	88	0
16	CP	701	0	720	91	0
17	AQ	824	0	891	46	0
17	CQ	824	0	891	49	0
18	AR	574	0	644	63	0
18	CR	574	0	644	64	0
19	AS	630	0	652	40	0
19	CS	630	0	652	34	0
20	AT	763	0	861	78	0
20	CT	763	0	861	75	0
21	AU	209	0	221	11	0
21	CU	209	0	221	11	0
22	B0	650	0	654	67	0
22	D0	650	0	654	64	0
23	B1	693	0	764	143	0
23	D1	693	0	764	144	0
24	B2	421	0	461	119	1
24	D2	421	0	461	125	0
25	B3	468	0	523	37	0
25	D3	468	0	523	56	0
26	B4	157	0	69	12	0
26	D4	157	0	69	12	0
27	B5	459	0	478	82	0
27	D5	459	0	480	85	0
28	B6	381	0	390	96	0
28	D6	381	0	390	92	0
29	B7	419	0	467	37	0
29	D7	419	0	467	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B8	508	0	576	156	0
30	D8	508	0	576	144	0
31	BA	58698	0	29590	2392	0
31	DA	58698	0	29591	2578	1
32	BB	2551	0	1295	156	0
32	DB	2551	0	1295	173	0
33	BD	2105	0	2182	336	0
33	DD	2105	0	2182	333	0
34	BE	1564	0	1629	214	0
34	DE	1564	0	1629	213	0
35	BF	1624	0	1677	171	0
35	DF	1624	0	1677	178	0
36	BG	1474	0	1534	149	0
36	DG	1474	0	1534	149	0
37	BH	1223	0	1282	141	0
37	DH	1223	0	1282	129	0
38	BI	1132	0	1218	142	0
38	DI	1132	0	1218	156	0
39	BN	1105	0	1180	184	0
39	DN	1105	0	1180	183	0
40	BO	933	0	996	86	0
40	DO	933	0	996	76	0
41	BP	1114	0	1187	271	0
41	DP	1114	0	1187	260	0
42	BQ	1080	0	1127	157	0
42	DQ	1080	0	1127	162	0
43	BR	960	0	1021	115	0
43	DR	960	0	1021	117	0
44	BS	771	0	832	148	0
44	DS	771	0	832	150	0
45	BT	1100	0	1164	173	0
45	DT	1100	0	1164	166	0
46	BU	958	0	1015	142	0
46	DU	958	0	1015	151	0
47	BV	779	0	851	210	0
47	DV	779	0	851	215	0
48	BW	896	0	953	76	0
48	DW	896	0	953	80	0
49	BX	726	0	778	163	0
49	DX	726	0	778	168	0
50	BY	776	0	870	179	0
50	DY	776	0	870	187	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	BZ	1404	0	1432	140	0
51	DZ	1404	0	1432	139	0
52	AA	51	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	B7	1	0	0	0	0
52	BA	349	0	0	0	0
52	BB	5	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	48	0	0	0	0
52	D0	1	0	0	0	0
52	D1	1	0	0	0	0
52	D5	2	0	0	0	0
52	D7	1	0	0	0	0
52	DA	309	0	0	0	0
52	DB	3	0	0	0	0
52	DD	1	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	52	0	72	3	0
55	DA	52	0	72	3	0
All	All	278000	0	189246	17418	1

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 17418 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:HG2	1.13	1.31
42:DQ:81:VAL:O	42:DQ:82:ARG:HG2	1.25	1.27
41:BP:59:LEU:HA	41:BP:61:ARG:NH1	1.49	1.25
41:DP:59:LEU:HA	41:DP:61:ARG:NH1	1.55	1.20
31:DA:2206:G:N2	31:DA:2207:G:H5'	1.58	1.19

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:B2:12:GLU:CB	31:DA:306:U:OP1[1_455]	2.15	0.05

## 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%)	178 (76%)	38 (16%)	17 (7%)	2	8
2	CB	233/256 (91%)	177 (76%)	39 (17%)	17 (7%)	2	8
3	AC	205/239 (86%)	155 (76%)	36 (18%)	14 (7%)	2	10
3	CC	205/239 (86%)	155 (76%)	37 (18%)	13 (6%)	2	12
4	AD	206/209 (99%)	138 (67%)	52 (25%)	16 (8%)	1	7
4	CD	206/209 (99%)	137 (66%)	55 (27%)	14 (7%)	2	10
5	AE	149/162 (92%)	105 (70%)	31 (21%)	13 (9%)	1	5
5	CE	149/162 (92%)	103 (69%)	33 (22%)	13 (9%)	1	5
6	AF	99/101 (98%)	76 (77%)	15 (15%)	8 (8%)	1	7
6	CF	99/101 (98%)	76 (77%)	14 (14%)	9 (9%)	1	5
7	AG	153/156 (98%)	130 (85%)	19 (12%)	4 (3%)	8	39
7	CG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	8	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AH	136/138 (99%)	98 (72%)	31 (23%)	7 (5%)	3	18
8	CH	136/138 (99%)	98 (72%)	31 (23%)	7 (5%)	3	18
9	AI	123/128 (96%)	92 (75%)	24 (20%)	7 (6%)	3	16
9	CI	123/128 (96%)	94 (76%)	22 (18%)	7 (6%)	3	16
10	AJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	3	18
10	CJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	3	18
11	AK	117/129 (91%)	87 (74%)	26 (22%)	4 (3%)	6	31
11	CK	117/129 (91%)	86 (74%)	27 (23%)	4 (3%)	6	31
12	AL	123/135 (91%)	82 (67%)	31 (25%)	10 (8%)	1	7
12	CL	123/135 (91%)	83 (68%)	29 (24%)	11 (9%)	1	5
13	AM	107/126 (85%)	84 (78%)	17 (16%)	6 (6%)	3	16
13	CM	107/126 (85%)	84 (78%)	17 (16%)	6 (6%)	3	16
14	AN	58/61 (95%)	45 (78%)	11 (19%)	2 (3%)	6	31
14	CN	58/61 (95%)	44 (76%)	12 (21%)	2 (3%)	6	31
15	AO	86/89 (97%)	62 (72%)	19 (22%)	5 (6%)	3	15
15	CO	86/89 (97%)	61 (71%)	21 (24%)	4 (5%)	4	21
16	AP	82/88 (93%)	48 (58%)	27 (33%)	7 (8%)	1	6
16	CP	82/88 (93%)	47 (57%)	29 (35%)	6 (7%)	2	8
17	AQ	98/105 (93%)	74 (76%)	18 (18%)	6 (6%)	2	14
17	CQ	98/105 (93%)	73 (74%)	19 (19%)	6 (6%)	2	14
18	AR	68/88 (77%)	52 (76%)	11 (16%)	5 (7%)	2	8
18	CR	68/88 (77%)	51 (75%)	13 (19%)	4 (6%)	2	14
19	AS	77/93 (83%)	58 (75%)	13 (17%)	6 (8%)	1	7
19	CS	77/93 (83%)	59 (77%)	12 (16%)	6 (8%)	1	7
20	AT	97/106 (92%)	69 (71%)	19 (20%)	9 (9%)	1	5
20	CT	97/106 (92%)	65 (67%)	23 (24%)	9 (9%)	1	5
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%)	65 (78%)	14 (17%)	4 (5%)	4	20
22	D0	83/85 (98%)	64 (77%)	15 (18%)	4 (5%)	4	20
23	B1	87/98 (89%)	48 (55%)	17 (20%)	22 (25%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	D1	87/98 (89%)	45 (52%)	19 (22%)	23 (26%)	0	0
24	B2	49/72 (68%)	23 (47%)	19 (39%)	7 (14%)	0	1
24	D2	49/72 (68%)	23 (47%)	18 (37%)	8 (16%)	0	1
25	B3	58/60 (97%)	52 (90%)	4 (7%)	2 (3%)	6	31
25	D3	58/60 (97%)	51 (88%)	5 (9%)	2 (3%)	6	31
26	B4	30/71 (42%)	5 (17%)	11 (37%)	14 (47%)	0	0
26	D4	30/71 (42%)	5 (17%)	10 (33%)	15 (50%)	0	0
27	B5	57/60 (95%)	38 (67%)	11 (19%)	8 (14%)	0	2
27	D5	57/60 (95%)	36 (63%)	14 (25%)	7 (12%)	1	2
28	B6	41/54 (76%)	21 (51%)	6 (15%)	14 (34%)	0	0
28	D6	41/54 (76%)	19 (46%)	8 (20%)	14 (34%)	0	0
29	B7	47/49 (96%)	41 (87%)	4 (8%)	2 (4%)	4	23
29	D7	47/49 (96%)	40 (85%)	4 (8%)	3 (6%)	2	11
30	B8	62/65 (95%)	42 (68%)	11 (18%)	9 (14%)	0	1
30	D8	62/65 (95%)	41 (66%)	12 (19%)	9 (14%)	0	1
33	BD	270/276 (98%)	208 (77%)	45 (17%)	17 (6%)	2	12
33	DD	270/276 (98%)	207 (77%)	47 (17%)	16 (6%)	2	14
34	BE	203/206 (98%)	138 (68%)	37 (18%)	28 (14%)	0	2
34	DE	203/206 (98%)	138 (68%)	38 (19%)	27 (13%)	0	2
35	BF	206/210 (98%)	160 (78%)	30 (15%)	16 (8%)	1	7
35	DF	206/210 (98%)	156 (76%)	33 (16%)	17 (8%)	1	6
36	BG	177/182 (97%)	128 (72%)	35 (20%)	14 (8%)	1	7
36	DG	177/182 (97%)	127 (72%)	36 (20%)	14 (8%)	1	7
37	BH	158/180 (88%)	92 (58%)	41 (26%)	25 (16%)	0	1
37	DH	158/180 (88%)	93 (59%)	39 (25%)	26 (16%)	0	1
38	BI	144/148 (97%)	88 (61%)	32 (22%)	24 (17%)	0	1
38	DI	144/148 (97%)	87 (60%)	35 (24%)	22 (15%)	0	1
39	BN	137/140 (98%)	87 (64%)	32 (23%)	18 (13%)	0	2
39	DN	137/140 (98%)	88 (64%)	32 (23%)	17 (12%)	1	2
40	BO	120/122 (98%)	101 (84%)	16 (13%)	3 (2%)	9	40
40	DO	120/122 (98%)	99 (82%)	17 (14%)	4 (3%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	BP	144/150 (96%)	77 (54%)	17 (12%)	50 (35%)	0	0
41	DP	144/150 (96%)	76 (53%)	18 (12%)	50 (35%)	0	0
42	BQ	134/141 (95%)	92 (69%)	28 (21%)	14 (10%)	1	4
42	DQ	134/141 (95%)	96 (72%)	23 (17%)	15 (11%)	1	3
43	BR	115/118 (98%)	78 (68%)	29 (25%)	8 (7%)	2	9
43	DR	115/118 (98%)	82 (71%)	24 (21%)	9 (8%)	1	7
44	BS	97/112 (87%)	49 (50%)	24 (25%)	24 (25%)	0	0
44	DS	97/112 (87%)	49 (50%)	23 (24%)	25 (26%)	0	0
45	BT	130/146 (89%)	89 (68%)	21 (16%)	20 (15%)	0	1
45	DT	130/146 (89%)	90 (69%)	21 (16%)	19 (15%)	0	1
46	BU	115/118 (98%)	77 (67%)	27 (24%)	11 (10%)	1	4
46	DU	115/118 (98%)	74 (64%)	29 (25%)	12 (10%)	1	4
47	BV	97/101 (96%)	54 (56%)	15 (16%)	28 (29%)	0	0
47	DV	97/101 (96%)	52 (54%)	18 (19%)	27 (28%)	0	0
48	BW	111/113 (98%)	88 (79%)	15 (14%)	8 (7%)	2	8
48	DW	111/113 (98%)	89 (80%)	15 (14%)	7 (6%)	2	12
49	BX	91/96 (95%)	47 (52%)	22 (24%)	22 (24%)	0	0
49	DX	91/96 (95%)	48 (53%)	22 (24%)	21 (23%)	0	0
50	BY	99/110 (90%)	45 (46%)	22 (22%)	32 (32%)	0	0
50	DY	99/110 (90%)	46 (46%)	21 (21%)	32 (32%)	0	0
51	BZ	175/206 (85%)	113 (65%)	43 (25%)	19 (11%)	1	3
51	DZ	175/206 (85%)	113 (65%)	44 (25%)	18 (10%)	1	4
All	All	11148/12060 (92%)	7735 (69%)	2187 (20%)	1226 (11%)	1	3

5 of 1226 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	24	TRP
2	AB	154	LEU
2	AB	165	VAL
2	AB	194	PRO

### 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%)	176 (87%)	26 (13%)	6	26
2	CB	202/220 (92%)	176 (87%)	26 (13%)	6	26
3	AC	160/188 (85%)	152 (95%)	8 (5%)	34	77
3	CC	160/188 (85%)	152 (95%)	8 (5%)	34	77
4	AD	180/181 (99%)	157 (87%)	23 (13%)	6	27
4	CD	180/181 (99%)	156 (87%)	24 (13%)	6	25
5	AE	115/123 (94%)	100 (87%)	15 (13%)	6	26
5	CE	115/123 (94%)	100 (87%)	15 (13%)	6	26
6	AF	90/90 (100%)	79 (88%)	11 (12%)	7	29
6	CF	90/90 (100%)	79 (88%)	11 (12%)	7	29
7	AG	126/127 (99%)	121 (96%)	5 (4%)	42	84
7	CG	126/127 (99%)	121 (96%)	5 (4%)	42	84
8	AH	119/119 (100%)	107 (90%)	12 (10%)	11	39
8	CH	119/119 (100%)	107 (90%)	12 (10%)	11	39
9	AI	98/99 (99%)	88 (90%)	10 (10%)	11	38
9	CI	98/99 (99%)	88 (90%)	10 (10%)	11	38
10	AJ	88/92 (96%)	81 (92%)	7 (8%)	17	53
10	CJ	88/92 (96%)	81 (92%)	7 (8%)	17	53
11	AK	90/99 (91%)	79 (88%)	11 (12%)	7	29
11	CK	90/99 (91%)	80 (89%)	10 (11%)	9	34
12	AL	104/111 (94%)	96 (92%)	8 (8%)	18	56
12	CL	104/111 (94%)	96 (92%)	8 (8%)	18	56
13	AM	93/101 (92%)	86 (92%)	7 (8%)	19	57
13	CM	93/101 (92%)	86 (92%)	7 (8%)	19	57
14	AN	49/50 (98%)	46 (94%)	3 (6%)	26	68
14	CN	49/50 (98%)	47 (96%)	2 (4%)	41	83
15	AO	79/80 (99%)	69 (87%)	10 (13%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CO	79/80 (99%)	69 (87%)	10 (13%)	6	27
16	AP	72/74 (97%)	60 (83%)	12 (17%)	3	16
16	CP	72/74 (97%)	60 (83%)	12 (17%)	3	16
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	51	89
17	CQ	94/97 (97%)	91 (97%)	3 (3%)	51	89
18	AR	61/77 (79%)	56 (92%)	5 (8%)	17	52
18	CR	61/77 (79%)	55 (90%)	6 (10%)	12	41
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%)	66 (87%)	10 (13%)	6	25
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%)	49 (80%)	12 (20%)	2	11
22	D0	61/67 (91%)	47 (77%)	14 (23%)	1	6
23	B1	73/83 (88%)	55 (75%)	18 (25%)	1	4
23	D1	73/83 (88%)	55 (75%)	18 (25%)	1	4
24	B2	46/67 (69%)	29 (63%)	17 (37%)	0	1
24	D2	46/67 (69%)	30 (65%)	16 (35%)	0	1
25	B3	51/52 (98%)	44 (86%)	7 (14%)	5	24
25	D3	51/52 (98%)	44 (86%)	7 (14%)	5	24
27	B5	51/52 (98%)	38 (74%)	13 (26%)	1	4
27	D5	51/52 (98%)	36 (71%)	15 (29%)	0	2
28	B6	43/52 (83%)	27 (63%)	16 (37%)	0	1
28	D6	43/52 (83%)	27 (63%)	16 (37%)	0	1
29	B7	41/42 (98%)	35 (85%)	6 (15%)	5	21
29	D7	41/42 (98%)	35 (85%)	6 (15%)	5	21
30	B8	53/55 (96%)	38 (72%)	15 (28%)	0	3
30	D8	53/55 (96%)	41 (77%)	12 (23%)	1	6
33	BD	213/218 (98%)	163 (76%)	50 (24%)	1	5
33	DD	213/218 (98%)	162 (76%)	51 (24%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
34	BE	165/166 (99%)	126 (76%)	39 (24%)	1	5	
34	DE	165/166 (99%)	126 (76%)	39 (24%)	1	5	
35	BF	165/166 (99%)	132 (80%)	33 (20%)	2	10	
35	DF	165/166 (99%)	135 (82%)	30 (18%)	2	13	
36	BG	155/156 (99%)	132 (85%)	23 (15%)	4	21	
36	DG	155/156 (99%)	131 (84%)	24 (16%)	4	19	
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%)	103 (84%)	19 (16%)	4	18	
38	DI	122/124 (98%)	103 (84%)	19 (16%)	4	18	
39	BN	117/119 (98%)	93 (80%)	24 (20%)	2	9	
39	DN	117/119 (98%)	92 (79%)	25 (21%)	1	8	
40	BO	100/100 (100%)	75 (75%)	25 (25%)	1	4	
40	DO	100/100 (100%)	74 (74%)	26 (26%)	1	4	
41	BP	112/116 (97%)	63 (56%)	49 (44%)	0	0	
41	DP	112/116 (97%)	65 (58%)	47 (42%)	0	0	
42	BQ	106/111 (96%)	88 (83%)	18 (17%)	3	15	
42	DQ	106/111 (96%)	87 (82%)	19 (18%)	2	13	
43	BR	100/101 (99%)	76 (76%)	24 (24%)	1	5	
43	DR	100/101 (99%)	75 (75%)	25 (25%)	1	4	
44	BS	77/88 (88%)	54 (70%)	23 (30%)	0	2	
44	DS	77/88 (88%)	54 (70%)	23 (30%)	0	2	
45	BT	116/127 (91%)	84 (72%)	32 (28%)	0	3	
45	DT	116/127 (91%)	84 (72%)	32 (28%)	0	3	
46	BU	92/94 (98%)	75 (82%)	17 (18%)	2	13	
46	DU	92/94 (98%)	74 (80%)	18 (20%)	2	11	
47	BV	82/82 (100%)	53 (65%)	29 (35%)	0	1	
47	DV	82/82 (100%)	52 (63%)	30 (37%)	0	1	
48	BW	91/92 (99%)	70 (77%)	21 (23%)	1	6	
48	DW	91/92 (99%)	69 (76%)	22 (24%)	1	5	
49	BX	74/78 (95%)	54 (73%)	20 (27%)	1	3	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	59 (70%)	25 (30%)	0	2
51	BZ	155/179 (87%)	130 (84%)	25 (16%)	3	17
51	DZ	155/179 (87%)	130 (84%)	25 (16%)	3	17
All	All	9322/9876 (94%)	7681 (82%)	1641 (18%)	3	14

5 of 1641 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BW	76	VAL
8	CH	95	VAL
46	DU	102	GLU
49	BX	65	ARG
2	CB	130	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 272 such sidechains are listed below:

Mol	Chain	Res	Type
47	BV	89	GLN
6	CF	18	GLN
45	DT	123	GLN
48	BW	61	ASN
2	CB	40	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	287 (19%)	31 (2%)
1	CA	1503/1522 (98%)	288 (19%)	31 (2%)
31	BA	2723/2787 (97%)	735 (26%)	71 (2%)
31	DA	2723/2787 (97%)	729 (26%)	70 (2%)
32	BB	118/122 (96%)	35 (29%)	1 (0%)
32	DB	118/122 (96%)	35 (29%)	0
All	All	8688/8862 (98%)	2109 (24%)	204 (2%)

5 of 2109 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 204 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	BA	2506	U
1	CA	484	G
31	DA	1992	G
31	BA	2611	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 802 ligands modelled in this entry, 800 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	ZIT	BA	3351	-	54,54,54	1.30	5 (9%)	83,83,83	1.22	7 (8%)
55	ZIT	DA	3311	-	54,54,54	1.30	5 (9%)	83,83,83	1.22	7 (8%)

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	ZIT	BA	3351	-	-	0/72/107/107	0/3/3/3
55	ZIT	DA	3311	-	-	0/72/107/107	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BA	3351	ZIT	C22-C11	3.40	1.58	1.52
55	DA	3311	ZIT	C22-C11	3.38	1.58	1.52
55	DA	3311	ZIT	C13-C14	3.00	1.60	1.54
55	BA	3351	ZIT	C13-C14	2.96	1.60	1.54
55	DA	3311	ZIT	O13-C13	2.45	1.48	1.44

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BA	3351	ZIT	C12-C11-N10	-3.85	105.81	109.97
55	DA	3311	ZIT	C12-C11-N10	-3.82	105.84	109.97
55	BA	3351	ZIT	C9-N10-C11	-3.66	106.95	112.40
55	DA	3311	ZIT	C9-N10-C11	-3.63	106.99	112.40
55	BA	3351	ZIT	C2B-C3B-C4B	-2.75	104.59	107.91

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
47	DV	1

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Mol	Chain	Number of breaks
36	DG	1
36	BG	1
9	AI	1
9	CI	1
47	BV	1
28	D6	1
28	B6	1

The worst 5 of 14 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	5.29
1	AM	69:GLU	C	70:LEU	N	5.28
1	DG	112:PRO	C	113:ARG	N	4.77
1	BG	112:PRO	C	113:ARG	N	4.76
1	AM	112:GLY	C	113:PRO	N	4.20

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1504/1522 (98%)	0.41	163 (10%) 6 2	60, 125, 191, 194	0
1	CA	1504/1522 (98%)	0.42	167 (11%) 6 2	61, 125, 191, 194	0
2	AB	235/256 (91%)	0.30	12 (5%) 27 6	107, 156, 184, 191	0
2	CB	235/256 (91%)	0.49	20 (8%) 11 3	107, 158, 185, 191	0
3	AC	207/239 (86%)	0.24	7 (3%) 43 8	115, 163, 184, 189	0
3	CC	207/239 (86%)	0.76	27 (13%) 4 1	119, 166, 184, 191	0
4	AD	208/209 (99%)	0.28	7 (3%) 43 8	83, 131, 170, 181	0
4	CD	208/209 (99%)	0.22	10 (4%) 29 6	82, 131, 168, 182	0
5	AE	151/162 (93%)	0.35	10 (6%) 18 4	83, 116, 160, 188	0
5	CE	151/162 (93%)	0.38	4 (2%) 53 10	84, 117, 162, 189	0
6	AF	101/101 (100%)	0.05	1 (0%) 79 22	85, 132, 164, 180	0
6	CF	101/101 (100%)	0.05	3 (2%) 48 9	86, 132, 165, 182	0
7	AG	155/156 (99%)	0.70	28 (18%) 2 1	140, 171, 188, 191	0
7	CG	155/156 (99%)	1.49	48 (30%) 1 0	140, 171, 188, 190	0
8	AH	138/138 (100%)	-0.03	2 (1%) 72 18	85, 121, 155, 164	0
8	CH	138/138 (100%)	-0.05	2 (1%) 72 18	85, 123, 156, 162	0
9	AI	127/128 (99%)	1.83	53 (41%) 1 0	142, 182, 190, 192	0
9	CI	127/128 (99%)	1.63	42 (33%) 1 0	143, 183, 190, 191	0
10	AJ	99/105 (94%)	1.97	42 (42%) 1 0	130, 176, 189, 191	0
10	CJ	99/105 (94%)	2.14	46 (46%) 1 0	130, 177, 190, 193	0
11	AK	119/129 (92%)	0.47	8 (6%) 17 4	82, 123, 164, 187	0
11	CK	119/129 (92%)	0.57	10 (8%) 11 3	84, 123, 165, 186	0
12	AL	125/135 (92%)	0.42	9 (7%) 15 4	80, 108, 163, 189	0
12	CL	125/135 (92%)	0.43	6 (4%) 29 6	82, 109, 164, 189	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	115/126 (91%)	2.11	55 (47%) 1 0	150, 185, 190, 193	0
13	CM	115/126 (91%)	1.82	50 (43%) 1 0	149, 185, 190, 192	0
14	AN	60/61 (98%)	0.97	10 (16%) 2 1	131, 168, 185, 189	0
14	CN	60/61 (98%)	0.85	10 (16%) 2 1	132, 170, 186, 189	0
15	AO	88/89 (98%)	-0.07	1 (1%) 77 21	74, 111, 157, 162	0
15	CO	88/89 (98%)	0.23	1 (1%) 77 21	74, 112, 159, 165	0
16	AP	84/88 (95%)	0.80	15 (17%) 2 1	91, 118, 161, 179	0
16	CP	84/88 (95%)	0.77	10 (11%) 5 1	89, 116, 160, 180	0
17	AQ	100/105 (95%)	0.18	5 (5%) 28 6	80, 109, 153, 163	0
17	CQ	100/105 (95%)	0.27	3 (3%) 48 9	85, 110, 153, 159	0
18	AR	70/88 (79%)	0.62	6 (8%) 11 3	93, 121, 170, 183	0
18	CR	70/88 (79%)	1.50	16 (22%) 1 1	93, 122, 171, 183	0
19	AS	79/93 (84%)	1.90	27 (34%) 1 0	142, 186, 190, 191	0
19	CS	79/93 (84%)	1.84	31 (39%) 1 0	142, 186, 191, 192	0
20	AT	99/106 (93%)	0.47	11 (11%) 6 2	84, 119, 157, 177	0
20	CT	99/106 (93%)	0.25	7 (7%) 16 4	84, 119, 157, 179	0
21	AU	25/27 (92%)	2.55	14 (56%) 0 0	143, 174, 188, 190	0
21	CU	25/27 (92%)	2.55	15 (60%) 0 0	141, 172, 188, 189	0
22	B0	85/85 (100%)	0.35	8 (9%) 9 2	49, 70, 175, 187	0
22	D0	85/85 (100%)	0.37	7 (8%) 12 3	54, 74, 173, 188	0
23	B1	89/98 (90%)	0.09	1 (1%) 77 21	50, 79, 150, 187	0
23	D1	89/98 (90%)	0.16	3 (3%) 43 8	51, 81, 151, 190	0
24	B2	51/72 (70%)	0.55	5 (9%) 8 2	59, 99, 175, 186	0
24	D2	51/72 (70%)	0.47	7 (13%) 4 1	62, 100, 175, 188	0
25	B3	60/60 (100%)	-0.19	1 (1%) 67 15	46, 69, 132, 168	0
25	D3	60/60 (100%)	0.34	2 (3%) 44 8	51, 72, 136, 161	0
26	B4	32/71 (45%)	-0.23	0 100 100	133, 161, 182, 184	0
26	D4	32/71 (45%)	0.10	2 (6%) 19 5	133, 164, 182, 186	0
27	B5	58/60 (96%)	0.04	3 (5%) 26 6	34, 61, 165, 188	0
27	D5	58/60 (96%)	0.00	4 (6%) 17 4	39, 63, 163, 190	0
28	B6	45/54 (83%)	0.38	1 (2%) 59 12	49, 85, 141, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	D6	45/54 (83%)	0.57	5 (11%) 6 2	52, 87, 142, 172	0
29	B7	49/49 (100%)	0.39	4 (8%) 12 3	36, 45, 119, 172	0
29	D7	49/49 (100%)	0.43	5 (10%) 7 2	38, 49, 120, 173	0
30	B8	64/65 (98%)	0.14	2 (3%) 47 9	46, 68, 140, 165	0
30	D8	64/65 (98%)	0.14	1 (1%) 68 16	49, 73, 141, 169	0
31	BA	2725/2787 (97%)	-0.20	51 (1%) 64 13	33, 59, 153, 194	0
31	DA	2725/2787 (97%)	-0.31	92 (3%) 43 8	38, 64, 157, 194	0
32	BB	119/122 (97%)	0.02	5 (4%) 35 7	50, 101, 149, 184	0
32	DB	119/122 (97%)	0.20	7 (5%) 22 5	59, 105, 157, 184	0
33	BD	272/276 (98%)	-0.20	1 (0%) 90 41	37, 62, 120, 168	0
33	DD	272/276 (98%)	-0.15	4 (1%) 70 16	40, 65, 122, 165	0
34	BE	205/206 (99%)	-0.04	4 (1%) 62 12	36, 65, 153, 181	0
34	DE	205/206 (99%)	0.01	6 (2%) 49 9	40, 69, 154, 182	0
35	BF	208/210 (99%)	0.04	8 (3%) 38 7	35, 77, 175, 189	0
35	DF	208/210 (99%)	0.19	7 (3%) 43 8	39, 79, 176, 188	0
36	BG	181/182 (99%)	0.68	23 (12%) 4 1	100, 152, 186, 192	0
36	DG	181/182 (99%)	1.19	44 (24%) 1 1	106, 159, 189, 191	0
37	BH	160/180 (88%)	0.07	1 (0%) 86 32	69, 111, 151, 182	0
37	DH	160/180 (88%)	0.50	15 (9%) 9 2	74, 114, 157, 185	0
38	BI	146/148 (98%)	0.17	3 (2%) 60 12	67, 152, 187, 190	0
38	DI	146/148 (98%)	0.60	13 (8%) 10 3	69, 156, 189, 191	0
39	BN	139/140 (99%)	-0.11	2 (1%) 72 18	45, 75, 143, 182	0
39	DN	139/140 (99%)	-0.18	2 (1%) 72 18	49, 78, 143, 183	0
40	BO	122/122 (100%)	-0.21	0 100 100	45, 67, 123, 147	0
40	DO	122/122 (100%)	-0.42	0 100 100	48, 69, 125, 149	0
41	BP	146/150 (97%)	0.29	8 (5%) 24 5	29, 93, 149, 190	0
41	DP	146/150 (97%)	0.24	5 (3%) 43 8	38, 95, 152, 188	0
42	BQ	136/141 (96%)	0.15	5 (3%) 39 8	50, 77, 147, 183	0
42	DQ	136/141 (96%)	0.34	6 (4%) 33 7	52, 79, 147, 183	0
43	BR	117/118 (99%)	-0.13	0 100 100	40, 60, 130, 139	0
43	DR	117/118 (99%)	-0.20	1 (0%) 81 24	42, 62, 131, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BS	99/112 (88%)	0.25	2 (2%) 62 12	54, 111, 148, 165	0
44	DS	99/112 (88%)	0.72	11 (11%) 6 2	62, 113, 154, 170	0
45	BT	132/146 (90%)	0.08	5 (3%) 38 7	55, 87, 154, 181	0
45	DT	132/146 (90%)	0.12	9 (6%) 17 4	58, 90, 156, 179	0
46	BU	117/118 (99%)	0.00	2 (1%) 67 15	40, 62, 124, 176	0
46	DU	117/118 (99%)	0.13	3 (2%) 53 10	44, 67, 130, 175	0
47	BV	101/101 (100%)	0.25	5 (4%) 28 6	38, 103, 176, 189	0
47	DV	101/101 (100%)	0.25	6 (5%) 22 5	44, 109, 177, 188	0
48	BW	113/113 (100%)	-0.32	0 100 100	38, 51, 112, 179	0
48	DW	113/113 (100%)	-0.32	0 100 100	41, 54, 119, 181	0
49	BX	93/96 (96%)	0.03	0 100 100	47, 74, 145, 179	0
49	DX	93/96 (96%)	0.02	1 (1%) 77 21	52, 76, 146, 179	0
50	BY	101/110 (91%)	0.50	10 (9%) 8 2	57, 107, 184, 192	0
50	DY	101/110 (91%)	0.43	9 (8%) 10 3	60, 108, 183, 193	0
51	BZ	177/206 (85%)	0.10	3 (1%) 67 15	68, 113, 158, 169	0
51	DZ	177/206 (85%)	0.24	7 (3%) 36 7	74, 117, 161, 168	0
All	All	20062/20922 (95%)	0.22	1461 (7%) 15 3	29, 99, 187, 194	0

The worst 5 of 1461 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	DA	2802	G	18.9
1	CA	83	U	14.3
1	CA	84	U	13.6
1	AA	89	C	13.5
31	BA	2189	U	12.7

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
52	MG	DA	3279	1/1	0.28	-	64,64,64,64	0
52	MG	DA	3181	1/1	0.24	-	50,50,50,50	0
52	MG	BA	3243	1/1	0.10	-	58,58,58,58	0
52	MG	BA	3112	1/1	0.14	-	43,43,43,43	0
52	MG	DA	3153	1/1	0.56	-	59,59,59,59	0
52	MG	BA	3183	1/1	0.14	-	72,72,72,72	0
52	MG	DA	3239	1/1	0.08	-	59,59,59,59	0
52	MG	BA	3050	1/1	0.24	-	38,38,38,38	0
52	MG	DA	3070	1/1	0.59	-	74,74,74,74	0
52	MG	AA	1639	1/1	0.24	-	95,95,95,95	0
52	MG	BA	3295	1/1	0.22	-	70,70,70,70	0
52	MG	BA	3227	1/1	0.13	-	39,39,39,39	0
52	MG	BA	3302	1/1	0.20	-	72,72,72,72	0
53	ZN	AN	101	1/1	0.14	-	159,159,159,159	0
52	MG	BA	3333	1/1	0.18	-	80,80,80,80	0
52	MG	BA	3192	1/1	0.33	-	58,58,58,58	0
52	MG	DA	3225	1/1	0.14	-	54,54,54,54	0
52	MG	BA	3131	1/1	0.20	-	45,45,45,45	0
52	MG	BA	3343	1/1	0.47	-	58,58,58,58	0
52	MG	BP	202	1/1	0.26	-	58,58,58,58	0
52	MG	DA	3044	1/1	0.33	-	46,46,46,46	0
52	MG	BA	3034	1/1	0.26	-	62,62,62,62	0
52	MG	DA	3133	1/1	0.60	-	53,53,53,53	0
52	MG	B1	101	1/1	0.29	-	39,39,39,39	0
52	MG	DA	3085	1/1	0.28	-	54,54,54,54	0
52	MG	BA	3244	1/1	0.26	-	40,40,40,40	0
52	MG	DR	201	1/1	0.28	-	43,43,43,43	0
52	MG	DA	3302	1/1	0.70	-	86,86,86,86	0
52	MG	DA	3261	1/1	0.53	-	95,95,95,95	0
52	MG	BA	3260	1/1	0.36	-	42,42,42,42	0
52	MG	BA	3312	1/1	0.61	-	87,87,87,87	0
52	MG	BA	3325	1/1	0.36	-	43,43,43,43	0
52	MG	BA	3096	1/1	0.27	-	55,55,55,55	0
52	MG	AA	1627	1/1	0.41	-	66,66,66,66	0
52	MG	BA	3029	1/1	0.20	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	BE	301	1/1	0.42	-	29,29,29,29	0
52	MG	BA	3160	1/1	0.36	-	39,39,39,39	0
52	MG	BA	3107	1/1	0.15	-	34,34,34,34	0
52	MG	DA	3144	1/1	0.38	-	47,47,47,47	0
52	MG	DA	3287	1/1	0.12	-	51,51,51,51	0
52	MG	DA	3006	1/1	0.40	-	39,39,39,39	0
52	MG	D0	101	1/1	0.15	-	62,62,62,62	0
52	MG	BA	3080	1/1	0.49	-	34,34,34,34	0
52	MG	DA	3207	1/1	0.78	-	78,78,78,78	0
52	MG	DA	3146	1/1	0.32	-	69,69,69,69	0
52	MG	BA	3124	1/1	0.16	-	42,42,42,42	0
52	MG	DA	3027	1/1	0.39	-	61,61,61,61	0
52	MG	CA	1616	1/1	0.52	-	73,73,73,73	0
52	MG	BU	201	1/1	0.28	-	26,26,26,26	0
52	MG	BA	3013	1/1	0.33	-	21,21,21,21	0
52	MG	DA	3149	1/1	0.17	-	55,55,55,55	0
52	MG	AA	1626	1/1	0.46	-	76,76,76,76	0
52	MG	CA	1618	1/1	0.32	-	62,62,62,62	0
52	MG	BA	3309	1/1	0.89	-	61,61,61,61	0
52	MG	DA	3115	1/1	0.39	-	72,72,72,72	0
52	MG	AA	1651	1/1	0.27	-	75,75,75,75	0
52	MG	BA	3041	1/1	0.33	-	29,29,29,29	0
52	MG	DA	3136	1/1	0.47	-	59,59,59,59	0
52	MG	BA	3042	1/1	0.26	-	15,15,15,15	0
52	MG	BA	3119	1/1	0.24	-	52,52,52,52	0
52	MG	BA	3091	1/1	0.24	-	9,9,9,9	0
52	MG	BA	3225	1/1	0.23	-	33,33,33,33	0
52	MG	BF	301	1/1	0.18	-	62,62,62,62	0
52	MG	CA	1602	1/1	0.38	-	70,70,70,70	0
52	MG	BP	203	1/1	0.10	-	0,0,0,0	0
52	MG	DA	3248	1/1	0.34	-	74,74,74,74	0
52	MG	BA	3266	1/1	0.32	-	35,35,35,35	0
52	MG	DA	3180	1/1	0.45	-	52,52,52,52	0
52	MG	AA	1636	1/1	0.17	-	63,63,63,63	0
52	MG	BA	3222	1/1	0.23	-	23,23,23,23	0
52	MG	BA	3289	1/1	0.20	-	55,55,55,55	0
52	MG	BA	3231	1/1	0.59	-	52,52,52,52	0
52	MG	BA	3171	1/1	0.29	-	62,62,62,62	0
52	MG	CA	1603	1/1	0.46	-	63,63,63,63	0
52	MG	DA	3094	1/1	0.33	-	56,56,56,56	0
52	MG	BA	3338	1/1	0.20	-	73,73,73,73	0
52	MG	BA	3003	1/1	0.34	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	DA	3083	1/1	0.23	-	47,47,47,47	0
52	MG	DA	3139	1/1	0.38	-	68,68,68,68	0
52	MG	BA	3173	1/1	0.32	-	24,24,24,24	0
52	MG	DA	3137	1/1	0.40	-	38,38,38,38	0
52	MG	DA	3011	1/1	0.51	-	50,50,50,50	0
52	MG	BA	3300	1/1	0.26	-	59,59,59,59	0
52	MG	BA	3202	1/1	0.28	-	41,41,41,41	0
52	MG	DA	3292	1/1	0.58	-	75,75,75,75	0
52	MG	BA	3340	1/1	0.34	-	62,62,62,62	0
52	MG	BA	3102	1/1	0.26	-	24,24,24,24	0
52	MG	CA	1642	1/1	0.29	-	62,62,62,62	0
52	MG	DA	3198	1/1	0.79	-	70,70,70,70	0
52	MG	BA	3035	1/1	0.23	-	21,21,21,21	0
52	MG	DA	3269	1/1	0.13	-	61,61,61,61	0
52	MG	AA	1609	1/1	0.25	-	51,51,51,51	0
52	MG	BA	3327	1/1	0.24	-	47,47,47,47	0
52	MG	DA	3201	1/1	0.32	-	59,59,59,59	0
52	MG	AA	1625	1/1	0.17	-	73,73,73,73	0
52	MG	DA	3039	1/1	0.31	-	43,43,43,43	0
52	MG	DA	3134	1/1	0.51	-	47,47,47,47	0
52	MG	DA	3105	1/1	0.25	-	47,47,47,47	0
52	MG	DA	3275	1/1	0.38	-	62,62,62,62	0
52	MG	BA	3118	1/1	0.28	-	59,59,59,59	0
52	MG	BA	3264	1/1	0.18	-	35,35,35,35	0
52	MG	DA	3293	1/1	0.09	-	53,53,53,53	0
52	MG	DA	3212	1/1	0.10	-	68,68,68,68	0
52	MG	DA	3126	1/1	0.19	-	73,73,73,73	0
52	MG	DA	3024	1/1	0.41	-	61,61,61,61	0
52	MG	DA	3067	1/1	0.28	-	81,81,81,81	0
52	MG	DA	3259	1/1	0.57	-	74,74,74,74	0
52	MG	BA	3182	1/1	0.58	-	68,68,68,68	0
52	MG	DB	203	1/1	0.46	-	56,56,56,56	0
52	MG	DA	3195	1/1	0.51	-	56,56,56,56	0
52	MG	DA	3232	1/1	0.32	-	72,72,72,72	0
52	MG	DA	3267	1/1	0.51	-	72,72,72,72	0
52	MG	BA	3223	1/1	0.53	-	36,36,36,36	0
52	MG	DA	3012	1/1	0.32	-	23,23,23,23	0
52	MG	BA	3046	1/1	0.17	-	37,37,37,37	0
52	MG	BA	3026	1/1	0.10	-	49,49,49,49	0
52	MG	BA	3334	1/1	0.28	-	53,53,53,53	0
52	MG	BA	3033	1/1	0.09	-	20,20,20,20	0
52	MG	BA	3208	1/1	0.10	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	BA	3108	1/1	0.38	-	56,56,56,56	0
52	MG	DA	3242	1/1	0.25	-	69,69,69,69	0
52	MG	DA	3154	1/1	0.65	-	62,62,62,62	0
52	MG	DA	3204	1/1	0.37	-	45,45,45,45	0
52	MG	DA	3305	1/1	0.33	-	76,76,76,76	0
52	MG	DA	3141	1/1	0.41	-	61,61,61,61	0
52	MG	BA	3299	1/1	0.45	-	58,58,58,58	0
52	MG	BA	3234	1/1	0.38	-	45,45,45,45	0
52	MG	BA	3104	1/1	0.36	-	37,37,37,37	0
52	MG	DA	3037	1/1	0.66	-	74,74,74,74	0
52	MG	DA	3074	1/1	0.21	-	53,53,53,53	0
52	MG	AA	1632	1/1	0.58	-	72,72,72,72	0
52	MG	BA	3094	1/1	0.37	-	52,52,52,52	0
52	MG	DA	3065	1/1	0.20	-	49,49,49,49	0
52	MG	DX	101	1/1	0.28	-	77,77,77,77	0
52	MG	BA	3067	1/1	0.56	-	37,37,37,37	0
52	MG	BA	3224	1/1	0.12	-	40,40,40,40	0
52	MG	DA	3295	1/1	0.14	-	88,88,88,88	0
52	MG	DA	3078	1/1	0.65	-	46,46,46,46	0
52	MG	DA	3294	1/1	0.23	-	67,67,67,67	0
52	MG	CA	1636	1/1	0.32	-	79,79,79,79	0
52	MG	AA	1616	1/1	0.19	-	77,77,77,77	0
52	MG	DA	3021	1/1	0.35	-	47,47,47,47	0
52	MG	BB	201	1/1	0.43	-	42,42,42,42	0
52	MG	BA	3166	1/1	0.60	-	39,39,39,39	0
52	MG	DA	3255	1/1	0.44	-	75,75,75,75	0
52	MG	BA	3004	1/1	0.20	-	23,23,23,23	0
52	MG	DA	3174	1/1	0.55	-	63,63,63,63	0
52	MG	BA	3165	1/1	0.56	-	50,50,50,50	0
52	MG	DA	3161	1/1	0.67	-	72,72,72,72	0
52	MG	DB	202	1/1	0.35	-	63,63,63,63	0
52	MG	BA	3246	1/1	0.40	-	75,75,75,75	0
52	MG	DA	3163	1/1	0.47	-	68,68,68,68	0
52	MG	DA	3253	1/1	0.35	-	50,50,50,50	0
52	MG	BA	3011	1/1	0.27	-	7,7,7,7	0
52	MG	AA	1648	1/1	0.75	-	62,62,62,62	0
52	MG	BA	3211	1/1	0.11	-	39,39,39,39	0
52	MG	BA	3137	1/1	0.23	-	61,61,61,61	0
52	MG	DA	3150	1/1	0.51	-	77,77,77,77	0
52	MG	DA	3214	1/1	0.39	-	65,65,65,65	0
52	MG	BA	3261	1/1	0.23	-	38,38,38,38	0
52	MG	DA	3156	1/1	0.38	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	BA	3251	1/1	0.09	-	35,35,35,35	0
52	MG	DA	3303	1/1	0.64	-	49,49,49,49	0
52	MG	DA	3109	1/1	0.41	-	71,71,71,71	0
52	MG	DA	3032	1/1	0.36	-	69,69,69,69	0
52	MG	DA	3009	1/1	0.48	-	54,54,54,54	0
52	MG	DA	3224	1/1	0.08	-	68,68,68,68	0
52	MG	CA	1611	1/1	0.61	-	81,81,81,81	0
52	MG	BA	3235	1/1	0.34	-	72,72,72,72	0
52	MG	CA	1637	1/1	0.92	-	80,80,80,80	0
52	MG	BA	3172	1/1	0.21	-	64,64,64,64	0
52	MG	DA	3030	1/1	0.40	-	42,42,42,42	0
52	MG	DA	3249	1/1	0.73	-	79,79,79,79	0
52	MG	BA	3347	1/1	0.17	-	66,66,66,66	0
52	MG	DA	3005	1/1	0.25	-	73,73,73,73	0
52	MG	DA	3157	1/1	0.48	-	65,65,65,65	0
52	MG	DA	3131	1/1	0.54	-	47,47,47,47	0
52	MG	CA	1614	1/1	0.54	-	76,76,76,76	0
52	MG	DA	3081	1/1	0.28	-	43,43,43,43	0
52	MG	BA	3189	1/1	0.36	-	45,45,45,45	0
52	MG	AA	1603	1/1	0.32	-	62,62,62,62	0
52	MG	BA	3099	1/1	0.19	-	26,26,26,26	0
52	MG	DA	3285	1/1	0.55	-	66,66,66,66	0
52	MG	BA	3316	1/1	0.14	-	56,56,56,56	0
52	MG	BA	3001	1/1	0.33	-	49,49,49,49	0
52	MG	AA	1640	1/1	0.68	-	83,83,83,83	0
52	MG	AA	1645	1/1	0.37	-	81,81,81,81	0
52	MG	DQ	201	1/1	0.27	-	78,78,78,78	0
52	MG	CA	1645	1/1	0.46	-	97,97,97,97	0
52	MG	BA	3257	1/1	0.26	-	48,48,48,48	0
52	MG	BA	3270	1/1	0.14	-	50,50,50,50	0
52	MG	DA	3026	1/1	0.20	-	43,43,43,43	0
52	MG	BA	3282	1/1	0.07	-	67,67,67,67	0
52	MG	DA	3101	1/1	0.35	-	43,43,43,43	0
52	MG	BA	3305	1/1	0.33	-	54,54,54,54	0
52	MG	DA	3098	1/1	0.12	-	49,49,49,49	0
52	MG	DA	3301	1/1	0.26	-	57,57,57,57	0
52	MG	AA	1611	1/1	0.15	-	75,75,75,75	0
52	MG	BA	3037	1/1	0.29	-	14,14,14,14	0
52	MG	DA	3296	1/1	0.11	-	60,60,60,60	0
52	MG	CA	1628	1/1	0.42	-	75,75,75,75	0
52	MG	DA	3108	1/1	0.33	-	48,48,48,48	0
52	MG	DA	3164	1/1	0.15	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	BA	3293	1/1	0.21	-	55,55,55,55	0
52	MG	BA	3337	1/1	0.25	-	58,58,58,58	0
52	MG	BA	3060	1/1	0.36	-	40,40,40,40	0
52	MG	AA	1630	1/1	0.49	-	59,59,59,59	0
52	MG	DA	3092	1/1	0.23	-	61,61,61,61	0
52	MG	BA	3288	1/1	0.43	-	72,72,72,72	0
52	MG	BA	3247	1/1	0.08	-	40,40,40,40	0
52	MG	DA	3168	1/1	0.23	-	53,53,53,53	0
52	MG	DA	3252	1/1	0.49	-	66,66,66,66	0
52	MG	DA	3223	1/1	0.09	-	65,65,65,65	0
52	MG	DA	3142	1/1	0.42	-	41,41,41,41	0
52	MG	DA	3246	1/1	0.23	-	87,87,87,87	0
52	MG	DA	3062	1/1	0.61	-	65,65,65,65	0
52	MG	BA	3197	1/1	0.22	-	52,52,52,52	0
52	MG	DA	3176	1/1	0.20	-	78,78,78,78	0
52	MG	DA	3221	1/1	0.36	-	53,53,53,53	0
52	MG	DA	3140	1/1	0.18	-	49,49,49,49	0
52	MG	BA	3095	1/1	0.44	-	38,38,38,38	0
52	MG	BA	3259	1/1	0.49	-	46,46,46,46	0
52	MG	DA	3299	1/1	0.35	-	66,66,66,66	0
52	MG	BA	3341	1/1	0.67	-	63,63,63,63	0
52	MG	BB	204	1/1	0.51	-	56,56,56,56	0
52	MG	BA	3070	1/1	0.31	-	35,35,35,35	0
52	MG	BA	3322	1/1	0.17	-	20,20,20,20	0
52	MG	BA	3191	1/1	0.67	-	64,64,64,64	0
52	MG	BA	3252	1/1	0.29	-	50,50,50,50	0
52	MG	DA	3203	1/1	0.55	-	67,67,67,67	0
54	K	DA	3310	1/1	0.45	-	106,106,106,106	0
52	MG	DA	3159	1/1	0.46	-	61,61,61,61	0
52	MG	BA	3144	1/1	0.24	-	53,53,53,53	0
52	MG	DA	3231	1/1	0.32	-	79,79,79,79	0
52	MG	BA	3150	1/1	0.39	-	50,50,50,50	0
52	MG	CA	1635	1/1	0.14	-	86,86,86,86	0
52	MG	AA	1623	1/1	0.38	-	54,54,54,54	0
52	MG	BA	3098	1/1	0.28	-	46,46,46,46	0
52	MG	BA	3271	1/1	0.28	-	46,46,46,46	0
52	MG	DA	3119	1/1	0.08	-	64,64,64,64	0
52	MG	DA	3193	1/1	0.37	-	50,50,50,50	0
52	MG	BA	3103	1/1	0.15	-	42,42,42,42	0
52	MG	DA	3283	1/1	0.43	-	72,72,72,72	0
52	MG	DA	3251	1/1	0.37	-	63,63,63,63	0
52	MG	CA	1606	1/1	0.32	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	BA	3314	1/1	0.23	-	56,56,56,56	0
52	MG	BA	3329	1/1	0.69	-	68,68,68,68	0
52	MG	DA	3284	1/1	0.73	-	65,65,65,65	0
52	MG	CA	1605	1/1	0.44	-	61,61,61,61	0
54	K	BA	3350	1/1	0.44	-	95,95,95,95	0
52	MG	BA	3164	1/1	0.25	-	47,47,47,47	0
52	MG	BA	3281	1/1	0.33	-	46,46,46,46	0
52	MG	BA	3114	1/1	0.46	-	56,56,56,56	0
52	MG	DA	3208	1/1	0.67	-	62,62,62,62	0
52	MG	AA	1621	1/1	0.32	-	46,46,46,46	0
52	MG	AA	1617	1/1	0.35	-	64,64,64,64	0
52	MG	BA	3149	1/1	0.12	-	51,51,51,51	0
52	MG	BA	3032	1/1	0.29	-	15,15,15,15	0
52	MG	DA	3093	1/1	0.32	-	64,64,64,64	0
52	MG	DA	3247	1/1	0.62	-	87,87,87,87	0
52	MG	DA	3278	1/1	0.51	-	68,68,68,68	0
52	MG	BA	3006	1/1	0.38	-	29,29,29,29	0
52	MG	BA	3087	1/1	0.44	-	58,58,58,58	0
52	MG	DA	3132	1/1	0.42	-	43,43,43,43	0
52	MG	BA	3221	1/1	0.46	-	40,40,40,40	0
52	MG	DA	3238	1/1	0.44	-	73,73,73,73	0
52	MG	BD	301	1/1	0.16	-	43,43,43,43	0
52	MG	DA	3194	1/1	0.30	-	60,60,60,60	0
52	MG	DA	3013	1/1	0.49	-	77,77,77,77	0
52	MG	DA	3112	1/1	0.31	-	68,68,68,68	0
52	MG	BA	3134	1/1	0.12	-	46,46,46,46	0
52	MG	DA	3004	1/1	0.23	-	49,49,49,49	0
53	ZN	AD	301	1/1	0.29	-	108,108,108,108	0
52	MG	BA	3066	1/1	0.39	-	43,43,43,43	0
52	MG	BA	3122	1/1	0.28	-	40,40,40,40	0
52	MG	DA	3049	1/1	0.33	-	35,35,35,35	0
52	MG	BA	3328	1/1	0.18	-	65,65,65,65	0
52	MG	BA	3278	1/1	0.22	-	41,41,41,41	0
52	MG	DA	3125	1/1	0.63	-	58,58,58,58	0
52	MG	BA	3061	1/1	0.14	-	23,23,23,23	0
52	MG	BA	3057	1/1	0.34	-	44,44,44,44	0
52	MG	DA	3190	1/1	0.39	-	63,63,63,63	0
52	MG	BA	3238	1/1	0.44	-	49,49,49,49	0
52	MG	BA	3175	1/1	0.11	-	49,49,49,49	0
52	MG	BA	3344	1/1	0.60	-	48,48,48,48	0
52	MG	DA	3250	1/1	0.13	-	75,75,75,75	0
52	MG	BA	3051	1/1	0.29	-	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	DA	3281	1/1	0.16	-	30,30,30,30	0
52	MG	DA	3217	1/1	0.64	-	62,62,62,62	0
52	MG	CA	1627	1/1	0.09	-	66,66,66,66	0
52	MG	BA	3136	1/1	0.47	-	32,32,32,32	0
52	MG	BA	3321	1/1	0.42	-	75,75,75,75	0
52	MG	CA	1609	1/1	0.19	-	94,94,94,94	0
52	MG	BA	3254	1/1	0.23	-	53,53,53,53	0
52	MG	DA	3076	1/1	0.25	-	55,55,55,55	0
52	MG	BA	3019	1/1	0.37	-	24,24,24,24	0
52	MG	DA	3151	1/1	0.51	-	72,72,72,72	0
52	MG	DA	3002	1/1	0.37	-	38,38,38,38	0
52	MG	BB	203	1/1	0.28	-	41,41,41,41	0
52	MG	DA	3158	1/1	0.18	-	61,61,61,61	0
52	MG	AA	1646	1/1	0.68	-	82,82,82,82	0
52	MG	BA	3068	1/1	0.31	-	54,54,54,54	0
52	MG	BQ	201	1/1	0.17	-	32,32,32,32	0
52	MG	BA	3198	1/1	0.43	-	44,44,44,44	0
52	MG	BA	3180	1/1	0.47	-	64,64,64,64	0
52	MG	DA	3084	1/1	0.16	-	54,54,54,54	0
52	MG	BA	3017	1/1	0.37	-	32,32,32,32	0
52	MG	BA	3237	1/1	0.40	-	61,61,61,61	0
52	MG	BA	3151	1/1	0.22	-	74,74,74,74	0
52	MG	BA	3040	1/1	0.69	-	51,51,51,51	0
52	MG	BX	101	1/1	0.25	-	61,61,61,61	0
52	MG	DA	3075	1/1	0.50	-	55,55,55,55	0
52	MG	DA	3178	1/1	0.33	-	65,65,65,65	0
52	MG	BA	3097	1/1	0.25	-	70,70,70,70	0
52	MG	CA	1601	1/1	0.19	-	83,83,83,83	0
52	MG	BA	3074	1/1	0.46	-	36,36,36,36	0
52	MG	BA	3143	1/1	0.37	-	30,30,30,30	0
52	MG	AA	1635	1/1	0.59	-	63,63,63,63	0
52	MG	DA	3008	1/1	0.34	-	52,52,52,52	0
52	MG	DB	201	1/1	0.38	-	52,52,52,52	0
52	MG	DA	3053	1/1	0.55	-	51,51,51,51	0
52	MG	BA	3267	1/1	0.35	-	38,38,38,38	0
52	MG	BA	3217	1/1	0.43	-	50,50,50,50	0
52	MG	BA	3081	1/1	0.19	-	37,37,37,37	0
52	MG	CA	1631	1/1	0.75	-	70,70,70,70	0
52	MG	AA	1606	1/1	0.56	-	73,73,73,73	0
52	MG	DA	3016	1/1	0.46	-	56,56,56,56	0
52	MG	BA	3342	1/1	0.21	-	49,49,49,49	0
52	MG	BA	3127	1/1	0.15	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	BA	3159	1/1	0.44	-	45,45,45,45	0
52	MG	BA	3190	1/1	0.30	-	53,53,53,53	0
52	MG	DA	3061	1/1	0.21	-	57,57,57,57	0
52	MG	BB	205	1/1	0.24	-	78,78,78,78	0
52	MG	BA	3024	1/1	0.18	-	2,2,2,2	0
52	MG	BA	3007	1/1	0.51	-	48,48,48,48	0
52	MG	CA	1646	1/1	0.51	-	80,80,80,80	0
52	MG	BA	3079	1/1	0.31	-	0,0,0,0	0
52	MG	DA	3188	1/1	0.23	-	48,48,48,48	0
52	MG	AA	1629	1/1	0.56	-	67,67,67,67	0
52	MG	BA	3196	1/1	0.19	-	65,65,65,65	0
52	MG	BA	3276	1/1	0.35	-	55,55,55,55	0
52	MG	DA	3104	1/1	0.54	-	48,48,48,48	0
52	MG	BA	3280	1/1	0.30	-	75,75,75,75	0
52	MG	DA	3057	1/1	0.47	-	40,40,40,40	0
52	MG	DA	3291	1/1	1.03	-	86,86,86,86	0
52	MG	DA	3096	1/1	0.35	-	45,45,45,45	0
52	MG	BR	201	1/1	0.25	-	20,20,20,20	0
52	MG	BA	3232	1/1	0.36	-	70,70,70,70	0
52	MG	BA	3248	1/1	0.10	-	47,47,47,47	0
52	MG	BA	3053	1/1	0.36	-	15,15,15,15	0
52	MG	BA	3200	1/1	0.86	-	59,59,59,59	0
52	MG	BA	3002	1/1	0.23	-	20,20,20,20	0
52	MG	BA	3012	1/1	0.29	-	22,22,22,22	0
52	MG	BA	3206	1/1	0.47	-	29,29,29,29	0
52	MG	DA	3001	1/1	0.39	-	76,76,76,76	0
52	MG	DA	3233	1/1	0.45	-	68,68,68,68	0
52	MG	DA	3033	1/1	0.36	-	44,44,44,44	0
52	MG	BA	3331	1/1	0.43	-	46,46,46,46	0
52	MG	DA	3270	1/1	0.62	-	65,65,65,65	0
52	MG	AA	1610	1/1	0.49	-	65,65,65,65	0
52	MG	BA	3241	1/1	0.46	-	79,79,79,79	0
52	MG	BA	3162	1/1	0.15	-	47,47,47,47	0
52	MG	BA	3209	1/1	0.49	-	56,56,56,56	0
52	MG	DA	3082	1/1	0.18	-	17,17,17,17	0
52	MG	DA	3243	1/1	0.34	-	70,70,70,70	0
52	MG	BA	3157	1/1	0.66	-	74,74,74,74	0
52	MG	DA	3286	1/1	0.55	-	58,58,58,58	0
52	MG	DA	3169	1/1	0.78	-	51,51,51,51	0
52	MG	BA	3015	1/1	0.30	-	48,48,48,48	0
52	MG	DA	3069	1/1	0.48	-	51,51,51,51	0
52	MG	BA	3291	1/1	0.53	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	DA	3017	1/1	0.28	-	47,47,47,47	0
52	MG	DA	3191	1/1	0.20	-	91,91,91,91	0
52	MG	DA	3048	1/1	0.19	-	40,40,40,40	0
52	MG	CA	1622	1/1	0.25	-	78,78,78,78	0
52	MG	BA	3273	1/1	0.48	-	58,58,58,58	0
52	MG	DA	3192	1/1	0.51	-	55,55,55,55	0
52	MG	DA	3114	1/1	0.31	-	65,65,65,65	0
52	MG	BA	3121	1/1	0.36	-	57,57,57,57	0
52	MG	BA	3274	1/1	0.19	-	81,81,81,81	0
52	MG	DA	3300	1/1	0.09	-	75,75,75,75	0
52	MG	DA	3095	1/1	0.51	-	53,53,53,53	0
52	MG	BA	3139	1/1	0.27	-	24,24,24,24	0
52	MG	BA	3021	1/1	0.27	-	16,16,16,16	0
52	MG	DA	3185	1/1	0.42	-	61,61,61,61	0
52	MG	BA	3049	1/1	0.56	-	41,41,41,41	0
52	MG	BA	3249	1/1	0.22	-	40,40,40,40	0
52	MG	DA	3066	1/1	0.49	-	60,60,60,60	0
52	MG	DA	3129	1/1	0.16	-	87,87,87,87	0
52	MG	CA	1644	1/1	0.48	-	74,74,74,74	0
52	MG	DA	3290	1/1	0.33	-	52,52,52,52	0
52	MG	DA	3135	1/1	0.18	-	71,71,71,71	0
52	MG	AA	1649	1/1	0.47	-	86,86,86,86	0
52	MG	BA	3083	1/1	0.17	-	5,5,5,5	0
52	MG	DA	3241	1/1	0.24	-	60,60,60,60	0
52	MG	DA	3256	1/1	0.20	-	57,57,57,57	0
52	MG	DA	3187	1/1	0.17	-	52,52,52,52	0
52	MG	BA	3148	1/1	0.34	-	58,58,58,58	0
52	MG	BA	3170	1/1	0.37	-	69,69,69,69	0
52	MG	BA	3141	1/1	0.42	-	27,27,27,27	0
52	MG	CA	1630	1/1	0.27	-	77,77,77,77	0
52	MG	DA	3199	1/1	0.26	-	47,47,47,47	0
52	MG	DA	3218	1/1	0.20	-	78,78,78,78	0
52	MG	DA	3276	1/1	0.09	-	70,70,70,70	0
52	MG	B0	101	1/1	0.09	-	34,34,34,34	0
52	MG	BA	3220	1/1	0.43	-	27,27,27,27	0
52	MG	BA	3069	1/1	0.23	-	18,18,18,18	0
52	MG	DA	3107	1/1	0.38	-	38,38,38,38	0
52	MG	DA	3055	1/1	0.36	-	42,42,42,42	0
52	MG	DA	3215	1/1	0.41	-	59,59,59,59	0
52	MG	DA	3110	1/1	0.40	-	73,73,73,73	0
52	MG	DA	3306	1/1	0.38	-	87,87,87,87	0
52	MG	AA	1647	1/1	0.37	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	BA	3167	1/1	0.58	-	52,52,52,52	0
52	MG	BA	3115	1/1	0.25	-	49,49,49,49	0
52	MG	BA	3014	1/1	0.38	-	32,32,32,32	0
52	MG	DA	3117	1/1	0.09	-	59,59,59,59	0
52	MG	DA	3160	1/1	0.29	-	59,59,59,59	0
52	MG	DA	3019	1/1	0.27	-	42,42,42,42	0
52	MG	BA	3207	1/1	0.17	-	23,23,23,23	0
52	MG	B5	101	1/1	0.22	-	27,27,27,27	0
52	MG	BA	3084	1/1	0.09	-	14,14,14,14	0
52	MG	BA	3303	1/1	0.53	-	68,68,68,68	0
52	MG	AA	1637	1/1	0.31	-	69,69,69,69	0
52	MG	BA	3213	1/1	0.44	-	32,32,32,32	0
52	MG	CA	1624	1/1	0.42	-	65,65,65,65	0
52	MG	BA	3152	1/1	0.29	-	61,61,61,61	0
52	MG	BA	3027	1/1	0.44	-	42,42,42,42	0
52	MG	BA	3219	1/1	0.11	-	38,38,38,38	0
52	MG	DA	3189	1/1	0.49	-	63,63,63,63	0
52	MG	BA	3078	1/1	0.18	-	34,34,34,34	0
52	MG	BA	3292	1/1	0.73	-	60,60,60,60	0
52	MG	BA	3239	1/1	0.23	-	48,48,48,48	0
52	MG	BA	3228	1/1	0.65	-	69,69,69,69	0
52	MG	DA	3077	1/1	0.68	-	49,49,49,49	0
52	MG	CA	1610	1/1	0.26	-	61,61,61,61	0
52	MG	BA	3052	1/1	0.29	-	15,15,15,15	0
52	MG	BA	3256	1/1	0.31	-	63,63,63,63	0
52	MG	BA	3088	1/1	0.17	-	10,10,10,10	0
52	MG	DA	3184	1/1	0.37	-	63,63,63,63	0
52	MG	BA	3023	1/1	0.32	-	34,34,34,34	0
52	MG	DA	3227	1/1	0.26	-	74,74,74,74	0
52	MG	BA	3345	1/1	0.28	-	60,60,60,60	0
52	MG	DA	3102	1/1	0.24	-	80,80,80,80	0
52	MG	BA	3326	1/1	0.34	-	54,54,54,54	0
52	MG	BA	3204	1/1	0.18	-	46,46,46,46	0
52	MG	DA	3064	1/1	0.40	-	68,68,68,68	0
52	MG	DA	3219	1/1	0.44	-	75,75,75,75	0
52	MG	BA	3048	1/1	0.40	-	30,30,30,30	0
52	MG	BA	3075	1/1	0.17	-	26,26,26,26	0
55	ZIT	BA	3351	52/52	0.33	-	100,100,100,100	0
52	MG	DA	3073	1/1	0.24	-	42,42,42,42	0
52	MG	BA	3117	1/1	0.38	-	39,39,39,39	0
52	MG	AA	1644	1/1	1.19	-	99,99,99,99	0
52	MG	AA	1604	1/1	0.57	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	BA	3072	1/1	0.28	-	24,24,24,24	0
52	MG	BA	3307	1/1	0.49	-	76,76,76,76	0
52	MG	DP	201	1/1	0.19	-	50,50,50,50	0
52	MG	DA	3289	1/1	0.36	-	92,92,92,92	0
52	MG	DA	3210	1/1	0.23	-	63,63,63,63	0
52	MG	BA	3128	1/1	0.26	-	54,54,54,54	0
52	MG	BA	3301	1/1	0.12	-	57,57,57,57	0
52	MG	DA	3058	1/1	0.22	-	58,58,58,58	0
52	MG	BA	3154	1/1	0.20	-	32,32,32,32	0
52	MG	DA	3029	1/1	0.26	-	87,87,87,87	0
52	MG	DD	301	1/1	0.27	-	35,35,35,35	0
52	MG	BA	3195	1/1	0.61	-	58,58,58,58	0
52	MG	BA	3110	1/1	0.42	-	45,45,45,45	0
52	MG	DA	3209	1/1	0.46	-	59,59,59,59	0
52	MG	BA	3076	1/1	0.24	-	43,43,43,43	0
52	MG	BA	3287	1/1	0.40	-	58,58,58,58	0
52	MG	B7	101	1/1	0.14	-	37,37,37,37	0
52	MG	AA	1619	1/1	0.39	-	56,56,56,56	0
52	MG	BA	3028	1/1	0.32	-	28,28,28,28	0
52	MG	CA	1619	1/1	0.32	-	75,75,75,75	0
52	MG	BA	3332	1/1	0.28	-	61,61,61,61	0
52	MG	DA	3097	1/1	0.30	-	44,44,44,44	0
52	MG	DA	3205	1/1	0.46	-	54,54,54,54	0
52	MG	DA	3118	1/1	0.11	-	66,66,66,66	0
52	MG	BA	3285	1/1	0.49	-	57,57,57,57	0
52	MG	DA	3080	1/1	0.43	-	40,40,40,40	0
52	MG	AA	1631	1/1	0.12	-	60,60,60,60	0
52	MG	DA	3130	1/1	0.30	-	43,43,43,43	0
52	MG	DA	3271	1/1	0.15	-	46,46,46,46	0
52	MG	DA	3086	1/1	0.43	-	38,38,38,38	0
52	MG	BA	3005	1/1	0.36	-	47,47,47,47	0
52	MG	BA	3205	1/1	0.36	-	55,55,55,55	0
52	MG	BA	3324	1/1	0.44	-	59,59,59,59	0
52	MG	BA	3242	1/1	0.14	-	48,48,48,48	0
52	MG	DA	3268	1/1	1.42	-	81,81,81,81	0
52	MG	BA	3330	1/1	0.83	-	71,71,71,71	0
52	MG	AA	1650	1/1	0.43	-	68,68,68,68	0
52	MG	BA	3258	1/1	0.32	-	61,61,61,61	0
52	MG	AA	1638	1/1	0.32	-	82,82,82,82	0
52	MG	BA	3038	1/1	0.42	-	25,25,25,25	0
52	MG	BA	3065	1/1	0.31	-	32,32,32,32	0
52	MG	DE	301	1/1	0.29	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	DA	3182	1/1	0.22	-	55,55,55,55	0
52	MG	BA	3156	1/1	0.41	-	53,53,53,53	0
52	MG	BA	3030	1/1	0.22	-	17,17,17,17	0
52	MG	DA	3254	1/1	0.11	-	65,65,65,65	0
52	MG	DA	3235	1/1	0.23	-	79,79,79,79	0
52	MG	AA	1622	1/1	0.51	-	75,75,75,75	0
52	MG	CA	1639	1/1	0.17	-	64,64,64,64	0
52	MG	DA	3015	1/1	0.33	-	23,23,23,23	0
52	MG	CA	1607	1/1	0.46	-	82,82,82,82	0
52	MG	DA	3155	1/1	0.16	-	62,62,62,62	0
52	MG	BA	3185	1/1	0.27	-	14,14,14,14	0
52	MG	BA	3111	1/1	0.12	-	19,19,19,19	0
52	MG	BA	3086	1/1	0.16	-	18,18,18,18	0
52	MG	BA	3179	1/1	0.14	-	59,59,59,59	0
52	MG	BA	3348	1/1	0.09	-	61,61,61,61	0
52	MG	DA	3047	1/1	0.48	-	45,45,45,45	0
52	MG	DA	3222	1/1	0.75	-	67,67,67,67	0
52	MG	DA	3197	1/1	0.47	-	75,75,75,75	0
52	MG	DA	3272	1/1	0.16	-	74,74,74,74	0
52	MG	DA	3213	1/1	0.43	-	36,36,36,36	0
52	MG	BA	3236	1/1	0.31	-	70,70,70,70	0
52	MG	DA	3035	1/1	0.77	-	54,54,54,54	0
52	MG	BA	3311	1/1	0.33	-	46,46,46,46	0
52	MG	DA	3266	1/1	0.37	-	75,75,75,75	0
52	MG	BA	3055	1/1	0.24	-	19,19,19,19	0
52	MG	BA	3092	1/1	0.61	-	52,52,52,52	0
52	MG	BA	3193	1/1	0.23	-	28,28,28,28	0
52	MG	BQ	202	1/1	0.26	-	59,59,59,59	0
52	MG	DA	3200	1/1	0.31	-	50,50,50,50	0
52	MG	BA	3313	1/1	0.42	-	54,54,54,54	0
52	MG	DA	3170	1/1	0.44	-	53,53,53,53	0
52	MG	DA	3240	1/1	0.45	-	89,89,89,89	0
52	MG	DA	3298	1/1	0.61	-	71,71,71,71	0
52	MG	DA	3103	1/1	0.70	-	70,70,70,70	0
52	MG	DA	3059	1/1	0.38	-	53,53,53,53	0
52	MG	DA	3138	1/1	0.38	-	50,50,50,50	0
52	MG	BA	3018	1/1	0.14	-	26,26,26,26	0
52	MG	DA	3056	1/1	0.29	-	60,60,60,60	0
52	MG	BA	3116	1/1	0.19	-	51,51,51,51	0
52	MG	AA	1628	1/1	0.51	-	66,66,66,66	0
52	MG	BA	3064	1/1	0.21	-	28,28,28,28	0
52	MG	BA	3100	1/1	0.27	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	D1	101	1/1	0.29	-	50,50,50,50	0
52	MG	DA	3010	1/1	0.36	-	31,31,31,31	0
52	MG	BA	3020	1/1	0.39	-	38,38,38,38	0
52	MG	BA	3168	1/1	0.06	-	43,43,43,43	0
52	MG	BA	3294	1/1	0.50	-	65,65,65,65	0
52	MG	DA	3309	1/1	0.16	-	84,84,84,84	0
52	MG	DA	3127	1/1	0.41	-	35,35,35,35	0
52	MG	CA	1643	1/1	0.73	-	62,62,62,62	0
52	MG	BA	3297	1/1	0.16	-	61,61,61,61	0
52	MG	BA	3130	1/1	0.22	-	26,26,26,26	0
52	MG	DA	3054	1/1	0.35	-	36,36,36,36	0
52	MG	BA	3089	1/1	0.35	-	26,26,26,26	0
52	MG	DA	3100	1/1	0.64	-	50,50,50,50	0
52	MG	BA	3194	1/1	0.49	-	44,44,44,44	0
52	MG	DA	3230	1/1	0.23	-	56,56,56,56	0
52	MG	BA	3031	1/1	0.34	-	77,77,77,77	0
52	MG	BA	3043	1/1	0.15	-	36,36,36,36	0
52	MG	DA	3121	1/1	0.13	-	37,37,37,37	0
52	MG	DA	3179	1/1	0.83	-	77,77,77,77	0
52	MG	DA	3166	1/1	0.35	-	46,46,46,46	0
52	MG	DA	3262	1/1	0.40	-	77,77,77,77	0
52	MG	DA	3196	1/1	0.24	-	51,51,51,51	0
52	MG	BA	3153	1/1	0.45	-	25,25,25,25	0
52	MG	BA	3216	1/1	0.40	-	43,43,43,43	0
52	MG	DA	3244	1/1	0.24	-	86,86,86,86	0
52	MG	BA	3009	1/1	0.35	-	38,38,38,38	0
52	MG	BA	3123	1/1	0.39	-	22,22,22,22	0
52	MG	BA	3323	1/1	0.30	-	64,64,64,64	0
52	MG	BA	3016	1/1	0.27	-	21,21,21,21	0
52	MG	AA	1612	1/1	0.29	-	66,66,66,66	0
52	MG	DA	3237	1/1	0.21	-	53,53,53,53	0
52	MG	DA	3245	1/1	0.15	-	78,78,78,78	0
52	MG	BP	201	1/1	0.21	-	13,13,13,13	0
52	MG	BA	3133	1/1	0.49	-	35,35,35,35	0
52	MG	DA	3116	1/1	0.54	-	41,41,41,41	0
52	MG	DA	3007	1/1	0.33	-	39,39,39,39	0
52	MG	DA	3288	1/1	0.19	-	72,72,72,72	0
52	MG	BA	3071	1/1	0.42	-	47,47,47,47	0
52	MG	BA	3284	1/1	0.27	-	71,71,71,71	0
52	MG	DA	3087	1/1	0.27	-	55,55,55,55	0
52	MG	D5	102	1/1	0.57	-	79,79,79,79	0
52	MG	CA	1613	1/1	0.17	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	DA	3265	1/1	1.07	-	79,79,79,79	0
52	MG	DA	3206	1/1	0.15	-	48,48,48,48	0
52	MG	CA	1633	1/1	1.26	-	87,87,87,87	0
52	MG	BA	3310	1/1	0.15	-	47,47,47,47	0
52	MG	BA	3025	1/1	0.31	-	54,54,54,54	0
52	MG	DA	3229	1/1	0.15	-	45,45,45,45	0
52	MG	DA	3173	1/1	0.37	-	65,65,65,65	0
52	MG	BA	3298	1/1	0.33	-	61,61,61,61	0
52	MG	AA	1602	1/1	0.41	-	37,37,37,37	0
52	MG	BA	3073	1/1	0.38	-	53,53,53,53	0
52	MG	BA	3169	1/1	0.33	-	46,46,46,46	0
52	MG	BA	3214	1/1	0.48	-	66,66,66,66	0
52	MG	BA	3125	1/1	0.18	-	46,46,46,46	0
52	MG	BA	3203	1/1	0.35	-	35,35,35,35	0
52	MG	BA	3146	1/1	0.49	-	42,42,42,42	0
53	ZN	CD	301	1/1	0.24	-	93,93,93,93	0
52	MG	BA	3306	1/1	0.22	-	56,56,56,56	0
52	MG	BA	3174	1/1	0.61	-	57,57,57,57	0
52	MG	CA	1632	1/1	0.26	-	79,79,79,79	0
52	MG	DF	301	1/1	0.32	-	92,92,92,92	0
52	MG	AA	1634	1/1	0.31	-	58,58,58,58	0
52	MG	DA	3216	1/1	0.62	-	85,85,85,85	0
52	MG	DA	3028	1/1	0.25	-	39,39,39,39	0
52	MG	BA	3240	1/1	0.47	-	60,60,60,60	0
52	MG	DA	3148	1/1	0.35	-	48,48,48,48	0
52	MG	DA	3050	1/1	0.39	-	42,42,42,42	0
52	MG	DA	3090	1/1	0.41	-	76,76,76,76	0
52	MG	DA	3183	1/1	0.29	-	44,44,44,44	0
52	MG	DA	3273	1/1	0.67	-	75,75,75,75	0
52	MG	DA	3236	1/1	0.38	-	67,67,67,67	0
52	MG	BA	3135	1/1	0.26	-	8,8,8,8	0
52	MG	BA	3161	1/1	0.26	-	42,42,42,42	0
52	MG	BA	3105	1/1	0.52	-	46,46,46,46	0
55	ZIT	DA	3311	52/52	0.28	-	100,100,100,100	0
52	MG	BA	3077	1/1	0.36	-	28,28,28,28	0
52	MG	B5	102	1/1	0.38	-	56,56,56,56	0
52	MG	DA	3120	1/1	0.28	-	71,71,71,71	0
52	MG	DA	3211	1/1	0.15	-	79,79,79,79	0
52	MG	DA	3111	1/1	0.44	-	71,71,71,71	0
52	MG	BA	3058	1/1	0.40	-	39,39,39,39	0
52	MG	BA	3129	1/1	0.13	-	18,18,18,18	0
52	MG	BA	3056	1/1	0.17	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	CA	1629	1/1	0.10	-	82,82,82,82	0
52	MG	DA	3031	1/1	0.23	-	47,47,47,47	0
52	MG	BA	3318	1/1	0.43	-	60,60,60,60	0
52	MG	BA	3158	1/1	0.41	-	49,49,49,49	0
52	MG	DA	3280	1/1	0.49	-	77,77,77,77	0
52	MG	DA	3113	1/1	0.47	-	62,62,62,62	0
52	MG	BA	3187	1/1	0.52	-	42,42,42,42	0
52	MG	BA	3054	1/1	0.15	-	68,68,68,68	0
52	MG	AA	1613	1/1	0.14	-	70,70,70,70	0
52	MG	DA	3020	1/1	0.42	-	64,64,64,64	0
52	MG	BA	3008	1/1	0.49	-	34,34,34,34	0
52	MG	CA	1620	1/1	0.36	-	66,66,66,66	0
52	MG	BA	3120	1/1	0.47	-	52,52,52,52	0
52	MG	DA	3308	1/1	0.10	-	81,81,81,81	0
52	MG	BA	3093	1/1	0.59	-	43,43,43,43	0
52	MG	BA	3063	1/1	0.39	-	48,48,48,48	0
52	MG	BA	3272	1/1	0.31	-	51,51,51,51	0
52	MG	CA	1634	1/1	0.55	-	87,87,87,87	0
52	MG	BA	3262	1/1	0.12	-	75,75,75,75	0
52	MG	BA	3147	1/1	0.15	-	12,12,12,12	0
52	MG	AA	1643	1/1	0.10	-	78,78,78,78	0
52	MG	BA	3186	1/1	0.40	-	66,66,66,66	0
52	MG	CA	1608	1/1	0.23	-	51,51,51,51	0
52	MG	DA	3123	1/1	0.12	-	61,61,61,61	0
52	MG	AA	1624	1/1	0.37	-	56,56,56,56	0
52	MG	DA	3172	1/1	0.54	-	64,64,64,64	0
52	MG	CA	1623	1/1	0.50	-	67,67,67,67	0
52	MG	DA	3046	1/1	0.28	-	28,28,28,28	0
52	MG	CA	1621	1/1	0.21	-	68,68,68,68	0
52	MG	DA	3088	1/1	0.48	-	34,34,34,34	0
52	MG	DA	3023	1/1	0.21	-	47,47,47,47	0
52	MG	DA	3162	1/1	0.21	-	69,69,69,69	0
52	MG	BA	3296	1/1	0.70	-	67,67,67,67	0
52	MG	D7	101	1/1	0.35	-	62,62,62,62	0
52	MG	BA	3177	1/1	0.42	-	52,52,52,52	0
52	MG	BA	3226	1/1	0.15	-	32,32,32,32	0
52	MG	DA	3041	1/1	0.18	-	37,37,37,37	0
52	MG	BA	3085	1/1	0.21	-	40,40,40,40	0
52	MG	DA	3258	1/1	0.18	-	61,61,61,61	0
52	MG	BA	3045	1/1	0.29	-	26,26,26,26	0
52	MG	BA	3245	1/1	0.52	-	45,45,45,45	0
52	MG	DA	3260	1/1	0.78	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	BA	3279	1/1	0.31	-	50,50,50,50	0
52	MG	DA	3297	1/1	0.24	-	74,74,74,74	0
52	MG	CA	1641	1/1	0.77	-	87,87,87,87	0
52	MG	BA	3113	1/1	0.32	-	26,26,26,26	0
52	MG	DA	3106	1/1	0.46	-	76,76,76,76	0
52	MG	AA	1601	1/1	0.16	-	58,58,58,58	0
52	MG	DA	3045	1/1	0.45	-	39,39,39,39	0
52	MG	BA	3349	1/1	0.07	-	61,61,61,61	0
52	MG	BA	3044	1/1	0.33	-	26,26,26,26	0
52	MG	DA	3220	1/1	0.14	-	62,62,62,62	0
52	MG	BA	3188	1/1	0.61	-	62,62,62,62	0
52	MG	DA	3165	1/1	0.32	-	52,52,52,52	0
52	MG	CA	1612	1/1	0.09	-	77,77,77,77	0
52	MG	DA	3175	1/1	0.71	-	67,67,67,67	0
52	MG	BA	3250	1/1	0.20	-	54,54,54,54	0
52	MG	BA	3022	1/1	0.36	-	49,49,49,49	0
52	MG	DA	3072	1/1	0.35	-	46,46,46,46	0
52	MG	BA	3233	1/1	0.19	-	63,63,63,63	0
52	MG	DA	3257	1/1	0.84	-	63,63,63,63	0
52	MG	DA	3143	1/1	0.45	-	57,57,57,57	0
52	MG	AA	1607	1/1	0.25	-	74,74,74,74	0
52	MG	BA	3106	1/1	0.16	-	12,12,12,12	0
52	MG	BA	3283	1/1	0.08	-	53,53,53,53	0
53	ZN	CN	101	1/1	0.18	-	157,157,157,157	0
52	MG	DA	3122	1/1	0.23	-	61,61,61,61	0
52	MG	DA	3145	1/1	0.73	-	88,88,88,88	0
52	MG	DA	3177	1/1	0.15	-	61,61,61,61	0
52	MG	DA	3167	1/1	0.37	-	48,48,48,48	0
52	MG	CA	1626	1/1	0.52	-	78,78,78,78	0
52	MG	DA	3282	1/1	0.39	-	62,62,62,62	0
52	MG	BA	3126	1/1	0.55	-	50,50,50,50	0
52	MG	AA	1605	1/1	0.28	-	75,75,75,75	0
52	MG	DA	3071	1/1	0.30	-	40,40,40,40	0
52	MG	DA	3263	1/1	0.25	-	67,67,67,67	0
52	MG	BA	3138	1/1	0.09	-	74,74,74,74	0
52	MG	DA	3060	1/1	0.09	-	34,34,34,34	0
52	MG	DA	3022	1/1	0.39	-	47,47,47,47	0
52	MG	BA	3062	1/1	0.33	-	44,44,44,44	0
52	MG	DA	3152	1/1	0.52	-	43,43,43,43	0
52	MG	DA	3052	1/1	0.38	-	63,63,63,63	0
52	MG	BA	3201	1/1	0.30	-	29,29,29,29	0
52	MG	DA	3128	1/1	0.62	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	BA	3304	1/1	1.14	-	86,86,86,86	0
52	MG	DA	3171	1/1	0.32	-	43,43,43,43	0
52	MG	BA	3317	1/1	0.13	-	41,41,41,41	0
52	MG	BA	3109	1/1	0.35	-	34,34,34,34	0
52	MG	BA	3263	1/1	0.55	-	62,62,62,62	0
52	MG	DA	3264	1/1	0.84	-	80,80,80,80	0
52	MG	BA	3010	1/1	0.42	-	38,38,38,38	0
52	MG	DA	3099	1/1	0.49	-	46,46,46,46	0
52	MG	DA	3043	1/1	0.35	-	35,35,35,35	0
52	MG	BA	3230	1/1	0.48	-	38,38,38,38	0
52	MG	CA	1615	1/1	0.61	-	67,67,67,67	0
52	MG	BA	3275	1/1	0.27	-	47,47,47,47	0
52	MG	DA	3274	1/1	0.27	-	63,63,63,63	0
52	MG	BA	3132	1/1	0.19	-	55,55,55,55	0
52	MG	DA	3089	1/1	0.59	-	47,47,47,47	0
52	MG	AA	1618	1/1	0.56	-	72,72,72,72	0
52	MG	DA	3014	1/1	0.38	-	68,68,68,68	0
52	MG	BA	3155	1/1	0.39	-	41,41,41,41	0
52	MG	BA	3269	1/1	0.16	-	55,55,55,55	0
52	MG	BA	3320	1/1	0.36	-	54,54,54,54	0
52	MG	AA	1633	1/1	0.16	-	81,81,81,81	0
52	MG	BA	3082	1/1	0.49	-	49,49,49,49	0
52	MG	DA	3068	1/1	0.38	-	49,49,49,49	0
52	MG	DA	3018	1/1	0.54	-	32,32,32,32	0
52	MG	BA	3255	1/1	0.27	-	45,45,45,45	0
52	MG	DA	3063	1/1	0.23	-	47,47,47,47	0
52	MG	BB	202	1/1	0.24	-	30,30,30,30	0
52	MG	BA	3215	1/1	0.37	-	36,36,36,36	0
52	MG	BA	3047	1/1	0.41	-	21,21,21,21	0
52	MG	DU	201	1/1	0.22	-	60,60,60,60	0
52	MG	CA	1640	1/1	0.28	-	68,68,68,68	0
52	MG	BA	3286	1/1	0.07	-	45,45,45,45	0
52	MG	DA	3186	1/1	0.53	-	63,63,63,63	0
52	MG	BA	3315	1/1	0.36	-	69,69,69,69	0
52	MG	DA	3038	1/1	0.53	-	48,48,48,48	0
52	MG	BA	3140	1/1	0.55	-	40,40,40,40	0
52	MG	BA	3176	1/1	0.48	-	48,48,48,48	0
52	MG	DA	3307	1/1	0.23	-	80,80,80,80	0
52	MG	BA	3346	1/1	0.42	-	80,80,80,80	0
52	MG	DA	3228	1/1	0.10	-	60,60,60,60	0
52	MG	BA	3229	1/1	0.28	-	50,50,50,50	0
52	MG	DA	3277	1/1	0.54	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	DA	3147	1/1	0.21	-	63,63,63,63	0
52	MG	AA	1620	1/1	0.44	-	73,73,73,73	0
52	MG	BA	3336	1/1	0.52	-	65,65,65,65	0
52	MG	CA	1647	1/1	0.22	-	84,84,84,84	0
52	MG	CA	1648	1/1	0.14	-	79,79,79,79	0
52	MG	CA	1604	1/1	0.36	-	86,86,86,86	0
52	MG	AA	1608	1/1	0.30	-	54,54,54,54	0
52	MG	CA	1617	1/1	0.28	-	61,61,61,61	0
52	MG	D5	101	1/1	0.40	-	47,47,47,47	0
52	MG	BA	3036	1/1	0.17	-	0,0,0,0	0
52	MG	AA	1614	1/1	0.13	-	77,77,77,77	0
52	MG	BA	3290	1/1	0.34	-	47,47,47,47	0
52	MG	BA	3319	1/1	0.43	-	40,40,40,40	0
52	MG	DA	3034	1/1	0.45	-	39,39,39,39	0
52	MG	BA	3265	1/1	0.44	-	63,63,63,63	0
52	MG	DA	3051	1/1	0.37	-	26,26,26,26	0
52	MG	AA	1615	1/1	0.55	-	76,76,76,76	0
52	MG	DA	3079	1/1	0.31	-	59,59,59,59	0
52	MG	BA	3059	1/1	0.26	-	39,39,39,39	0
52	MG	DA	3234	1/1	0.46	-	60,60,60,60	0
52	MG	BA	3199	1/1	0.51	-	49,49,49,49	0
52	MG	DA	3025	1/1	0.54	-	50,50,50,50	0
52	MG	BA	3090	1/1	0.13	-	38,38,38,38	0
52	MG	BA	3210	1/1	0.33	-	37,37,37,37	0
52	MG	DA	3091	1/1	0.50	-	41,41,41,41	0
52	MG	BA	3335	1/1	0.15	-	52,52,52,52	0
52	MG	BA	3163	1/1	0.39	-	47,47,47,47	0
52	MG	DA	3304	1/1	0.34	-	52,52,52,52	0
52	MG	DA	3042	1/1	0.33	-	47,47,47,47	0
52	MG	BA	3145	1/1	0.52	-	40,40,40,40	0
52	MG	AA	1641	1/1	0.16	-	69,69,69,69	0
52	MG	BA	3212	1/1	0.43	-	30,30,30,30	0
52	MG	BA	3101	1/1	0.42	-	39,39,39,39	0
52	MG	BA	3339	1/1	0.14	-	41,41,41,41	0
52	MG	DA	3226	1/1	0.30	-	64,64,64,64	0
52	MG	BA	3253	1/1	0.14	-	51,51,51,51	0
52	MG	BA	3039	1/1	0.71	-	60,60,60,60	0
52	MG	BA	3142	1/1	0.63	-	39,39,39,39	0
52	MG	BA	3268	1/1	0.25	-	40,40,40,40	0
52	MG	DA	3003	1/1	0.63	-	56,56,56,56	0
52	MG	BA	3181	1/1	0.31	-	51,51,51,51	0
52	MG	CA	1638	1/1	0.29	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
52	MG	DA	3040	1/1	0.24	-	43,43,43,43	0
52	MG	CA	1625	1/1	0.70	-	74,74,74,74	0
52	MG	BA	3218	1/1	0.41	-	33,33,33,33	0
52	MG	DA	3036	1/1	0.41	-	39,39,39,39	0
52	MG	DA	3202	1/1	0.24	-	40,40,40,40	0
52	MG	DA	3124	1/1	0.31	-	83,83,83,83	0
52	MG	BA	3308	1/1	0.43	-	64,64,64,64	0
52	MG	AA	1642	1/1	0.34	-	51,51,51,51	0
52	MG	BA	3178	1/1	0.54	-	78,78,78,78	0
52	MG	BA	3277	1/1	0.42	-	62,62,62,62	0
52	MG	BA	3184	1/1	0.41	-	50,50,50,50	0

## 6.5 Other polymers

There are no such residues in this entry.