



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 03:21 am BST

PDB ID : 4V7L  
Title : The structures of viomycin bound to the 70S ribosome.  
Authors : Stanley, R.E.; Blaha, G.  
Deposited on : 2009-11-12  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

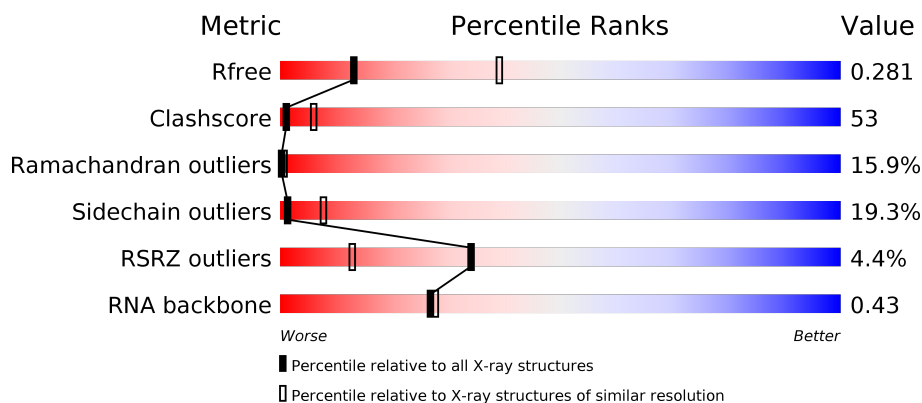
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1509	<div> <div>2%</div> <div>14%</div> <div>58%</div> <div>23%</div> <div>• •</div> </div>
1	CA	1509	<div> <div>2%</div> <div>9%</div> <div>64%</div> <div>23%</div> <div>• •</div> </div>
2	AB	256	<div> <div>6%</div> <div>15%</div> <div>56%</div> <div>18%</div> <div>• 8%</div> </div>
2	CB	256	<div> <div>5%</div> <div>15%</div> <div>60%</div> <div>16%</div> <div>• 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
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	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
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	AV	30	
22	CV	30	
23	AW	75	
23	CW	75	
24	AX	77	
24	CX	77	
25	AY	75	
25	CY	75	
26	AZ	6	
26	CZ	6	
27	BA	2915	
27	DA	2915	

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Mol	Chain	Length	Quality of chain
28	BB	122	
28	DB	122	
29	BC	229	
29	DC	229	
30	BD	276	
30	DD	276	
31	BE	206	
31	DE	206	
32	BF	210	
32	DF	210	
33	BG	182	
33	DG	182	
34	BH	180	
34	DH	180	
35	BI	148	
35	DI	148	
36	BN	140	
36	DN	140	
37	BO	122	
37	DO	122	
38	BP	150	
38	DP	150	
39	BQ	141	
39	DQ	141	
40	BR	118	

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Mol	Chain	Length	Quality of chain
40	DR	118	
41	BS	112	
41	DS	112	
42	BT	146	
42	DT	146	
43	BU	118	
43	DU	118	
44	BV	101	
44	DV	101	
45	BW	113	
45	DW	113	
46	BX	96	
46	DX	96	
47	BY	110	
47	DY	110	
48	BZ	206	
48	DZ	206	
49	B0	85	
49	D0	85	
50	B1	98	
50	D1	98	
51	B2	72	
51	D2	72	
52	B3	60	
52	D3	60	

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Mol	Chain	Length	Quality of chain
53	B4	71	
53	D4	71	
54	B5	60	
54	D5	60	
55	B6	54	
55	D6	54	
56	B7	49	
56	D7	49	
57	B8	65	
57	D8	65	
58	B9	37	
58	D9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	UAL	CZ	5	-	-	X	-
26	5OH	CZ	6	-	-	X	-
59	MG	AA	1707	-	-	-	X
59	MG	AA	1710	-	-	-	X
59	MG	AA	1727	-	-	-	X
59	MG	AW	101	-	-	-	X
59	MG	AW	106	-	-	-	X
59	MG	AX	107	-	-	-	X
59	MG	BA	3004	-	-	-	X
59	MG	BA	3134	-	-	-	X
59	MG	BA	3162	-	-	-	X
59	MG	BA	3165	-	-	-	X
59	MG	BA	3269	-	-	-	X
59	MG	BA	3294	-	-	-	X
59	MG	BA	3297	-	-	-	X
59	MG	BA	3298	-	-	-	X
59	MG	BA	3303	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3307	-	-	-	X
59	MG	BA	3317	-	-	-	X
59	MG	BA	3320	-	-	-	X
59	MG	BA	3332	-	-	-	X
59	MG	BA	3333	-	-	-	X
59	MG	BA	3347	-	-	-	X
59	MG	BX	101	-	-	-	X
59	MG	CA	1603	-	-	-	X
59	MG	CA	1605	-	-	-	X
59	MG	CA	1644	-	-	-	X
59	MG	CA	1675	-	-	-	X
59	MG	CA	1683	-	-	-	X
59	MG	DA	3069	-	-	-	X
59	MG	DA	3095	-	-	-	X
59	MG	DA	3119	-	-	-	X
59	MG	DA	3203	-	-	-	X
59	MG	DA	3211	-	-	-	X
59	MG	DA	3213	-	-	-	X
59	MG	DA	3238	-	-	-	X
59	MG	DA	3273	-	-	-	X
59	MG	DD	301	-	-	-	X



## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 294559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1495	Total	C	N	O	P	0	0	0
			32141	14306	5964	10377	1494			
1	CA	1495	Total	C	N	O	P	0	0	0
			32141	14306	5964	10377	1494			

- 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
			1005	636	195	174			
9	CI	127	Total	C	N	O	0	0	0
			1006	637	195	174			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	120	Total	C	N	O	S	0	0	0
			947	585	195	165	2			
13	CM	119	Total	C	N	O	S	0	0	0
			910	564	180	164	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			
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 RNA chain called RNA (5'-R(\*AP\*AP\*AP\*AP\*AP\*GP\*GP\*AP\*AP\*AP\*UP\*A\*AP\*AP\*AP\*AP\*UP\*GP\*CP\*AP\*GP\*UP\*UP\*CP\*AP\*AP\*UP\*CP\*UP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0	0
			213	97	42	65	9			
22	CV	10	Total	C	N	O	P	0	0	0
			213	97	42	65	9			

- Molecule 23 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	75	Total	C	N	O	P	0	0	0
			1593	711	281	526	75			
23	CW	75	Total	C	N	O	P	0	0	0
			1593	711	281	526	75			

- Molecule 24 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
24	CX	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 25 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			
25	CY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	33	G	C	CONFLICT	GB CP001637.1
AY	44	U	A	CONFLICT	GB CP001637.1

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Chain	Residue	Modelled	Actual	Comment	Reference
CY	33	G	C	CONFLICT	GB CP001637.1
CY	44	U	A	CONFLICT	GB CP001637.1

- Molecule 26 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AZ	6	Total	C	N	O	0	0	0
			48	25	13	10			
26	CZ	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BA	2800	Total	C	N	O	P	0	0	0
			60311	26841	11284	19387	2799			
27	DA	2800	Total	C	N	O	P	0	0	0
			60313	26842	11286	19386	2799			

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BB	118	Total	C	N	O	P	0	0	0
			2528	1126	466	819	117			
28	DB	118	Total	C	N	O	P	0	0	0
			2528	1126	466	819	117			

- Molecule 29 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			
29	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 30 is a protein called 50S ribosomal protein L2.

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

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BH	164	Total	C	N	O	S	0	0	1
			1252	794	233	224	1			
34	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BI	146	Total	C	N	O	S	0	0	1
			1042	668	175	198	1			
35	DI	146	Total	C	N	O	S	0	0	1
			1046	670	175	200	1			

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
39	DQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	DS	101	Total	C	N	O	0	0	1
			777	489	156	132			

- Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BT	138	Total 1142	C 710	N 235	O 196	S 1	0	0	1
42	DT	138	Total 1142	C 710	N 235	O 196	S 1	0	0	1

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

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

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
49	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B1	94	Total	C	N	O	S	0	0	1
			715	448	141	125	1			
50	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
51	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 52 is a protein called 50S ribosomal protein L30.

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

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
53	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 54 is a protein called 50S ribosomal protein L32.

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

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B6	51	Total	C	N	O	S	0	0	1
			411	253	84	70	4			
55	D6	46	Total	C	N	O	S	0	0	1
			390	241	80	65	4			

- Molecule 56 is a protein called 50S ribosomal protein L34.

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

- Molecule 57 is a protein called 50S ribosomal protein L35.

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

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

- Molecule 58 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
58	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BA	400	Total	Mg	0	0
			400	400		
59	AK	2	Total	Mg	0	0
			2	2		
59	DF	1	Total	Mg	0	0
			1	1		
59	CV	2	Total	Mg	0	0
			2	2		
59	BE	1	Total	Mg	0	0
			1	1		
59	AW	7	Total	Mg	0	0
			7	7		
59	BP	1	Total	Mg	0	0
			1	1		
59	AX	7	Total	Mg	0	0
			7	7		
59	DR	1	Total	Mg	0	0
			1	1		
59	CA	92	Total	Mg	0	0
			92	92		
59	B5	1	Total	Mg	0	0
			1	1		
59	BB	1	Total	Mg	0	0
			1	1		
59	D6	1	Total	Mg	0	0
			1	1		
59	AE	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BF	2	Total 2	Mg 2	0	0
59	BX	1	Total 1	Mg 1	0	0
59	AA	133	Total 133	Mg 133	0	0
59	BQ	1	Total 1	Mg 1	0	0
59	CQ	1	Total 1	Mg 1	0	0
59	CX	3	Total 3	Mg 3	0	0
59	BU	1	Total 1	Mg 1	0	0
59	AD	1	Total 1	Mg 1	0	0
59	BN	1	Total 1	Mg 1	0	0
59	BY	1	Total 1	Mg 1	0	0
59	BR	1	Total 1	Mg 1	0	0
59	DA	275	Total 275	Mg 275	0	0
59	CE	2	Total 2	Mg 2	0	0
59	DD	3	Total 3	Mg 3	0	0
59	AL	1	Total 1	Mg 1	0	0
59	DE	3	Total 3	Mg 3	0	0
59	AH	1	Total 1	Mg 1	0	0
59	BZ	1	Total 1	Mg 1	0	0
59	DZ	1	Total 1	Mg 1	0	0
59	AC	1	Total 1	Mg 1	0	0
59	DB	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D5	2	Total 2	Mg 2	0	0
59	BD	1	Total 1	Mg 1	0	0
59	AT	2	Total 2	Mg 2	0	0
59	B0	2	Total 2	Mg 2	0	0
59	AO	1	Total 1	Mg 1	0	0
59	AY	2	Total 2	Mg 2	0	0
59	AF	1	Total 1	Mg 1	0	0
59	BH	1	Total 1	Mg 1	0	0

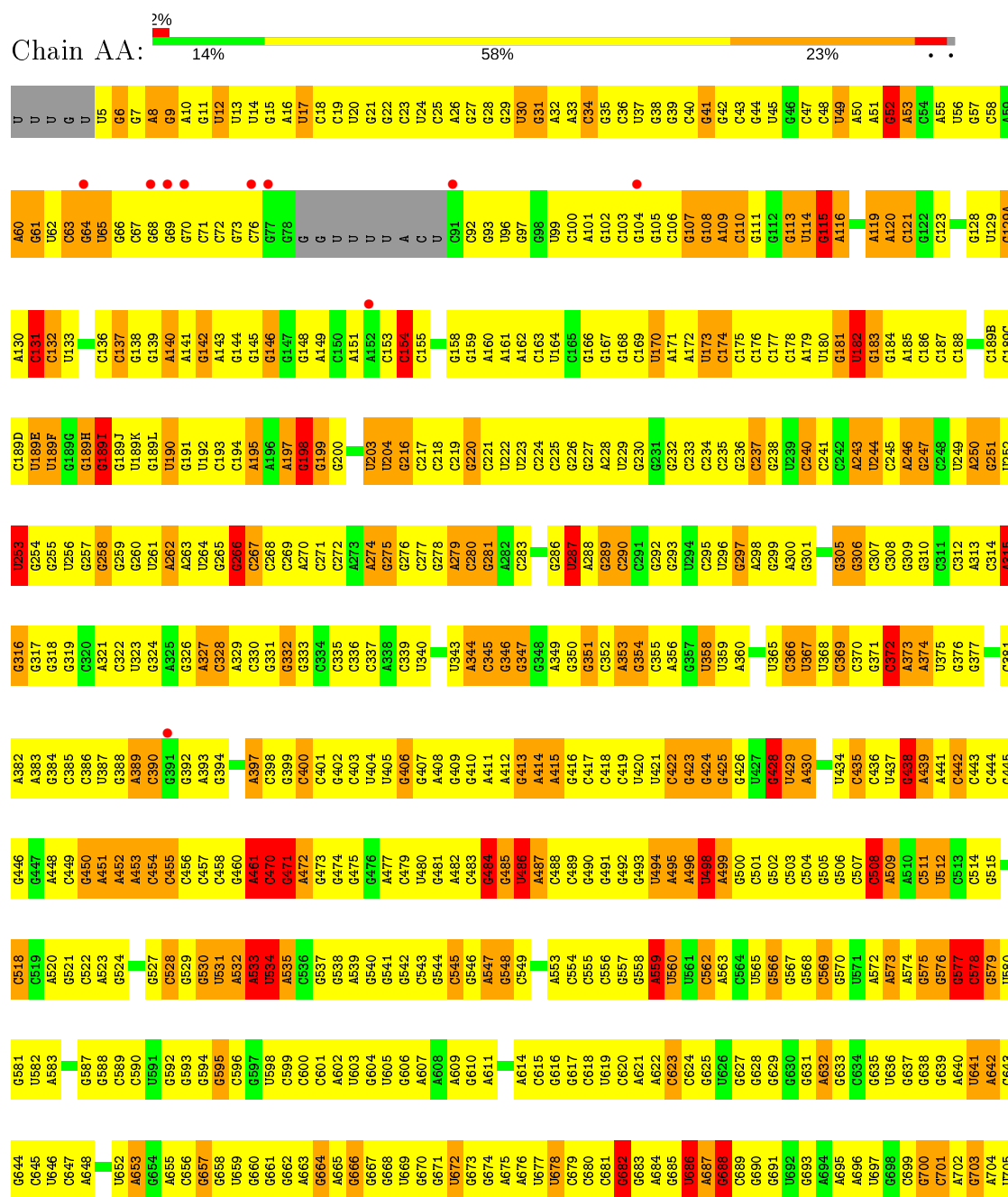
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	B5	1	Total 1	Zn 1	0	0
60	B4	1	Total 1	Zn 1	0	0
60	AD	1	Total 1	Zn 1	0	0
60	B9	1	Total 1	Zn 1	0	0
60	D9	1	Total 1	Zn 1	0	0
60	D5	1	Total 1	Zn 1	0	0
60	D4	1	Total 1	Zn 1	0	0
60	CD	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

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

- Molecule 1: 16S ribosomal RNA



A1519	A1447	G1385	C1326	G1265	G1204	U1078	C1140	U1078	G1022	G962	A900	G829	A766	A706
G1520	C1452	G1386	C1327	G1266	G1023	G1079	C1141	G1079	G1023	G963	A901	G830	A767	C707
G1521	G1456	G1328	G1329	G1267	U1024	A1080	G1432	A1080	U1024	A964	G902	G831	A768	G709
G1522	C1457	A1329	A1328	A1268	G1025	G1081	G1433	G1081	G1025	A965	G903	G832	A769	G710
G1523	G1458	U1390	U1329	A1269	G1026	U1082	G1434	U1082	G1026	G966	G904	G833	G770	G711
G1524	C1459	G1391	G1330	C1270	G1027	U1083	G1435	U1083	G1027	G967	G905	G834	G771	G712
G1525	A1460	G1392	A1332	G1271	C1028	G1084	A1436	G1084	C1028	A968	U905	G835	G772	A713
G1526	G1461	U1393	A1333	G1272	U1085	U1085	A1437	U1085	U1085	A969	G906	G836	G773	G714
G1527	G1462	C1395	G1334	G1273	C1029	U1086	U1438	U1086	C1029	G970	G907	G837	G774	G715
G1528	A1396	A1396	C1335	G1274	C1030	G1087	G1439	G1087	C1030	G971	A909	G838	G775	A716
G1529	C1463	C1397	C1336	A1275	G1030A	U1088	U1440	U1088	G1030A	G972	A909	U839	G776	A717
G1530	G1464	A1398	A1337	G1276	C1030B	U1089	U1441	U1089	C1030B	G973	U911	U841	G777	C717
G1531	C1465	C1399	G1338	C1277	A1030C	U1090	A1151	U1090	A1030C	G974	C912	C848	G778	G718
	C1466	C1400	A1339	U1278	A1030D	U1091	A1152	U1091	A1030D	A975	A913	C849	G779	C719
	G1467	G1401	A1340	A1279	G1031	U1092	C1153	U1092	G1031	G976	A914	U850	A780	C720
	A1468	C1402	G1341	C1280	G1032	A1093	G1154	A1093	G1032	G977	A915	U851	A781	C721
	G1471	C1403	G1342	U1281	G1033	U1094	G1155	U1094	G1033	A978	A916	G852	A782	U722
	U1472	G1404	C1343	G1282	A1034	U1095	G1156	U1095	A1034	G979	G917	G853	C783	U723
	A1473	G1405	C1344	G1222	G1035	U1096	A1157	U1096	G1035	C980	A918	G854	C784	U724
		U1406	U1345	G1223	G1036	C1097	C1158	U1097	G1036	G981	A919	G855	C785	G725
	G1476	C1407	A1346	G1224	C1037		U1159	C1097	C1037	U982	A920	G856	G786	C726
	C1477	A1408	G1347	A1225	U1038	C1100	C1160	C1097	U1038	U983	U921	G857	U788	C727
	C1478	C1409	U1348	C1226	A1101	A1101	C1161	A1101	U1040	C984	U922	C858	U789	A728
	C1479	G1410	A1349	A1227	C1102	C1102	G1162	C1102	A1041	C985	A923	A859	A790	A729
		C1411	A1350	C1228	C1103	C1103	G1163	C1103	G1042	A986	A924	A860	G791	G730
	G1482	C1412	U1351	A1229	C1104	G1104	C1164	G1104	C1043	G987	G925	G861	A792	G731
	A1483	A1413	C1352	A1230	G1105	A1105	G1165	A1105	A1044		G926	C862	U793	C732
	C1484	U1414	G1353	G1231	A1168	C1106	C1166	C1106	A1046	C998	G927	U863	A802	A733
	U1485	G1415	C1354	U1232	A1169	C1107	A1168	C1107	A1047	C999	C936	G874	A803	G742
	G1486	G1416	C1355	G1233	A1170	G1108	A1169	G1108	U1047	U992	G929	C875	G804	G743
	G1487	G1417	G1356	C1234	G1171	C1109	G1170	G1109	G1048	G993	C930	G876	A807	C744
	C1488	A1418	A1357	U1235	C1172		C1171		U1049	A994	C931	G877	C808	C745
		G1419	U1358	U1236	C1173		C1172		G1050	U994	G932	G878	C809	A746
	A1492	C1420	C1359	A1237	G1174		C1173		U1051	A996	G933	U879	C810	C747
	C1493	G1421	A1360	C1238			C1174		G1052	G997	C934	A872	C812	C748
	G1494	G1422	G1361	A1239	G1178	G1115	G1178	G1115	G1053	C998	A935	A873	U813	G749
	C1495	C1423	C1362	U1240	G1179	C1116	A1179	C1116	C1054	C999	C936	G874	A814	G750
	C1496	U1424	C1363	G1241	A1180	G1117	A1180	G1117	A1055	U1000	A937	C875	A815	A751
	G1497	U1425	A1363A	C1242	G1181	C1118	G1181	C1118	U1056	A1001	A938	G876	A816	G752
	U1498	C1426	U1364	C1243	G1182	C1119	G1182	C1119	G1057	G1001A	A939	C877	A817	C753
	A1499	U1427	G1365	C1244	A1183	G1120	G1183	G1120	G1058	G1002	C940	G878	C817	A754
	C1500	A1428	C1366	C1245	G1184	U1121	G1184	U1121	C1059	G1003	G941	C879	G818	G755
	G1501	C1429	C1367	C1246	G1185	U1122	G1185	U1122	G1060	A1004	G942	C880	A819	C756
	C1502	G1430	G1368	U1247	G1186	A1123	G1186	A1123	G1061	A1005	U943	C881	U820	G757
	A1503	C1431	C1369	A1248	G1187	G1124	G1187	G1124	U1062	C1006	G944	C882	G821	A758
	G1504	G1432	G1370	C1249	G1188	U1125	G1188	U1125	C1063	C1007	A946	C883	A816	A759
	C1505	A1433	G1371		C1189	G1126	C1189	G1126	G1064	G1008	G945	U884	G822	G760
	U1506	A1434	U1372	G1253	G1190	G1127	G1190	G1127	U1065	G1009	G950	G885	G823	G761
	G1435	G1435	G1373	G1254	A1191	C1128	A1191	C1128	U1066	G1010	U951	G886	G824	C762
	U1436	U1436	A1374	G1255	C1192	C1129	C1192	C1129	A1067	G1011	U952	G887	G825	C763
	C1437	A1375	A1376	G1256	G1193		G1193		G1068	U1012	U953	G888	G826	U827
	C1509	U1376	U1377	A1257	U1196	G1131	U1196	G1131	C1069	G1013	G954	A889	U827	A828
	G1510	G1511	C1377	C1258	U1197	C1132	U1197	C1132	U1070	A1014	G955	G890	U820	
	U1512	A1513	C1378	G1259	G1197	C1133	G1197	C1133	A1015	A1015	U956	G891	G821	
	C1514	A1442B	G1379	C1260	U1198	G1134	U1198	G1134	A1016	A1016	U957	G892	G822	
	C1515	U1381	U1380	A1261	U1199	G1135	U1199	G1135	U1073	G1017	G958	G893	G823	
	G1516	C1382	U1382	A1262	C1200	G1074	C1200	G1074	G1018	A956	A956	G894	G824	
	C1517	C1383	C1382	C1262	A1201	G1075	A1201	G1075	C1019	A959	A959	G895	G825	
	A1518	U1446	C1384	C1264	C1202	C1076	C1202	C1076	U1020	U1020	U960	G896	G826	
					G1203	G1077	G1203	G1077	G1021	G1021	U961	C897	U827	

● Molecule 1: 16S ribosomal RNA

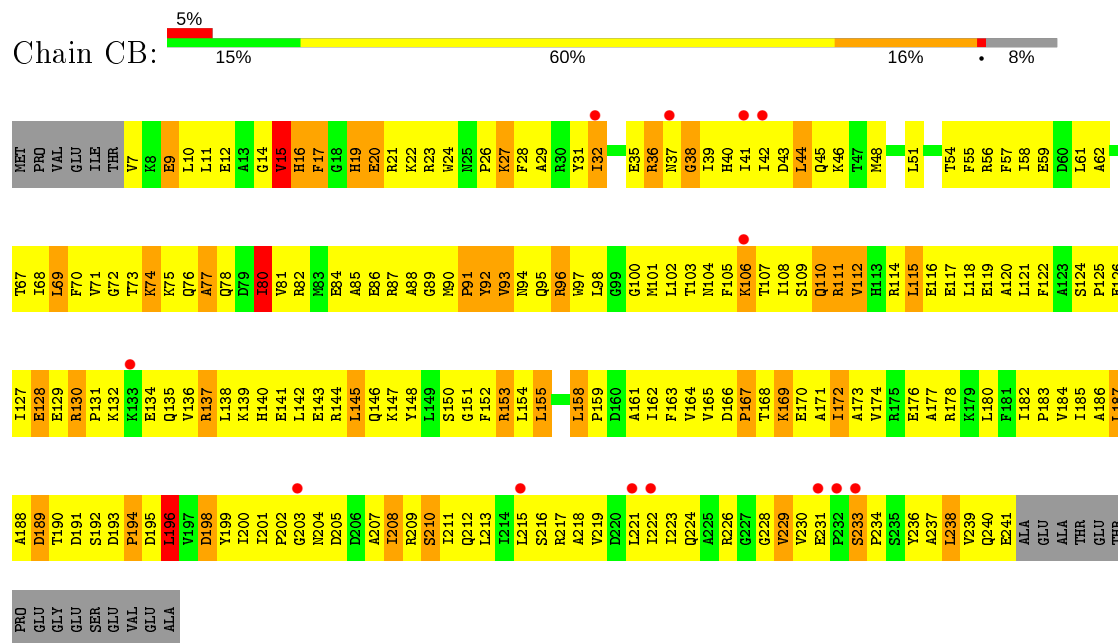




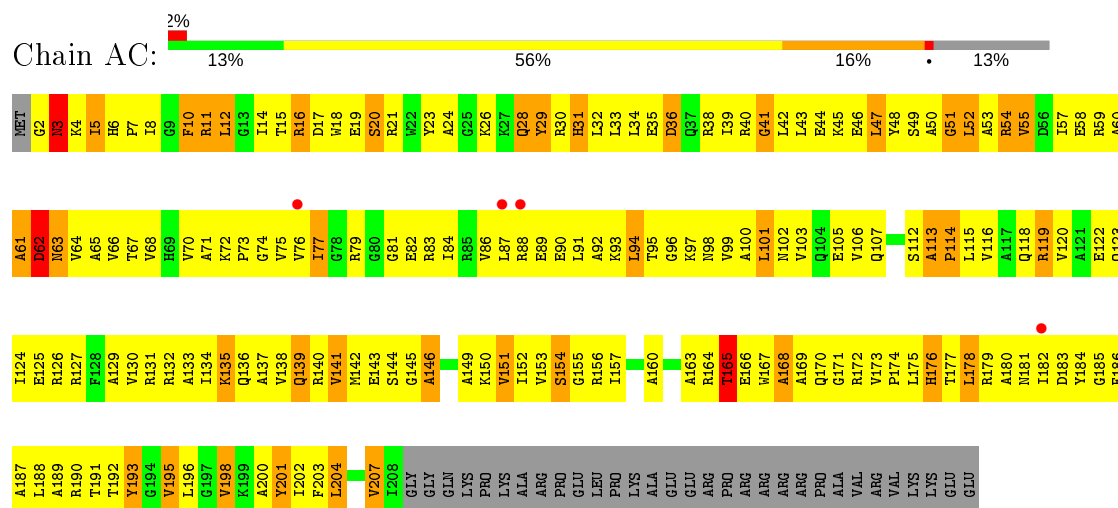


ALA  
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GLU  
THR  
GLU  
PRO  
GLU  
GLY  
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ALA

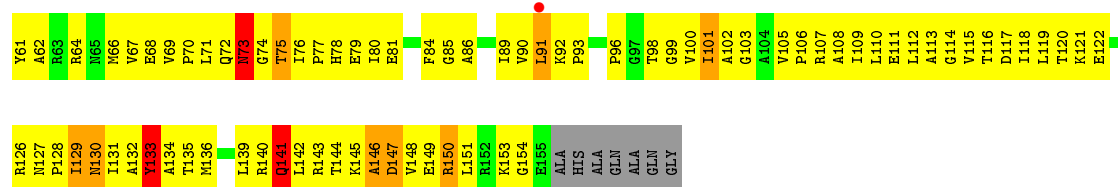
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3

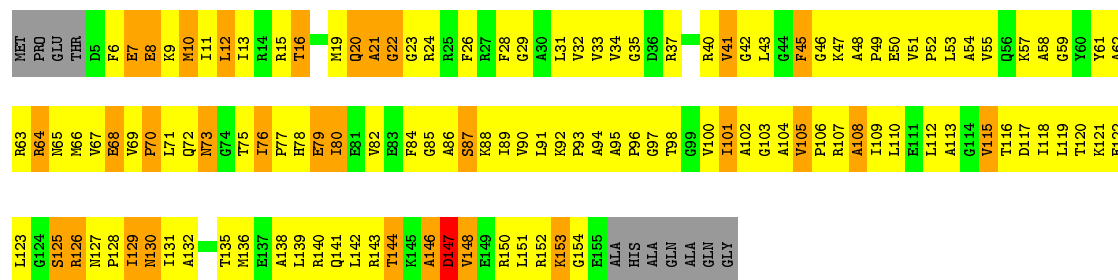






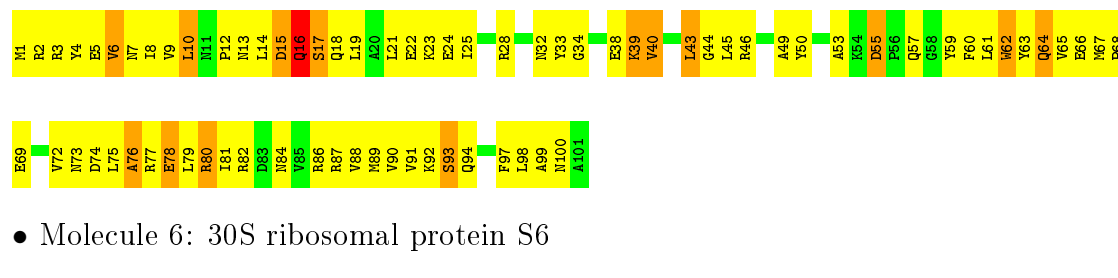
• Molecule 5: 30S ribosomal protein S5

Chain CE: 16% 58% 19% 7%



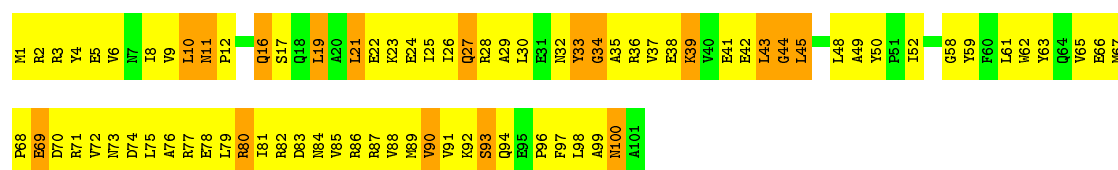
• Molecule 6: 30S ribosomal protein S6

Chain AF: 26% 59% 14% 1%



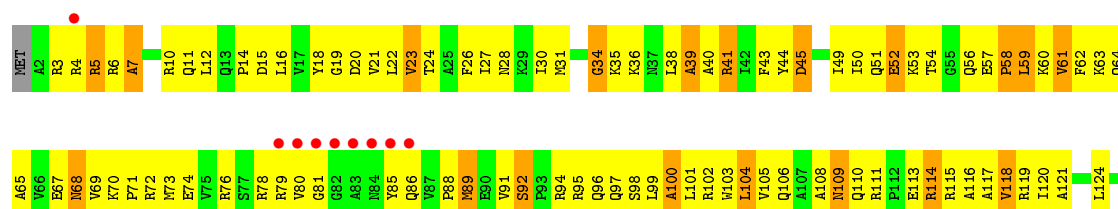
• Molecule 7: 30S ribosomal protein S7

Chain CF: 20% 63% 17% 1%



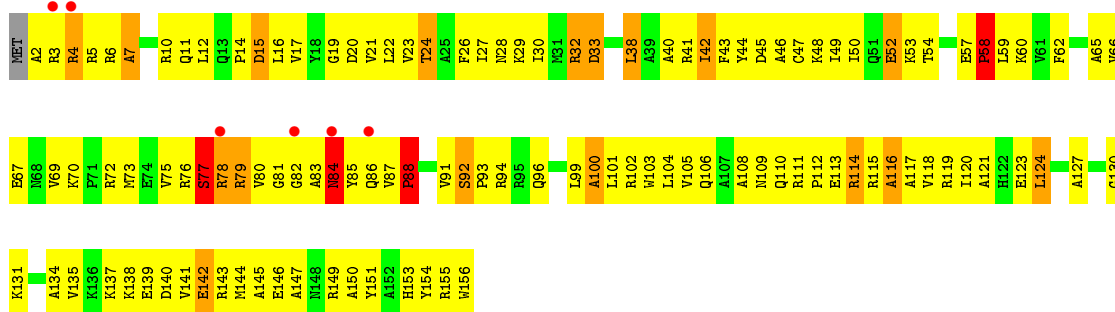
• Molecule 8: 30S ribosomal protein S8

Chain AG: 6% 58% 15% 1%

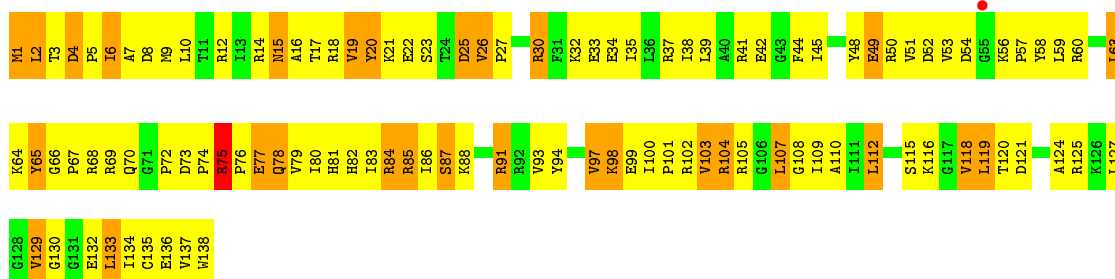




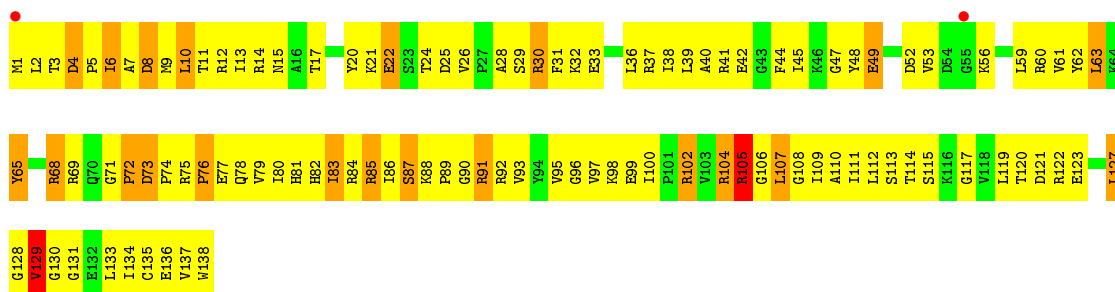
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

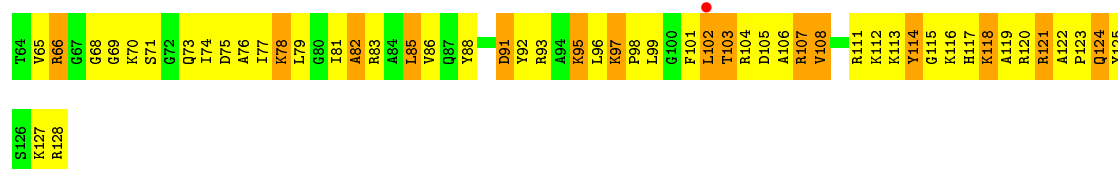


• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

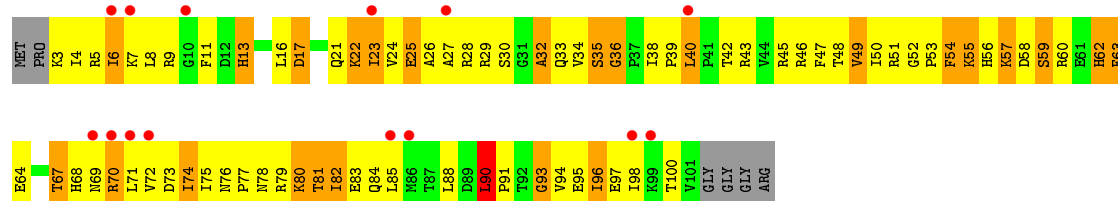
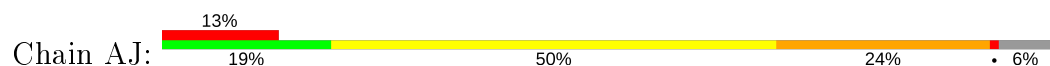




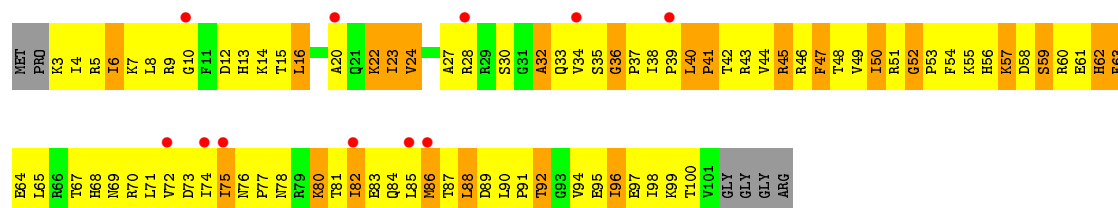
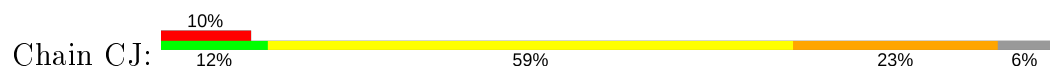
• Molecule 9: 30S ribosomal protein S9



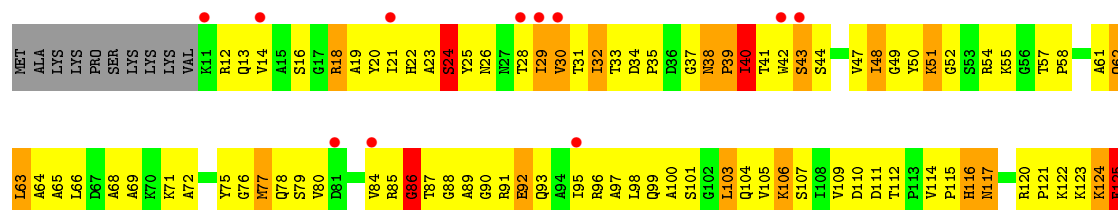
• Molecule 10: 30S ribosomal protein S10

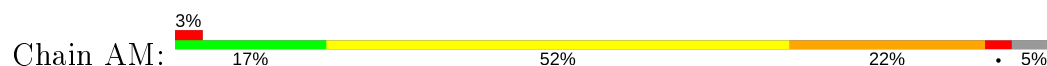


• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

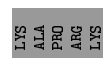
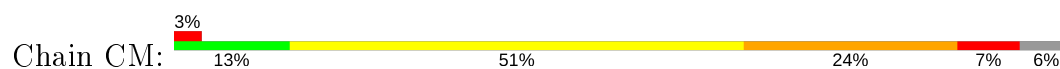




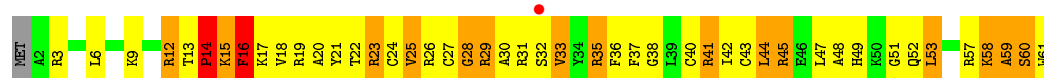




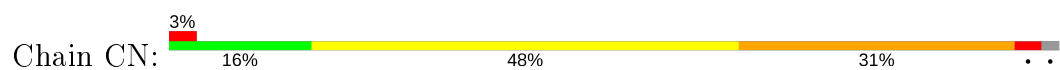
• Molecule 13: 30S ribosomal protein S13



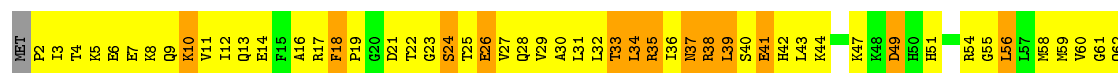
• Molecule 14: 30S ribosomal protein S14



• Molecule 14: 30S ribosomal protein S14

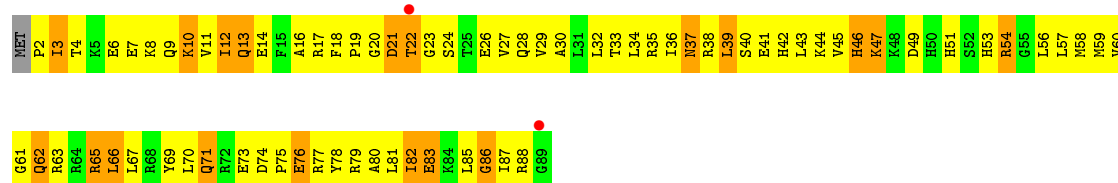


• Molecule 15: 30S ribosomal protein S15

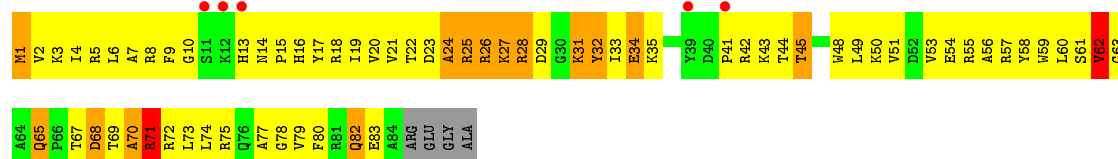


• Molecule 15: 30S ribosomal protein S15

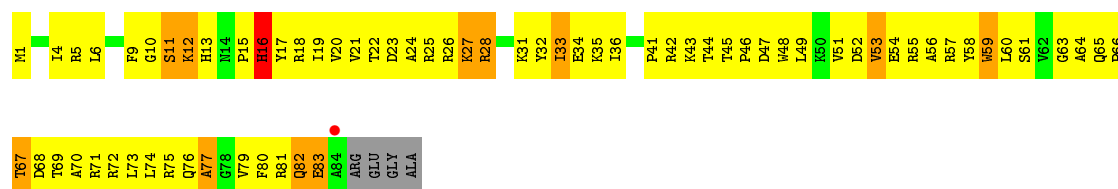




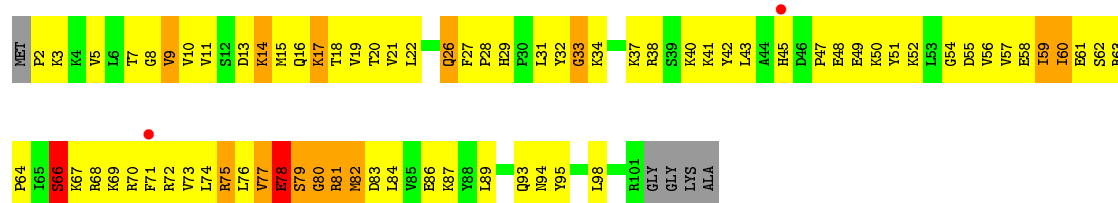
• Molecule 16: 30S ribosomal protein S16



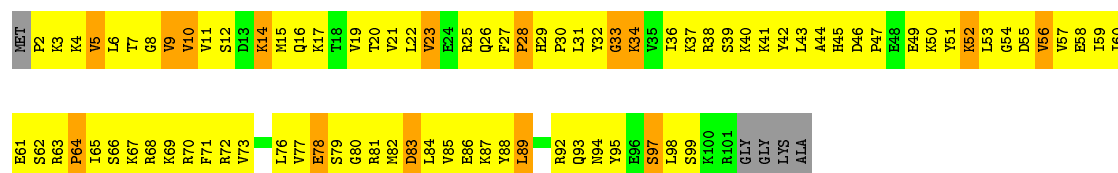
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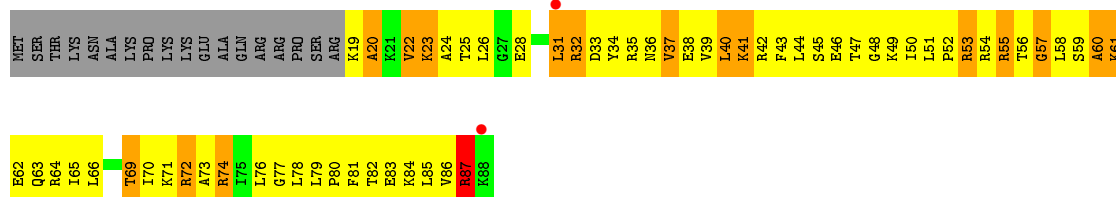
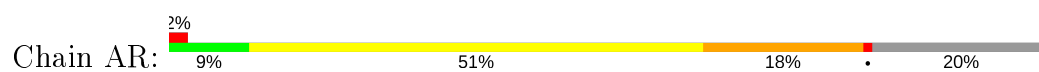
• Molecule 17: 30S ribosomal protein S17



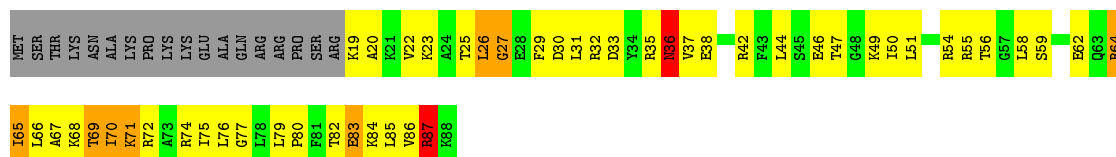
• Molecule 17: 30S ribosomal protein S17



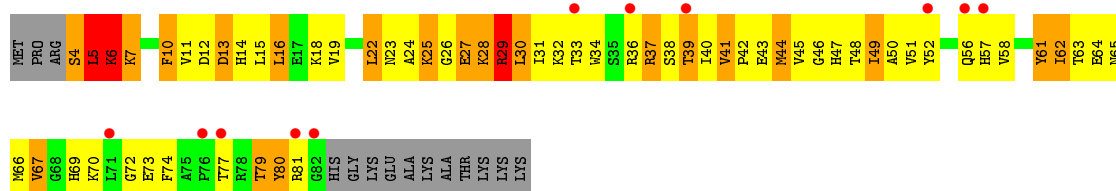
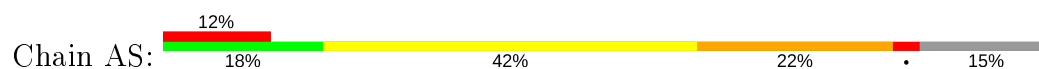
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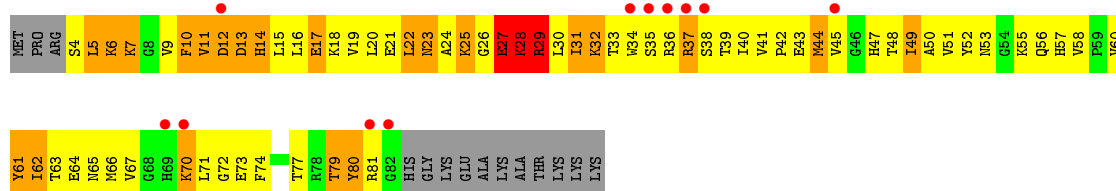
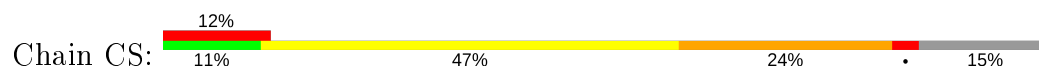
- Molecule 18: 30S ribosomal protein S18



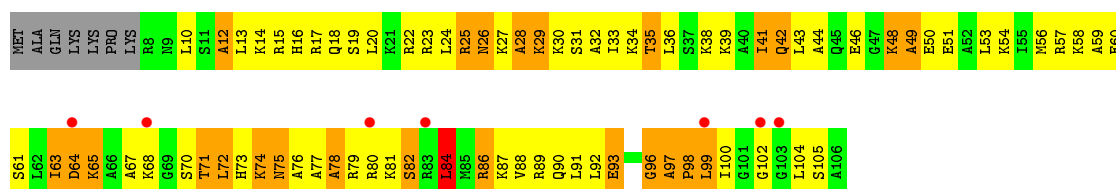
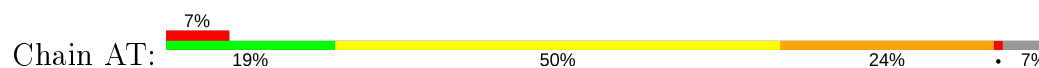
- Molecule 19: 30S ribosomal protein S19



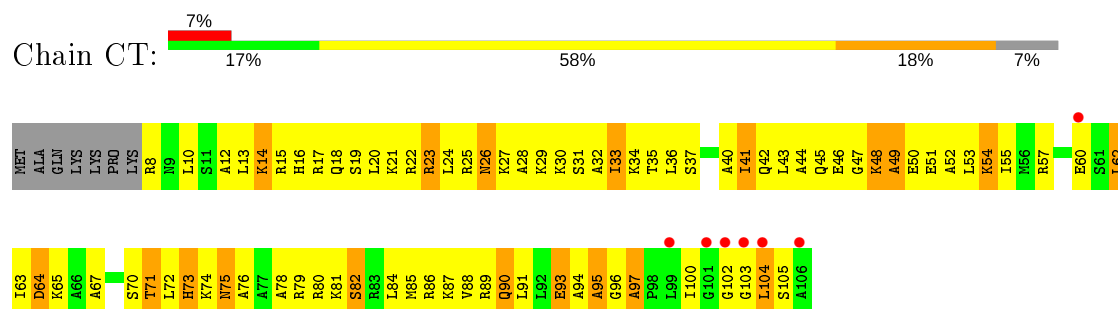
- Molecule 19: 30S ribosomal protein S19



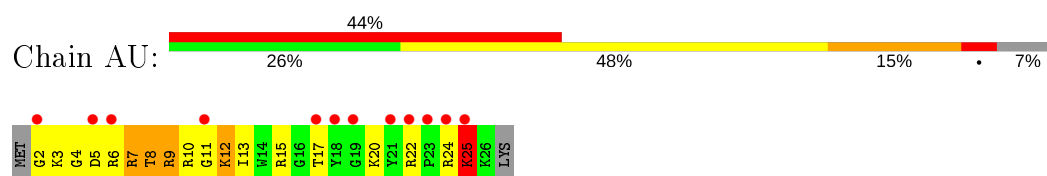
- Molecule 20: 30S ribosomal protein S20



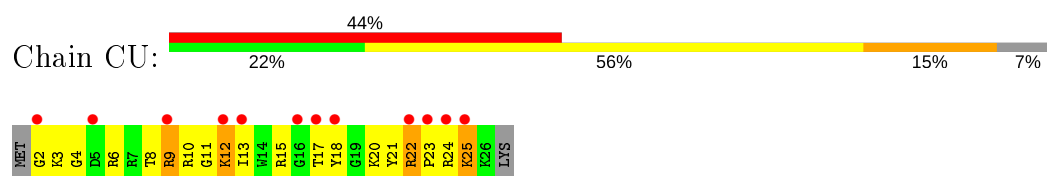
- Molecule 20: 30S ribosomal protein S20



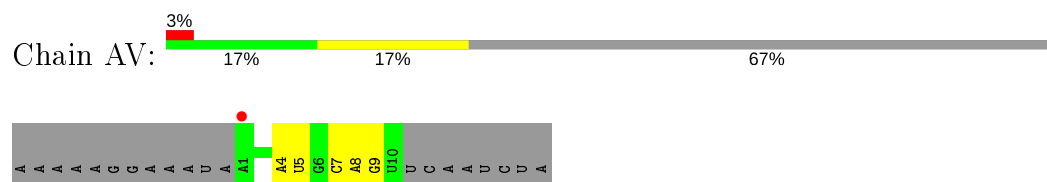
- Molecule 21: 30S ribosomal protein Thx



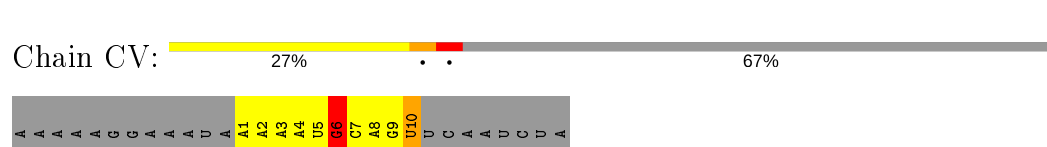
- Molecule 21: 30S ribosomal protein Thx



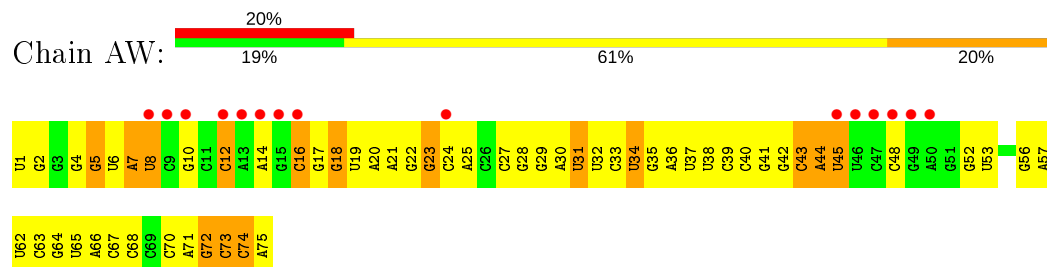
- Molecule 22: RNA (5'-R(\*AP\*AP\*AP\*AP\*AP\*GP\*GP\*AP\*AP\*AP\*UP\*A\*AP\*AP\*AP\*AP\*UP\*GP\*CP\*AP\*GP\*UP\*UP\*CP\*AP\*AP\*UP\*CP\*UP\*A)-3')



- Molecule 22: RNA (5'-R(\*AP\*AP\*AP\*AP\*AP\*GP\*GP\*AP\*AP\*AP\*UP\*A\*AP\*AP\*AP\*AP\*UP\*GP\*CP\*AP\*GP\*UP\*UP\*CP\*AP\*AP\*UP\*CP\*UP\*A)-3')

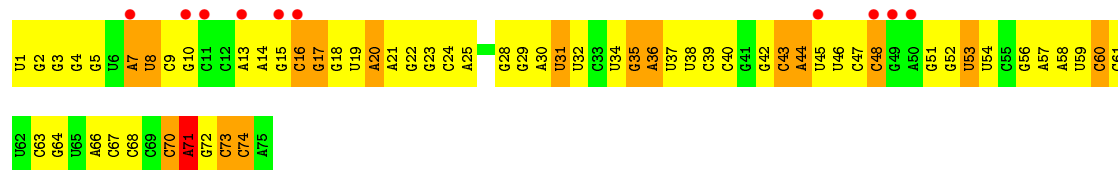


- Molecule 23: tRNA-Gln



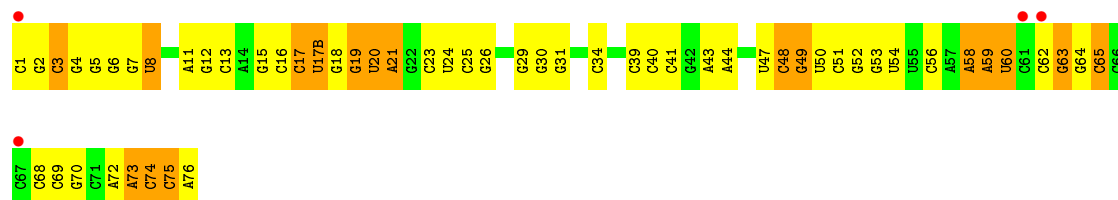
## ● Molecule 23: tRNA-Gln

Chain CW: 



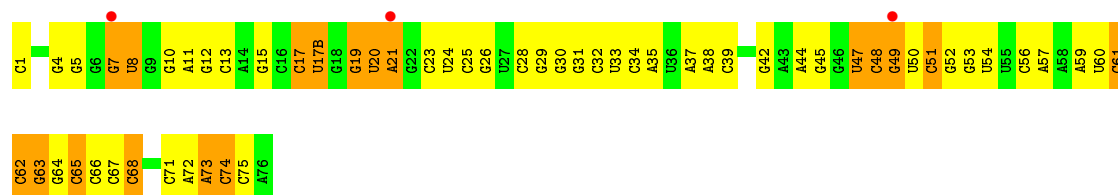
## ● Molecule 24: tRNA-Met

Chain AX: 




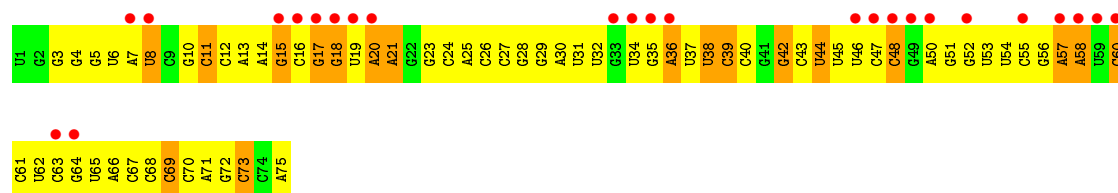
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Chain CX: 

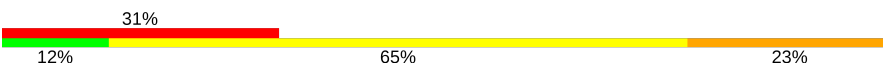


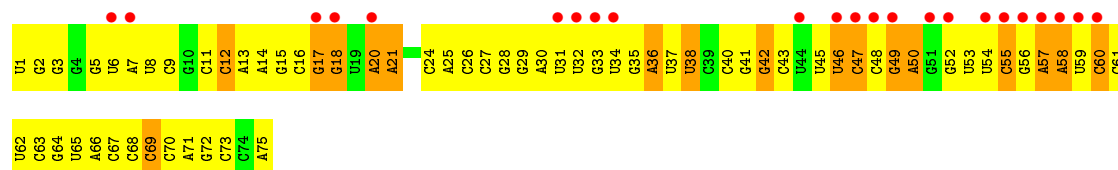
## ● Molecule 25: tRNA-Gln

Chain AY: 



## ● Molecule 25: tRNA-Gln

Chain CY: 



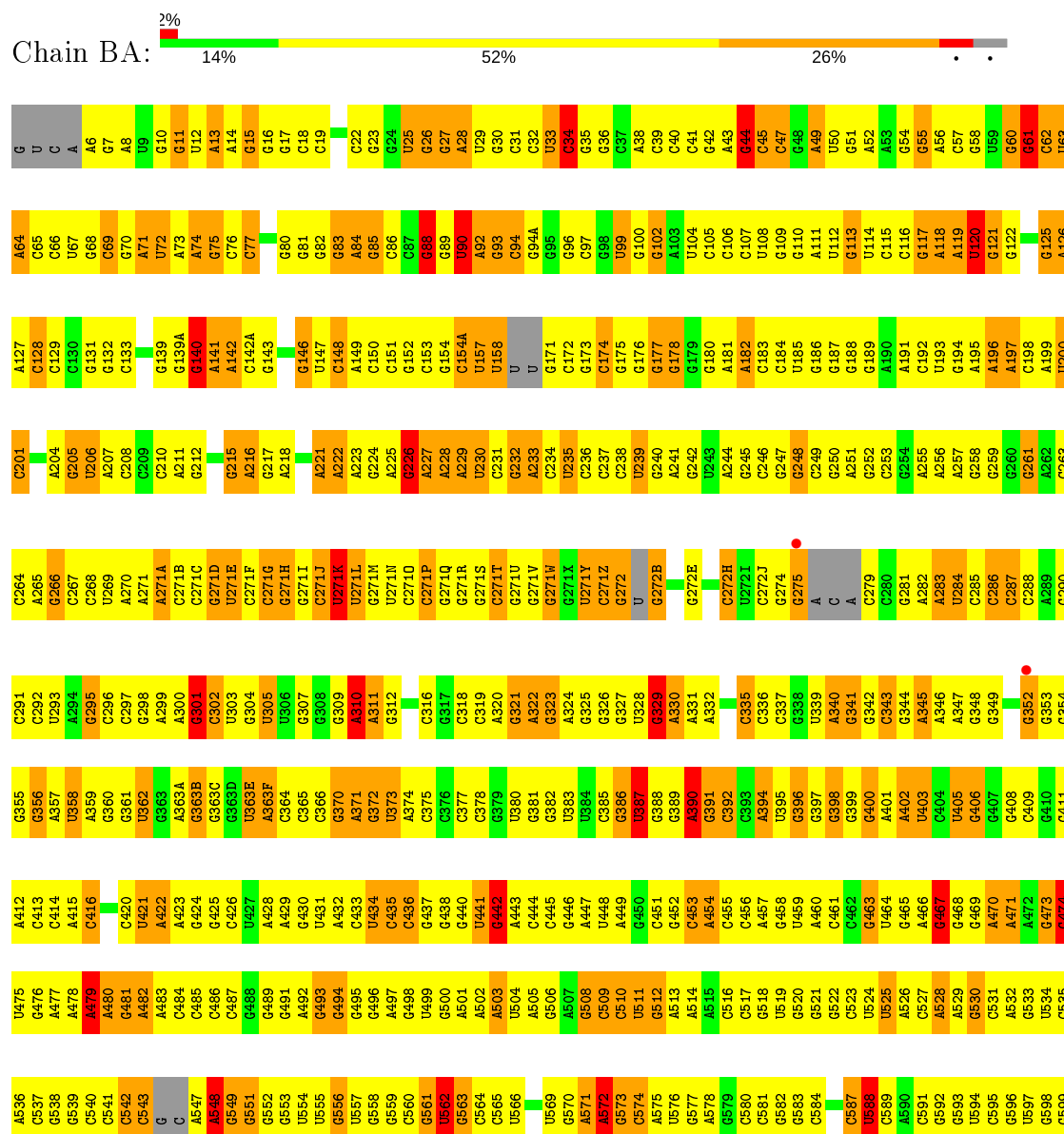
## ● Molecule 26: Viomycin



## ● Molecule 26: Viomycin



## ● Molecule 27: 23S ribosomal RNA



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C1407	G1345	G1219	G1281	C1158	C967	G906	C840	U773	G711	C	U614
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G1450	U1391	A1265	C1140	G1203	C1013	C951	C888		U757		G
C1450A	A1392	G1266	U1141	A1204	U1014	G952	C889	C825	C758		G
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U1394	A1393	A1268	G1142A	G1206	G1016	G954	G892	U827	G760		G
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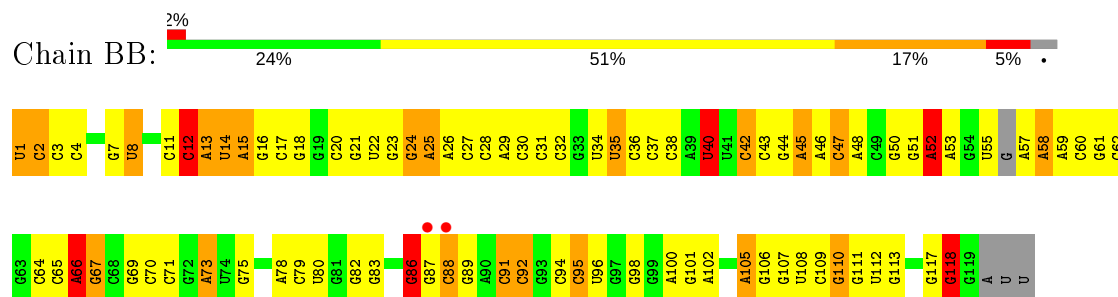


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C	G1014	C955	G826	G765	G699	G	G599	C535	G473	A412	G354	C292	A265
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G	A1027	G968	G778	G778	A716	C	G612	G551	A480	G425	G363D	U305	G271J
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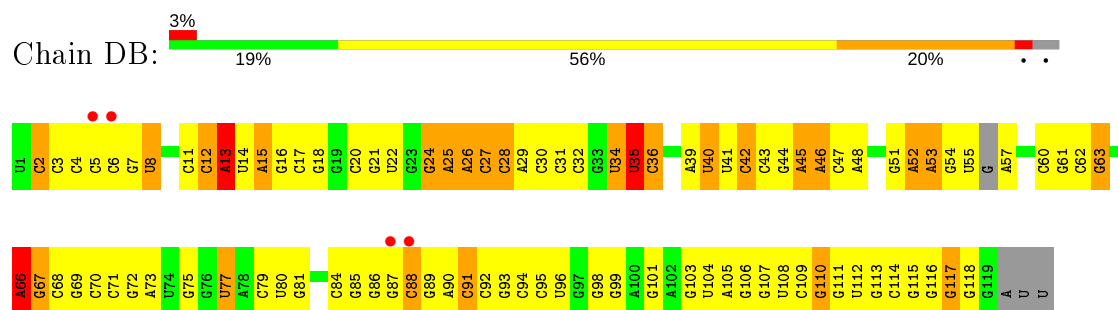
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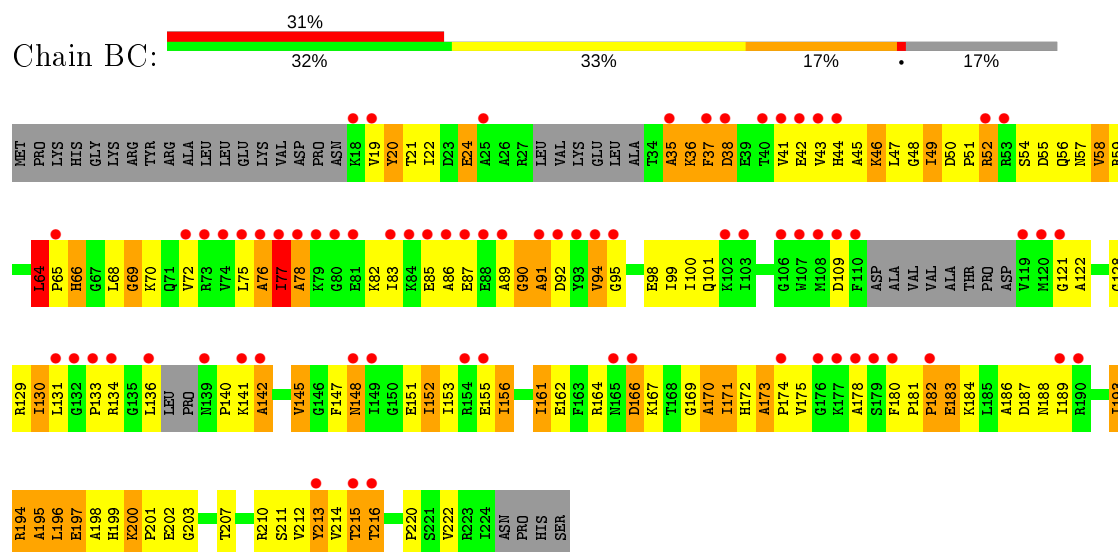
• Molecule 28: 5S ribosomal RNA



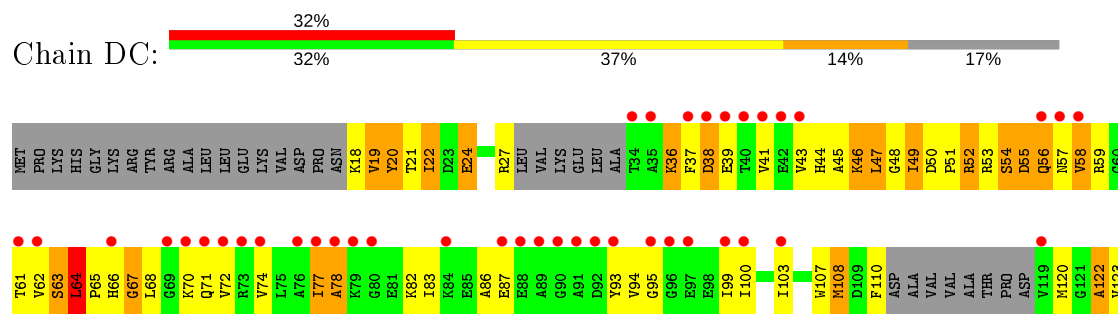
- Molecule 28: 5S ribosomal RNA

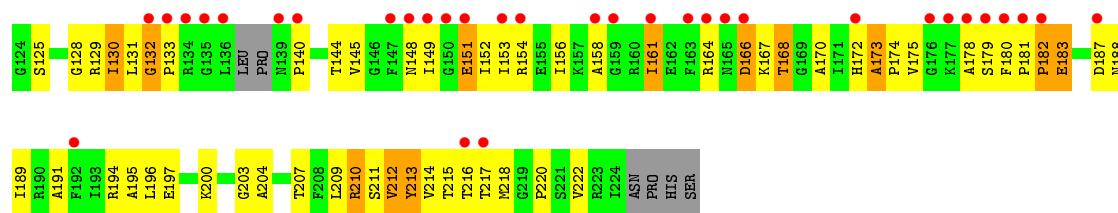


- Molecule 29: 50S ribosomal protein L1

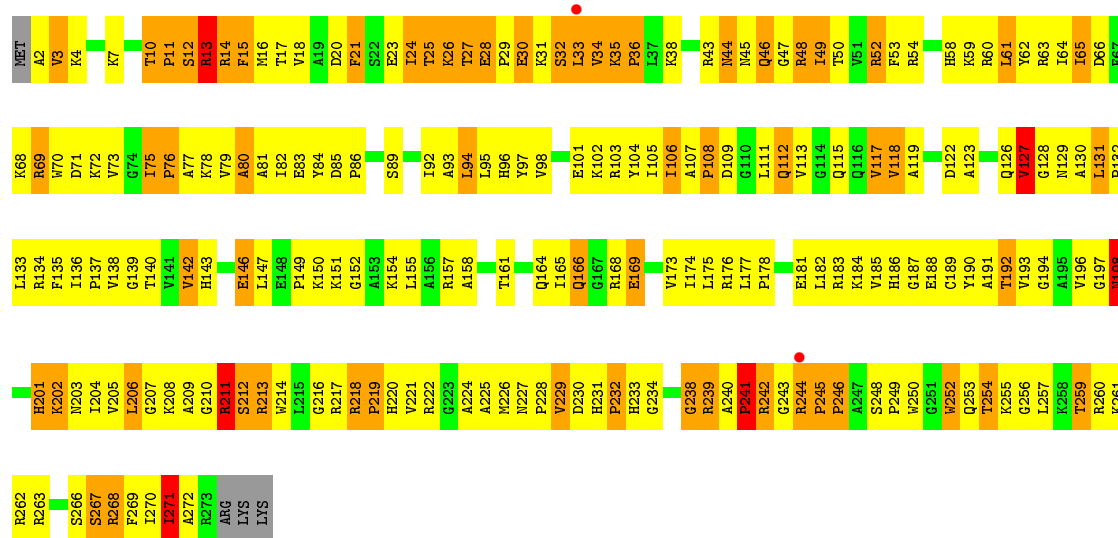


- Molecule 29: 50S ribosomal protein L1

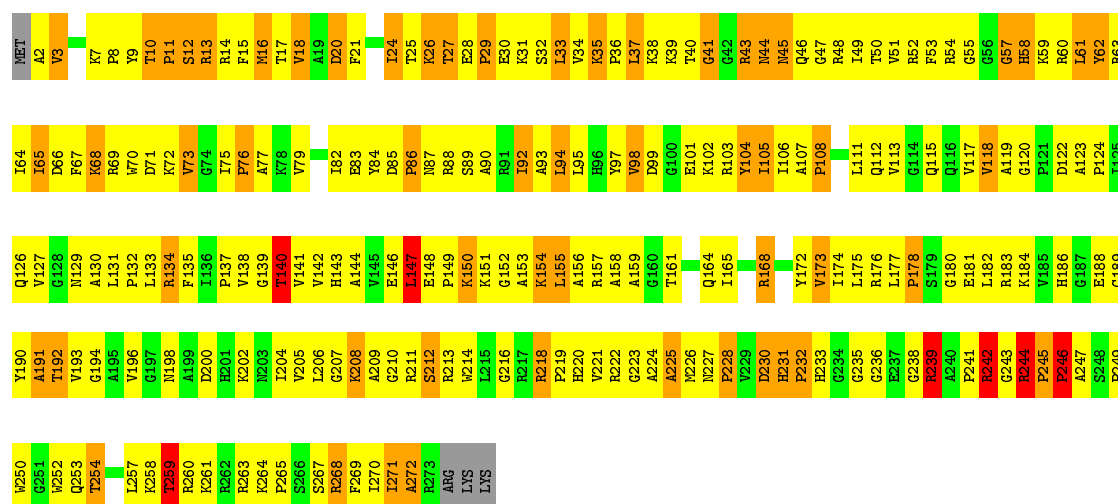




• Molecule 30: 50S ribosomal protein L2

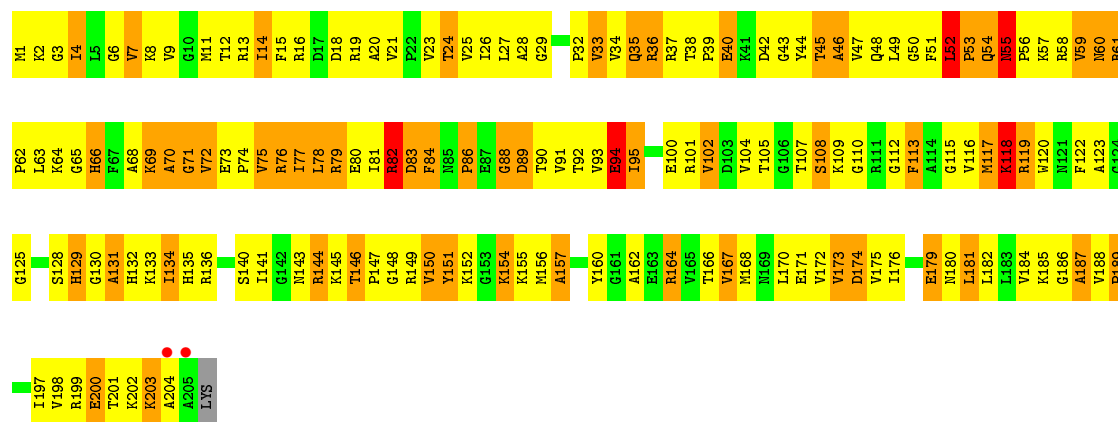


• Molecule 30: 50S ribosomal protein L2

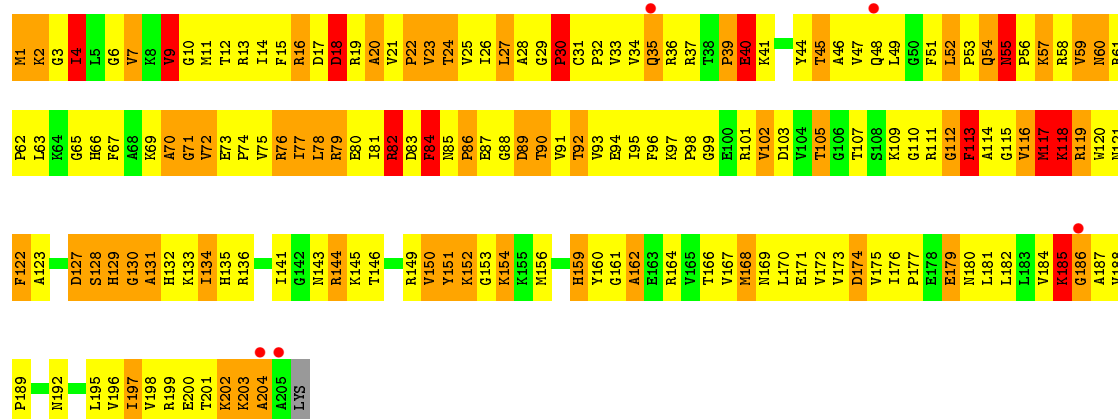
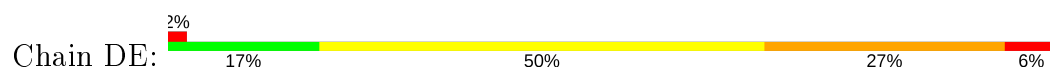


• Molecule 31: 50S ribosomal protein L3

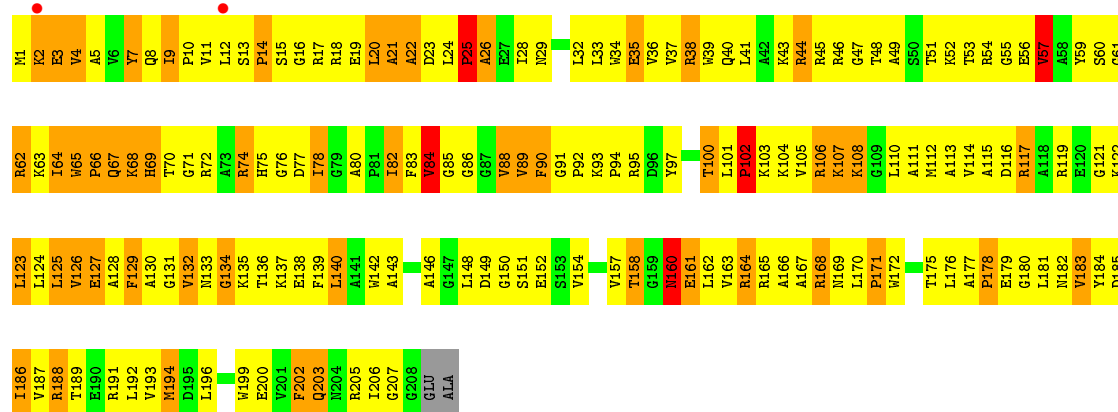
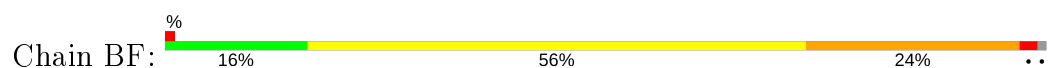




• Molecule 31: 50S ribosomal protein L3

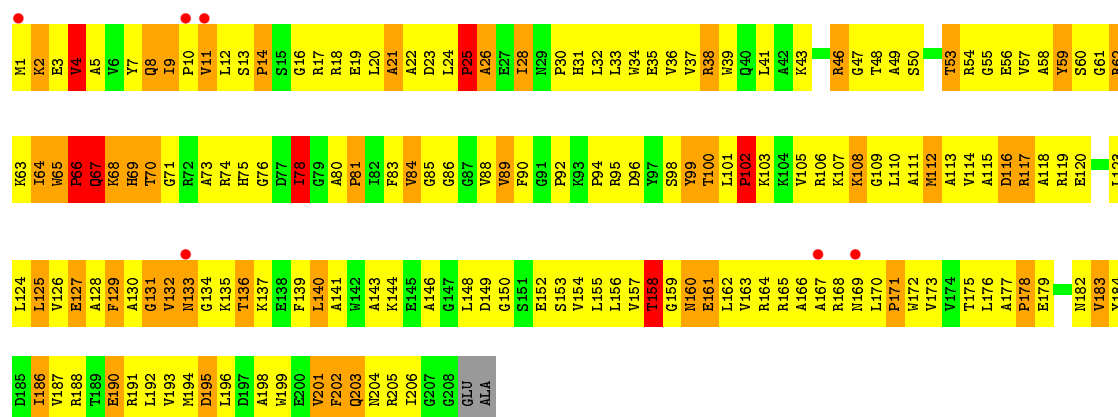


• Molecule 32: 50S ribosomal protein L4

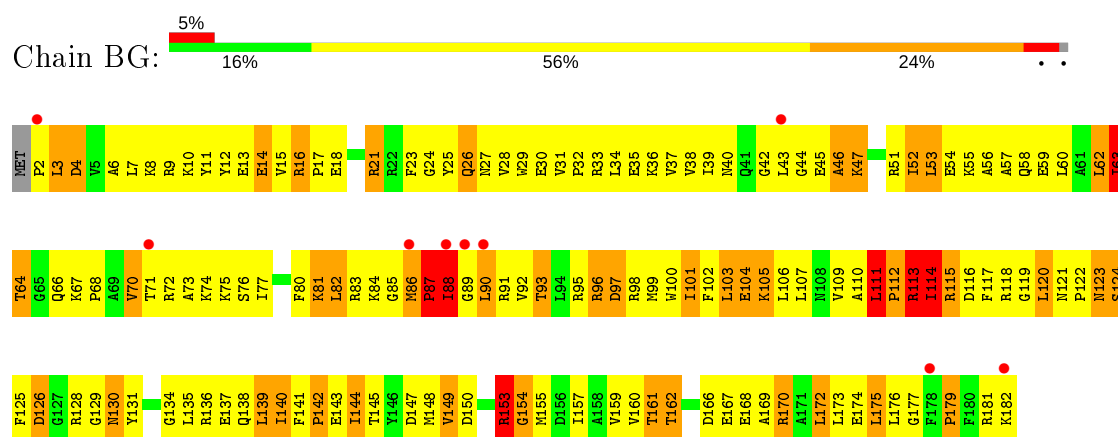


• Molecule 32: 50S ribosomal protein L4

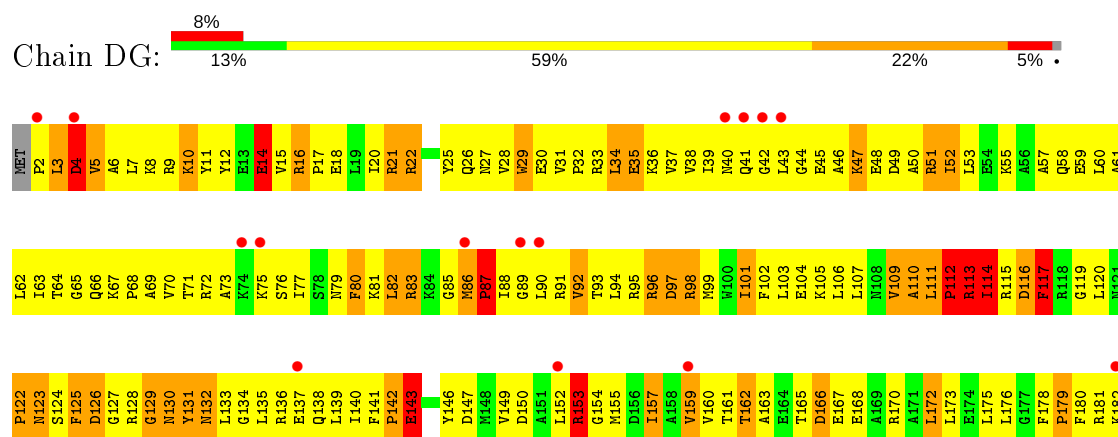




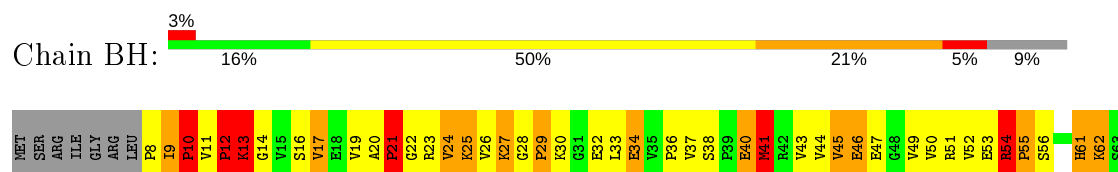
• Molecule 33: 50S ribosomal protein L5



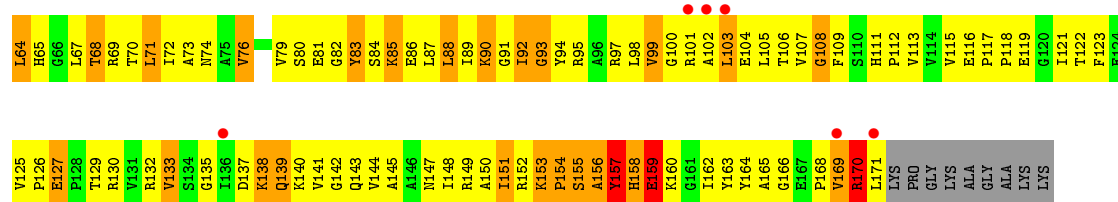
• Molecule 33: 50S ribosomal protein L5



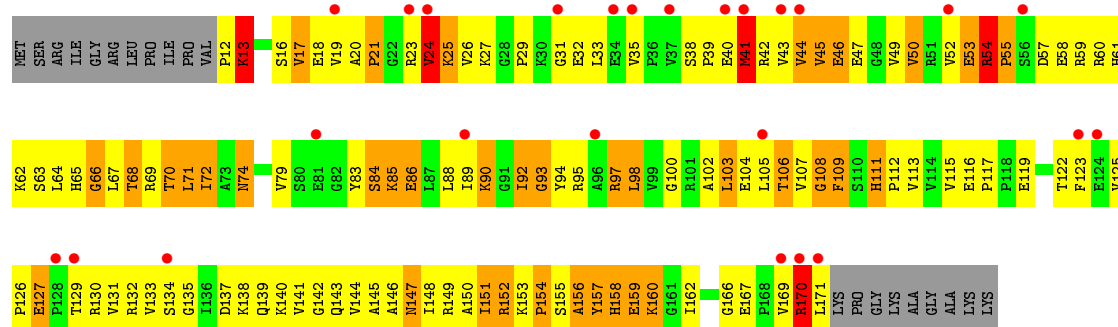
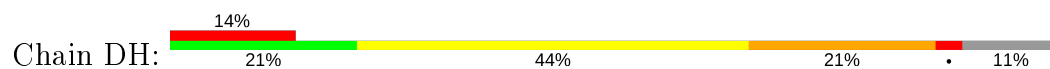
• Molecule 34: 50S ribosomal protein L6



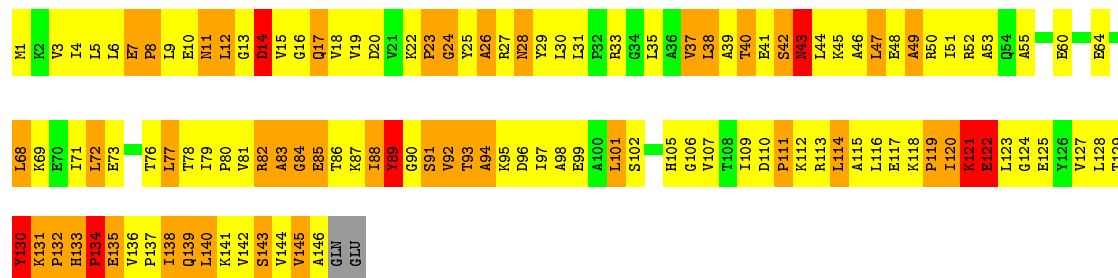
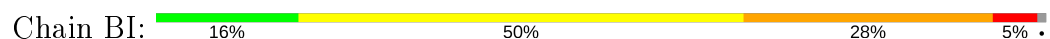




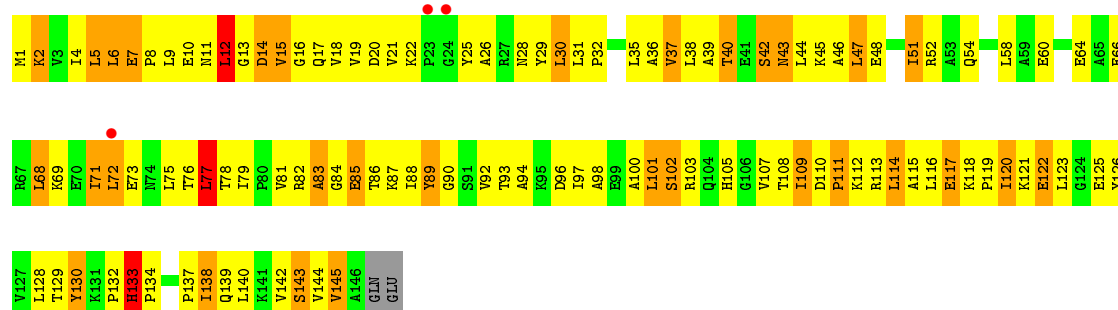
• Molecule 34: 50S ribosomal protein L6



• Molecule 35: 50S ribosomal protein L9

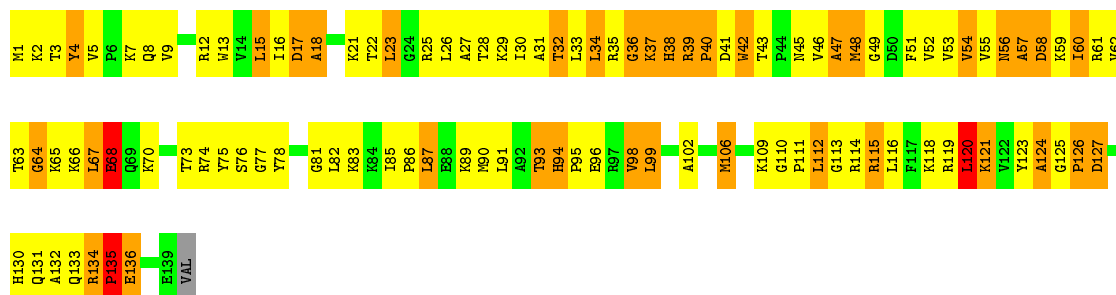


• Molecule 35: 50S ribosomal protein L9




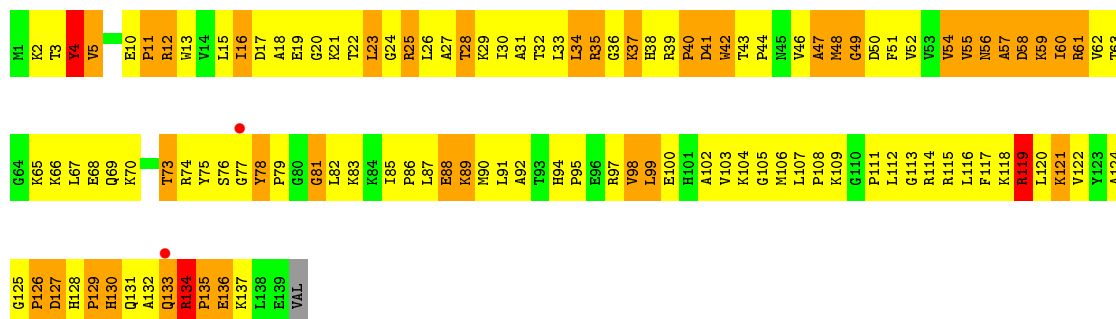
• Molecule 36: 50S ribosomal protein L13

Chain BN:  23% 49% 26% ..



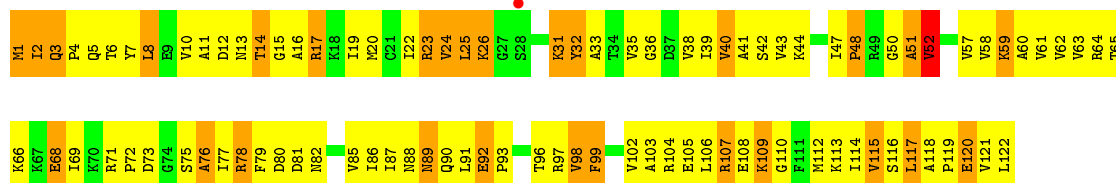
- Molecule 36: 50S ribosomal protein L13

Chain DN:  14% 55% 28% ..

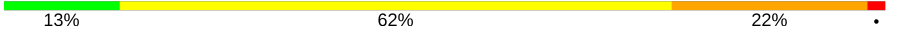


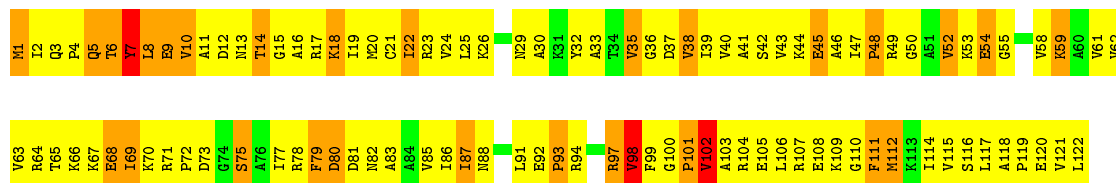
- Molecule 37: 50S ribosomal protein L14

Chain BO:  21% 55% 23% .




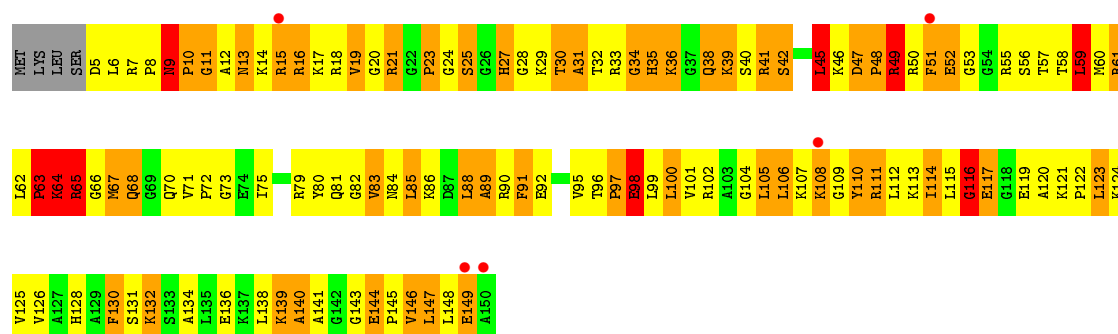
- Molecule 37: 50S ribosomal protein L14

Chain DO:  13% 62% 22% .

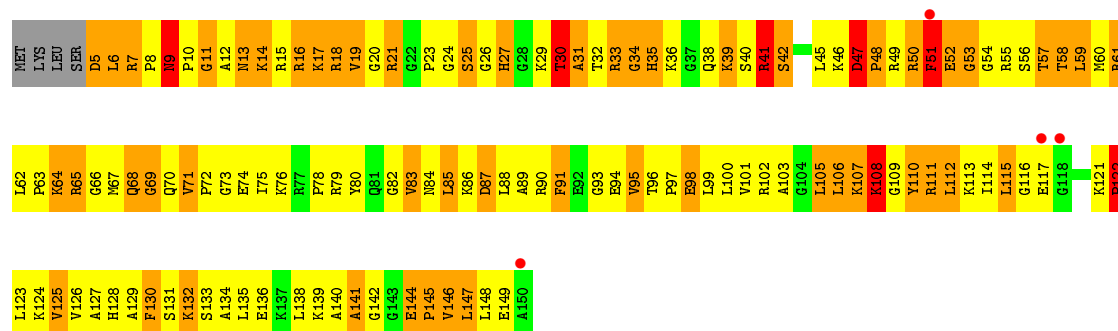


- Molecule 38: 50S ribosomal protein L15

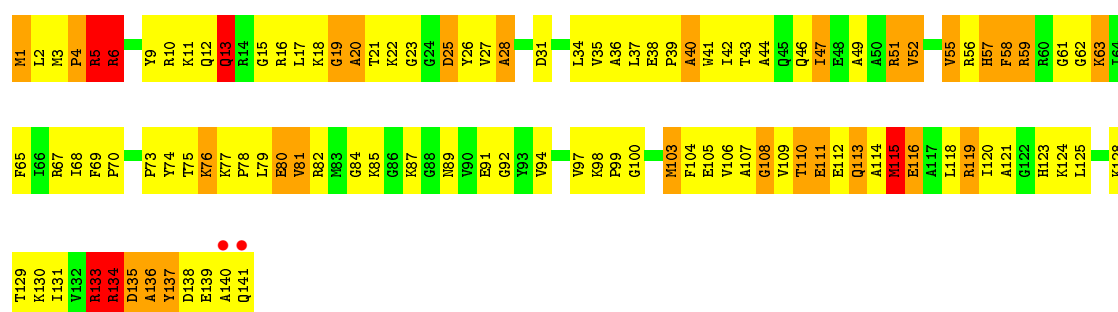
Chain BP:  3% 15% 43% 33% 6% .



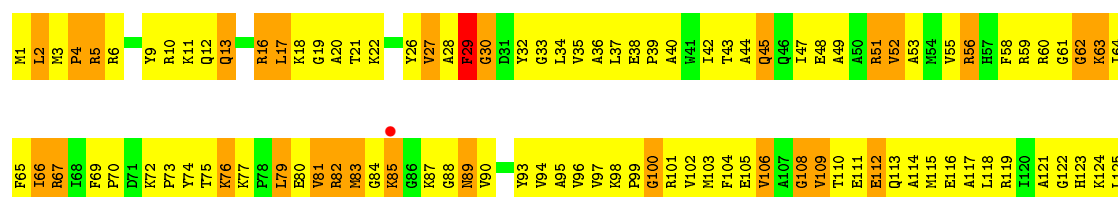
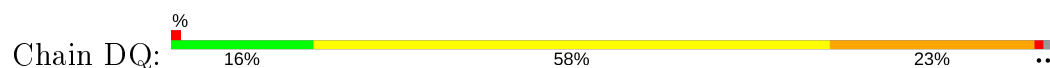
• Molecule 38: 50S ribosomal protein L15

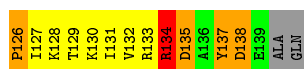


• Molecule 39: 50S ribosomal protein L16



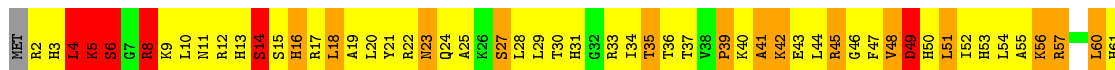
• Molecule 39: 50S ribosomal protein L16





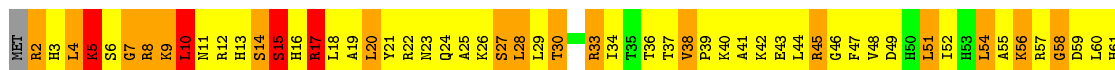
- Molecule 40: 50S ribosomal protein L17

Chain BR: 17% 56% 21% 5% •



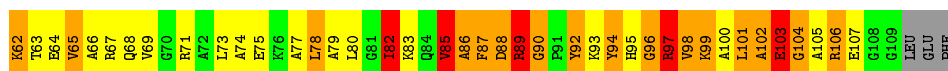
- Molecule 40: 50S ribosomal protein L17

Chain DR: 13% 51% 31% 5% •



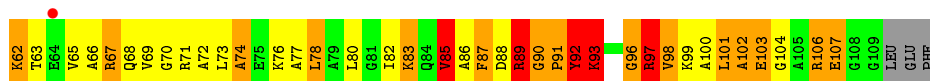
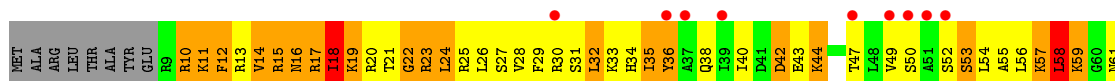
- Molecule 41: 50S ribosomal protein L18

Chain BS: 13% 42% 26% 7% 12%



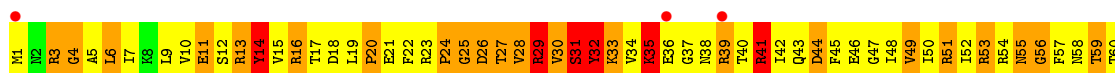
- Molecule 41: 50S ribosomal protein L18

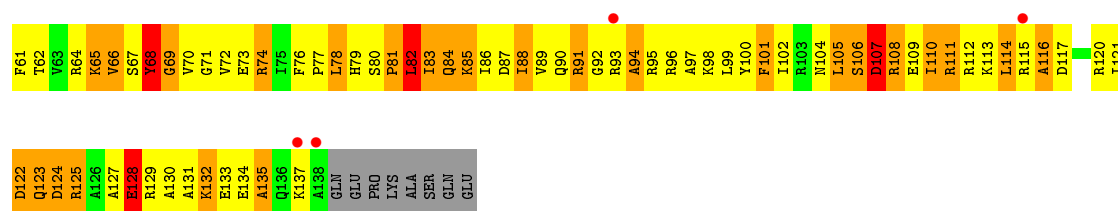
Chain DS: 9% 17% 37% 30% 6% 10%



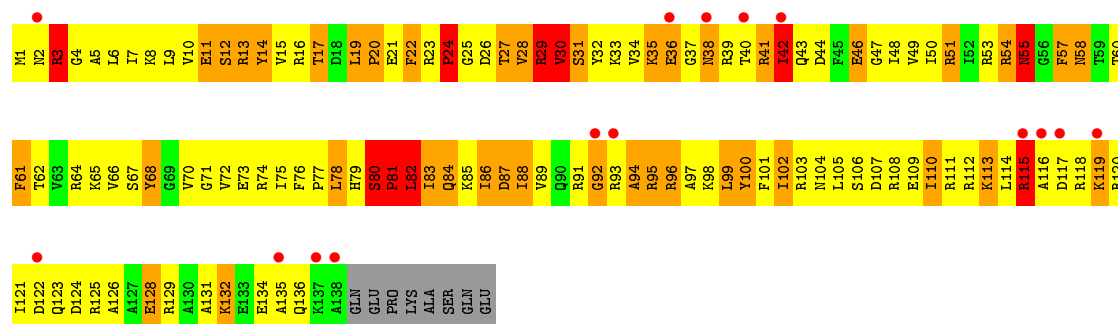
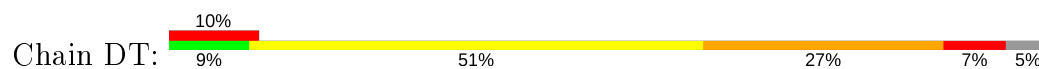
- Molecule 42: 50S ribosomal protein L19

Chain BT: 5% 7% 48% 33% 7% 5%

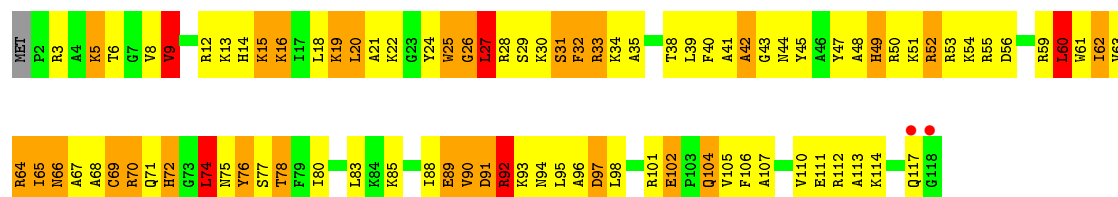




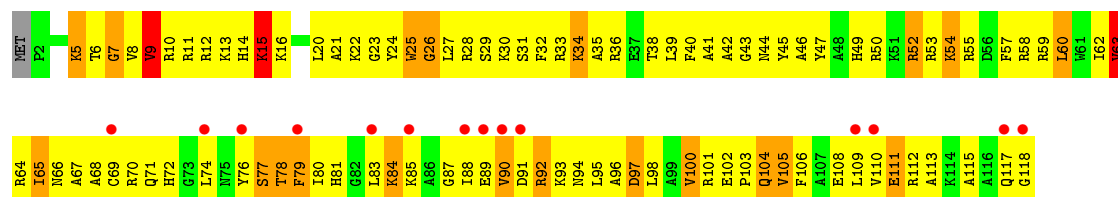
• Molecule 42: 50S ribosomal protein L19



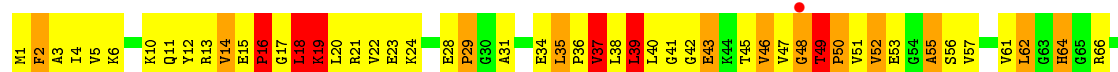
• Molecule 43: 50S ribosomal protein L20



• Molecule 43: 50S ribosomal protein L20

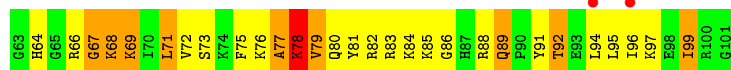
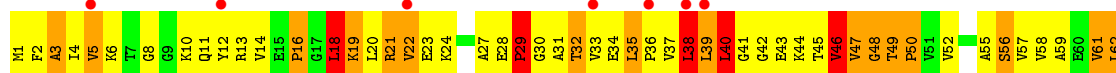
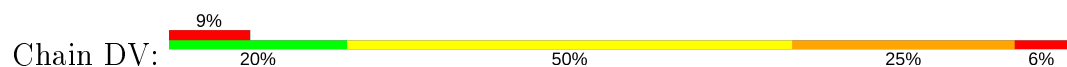


• Molecule 44: 50S ribosomal protein L21

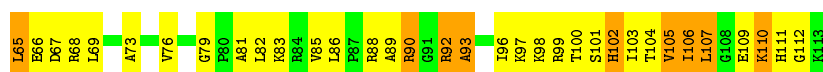
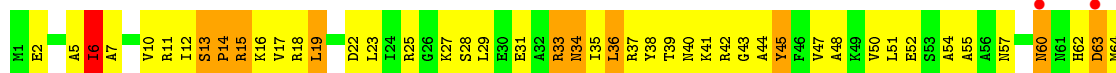




- Molecule 44: 50S ribosomal protein L21



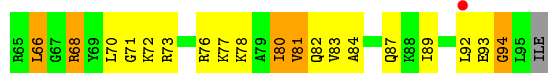
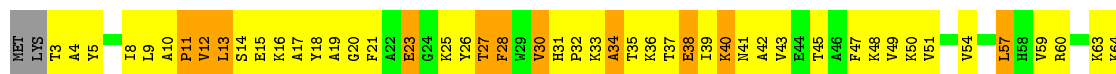
- Molecule 45: 50S ribosomal protein L22



- Molecule 45: 50S ribosomal protein L22

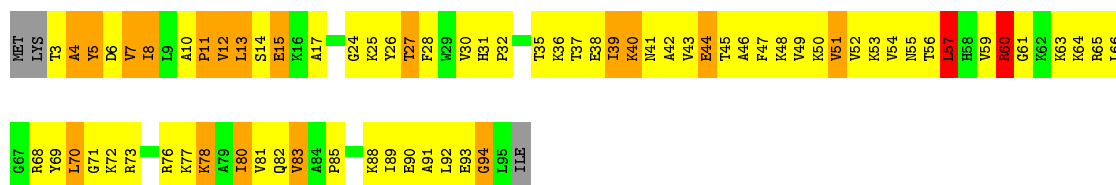


- Molecule 46: 50S ribosomal protein L23

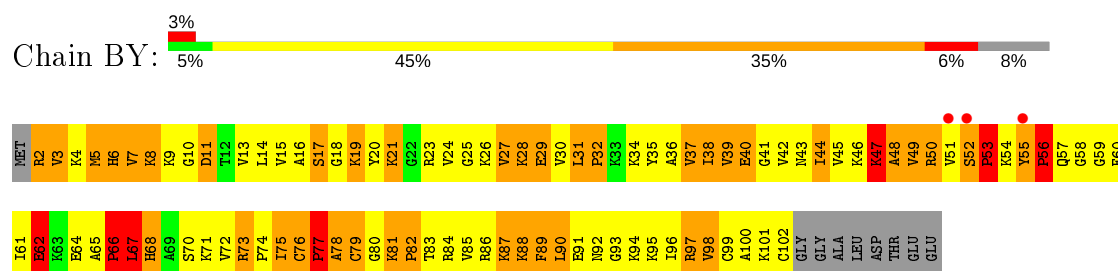


- Molecule 46: 50S ribosomal protein L23

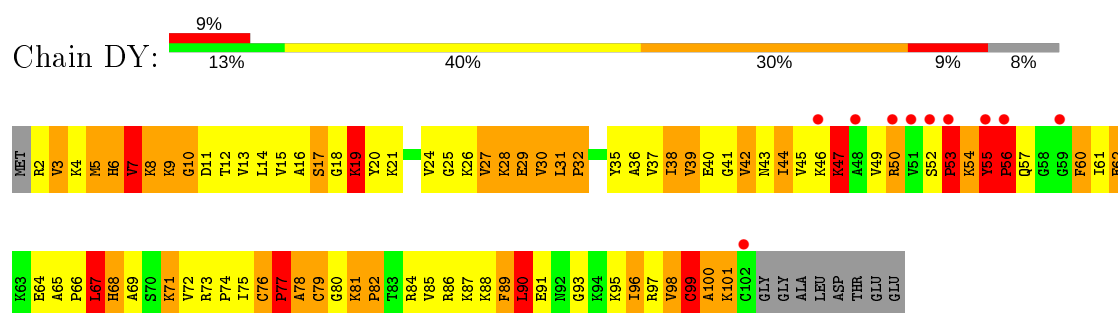




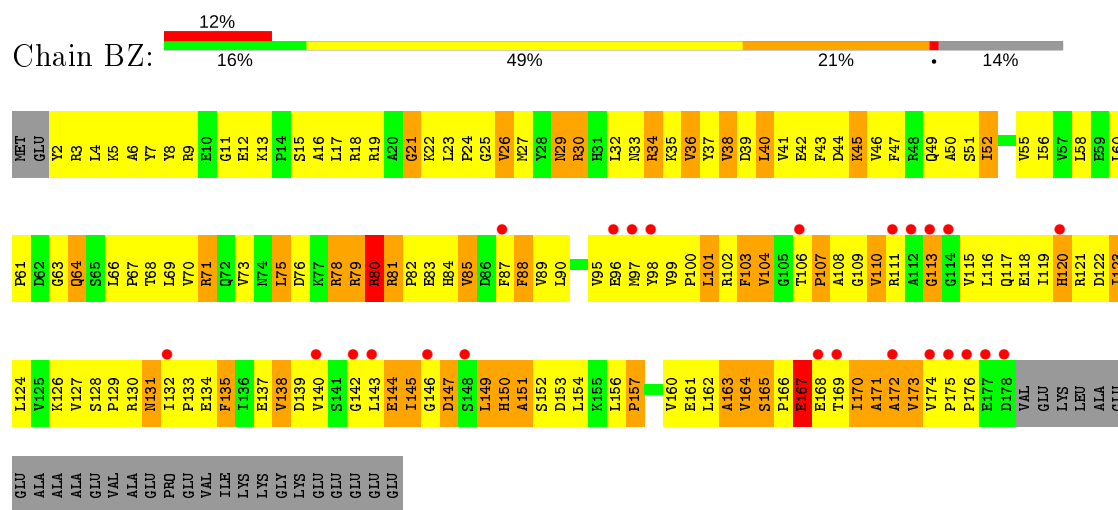
- Molecule 47: 50S ribosomal protein L24



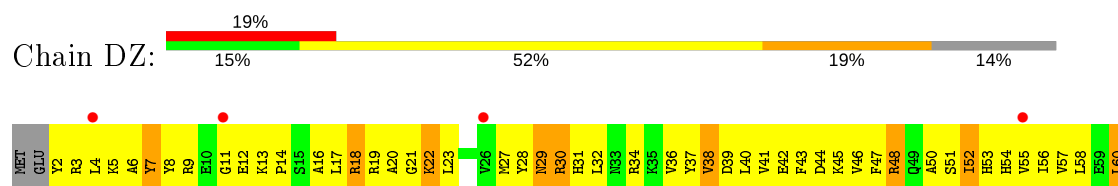
- Molecule 47: 50S ribosomal protein L24

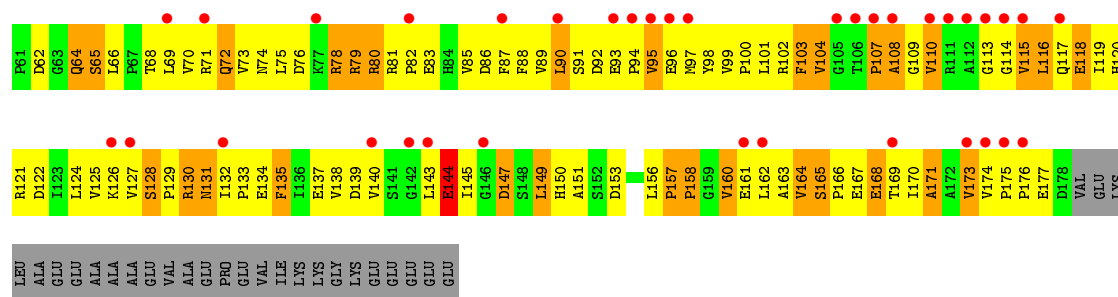


- Molecule 48: 50S ribosomal protein L25

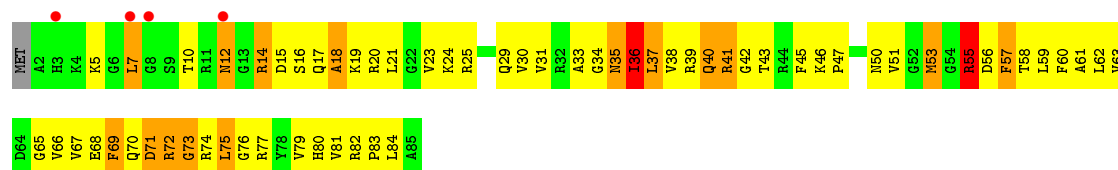


- Molecule 48: 50S ribosomal protein L25

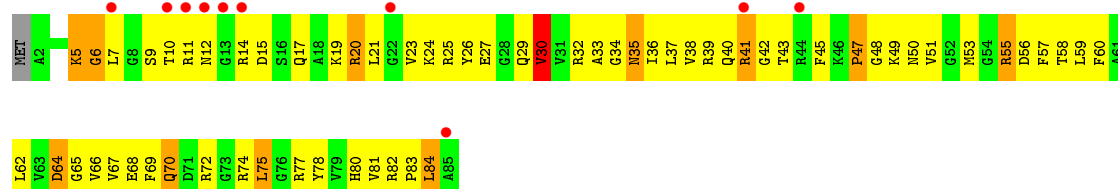




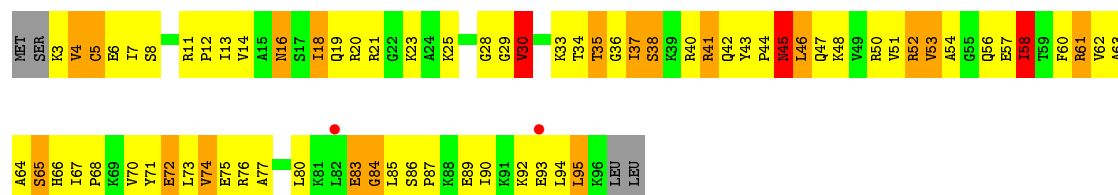
- Molecule 49: 50S ribosomal protein L27



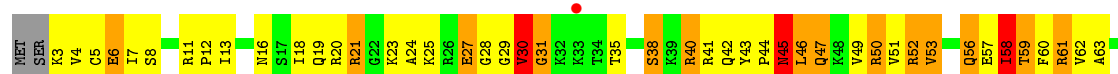
- Molecule 49: 50S ribosomal protein L27



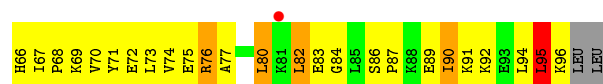
- Molecule 50: 50S ribosomal protein L28



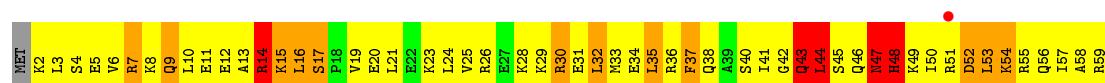
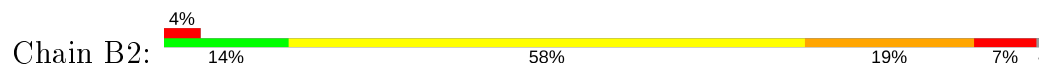
- Molecule 50: 50S ribosomal protein L28







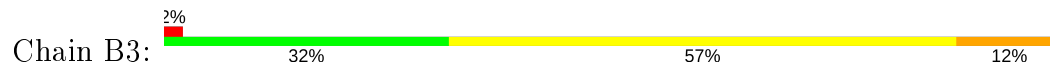
- Molecule 51: 50S ribosomal protein L29



- Molecule 51: 50S ribosomal protein L29



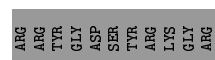
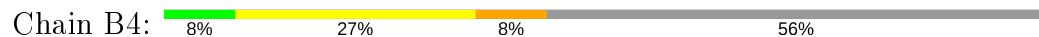
- Molecule 52: 50S ribosomal protein L30




- Molecule 52: 50S ribosomal protein L30

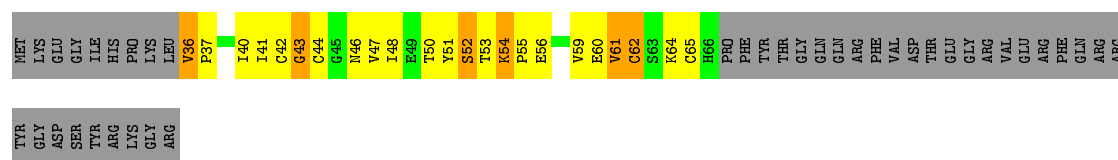


- Molecule 53: 50S ribosomal protein L31



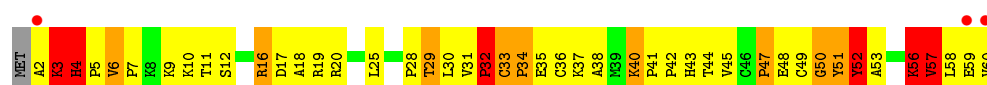
- Molecule 53: 50S ribosomal protein L31

Chain D4: 



- Molecule 54: 50S ribosomal protein L32

Chain B5: 



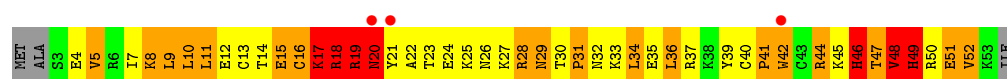
- Molecule 54: 50S ribosomal protein L32

Chain D5: 



- Molecule 55: 50S ribosomal protein L33

Chain B6: 



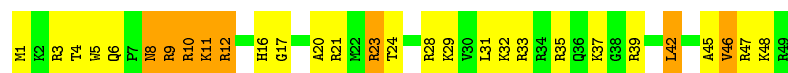
- Molecule 55: 50S ribosomal protein L33

Chain D6: 



- Molecule 56: 50S ribosomal protein L34

Chain B7: 

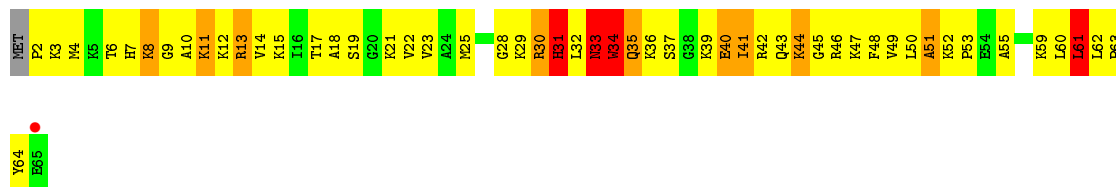


- Molecule 56: 50S ribosomal protein L34

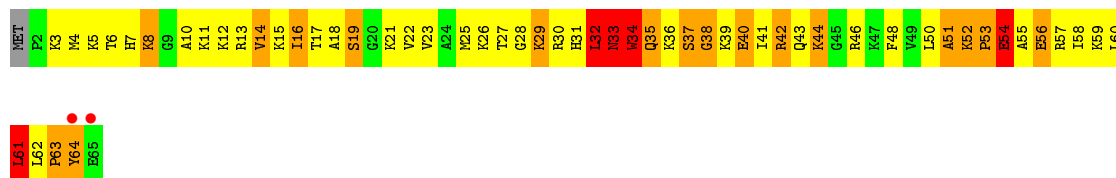
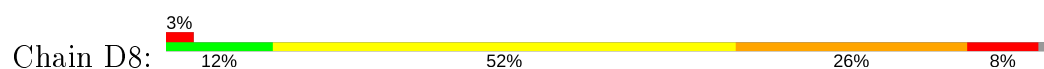
Chain D7: 



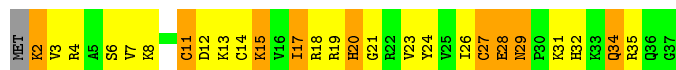
- Molecule 57: 50S ribosomal protein L35



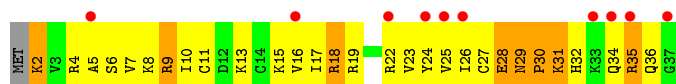
- Molecule 57: 50S ribosomal protein L35



- Molecule 58: 50S ribosomal protein L36



- Molecule 58: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.23Å 448.51Å 633.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.93 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 94.2 (49.93-3.00)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.248 , 0.272 0.250 , 0.281	Depositor DCC
$R_{free}$ test set	55515 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.5	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 91.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	294559	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DPP, MG, KBE, UAL, 5OH

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	0.52	0/35980	0.82	47/56157 (0.1%)
1	CA	0.50	0/35980	0.82	32/56157 (0.1%)
2	AB	0.38	0/1936	0.73	0/2611
2	CB	0.37	0/1936	0.71	0/2611
3	AC	0.37	0/1637	0.74	1/2207 (0.0%)
3	CC	0.37	0/1637	0.73	0/2207
4	AD	0.45	0/1733	0.76	1/2318 (0.0%)
4	CD	0.44	0/1733	0.80	2/2318 (0.1%)
5	AE	0.43	0/1163	0.77	0/1566
5	CE	0.43	0/1163	0.77	0/1566
6	AF	0.41	0/856	0.71	0/1154
6	CF	0.41	0/856	0.72	0/1154
7	AG	0.39	0/1276	0.75	1/1709 (0.1%)
7	CG	0.40	0/1276	0.69	0/1709
8	AH	0.42	0/1136	0.76	0/1527
8	CH	0.40	0/1136	0.73	0/1527
9	AI	0.36	0/1023	0.71	0/1371
9	CI	0.37	0/1024	0.68	0/1372
10	AJ	0.37	0/808	0.68	0/1087
10	CJ	0.39	0/808	0.72	0/1087
11	AK	0.40	0/900	0.77	1/1213 (0.1%)
11	CK	0.41	0/900	0.77	1/1213 (0.1%)
12	AL	0.47	0/987	0.89	0/1322
12	CL	0.43	0/987	0.79	0/1322
13	AM	0.44	0/957	0.80	0/1284
13	CM	0.89	5/920 (0.5%)	1.22	13/1241 (1.0%)
14	AN	0.43	0/501	0.73	0/664
14	CN	0.42	0/501	0.72	1/664 (0.2%)
15	AO	0.43	0/745	0.71	0/992
15	CO	0.41	0/745	0.67	0/992
16	AP	0.43	0/717	0.78	1/965 (0.1%)
16	CP	0.40	0/717	0.70	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.44	0/837	0.77	0/1119
17	CQ	0.40	0/837	0.74	0/1119
18	AR	0.45	0/579	0.82	0/768
18	CR	0.44	0/579	0.82	0/768
19	AS	0.41	0/643	0.71	0/867
19	CS	0.39	0/643	0.69	0/867
20	AT	0.38	0/765	0.80	0/1007
20	CT	0.39	0/765	0.77	0/1007
21	AU	0.46	0/213	0.77	0/279
21	CU	0.36	0/213	0.66	0/279
22	AV	0.56	0/239	0.66	0/371
22	CV	0.49	0/239	0.81	1/371 (0.3%)
23	AW	0.50	0/1778	0.76	0/2768
23	CW	0.43	0/1778	0.74	0/2768
24	AX	0.50	0/1832	0.74	0/2855
24	CX	0.49	0/1832	0.73	1/2855 (0.0%)
25	AY	0.36	0/1776	0.71	0/2766
25	CY	0.39	0/1776	0.73	0/2766
26	AZ	0.95	0/11	0.62	0/13
26	CZ	1.05	0/11	0.87	0/13
27	BA	0.64	0/67544	0.87	94/105433 (0.1%)
27	DA	0.55	0/67547	0.85	93/105438 (0.1%)
28	BB	0.58	0/2826	0.85	4/4406 (0.1%)
28	DB	0.50	0/2826	0.85	4/4406 (0.1%)
29	BC	0.29	0/1145	0.64	0/1556
29	DC	0.30	0/1145	0.67	0/1556
30	BD	0.60	2/2155 (0.1%)	0.94	3/2907 (0.1%)
30	DD	0.52	0/2155	0.90	5/2907 (0.2%)
31	BE	0.55	0/1597	0.92	0/2155
31	DE	0.46	0/1597	0.89	3/2155 (0.1%)
32	BF	0.50	0/1659	0.83	0/2246
32	DF	0.44	0/1659	0.81	1/2246 (0.0%)
33	BG	0.52	1/1499 (0.1%)	0.91	5/2016 (0.2%)
33	DG	0.50	1/1499 (0.1%)	0.89	5/2016 (0.2%)
34	BH	0.54	1/1277 (0.1%)	0.89	3/1729 (0.2%)
34	DH	0.35	0/1246	0.76	0/1684
35	BI	0.37	0/1057	0.81	0/1453
35	DI	0.38	0/1061	0.81	0/1458
36	BN	0.54	0/1132	0.89	2/1527 (0.1%)
36	DN	0.41	0/1132	0.79	0/1527
37	BO	0.50	0/943	0.90	4/1269 (0.3%)
37	DO	0.48	0/943	0.79	0/1269
38	BP	0.60	0/1131	1.14	9/1504 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DP	0.49	0/1131	0.97	5/1504 (0.3%)
39	BQ	0.52	0/1143	0.79	0/1527
39	DQ	0.41	0/1128	0.73	0/1508
40	BR	0.53	0/974	0.94	6/1302 (0.5%)
40	DR	0.45	0/974	0.87	2/1302 (0.2%)
41	BS	0.50	0/779	1.01	4/1038 (0.4%)
41	DS	0.42	0/785	0.92	3/1048 (0.3%)
42	BT	0.54	0/1156	0.99	5/1544 (0.3%)
42	DT	0.48	0/1156	0.89	2/1544 (0.1%)
43	BU	0.57	0/975	0.86	2/1297 (0.2%)
43	DU	0.42	0/975	0.84	3/1297 (0.2%)
44	BV	0.51	0/790	0.95	3/1057 (0.3%)
44	DV	0.42	0/790	0.82	0/1057
45	BW	0.52	0/907	0.88	2/1216 (0.2%)
45	DW	0.50	0/907	0.85	0/1216
46	BX	0.53	0/740	0.89	0/995
46	DX	0.48	0/740	0.81	1/995 (0.1%)
47	BY	0.56	0/789	1.06	3/1053 (0.3%)
47	DY	0.48	0/789	0.93	3/1053 (0.3%)
48	BZ	0.42	0/1436	0.74	0/1951
48	DZ	0.36	0/1436	0.70	0/1951
49	B0	0.53	0/671	0.81	1/892 (0.1%)
49	D0	0.45	0/671	0.73	0/892
50	B1	0.49	0/722	0.82	0/964
50	D1	0.47	0/739	0.79	0/983
51	B2	0.55	0/600	0.86	1/793 (0.1%)
51	D2	0.42	0/600	0.74	0/793
52	B3	0.52	0/473	0.84	0/636
52	D3	0.41	0/473	0.81	0/636
53	B4	0.42	0/229	0.86	0/311
53	D4	0.50	0/229	1.01	2/311 (0.6%)
54	B5	0.53	0/473	0.95	2/639 (0.3%)
54	D5	0.46	0/473	0.79	0/639
55	B6	0.75	0/418	1.17	3/562 (0.5%)
55	D6	0.80	1/397 (0.3%)	1.20	4/531 (0.8%)
56	B7	0.59	0/427	0.92	1/563 (0.2%)
56	D7	0.50	0/427	0.85	0/563
57	B8	0.59	0/516	1.01	1/681 (0.1%)
57	D8	0.50	0/516	0.95	3/681 (0.4%)
58	B9	0.54	0/302	0.88	0/397
58	D9	0.33	0/302	0.74	0/397
All	All	0.54	11/318953 (0.0%)	0.84	400/477060 (0.1%)

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
1	AA	0	90
1	CA	1	81
13	CM	0	1
22	CV	0	2
23	AW	0	1
23	CW	0	2
27	BA	0	223
27	DA	0	164
28	BB	0	6
28	DB	0	6
30	DD	0	1
36	DN	0	1
47	BY	0	1
54	D5	0	1
55	B6	0	1
55	D6	0	1
All	All	1	582

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	CM	113	PRO	N-CD	-7.63	1.37	1.47
55	D6	46	HIS	C-N	-6.65	1.18	1.34
34	BH	11	VAL	C-N	6.53	1.46	1.34
13	CM	65	LYS	C-N	6.24	1.48	1.34
33	BG	111	LEU	C-N	5.78	1.45	1.34

The worst 5 of 400 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	CM	70	LEU	N-CA-C	-12.04	78.50	111.00
27	BA	2424	C	N1-C1'-C2'	-11.64	98.86	114.00
55	B6	46	HIS	N-CA-C	11.54	142.16	111.00
38	BP	52	GLU	N-CA-C	11.01	140.73	111.00
27	DA	1782	C	N1-C1'-C2'	-10.49	100.36	114.00

All (1) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	CA	517	G	C3'

5 of 582 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	34	C	Sidechain
1	AA	49	U	Sidechain
1	AA	52	G	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32141	0	16225	1910	0
1	CA	32141	0	16225	2201	0
2	AB	1901	0	1951	267	0
2	CB	1901	0	1951	267	0
3	AC	1613	0	1677	233	0
3	CC	1613	0	1677	215	0
4	AD	1703	0	1764	222	0
4	CD	1703	0	1764	256	0
5	AE	1147	0	1207	175	0
5	CE	1147	0	1207	184	0
6	AF	843	0	857	110	0
6	CF	843	0	857	121	0
7	AG	1257	0	1296	180	0
7	CG	1257	0	1296	149	0
8	AH	1116	0	1177	206	0
8	CH	1116	0	1177	178	0
9	AI	1005	0	1032	145	0
9	CI	1006	0	1034	145	0
10	AJ	795	0	840	164	0
10	CJ	795	0	840	157	0
11	AK	885	0	904	123	0
11	CK	885	0	904	113	0
12	AL	971	0	1057	167	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	CL	971	0	1057	185	0
13	AM	947	0	999	196	0
13	CM	910	0	931	185	0
14	AN	492	0	533	99	0
14	CN	492	0	533	106	0
15	AO	734	0	771	116	0
15	CO	734	0	771	104	0
16	AP	701	0	720	113	0
16	CP	701	0	720	96	0
17	AQ	824	0	891	109	0
17	CQ	824	0	891	121	0
18	AR	574	0	644	90	0
18	CR	574	0	644	73	0
19	AS	630	0	652	109	0
19	CS	630	0	652	106	0
20	AT	763	0	861	118	0
20	CT	763	0	861	132	0
21	AU	209	0	221	24	0
21	CU	209	0	221	33	0
22	AV	213	0	110	6	0
22	CV	213	0	110	12	0
23	AW	1593	0	810	80	0
23	CW	1593	0	810	75	0
24	AX	1640	0	837	69	0
24	CX	1640	0	837	74	0
25	AY	1591	0	810	83	0
25	CY	1591	0	810	87	0
26	AZ	48	0	40	12	0
26	CZ	48	0	40	19	0
27	BA	60311	0	30410	3525	0
27	DA	60313	0	30409	3995	0
28	BB	2528	0	1285	121	0
28	DB	2528	0	1285	140	0
29	BC	1142	0	865	101	0
29	DC	1142	0	865	133	0
30	BD	2105	0	2182	414	0
30	DD	2105	0	2182	386	0
31	BE	1564	0	1629	294	0
31	DE	1564	0	1629	325	0
32	BF	1624	0	1677	321	0
32	DF	1624	0	1677	262	0
33	BG	1474	0	1535	226	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DG	1474	0	1535	259	0
34	BH	1252	0	1316	235	0
34	DH	1223	0	1282	194	0
35	BI	1042	0	1031	193	0
35	DI	1046	0	1035	152	0
36	BN	1105	0	1180	171	0
36	DN	1105	0	1180	214	0
37	BO	933	0	996	170	0
37	DO	933	0	996	165	0
38	BP	1114	0	1187	295	0
38	DP	1114	0	1187	327	0
39	BQ	1122	0	1179	176	0
39	DQ	1107	0	1166	203	0
40	BR	960	0	1021	164	0
40	DR	960	0	1021	179	0
41	BS	771	0	832	160	0
41	DS	777	0	825	148	0
42	BT	1142	0	1202	279	0
42	DT	1142	0	1202	273	0
43	BU	958	0	1015	185	0
43	DU	958	0	1015	196	0
44	BV	779	0	852	166	0
44	DV	779	0	852	168	0
45	BW	896	0	953	103	0
45	DW	896	0	953	157	0
46	BX	726	0	778	103	0
46	DX	726	0	778	127	0
47	BY	776	0	870	215	0
47	DY	776	0	870	191	0
48	BZ	1404	0	1432	184	0
48	DZ	1404	0	1432	221	0
49	B0	662	0	688	89	0
49	D0	662	0	688	103	0
50	B1	715	0	766	118	0
50	D1	732	0	808	98	0
51	B2	598	0	653	112	0
51	D2	598	0	653	84	0
52	B3	468	0	523	56	0
52	D3	468	0	523	84	0
53	B4	226	0	226	40	0
53	D4	226	0	227	33	0
54	B5	459	0	476	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	D5	459	0	476	70	0
55	B6	411	0	403	122	0
55	D6	390	0	403	103	0
56	B7	419	0	467	49	0
56	D7	419	0	467	80	0
57	B8	508	0	576	122	0
57	D8	508	0	576	135	0
58	B9	299	0	323	50	0
58	D9	299	0	323	49	0
59	AA	133	0	0	0	0
59	AC	1	0	0	0	0
59	AD	1	0	0	0	0
59	AE	1	0	0	0	0
59	AF	1	0	0	0	0
59	AH	1	0	0	0	0
59	AK	2	0	0	0	0
59	AL	1	0	0	0	0
59	AO	1	0	0	0	0
59	AT	2	0	0	0	0
59	AW	7	0	0	0	0
59	AX	7	0	0	0	0
59	AY	2	0	0	0	0
59	B0	2	0	0	0	0
59	B5	1	0	0	0	0
59	BA	400	0	0	0	0
59	BB	1	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	2	0	0	0	0
59	BH	1	0	0	0	0
59	BN	1	0	0	0	0
59	BP	1	0	0	0	0
59	BQ	1	0	0	0	0
59	BR	1	0	0	0	0
59	BU	1	0	0	0	0
59	BX	1	0	0	0	0
59	BY	1	0	0	1	0
59	BZ	1	0	0	0	0
59	CA	92	0	0	0	0
59	CE	2	0	0	0	0
59	CQ	1	0	0	0	0
59	CV	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	CX	3	0	0	0	0
59	D5	2	0	0	0	0
59	D6	1	0	0	0	0
59	DA	275	0	0	0	0
59	DB	1	0	0	0	0
59	DD	3	0	0	0	0
59	DE	3	0	0	0	0
59	DF	1	0	0	0	0
59	DR	1	0	0	0	0
59	DZ	1	0	0	0	0
60	AD	1	0	0	1	0
60	B4	1	0	0	0	0
60	B5	1	0	0	0	0
60	B9	1	0	0	0	0
60	CD	1	0	0	1	0
60	D4	1	0	0	0	0
60	D5	1	0	0	0	0
60	D9	1	0	0	0	0
All	All	294559	0	198754	25938	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

The worst 5 of 25938 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BP:59:LEU:HA	38:BP:61:ARG:CZ	1.58	1.32
30:DD:231:HIS:ND1	30:DD:232:PRO:HD2	1.55	1.20
1:CA:1363(A):A:H1'	1:CA:1365:G:N7	1.57	1.19
40:BR:100:LEU:HD21	40:BR:113:LEU:HD13	1.24	1.19
27:BA:2787:C:H1'	31:BE:61:ARG:HG3	1.25	1.18

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	126 (54%)	73 (31%)	34 (15%)	0	1
2	CB	233/256 (91%)	151 (65%)	50 (22%)	32 (14%)	0	1
3	AC	205/239 (86%)	123 (60%)	54 (26%)	28 (14%)	0	1
3	CC	205/239 (86%)	121 (59%)	59 (29%)	25 (12%)	0	1
4	AD	206/209 (99%)	129 (63%)	52 (25%)	25 (12%)	0	1
4	CD	206/209 (99%)	126 (61%)	51 (25%)	29 (14%)	0	1
5	AE	149/162 (92%)	94 (63%)	38 (26%)	17 (11%)	0	2
5	CE	149/162 (92%)	103 (69%)	27 (18%)	19 (13%)	0	1
6	AF	99/101 (98%)	71 (72%)	18 (18%)	10 (10%)	0	2
6	CF	99/101 (98%)	76 (77%)	16 (16%)	7 (7%)	1	5
7	AG	153/156 (98%)	101 (66%)	39 (26%)	13 (8%)	1	4
7	CG	153/156 (98%)	102 (67%)	38 (25%)	13 (8%)	1	4
8	AH	136/138 (99%)	98 (72%)	27 (20%)	11 (8%)	1	4
8	CH	136/138 (99%)	81 (60%)	38 (28%)	17 (12%)	0	1
9	AI	125/128 (98%)	83 (66%)	29 (23%)	13 (10%)	0	2
9	CI	125/128 (98%)	82 (66%)	26 (21%)	17 (14%)	0	1
10	AJ	97/105 (92%)	64 (66%)	26 (27%)	7 (7%)	1	5
10	CJ	97/105 (92%)	55 (57%)	28 (29%)	14 (14%)	0	1
11	AK	117/129 (91%)	70 (60%)	34 (29%)	13 (11%)	0	2
11	CK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	6
12	AL	123/132 (93%)	75 (61%)	25 (20%)	23 (19%)	0	0
12	CL	123/132 (93%)	76 (62%)	24 (20%)	23 (19%)	0	0
13	AM	118/126 (94%)	64 (54%)	33 (28%)	21 (18%)	0	0
13	CM	117/126 (93%)	64 (55%)	29 (25%)	24 (20%)	0	0
14	AN	58/61 (95%)	29 (50%)	19 (33%)	10 (17%)	0	0
14	CN	58/61 (95%)	35 (60%)	12 (21%)	11 (19%)	0	0
15	AO	86/89 (97%)	56 (65%)	19 (22%)	11 (13%)	0	1
15	CO	86/89 (97%)	49 (57%)	28 (33%)	9 (10%)	0	2
16	AP	82/88 (93%)	49 (60%)	21 (26%)	12 (15%)	0	1
16	CP	82/88 (93%)	45 (55%)	28 (34%)	9 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	98/105 (93%)	73 (74%)	15 (15%)	10 (10%)	0	2
17	CQ	98/105 (93%)	70 (71%)	22 (22%)	6 (6%)	1	8
18	AR	68/88 (77%)	35 (52%)	21 (31%)	12 (18%)	0	0
18	CR	68/88 (77%)	41 (60%)	16 (24%)	11 (16%)	0	1
19	AS	77/93 (83%)	51 (66%)	15 (20%)	11 (14%)	0	1
19	CS	77/93 (83%)	46 (60%)	18 (23%)	13 (17%)	0	0
20	AT	97/106 (92%)	59 (61%)	20 (21%)	18 (19%)	0	0
20	CT	97/106 (92%)	52 (54%)	36 (37%)	9 (9%)	0	3
21	AU	23/27 (85%)	16 (70%)	4 (17%)	3 (13%)	0	1
21	CU	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	0
26	AZ	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
26	CZ	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
29	BC	183/229 (80%)	69 (38%)	49 (27%)	65 (36%)	0	0
29	DC	183/229 (80%)	69 (38%)	59 (32%)	55 (30%)	0	0
30	BD	270/276 (98%)	172 (64%)	66 (24%)	32 (12%)	0	1
30	DD	270/276 (98%)	180 (67%)	57 (21%)	33 (12%)	0	1
31	BE	203/206 (98%)	130 (64%)	38 (19%)	35 (17%)	0	0
31	DE	203/206 (98%)	125 (62%)	34 (17%)	44 (22%)	0	0
32	BF	206/210 (98%)	137 (66%)	31 (15%)	38 (18%)	0	0
32	DF	206/210 (98%)	125 (61%)	40 (19%)	41 (20%)	0	0
33	BG	179/182 (98%)	107 (60%)	47 (26%)	25 (14%)	0	1
33	DG	179/182 (98%)	109 (61%)	42 (24%)	28 (16%)	0	1
34	BH	162/180 (90%)	87 (54%)	43 (26%)	32 (20%)	0	0
34	DH	158/180 (88%)	88 (56%)	35 (22%)	35 (22%)	0	0
35	BI	144/148 (97%)	73 (51%)	33 (23%)	38 (26%)	0	0
35	DI	144/148 (97%)	80 (56%)	41 (28%)	23 (16%)	0	1
36	BN	137/140 (98%)	91 (66%)	27 (20%)	19 (14%)	0	1
36	DN	137/140 (98%)	82 (60%)	28 (20%)	27 (20%)	0	0
37	BO	120/122 (98%)	84 (70%)	25 (21%)	11 (9%)	1	3
37	DO	120/122 (98%)	80 (67%)	23 (19%)	17 (14%)	0	1
38	BP	144/150 (96%)	71 (49%)	42 (29%)	31 (22%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DP	144/150 (96%)	72 (50%)	36 (25%)	36 (25%)	0	0
39	BQ	139/141 (99%)	98 (70%)	21 (15%)	20 (14%)	0	1
39	DQ	137/141 (97%)	88 (64%)	29 (21%)	20 (15%)	0	1
40	BR	115/118 (98%)	75 (65%)	25 (22%)	15 (13%)	0	1
40	DR	115/118 (98%)	66 (57%)	31 (27%)	18 (16%)	0	1
41	BS	97/112 (87%)	45 (46%)	24 (25%)	28 (29%)	0	0
41	DS	99/112 (88%)	51 (52%)	14 (14%)	34 (34%)	0	0
42	BT	136/146 (93%)	78 (57%)	26 (19%)	32 (24%)	0	0
42	DT	136/146 (93%)	68 (50%)	32 (24%)	36 (26%)	0	0
43	BU	115/118 (98%)	70 (61%)	27 (24%)	18 (16%)	0	1
43	DU	115/118 (98%)	69 (60%)	30 (26%)	16 (14%)	0	1
44	BV	99/101 (98%)	61 (62%)	24 (24%)	14 (14%)	0	1
44	DV	99/101 (98%)	61 (62%)	19 (19%)	19 (19%)	0	0
45	BW	111/113 (98%)	77 (69%)	23 (21%)	11 (10%)	0	2
45	DW	111/113 (98%)	71 (64%)	29 (26%)	11 (10%)	0	2
46	BX	91/96 (95%)	67 (74%)	16 (18%)	8 (9%)	1	3
46	DX	91/96 (95%)	60 (66%)	17 (19%)	14 (15%)	0	1
47	BY	99/110 (90%)	42 (42%)	22 (22%)	35 (35%)	0	0
47	DY	99/110 (90%)	37 (37%)	29 (29%)	33 (33%)	0	0
48	BZ	175/206 (85%)	99 (57%)	49 (28%)	27 (15%)	0	1
48	DZ	175/206 (85%)	97 (55%)	51 (29%)	27 (15%)	0	1
49	B0	82/85 (96%)	62 (76%)	12 (15%)	8 (10%)	0	2
49	D0	82/85 (96%)	61 (74%)	14 (17%)	7 (8%)	1	4
50	B1	92/98 (94%)	60 (65%)	20 (22%)	12 (13%)	0	1
50	D1	92/98 (94%)	65 (71%)	16 (17%)	11 (12%)	0	1
51	B2	69/72 (96%)	46 (67%)	14 (20%)	9 (13%)	0	1
51	D2	69/72 (96%)	37 (54%)	20 (29%)	12 (17%)	0	0
52	B3	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	3	20
52	D3	58/60 (97%)	46 (79%)	10 (17%)	2 (3%)	3	20
53	B4	29/71 (41%)	18 (62%)	6 (21%)	5 (17%)	0	0
53	D4	29/71 (41%)	17 (59%)	9 (31%)	3 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	B5	57/60 (95%)	34 (60%)	13 (23%)	10 (18%)	0	0
54	D5	57/60 (95%)	33 (58%)	14 (25%)	10 (18%)	0	0
55	B6	49/54 (91%)	17 (35%)	14 (29%)	18 (37%)	0	0
55	D6	44/54 (82%)	16 (36%)	11 (25%)	17 (39%)	0	0
56	B7	47/49 (96%)	35 (74%)	8 (17%)	4 (8%)	1	4
56	D7	47/49 (96%)	30 (64%)	13 (28%)	4 (8%)	1	4
57	B8	62/65 (95%)	34 (55%)	19 (31%)	9 (14%)	0	1
57	D8	62/65 (95%)	32 (52%)	15 (24%)	15 (24%)	0	0
58	B9	34/37 (92%)	25 (74%)	8 (24%)	1 (3%)	4	24
58	D9	34/37 (92%)	18 (53%)	13 (38%)	3 (9%)	1	3
All	All	11702/12598 (93%)	7090 (61%)	2747 (24%)	1865 (16%)	0	1

5 of 1865 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	20	GLU
2	AB	96	ARG
2	AB	101	MET

### 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%)	169 (84%)	33 (16%)	2	11
2	CB	202/220 (92%)	174 (86%)	28 (14%)	3	16
3	AC	160/188 (85%)	129 (81%)	31 (19%)	1	7
3	CC	160/188 (85%)	140 (88%)	20 (12%)	4	20
4	AD	180/181 (99%)	147 (82%)	33 (18%)	1	9
4	CD	180/181 (99%)	147 (82%)	33 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	115/123 (94%)	101 (88%)	14 (12%)	5	21
5	CE	115/123 (94%)	96 (84%)	19 (16%)	2	11
6	AF	90/90 (100%)	80 (89%)	10 (11%)	6	25
6	CF	90/90 (100%)	78 (87%)	12 (13%)	4	17
7	AG	126/127 (99%)	106 (84%)	20 (16%)	2	12
7	CG	126/127 (99%)	106 (84%)	20 (16%)	2	12
8	AH	119/119 (100%)	96 (81%)	23 (19%)	1	8
8	CH	119/119 (100%)	105 (88%)	14 (12%)	5	22
9	AI	97/99 (98%)	80 (82%)	17 (18%)	2	10
9	CI	97/99 (98%)	85 (88%)	12 (12%)	4	20
10	AJ	88/92 (96%)	68 (77%)	20 (23%)	1	4
10	CJ	88/92 (96%)	74 (84%)	14 (16%)	2	12
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	9
11	CK	90/99 (91%)	78 (87%)	12 (13%)	4	17
12	AL	104/109 (95%)	87 (84%)	17 (16%)	2	11
12	CL	104/109 (95%)	90 (86%)	14 (14%)	4	17
13	AM	94/101 (93%)	75 (80%)	19 (20%)	1	6
13	CM	88/101 (87%)	69 (78%)	19 (22%)	1	5
14	AN	49/50 (98%)	39 (80%)	10 (20%)	1	6
14	CN	49/50 (98%)	37 (76%)	12 (24%)	0	3
15	AO	79/80 (99%)	63 (80%)	16 (20%)	1	6
15	CO	79/80 (99%)	65 (82%)	14 (18%)	2	9
16	AP	72/74 (97%)	63 (88%)	9 (12%)	4	20
16	CP	72/74 (97%)	60 (83%)	12 (17%)	2	11
17	AQ	94/97 (97%)	80 (85%)	14 (15%)	3	14
17	CQ	94/97 (97%)	84 (89%)	10 (11%)	6	26
18	AR	61/77 (79%)	53 (87%)	8 (13%)	4	18
18	CR	61/77 (79%)	55 (90%)	6 (10%)	8	30
19	AS	69/80 (86%)	53 (77%)	16 (23%)	1	4
19	CS	69/80 (86%)	51 (74%)	18 (26%)	0	2
20	AT	76/82 (93%)	63 (83%)	13 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	CT	76/82 (93%)	65 (86%)	11 (14%)	3	15
21	AU	19/22 (86%)	16 (84%)	3 (16%)	2	12
21	CU	19/22 (86%)	18 (95%)	1 (5%)	22	58
26	AZ	2/2 (100%)	2 (100%)	0	100	100
26	CZ	2/2 (100%)	2 (100%)	0	100	100
29	BC	61/181 (34%)	56 (92%)	5 (8%)	11	39
29	DC	61/181 (34%)	51 (84%)	10 (16%)	2	11
30	BD	213/218 (98%)	162 (76%)	51 (24%)	0	3
30	DD	213/218 (98%)	173 (81%)	40 (19%)	1	8
31	BE	165/166 (99%)	127 (77%)	38 (23%)	1	4
31	DE	165/166 (99%)	121 (73%)	44 (27%)	0	2
32	BF	165/166 (99%)	136 (82%)	29 (18%)	2	10
32	DF	165/166 (99%)	138 (84%)	27 (16%)	2	11
33	BG	155/156 (99%)	117 (76%)	38 (24%)	0	3
33	DG	155/156 (99%)	125 (81%)	30 (19%)	1	7
34	BH	136/148 (92%)	111 (82%)	25 (18%)	1	9
34	DH	132/148 (89%)	111 (84%)	21 (16%)	2	12
35	BI	102/124 (82%)	79 (78%)	23 (22%)	1	4
35	DI	103/124 (83%)	85 (82%)	18 (18%)	2	10
36	BN	117/119 (98%)	88 (75%)	29 (25%)	0	3
36	DN	117/119 (98%)	92 (79%)	25 (21%)	1	5
37	BO	100/100 (100%)	81 (81%)	19 (19%)	1	8
37	DO	100/100 (100%)	75 (75%)	25 (25%)	0	3
38	BP	112/116 (97%)	76 (68%)	36 (32%)	0	1
38	DP	112/116 (97%)	79 (70%)	33 (30%)	0	1
39	BQ	111/111 (100%)	85 (77%)	26 (23%)	1	4
39	DQ	110/111 (99%)	91 (83%)	19 (17%)	2	10
40	BR	100/101 (99%)	77 (77%)	23 (23%)	1	4
40	DR	100/101 (99%)	67 (67%)	33 (33%)	0	1
41	BS	77/88 (88%)	60 (78%)	17 (22%)	1	4
41	DS	76/88 (86%)	62 (82%)	14 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BT	120/127 (94%)	81 (68%)	39 (32%)	0	1
42	DT	120/127 (94%)	88 (73%)	32 (27%)	0	2
43	BU	92/94 (98%)	71 (77%)	21 (23%)	1	4
43	DU	92/94 (98%)	81 (88%)	11 (12%)	5	22
44	BV	82/82 (100%)	59 (72%)	23 (28%)	0	2
44	DV	82/82 (100%)	60 (73%)	22 (27%)	0	2
45	BW	91/92 (99%)	74 (81%)	17 (19%)	1	8
45	DW	91/92 (99%)	72 (79%)	19 (21%)	1	5
46	BX	74/78 (95%)	60 (81%)	14 (19%)	1	8
46	DX	74/78 (95%)	58 (78%)	16 (22%)	1	5
47	BY	84/91 (92%)	62 (74%)	22 (26%)	0	2
47	DY	84/91 (92%)	63 (75%)	21 (25%)	0	3
48	BZ	155/179 (87%)	127 (82%)	28 (18%)	1	9
48	DZ	155/179 (87%)	135 (87%)	20 (13%)	4	19
49	B0	66/67 (98%)	53 (80%)	13 (20%)	1	7
49	D0	66/67 (98%)	58 (88%)	8 (12%)	5	21
50	B1	74/83 (89%)	56 (76%)	18 (24%)	0	3
50	D1	78/83 (94%)	63 (81%)	15 (19%)	1	8
51	B2	66/67 (98%)	50 (76%)	16 (24%)	0	3
51	D2	66/67 (98%)	53 (80%)	13 (20%)	1	7
52	B3	51/52 (98%)	42 (82%)	9 (18%)	2	10
52	D3	51/52 (98%)	44 (86%)	7 (14%)	3	17
53	B4	27/63 (43%)	23 (85%)	4 (15%)	3	14
53	D4	27/63 (43%)	25 (93%)	2 (7%)	13	44
54	B5	51/52 (98%)	39 (76%)	12 (24%)	1	3
54	D5	51/52 (98%)	42 (82%)	9 (18%)	2	10
55	B6	43/52 (83%)	30 (70%)	13 (30%)	0	1
55	D6	44/52 (85%)	28 (64%)	16 (36%)	0	1
56	B7	41/42 (98%)	34 (83%)	7 (17%)	2	10
56	D7	41/42 (98%)	36 (88%)	5 (12%)	5	21
57	B8	53/55 (96%)	44 (83%)	9 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	D8	53/55 (96%)	39 (74%)	14 (26%)	0	2
58	B9	33/34 (97%)	24 (73%)	9 (27%)	0	2
58	D9	33/34 (97%)	28 (85%)	5 (15%)	3	14
All	All	9600/10432 (92%)	7750 (81%)	1850 (19%)	1	8

5 of 1850 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BY	97	ARG
4	CD	78	LEU
46	DX	68	ARG
48	BZ	153	ASP
55	B6	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 293 such sidechains are listed below:

Mol	Chain	Res	Type
48	BZ	33	ASN
3	CC	28	GLN
48	DZ	72	GLN
49	B0	29	GLN
55	B6	20	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1493/1509 (98%)	351 (23%)	136 (9%)
1	CA	1493/1509 (98%)	365 (24%)	120 (8%)
22	AV	9/30 (30%)	0	0
22	CV	9/30 (30%)	0	0
23	AW	74/75 (98%)	17 (22%)	2 (2%)
23	CW	74/75 (98%)	16 (21%)	4 (5%)
24	AX	76/77 (98%)	19 (25%)	1 (1%)
24	CX	76/77 (98%)	19 (25%)	0
25	AY	74/75 (98%)	23 (31%)	1 (1%)
25	CY	74/75 (98%)	22 (29%)	1 (1%)
27	BA	2792/2915 (95%)	798 (28%)	220 (7%)
27	DA	2793/2915 (95%)	905 (32%)	280 (10%)
28	BB	116/122 (95%)	26 (22%)	5 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	DB	116/122 (95%)	28 (24%)	8 (6%)
All	All	9269/9606 (96%)	2589 (27%)	778 (8%)

5 of 2589 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	31	G
1	AA	32	A

5 of 778 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	2792	G
1	CA	967	C
27	DA	2296	U
28	BB	25	A
1	CA	389	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
26	DPP	CZ	2	26	3,5,6	0.84	0	1,5,7	0.02	0
26	UAL	AZ	5	26	7,8,9	2.47	2 (28%)	5,9,11	1.47	1 (20%)
26	DPP	AZ	2	26	3,5,6	0.41	0	1,5,7	0.16	0
26	UAL	CZ	5	26	7,8,9	3.02	2 (28%)	5,9,11	3.74	4 (80%)
26	5OH	AZ	6	26	8,12,13	0.60	0	3,16,18	0.82	0
26	KBE	AZ	1	26	8,8,9	0.59	0	7,8,10	1.29	1 (14%)
26	5OH	CZ	6	26	8,12,13	0.76	0	3,16,18	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	KBE	CZ	1	26	8,8,9	0.65	0	7,8,10	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DPP	CZ	2	26	-	0/2/4/6	-
26	UAL	AZ	5	26	-	0/3/7/9	-
26	DPP	AZ	2	26	-	0/2/4/6	-
26	UAL	CZ	5	26	-	0/3/7/9	-
26	5OH	AZ	6	26	-	0/2/18/20	0/1/1/1
26	KBE	AZ	1	26	-	1/7/7/8	-
26	5OH	CZ	6	26	-	0/2/18/20	0/1/1/1
26	KBE	CZ	1	26	-	0/7/7/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	CZ	5	UAL	C1-N1	-6.66	1.29	1.40
26	AZ	5	UAL	C-CA	5.14	1.53	1.45
26	CZ	5	UAL	C-CA	3.71	1.51	1.45
26	AZ	5	UAL	C1-N1	-3.10	1.35	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	CZ	5	UAL	O2-C1-N2	-6.58	111.92	123.22
26	CZ	5	UAL	CA-CB-N1	-3.05	119.84	125.60
26	AZ	1	KBE	CB-CA-C	2.78	116.35	112.25
26	CZ	5	UAL	N2-C1-N1	2.73	121.55	115.50
26	CZ	5	UAL	O2-C1-N1	2.65	126.51	120.23

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	AZ	1	KBE	C-CA-CB-N

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	AZ	5	UAL	3	0
26	CZ	5	UAL	4	0
26	AZ	6	5OH	3	0
26	AZ	1	KBE	3	0
26	CZ	6	5OH	11	0
26	CZ	1	KBE	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 973 ligands modelled in this entry, 973 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	D6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D6	46:HIS	C	47:THR	N	1.18



## 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	1495/1509 (99%)	-0.10	29 (1%) 66 37	48, 83, 149, 196	0
1	CA	1495/1509 (99%)	-0.03	32 (2%) 63 34	59, 91, 155, 196	0
2	AB	235/256 (91%)	0.18	15 (6%) 19 6	80, 114, 144, 161	0
2	CB	235/256 (91%)	0.07	13 (5%) 25 9	81, 118, 152, 171	0
3	AC	207/239 (86%)	-0.09	4 (1%) 66 37	76, 101, 140, 153	0
3	CC	207/239 (86%)	0.02	9 (4%) 35 13	89, 109, 136, 147	0
4	AD	208/209 (99%)	-0.08	9 (4%) 35 13	65, 84, 101, 114	0
4	CD	208/209 (99%)	-0.26	2 (0%) 82 59	55, 77, 98, 107	0
5	AE	151/162 (93%)	-0.17	2 (1%) 77 51	59, 81, 107, 122	0
5	CE	151/162 (93%)	-0.03	0 100 100	72, 88, 109, 145	0
6	AF	101/101 (100%)	-0.30	0 100 100	63, 84, 93, 110	0
6	CF	101/101 (100%)	-0.24	0 100 100	76, 88, 101, 134	0
7	AG	155/156 (99%)	-0.06	9 (5%) 23 7	74, 94, 129, 151	0
7	CG	155/156 (99%)	-0.11	6 (3%) 39 15	84, 103, 128, 140	0
8	AH	138/138 (100%)	-0.33	1 (0%) 87 69	69, 84, 96, 107	0
8	CH	138/138 (100%)	-0.18	2 (1%) 75 49	74, 91, 102, 117	0
9	AI	127/128 (99%)	0.34	9 (7%) 16 5	76, 115, 136, 144	0
9	CI	127/128 (99%)	0.20	9 (7%) 16 5	89, 121, 139, 143	0
10	AJ	99/105 (94%)	0.81	14 (14%) 2 1	80, 127, 152, 164	0
10	CJ	99/105 (94%)	0.78	11 (11%) 5 1	88, 125, 148, 154	0
11	AK	119/129 (92%)	0.30	12 (10%) 7 2	55, 79, 107, 127	0
11	CK	119/129 (92%)	0.15	10 (8%) 11 3	69, 88, 108, 124	0
12	AL	125/132 (94%)	-0.15	0 100 100	55, 69, 91, 126	0
12	CL	125/132 (94%)	0.17	7 (5%) 24 8	66, 82, 98, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	120/126 (95%)	-0.26	4 (3%)	46	20	58, 86, 98, 107	0
13	CM	119/126 (94%)	-0.15	4 (3%)	45	19	80, 108, 125, 136	0
14	AN	60/61 (98%)	-0.02	1 (1%)	70	41	76, 92, 110, 122	0
14	CN	60/61 (98%)	0.30	2 (3%)	46	20	90, 105, 120, 123	0
15	AO	88/89 (98%)	-0.05	4 (4%)	33	12	64, 76, 99, 114	0
15	CO	88/89 (98%)	0.15	2 (2%)	60	31	71, 84, 106, 117	0
16	AP	84/88 (95%)	0.00	5 (5%)	21	7	68, 86, 108, 124	0
16	CP	84/88 (95%)	0.12	1 (1%)	79	54	71, 81, 105, 136	0
17	AQ	100/105 (95%)	0.16	2 (2%)	65	36	62, 79, 95, 99	0
17	CQ	100/105 (95%)	-0.23	0	100	100	64, 85, 100, 103	0
18	AR	70/88 (79%)	-0.12	2 (2%)	51	23	67, 83, 106, 134	0
18	CR	70/88 (79%)	-0.08	0	100	100	73, 86, 107, 134	0
19	AS	79/93 (84%)	0.66	11 (13%)	2	1	87, 105, 127, 134	0
19	CS	79/93 (84%)	0.71	11 (13%)	2	1	101, 122, 143, 154	0
20	AT	99/106 (93%)	0.06	7 (7%)	16	5	71, 89, 118, 130	0
20	CT	99/106 (93%)	0.03	7 (7%)	16	5	74, 90, 114, 125	0
21	AU	25/27 (92%)	2.00	12 (48%)	0	0	86, 92, 100, 118	0
21	CU	25/27 (92%)	2.32	12 (48%)	0	0	89, 104, 117, 119	0
22	AV	10/30 (33%)	0.45	1 (10%)	7	2	63, 73, 124, 133	0
22	CV	10/30 (33%)	-0.03	0	100	100	68, 85, 125, 130	0
23	AW	75/75 (100%)	0.73	15 (20%)	1	0	46, 119, 161, 185	0
23	CW	75/75 (100%)	0.50	10 (13%)	3	1	79, 141, 174, 184	0
24	AX	77/77 (100%)	0.06	4 (5%)	27	10	48, 89, 121, 130	0
24	CX	77/77 (100%)	0.07	3 (3%)	39	15	69, 98, 125, 132	0
25	AY	75/75 (100%)	1.25	25 (33%)	0	0	51, 157, 193, 194	0
25	CY	75/75 (100%)	1.32	23 (30%)	0	0	67, 167, 194, 194	0
26	AZ	2/6 (33%)	0.41	0	100	100	85, 85, 85, 88	0
26	CZ	2/6 (33%)	0.76	0	100	100	99, 99, 99, 100	0
27	BA	2800/2915 (96%)	-0.12	49 (1%)	68	40	30, 56, 157, 198	0
27	DA	2800/2915 (96%)	-0.01	73 (2%)	56	27	49, 77, 168, 197	0
28	BB	118/122 (96%)	-0.22	2 (1%)	70	41	47, 76, 119, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DB	118/122 (96%)	0.00	4 (3%) 45 19	80, 104, 136, 162	0
29	BC	191/229 (83%)	1.64	72 (37%) 0 0	130, 167, 187, 195	0
29	DC	191/229 (83%)	2.08	74 (38%) 0 0	122, 173, 188, 191	0
30	BD	272/276 (98%)	-0.38	2 (0%) 87 69	32, 52, 68, 79	0
30	DD	272/276 (98%)	-0.32	0 100 100	46, 61, 78, 92	0
31	BE	205/206 (99%)	-0.24	2 (0%) 82 59	33, 58, 93, 104	0
31	DE	205/206 (99%)	0.01	5 (2%) 59 30	57, 84, 112, 121	0
32	BF	208/210 (99%)	-0.34	2 (0%) 82 59	29, 60, 125, 149	0
32	DF	208/210 (99%)	-0.03	6 (2%) 51 23	54, 86, 132, 152	0
33	BG	181/182 (99%)	-0.02	9 (4%) 28 10	64, 83, 116, 146	0
33	DG	181/182 (99%)	0.34	15 (8%) 11 3	79, 106, 132, 153	0
34	BH	164/180 (91%)	0.06	6 (3%) 41 17	68, 97, 124, 142	0
34	DH	160/180 (88%)	0.87	25 (15%) 2 1	110, 139, 159, 163	0
35	BI	146/148 (98%)	-0.22	0 100 100	62, 119, 140, 144	0
35	DI	146/148 (98%)	-0.03	3 (2%) 63 34	67, 105, 128, 136	0
36	BN	139/140 (99%)	-0.43	0 100 100	42, 57, 86, 104	0
36	DN	139/140 (99%)	-0.26	2 (1%) 75 49	65, 91, 115, 124	0
37	BO	122/122 (100%)	-0.54	1 (0%) 86 65	38, 57, 75, 88	0
37	DO	122/122 (100%)	-0.37	0 100 100	60, 77, 93, 100	0
38	BP	146/150 (97%)	0.13	5 (3%) 45 19	37, 69, 102, 156	0
38	DP	146/150 (97%)	0.28	4 (2%) 54 26	61, 93, 122, 148	0
39	BQ	141/141 (100%)	-0.18	2 (1%) 75 49	42, 60, 92, 118	0
39	DQ	139/141 (98%)	-0.18	1 (0%) 87 69	68, 90, 120, 134	0
40	BR	117/118 (99%)	-0.36	0 100 100	35, 52, 69, 82	0
40	DR	117/118 (99%)	-0.12	0 100 100	58, 71, 83, 96	0
41	BS	99/112 (88%)	-0.19	0 100 100	48, 76, 94, 105	0
41	DS	101/112 (90%)	0.30	10 (9%) 7 2	69, 100, 117, 122	0
42	BT	138/146 (94%)	-0.13	7 (5%) 28 10	51, 70, 126, 152	0
42	DT	138/146 (94%)	0.13	15 (10%) 5 2	61, 90, 149, 175	0
43	BU	117/118 (99%)	-0.22	2 (1%) 70 41	37, 49, 73, 95	0
43	DU	117/118 (99%)	0.32	14 (11%) 4 1	60, 91, 111, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BV	101/101 (100%)	-0.46	1 (0%) 82 59	35, 65, 90, 116	0
44	DV	101/101 (100%)	0.29	9 (8%) 9 3	59, 106, 121, 129	0
45	BW	113/113 (100%)	-0.31	2 (1%) 68 40	32, 46, 76, 136	0
45	DW	113/113 (100%)	-0.36	1 (0%) 84 63	43, 64, 95, 130	0
46	BX	93/96 (96%)	-0.32	1 (1%) 80 56	43, 53, 70, 91	0
46	DX	93/96 (96%)	-0.28	0 100 100	56, 71, 89, 95	0
47	BY	101/110 (91%)	-0.05	3 (2%) 50 22	58, 78, 145, 163	0
47	DY	101/110 (91%)	0.26	10 (9%) 7 2	73, 94, 149, 156	0
48	BZ	177/206 (85%)	0.57	24 (13%) 3 1	65, 107, 169, 177	0
48	DZ	177/206 (85%)	1.28	40 (22%) 0 0	104, 130, 177, 191	0
49	B0	84/85 (98%)	-0.15	4 (4%) 30 11	43, 56, 83, 103	0
49	D0	84/85 (98%)	0.48	10 (11%) 4 1	71, 83, 100, 118	0
50	B1	94/98 (95%)	-0.21	2 (2%) 63 34	44, 61, 92, 109	0
50	D1	94/98 (95%)	0.06	2 (2%) 63 34	54, 70, 94, 110	0
51	B2	71/72 (98%)	-0.37	3 (4%) 36 14	46, 66, 86, 117	0
51	D2	71/72 (98%)	-0.30	0 100 100	65, 86, 103, 107	0
52	B3	60/60 (100%)	-0.25	1 (1%) 70 41	43, 58, 85, 110	0
52	D3	60/60 (100%)	0.14	2 (3%) 46 20	75, 90, 112, 116	0
53	B4	31/71 (43%)	-0.43	0 100 100	92, 107, 120, 126	0
53	D4	31/71 (43%)	-0.13	0 100 100	108, 119, 128, 135	0
54	B5	59/60 (98%)	-0.23	3 (5%) 28 10	33, 51, 115, 135	0
54	D5	59/60 (98%)	-0.01	4 (6%) 17 5	60, 71, 143, 177	0
55	B6	51/54 (94%)	0.17	3 (5%) 22 7	59, 83, 106, 112	0
55	D6	46/54 (85%)	0.80	9 (19%) 1 0	56, 103, 116, 117	0
56	B7	49/49 (100%)	-0.17	0 100 100	28, 44, 84, 115	0
56	D7	49/49 (100%)	0.49	4 (8%) 11 3	46, 59, 90, 101	0
57	B8	64/65 (98%)	-0.18	1 (1%) 72 44	40, 56, 73, 97	0
57	D8	64/65 (98%)	0.11	2 (3%) 49 21	60, 74, 87, 118	0
58	B9	36/37 (97%)	0.31	0 100 100	46, 63, 80, 93	0
58	D9	36/37 (97%)	1.07	10 (27%) 0 0	88, 122, 133, 137	0
All	All	21214/22204 (95%)	0.03	936 (4%) 34 13	28, 83, 154, 198	0

The worst 5 of 936 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
48	DZ	111	ARG	15.7
27	BA	2802	G	15.7
48	DZ	175	PRO	14.5
27	DA	2802	G	13.1
29	DC	165	ASN	13.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
26	UAL	CZ	5	9/10	0.78	0.28	97,99,99,99	0
26	KBE	CZ	1	9/10	0.79	0.36	89,91,93,94	0
26	UAL	AZ	5	9/10	0.81	0.20	81,82,83,84	0
26	DPP	CZ	2	6/7	0.83	0.15	94,96,97,97	0
26	KBE	AZ	1	9/10	0.85	0.33	78,79,82,82	0
26	5OH	AZ	6	12/13	0.87	0.18	84,89,92,94	0
26	5OH	CZ	6	12/13	0.89	0.28	99,101,102,102	0
26	DPP	AZ	2	6/7	0.93	0.16	79,82,82,84	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
59	MG	DD	301	1/1	0.12	0.57	110,110,110,110	0
59	MG	CA	1605	1/1	0.23	0.47	99,99,99,99	0
59	MG	BA	3332	1/1	0.42	0.45	105,105,105,105	0
59	MG	AT	201	1/1	0.43	0.13	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3069	1/1	0.45	0.83	78,78,78,78	0
59	MG	BA	3297	1/1	0.48	0.69	95,95,95,95	0
59	MG	DA	3203	1/1	0.50	0.91	97,97,97,97	0
59	MG	AA	1710	1/1	0.53	0.65	113,113,113,113	0
59	MG	AA	1620	1/1	0.57	0.34	45,45,45,45	0
59	MG	CA	1672	1/1	0.57	0.27	45,45,45,45	0
59	MG	CA	1630	1/1	0.62	0.37	55,55,55,55	0
59	MG	DA	3247	1/1	0.62	0.35	82,82,82,82	0
59	MG	BA	3290	1/1	0.63	0.17	69,69,69,69	0
59	MG	DA	3181	1/1	0.64	0.25	52,52,52,52	0
59	MG	BA	3307	1/1	0.66	0.45	64,64,64,64	0
59	MG	DA	3183	1/1	0.67	0.11	100,100,100,100	0
59	MG	AA	1676	1/1	0.68	0.19	77,77,77,77	0
59	MG	DA	3108	1/1	0.68	0.34	51,51,51,51	0
59	MG	BA	3294	1/1	0.68	1.08	72,72,72,72	0
59	MG	AX	105	1/1	0.69	0.40	82,82,82,82	0
59	MG	DA	3211	1/1	0.69	1.14	78,78,78,78	0
59	MG	DA	3273	1/1	0.70	0.96	106,106,106,106	0
59	MG	BA	3134	1/1	0.70	0.57	39,39,39,39	0
59	MG	BX	101	1/1	0.70	0.53	53,53,53,53	0
59	MG	AA	1707	1/1	0.70	0.55	59,59,59,59	0
59	MG	DA	3245	1/1	0.71	0.33	86,86,86,86	0
59	MG	AK	202	1/1	0.72	0.29	90,90,90,90	0
59	MG	AA	1727	1/1	0.72	0.53	71,71,71,71	0
59	MG	BA	3296	1/1	0.72	0.27	61,61,61,61	0
59	MG	CA	1670	1/1	0.73	0.29	67,67,67,67	0
59	MG	BA	3004	1/1	0.73	0.50	81,81,81,81	0
59	MG	AA	1647	1/1	0.73	0.29	80,80,80,80	0
59	MG	DA	3077	1/1	0.73	0.33	73,73,73,73	0
59	MG	BA	3347	1/1	0.73	0.84	78,78,78,78	0
59	MG	BA	3177	1/1	0.74	0.25	65,65,65,65	0
59	MG	BA	3224	1/1	0.74	0.27	63,63,63,63	0
59	MG	BA	3265	1/1	0.74	0.24	28,28,28,28	0
59	MG	DA	3238	1/1	0.74	0.53	101,101,101,101	0
59	MG	BA	3298	1/1	0.74	1.43	178,178,178,178	0
59	MG	BA	3165	1/1	0.74	0.63	60,60,60,60	0
59	MG	DA	3166	1/1	0.74	0.12	41,41,41,41	0
59	MG	AX	107	1/1	0.74	0.58	80,80,80,80	0
59	MG	CA	1675	1/1	0.74	0.51	150,150,150,150	0
59	MG	AA	1659	1/1	0.75	0.25	73,73,73,73	0
59	MG	AA	1667	1/1	0.75	0.38	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AW	101	1/1	0.75	0.43	135,135,135,135	0
59	MG	CA	1683	1/1	0.75	0.55	55,55,55,55	0
59	MG	AA	1624	1/1	0.76	0.18	54,54,54,54	0
59	MG	BA	3162	1/1	0.76	0.64	66,66,66,66	0
59	MG	CA	1623	1/1	0.76	0.21	91,91,91,91	0
59	MG	DA	3190	1/1	0.76	0.14	33,33,33,33	0
59	MG	DA	3213	1/1	0.76	0.64	62,62,62,62	0
59	MG	AA	1627	1/1	0.76	0.40	55,55,55,55	0
59	MG	CA	1686	1/1	0.76	0.30	64,64,64,64	0
59	MG	CA	1644	1/1	0.77	0.80	68,68,68,68	0
59	MG	BA	3269	1/1	0.77	0.95	83,83,83,83	0
59	MG	DA	3271	1/1	0.78	0.16	80,80,80,80	0
59	MG	DA	3119	1/1	0.78	0.46	62,62,62,62	0
59	MG	AW	106	1/1	0.78	0.47	94,94,94,94	0
59	MG	DA	3217	1/1	0.78	0.39	85,85,85,85	0
59	MG	AA	1700	1/1	0.78	0.31	58,58,58,58	0
59	MG	BA	3320	1/1	0.78	1.92	89,89,89,89	0
59	MG	AA	1641	1/1	0.78	0.20	62,62,62,62	0
59	MG	BA	3323	1/1	0.79	0.17	61,61,61,61	0
59	MG	DA	3095	1/1	0.79	1.16	64,64,64,64	0
59	MG	BA	3154	1/1	0.79	0.30	44,44,44,44	0
59	MG	BA	3346	1/1	0.79	0.34	35,35,35,35	0
59	MG	BA	3303	1/1	0.79	0.86	91,91,91,91	0
59	MG	BA	3317	1/1	0.79	0.41	50,50,50,50	0
59	MG	AA	1646	1/1	0.79	0.30	61,61,61,61	0
59	MG	BA	3219	1/1	0.79	0.25	43,43,43,43	0
59	MG	DA	3099	1/1	0.79	0.30	45,45,45,45	0
59	MG	DA	3112	1/1	0.80	0.21	70,70,70,70	0
59	MG	DA	3186	1/1	0.80	0.16	41,41,41,41	0
59	MG	BA	3333	1/1	0.80	0.66	55,55,55,55	0
59	MG	AA	1729	1/1	0.80	0.26	57,57,57,57	0
59	MG	BA	3182	1/1	0.80	0.86	81,81,81,81	0
59	MG	BA	3010	1/1	0.80	0.32	29,29,29,29	0
59	MG	CA	1603	1/1	0.80	0.45	113,113,113,113	0
59	MG	BA	3351	1/1	0.80	0.30	60,60,60,60	0
59	MG	CA	1612	1/1	0.81	0.50	80,80,80,80	0
59	MG	DA	3250	1/1	0.81	0.41	61,61,61,61	0
59	MG	AA	1711	1/1	0.81	0.27	68,68,68,68	0
59	MG	AY	102	1/1	0.81	0.52	96,96,96,96	0
59	MG	DA	3132	1/1	0.81	0.22	60,60,60,60	0
59	MG	DA	3251	1/1	0.81	0.17	44,44,44,44	0
59	MG	DA	3207	1/1	0.81	0.95	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1689	1/1	0.81	0.21	73,73,73,73	0
59	MG	DA	3171	1/1	0.81	0.45	75,75,75,75	0
59	MG	AW	102	1/1	0.81	0.12	53,53,53,53	0
59	MG	AA	1665	1/1	0.81	0.26	49,49,49,49	0
59	MG	BA	3360	1/1	0.82	0.40	68,68,68,68	0
59	MG	BA	3159	1/1	0.82	0.19	46,46,46,46	0
59	MG	DA	3007	1/1	0.82	0.33	42,42,42,42	0
59	MG	DD	303	1/1	0.82	0.51	95,95,95,95	0
59	MG	CQ	201	1/1	0.82	0.12	94,94,94,94	0
59	MG	BA	3116	1/1	0.83	0.21	54,54,54,54	0
59	MG	BA	3357	1/1	0.83	0.23	54,54,54,54	0
59	MG	BA	3337	1/1	0.83	0.36	61,61,61,61	0
59	MG	DA	3152	1/1	0.83	0.39	54,54,54,54	0
59	MG	BA	3374	1/1	0.83	0.42	31,31,31,31	0
59	MG	DR	201	1/1	0.83	0.32	65,65,65,65	0
59	MG	BA	3184	1/1	0.83	0.26	56,56,56,56	0
59	MG	DA	3189	1/1	0.83	1.16	92,92,92,92	0
59	MG	BA	3087	1/1	0.83	0.21	39,39,39,39	0
59	MG	DA	3126	1/1	0.83	0.30	48,48,48,48	0
59	MG	AA	1621	1/1	0.83	0.37	54,54,54,54	0
59	MG	DA	3253	1/1	0.83	0.22	46,46,46,46	0
59	MG	BA	3127	1/1	0.83	0.24	48,48,48,48	0
59	MG	AK	201	1/1	0.83	0.31	66,66,66,66	0
59	MG	BA	3270	1/1	0.83	0.27	64,64,64,64	0
59	MG	AW	103	1/1	0.83	0.40	73,73,73,73	0
59	MG	BA	3164	1/1	0.83	0.49	37,37,37,37	0
59	MG	AA	1634	1/1	0.83	0.12	72,72,72,72	0
59	MG	BN	201	1/1	0.83	0.35	67,67,67,67	0
59	MG	AA	1725	1/1	0.83	0.26	84,84,84,84	0
59	MG	CA	1643	1/1	0.84	0.62	51,51,51,51	0
59	MG	AA	1699	1/1	0.84	0.41	61,61,61,61	0
59	MG	DA	3227	1/1	0.84	0.20	72,72,72,72	0
59	MG	BA	3392	1/1	0.84	0.30	63,63,63,63	0
59	MG	BZ	301	1/1	0.84	0.15	42,42,42,42	0
59	MG	DA	3235	1/1	0.84	0.23	68,68,68,68	0
59	MG	BA	3185	1/1	0.84	0.33	62,62,62,62	0
59	MG	AA	1717	1/1	0.84	0.18	50,50,50,50	0
59	MG	BR	201	1/1	0.84	0.44	41,41,41,41	0
59	MG	AA	1637	1/1	0.85	0.21	40,40,40,40	0
59	MG	BA	3237	1/1	0.85	0.47	32,32,32,32	0
59	MG	DA	3234	1/1	0.85	0.41	84,84,84,84	0
59	MG	BA	3166	1/1	0.85	0.20	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3224	1/1	0.85	0.12	53,53,53,53	0
59	MG	BA	3216	1/1	0.85	0.41	42,42,42,42	0
59	MG	BA	3231	1/1	0.85	0.07	54,54,54,54	0
59	MG	BA	3259	1/1	0.85	0.16	35,35,35,35	0
59	MG	DB	201	1/1	0.85	0.15	44,44,44,44	0
59	MG	BA	3382	1/1	0.85	0.34	37,37,37,37	0
59	MG	BA	3156	1/1	0.85	0.29	25,25,25,25	0
59	MG	DA	3043	1/1	0.85	0.33	48,48,48,48	0
59	MG	DA	3226	1/1	0.85	0.71	70,70,70,70	0
59	MG	DA	3030	1/1	0.85	0.10	17,17,17,17	0
59	MG	CA	1689	1/1	0.85	0.15	63,63,63,63	0
59	MG	CA	1638	1/1	0.85	0.20	46,46,46,46	0
59	MG	CA	1651	1/1	0.85	0.15	50,50,50,50	0
59	MG	DA	3137	1/1	0.85	0.13	28,28,28,28	0
59	MG	AA	1678	1/1	0.85	0.21	52,52,52,52	0
59	MG	BA	3002	1/1	0.85	0.17	59,59,59,59	0
59	MG	DA	3270	1/1	0.85	0.27	61,61,61,61	0
59	MG	CA	1677	1/1	0.85	0.15	53,53,53,53	0
59	MG	DA	3170	1/1	0.85	0.14	52,52,52,52	0
59	MG	BA	3037	1/1	0.85	0.46	27,27,27,27	0
59	MG	CA	1652	1/1	0.85	0.37	86,86,86,86	0
59	MG	DA	3121	1/1	0.85	0.18	37,37,37,37	0
59	MG	BA	3362	1/1	0.85	0.35	51,51,51,51	0
59	MG	BA	3205	1/1	0.85	0.27	86,86,86,86	0
59	MG	B0	102	1/1	0.86	0.32	49,49,49,49	0
59	MG	AX	102	1/1	0.86	0.12	51,51,51,51	0
59	MG	BA	3099	1/1	0.86	0.87	51,51,51,51	0
59	MG	AA	1655	1/1	0.86	0.40	28,28,28,28	0
59	MG	DA	3176	1/1	0.86	0.18	51,51,51,51	0
59	MG	BA	3028	1/1	0.86	0.22	41,41,41,41	0
59	MG	BA	3176	1/1	0.86	0.27	27,27,27,27	0
59	MG	BA	3302	1/1	0.86	0.15	42,42,42,42	0
59	MG	AA	1724	1/1	0.86	0.35	56,56,56,56	0
59	MG	DA	3005	1/1	0.86	0.25	50,50,50,50	0
59	MG	BA	3232	1/1	0.86	0.32	25,25,25,25	0
59	MG	CA	1671	1/1	0.86	0.30	54,54,54,54	0
59	MG	BA	3112	1/1	0.86	0.13	52,52,52,52	0
59	MG	BA	3352	1/1	0.86	0.47	51,51,51,51	0
59	MG	DA	3218	1/1	0.86	0.80	75,75,75,75	0
59	MG	BA	3147	1/1	0.86	0.25	33,33,33,33	0
59	MG	DA	3053	1/1	0.86	0.19	47,47,47,47	0
59	MG	BA	3315	1/1	0.86	0.39	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1652	1/1	0.86	0.43	55,55,55,55	0
59	MG	AX	106	1/1	0.86	0.14	43,43,43,43	0
59	MG	BA	3261	1/1	0.86	0.19	53,53,53,53	0
59	MG	BA	3227	1/1	0.86	0.15	69,69,69,69	0
59	MG	DA	3098	1/1	0.86	0.17	37,37,37,37	0
59	MG	BA	3299	1/1	0.86	1.44	85,85,85,85	0
59	MG	AC	301	1/1	0.86	0.15	64,64,64,64	0
59	MG	DA	3123	1/1	0.86	0.26	32,32,32,32	0
59	MG	BA	3126	1/1	0.87	0.33	52,52,52,52	0
59	MG	DA	3229	1/1	0.87	0.25	76,76,76,76	0
59	MG	B0	101	1/1	0.87	0.25	58,58,58,58	0
59	MG	AA	1714	1/1	0.87	0.37	66,66,66,66	0
59	MG	DA	3197	1/1	0.87	0.34	84,84,84,84	0
59	MG	CA	1659	1/1	0.87	0.10	64,64,64,64	0
59	MG	DA	3175	1/1	0.87	0.54	53,53,53,53	0
59	MG	AA	1648	1/1	0.87	0.24	48,48,48,48	0
59	MG	DA	3068	1/1	0.87	0.20	60,60,60,60	0
59	MG	DA	3220	1/1	0.87	0.18	64,64,64,64	0
59	MG	AA	1643	1/1	0.87	0.20	51,51,51,51	0
59	MG	DA	3210	1/1	0.87	0.46	57,57,57,57	0
59	MG	BA	3027	1/1	0.87	0.24	35,35,35,35	0
59	MG	CA	1608	1/1	0.87	0.79	57,57,57,57	0
59	MG	DA	3049	1/1	0.87	0.14	41,41,41,41	0
59	MG	CA	1631	1/1	0.87	0.47	45,45,45,45	0
59	MG	AW	104	1/1	0.87	0.14	57,57,57,57	0
59	MG	AA	1695	1/1	0.87	0.17	55,55,55,55	0
59	MG	DA	3084	1/1	0.87	0.14	48,48,48,48	0
59	MG	AA	1723	1/1	0.87	0.14	36,36,36,36	0
59	MG	BA	3249	1/1	0.87	0.61	50,50,50,50	0
59	MG	DA	3274	1/1	0.87	0.18	62,62,62,62	0
59	MG	DA	3236	1/1	0.87	1.01	91,91,91,91	0
59	MG	AW	105	1/1	0.87	0.21	41,41,41,41	0
59	MG	CA	1657	1/1	0.88	0.69	62,62,62,62	0
59	MG	DA	3193	1/1	0.88	0.18	40,40,40,40	0
59	MG	BA	3386	1/1	0.88	0.18	20,20,20,20	0
59	MG	BA	3230	1/1	0.88	0.17	48,48,48,48	0
59	MG	CE	201	1/1	0.88	0.08	71,71,71,71	0
59	MG	BA	3331	1/1	0.88	0.12	52,52,52,52	0
59	MG	BA	3394	1/1	0.88	0.25	49,49,49,49	0
59	MG	AA	1635	1/1	0.88	0.21	46,46,46,46	0
59	MG	DA	3265	1/1	0.88	0.44	51,51,51,51	0
59	MG	BA	3210	1/1	0.88	0.25	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3120	1/1	0.88	0.15	55,55,55,55	0
59	MG	DA	3078	1/1	0.88	0.24	58,58,58,58	0
59	MG	BA	3348	1/1	0.88	0.38	62,62,62,62	0
59	MG	DA	3240	1/1	0.88	0.19	49,49,49,49	0
59	MG	BA	3003	1/1	0.88	0.39	42,42,42,42	0
60	ZN	D5	103	1/1	0.88	0.05	92,92,92,92	0
59	MG	BA	3397	1/1	0.88	0.47	66,66,66,66	0
59	MG	BA	3256	1/1	0.88	0.18	56,56,56,56	0
59	MG	DA	3097	1/1	0.88	0.37	65,65,65,65	0
59	MG	DA	3200	1/1	0.88	0.31	46,46,46,46	0
59	MG	BA	3366	1/1	0.88	0.40	64,64,64,64	0
59	MG	BA	3214	1/1	0.88	0.33	87,87,87,87	0
59	MG	AA	1654	1/1	0.88	0.25	100,100,100,100	0
59	MG	DA	3168	1/1	0.88	0.26	43,43,43,43	0
59	MG	BA	3167	1/1	0.88	0.20	31,31,31,31	0
59	MG	DA	3212	1/1	0.88	0.43	61,61,61,61	0
59	MG	BA	3260	1/1	0.88	0.17	58,58,58,58	0
59	MG	DA	3136	1/1	0.88	0.30	47,47,47,47	0
59	MG	BA	3196	1/1	0.88	0.30	49,49,49,49	0
59	MG	CA	1607	1/1	0.88	0.41	36,36,36,36	0
59	MG	CA	1618	1/1	0.88	0.47	69,69,69,69	0
59	MG	BA	3316	1/1	0.88	0.43	68,68,68,68	0
59	MG	BA	3310	1/1	0.88	0.37	55,55,55,55	0
59	MG	BA	3120	1/1	0.88	0.29	49,49,49,49	0
59	MG	BA	3174	1/1	0.88	0.14	43,43,43,43	0
59	MG	DA	3109	1/1	0.88	0.73	65,65,65,65	0
59	MG	DA	3254	1/1	0.89	0.17	54,54,54,54	0
59	MG	BA	3389	1/1	0.89	0.20	44,44,44,44	0
59	MG	DA	3014	1/1	0.89	0.22	79,79,79,79	0
59	MG	DA	3102	1/1	0.89	0.13	84,84,84,84	0
59	MG	BA	3334	1/1	0.89	0.17	32,32,32,32	0
59	MG	BA	3133	1/1	0.89	0.17	20,20,20,20	0
59	MG	AA	1656	1/1	0.89	0.21	42,42,42,42	0
59	MG	BA	3308	1/1	0.89	0.83	49,49,49,49	0
59	MG	DA	3196	1/1	0.89	0.40	48,48,48,48	0
59	MG	BA	3295	1/1	0.89	0.42	47,47,47,47	0
59	MG	DA	3088	1/1	0.89	0.15	36,36,36,36	0
59	MG	BA	3191	1/1	0.89	0.19	31,31,31,31	0
59	MG	BA	3252	1/1	0.89	0.12	18,18,18,18	0
59	MG	BF	302	1/1	0.89	0.18	26,26,26,26	0
59	MG	CA	1666	1/1	0.89	0.08	68,68,68,68	0
59	MG	CA	1619	1/1	0.89	0.43	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3398	1/1	0.89	0.40	66,66,66,66	0
59	MG	BA	3197	1/1	0.89	0.36	45,45,45,45	0
59	MG	BA	3373	1/1	0.89	0.34	55,55,55,55	0
59	MG	BA	3272	1/1	0.89	0.31	30,30,30,30	0
59	MG	BA	3103	1/1	0.89	0.65	65,65,65,65	0
59	MG	BA	3094	1/1	0.89	0.13	12,12,12,12	0
59	MG	DA	3223	1/1	0.89	0.17	61,61,61,61	0
59	MG	AA	1617	1/1	0.89	0.09	48,48,48,48	0
59	MG	BA	3344	1/1	0.89	0.10	37,37,37,37	0
59	MG	DA	3061	1/1	0.89	0.31	28,28,28,28	0
59	MG	AA	1688	1/1	0.89	0.26	47,47,47,47	0
59	MG	DA	3198	1/1	0.89	0.49	56,56,56,56	0
59	MG	AA	1684	1/1	0.89	0.09	42,42,42,42	0
59	MG	DE	303	1/1	0.89	0.11	32,32,32,32	0
59	MG	CA	1639	1/1	0.89	0.31	74,74,74,74	0
59	MG	CA	1669	1/1	0.89	0.17	36,36,36,36	0
59	MG	BA	3245	1/1	0.89	0.67	48,48,48,48	0
59	MG	AA	1603	1/1	0.89	0.51	58,58,58,58	0
59	MG	CA	1645	1/1	0.90	0.05	27,27,27,27	0
59	MG	AX	101	1/1	0.90	0.41	57,57,57,57	0
59	MG	BA	3246	1/1	0.90	0.51	46,46,46,46	0
59	MG	BA	3208	1/1	0.90	0.20	54,54,54,54	0
59	MG	BA	3148	1/1	0.90	0.17	27,27,27,27	0
59	MG	CA	1679	1/1	0.90	0.18	46,46,46,46	0
59	MG	AX	104	1/1	0.90	0.26	45,45,45,45	0
59	MG	BA	3288	1/1	0.90	0.16	33,33,33,33	0
59	MG	BA	3257	1/1	0.90	0.21	21,21,21,21	0
59	MG	AA	1671	1/1	0.90	0.18	83,83,83,83	0
59	MG	BA	3400	1/1	0.90	0.17	39,39,39,39	0
59	MG	BA	3228	1/1	0.90	0.46	21,21,21,21	0
59	MG	BA	3326	1/1	0.90	0.15	35,35,35,35	0
59	MG	BA	3292	1/1	0.90	0.31	40,40,40,40	0
59	MG	CA	1692	1/1	0.90	0.38	73,73,73,73	0
59	MG	DA	3163	1/1	0.90	0.62	62,62,62,62	0
59	MG	CA	1688	1/1	0.90	0.14	59,59,59,59	0
59	MG	BA	3305	1/1	0.90	0.29	32,32,32,32	0
59	MG	DA	3257	1/1	0.90	0.49	40,40,40,40	0
59	MG	DA	3080	1/1	0.90	0.17	41,41,41,41	0
59	MG	BA	3053	1/1	0.90	0.22	11,11,11,11	0
59	MG	AA	1639	1/1	0.90	0.16	54,54,54,54	0
59	MG	DA	3187	1/1	0.90	0.51	51,51,51,51	0
59	MG	AT	202	1/1	0.90	0.42	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1686	1/1	0.90	0.14	58,58,58,58	0
59	MG	CA	1661	1/1	0.90	0.45	42,42,42,42	0
59	MG	BA	3235	1/1	0.90	0.36	51,51,51,51	0
59	MG	CX	101	1/1	0.90	0.12	42,42,42,42	0
59	MG	AA	1640	1/1	0.90	0.35	37,37,37,37	0
59	MG	DA	3215	1/1	0.90	0.56	63,63,63,63	0
59	MG	DA	3178	1/1	0.90	0.57	36,36,36,36	0
59	MG	BA	3084	1/1	0.90	0.26	19,19,19,19	0
59	MG	BA	3335	1/1	0.90	0.42	52,52,52,52	0
59	MG	DA	3052	1/1	0.90	0.15	30,30,30,30	0
59	MG	BA	3381	1/1	0.90	0.16	43,43,43,43	0
59	MG	DA	3045	1/1	0.90	0.13	41,41,41,41	0
59	MG	AO	101	1/1	0.90	0.12	62,62,62,62	0
59	MG	DA	3192	1/1	0.90	0.22	39,39,39,39	0
59	MG	DA	3167	1/1	0.90	0.15	42,42,42,42	0
59	MG	DZ	301	1/1	0.90	0.21	55,55,55,55	0
59	MG	DA	3219	1/1	0.90	0.17	40,40,40,40	0
59	MG	BA	3019	1/1	0.90	0.31	21,21,21,21	0
59	MG	BA	3253	1/1	0.90	0.29	56,56,56,56	0
59	MG	DA	3164	1/1	0.90	0.38	51,51,51,51	0
59	MG	AA	1672	1/1	0.90	0.15	51,51,51,51	0
59	MG	CA	1625	1/1	0.90	0.55	54,54,54,54	0
59	MG	CA	1621	1/1	0.91	0.40	42,42,42,42	0
59	MG	AA	1732	1/1	0.91	0.16	32,32,32,32	0
59	MG	AA	1685	1/1	0.91	0.55	50,50,50,50	0
59	MG	DA	3268	1/1	0.91	0.21	47,47,47,47	0
59	MG	BA	3341	1/1	0.91	0.28	86,86,86,86	0
59	MG	BA	3276	1/1	0.91	0.24	45,45,45,45	0
59	MG	AA	1731	1/1	0.91	0.17	22,22,22,22	0
59	MG	DA	3144	1/1	0.91	0.57	57,57,57,57	0
59	MG	BA	3026	1/1	0.91	0.29	29,29,29,29	0
59	MG	BA	3396	1/1	0.91	0.18	37,37,37,37	0
59	MG	BA	3119	1/1	0.91	0.16	20,20,20,20	0
59	MG	CA	1642	1/1	0.91	0.24	29,29,29,29	0
59	MG	BA	3057	1/1	0.91	0.15	23,23,23,23	0
59	MG	BA	3104	1/1	0.91	0.40	52,52,52,52	0
59	MG	AF	201	1/1	0.91	0.18	39,39,39,39	0
59	MG	BA	3108	1/1	0.91	0.14	44,44,44,44	0
59	MG	BA	3293	1/1	0.91	0.64	44,44,44,44	0
59	MG	AA	1698	1/1	0.91	0.19	49,49,49,49	0
59	MG	BA	3309	1/1	0.91	0.05	41,41,41,41	0
59	MG	BA	3274	1/1	0.91	0.15	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3082	1/1	0.91	0.47	37,37,37,37	0
59	MG	BA	3359	1/1	0.91	0.32	51,51,51,51	0
59	MG	DA	3275	1/1	0.91	0.34	54,54,54,54	0
59	MG	BA	3376	1/1	0.91	0.91	66,66,66,66	0
59	MG	BA	3179	1/1	0.91	0.33	31,31,31,31	0
59	MG	BA	3291	1/1	0.91	0.15	42,42,42,42	0
59	MG	BA	3371	1/1	0.91	0.25	57,57,57,57	0
59	MG	BA	3049	1/1	0.91	0.11	12,12,12,12	0
59	MG	BA	3043	1/1	0.91	0.32	22,22,22,22	0
59	MG	BA	3281	1/1	0.91	0.21	41,41,41,41	0
59	MG	DA	3209	1/1	0.91	0.44	69,69,69,69	0
59	MG	DA	3261	1/1	0.91	0.32	50,50,50,50	0
59	MG	DA	3145	1/1	0.91	0.31	45,45,45,45	0
59	MG	BA	3349	1/1	0.91	0.18	53,53,53,53	0
59	MG	BA	3240	1/1	0.91	0.13	60,60,60,60	0
59	MG	AA	1605	1/1	0.91	0.28	54,54,54,54	0
59	MG	DA	3172	1/1	0.91	0.30	55,55,55,55	0
59	MG	BA	3114	1/1	0.91	0.35	53,53,53,53	0
59	MG	AA	1693	1/1	0.92	0.16	41,41,41,41	0
59	MG	CA	1674	1/1	0.92	0.33	63,63,63,63	0
59	MG	AA	1638	1/1	0.92	0.18	50,50,50,50	0
59	MG	DA	3035	1/1	0.92	0.64	63,63,63,63	0
59	MG	DA	3243	1/1	0.92	0.38	35,35,35,35	0
59	MG	DA	3230	1/1	0.92	0.51	46,46,46,46	0
59	MG	AA	1702	1/1	0.92	0.52	59,59,59,59	0
59	MG	AA	1666	1/1	0.92	0.81	75,75,75,75	0
59	MG	BA	3089	1/1	0.92	0.15	55,55,55,55	0
59	MG	DA	3027	1/1	0.92	0.46	28,28,28,28	0
59	MG	BA	3078	1/1	0.92	0.12	20,20,20,20	0
59	MG	DA	3087	1/1	0.92	0.84	59,59,59,59	0
59	MG	DA	3262	1/1	0.92	0.08	58,58,58,58	0
59	MG	BA	3233	1/1	0.92	0.13	32,32,32,32	0
59	MG	DA	3140	1/1	0.92	0.41	38,38,38,38	0
59	MG	BA	3056	1/1	0.92	0.67	59,59,59,59	0
59	MG	BA	3079	1/1	0.92	0.15	23,23,23,23	0
59	MG	DA	3244	1/1	0.92	0.20	33,33,33,33	0
60	ZN	B5	102	1/1	0.92	0.07	75,75,75,75	0
59	MG	BA	3379	1/1	0.92	0.51	52,52,52,52	0
59	MG	BA	3383	1/1	0.92	0.34	36,36,36,36	0
59	MG	DA	3057	1/1	0.92	0.11	21,21,21,21	0
60	ZN	B4	101	1/1	0.92	0.06	117,117,117,117	0
59	MG	AA	1712	1/1	0.92	0.43	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3128	1/1	0.92	0.14	26,26,26,26	0
59	MG	BA	3153	1/1	0.92	0.17	37,37,37,37	0
59	MG	BA	3268	1/1	0.92	0.47	44,44,44,44	0
59	MG	BF	301	1/1	0.92	0.15	37,37,37,37	0
59	MG	BA	3229	1/1	0.92	0.36	37,37,37,37	0
59	MG	CA	1615	1/1	0.92	0.63	51,51,51,51	0
59	MG	CA	1687	1/1	0.92	0.15	56,56,56,56	0
59	MG	AA	1719	1/1	0.92	0.29	58,58,58,58	0
59	MG	DA	3103	1/1	0.92	0.07	38,38,38,38	0
59	MG	BA	3183	1/1	0.92	0.23	37,37,37,37	0
59	MG	BA	3067	1/1	0.92	0.37	36,36,36,36	0
59	MG	DA	3091	1/1	0.92	0.18	67,67,67,67	0
59	MG	DA	3011	1/1	0.92	0.42	37,37,37,37	0
59	MG	CA	1636	1/1	0.92	0.17	55,55,55,55	0
59	MG	AA	1642	1/1	0.92	0.12	55,55,55,55	0
59	MG	AA	1633	1/1	0.92	0.08	37,37,37,37	0
59	MG	DA	3017	1/1	0.92	0.22	16,16,16,16	0
59	MG	CA	1653	1/1	0.92	0.15	46,46,46,46	0
59	MG	BA	3128	1/1	0.92	0.43	34,34,34,34	0
59	MG	DA	3184	1/1	0.92	0.11	50,50,50,50	0
59	MG	BA	3102	1/1	0.92	0.31	49,49,49,49	0
59	MG	AA	1649	1/1	0.92	0.36	71,71,71,71	0
59	MG	DA	3146	1/1	0.92	0.20	70,70,70,70	0
59	MG	CV	101	1/1	0.92	0.24	36,36,36,36	0
59	MG	CX	102	1/1	0.92	0.51	78,78,78,78	0
59	MG	CA	1622	1/1	0.92	0.26	49,49,49,49	0
59	MG	DA	3232	1/1	0.92	0.30	80,80,80,80	0
59	MG	AA	1728	1/1	0.92	0.11	59,59,59,59	0
59	MG	DA	3065	1/1	0.92	0.32	51,51,51,51	0
59	MG	BA	3144	1/1	0.92	0.14	37,37,37,37	0
59	MG	AA	1691	1/1	0.92	0.44	56,56,56,56	0
59	MG	DA	3079	1/1	0.92	0.28	16,16,16,16	0
59	MG	DA	3100	1/1	0.92	0.37	57,57,57,57	0
59	MG	DA	3125	1/1	0.92	0.39	59,59,59,59	0
59	MG	AD	301	1/1	0.92	0.12	49,49,49,49	0
59	MG	BA	3271	1/1	0.93	0.49	64,64,64,64	0
59	MG	DA	3133	1/1	0.93	0.15	69,69,69,69	0
59	MG	BA	3175	1/1	0.93	0.24	43,43,43,43	0
59	MG	BA	3340	1/1	0.93	0.13	42,42,42,42	0
59	MG	DA	3089	1/1	0.93	0.36	26,26,26,26	0
59	MG	DA	3111	1/1	0.93	0.62	71,71,71,71	0
59	MG	BA	3131	1/1	0.93	0.84	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	CA	1609	1/1	0.93	0.48	52,52,52,52	0
59	MG	DA	3101	1/1	0.93	0.09	28,28,28,28	0
59	MG	DA	3162	1/1	0.93	0.11	40,40,40,40	0
59	MG	DA	3160	1/1	0.93	0.33	28,28,28,28	0
59	MG	AA	1651	1/1	0.93	0.30	37,37,37,37	0
59	MG	BA	3170	1/1	0.93	0.26	57,57,57,57	0
59	MG	BA	3110	1/1	0.93	0.20	39,39,39,39	0
59	MG	AA	1623	1/1	0.93	0.21	27,27,27,27	0
59	MG	BA	3324	1/1	0.93	0.45	35,35,35,35	0
59	MG	AA	1718	1/1	0.93	0.14	36,36,36,36	0
59	MG	DA	3252	1/1	0.93	0.35	47,47,47,47	0
59	MG	DA	3022	1/1	0.93	0.17	14,14,14,14	0
59	MG	BA	3117	1/1	0.93	0.24	38,38,38,38	0
59	MG	BA	3266	1/1	0.93	0.31	27,27,27,27	0
59	MG	DA	3161	1/1	0.93	0.50	32,32,32,32	0
59	MG	BA	3135	1/1	0.93	0.25	38,38,38,38	0
59	MG	DA	3157	1/1	0.93	0.41	62,62,62,62	0
59	MG	CA	1617	1/1	0.93	0.28	39,39,39,39	0
59	MG	BA	3200	1/1	0.93	0.21	51,51,51,51	0
59	MG	AA	1658	1/1	0.93	0.58	42,42,42,42	0
59	MG	BA	3038	1/1	0.93	0.25	20,20,20,20	0
59	MG	BA	3244	1/1	0.93	0.17	31,31,31,31	0
59	MG	DA	3199	1/1	0.93	0.50	38,38,38,38	0
59	MG	BA	3157	1/1	0.93	0.13	42,42,42,42	0
59	MG	BA	3255	1/1	0.93	0.11	22,22,22,22	0
59	MG	AE	201	1/1	0.93	0.21	87,87,87,87	0
59	MG	BA	3234	1/1	0.93	0.33	35,35,35,35	0
59	MG	DA	3093	1/1	0.93	0.25	40,40,40,40	0
59	MG	BA	3109	1/1	0.93	0.14	34,34,34,34	0
59	MG	AA	1610	1/1	0.93	0.09	29,29,29,29	0
59	MG	AA	1716	1/1	0.93	0.23	44,44,44,44	0
59	MG	BA	3054	1/1	0.93	0.12	22,22,22,22	0
59	MG	BA	3363	1/1	0.93	0.26	56,56,56,56	0
59	MG	AA	1662	1/1	0.93	0.22	23,23,23,23	0
59	MG	DA	3239	1/1	0.93	1.00	78,78,78,78	0
59	MG	AA	1721	1/1	0.93	0.14	54,54,54,54	0
59	MG	DA	3153	1/1	0.93	0.18	28,28,28,28	0
59	MG	CA	1649	1/1	0.93	0.09	48,48,48,48	0
59	MG	BA	3058	1/1	0.93	0.21	20,20,20,20	0
59	MG	BA	3181	1/1	0.93	0.10	46,46,46,46	0
59	MG	AA	1660	1/1	0.93	0.41	40,40,40,40	0
59	MG	DA	3113	1/1	0.93	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3313	1/1	0.93	0.42	55,55,55,55	0
59	MG	DA	3003	1/1	0.93	0.22	36,36,36,36	0
59	MG	BA	3350	1/1	0.93	0.13	20,20,20,20	0
59	MG	DA	3076	1/1	0.93	0.28	48,48,48,48	0
59	MG	BA	3073	1/1	0.93	0.16	10,10,10,10	0
59	MG	BA	3273	1/1	0.93	0.21	26,26,26,26	0
59	MG	BA	3280	1/1	0.93	0.37	54,54,54,54	0
59	MG	AA	1722	1/1	0.93	0.15	35,35,35,35	0
59	MG	BA	3287	1/1	0.93	0.57	56,56,56,56	0
59	MG	BA	3306	1/1	0.93	0.15	29,29,29,29	0
59	MG	BA	3239	1/1	0.93	0.21	25,25,25,25	0
59	MG	BA	3391	1/1	0.93	0.19	31,31,31,31	0
59	MG	BA	3138	1/1	0.93	0.17	17,17,17,17	0
59	MG	DA	3021	1/1	0.93	0.17	28,28,28,28	0
59	MG	AA	1645	1/1	0.93	0.41	64,64,64,64	0
59	MG	DA	3009	1/1	0.93	0.15	20,20,20,20	0
59	MG	CA	1641	1/1	0.93	0.15	28,28,28,28	0
59	MG	BA	3143	1/1	0.93	0.25	37,37,37,37	0
59	MG	DA	3051	1/1	0.93	0.46	51,51,51,51	0
59	MG	BA	3064	1/1	0.93	0.28	32,32,32,32	0
59	MG	BA	3139	1/1	0.94	0.15	15,15,15,15	0
59	MG	CA	1691	1/1	0.94	0.15	55,55,55,55	0
59	MG	AY	101	1/1	0.94	0.17	71,71,71,71	0
59	MG	BA	3189	1/1	0.94	0.31	18,18,18,18	0
59	MG	DA	3214	1/1	0.94	0.15	34,34,34,34	0
59	MG	DA	3094	1/1	0.94	0.24	27,27,27,27	0
59	MG	BA	3075	1/1	0.94	0.29	32,32,32,32	0
59	MG	BA	3338	1/1	0.94	0.07	60,60,60,60	0
59	MG	BA	3223	1/1	0.94	0.25	46,46,46,46	0
59	MG	BA	3173	1/1	0.94	0.11	17,17,17,17	0
59	MG	BA	3388	1/1	0.94	0.13	13,13,13,13	0
59	MG	BU	201	1/1	0.94	0.27	22,22,22,22	0
59	MG	AA	1663	1/1	0.94	0.44	53,53,53,53	0
59	MG	DA	3208	1/1	0.94	0.40	62,62,62,62	0
59	MG	BA	3031	1/1	0.94	0.22	12,12,12,12	0
59	MG	AA	1629	1/1	0.94	0.15	78,78,78,78	0
59	MG	DA	3256	1/1	0.94	0.12	27,27,27,27	0
59	MG	BA	3180	1/1	0.94	0.35	22,22,22,22	0
59	MG	DA	3231	1/1	0.94	0.21	43,43,43,43	0
59	MG	CA	1681	1/1	0.94	0.07	58,58,58,58	0
59	MG	AA	1661	1/1	0.94	0.13	34,34,34,34	0
59	MG	BA	3125	1/1	0.94	0.48	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3020	1/1	0.94	0.23	22,22,22,22	0
59	MG	AA	1715	1/1	0.94	0.14	34,34,34,34	0
59	MG	CA	1626	1/1	0.94	0.33	46,46,46,46	0
59	MG	BA	3339	1/1	0.94	0.39	66,66,66,66	0
59	MG	AA	1733	1/1	0.94	0.13	30,30,30,30	0
59	MG	AA	1618	1/1	0.94	0.23	22,22,22,22	0
59	MG	DF	301	1/1	0.94	0.09	31,31,31,31	0
59	MG	BA	3312	1/1	0.94	0.13	42,42,42,42	0
59	MG	DA	3248	1/1	0.94	0.46	60,60,60,60	0
59	MG	CA	1647	1/1	0.94	0.43	51,51,51,51	0
59	MG	BA	3301	1/1	0.94	0.11	21,21,21,21	0
59	MG	BA	3248	1/1	0.94	0.27	37,37,37,37	0
59	MG	DA	3134	1/1	0.94	0.26	42,42,42,42	0
59	MG	BA	3098	1/1	0.94	0.31	18,18,18,18	0
59	MG	BA	3372	1/1	0.94	0.21	26,26,26,26	0
59	MG	AX	103	1/1	0.94	0.14	32,32,32,32	0
59	MG	DA	3148	1/1	0.94	0.62	40,40,40,40	0
59	MG	BA	3052	1/1	0.94	0.43	37,37,37,37	0
59	MG	AA	1604	1/1	0.94	0.30	56,56,56,56	0
59	MG	BA	3061	1/1	0.94	0.28	21,21,21,21	0
59	MG	BA	3211	1/1	0.94	0.18	16,16,16,16	0
59	MG	BA	3393	1/1	0.94	0.15	40,40,40,40	0
59	MG	BA	3091	1/1	0.94	0.23	34,34,34,34	0
59	MG	DA	3074	1/1	0.94	0.35	59,59,59,59	0
59	MG	DA	3191	1/1	0.94	0.08	77,77,77,77	0
59	MG	BA	3319	1/1	0.94	0.41	25,25,25,25	0
59	MG	BA	3343	1/1	0.94	0.20	34,34,34,34	0
59	MG	BA	3095	1/1	0.94	0.25	30,30,30,30	0
59	MG	AA	1608	1/1	0.94	0.07	26,26,26,26	0
59	MG	BA	3322	1/1	0.94	0.68	147,147,147,147	0
59	MG	BA	3384	1/1	0.94	0.10	39,39,39,39	0
59	MG	DA	3042	1/1	0.94	0.29	41,41,41,41	0
59	MG	BA	3093	1/1	0.94	0.15	10,10,10,10	0
59	MG	BA	3195	1/1	0.94	0.15	79,79,79,79	0
59	MG	BA	3146	1/1	0.94	0.36	12,12,12,12	0
59	MG	CA	1627	1/1	0.94	0.15	62,62,62,62	0
59	MG	CA	1614	1/1	0.94	0.16	49,49,49,49	0
59	MG	AA	1607	1/1	0.94	0.44	43,43,43,43	0
59	MG	BA	3354	1/1	0.94	0.11	41,41,41,41	0
59	MG	DA	3124	1/1	0.94	0.05	43,43,43,43	0
59	MG	AA	1726	1/1	0.94	0.29	32,32,32,32	0
59	MG	BA	3369	1/1	0.94	0.28	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AL	201	1/1	0.94	0.46	44,44,44,44	0
59	MG	AW	107	1/1	0.94	0.14	41,41,41,41	0
59	MG	DA	3173	1/1	0.94	0.20	57,57,57,57	0
59	MG	CA	1668	1/1	0.94	0.08	42,42,42,42	0
59	MG	AA	1703	1/1	0.94	0.08	41,41,41,41	0
59	MG	DA	3039	1/1	0.94	0.32	58,58,58,58	0
59	MG	BA	3241	1/1	0.94	0.27	38,38,38,38	0
59	MG	BA	3034	1/1	0.94	0.32	37,37,37,37	0
59	MG	BA	3367	1/1	0.94	0.44	35,35,35,35	0
59	MG	DA	3155	1/1	0.94	0.18	56,56,56,56	0
59	MG	BA	3325	1/1	0.94	0.15	61,61,61,61	0
59	MG	BA	3336	1/1	0.94	0.30	23,23,23,23	0
59	MG	DA	3259	1/1	0.94	0.36	43,43,43,43	0
59	MG	DA	3241	1/1	0.94	0.30	42,42,42,42	0
59	MG	DA	3260	1/1	0.94	0.28	35,35,35,35	0
59	MG	CA	1665	1/1	0.94	0.27	34,34,34,34	0
59	MG	BA	3365	1/1	0.94	0.15	36,36,36,36	0
59	MG	AA	1619	1/1	0.94	0.55	47,47,47,47	0
60	ZN	D4	101	1/1	0.94	0.17	147,147,147,147	0
59	MG	DA	3029	1/1	0.94	0.34	34,34,34,34	0
59	MG	DA	3002	1/1	0.94	0.23	31,31,31,31	0
59	MG	DA	3142	1/1	0.94	0.15	44,44,44,44	0
59	MG	DE	302	1/1	0.94	0.65	65,65,65,65	0
59	MG	DA	3169	1/1	0.94	0.14	37,37,37,37	0
59	MG	AA	1653	1/1	0.95	0.25	47,47,47,47	0
59	MG	AA	1644	1/1	0.95	0.25	48,48,48,48	0
59	MG	BA	3171	1/1	0.95	0.50	51,51,51,51	0
59	MG	BA	3145	1/1	0.95	0.31	13,13,13,13	0
59	MG	BA	3380	1/1	0.95	0.19	47,47,47,47	0
59	MG	CA	1684	1/1	0.95	0.51	49,49,49,49	0
59	MG	CA	1637	1/1	0.95	0.07	29,29,29,29	0
59	MG	CV	102	1/1	0.95	0.35	44,44,44,44	0
59	MG	BA	3254	1/1	0.95	0.08	43,43,43,43	0
59	MG	BA	3150	1/1	0.95	0.14	33,33,33,33	0
59	MG	DA	3165	1/1	0.95	0.07	49,49,49,49	0
59	MG	BA	3106	1/1	0.95	0.30	29,29,29,29	0
59	MG	BA	3069	1/1	0.95	0.22	20,20,20,20	0
59	MG	AA	1611	1/1	0.95	0.16	52,52,52,52	0
60	ZN	AD	302	1/1	0.95	0.24	67,67,67,67	0
59	MG	BA	3209	1/1	0.95	0.11	27,27,27,27	0
59	MG	BA	3086	1/1	0.95	0.53	46,46,46,46	0
59	MG	BA	3070	1/1	0.95	0.08	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3284	1/1	0.95	0.37	33,33,33,33	0
59	MG	BA	3035	1/1	0.95	0.17	22,22,22,22	0
59	MG	BA	3311	1/1	0.95	0.87	54,54,54,54	0
59	MG	BA	3206	1/1	0.95	0.16	36,36,36,36	0
59	MG	BA	3361	1/1	0.95	0.11	25,25,25,25	0
59	MG	DA	3237	1/1	0.95	0.09	39,39,39,39	0
59	MG	BA	3243	1/1	0.95	0.29	35,35,35,35	0
59	MG	DA	3249	1/1	0.95	0.41	54,54,54,54	0
59	MG	BA	3218	1/1	0.95	0.12	21,21,21,21	0
59	MG	CA	1613	1/1	0.95	0.06	66,66,66,66	0
59	MG	AA	1674	1/1	0.95	0.05	42,42,42,42	0
59	MG	DA	3216	1/1	0.95	0.29	35,35,35,35	0
59	MG	BA	3122	1/1	0.95	0.20	38,38,38,38	0
59	MG	AA	1730	1/1	0.95	0.50	60,60,60,60	0
59	MG	AA	1628	1/1	0.95	0.47	46,46,46,46	0
59	MG	BA	3151	1/1	0.95	0.29	22,22,22,22	0
59	MG	BA	3199	1/1	0.95	0.25	54,54,54,54	0
59	MG	BA	3142	1/1	0.95	0.26	18,18,18,18	0
59	MG	DA	3028	1/1	0.95	0.33	35,35,35,35	0
59	MG	BA	3137	1/1	0.95	0.17	34,34,34,34	0
59	MG	DA	3201	1/1	0.95	0.12	33,33,33,33	0
59	MG	D6	101	1/1	0.95	0.30	37,37,37,37	0
59	MG	BA	3083	1/1	0.95	0.17	6,6,6,6	0
59	MG	BA	3132	1/1	0.95	0.17	87,87,87,87	0
59	MG	BA	3082	1/1	0.95	0.12	15,15,15,15	0
59	MG	BA	3238	1/1	0.95	0.14	26,26,26,26	0
59	MG	DA	3255	1/1	0.95	0.15	13,13,13,13	0
59	MG	D5	102	1/1	0.95	0.22	91,91,91,91	0
59	MG	AA	1614	1/1	0.95	0.20	45,45,45,45	0
59	MG	DA	3044	1/1	0.95	0.13	22,22,22,22	0
59	MG	BA	3375	1/1	0.95	0.20	38,38,38,38	0
59	MG	BA	3286	1/1	0.95	0.20	26,26,26,26	0
59	MG	BA	3283	1/1	0.95	0.27	46,46,46,46	0
60	ZN	D9	101	1/1	0.95	0.02	109,109,109,109	0
59	MG	BA	3193	1/1	0.95	0.36	58,58,58,58	0
59	MG	BA	3213	1/1	0.95	0.54	54,54,54,54	0
59	MG	BA	3201	1/1	0.95	0.17	111,111,111,111	0
59	MG	DA	3272	1/1	0.95	0.52	60,60,60,60	0
59	MG	AA	1697	1/1	0.95	0.34	73,73,73,73	0
59	MG	DA	3202	1/1	0.95	0.11	34,34,34,34	0
59	MG	DA	3221	1/1	0.95	0.39	59,59,59,59	0
59	MG	BA	3202	1/1	0.95	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3127	1/1	0.95	0.28	48,48,48,48	0
59	MG	AA	1622	1/1	0.95	0.29	44,44,44,44	0
59	MG	DA	3020	1/1	0.95	0.26	45,45,45,45	0
59	MG	BA	3024	1/1	0.95	0.18	22,22,22,22	0
59	MG	BA	3378	1/1	0.95	0.29	25,25,25,25	0
59	MG	CA	1648	1/1	0.95	0.18	56,56,56,56	0
59	MG	CA	1682	1/1	0.95	0.50	61,61,61,61	0
59	MG	CA	1654	1/1	0.95	0.12	63,63,63,63	0
59	MG	D5	101	1/1	0.95	0.14	28,28,28,28	0
59	MG	AA	1670	1/1	0.95	0.22	36,36,36,36	0
59	MG	BA	3300	1/1	0.95	0.13	40,40,40,40	0
59	MG	CA	1629	1/1	0.95	0.29	52,52,52,52	0
59	MG	BA	3278	1/1	0.95	0.31	50,50,50,50	0
59	MG	BQ	201	1/1	0.95	0.13	48,48,48,48	0
59	MG	DA	3116	1/1	0.95	0.13	43,43,43,43	0
59	MG	BA	3247	1/1	0.95	0.08	29,29,29,29	0
59	MG	BA	3395	1/1	0.95	0.18	46,46,46,46	0
59	MG	DA	3158	1/1	0.95	0.33	38,38,38,38	0
59	MG	DA	3138	1/1	0.95	0.12	19,19,19,19	0
59	MG	AA	1687	1/1	0.95	0.06	27,27,27,27	0
59	MG	CA	1660	1/1	0.95	0.11	45,45,45,45	0
59	MG	DA	3149	1/1	0.95	0.36	42,42,42,42	0
59	MG	DA	3242	1/1	0.95	0.17	34,34,34,34	0
59	MG	DA	3269	1/1	0.95	0.15	43,43,43,43	0
59	MG	CA	1620	1/1	0.95	0.40	40,40,40,40	0
59	MG	AA	1680	1/1	0.95	0.41	63,63,63,63	0
59	MG	BP	201	1/1	0.95	0.11	21,21,21,21	0
59	MG	BA	3158	1/1	0.95	0.12	40,40,40,40	0
59	MG	BH	201	1/1	0.96	0.13	71,71,71,71	0
59	MG	DA	3054	1/1	0.96	0.11	42,42,42,42	0
59	MG	CA	1616	1/1	0.96	0.23	46,46,46,46	0
59	MG	BA	3377	1/1	0.96	0.36	43,43,43,43	0
59	MG	DA	3081	1/1	0.96	0.20	48,48,48,48	0
59	MG	CA	1690	1/1	0.96	0.14	46,46,46,46	0
59	MG	CA	1664	1/1	0.96	0.41	44,44,44,44	0
59	MG	BA	3186	1/1	0.96	0.21	30,30,30,30	0
59	MG	DA	3222	1/1	0.96	0.11	50,50,50,50	0
59	MG	DA	3034	1/1	0.96	0.07	30,30,30,30	0
59	MG	AA	1630	1/1	0.96	0.07	26,26,26,26	0
59	MG	BA	3149	1/1	0.96	0.43	31,31,31,31	0
59	MG	BA	3321	1/1	0.96	0.23	51,51,51,51	0
59	MG	BA	3047	1/1	0.96	0.22	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3370	1/1	0.96	0.15	28,28,28,28	0
59	MG	BA	3123	1/1	0.96	0.17	45,45,45,45	0
59	MG	BA	3042	1/1	0.96	0.20	22,22,22,22	0
59	MG	CA	1610	1/1	0.96	0.34	27,27,27,27	0
59	MG	CA	1656	1/1	0.96	0.22	51,51,51,51	0
59	MG	DA	3139	1/1	0.96	0.08	18,18,18,18	0
59	MG	DA	3118	1/1	0.96	0.16	41,41,41,41	0
59	MG	BA	3198	1/1	0.96	0.08	16,16,16,16	0
59	MG	BA	3314	1/1	0.96	0.18	68,68,68,68	0
59	MG	BA	3221	1/1	0.96	0.24	25,25,25,25	0
59	MG	AA	1632	1/1	0.96	0.37	53,53,53,53	0
59	MG	CA	1685	1/1	0.96	0.08	36,36,36,36	0
59	MG	CA	1611	1/1	0.96	0.21	38,38,38,38	0
59	MG	DA	3225	1/1	0.96	0.76	55,55,55,55	0
59	MG	BA	3001	1/1	0.96	0.18	72,72,72,72	0
59	MG	DA	3150	1/1	0.96	0.18	43,43,43,43	0
59	MG	DA	3110	1/1	0.96	0.09	38,38,38,38	0
59	MG	BA	3011	1/1	0.96	0.14	31,31,31,31	0
59	MG	BA	3275	1/1	0.96	0.12	93,93,93,93	0
59	MG	BA	3345	1/1	0.96	0.24	31,31,31,31	0
59	MG	DA	3107	1/1	0.96	0.11	32,32,32,32	0
59	MG	DA	3073	1/1	0.96	0.22	18,18,18,18	0
59	MG	DA	3131	1/1	0.96	0.17	38,38,38,38	0
59	MG	DA	3264	1/1	0.96	0.36	41,41,41,41	0
59	MG	DA	3156	1/1	0.96	0.29	28,28,28,28	0
59	MG	DA	3013	1/1	0.96	0.42	32,32,32,32	0
59	MG	AA	1606	1/1	0.96	0.28	63,63,63,63	0
59	MG	BA	3304	1/1	0.96	0.46	22,22,22,22	0
59	MG	BA	3160	1/1	0.96	0.27	13,13,13,13	0
59	MG	CX	103	1/1	0.96	0.21	50,50,50,50	0
59	MG	CA	1604	1/1	0.96	0.11	21,21,21,21	0
59	MG	BA	3267	1/1	0.96	0.12	31,31,31,31	0
59	MG	BA	3060	1/1	0.96	0.13	13,13,13,13	0
59	MG	BA	3390	1/1	0.96	0.19	53,53,53,53	0
59	MG	BA	3190	1/1	0.96	0.18	29,29,29,29	0
59	MG	DA	3062	1/1	0.96	0.18	24,24,24,24	0
59	MG	CA	1650	1/1	0.96	0.43	69,69,69,69	0
59	MG	DA	3016	1/1	0.96	0.12	54,54,54,54	0
59	MG	BA	3222	1/1	0.96	0.20	18,18,18,18	0
59	MG	AA	1682	1/1	0.96	0.12	53,53,53,53	0
59	MG	BA	3030	1/1	0.96	0.13	18,18,18,18	0
59	MG	DA	3188	1/1	0.96	0.34	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	CA	1628	1/1	0.96	0.08	27,27,27,27	0
59	MG	AA	1669	1/1	0.96	0.16	36,36,36,36	0
59	MG	BA	3029	1/1	0.96	0.15	23,23,23,23	0
59	MG	AA	1720	1/1	0.96	0.16	52,52,52,52	0
59	MG	BA	3014	1/1	0.96	0.24	63,63,63,63	0
59	MG	BA	3033	1/1	0.96	0.29	26,26,26,26	0
59	MG	DA	3004	1/1	0.96	0.23	54,54,54,54	0
59	MG	DA	3058	1/1	0.96	0.07	33,33,33,33	0
59	MG	DA	3141	1/1	0.96	0.14	46,46,46,46	0
59	MG	CA	1646	1/1	0.96	0.32	40,40,40,40	0
59	MG	CA	1667	1/1	0.96	0.26	37,37,37,37	0
59	MG	BA	3399	1/1	0.96	0.19	41,41,41,41	0
59	MG	AA	1601	1/1	0.96	0.08	38,38,38,38	0
59	MG	AA	1681	1/1	0.96	0.07	30,30,30,30	0
59	MG	BA	3204	1/1	0.96	0.10	2,2,2,2	0
59	MG	BA	3051	1/1	0.96	0.22	1,1,1,1	0
59	MG	DA	3179	1/1	0.96	0.15	33,33,33,33	0
59	MG	BA	3282	1/1	0.96	0.22	48,48,48,48	0
59	MG	CA	1606	1/1	0.96	0.66	52,52,52,52	0
59	MG	BA	3318	1/1	0.96	0.35	41,41,41,41	0
59	MG	BA	3220	1/1	0.96	0.52	52,52,52,52	0
59	MG	BA	3251	1/1	0.96	0.27	34,34,34,34	0
59	MG	DA	3046	1/1	0.96	0.18	15,15,15,15	0
59	MG	BA	3121	1/1	0.96	0.16	38,38,38,38	0
59	MG	BA	3385	1/1	0.96	0.11	32,32,32,32	0
59	MG	BA	3068	1/1	0.96	0.22	15,15,15,15	0
59	MG	CA	1640	1/1	0.96	0.10	47,47,47,47	0
59	MG	AA	1626	1/1	0.96	0.11	48,48,48,48	0
59	MG	BA	3022	1/1	0.96	0.16	12,12,12,12	0
59	MG	BA	3226	1/1	0.96	0.09	33,33,33,33	0
59	MG	DA	3263	1/1	0.96	0.43	62,62,62,62	0
59	MG	CE	202	1/1	0.96	0.21	40,40,40,40	0
59	MG	BA	3168	1/1	0.96	0.14	37,37,37,37	0
59	MG	BA	3277	1/1	0.96	0.32	60,60,60,60	0
59	MG	BA	3187	1/1	0.96	0.37	35,35,35,35	0
59	MG	DA	3050	1/1	0.96	0.35	70,70,70,70	0
59	MG	CA	1673	1/1	0.96	0.32	71,71,71,71	0
59	MG	DA	3037	1/1	0.96	0.17	26,26,26,26	0
59	MG	BA	3329	1/1	0.96	0.09	48,48,48,48	0
59	MG	DA	3083	1/1	0.96	0.31	35,35,35,35	0
59	MG	AA	1664	1/1	0.96	0.10	20,20,20,20	0
59	MG	CA	1602	1/1	0.96	0.37	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3258	1/1	0.96	0.13	26,26,26,26	0
59	MG	DA	3012	1/1	0.96	0.25	33,33,33,33	0
59	MG	AA	1683	1/1	0.96	0.10	31,31,31,31	0
59	MG	BA	3163	1/1	0.96	0.12	22,22,22,22	0
59	MG	DA	3159	1/1	0.96	0.14	16,16,16,16	0
59	MG	DA	3151	1/1	0.96	0.13	14,14,14,14	0
59	MG	BA	3285	1/1	0.96	0.20	28,28,28,28	0
59	MG	BA	3289	1/1	0.96	0.18	36,36,36,36	0
59	MG	DA	3267	1/1	0.96	0.28	53,53,53,53	0
59	MG	BA	3327	1/1	0.96	0.35	44,44,44,44	0
59	MG	BA	3113	1/1	0.97	0.40	34,34,34,34	0
59	MG	DA	3024	1/1	0.97	0.17	29,29,29,29	0
59	MG	BA	3203	1/1	0.97	0.16	38,38,38,38	0
59	MG	AA	1673	1/1	0.97	0.20	35,35,35,35	0
59	MG	BA	3105	1/1	0.97	0.22	14,14,14,14	0
59	MG	DA	3182	1/1	0.97	0.16	33,33,33,33	0
59	MG	DA	3122	1/1	0.97	0.20	31,31,31,31	0
59	MG	BA	3262	1/1	0.97	0.23	27,27,27,27	0
59	MG	BA	3368	1/1	0.97	0.10	24,24,24,24	0
59	MG	BA	3013	1/1	0.97	0.24	6,6,6,6	0
59	MG	BE	301	1/1	0.97	0.23	12,12,12,12	0
59	MG	BA	3130	1/1	0.97	0.08	13,13,13,13	0
59	MG	DA	3066	1/1	0.97	0.27	31,31,31,31	0
59	MG	BA	3115	1/1	0.97	0.27	22,22,22,22	0
59	MG	AA	1636	1/1	0.97	0.25	21,21,21,21	0
59	MG	DA	3015	1/1	0.97	0.42	37,37,37,37	0
59	MG	BA	3046	1/1	0.97	0.14	30,30,30,30	0
59	MG	DA	3072	1/1	0.97	0.29	28,28,28,28	0
59	MG	BA	3107	1/1	0.97	0.16	13,13,13,13	0
59	MG	DA	3185	1/1	0.97	0.08	42,42,42,42	0
59	MG	DA	3195	1/1	0.97	0.30	38,38,38,38	0
59	MG	B5	101	1/1	0.97	0.48	37,37,37,37	0
59	MG	AA	1694	1/1	0.97	0.27	24,24,24,24	0
59	MG	DA	3033	1/1	0.97	0.12	10,10,10,10	0
59	MG	AA	1677	1/1	0.97	0.38	75,75,75,75	0
59	MG	BA	3048	1/1	0.97	0.10	6,6,6,6	0
59	MG	BA	3194	1/1	0.97	0.31	33,33,33,33	0
59	MG	BD	301	1/1	0.97	0.16	13,13,13,13	0
59	MG	BA	3215	1/1	0.97	0.15	12,12,12,12	0
59	MG	BA	3118	1/1	0.97	0.25	18,18,18,18	0
59	MG	BA	3050	1/1	0.97	0.28	4,4,4,4	0
59	MG	DA	3041	1/1	0.97	0.29	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3036	1/1	0.97	0.32	20,20,20,20	0
59	MG	BA	3088	1/1	0.97	0.34	22,22,22,22	0
59	MG	BA	3085	1/1	0.97	0.41	18,18,18,18	0
59	MG	AA	1675	1/1	0.97	0.49	38,38,38,38	0
59	MG	BA	3172	1/1	0.97	0.39	40,40,40,40	0
59	MG	DA	3258	1/1	0.97	0.19	29,29,29,29	0
59	MG	CA	1624	1/1	0.97	0.15	24,24,24,24	0
59	MG	BA	3178	1/1	0.97	0.37	11,11,11,11	0
59	MG	BA	3353	1/1	0.97	0.38	50,50,50,50	0
59	MG	DA	3047	1/1	0.97	0.17	25,25,25,25	0
59	MG	DA	3038	1/1	0.97	0.14	25,25,25,25	0
59	MG	BA	3066	1/1	0.97	0.29	20,20,20,20	0
59	MG	CA	1658	1/1	0.97	0.13	40,40,40,40	0
59	MG	CA	1676	1/1	0.97	0.17	55,55,55,55	0
59	MG	DA	3106	1/1	0.97	0.21	51,51,51,51	0
59	MG	DA	3104	1/1	0.97	0.11	36,36,36,36	0
59	MG	BA	3364	1/1	0.97	0.18	8,8,8,8	0
59	MG	DA	3086	1/1	0.97	0.16	26,26,26,26	0
59	MG	BA	3016	1/1	0.97	0.41	27,27,27,27	0
59	MG	DA	3228	1/1	0.97	0.05	16,16,16,16	0
59	MG	BA	3100	1/1	0.97	0.21	22,22,22,22	0
59	MG	AA	1625	1/1	0.97	0.20	32,32,32,32	0
59	MG	BA	3355	1/1	0.97	0.17	33,33,33,33	0
59	MG	DA	3180	1/1	0.97	0.50	27,27,27,27	0
59	MG	BA	3101	1/1	0.97	0.11	25,25,25,25	0
59	MG	DA	3204	1/1	0.97	0.14	41,41,41,41	0
59	MG	DA	3194	1/1	0.97	0.33	52,52,52,52	0
59	MG	BA	3059	1/1	0.97	0.06	33,33,33,33	0
59	MG	AA	1657	1/1	0.97	0.16	53,53,53,53	0
59	MG	CA	1601	1/1	0.97	0.17	29,29,29,29	0
59	MG	BA	3080	1/1	0.97	0.24	26,26,26,26	0
59	MG	BA	3074	1/1	0.97	0.18	12,12,12,12	0
59	MG	BA	3358	1/1	0.97	0.09	49,49,49,49	0
59	MG	BA	3097	1/1	0.97	0.10	21,21,21,21	0
59	MG	BA	3188	1/1	0.97	0.42	22,22,22,22	0
59	MG	BA	3217	1/1	0.97	0.17	11,11,11,11	0
59	MG	DA	3018	1/1	0.97	0.17	14,14,14,14	0
59	MG	DA	3105	1/1	0.97	0.22	28,28,28,28	0
59	MG	BA	3090	1/1	0.97	0.14	32,32,32,32	0
59	MG	DA	3117	1/1	0.97	0.08	32,32,32,32	0
59	MG	CA	1678	1/1	0.97	0.17	45,45,45,45	0
59	MG	DA	3006	1/1	0.97	0.31	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	CA	1662	1/1	0.97	0.08	23,23,23,23	0
59	MG	BA	3236	1/1	0.97	0.22	23,23,23,23	0
59	MG	BA	3242	1/1	0.97	0.58	44,44,44,44	0
59	MG	BA	3342	1/1	0.97	0.21	21,21,21,21	0
59	MG	CA	1632	1/1	0.97	0.30	47,47,47,47	0
59	MG	BA	3225	1/1	0.97	0.25	43,43,43,43	0
59	MG	DA	3063	1/1	0.97	0.15	53,53,53,53	0
59	MG	DA	3233	1/1	0.97	0.34	58,58,58,58	0
59	MG	BA	3264	1/1	0.97	0.26	34,34,34,34	0
59	MG	AH	201	1/1	0.97	0.29	31,31,31,31	0
59	MG	DA	3085	1/1	0.97	0.25	22,22,22,22	0
59	MG	DD	302	1/1	0.97	0.48	34,34,34,34	0
59	MG	DA	3177	1/1	0.97	0.42	29,29,29,29	0
59	MG	DA	3055	1/1	0.97	0.39	42,42,42,42	0
59	MG	BA	3005	1/1	0.97	0.08	17,17,17,17	0
60	ZN	CD	301	1/1	0.97	0.25	61,61,61,61	0
59	MG	DA	3070	1/1	0.97	0.14	10,10,10,10	0
59	MG	BA	3025	1/1	0.97	0.17	20,20,20,20	0
59	MG	BA	3328	1/1	0.97	0.21	35,35,35,35	0
59	MG	BA	3071	1/1	0.97	0.05	42,42,42,42	0
59	MG	DA	3060	1/1	0.97	0.12	16,16,16,16	0
59	MG	BA	3330	1/1	0.98	0.09	21,21,21,21	0
59	MG	DA	3031	1/1	0.98	0.16	31,31,31,31	0
59	MG	DA	3067	1/1	0.98	0.27	50,50,50,50	0
59	MG	DA	3092	1/1	0.98	0.36	51,51,51,51	0
59	MG	BA	3169	1/1	0.98	0.12	51,51,51,51	0
59	MG	DA	3266	1/1	0.98	0.38	72,72,72,72	0
59	MG	AA	1704	1/1	0.98	0.06	40,40,40,40	0
59	MG	BA	3040	1/1	0.98	0.06	9,9,9,9	0
59	MG	BA	3065	1/1	0.98	0.10	13,13,13,13	0
59	MG	BA	3012	1/1	0.98	0.29	31,31,31,31	0
59	MG	BA	3111	1/1	0.98	0.27	28,28,28,28	0
59	MG	DA	3174	1/1	0.98	0.04	47,47,47,47	0
59	MG	AA	1692	1/1	0.98	0.04	55,55,55,55	0
59	MG	DE	301	1/1	0.98	0.20	43,43,43,43	0
59	MG	AA	1616	1/1	0.98	0.08	16,16,16,16	0
59	MG	CA	1680	1/1	0.98	0.17	59,59,59,59	0
59	MG	DA	3114	1/1	0.98	0.08	42,42,42,42	0
59	MG	DA	3056	1/1	0.98	0.21	31,31,31,31	0
59	MG	AA	1701	1/1	0.98	0.29	36,36,36,36	0
59	MG	BA	3124	1/1	0.98	0.15	27,27,27,27	0
59	MG	BA	3032	1/1	0.98	0.15	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3135	1/1	0.98	0.33	58,58,58,58	0
59	MG	BA	3279	1/1	0.98	0.16	62,62,62,62	0
59	MG	BA	3152	1/1	0.98	0.39	18,18,18,18	0
60	ZN	B9	101	1/1	0.98	0.06	64,64,64,64	0
59	MG	DA	3001	1/1	0.98	0.09	25,25,25,25	0
59	MG	AA	1708	1/1	0.98	0.04	64,64,64,64	0
59	MG	AA	1612	1/1	0.98	0.04	32,32,32,32	0
59	MG	DA	3040	1/1	0.98	0.07	34,34,34,34	0
59	MG	CA	1663	1/1	0.98	0.20	50,50,50,50	0
59	MG	BA	3092	1/1	0.98	0.08	20,20,20,20	0
59	MG	BA	3007	1/1	0.98	0.57	39,39,39,39	0
59	MG	AA	1696	1/1	0.98	0.20	34,34,34,34	0
59	MG	AA	1602	1/1	0.98	0.16	44,44,44,44	0
59	MG	BA	3018	1/1	0.98	0.25	23,23,23,23	0
59	MG	BB	201	1/1	0.98	0.07	18,18,18,18	0
59	MG	BA	3045	1/1	0.98	0.14	23,23,23,23	0
59	MG	BA	3356	1/1	0.98	0.17	41,41,41,41	0
59	MG	BA	3140	1/1	0.98	0.04	30,30,30,30	0
59	MG	DA	3071	1/1	0.98	0.18	27,27,27,27	0
59	MG	DA	3096	1/1	0.98	0.19	38,38,38,38	0
59	MG	BA	3207	1/1	0.98	0.19	24,24,24,24	0
59	MG	BA	3021	1/1	0.98	0.24	3,3,3,3	0
59	MG	BA	3263	1/1	0.98	0.16	37,37,37,37	0
59	MG	BA	3192	1/1	0.98	0.25	29,29,29,29	0
59	MG	CA	1634	1/1	0.98	0.04	17,17,17,17	0
59	MG	BA	3039	1/1	0.98	0.24	18,18,18,18	0
59	MG	DA	3026	1/1	0.98	0.16	36,36,36,36	0
59	MG	BA	3044	1/1	0.98	0.28	28,28,28,28	0
59	MG	DA	3129	1/1	0.98	0.40	35,35,35,35	0
59	MG	DA	3036	1/1	0.98	0.35	31,31,31,31	0
59	MG	DA	3090	1/1	0.98	0.19	24,24,24,24	0
59	MG	BA	3017	1/1	0.98	0.19	14,14,14,14	0
59	MG	BA	3077	1/1	0.98	0.07	23,23,23,23	0
59	MG	BA	3076	1/1	0.98	0.42	34,34,34,34	0
59	MG	BA	3009	1/1	0.98	0.25	30,30,30,30	0
59	MG	AA	1690	1/1	0.98	0.21	40,40,40,40	0
59	MG	CA	1633	1/1	0.98	0.22	38,38,38,38	0
59	MG	DA	3010	1/1	0.98	0.26	39,39,39,39	0
59	MG	BA	3155	1/1	0.98	0.08	9,9,9,9	0
59	MG	DA	3048	1/1	0.98	0.18	48,48,48,48	0
59	MG	BA	3015	1/1	0.98	0.38	25,25,25,25	0
59	MG	BA	3081	1/1	0.98	0.33	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3250	1/1	0.98	0.13	21,21,21,21	0
59	MG	DA	3147	1/1	0.98	0.40	44,44,44,44	0
59	MG	AA	1613	1/1	0.98	0.08	51,51,51,51	0
59	MG	AA	1713	1/1	0.98	0.16	57,57,57,57	0
59	MG	AA	1705	1/1	0.98	0.10	47,47,47,47	0
59	MG	AA	1609	1/1	0.98	0.11	23,23,23,23	0
59	MG	BA	3023	1/1	0.98	0.25	23,23,23,23	0
59	MG	CA	1655	1/1	0.99	0.29	41,41,41,41	0
59	MG	DA	3205	1/1	0.99	0.25	27,27,27,27	0
59	MG	AA	1706	1/1	0.99	0.29	43,43,43,43	0
59	MG	DA	3115	1/1	0.99	0.15	59,59,59,59	0
59	MG	AA	1650	1/1	0.99	0.20	26,26,26,26	0
59	MG	AA	1668	1/1	0.99	0.19	194,194,194,194	0
59	MG	DA	3143	1/1	0.99	0.27	30,30,30,30	0
59	MG	BA	3161	1/1	0.99	0.44	16,16,16,16	0
59	MG	AA	1631	1/1	0.99	0.10	25,25,25,25	0
59	MG	CA	1635	1/1	0.99	0.28	32,32,32,32	0
59	MG	BA	3055	1/1	0.99	0.18	21,21,21,21	0
59	MG	BA	3136	1/1	0.99	0.07	30,30,30,30	0
59	MG	DA	3246	1/1	0.99	0.14	23,23,23,23	0
59	MG	DA	3023	1/1	0.99	0.05	33,33,33,33	0
59	MG	BA	3387	1/1	0.99	0.13	46,46,46,46	0
59	MG	BA	3096	1/1	0.99	0.11	17,17,17,17	0
59	MG	DA	3206	1/1	0.99	0.26	27,27,27,27	0
59	MG	DA	3059	1/1	0.99	0.03	28,28,28,28	0
59	MG	BA	3129	1/1	0.99	0.13	27,27,27,27	0
59	MG	BA	3006	1/1	0.99	0.33	16,16,16,16	0
59	MG	DA	3032	1/1	0.99	0.09	9,9,9,9	0
59	MG	AA	1709	1/1	0.99	0.10	44,44,44,44	0
59	MG	BA	3141	1/1	0.99	0.23	1,1,1,1	0
59	MG	BA	3212	1/1	0.99	0.14	25,25,25,25	0
59	MG	BA	3072	1/1	0.99	0.23	16,16,16,16	0
59	MG	DA	3008	1/1	0.99	0.05	39,39,39,39	0
59	MG	BY	201	1/1	0.99	0.16	32,32,32,32	0
59	MG	BA	3062	1/1	0.99	0.14	14,14,14,14	0
59	MG	AA	1615	1/1	0.99	0.22	42,42,42,42	0
59	MG	BA	3008	1/1	0.99	0.20	13,13,13,13	0
59	MG	AA	1679	1/1	0.99	0.04	27,27,27,27	0
59	MG	DA	3019	1/1	0.99	0.19	13,13,13,13	0
59	MG	DA	3154	1/1	0.99	0.07	64,64,64,64	0
59	MG	DA	3130	1/1	0.99	0.31	27,27,27,27	0
59	MG	DA	3075	1/1	0.99	0.13	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3063	1/1	0.99	0.23	19,19,19,19	0
59	MG	BA	3041	1/1	0.99	0.21	20,20,20,20	0
59	MG	DA	3064	1/1	0.99	0.15	48,48,48,48	0
59	MG	DA	3025	1/1	1.00	0.16	5,5,5,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.