



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 05:47 am BST

PDB ID : 4V7W
Title : Structure of the *Thermus thermophilus* ribosome complexed with chloramphenicol.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-16
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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
buster-report : 1.1.7 (2018)
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

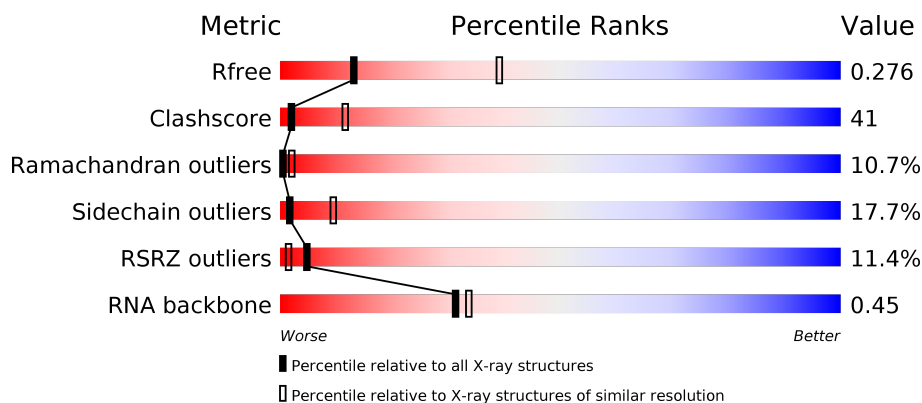
1 Overall quality at a glance ⓘ

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 ≥ 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	1522	<div> <div>19%</div> <div>22% 61% 15% ..</div> </div>
1	CA	1522	<div> <div>16%</div> <div>22% 60% 16% .</div> </div>
2	AB	256	<div> <div>14%</div> <div>25% 53% 11% . 8%</div> </div>
2	CB	256	<div> <div>20%</div> <div>27% 50% 13% . 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	135	
12	CL	135	
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	B0	85	
22	D0	85	
23	B1	98	
23	D1	98	
24	B2	72	
24	D2	72	
25	B3	60	
25	D3	60	
26	B4	71	
26	D4	71	
27	B5	60	
27	D5	60	



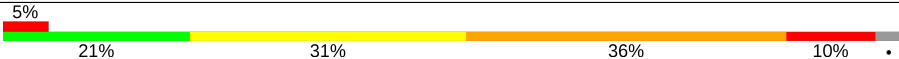
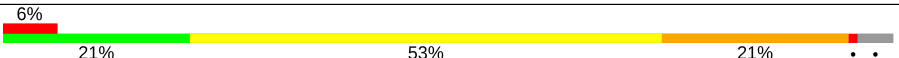
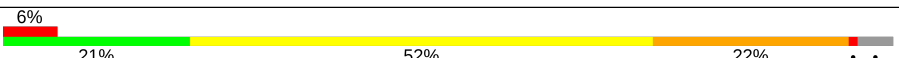
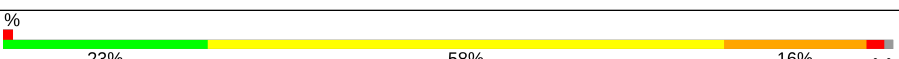
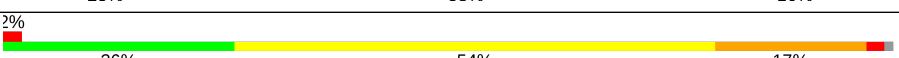
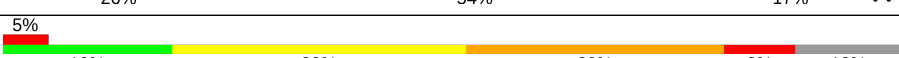

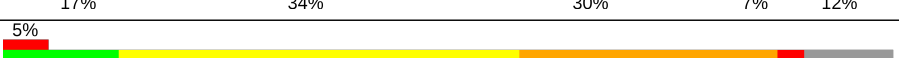
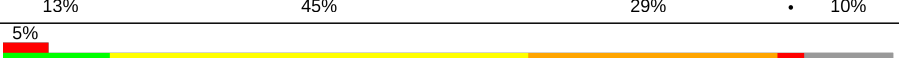
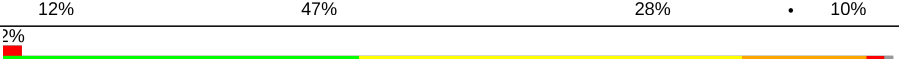



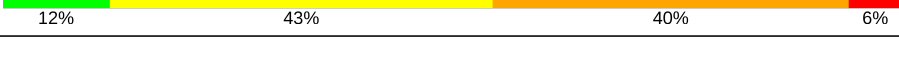
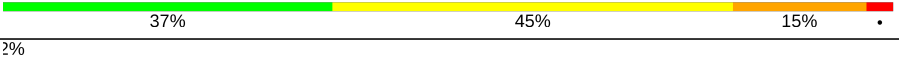

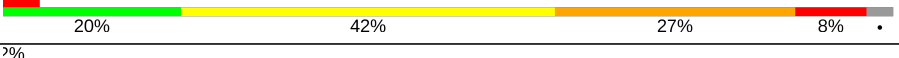
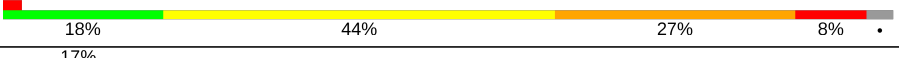

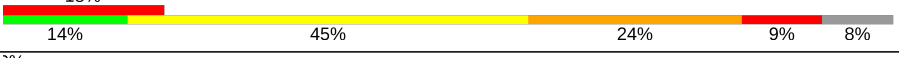
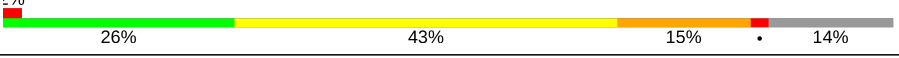
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Mol	Chain	Length	Quality of chain
28	B6	54	
28	D6	54	
29	B7	49	
29	D7	49	
30	B8	65	
30	D8	65	
31	BA	2787	
31	DA	2787	
32	BB	122	
32	DB	122	
33	BD	276	
33	DD	276	
34	BE	206	
34	DE	206	
35	BF	210	
35	DF	210	
36	BG	182	
36	DG	182	
37	BH	180	
37	DH	180	
38	BI	148	
38	DI	148	
39	BN	140	
39	DN	140	
40	BO	122	

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Mol	Chain	Length	Quality of chain
40	DO	122	
41	BP	150	
41	DP	150	
42	BQ	141	
42	DQ	141	
43	BR	118	
43	DR	118	
44	BS	112	
44	DS	112	
45	BT	146	
45	DT	146	
46	BU	118	
46	DU	118	
47	BV	101	
47	DV	101	
48	BW	113	
48	DW	113	
49	BX	96	
49	DX	96	
50	BY	110	
50	DY	110	
51	BZ	206	
51	DZ	206	

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
52	MG	AA	1637	-	-	-	X
52	MG	AA	1643	-	-	-	X
52	MG	AA	1644	-	-	-	X
52	MG	AA	1654	-	-	-	X
52	MG	BA	3007	-	-	-	X
52	MG	BA	3072	-	-	-	X
52	MG	BA	3074	-	-	-	X
52	MG	BA	3088	-	-	-	X
52	MG	BA	3128	-	-	-	X
52	MG	BA	3131	-	-	-	X
52	MG	BA	3150	-	-	-	X
52	MG	BA	3159	-	-	-	X
52	MG	BA	3167	-	-	-	X
52	MG	BA	3171	-	-	-	X
52	MG	BA	3175	-	-	-	X
52	MG	BA	3176	-	-	-	X
52	MG	BA	3180	-	-	-	X
52	MG	BA	3247	-	-	-	X
52	MG	BA	3313	-	-	-	X
52	MG	BA	3330	-	-	-	X
52	MG	BA	3337	-	-	-	X
52	MG	BA	3349	-	-	-	X
52	MG	BA	3355	-	-	-	X
52	MG	BA	3358	-	-	-	X
52	MG	CA	1626	-	-	-	X
52	MG	CA	1627	-	-	-	X
52	MG	CA	1630	-	-	-	X
52	MG	CA	1638	-	-	-	X
52	MG	DA	3025	-	-	-	X
52	MG	DA	3074	-	-	-	X
52	MG	DA	3075	-	-	-	X
52	MG	DA	3106	-	-	-	X
52	MG	DA	3149	-	-	-	X
52	MG	DA	3153	-	-	-	X
52	MG	DA	3166	-	-	-	X
52	MG	DA	3180	-	-	-	X
52	MG	DA	3187	-	-	-	X
52	MG	DA	3195	-	-	-	X
52	MG	DA	3208	-	-	-	X
52	MG	DA	3232	-	-	-	X
52	MG	DA	3236	-	-	-	X
52	MG	DA	3243	-	-	-	X
52	MG	DA	3252	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	DA	3267	-	-	-	X
52	MG	DA	3271	-	-	-	X
52	MG	DA	3274	-	-	-	X
52	MG	DA	3280	-	-	-	X
52	MG	DA	3281	-	-	-	X
52	MG	DA	3283	-	-	-	X
52	MG	DA	3289	-	-	-	X
52	MG	DA	3290	-	-	-	X
52	MG	DA	3295	-	-	-	X
52	MG	DA	3297	-	-	-	X
52	MG	DA	3305	-	-	-	X
52	MG	DA	3310	-	-	-	X
52	MG	DA	3325	-	-	-	X
52	MG	DA	3328	-	-	-	X
52	MG	DU	201	-	-	-	X
53	ZN	CD	301	-	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 277987 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 rRNA.

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

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

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

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

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

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

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

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

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

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

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

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

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

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

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	BA	368	Total	Mg	0	0
			368	368		
52	CA	53	Total	Mg	0	0
			53	53		
52	DQ	1	Total	Mg	0	0
			1	1		
52	DF	1	Total	Mg	0	0
			1	1		
52	BE	1	Total	Mg	0	0
			1	1		
52	DU	1	Total	Mg	0	0
			1	1		
52	B1	1	Total	Mg	0	0
			1	1		
52	BP	2	Total	Mg	0	0
			2	2		
52	DR	1	Total	Mg	0	0
			1	1		
52	B5	2	Total	Mg	0	0
			2	2		
52	BB	7	Total	Mg	0	0
			7	7		
52	BF	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	AA	56	Total	Mg	0	0
			56	56		
52	BQ	2	Total	Mg	0	0
			2	2		
52	BU	1	Total	Mg	0	0
			1	1		
52	DD	1	Total	Mg	0	0
			1	1		
52	BR	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	DA	332	Total 332	Mg 332	0	0
52	DE	1	Total 1	Mg 1	0	0
52	D1	1	Total 1	Mg 1	0	0
52	DX	1	Total 1	Mg 1	0	0
52	DP	1	Total 1	Mg 1	0	0
52	D5	2	Total 2	Mg 2	0	0
52	BD	1	Total 1	Mg 1	0	0
52	DB	4	Total 4	Mg 4	0	0

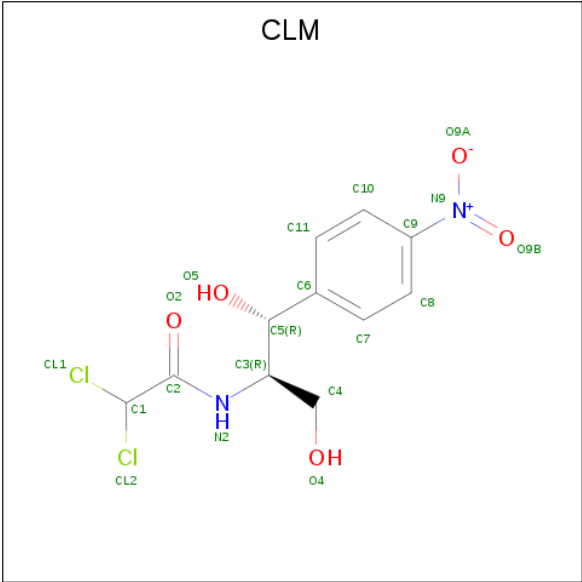
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 55 is CHLORAMPHENICOL (three-letter code: CLM) (formula: C₁₁H₁₂Cl₂N₂O₅).

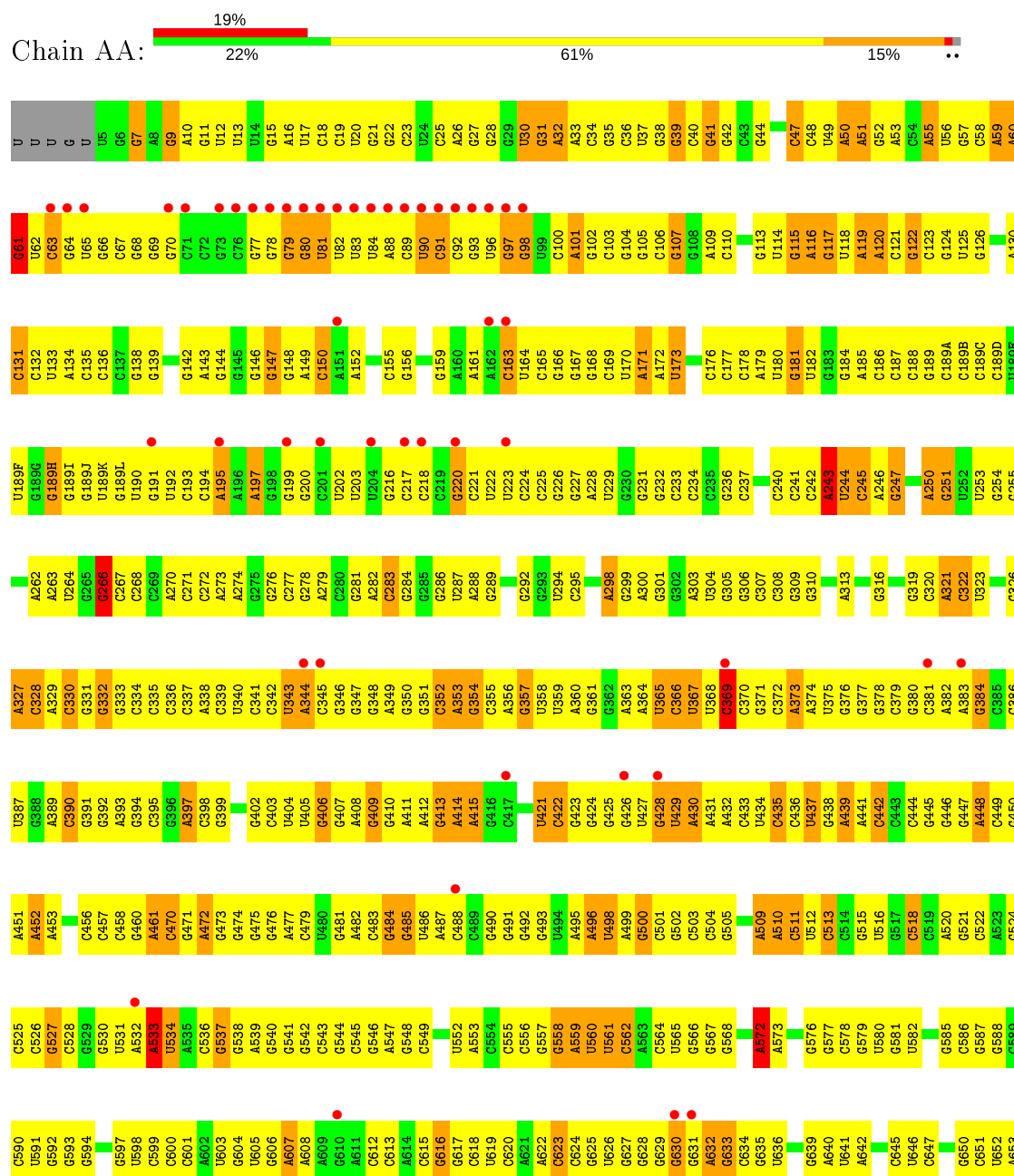


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	BA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
55	DA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

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.

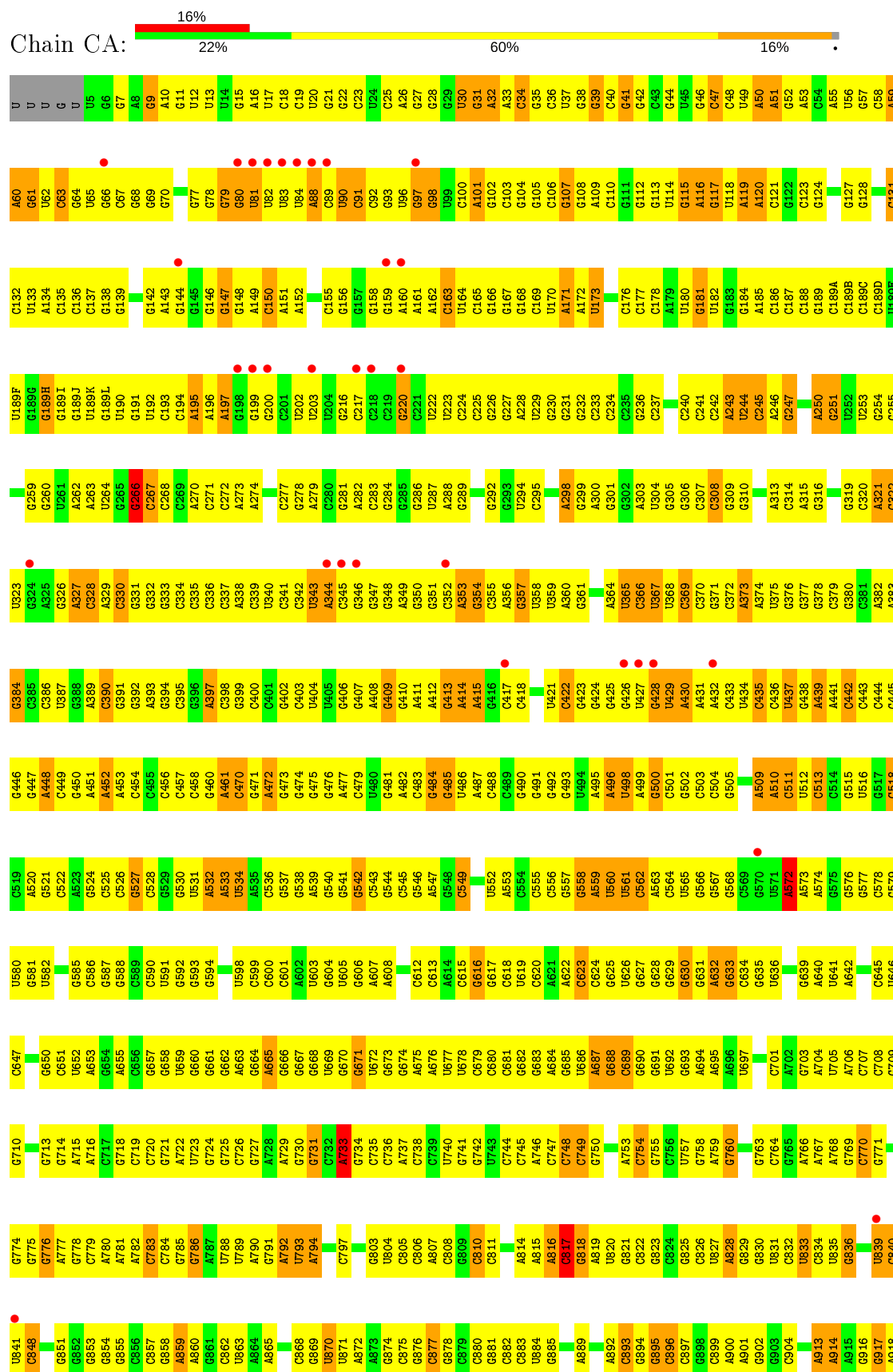
• Molecule 1: 16S rRNA

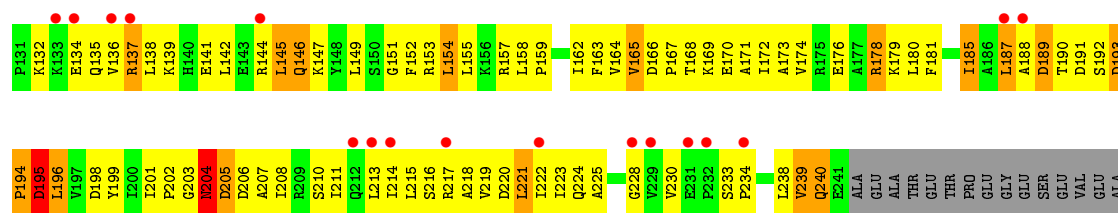




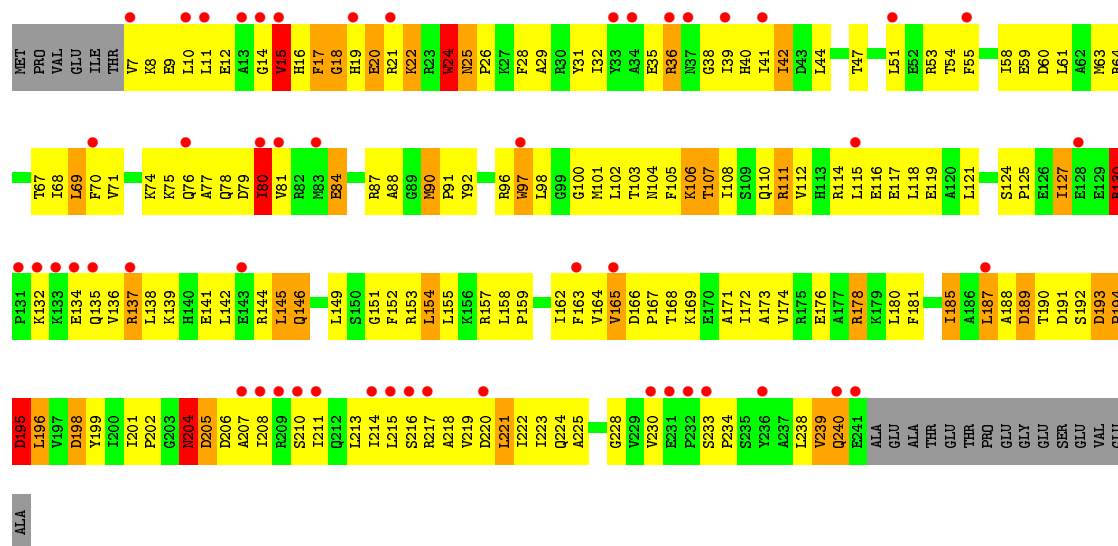
● Molecule 1: 16S rRNA

Chain CA:

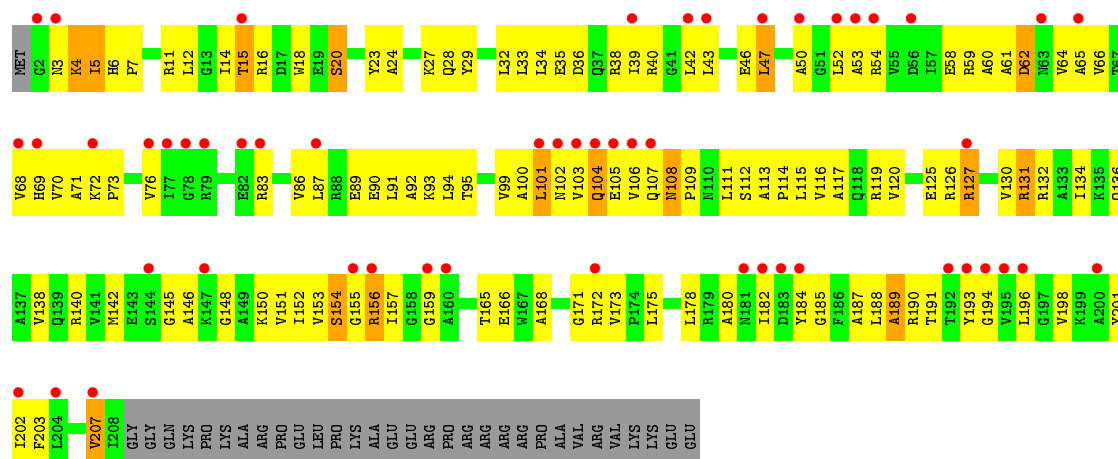




• Molecule 2: 30S ribosomal protein S2



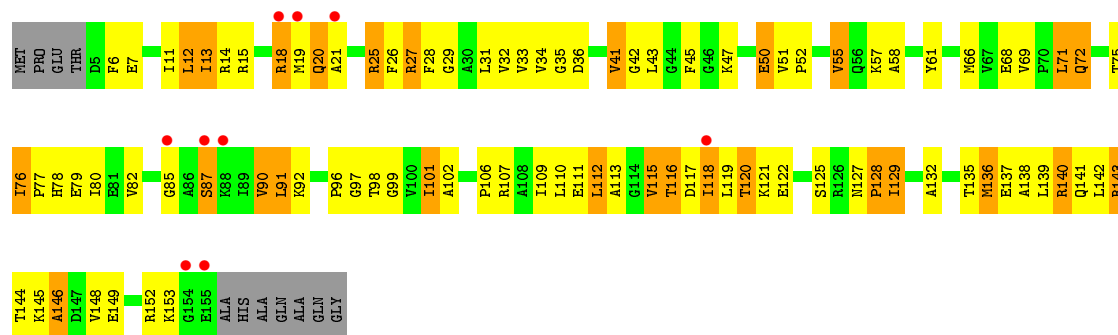
• Molecule 3: 30S ribosomal protein S3

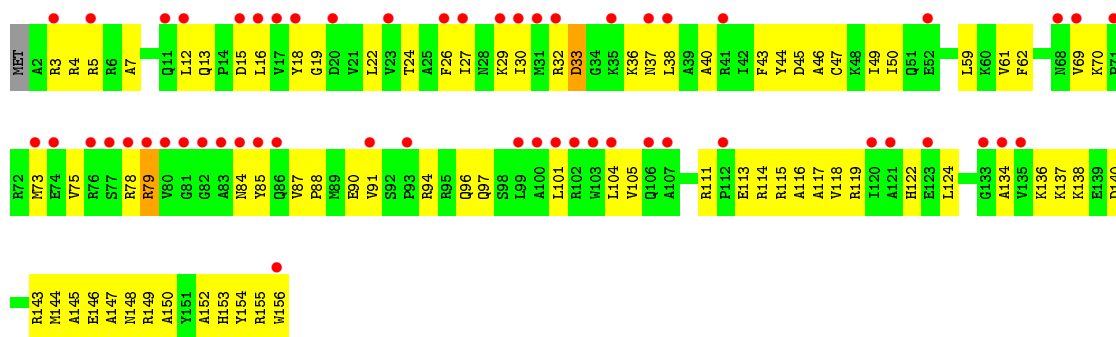


• Molecule 3: 30S ribosomal protein S3

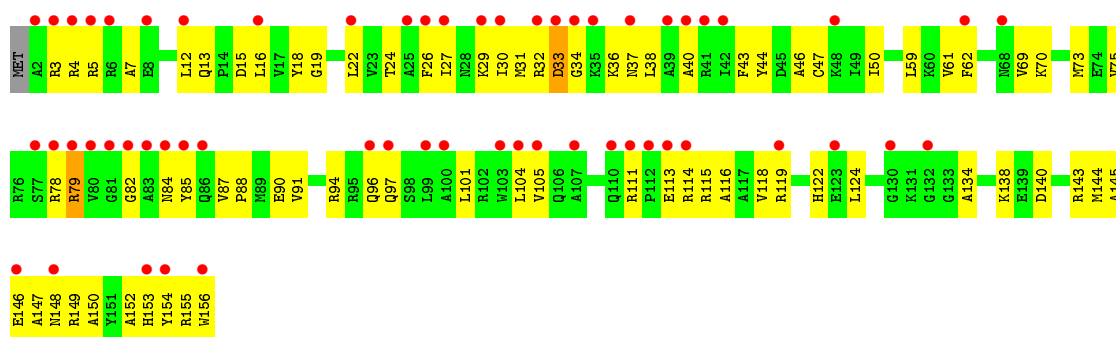
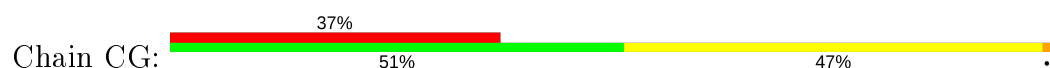




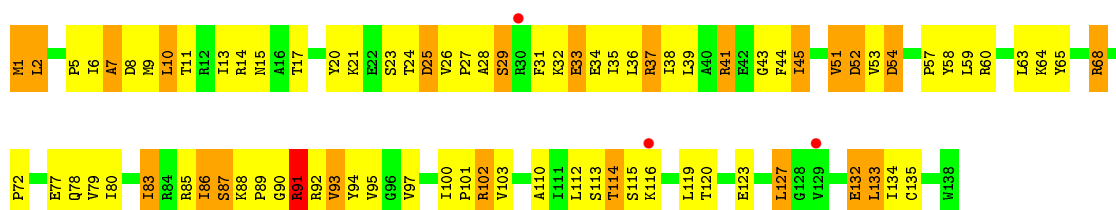




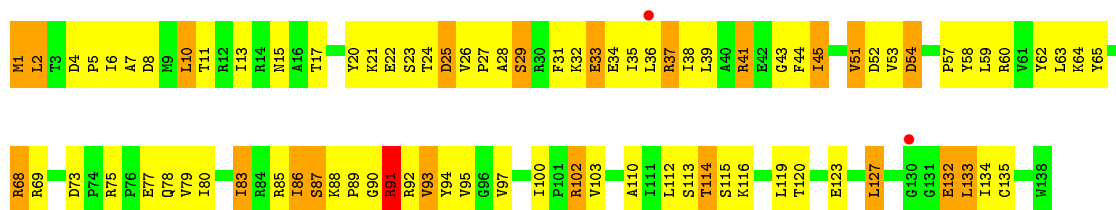
• Molecule 7: 30S ribosomal protein S7



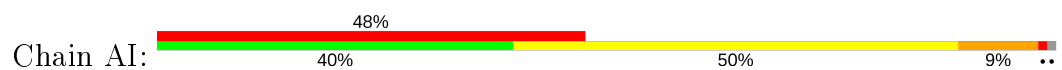
• Molecule 8: 30S ribosomal protein S8

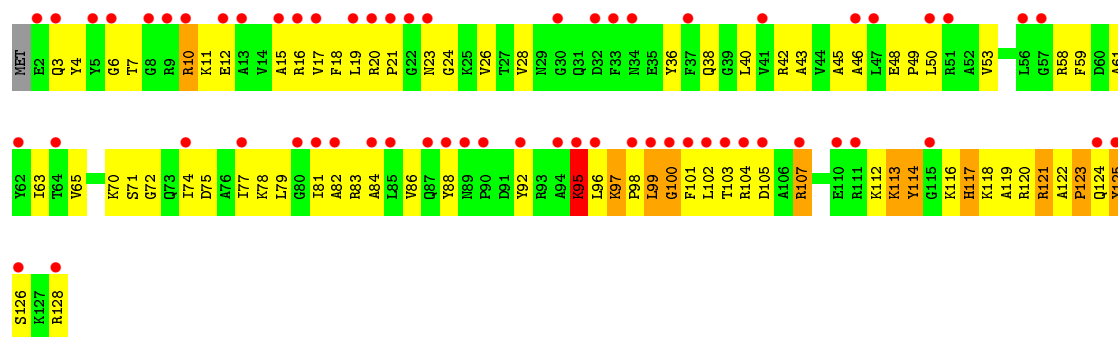


• Molecule 8: 30S ribosomal protein S8

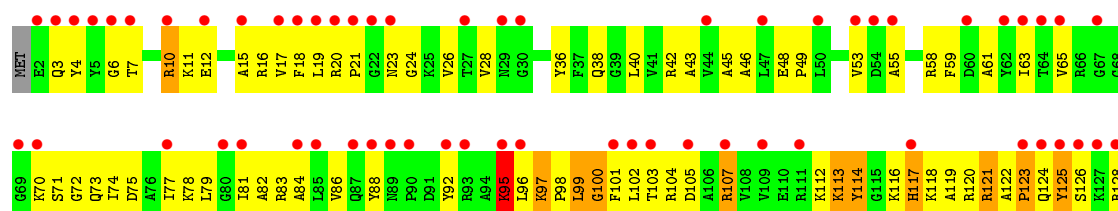


• Molecule 9: 30S ribosomal protein S9

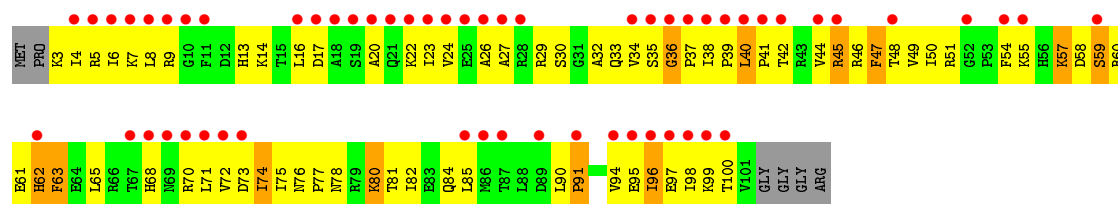




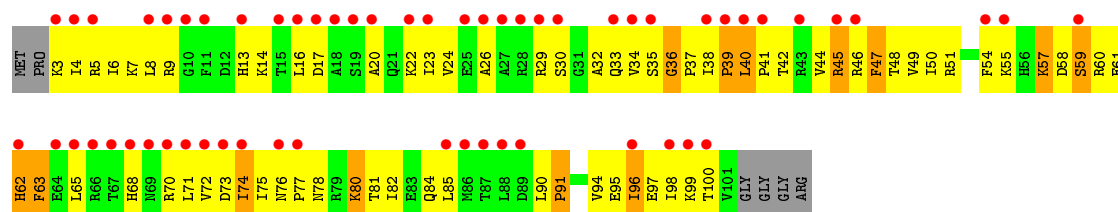
• Molecule 9: 30S ribosomal protein S9



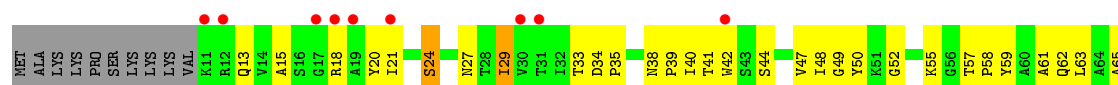
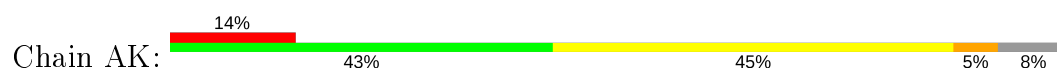
• Molecule 10: 30S ribosomal protein S10

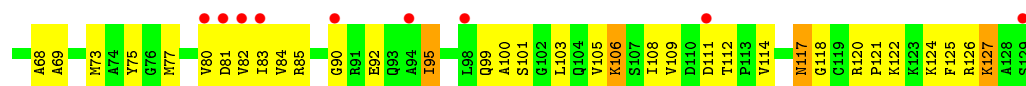


• Molecule 10: 30S ribosomal protein S10

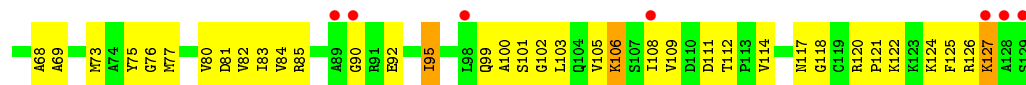
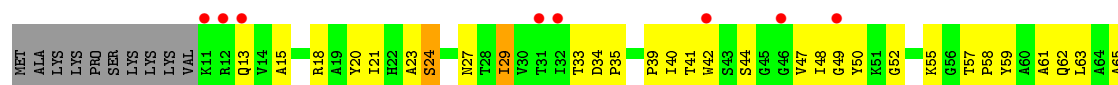
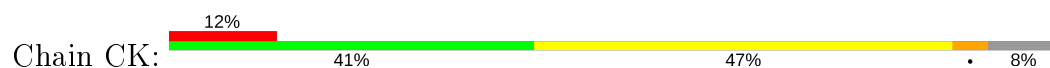


• Molecule 11: 30S ribosomal protein S11

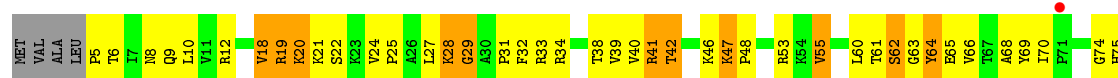
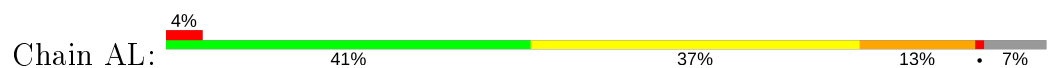




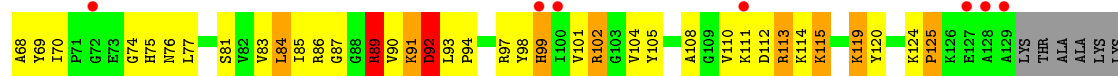
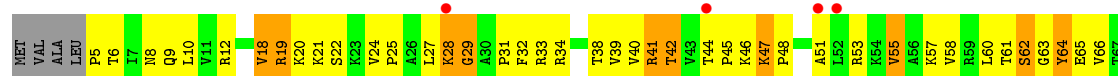
• Molecule 11: 30S ribosomal protein S11



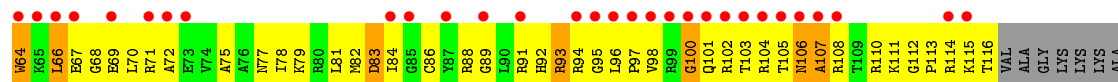
• Molecule 12: 30S ribosomal protein S12



• Molecule 12: 30S ribosomal protein S12

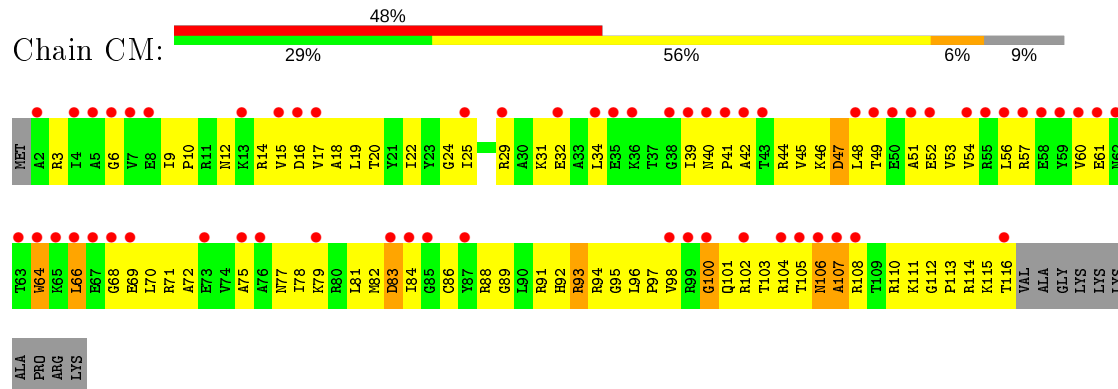


• Molecule 13: 30S ribosomal protein S13

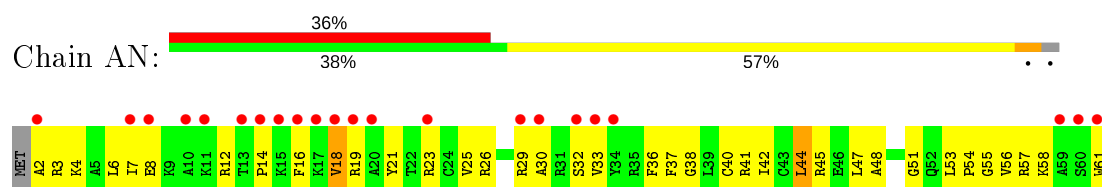


PRO
ARG
LYS

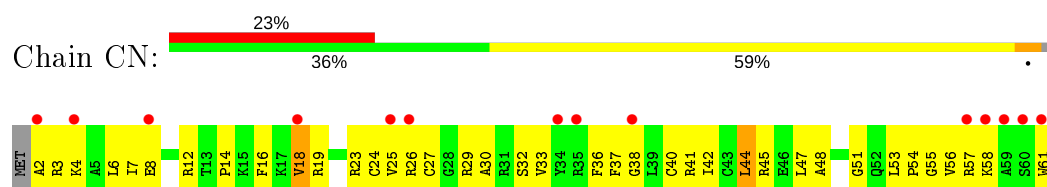
- Molecule 13: 30S ribosomal protein S13



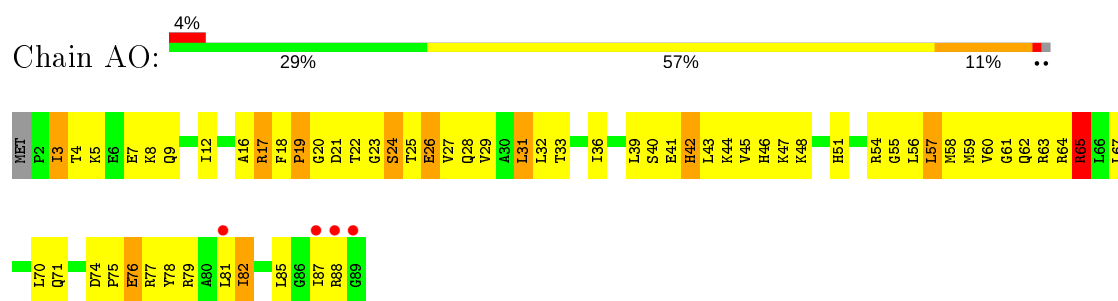
- Molecule 14: 30S ribosomal protein S14



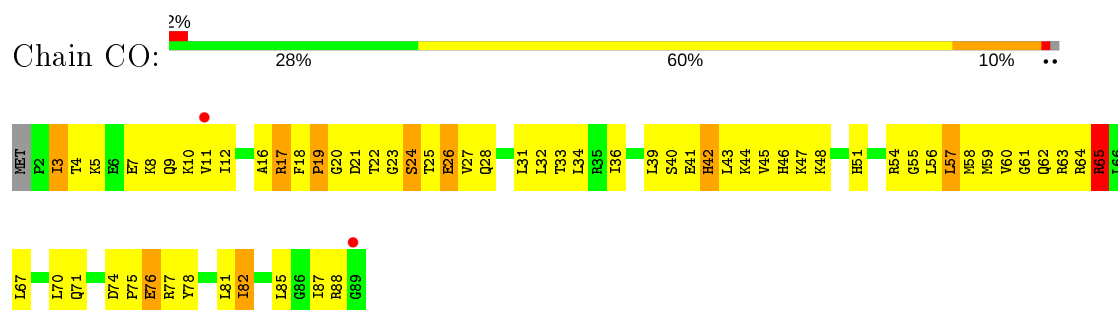
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

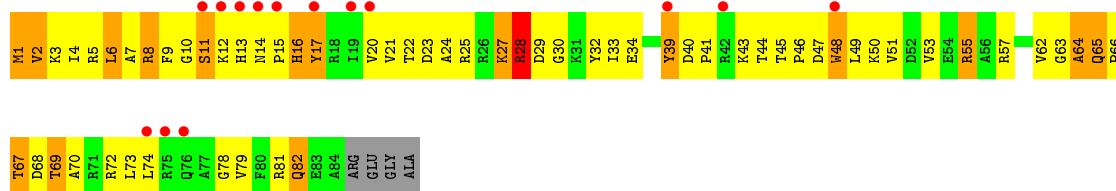


- Molecule 15: 30S ribosomal protein S15



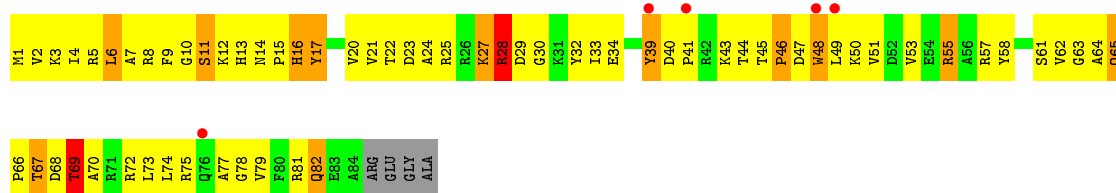
- Molecule 16: 30S ribosomal protein S16

Chain AP: 



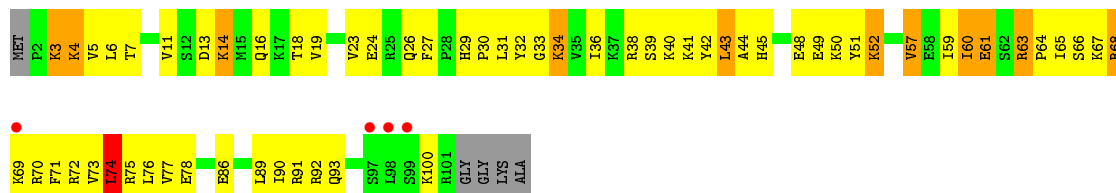
- Molecule 16: 30S ribosomal protein S16

Chain CP: 



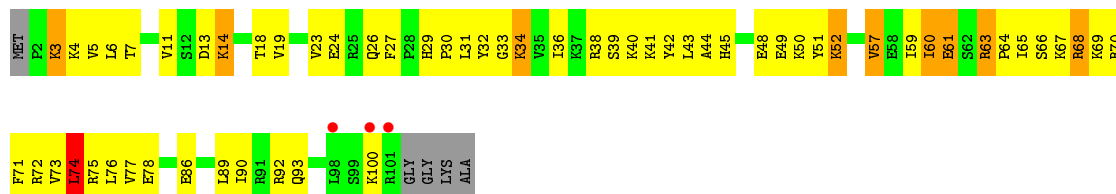
- Molecule 17: 30S ribosomal protein S17

Chain AQ: 



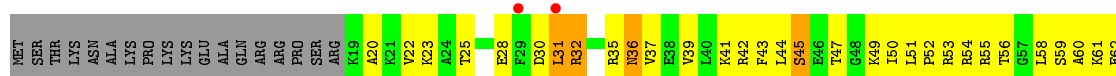
- Molecule 17: 30S ribosomal protein S17

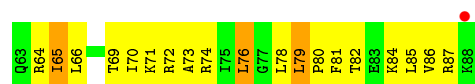
Chain CQ: 



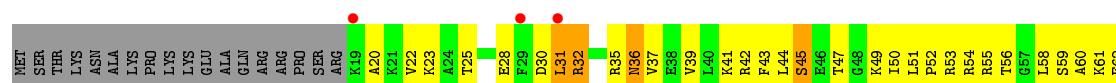
- Molecule 18: 30S ribosomal protein S18

Chain AR: 

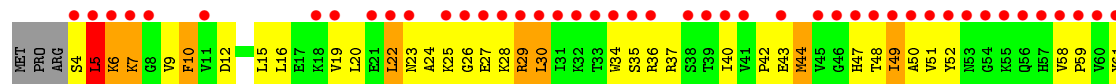




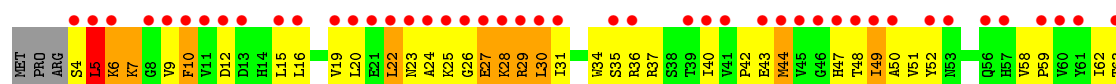
- Molecule 18: 30S ribosomal protein S18



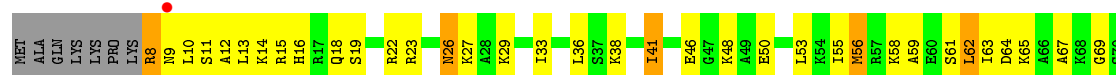
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19

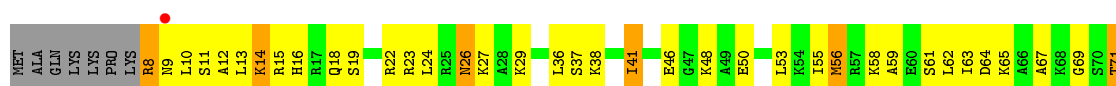


- Molecule 20: 30S ribosomal protein S20

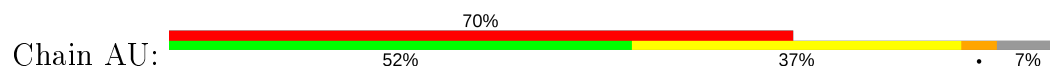


- Molecule 20: 30S ribosomal protein S20





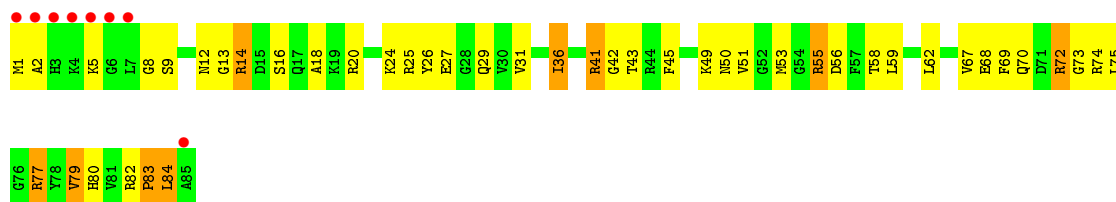
• Molecule 21: 30S ribosomal protein Thx



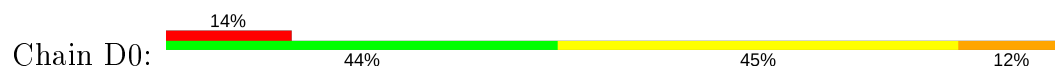
• Molecule 21: 30S ribosomal protein Thx



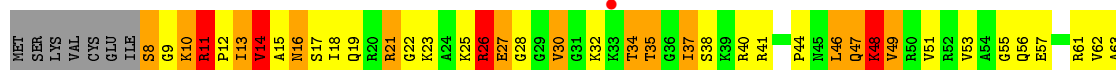
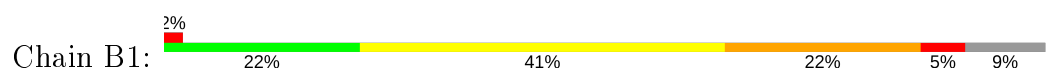
• Molecule 22: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L27

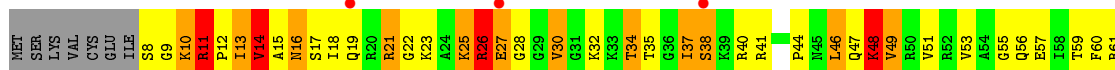
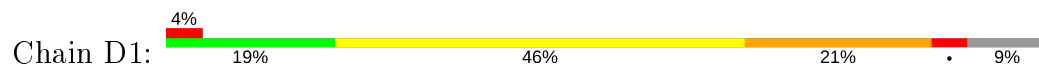


• Molecule 23: 50S ribosomal protein L28

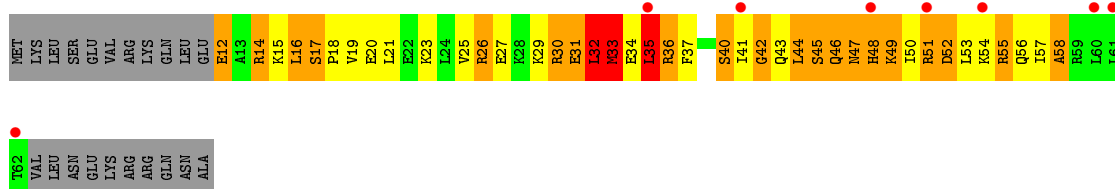




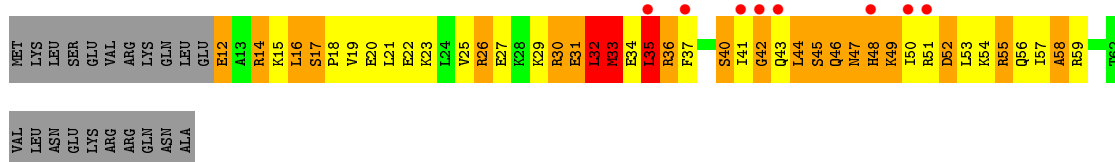
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



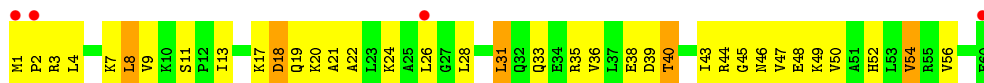
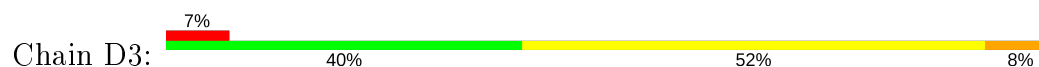
- Molecule 24: 50S ribosomal protein L29



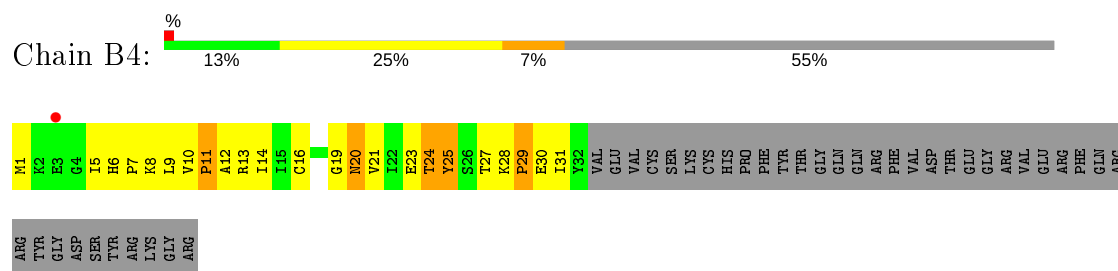
- Molecule 25: 50S ribosomal protein L30



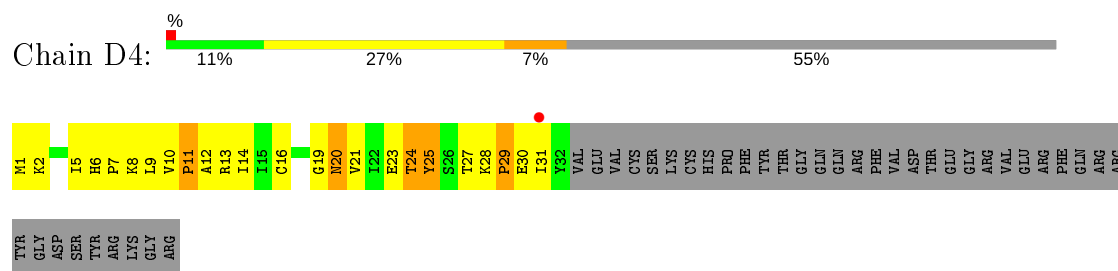
- Molecule 25: 50S ribosomal protein L30



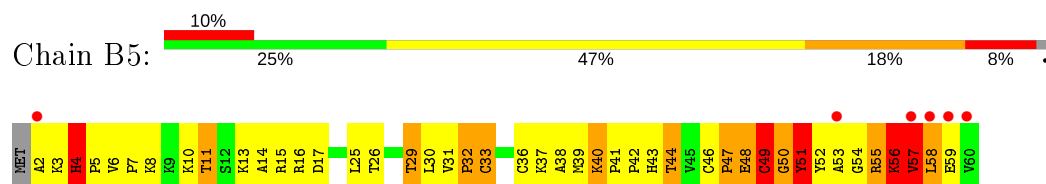
• Molecule 26: 50S ribosomal protein L31



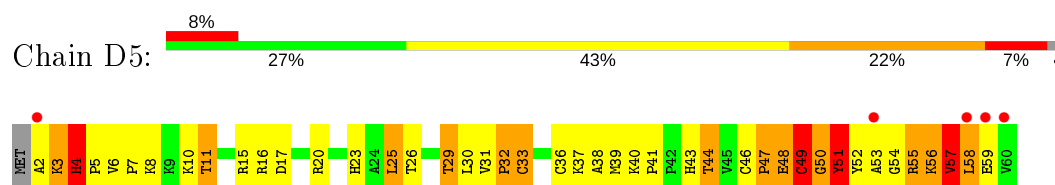
• Molecule 26: 50S ribosomal protein L31



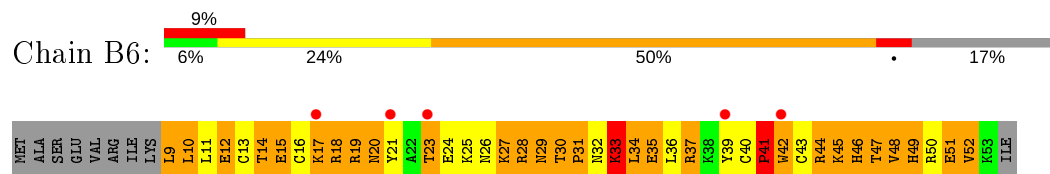
• Molecule 27: 50S ribosomal protein L32



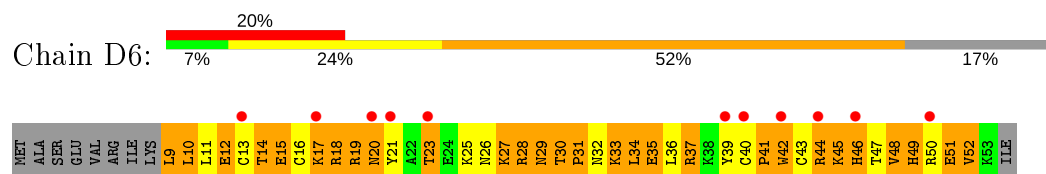
• Molecule 27: 50S ribosomal protein L32



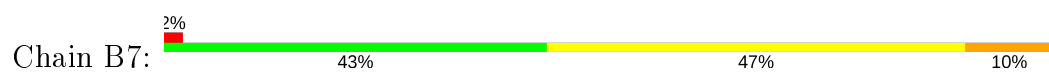
• Molecule 28: 50S ribosomal protein L33



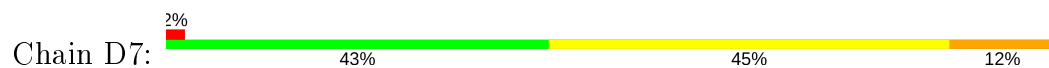
• Molecule 28: 50S ribosomal protein L33



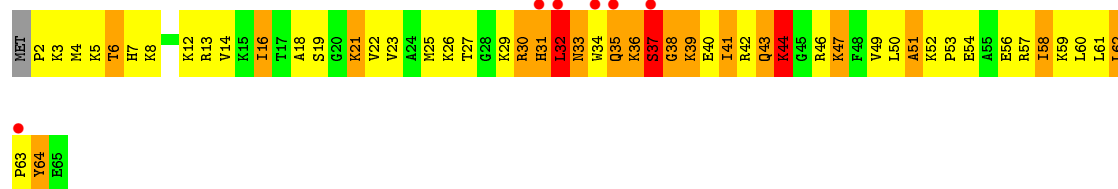
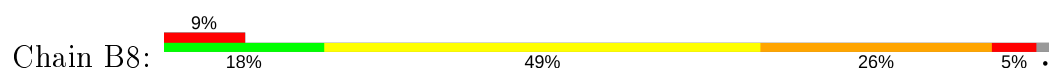
• Molecule 29: 50S ribosomal protein L34



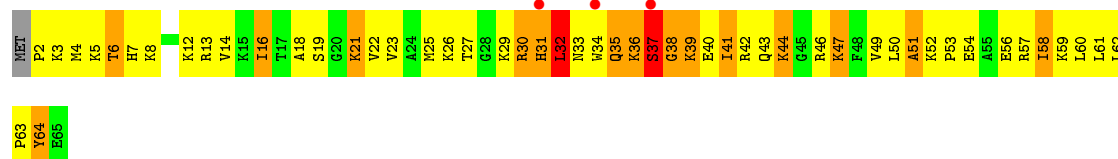
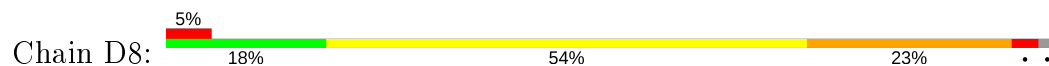
• Molecule 29: 50S ribosomal protein L34



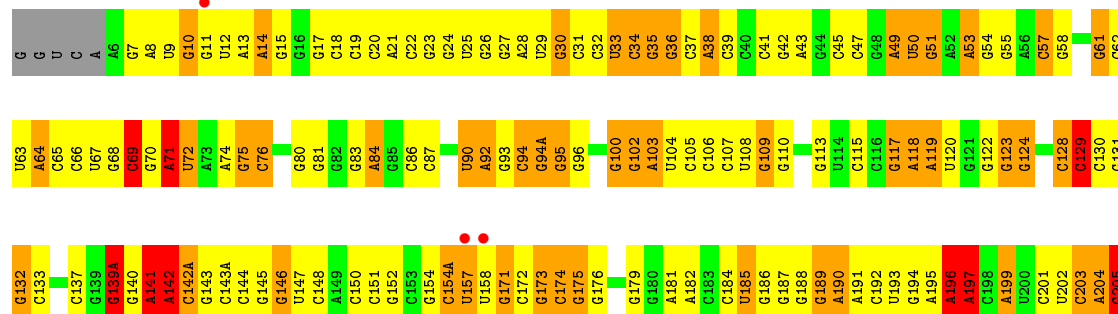
• Molecule 30: 50S ribosomal protein L35



• Molecule 30: 50S ribosomal protein L35

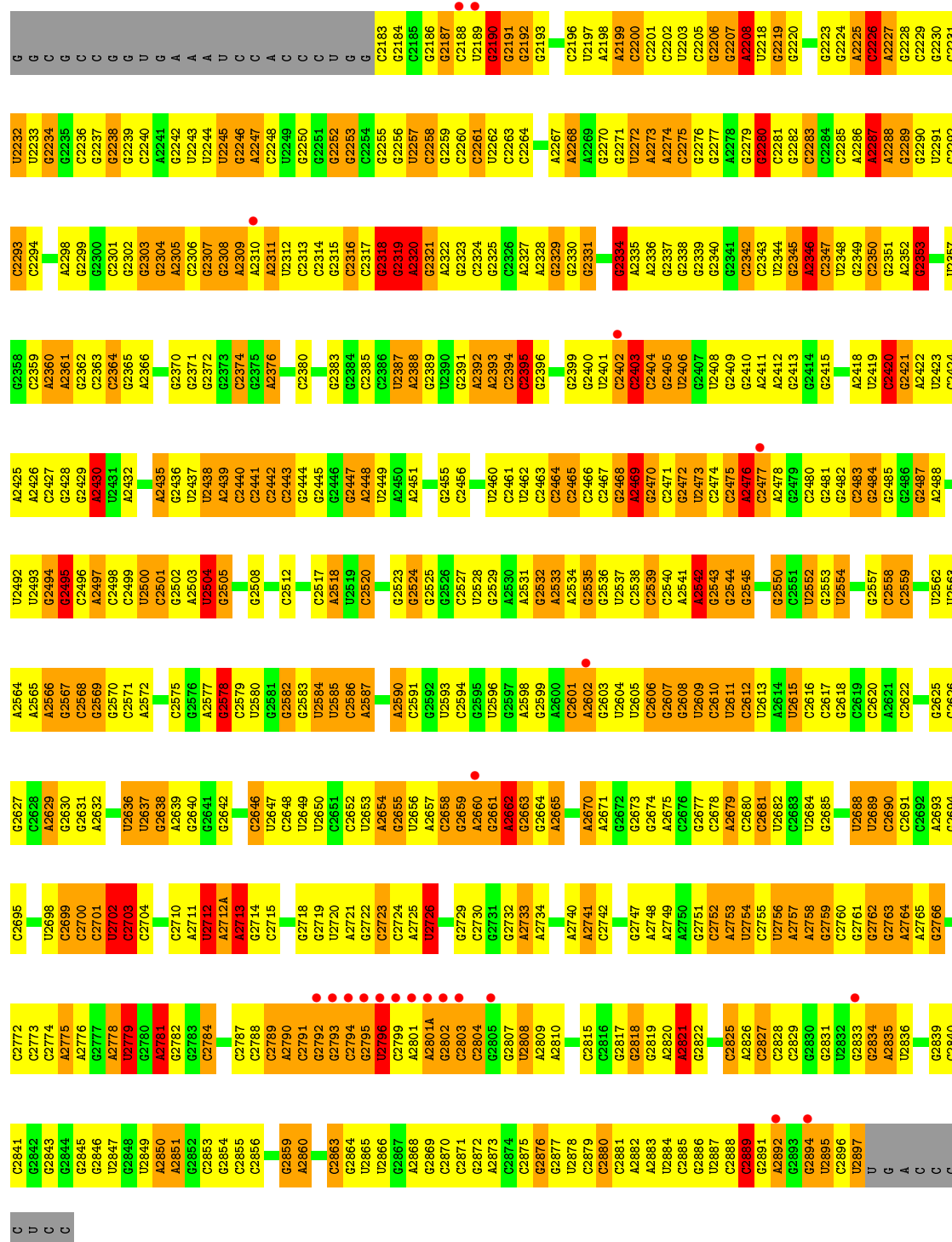


• Molecule 31: 23S ribosomal RNA

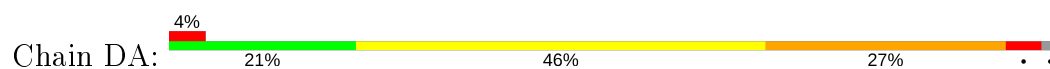


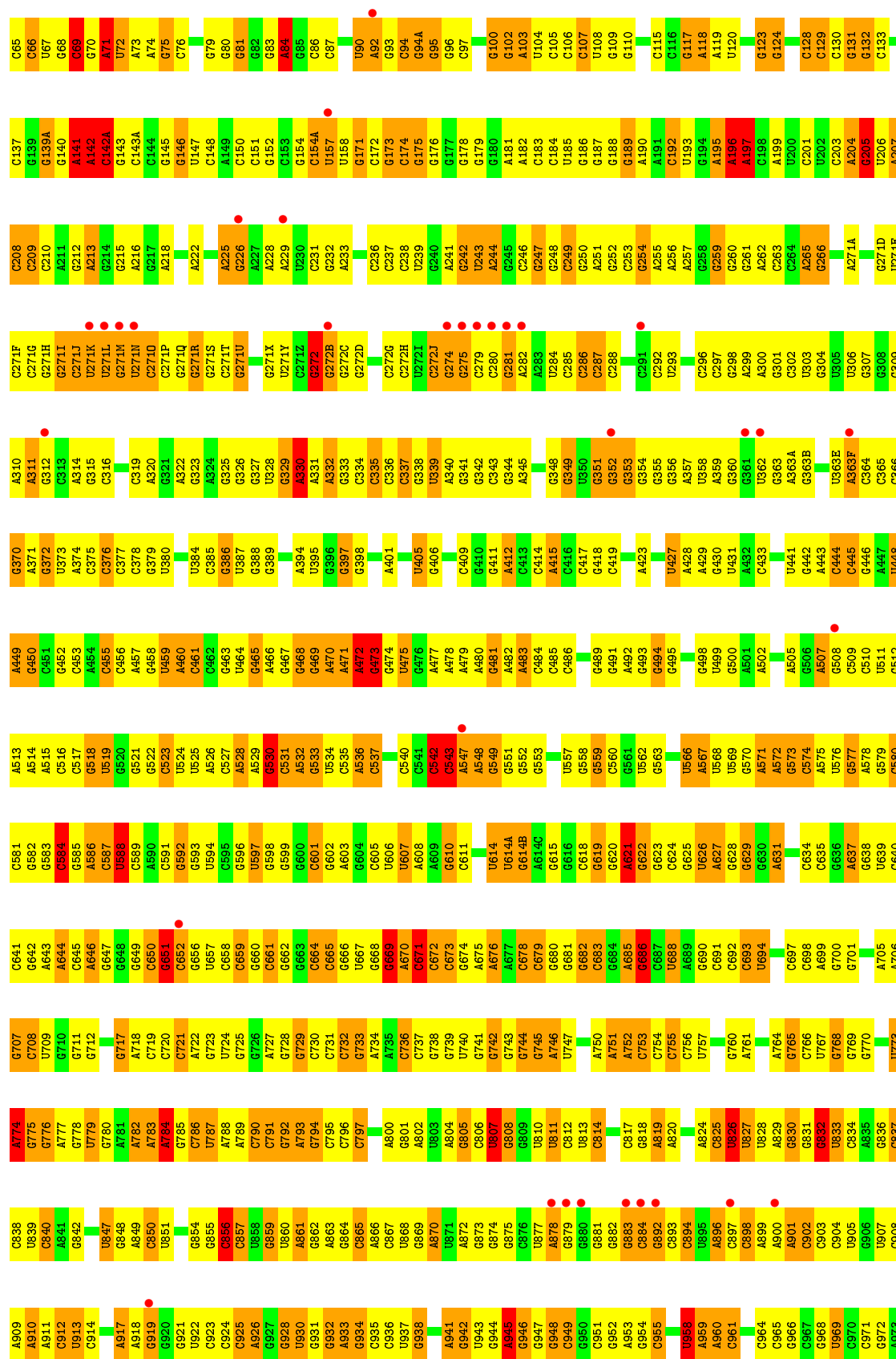
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A1046	A984	A849	A781	A644	C584	A514	A449	U373	G312	C271G	C209
G1047	C985	C850	A782	C645	G585	A515	G450	A374	C313	G271H	C210
A1048	G921	U851	C783	A646	A586	C516	G451	C375	A314	G271I	A211
C1049	C987	U852	A784	G647	C587	C517	G452	C376	G315	C271J	C212
A1050	A988	G854	G785	G651	U588	G518	G455	C377	C316	U271K	A213
G1051	G855	C924	G786	G652	C589	U519	C456	C378	G319	U271L	G214
C1052	C925	C856	A787	G656	A590	G520	C457	G379	A320	G271M	G215
C1053	C991	C857	A788	G657	C591	G521	A458	U380	A321	U271N	A216
A1106	G927	U858	A789	C658	G592	G522	G458	U384	G321	C271O	G217
G1107	G928	G859	C790	C659	U594	C523	U459	C385	A322	C271P	A218
U1108	U930	U860	C791	G660	C595	U524	A460	G323	G324	G271Q	G219
C1109	G931	A861	G792	C661	G596	A526	C461	G325	A324	G271R	A222
G1110	C932	G862	A793	G662	U597	C527	G462	G326	G327	C271S	
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G1114	A866	A867	A797	G668	C601	C531	G467	U395	A330	G271Y	G226
G1115	C937	C867	G798	G669	G602	A532	G468	G396	A331	U271Z	A227
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G1117	C939	G869	A800	G671	G604	U534	A470	G398	G333	G272A	C231
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G1119	G942	A872	G803	C673	U606	A536	A472	C336	C335	G272C	A233
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U1131	G952	G882	A751	G683	A614C	G551	A482	A415	A346	G281	G245
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G1137	U958	C898	U757	G688	G620	U562	A491	G352	G352	C287	G252
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A1143A	C964	A901	G708	U694	U626	U568	A497	U358	C297	G297	G260
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G1157	A909	C837	C708	G715	G635	A576	A505	G442	A363F	G304	
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WORLDWIDE
PDB
PROTEIN DATA BANK



● Molecule 31: 23S ribosomal RNA

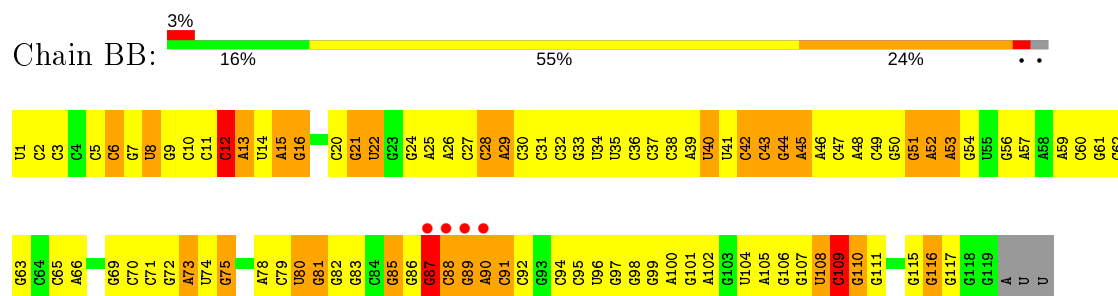




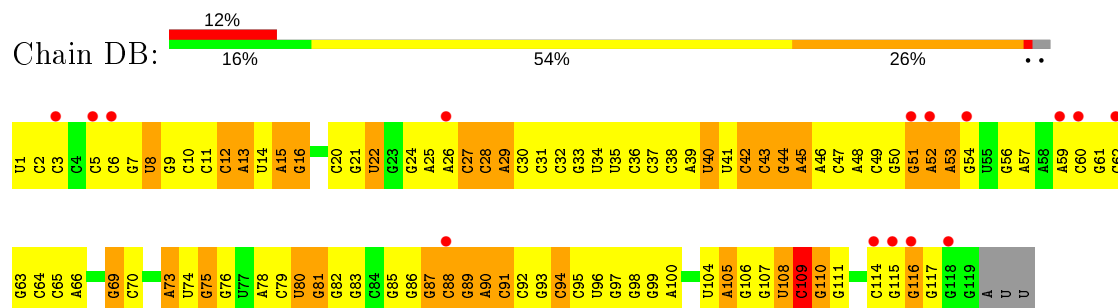
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	A1847	A1784	G1703	C1638	A1572	C1501	A1439	C1370	C1304	G1244	C1179	U1108	C994
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	A1883	A1809	G1745A	C1662	C1599	G1527	G1463	U1406	A1336	U1275	A1213	A1143	U1026
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U1955	A1749	G1813	A1749	G1667	A1603	C1529	C1467	C1409	G1339	A1278	C1218	C1152	G1030
U1956	G1814	G1750	C1751	A1668	C1604	C1530	C1468	G1404	U1340	G1279	G1219	C1153	
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G1958	G1816	G1816	C1752	C1670	C1607	C1532	G1470	U1406		G1281	C1221	A1155	G1034
G1959			G1753		A1608	G1533	A1471	C1407	G1337	A1276	C1222A	A1156	G1036
A1960	A1819	A1819	C1754	G1674	A1609	C1543	A1472	C1408	U1347	G1282	G1223	G1157	G1037
C1961	U1820	U1820	A1755	C1675	A1610	A1544	G1473	C1409	G1339	A1283			
C1962	C1894	A1821	G1756	A1676	C1611	A1545	C1474	G1410	U1340	G1284			
U1963	G1822	G1822	U1757	A1677	C1612	C1546	G1475	C1411	U1341	G1285			
G1964			G1758	G1678	G1613	C1547		A1412					
C1965		A1825	U1679	U1679	A1614	C1548	G1478	G1413	C1345	U1282			
A1966	G1826	G1826	A1762	U1680	C1615	C1549	G1479	G1416	G1346	G1283			
C1967	A1900	G1827	G1763	A1681	A1616	C1550	G1480	G1417	G1347	A1284			
G1968	A1901	G1828	G1764	G1682	C1617	C1551	U1481		G1348				

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A2851		G2717	U2648	G2517	A2450	A2388	G2323	C2039	A1972
G2852	G2785	G2718	U2649	A2518	A2451	G2389	G2324	G2040	G1973
G2789	G2786	G2719	U2650	U2519	G2455	U2390	G2325	U2041	C1974
A2790	G2787	U2720	C2651	C2520	G2456	G2391	G2326	A2042	
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	G2794	U2726	A2657		G2464	G2399	A2333	G2049	A1986
	U2786		A2657		G2465	G2400	G2334	C2050	G1987
G2863	G2789	G2729	C2658	G2529	C2466	U2401	A2335	A2051	G1988
G2864	A2801	C2730	G2659	A2530	C2467	G2402	G2336	G2052	G1989
U2865	A2801.A	G2731	A2660	A2531	G2468	C2403	G2337	G2053	G1990
U2866	G2802	G2732	G2661	G2532	U2469	G2404	G2338	G2054	G1991
G2867	G2803	A2733	A2662	A2533	A2469	G2405	G2339	G2055	U1991
G2868	G2804	A2734	G2663	G2534	G2470	U2406	G2340	G2056	G1992
			G2664	G2535	C2471	G2407	G2341	A2057	U1993
G2869	G2807	A2738	A2665	U2536	U2472	U2408	G2342	A2058	G1994
C2871	U2808	G2739		U2537	C2473	G2409	C2343		
A2809	A2809	A2740	A2670	C2538	C2474	G2410	G2344		G1997
A2810	A2810	A2741	A2671	C2539	C2475	G2411	U2345	A2060	G1998
G2872		C2742	G2672	G2540	A2476	A2411	G2346	G2061	C1999
G2874			G2673	A2541	C2477	A2412	A2347	A2062	A2000
	C2814	G2744		A2542	A2478	G2413	G2348	G2063	G2001
C2875	C2815		G2677	G2543	G2479	G2414	U2349	G2064	G2002
G2876	G2816	G2747	C2678	G2544	C2480	G2415	G2349	G2065	A2005
U2878	G2817	A2748	A2679	G2545	G2481	C2416	G2350	G2066	C2006
G2879	G2818	A2749	A2680	U2546	G2482	C2417	G2351	G2067	C2007
C2880	G2819	A2750	C2681	G2547	C2483	A2418	G2352	U2068	C2008
A2882	A2820	G2751	U2682		G2484	U2419	G2353	G2069	G2009
U2883	G2821	C2752		G2550	G2485	C2420	G2354	G2070	G2010
U2884	G2822	C2753		G2551	G2486	G2421		A2071	G2011
G2885	A2823	U2754	G2685	G2552	G2487	A2422	U2357	G2072	U2011
G2886	C2824	G2755	U2686	G2553	A2488	U2423	G2358	C2073	G2012
U2887	C2825	U2756	U2687	U2554		C2424	A2359	U2074	A2013
C2888	A2826	A2757	U2688		U2492	A2425	A2360	U2075	A2014
G2889	G2827	A2758	G2689	G2557	U2493	A2426	A2361	U2076	A2015
C2891	C2828	C2759	C2690	C2558	G2494	C2427	G2362	A2077	U2016
G2892	C2829	C2760	C2691	C2559	G2495	G2428	G2363	G2078	U2017
G2893	G2830	G2761	A2692	C2560	C2496	G2429	G2364	U2079	G2018
U2894	G2831	G2762	G2693	A2561	A2497	A2430	G2365	G2080	A2019
G2895	U2832	G2763		U2562	C2498	U2431	A2366	C2081	A2020
G2896	G2833	A2764	U2698	U2563	C2499	A2432		A2082	C2021
U2897	G2834	A2765	C2699	A2564	U2500	A2433	G2370	G2083	U2022
	A2835	G2766	C2700	A2565	C2501	A2434	U2443	C2084	G2023
	U2836		C2701	A2566	G2502	A2435		G2085	G2024
G2897	G2837		G2702	G2567	A2503		G2374	U2086	C2025
	C2838	C2772	U2703	C2568	U2504	U2438	A2311	G2087	C2026
C2899	G2839	C2773	G2704	G2569	G2505	A2439	U2312	G2088	G2027
G2900	C2840	A2774	C2705	G2570	U2506	C2440	A2377	U2089	U2028
G2901	G2841	G2775	C2706	C2571	C2507	C2441	G2378	G2090	G2029
G2902	G2842	A2776		A2572	G2508	C2442	G2379	U2091	A2030
G2903	G2843	G2777	C2710			C2443	C2380	U2092	A2031
G2904	G2844	A2778	A2711		U2511	G2444	G2381	G2093	A2032
G2905	G2845	U2779	U2712	G2575	G2512	G2445	G2382	G2094	A2033
	G2846	G2780	A2712.A	G2576	G2513	G2446	G2383	G2095	
		A2781	A2713	A2577	G2514	G2446	G2384		

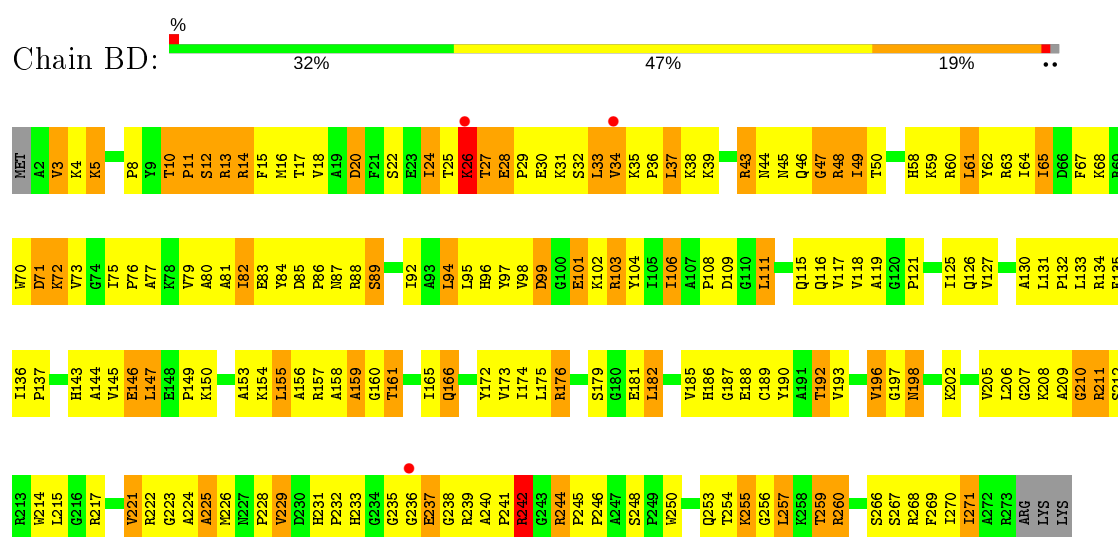
- Molecule 32: 5S ribosomal RNA

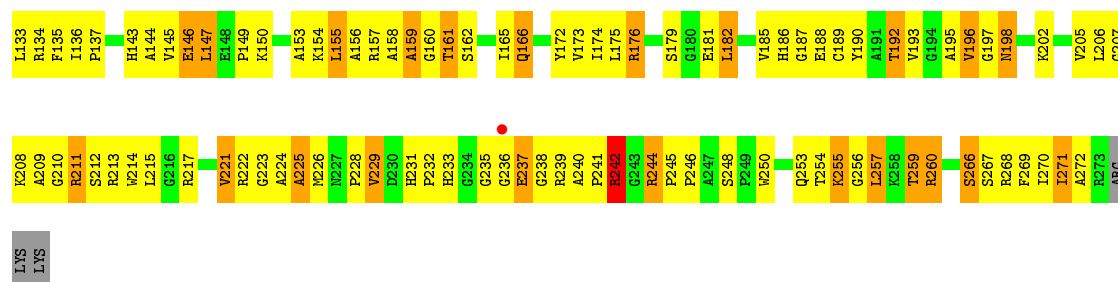


- Molecule 32: 5S ribosomal RNA

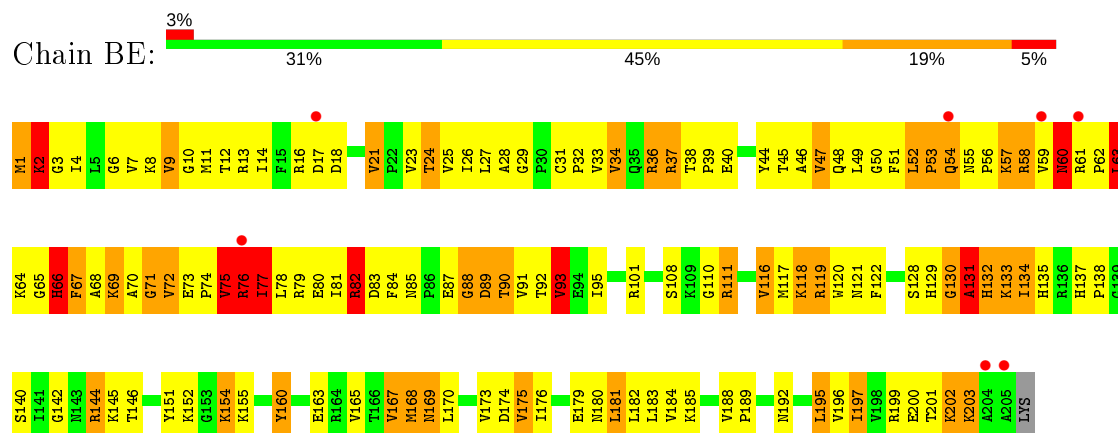


- Molecule 33: 50S ribosomal protein L2

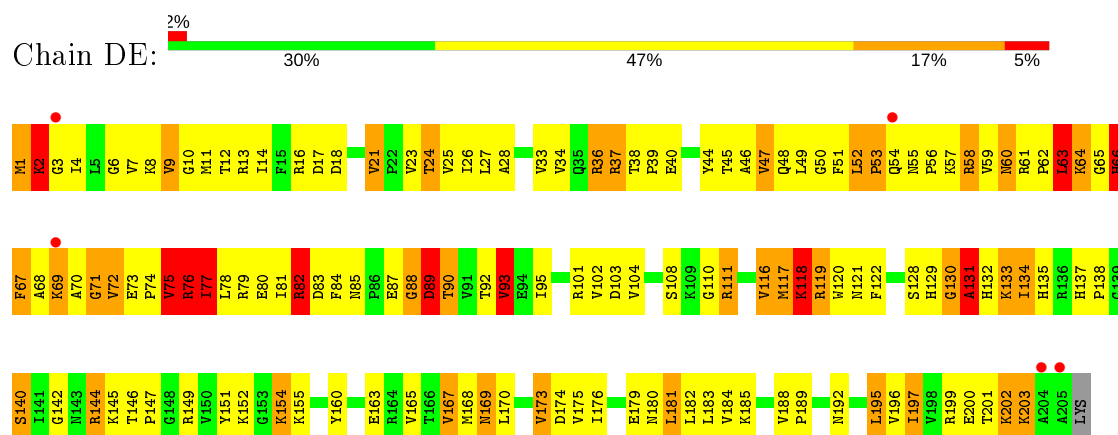




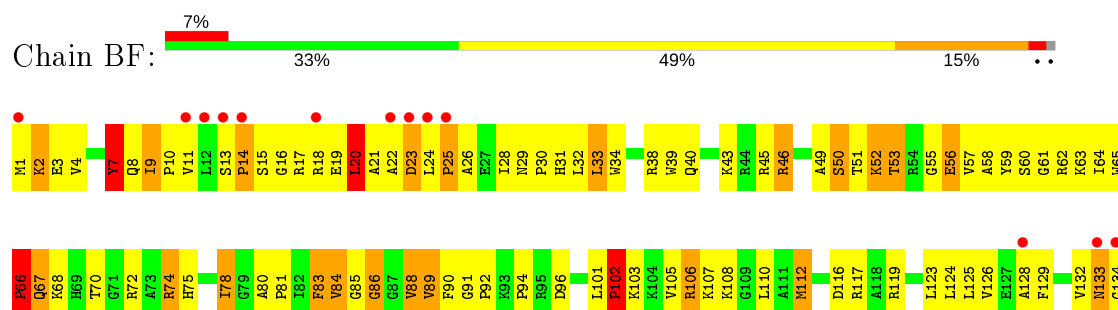
• Molecule 34: 50S ribosomal protein L3

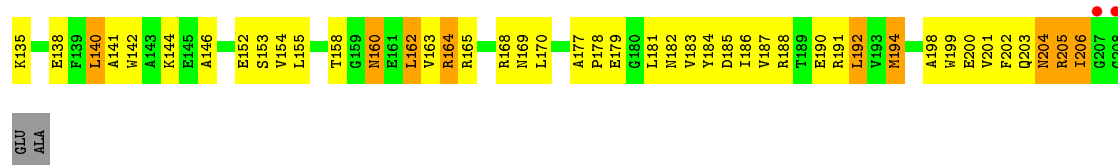


• Molecule 34: 50S ribosomal protein L3

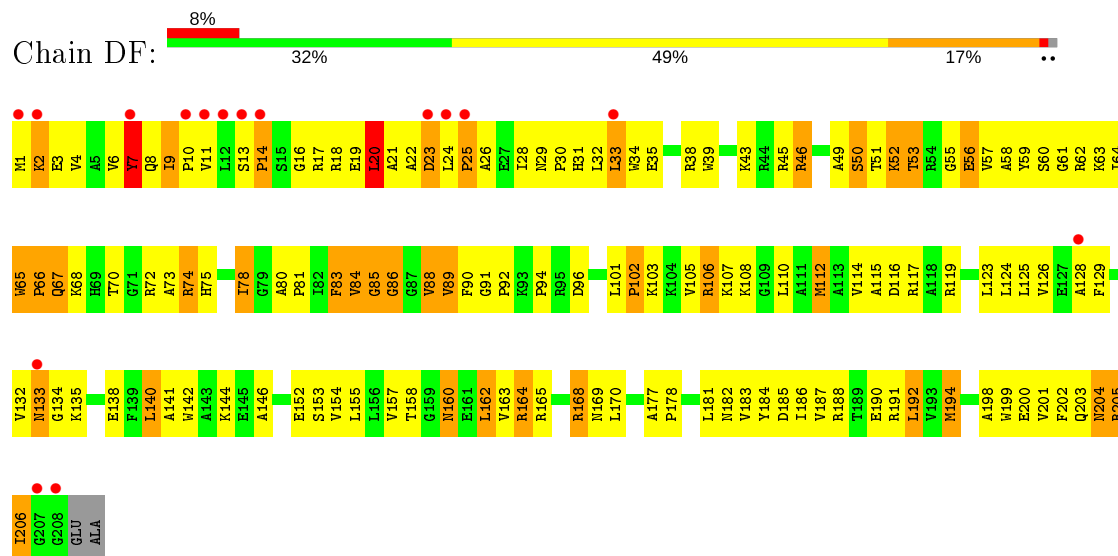


• Molecule 35: 50S ribosomal protein L4

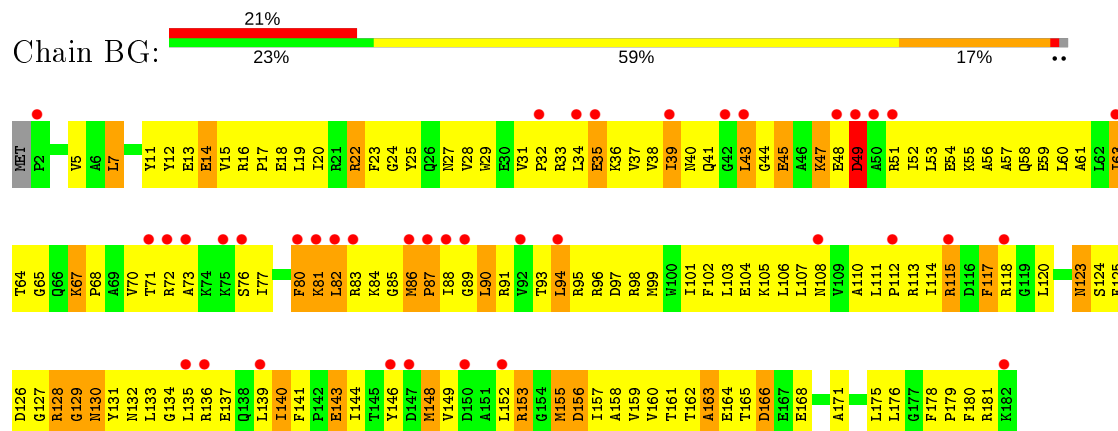




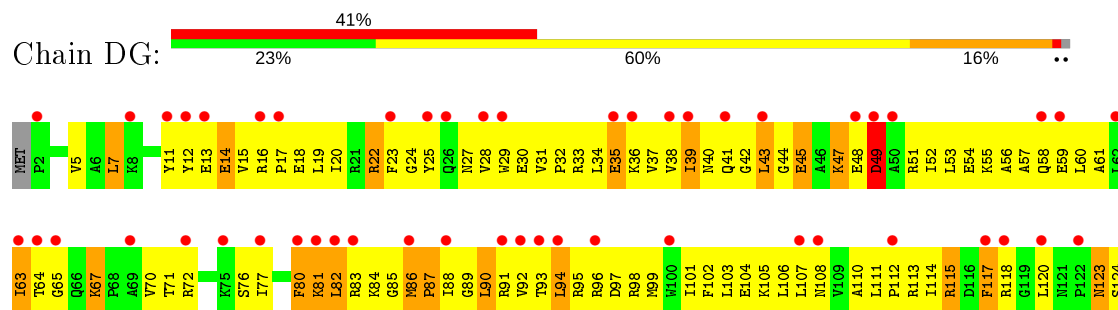
• Molecule 35: 50S ribosomal protein L4

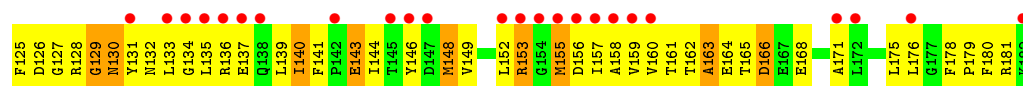


• Molecule 36: 50S ribosomal protein L5

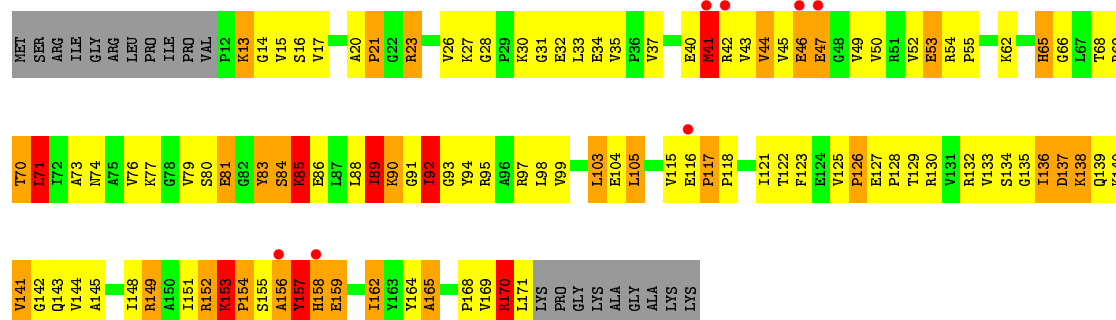


• Molecule 36: 50S ribosomal protein L5

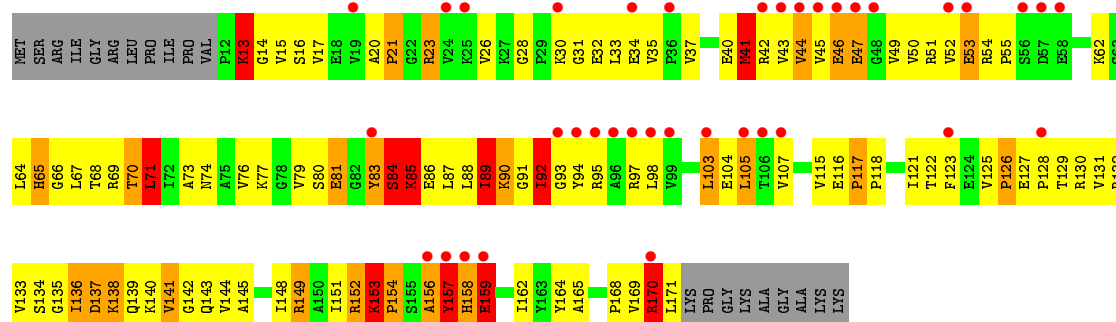




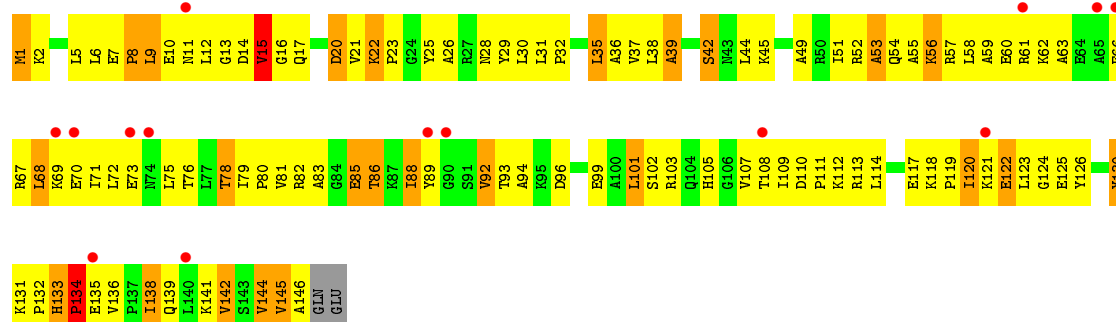
• Molecule 37: 50S ribosomal protein L6



• Molecule 37: 50S ribosomal protein L6

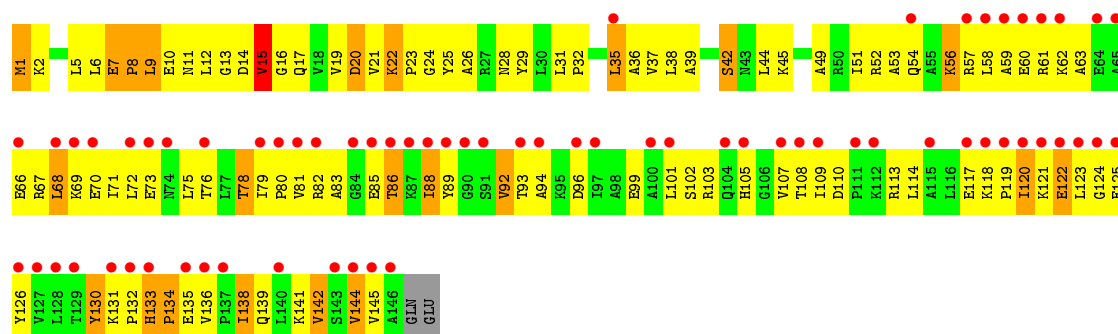


• Molecule 38: 50S ribosomal protein L9

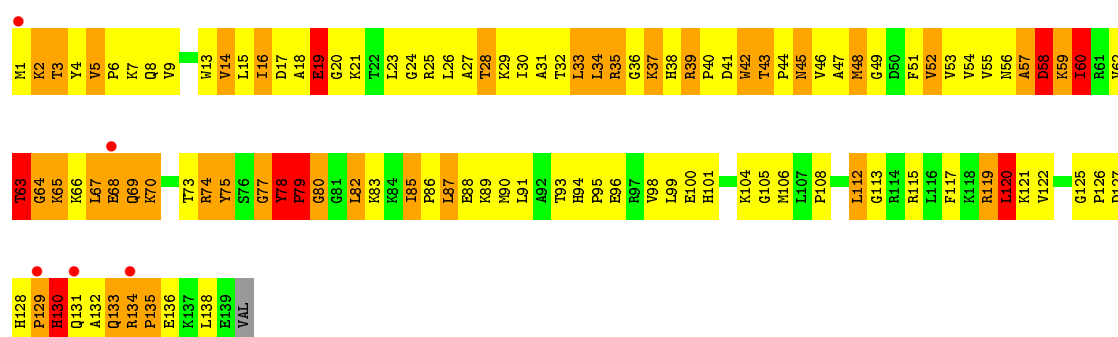
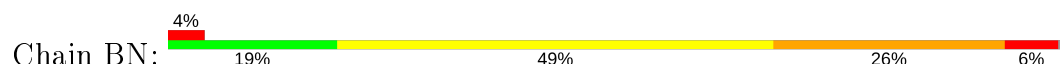


• Molecule 38: 50S ribosomal protein L9

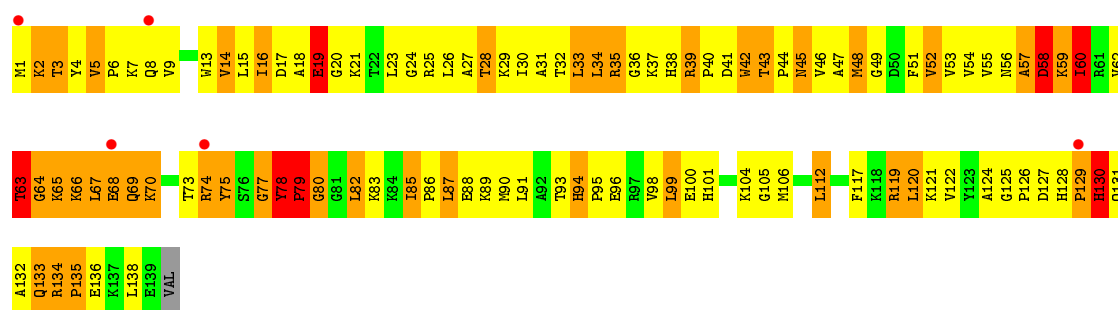
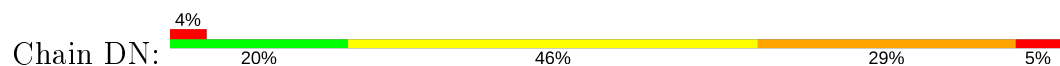




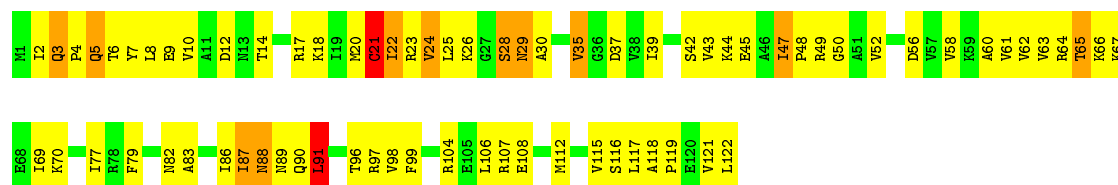
● Molecule 39: 50S ribosomal protein L13



● Molecule 39: 50S ribosomal protein L13

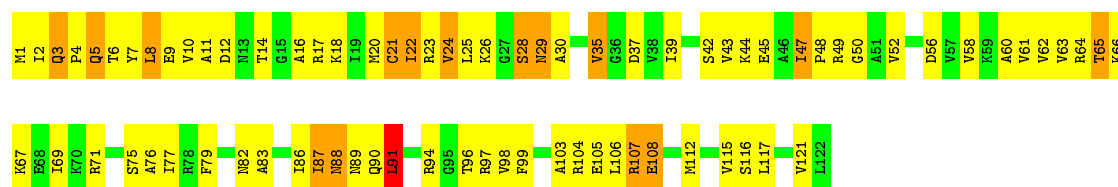


● Molecule 40: 50S ribosomal protein L14




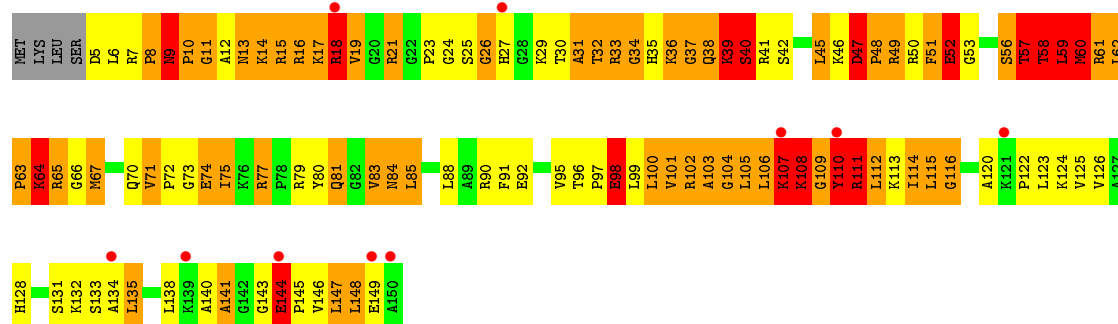
● Molecule 40: 50S ribosomal protein L14

Chain DO: 




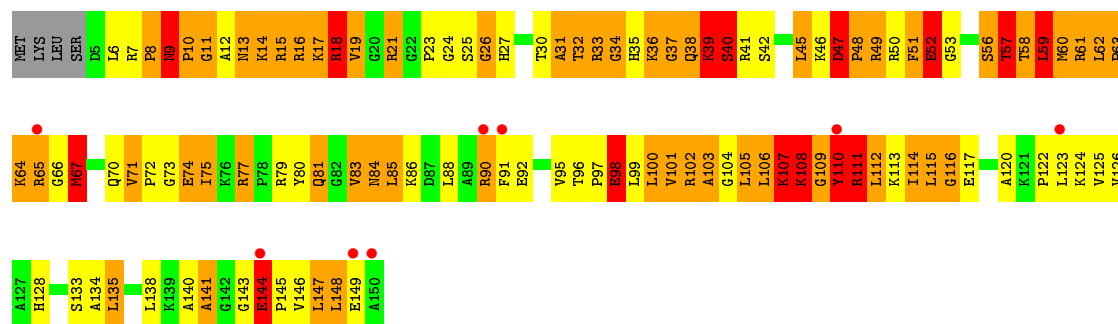
• Molecule 41: 50S ribosomal protein L15

Chain BP: 



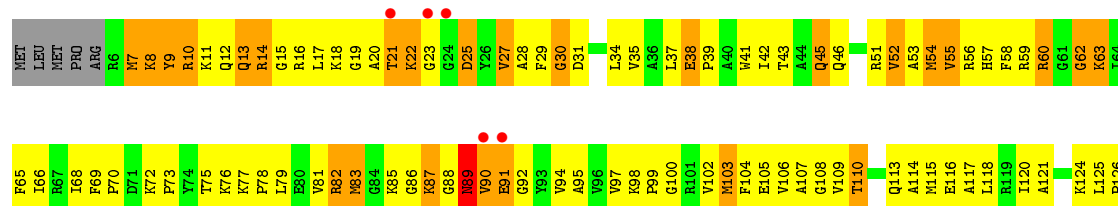
• Molecule 41: 50S ribosomal protein L15

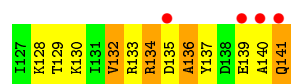
Chain DP: 



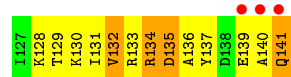
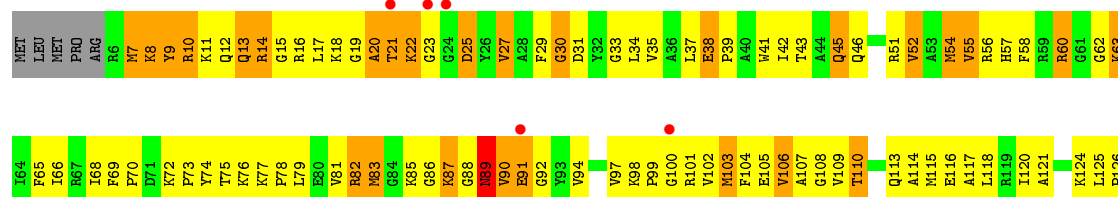
• Molecule 42: 50S ribosomal protein L16

Chain BQ: 

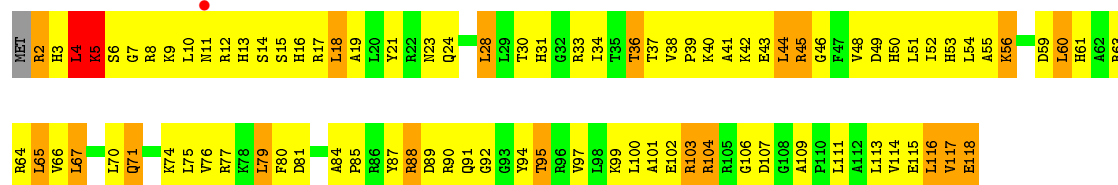




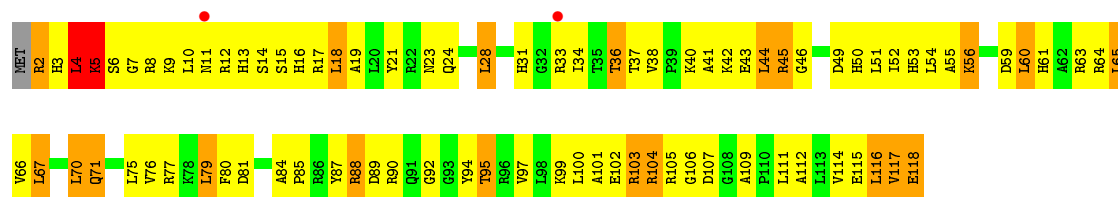
- Molecule 42: 50S ribosomal protein L16



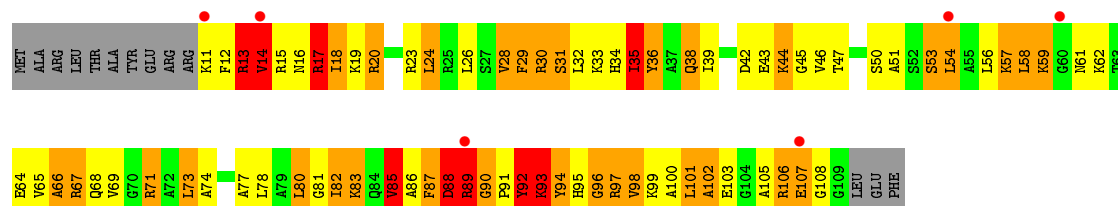
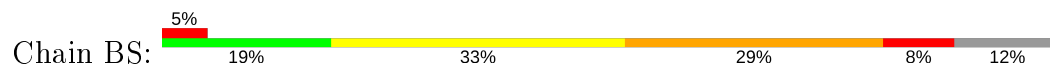
- Molecule 43: 50S ribosomal protein L17



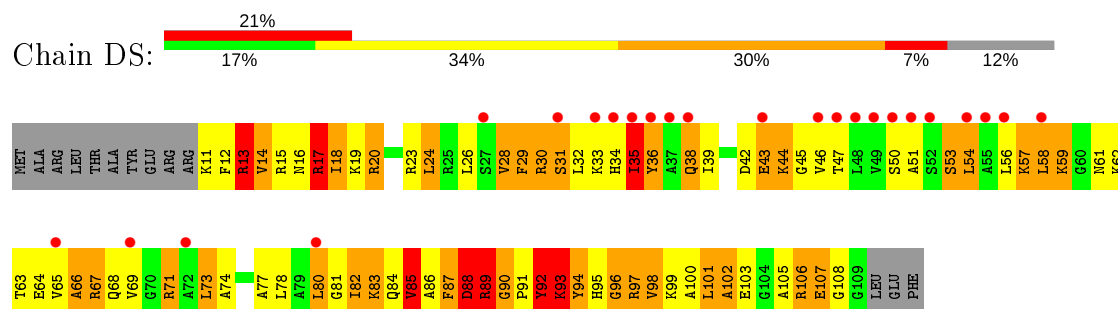
- Molecule 43: 50S ribosomal protein L17



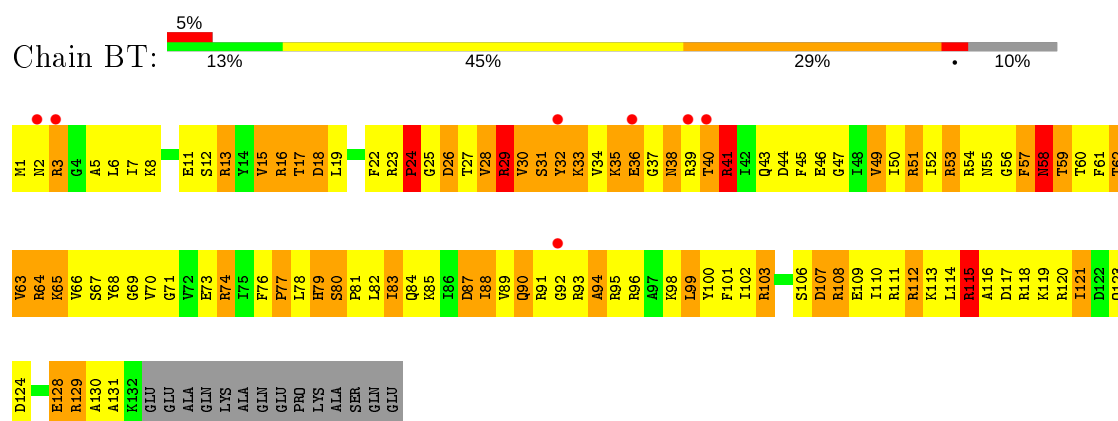
- Molecule 44: 50S ribosomal protein L18



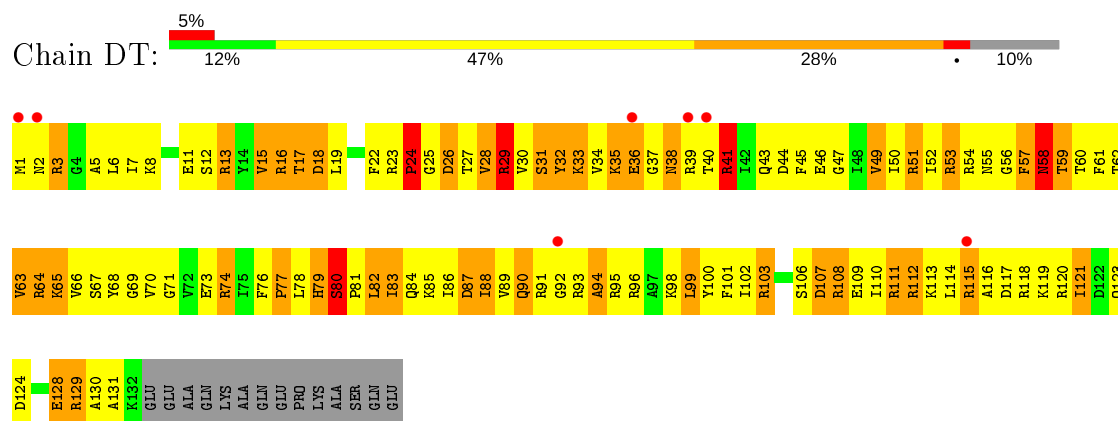
• Molecule 44: 50S ribosomal protein L18



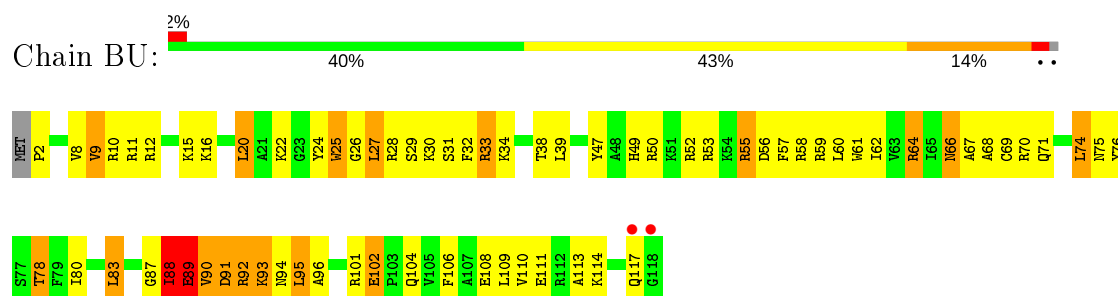
• Molecule 45: 50S ribosomal protein L19



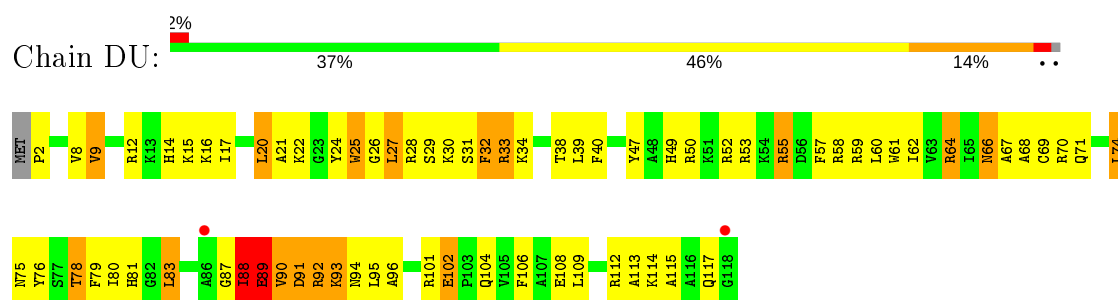
• Molecule 45: 50S ribosomal protein L19



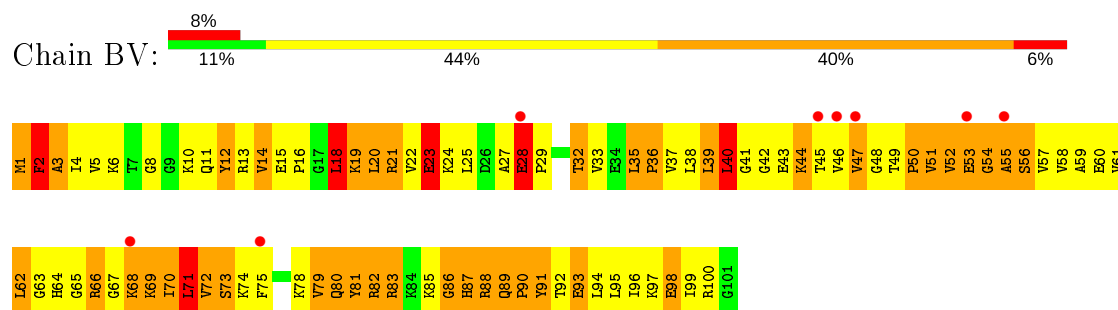
• Molecule 46: 50S ribosomal protein L20



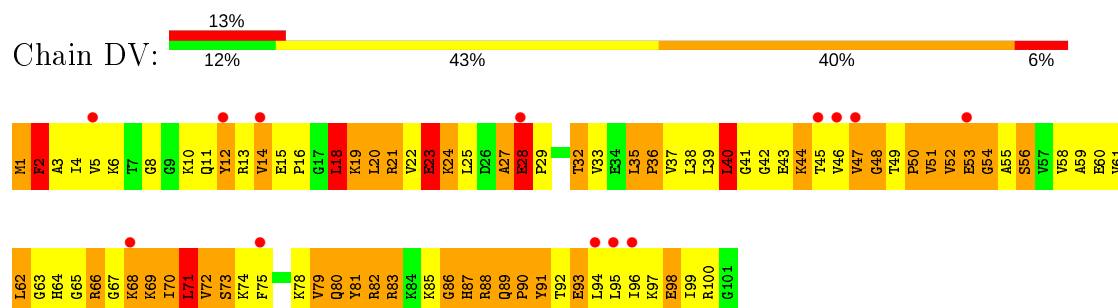
• Molecule 46: 50S ribosomal protein L20



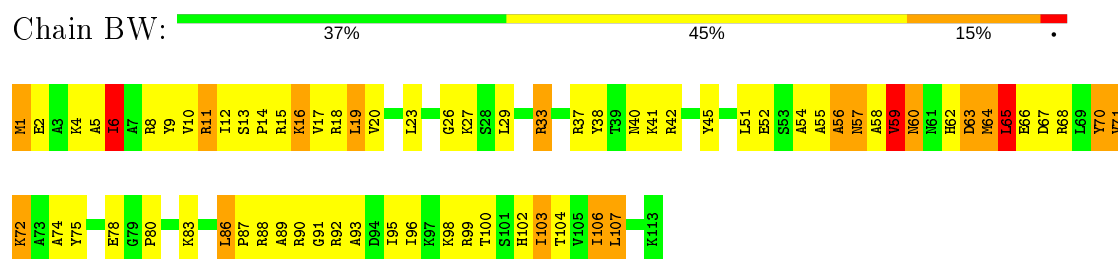
• Molecule 47: 50S ribosomal protein L21



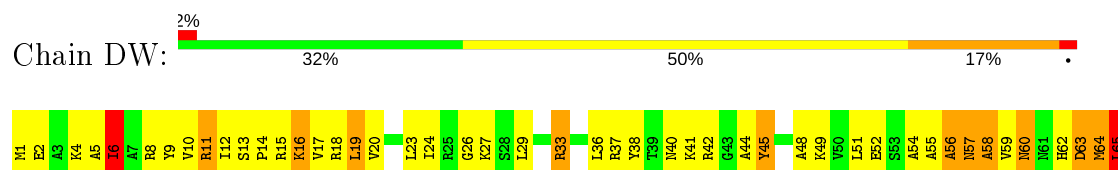
• Molecule 47: 50S ribosomal protein L21

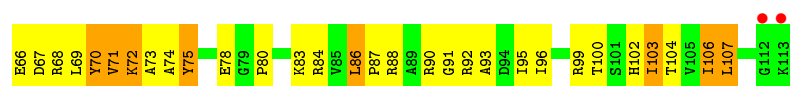


• Molecule 48: 50S ribosomal protein L22

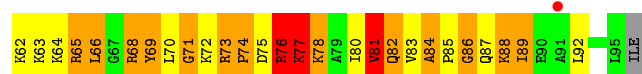
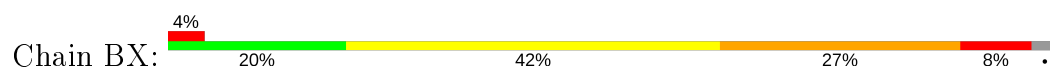


• Molecule 48: 50S ribosomal protein L22

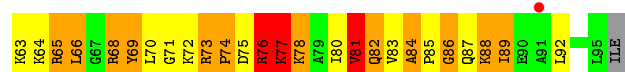
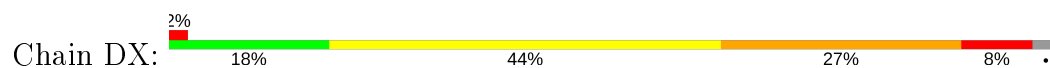




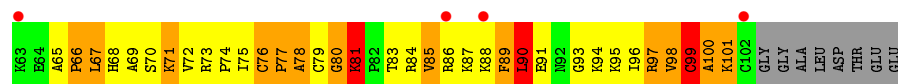
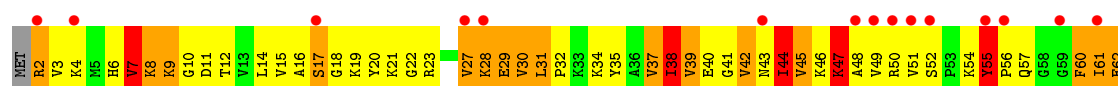
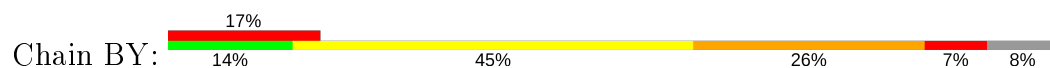
• Molecule 49: 50S ribosomal protein L23



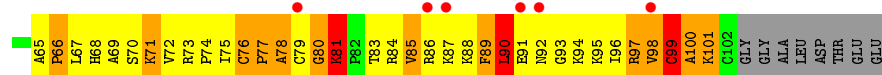
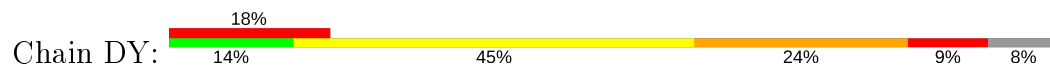
• Molecule 49: 50S ribosomal protein L23



• Molecule 50: 50S ribosomal protein L24

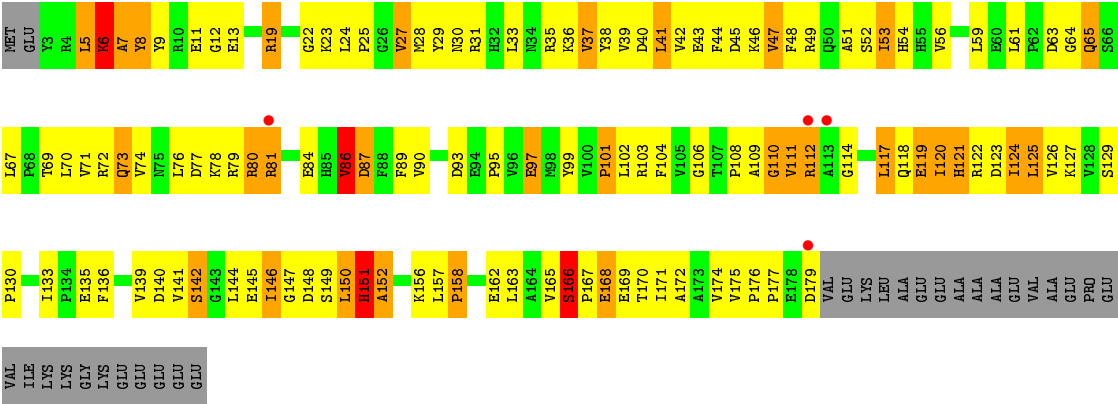


• Molecule 50: 50S ribosomal protein L24

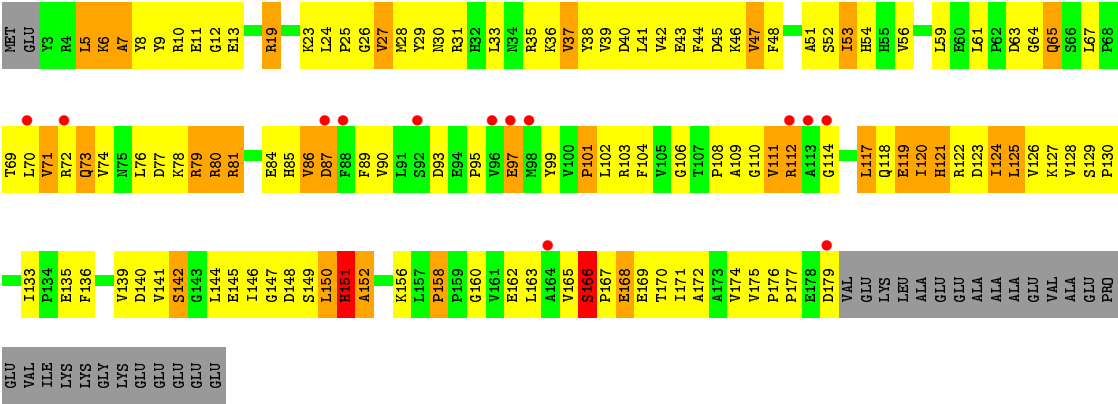


• Molecule 51: 50S ribosomal protein L25





• Molecule 51: 50S ribosomal protein L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.18Å 448.40Å 621.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.00 49.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.57-3.00) 98.6 (49.57-3.00)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.244 , 0.281 0.242 , 0.276	Depositor DCC
R_{free} test set	57089 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 86.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	277987	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: K, CLM, MG, ZN

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	0.54	0/36190	0.92	37/56486 (0.1%)
1	CA	0.53	0/36190	0.93	55/56486 (0.1%)
2	AB	0.29	0/1936	0.51	0/2611
2	CB	0.29	0/1936	0.50	0/2611
3	AC	0.27	0/1637	0.44	0/2207
3	CC	0.26	0/1637	0.44	0/2207
4	AD	0.36	0/1733	0.54	0/2318
4	CD	0.38	1/1733 (0.1%)	0.55	0/2318
5	AE	0.38	0/1163	0.58	0/1566
5	CE	0.37	0/1163	0.59	0/1566
6	AF	0.38	0/856	0.58	0/1154
6	CF	0.36	0/856	0.58	0/1154
7	AG	0.25	0/1276	0.44	0/1709
7	CG	0.25	0/1276	0.44	0/1709
8	AH	0.34	0/1136	0.56	0/1527
8	CH	0.34	0/1136	0.55	0/1527
9	AI	0.25	0/1028	0.44	0/1375
9	CI	0.25	0/1028	0.44	0/1375
10	AJ	0.27	0/808	0.48	0/1087
10	CJ	0.26	0/808	0.49	0/1087
11	AK	0.33	0/900	0.55	0/1213
11	CK	0.35	0/900	0.54	0/1213
12	AL	0.42	0/987	0.65	0/1322
12	CL	0.42	0/987	0.65	0/1322
13	AM	0.26	0/928	0.47	0/1238
13	CM	0.26	0/928	0.46	0/1238
14	AN	0.26	0/501	0.42	0/664
14	CN	0.26	0/501	0.42	0/664
15	AO	0.36	0/745	0.59	0/992
15	CO	0.35	0/745	0.58	0/992
16	AP	0.34	0/717	0.59	0/965
16	CP	0.35	0/717	0.60	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.36	0/837	0.58	0/1119
17	CQ	0.37	0/837	0.59	0/1119
18	AR	0.35	0/579	0.58	0/768
18	CR	0.36	0/579	0.57	0/768
19	AS	0.26	0/643	0.43	0/867
19	CS	0.26	0/643	0.44	0/867
20	AT	0.36	0/765	0.57	0/1007
20	CT	0.35	0/765	0.56	0/1007
21	AU	0.26	0/213	0.43	0/279
21	CU	0.26	0/213	0.43	0/279
22	B0	0.53	0/658	0.70	0/878
22	D0	0.49	0/658	0.70	0/878
23	B1	0.78	0/700	0.99	2/931 (0.2%)
23	D1	0.67	0/700	0.95	1/931 (0.1%)
24	B2	0.66	0/423	0.94	0/560
24	D2	0.55	0/423	0.89	0/560
25	B3	0.61	0/473	0.69	0/636
25	D3	0.49	0/473	0.67	0/636
26	B4	0.30	0/156	0.68	0/215
26	D4	0.30	0/156	0.65	0/215
27	B5	0.84	1/473 (0.2%)	1.02	2/639 (0.3%)
27	D5	0.77	0/473	0.97	1/639 (0.2%)
28	B6	0.89	0/387	1.07	0/517
28	D6	0.71	0/387	1.01	0/517
29	B7	0.64	0/427	0.79	0/563
29	D7	0.67	0/427	0.76	0/563
30	B8	0.72	0/516	1.09	2/681 (0.3%)
30	D8	0.64	0/516	1.04	0/681
31	BA	1.06	84/65745 (0.1%)	1.42	971/102639 (0.9%)
31	DA	0.85	35/65745 (0.1%)	1.41	1008/102639 (1.0%)
32	BB	0.83	0/2853	1.18	23/4451 (0.5%)
32	DB	0.66	0/2853	1.13	19/4451 (0.4%)
33	BD	0.63	0/2155	0.85	2/2907 (0.1%)
33	DD	0.59	0/2155	0.83	1/2907 (0.0%)
34	BE	0.63	0/1597	0.82	0/2155
34	DE	0.56	0/1597	0.81	0/2155
35	BF	0.60	0/1659	0.76	0/2246
35	DF	0.52	1/1659 (0.1%)	0.74	0/2246
36	BG	0.34	0/1498	0.55	0/2013
36	DG	0.30	0/1498	0.54	0/2013
37	BH	0.60	0/1246	0.74	0/1684
37	DH	0.44	0/1246	0.69	0/1684
38	BI	0.38	0/1147	0.61	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.40	0/1147	0.61	0/1553
39	BN	0.71	0/1132	0.93	2/1527 (0.1%)
39	DN	0.59	0/1132	0.87	1/1527 (0.1%)
40	BO	0.59	1/943 (0.1%)	0.73	0/1269
40	DO	0.52	0/943	0.73	1/1269 (0.1%)
41	BP	0.69	0/1131	1.03	8/1504 (0.5%)
41	DP	0.60	0/1131	0.98	6/1504 (0.4%)
42	BQ	0.70	0/1100	0.85	1/1470 (0.1%)
42	DQ	0.60	0/1100	0.83	0/1470
43	BR	0.63	0/974	0.82	1/1302 (0.1%)
43	DR	0.56	0/974	0.80	1/1302 (0.1%)
44	BS	0.50	0/779	0.77	0/1038
44	DS	0.43	0/779	0.73	0/1038
45	BT	0.59	0/1114	0.85	2/1488 (0.1%)
45	DT	0.52	0/1114	0.83	1/1488 (0.1%)
46	BU	0.69	0/975	0.76	0/1297
46	DU	0.56	0/975	0.72	0/1297
47	BV	0.72	0/789	0.95	1/1054 (0.1%)
47	DV	0.58	0/789	0.89	1/1054 (0.1%)
48	BW	0.68	0/907	0.84	2/1216 (0.2%)
48	DW	0.58	0/907	0.81	2/1216 (0.2%)
49	BX	0.70	0/740	0.96	2/995 (0.2%)
49	DX	0.63	0/740	0.94	2/995 (0.2%)
50	BY	0.70	1/789 (0.1%)	0.91	0/1053
50	DY	0.60	0/789	0.87	1/1053 (0.1%)
51	BZ	0.47	0/1436	0.67	2/1951 (0.1%)
51	DZ	0.41	0/1436	0.66	1/1951 (0.1%)
All	All	0.75	124/301000 (0.0%)	1.13	2162/449812 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	B1	0	1
23	D1	0	1
24	B2	0	1
24	D2	0	1
27	B5	0	1
27	D5	0	1
28	B6	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	BA	19	0
31	DA	19	0
33	BD	0	3
33	DD	0	3
34	BE	0	2
34	DE	0	2
37	BH	0	1
37	DH	0	1
41	BP	0	5
41	DP	0	4
42	BQ	0	1
42	DQ	0	1
43	BR	0	2
43	DR	0	2
44	BS	0	1
44	DS	0	1
45	BT	0	2
45	DT	0	2
46	BU	0	1
47	BV	0	3
47	DV	0	3
49	BX	0	4
49	DX	0	4
All	All	38	55

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	669	G	C4'-C3'	-11.30	1.40	1.53
31	DA	669	G	C4'-C3'	-10.33	1.41	1.53
31	BA	1300	U	C4'-C3'	-9.89	1.42	1.53
31	BA	1332	G	N9-C4	-9.70	1.30	1.38
31	DA	783	A	N9-C4	-9.28	1.32	1.37

The worst 5 of 2162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BA	1332	G	N3-C4-C5	18.18	137.69	128.60
31	DA	1779	U	C5-C6-N1	-17.02	114.19	122.70
31	BA	1779	U	C5-C6-N1	-16.17	114.61	122.70
31	BA	1332	G	N3-C4-N9	-15.97	116.42	126.00
31	BA	1332	G	C2-N3-C4	-15.30	104.25	111.90

5 of 38 chirality outliers are listed below:

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

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	B1	30	VAL	Peptide
24	B2	55	ARG	Peptide
27	B5	51	TYR	Peptide
28	B6	47	THR	Peptide
33	BD	47	GLY	Peptide

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	32329	0	16318	1597	0
1	CA	32329	0	16318	1553	0
2	AB	1901	0	1951	215	0
2	CB	1901	0	1951	207	0
3	AC	1613	0	1677	116	0
3	CC	1613	0	1677	116	0
4	AD	1703	0	1765	190	0
4	CD	1703	0	1764	192	0
5	AE	1147	0	1207	101	0
5	CE	1147	0	1207	100	0
6	AF	843	0	857	96	0
6	CF	843	0	857	98	0
7	AG	1257	0	1296	75	0
7	CG	1257	0	1296	75	0
8	AH	1116	0	1177	101	0
8	CH	1116	0	1177	99	0
9	AI	1011	0	1042	101	0
9	CI	1011	0	1042	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	105	0
10	CJ	795	0	840	102	0
11	AK	885	0	904	63	0
11	CK	885	0	904	68	0
12	AL	971	0	1057	100	0
12	CL	971	0	1057	103	0
13	AM	921	0	976	88	0
13	CM	921	0	976	91	0
14	AN	492	0	530	47	0
14	CN	492	0	529	46	0
15	AO	734	0	771	76	0
15	CO	734	0	771	78	0
16	AP	701	0	720	91	0
16	CP	701	0	720	97	0
17	AQ	824	0	891	66	0
17	CQ	824	0	891	55	0
18	AR	574	0	644	76	0
18	CR	574	0	644	78	0
19	AS	630	0	652	51	0
19	CS	630	0	652	52	0
20	AT	763	0	861	82	0
20	CT	763	0	861	73	0
21	AU	209	0	221	9	0
21	CU	209	0	221	9	0
22	B0	650	0	654	55	0
22	D0	650	0	654	57	0
23	B1	693	0	764	146	0
23	D1	693	0	764	143	0
24	B2	421	0	461	119	0
24	D2	421	0	461	123	0
25	B3	468	0	523	32	0
25	D3	468	0	523	41	0
26	B4	157	0	69	20	0
26	D4	157	0	69	21	0
27	B5	459	0	480	94	0
27	D5	459	0	480	86	0
28	B6	381	0	390	102	0
28	D6	381	0	390	97	0
29	B7	419	0	467	37	0
29	D7	419	0	467	39	0
30	B8	508	0	576	158	0
30	D8	508	0	576	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BA	58698	0	29590	2607	0
31	DA	58698	0	29591	2784	0
32	BB	2551	0	1295	145	0
32	DB	2551	0	1295	156	0
33	BD	2105	0	2182	325	0
33	DD	2105	0	2182	333	0
34	BE	1564	0	1629	240	0
34	DE	1564	0	1629	249	0
35	BF	1624	0	1677	182	0
35	DF	1624	0	1677	185	0
36	BG	1474	0	1534	190	0
36	DG	1474	0	1534	187	0
37	BH	1223	0	1282	162	0
37	DH	1223	0	1282	157	0
38	BI	1132	0	1218	120	0
38	DI	1132	0	1218	125	0
39	BN	1105	0	1180	218	0
39	DN	1105	0	1180	229	0
40	BO	933	0	996	77	0
40	DO	933	0	996	86	0
41	BP	1114	0	1187	302	0
41	DP	1114	0	1187	289	0
42	BQ	1080	0	1127	165	0
42	DQ	1080	0	1127	176	0
43	BR	960	0	1021	135	0
43	DR	960	0	1021	132	0
44	BS	771	0	832	149	0
44	DS	771	0	832	139	0
45	BT	1100	0	1164	210	0
45	DT	1100	0	1164	201	0
46	BU	958	0	1015	145	0
46	DU	958	0	1015	151	0
47	BV	779	0	851	224	0
47	DV	779	0	851	225	0
48	BW	896	0	953	76	0
48	DW	896	0	953	84	0
49	BX	726	0	778	168	0
49	DX	726	0	778	164	0
50	BY	776	0	870	177	0
50	DY	776	0	870	178	0
51	BZ	1404	0	1432	153	0
51	DZ	1404	0	1432	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AA	56	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	BA	368	0	0	0	0
52	BB	7	0	0	0	0
52	BD	1	0	0	0	0
52	BE	1	0	0	0	0
52	BF	1	0	0	0	0
52	BP	2	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	2	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	53	0	0	0	0
52	D1	1	0	0	0	0
52	D5	2	0	0	0	0
52	DA	332	0	0	0	0
52	DB	4	0	0	0	0
52	DD	1	0	0	0	0
52	DE	1	0	0	0	0
52	DF	1	0	0	0	0
52	DP	1	0	0	0	0
52	DQ	1	0	0	0	0
52	DR	1	0	0	0	0
52	DU	1	0	0	0	0
52	DX	1	0	0	0	0
53	AD	1	0	0	0	0
53	AN	1	0	0	0	0
53	CD	1	0	0	2	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	20	0	10	0	0
55	DA	20	0	10	0	0
All	All	277987	0	189127	18994	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 41.

The worst 5 of 18994 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)
27:B5:46:CYS:SG	27:B5:47:PRO:HD2	1.78	1.22
31:BA:1899:G:H22	31:BA:1902:C:N4	1.41	1.18
30:B8:32:LEU:CB	30:B8:35:GLN:H	1.57	1.17
32:DB:20:C:H2'	32:DB:21:G:H5''	1.25	1.17
41:BP:141:ALA:HB3	25:D3:1:MET:SD	1.86	1.16

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	155 (66%)	61 (26%)	17 (7%)	1	5
2	CB	233/256 (91%)	155 (66%)	60 (26%)	18 (8%)	1	5
3	AC	205/239 (86%)	148 (72%)	46 (22%)	11 (5%)	2	11
3	CC	205/239 (86%)	148 (72%)	45 (22%)	12 (6%)	1	9
4	AD	206/209 (99%)	129 (63%)	57 (28%)	20 (10%)	0	2
4	CD	206/209 (99%)	131 (64%)	55 (27%)	20 (10%)	0	2
5	AE	149/162 (92%)	103 (69%)	36 (24%)	10 (7%)	1	6
5	CE	149/162 (92%)	104 (70%)	36 (24%)	9 (6%)	1	9
6	AF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	2	12
6	CF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	2	12
7	AG	153/156 (98%)	123 (80%)	28 (18%)	2 (1%)	12	45
7	CG	153/156 (98%)	124 (81%)	27 (18%)	2 (1%)	12	45
8	AH	136/138 (99%)	98 (72%)	25 (18%)	13 (10%)	0	3
8	CH	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	1	3
9	AI	123/128 (96%)	89 (72%)	26 (21%)	8 (6%)	1	7
9	CI	123/128 (96%)	91 (74%)	24 (20%)	8 (6%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	97/105 (92%)	78 (80%)	15 (16%)	4 (4%)	3	16
10	CJ	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	2	12
11	AK	117/129 (91%)	92 (79%)	23 (20%)	2 (2%)	9	39
11	CK	117/129 (91%)	90 (77%)	25 (21%)	2 (2%)	9	39
12	AL	123/135 (91%)	85 (69%)	25 (20%)	13 (11%)	0	2
12	CL	123/135 (91%)	82 (67%)	27 (22%)	14 (11%)	0	2
13	AM	107/126 (85%)	80 (75%)	21 (20%)	6 (6%)	2	10
13	CM	107/126 (85%)	81 (76%)	19 (18%)	7 (6%)	1	7
14	AN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	39
14	CN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	39
15	AO	86/89 (97%)	65 (76%)	14 (16%)	7 (8%)	1	4
15	CO	86/89 (97%)	64 (74%)	16 (19%)	6 (7%)	1	6
16	AP	82/88 (93%)	51 (62%)	18 (22%)	13 (16%)	0	1
16	CP	82/88 (93%)	52 (63%)	18 (22%)	12 (15%)	0	1
17	AQ	98/105 (93%)	79 (81%)	11 (11%)	8 (8%)	1	4
17	CQ	98/105 (93%)	78 (80%)	13 (13%)	7 (7%)	1	5
18	AR	68/88 (77%)	49 (72%)	14 (21%)	5 (7%)	1	5
18	CR	68/88 (77%)	46 (68%)	16 (24%)	6 (9%)	1	3
19	AS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	1	3
19	CS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	1	3
20	AT	97/106 (92%)	70 (72%)	18 (19%)	9 (9%)	0	3
20	CT	97/106 (92%)	68 (70%)	20 (21%)	9 (9%)	0	3
21	AU	23/27 (85%)	17 (74%)	5 (22%)	1 (4%)	2	15
21	CU	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1	3
22	B0	83/85 (98%)	69 (83%)	10 (12%)	4 (5%)	2	13
22	D0	83/85 (98%)	68 (82%)	11 (13%)	4 (5%)	2	13
23	B1	87/98 (89%)	47 (54%)	24 (28%)	16 (18%)	0	0
23	D1	87/98 (89%)	46 (53%)	24 (28%)	17 (20%)	0	0
24	B2	49/72 (68%)	23 (47%)	14 (29%)	12 (24%)	0	0
24	D2	49/72 (68%)	22 (45%)	15 (31%)	12 (24%)	0	0
25	B3	58/60 (97%)	50 (86%)	8 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	D3	58/60 (97%)	48 (83%)	10 (17%)	0	100	100
26	B4	30/71 (42%)	4 (13%)	14 (47%)	12 (40%)	0	0
26	D4	30/71 (42%)	3 (10%)	15 (50%)	12 (40%)	0	0
27	B5	57/60 (95%)	43 (75%)	4 (7%)	10 (18%)	0	0
27	D5	57/60 (95%)	42 (74%)	6 (10%)	9 (16%)	0	1
28	B6	41/54 (76%)	21 (51%)	6 (15%)	14 (34%)	0	0
28	D6	41/54 (76%)	21 (51%)	7 (17%)	13 (32%)	0	0
29	B7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
29	D7	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
30	B8	62/65 (95%)	41 (66%)	12 (19%)	9 (14%)	0	1
30	D8	62/65 (95%)	42 (68%)	12 (19%)	8 (13%)	0	1
33	BD	270/276 (98%)	211 (78%)	44 (16%)	15 (6%)	2	10
33	DD	270/276 (98%)	208 (77%)	46 (17%)	16 (6%)	1	9
34	BE	203/206 (98%)	147 (72%)	31 (15%)	25 (12%)	0	1
34	DE	203/206 (98%)	144 (71%)	37 (18%)	22 (11%)	0	2
35	BF	206/210 (98%)	158 (77%)	34 (16%)	14 (7%)	1	6
35	DF	206/210 (98%)	154 (75%)	36 (18%)	16 (8%)	1	4
36	BG	177/182 (97%)	125 (71%)	35 (20%)	17 (10%)	0	3
36	DG	177/182 (97%)	126 (71%)	34 (19%)	17 (10%)	0	3
37	BH	158/180 (88%)	102 (65%)	31 (20%)	25 (16%)	0	1
37	DH	158/180 (88%)	101 (64%)	31 (20%)	26 (16%)	0	0
38	BI	144/148 (97%)	98 (68%)	30 (21%)	16 (11%)	0	2
38	DI	144/148 (97%)	99 (69%)	33 (23%)	12 (8%)	1	4
39	BN	137/140 (98%)	89 (65%)	28 (20%)	20 (15%)	0	1
39	DN	137/140 (98%)	92 (67%)	25 (18%)	20 (15%)	0	1
40	BO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9	39
40	DO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	5	28
41	BP	144/150 (96%)	71 (49%)	33 (23%)	40 (28%)	0	0
41	DP	144/150 (96%)	70 (49%)	33 (23%)	41 (28%)	0	0
42	BQ	134/141 (95%)	97 (72%)	21 (16%)	16 (12%)	0	1
42	DQ	134/141 (95%)	92 (69%)	25 (19%)	17 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BR	115/118 (98%)	86 (75%)	22 (19%)	7 (6%)	1	8
43	DR	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	1	8
44	BS	97/112 (87%)	45 (46%)	22 (23%)	30 (31%)	0	0
44	DS	97/112 (87%)	44 (45%)	22 (23%)	31 (32%)	0	0
45	BT	130/146 (89%)	91 (70%)	21 (16%)	18 (14%)	0	1
45	DT	130/146 (89%)	91 (70%)	21 (16%)	18 (14%)	0	1
46	BU	115/118 (98%)	89 (77%)	18 (16%)	8 (7%)	1	6
46	DU	115/118 (98%)	86 (75%)	21 (18%)	8 (7%)	1	6
47	BV	97/101 (96%)	54 (56%)	18 (19%)	25 (26%)	0	0
47	DV	97/101 (96%)	53 (55%)	19 (20%)	25 (26%)	0	0
48	BW	111/113 (98%)	85 (77%)	17 (15%)	9 (8%)	1	4
48	DW	111/113 (98%)	83 (75%)	19 (17%)	9 (8%)	1	4
49	BX	91/96 (95%)	47 (52%)	23 (25%)	21 (23%)	0	0
49	DX	91/96 (95%)	48 (53%)	23 (25%)	20 (22%)	0	0
50	BY	99/110 (90%)	47 (48%)	22 (22%)	30 (30%)	0	0
50	DY	99/110 (90%)	44 (44%)	25 (25%)	30 (30%)	0	0
51	BZ	175/206 (85%)	123 (70%)	32 (18%)	20 (11%)	0	2
51	DZ	175/206 (85%)	121 (69%)	36 (21%)	18 (10%)	0	2
All	All	11148/12060 (92%)	7786 (70%)	2170 (20%)	1192 (11%)	0	2

5 of 1192 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	18	GLY
2	AB	20	GLU
2	AB	106	LYS
2	AB	165	VAL
2	AB	195	ASP

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	170 (84%)	32 (16%)	2	12
2	CB	202/220 (92%)	168 (83%)	34 (17%)	2	11
3	AC	160/188 (85%)	153 (96%)	7 (4%)	28	65
3	CC	160/188 (85%)	153 (96%)	7 (4%)	28	65
4	AD	180/181 (99%)	156 (87%)	24 (13%)	4	17
4	CD	180/181 (99%)	156 (87%)	24 (13%)	4	17
5	AE	115/123 (94%)	95 (83%)	20 (17%)	2	10
5	CE	115/123 (94%)	95 (83%)	20 (17%)	2	10
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	21
6	CF	90/90 (100%)	78 (87%)	12 (13%)	4	17
7	AG	126/127 (99%)	122 (97%)	4 (3%)	39	74
7	CG	126/127 (99%)	122 (97%)	4 (3%)	39	74
8	AH	119/119 (100%)	106 (89%)	13 (11%)	6	25
8	CH	119/119 (100%)	106 (89%)	13 (11%)	6	25
9	AI	98/99 (99%)	90 (92%)	8 (8%)	11	39
9	CI	98/99 (99%)	90 (92%)	8 (8%)	11	39
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	5	24
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	5	24
11	AK	90/99 (91%)	82 (91%)	8 (9%)	9	35
11	CK	90/99 (91%)	83 (92%)	7 (8%)	12	42
12	AL	104/111 (94%)	92 (88%)	12 (12%)	5	24
12	CL	104/111 (94%)	91 (88%)	13 (12%)	4	20
13	AM	93/101 (92%)	87 (94%)	6 (6%)	17	50
13	CM	93/101 (92%)	87 (94%)	6 (6%)	17	50
14	AN	49/50 (98%)	45 (92%)	4 (8%)	11	39
14	CN	49/50 (98%)	45 (92%)	4 (8%)	11	39
15	AO	79/80 (99%)	68 (86%)	11 (14%)	3	16
15	CO	79/80 (99%)	68 (86%)	11 (14%)	3	16
16	AP	72/74 (97%)	58 (81%)	14 (19%)	1	7
16	CP	72/74 (97%)	59 (82%)	13 (18%)	1	9
17	AQ	94/97 (97%)	82 (87%)	12 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	82 (87%)	12 (13%)	4	19
18	AR	61/77 (79%)	55 (90%)	6 (10%)	8	30
18	CR	61/77 (79%)	55 (90%)	6 (10%)	8	30
19	AS	69/80 (86%)	62 (90%)	7 (10%)	7	29
19	CS	69/80 (86%)	62 (90%)	7 (10%)	7	29
20	AT	76/82 (93%)	68 (90%)	8 (10%)	7	27
20	CT	76/82 (93%)	68 (90%)	8 (10%)	7	27
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
22	B0	61/67 (91%)	53 (87%)	8 (13%)	4	18
22	D0	61/67 (91%)	53 (87%)	8 (13%)	4	18
23	B1	73/83 (88%)	53 (73%)	20 (27%)	0	2
23	D1	73/83 (88%)	55 (75%)	18 (25%)	0	3
24	B2	46/67 (69%)	33 (72%)	13 (28%)	0	2
24	D2	46/67 (69%)	33 (72%)	13 (28%)	0	2
25	B3	51/52 (98%)	45 (88%)	6 (12%)	5	22
25	D3	51/52 (98%)	44 (86%)	7 (14%)	3	17
27	B5	51/52 (98%)	40 (78%)	11 (22%)	1	5
27	D5	51/52 (98%)	38 (74%)	13 (26%)	0	3
28	B6	43/52 (83%)	27 (63%)	16 (37%)	0	0
28	D6	43/52 (83%)	28 (65%)	15 (35%)	0	1
29	B7	41/42 (98%)	33 (80%)	8 (20%)	1	7
29	D7	41/42 (98%)	32 (78%)	9 (22%)	1	4
30	B8	53/55 (96%)	40 (76%)	13 (24%)	0	3
30	D8	53/55 (96%)	41 (77%)	12 (23%)	1	4
33	BD	213/218 (98%)	166 (78%)	47 (22%)	1	4
33	DD	213/218 (98%)	165 (78%)	48 (22%)	1	4
34	BE	165/166 (99%)	122 (74%)	43 (26%)	0	2
34	DE	165/166 (99%)	122 (74%)	43 (26%)	0	2
35	BF	165/166 (99%)	134 (81%)	31 (19%)	1	8
35	DF	165/166 (99%)	137 (83%)	28 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BG	155/156 (99%)	134 (86%)	21 (14%)	4	17
36	DG	155/156 (99%)	134 (86%)	21 (14%)	4	17
37	BH	132/148 (89%)	105 (80%)	27 (20%)	1	6
37	DH	132/148 (89%)	105 (80%)	27 (20%)	1	6
38	BI	122/124 (98%)	104 (85%)	18 (15%)	3	14
38	DI	122/124 (98%)	104 (85%)	18 (15%)	3	14
39	BN	117/119 (98%)	79 (68%)	38 (32%)	0	1
39	DN	117/119 (98%)	79 (68%)	38 (32%)	0	1
40	BO	100/100 (100%)	81 (81%)	19 (19%)	1	8
40	DO	100/100 (100%)	81 (81%)	19 (19%)	1	8
41	BP	112/116 (97%)	72 (64%)	40 (36%)	0	1
41	DP	112/116 (97%)	72 (64%)	40 (36%)	0	1
42	BQ	106/111 (96%)	86 (81%)	20 (19%)	1	8
42	DQ	106/111 (96%)	85 (80%)	21 (20%)	1	7
43	BR	100/101 (99%)	81 (81%)	19 (19%)	1	8
43	DR	100/101 (99%)	80 (80%)	20 (20%)	1	7
44	BS	77/88 (88%)	53 (69%)	24 (31%)	0	1
44	DS	77/88 (88%)	54 (70%)	23 (30%)	0	1
45	BT	116/127 (91%)	81 (70%)	35 (30%)	0	1
45	DT	116/127 (91%)	81 (70%)	35 (30%)	0	1
46	BU	92/94 (98%)	79 (86%)	13 (14%)	3	16
46	DU	92/94 (98%)	79 (86%)	13 (14%)	3	16
47	BV	82/82 (100%)	53 (65%)	29 (35%)	0	1
47	DV	82/82 (100%)	53 (65%)	29 (35%)	0	1
48	BW	91/92 (99%)	70 (77%)	21 (23%)	1	4
48	DW	91/92 (99%)	71 (78%)	20 (22%)	1	4
49	BX	74/78 (95%)	54 (73%)	20 (27%)	0	2
49	DX	74/78 (95%)	53 (72%)	21 (28%)	0	2
50	BY	84/91 (92%)	60 (71%)	24 (29%)	0	2
50	DY	84/91 (92%)	61 (73%)	23 (27%)	0	2
51	BZ	155/179 (87%)	130 (84%)	25 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	DZ	155/179 (87%)	130 (84%)	25 (16%)	2 12
All	All	9322/9876 (94%)	7670 (82%)	1652 (18%)	2 9

5 of 1652 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BW	60	ASN
7	CG	36	LYS
46	DU	66	ASN
49	BX	49	VAL
2	CB	90	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 277 such sidechains are listed below:

Mol	Chain	Res	Type
48	BW	40	ASN
6	CF	18	GLN
45	DT	90	GLN
48	BW	62	HIS
2	CB	204	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	280 (18%)	31 (2%)
1	CA	1503/1522 (98%)	283 (18%)	31 (2%)
31	BA	2723/2787 (97%)	712 (26%)	70 (2%)
31	DA	2723/2787 (97%)	706 (25%)	69 (2%)
32	BB	118/122 (96%)	34 (28%)	1 (0%)
32	DB	118/122 (96%)	35 (29%)	1 (0%)
All	All	8688/8862 (98%)	2050 (23%)	203 (2%)

5 of 2050 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	41	G

5 of 203 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	BA	2439	A
1	CA	429	U
31	DA	1934	C
31	BA	2689	U
1	CA	60	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 853 ligands modelled in this entry, 851 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	CLM	DA	3334	54	19,20,20	1.22	1 (5%)	23,27,27	0.90	0
55	CLM	BA	3370	54	19,20,20	1.22	1 (5%)	23,27,27	0.90	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
55	CLM	DA	3334	54	-	0/20/22/22	0/1/1/1
55	CLM	BA	3370	54	-	0/20/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	3334	CLM	C9-N9	-4.29	1.34	1.45
55	BA	3370	CLM	C9-N9	-4.26	1.34	1.45

There are no bond angle outliers.

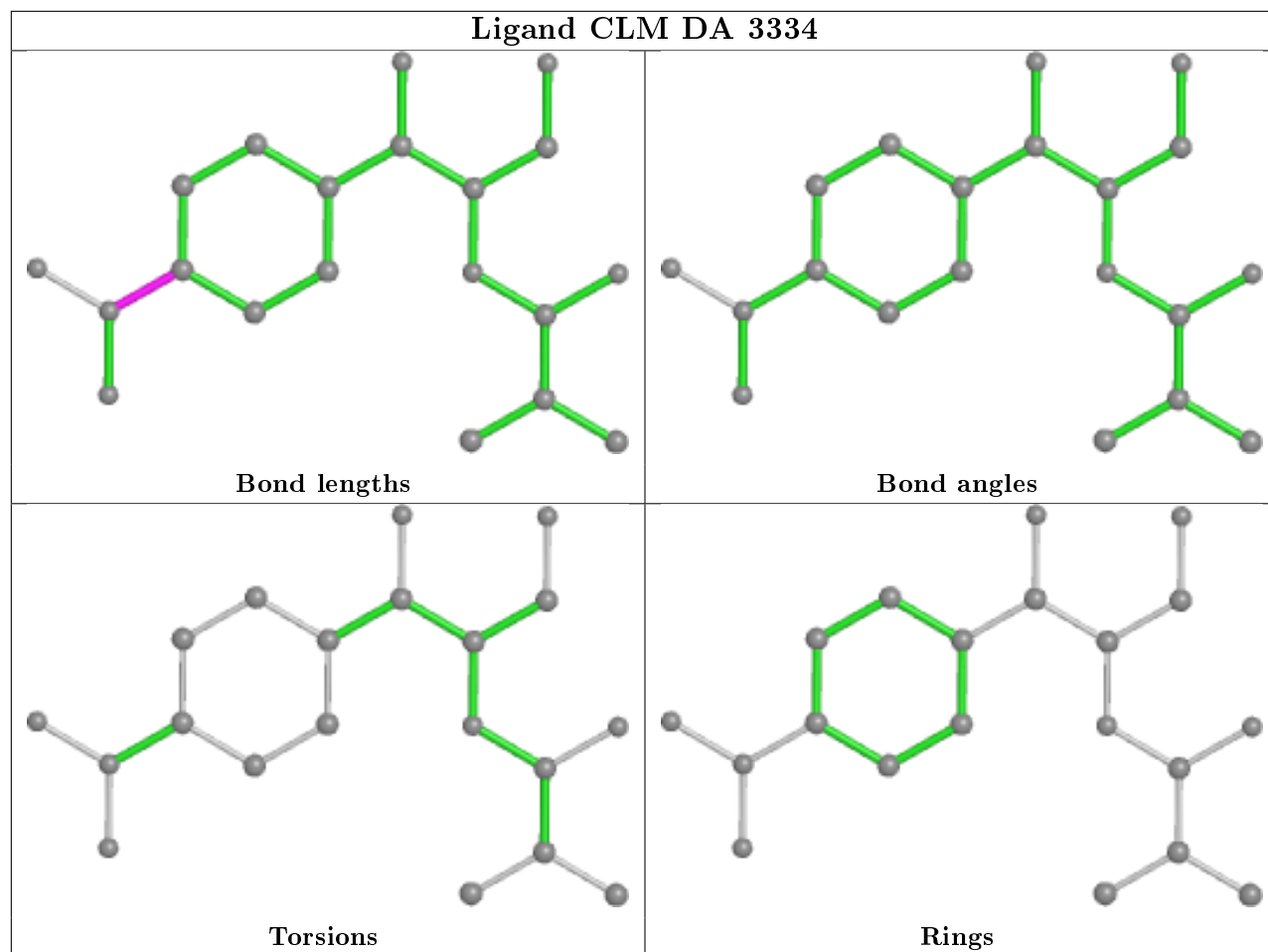
There are no chirality outliers.

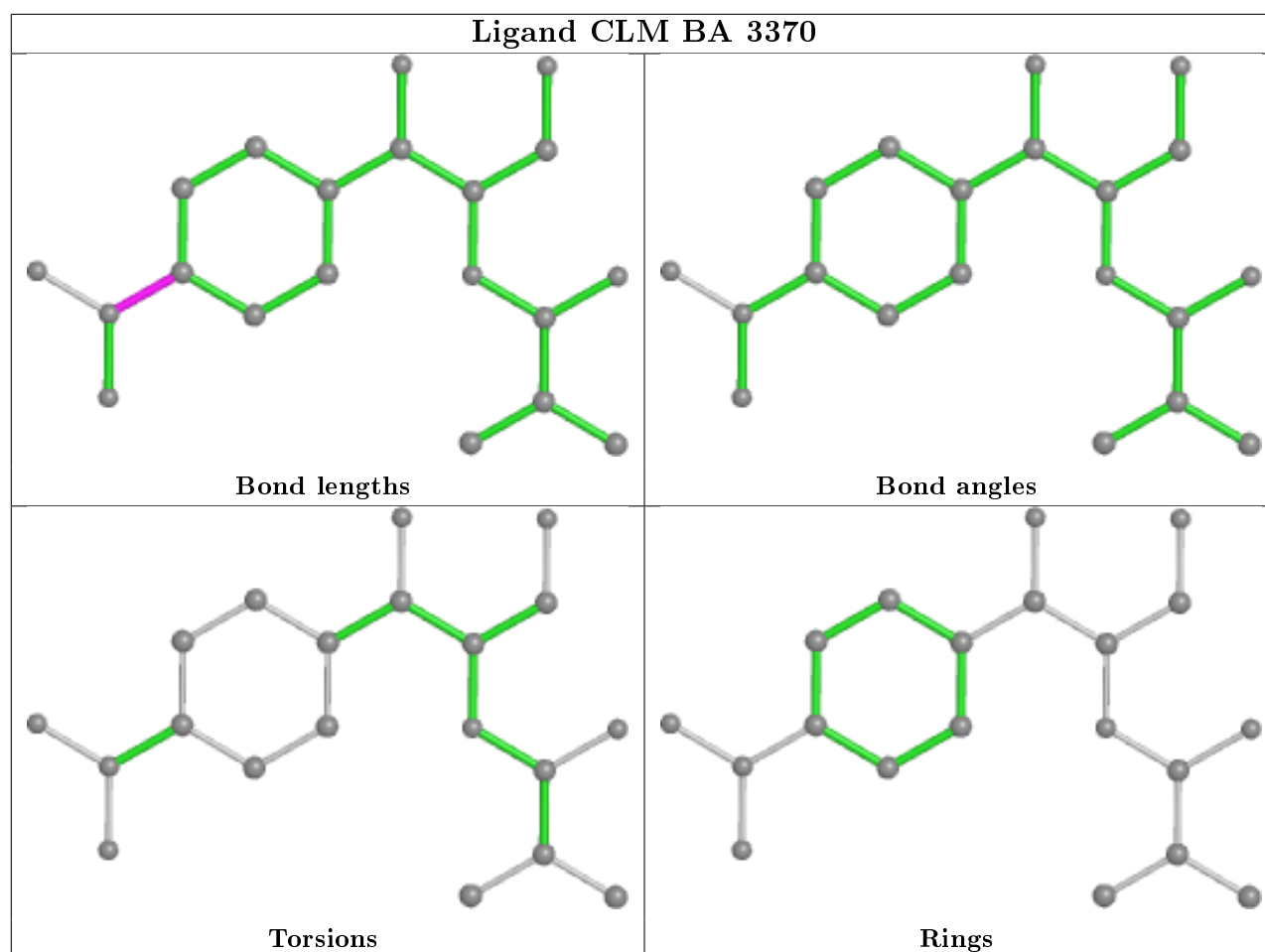
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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
13	CM	3
13	AM	3
47	DV	1
36	DG	1
36	BG	1
9	AI	1
9	CI	1
47	BV	1
28	D6	1

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Mol	Chain	Number of breaks
28	B6	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CM	69:GLU	C	70:LEU	N	5.35
1	AM	69:GLU	C	70:LEU	N	5.34
1	BG	112:PRO	C	113:ARG	N	4.53
1	DG	112:PRO	C	113:ARG	N	4.53
1	CM	112:GLY	C	113:PRO	N	4.49

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	1.11	291 (19%) 1 0	42, 106, 199, 201	0
1	CA	1504/1522 (98%)	0.93	239 (15%) 1 1	46, 105, 198, 201	0
2	AB	235/256 (91%)	0.71	35 (14%) 2 1	83, 146, 188, 195	0
2	CB	235/256 (91%)	0.90	51 (21%) 0 0	84, 149, 187, 196	0
3	AC	207/239 (86%)	1.13	52 (25%) 0 0	97, 158, 187, 194	0
3	CC	207/239 (86%)	1.19	51 (24%) 0 0	98, 160, 187, 194	0
4	AD	208/209 (99%)	0.35	9 (4%) 35 13	72, 112, 165, 186	0
4	CD	208/209 (99%)	0.19	4 (1%) 66 37	70, 111, 164, 185	0
5	AE	151/162 (93%)	0.43	9 (5%) 21 7	59, 97, 151, 194	0
5	CE	151/162 (93%)	0.45	8 (5%) 26 10	64, 98, 153, 194	0
6	AF	101/101 (100%)	0.21	6 (5%) 22 7	66, 111, 160, 183	0
6	CF	101/101 (100%)	0.17	4 (3%) 38 15	67, 113, 160, 188	0
7	AG	155/156 (99%)	1.77	55 (35%) 0 0	124, 172, 192, 197	0
7	CG	155/156 (99%)	1.93	58 (37%) 0 0	125, 172, 192, 198	0
8	AH	138/138 (100%)	0.06	3 (2%) 62 33	67, 102, 147, 162	0
8	CH	138/138 (100%)	0.13	2 (1%) 75 49	66, 102, 147, 163	0
9	AI	127/128 (99%)	2.47	62 (48%) 0 0	125, 179, 196, 199	0
9	CI	127/128 (99%)	2.38	60 (47%) 0 0	126, 180, 197, 199	0
10	AJ	99/105 (94%)	3.03	57 (57%) 0 0	122, 175, 196, 198	0
10	CJ	99/105 (94%)	2.81	58 (58%) 0 0	121, 176, 197, 199	0
11	AK	119/129 (92%)	0.67	18 (15%) 2 1	63, 105, 164, 188	0
11	CK	119/129 (92%)	0.79	15 (12%) 3 1	65, 104, 168, 191	0
12	AL	125/135 (92%)	0.33	5 (4%) 38 15	57, 89, 154, 198	0
12	CL	125/135 (92%)	0.57	11 (8%) 10 3	55, 89, 158, 198	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	AM	115/126 (91%)	2.67	65 (56%)	0	0	136, 190, 198, 200	0
13	CM	115/126 (91%)	2.58	61 (53%)	0	0	136, 188, 197, 199	0
14	AN	60/61 (98%)	1.68	22 (36%)	0	0	113, 167, 193, 196	0
14	CN	60/61 (98%)	1.31	14 (23%)	0	0	112, 168, 191, 196	0
15	AO	88/89 (98%)	0.11	4 (4%)	33	12	59, 91, 149, 155	0
15	CO	88/89 (98%)	0.12	2 (2%)	60	31	63, 92, 150, 157	0
16	AP	84/88 (95%)	0.94	14 (16%)	1	0	77, 101, 161, 188	0
16	CP	84/88 (95%)	0.49	5 (5%)	21	7	78, 100, 154, 186	0
17	AQ	100/105 (95%)	0.17	4 (4%)	38	15	62, 93, 138, 158	0
17	CQ	100/105 (95%)	0.14	3 (3%)	50	22	59, 92, 140, 157	0
18	AR	70/88 (79%)	0.36	3 (4%)	35	13	73, 98, 167, 197	0
18	CR	70/88 (79%)	0.93	7 (10%)	7	2	74, 100, 167, 196	0
19	AS	79/93 (84%)	4.19	61 (77%)	0	0	142, 191, 198, 199	0
19	CS	79/93 (84%)	3.55	59 (74%)	0	0	142, 190, 198, 199	0
20	AT	99/106 (93%)	0.18	4 (4%)	38	15	73, 110, 157, 186	0
20	CT	99/106 (93%)	0.39	9 (9%)	9	3	74, 108, 156, 189	0
21	AU	25/27 (92%)	4.40	19 (76%)	0	0	138, 175, 193, 196	0
21	CU	25/27 (92%)	3.38	17 (68%)	0	0	135, 172, 193, 195	0
22	B0	85/85 (100%)	0.69	8 (9%)	8	3	34, 59, 182, 197	0
22	D0	85/85 (100%)	0.62	12 (14%)	2	1	40, 64, 178, 197	0
23	B1	89/98 (90%)	0.36	2 (2%)	62	33	37, 64, 141, 187	0
23	D1	89/98 (90%)	0.17	4 (4%)	33	12	40, 66, 142, 191	0
24	B2	51/72 (70%)	0.87	8 (15%)	2	1	49, 87, 184, 193	0
24	D2	51/72 (70%)	0.52	8 (15%)	2	1	50, 91, 183, 195	0
25	B3	60/60 (100%)	0.05	1 (1%)	70	41	36, 56, 132, 180	0
25	D3	60/60 (100%)	0.40	4 (6%)	17	5	42, 61, 138, 178	0
26	B4	32/71 (45%)	0.00	1 (3%)	49	21	109, 156, 186, 191	0
26	D4	32/71 (45%)	0.21	1 (3%)	49	21	112, 161, 188, 195	0
27	B5	59/60 (98%)	0.68	6 (10%)	6	2	25, 47, 180, 195	0
27	D5	59/60 (98%)	0.35	5 (8%)	10	3	28, 50, 184, 195	0
28	B6	45/54 (83%)	0.77	5 (11%)	5	1	36, 70, 133, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	0.89	11 (24%) 0 0	42, 74, 138, 184	0
29	B7	49/49 (100%)	0.29	1 (2%) 65 36	26, 33, 117, 170	0
29	D7	49/49 (100%)	0.33	1 (2%) 65 36	27, 37, 118, 170	0
30	B8	64/65 (98%)	0.45	6 (9%) 8 3	34, 57, 138, 181	0
30	D8	64/65 (98%)	0.18	3 (4%) 31 11	38, 59, 139, 183	0
31	BA	2725/2787 (97%)	0.40	76 (2%) 53 25	26, 46, 145, 201	0
31	DA	2725/2787 (97%)	0.21	103 (3%) 40 16	27, 51, 149, 201	0
32	BB	119/122 (97%)	0.55	4 (3%) 45 19	39, 91, 140, 185	0
32	DB	119/122 (97%)	0.78	15 (12%) 3 1	48, 95, 154, 190	0
33	BD	272/276 (98%)	-0.10	3 (1%) 80 56	27, 47, 100, 177	0
33	DD	272/276 (98%)	-0.15	3 (1%) 80 56	29, 50, 104, 181	0
34	BE	205/206 (99%)	0.16	7 (3%) 45 19	25, 52, 145, 189	0
34	DE	205/206 (99%)	-0.03	5 (2%) 59 30	29, 56, 142, 189	0
35	BF	208/210 (99%)	0.45	15 (7%) 15 4	24, 58, 180, 197	0
35	DF	208/210 (99%)	0.38	16 (7%) 13 4	27, 63, 178, 197	0
36	BG	181/182 (99%)	1.17	39 (21%) 0 0	87, 145, 189, 199	0
36	DG	181/182 (99%)	1.94	74 (40%) 0 0	91, 153, 193, 199	0
37	BH	160/180 (88%)	0.38	7 (4%) 34 13	62, 102, 150, 193	0
37	DH	160/180 (88%)	1.08	37 (23%) 0 0	70, 110, 157, 195	0
38	BI	146/148 (98%)	0.50	14 (9%) 8 2	52, 143, 185, 195	0
38	DI	146/148 (98%)	3.26	68 (46%) 0 0	56, 156, 188, 198	0
39	BN	139/140 (99%)	0.20	5 (3%) 42 17	32, 60, 140, 187	0
39	DN	139/140 (99%)	-0.07	5 (3%) 42 17	38, 65, 142, 188	0
40	BO	122/122 (100%)	-0.20	0 100 100	32, 52, 105, 141	0
40	DO	122/122 (100%)	-0.45	0 100 100	35, 55, 111, 146	0
41	BP	146/150 (97%)	0.78	10 (6%) 17 5	22, 79, 148, 199	0
41	DP	146/150 (97%)	0.46	8 (5%) 25 9	27, 81, 150, 198	0
42	BQ	136/141 (96%)	0.52	9 (6%) 18 5	39, 64, 150, 189	0
42	DQ	136/141 (96%)	0.38	8 (5%) 22 7	43, 69, 149, 190	0
43	BR	117/118 (99%)	-0.02	1 (0%) 84 63	28, 44, 113, 143	0
43	DR	117/118 (99%)	-0.17	2 (1%) 70 41	30, 49, 115, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	0.44	6 (6%) 21 7	53, 98, 141, 178	0
44	DS	99/112 (88%)	1.12	24 (24%) 0 0	63, 103, 146, 180	0
45	BT	132/146 (90%)	0.31	7 (5%) 26 10	42, 73, 157, 191	0
45	DT	132/146 (90%)	0.14	7 (5%) 26 10	46, 77, 159, 194	0
46	BU	117/118 (99%)	0.24	2 (1%) 70 41	23, 50, 114, 190	0
46	DU	117/118 (99%)	0.12	2 (1%) 70 41	32, 56, 119, 193	0
47	BV	101/101 (100%)	0.80	8 (7%) 12 4	32, 91, 171, 194	0
47	DV	101/101 (100%)	0.76	13 (12%) 3 1	35, 97, 169, 195	0
48	BW	113/113 (100%)	-0.20	0 100 100	28, 40, 101, 168	0
48	DW	113/113 (100%)	-0.33	2 (1%) 68 40	31, 43, 106, 175	0
49	BX	93/96 (96%)	0.34	4 (4%) 35 13	36, 65, 142, 184	0
49	DX	93/96 (96%)	0.01	2 (2%) 62 33	42, 69, 147, 185	0
50	BY	101/110 (91%)	1.12	19 (18%) 1 0	39, 91, 191, 199	0
50	DY	101/110 (91%)	0.93	20 (19%) 1 0	40, 96, 191, 199	0
51	BZ	177/206 (85%)	0.22	4 (2%) 60 31	56, 100, 150, 175	0
51	DZ	177/206 (85%)	0.49	13 (7%) 15 4	63, 103, 153, 179	0
All	All	20064/20922 (95%)	0.64	2290 (11%) 5 1	22, 84, 190, 201	0

The worst 5 of 2290 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BF	208	GLY	23.7
42	BQ	140	ALA	18.8
38	DI	100	ALA	18.7
42	DQ	140	ALA	17.0
1	AA	88	A	16.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
52	MG	DA	3309	1/1	0.36	0.17	66,66,66,66	0
52	MG	DA	3232	1/1	0.48	0.87	63,63,63,63	0
52	MG	BA	3362	1/1	0.48	0.38	50,50,50,50	0
52	MG	AA	1643	1/1	0.49	1.02	66,66,66,66	0
52	MG	DA	3124	1/1	0.56	0.29	49,49,49,49	0
52	MG	DA	3297	1/1	0.56	0.51	55,55,55,55	0
52	MG	DA	3310	1/1	0.59	0.45	56,56,56,56	0
52	MG	DA	3133	1/1	0.62	0.12	55,55,55,55	0
52	MG	BA	3128	1/1	0.62	0.91	45,45,45,45	0
52	MG	BA	3349	1/1	0.62	0.78	65,65,65,65	0
52	MG	AA	1654	1/1	0.63	0.83	64,64,64,64	0
52	MG	BA	3167	1/1	0.65	0.54	51,51,51,51	0
52	MG	BA	3175	1/1	0.65	0.64	43,43,43,43	0
52	MG	BA	3098	1/1	0.66	0.34	59,59,59,59	0
52	MG	BF	301	1/1	0.66	0.40	43,43,43,43	0
52	MG	AA	1635	1/1	0.66	0.14	53,53,53,53	0
52	MG	BA	3072	1/1	0.66	0.56	41,41,41,41	0
52	MG	DA	3305	1/1	0.67	0.99	46,46,46,46	0
52	MG	DA	3236	1/1	0.67	0.57	71,71,71,71	0
52	MG	BA	3150	1/1	0.69	0.43	40,40,40,40	0
52	MG	DA	3074	1/1	0.69	0.59	54,54,54,54	0
52	MG	BA	3088	1/1	0.69	0.40	33,33,33,33	0
52	MG	DA	3167	1/1	0.70	0.26	63,63,63,63	0
52	MG	AA	1604	1/1	0.70	0.32	62,62,62,62	0
52	MG	BA	3151	1/1	0.71	0.39	47,47,47,47	0
52	MG	BA	3346	1/1	0.71	0.12	63,63,63,63	0
52	MG	DA	3280	1/1	0.71	0.42	70,70,70,70	0
52	MG	BA	3313	1/1	0.72	0.66	56,56,56,56	0
52	MG	CA	1626	1/1	0.72	0.48	68,68,68,68	0
52	MG	BA	3007	1/1	0.72	0.70	40,40,40,40	0
52	MG	BA	3271	1/1	0.72	0.16	53,53,53,53	0
52	MG	DA	3303	1/1	0.72	0.28	43,43,43,43	0
52	MG	DA	3252	1/1	0.73	0.47	57,57,57,57	0
52	MG	BA	3292	1/1	0.73	0.14	41,41,41,41	0
52	MG	DA	3295	1/1	0.73	0.65	73,73,73,73	0
52	MG	DA	3243	1/1	0.73	0.52	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	AA	1649	1/1	0.73	0.26	76,76,76,76	0
52	MG	DA	3290	1/1	0.73	0.55	55,55,55,55	0
52	MG	BA	3171	1/1	0.73	0.77	35,35,35,35	0
52	MG	BA	3363	1/1	0.74	0.20	54,54,54,54	0
52	MG	BA	3154	1/1	0.74	0.37	77,77,77,77	0
52	MG	DA	3328	1/1	0.74	0.52	61,61,61,61	0
52	MG	DA	3166	1/1	0.74	0.62	64,64,64,64	0
52	MG	CA	1608	1/1	0.74	0.33	68,68,68,68	0
52	MG	BA	3203	1/1	0.75	0.13	47,47,47,47	0
52	MG	BA	3307	1/1	0.75	0.36	38,38,38,38	0
52	MG	BA	3131	1/1	0.75	0.52	45,45,45,45	0
52	MG	BA	3247	1/1	0.75	0.56	35,35,35,35	0
52	MG	DA	3331	1/1	0.76	0.15	67,67,67,67	0
52	MG	BA	3141	1/1	0.76	0.18	47,47,47,47	0
52	MG	BA	3180	1/1	0.76	0.64	46,46,46,46	0
52	MG	BA	3336	1/1	0.76	0.34	49,49,49,49	0
52	MG	DA	3153	1/1	0.77	0.77	73,73,73,73	0
52	MG	DA	3184	1/1	0.77	0.29	32,32,32,32	0
52	MG	DA	3187	1/1	0.77	0.57	44,44,44,44	0
52	MG	AA	1644	1/1	0.77	0.41	68,68,68,68	0
52	MG	BA	3361	1/1	0.77	0.33	52,52,52,52	0
52	MG	AA	1637	1/1	0.77	0.69	51,51,51,51	0
52	MG	AA	1611	1/1	0.77	0.17	72,72,72,72	0
52	MG	DA	3195	1/1	0.77	0.48	36,36,36,36	0
52	MG	DA	3281	1/1	0.77	0.81	63,63,63,63	0
52	MG	BA	3355	1/1	0.77	0.85	51,51,51,51	0
52	MG	BA	3159	1/1	0.77	0.70	52,52,52,52	0
52	MG	DA	3283	1/1	0.78	0.65	52,52,52,52	0
52	MG	BA	3176	1/1	0.78	0.42	58,58,58,58	0
52	MG	DA	3201	1/1	0.78	0.23	43,43,43,43	0
52	MG	DA	3249	1/1	0.78	0.23	48,48,48,48	0
52	MG	CA	1630	1/1	0.78	0.62	66,66,66,66	0
52	MG	DA	3274	1/1	0.78	0.42	71,71,71,71	0
52	MG	DA	3289	1/1	0.78	0.45	53,53,53,53	0
52	MG	BA	3181	1/1	0.78	0.15	32,32,32,32	0
52	MG	DA	3322	1/1	0.78	0.39	45,45,45,45	0
52	MG	DA	3264	1/1	0.78	0.26	58,58,58,58	0
52	MG	BA	3113	1/1	0.78	0.21	26,26,26,26	0
52	MG	BA	3291	1/1	0.78	0.21	54,54,54,54	0
52	MG	DA	3325	1/1	0.79	0.56	46,46,46,46	0
52	MG	BA	3074	1/1	0.79	0.50	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3351	1/1	0.79	0.30	48,48,48,48	0
52	MG	BA	3358	1/1	0.79	0.50	59,59,59,59	0
52	MG	CA	1638	1/1	0.79	1.28	64,64,64,64	0
52	MG	DA	3208	1/1	0.79	0.57	34,34,34,34	0
52	MG	DA	3271	1/1	0.79	0.56	56,56,56,56	0
52	MG	BA	3330	1/1	0.79	0.55	48,48,48,48	0
52	MG	DA	3106	1/1	0.79	0.91	53,53,53,53	0
52	MG	BA	3337	1/1	0.79	0.47	32,32,32,32	0
52	MG	DA	3180	1/1	0.79	0.50	38,38,38,38	0
52	MG	DA	3149	1/1	0.79	0.58	54,54,54,54	0
52	MG	BA	3246	1/1	0.79	0.37	40,40,40,40	0
52	MG	DA	3159	1/1	0.79	0.24	40,40,40,40	0
52	MG	DU	201	1/1	0.79	0.47	60,60,60,60	0
52	MG	DA	3025	1/1	0.79	0.44	46,46,46,46	0
52	MG	AA	1656	1/1	0.80	0.17	62,62,62,62	0
52	MG	BA	3259	1/1	0.80	0.41	40,40,40,40	0
52	MG	DA	3075	1/1	0.80	0.45	38,38,38,38	0
52	MG	DA	3225	1/1	0.80	0.20	37,37,37,37	0
52	MG	DA	3304	1/1	0.80	0.79	63,63,63,63	0
52	MG	CA	1627	1/1	0.80	0.75	81,81,81,81	0
52	MG	DA	3221	1/1	0.80	0.68	43,43,43,43	0
52	MG	DA	3267	1/1	0.80	0.45	46,46,46,46	0
52	MG	DA	3298	1/1	0.80	0.64	59,59,59,59	0
52	MG	BA	3215	1/1	0.80	0.20	10,10,10,10	0
52	MG	BA	3282	1/1	0.80	0.59	46,46,46,46	0
52	MG	BA	3289	1/1	0.80	0.27	44,44,44,44	0
52	MG	BA	3237	1/1	0.80	0.50	42,42,42,42	0
52	MG	BA	3116	1/1	0.81	0.11	41,41,41,41	0
52	MG	BA	3127	1/1	0.81	0.50	44,44,44,44	0
52	MG	DA	3293	1/1	0.81	0.74	54,54,54,54	0
52	MG	DA	3123	1/1	0.81	0.22	38,38,38,38	0
52	MG	CA	1625	1/1	0.81	0.56	59,59,59,59	0
52	MG	BA	3234	1/1	0.81	0.19	16,16,16,16	0
52	MG	DA	3173	1/1	0.81	0.77	57,57,57,57	0
52	MG	DA	3329	1/1	0.81	0.34	51,51,51,51	0
52	MG	DA	3222	1/1	0.81	0.52	41,41,41,41	0
52	MG	CA	1642	1/1	0.81	1.23	71,71,71,71	0
52	MG	DA	3245	1/1	0.81	0.19	65,65,65,65	0
52	MG	BA	3326	1/1	0.82	0.43	40,40,40,40	0
52	MG	BA	3198	1/1	0.82	0.89	62,62,62,62	0
52	MG	DA	3009	1/1	0.82	0.43	47,47,47,47	0
52	MG	CA	1611	1/1	0.82	0.84	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	CLM	DA	3334	20/20	0.82	0.50	90,90,90,90	0
52	MG	BA	3323	1/1	0.82	0.63	42,42,42,42	0
52	MG	DA	3265	1/1	0.82	0.14	38,38,38,38	0
52	MG	DA	3263	1/1	0.82	0.29	65,65,65,65	0
52	MG	BA	3062	1/1	0.82	0.17	30,30,30,30	0
52	MG	BA	3009	1/1	0.82	0.55	38,38,38,38	0
52	MG	AA	1612	1/1	0.82	0.59	56,56,56,56	0
52	MG	BA	3360	1/1	0.82	0.51	48,48,48,48	0
52	MG	CA	1649	1/1	0.82	0.36	55,55,55,55	0
52	MG	DA	3287	1/1	0.82	1.20	61,61,61,61	0
52	MG	DA	3054	1/1	0.82	0.28	55,55,55,55	0
52	MG	DA	3175	1/1	0.82	0.48	51,51,51,51	0
52	MG	BA	3094	1/1	0.82	0.57	30,30,30,30	0
52	MG	DA	3170	1/1	0.82	0.15	42,42,42,42	0
52	MG	AA	1638	1/1	0.82	0.52	69,69,69,69	0
52	MG	BA	3093	1/1	0.82	1.00	50,50,50,50	0
52	MG	DA	3090	1/1	0.82	0.34	33,33,33,33	0
52	MG	BA	3274	1/1	0.83	0.46	33,33,33,33	0
52	MG	BA	3338	1/1	0.83	0.38	50,50,50,50	0
52	MG	BA	3320	1/1	0.83	1.17	52,52,52,52	0
52	MG	AA	1624	1/1	0.83	0.49	59,59,59,59	0
52	MG	BB	203	1/1	0.83	0.11	55,55,55,55	0
52	MG	DA	3278	1/1	0.83	0.52	54,54,54,54	0
52	MG	BA	3238	1/1	0.83	0.77	43,43,43,43	0
52	MG	DA	3312	1/1	0.83	0.59	45,45,45,45	0
52	MG	BA	3305	1/1	0.83	0.27	54,54,54,54	0
52	MG	AA	1620	1/1	0.83	0.61	52,52,52,52	0
52	MG	BA	3278	1/1	0.83	0.16	31,31,31,31	0
52	MG	DA	3206	1/1	0.83	0.64	45,45,45,45	0
52	MG	AA	1629	1/1	0.83	0.34	49,49,49,49	0
52	MG	BA	3350	1/1	0.83	0.38	54,54,54,54	0
52	MG	CA	1610	1/1	0.83	0.27	66,66,66,66	0
52	MG	DA	3137	1/1	0.83	0.17	69,69,69,69	0
52	MG	AA	1613	1/1	0.83	0.29	62,62,62,62	0
52	MG	BA	3318	1/1	0.83	0.38	34,34,34,34	0
52	MG	DA	3327	1/1	0.83	0.14	41,41,41,41	0
52	MG	DA	3085	1/1	0.83	0.17	19,19,19,19	0
52	MG	BA	3056	1/1	0.83	0.16	20,20,20,20	0
52	MG	DA	3270	1/1	0.84	0.43	55,55,55,55	0
52	MG	DA	3127	1/1	0.84	0.21	33,33,33,33	0
52	MG	DX	101	1/1	0.84	0.25	45,45,45,45	0
52	MG	BA	3207	1/1	0.84	0.72	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	AA	1632	1/1	0.84	0.65	51,51,51,51	0
54	K	DA	3333	1/1	0.84	0.30	62,62,62,62	0
52	MG	BA	3345	1/1	0.84	0.25	43,43,43,43	0
52	MG	BA	3221	1/1	0.84	0.25	31,31,31,31	0
52	MG	DA	3029	1/1	0.84	0.23	43,43,43,43	0
52	MG	DA	3101	1/1	0.84	0.33	34,34,34,34	0
52	MG	DA	3165	1/1	0.84	0.28	38,38,38,38	0
52	MG	BP	201	1/1	0.84	0.56	35,35,35,35	0
52	MG	DA	3234	1/1	0.84	0.72	60,60,60,60	0
52	MG	BA	3075	1/1	0.84	0.47	38,38,38,38	0
52	MG	AA	1630	1/1	0.84	0.53	49,49,49,49	0
52	MG	DA	3257	1/1	0.84	0.36	46,46,46,46	0
52	MG	BA	3276	1/1	0.84	0.36	35,35,35,35	0
52	MG	DA	3072	1/1	0.84	0.89	71,71,71,71	0
52	MG	DB	201	1/1	0.84	0.46	57,57,57,57	0
52	MG	BA	3300	1/1	0.84	0.41	45,45,45,45	0
52	MG	DA	3259	1/1	0.84	0.51	79,79,79,79	0
52	MG	BA	3359	1/1	0.84	0.58	39,39,39,39	0
52	MG	DB	204	1/1	0.84	0.47	37,37,37,37	0
52	MG	BA	3139	1/1	0.84	0.68	30,30,30,30	0
52	MG	DA	3214	1/1	0.85	0.43	39,39,39,39	0
52	MG	CA	1628	1/1	0.85	0.63	50,50,50,50	0
52	MG	DF	301	1/1	0.85	0.41	53,53,53,53	0
52	MG	BA	3229	1/1	0.85	0.36	26,26,26,26	0
52	MG	DA	3177	1/1	0.85	0.41	37,37,37,37	0
52	MG	CA	1606	1/1	0.85	0.86	52,52,52,52	0
52	MG	DA	3047	1/1	0.85	0.55	33,33,33,33	0
52	MG	BA	3248	1/1	0.85	0.35	33,33,33,33	0
52	MG	BA	3365	1/1	0.85	0.36	43,43,43,43	0
52	MG	BA	3209	1/1	0.85	0.39	36,36,36,36	0
52	MG	BA	3249	1/1	0.85	0.33	54,54,54,54	0
52	MG	DD	301	1/1	0.85	0.44	32,32,32,32	0
52	MG	AA	1651	1/1	0.85	0.32	45,45,45,45	0
52	MG	BA	3356	1/1	0.85	0.08	60,60,60,60	0
52	MG	BA	3118	1/1	0.85	0.20	38,38,38,38	0
52	MG	DA	3239	1/1	0.85	0.78	41,41,41,41	0
52	MG	DA	3210	1/1	0.85	0.23	46,46,46,46	0
52	MG	BA	3199	1/1	0.85	0.40	42,42,42,42	0
52	MG	CA	1631	1/1	0.85	0.08	71,71,71,71	0
52	MG	BA	3255	1/1	0.85	0.44	54,54,54,54	0
52	MG	DQ	201	1/1	0.85	0.36	42,42,42,42	0
52	MG	CA	1614	1/1	0.86	0.63	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3105	1/1	0.86	0.20	39,39,39,39	0
52	MG	BA	3258	1/1	0.86	0.24	21,21,21,21	0
52	MG	BA	3325	1/1	0.86	0.63	53,53,53,53	0
52	MG	DA	3164	1/1	0.86	0.56	41,41,41,41	0
52	MG	BA	3115	1/1	0.86	0.44	34,34,34,34	0
52	MG	DA	3126	1/1	0.86	0.16	36,36,36,36	0
52	MG	CA	1637	1/1	0.86	0.35	65,65,65,65	0
52	MG	DA	3216	1/1	0.86	0.56	45,45,45,45	0
52	MG	BA	3003	1/1	0.86	0.80	44,44,44,44	0
52	MG	BA	3279	1/1	0.86	0.36	39,39,39,39	0
52	MG	DA	3132	1/1	0.86	0.77	53,53,53,53	0
52	MG	DA	3156	1/1	0.86	0.35	51,51,51,51	0
52	MG	BA	3240	1/1	0.86	0.38	50,50,50,50	0
52	MG	BA	3367	1/1	0.86	0.10	47,47,47,47	0
52	MG	BA	3314	1/1	0.86	0.50	41,41,41,41	0
52	MG	BA	3368	1/1	0.86	0.07	60,60,60,60	0
52	MG	BA	3366	1/1	0.86	0.14	52,52,52,52	0
52	MG	AA	1646	1/1	0.86	0.12	48,48,48,48	0
52	MG	DA	3302	1/1	0.86	0.24	39,39,39,39	0
52	MG	BR	202	1/1	0.86	0.68	31,31,31,31	0
52	MG	AA	1648	1/1	0.86	1.32	80,80,80,80	0
52	MG	BA	3243	1/1	0.86	0.20	30,30,30,30	0
52	MG	BA	3347	1/1	0.86	0.43	47,47,47,47	0
52	MG	D5	102	1/1	0.86	0.51	58,58,58,58	0
52	MG	BA	3111	1/1	0.87	0.55	41,41,41,41	0
52	MG	BA	3317	1/1	0.87	0.36	53,53,53,53	0
52	MG	BA	3160	1/1	0.87	0.58	41,41,41,41	0
52	MG	BA	3352	1/1	0.87	0.27	51,51,51,51	0
52	MG	DA	3055	1/1	0.87	0.52	34,34,34,34	0
52	MG	DA	3136	1/1	0.87	0.36	48,48,48,48	0
52	MG	BA	3331	1/1	0.87	0.53	37,37,37,37	0
52	MG	BA	3286	1/1	0.87	0.51	44,44,44,44	0
52	MG	CA	1604	1/1	0.87	0.32	67,67,67,67	0
52	MG	DA	3233	1/1	0.87	0.56	51,51,51,51	0
52	MG	BA	3341	1/1	0.87	0.65	66,66,66,66	0
52	MG	BA	3299	1/1	0.87	0.38	37,37,37,37	0
52	MG	DA	3250	1/1	0.87	0.35	56,56,56,56	0
52	MG	CA	1635	1/1	0.87	0.79	73,73,73,73	0
52	MG	DA	3176	1/1	0.87	0.20	66,66,66,66	0
52	MG	DA	3285	1/1	0.87	0.20	33,33,33,33	0
52	MG	BA	3225	1/1	0.87	0.60	32,32,32,32	0
52	MG	BA	3244	1/1	0.87	0.36	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BQ	202	1/1	0.87	0.35	37,37,37,37	0
52	MG	CA	1652	1/1	0.87	0.15	61,61,61,61	0
52	MG	DA	3115	1/1	0.87	0.27	47,47,47,47	0
52	MG	BA	3049	1/1	0.87	0.56	23,23,23,23	0
52	MG	BA	3364	1/1	0.88	0.35	64,64,64,64	0
52	MG	DA	3332	1/1	0.88	0.15	69,69,69,69	0
52	MG	BA	3112	1/1	0.88	0.25	14,14,14,14	0
52	MG	BA	3124	1/1	0.88	0.43	39,39,39,39	0
52	MG	BA	3205	1/1	0.88	0.50	34,34,34,34	0
52	MG	DA	3306	1/1	0.88	0.44	54,54,54,54	0
52	MG	DA	3299	1/1	0.88	0.18	41,41,41,41	0
52	MG	CA	1622	1/1	0.88	0.45	46,46,46,46	0
52	MG	DA	3007	1/1	0.88	0.49	48,48,48,48	0
52	MG	BA	3332	1/1	0.88	0.41	35,35,35,35	0
52	MG	BA	3250	1/1	0.88	0.70	48,48,48,48	0
52	MG	DA	3006	1/1	0.88	0.58	38,38,38,38	0
52	MG	AA	1652	1/1	0.88	0.73	44,44,44,44	0
52	MG	BA	3148	1/1	0.88	0.48	23,23,23,23	0
52	MG	DA	3021	1/1	0.88	0.35	38,38,38,38	0
52	MG	DA	3086	1/1	0.88	0.20	34,34,34,34	0
52	MG	BA	3296	1/1	0.88	0.07	36,36,36,36	0
52	MG	DA	3103	1/1	0.88	0.56	33,33,33,33	0
52	MG	DA	3116	1/1	0.88	0.28	45,45,45,45	0
52	MG	DA	3118	1/1	0.88	0.33	43,43,43,43	0
52	MG	DA	3014	1/1	0.88	0.40	71,71,71,71	0
52	MG	DA	3326	1/1	0.88	0.22	49,49,49,49	0
52	MG	DA	3110	1/1	0.88	0.22	50,50,50,50	0
52	MG	CA	1645	1/1	0.88	0.35	45,45,45,45	0
52	MG	BB	205	1/1	0.88	0.16	59,59,59,59	0
52	MG	BA	3315	1/1	0.88	0.23	43,43,43,43	0
52	MG	BA	3155	1/1	0.88	0.32	39,39,39,39	0
52	MG	BA	3232	1/1	0.88	0.31	27,27,27,27	0
52	MG	BA	3319	1/1	0.88	0.48	46,46,46,46	0
52	MG	BA	3340	1/1	0.88	0.23	39,39,39,39	0
52	MG	BA	3200	1/1	0.88	0.33	12,12,12,12	0
52	MG	DA	3016	1/1	0.88	0.59	29,29,29,29	0
52	MG	BA	3288	1/1	0.88	0.52	46,46,46,46	0
52	MG	DB	202	1/1	0.88	0.41	60,60,60,60	0
52	MG	DA	3135	1/1	0.88	0.68	39,39,39,39	0
52	MG	BA	3335	1/1	0.88	0.42	57,57,57,57	0
52	MG	BA	3089	1/1	0.88	0.39	15,15,15,15	0
52	MG	BA	3269	1/1	0.89	0.44	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	CA	1633	1/1	0.89	0.87	50,50,50,50	0
52	MG	DA	3211	1/1	0.89	0.90	50,50,50,50	0
52	MG	DA	3065	1/1	0.89	0.19	30,30,30,30	0
52	MG	CA	1613	1/1	0.89	0.35	58,58,58,58	0
52	MG	DA	3277	1/1	0.89	0.17	38,38,38,38	0
52	MG	DA	3235	1/1	0.89	0.28	48,48,48,48	0
52	MG	DA	3220	1/1	0.89	0.21	40,40,40,40	0
52	MG	DA	3262	1/1	0.89	0.71	60,60,60,60	0
52	MG	DA	3215	1/1	0.89	0.28	27,27,27,27	0
52	MG	DA	3260	1/1	0.89	0.48	34,34,34,34	0
52	MG	DA	3301	1/1	0.89	0.20	15,15,15,15	0
52	MG	BA	3161	1/1	0.89	0.27	32,32,32,32	0
52	MG	BA	3026	1/1	0.89	0.39	45,45,45,45	0
52	MG	BA	3322	1/1	0.89	0.50	41,41,41,41	0
52	MG	AA	1622	1/1	0.89	0.47	40,40,40,40	0
52	MG	DA	3001	1/1	0.89	0.43	45,45,45,45	0
52	MG	DA	3272	1/1	0.89	0.47	47,47,47,47	0
52	MG	DA	3242	1/1	0.89	0.33	35,35,35,35	0
52	MG	BA	3354	1/1	0.89	0.39	40,40,40,40	0
52	MG	DA	3276	1/1	0.89	0.85	44,44,44,44	0
52	MG	DA	3061	1/1	0.89	0.42	34,34,34,34	0
52	MG	DA	3223	1/1	0.89	0.62	37,37,37,37	0
52	MG	AA	1650	1/1	0.89	0.56	49,49,49,49	0
52	MG	BA	3277	1/1	0.89	0.34	10,10,10,10	0
52	MG	BA	3097	1/1	0.89	0.41	32,32,32,32	0
52	MG	BA	3196	1/1	0.89	0.40	26,26,26,26	0
52	MG	BA	3025	1/1	0.89	0.27	29,29,29,29	0
52	MG	DA	3193	1/1	0.89	0.74	40,40,40,40	0
52	MG	BA	3321	1/1	0.90	0.31	33,33,33,33	0
52	MG	BA	3177	1/1	0.90	0.87	67,67,67,67	0
52	MG	DA	3313	1/1	0.90	0.67	48,48,48,48	0
52	MG	AA	1641	1/1	0.90	0.22	64,64,64,64	0
55	CLM	BA	3370	20/20	0.90	0.46	90,90,90,90	0
52	MG	CA	1648	1/1	0.90	0.90	53,53,53,53	0
52	MG	DA	3154	1/1	0.90	0.53	51,51,51,51	0
52	MG	BA	3309	1/1	0.90	0.58	49,49,49,49	0
52	MG	BA	3184	1/1	0.90	0.52	40,40,40,40	0
52	MG	BB	201	1/1	0.90	0.54	35,35,35,35	0
52	MG	BA	3204	1/1	0.90	0.26	36,36,36,36	0
52	MG	AA	1631	1/1	0.90	0.62	52,52,52,52	0
52	MG	DA	3316	1/1	0.90	0.21	62,62,62,62	0
52	MG	DA	3008	1/1	0.90	0.40	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	CA	1653	1/1	0.90	0.19	47,47,47,47	0
52	MG	DA	3198	1/1	0.90	0.31	37,37,37,37	0
52	MG	CA	1650	1/1	0.90	0.31	45,45,45,45	0
52	MG	DA	3296	1/1	0.90	0.31	45,45,45,45	0
52	MG	DA	3251	1/1	0.90	0.19	72,72,72,72	0
52	MG	DA	3246	1/1	0.90	0.10	43,43,43,43	0
52	MG	DA	3107	1/1	0.90	0.44	15,15,15,15	0
52	MG	DB	203	1/1	0.90	0.14	73,73,73,73	0
52	MG	DA	3227	1/1	0.90	0.24	47,47,47,47	0
52	MG	DA	3188	1/1	0.90	0.62	43,43,43,43	0
52	MG	BA	3283	1/1	0.90	0.36	50,50,50,50	0
52	MG	BA	3188	1/1	0.90	0.51	36,36,36,36	0
52	MG	CA	1621	1/1	0.90	0.43	50,50,50,50	0
52	MG	BA	3304	1/1	0.90	0.53	49,49,49,49	0
52	MG	DA	3282	1/1	0.90	0.23	61,61,61,61	0
52	MG	DA	3266	1/1	0.90	0.61	45,45,45,45	0
52	MG	BA	3228	1/1	0.90	0.42	27,27,27,27	0
52	MG	DA	3207	1/1	0.90	0.46	54,54,54,54	0
52	MG	DA	3288	1/1	0.90	0.22	42,42,42,42	0
52	MG	CA	1639	1/1	0.91	0.56	50,50,50,50	0
52	MG	DA	3058	1/1	0.91	0.34	42,42,42,42	0
52	MG	BA	3108	1/1	0.91	0.18	31,31,31,31	0
52	MG	DA	3269	1/1	0.91	0.20	61,61,61,61	0
52	MG	DA	3003	1/1	0.91	0.71	39,39,39,39	0
52	MG	BA	3103	1/1	0.91	0.36	27,27,27,27	0
52	MG	DA	3191	1/1	0.91	0.44	38,38,38,38	0
52	MG	DA	3231	1/1	0.91	0.55	54,54,54,54	0
52	MG	BA	3235	1/1	0.91	0.56	38,38,38,38	0
52	MG	DA	3323	1/1	0.91	0.67	62,62,62,62	0
52	MG	BA	3110	1/1	0.91	0.52	27,27,27,27	0
52	MG	BA	3109	1/1	0.91	0.82	40,40,40,40	0
52	MG	AA	1618	1/1	0.91	0.19	53,53,53,53	0
52	MG	BA	3272	1/1	0.91	0.44	36,36,36,36	0
52	MG	BA	3013	1/1	0.91	0.41	7,7,7,7	0
52	MG	BA	3046	1/1	0.91	0.37	24,24,24,24	0
52	MG	DA	3268	1/1	0.91	0.94	63,63,63,63	0
52	MG	DA	3109	1/1	0.91	0.34	48,48,48,48	0
52	MG	BA	3169	1/1	0.91	0.34	33,33,33,33	0
52	MG	DA	3315	1/1	0.91	0.17	43,43,43,43	0
52	MG	DA	3067	1/1	0.91	0.29	35,35,35,35	0
52	MG	CA	1618	1/1	0.91	0.46	58,58,58,58	0
52	MG	BA	3117	1/1	0.91	0.31	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3292	1/1	0.91	0.32	52,52,52,52	0
52	MG	AA	1609	1/1	0.91	0.45	52,52,52,52	0
52	MG	DA	3150	1/1	0.91	0.51	32,32,32,32	0
52	MG	DA	3032	1/1	0.91	0.37	31,31,31,31	0
52	MG	AA	1605	1/1	0.91	0.39	71,71,71,71	0
52	MG	AA	1615	1/1	0.91	0.21	35,35,35,35	0
52	MG	DA	3169	1/1	0.91	0.55	45,45,45,45	0
52	MG	BA	3004	1/1	0.91	0.35	14,14,14,14	0
52	MG	CA	1643	1/1	0.91	0.29	42,42,42,42	0
52	MG	CA	1602	1/1	0.91	0.58	40,40,40,40	0
52	MG	AA	1653	1/1	0.91	0.33	46,46,46,46	0
52	MG	BA	3324	1/1	0.91	0.45	53,53,53,53	0
52	MG	CA	1651	1/1	0.91	0.69	51,51,51,51	0
52	MG	DA	3125	1/1	0.91	0.16	33,33,33,33	0
54	K	BA	3369	1/1	0.91	0.16	41,41,41,41	0
52	MG	DA	3096	1/1	0.91	0.47	61,61,61,61	0
52	MG	AA	1634	1/1	0.91	0.64	51,51,51,51	0
52	MG	BA	3260	1/1	0.91	0.30	13,13,13,13	0
52	MG	CA	1601	1/1	0.91	0.20	61,61,61,61	0
52	MG	DA	3069	1/1	0.91	0.29	63,63,63,63	0
52	MG	DA	3241	1/1	0.91	0.12	54,54,54,54	0
52	MG	BA	3085	1/1	0.91	0.17	9,9,9,9	0
52	MG	BA	3166	1/1	0.91	0.19	27,27,27,27	0
52	MG	BA	3201	1/1	0.91	0.63	31,31,31,31	0
52	MG	BA	3202	1/1	0.91	0.61	35,35,35,35	0
52	MG	DA	3160	1/1	0.91	0.59	51,51,51,51	0
52	MG	BA	3333	1/1	0.91	0.48	50,50,50,50	0
52	MG	BA	3146	1/1	0.91	0.40	33,33,33,33	0
52	MG	CA	1636	1/1	0.91	0.26	77,77,77,77	0
52	MG	DA	3052	1/1	0.91	0.51	36,36,36,36	0
52	MG	AA	1628	1/1	0.91	0.70	70,70,70,70	0
52	MG	AA	1621	1/1	0.91	0.49	37,37,37,37	0
52	MG	BA	3236	1/1	0.92	0.26	31,31,31,31	0
52	MG	BA	3090	1/1	0.92	0.42	14,14,14,14	0
52	MG	BA	3162	1/1	0.92	0.30	45,45,45,45	0
52	MG	BA	3357	1/1	0.92	0.41	44,44,44,44	0
52	MG	DA	3200	1/1	0.92	0.19	37,37,37,37	0
52	MG	DA	3035	1/1	0.92	0.45	31,31,31,31	0
52	MG	DA	3185	1/1	0.92	0.47	49,49,49,49	0
52	MG	DA	3094	1/1	0.92	0.69	38,38,38,38	0
52	MG	CA	1605	1/1	0.92	0.29	68,68,68,68	0
52	MG	AA	1645	1/1	0.92	0.59	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3033	1/1	0.92	0.30	18,18,18,18	0
53	ZN	AN	101	1/1	0.92	0.15	144,144,144,144	0
52	MG	BA	3227	1/1	0.92	0.61	22,22,22,22	0
52	MG	DA	3095	1/1	0.92	0.41	47,47,47,47	0
52	MG	BA	3287	1/1	0.92	0.34	27,27,27,27	0
52	MG	DA	3121	1/1	0.92	0.28	49,49,49,49	0
52	MG	DA	3157	1/1	0.92	0.24	48,48,48,48	0
52	MG	BA	3083	1/1	0.92	0.55	34,34,34,34	0
52	MG	DA	3051	1/1	0.92	0.51	29,29,29,29	0
52	MG	BA	3245	1/1	0.92	0.52	52,52,52,52	0
52	MG	BA	3206	1/1	0.92	0.56	29,29,29,29	0
52	MG	BA	3170	1/1	0.92	0.65	36,36,36,36	0
52	MG	BA	3069	1/1	0.92	0.31	26,26,26,26	0
52	MG	BA	3298	1/1	0.92	0.36	41,41,41,41	0
52	MG	BX	101	1/1	0.92	0.26	21,21,21,21	0
52	MG	DA	3284	1/1	0.92	0.72	49,49,49,49	0
52	MG	BA	3230	1/1	0.92	0.76	37,37,37,37	0
52	MG	DA	3226	1/1	0.92	0.65	55,55,55,55	0
52	MG	BA	3041	1/1	0.92	0.44	24,24,24,24	0
52	MG	DA	3319	1/1	0.92	0.63	55,55,55,55	0
52	MG	CA	1612	1/1	0.92	0.34	48,48,48,48	0
52	MG	BA	3327	1/1	0.92	0.30	48,48,48,48	0
52	MG	DA	3070	1/1	0.92	0.32	35,35,35,35	0
52	MG	BA	3239	1/1	0.92	0.17	32,32,32,32	0
52	MG	DA	3131	1/1	0.92	0.28	55,55,55,55	0
52	MG	DA	3318	1/1	0.92	0.36	43,43,43,43	0
52	MG	BA	3226	1/1	0.92	0.20	14,14,14,14	0
52	MG	DA	3026	1/1	0.92	0.43	55,55,55,55	0
52	MG	BE	301	1/1	0.92	0.49	16,16,16,16	0
52	MG	DA	3330	1/1	0.92	0.28	53,53,53,53	0
52	MG	BA	3312	1/1	0.92	0.20	41,41,41,41	0
52	MG	DA	3049	1/1	0.92	0.55	42,42,42,42	0
52	MG	BA	3241	1/1	0.92	0.18	44,44,44,44	0
52	MG	B1	101	1/1	0.92	0.32	25,25,25,25	0
52	MG	DA	3202	1/1	0.92	0.54	46,46,46,46	0
52	MG	DA	3030	1/1	0.92	0.26	37,37,37,37	0
52	MG	BA	3344	1/1	0.92	0.09	56,56,56,56	0
52	MG	DA	3248	1/1	0.92	0.33	33,33,33,33	0
52	MG	BA	3063	1/1	0.92	0.54	45,45,45,45	0
52	MG	DA	3063	1/1	0.92	0.39	38,38,38,38	0
52	MG	BB	204	1/1	0.92	0.43	41,41,41,41	0
52	MG	DA	3143	1/1	0.92	0.43	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3089	1/1	0.92	0.61	31,31,31,31	0
52	MG	CA	1607	1/1	0.92	0.46	46,46,46,46	0
52	MG	BA	3134	1/1	0.92	0.27	36,36,36,36	0
52	MG	BA	3061	1/1	0.92	0.38	35,35,35,35	0
52	MG	CA	1634	1/1	0.92	0.16	47,47,47,47	0
52	MG	CA	1624	1/1	0.93	0.40	50,50,50,50	0
52	MG	DA	3183	1/1	0.93	0.45	35,35,35,35	0
52	MG	BA	3256	1/1	0.93	0.12	24,24,24,24	0
52	MG	BA	3189	1/1	0.93	0.19	46,46,46,46	0
52	MG	AA	1608	1/1	0.93	0.45	70,70,70,70	0
52	MG	DA	3314	1/1	0.93	0.23	40,40,40,40	0
52	MG	AA	1642	1/1	0.93	0.34	46,46,46,46	0
52	MG	DA	3040	1/1	0.93	0.95	58,58,58,58	0
52	MG	BA	3001	1/1	0.93	0.38	36,36,36,36	0
52	MG	BA	3308	1/1	0.93	0.37	45,45,45,45	0
52	MG	DA	3113	1/1	0.93	0.09	59,59,59,59	0
52	MG	DA	3244	1/1	0.93	0.62	36,36,36,36	0
52	MG	DA	3179	1/1	0.93	0.33	29,29,29,29	0
52	MG	DA	3048	1/1	0.93	0.48	30,30,30,30	0
52	MG	DA	3148	1/1	0.93	0.29	51,51,51,51	0
52	MG	BA	3080	1/1	0.93	0.68	14,14,14,14	0
52	MG	BA	3218	1/1	0.93	0.33	30,30,30,30	0
52	MG	CA	1620	1/1	0.93	0.34	45,45,45,45	0
52	MG	DA	3212	1/1	0.93	0.21	33,33,33,33	0
52	MG	DA	3182	1/1	0.93	0.55	41,41,41,41	0
52	MG	BA	3306	1/1	0.93	0.56	35,35,35,35	0
52	MG	DA	3254	1/1	0.93	0.19	46,46,46,46	0
52	MG	CA	1641	1/1	0.93	0.40	45,45,45,45	0
52	MG	BA	3193	1/1	0.93	0.55	46,46,46,46	0
52	MG	DA	3128	1/1	0.93	0.23	29,29,29,29	0
52	MG	DA	3145	1/1	0.93	0.55	40,40,40,40	0
52	MG	BA	3122	1/1	0.93	0.51	37,37,37,37	0
52	MG	BA	3265	1/1	0.93	0.31	43,43,43,43	0
52	MG	D5	101	1/1	0.93	0.47	30,30,30,30	0
52	MG	DA	3120	1/1	0.93	0.29	36,36,36,36	0
52	MG	BA	3152	1/1	0.93	0.12	49,49,49,49	0
52	MG	DA	3256	1/1	0.93	0.30	46,46,46,46	0
52	MG	DA	3308	1/1	0.93	0.15	43,43,43,43	0
52	MG	AA	1603	1/1	0.93	0.38	43,43,43,43	0
52	MG	DR	201	1/1	0.93	0.45	34,34,34,34	0
52	MG	BA	3263	1/1	0.93	0.17	29,29,29,29	0
52	MG	DA	3027	1/1	0.93	0.60	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3018	1/1	0.93	0.29	27,27,27,27	0
52	MG	DA	3088	1/1	0.93	0.48	40,40,40,40	0
52	MG	BA	3039	1/1	0.93	0.72	37,37,37,37	0
52	MG	D1	101	1/1	0.93	0.34	47,47,47,47	0
52	MG	AA	1639	1/1	0.93	0.35	48,48,48,48	0
52	MG	BA	3329	1/1	0.93	0.33	49,49,49,49	0
52	MG	DA	3286	1/1	0.93	0.43	43,43,43,43	0
52	MG	AA	1636	1/1	0.93	0.52	47,47,47,47	0
52	MG	AA	1626	1/1	0.93	0.44	46,46,46,46	0
52	MG	BA	3104	1/1	0.93	0.19	22,22,22,22	0
52	MG	BP	202	1/1	0.94	0.28	0,0,0,0	0
52	MG	AA	1647	1/1	0.94	0.47	46,46,46,46	0
52	MG	AA	1619	1/1	0.94	0.37	44,44,44,44	0
52	MG	BA	3153	1/1	0.94	0.41	34,34,34,34	0
52	MG	DA	3218	1/1	0.94	0.31	24,24,24,24	0
52	MG	BA	3101	1/1	0.94	0.35	24,24,24,24	0
52	MG	AA	1640	1/1	0.94	0.47	60,60,60,60	0
52	MG	BA	3281	1/1	0.94	0.21	41,41,41,41	0
52	MG	DA	3174	1/1	0.94	0.34	54,54,54,54	0
52	MG	BA	3048	1/1	0.94	0.55	22,22,22,22	0
52	MG	BA	3042	1/1	0.94	0.31	7,7,7,7	0
52	MG	BA	3091	1/1	0.94	0.25	14,14,14,14	0
52	MG	DA	3300	1/1	0.94	0.47	54,54,54,54	0
52	MG	DA	3258	1/1	0.94	0.24	38,38,38,38	0
52	MG	DA	3005	1/1	0.94	0.19	49,49,49,49	0
52	MG	BA	3102	1/1	0.94	0.44	38,38,38,38	0
52	MG	BA	3339	1/1	0.94	0.34	31,31,31,31	0
52	MG	DA	3117	1/1	0.94	0.12	54,54,54,54	0
52	MG	BA	3105	1/1	0.94	0.54	19,19,19,19	0
52	MG	BA	3040	1/1	0.94	0.65	37,37,37,37	0
52	MG	BA	3219	1/1	0.94	0.59	24,24,24,24	0
52	MG	DA	3279	1/1	0.94	0.59	44,44,44,44	0
52	MG	B5	102	1/1	0.94	0.59	44,44,44,44	0
52	MG	DA	3140	1/1	0.94	0.47	42,42,42,42	0
52	MG	AA	1616	1/1	0.94	0.08	57,57,57,57	0
52	MG	BA	3106	1/1	0.94	0.57	37,37,37,37	0
52	MG	BA	3132	1/1	0.94	0.27	15,15,15,15	0
52	MG	BA	3328	1/1	0.94	0.29	27,27,27,27	0
52	MG	DA	3168	1/1	0.94	0.55	32,32,32,32	0
52	MG	BA	3059	1/1	0.94	0.34	25,25,25,25	0
52	MG	DA	3042	1/1	0.94	0.25	29,29,29,29	0
52	MG	BA	3137	1/1	0.94	0.32	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3029	1/1	0.94	0.32	25,25,25,25	0
52	MG	BA	3119	1/1	0.94	0.40	34,34,34,34	0
52	MG	BA	3342	1/1	0.94	1.39	69,69,69,69	0
52	MG	AA	1607	1/1	0.94	0.72	47,47,47,47	0
52	MG	CA	1617	1/1	0.94	0.53	48,48,48,48	0
52	MG	BA	3267	1/1	0.94	0.19	41,41,41,41	0
52	MG	DA	3144	1/1	0.94	0.60	43,43,43,43	0
52	MG	BA	3143	1/1	0.94	0.63	29,29,29,29	0
52	MG	BA	3254	1/1	0.94	0.70	34,34,34,34	0
52	MG	DA	3230	1/1	0.94	0.15	25,25,25,25	0
52	MG	BA	3270	1/1	0.94	0.55	26,26,26,26	0
52	MG	BA	3038	1/1	0.94	0.48	17,17,17,17	0
52	MG	DA	3294	1/1	0.94	0.18	46,46,46,46	0
52	MG	BA	3252	1/1	0.94	0.22	50,50,50,50	0
52	MG	BA	3186	1/1	0.94	0.50	38,38,38,38	0
52	MG	BA	3266	1/1	0.94	0.44	37,37,37,37	0
52	MG	DA	3114	1/1	0.94	0.22	46,46,46,46	0
52	MG	DA	3275	1/1	0.94	0.60	51,51,51,51	0
52	MG	DA	3098	1/1	0.94	0.47	34,34,34,34	0
52	MG	DA	3056	1/1	0.94	0.30	24,24,24,24	0
52	MG	BA	3016	1/1	0.94	0.34	11,11,11,11	0
52	MG	CA	1609	1/1	0.94	0.34	41,41,41,41	0
52	MG	CA	1646	1/1	0.94	0.79	58,58,58,58	0
52	MG	BA	3099	1/1	0.94	0.30	34,34,34,34	0
52	MG	BA	3071	1/1	0.94	0.44	22,22,22,22	0
52	MG	BA	3224	1/1	0.94	0.31	27,27,27,27	0
52	MG	BA	3195	1/1	0.94	0.42	49,49,49,49	0
52	MG	BA	3284	1/1	0.94	0.28	39,39,39,39	0
52	MG	BA	3057	1/1	0.94	0.29	37,37,37,37	0
52	MG	DA	3219	1/1	0.94	0.37	25,25,25,25	0
52	MG	BA	3311	1/1	0.94	0.20	38,38,38,38	0
52	MG	BA	3145	1/1	0.94	0.52	33,33,33,33	0
52	MG	BA	3197	1/1	0.94	0.18	27,27,27,27	0
52	MG	DA	3060	1/1	0.95	0.31	46,46,46,46	0
52	MG	BA	3220	1/1	0.95	0.69	22,22,22,22	0
52	MG	BA	3303	1/1	0.95	0.23	37,37,37,37	0
52	MG	DA	3038	1/1	0.95	0.57	25,25,25,25	0
52	MG	BA	3231	1/1	0.95	0.11	26,26,26,26	0
52	MG	BA	3120	1/1	0.95	0.42	25,25,25,25	0
52	MG	BA	3163	1/1	0.95	0.51	53,53,53,53	0
52	MG	BA	3334	1/1	0.95	0.40	39,39,39,39	0
52	MG	DA	3311	1/1	0.95	0.28	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3324	1/1	0.95	0.17	38,38,38,38	0
52	MG	BA	3316	1/1	0.95	0.36	41,41,41,41	0
52	MG	BA	3157	1/1	0.95	0.44	13,13,13,13	0
52	MG	DA	3002	1/1	0.95	0.48	22,22,22,22	0
52	MG	DA	3057	1/1	0.95	0.32	32,32,32,32	0
52	MG	BA	3280	1/1	0.95	0.40	41,41,41,41	0
52	MG	CA	1615	1/1	0.95	0.39	64,64,64,64	0
52	MG	DA	3129	1/1	0.95	0.32	36,36,36,36	0
52	MG	DP	201	1/1	0.95	0.18	19,19,19,19	0
52	MG	BA	3301	1/1	0.95	0.66	36,36,36,36	0
52	MG	AA	1655	1/1	0.95	0.21	45,45,45,45	0
52	MG	DA	3119	1/1	0.95	0.40	36,36,36,36	0
52	MG	AA	1627	1/1	0.95	0.20	60,60,60,60	0
52	MG	DA	3018	1/1	0.95	0.33	29,29,29,29	0
52	MG	AA	1625	1/1	0.95	0.58	40,40,40,40	0
52	MG	DA	3083	1/1	0.95	0.45	37,37,37,37	0
52	MG	BA	3054	1/1	0.95	0.29	48,48,48,48	0
52	MG	DA	3019	1/1	0.95	0.63	25,25,25,25	0
52	MG	BA	3008	1/1	0.95	0.45	27,27,27,27	0
52	MG	DA	3199	1/1	0.95	0.57	43,43,43,43	0
52	MG	BA	3052	1/1	0.95	0.53	23,23,23,23	0
52	MG	BB	207	1/1	0.95	0.20	58,58,58,58	0
52	MG	DA	3122	1/1	0.95	0.67	40,40,40,40	0
52	MG	CA	1619	1/1	0.95	0.53	40,40,40,40	0
52	MG	CA	1632	1/1	0.95	0.35	56,56,56,56	0
52	MG	DA	3228	1/1	0.95	0.23	38,38,38,38	0
52	MG	BA	3036	1/1	0.95	0.45	8,8,8,8	0
52	MG	DA	3163	1/1	0.95	0.66	30,30,30,30	0
52	MG	BA	3070	1/1	0.95	0.35	24,24,24,24	0
52	MG	BA	3044	1/1	0.95	0.28	9,9,9,9	0
52	MG	DA	3023	1/1	0.95	0.48	27,27,27,27	0
52	MG	DE	301	1/1	0.95	0.43	31,31,31,31	0
52	MG	DA	3112	1/1	0.95	0.44	28,28,28,28	0
52	MG	BA	3144	1/1	0.95	0.60	29,29,29,29	0
52	MG	DA	3291	1/1	0.95	0.20	36,36,36,36	0
52	MG	BA	3158	1/1	0.95	0.35	9,9,9,9	0
52	MG	CA	1629	1/1	0.95	0.16	57,57,57,57	0
52	MG	BA	3140	1/1	0.95	0.54	44,44,44,44	0
52	MG	DA	3139	1/1	0.95	0.83	43,43,43,43	0
52	MG	BA	3348	1/1	0.95	0.26	34,34,34,34	0
52	MG	DA	3080	1/1	0.95	0.82	30,30,30,30	0
52	MG	DA	3147	1/1	0.95	0.26	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3060	1/1	0.95	0.36	31,31,31,31	0
52	MG	BA	3264	1/1	0.95	0.25	11,11,11,11	0
52	MG	DA	3022	1/1	0.95	0.29	38,38,38,38	0
52	MG	BA	3021	1/1	0.95	0.44	19,19,19,19	0
52	MG	B5	101	1/1	0.95	0.39	28,28,28,28	0
52	MG	BA	3223	1/1	0.95	0.43	25,25,25,25	0
52	MG	BA	3217	1/1	0.95	0.35	34,34,34,34	0
52	MG	DA	3224	1/1	0.95	0.61	41,41,41,41	0
52	MG	DA	3013	1/1	0.95	0.46	10,10,10,10	0
52	MG	BA	3064	1/1	0.95	0.48	41,41,41,41	0
52	MG	AA	1610	1/1	0.95	0.21	33,33,33,33	0
52	MG	DA	3146	1/1	0.95	0.34	37,37,37,37	0
52	MG	DA	3192	1/1	0.95	0.65	36,36,36,36	0
52	MG	BA	3293	1/1	0.95	0.36	47,47,47,47	0
52	MG	DA	3152	1/1	0.95	0.40	36,36,36,36	0
52	MG	DA	3197	1/1	0.95	0.47	46,46,46,46	0
52	MG	DA	3050	1/1	0.95	0.34	33,33,33,33	0
52	MG	DA	3161	1/1	0.95	0.15	44,44,44,44	0
52	MG	AA	1617	1/1	0.95	0.52	57,57,57,57	0
52	MG	BA	3076	1/1	0.95	0.24	21,21,21,21	0
52	MG	DA	3237	1/1	0.95	0.26	57,57,57,57	0
52	MG	BA	3023	1/1	0.95	0.39	13,13,13,13	0
52	MG	DA	3213	1/1	0.95	0.42	26,26,26,26	0
52	MG	BA	3147	1/1	0.95	0.57	28,28,28,28	0
52	MG	BA	3182	1/1	0.95	0.49	37,37,37,37	0
52	MG	DA	3204	1/1	0.95	0.30	42,42,42,42	0
52	MG	DA	3099	1/1	0.95	0.63	34,34,34,34	0
52	MG	BA	3022	1/1	0.95	0.36	37,37,37,37	0
52	MG	BA	3130	1/1	0.95	0.13	36,36,36,36	0
52	MG	BA	3165	1/1	0.95	0.30	26,26,26,26	0
52	MG	BA	3027	1/1	0.95	0.49	25,25,25,25	0
52	MG	DA	3273	1/1	0.95	0.28	39,39,39,39	0
52	MG	BA	3285	1/1	0.95	0.42	35,35,35,35	0
52	MG	DA	3010	1/1	0.96	0.36	35,35,35,35	0
52	MG	BA	3190	1/1	0.96	0.55	36,36,36,36	0
52	MG	DA	3240	1/1	0.96	0.18	40,40,40,40	0
52	MG	BA	3034	1/1	0.96	0.23	45,45,45,45	0
52	MG	BA	3014	1/1	0.96	0.54	30,30,30,30	0
52	MG	BA	3290	1/1	0.96	0.28	40,40,40,40	0
52	MG	BA	3082	1/1	0.96	0.33	6,6,6,6	0
52	MG	BA	3257	1/1	0.96	0.22	35,35,35,35	0
52	MG	BA	3066	1/1	0.96	0.44	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3295	1/1	0.96	0.23	35,35,35,35	0
52	MG	DA	3155	1/1	0.96	0.13	41,41,41,41	0
52	MG	DA	3229	1/1	0.96	0.55	36,36,36,36	0
52	MG	DA	3138	1/1	0.96	0.38	31,31,31,31	0
52	MG	DA	3011	1/1	0.96	0.51	27,27,27,27	0
52	MG	DA	3071	1/1	0.96	0.54	31,31,31,31	0
52	MG	BA	3164	1/1	0.96	0.33	33,33,33,33	0
52	MG	BA	3222	1/1	0.96	0.58	20,20,20,20	0
52	MG	BD	301	1/1	0.96	0.43	25,25,25,25	0
52	MG	BA	3185	1/1	0.96	0.27	45,45,45,45	0
52	MG	BA	3172	1/1	0.96	0.53	18,18,18,18	0
53	ZN	CD	301	1/1	0.96	0.28	107,107,107,107	0
52	MG	BA	3030	1/1	0.96	0.26	17,17,17,17	0
52	MG	BA	3253	1/1	0.96	0.30	17,17,17,17	0
52	MG	DA	3041	1/1	0.96	0.34	29,29,29,29	0
52	MG	DA	3004	1/1	0.96	0.25	19,19,19,19	0
52	MG	BB	202	1/1	0.96	0.34	27,27,27,27	0
52	MG	BA	3268	1/1	0.96	0.52	38,38,38,38	0
52	MG	BA	3035	1/1	0.96	0.33	18,18,18,18	0
52	MG	BA	3297	1/1	0.96	0.34	31,31,31,31	0
52	MG	DA	3141	1/1	0.96	0.54	35,35,35,35	0
52	MG	BA	3002	1/1	0.96	0.54	23,23,23,23	0
52	MG	AA	1601	1/1	0.96	0.22	50,50,50,50	0
52	MG	DA	3320	1/1	0.96	0.42	31,31,31,31	0
52	MG	CA	1616	1/1	0.96	0.50	45,45,45,45	0
52	MG	BA	3006	1/1	0.96	0.62	33,33,33,33	0
52	MG	BA	3031	1/1	0.96	0.22	39,39,39,39	0
52	MG	DA	3017	1/1	0.96	0.45	37,37,37,37	0
52	MG	BA	3095	1/1	0.96	0.44	38,38,38,38	0
52	MG	AA	1614	1/1	0.96	0.34	47,47,47,47	0
52	MG	CA	1640	1/1	0.96	0.12	53,53,53,53	0
52	MG	DA	3097	1/1	0.96	0.37	30,30,30,30	0
52	MG	BA	3129	1/1	0.96	0.19	33,33,33,33	0
52	MG	BA	3192	1/1	0.96	0.35	17,17,17,17	0
52	MG	DA	3190	1/1	0.96	0.40	43,43,43,43	0
52	MG	DA	3077	1/1	0.96	0.27	38,38,38,38	0
52	MG	CA	1623	1/1	0.96	0.12	50,50,50,50	0
52	MG	BA	3233	1/1	0.96	0.29	20,20,20,20	0
52	MG	BA	3173	1/1	0.96	0.29	50,50,50,50	0
52	MG	DA	3068	1/1	0.96	0.44	57,57,57,57	0
52	MG	BA	3114	1/1	0.96	0.49	21,21,21,21	0
52	MG	BA	3058	1/1	0.96	0.29	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3108	1/1	0.96	0.47	39,39,39,39	0
52	MG	BA	3136	1/1	0.96	0.50	22,22,22,22	0
52	MG	BA	3212	1/1	0.96	0.33	30,30,30,30	0
52	MG	BA	3211	1/1	0.96	0.29	30,30,30,30	0
52	MG	BA	3020	1/1	0.96	0.35	8,8,8,8	0
52	MG	DA	3261	1/1	0.96	0.06	51,51,51,51	0
52	MG	DA	3028	1/1	0.96	0.33	34,34,34,34	0
52	MG	BA	3343	1/1	0.96	0.55	40,40,40,40	0
52	MG	BA	3065	1/1	0.96	0.29	28,28,28,28	0
52	MG	DA	3024	1/1	0.96	0.40	47,47,47,47	0
52	MG	DA	3045	1/1	0.97	0.40	30,30,30,30	0
52	MG	DA	3087	1/1	0.97	0.12	24,24,24,24	0
52	MG	BA	3138	1/1	0.97	0.38	4,4,4,4	0
52	MG	BR	201	1/1	0.97	0.39	7,7,7,7	0
52	MG	DA	3162	1/1	0.97	0.53	50,50,50,50	0
52	MG	DA	3092	1/1	0.97	0.70	47,47,47,47	0
52	MG	BA	3068	1/1	0.97	0.60	35,35,35,35	0
52	MG	DA	3033	1/1	0.97	0.29	31,31,31,31	0
52	MG	BA	3174	1/1	0.97	0.48	29,29,29,29	0
52	MG	DA	3062	1/1	0.97	0.16	24,24,24,24	0
52	MG	BA	3216	1/1	0.97	0.53	35,35,35,35	0
52	MG	DA	3151	1/1	0.97	0.44	40,40,40,40	0
52	MG	BA	3067	1/1	0.97	0.57	28,28,28,28	0
52	MG	BA	3242	1/1	0.97	0.40	33,33,33,33	0
52	MG	DA	3178	1/1	0.97	0.41	30,30,30,30	0
52	MG	BA	3142	1/1	0.97	0.41	26,26,26,26	0
52	MG	AA	1606	1/1	0.97	0.60	86,86,86,86	0
52	MG	BA	3353	1/1	0.97	0.12	31,31,31,31	0
52	MG	DA	3307	1/1	0.97	0.32	42,42,42,42	0
52	MG	BA	3125	1/1	0.97	0.53	18,18,18,18	0
52	MG	BA	3053	1/1	0.97	0.44	6,6,6,6	0
52	MG	BA	3126	1/1	0.97	0.21	29,29,29,29	0
52	MG	BA	3123	1/1	0.97	0.38	40,40,40,40	0
52	MG	BA	3019	1/1	0.97	0.58	13,13,13,13	0
52	MG	DA	3217	1/1	0.97	0.13	36,36,36,36	0
52	MG	BA	3179	1/1	0.97	0.46	25,25,25,25	0
52	MG	BU	201	1/1	0.97	0.36	25,25,25,25	0
52	MG	DA	3134	1/1	0.97	0.54	28,28,28,28	0
52	MG	DA	3039	1/1	0.97	0.53	48,48,48,48	0
52	MG	DA	3036	1/1	0.97	0.46	12,12,12,12	0
52	MG	BA	3262	1/1	0.97	0.15	30,30,30,30	0
52	MG	DA	3255	1/1	0.97	0.45	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3081	1/1	0.97	0.56	24,24,24,24	0
52	MG	BA	3010	1/1	0.97	0.40	37,37,37,37	0
52	MG	BA	3050	1/1	0.97	0.31	21,21,21,21	0
52	MG	BA	3294	1/1	0.97	0.56	40,40,40,40	0
52	MG	BA	3210	1/1	0.97	0.51	29,29,29,29	0
52	MG	DA	3044	1/1	0.97	0.36	35,35,35,35	0
52	MG	DA	3076	1/1	0.97	0.24	23,23,23,23	0
52	MG	BA	3015	1/1	0.97	0.36	29,29,29,29	0
52	MG	CA	1647	1/1	0.97	0.28	49,49,49,49	0
52	MG	DA	3130	1/1	0.97	0.20	53,53,53,53	0
52	MG	DA	3043	1/1	0.97	0.25	49,49,49,49	0
52	MG	BA	3077	1/1	0.97	0.28	20,20,20,20	0
52	MG	BA	3156	1/1	0.97	0.49	12,12,12,12	0
52	MG	BA	3047	1/1	0.97	0.56	22,22,22,22	0
52	MG	DA	3186	1/1	0.97	0.25	42,42,42,42	0
52	MG	DA	3172	1/1	0.97	0.32	48,48,48,48	0
52	MG	BA	3251	1/1	0.97	0.17	40,40,40,40	0
52	MG	BA	3073	1/1	0.97	0.28	7,7,7,7	0
52	MG	BA	3107	1/1	0.97	0.25	7,7,7,7	0
52	MG	BA	3086	1/1	0.97	0.35	27,27,27,27	0
52	MG	BA	3168	1/1	0.97	0.45	21,21,21,21	0
52	MG	BA	3096	1/1	0.97	0.43	16,16,16,16	0
52	MG	BA	3178	1/1	0.97	0.28	32,32,32,32	0
52	MG	CA	1644	1/1	0.97	0.25	43,43,43,43	0
52	MG	DA	3181	1/1	0.97	0.67	29,29,29,29	0
52	MG	BA	3187	1/1	0.97	0.61	33,33,33,33	0
52	MG	BA	3261	1/1	0.97	0.26	27,27,27,27	0
52	MG	DA	3059	1/1	0.97	0.41	24,24,24,24	0
52	MG	DA	3196	1/1	0.97	0.48	33,33,33,33	0
52	MG	DA	3194	1/1	0.97	0.35	22,22,22,22	0
52	MG	BA	3012	1/1	0.97	0.47	38,38,38,38	0
52	MG	BA	3214	1/1	0.97	0.20	23,23,23,23	0
52	MG	BA	3011	1/1	0.97	0.47	17,17,17,17	0
52	MG	BA	3087	1/1	0.97	0.20	10,10,10,10	0
52	MG	BA	3135	1/1	0.97	0.24	30,30,30,30	0
52	MG	BA	3208	1/1	0.97	0.32	17,17,17,17	0
52	MG	BB	206	1/1	0.97	0.74	48,48,48,48	0
52	MG	DA	3082	1/1	0.97	0.48	44,44,44,44	0
52	MG	DA	3015	1/1	0.97	0.39	52,52,52,52	0
52	MG	BA	3051	1/1	0.98	0.50	19,19,19,19	0
52	MG	BA	3191	1/1	0.98	0.42	19,19,19,19	0
52	MG	DA	3142	1/1	0.98	0.57	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3238	1/1	0.98	0.30	36,36,36,36	0
52	MG	DA	3031	1/1	0.98	0.17	51,51,51,51	0
52	MG	DA	3205	1/1	0.98	0.70	39,39,39,39	0
52	MG	DA	3084	1/1	0.98	0.45	31,31,31,31	0
52	MG	DA	3111	1/1	0.98	0.63	39,39,39,39	0
52	MG	BA	3149	1/1	0.98	0.19	8,8,8,8	0
52	MG	BA	3079	1/1	0.98	0.24	36,36,36,36	0
52	MG	DA	3034	1/1	0.98	0.37	38,38,38,38	0
52	MG	DA	3053	1/1	0.98	0.46	21,21,21,21	0
52	MG	BA	3055	1/1	0.98	0.41	19,19,19,19	0
52	MG	AA	1633	1/1	0.98	0.10	42,42,42,42	0
52	MG	DA	3104	1/1	0.98	0.43	41,41,41,41	0
52	MG	BA	3092	1/1	0.98	0.50	19,19,19,19	0
52	MG	CA	1603	1/1	0.98	0.42	32,32,32,32	0
52	MG	DA	3317	1/1	0.98	0.06	48,48,48,48	0
53	ZN	CN	101	1/1	0.98	0.16	136,136,136,136	0
52	MG	DA	3100	1/1	0.98	0.48	35,35,35,35	0
52	MG	DA	3079	1/1	0.98	0.22	36,36,36,36	0
52	MG	DA	3093	1/1	0.98	0.48	44,44,44,44	0
52	MG	DA	3046	1/1	0.98	0.51	34,34,34,34	0
52	MG	BQ	201	1/1	0.98	0.22	18,18,18,18	0
52	MG	BA	3005	1/1	0.98	0.36	26,26,26,26	0
52	MG	BA	3302	1/1	0.98	0.72	31,31,31,31	0
52	MG	DA	3253	1/1	0.98	0.59	32,32,32,32	0
52	MG	AA	1602	1/1	0.98	0.56	32,32,32,32	0
52	MG	BA	3275	1/1	0.98	0.46	29,29,29,29	0
52	MG	BA	3183	1/1	0.98	0.39	43,43,43,43	0
52	MG	DA	3073	1/1	0.98	0.30	27,27,27,27	0
52	MG	DA	3066	1/1	0.98	0.42	29,29,29,29	0
52	MG	DA	3203	1/1	0.98	0.32	38,38,38,38	0
52	MG	DA	3020	1/1	0.98	0.60	33,33,33,33	0
52	MG	DA	3209	1/1	0.98	0.40	51,51,51,51	0
52	MG	DA	3091	1/1	0.98	0.43	11,11,11,11	0
52	MG	BA	3310	1/1	0.98	0.52	31,31,31,31	0
52	MG	DA	3189	1/1	0.98	0.14	42,42,42,42	0
52	MG	DA	3102	1/1	0.98	0.55	24,24,24,24	0
52	MG	BA	3100	1/1	0.98	0.39	23,23,23,23	0
52	MG	BA	3037	1/1	0.98	0.50	1,1,1,1	0
52	MG	DA	3037	1/1	0.98	0.76	33,33,33,33	0
52	MG	BA	3032	1/1	0.98	0.34	15,15,15,15	0
52	MG	BA	3213	1/1	0.98	0.47	17,17,17,17	0
52	MG	AA	1623	1/1	0.98	0.46	31,31,31,31	0

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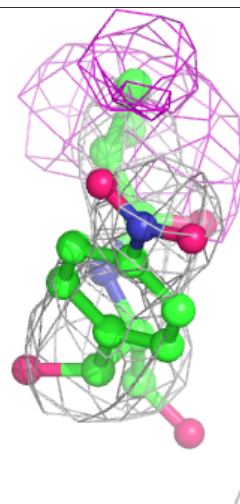
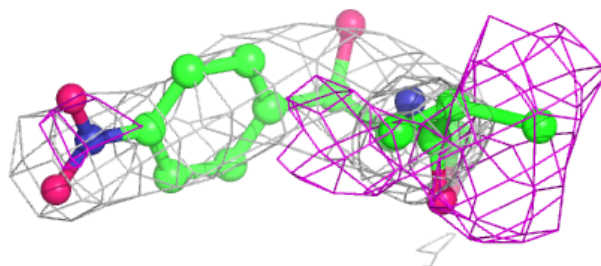
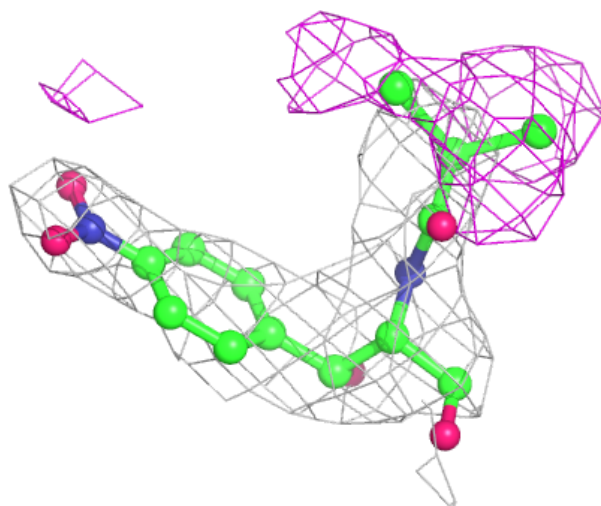
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3012	1/1	0.98	0.48	26,26,26,26	0
52	MG	BA	3121	1/1	0.98	0.27	34,34,34,34	0
52	MG	BA	3078	1/1	0.98	0.45	22,22,22,22	0
52	MG	DA	3158	1/1	0.98	0.31	33,33,33,33	0
52	MG	BA	3028	1/1	0.98	0.48	24,24,24,24	0
52	MG	BA	3024	1/1	0.99	0.33	20,20,20,20	0
52	MG	BA	3045	1/1	0.99	0.41	14,14,14,14	0
52	MG	DA	3171	1/1	0.99	0.35	26,26,26,26	0
52	MG	BA	3043	1/1	0.99	0.18	32,32,32,32	0
52	MG	DA	3321	1/1	0.99	0.07	41,41,41,41	0
52	MG	DA	3078	1/1	0.99	0.50	31,31,31,31	0
53	ZN	AD	301	1/1	0.99	0.28	109,109,109,109	0
52	MG	BA	3081	1/1	0.99	0.43	7,7,7,7	0
52	MG	DA	3064	1/1	0.99	0.51	44,44,44,44	0
52	MG	BA	3084	1/1	0.99	0.37	5,5,5,5	0
52	MG	BA	3273	1/1	0.99	0.20	3,3,3,3	0
52	MG	DA	3247	1/1	0.99	0.15	37,37,37,37	0
52	MG	BA	3017	1/1	0.99	0.46	27,27,27,27	0
52	MG	BA	3194	1/1	0.99	0.50	30,30,30,30	0
52	MG	BA	3133	1/1	0.99	0.31	25,25,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

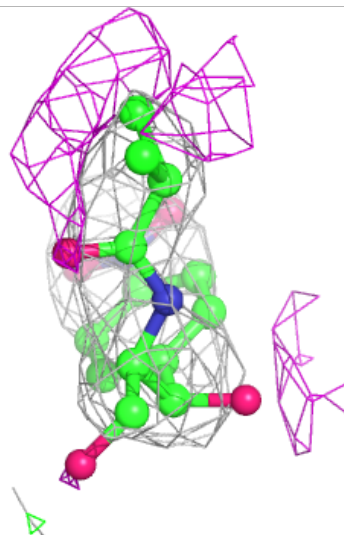
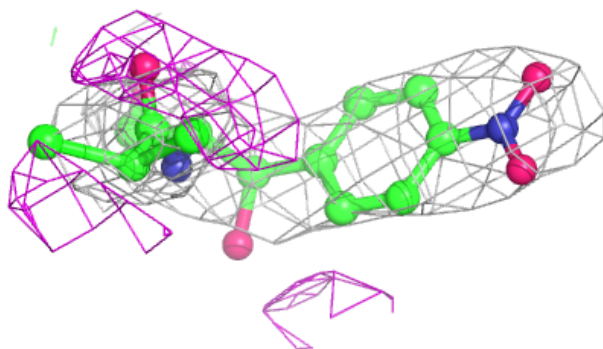
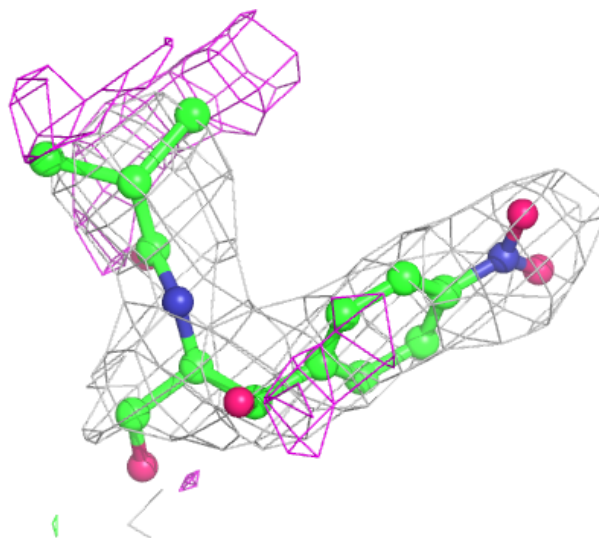
Electron density around CLM DA 3334:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLM BA 3370:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.