



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 22, 2024 – 11:07 PM EDT

PDB ID : 4V7Z
Title : Structure of the *Thermus thermophilus* 70S ribosome complexed with telithromycin.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-18
Resolution : 3.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

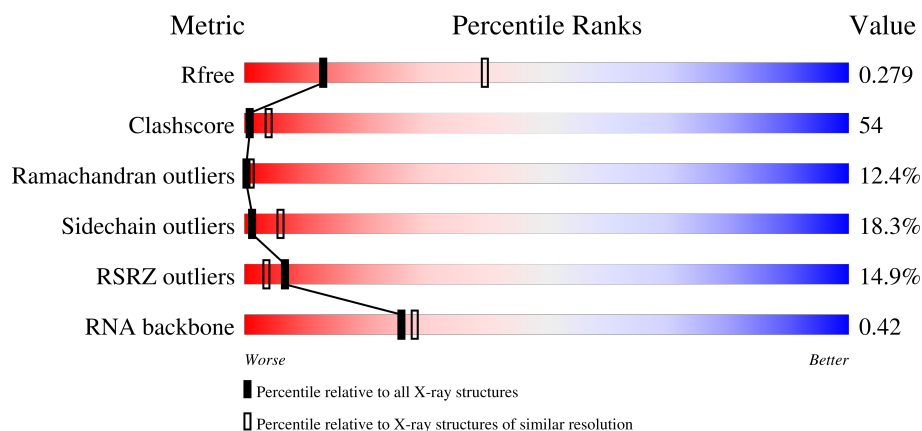
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

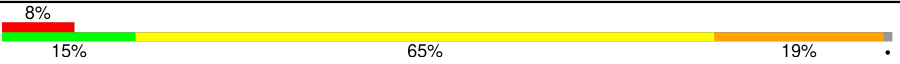
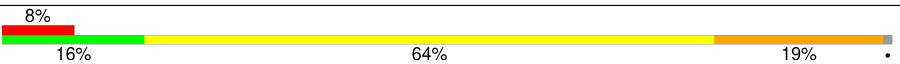
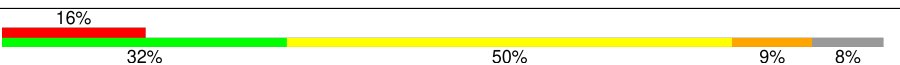
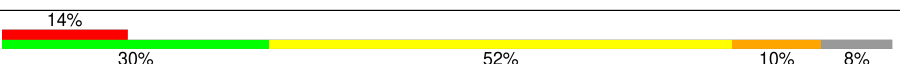
The reported resolution of this entry is 3.10 Å.

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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)
RNA backbone	3690	1021 (3.36-2.84)

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 of 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	
1	CA	1522	
2	AB	256	
2	CB	256	

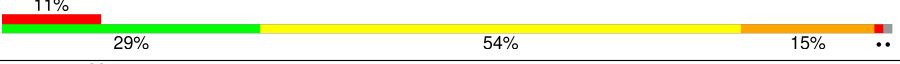
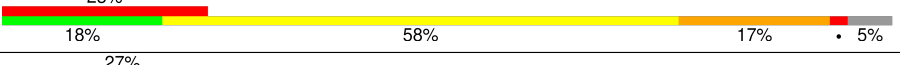
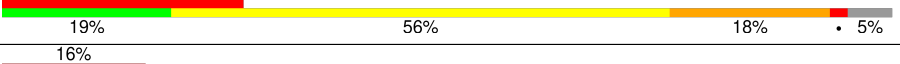
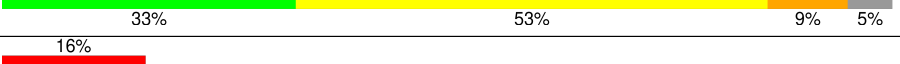
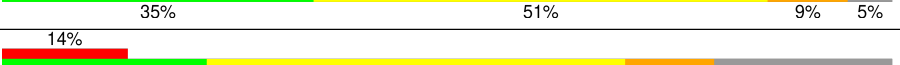
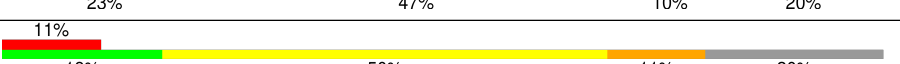
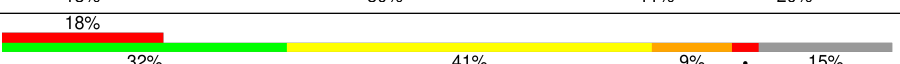
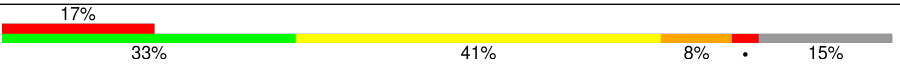
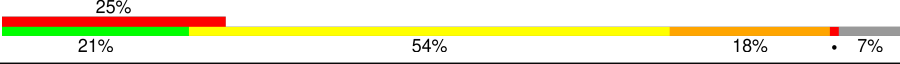
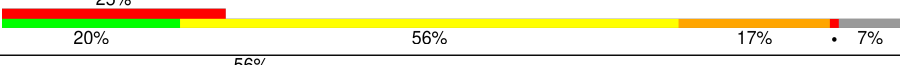



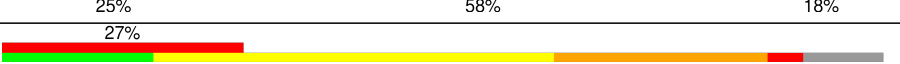
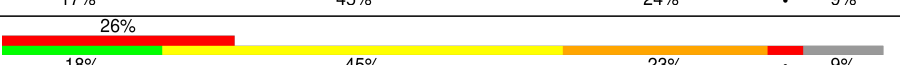
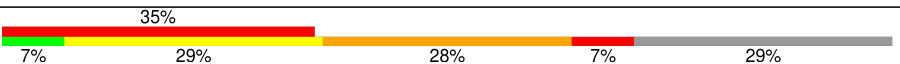
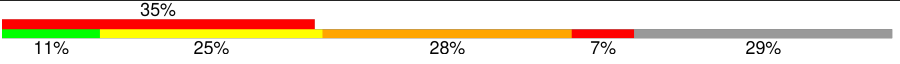
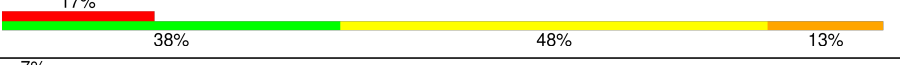
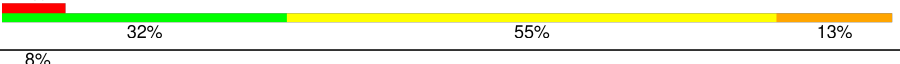


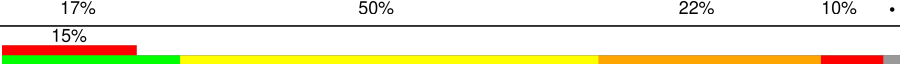



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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
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	

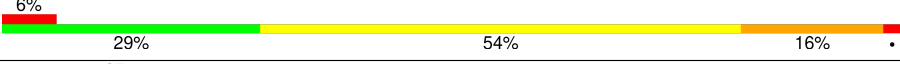


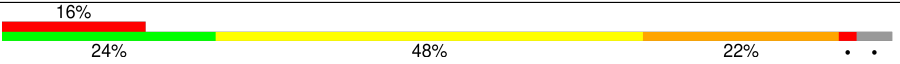
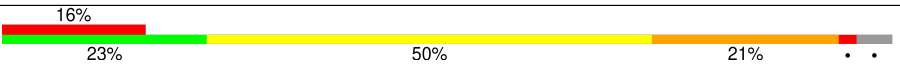
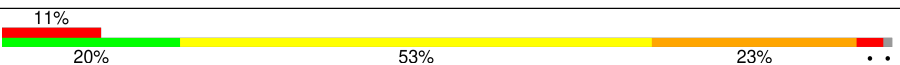
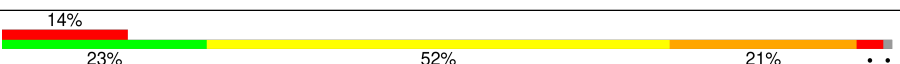
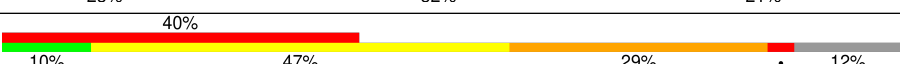
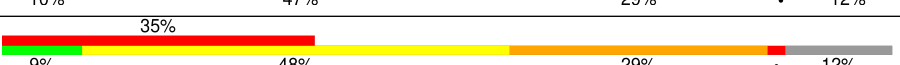
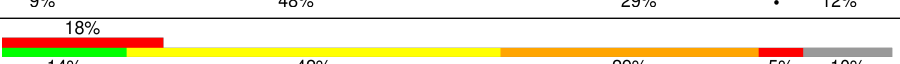
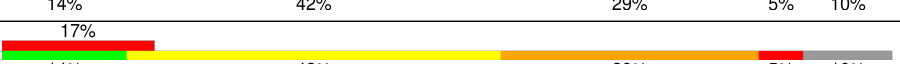
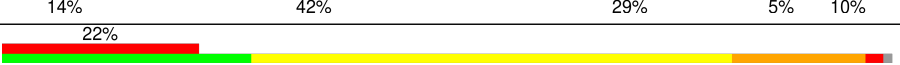
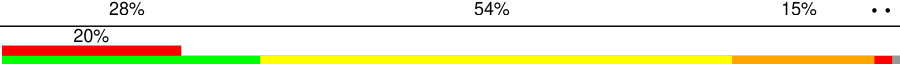



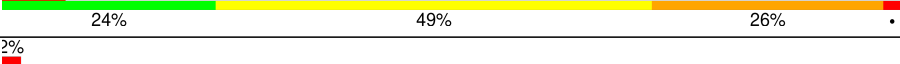
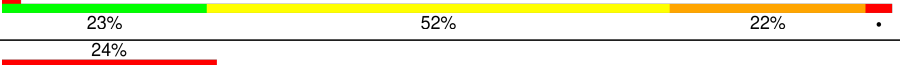

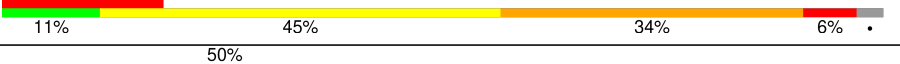

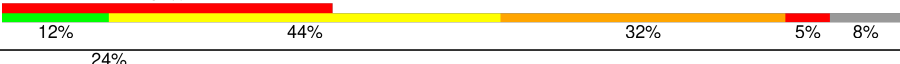
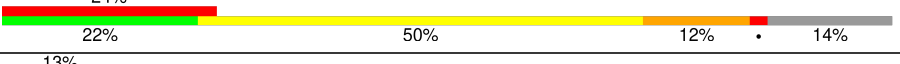
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Mol	Chain	Length	Quality of chain
28	B6	54	
28	D6	54	
29	B7	49	
29	D7	49	
30	B8	65	
30	D8	65	
31	BA	2787	
31	DA	2787	
32	BB	122	
32	DB	122	
33	BD	276	
33	DD	276	
34	BE	206	
34	DE	206	
35	BF	210	
35	DF	210	
36	BG	182	
36	DG	182	
37	BH	180	
37	DH	180	
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	1618	-	-	-	X
52	MG	BA	3039	-	-	-	X
52	MG	BA	3166	-	-	-	X
52	MG	BA	3219	-	-	-	X
52	MG	CA	1626	-	-	-	X
52	MG	CA	1643	-	-	-	X
52	MG	DA	3071	-	-	-	X
52	MG	DA	3090	-	-	-	X
52	MG	DA	3131	-	-	-	X
52	MG	DA	3150	-	-	-	X
52	MG	DA	3236	-	-	-	X
52	MG	DA	3311	-	-	-	X
55	TEL	BA	3362	-	-	X	-
55	TEL	DA	3320	-	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 278037 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	9	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	9	0	0
			459	288	90	76	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	AA	52	Total	Mg	0	0
			52	52		
52	B0	1	Total	Mg	0	0
			1	1		
52	B1	1	Total	Mg	0	0
			1	1		
52	B5	2	Total	Mg	0	0
			2	2		
52	B7	1	Total	Mg	0	0
			1	1		
52	BA	360	Total	Mg	0	0
			360	360		
52	BB	7	Total	Mg	0	0
			7	7		
52	BD	2	Total	Mg	0	0
			2	2		
52	BF	1	Total	Mg	0	0
			1	1		
52	BP	3	Total	Mg	0	0
			3	3		
52	BQ	2	Total	Mg	0	0
			2	2		
52	BR	1	Total	Mg	0	0
			1	1		
52	BU	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	CA	50	Total	Mg	0	0
			50	50		
52	D5	1	Total	Mg	0	0
			1	1		
52	D7	1	Total	Mg	0	0
			1	1		
52	D8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	DA	318	Total 318	Mg 318	0	0
52	DB	3	Total 3	Mg 3	0	0
52	DD	2	Total 2	Mg 2	0	0
52	DE	1	Total 1	Mg 1	0	0
52	DF	1	Total 1	Mg 1	0	0
52	DP	1	Total 1	Mg 1	0	0
52	DQ	1	Total 1	Mg 1	0	0
52	DR	2	Total 2	Mg 2	0	0
52	DU	1	Total 1	Mg 1	0	0
52	DX	1	Total 1	Mg 1	0	0

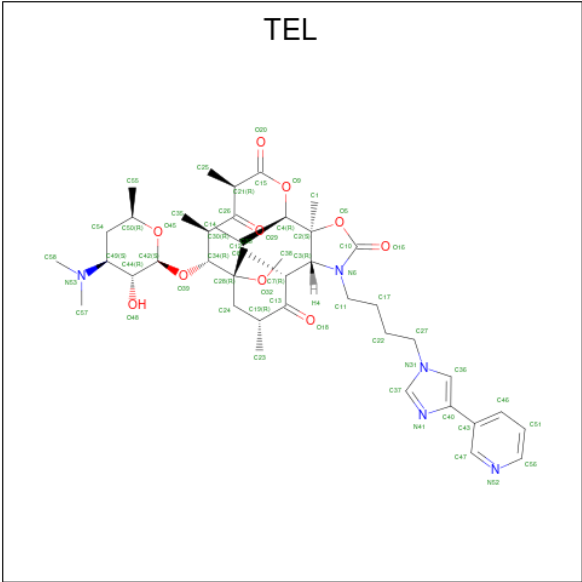
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	AD	1	Total 1	Zn 1	0	0
53	AN	1	Total 1	Zn 1	0	0
53	CD	1	Total 1	Zn 1	0	0
53	CN	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 TELITHROMYCIN (three-letter code: TEL) (formula: C₄₃H₆₅N₅O₁₀).

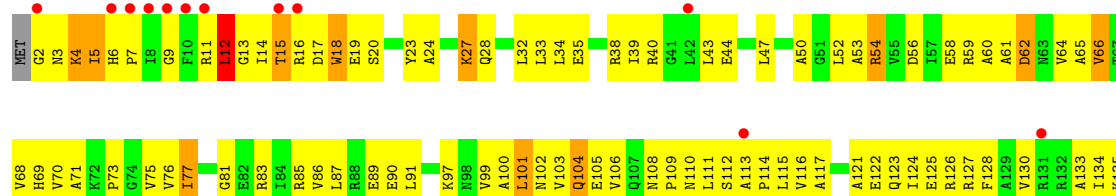


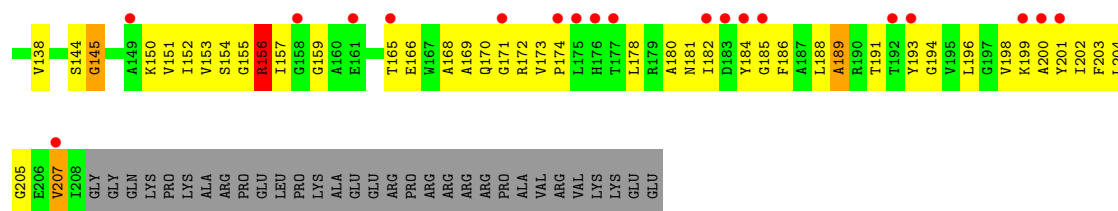
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BA	1	Total	C	N	O	0	0
			58	43	5	10		
55	DA	1	Total	C	N	O	0	0
			58	43	5	10		

A1396	A1397	G1337	G1276	U1211	G1144	U1083	A1014	G951	G818	U757	A696	U636
C1398	C1399	G1338	C1277	U1212	C1145	G1084	A1015	U952	A819	G758	U697	G637
A1340	A1341	A1146	U1278	A1213	A1147	U1085	G1016	G953	U820	A759	G698	G638
G1401	G1402	C1148	A1280	G1214	C1149	G1087	C1017	G954	G821	G760	G699	G639
C1403	C1404	U1150	G1281	G1215	U1148	U1088	G1018	U955	C822	G761	G700	A640
G1405	G1406	U1151	C1282	G1216	U1149	U1089	G1019	U956	G823	G762	G701	U641
A1407	A1408	A1152	C1217	G1217	U1150	U1090	U1025	U957	C824	A763	A702	A642
C1409	C1410	A1153	U1219	U1218	A1151	U1091	G1026	U958	G825	G764	G703	G643
G1411	G1412	C1153	G1220	C1219	A1152	A1092	U1029	U959	U826	G765	A704	G644
C1413	C1414	A1286	G1221	G1220	G1154	A1093	C1030	U960	A828	A767	U706	U645
A1415	A1416	U1155	G1222	G1221	G1155	G1094	G1030	G962	G829	A768	C707	U646
G1417	G1418	C1156	C1223	G1222	G1156	U1095	G1030A	G963	G830	G769	C708	A648
C1419	C1420	A1157	G1224	G1223	A1157	C1096	G1030C	G964	U831	C770	G709	G649
G1421	G1422	U1158	A1225	C1224	U1158	C1097	G1030D	U965	G832	G771	G711	G650
A1423	A1424	C1159	A1226	U1232	U1159	C1098	G1030E	U966	U833	G772	G712	C651
C1425	C1426	G1160	A1227	G1232	U1160	G1099	G1031	U967	U834	G773	A713	U652
A1427	A1428	C1161	C1234	G1233	C1161	C1100	G1036	U968	U835	G774	G714	G653
G1429	G1430	U1162	U1235	G1234	C1162	A1101	G1037	A969	G836	G775	G715	G654
C1431	C1432	C1163	A1236	U1242	U1163	A1102	C1038	G970	G837	G776	A716	A655
A1433	A1434	G1164	G1237	C1237	C1164	C1103	C1039	G971	U838	G777	G717	G656
G1435	G1436	C1165	U1238	G1238	U1165	G1104	G1046	G972	U839	G778	C718	G657
C1437	C1438	G1166	U1239	G1239	G1166	A1105	A1047	G973	U840	C779	C719	U659
A1439	A1440	U1167	U1240	G1240	U1167	G1106	G1048	G974	U841	A780	C720	G660
G1441	G1442	C1168	G1241	C1242	U1168	G1107	G1049	A975	C848	A781	G721	G661
C1442A	C1442B	G1169	C1242	G1242	U1169	G1108	G1050	A976	G851	A782	A722	G662
G1443	G1444	U1170	U1243	G1243	U1170	G1109	G1051	A977	G852	C783	U723	G663
U1445	U1446	C1171	A1244	G1244	A1171	A1110	G1052	A978	G853	C784	G724	G664
A1447	A1448	G1172	U1245	G1245	C1172	G1111	U1053	A979	G854	C785	G725	A665
C1449	C1450	U1173	C1246	G1246	G1173	C1112	U1054	A980	G855	C786	G726	G666
G1451	G1452	C1174	U1247	G1247	U1174	G1113	G1055	A981	C856	C787	G727	G667
C1453	C1454	G1175	U1248	G1248	U1175	C1114	G1056	U982	C857	C788	A728	G668
A1455	A1456	U1176	C1249	G1249	U1176	G1115	A1057	G922	C858	C789	G730	U669
G1457	G1458	C1177	U1250	G1250	U1177	C1116	U1058	A923	G859	C790	G731	G671
U1459	U1460	G1178	A1251	G1251	U1178	G1117	G1059	C924	A860	A792	G732	U672
A1461	A1462	U1179	U1252	G1252	U1179	G1118	C1060	A925	C861	C793	A733	G673
G1463	G1464	C1180	C1253	G1253	U1180	C1119	G1061	G926	C862	A794	G734	G674
C1465	C1466	G1181	U1254	G1254	U1181	G1120	G1062	U927	U863	C795	G735	A675
A1467	A1468	U1182	C1255	G1255	U1182	C1121	C1063	C930	A864	C796	G736	U676
G1469	G1470	C1183	U1256	G1256	U1183	G1122	C1064	C931	A865	C797	A737	U677
C1471	C1472	G1184	A1257	G1257	U1184	U1123	U1065	C932	C868	C798	G738	U678
A1473	A1474	U1185	U1258	G1258	U1185	G1124	U1066	C933	C869	C799	C739	C679
G1475	G1476	C1186	C1259	G1259	U1186	U1125	U1067	C934	U870	U800	U740	G680
C1477	C1478	G1187	U1260	G1260	U1187	C1126	A1067	C935	U871	A802	G741	C681
A1479	A1480	U1188	C1261	G1261	U1188	C1127	G1068	U936	U872	G803	G742	G682
G1481	G1482	C1189	U1262	G1262	U1189	C1128	C1069	A937	A873	U804	U751	C683
C1483	C1484	G1190	C1263	G1263	U1190	C1129	U1070	A938	G874	C805	G752	G684
U1485	U1486	U1191	U1264	G1264	U1191	G1130	G1071	G939	C875	C806	A753	U685
A1487	A1488	C1192	C1265	G1265	U1192	C1131	U1072	C940	G876	C807	C747	U686
G1489	G1490	U1193	A1266	G1266	U1193	C1132	U1073	G941	C877	G809	C748	A687
C1491	C1492	C1194	U1267	G1267	U1194	G1133	G1074	G942	C878	C910	C749	G688
A1493	A1494	G1195	C1268	G1268	U1195	C1134	C1075	U943	C879	C811	G750	C689
G1495	G1496	U1196	U1269	G1269	U1196	U1135	C1076	G944	C880	C812	U751	G690
C1497	C1498	C1197	C1270	G1270	U1197	C1136	G1077	G945	C881	G813	G752	G691
A1499	A1500	G1198	G1271	G1271	U1198	G1137	U1078	A946	C882	A814	A754	U692
G1501	G1502	U1199	U1272	G1272	U1199	C1138	G1079	G947	C883	A815	C755	A693
C1503	C1504	C1200	C1273	G1273	U1200	G1139	A1080	C948	U884	A694	G756	A695
A1505	A1506	A1201	U1274	G1274	U1201	G1142	U1012	C949	G885	A816		
G1507	G1508	C1202	A1275	G1275	U1202	G1143	G1013	U950				

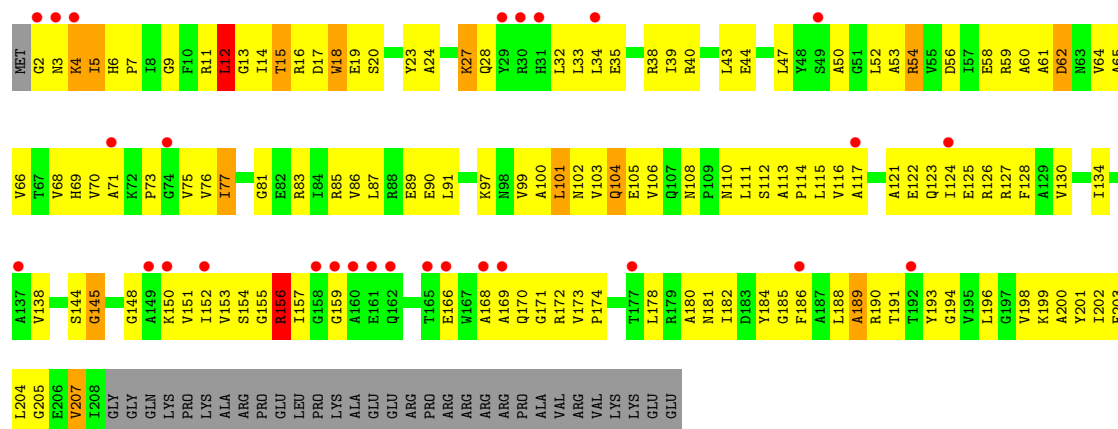




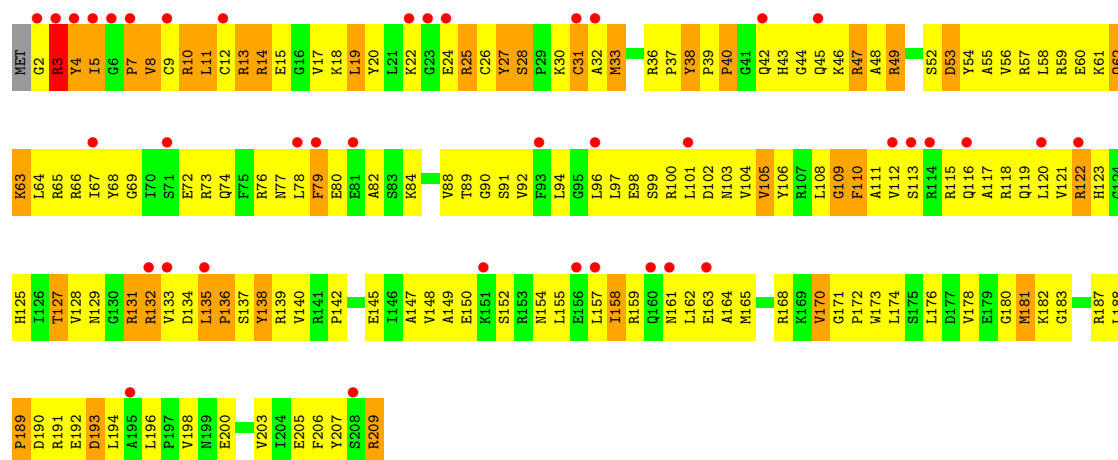




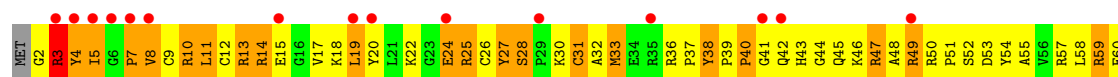
• Molecule 3: 30S ribosomal protein S3

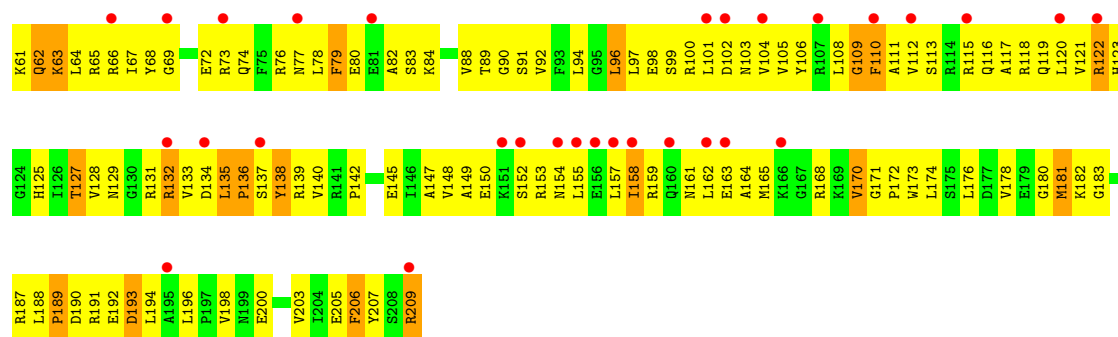


• Molecule 4: 30S ribosomal protein S4

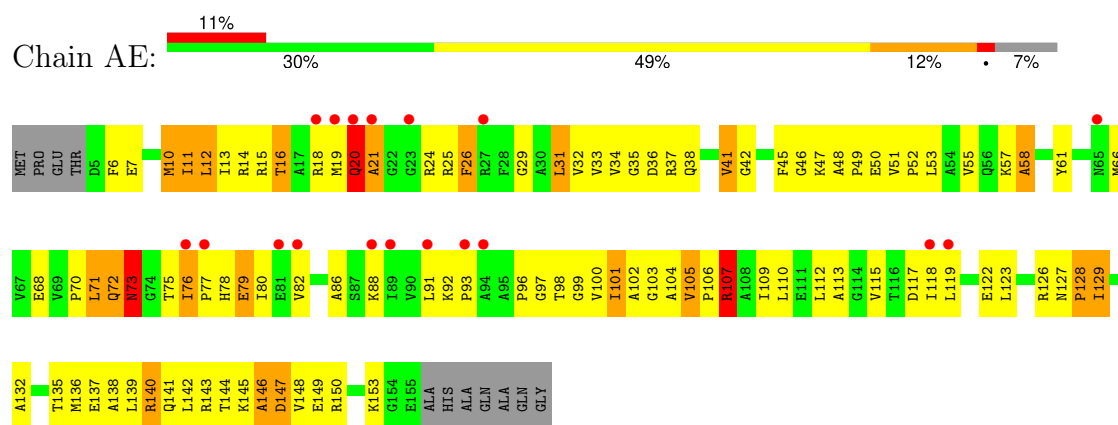


• Molecule 4: 30S ribosomal protein S4

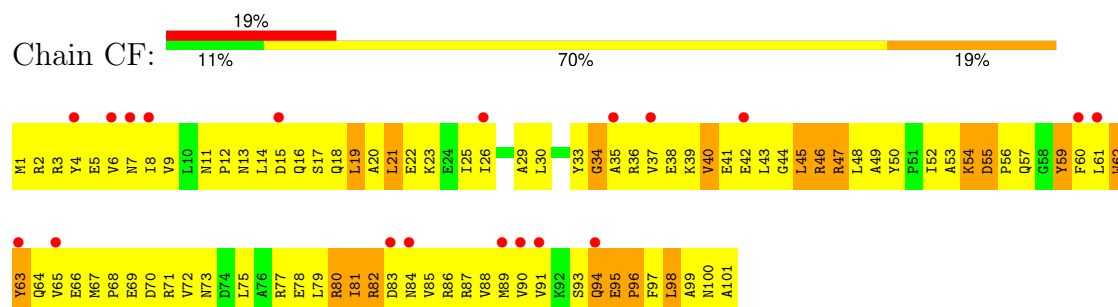




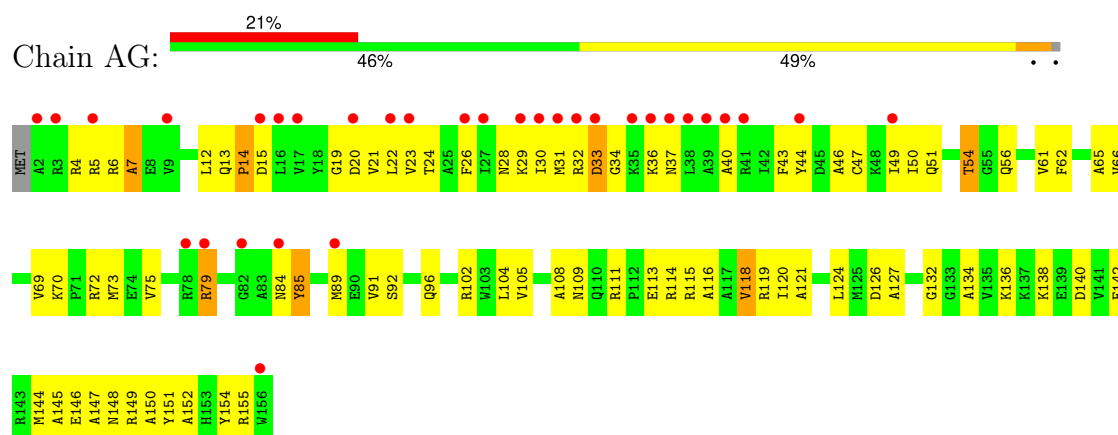
• Molecule 5: 30S ribosomal protein S5



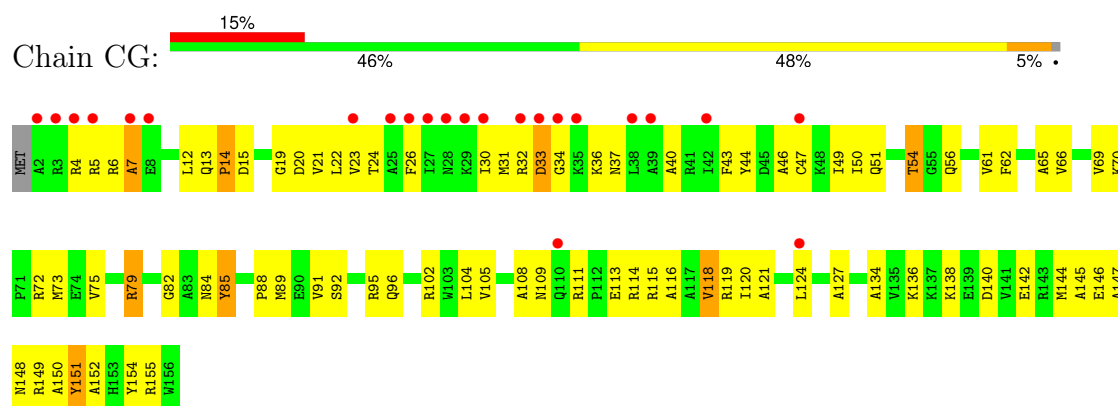
- Molecule 6: 30S ribosomal protein S6



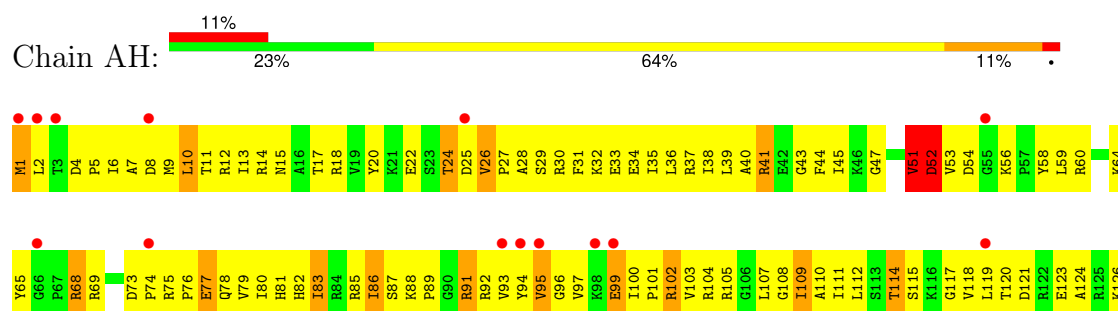
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7

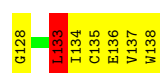
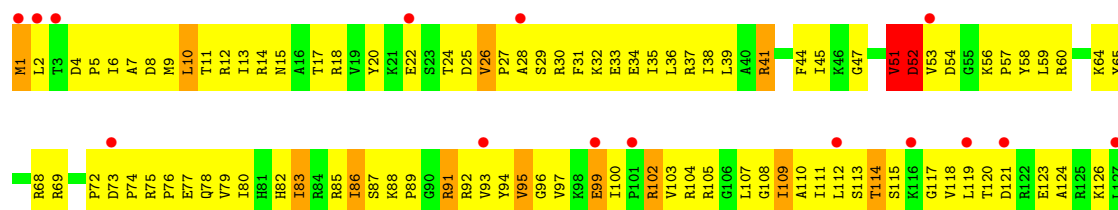


- Molecule 8: 30S ribosomal protein S8

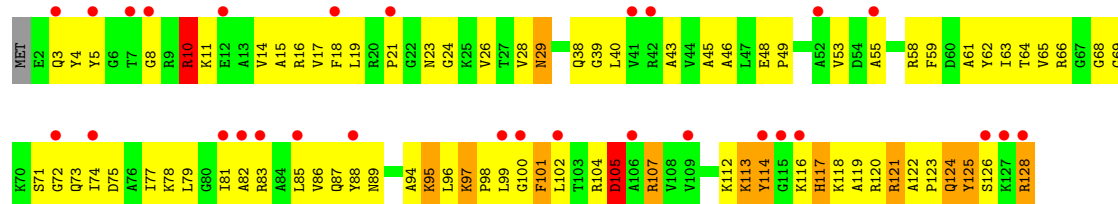




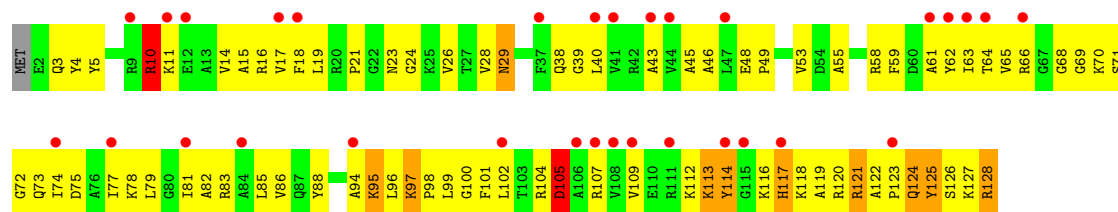
• Molecule 8: 30S ribosomal protein S8



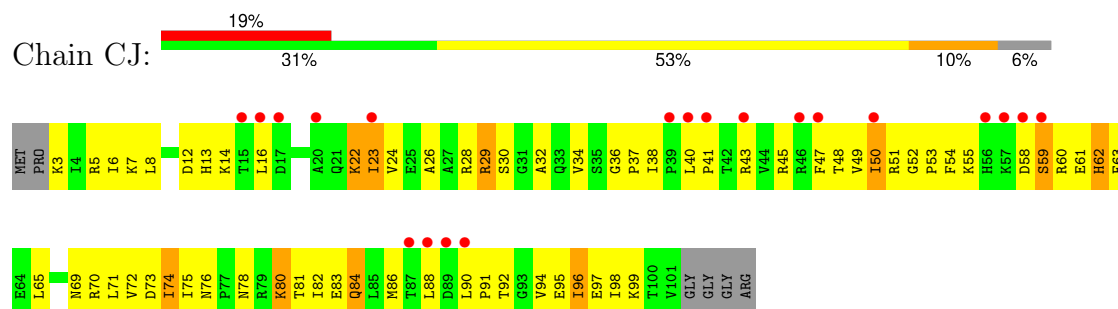
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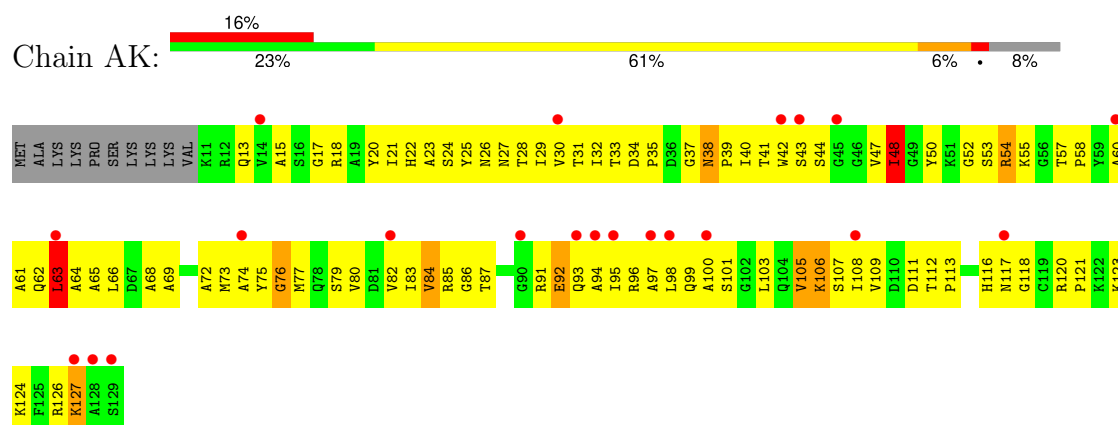
• Molecule 9: 30S ribosomal protein S9



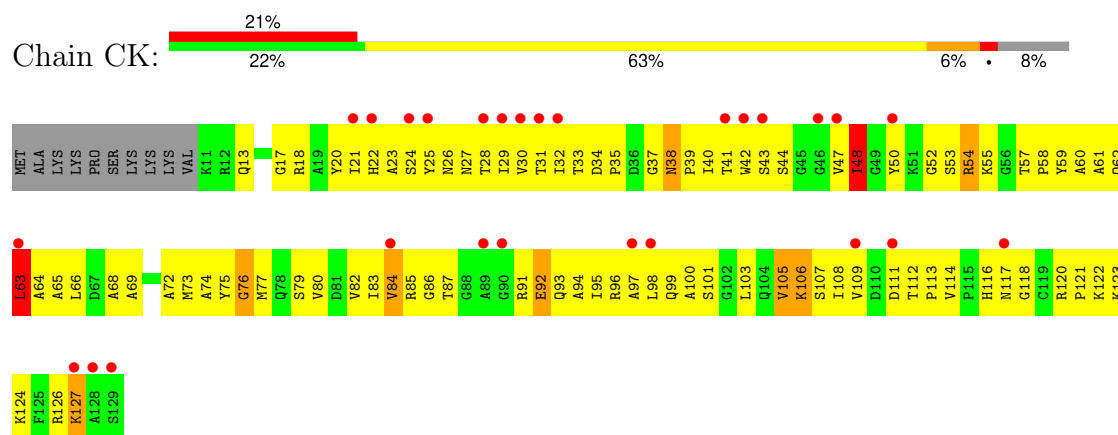
- Molecule 10: 30S ribosomal protein S10



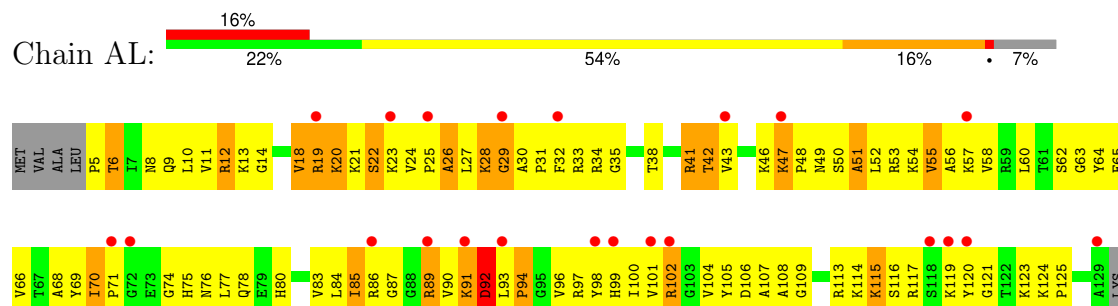
- Molecule 11: 30S ribosomal protein S11



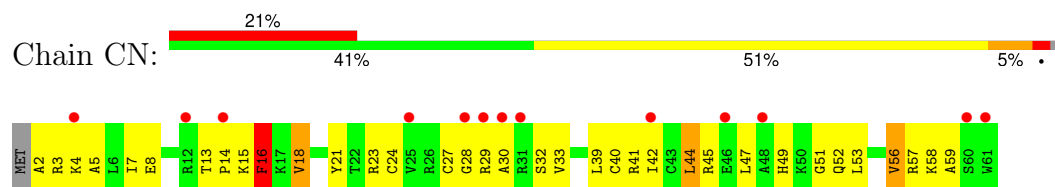
- Molecule 11: 30S ribosomal protein S11



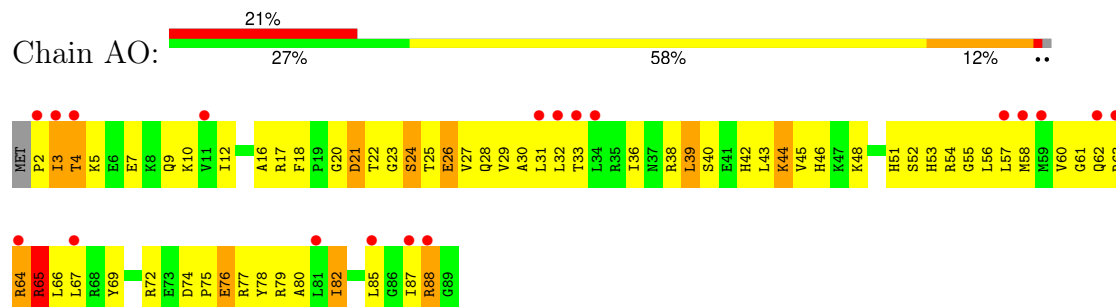
- Molecule 12: 30S ribosomal protein S12



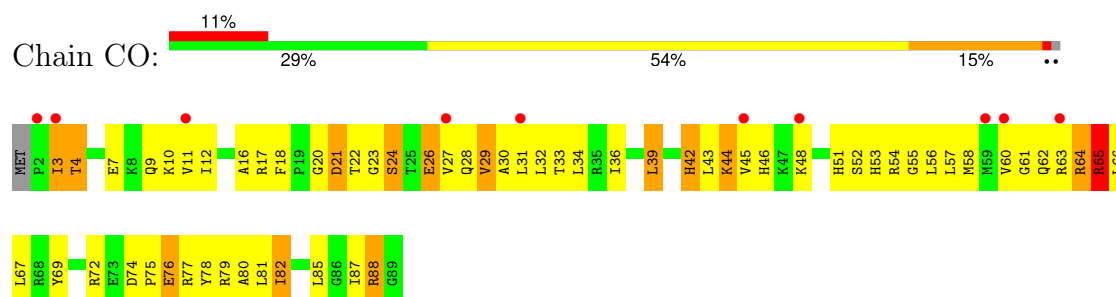
- Molecule 14: 30S ribosomal protein S14



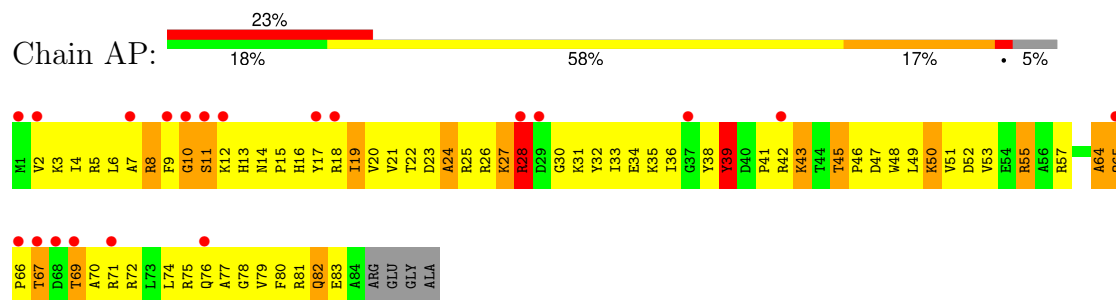
- Molecule 15: 30S ribosomal protein S15



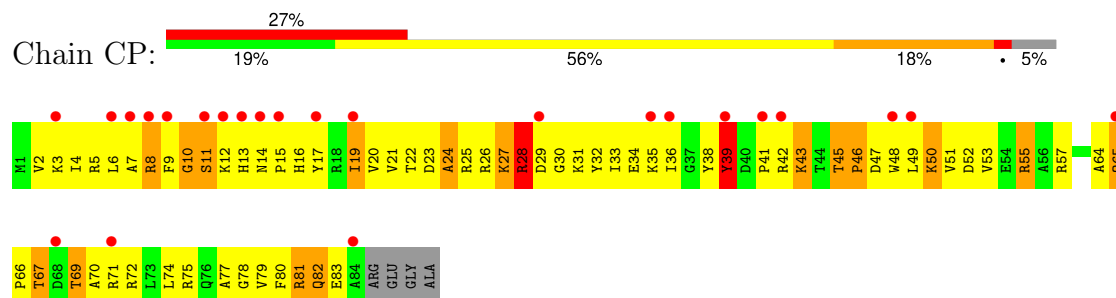
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

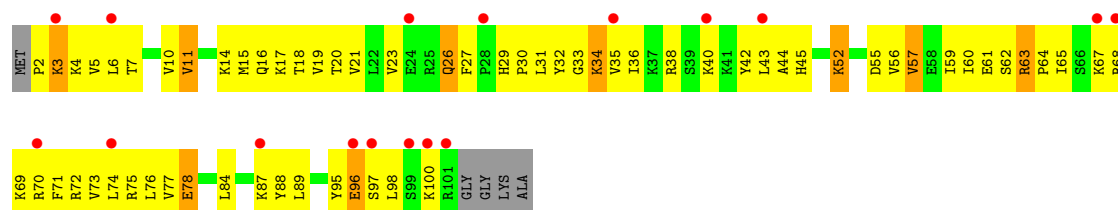


- Molecule 16: 30S ribosomal protein S16



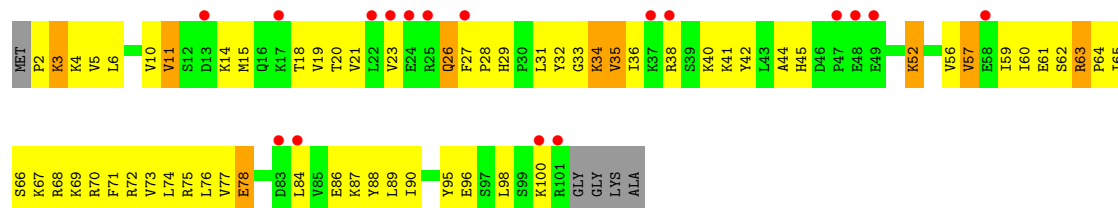
- Molecule 17: 30S ribosomal protein S17

Chain AQ: 



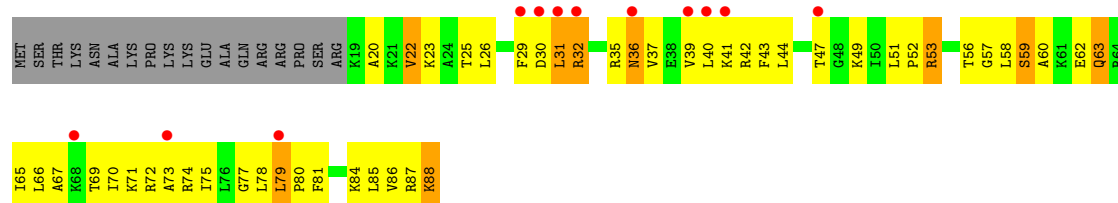
- Molecule 17: 30S ribosomal protein S17

Chain CQ: 




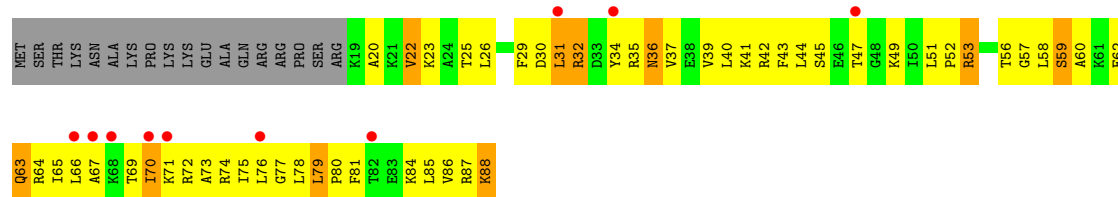
- Molecule 18: 30S ribosomal protein S18

Chain AR: 



- Molecule 18: 30S ribosomal protein S18

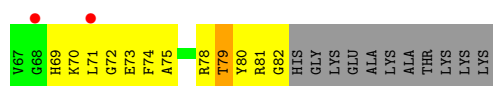
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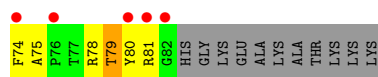
- Molecule 19: 30S ribosomal protein S19

Chain AS: 

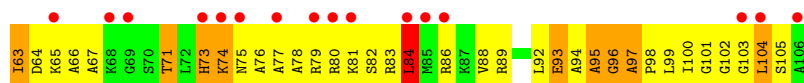
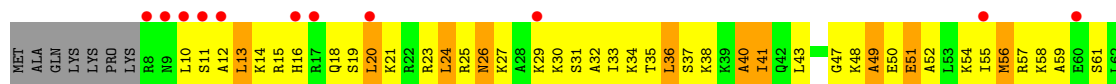




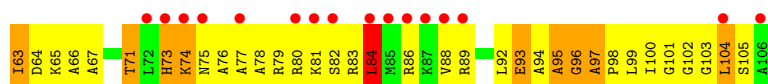
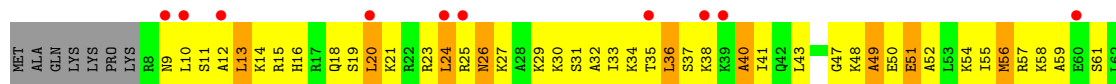
- Molecule 19: 30S ribosomal protein S19



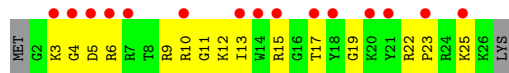
- Molecule 20: 30S ribosomal protein S20



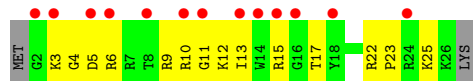
- Molecule 20: 30S ribosomal protein S20



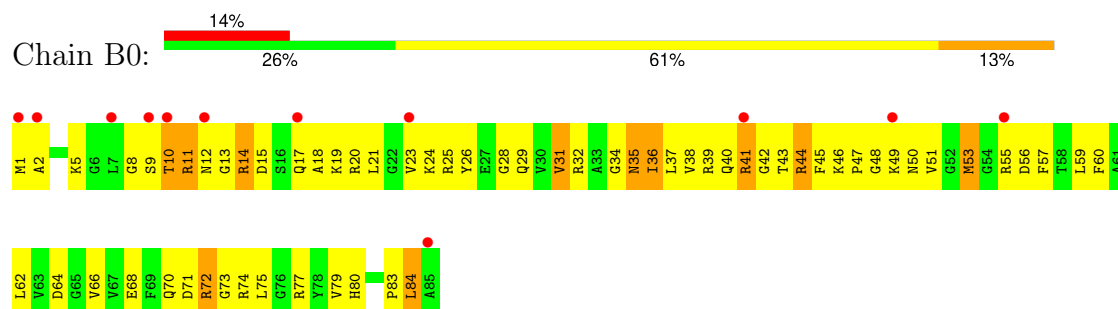
- Molecule 21: 30S ribosomal protein Thx



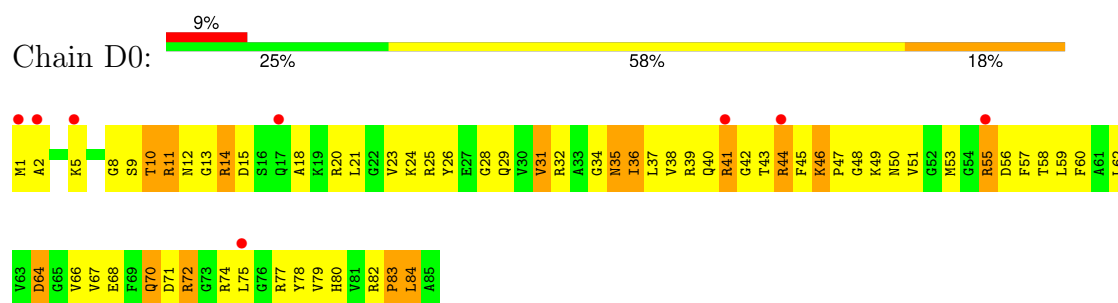
- Molecule 21: 30S ribosomal protein Thx



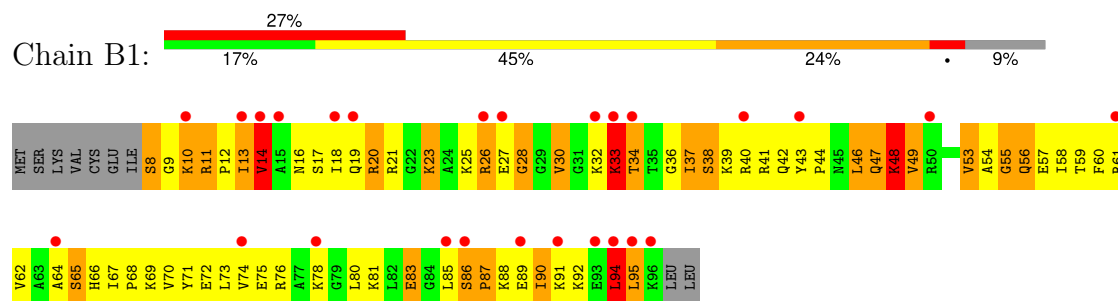
- Molecule 22: 50S ribosomal protein L27



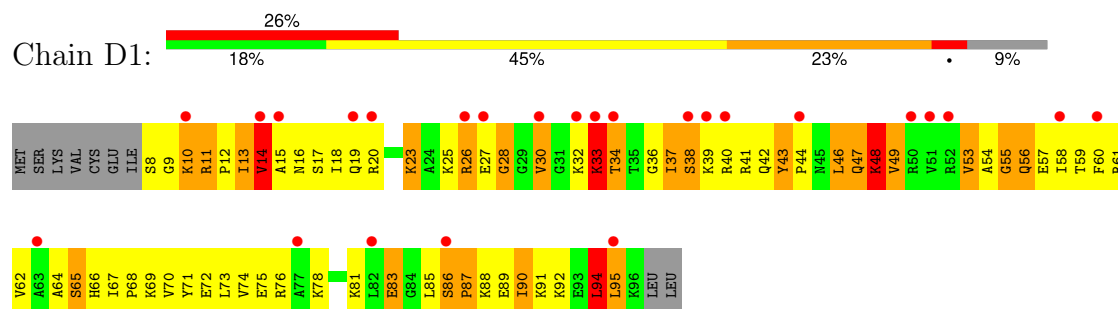
- Molecule 22: 50S ribosomal protein L27



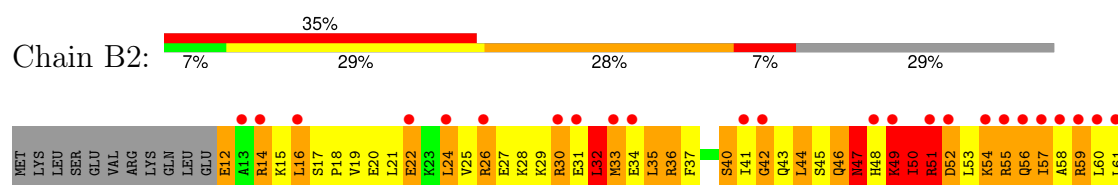
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28

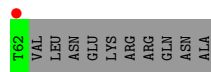


- Molecule 24: 50S ribosomal protein L29





- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



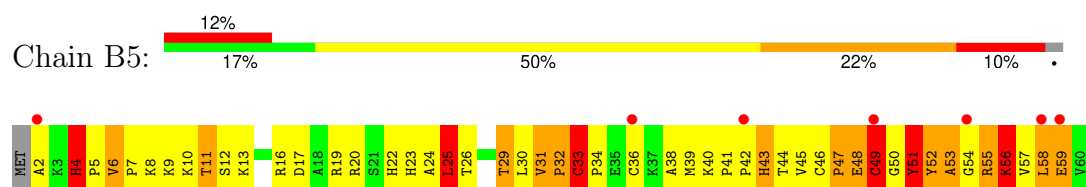
- Molecule 26: 50S ribosomal protein L31



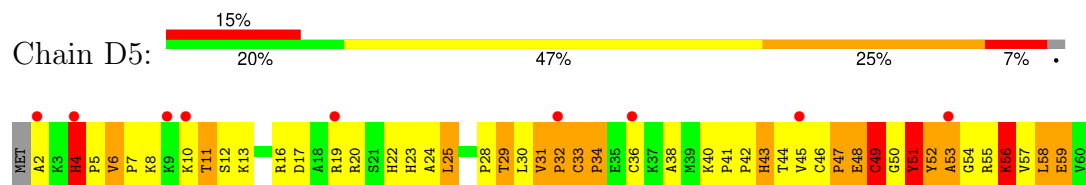
- Molecule 26: 50S ribosomal protein L31



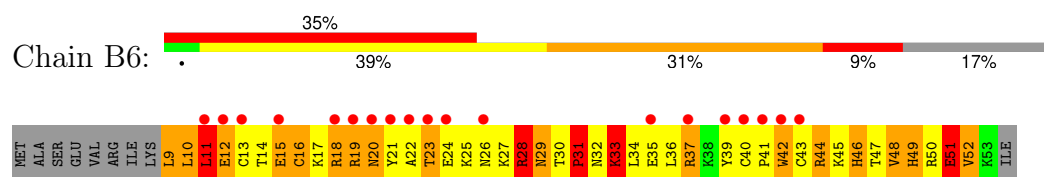
- Molecule 27: 50S ribosomal protein L32



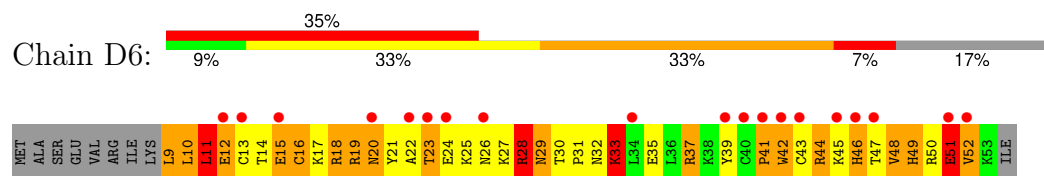
- Molecule 27: 50S ribosomal protein L32



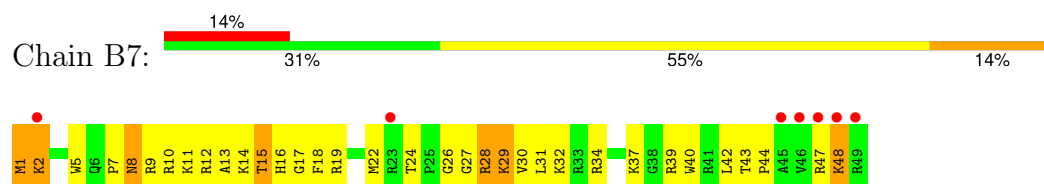
- Molecule 28: 50S ribosomal protein L33



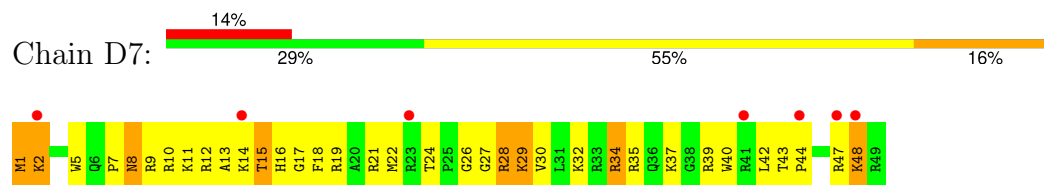
- Molecule 28: 50S ribosomal protein L33



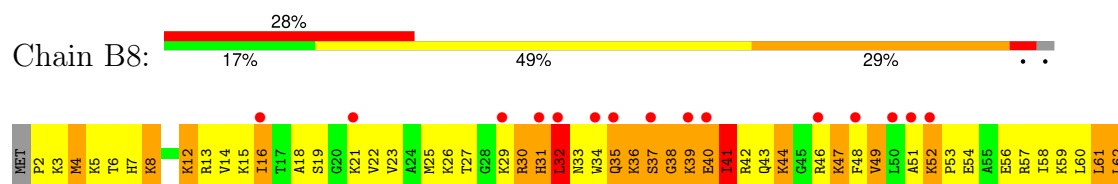
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



P63
Y64
E65

• Molecule 30: 50S ribosomal protein L35

Chain D8: 18% 31% 43% 32% 5%

MET P2 P3 K3 M4 K5 T6 H7 K8 K12 R13 K14 V14 V15 I16 I17 T18 A18 S19 G20 G21 K21 V22 V23 V24 M25 M26 K27 T27 G28 K29 R30 R31 H31 L32 N33 K34 K35 Q35 K36 K37 S37 G38 K39 E40 E41 R42 Q43 K44 K45 G45 R46 K47 F48 V49 L50 A51 K52 P53 E54 A55 E56 R57 T58 K59 L60 L61 L62

P63
Y64
E65

• Molecule 31: 23S ribosomal RNA

Chain BA: 5% 10% 47% 34% 7%

G G U C A G G A8 U9 G10 G11 G12 G13 G14 G15 G16 G17 G18 G19 G20 A21 G22 G23 G24 G25 G26 G27 A28 U29 G30 G31 C32 U33 G34 G35 G36 G37 A38 C39 C40 C41 C42 A43 G44 C45 C47 C48 A49 U50 G51 A52 A53 G54 G55 G56 A57 G58 U59 G60 G61

C62 U63 A64 C65 C66 U67 G68 C69 G70 U71 U72 A73 A74 G75 G76 G77 A78 G79 G80 G81 G82 G83 G84 G85 C86 G88 G89 U90 A92 G93 G94 G95 G96 G98 G99 G100 G102 U103 C104 C105 C106 C107 U108 G109 G110 A111 U112 U113 U114 C115 C116 A117 A118 A119 U120 G121 G122 G123 G124

G125 A126 A127 C128 C129 C130 C131 G132 C133 G136 G137 A138 G139 G140 A141 A142 A143 A144 A145 A146 U147 C148 A149 C150 C151 G152 C153 C154 C155 U156 U157 U158 G171 C172 C173 C174 G175 G176 G177 A181 A182 C183 C184 U185 U186 G187 G188 G189 A190 A191 C192 C193 U194 A195 A196 A197 C198

A199 U200 C201 U202 C203 C204 G205 U206 A207 U208 C209 C210 C211 A212 G212 A213 G214 G215 A216 A217 G218 A219 G220 A221 A222 A225 G226 A227 A228 A229 C230 C231 G232 C233 C234 U235 C236 C237 C238 U239 G240 A241 G242 G243 A244 G245 C246 G247 G248 C249 G250 A251 G252 C253 G254 A255 A256 A257 G258 G259

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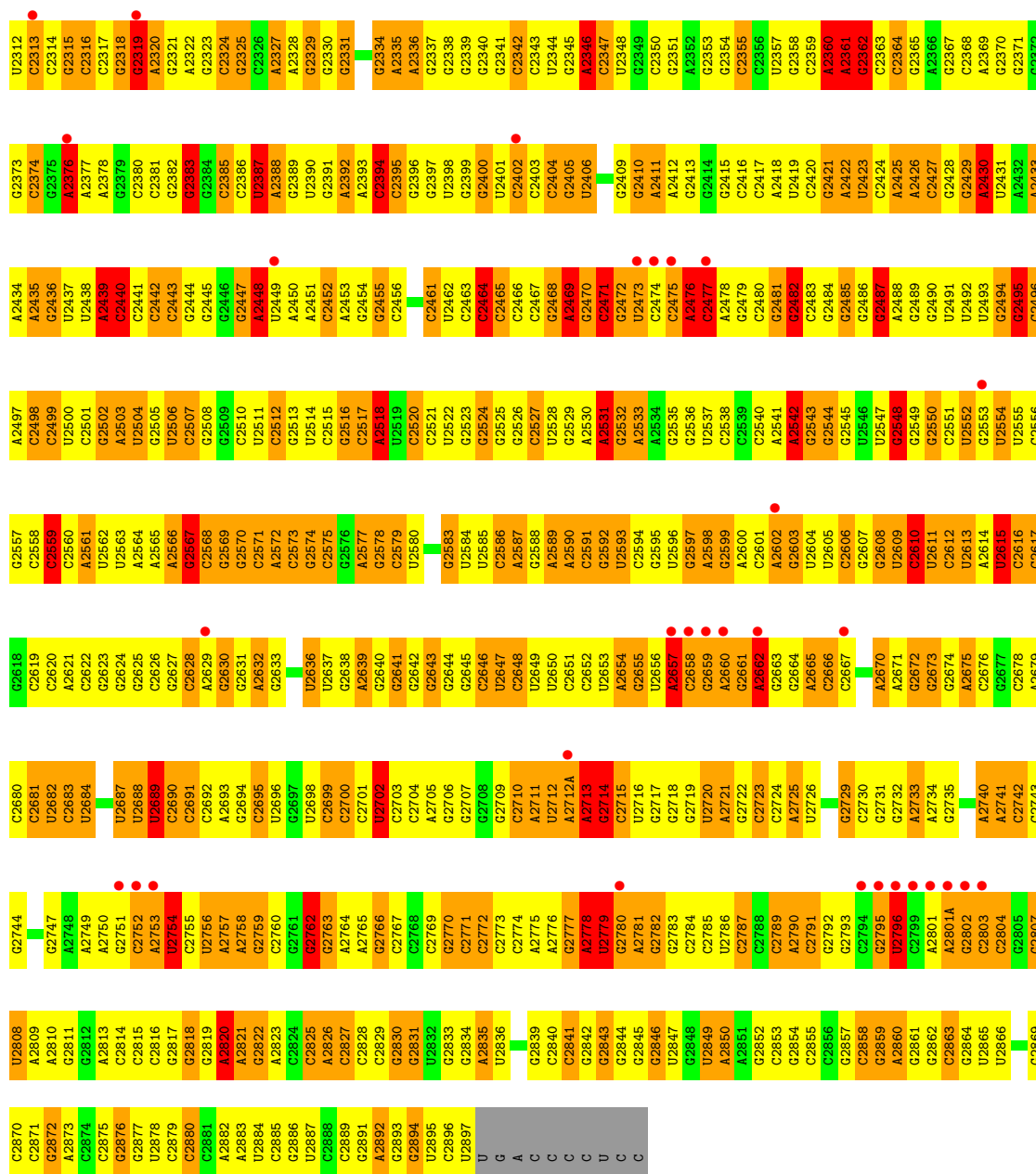
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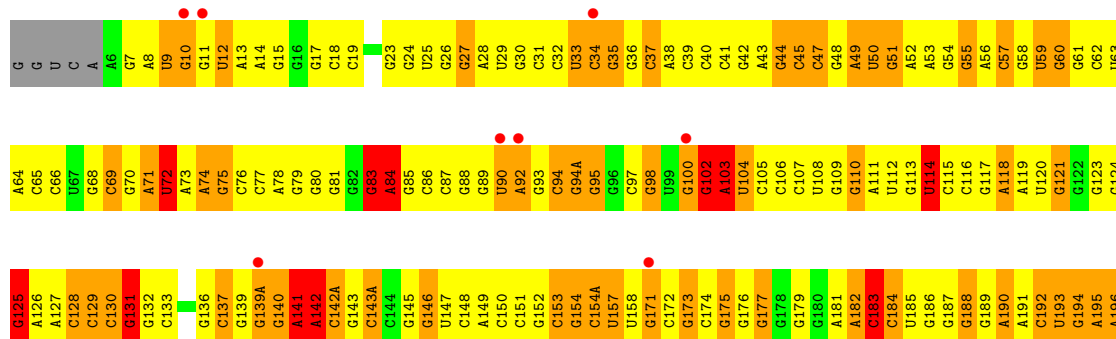
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U1394	G1332	C1270	U1211	G1036	C976	G916	C849	A787	G729	G666	A603	G539
A1395	C1333	G1271	G1212	G1037	C977	A917	C850	C790	C730	G667	G604	C540
U1396	U1334	A1272	A1213	G1038	G978	A918	U851	C791	C731	G668	C605	C541
U1397	U1335	A1273	A1214	C1039	G979	G919	G852	G792	G732	G669	U606	C542
C1398	A1336	A1274	G1215	C1040	A980	G920	G853	A793	G733	A670	C543	C543
C1399	G1337	A1275	G1216	C1041	A981	G921	G854	G794	A734	C671	A547	A547
G1400	G1338	A1276	C1217	G1042	C982	U922	G855	C795	A735	C672	G610	A548
G1401	G1339	A1277	C1218	C1043	A983	U923	C856	C796	C736	C673	C611	C611
C1402	U1340	A1278	G1219	G1044	A984	C924	C857	C797	C737	C674	C612	C551
C1403	U1341	G1279	U1159	A1045	C985	U925	U858	G798	G738	A675	G613	G552
C1404	A1342	G1280	G1160	A1046	C986	A926	G859	G799	G739	A676	U614	G553
U1405	G1343	G1281	G1161	G1047	G987	G927	U860	A800	U740	A677	U614A	U554
U1406	C1344	U1282	G1162	A1048	A988	G928	A861	G801	G741	C678	G614B	U555
C1407	C1345	G1283	G1163	C1049	G989	U930	G862	A802	G742	C679	A614C	G556
C1408	G1346	C1278	G1164	A1050	A990	G931	C863	U803	G743	G680	G615	U557
C1409	G1347	G1279	U1165	G1051	C991	G932	G864	A804	G744	G681	G558	U558
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C1412	C1350	G1289	G1168	A1106	C994	C935	C867	U807	U747	G684	A621	G561
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G1414	U1352	C1291	G1170	U1108	A996	U937	C869	G809	C749	G686	G623	G563
U1415	A1353	U1292	G1171	C1109	G997	G938	U870	U810	A750	C687	C624	C564
G1416	G1354	C1293	G1173	G1110	C998	G939	U871	U811	A751	U688	G625	C565
C1417	G1355	U1294	A1174	A1111	U999	G940	A872	C812	A752	A689	U626	U566
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	G2097	G2035	C1974	C1914	G1845	A1785	U1709	G1649	C1590	U1518	G1459
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	G2100	G2038	A1977	U1917	A1848	G1788	C1712	A1852	G1593		C1462
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	U2102	C2040	C1979	A1919	G1850	G1790	G1714	A1854	G1595	G1526	C1464
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				C1928	A1859	G1799	A1741	C1663	C1604	C1543	G1473
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				U1930	G1861	G1801	C1743	A1665	G1606	A1545	G1475
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				U1935	C1866	G1806	G1747	C1670	C1611	C1550	G1480
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				C1943	G1883	G1814	C1754	G1678	G1619	A1558	U1489
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				U1956	G1896	C1827	C1767	C1691	A1631A	A1571	C1502
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				G1959	G1899	G1830	G1770	C1694	A1634	C1574	C1505
				A1960	A1900	C2021	G1771	G1695	G1635	C1575	C1506
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				G1963	G1903	U1834	C1774	A1698	C1638	U1578	C1509
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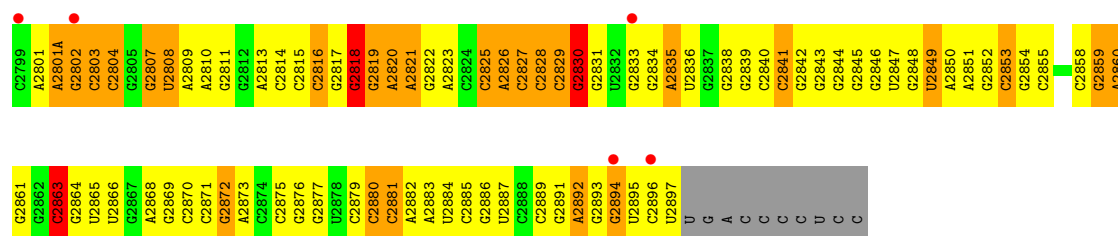
• Molecule 31: 23S ribosomal RNA



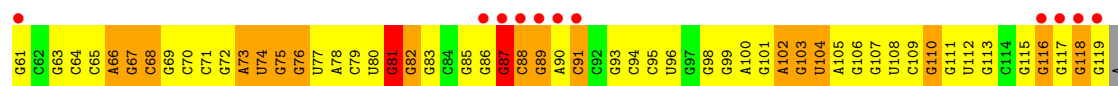
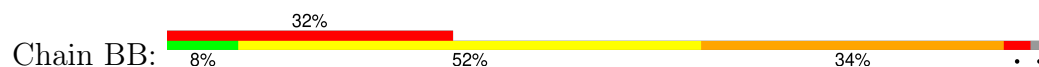
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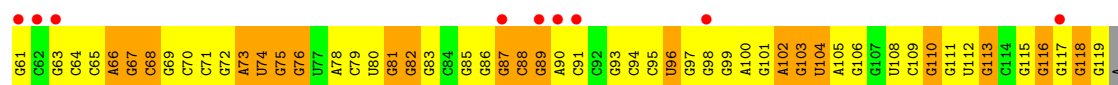
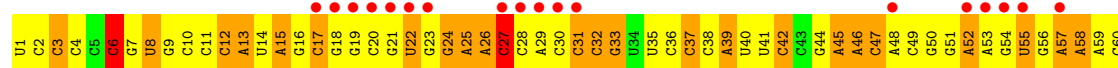


• Molecule 32: 5S ribosomal RNA



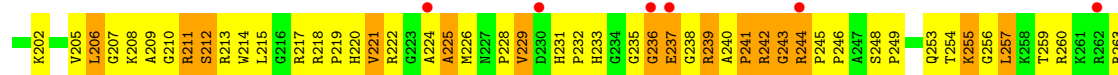
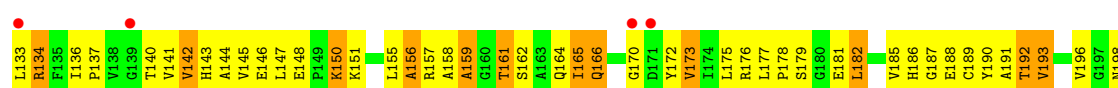
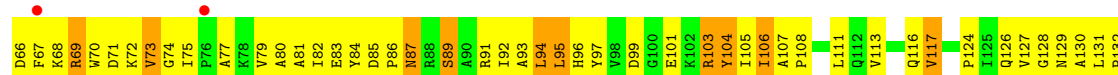
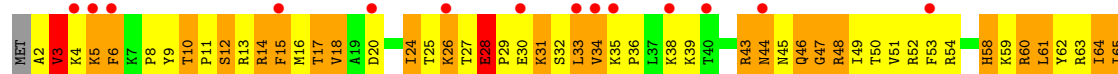
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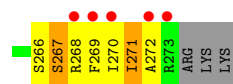
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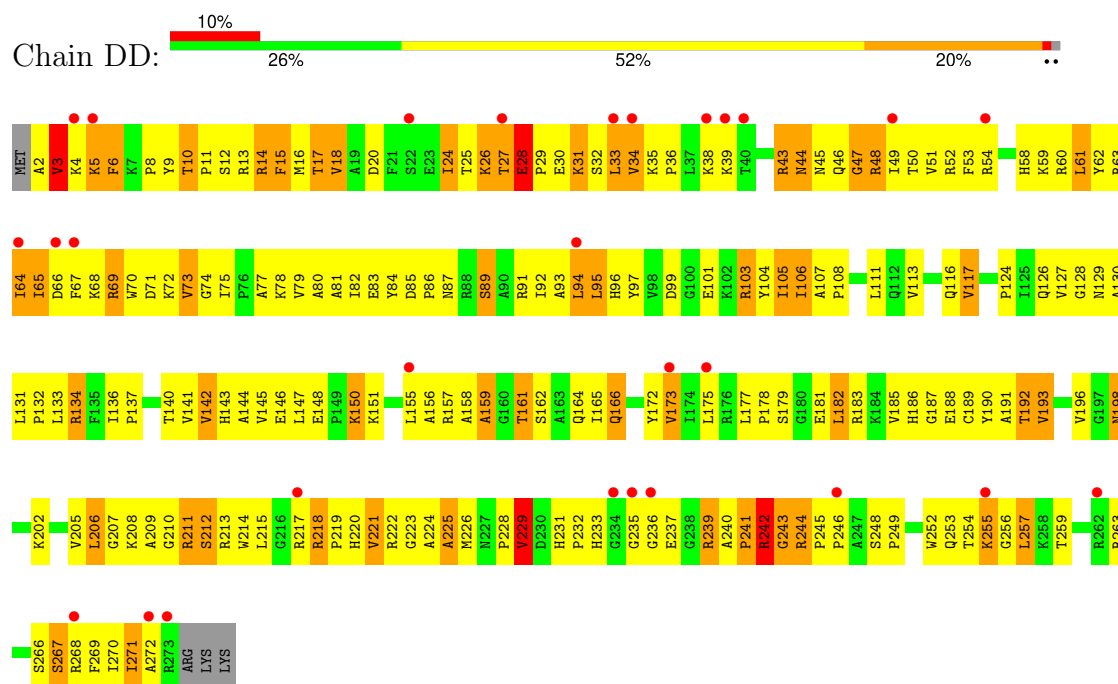
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• Molecule 33: 50S ribosomal protein L2

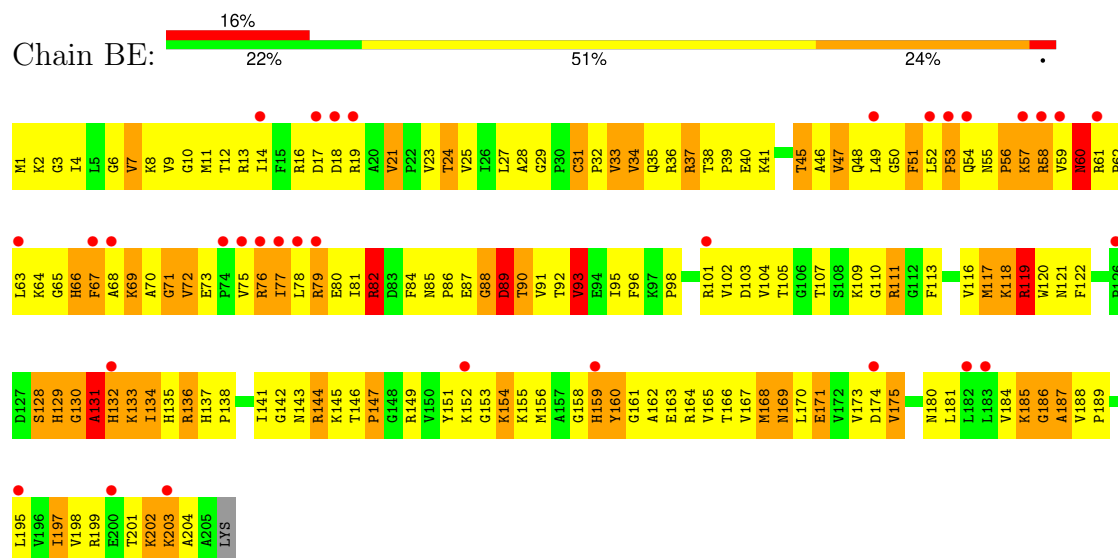




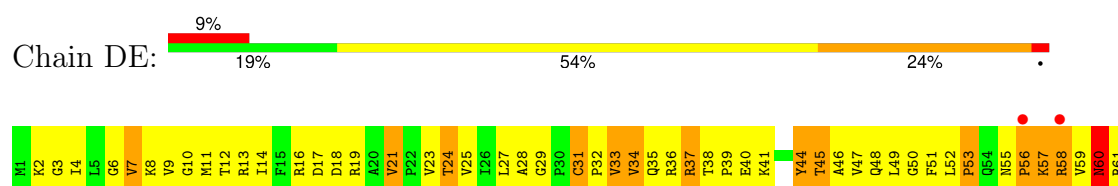
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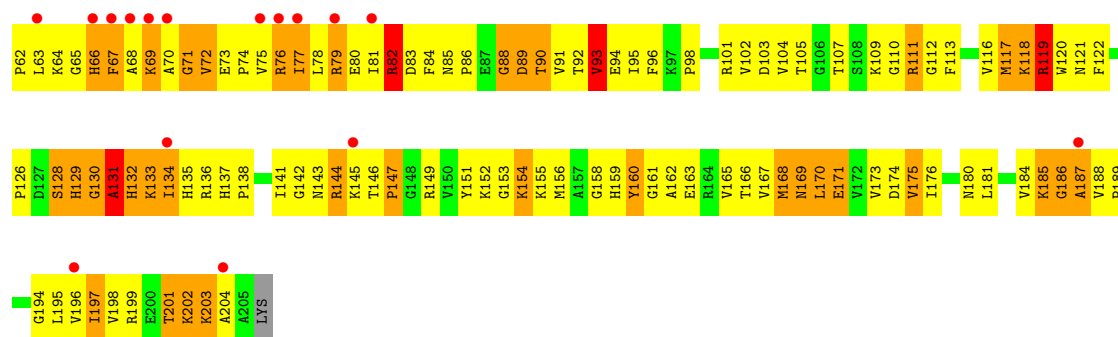


• Molecule 34: 50S ribosomal protein L3

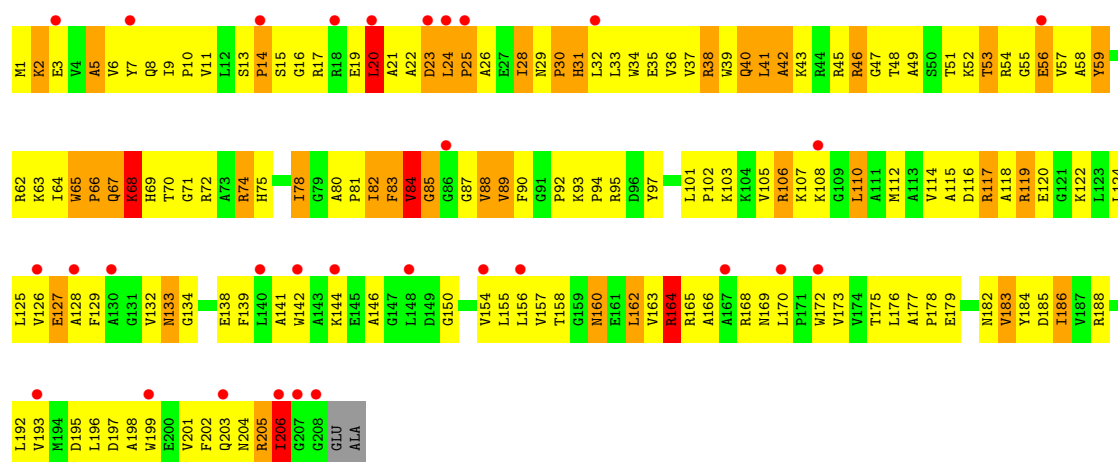


• Molecule 34: 50S ribosomal protein L3

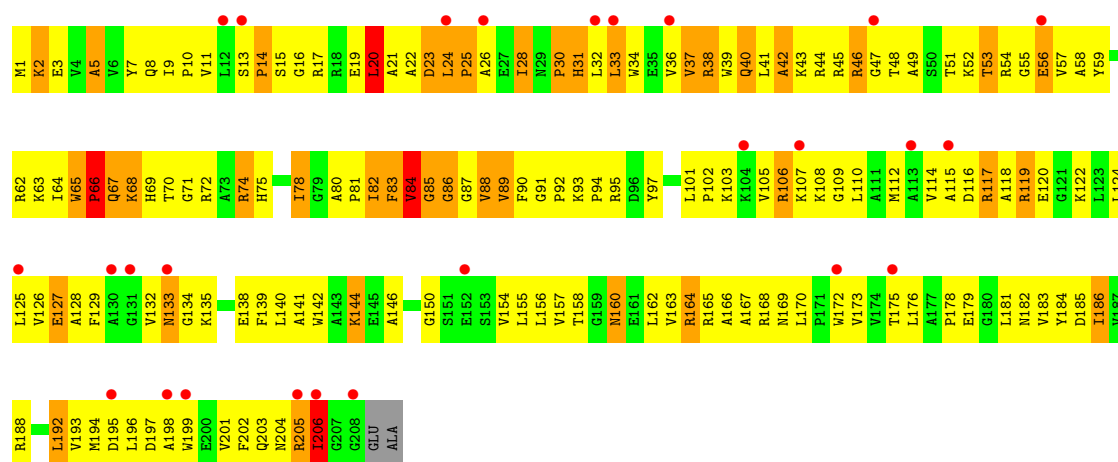




• Molecule 35: 50S ribosomal protein L4

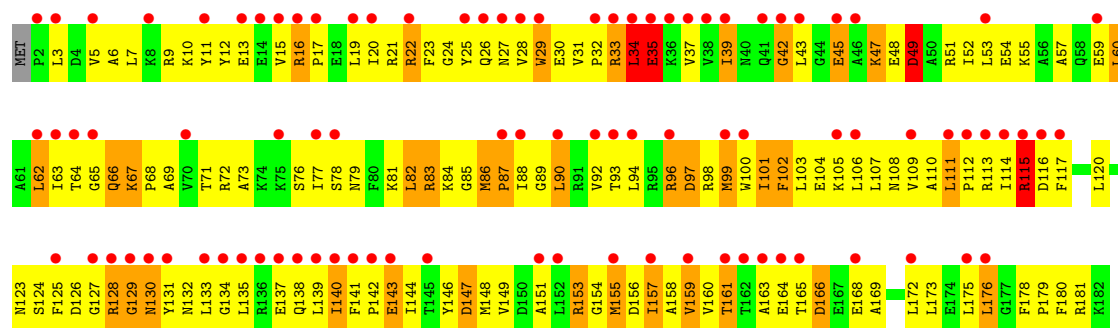


• Molecule 35: 50S ribosomal protein L4

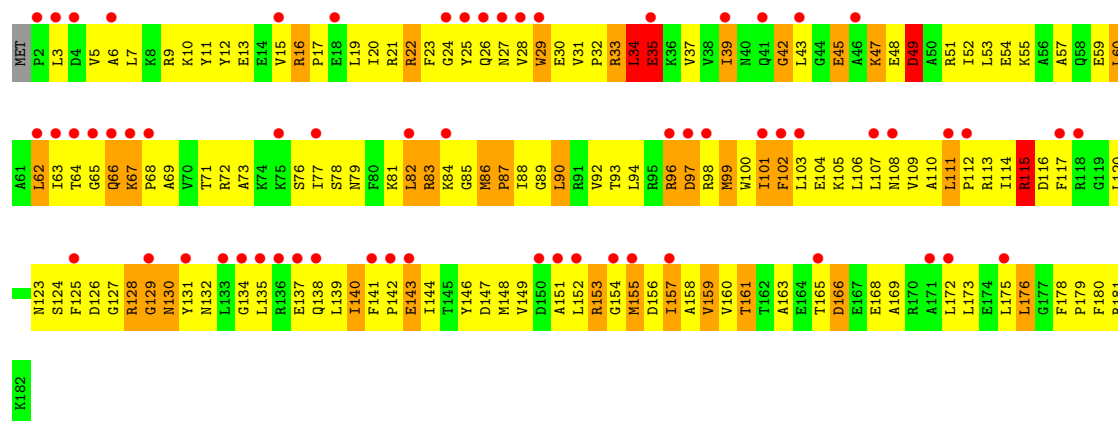


• Molecule 36: 50S ribosomal protein L5

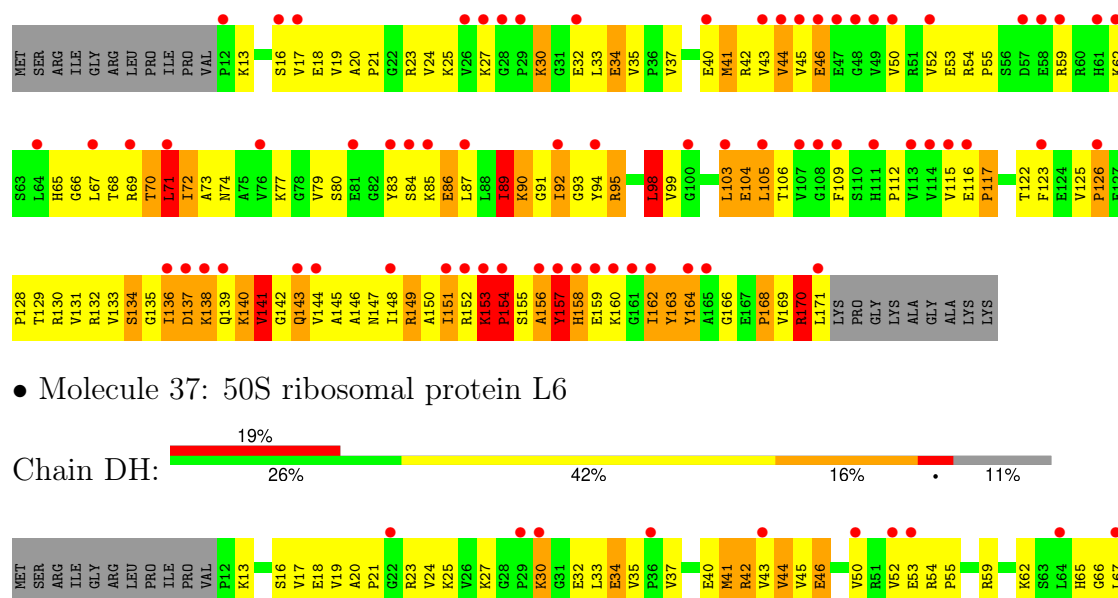


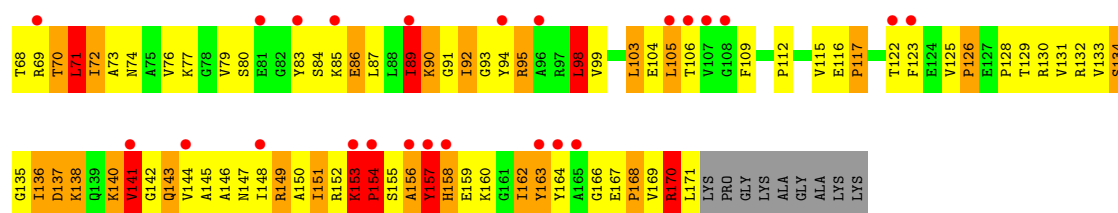


• Molecule 36: 50S ribosomal protein L5

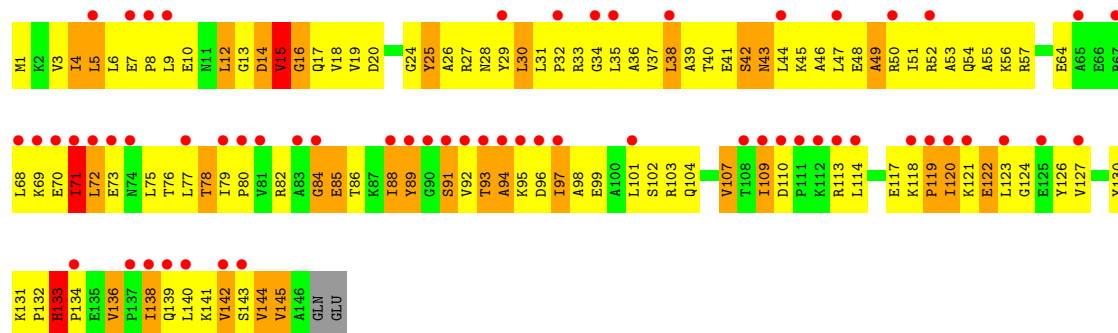
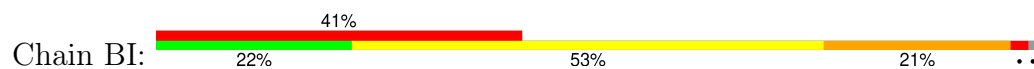


• Molecule 37: 50S ribosomal protein L6

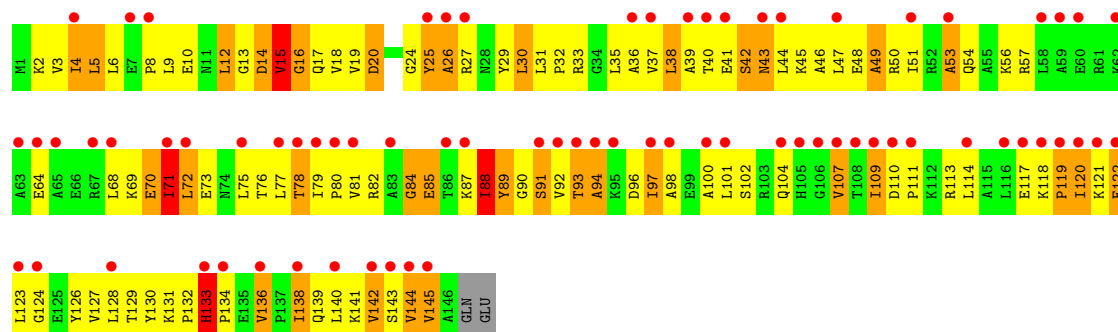




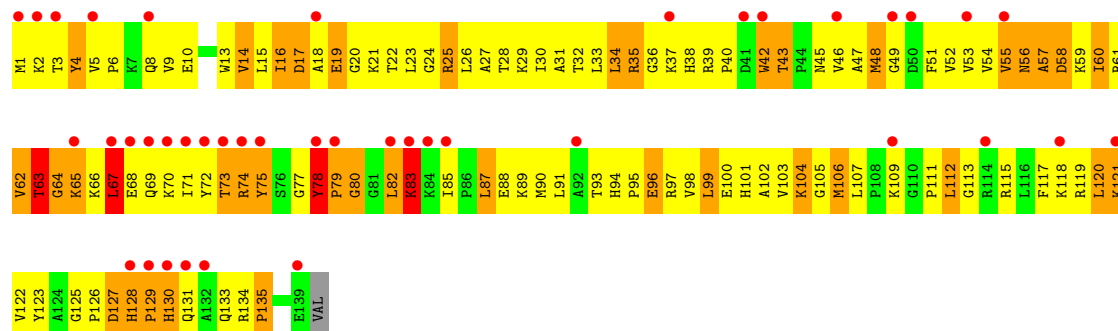
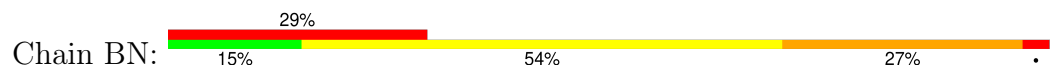
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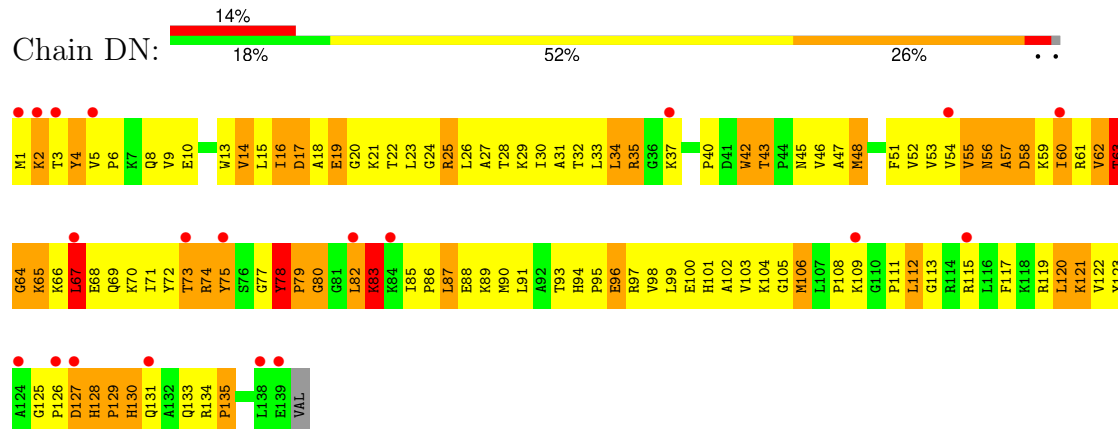
● Molecule 38: 50S ribosomal protein L9



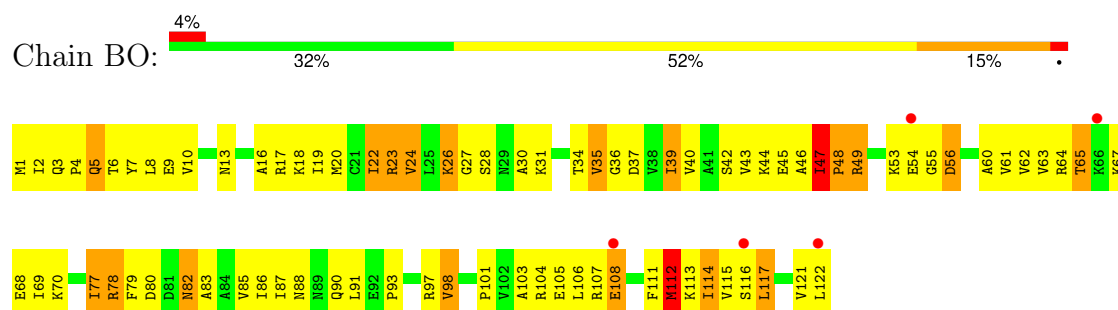
● Molecule 39: 50S ribosomal protein L13



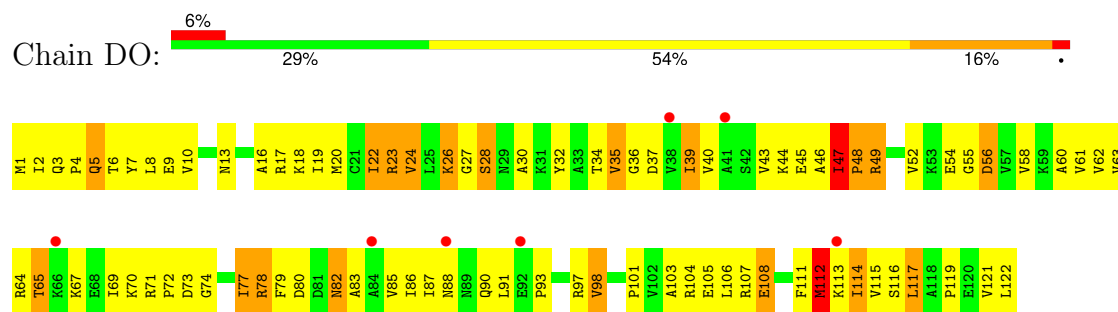
- Molecule 39: 50S ribosomal protein L13



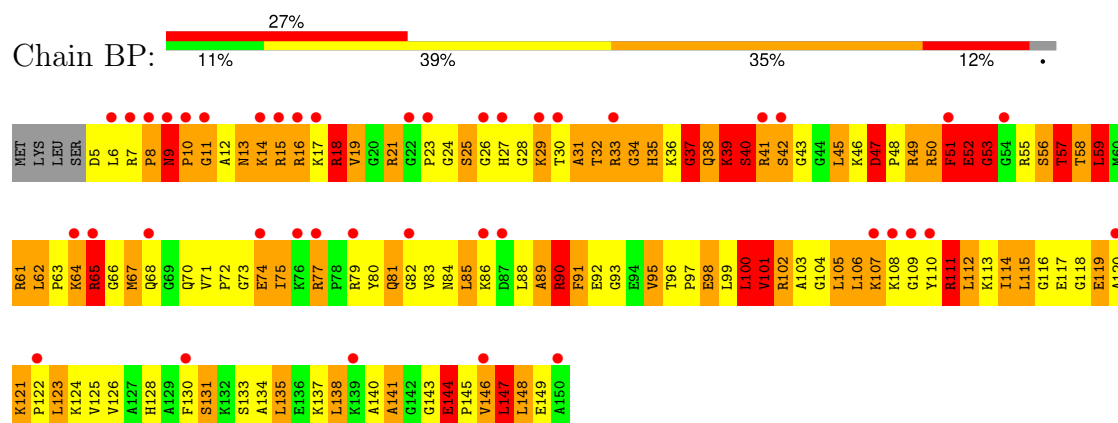
- Molecule 40: 50S ribosomal protein L14



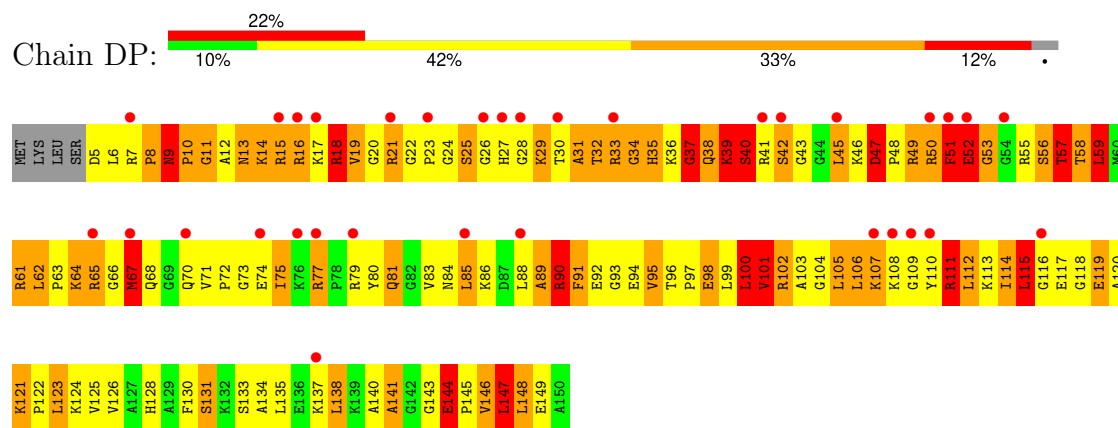
- Molecule 40: 50S ribosomal protein L14



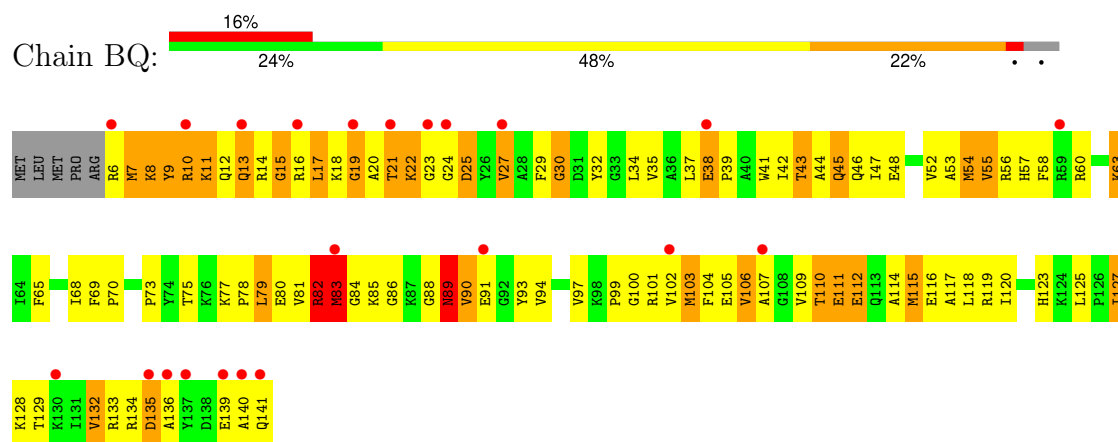
- Molecule 41: 50S ribosomal protein L15



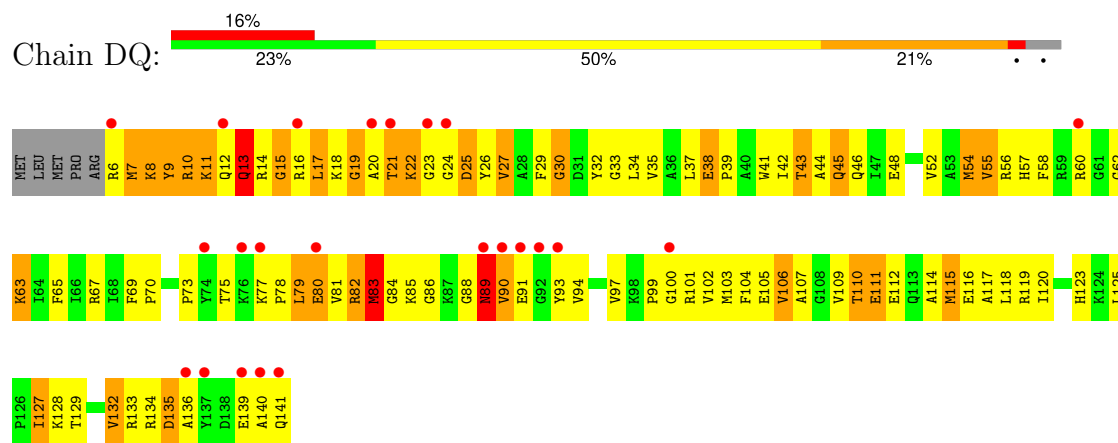
- Molecule 41: 50S ribosomal protein L15



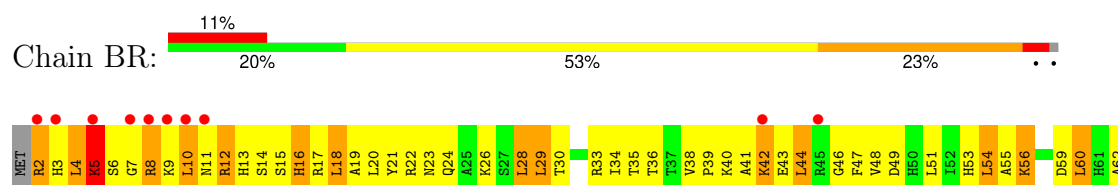
- Molecule 42: 50S ribosomal protein L16

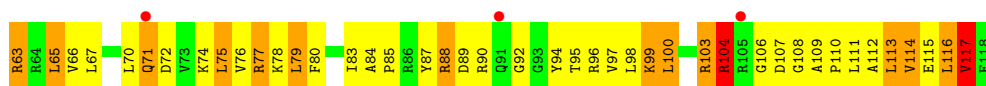


- Molecule 42: 50S ribosomal protein L16



- Molecule 43: 50S ribosomal protein L17

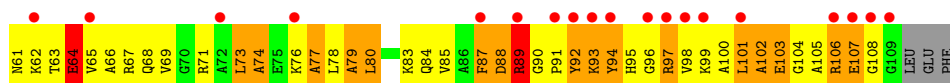




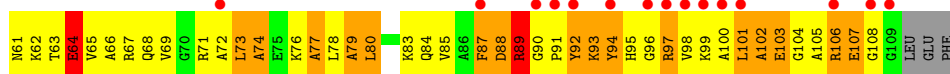
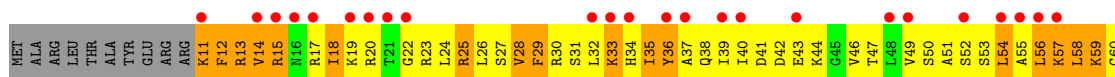
• Molecule 43: 50S ribosomal protein L17



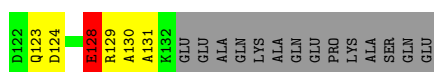
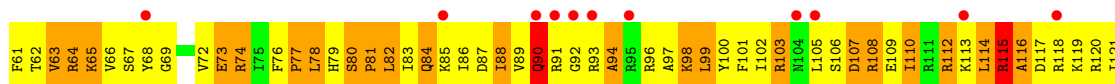
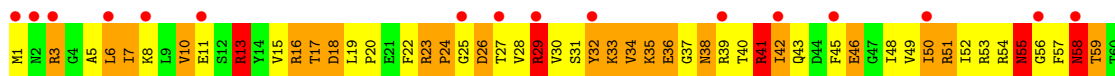
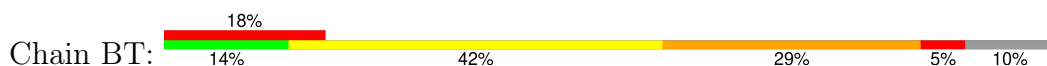
• Molecule 44: 50S ribosomal protein L18



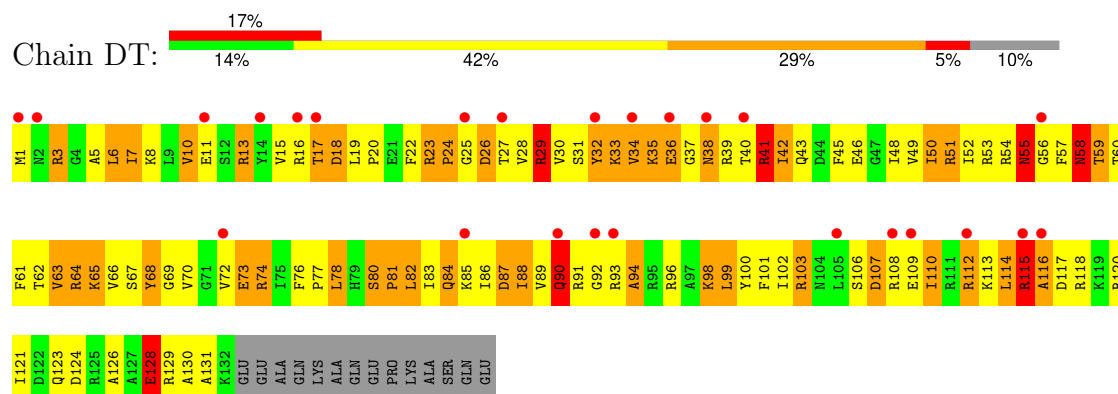
• Molecule 44: 50S ribosomal protein L18



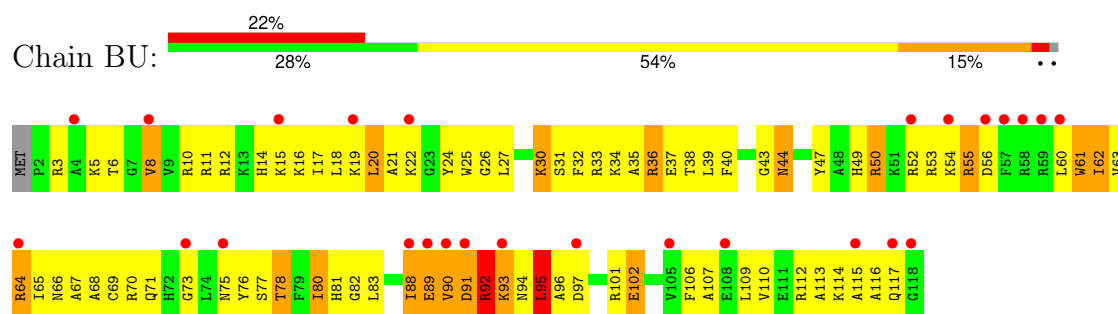
• Molecule 45: 50S ribosomal protein L19



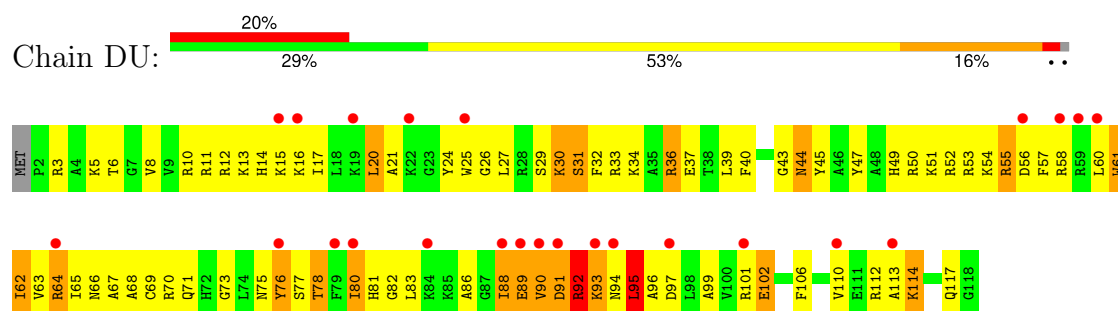
- Molecule 45: 50S ribosomal protein L19



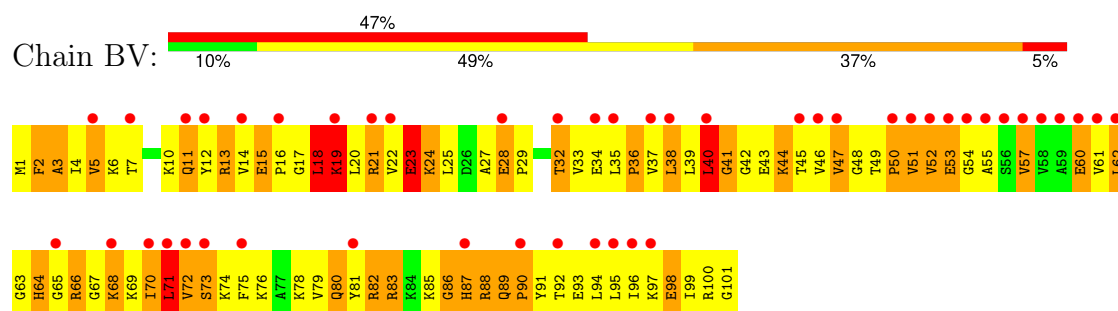
- Molecule 46: 50S ribosomal protein L20



- Molecule 46: 50S ribosomal protein L20

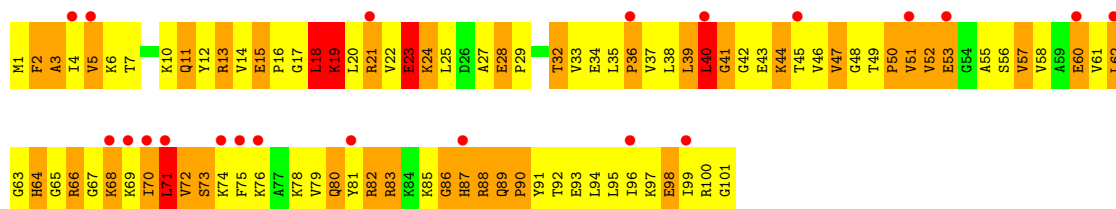


- Molecule 47: 50S ribosomal protein L21

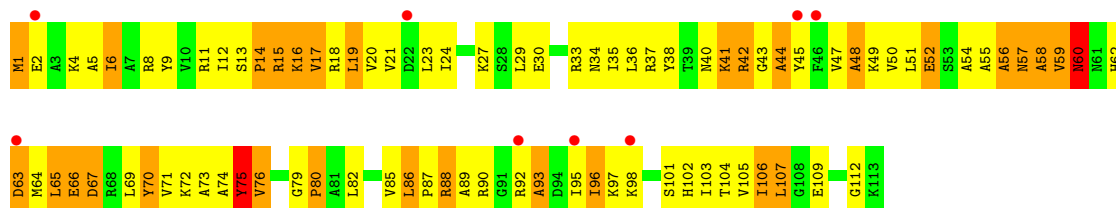


- Molecule 47: 50S ribosomal protein L21

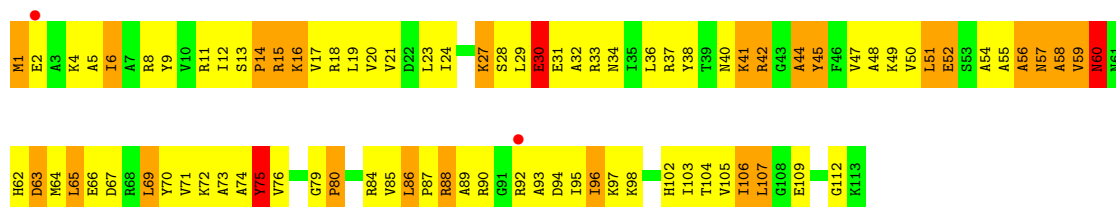




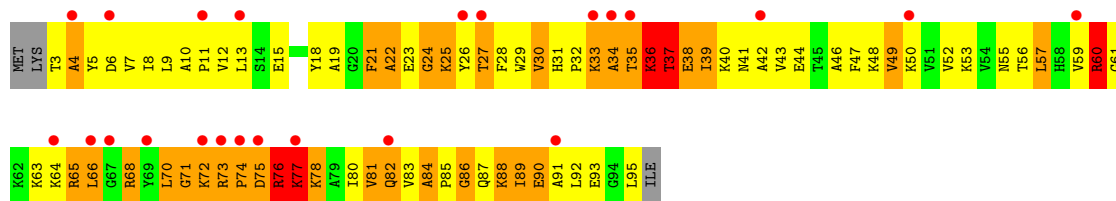
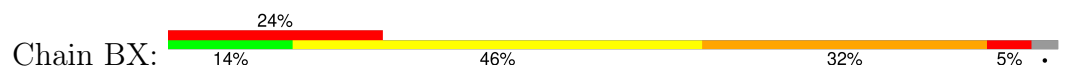
• Molecule 48: 50S ribosomal protein L22



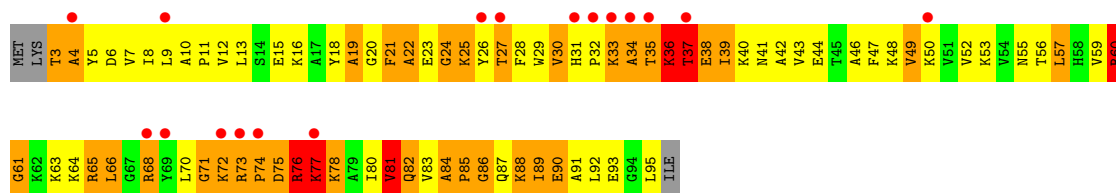
• Molecule 48: 50S ribosomal protein L22



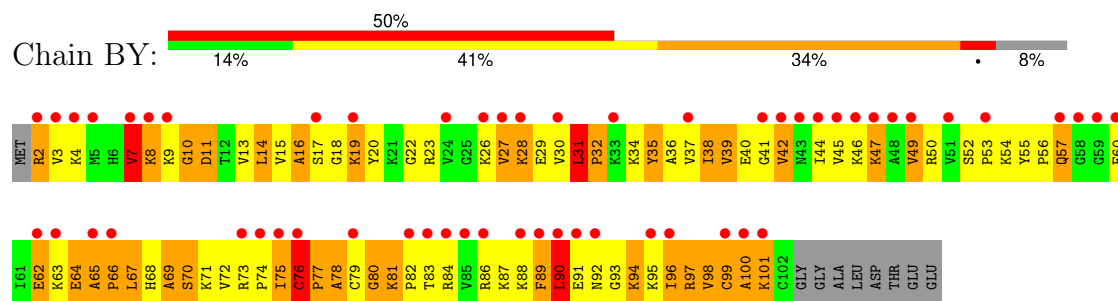
• Molecule 49: 50S ribosomal protein L23



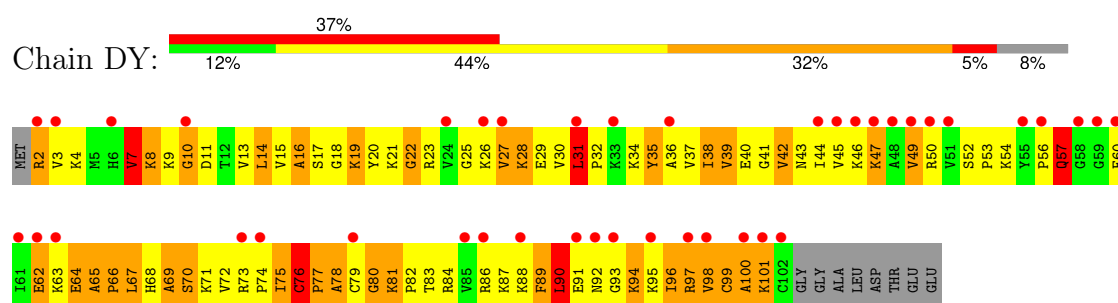
• Molecule 49: 50S ribosomal protein L23



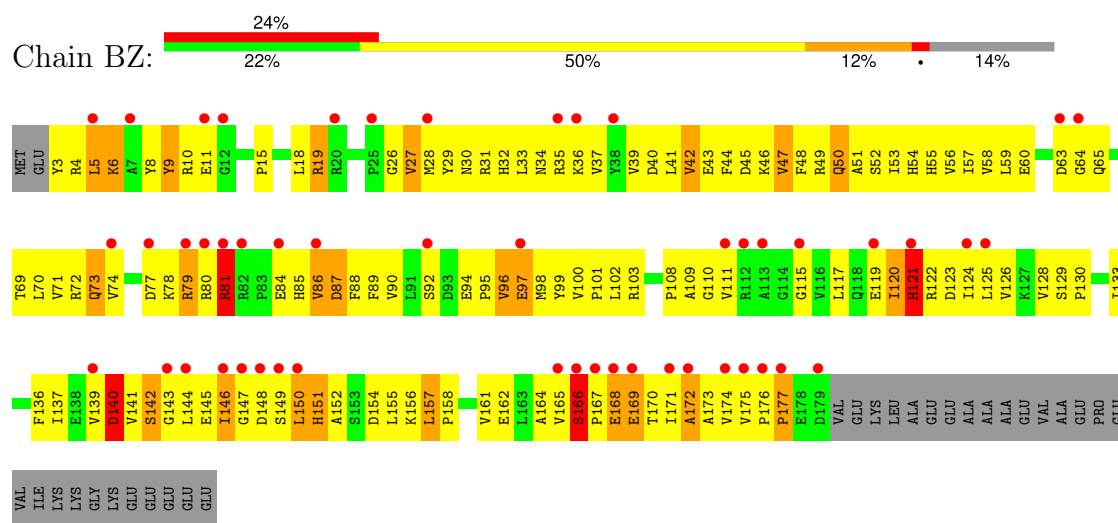
- Molecule 50: 50S ribosomal protein L24



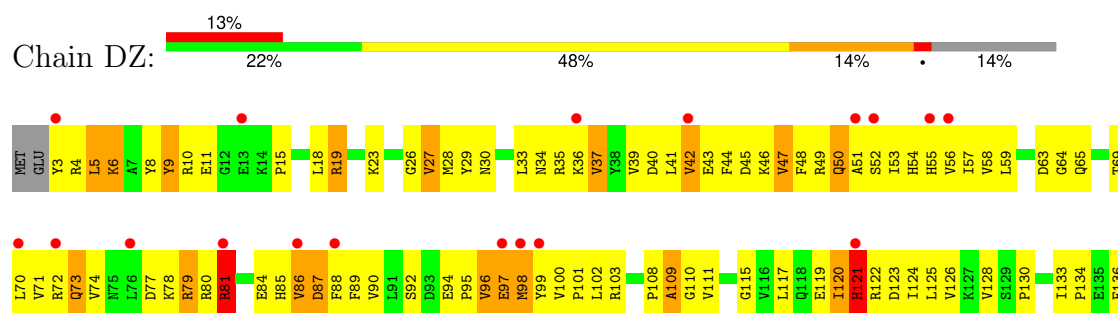
- Molecule 50: 50S ribosomal protein L24

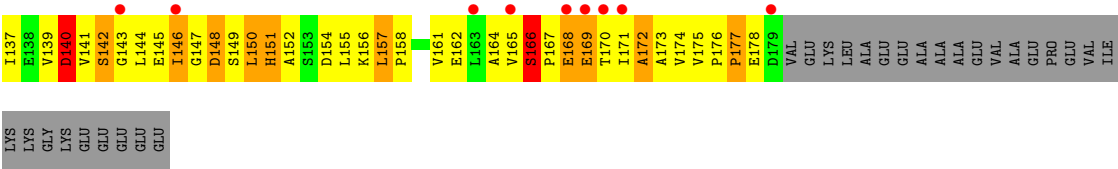


- Molecule 51: 50S ribosomal protein L25



- 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	207.32Å 437.99Å 614.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 3.10 48.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.97-3.10) 91.3 (48.97-3.10)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.246 , 0.284 0.242 , 0.279	Depositor DCC
R_{free} test set	45926 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	88.4	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 112.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	278037	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

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

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, ZN, TEL, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.54	2/36190 (0.0%)	0.91	51/56486 (0.1%)
1	CA	0.52	2/36190 (0.0%)	0.92	61/56486 (0.1%)
2	AB	0.28	0/1936	0.49	0/2611
2	CB	0.28	0/1936	0.48	0/2611
3	AC	0.27	0/1637	0.45	0/2207
3	CC	0.27	0/1637	0.44	0/2207
4	AD	0.32	0/1733	0.54	0/2318
4	CD	0.34	0/1733	0.55	0/2318
5	AE	0.36	0/1163	0.55	0/1566
5	CE	0.34	0/1163	0.55	0/1566
6	AF	0.35	0/856	0.57	0/1154
6	CF	0.35	0/856	0.56	0/1154
7	AG	0.26	0/1276	0.43	0/1709
7	CG	0.26	0/1276	0.43	0/1709
8	AH	0.36	0/1136	0.56	0/1527
8	CH	0.35	0/1136	0.56	0/1527
9	AI	0.28	0/1028	0.44	0/1375
9	CI	0.28	0/1028	0.44	0/1375
10	AJ	0.27	0/808	0.48	0/1087
10	CJ	0.27	0/808	0.48	0/1087
11	AK	0.34	0/900	0.55	0/1213
11	CK	0.33	0/900	0.55	0/1213
12	AL	0.40	0/987	0.65	0/1322
12	CL	0.40	0/987	0.66	0/1322
13	AM	0.28	0/928	0.48	0/1238
13	CM	0.28	0/928	0.48	0/1238
14	AN	0.28	0/501	0.46	0/664
14	CN	0.29	0/501	0.46	0/664
15	AO	0.35	0/745	0.55	0/992
15	CO	0.34	0/745	0.54	0/992
16	AP	0.34	0/717	0.55	0/965
16	CP	0.34	0/717	0.56	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.35	0/837	0.56	0/1119
17	CQ	0.35	0/837	0.55	0/1119
18	AR	0.35	0/579	0.57	0/768
18	CR	0.34	0/579	0.57	0/768
19	AS	0.28	0/643	0.45	0/867
19	CS	0.29	0/643	0.45	0/867
20	AT	0.34	0/765	0.53	0/1007
20	CT	0.34	0/765	0.54	0/1007
21	AU	0.26	0/213	0.42	0/279
21	CU	0.28	0/213	0.43	0/279
22	B0	0.60	0/658	0.75	0/878
22	D0	0.54	0/658	0.73	0/878
23	B1	0.69	0/700	0.97	0/931
23	D1	0.61	0/700	0.92	1/931 (0.1%)
24	B2	0.61	0/423	0.92	1/560 (0.2%)
24	D2	0.55	0/423	0.88	1/560 (0.2%)
25	B3	0.62	0/473	0.71	0/636
25	D3	0.45	0/473	0.66	0/636
26	B4	0.26	0/156	0.53	0/215
26	D4	0.28	0/156	0.52	0/215
27	B5	0.83	2/473 (0.4%)	1.04	3/639 (0.5%)
27	D5	0.67	0/473	1.01	3/639 (0.5%)
28	B6	0.73	0/387	0.91	2/517 (0.4%)
28	D6	0.60	0/387	0.85	1/517 (0.2%)
29	B7	0.67	0/427	0.83	0/563
29	D7	0.61	0/427	0.81	0/563
30	B8	0.72	0/516	0.98	1/681 (0.1%)
30	D8	0.61	0/516	0.94	1/681 (0.1%)
31	BA	1.17	111/65745 (0.2%)	1.49	1343/102639 (1.3%)
31	DA	0.89	28/65745 (0.0%)	1.45	1209/102639 (1.2%)
32	BB	0.87	0/2853	1.26	35/4451 (0.8%)
32	DB	0.63	0/2853	1.18	25/4451 (0.6%)
33	BD	0.63	0/2155	0.85	3/2907 (0.1%)
33	DD	0.58	0/2155	0.82	2/2907 (0.1%)
34	BE	0.69	0/1597	0.87	2/2155 (0.1%)
34	DE	0.58	0/1597	0.83	0/2155
35	BF	0.65	2/1659 (0.1%)	0.77	0/2246
35	DF	0.53	1/1659 (0.1%)	0.74	0/2246
36	BG	0.37	0/1498	0.61	1/2013 (0.0%)
36	DG	0.35	0/1498	0.59	1/2013 (0.0%)
37	BH	0.57	0/1246	0.71	0/1684
37	DH	0.41	0/1246	0.66	0/1684
38	BI	0.40	0/1147	0.65	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.43	0/1147	0.66	1/1553 (0.1%)
39	BN	0.71	0/1132	0.83	0/1527
39	DN	0.56	0/1132	0.76	0/1527
40	BO	0.62	0/943	0.74	0/1269
40	DO	0.53	0/943	0.73	0/1269
41	BP	0.65	0/1131	0.98	5/1504 (0.3%)
41	DP	0.56	0/1131	0.94	4/1504 (0.3%)
42	BQ	0.66	0/1100	0.80	1/1470 (0.1%)
42	DQ	0.55	0/1100	0.74	0/1470
43	BR	0.69	0/974	0.82	1/1302 (0.1%)
43	DR	0.57	0/974	0.80	2/1302 (0.2%)
44	BS	0.52	0/779	0.75	0/1038
44	DS	0.43	0/779	0.72	0/1038
45	BT	0.58	0/1114	0.82	0/1488
45	DT	0.52	0/1114	0.79	0/1488
46	BU	0.70	0/975	0.80	2/1297 (0.2%)
46	DU	0.56	0/975	0.74	1/1297 (0.1%)
47	BV	0.69	0/789	0.89	0/1054
47	DV	0.54	0/789	0.84	1/1054 (0.1%)
48	BW	0.76	0/907	0.91	1/1216 (0.1%)
48	DW	0.61	0/907	0.88	0/1216
49	BX	0.72	0/740	0.92	0/995
49	DX	0.63	0/740	0.90	0/995
50	BY	0.65	0/789	0.86	0/1053
50	DY	0.53	0/789	0.81	0/1053
51	BZ	0.46	0/1436	0.62	1/1951 (0.1%)
51	DZ	0.40	0/1436	0.61	1/1951 (0.1%)
All	All	0.79	148/301000 (0.0%)	1.17	2768/449812 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	CA	1	0
22	B0	0	1
22	D0	0	1
23	B1	0	1
23	D1	0	1
24	B2	0	1
24	D2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	B5	0	1
27	D5	0	1
31	BA	18	0
31	DA	18	0
33	BD	0	4
33	DD	0	2
34	BE	0	2
34	DE	0	2
37	BH	0	1
37	DH	0	1
41	BP	0	5
41	DP	0	3
42	BQ	0	1
42	DQ	0	1
43	BR	0	1
43	DR	0	1
45	BT	0	1
45	DT	0	1
47	BV	0	1
47	DV	0	2
49	BX	0	2
49	DX	0	3
All	All	37	42

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	1142(A)	A	N9-C4	-11.15	1.31	1.37
31	BA	783	A	N9-C4	-10.64	1.31	1.37
31	BA	669	G	C4'-C3'	-10.15	1.42	1.53
31	BA	774	A	N9-C4	-9.61	1.32	1.37
31	DA	1142(A)	A	N9-C4	-9.23	1.32	1.37

The worst 5 of 2768 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	55	A	C8-N9-C4	-18.55	98.38	105.80
1	AA	55	A	N7-C8-N9	17.45	122.53	113.80
31	BA	1332	G	N3-C4-C5	16.73	136.96	128.60
31	BA	1332	G	N3-C4-N9	-16.73	115.96	126.00
31	BA	814	C	C6-N1-C2	15.82	126.63	120.30

5 of 37 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	BA	472	A	C3'
31	BA	669	G	C1',C4',C3'
31	BA	945	A	C1'
31	BA	1300	U	C4',C3'
31	BA	1379	A	C1'

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	B0	11	ARG	Peptide
23	B1	30	VAL	Peptide
24	B2	54	LYS	Peptide
27	B5	51	TYR	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	2214	12
1	CA	32329	0	16318	2202	2
2	AB	1901	0	1951	203	0
2	CB	1901	0	1951	204	0
3	AC	1613	0	1677	143	0
3	CC	1613	0	1677	145	0
4	AD	1703	0	1763	229	0
4	CD	1703	0	1764	232	0
5	AE	1147	0	1207	126	0
5	CE	1147	0	1207	145	0
6	AF	843	0	857	116	0
6	CF	843	0	857	125	0
7	AG	1257	0	1296	77	0
7	CG	1257	0	1296	81	0
8	AH	1116	0	1177	144	0
8	CH	1116	0	1177	137	0
9	AI	1011	0	1042	112	0
9	CI	1011	0	1042	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	102	0
10	CJ	795	0	840	105	0
11	AK	885	0	904	109	0
11	CK	885	0	904	116	0
12	AL	971	0	1057	136	0
12	CL	971	0	1057	131	0
13	AM	921	0	976	97	0
13	CM	921	0	976	91	0
14	AN	492	0	532	46	0
14	CN	492	0	529	49	0
15	AO	734	0	771	81	0
15	CO	734	0	771	79	0
16	AP	701	0	720	103	0
16	CP	701	0	720	110	0
17	AQ	824	0	891	81	0
17	CQ	824	0	891	78	0
18	AR	574	0	644	86	0
18	CR	574	0	644	86	0
19	AS	630	0	652	53	0
19	CS	630	0	652	50	0
20	AT	763	0	861	93	0
20	CT	763	0	861	94	0
21	AU	209	0	221	14	0
21	CU	209	0	221	12	0
22	B0	650	0	654	90	0
22	D0	650	0	654	95	0
23	B1	693	0	764	149	0
23	D1	693	0	764	156	0
24	B2	421	0	461	141	0
24	D2	421	0	461	136	0
25	B3	468	0	523	47	0
25	D3	468	0	523	70	0
26	B4	157	0	69	7	0
26	D4	157	0	69	8	0
27	B5	459	0	480	100	0
27	D5	459	0	480	100	0
28	B6	381	0	390	102	0
28	D6	381	0	390	95	0
29	B7	419	0	467	54	0
29	D7	419	0	467	57	0
30	B8	508	0	576	156	0
30	D8	508	0	576	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BA	58698	0	29589	4119	0
31	DA	58698	0	29591	4387	0
32	BB	2551	0	1295	239	0
32	DB	2551	0	1295	231	0
33	BD	2105	0	2182	402	0
33	DD	2105	0	2182	406	0
34	BE	1564	0	1629	278	0
34	DE	1564	0	1629	278	0
35	BF	1624	0	1677	214	0
35	DF	1624	0	1677	209	0
36	BG	1474	0	1534	220	0
36	DG	1474	0	1534	223	0
37	BH	1223	0	1282	170	0
37	DH	1223	0	1282	162	0
38	BI	1132	0	1218	167	2
38	DI	1132	0	1218	158	12
39	BN	1105	0	1180	231	0
39	DN	1105	0	1180	231	0
40	BO	933	0	996	138	0
40	DO	933	0	996	133	0
41	BP	1114	0	1187	372	0
41	DP	1114	0	1187	345	0
42	BQ	1080	0	1127	195	0
42	DQ	1080	0	1127	195	0
43	BR	960	0	1021	136	0
43	DR	960	0	1021	146	0
44	BS	771	0	832	166	0
44	DS	771	0	832	172	0
45	BT	1100	0	1164	210	0
45	DT	1100	0	1164	213	0
46	BU	958	0	1015	171	0
46	DU	958	0	1015	177	0
47	BV	779	0	851	265	0
47	DV	779	0	851	258	0
48	BW	896	0	953	110	0
48	DW	896	0	953	128	0
49	BX	726	0	778	203	0
49	DX	726	0	777	199	0
50	BY	776	0	870	193	0
50	DY	776	0	870	191	0
51	BZ	1404	0	1432	190	0
51	DZ	1404	0	1432	196	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AA	52	0	0	0	0
52	B0	1	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	B7	1	0	0	0	0
52	BA	360	0	0	0	0
52	BB	7	0	0	0	0
52	BD	2	0	0	0	0
52	BF	1	0	0	0	0
52	BP	3	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	1	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	50	0	0	0	0
52	D5	1	0	0	0	0
52	D7	1	0	0	0	0
52	D8	1	0	0	0	0
52	DA	318	0	0	0	0
52	DB	3	0	0	0	0
52	DD	2	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	2	0	0	0	0
52	DU	1	0	0	0	0
52	DX	1	0	0	0	0
53	AD	1	0	0	0	0
53	AN	1	0	0	0	0
53	CD	1	0	0	0	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	58	0	65	32	0
55	DA	58	0	65	34	0
All	All	278037	0	189235	24925	14

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 54.

The worst 5 of 24925 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)
1:CA:921:U:H1'	1:CA:922:G:C4	1.55	1.40
55:DA:3320:TEL:H11	55:DA:3320:TEL:C14	1.64	1.28
55:BA:3362:TEL:H11	55:BA:3362:TEL:C14	1.64	1.24
33:BD:35:LYS:HD2	33:BD:104:TYR:CD1	1.73	1.22
26:B4:13:ARG:HA	36:BG:101:ILE:HG13	1.22	1.19

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:358:U:OP2	38:DI:90:GLY:N[2_655]	1.80	0.40
1:AA:55:A:C8	38:DI:82:ARG:NE[2_655]	1.98	0.22
1:AA:55:A:O4'	38:DI:82:ARG:NE[2_655]	1.98	0.22
1:AA:358:U:O4'	38:DI:89:TYR:CD1[2_655]	1.99	0.21
1:AA:359:U:O5'	38:DI:87:LYS:O[2_655]	1.99	0.21

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	168 (72%)	49 (21%)	16 (7%)	1	5
2	CB	233/256 (91%)	169 (72%)	48 (21%)	16 (7%)	1	5
3	AC	205/239 (86%)	152 (74%)	40 (20%)	13 (6%)	1	7
3	CC	205/239 (86%)	153 (75%)	40 (20%)	12 (6%)	1	8
4	AD	206/209 (99%)	131 (64%)	49 (24%)	26 (13%)	0	1
4	CD	206/209 (99%)	130 (63%)	48 (23%)	28 (14%)	0	1
5	AE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	0	3
5	CE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	0	3
6	AF	99/101 (98%)	69 (70%)	18 (18%)	12 (12%)	0	1
6	CF	99/101 (98%)	66 (67%)	20 (20%)	13 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	153/156 (98%)	126 (82%)	22 (14%)	5 (3%)	3	17
7	CG	153/156 (98%)	127 (83%)	21 (14%)	5 (3%)	3	17
8	AH	136/138 (99%)	100 (74%)	26 (19%)	10 (7%)	1	5
8	CH	136/138 (99%)	99 (73%)	28 (21%)	9 (7%)	1	6
9	AI	123/128 (96%)	85 (69%)	27 (22%)	11 (9%)	0	3
9	CI	123/128 (96%)	86 (70%)	26 (21%)	11 (9%)	0	3
10	AJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	3	19
10	CJ	97/105 (92%)	76 (78%)	18 (19%)	3 (3%)	3	19
11	AK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	6
11	CK	117/129 (91%)	86 (74%)	23 (20%)	8 (7%)	1	6
12	AL	123/135 (91%)	76 (62%)	26 (21%)	21 (17%)	0	0
12	CL	123/135 (91%)	77 (63%)	24 (20%)	22 (18%)	0	0
13	AM	107/126 (85%)	75 (70%)	26 (24%)	6 (6%)	1	8
13	CM	107/126 (85%)	74 (69%)	27 (25%)	6 (6%)	1	8
14	AN	58/61 (95%)	48 (83%)	5 (9%)	5 (9%)	0	4
14	CN	58/61 (95%)	48 (83%)	5 (9%)	5 (9%)	0	4
15	AO	86/89 (97%)	56 (65%)	21 (24%)	9 (10%)	0	2
15	CO	86/89 (97%)	56 (65%)	21 (24%)	9 (10%)	0	2
16	AP	82/88 (93%)	48 (58%)	21 (26%)	13 (16%)	0	0
16	CP	82/88 (93%)	48 (58%)	21 (26%)	13 (16%)	0	0
17	AQ	98/105 (93%)	76 (78%)	17 (17%)	5 (5%)	1	10
17	CQ	98/105 (93%)	76 (78%)	17 (17%)	5 (5%)	1	10
18	AR	68/88 (77%)	43 (63%)	20 (29%)	5 (7%)	1	5
18	CR	68/88 (77%)	42 (62%)	19 (28%)	7 (10%)	0	3
19	AS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1	4
19	CS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1	4
20	AT	97/106 (92%)	58 (60%)	24 (25%)	15 (16%)	0	0
20	CT	97/106 (92%)	53 (55%)	29 (30%)	15 (16%)	0	0
21	AU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	13
21	CU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	13
22	B0	83/85 (98%)	67 (81%)	9 (11%)	7 (8%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	D0	83/85 (98%)	62 (75%)	14 (17%)	7 (8%)	0	4
23	B1	87/98 (89%)	43 (49%)	27 (31%)	17 (20%)	0	0
23	D1	87/98 (89%)	44 (51%)	26 (30%)	17 (20%)	0	0
24	B2	49/72 (68%)	25 (51%)	14 (29%)	10 (20%)	0	0
24	D2	49/72 (68%)	26 (53%)	13 (26%)	10 (20%)	0	0
25	B3	58/60 (97%)	48 (83%)	9 (16%)	1 (2%)	7	30
25	D3	58/60 (97%)	44 (76%)	13 (22%)	1 (2%)	7	30
26	B4	30/71 (42%)	7 (23%)	11 (37%)	12 (40%)	0	0
26	D4	30/71 (42%)	6 (20%)	11 (37%)	13 (43%)	0	0
27	B5	57/60 (95%)	37 (65%)	8 (14%)	12 (21%)	0	0
27	D5	57/60 (95%)	36 (63%)	8 (14%)	13 (23%)	0	0
28	B6	41/54 (76%)	19 (46%)	10 (24%)	12 (29%)	0	0
28	D6	41/54 (76%)	18 (44%)	11 (27%)	12 (29%)	0	0
29	B7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	5	25
29	D7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	5	25
30	B8	62/65 (95%)	37 (60%)	15 (24%)	10 (16%)	0	0
30	D8	62/65 (95%)	38 (61%)	13 (21%)	11 (18%)	0	0
33	BD	270/276 (98%)	203 (75%)	50 (18%)	17 (6%)	1	7
33	DD	270/276 (98%)	202 (75%)	52 (19%)	16 (6%)	1	8
34	BE	203/206 (98%)	133 (66%)	43 (21%)	27 (13%)	0	1
34	DE	203/206 (98%)	136 (67%)	39 (19%)	28 (14%)	0	1
35	BF	206/210 (98%)	138 (67%)	44 (21%)	24 (12%)	0	1
35	DF	206/210 (98%)	137 (66%)	45 (22%)	24 (12%)	0	1
36	BG	177/182 (97%)	110 (62%)	46 (26%)	21 (12%)	0	1
36	DG	177/182 (97%)	109 (62%)	47 (27%)	21 (12%)	0	1
37	BH	158/180 (88%)	98 (62%)	38 (24%)	22 (14%)	0	1
37	DH	158/180 (88%)	97 (61%)	37 (23%)	24 (15%)	0	0
38	BI	144/148 (97%)	86 (60%)	36 (25%)	22 (15%)	0	0
38	DI	144/148 (97%)	83 (58%)	38 (26%)	23 (16%)	0	0
39	BN	137/140 (98%)	93 (68%)	29 (21%)	15 (11%)	0	2
39	DN	137/140 (98%)	97 (71%)	25 (18%)	15 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BO	120/122 (98%)	96 (80%)	19 (16%)	5 (4%)	2	13
40	DO	120/122 (98%)	98 (82%)	17 (14%)	5 (4%)	2	13
41	BP	144/150 (96%)	72 (50%)	31 (22%)	41 (28%)	0	0
41	DP	144/150 (96%)	72 (50%)	29 (20%)	43 (30%)	0	0
42	BQ	134/141 (95%)	92 (69%)	29 (22%)	13 (10%)	0	3
42	DQ	134/141 (95%)	91 (68%)	29 (22%)	14 (10%)	0	2
43	BR	115/118 (98%)	70 (61%)	34 (30%)	11 (10%)	0	3
43	DR	115/118 (98%)	71 (62%)	34 (30%)	10 (9%)	0	4
44	BS	97/112 (87%)	43 (44%)	26 (27%)	28 (29%)	0	0
44	DS	97/112 (87%)	41 (42%)	29 (30%)	27 (28%)	0	0
45	BT	130/146 (89%)	80 (62%)	25 (19%)	25 (19%)	0	0
45	DT	130/146 (89%)	80 (62%)	26 (20%)	24 (18%)	0	0
46	BU	115/118 (98%)	78 (68%)	29 (25%)	8 (7%)	1	5
46	DU	115/118 (98%)	82 (71%)	24 (21%)	9 (8%)	1	4
47	BV	97/101 (96%)	49 (50%)	24 (25%)	24 (25%)	0	0
47	DV	97/101 (96%)	47 (48%)	25 (26%)	25 (26%)	0	0
48	BW	111/113 (98%)	81 (73%)	11 (10%)	19 (17%)	0	0
48	DW	111/113 (98%)	78 (70%)	15 (14%)	18 (16%)	0	0
49	BX	91/96 (95%)	45 (50%)	22 (24%)	24 (26%)	0	0
49	DX	91/96 (95%)	45 (50%)	21 (23%)	25 (28%)	0	0
50	BY	99/110 (90%)	41 (41%)	25 (25%)	33 (33%)	0	0
50	DY	99/110 (90%)	41 (41%)	27 (27%)	31 (31%)	0	0
51	BZ	175/206 (85%)	117 (67%)	41 (23%)	17 (10%)	0	3
51	DZ	175/206 (85%)	116 (66%)	41 (23%)	18 (10%)	0	3
All	All	11148/12060 (92%)	7385 (66%)	2386 (21%)	1377 (12%)	0	1

5 of 1377 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	34	ALA
2	AB	165	VAL
2	AB	194	PRO
3	AC	54	ARG

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%)	182 (90%)	20 (10%)	6	24
2	CB	202/220 (92%)	183 (91%)	19 (9%)	7	27
3	AC	160/188 (85%)	154 (96%)	6 (4%)	28	59
3	CC	160/188 (85%)	154 (96%)	6 (4%)	28	59
4	AD	180/181 (99%)	157 (87%)	23 (13%)	3	15
4	CD	180/181 (99%)	156 (87%)	24 (13%)	3	13
5	AE	115/123 (94%)	101 (88%)	14 (12%)	4	16
5	CE	115/123 (94%)	101 (88%)	14 (12%)	4	16
6	AF	90/90 (100%)	80 (89%)	10 (11%)	5	20
6	CF	90/90 (100%)	80 (89%)	10 (11%)	5	20
7	AG	126/127 (99%)	120 (95%)	6 (5%)	21	51
7	CG	126/127 (99%)	120 (95%)	6 (5%)	21	51
8	AH	119/119 (100%)	104 (87%)	15 (13%)	3	15
8	CH	119/119 (100%)	105 (88%)	14 (12%)	4	17
9	AI	98/99 (99%)	87 (89%)	11 (11%)	5	20
9	CI	98/99 (99%)	88 (90%)	10 (10%)	6	23
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	2	10
10	CJ	88/92 (96%)	76 (86%)	12 (14%)	3	13
11	AK	90/99 (91%)	83 (92%)	7 (8%)	10	35
11	CK	90/99 (91%)	83 (92%)	7 (8%)	10	35
12	AL	104/111 (94%)	94 (90%)	10 (10%)	7	26
12	CL	104/111 (94%)	94 (90%)	10 (10%)	7	26
13	AM	93/101 (92%)	85 (91%)	8 (9%)	8	31
13	CM	93/101 (92%)	85 (91%)	8 (9%)	8	31
14	AN	49/50 (98%)	46 (94%)	3 (6%)	15	43
14	CN	49/50 (98%)	46 (94%)	3 (6%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	79/80 (99%)	71 (90%)	8 (10%)	6	23
15	CO	79/80 (99%)	71 (90%)	8 (10%)	6	23
16	AP	72/74 (97%)	61 (85%)	11 (15%)	2	10
16	CP	72/74 (97%)	61 (85%)	11 (15%)	2	10
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	8	32
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	8	32
18	AR	61/77 (79%)	55 (90%)	6 (10%)	6	25
18	CR	61/77 (79%)	55 (90%)	6 (10%)	6	25
19	AS	69/80 (86%)	60 (87%)	9 (13%)	3	14
19	CS	69/80 (86%)	60 (87%)	9 (13%)	3	14
20	AT	76/82 (93%)	65 (86%)	11 (14%)	2	11
20	CT	76/82 (93%)	64 (84%)	12 (16%)	2	9
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%)	48 (79%)	13 (21%)	1	4
22	D0	61/67 (91%)	48 (79%)	13 (21%)	1	4
23	B1	73/83 (88%)	51 (70%)	22 (30%)	0	0
23	D1	73/83 (88%)	53 (73%)	20 (27%)	0	1
24	B2	46/67 (69%)	28 (61%)	18 (39%)	0	0
24	D2	46/67 (69%)	28 (61%)	18 (39%)	0	0
25	B3	51/52 (98%)	41 (80%)	10 (20%)	1	5
25	D3	51/52 (98%)	42 (82%)	9 (18%)	1	7
27	B5	51/52 (98%)	39 (76%)	12 (24%)	0	2
27	D5	51/52 (98%)	41 (80%)	10 (20%)	1	5
28	B6	43/52 (83%)	27 (63%)	16 (37%)	0	0
28	D6	43/52 (83%)	28 (65%)	15 (35%)	0	0
29	B7	41/42 (98%)	32 (78%)	9 (22%)	1	3
29	D7	41/42 (98%)	31 (76%)	10 (24%)	0	2
30	B8	53/55 (96%)	36 (68%)	17 (32%)	0	0
30	D8	53/55 (96%)	35 (66%)	18 (34%)	0	0
33	BD	213/218 (98%)	160 (75%)	53 (25%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
33	DD	213/218 (98%)	157 (74%)	56 (26%)	0	1	
34	BE	165/166 (99%)	127 (77%)	38 (23%)	0	3	
34	DE	165/166 (99%)	126 (76%)	39 (24%)	0	2	
35	BF	165/166 (99%)	130 (79%)	35 (21%)	1	4	
35	DF	165/166 (99%)	132 (80%)	33 (20%)	1	4	
36	BG	155/156 (99%)	126 (81%)	29 (19%)	1	5	
36	DG	155/156 (99%)	126 (81%)	29 (19%)	1	5	
37	BH	132/148 (89%)	105 (80%)	27 (20%)	1	4	
37	DH	132/148 (89%)	107 (81%)	25 (19%)	1	5	
38	BI	122/124 (98%)	99 (81%)	23 (19%)	1	5	
38	DI	122/124 (98%)	100 (82%)	22 (18%)	1	6	
39	BN	117/119 (98%)	80 (68%)	37 (32%)	0	0	
39	DN	117/119 (98%)	81 (69%)	36 (31%)	0	0	
40	BO	100/100 (100%)	82 (82%)	18 (18%)	1	6	
40	DO	100/100 (100%)	80 (80%)	20 (20%)	1	4	
41	BP	112/116 (97%)	67 (60%)	45 (40%)	0	0	
41	DP	112/116 (97%)	67 (60%)	45 (40%)	0	0	
42	BQ	106/111 (96%)	81 (76%)	25 (24%)	0	2	
42	DQ	106/111 (96%)	82 (77%)	24 (23%)	1	3	
43	BR	100/101 (99%)	76 (76%)	24 (24%)	0	2	
43	DR	100/101 (99%)	76 (76%)	24 (24%)	0	2	
44	BS	77/88 (88%)	59 (77%)	18 (23%)	0	2	
44	DS	77/88 (88%)	59 (77%)	18 (23%)	0	2	
45	BT	116/127 (91%)	76 (66%)	40 (34%)	0	0	
45	DT	116/127 (91%)	77 (66%)	39 (34%)	0	0	
46	BU	92/94 (98%)	74 (80%)	18 (20%)	1	5	
46	DU	92/94 (98%)	71 (77%)	21 (23%)	0	3	
47	BV	82/82 (100%)	56 (68%)	26 (32%)	0	0	
47	DV	82/82 (100%)	57 (70%)	25 (30%)	0	0	
48	BW	91/92 (99%)	67 (74%)	24 (26%)	0	1	
48	DW	91/92 (99%)	69 (76%)	22 (24%)	0	2	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BX	74/78 (95%)	55 (74%)	19 (26%)	0	1
49	DX	74/78 (95%)	54 (73%)	20 (27%)	0	1
50	BY	84/91 (92%)	67 (80%)	17 (20%)	1	4
50	DY	84/91 (92%)	66 (79%)	18 (21%)	1	4
51	BZ	155/179 (87%)	132 (85%)	23 (15%)	2	10
51	DZ	155/179 (87%)	131 (84%)	24 (16%)	2	9
All	All	9322/9876 (94%)	7617 (82%)	1705 (18%)	1	6

5 of 1705 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	CF	97	PHE
29	D7	48	LYS
47	DV	13	ARG
9	CI	113	LYS
6	CF	94	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 256 such sidechains are listed below:

Mol	Chain	Res	Type
42	DQ	141	GLN
43	DR	61	HIS
42	BQ	13	GLN
41	BP	81	GLN
45	DT	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	307 (20%)	30 (1%)
1	CA	1503/1522 (98%)	307 (20%)	30 (1%)
31	BA	2723/2787 (97%)	822 (30%)	77 (2%)
31	DA	2723/2787 (97%)	827 (30%)	75 (2%)
32	BB	118/122 (96%)	42 (35%)	0
32	DB	118/122 (96%)	42 (35%)	0
All	All	8688/8862 (98%)	2347 (27%)	212 (2%)

5 of 2347 RNA backbone outliers are listed below:

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

5 of 212 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	366	C
31	DA	272	G
31	DA	2422	A
1	CA	509	A
1	CA	1064	G

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 827 ligands modelled in this entry, 825 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	TEL	BA	3362	-	58,62,62	1.77	7 (12%)	74,92,92	3.11	23 (31%)
55	TEL	DA	3320	-	58,62,62	1.77	7 (12%)	74,92,92	3.11	23 (31%)

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	TEL	BA	3362	-	-	31/73/108/108	0/4/5/5
55	TEL	DA	3320	-	-	31/73/108/108	0/4/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	3320	TEL	C43-C40	-7.29	1.37	1.49
55	BA	3362	TEL	C43-C40	-7.23	1.37	1.49
55	BA	3362	TEL	O5-C2	-4.94	1.40	1.47
55	DA	3320	TEL	O5-C2	-4.93	1.40	1.47
55	BA	3362	TEL	C36-N31	-4.30	1.31	1.38

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BA	3362	TEL	C8-C4-C2	-16.47	92.52	115.23
55	DA	3320	TEL	C8-C4-C2	-16.47	92.52	115.23
55	DA	3320	TEL	O9-C15-C21	10.31	121.11	110.93
55	BA	3362	TEL	O9-C15-C21	10.31	121.11	110.93
55	BA	3362	TEL	C2-O5-C10	-7.20	102.94	109.23

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

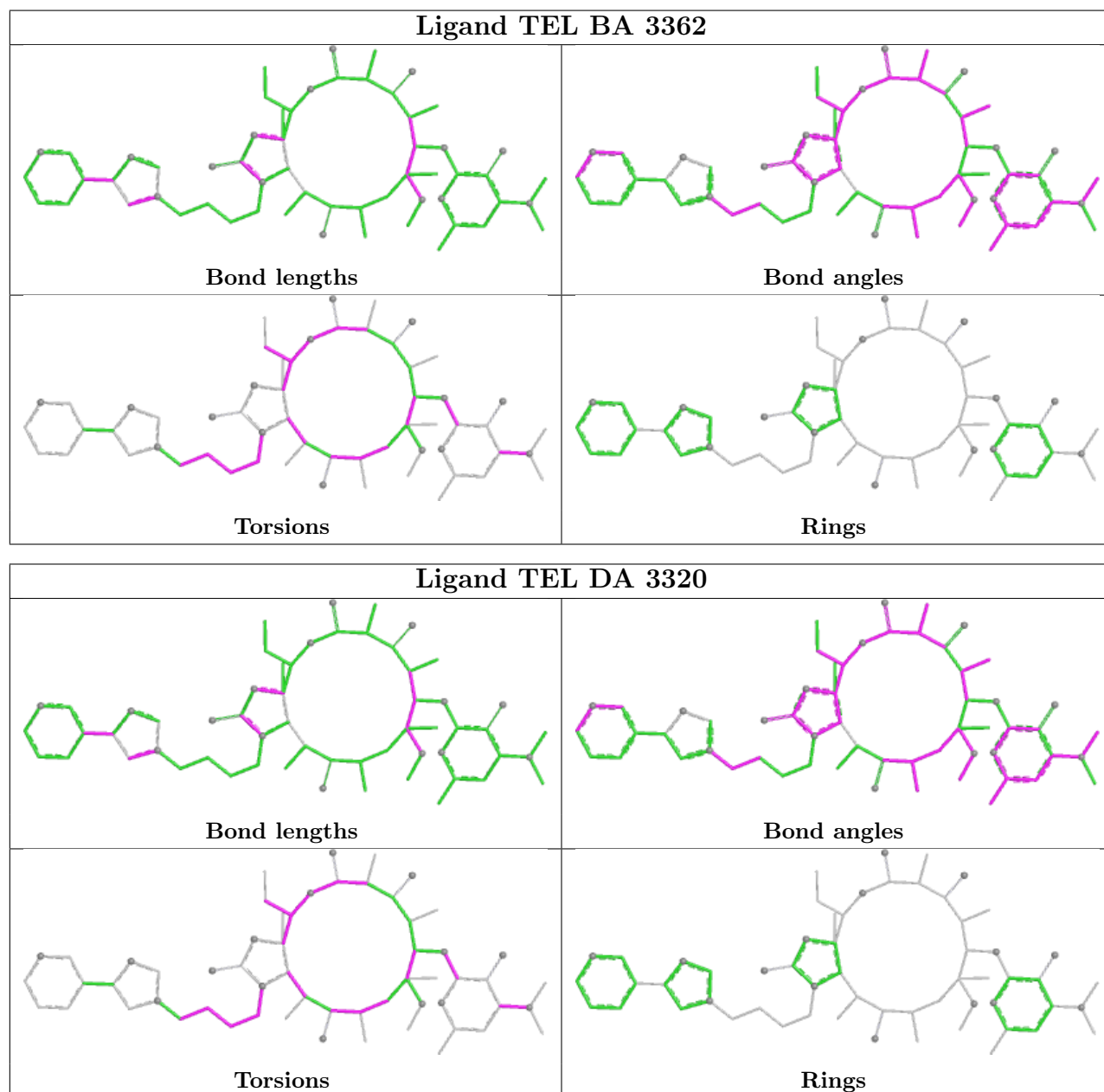
Mol	Chain	Res	Type	Atoms
55	BA	3362	TEL	C1-C2-C4-C8
55	BA	3362	TEL	C1-C2-C4-O9
55	BA	3362	TEL	C3-C2-C4-O9
55	BA	3362	TEL	O5-C2-C4-O9
55	BA	3362	TEL	C2-C3-C7-C13

There are no ring outliers.

2 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	BA	3362	TEL	32	0
55	DA	3320	TEL	34	0

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
36	DG	1
36	BG	1
28	D6	1
28	B6	1
9	AI	1
47	BV	1
9	CI	1
47	DV	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DG	112:PRO	C	113:ARG	N	5.74
1	BG	112:PRO	C	113:ARG	N	5.73
1	CM	69:GLU	C	70:LEU	N	4.94
1	AM	69:GLU	C	70:LEU	N	4.93
1	D6	46:HIS	C	47:THR	N	4.90

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.66	127 (8%) 18 10	64, 134, 200, 203	0
1	CA	1504/1522 (98%)	0.63	122 (8%) 19 11	67, 134, 200, 203	0
2	AB	235/256 (91%)	1.08	42 (17%) 4 2	122, 175, 196, 201	0
2	CB	235/256 (91%)	0.96	36 (15%) 6 3	123, 175, 196, 202	0
3	AC	207/239 (86%)	0.91	31 (14%) 6 3	122, 174, 194, 197	0
3	CC	207/239 (86%)	0.84	28 (13%) 8 5	122, 175, 195, 199	0
4	AD	208/209 (99%)	1.14	40 (19%) 4 2	89, 149, 187, 193	0
4	CD	208/209 (99%)	1.31	45 (21%) 3 1	86, 148, 186, 193	0
5	AE	151/162 (93%)	0.74	18 (11%) 10 6	88, 127, 174, 197	0
5	CE	151/162 (93%)	0.73	19 (12%) 9 5	90, 128, 174, 197	0
6	AF	101/101 (100%)	0.93	15 (14%) 7 3	95, 151, 183, 196	0
6	CF	101/101 (100%)	1.28	19 (18%) 4 2	96, 154, 184, 198	0
7	AG	155/156 (99%)	1.19	32 (20%) 3 2	146, 184, 197, 200	0
7	CG	155/156 (99%)	0.95	23 (14%) 7 4	146, 185, 197, 199	0
8	AH	138/138 (100%)	0.68	15 (10%) 12 7	92, 129, 167, 189	0
8	CH	138/138 (100%)	0.75	15 (10%) 12 7	92, 129, 166, 189	0
9	AI	127/128 (99%)	1.28	29 (22%) 2 1	143, 190, 200, 202	0
9	CI	127/128 (99%)	1.29	31 (24%) 2 1	144, 190, 199, 202	0
10	AJ	99/105 (94%)	1.23	23 (23%) 2 1	130, 184, 199, 200	0
10	CJ	99/105 (94%)	1.19	20 (20%) 3 2	134, 185, 199, 202	0
11	AK	119/129 (92%)	0.92	21 (17%) 4 3	87, 142, 187, 200	0
11	CK	119/129 (92%)	1.26	27 (22%) 3 1	86, 144, 189, 200	0
12	AL	125/135 (92%)	0.96	22 (17%) 4 3	76, 114, 168, 200	0
12	CL	125/135 (92%)	1.10	24 (19%) 4 2	80, 114, 169, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	115/126 (91%)	1.52	31 (26%)	2	1	147, 192, 199, 201	0
13	CM	115/126 (91%)	1.34	31 (26%)	2	1	148, 192, 199, 202	0
14	AN	60/61 (98%)	1.09	10 (16%)	5	3	141, 183, 196, 199	0
14	CN	60/61 (98%)	1.39	13 (21%)	3	1	142, 182, 196, 198	0
15	AO	88/89 (98%)	1.09	19 (21%)	3	1	85, 123, 173, 189	0
15	CO	88/89 (98%)	0.85	10 (11%)	11	7	87, 124, 176, 186	0
16	AP	84/88 (95%)	1.44	20 (23%)	2	1	97, 128, 177, 192	0
16	CP	84/88 (95%)	1.68	24 (28%)	1	1	97, 126, 175, 191	0
17	AQ	100/105 (95%)	0.92	17 (17%)	5	3	82, 113, 158, 175	0
17	CQ	100/105 (95%)	0.96	17 (17%)	5	3	82, 114, 158, 176	0
18	AR	70/88 (79%)	1.05	12 (17%)	5	3	102, 140, 183, 193	0
18	CR	70/88 (79%)	0.98	10 (14%)	7	4	103, 140, 182, 196	0
19	AS	79/93 (84%)	1.23	17 (21%)	3	1	160, 194, 199, 199	0
19	CS	79/93 (84%)	1.13	16 (20%)	3	2	158, 193, 199, 200	0
20	AT	99/106 (93%)	1.51	27 (27%)	2	1	97, 133, 181, 196	0
20	CT	99/106 (93%)	1.32	26 (26%)	2	1	97, 132, 180, 197	0
21	AU	25/27 (92%)	2.44	15 (60%)	0	0	153, 185, 194, 195	0
21	CU	25/27 (92%)	3.08	13 (52%)	0	0	156, 186, 195, 196	0
22	B0	85/85 (100%)	0.60	12 (14%)	7	4	56, 78, 183, 200	0
22	D0	85/85 (100%)	0.57	8 (9%)	15	9	62, 82, 179, 199	0
23	B1	89/98 (90%)	1.51	26 (29%)	1	1	54, 86, 160, 184	0
23	D1	89/98 (90%)	1.38	25 (28%)	2	1	57, 88, 162, 191	0
24	B2	51/72 (70%)	2.19	25 (49%)	0	0	63, 105, 166, 192	0
24	D2	51/72 (70%)	2.12	25 (49%)	0	0	68, 110, 167, 192	0
25	B3	60/60 (100%)	0.83	10 (16%)	5	3	49, 77, 143, 193	0
25	D3	60/60 (100%)	0.34	4 (6%)	25	15	54, 79, 145, 186	0
26	B4	32/71 (45%)	1.48	6 (18%)	4	2	140, 177, 199, 200	0
26	D4	32/71 (45%)	1.80	12 (37%)	1	0	139, 180, 199, 201	0
27	B5	58/60 (96%)	0.89	7 (12%)	10	6	40, 65, 182, 197	0
27	D5	58/60 (96%)	0.84	9 (15%)	6	3	42, 69, 186, 197	0
28	B6	45/54 (83%)	2.04	19 (42%)	1	0	52, 100, 167, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	1.83	19 (42%) 1 0	57, 102, 169, 189	0
29	B7	49/49 (100%)	0.54	7 (14%) 7 4	42, 51, 132, 180	0
29	D7	49/49 (100%)	0.34	7 (14%) 7 4	45, 54, 132, 180	0
30	B8	64/65 (98%)	1.73	18 (28%) 2 1	53, 76, 137, 169	0
30	D8	64/65 (98%)	1.64	20 (31%) 1 1	55, 79, 140, 168	0
31	BA	2725/2787 (97%)	0.20	134 (4%) 36 21	38, 66, 177, 204	0
31	DA	2725/2787 (97%)	0.20	122 (4%) 39 23	44, 71, 181, 203	0
32	BB	119/122 (97%)	1.60	39 (32%) 1 0	56, 123, 191, 200	0
32	DB	119/122 (97%)	1.08	27 (22%) 3 1	64, 127, 194, 203	0
33	BD	272/276 (98%)	0.62	31 (11%) 11 7	42, 70, 130, 172	0
33	DD	272/276 (98%)	0.69	28 (10%) 13 8	47, 73, 128, 175	0
34	BE	205/206 (99%)	0.95	32 (15%) 6 3	40, 75, 166, 194	0
34	DE	205/206 (99%)	0.56	18 (8%) 17 10	46, 78, 169, 195	0
35	BF	208/210 (99%)	0.92	30 (14%) 7 4	39, 86, 178, 198	0
35	DF	208/210 (99%)	0.73	26 (12%) 9 6	44, 89, 182, 199	0
36	BG	181/182 (99%)	2.33	92 (50%) 0 0	116, 186, 200, 203	0
36	DG	181/182 (99%)	1.95	62 (34%) 1 0	119, 188, 200, 203	0
37	BH	160/180 (88%)	1.98	69 (43%) 1 0	81, 136, 181, 190	0
37	DH	160/180 (88%)	1.36	34 (21%) 3 2	87, 142, 186, 195	0
38	BI	146/148 (98%)	2.07	60 (41%) 1 0	74, 178, 197, 200	0
38	DI	146/148 (98%)	2.47	73 (50%) 0 0	76, 180, 198, 201	0
39	BN	139/140 (99%)	1.43	41 (29%) 1 1	51, 86, 154, 186	0
39	DN	139/140 (99%)	0.78	20 (14%) 7 4	56, 90, 155, 190	0
40	BO	122/122 (100%)	0.52	5 (4%) 42 24	51, 79, 133, 168	0
40	DO	122/122 (100%)	0.65	7 (5%) 30 18	54, 84, 136, 173	0
41	BP	146/150 (97%)	1.58	41 (28%) 2 1	43, 106, 165, 199	0
41	DP	146/150 (97%)	1.30	33 (22%) 3 1	42, 109, 168, 198	0
42	BQ	136/141 (96%)	1.06	22 (16%) 5 3	55, 88, 159, 190	0
42	DQ	136/141 (96%)	1.07	23 (16%) 5 3	59, 90, 160, 191	0
43	BR	117/118 (99%)	0.60	13 (11%) 12 7	43, 65, 134, 180	0
43	DR	117/118 (99%)	0.63	17 (14%) 7 4	47, 68, 136, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	2.16	45 (45%)	1	0	79, 134, 189, 198	0
44	DS	99/112 (88%)	1.95	39 (39%)	1	0	83, 136, 192, 198	0
45	BT	132/146 (90%)	1.32	27 (20%)	3	2	60, 105, 179, 192	0
45	DT	132/146 (90%)	1.20	25 (18%)	4	2	65, 107, 179, 195	0
46	BU	117/118 (99%)	1.04	26 (22%)	3	1	43, 71, 142, 190	0
46	DU	117/118 (99%)	1.05	24 (20%)	3	2	48, 76, 145, 194	0
47	BV	101/101 (100%)	2.08	47 (46%)	0	0	44, 117, 183, 198	0
47	DV	101/101 (100%)	1.10	21 (20%)	3	2	49, 120, 186, 197	0
48	BW	113/113 (100%)	0.34	8 (7%)	23	14	41, 58, 127, 188	0
48	DW	113/113 (100%)	0.21	2 (1%)	67	49	43, 62, 130, 191	0
49	BX	93/96 (96%)	1.21	23 (24%)	2	1	50, 82, 151, 186	0
49	DX	93/96 (96%)	1.01	17 (18%)	4	2	57, 84, 153, 186	0
50	BY	101/110 (91%)	2.55	55 (54%)	0	0	61, 120, 197, 199	0
50	DY	101/110 (91%)	2.01	41 (40%)	1	0	68, 121, 195, 199	0
51	BZ	177/206 (85%)	1.49	50 (28%)	1	1	76, 129, 182, 196	0
51	DZ	177/206 (85%)	1.02	27 (15%)	6	3	80, 133, 185, 196	0
All	All	20062/20922 (95%)	0.83	2987 (14%)	7	3	38, 110, 197, 204	0

The worst 5 of 2987 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	CD	6	GLY	14.8
13	CM	102	ARG	13.5
17	CQ	24	GLU	13.3
38	DI	120	ILE	13.2
27	B5	2	ALA	13.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	CA	1648	1/1	0.53	0.30	69,69,69,69	0
52	MG	AA	1645	1/1	0.54	0.30	104,104,104,104	0
52	MG	DA	3229	1/1	0.59	0.27	78,78,78,78	0
52	MG	DA	3270	1/1	0.61	0.34	92,92,92,92	0
52	MG	DA	3114	1/1	0.62	0.14	75,75,75,75	0
52	MG	BA	3290	1/1	0.63	0.33	87,87,87,87	0
52	MG	BA	3219	1/1	0.64	0.42	75,75,75,75	0
52	MG	CA	1633	1/1	0.64	0.26	77,77,77,77	0
52	MG	DA	3238	1/1	0.66	0.19	80,80,80,80	0
52	MG	DA	3311	1/1	0.66	0.46	86,86,86,86	0
52	MG	DA	3255	1/1	0.68	0.39	91,91,91,91	0
52	MG	DA	3150	1/1	0.69	0.55	80,80,80,80	0
52	MG	DA	3060	1/1	0.70	0.37	50,50,50,50	0
52	MG	AA	1612	1/1	0.70	0.26	84,84,84,84	0
52	MG	CA	1634	1/1	0.71	0.29	88,88,88,88	0
52	MG	AA	1614	1/1	0.71	0.22	81,81,81,81	0
52	MG	BA	3359	1/1	0.72	0.16	81,81,81,81	0
52	MG	DA	3236	1/1	0.72	0.59	76,76,76,76	0
52	MG	CA	1627	1/1	0.72	0.23	76,76,76,76	0
52	MG	DA	3242	1/1	0.72	0.20	84,84,84,84	0
52	MG	DA	3076	1/1	0.72	0.27	56,56,56,56	0
52	MG	AA	1626	1/1	0.72	0.20	84,84,84,84	0
52	MG	BA	3039	1/1	0.72	0.41	57,57,57,57	0
52	MG	CA	1631	1/1	0.73	0.24	95,95,95,95	0
52	MG	BA	3327	1/1	0.73	0.37	70,70,70,70	0
52	MG	DA	3296	1/1	0.73	0.35	104,104,104,104	0
52	MG	CA	1630	1/1	0.73	0.34	74,74,74,74	0
52	MG	DA	3203	1/1	0.74	0.17	55,55,55,55	0
52	MG	DA	3292	1/1	0.74	0.32	60,60,60,60	0
52	MG	BA	3326	1/1	0.75	0.14	60,60,60,60	0
52	MG	DA	3071	1/1	0.75	0.42	85,85,85,85	0
52	MG	CA	1614	1/1	0.75	0.23	80,80,80,80	0
52	MG	AA	1604	1/1	0.76	0.24	100,100,100,100	0
52	MG	CA	1612	1/1	0.76	0.18	70,70,70,70	0
52	MG	BA	3112	1/1	0.76	0.20	43,43,43,43	0
52	MG	DA	3251	1/1	0.76	0.35	91,91,91,91	0
52	MG	CA	1625	1/1	0.76	0.31	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3154	1/1	0.76	0.29	66,66,66,66	0
52	MG	DA	3273	1/1	0.76	0.22	80,80,80,80	0
52	MG	DA	3157	1/1	0.76	0.21	72,72,72,72	0
52	MG	CA	1626	1/1	0.76	0.41	70,70,70,70	0
52	MG	AA	1618	1/1	0.76	0.52	81,81,81,81	0
52	MG	BA	3166	1/1	0.77	0.51	75,75,75,75	0
52	MG	DA	3159	1/1	0.77	0.22	39,39,39,39	0
52	MG	BA	3237	1/1	0.78	0.35	60,60,60,60	0
52	MG	BA	3348	1/1	0.78	0.19	73,73,73,73	0
52	MG	CA	1632	1/1	0.78	0.21	76,76,76,76	0
52	MG	DA	3182	1/1	0.78	0.35	54,54,54,54	0
52	MG	BA	3093	1/1	0.78	0.33	57,57,57,57	0
52	MG	AA	1633	1/1	0.78	0.09	90,90,90,90	0
52	MG	DA	3123	1/1	0.78	0.09	67,67,67,67	0
52	MG	CA	1643	1/1	0.78	0.47	93,93,93,93	0
52	MG	BF	301	1/1	0.79	0.11	59,59,59,59	0
52	MG	CA	1608	1/1	0.79	0.26	90,90,90,90	0
52	MG	CA	1610	1/1	0.79	0.10	106,106,106,106	0
52	MG	CA	1636	1/1	0.79	0.28	74,74,74,74	0
52	MG	DA	3119	1/1	0.79	0.21	56,56,56,56	0
52	MG	BA	3285	1/1	0.79	0.27	56,56,56,56	0
52	MG	DA	3131	1/1	0.79	0.41	66,66,66,66	0
52	MG	BA	3238	1/1	0.79	0.16	70,70,70,70	0
52	MG	DA	3109	1/1	0.80	0.09	60,60,60,60	0
52	MG	BA	3302	1/1	0.80	0.20	67,67,67,67	0
52	MG	CA	1617	1/1	0.80	0.39	74,74,74,74	0
52	MG	DA	3163	1/1	0.80	0.17	77,77,77,77	0
52	MG	DA	3179	1/1	0.80	0.33	67,67,67,67	0
52	MG	DA	3120	1/1	0.80	0.22	84,84,84,84	0
52	MG	DA	3285	1/1	0.80	0.24	70,70,70,70	0
52	MG	BA	3098	1/1	0.80	0.22	76,76,76,76	0
52	MG	BA	3246	1/1	0.80	0.36	68,68,68,68	0
52	MG	DA	3090	1/1	0.80	0.43	53,53,53,53	0
52	MG	DR	201	1/1	0.80	0.39	45,45,45,45	0
52	MG	BA	3162	1/1	0.81	0.28	69,69,69,69	0
52	MG	CA	1606	1/1	0.81	0.34	73,73,73,73	0
52	MG	DA	3183	1/1	0.81	0.47	80,80,80,80	0
52	MG	DA	3187	1/1	0.81	0.36	53,53,53,53	0
52	MG	BA	3343	1/1	0.81	0.14	51,51,51,51	0
52	MG	BA	3305	1/1	0.81	0.26	72,72,72,72	0
52	MG	CA	1628	1/1	0.81	0.24	92,92,92,92	0
52	MG	DA	3297	1/1	0.81	0.25	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3211	1/1	0.81	0.30	38,38,38,38	0
52	MG	BB	206	1/1	0.81	0.33	66,66,66,66	0
52	MG	BA	3151	1/1	0.82	0.27	68,68,68,68	0
52	MG	CA	1635	1/1	0.82	0.37	80,80,80,80	0
52	MG	DA	3260	1/1	0.82	0.26	73,73,73,73	0
52	MG	BA	3289	1/1	0.82	0.10	66,66,66,66	0
52	MG	AA	1632	1/1	0.82	0.33	70,70,70,70	0
52	MG	DA	3093	1/1	0.82	0.45	49,49,49,49	0
52	MG	DA	3104	1/1	0.82	0.20	85,85,85,85	0
52	MG	CA	1618	1/1	0.82	0.27	84,84,84,84	0
52	MG	DA	3237	1/1	0.82	0.16	56,56,56,56	0
52	MG	DA	3014	1/1	0.82	0.28	76,76,76,76	0
52	MG	DF	301	1/1	0.82	0.18	83,83,83,83	0
52	MG	DA	3116	1/1	0.82	0.17	65,65,65,65	0
52	MG	DA	3094	1/1	0.83	0.36	75,75,75,75	0
52	MG	BA	3296	1/1	0.83	0.12	54,54,54,54	0
52	MG	DA	3028	1/1	0.83	0.27	68,68,68,68	0
52	MG	DA	3037	1/1	0.83	0.32	39,39,39,39	0
52	MG	DA	3053	1/1	0.83	0.29	90,90,90,90	0
52	MG	DA	3264	1/1	0.83	0.14	87,87,87,87	0
52	MG	DA	3269	1/1	0.83	0.26	64,64,64,64	0
52	MG	AA	1625	1/1	0.83	0.20	73,73,73,73	0
52	MG	DA	3271	1/1	0.83	0.34	67,67,67,67	0
52	MG	DA	3184	1/1	0.83	0.27	96,96,96,96	0
52	MG	DA	3284	1/1	0.83	0.36	70,70,70,70	0
52	MG	BA	3286	1/1	0.83	0.21	72,72,72,72	0
52	MG	DA	3192	1/1	0.83	0.24	71,71,71,71	0
52	MG	BA	3160	1/1	0.83	0.47	78,78,78,78	0
52	MG	DA	3205	1/1	0.83	0.23	64,64,64,64	0
52	MG	DA	3299	1/1	0.83	0.18	64,64,64,64	0
52	MG	DA	3086	1/1	0.83	0.30	61,61,61,61	0
52	MG	AA	1650	1/1	0.83	0.28	86,86,86,86	0
52	MG	CA	1649	1/1	0.83	0.20	80,80,80,80	0
52	MG	BA	3307	1/1	0.84	0.38	70,70,70,70	0
52	MG	DA	3113	1/1	0.84	0.18	75,75,75,75	0
52	MG	DA	3222	1/1	0.84	0.24	72,72,72,72	0
52	MG	DA	3224	1/1	0.84	0.39	47,47,47,47	0
52	MG	BA	3309	1/1	0.84	0.24	70,70,70,70	0
52	MG	DA	3085	1/1	0.84	0.25	62,62,62,62	0
52	MG	DA	3176	1/1	0.84	0.36	41,41,41,41	0
52	MG	DA	3034	1/1	0.84	0.37	51,51,51,51	0
52	MG	AA	1636	1/1	0.84	0.17	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3255	1/1	0.84	0.16	46,46,46,46	0
52	MG	DA	3300	1/1	0.84	0.26	58,58,58,58	0
52	MG	DA	3128	1/1	0.84	0.33	62,62,62,62	0
52	MG	DA	3318	1/1	0.84	0.20	83,83,83,83	0
52	MG	DB	202	1/1	0.84	0.36	80,80,80,80	0
52	MG	B0	101	1/1	0.84	0.15	48,48,48,48	0
52	MG	DA	3063	1/1	0.84	0.34	72,72,72,72	0
52	MG	DU	201	1/1	0.84	0.25	75,75,75,75	0
52	MG	CA	1604	1/1	0.85	0.16	98,98,98,98	0
52	MG	DA	3194	1/1	0.85	0.18	56,56,56,56	0
52	MG	AA	1622	1/1	0.85	0.32	64,64,64,64	0
52	MG	DA	3115	1/1	0.85	0.29	58,58,58,58	0
52	MG	DA	3087	1/1	0.85	0.23	53,53,53,53	0
52	MG	DA	3118	1/1	0.85	0.30	72,72,72,72	0
52	MG	DA	3286	1/1	0.85	0.12	63,63,63,63	0
52	MG	DA	3289	1/1	0.85	0.29	71,71,71,71	0
52	MG	DA	3171	1/1	0.85	0.21	73,73,73,73	0
52	MG	CA	1646	1/1	0.85	0.23	68,68,68,68	0
52	MG	BA	3228	1/1	0.85	0.35	56,56,56,56	0
52	MG	DA	3180	1/1	0.85	0.34	56,56,56,56	0
52	MG	DA	3122	1/1	0.85	0.13	61,61,61,61	0
52	MG	BA	3251	1/1	0.85	0.22	44,44,44,44	0
52	MG	DA	3316	1/1	0.85	0.32	75,75,75,75	0
52	MG	BA	3232	1/1	0.85	0.20	43,43,43,43	0
52	MG	DA	3186	1/1	0.85	0.14	58,58,58,58	0
52	MG	DA	3261	1/1	0.85	0.28	38,38,38,38	0
52	MG	AA	1610	1/1	0.85	0.15	115,115,115,115	0
52	MG	DA	3268	1/1	0.85	0.40	72,72,72,72	0
52	MG	BA	3188	1/1	0.86	0.19	80,80,80,80	0
52	MG	DA	3256	1/1	0.86	0.31	77,77,77,77	0
52	MG	DA	3259	1/1	0.86	0.35	60,60,60,60	0
52	MG	AA	1637	1/1	0.86	0.21	54,54,54,54	0
52	MG	DA	3112	1/1	0.86	0.09	76,76,76,76	0
52	MG	BA	3292	1/1	0.86	0.12	67,67,67,67	0
52	MG	BA	3295	1/1	0.86	0.30	79,79,79,79	0
52	MG	AA	1644	1/1	0.86	0.33	94,94,94,94	0
52	MG	BA	3350	1/1	0.86	0.32	64,64,64,64	0
52	MG	BA	3086	1/1	0.86	0.14	28,28,28,28	0
52	MG	BA	3360	1/1	0.86	0.20	68,68,68,68	0
52	MG	DA	3276	1/1	0.86	0.41	87,87,87,87	0
52	MG	CA	1639	1/1	0.86	0.33	87,87,87,87	0
52	MG	DA	3079	1/1	0.86	0.27	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	CA	1621	1/1	0.86	0.26	78,78,78,78	0
52	MG	DA	3204	1/1	0.86	0.19	48,48,48,48	0
52	MG	BA	3126	1/1	0.86	0.19	56,56,56,56	0
52	MG	DA	3210	1/1	0.86	0.17	49,49,49,49	0
52	MG	DA	3130	1/1	0.86	0.27	83,83,83,83	0
52	MG	DA	3223	1/1	0.86	0.35	62,62,62,62	0
52	MG	BD	302	1/1	0.86	0.17	47,47,47,47	0
52	MG	DA	3148	1/1	0.86	0.34	61,61,61,61	0
52	MG	BA	3176	1/1	0.86	0.41	68,68,68,68	0
52	MG	DA	3007	1/1	0.86	0.25	40,40,40,40	0
52	MG	DA	3013	1/1	0.86	0.23	77,77,77,77	0
52	MG	DA	3102	1/1	0.86	0.22	54,54,54,54	0
52	MG	DA	3250	1/1	0.86	0.19	62,62,62,62	0
52	MG	DA	3103	1/1	0.86	0.46	58,58,58,58	0
52	MG	CA	1616	1/1	0.87	0.21	74,74,74,74	0
52	MG	AA	1651	1/1	0.87	0.24	81,81,81,81	0
52	MG	BA	3165	1/1	0.87	0.12	57,57,57,57	0
52	MG	DA	3206	1/1	0.87	0.45	74,74,74,74	0
52	MG	DA	3155	1/1	0.87	0.21	59,59,59,59	0
52	MG	AA	1640	1/1	0.87	0.31	77,77,77,77	0
52	MG	DA	3278	1/1	0.87	0.53	83,83,83,83	0
52	MG	DA	3068	1/1	0.87	0.12	80,80,80,80	0
52	MG	CA	1640	1/1	0.87	0.27	74,74,74,74	0
52	MG	CA	1624	1/1	0.87	0.22	69,69,69,69	0
52	MG	DA	3287	1/1	0.87	0.16	64,64,64,64	0
52	MG	AA	1648	1/1	0.87	0.25	57,57,57,57	0
52	MG	BA	3115	1/1	0.87	0.10	71,71,71,71	0
52	MG	BA	3122	1/1	0.87	0.26	61,61,61,61	0
52	MG	BA	3074	1/1	0.87	0.22	67,67,67,67	0
52	MG	BA	3337	1/1	0.87	0.38	61,61,61,61	0
52	MG	AA	1613	1/1	0.87	0.23	76,76,76,76	0
52	MG	DA	3309	1/1	0.87	0.15	76,76,76,76	0
52	MG	DA	3254	1/1	0.87	0.15	61,61,61,61	0
52	MG	DA	3185	1/1	0.87	0.33	65,65,65,65	0
52	MG	BA	3088	1/1	0.87	0.21	60,60,60,60	0
52	MG	DA	3095	1/1	0.87	0.14	56,56,56,56	0
52	MG	BA	3161	1/1	0.87	0.24	65,65,65,65	0
52	MG	DA	3142	1/1	0.87	0.29	69,69,69,69	0
52	MG	DA	3197	1/1	0.87	0.20	59,59,59,59	0
52	MG	BA	3034	1/1	0.88	0.27	69,69,69,69	0
52	MG	AA	1617	1/1	0.88	0.27	55,55,55,55	0
52	MG	DA	3211	1/1	0.88	0.36	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3217	1/1	0.88	0.30	55,55,55,55	0
52	MG	BA	3072	1/1	0.88	0.46	59,59,59,59	0
52	MG	DA	3173	1/1	0.88	0.31	48,48,48,48	0
52	MG	DA	3174	1/1	0.88	0.27	35,35,35,35	0
52	MG	DA	3225	1/1	0.88	0.28	81,81,81,81	0
52	MG	AA	1627	1/1	0.88	0.09	71,71,71,71	0
52	MG	DA	3235	1/1	0.88	0.05	48,48,48,48	0
52	MG	AA	1608	1/1	0.88	0.22	71,71,71,71	0
52	MG	CA	1603	1/1	0.88	0.27	57,57,57,57	0
52	MG	BA	3181	1/1	0.88	0.28	54,54,54,54	0
52	MG	DA	3127	1/1	0.88	0.20	40,40,40,40	0
52	MG	BA	3147	1/1	0.88	0.22	55,55,55,55	0
52	MG	BA	3312	1/1	0.88	0.17	55,55,55,55	0
52	MG	DA	3307	1/1	0.88	0.10	65,65,65,65	0
52	MG	BA	3278	1/1	0.88	0.23	62,62,62,62	0
52	MG	BA	3283	1/1	0.88	0.33	70,70,70,70	0
52	MG	DA	3315	1/1	0.88	0.17	69,69,69,69	0
52	MG	DA	3144	1/1	0.88	0.27	65,65,65,65	0
52	MG	BA	3195	1/1	0.88	0.13	40,40,40,40	0
52	MG	DA	3062	1/1	0.88	0.37	76,76,76,76	0
52	MG	AA	1646	1/1	0.88	0.21	53,53,53,53	0
52	MG	BA	3214	1/1	0.88	0.33	55,55,55,55	0
52	MG	BA	3004	1/1	0.88	0.22	31,31,31,31	0
53	ZN	AN	101	1/1	0.88	0.08	181,181,181,181	0
52	MG	BA	3116	1/1	0.89	0.34	67,67,67,67	0
52	MG	DA	3153	1/1	0.89	0.12	80,80,80,80	0
52	MG	DA	3080	1/1	0.89	0.41	59,59,59,59	0
52	MG	DA	3239	1/1	0.89	0.09	65,65,65,65	0
52	MG	DA	3081	1/1	0.89	0.19	58,58,58,58	0
52	MG	DA	3082	1/1	0.89	0.20	50,50,50,50	0
52	MG	AA	1643	1/1	0.89	0.66	85,85,85,85	0
52	MG	DA	3161	1/1	0.89	0.15	72,72,72,72	0
52	MG	CA	1601	1/1	0.89	0.24	85,85,85,85	0
52	MG	DA	3166	1/1	0.89	0.07	55,55,55,55	0
52	MG	DA	3258	1/1	0.89	0.18	70,70,70,70	0
52	MG	DA	3169	1/1	0.89	0.19	49,49,49,49	0
52	MG	BA	3005	1/1	0.89	0.17	56,56,56,56	0
52	MG	DA	3089	1/1	0.89	0.30	54,54,54,54	0
52	MG	BA	3170	1/1	0.89	0.32	44,44,44,44	0
52	MG	CA	1605	1/1	0.89	0.20	102,102,102,102	0
52	MG	BA	3241	1/1	0.89	0.32	69,69,69,69	0
52	MG	CA	1642	1/1	0.89	0.18	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3130	1/1	0.89	0.50	65,65,65,65	0
52	MG	BA	3310	1/1	0.89	0.33	74,74,74,74	0
52	MG	BA	3146	1/1	0.89	0.27	56,56,56,56	0
52	MG	BA	3182	1/1	0.89	0.22	54,54,54,54	0
52	MG	DA	3283	1/1	0.89	0.32	57,57,57,57	0
52	MG	D7	101	1/1	0.89	0.17	58,58,58,58	0
52	MG	D8	101	1/1	0.89	0.26	66,66,66,66	0
52	MG	CA	1615	1/1	0.89	0.17	69,69,69,69	0
52	MG	BA	3276	1/1	0.89	0.26	76,76,76,76	0
52	MG	BA	3184	1/1	0.89	0.36	62,62,62,62	0
52	MG	DA	3199	1/1	0.89	0.23	74,74,74,74	0
52	MG	DA	3294	1/1	0.89	0.18	50,50,50,50	0
52	MG	DA	3016	1/1	0.89	0.41	54,54,54,54	0
52	MG	BA	3338	1/1	0.89	0.06	61,61,61,61	0
52	MG	BA	3064	1/1	0.89	0.25	45,45,45,45	0
52	MG	CA	1622	1/1	0.89	0.19	75,75,75,75	0
52	MG	BA	3027	1/1	0.89	0.26	19,19,19,19	0
52	MG	DA	3308	1/1	0.89	0.43	75,75,75,75	0
52	MG	BA	3209	1/1	0.89	0.16	51,51,51,51	0
52	MG	BA	3156	1/1	0.89	0.33	31,31,31,31	0
52	MG	BA	3031	1/1	0.89	0.28	66,66,66,66	0
52	MG	DA	3065	1/1	0.89	0.18	70,70,70,70	0
52	MG	BB	203	1/1	0.89	0.10	82,82,82,82	0
52	MG	BA	3076	1/1	0.89	0.11	29,29,29,29	0
52	MG	DA	3226	1/1	0.89	0.50	73,73,73,73	0
52	MG	DA	3145	1/1	0.89	0.19	57,57,57,57	0
52	MG	DA	3232	1/1	0.89	0.25	56,56,56,56	0
52	MG	BD	301	1/1	0.89	0.40	51,51,51,51	0
52	MG	AA	1629	1/1	0.90	0.39	83,83,83,83	0
52	MG	BA	3353	1/1	0.90	0.15	73,73,73,73	0
52	MG	DA	3083	1/1	0.90	0.19	43,43,43,43	0
52	MG	BA	3355	1/1	0.90	0.24	78,78,78,78	0
52	MG	AA	1630	1/1	0.90	0.33	75,75,75,75	0
52	MG	DA	3165	1/1	0.90	0.26	53,53,53,53	0
52	MG	BA	3185	1/1	0.90	0.20	61,61,61,61	0
52	MG	BA	3284	1/1	0.90	0.13	34,34,34,34	0
52	MG	CA	1638	1/1	0.90	0.19	62,62,62,62	0
52	MG	DA	3257	1/1	0.90	0.17	72,72,72,72	0
52	MG	DA	3092	1/1	0.90	0.18	61,61,61,61	0
52	MG	BA	3001	1/1	0.90	0.15	55,55,55,55	0
52	MG	BA	3101	1/1	0.90	0.22	17,17,17,17	0
52	MG	BA	3202	1/1	0.90	0.16	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	AA	1623	1/1	0.90	0.31	50,50,50,50	0
52	MG	DA	3265	1/1	0.90	0.18	61,61,61,61	0
52	MG	AA	1641	1/1	0.90	0.22	57,57,57,57	0
52	MG	BA	3010	1/1	0.90	0.34	53,53,53,53	0
52	MG	DA	3107	1/1	0.90	0.33	42,42,42,42	0
52	MG	BA	3164	1/1	0.90	0.23	40,40,40,40	0
52	MG	DA	3110	1/1	0.90	0.41	46,46,46,46	0
52	MG	BA	3301	1/1	0.90	0.22	52,52,52,52	0
52	MG	DA	3188	1/1	0.90	0.40	81,81,81,81	0
52	MG	DA	3280	1/1	0.90	0.19	67,67,67,67	0
52	MG	DA	3281	1/1	0.90	0.34	87,87,87,87	0
52	MG	DA	3282	1/1	0.90	0.14	59,59,59,59	0
52	MG	BA	3224	1/1	0.90	0.07	43,43,43,43	0
52	MG	DA	3004	1/1	0.90	0.18	39,39,39,39	0
52	MG	BA	3303	1/1	0.90	0.19	36,36,36,36	0
52	MG	DA	3198	1/1	0.90	0.19	53,53,53,53	0
52	MG	BA	3226	1/1	0.90	0.26	42,42,42,42	0
52	MG	BA	3025	1/1	0.90	0.25	64,64,64,64	0
52	MG	BA	3123	1/1	0.90	0.29	48,48,48,48	0
52	MG	BA	3234	1/1	0.90	0.15	40,40,40,40	0
52	MG	DA	3295	1/1	0.90	0.33	65,65,65,65	0
52	MG	BA	3168	1/1	0.90	0.18	59,59,59,59	0
52	MG	BA	3321	1/1	0.90	0.18	69,69,69,69	0
52	MG	DA	3046	1/1	0.90	0.33	49,49,49,49	0
52	MG	DA	3216	1/1	0.90	0.35	78,78,78,78	0
52	MG	DA	3301	1/1	0.90	0.41	67,67,67,67	0
52	MG	DA	3302	1/1	0.90	0.30	64,64,64,64	0
52	MG	BA	3081	1/1	0.90	0.27	39,39,39,39	0
52	MG	DA	3219	1/1	0.90	0.14	49,49,49,49	0
52	MG	CA	1620	1/1	0.90	0.21	70,70,70,70	0
52	MG	BA	3175	1/1	0.90	0.08	50,50,50,50	0
52	MG	DA	3314	1/1	0.90	0.23	54,54,54,54	0
52	MG	BA	3333	1/1	0.90	0.08	48,48,48,48	0
52	MG	BA	3335	1/1	0.90	0.19	55,55,55,55	0
52	MG	DA	3317	1/1	0.90	0.19	60,60,60,60	0
52	MG	BA	3243	1/1	0.90	0.21	39,39,39,39	0
52	MG	BA	3127	1/1	0.90	0.29	48,48,48,48	0
52	MG	BA	3341	1/1	0.90	0.16	67,67,67,67	0
52	MG	DA	3234	1/1	0.90	0.18	73,73,73,73	0
52	MG	BA	3179	1/1	0.90	0.36	55,55,55,55	0
52	MG	AA	1620	1/1	0.90	0.22	95,95,95,95	0
52	MG	AA	1628	1/1	0.91	0.29	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3077	1/1	0.91	0.20	46,46,46,46	0
52	MG	BA	3220	1/1	0.91	0.27	36,36,36,36	0
52	MG	BA	3038	1/1	0.91	0.31	25,25,25,25	0
52	MG	BA	3152	1/1	0.91	0.12	58,58,58,58	0
52	MG	BA	3356	1/1	0.91	0.23	75,75,75,75	0
52	MG	DA	3168	1/1	0.91	0.15	64,64,64,64	0
52	MG	BA	3180	1/1	0.91	0.29	68,68,68,68	0
52	MG	BA	3154	1/1	0.91	0.23	73,73,73,73	0
52	MG	AA	1638	1/1	0.91	0.23	91,91,91,91	0
52	MG	CA	1637	1/1	0.91	0.25	85,85,85,85	0
52	MG	BA	3117	1/1	0.91	0.28	58,58,58,58	0
52	MG	BA	3063	1/1	0.91	0.35	57,57,57,57	0
52	MG	BA	3090	1/1	0.91	0.17	22,22,22,22	0
52	MG	DA	3181	1/1	0.91	0.16	62,62,62,62	0
52	MG	BA	3304	1/1	0.91	0.22	41,41,41,41	0
52	MG	BP	203	1/1	0.91	0.10	29,29,29,29	0
52	MG	BA	3190	1/1	0.91	0.24	34,34,34,34	0
52	MG	DA	3274	1/1	0.91	0.14	68,68,68,68	0
52	MG	DA	3275	1/1	0.91	0.37	72,72,72,72	0
52	MG	AA	1639	1/1	0.91	0.45	77,77,77,77	0
52	MG	DA	3277	1/1	0.91	0.16	66,66,66,66	0
52	MG	BA	3308	1/1	0.91	0.12	55,55,55,55	0
52	MG	BA	3200	1/1	0.91	0.33	55,55,55,55	0
52	MG	BA	3252	1/1	0.91	0.17	72,72,72,72	0
52	MG	AA	1605	1/1	0.91	0.22	106,106,106,106	0
52	MG	DA	3006	1/1	0.91	0.35	40,40,40,40	0
52	MG	BA	3256	1/1	0.91	0.21	43,43,43,43	0
52	MG	BA	3264	1/1	0.91	0.16	58,58,58,58	0
52	MG	CA	1613	1/1	0.91	0.32	87,87,87,87	0
52	MG	DA	3201	1/1	0.91	0.22	46,46,46,46	0
52	MG	DA	3202	1/1	0.91	0.20	73,73,73,73	0
52	MG	DA	3291	1/1	0.91	0.42	88,88,88,88	0
52	MG	BA	3271	1/1	0.91	0.36	57,57,57,57	0
52	MG	DA	3017	1/1	0.91	0.15	55,55,55,55	0
52	MG	DA	3024	1/1	0.91	0.24	54,54,54,54	0
52	MG	BA	3329	1/1	0.91	0.28	65,65,65,65	0
52	MG	DA	3030	1/1	0.91	0.19	66,66,66,66	0
52	MG	DA	3033	1/1	0.91	0.26	63,63,63,63	0
52	MG	BA	3332	1/1	0.91	0.18	65,65,65,65	0
52	MG	BA	3203	1/1	0.91	0.19	53,53,53,53	0
52	MG	DA	3038	1/1	0.91	0.18	68,68,68,68	0
52	MG	BA	3128	1/1	0.91	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3336	1/1	0.91	0.28	61,61,61,61	0
52	MG	DA	3132	1/1	0.91	0.19	72,72,72,72	0
52	MG	DA	3136	1/1	0.91	0.20	81,81,81,81	0
52	MG	DA	3313	1/1	0.91	0.22	64,64,64,64	0
52	MG	DA	3055	1/1	0.91	0.19	38,38,38,38	0
52	MG	BA	3280	1/1	0.91	0.23	80,80,80,80	0
52	MG	DA	3231	1/1	0.91	0.10	42,42,42,42	0
52	MG	BA	3282	1/1	0.91	0.22	49,49,49,49	0
52	MG	DA	3146	1/1	0.91	0.33	59,59,59,59	0
52	MG	BA	3339	1/1	0.91	0.24	74,74,74,74	0
52	MG	AA	1615	1/1	0.91	0.25	72,72,72,72	0
52	MG	BA	3108	1/1	0.91	0.22	43,43,43,43	0
52	MG	DA	3070	1/1	0.91	0.36	52,52,52,52	0
52	MG	DX	101	1/1	0.91	0.17	76,76,76,76	0
52	MG	BA	3346	1/1	0.91	0.21	61,61,61,61	0
54	K	DA	3319	1/1	0.91	0.12	82,82,82,82	0
52	MG	BA	3331	1/1	0.92	0.16	52,52,52,52	0
52	MG	CA	1647	1/1	0.92	0.16	78,78,78,78	0
52	MG	BA	3216	1/1	0.92	0.14	46,46,46,46	0
52	MG	BA	3140	1/1	0.92	0.18	78,78,78,78	0
52	MG	CA	1611	1/1	0.92	0.15	72,72,72,72	0
52	MG	BA	3334	1/1	0.92	0.18	61,61,61,61	0
52	MG	BA	3173	1/1	0.92	0.32	46,46,46,46	0
52	MG	BA	3142	1/1	0.92	0.25	47,47,47,47	0
52	MG	BA	3144	1/1	0.92	0.35	43,43,43,43	0
52	MG	DA	3012	1/1	0.92	0.15	29,29,29,29	0
52	MG	DA	3098	1/1	0.92	0.17	38,38,38,38	0
52	MG	AA	1635	1/1	0.92	0.23	50,50,50,50	0
52	MG	BA	3105	1/1	0.92	0.24	32,32,32,32	0
52	MG	BA	3150	1/1	0.92	0.21	50,50,50,50	0
52	MG	DA	3106	1/1	0.92	0.44	50,50,50,50	0
52	MG	AA	1619	1/1	0.92	0.28	55,55,55,55	0
52	MG	DA	3272	1/1	0.92	0.35	78,78,78,78	0
52	MG	DA	3022	1/1	0.92	0.22	38,38,38,38	0
52	MG	AA	1652	1/1	0.92	0.14	83,83,83,83	0
52	MG	BA	3239	1/1	0.92	0.17	61,61,61,61	0
52	MG	CA	1623	1/1	0.92	0.20	79,79,79,79	0
52	MG	BA	3153	1/1	0.92	0.28	62,62,62,62	0
52	MG	BA	3242	1/1	0.92	0.33	71,71,71,71	0
52	MG	AA	1607	1/1	0.92	0.29	81,81,81,81	0
52	MG	DA	3117	1/1	0.92	0.20	59,59,59,59	0
52	MG	BA	3244	1/1	0.92	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3083	1/1	0.92	0.33	45,45,45,45	0
52	MG	CA	1629	1/1	0.92	0.09	69,69,69,69	0
52	MG	BA	3192	1/1	0.92	0.30	42,42,42,42	0
52	MG	DA	3057	1/1	0.92	0.19	60,60,60,60	0
52	MG	DA	3058	1/1	0.92	0.28	42,42,42,42	0
52	MG	BA	3047	1/1	0.92	0.33	41,41,41,41	0
52	MG	DA	3290	1/1	0.92	0.30	74,74,74,74	0
52	MG	BB	205	1/1	0.92	0.14	90,90,90,90	0
52	MG	BA	3053	1/1	0.92	0.27	33,33,33,33	0
52	MG	DA	3214	1/1	0.92	0.20	33,33,33,33	0
52	MG	BA	3055	1/1	0.92	0.20	31,31,31,31	0
52	MG	DA	3066	1/1	0.92	0.16	52,52,52,52	0
52	MG	DA	3218	1/1	0.92	0.31	53,53,53,53	0
52	MG	DA	3140	1/1	0.92	0.23	46,46,46,46	0
52	MG	DA	3067	1/1	0.92	0.26	57,57,57,57	0
52	MG	AA	1616	1/1	0.92	0.16	68,68,68,68	0
52	MG	BA	3313	1/1	0.92	0.37	61,61,61,61	0
52	MG	BP	201	1/1	0.92	0.13	17,17,17,17	0
52	MG	DA	3075	1/1	0.92	0.21	50,50,50,50	0
52	MG	DA	3149	1/1	0.92	0.27	51,51,51,51	0
52	MG	DA	3230	1/1	0.92	0.10	69,69,69,69	0
52	MG	BA	3314	1/1	0.92	0.31	63,63,63,63	0
52	MG	DA	3152	1/1	0.92	0.19	66,66,66,66	0
52	MG	BA	3096	1/1	0.92	0.25	33,33,33,33	0
52	MG	BA	3029	1/1	0.92	0.19	30,30,30,30	0
52	MG	BA	3100	1/1	0.92	0.30	40,40,40,40	0
52	MG	DA	3156	1/1	0.92	0.20	44,44,44,44	0
52	MG	BA	3279	1/1	0.92	0.33	62,62,62,62	0
52	MG	CA	1645	1/1	0.92	0.26	64,64,64,64	0
52	MG	DA	3240	1/1	0.92	0.05	47,47,47,47	0
52	MG	DA	3241	1/1	0.92	0.14	48,48,48,48	0
52	MG	DA	3160	1/1	0.92	0.29	51,51,51,51	0
52	MG	DA	3243	1/1	0.92	0.10	94,94,94,94	0
52	MG	DA	3247	1/1	0.92	0.14	61,61,61,61	0
52	MG	BA	3347	1/1	0.93	0.14	58,58,58,58	0
52	MG	DA	3190	1/1	0.93	0.06	49,49,49,49	0
52	MG	BA	3269	1/1	0.93	0.24	45,45,45,45	0
52	MG	DA	3262	1/1	0.93	0.30	55,55,55,55	0
52	MG	DA	3263	1/1	0.93	0.29	55,55,55,55	0
52	MG	BA	3077	1/1	0.93	0.19	40,40,40,40	0
52	MG	DA	3135	1/1	0.93	0.19	74,74,74,74	0
52	MG	DA	3266	1/1	0.93	0.35	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3009	1/1	0.93	0.27	44,44,44,44	0
52	MG	DA	3138	1/1	0.93	0.16	35,35,35,35	0
52	MG	DA	3139	1/1	0.93	0.26	48,48,48,48	0
52	MG	BA	3163	1/1	0.93	0.22	45,45,45,45	0
52	MG	BA	3311	1/1	0.93	0.35	69,69,69,69	0
52	MG	BA	3357	1/1	0.93	0.11	66,66,66,66	0
52	MG	AA	1634	1/1	0.93	0.26	54,54,54,54	0
52	MG	BA	3111	1/1	0.93	0.10	19,19,19,19	0
52	MG	BA	3281	1/1	0.93	0.10	45,45,45,45	0
52	MG	BA	3315	1/1	0.93	0.24	62,62,62,62	0
52	MG	DA	3212	1/1	0.93	0.09	71,71,71,71	0
52	MG	DA	3025	1/1	0.93	0.27	61,61,61,61	0
52	MG	DA	3151	1/1	0.93	0.13	66,66,66,66	0
52	MG	DA	3091	1/1	0.93	0.32	44,44,44,44	0
52	MG	DA	3027	1/1	0.93	0.31	43,43,43,43	0
52	MG	BA	3318	1/1	0.93	0.09	55,55,55,55	0
52	MG	BA	3319	1/1	0.93	0.35	60,60,60,60	0
52	MG	DA	3032	1/1	0.93	0.18	51,51,51,51	0
52	MG	BA	3059	1/1	0.93	0.26	46,46,46,46	0
52	MG	BA	3196	1/1	0.93	0.27	66,66,66,66	0
52	MG	BA	3198	1/1	0.93	0.22	24,24,24,24	0
52	MG	DA	3227	1/1	0.93	0.26	79,79,79,79	0
52	MG	DA	3228	1/1	0.93	0.17	57,57,57,57	0
52	MG	DA	3293	1/1	0.93	0.13	60,60,60,60	0
52	MG	BA	3199	1/1	0.93	0.28	39,39,39,39	0
52	MG	DA	3162	1/1	0.93	0.21	80,80,80,80	0
52	MG	BA	3114	1/1	0.93	0.18	49,49,49,49	0
52	MG	AA	1603	1/1	0.93	0.21	45,45,45,45	0
52	MG	DA	3233	1/1	0.93	0.06	57,57,57,57	0
52	MG	BA	3089	1/1	0.93	0.09	20,20,20,20	0
52	MG	DA	3167	1/1	0.93	0.07	45,45,45,45	0
52	MG	AA	1621	1/1	0.93	0.38	51,51,51,51	0
52	MG	DA	3305	1/1	0.93	0.07	80,80,80,80	0
52	MG	BA	3120	1/1	0.93	0.18	65,65,65,65	0
52	MG	DA	3170	1/1	0.93	0.38	76,76,76,76	0
52	MG	CA	1607	1/1	0.93	0.29	74,74,74,74	0
52	MG	DA	3310	1/1	0.93	0.22	54,54,54,54	0
52	MG	BA	3070	1/1	0.93	0.18	25,25,25,25	0
52	MG	DA	3312	1/1	0.93	0.10	53,53,53,53	0
52	MG	BA	3300	1/1	0.93	0.17	56,56,56,56	0
52	MG	BA	3041	1/1	0.93	0.17	22,22,22,22	0
52	MG	AA	1647	1/1	0.93	0.10	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3244	1/1	0.93	0.21	69,69,69,69	0
52	MG	BA	3340	1/1	0.93	0.09	83,83,83,83	0
52	MG	BA	3259	1/1	0.93	0.12	47,47,47,47	0
52	MG	DA	3069	1/1	0.93	0.34	54,54,54,54	0
52	MG	DA	3253	1/1	0.93	0.08	51,51,51,51	0
52	MG	BA	3262	1/1	0.93	0.33	68,68,68,68	0
52	MG	DR	202	1/1	0.93	0.12	50,50,50,50	0
52	MG	D5	101	1/1	0.93	0.41	51,51,51,51	0
52	MG	DA	3073	1/1	0.93	0.42	55,55,55,55	0
52	MG	BA	3049	1/1	0.93	0.25	26,26,26,26	0
54	K	BA	3361	1/1	0.93	0.09	69,69,69,69	0
52	MG	DA	3129	1/1	0.93	0.09	48,48,48,48	0
55	TEL	DA	3320	58/58	0.93	0.25	110,110,110,110	0
52	MG	BA	3028	1/1	0.94	0.32	30,30,30,30	0
52	MG	B7	101	1/1	0.94	0.10	42,42,42,42	0
52	MG	DA	3252	1/1	0.94	0.15	55,55,55,55	0
52	MG	DA	3088	1/1	0.94	0.19	53,53,53,53	0
52	MG	BA	3050	1/1	0.94	0.18	34,34,34,34	0
52	MG	BA	3052	1/1	0.94	0.12	17,17,17,17	0
52	MG	BA	3257	1/1	0.94	0.07	19,19,19,19	0
52	MG	DA	3008	1/1	0.94	0.34	50,50,50,50	0
52	MG	AA	1611	1/1	0.94	0.18	50,50,50,50	0
52	MG	BA	3201	1/1	0.94	0.18	52,52,52,52	0
52	MG	DA	3175	1/1	0.94	0.13	68,68,68,68	0
52	MG	BA	3263	1/1	0.94	0.27	54,54,54,54	0
52	MG	DA	3178	1/1	0.94	0.44	52,52,52,52	0
52	MG	DA	3097	1/1	0.94	0.18	51,51,51,51	0
52	MG	BA	3032	1/1	0.94	0.23	39,39,39,39	0
52	MG	DA	3101	1/1	0.94	0.39	57,57,57,57	0
52	MG	BA	3057	1/1	0.94	0.07	40,40,40,40	0
52	MG	DA	3020	1/1	0.94	0.22	74,74,74,74	0
52	MG	DA	3021	1/1	0.94	0.17	42,42,42,42	0
52	MG	BA	3205	1/1	0.94	0.43	68,68,68,68	0
52	MG	BA	3274	1/1	0.94	0.14	36,36,36,36	0
52	MG	BA	3330	1/1	0.94	0.35	64,64,64,64	0
52	MG	BA	3207	1/1	0.94	0.15	34,34,34,34	0
52	MG	DA	3111	1/1	0.94	0.17	56,56,56,56	0
52	MG	BA	3277	1/1	0.94	0.24	49,49,49,49	0
52	MG	BA	3011	1/1	0.94	0.22	22,22,22,22	0
52	MG	DA	3031	1/1	0.94	0.33	61,61,61,61	0
52	MG	BA	3132	1/1	0.94	0.17	59,59,59,59	0
52	MG	DA	3279	1/1	0.94	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3135	1/1	0.94	0.21	30,30,30,30	0
52	MG	BA	3174	1/1	0.94	0.05	51,51,51,51	0
52	MG	DA	3036	1/1	0.94	0.29	54,54,54,54	0
52	MG	BA	3060	1/1	0.94	0.27	59,59,59,59	0
52	MG	BA	3099	1/1	0.94	0.16	45,45,45,45	0
52	MG	DA	3040	1/1	0.94	0.18	36,36,36,36	0
52	MG	DA	3042	1/1	0.94	0.16	48,48,48,48	0
52	MG	DA	3208	1/1	0.94	0.21	43,43,43,43	0
52	MG	DA	3288	1/1	0.94	0.10	32,32,32,32	0
52	MG	BA	3177	1/1	0.94	0.28	57,57,57,57	0
52	MG	DA	3050	1/1	0.94	0.21	39,39,39,39	0
52	MG	DA	3052	1/1	0.94	0.15	44,44,44,44	0
52	MG	BA	3178	1/1	0.94	0.17	25,25,25,25	0
52	MG	DA	3215	1/1	0.94	0.20	61,61,61,61	0
52	MG	BA	3036	1/1	0.94	0.06	0,0,0,0	0
52	MG	BA	3287	1/1	0.94	0.30	59,59,59,59	0
52	MG	DA	3134	1/1	0.94	0.34	61,61,61,61	0
52	MG	BA	3344	1/1	0.94	0.08	43,43,43,43	0
52	MG	DA	3220	1/1	0.94	0.13	68,68,68,68	0
52	MG	DA	3221	1/1	0.94	0.13	62,62,62,62	0
52	MG	BA	3230	1/1	0.94	0.24	44,44,44,44	0
52	MG	DA	3061	1/1	0.94	0.11	40,40,40,40	0
52	MG	DA	3303	1/1	0.94	0.25	57,57,57,57	0
52	MG	DA	3304	1/1	0.94	0.12	67,67,67,67	0
52	MG	BA	3037	1/1	0.94	0.14	14,14,14,14	0
52	MG	BA	3233	1/1	0.94	0.17	54,54,54,54	0
52	MG	BA	3066	1/1	0.94	0.21	36,36,36,36	0
52	MG	BA	3352	1/1	0.94	0.19	53,53,53,53	0
52	MG	BA	3235	1/1	0.94	0.22	43,43,43,43	0
52	MG	BA	3298	1/1	0.94	0.36	65,65,65,65	0
52	MG	BA	3299	1/1	0.94	0.23	43,43,43,43	0
52	MG	BA	3067	1/1	0.94	0.19	38,38,38,38	0
52	MG	BA	3013	1/1	0.94	0.23	33,33,33,33	0
52	MG	AA	1642	1/1	0.94	0.07	58,58,58,58	0
52	MG	DA	3074	1/1	0.94	0.28	56,56,56,56	0
52	MG	BB	201	1/1	0.94	0.25	47,47,47,47	0
52	MG	BB	202	1/1	0.94	0.33	44,44,44,44	0
52	MG	DB	201	1/1	0.94	0.28	59,59,59,59	0
52	MG	BA	3186	1/1	0.94	0.15	44,44,44,44	0
52	MG	DA	3078	1/1	0.94	0.14	62,62,62,62	0
52	MG	AA	1609	1/1	0.94	0.20	65,65,65,65	0
52	MG	DA	3158	1/1	0.94	0.32	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3043	1/1	0.94	0.11	39,39,39,39	0
52	MG	BA	3306	1/1	0.94	0.26	70,70,70,70	0
52	MG	BA	3191	1/1	0.94	0.17	59,59,59,59	0
52	MG	BA	3045	1/1	0.94	0.15	22,22,22,22	0
52	MG	BA	3250	1/1	0.94	0.10	40,40,40,40	0
52	MG	DA	3249	1/1	0.94	0.21	69,69,69,69	0
52	MG	BA	3231	1/1	0.95	0.11	31,31,31,31	0
52	MG	BA	3288	1/1	0.95	0.12	55,55,55,55	0
52	MG	BA	3054	1/1	0.95	0.15	50,50,50,50	0
52	MG	DA	3044	1/1	0.95	0.23	39,39,39,39	0
52	MG	BA	3102	1/1	0.95	0.14	41,41,41,41	0
52	MG	DA	3048	1/1	0.95	0.21	51,51,51,51	0
52	MG	DA	3049	1/1	0.95	0.07	54,54,54,54	0
52	MG	BA	3291	1/1	0.95	0.18	45,45,45,45	0
52	MG	DA	3191	1/1	0.95	0.29	48,48,48,48	0
52	MG	BA	3103	1/1	0.95	0.12	31,31,31,31	0
52	MG	DA	3193	1/1	0.95	0.23	54,54,54,54	0
52	MG	BA	3145	1/1	0.95	0.20	54,54,54,54	0
52	MG	DA	3121	1/1	0.95	0.45	64,64,64,64	0
52	MG	BA	3236	1/1	0.95	0.26	38,38,38,38	0
52	MG	DA	3056	1/1	0.95	0.36	51,51,51,51	0
52	MG	DA	3126	1/1	0.95	0.10	57,57,57,57	0
52	MG	BA	3104	1/1	0.95	0.07	45,45,45,45	0
52	MG	AA	1624	1/1	0.95	0.24	55,55,55,55	0
52	MG	BA	3187	1/1	0.95	0.30	60,60,60,60	0
52	MG	BA	3106	1/1	0.95	0.26	43,43,43,43	0
52	MG	BA	3189	1/1	0.95	0.26	40,40,40,40	0
52	MG	BA	3040	1/1	0.95	0.28	49,49,49,49	0
52	MG	DA	3209	1/1	0.95	0.31	58,58,58,58	0
52	MG	BA	3079	1/1	0.95	0.13	48,48,48,48	0
52	MG	BA	3012	1/1	0.95	0.34	61,61,61,61	0
52	MG	CA	1641	1/1	0.95	0.11	54,54,54,54	0
52	MG	DA	3213	1/1	0.95	0.22	44,44,44,44	0
52	MG	BA	3248	1/1	0.95	0.14	57,57,57,57	0
52	MG	BA	3194	1/1	0.95	0.18	27,27,27,27	0
52	MG	CA	1644	1/1	0.95	0.16	86,86,86,86	0
52	MG	DA	3141	1/1	0.95	0.10	65,65,65,65	0
52	MG	B5	102	1/1	0.95	0.25	80,80,80,80	0
52	MG	DA	3072	1/1	0.95	0.17	42,42,42,42	0
52	MG	BA	3061	1/1	0.95	0.20	36,36,36,36	0
52	MG	BA	3159	1/1	0.95	0.37	58,58,58,58	0
52	MG	DA	3147	1/1	0.95	0.29	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3087	1/1	0.95	0.07	18,18,18,18	0
52	MG	BA	3014	1/1	0.95	0.36	46,46,46,46	0
52	MG	BA	3258	1/1	0.95	0.15	57,57,57,57	0
52	MG	BX	101	1/1	0.95	0.09	58,58,58,58	0
52	MG	BA	3118	1/1	0.95	0.19	44,44,44,44	0
52	MG	CA	1602	1/1	0.95	0.45	73,73,73,73	0
52	MG	BA	3119	1/1	0.95	0.17	47,47,47,47	0
52	MG	BA	3033	1/1	0.95	0.06	27,27,27,27	0
52	MG	BA	3121	1/1	0.95	0.20	51,51,51,51	0
52	MG	BA	3268	1/1	0.95	0.16	60,60,60,60	0
52	MG	DA	3306	1/1	0.95	0.20	63,63,63,63	0
52	MG	BA	3324	1/1	0.95	0.38	64,64,64,64	0
52	MG	BA	3325	1/1	0.95	0.18	49,49,49,49	0
52	MG	CA	1609	1/1	0.95	0.12	48,48,48,48	0
52	MG	BA	3206	1/1	0.95	0.12	36,36,36,36	0
52	MG	DA	3019	1/1	0.95	0.33	42,42,42,42	0
52	MG	BA	3019	1/1	0.95	0.26	26,26,26,26	0
52	MG	BA	3023	1/1	0.95	0.19	31,31,31,31	0
52	MG	BA	3210	1/1	0.95	0.20	46,46,46,46	0
52	MG	BA	3125	1/1	0.95	0.06	53,53,53,53	0
52	MG	BA	3171	1/1	0.95	0.27	45,45,45,45	0
52	MG	DA	3026	1/1	0.95	0.26	32,32,32,32	0
52	MG	BA	3094	1/1	0.95	0.43	47,47,47,47	0
52	MG	DA	3246	1/1	0.95	0.16	70,70,70,70	0
52	MG	BA	3095	1/1	0.95	0.14	43,43,43,43	0
52	MG	DB	203	1/1	0.95	0.27	47,47,47,47	0
52	MG	DD	302	1/1	0.95	0.12	38,38,38,38	0
52	MG	AA	1606	1/1	0.95	0.24	63,63,63,63	0
52	MG	CA	1619	1/1	0.95	0.21	61,61,61,61	0
52	MG	BA	3222	1/1	0.95	0.18	58,58,58,58	0
52	MG	BA	3071	1/1	0.95	0.16	32,32,32,32	0
52	MG	DA	3177	1/1	0.95	0.36	48,48,48,48	0
52	MG	AA	1649	1/1	0.95	0.15	68,68,68,68	0
52	MG	DA	3108	1/1	0.95	0.07	56,56,56,56	0
52	MG	BA	3134	1/1	0.95	0.25	52,52,52,52	0
55	TEL	BA	3362	58/58	0.95	0.22	110,110,110,110	0
52	MG	BA	3073	1/1	0.95	0.19	24,24,24,24	0
52	MG	DA	3011	1/1	0.96	0.19	43,43,43,43	0
52	MG	BA	3078	1/1	0.96	0.28	39,39,39,39	0
52	MG	BA	3021	1/1	0.96	0.13	30,30,30,30	0
52	MG	BA	3247	1/1	0.96	0.14	77,77,77,77	0
52	MG	DA	3015	1/1	0.96	0.20	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	BA	3208	1/1	0.96	0.29	36,36,36,36	0
52	MG	AA	1602	1/1	0.96	0.26	50,50,50,50	0
52	MG	DA	3018	1/1	0.96	0.25	34,34,34,34	0
52	MG	BA	3065	1/1	0.96	0.14	37,37,37,37	0
52	MG	BA	3124	1/1	0.96	0.11	12,12,12,12	0
52	MG	BA	3254	1/1	0.96	0.20	58,58,58,58	0
52	MG	BA	3212	1/1	0.96	0.06	29,29,29,29	0
52	MG	BA	3213	1/1	0.96	0.07	34,34,34,34	0
52	MG	BA	3085	1/1	0.96	0.10	0,0,0,0	0
52	MG	BA	3155	1/1	0.96	0.19	42,42,42,42	0
52	MG	BA	3354	1/1	0.96	0.18	71,71,71,71	0
52	MG	BA	3218	1/1	0.96	0.35	38,38,38,38	0
52	MG	DA	3029	1/1	0.96	0.15	36,36,36,36	0
52	MG	BA	3260	1/1	0.96	0.14	46,46,46,46	0
52	MG	BA	3006	1/1	0.96	0.24	27,27,27,27	0
52	MG	BA	3008	1/1	0.96	0.20	36,36,36,36	0
52	MG	BA	3003	1/1	0.96	0.11	34,34,34,34	0
52	MG	DA	3099	1/1	0.96	0.15	56,56,56,56	0
52	MG	BA	3265	1/1	0.96	0.20	51,51,51,51	0
52	MG	BA	3267	1/1	0.96	0.07	40,40,40,40	0
52	MG	BA	3223	1/1	0.96	0.32	45,45,45,45	0
52	MG	BB	204	1/1	0.96	0.28	47,47,47,47	0
52	MG	DA	3105	1/1	0.96	0.16	74,74,74,74	0
52	MG	DA	3298	1/1	0.96	0.17	46,46,46,46	0
52	MG	DA	3039	1/1	0.96	0.47	69,69,69,69	0
52	MG	BA	3129	1/1	0.96	0.06	55,55,55,55	0
52	MG	BA	3015	1/1	0.96	0.08	46,46,46,46	0
52	MG	BB	207	1/1	0.96	0.17	80,80,80,80	0
52	MG	BA	3273	1/1	0.96	0.19	44,44,44,44	0
52	MG	BA	3017	1/1	0.96	0.32	46,46,46,46	0
52	MG	BA	3275	1/1	0.96	0.11	47,47,47,47	0
52	MG	BA	3133	1/1	0.96	0.14	38,38,38,38	0
52	MG	BP	202	1/1	0.96	0.39	66,66,66,66	0
52	MG	BA	3323	1/1	0.96	0.11	51,51,51,51	0
52	MG	DA	3245	1/1	0.96	0.14	44,44,44,44	0
52	MG	DA	3054	1/1	0.96	0.29	47,47,47,47	0
52	MG	BA	3091	1/1	0.96	0.15	44,44,44,44	0
52	MG	DA	3248	1/1	0.96	0.12	72,72,72,72	0
52	MG	BA	3042	1/1	0.96	0.15	31,31,31,31	0
52	MG	BA	3139	1/1	0.96	0.19	60,60,60,60	0
52	MG	BA	3169	1/1	0.96	0.40	49,49,49,49	0
52	MG	BA	3018	1/1	0.96	0.12	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3075	1/1	0.96	0.22	56,56,56,56	0
52	MG	CA	1650	1/1	0.96	0.21	66,66,66,66	0
52	MG	DA	3124	1/1	0.96	0.14	63,63,63,63	0
52	MG	DA	3125	1/1	0.96	0.06	54,54,54,54	0
52	MG	BA	3172	1/1	0.96	0.12	50,50,50,50	0
52	MG	DD	301	1/1	0.96	0.21	56,56,56,56	0
52	MG	BA	3143	1/1	0.96	0.19	34,34,34,34	0
52	MG	BA	3044	1/1	0.96	0.20	19,19,19,19	0
52	MG	DA	3001	1/1	0.96	0.27	66,66,66,66	0
52	MG	DA	3003	1/1	0.96	0.25	61,61,61,61	0
52	MG	BA	3240	1/1	0.96	0.25	39,39,39,39	0
52	MG	DA	3005	1/1	0.96	0.05	69,69,69,69	0
52	MG	DA	3133	1/1	0.96	0.17	31,31,31,31	0
52	MG	BA	3097	1/1	0.96	0.28	53,53,53,53	0
52	MG	BA	3204	1/1	0.96	0.29	49,49,49,49	0
52	MG	B5	101	1/1	0.96	0.20	54,54,54,54	0
52	MG	DA	3010	1/1	0.96	0.31	45,45,45,45	0
52	MG	BA	3245	1/1	0.97	0.23	48,48,48,48	0
52	MG	DA	3084	1/1	0.97	0.12	27,27,27,27	0
52	MG	BA	3215	1/1	0.97	0.21	37,37,37,37	0
52	MG	BA	3320	1/1	0.97	0.05	48,48,48,48	0
52	MG	BA	3107	1/1	0.97	0.05	20,20,20,20	0
52	MG	BA	3322	1/1	0.97	0.10	44,44,44,44	0
52	MG	BA	3217	1/1	0.97	0.22	34,34,34,34	0
52	MG	BA	3249	1/1	0.97	0.08	56,56,56,56	0
52	MG	BA	3068	1/1	0.97	0.17	47,47,47,47	0
52	MG	DA	3035	1/1	0.97	0.14	41,41,41,41	0
52	MG	BA	3193	1/1	0.97	0.23	51,51,51,51	0
52	MG	BA	3080	1/1	0.97	0.35	23,23,23,23	0
52	MG	BA	3328	1/1	0.97	0.17	41,41,41,41	0
52	MG	BA	3253	1/1	0.97	0.04	42,42,42,42	0
52	MG	BQ	201	1/1	0.97	0.06	32,32,32,32	0
52	MG	DA	3041	1/1	0.97	0.20	55,55,55,55	0
52	MG	BQ	202	1/1	0.97	0.16	49,49,49,49	0
52	MG	DA	3043	1/1	0.97	0.14	43,43,43,43	0
52	MG	BU	201	1/1	0.97	0.10	29,29,29,29	0
52	MG	DA	3045	1/1	0.97	0.35	51,51,51,51	0
52	MG	DA	3164	1/1	0.97	0.20	50,50,50,50	0
52	MG	BA	3221	1/1	0.97	0.25	47,47,47,47	0
52	MG	DA	3047	1/1	0.97	0.08	28,28,28,28	0
52	MG	BA	3069	1/1	0.97	0.18	46,46,46,46	0
52	MG	BA	3113	1/1	0.97	0.19	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3197	1/1	0.97	0.18	46,46,46,46	0
52	MG	DA	3051	1/1	0.97	0.12	53,53,53,53	0
52	MG	BA	3294	1/1	0.97	0.13	40,40,40,40	0
52	MG	DA	3172	1/1	0.97	0.24	59,59,59,59	0
52	MG	BA	3082	1/1	0.97	0.20	37,37,37,37	0
52	MG	BA	3058	1/1	0.97	0.14	47,47,47,47	0
52	MG	BA	3297	1/1	0.97	0.35	68,68,68,68	0
52	MG	BA	3229	1/1	0.97	0.05	30,30,30,30	0
52	MG	BA	3261	1/1	0.97	0.10	34,34,34,34	0
52	MG	BA	3131	1/1	0.97	0.09	17,17,17,17	0
52	MG	DA	3059	1/1	0.97	0.14	55,55,55,55	0
52	MG	BA	3030	1/1	0.97	0.08	26,26,26,26	0
52	MG	BA	3342	1/1	0.97	0.16	39,39,39,39	0
52	MG	BA	3051	1/1	0.97	0.14	22,22,22,22	0
52	MG	BA	3026	1/1	0.97	0.13	58,58,58,58	0
52	MG	DA	3064	1/1	0.97	0.20	46,46,46,46	0
52	MG	DA	3009	1/1	0.97	0.16	52,52,52,52	0
52	MG	BA	3345	1/1	0.97	0.13	70,70,70,70	0
52	MG	BA	3266	1/1	0.97	0.31	63,63,63,63	0
52	MG	BA	3158	1/1	0.97	0.12	32,32,32,32	0
52	MG	DA	3189	1/1	0.97	0.09	45,45,45,45	0
52	MG	BA	3016	1/1	0.97	0.13	30,30,30,30	0
52	MG	BA	3136	1/1	0.97	0.30	51,51,51,51	0
52	MG	BA	3351	1/1	0.97	0.12	53,53,53,53	0
52	MG	BA	3183	1/1	0.97	0.18	55,55,55,55	0
52	MG	BA	3137	1/1	0.97	0.14	16,16,16,16	0
52	MG	DA	3195	1/1	0.97	0.16	62,62,62,62	0
52	MG	DE	301	1/1	0.97	0.07	34,34,34,34	0
52	MG	BA	3138	1/1	0.97	0.42	42,42,42,42	0
52	MG	DP	201	1/1	0.97	0.05	42,42,42,42	0
52	MG	AA	1601	1/1	0.97	0.14	68,68,68,68	0
52	MG	BA	3020	1/1	0.97	0.11	24,24,24,24	0
52	MG	BA	3141	1/1	0.97	0.20	19,19,19,19	0
52	MG	DA	3137	1/1	0.97	0.40	49,49,49,49	0
52	MG	BA	3358	1/1	0.97	0.04	34,34,34,34	0
53	ZN	CN	101	1/1	0.97	0.05	164,164,164,164	0
52	MG	DA	3023	1/1	0.97	0.12	39,39,39,39	0
52	MG	BA	3056	1/1	0.97	0.05	31,31,31,31	0
52	MG	BA	3035	1/1	0.97	0.15	23,23,23,23	0
52	MG	BA	3317	1/1	0.97	0.10	49,49,49,49	0
52	MG	DA	3100	1/1	0.98	0.07	59,59,59,59	0
52	MG	DA	3143	1/1	0.98	0.21	43,43,43,43	0

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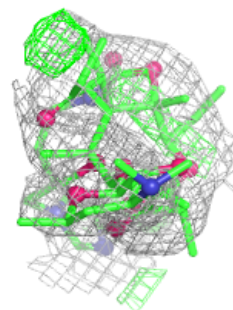
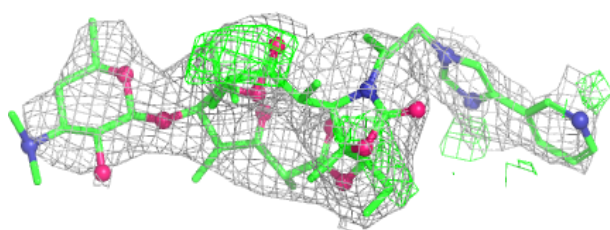
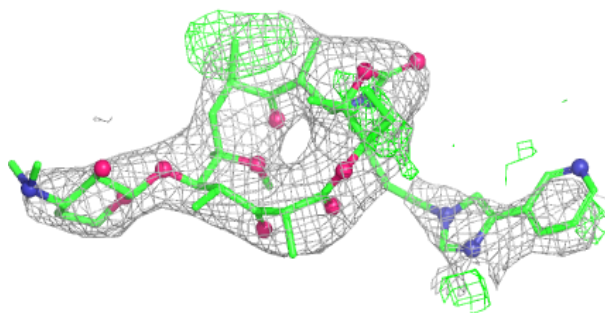
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3062	1/1	0.98	0.07	38,38,38,38	0
52	MG	BA	3092	1/1	0.98	0.18	22,22,22,22	0
52	MG	BA	3167	1/1	0.98	0.10	27,27,27,27	0
52	MG	BA	3084	1/1	0.98	0.16	25,25,25,25	0
52	MG	BA	3349	1/1	0.98	0.22	51,51,51,51	0
52	MG	AA	1631	1/1	0.98	0.05	63,63,63,63	0
52	MG	BA	3157	1/1	0.98	0.04	24,24,24,24	0
52	MG	BA	3024	1/1	0.98	0.05	37,37,37,37	0
52	MG	DA	3196	1/1	0.98	0.06	41,41,41,41	0
52	MG	B1	101	1/1	0.98	0.09	41,41,41,41	0
52	MG	BA	3270	1/1	0.98	0.06	24,24,24,24	0
52	MG	BA	3225	1/1	0.98	0.18	23,23,23,23	0
52	MG	DA	3200	1/1	0.98	0.17	47,47,47,47	0
52	MG	DQ	201	1/1	0.98	0.12	63,63,63,63	0
52	MG	BA	3002	1/1	0.98	0.32	31,31,31,31	0
52	MG	BA	3227	1/1	0.98	0.13	21,21,21,21	0
52	MG	BA	3148	1/1	0.98	0.14	28,28,28,28	0
52	MG	BR	201	1/1	0.98	0.13	27,27,27,27	0
53	ZN	AD	301	1/1	0.98	0.18	110,110,110,110	0
52	MG	BA	3048	1/1	0.98	0.15	20,20,20,20	0
52	MG	DA	3096	1/1	0.98	0.20	42,42,42,42	0
52	MG	DA	3207	1/1	0.98	0.06	53,53,53,53	0
52	MG	BA	3022	1/1	0.98	0.12	45,45,45,45	0
52	MG	DA	3002	1/1	0.98	0.32	41,41,41,41	0
52	MG	BA	3110	1/1	0.98	0.20	23,23,23,23	0
52	MG	DA	3267	1/1	0.99	0.09	57,57,57,57	0
52	MG	BA	3149	1/1	0.99	0.05	24,24,24,24	0
52	MG	BA	3007	1/1	0.99	0.29	57,57,57,57	0
53	ZN	CD	301	1/1	0.99	0.12	105,105,105,105	0
52	MG	BA	3046	1/1	0.99	0.15	38,38,38,38	0
52	MG	BA	3316	1/1	0.99	0.04	43,43,43,43	0
52	MG	BA	3272	1/1	0.99	0.26	38,38,38,38	0
52	MG	BA	3293	1/1	0.99	0.03	51,51,51,51	0
52	MG	BA	3109	1/1	0.99	0.05	36,36,36,36	0

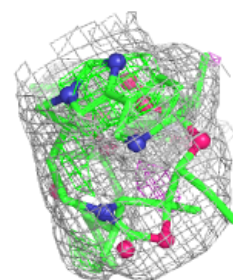
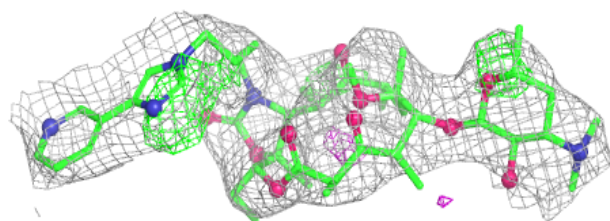
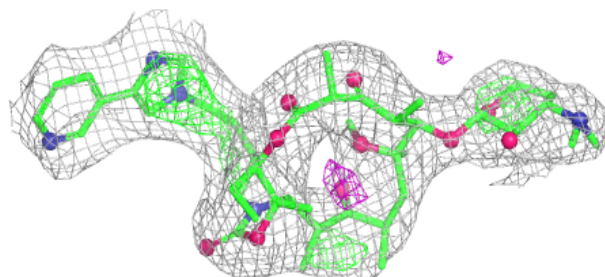
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TEL DA 3320:

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

**Electron density around TEL BA 3362:**

$2mF_o-DF_c$ (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.