



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:05 PM GMT

PDB ID : 4V7Y
Title : Structure of the *Thermus thermophilus* 70S ribosome complexed with azithromycin.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-18
Resolution : 3.00 Å(reported)

This is a wwPDB 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

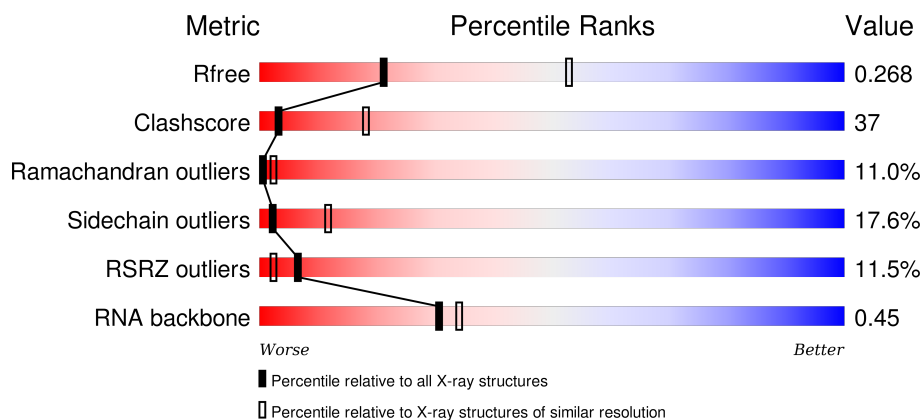
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>13%</div> <div>26% 57% 15%</div> </div>
1	CA	1522	<div> <div>14%</div> <div>26% 56% 16%</div> </div>
2	AB	256	<div> <div>14%</div> <div>34% 44% 12% 8%</div> </div>
2	CB	256	<div> <div>18%</div> <div>36% 43% 12% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	B0	85	
22	D0	85	
23	B1	98	
23	D1	98	
24	B2	72	
24	D2	72	
25	B3	60	
25	D3	60	
26	B4	71	
26	D4	71	
27	B5	60	
27	D5	60	

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	AA	1606	-	-	-	X
52	MG	AA	1609	-	-	-	X
52	MG	AA	1612	-	-	-	X
52	MG	AA	1621	-	-	-	X
52	MG	AA	1622	-	-	-	X
52	MG	AA	1623	-	-	-	X
52	MG	AA	1627	-	-	-	X
52	MG	AA	1629	-	-	-	X
52	MG	AA	1647	-	-	-	X
52	MG	AA	1648	-	-	-	X
52	MG	AA	1649	-	-	-	X
52	MG	AA	1651	-	-	-	X
52	MG	BA	3001	-	-	-	X
52	MG	BA	3002	-	-	-	X
52	MG	BA	3006	-	-	-	X
52	MG	BA	3008	-	-	-	X
52	MG	BA	3009	-	-	-	X
52	MG	BA	3010	-	-	-	X
52	MG	BA	3012	-	-	-	X
52	MG	BA	3016	-	-	-	X
52	MG	BA	3017	-	-	-	X
52	MG	BA	3020	-	-	-	X
52	MG	BA	3021	-	-	-	X
52	MG	BA	3023	-	-	-	X
52	MG	BA	3028	-	-	-	X
52	MG	BA	3032	-	-	-	X
52	MG	BA	3034	-	-	-	X
52	MG	BA	3037	-	-	-	X
52	MG	BA	3038	-	-	-	X
52	MG	BA	3039	-	-	-	X
52	MG	BA	3040	-	-	-	X
52	MG	BA	3041	-	-	-	X
52	MG	BA	3044	-	-	-	X
52	MG	BA	3046	-	-	-	X
52	MG	BA	3047	-	-	-	X
52	MG	BA	3049	-	-	-	X
52	MG	BA	3051	-	-	-	X
52	MG	BA	3052	-	-	-	X
52	MG	BA	3055	-	-	-	X
52	MG	BA	3057	-	-	-	X
52	MG	BA	3059	-	-	-	X
52	MG	BA	3060	-	-	-	X
52	MG	BA	3062	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	BA	3065	-	-	-	X
52	MG	BA	3069	-	-	-	X
52	MG	BA	3071	-	-	-	X
52	MG	BA	3073	-	-	-	X
52	MG	BA	3074	-	-	-	X
52	MG	BA	3079	-	-	-	X
52	MG	BA	3085	-	-	-	X
52	MG	BA	3087	-	-	-	X
52	MG	BA	3091	-	-	-	X
52	MG	BA	3093	-	-	-	X
52	MG	BA	3095	-	-	-	X
52	MG	BA	3099	-	-	-	X
52	MG	BA	3100	-	-	-	X
52	MG	BA	3108	-	-	-	X
52	MG	BA	3110	-	-	-	X
52	MG	BA	3115	-	-	-	X
52	MG	BA	3121	-	-	-	X
52	MG	BA	3123	-	-	-	X
52	MG	BA	3126	-	-	-	X
52	MG	BA	3139	-	-	-	X
52	MG	BA	3141	-	-	-	X
52	MG	BA	3142	-	-	-	X
52	MG	BA	3146	-	-	-	X
52	MG	BA	3148	-	-	-	X
52	MG	BA	3153	-	-	-	X
52	MG	BA	3158	-	-	-	X
52	MG	BA	3161	-	-	-	X
52	MG	BA	3169	-	-	-	X
52	MG	BA	3173	-	-	-	X
52	MG	BA	3176	-	-	-	X
52	MG	BA	3185	-	-	-	X
52	MG	BA	3189	-	-	-	X
52	MG	BA	3190	-	-	-	X
52	MG	BA	3193	-	-	-	X
52	MG	BA	3195	-	-	-	X
52	MG	BA	3200	-	-	-	X
52	MG	BA	3209	-	-	-	X
52	MG	BA	3217	-	-	-	X
52	MG	BA	3221	-	-	-	X
52	MG	BA	3223	-	-	-	X
52	MG	BA	3229	-	-	-	X
52	MG	BA	3230	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	BA	3241	-	-	-	X
52	MG	BA	3252	-	-	-	X
52	MG	BA	3254	-	-	-	X
52	MG	BA	3255	-	-	-	X
52	MG	BA	3268	-	-	-	X
52	MG	BA	3271	-	-	-	X
52	MG	BA	3275	-	-	-	X
52	MG	BA	3276	-	-	-	X
52	MG	BA	3285	-	-	-	X
52	MG	BA	3298	-	-	-	X
52	MG	BA	3302	-	-	-	X
52	MG	BA	3303	-	-	-	X
52	MG	BA	3311	-	-	-	X
52	MG	BA	3313	-	-	-	X
52	MG	BA	3315	-	-	-	X
52	MG	BA	3326	-	-	-	X
52	MG	BA	3331	-	-	-	X
52	MG	BA	3345	-	-	-	X
52	MG	BA	3347	-	-	-	X
52	MG	BQ	202	-	-	-	X
52	MG	BU	201	-	-	-	X
52	MG	CA	1605	-	-	-	X
52	MG	CA	1606	-	-	-	X
52	MG	CA	1609	-	-	-	X
52	MG	CA	1610	-	-	-	X
52	MG	CA	1617	-	-	-	X
52	MG	CA	1618	-	-	-	X
52	MG	CA	1619	-	-	-	X
52	MG	CA	1623	-	-	-	X
52	MG	CA	1625	-	-	-	X
52	MG	CA	1641	-	-	-	X
52	MG	CA	1642	-	-	-	X
52	MG	CA	1643	-	-	-	X
52	MG	CA	1644	-	-	-	X
52	MG	CA	1645	-	-	-	X
52	MG	CA	1647	-	-	-	X
52	MG	D1	101	-	-	-	X
52	MG	D5	101	-	-	-	X
52	MG	D7	101	-	-	-	X
52	MG	DA	3002	-	-	-	X
52	MG	DA	3006	-	-	-	X
52	MG	DA	3007	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	DA	3008	-	-	-	X
52	MG	DA	3009	-	-	-	X
52	MG	DA	3011	-	-	-	X
52	MG	DA	3015	-	-	-	X
52	MG	DA	3016	-	-	-	X
52	MG	DA	3019	-	-	-	X
52	MG	DA	3022	-	-	-	X
52	MG	DA	3026	-	-	-	X
52	MG	DA	3030	-	-	-	X
52	MG	DA	3032	-	-	-	X
52	MG	DA	3036	-	-	-	X
52	MG	DA	3039	-	-	-	X
52	MG	DA	3042	-	-	-	X
52	MG	DA	3044	-	-	-	X
52	MG	DA	3045	-	-	-	X
52	MG	DA	3047	-	-	-	X
52	MG	DA	3049	-	-	-	X
52	MG	DA	3053	-	-	-	X
52	MG	DA	3054	-	-	-	X
52	MG	DA	3055	-	-	-	X
52	MG	DA	3056	-	-	-	X
52	MG	DA	3059	-	-	-	X
52	MG	DA	3061	-	-	-	X
52	MG	DA	3063	-	-	-	X
52	MG	DA	3064	-	-	-	X
52	MG	DA	3067	-	-	-	X
52	MG	DA	3068	-	-	-	X
52	MG	DA	3070	-	-	-	X
52	MG	DA	3072	-	-	-	X
52	MG	DA	3077	-	-	-	X
52	MG	DA	3087	-	-	-	X
52	MG	DA	3088	-	-	-	X
52	MG	DA	3089	-	-	-	X
52	MG	DA	3091	-	-	-	X
52	MG	DA	3094	-	-	-	X
52	MG	DA	3095	-	-	-	X
52	MG	DA	3097	-	-	-	X
52	MG	DA	3103	-	-	-	X
52	MG	DA	3105	-	-	-	X
52	MG	DA	3106	-	-	-	X
52	MG	DA	3110	-	-	-	X
52	MG	DA	3111	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	DA	3112	-	-	-	X
52	MG	DA	3114	-	-	-	X
52	MG	DA	3115	-	-	-	X
52	MG	DA	3116	-	-	-	X
52	MG	DA	3130	-	-	-	X
52	MG	DA	3132	-	-	-	X
52	MG	DA	3133	-	-	-	X
52	MG	DA	3135	-	-	-	X
52	MG	DA	3137	-	-	-	X
52	MG	DA	3138	-	-	-	X
52	MG	DA	3140	-	-	-	X
52	MG	DA	3142	-	-	-	X
52	MG	DA	3146	-	-	-	X
52	MG	DA	3147	-	-	-	X
52	MG	DA	3149	-	-	-	X
52	MG	DA	3154	-	-	-	X
52	MG	DA	3156	-	-	-	X
52	MG	DA	3159	-	-	-	X
52	MG	DA	3166	-	-	-	X
52	MG	DA	3171	-	-	-	X
52	MG	DA	3173	-	-	-	X
52	MG	DA	3187	-	-	-	X
52	MG	DA	3188	-	-	-	X
52	MG	DA	3189	-	-	-	X
52	MG	DA	3197	-	-	-	X
52	MG	DA	3203	-	-	-	X
52	MG	DA	3208	-	-	-	X
52	MG	DA	3213	-	-	-	X
52	MG	DA	3214	-	-	-	X
52	MG	DA	3217	-	-	-	X
52	MG	DA	3227	-	-	-	X
52	MG	DA	3241	-	-	-	X
52	MG	DA	3246	-	-	-	X
52	MG	DA	3248	-	-	-	X
52	MG	DA	3264	-	-	-	X
52	MG	DA	3266	-	-	-	X
52	MG	DA	3270	-	-	-	X
52	MG	DA	3283	-	-	-	X
52	MG	DA	3285	-	-	-	X
52	MG	DA	3294	-	-	-	X
52	MG	DA	3304	-	-	-	X
54	K	BA	3350	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	K	DA	3310	-	-	-	X
55	ZIT	BA	3351	-	-	-	X
55	ZIT	DA	3311	-	-	-	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 278000 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	BA	349	Total	Mg	0	0
			349	349		
52	CA	48	Total	Mg	0	0
			48	48		
52	DQ	1	Total	Mg	0	0
			1	1		
52	DF	1	Total	Mg	0	0
			1	1		
52	BE	1	Total	Mg	0	0
			1	1		
52	DU	1	Total	Mg	0	0
			1	1		
52	B1	1	Total	Mg	0	0
			1	1		
52	BP	3	Total	Mg	0	0
			3	3		
52	DR	1	Total	Mg	0	0
			1	1		
52	B5	2	Total	Mg	0	0
			2	2		
52	BB	5	Total	Mg	0	0
			5	5		
52	BF	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	AA	51	Total	Mg	0	0
			51	51		
52	BQ	2	Total	Mg	0	0
			2	2		
52	D7	1	Total	Mg	0	0
			1	1		
52	BU	1	Total	Mg	0	0
			1	1		
52	DD	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	D0	1	Total 1	Mg 1	0	0
52	BR	1	Total 1	Mg 1	0	0
52	DA	309	Total 309	Mg 309	0	0
52	B7	1	Total 1	Mg 1	0	0
52	DE	1	Total 1	Mg 1	0	0
52	D1	1	Total 1	Mg 1	0	0
52	DX	1	Total 1	Mg 1	0	0
52	DP	1	Total 1	Mg 1	0	0
52	D5	2	Total 2	Mg 2	0	0
52	BD	1	Total 1	Mg 1	0	0
52	B0	1	Total 1	Mg 1	0	0
52	DB	3	Total 3	Mg 3	0	0

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

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

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

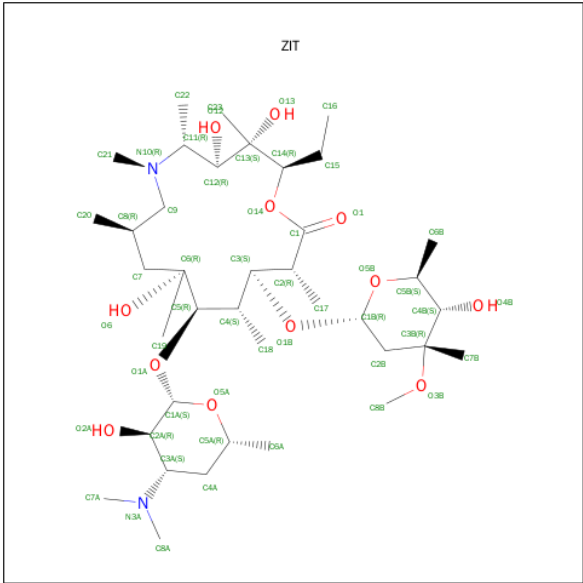
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	1	Total 1	K 1	0	0

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

- Molecule 55 is AZITHROMYCIN (three-letter code: ZIT) (formula: C₃₈H₇₂N₂O₁₂).

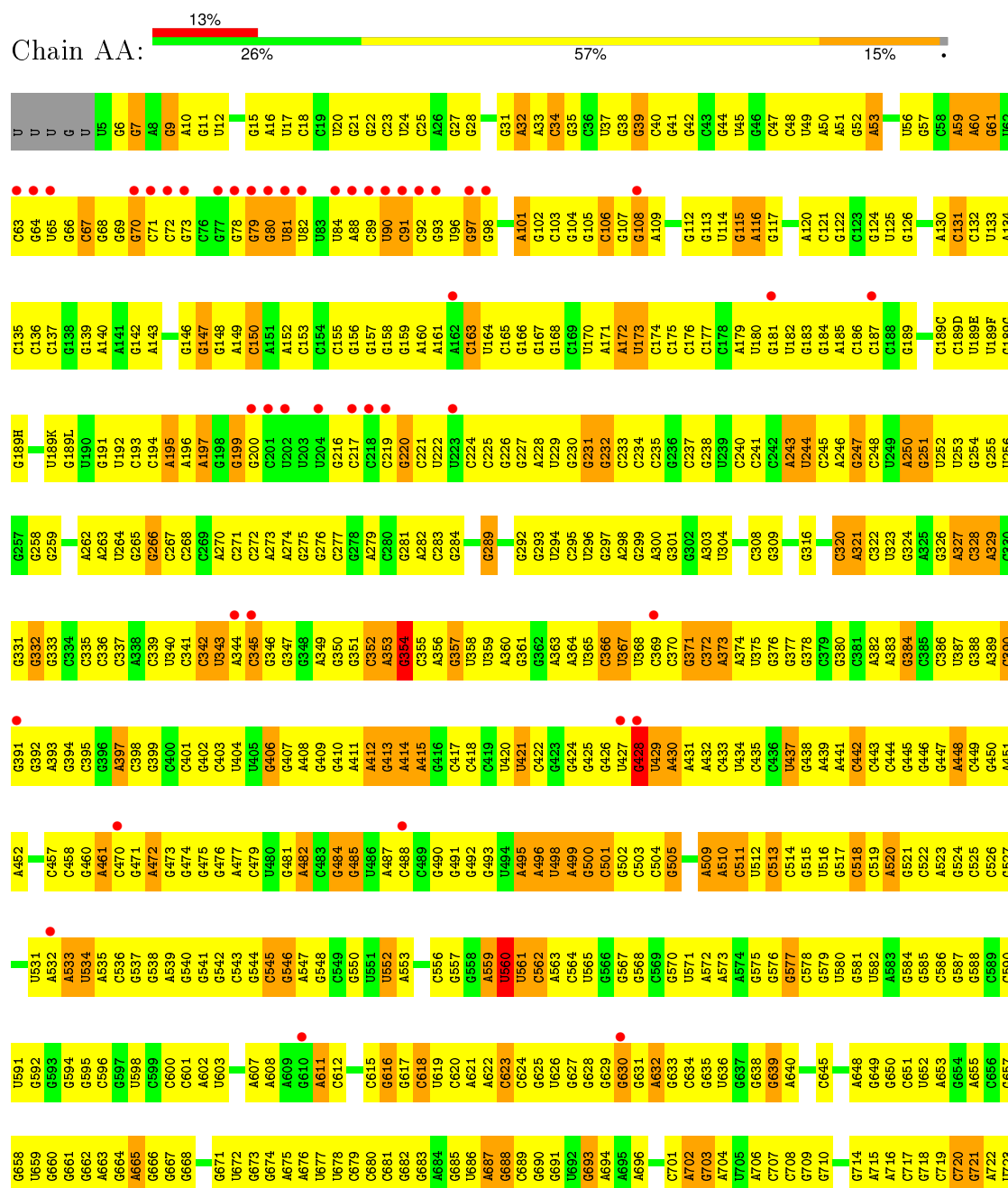


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BA	1	Total	C	N	O	0	0
			52	38	2	12		
55	DA	1	Total	C	N	O	0	0
			52	38	2	12		

3 Residue-property plots

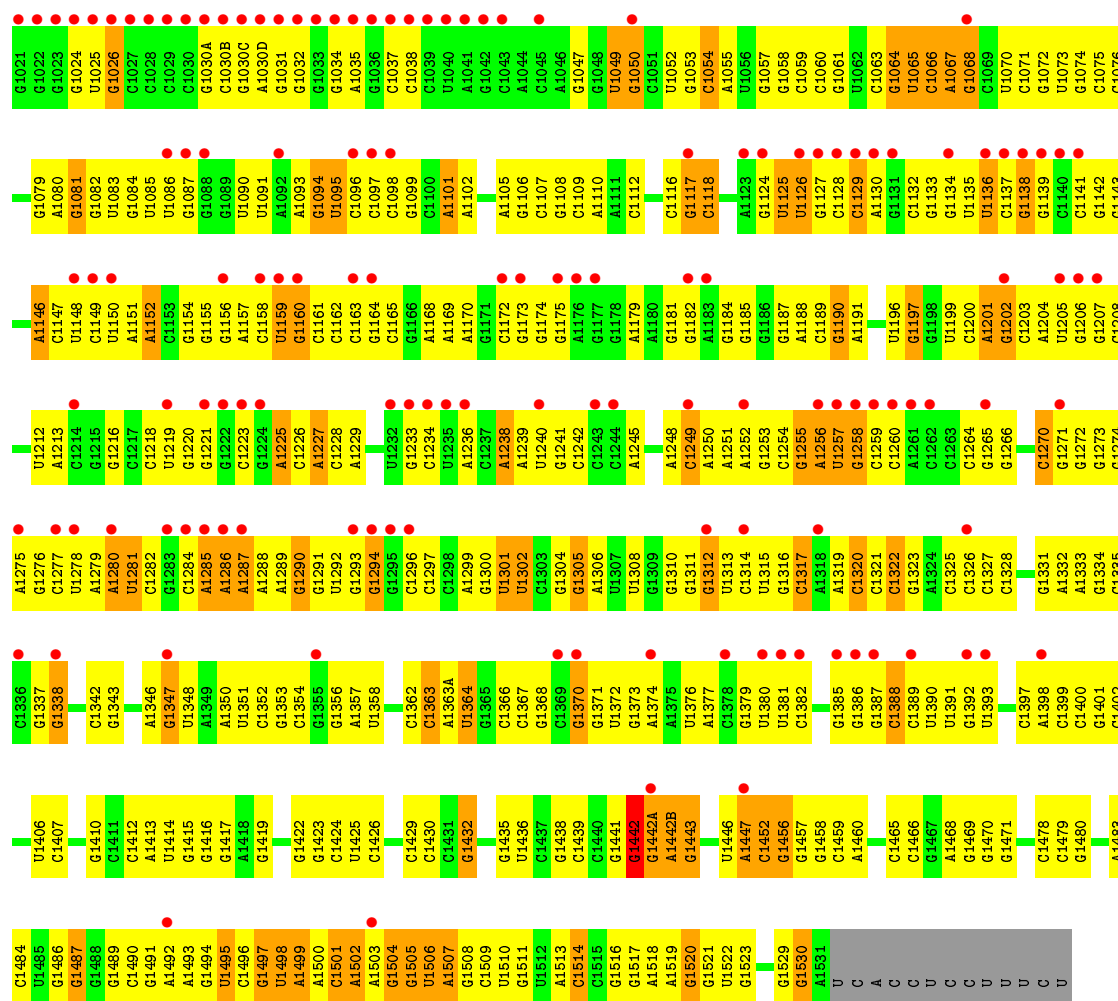
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA

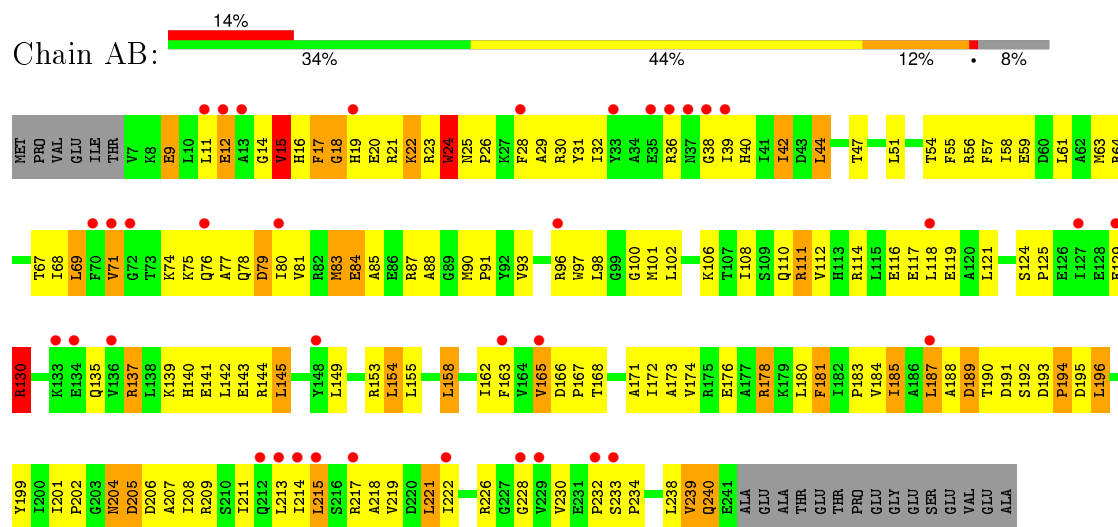






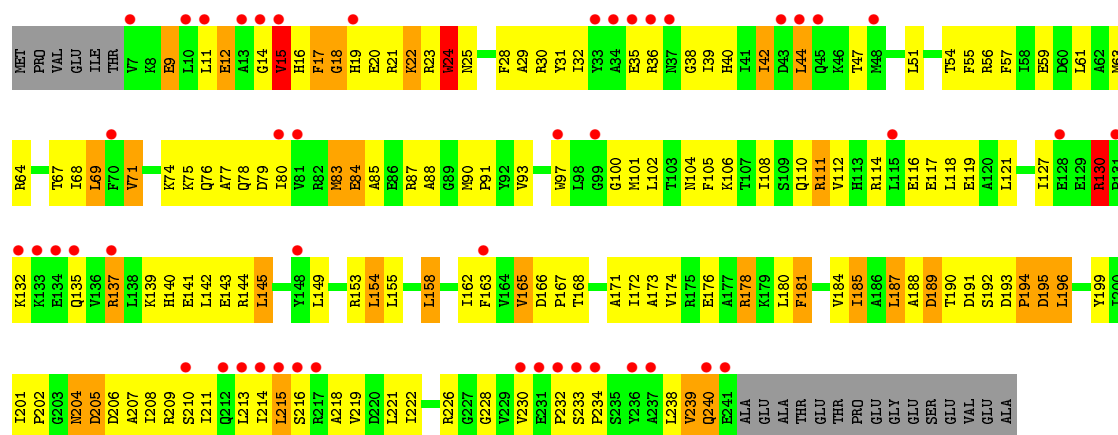


• Molecule 2: 30S ribosomal protein S2

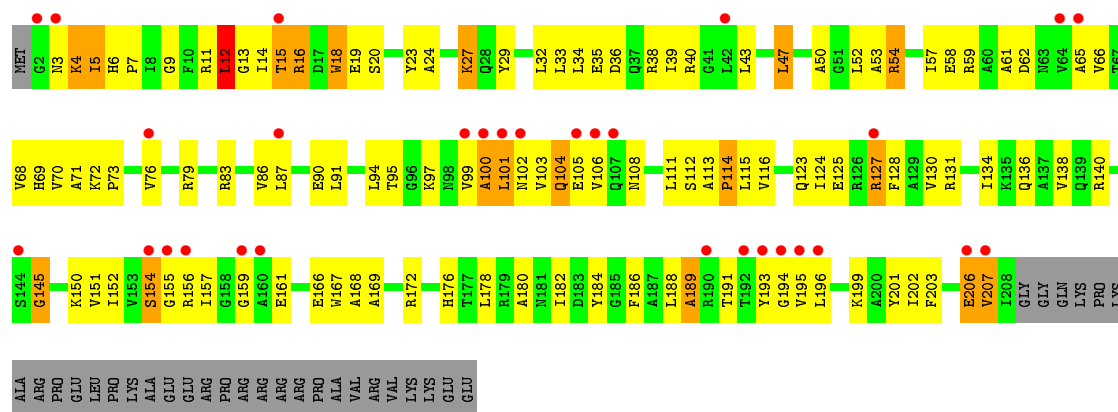
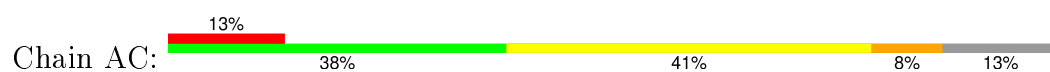


• Molecule 2: 30S ribosomal protein S2

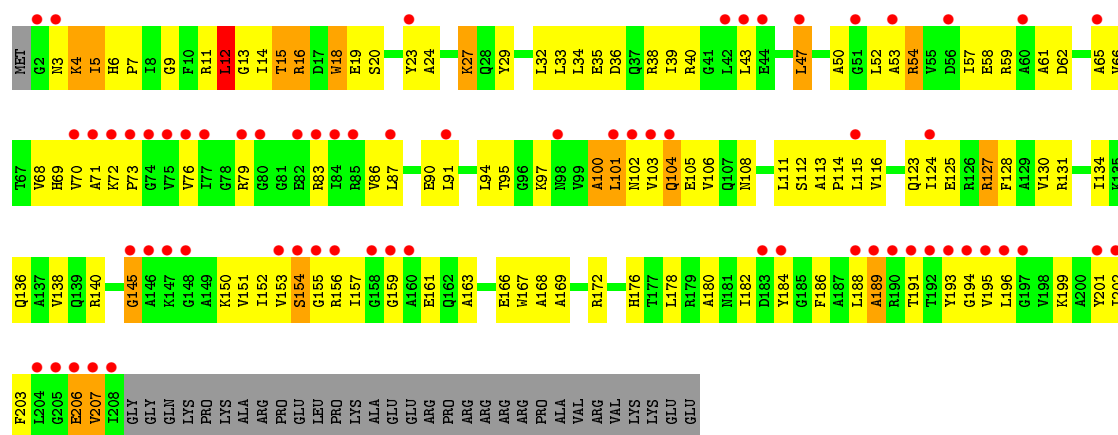




• Molecule 3: 30S ribosomal protein S3

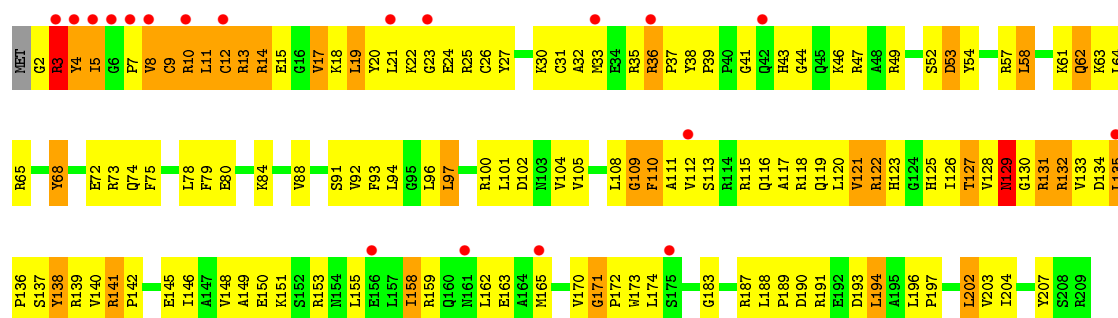


• Molecule 3: 30S ribosomal protein S3

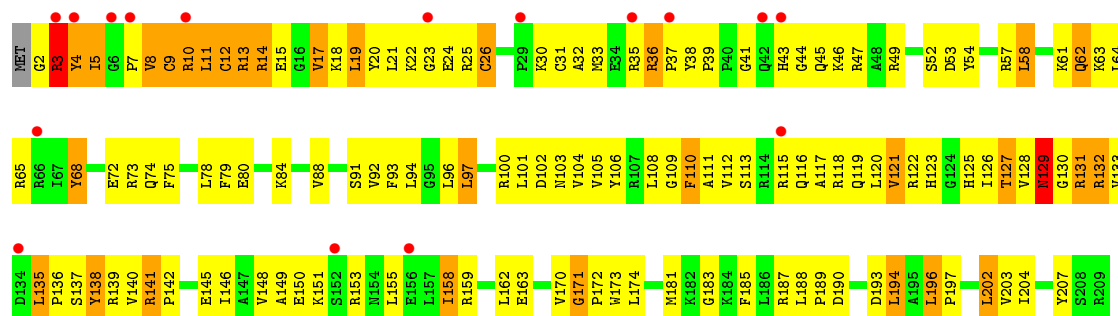


• Molecule 4: 30S ribosomal protein S4

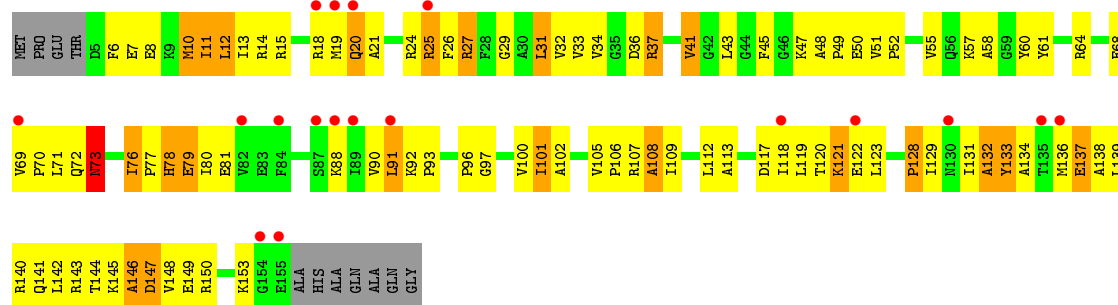




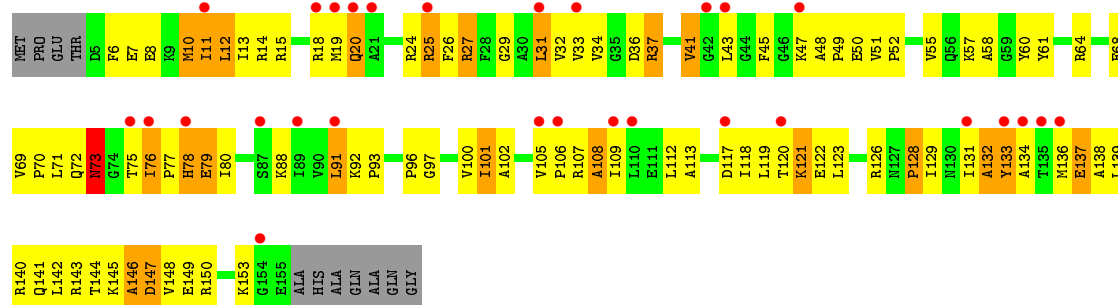
• Molecule 4: 30S ribosomal protein S4



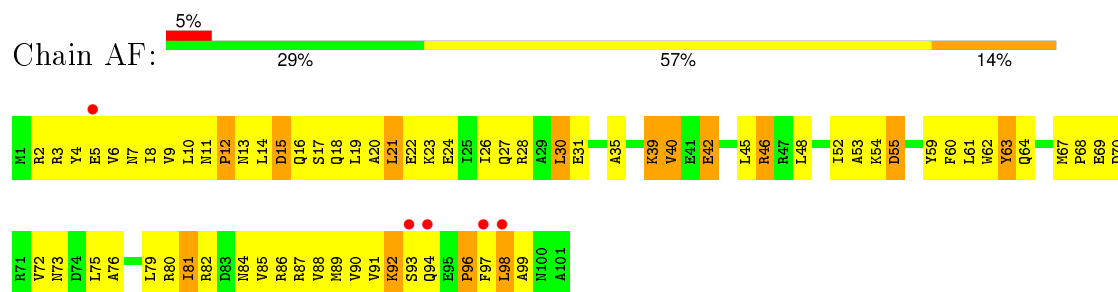
• Molecule 5: 30S ribosomal protein S5



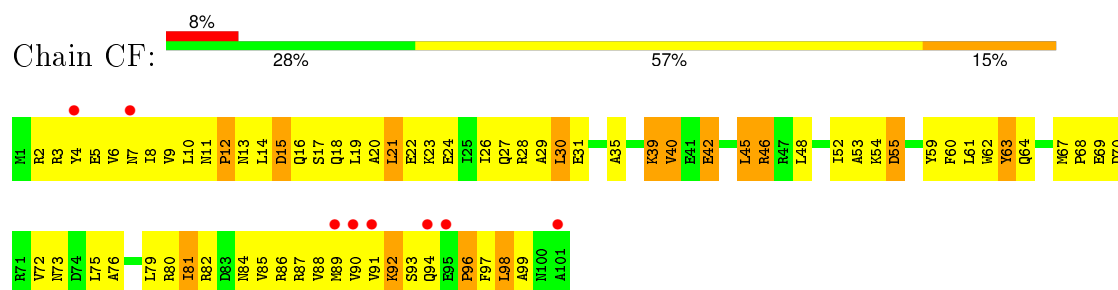
• Molecule 5: 30S ribosomal protein S5



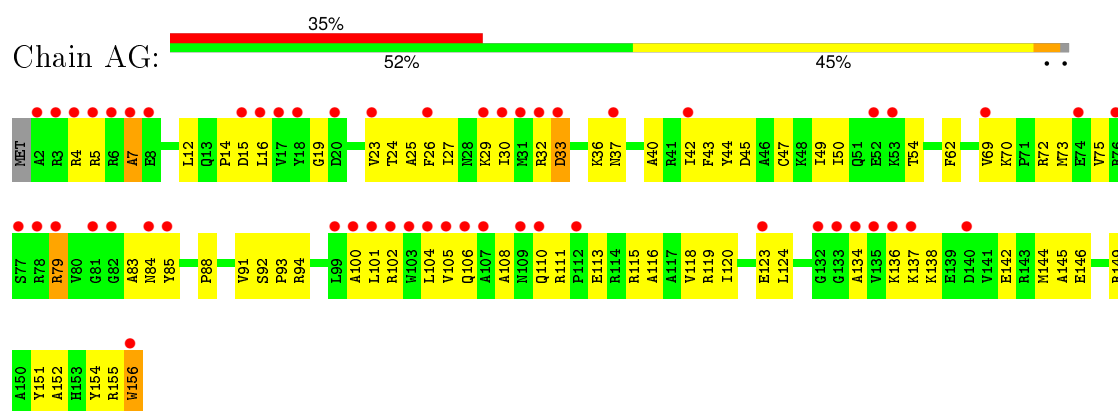
- Molecule 6: 30S ribosomal protein S6



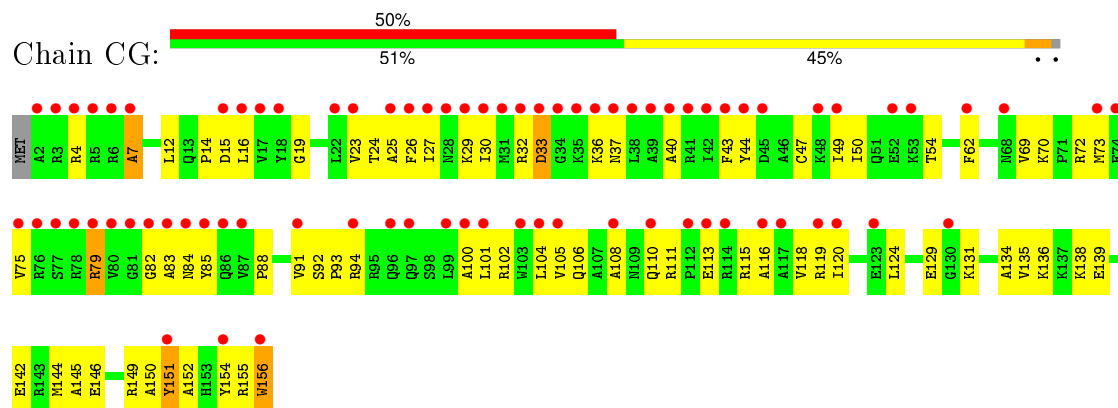
- Molecule 6: 30S ribosomal protein S6



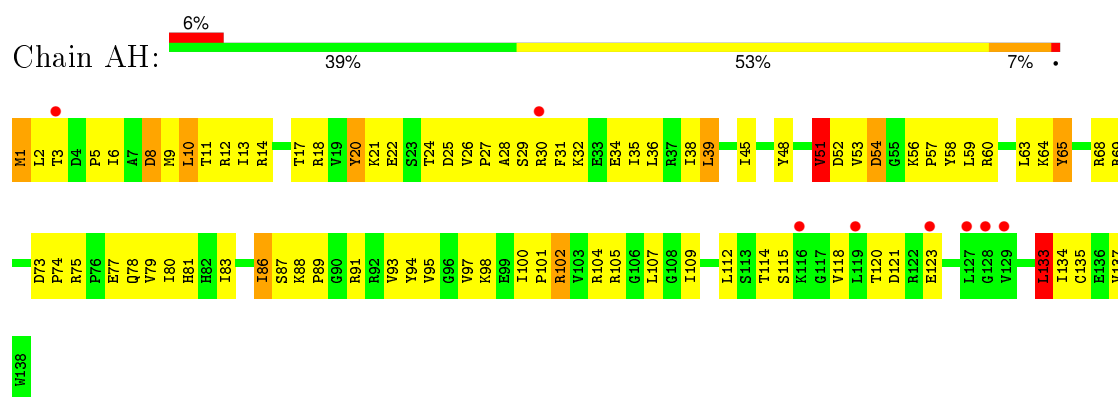
- Molecule 7: 30S ribosomal protein S7



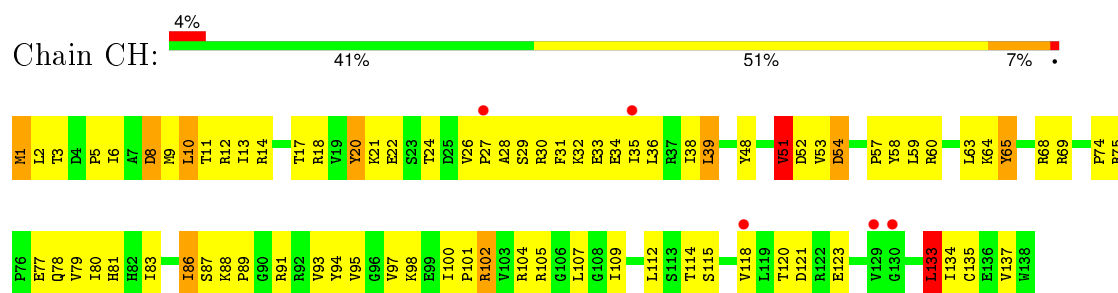
- Molecule 7: 30S ribosomal protein S7



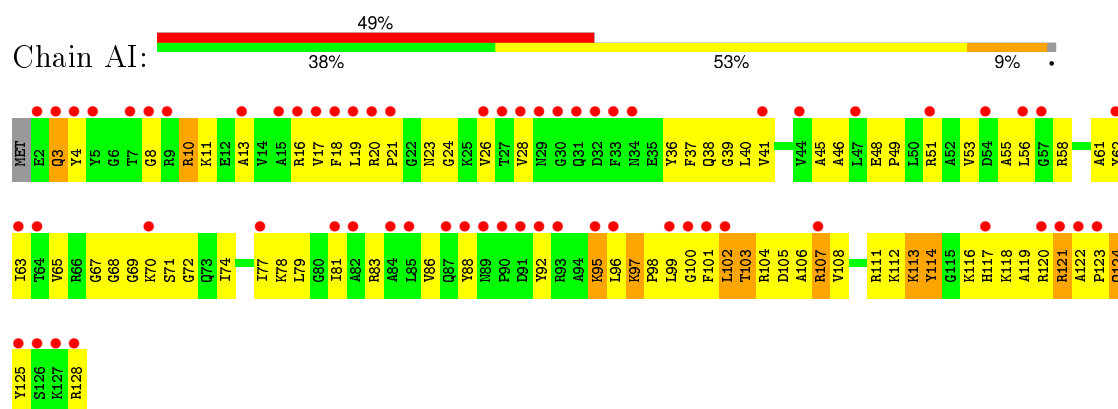
- Molecule 8: 30S ribosomal protein S8



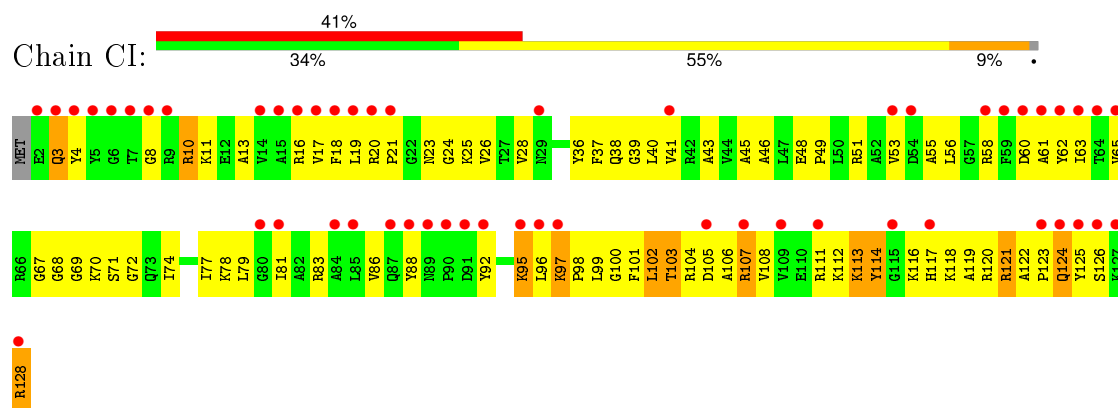
- Molecule 8: 30S ribosomal protein S8



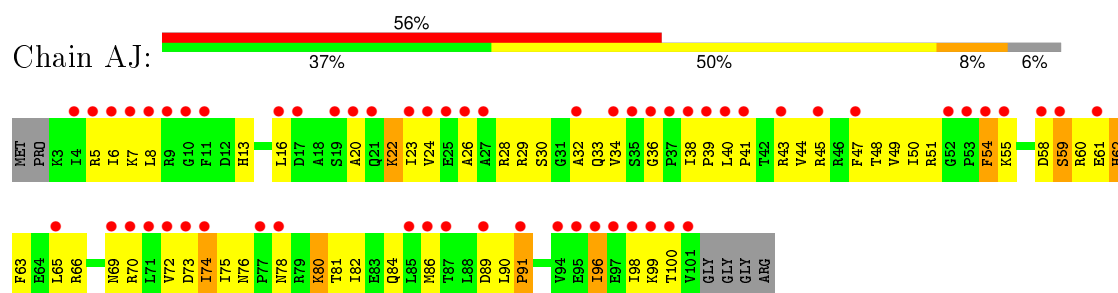
- Molecule 9: 30S ribosomal protein S9



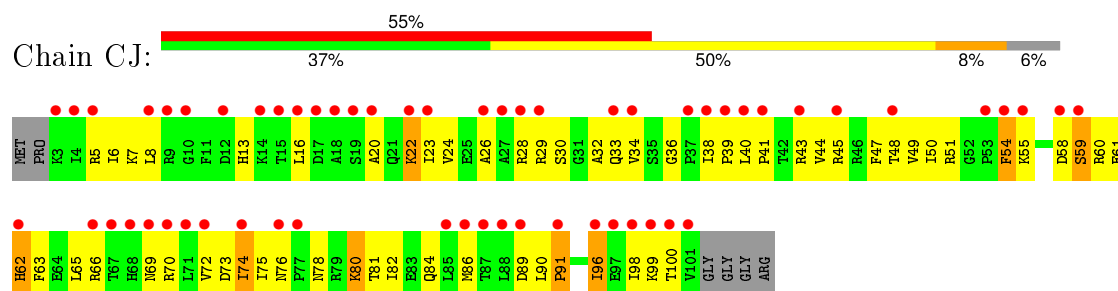
- Molecule 9: 30S ribosomal protein S9



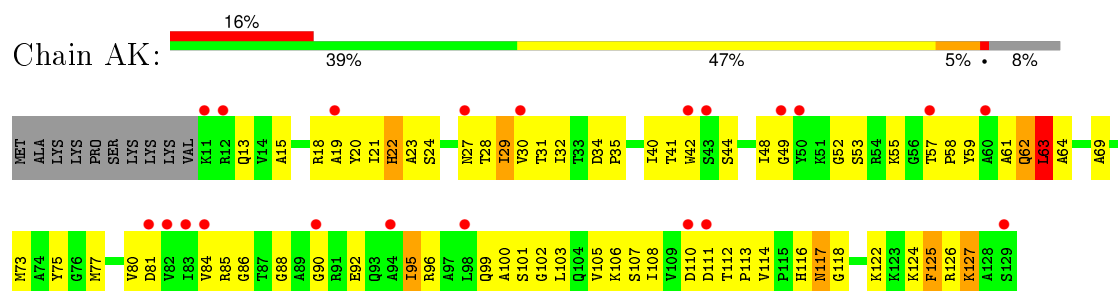
- Molecule 10: 30S ribosomal protein S10



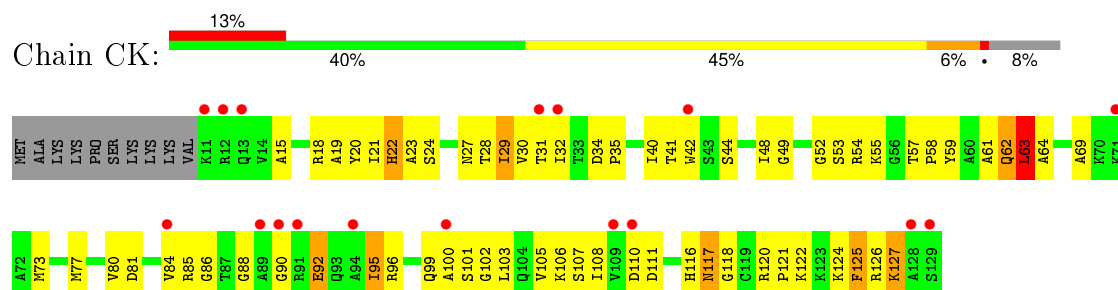
- Molecule 10: 30S ribosomal protein S10



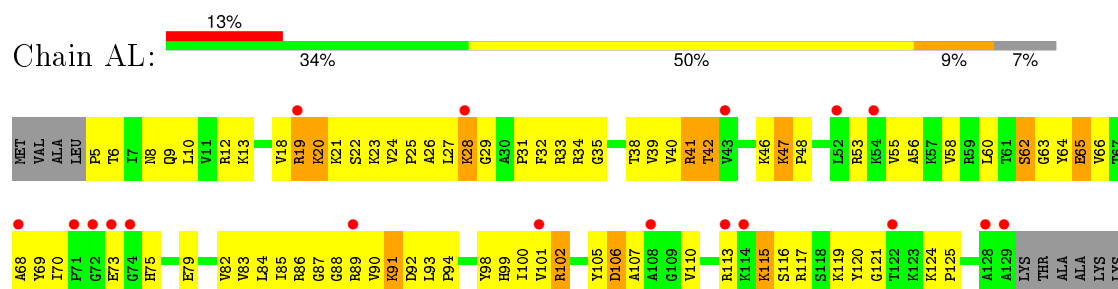
- Molecule 11: 30S ribosomal protein S11



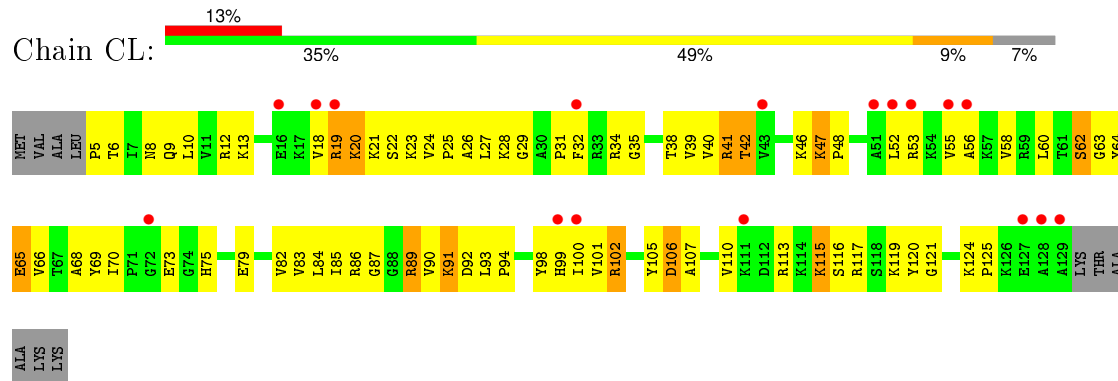
- Molecule 11: 30S ribosomal protein S11



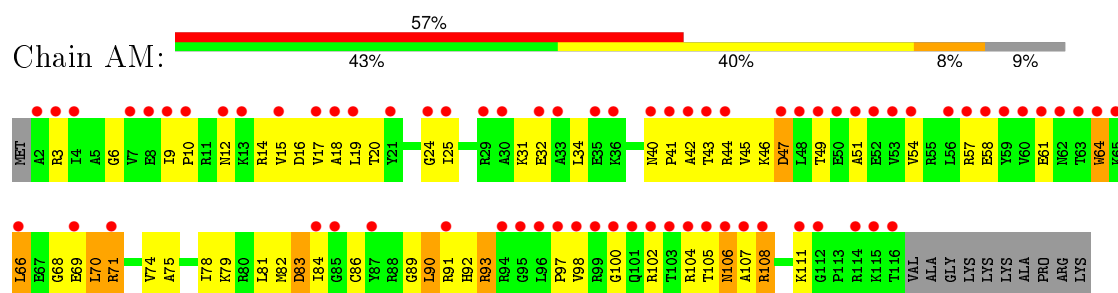
- Molecule 12: 30S ribosomal protein S12



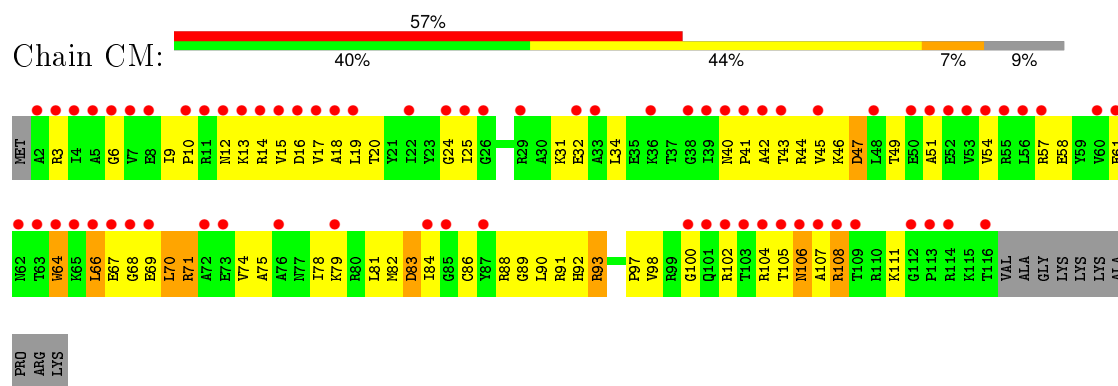
- Molecule 12: 30S ribosomal protein S12



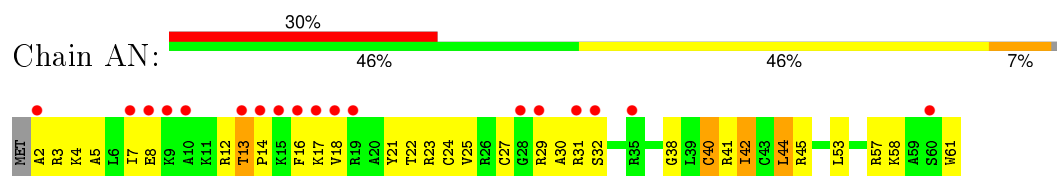
- Molecule 13: 30S ribosomal protein S13



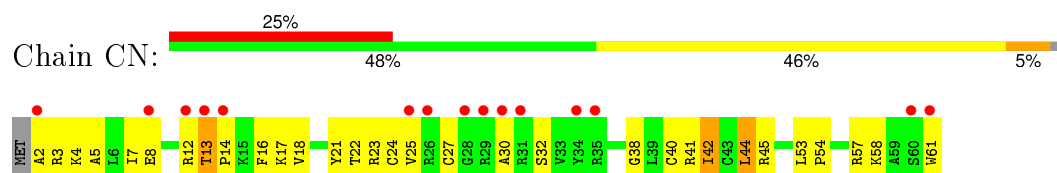
- Molecule 13: 30S ribosomal protein S13



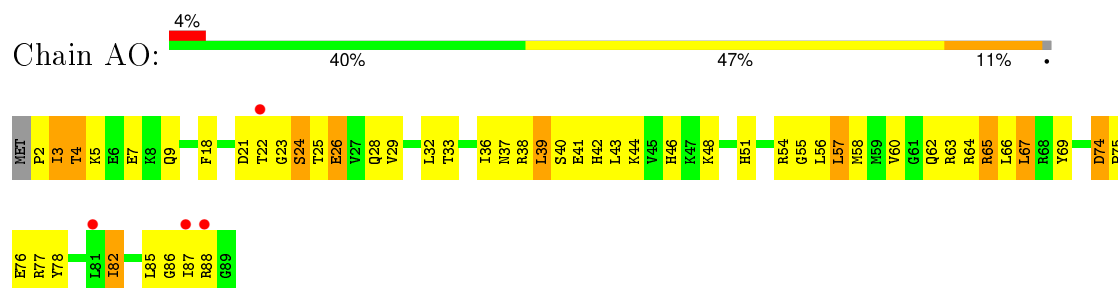
- Molecule 14: 30S ribosomal protein S14



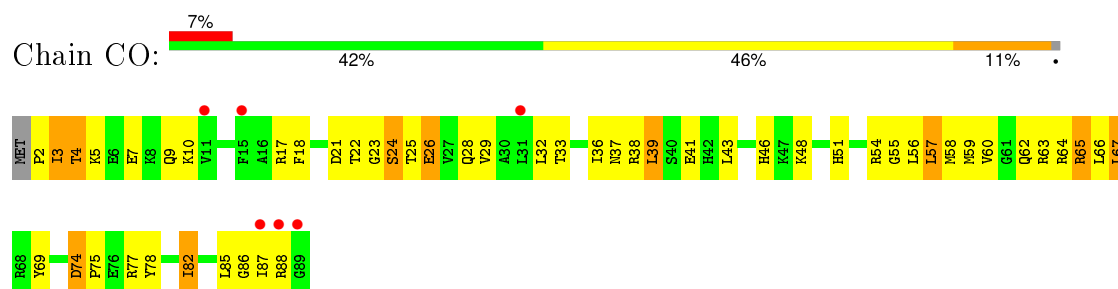
- Molecule 14: 30S ribosomal protein S14



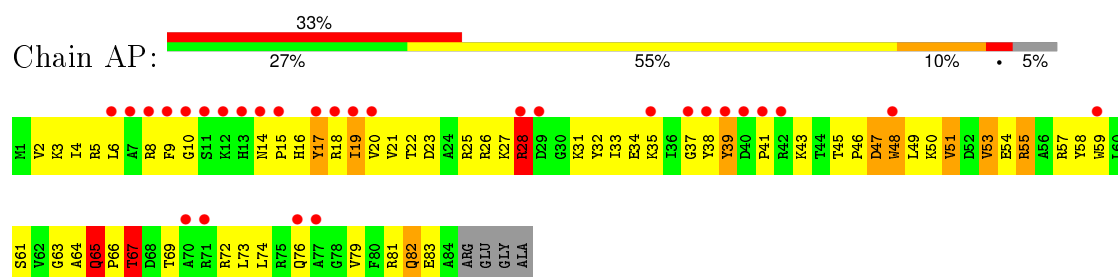
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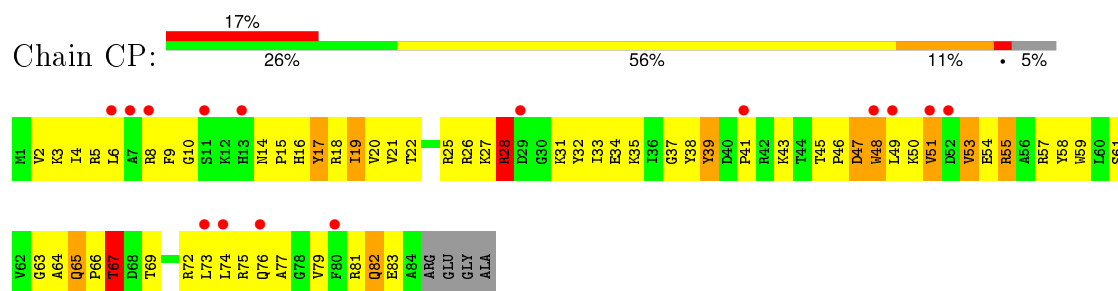
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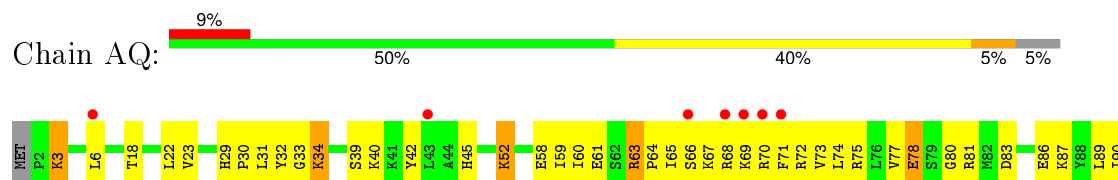
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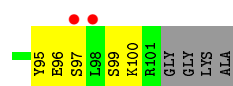


- Molecule 16: 30S ribosomal protein S16

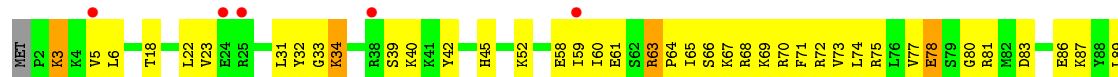


- Molecule 17: 30S ribosomal protein S17

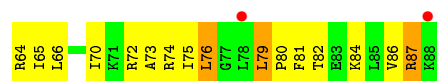
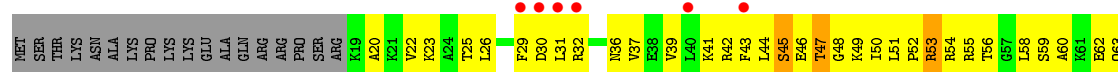




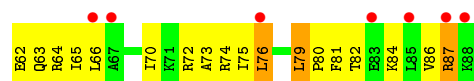
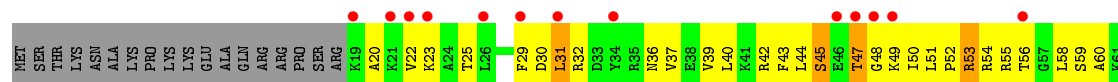
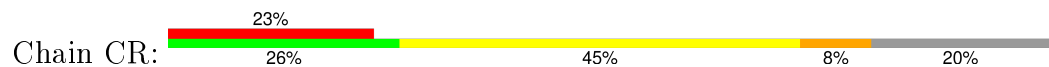
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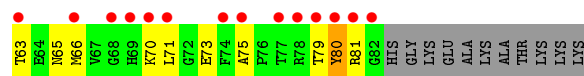
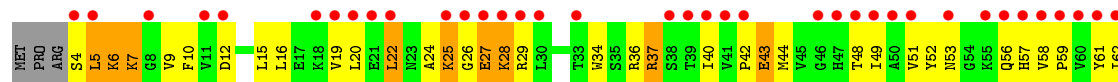
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

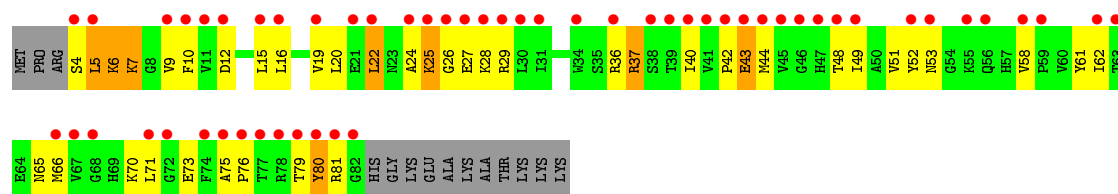


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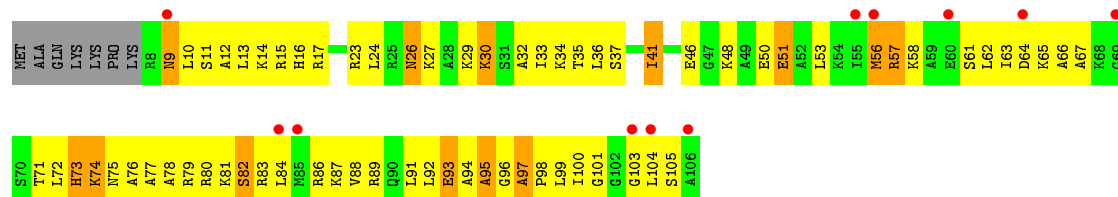


- Molecule 19: 30S ribosomal protein S19

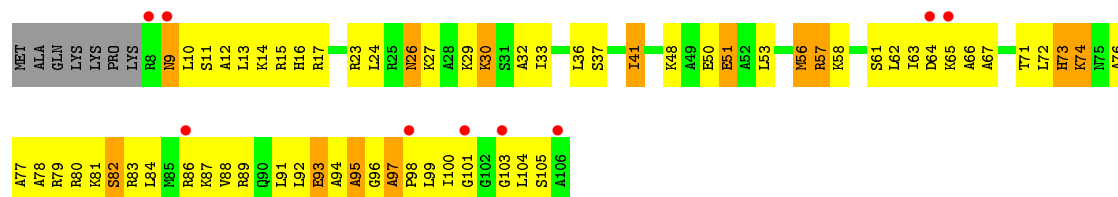




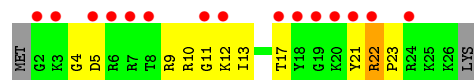
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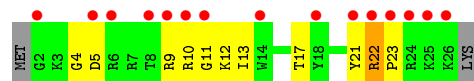
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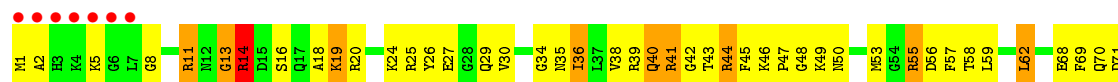
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx

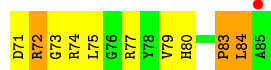


- Molecule 22: 50S ribosomal protein L27

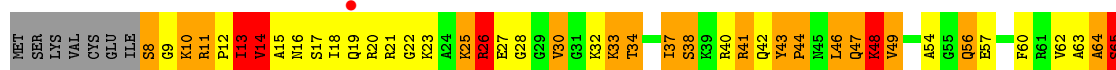
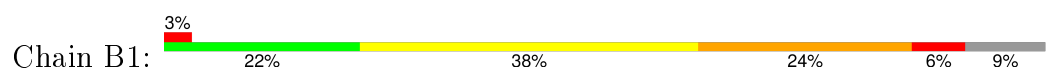




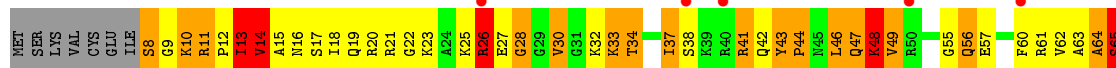
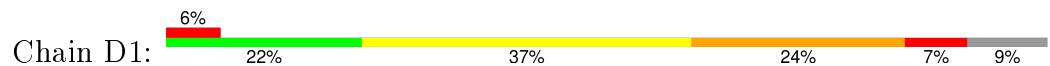
- Molecule 22: 50S ribosomal protein L27



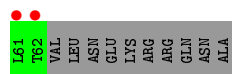
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29

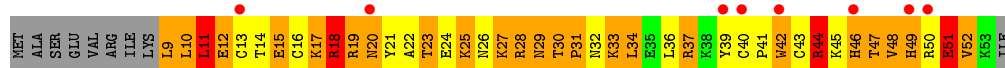




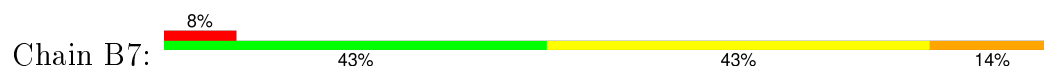
- Molecule 28: 50S ribosomal protein L33



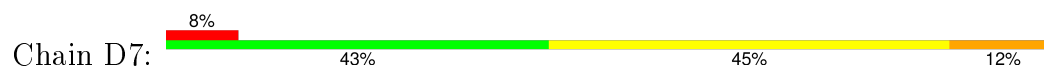
- Molecule 28: 50S ribosomal protein L33



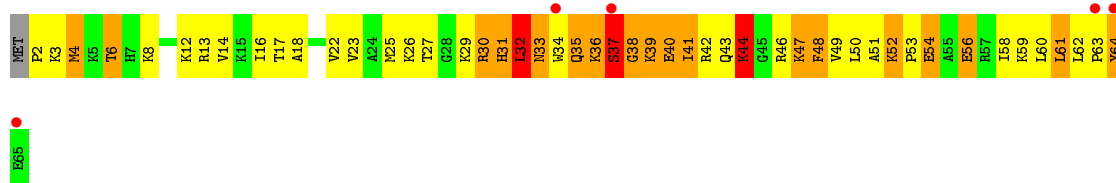
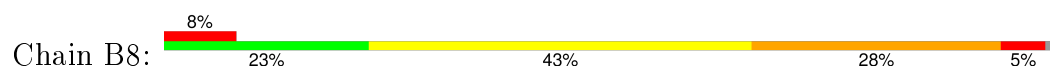
- Molecule 29: 50S ribosomal protein L34



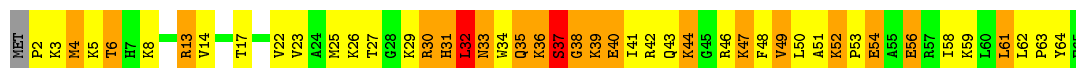
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



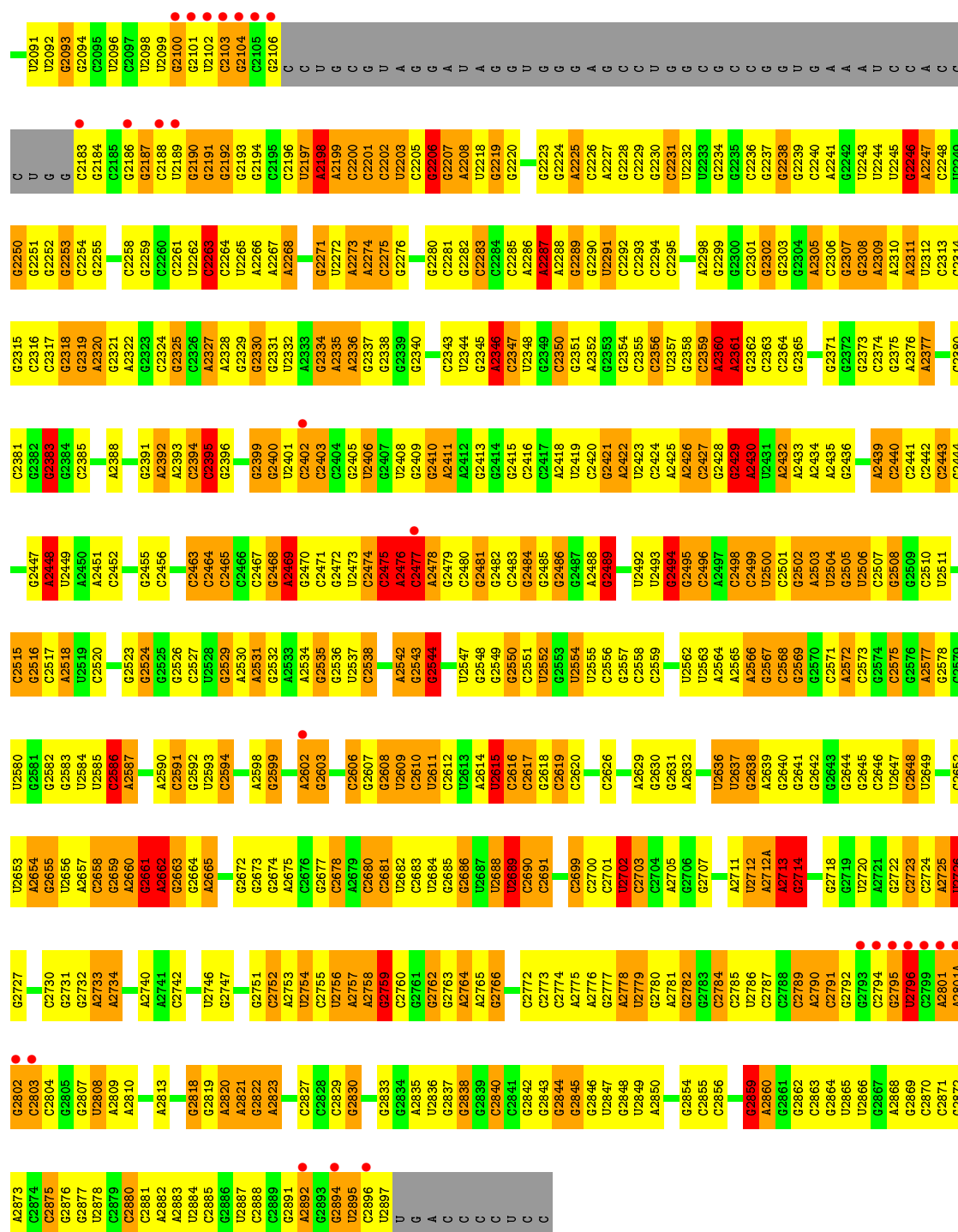
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 23S ribosomal RNA



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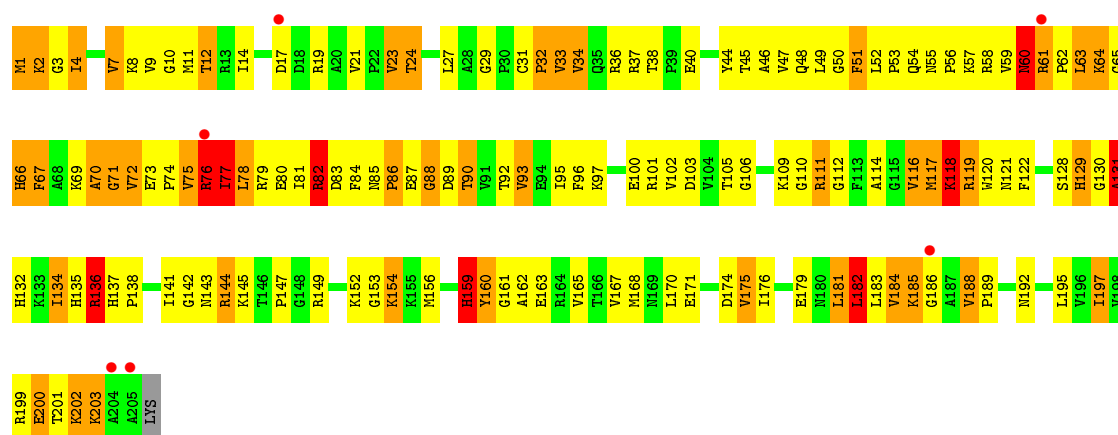




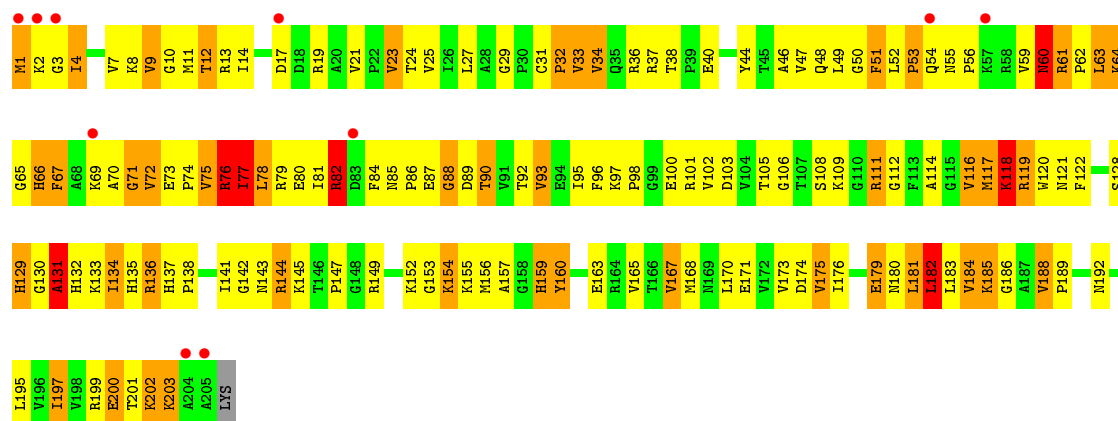
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C		C2044		C1908	U1768	G1680	G1613	C1549	G1479	G1410	G1344		
C		C2045	G1950	C1909	G1771	G1681	A1614	C1550	G1480	C1411	G1345	A1284	G1218
C			A1981	G1910	G1772	G1682	C1615	C1551	G1481	A1412		A1285	G1219
G			C1982	U1911	C1773	C1683	A1616	G1552	G1482		A1349	A1286	A1220
C	G2048	G2049	C1983	A1912	C1774	C1684	C1617	A1553	G1484		C1350	A1287	C1221A
C	A2050	A2051	G1984	A1913	U1775	C1685	A1618	A1554	G1485	G1416	C1351	U1288	G1224
A	A2051	G2052	G1985	C1914	G1776	G1686	G1619		A1486	C1417	U1352	C1289	G1225
G	G2053	G2054	A1986	U1915	U1777	G1687			G1487	G1418	U1353	C1290	G1226
G	A2054	C2055	G1987	A1916	U1778	A1688			U1489	A1419	A1354	U1291	A1227
A	C2056	G2057	U1917	G1917	U1779	A1689			G1490	U1420	G1355	U1292	G1227
U	G2057		C1918	A1918	U1780	U1693			G1491		G1356	C1293	G1228
A	U2058		A1919	C1919	C1781	C1694			G1492	A1427	U1357		G1229
A	C2059		C1920	C1920	C1782	G1695			C1493	C1428	G1358		
G	A2060		G1921	A1921	A1783	G1696			A1494	G1429	A1359		U1234
G	G2061		G1922	G1922	U1784	G1697			A1495	C1430	A1360		G1235
G	A2062		U1923	U1923	A1785	A1698			A1496	U1431	G1361		G1236
G	C2063		C1924	C1924	U1786	G1699			U1497	C1432	C1362		A1237
A	G2064		C1925	C1925	A1787	A1700			C1498	U1433	C1363		G1238
A	C2065		U1926	U1926	G1788	A1701			A1499	A1434	A1302		G1239
A	U2066		A1927	A1927	A1789	G1702			G1500	G1435	C1304		U1240
C	C2067		G1928	G1928	C1790	G1703			C1501	G1436	A1365		A1241
C			G1929	G1929	A1791	C1637			C1502	C1437	A1367		A1242
C			G1930	G1930	G1792	C1638			U1503	U1438	G1368		G1243
U			U1931	U1931	C1793	U1639			C1504	A1439	G1369		G1244



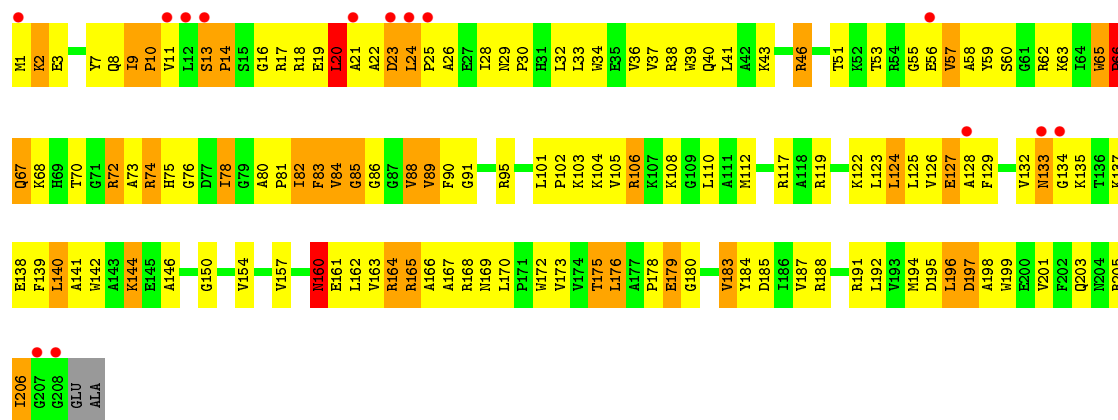




• Molecule 34: 50S ribosomal protein L3

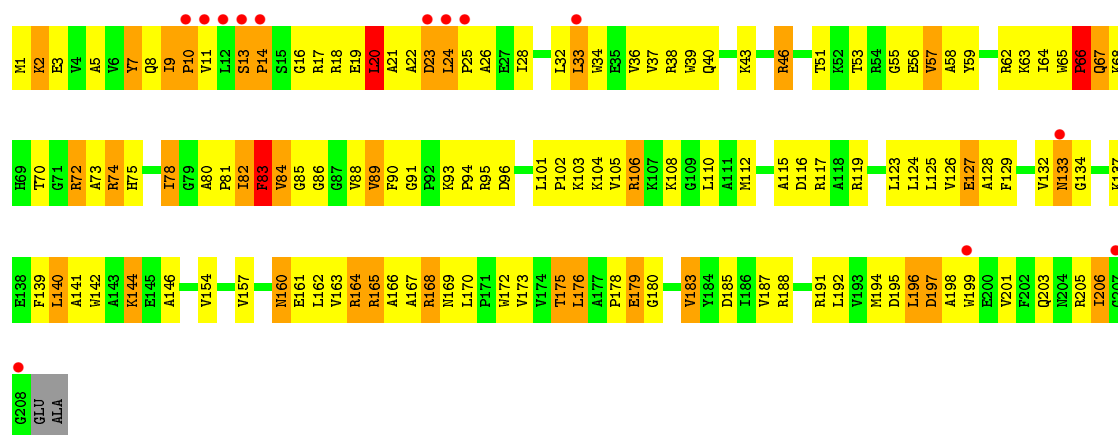


• Molecule 35: 50S ribosomal protein L4

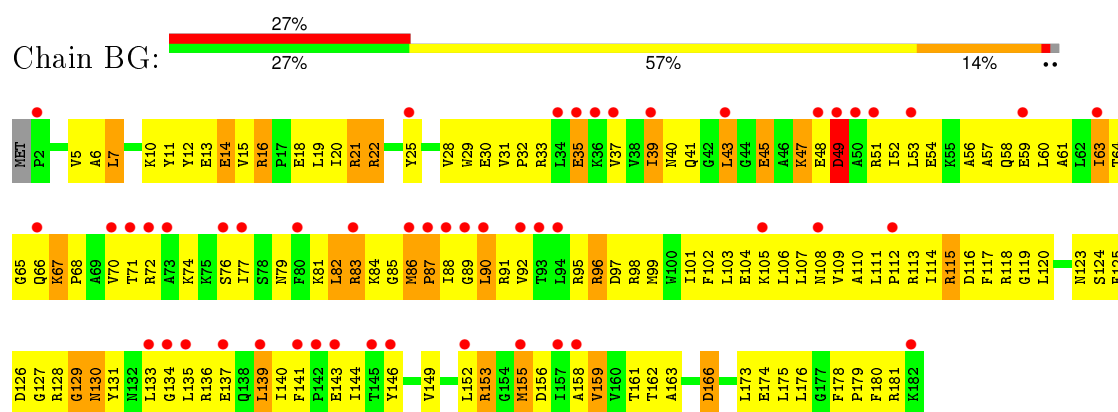


• Molecule 35: 50S ribosomal protein L4

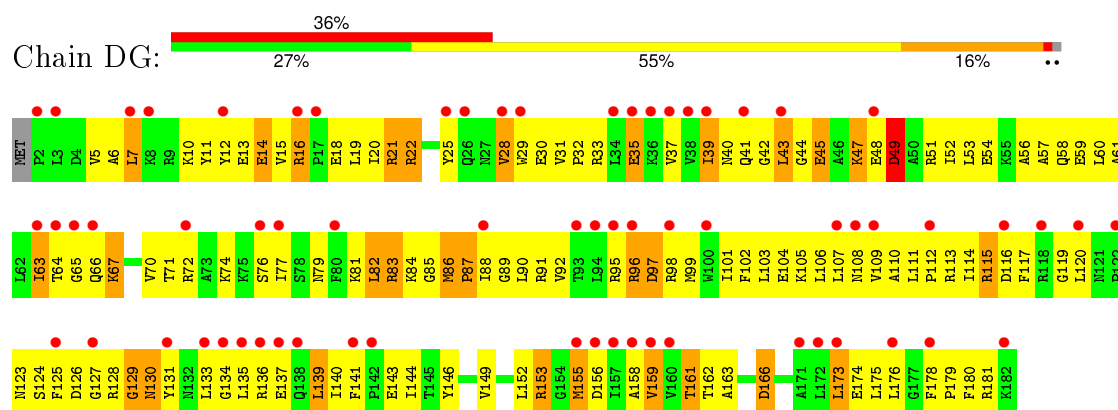




• Molecule 36: 50S ribosomal protein L5



• Molecule 36: 50S ribosomal protein L5

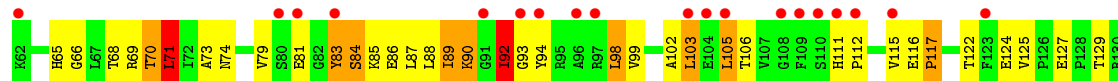


• Molecule 37: 50S ribosomal protein L6

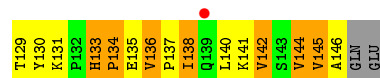
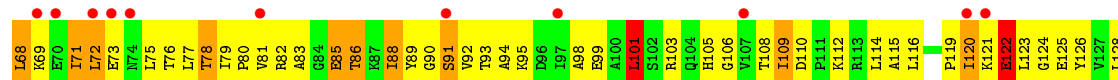
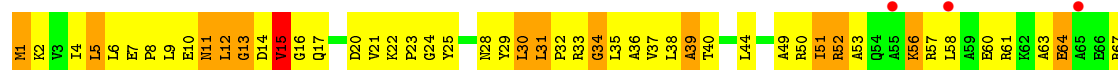




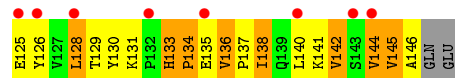
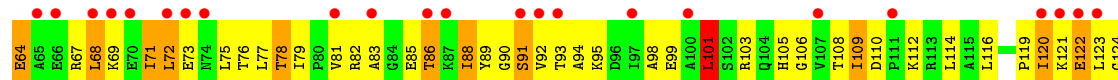
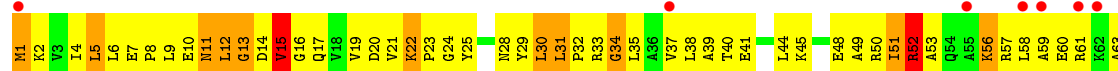
• Molecule 37: 50S ribosomal protein L6



• Molecule 38: 50S ribosomal protein L9

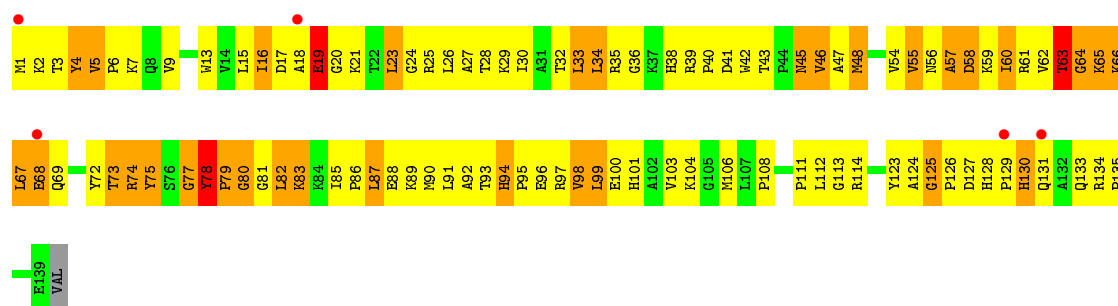


• Molecule 38: 50S ribosomal protein L9

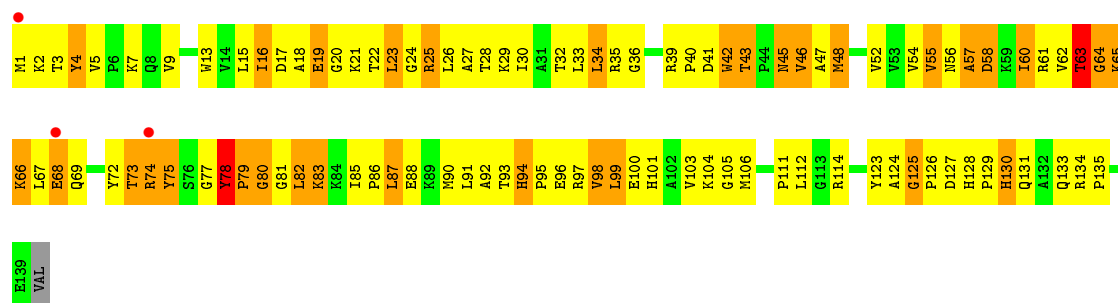


• Molecule 39: 50S ribosomal protein L13

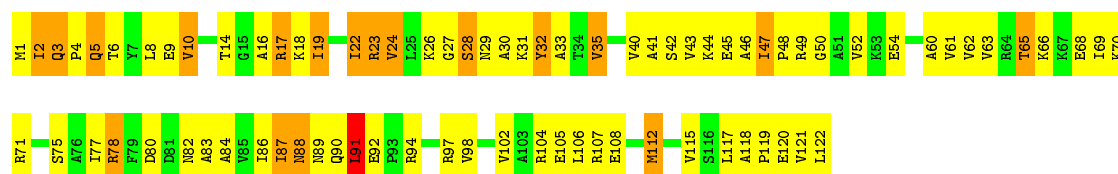




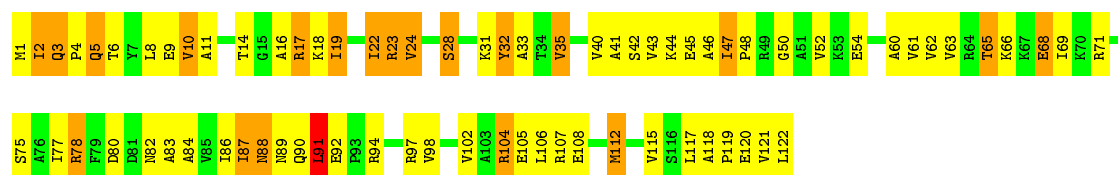
- Molecule 39: 50S ribosomal protein L13



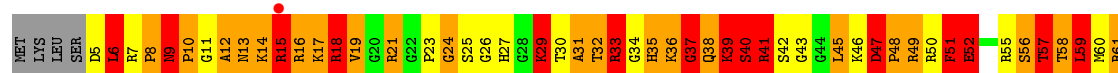
- Molecule 40: 50S ribosomal protein L14

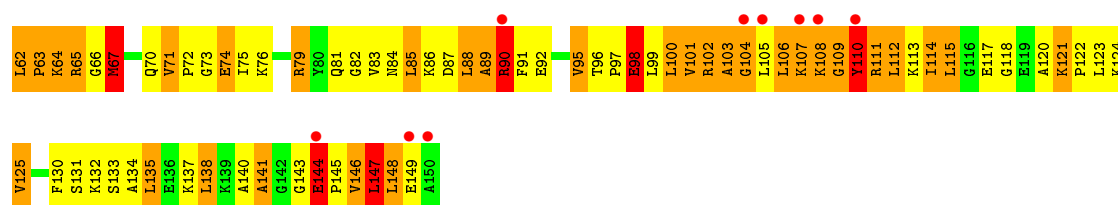


- Molecule 40: 50S ribosomal protein L14

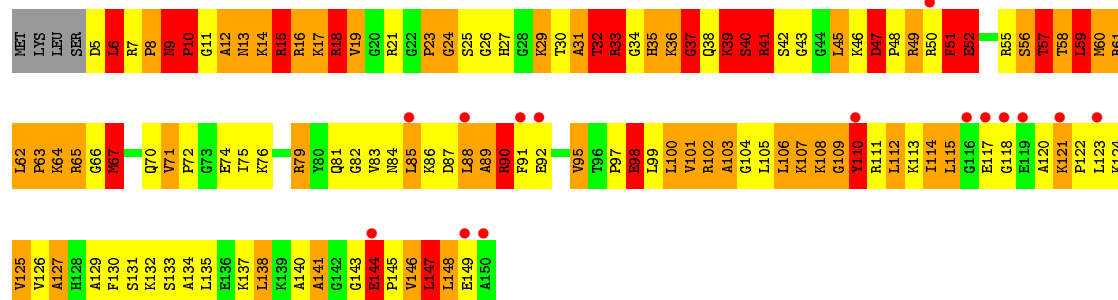


- Molecule 41: 50S ribosomal protein L15

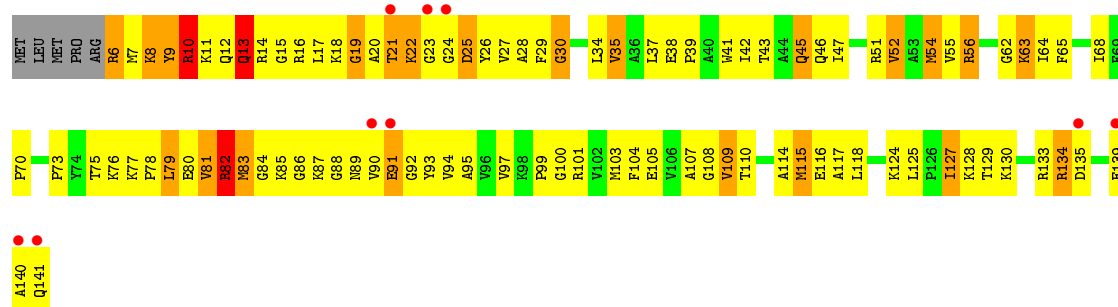




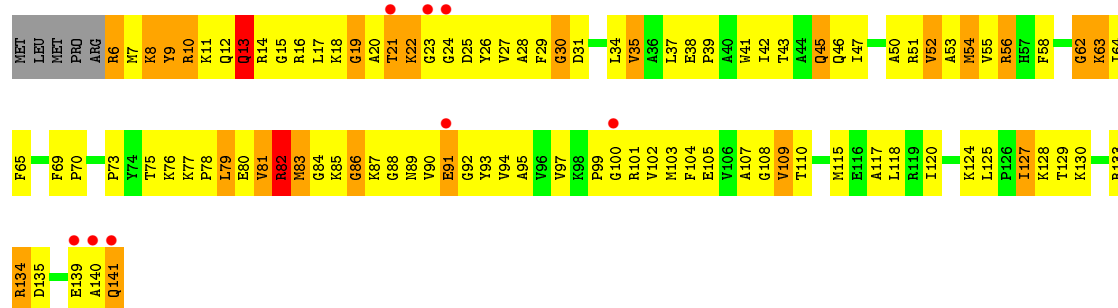
• Molecule 41: 50S ribosomal protein L15



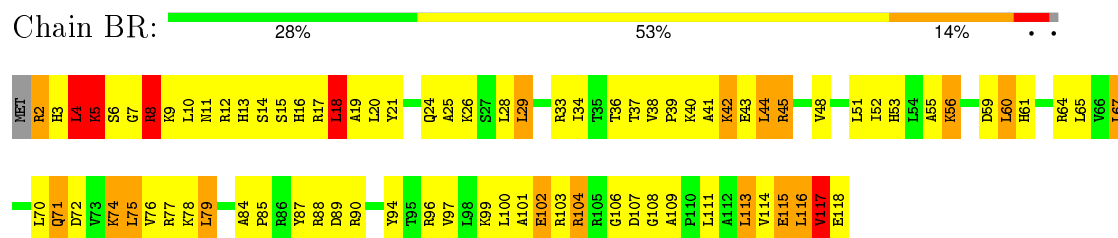
• Molecule 42: 50S ribosomal protein L16



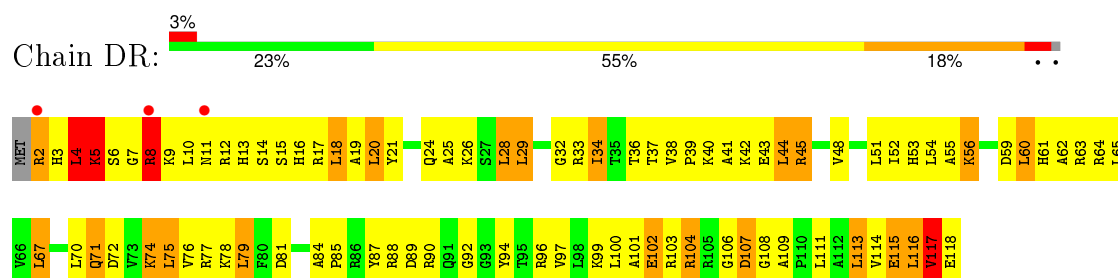
• Molecule 42: 50S ribosomal protein L16



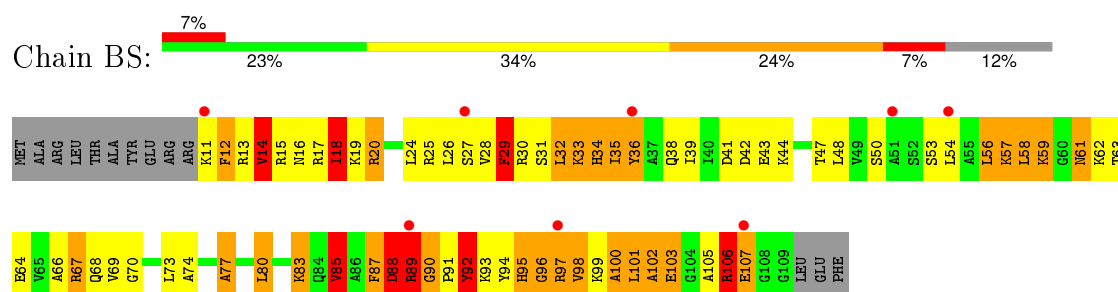
• Molecule 43: 50S ribosomal protein L17



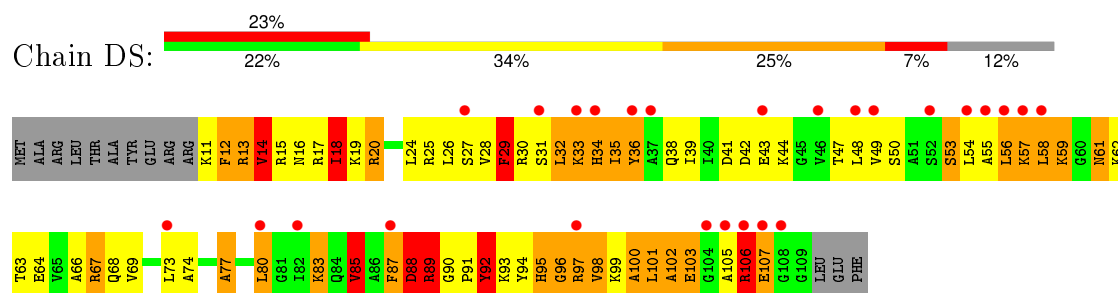
• Molecule 43: 50S ribosomal protein L17



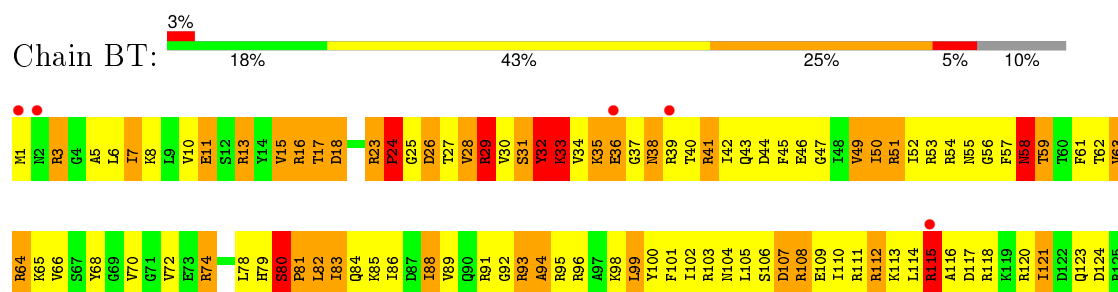
• Molecule 44: 50S ribosomal protein L18

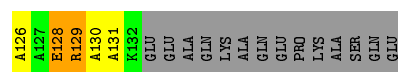


• Molecule 44: 50S ribosomal protein L18

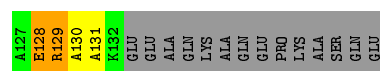
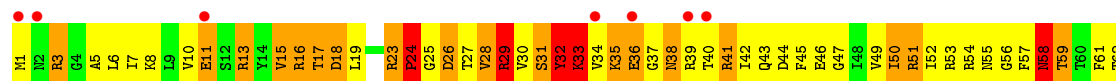
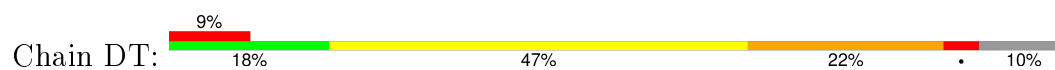


• Molecule 45: 50S ribosomal protein L19

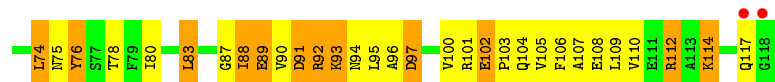




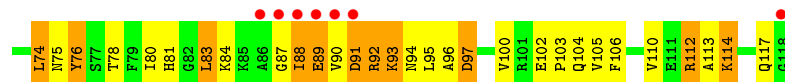
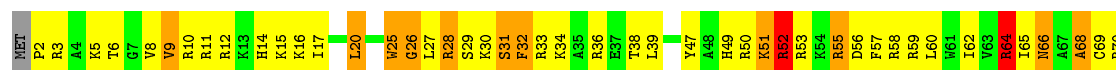
- Molecule 45: 50S ribosomal protein L19



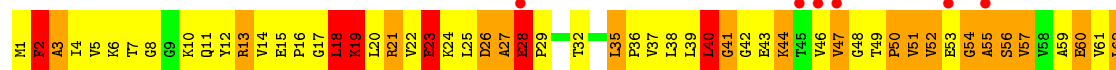
- Molecule 46: 50S ribosomal protein L20



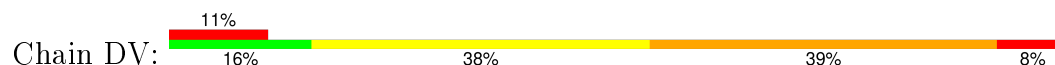
- Molecule 46: 50S ribosomal protein L20

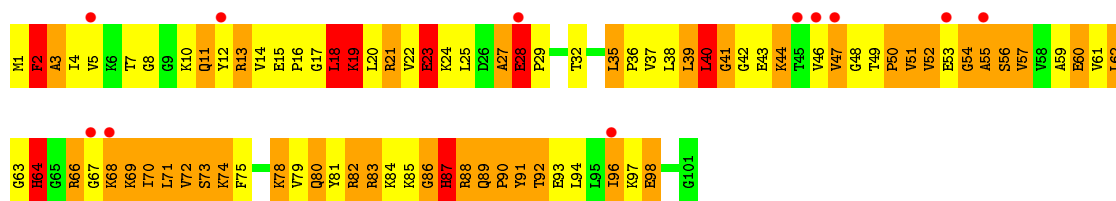


- Molecule 47: 50S ribosomal protein L21



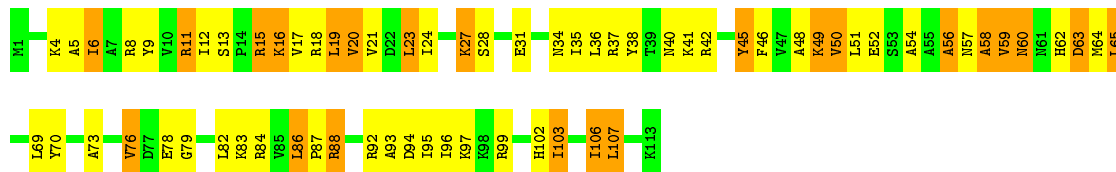
- Molecule 47: 50S ribosomal protein L21





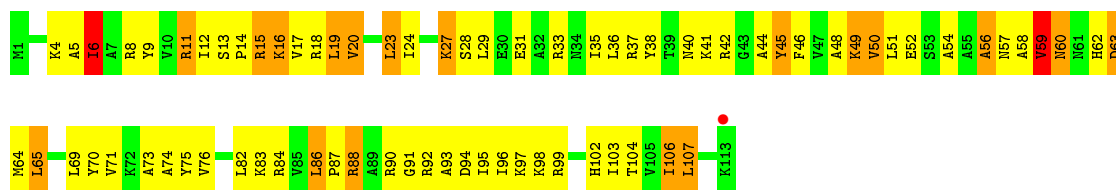
• Molecule 48: 50S ribosomal protein L22

Chain BW: 40% 40% 20%



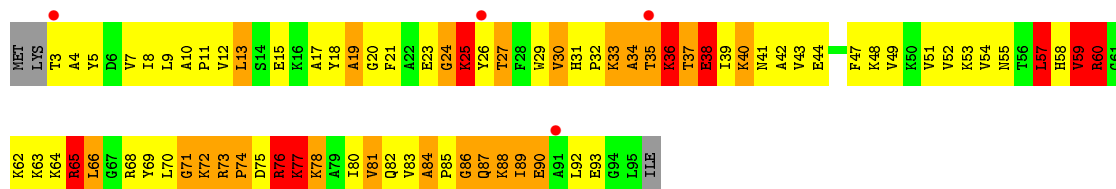
• Molecule 48: 50S ribosomal protein L22

Chain DW: 34% 49% 16%



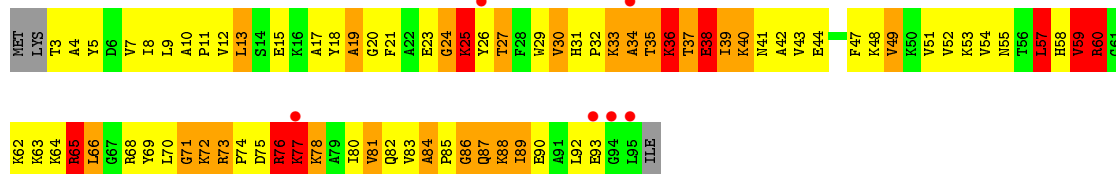
• Molecule 49: 50S ribosomal protein L23

Chain BX: 4% 16% 48% 24% 9%



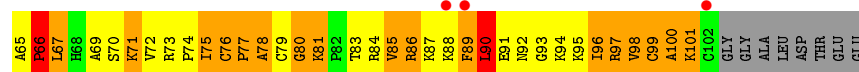
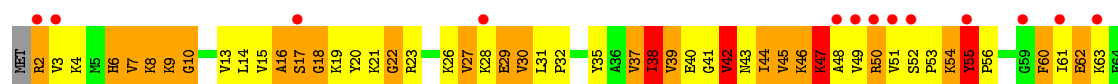
• Molecule 49: 50S ribosomal protein L23

Chain DX: 6% 16% 48% 24% 9%

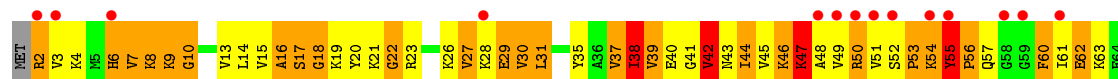


• Molecule 50: 50S ribosomal protein L24

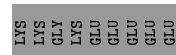
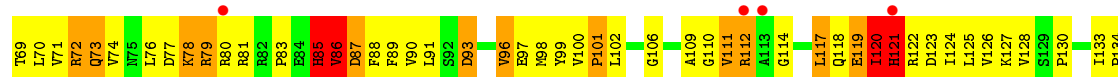
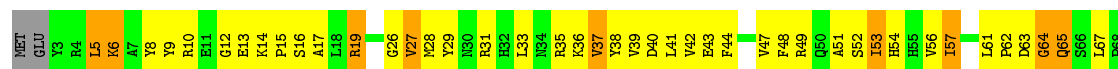
Chain BY: 15% 14% 37% 35% 5% 8%



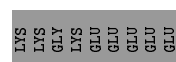
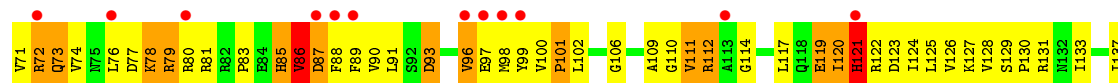
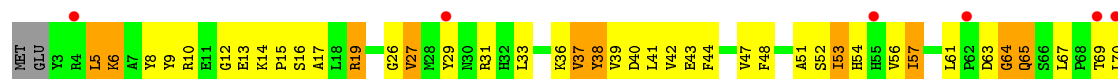
• Molecule 50: 50S ribosomal protein L24



• Molecule 51: 50S ribosomal protein L25



• Molecule 51: 50S ribosomal protein L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.22Å 450.25Å 623.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 3.00 49.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.80-3.00) 88.7 (49.80-3.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.01Å)	Xtriage
Refinement program	Phenix	Depositor
R, R_{free}	0.235 , 0.269 0.235 , 0.268	Depositor DCC
R_{free} test set	51892 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 92.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1035238 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	278000	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, ZIT, MG

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.38	0/1147	0.63	0/1553
39	BN	0.70	0/1132	0.88	1/1527 (0.1%)
39	DN	0.54	0/1132	0.79	0/1527
40	BO	0.57	0/943	0.71	0/1269
40	DO	0.50	0/943	0.69	0/1269
41	BP	0.72	1/1131 (0.1%)	1.03	4/1504 (0.3%)
41	DP	0.63	0/1131	0.95	4/1504 (0.3%)
42	BQ	0.65	0/1100	0.84	1/1470 (0.1%)
42	DQ	0.58	0/1100	0.80	0/1470
43	BR	0.63	0/974	0.91	4/1302 (0.3%)
43	DR	0.56	0/974	0.87	3/1302 (0.2%)
44	BS	0.56	0/779	0.83	0/1038
44	DS	0.49	0/779	0.78	0/1038
45	BT	0.58	0/1114	0.83	1/1488 (0.1%)
45	DT	0.53	0/1114	0.80	0/1488
46	BU	0.71	0/975	0.77	0/1297
46	DU	0.59	0/975	0.71	0/1297
47	BV	0.76	0/789	0.96	1/1054 (0.1%)
47	DV	0.58	0/789	0.89	1/1054 (0.1%)
48	BW	0.67	0/907	0.84	0/1216
48	DW	0.58	0/907	0.79	0/1216
49	BX	0.74	0/740	0.99	3/995 (0.3%)
49	DX	0.64	0/740	0.90	2/995 (0.2%)
50	BY	0.67	1/789 (0.1%)	0.88	1/1053 (0.1%)
50	DY	0.56	0/789	0.82	1/1053 (0.1%)
51	BZ	0.46	0/1436	0.64	2/1951 (0.1%)
51	DZ	0.40	0/1436	0.62	2/1951 (0.1%)
All	All	0.75	139/301000 (0.0%)	1.13	2159/449812 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	B1	0	1
23	D1	0	1
24	B2	0	3
24	D2	0	1
27	B5	0	1
27	D5	0	1
31	BA	21	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	DA	21	0
33	BD	0	2
33	DD	0	2
34	BE	0	2
34	DE	0	2
35	BF	0	1
37	BH	0	2
37	DH	0	2
41	BP	0	5
41	DP	0	4
42	BQ	0	1
42	DQ	0	1
43	BR	0	1
43	DR	0	1
44	BS	0	1
44	DS	0	1
45	BT	0	1
45	DT	0	1
47	BV	0	1
47	DV	0	2
49	BX	0	3
49	DX	0	3
All	All	42	47

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

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

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

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

5 of 42 chirality outliers are listed below:

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

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	B1	30	VAL	Peptide
24	B2	55	ARG	Peptide
24	B2	56	GLN	Peptide
24	B2	57	ILE	Peptide
27	B5	51	TYR	Peptide

5.2 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	1409	0
1	CA	32329	0	16318	1381	0
2	AB	1901	0	1951	169	0
2	CB	1901	0	1951	167	0
3	AC	1613	0	1677	116	0
3	CC	1613	0	1677	117	0
4	AD	1703	0	1763	158	0
4	CD	1703	0	1763	160	0
5	AE	1147	0	1207	103	0
5	CE	1147	0	1207	107	0
6	AF	843	0	857	80	0
6	CF	843	0	857	86	0
7	AG	1257	0	1296	60	0
7	CG	1257	0	1296	62	0
8	AH	1116	0	1177	83	0
8	CH	1116	0	1177	82	0
9	AI	1011	0	1042	84	0
9	CI	1011	0	1042	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	80	0
10	CJ	795	0	840	82	0
11	AK	885	0	904	64	0
11	CK	885	0	904	69	0
12	AL	971	0	1057	104	0
12	CL	971	0	1057	106	0
13	AM	921	0	976	60	0
13	CM	921	0	976	63	0
14	AN	492	0	530	35	0
14	CN	492	0	529	33	0
15	AO	734	0	771	54	0
15	CO	734	0	771	56	0
16	AP	701	0	720	88	0
16	CP	701	0	720	91	0
17	AQ	824	0	891	46	0
17	CQ	824	0	891	49	0
18	AR	574	0	644	63	0
18	CR	574	0	644	64	0
19	AS	630	0	652	40	0
19	CS	630	0	652	34	0
20	AT	763	0	861	78	0
20	CT	763	0	861	75	0
21	AU	209	0	221	11	0
21	CU	209	0	221	11	0
22	B0	650	0	654	67	0
22	D0	650	0	654	64	0
23	B1	693	0	764	143	0
23	D1	693	0	764	144	0
24	B2	421	0	461	119	1
24	D2	421	0	461	125	0
25	B3	468	0	523	37	0
25	D3	468	0	523	56	0
26	B4	157	0	69	12	0
26	D4	157	0	69	12	0
27	B5	459	0	478	82	0
27	D5	459	0	480	85	0
28	B6	381	0	390	96	0
28	D6	381	0	390	92	0
29	B7	419	0	467	37	0
29	D7	419	0	467	38	0
30	B8	508	0	576	156	0
30	D8	508	0	576	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BA	58698	0	29590	2392	0
31	DA	58698	0	29591	2578	1
32	BB	2551	0	1295	156	0
32	DB	2551	0	1295	173	0
33	BD	2105	0	2182	336	0
33	DD	2105	0	2182	333	0
34	BE	1564	0	1629	214	0
34	DE	1564	0	1629	213	0
35	BF	1624	0	1677	171	0
35	DF	1624	0	1677	178	0
36	BG	1474	0	1534	149	0
36	DG	1474	0	1534	149	0
37	BH	1223	0	1282	141	0
37	DH	1223	0	1282	129	0
38	BI	1132	0	1218	142	0
38	DI	1132	0	1218	156	0
39	BN	1105	0	1180	184	0
39	DN	1105	0	1180	183	0
40	BO	933	0	996	86	0
40	DO	933	0	996	76	0
41	BP	1114	0	1187	271	0
41	DP	1114	0	1187	260	0
42	BQ	1080	0	1127	157	0
42	DQ	1080	0	1127	162	0
43	BR	960	0	1021	115	0
43	DR	960	0	1021	117	0
44	BS	771	0	832	148	0
44	DS	771	0	832	150	0
45	BT	1100	0	1164	173	0
45	DT	1100	0	1164	166	0
46	BU	958	0	1015	142	0
46	DU	958	0	1015	151	0
47	BV	779	0	851	210	0
47	DV	779	0	851	215	0
48	BW	896	0	953	76	0
48	DW	896	0	953	80	0
49	BX	726	0	778	163	0
49	DX	726	0	778	168	0
50	BY	776	0	870	179	0
50	DY	776	0	870	187	0
51	BZ	1404	0	1432	140	0
51	DZ	1404	0	1432	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AA	51	0	0	0	0
52	B0	1	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	B7	1	0	0	0	0
52	BA	349	0	0	0	0
52	BB	5	0	0	0	0
52	BD	1	0	0	0	0
52	BE	1	0	0	0	0
52	BF	1	0	0	0	0
52	BP	3	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	1	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	48	0	0	0	0
52	D0	1	0	0	0	0
52	D1	1	0	0	0	0
52	D5	2	0	0	0	0
52	D7	1	0	0	0	0
52	DA	309	0	0	0	0
52	DB	3	0	0	0	0
52	DD	1	0	0	0	0
52	DE	1	0	0	0	0
52	DF	1	0	0	0	0
52	DP	1	0	0	0	0
52	DQ	1	0	0	0	0
52	DR	1	0	0	0	0
52	DU	1	0	0	0	0
52	DX	1	0	0	0	0
53	AD	1	0	0	0	0
53	AN	1	0	0	0	0
53	CD	1	0	0	0	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	52	0	72	3	0
55	DA	52	0	72	3	0
All	All	278000	0	189246	17418	1

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 37.

The worst 5 of 17418 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)
42:BQ:81:VAL:O	42:BQ:82:ARG:HG2	1.13	1.31
42:DQ:81:VAL:O	42:DQ:82:ARG:HG2	1.25	1.27
41:BP:59:LEU:HA	41:BP:61:ARG:NH1	1.49	1.25
41:DP:59:LEU:HA	41:DP:61:ARG:NH1	1.55	1.20
31:DA:2206:G:N2	31:DA:2207:G:H5'	1.58	1.19

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	7	33
8	AH	136/138 (99%)	98 (72%)	31 (23%)	7 (5%)	2	15
8	CH	136/138 (99%)	98 (72%)	31 (23%)	7 (5%)	2	15
9	AI	123/128 (96%)	92 (75%)	24 (20%)	7 (6%)	2	12
9	CI	123/128 (96%)	94 (76%)	22 (18%)	7 (6%)	2	12
10	AJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	2	15
10	CJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	2	15
11	AK	117/129 (91%)	87 (74%)	26 (22%)	4 (3%)	5	25
11	CK	117/129 (91%)	86 (74%)	27 (23%)	4 (3%)	5	25
12	AL	123/135 (91%)	82 (67%)	31 (25%)	10 (8%)	1	5
12	CL	123/135 (91%)	83 (68%)	29 (24%)	11 (9%)	1	4
13	AM	107/126 (85%)	84 (78%)	17 (16%)	6 (6%)	2	13
13	CM	107/126 (85%)	84 (78%)	17 (16%)	6 (6%)	2	13
14	AN	58/61 (95%)	45 (78%)	11 (19%)	2 (3%)	5	25
14	CN	58/61 (95%)	44 (76%)	12 (21%)	2 (3%)	5	25
15	AO	86/89 (97%)	62 (72%)	19 (22%)	5 (6%)	2	12
15	CO	86/89 (97%)	61 (71%)	21 (24%)	4 (5%)	3	17
16	AP	82/88 (93%)	48 (58%)	27 (33%)	7 (8%)	1	5
16	CP	82/88 (93%)	47 (57%)	29 (35%)	6 (7%)	1	6
17	AQ	98/105 (93%)	74 (76%)	18 (18%)	6 (6%)	2	11
17	CQ	98/105 (93%)	73 (74%)	19 (19%)	6 (6%)	2	11
18	AR	68/88 (77%)	52 (76%)	11 (16%)	5 (7%)	1	6
18	CR	68/88 (77%)	51 (75%)	13 (19%)	4 (6%)	2	11
19	AS	77/93 (83%)	58 (75%)	13 (17%)	6 (8%)	1	6
19	CS	77/93 (83%)	59 (77%)	12 (16%)	6 (8%)	1	6
20	AT	97/106 (92%)	69 (71%)	19 (20%)	9 (9%)	1	4
20	CT	97/106 (92%)	65 (67%)	23 (24%)	9 (9%)	1	4
21	AU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	3	19
21	CU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	3	19
22	B0	83/85 (98%)	65 (78%)	14 (17%)	4 (5%)	3	17
22	D0	83/85 (98%)	64 (77%)	15 (18%)	4 (5%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	B1	87/98 (89%)	48 (55%)	17 (20%)	22 (25%)	0	0
23	D1	87/98 (89%)	45 (52%)	19 (22%)	23 (26%)	0	0
24	B2	49/72 (68%)	23 (47%)	19 (39%)	7 (14%)	0	1
24	D2	49/72 (68%)	23 (47%)	18 (37%)	8 (16%)	0	1
25	B3	58/60 (97%)	52 (90%)	4 (7%)	2 (3%)	5	25
25	D3	58/60 (97%)	51 (88%)	5 (9%)	2 (3%)	5	25
26	B4	30/71 (42%)	5 (17%)	11 (37%)	14 (47%)	0	0
26	D4	30/71 (42%)	5 (17%)	10 (33%)	15 (50%)	0	0
27	B5	57/60 (95%)	38 (67%)	11 (19%)	8 (14%)	0	1
27	D5	57/60 (95%)	36 (63%)	14 (25%)	7 (12%)	0	2
28	B6	41/54 (76%)	21 (51%)	6 (15%)	14 (34%)	0	0
28	D6	41/54 (76%)	19 (46%)	8 (20%)	14 (34%)	0	0
29	B7	47/49 (96%)	41 (87%)	4 (8%)	2 (4%)	3	19
29	D7	47/49 (96%)	40 (85%)	4 (8%)	3 (6%)	2	9
30	B8	62/65 (95%)	42 (68%)	11 (18%)	9 (14%)	0	1
30	D8	62/65 (95%)	41 (66%)	12 (19%)	9 (14%)	0	1
33	BD	270/276 (98%)	208 (77%)	45 (17%)	17 (6%)	2	9
33	DD	270/276 (98%)	207 (77%)	47 (17%)	16 (6%)	2	11
34	BE	203/206 (98%)	138 (68%)	37 (18%)	28 (14%)	0	1
34	DE	203/206 (98%)	138 (68%)	38 (19%)	27 (13%)	0	1
35	BF	206/210 (98%)	160 (78%)	30 (15%)	16 (8%)	1	6
35	DF	206/210 (98%)	156 (76%)	33 (16%)	17 (8%)	1	5
36	BG	177/182 (97%)	128 (72%)	35 (20%)	14 (8%)	1	5
36	DG	177/182 (97%)	127 (72%)	36 (20%)	14 (8%)	1	5
37	BH	158/180 (88%)	92 (58%)	41 (26%)	25 (16%)	0	1
37	DH	158/180 (88%)	93 (59%)	39 (25%)	26 (16%)	0	1
38	BI	144/148 (97%)	88 (61%)	32 (22%)	24 (17%)	0	1
38	DI	144/148 (97%)	87 (60%)	35 (24%)	22 (15%)	0	1
39	BN	137/140 (98%)	87 (64%)	32 (23%)	18 (13%)	0	1
39	DN	137/140 (98%)	88 (64%)	32 (23%)	17 (12%)	0	2
40	BO	120/122 (98%)	101 (84%)	16 (13%)	3 (2%)	7	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	DO	120/122 (98%)	99 (82%)	17 (14%)	4 (3%)	5	26
41	BP	144/150 (96%)	77 (54%)	17 (12%)	50 (35%)	0	0
41	DP	144/150 (96%)	76 (53%)	18 (12%)	50 (35%)	0	0
42	BQ	134/141 (95%)	92 (69%)	28 (21%)	14 (10%)	1	3
42	DQ	134/141 (95%)	96 (72%)	23 (17%)	15 (11%)	0	2
43	BR	115/118 (98%)	78 (68%)	29 (25%)	8 (7%)	1	7
43	DR	115/118 (98%)	82 (71%)	24 (21%)	9 (8%)	1	6
44	BS	97/112 (87%)	49 (50%)	24 (25%)	24 (25%)	0	0
44	DS	97/112 (87%)	49 (50%)	23 (24%)	25 (26%)	0	0
45	BT	130/146 (89%)	89 (68%)	21 (16%)	20 (15%)	0	1
45	DT	130/146 (89%)	90 (69%)	21 (16%)	19 (15%)	0	1
46	BU	115/118 (98%)	77 (67%)	27 (24%)	11 (10%)	1	3
46	DU	115/118 (98%)	74 (64%)	29 (25%)	12 (10%)	1	3
47	BV	97/101 (96%)	54 (56%)	15 (16%)	28 (29%)	0	0
47	DV	97/101 (96%)	52 (54%)	18 (19%)	27 (28%)	0	0
48	BW	111/113 (98%)	88 (79%)	15 (14%)	8 (7%)	1	7
48	DW	111/113 (98%)	89 (80%)	15 (14%)	7 (6%)	2	9
49	BX	91/96 (95%)	47 (52%)	22 (24%)	22 (24%)	0	0
49	DX	91/96 (95%)	48 (53%)	22 (24%)	21 (23%)	0	0
50	BY	99/110 (90%)	45 (46%)	22 (22%)	32 (32%)	0	0
50	DY	99/110 (90%)	46 (46%)	21 (21%)	32 (32%)	0	0
51	BZ	175/206 (85%)	113 (65%)	43 (25%)	19 (11%)	0	2
51	DZ	175/206 (85%)	113 (65%)	44 (25%)	18 (10%)	1	3
All	All	11148/12060 (92%)	7735 (69%)	2187 (20%)	1226 (11%)	0	2

5 of 1226 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	176 (87%)	26 (13%)	5	23
2	CB	202/220 (92%)	176 (87%)	26 (13%)	5	23
3	AC	160/188 (85%)	152 (95%)	8 (5%)	30	70
3	CC	160/188 (85%)	152 (95%)	8 (5%)	30	70
4	AD	180/181 (99%)	157 (87%)	23 (13%)	5	23
4	CD	180/181 (99%)	156 (87%)	24 (13%)	5	21
5	AE	115/123 (94%)	100 (87%)	15 (13%)	5	22
5	CE	115/123 (94%)	100 (87%)	15 (13%)	5	22
6	AF	90/90 (100%)	79 (88%)	11 (12%)	6	25
6	CF	90/90 (100%)	79 (88%)	11 (12%)	6	25
7	AG	126/127 (99%)	121 (96%)	5 (4%)	38	77
7	CG	126/127 (99%)	121 (96%)	5 (4%)	38	77
8	AH	119/119 (100%)	107 (90%)	12 (10%)	9	34
8	CH	119/119 (100%)	107 (90%)	12 (10%)	9	34
9	AI	98/99 (99%)	88 (90%)	10 (10%)	9	33
9	CI	98/99 (99%)	88 (90%)	10 (10%)	9	33
10	AJ	88/92 (96%)	81 (92%)	7 (8%)	15	47
10	CJ	88/92 (96%)	81 (92%)	7 (8%)	15	47
11	AK	90/99 (91%)	79 (88%)	11 (12%)	6	25
11	CK	90/99 (91%)	80 (89%)	10 (11%)	8	29
12	AL	104/111 (94%)	96 (92%)	8 (8%)	16	50
12	CL	104/111 (94%)	96 (92%)	8 (8%)	16	50
13	AM	93/101 (92%)	86 (92%)	7 (8%)	17	51
13	CM	93/101 (92%)	86 (92%)	7 (8%)	17	51
14	AN	49/50 (98%)	46 (94%)	3 (6%)	23	61
14	CN	49/50 (98%)	47 (96%)	2 (4%)	37	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	79/80 (99%)	69 (87%)	10 (13%)	5	23
15	CO	79/80 (99%)	69 (87%)	10 (13%)	5	23
16	AP	72/74 (97%)	60 (83%)	12 (17%)	3	13
16	CP	72/74 (97%)	60 (83%)	12 (17%)	3	13
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	46	82
17	CQ	94/97 (97%)	91 (97%)	3 (3%)	46	82
18	AR	61/77 (79%)	56 (92%)	5 (8%)	14	46
18	CR	61/77 (79%)	55 (90%)	6 (10%)	10	36
19	AS	69/80 (86%)	62 (90%)	7 (10%)	9	34
19	CS	69/80 (86%)	62 (90%)	7 (10%)	9	34
20	AT	76/82 (93%)	65 (86%)	11 (14%)	4	18
20	CT	76/82 (93%)	66 (87%)	10 (13%)	5	22
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
22	B0	61/67 (91%)	49 (80%)	12 (20%)	1	9
22	D0	61/67 (91%)	47 (77%)	14 (23%)	1	5
23	B1	73/83 (88%)	55 (75%)	18 (25%)	1	3
23	D1	73/83 (88%)	55 (75%)	18 (25%)	1	3
24	B2	46/67 (69%)	29 (63%)	17 (37%)	0	1
24	D2	46/67 (69%)	30 (65%)	16 (35%)	0	1
25	B3	51/52 (98%)	44 (86%)	7 (14%)	4	20
25	D3	51/52 (98%)	44 (86%)	7 (14%)	4	20
27	B5	51/52 (98%)	38 (74%)	13 (26%)	1	3
27	D5	51/52 (98%)	36 (71%)	15 (29%)	0	2
28	B6	43/52 (83%)	27 (63%)	16 (37%)	0	1
28	D6	43/52 (83%)	27 (63%)	16 (37%)	0	1
29	B7	41/42 (98%)	35 (85%)	6 (15%)	4	18
29	D7	41/42 (98%)	35 (85%)	6 (15%)	4	18
30	B8	53/55 (96%)	38 (72%)	15 (28%)	0	2
30	D8	53/55 (96%)	41 (77%)	12 (23%)	1	5
33	BD	213/218 (98%)	163 (76%)	50 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DD	213/218 (98%)	162 (76%)	51 (24%)	1	4
34	BE	165/166 (99%)	126 (76%)	39 (24%)	1	4
34	DE	165/166 (99%)	126 (76%)	39 (24%)	1	4
35	BF	165/166 (99%)	132 (80%)	33 (20%)	1	8
35	DF	165/166 (99%)	135 (82%)	30 (18%)	2	11
36	BG	155/156 (99%)	132 (85%)	23 (15%)	4	17
36	DG	155/156 (99%)	131 (84%)	24 (16%)	3	16
37	BH	132/148 (89%)	107 (81%)	25 (19%)	2	10
37	DH	132/148 (89%)	108 (82%)	24 (18%)	2	11
38	BI	122/124 (98%)	103 (84%)	19 (16%)	3	16
38	DI	122/124 (98%)	103 (84%)	19 (16%)	3	16
39	BN	117/119 (98%)	93 (80%)	24 (20%)	1	7
39	DN	117/119 (98%)	92 (79%)	25 (21%)	1	6
40	BO	100/100 (100%)	75 (75%)	25 (25%)	1	3
40	DO	100/100 (100%)	74 (74%)	26 (26%)	0	3
41	BP	112/116 (97%)	63 (56%)	49 (44%)	0	0
41	DP	112/116 (97%)	65 (58%)	47 (42%)	0	0
42	BQ	106/111 (96%)	88 (83%)	18 (17%)	2	13
42	DQ	106/111 (96%)	87 (82%)	19 (18%)	2	11
43	BR	100/101 (99%)	76 (76%)	24 (24%)	1	4
43	DR	100/101 (99%)	75 (75%)	25 (25%)	1	3
44	BS	77/88 (88%)	54 (70%)	23 (30%)	0	2
44	DS	77/88 (88%)	54 (70%)	23 (30%)	0	2
45	BT	116/127 (91%)	84 (72%)	32 (28%)	0	2
45	DT	116/127 (91%)	84 (72%)	32 (28%)	0	2
46	BU	92/94 (98%)	75 (82%)	17 (18%)	2	10
46	DU	92/94 (98%)	74 (80%)	18 (20%)	1	9
47	BV	82/82 (100%)	53 (65%)	29 (35%)	0	1
47	DV	82/82 (100%)	52 (63%)	30 (37%)	0	1
48	BW	91/92 (99%)	70 (77%)	21 (23%)	1	5
48	DW	91/92 (99%)	69 (76%)	22 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BX	74/78 (95%)	54 (73%)	20 (27%)	0	3
49	DX	74/78 (95%)	54 (73%)	20 (27%)	0	3
50	BY	84/91 (92%)	58 (69%)	26 (31%)	0	2
50	DY	84/91 (92%)	59 (70%)	25 (30%)	0	2
51	BZ	155/179 (87%)	130 (84%)	25 (16%)	3	14
51	DZ	155/179 (87%)	130 (84%)	25 (16%)	3	14
All	All	9322/9876 (94%)	7681 (82%)	1641 (18%)	2	12

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

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

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

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

5.3.3 RNA ⓘ

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

5 of 2109 RNA backbone outliers are listed below:

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

5 of 204 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	BA	2506	U
1	CA	484	G
31	DA	1992	G
31	BA	2611	U
1	CA	60	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 802 ligands modelled in this entry, 800 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	ZIT	BA	3351	-	54,54,54	1.32	5 (9%)	76,83,83	1.06	5 (6%)
55	ZIT	DA	3311	-	54,54,54	1.32	5 (9%)	76,83,83	1.06	5 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	ZIT	BA	3351	-	-	0/72/107/107	0/3/3/3
55	ZIT	DA	3311	-	-	0/72/107/107	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	3311	ZIT	C6-C5	2.09	1.60	1.55
55	BA	3351	ZIT	C6-C5	2.11	1.60	1.55
55	DA	3311	ZIT	C13-C12	2.19	1.61	1.55
55	BA	3351	ZIT	C13-C12	2.21	1.61	1.55
55	BA	3351	ZIT	O13-C13	2.48	1.48	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BA	3351	ZIT	C2B-C3B-C4B	-2.57	104.59	107.81
55	DA	3311	ZIT	C2B-C3B-C4B	-2.55	104.61	107.81
55	BA	3351	ZIT	C4A-C3A-C2A	-2.14	106.91	110.03
55	DA	3311	ZIT	C4A-C3A-C2A	-2.13	106.92	110.03
55	BA	3351	ZIT	O6-C6-C7	2.03	113.83	108.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	BA	3351	ZIT	3	0
55	DA	3311	ZIT	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CM	69:GLU	C	70:LEU	N	5.29
1	AM	69:GLU	C	70:LEU	N	5.28
1	DG	112:PRO	C	113:ARG	N	4.77
1	BG	112:PRO	C	113:ARG	N	4.76
1	AM	112:GLY	C	113:PRO	N	4.20

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.67	201 (13%) 4 1	60, 125, 191, 194	0
1	CA	1504/1522 (98%)	0.66	208 (13%) 4 1	61, 125, 191, 194	0
2	AB	235/256 (91%)	0.55	37 (15%) 3 1	107, 156, 184, 191	0
2	CB	235/256 (91%)	0.95	47 (20%) 1 1	107, 158, 185, 191	0
3	AC	207/239 (86%)	0.64	30 (14%) 3 1	115, 163, 184, 189	0
3	CC	207/239 (86%)	1.42	65 (31%) 1 0	119, 166, 184, 191	0
4	AD	208/209 (99%)	0.45	19 (9%) 11 4	83, 131, 170, 181	0
4	CD	208/209 (99%)	0.37	16 (7%) 16 6	82, 131, 168, 182	0
5	AE	151/162 (93%)	0.47	18 (11%) 6 2	83, 116, 160, 188	0
5	CE	151/162 (93%)	0.82	29 (19%) 2 1	84, 117, 162, 189	0
6	AF	101/101 (100%)	0.25	5 (4%) 32 13	85, 132, 164, 180	0
6	CF	101/101 (100%)	0.22	8 (7%) 15 5	86, 132, 165, 182	0
7	AG	155/156 (99%)	1.48	54 (34%) 0 0	140, 171, 188, 191	0
7	CG	155/156 (99%)	2.53	78 (50%) 0 0	140, 171, 188, 190	0
8	AH	138/138 (100%)	0.10	8 (5%) 26 10	85, 121, 155, 164	0
8	CH	138/138 (100%)	0.05	5 (3%) 46 20	85, 123, 156, 162	0
9	AI	127/128 (99%)	2.44	63 (49%) 0 0	142, 182, 190, 192	0
9	CI	127/128 (99%)	2.38	53 (41%) 0 0	143, 183, 190, 191	0
10	AJ	99/105 (94%)	3.11	59 (59%) 0 0	130, 176, 189, 191	0
10	CJ	99/105 (94%)	2.92	58 (58%) 0 0	130, 177, 190, 193	0
11	AK	119/129 (92%)	0.77	21 (17%) 2 1	82, 123, 164, 187	0
11	CK	119/129 (92%)	0.90	17 (14%) 4 1	84, 123, 165, 186	0
12	AL	125/135 (92%)	0.64	18 (14%) 3 1	80, 108, 163, 189	0
12	CL	125/135 (92%)	0.67	17 (13%) 4 1	82, 109, 164, 189	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	AM	115/126 (91%)	3.15	72 (62%)	0	0	150, 185, 190, 193	0
13	CM	115/126 (91%)	2.93	72 (62%)	0	0	149, 185, 190, 192	0
14	AN	60/61 (98%)	1.37	18 (30%)	1	0	131, 168, 185, 189	0
14	CN	60/61 (98%)	1.13	15 (25%)	1	1	132, 170, 186, 189	0
15	AO	88/89 (98%)	0.17	4 (4%)	37	15	74, 111, 157, 162	0
15	CO	88/89 (98%)	0.43	6 (6%)	20	7	74, 112, 159, 165	0
16	AP	84/88 (95%)	1.20	29 (34%)	0	0	91, 118, 161, 179	0
16	CP	84/88 (95%)	0.86	15 (17%)	2	1	89, 116, 160, 180	0
17	AQ	100/105 (95%)	0.38	9 (9%)	12	4	80, 109, 153, 163	0
17	CQ	100/105 (95%)	0.26	7 (7%)	19	7	85, 110, 153, 159	0
18	AR	70/88 (79%)	0.66	8 (11%)	7	2	93, 121, 170, 183	0
18	CR	70/88 (79%)	1.54	20 (28%)	1	0	93, 122, 171, 183	0
19	AS	79/93 (84%)	3.49	51 (64%)	0	0	142, 186, 190, 191	0
19	CS	79/93 (84%)	3.44	55 (69%)	0	0	142, 186, 191, 192	0
20	AT	99/106 (93%)	0.69	11 (11%)	7	3	84, 119, 157, 177	0
20	CT	99/106 (93%)	0.42	9 (9%)	11	4	84, 119, 157, 179	0
21	AU	25/27 (92%)	3.35	15 (60%)	0	0	143, 174, 188, 190	0
21	CU	25/27 (92%)	2.75	15 (60%)	0	0	141, 172, 188, 189	0
22	B0	85/85 (100%)	0.43	8 (9%)	11	4	49, 70, 175, 187	0
22	D0	85/85 (100%)	0.55	9 (10%)	8	3	54, 74, 173, 188	0
23	B1	89/98 (90%)	0.24	3 (3%)	49	21	50, 79, 150, 187	0
23	D1	89/98 (90%)	0.15	6 (6%)	21	7	51, 81, 151, 190	0
24	B2	51/72 (70%)	0.79	7 (13%)	4	1	59, 99, 175, 186	0
24	D2	51/72 (70%)	0.56	7 (13%)	4	1	62, 100, 175, 188	0
25	B3	60/60 (100%)	-0.11	1 (1%)	73	45	46, 69, 132, 168	0
25	D3	60/60 (100%)	0.32	3 (5%)	32	13	51, 72, 136, 161	0
26	B4	32/71 (45%)	-0.20	0	100	100	133, 161, 182, 184	0
26	D4	32/71 (45%)	0.34	6 (18%)	2	1	133, 164, 182, 186	0
27	B5	58/60 (96%)	0.37	4 (6%)	20	7	34, 61, 165, 188	0
27	D5	58/60 (96%)	0.08	5 (8%)	13	4	39, 63, 163, 190	0
28	B6	45/54 (83%)	0.73	3 (6%)	21	7	49, 85, 141, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	0.64	8 (17%) 2 1	52, 87, 142, 172	0
29	B7	49/49 (100%)	0.30	4 (8%) 14 5	36, 45, 119, 172	0
29	D7	49/49 (100%)	0.39	4 (8%) 14 5	38, 49, 120, 173	0
30	B8	64/65 (98%)	0.33	5 (7%) 16 6	46, 68, 140, 165	0
30	D8	64/65 (98%)	0.11	0 100 100	49, 73, 141, 169	0
31	BA	2725/2787 (97%)	0.04	64 (2%) 64 33	33, 59, 153, 194	0
31	DA	2725/2787 (97%)	-0.14	110 (4%) 42 17	38, 64, 157, 194	0
32	BB	119/122 (97%)	0.19	4 (3%) 49 21	50, 101, 149, 184	0
32	DB	119/122 (97%)	0.42	10 (8%) 14 5	59, 105, 157, 184	0
33	BD	272/276 (98%)	-0.17	4 (1%) 76 49	37, 62, 120, 168	0
33	DD	272/276 (98%)	-0.27	4 (1%) 76 49	40, 65, 122, 165	0
34	BE	205/206 (99%)	0.01	6 (2%) 55 26	36, 65, 153, 181	0
34	DE	205/206 (99%)	0.08	10 (4%) 33 13	40, 69, 154, 182	0
35	BF	208/210 (99%)	0.17	14 (6%) 21 7	35, 77, 175, 189	0
35	DF	208/210 (99%)	0.32	13 (6%) 23 9	39, 79, 176, 188	0
36	BG	181/182 (99%)	1.21	50 (27%) 1 0	100, 152, 186, 192	0
36	DG	181/182 (99%)	1.90	66 (36%) 0 0	106, 159, 189, 191	0
37	BH	160/180 (88%)	0.25	4 (2%) 61 30	69, 111, 151, 182	0
37	DH	160/180 (88%)	0.98	37 (23%) 1 1	74, 114, 157, 185	0
38	BI	146/148 (98%)	0.50	15 (10%) 9 3	67, 152, 187, 190	0
38	DI	146/148 (98%)	1.12	38 (26%) 1 1	69, 156, 189, 191	0
39	BN	139/140 (99%)	0.03	5 (3%) 46 20	45, 75, 143, 182	0
39	DN	139/140 (99%)	-0.14	3 (2%) 65 35	49, 78, 143, 183	0
40	BO	122/122 (100%)	-0.23	0 100 100	45, 67, 123, 147	0
40	DO	122/122 (100%)	-0.54	0 100 100	48, 69, 125, 149	0
41	BP	146/150 (97%)	0.49	10 (6%) 20 7	29, 93, 149, 190	0
41	DP	146/150 (97%)	0.49	15 (10%) 9 3	38, 95, 152, 188	0
42	BQ	136/141 (96%)	0.45	9 (6%) 22 7	50, 77, 147, 183	0
42	DQ	136/141 (96%)	0.41	8 (5%) 26 10	52, 79, 147, 183	0
43	BR	117/118 (99%)	-0.05	0 100 100	40, 60, 130, 139	0
43	DR	117/118 (99%)	-0.27	3 (2%) 59 29	42, 62, 131, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	0.43	8 (8%) 15 5	54, 111, 148, 165	0
44	DS	99/112 (88%)	1.24	26 (26%) 1 1	62, 113, 154, 170	0
45	BT	132/146 (90%)	0.20	5 (3%) 44 18	55, 87, 154, 181	0
45	DT	132/146 (90%)	0.17	13 (9%) 10 4	58, 90, 156, 179	0
46	BU	117/118 (99%)	0.12	2 (1%) 73 45	40, 62, 124, 176	0
46	DU	117/118 (99%)	0.17	7 (5%) 25 9	44, 67, 130, 175	0
47	BV	101/101 (100%)	0.63	9 (8%) 12 4	38, 103, 176, 189	0
47	DV	101/101 (100%)	0.67	11 (10%) 7 3	44, 109, 177, 188	0
48	BW	113/113 (100%)	-0.36	0 100 100	38, 51, 112, 179	0
48	DW	113/113 (100%)	-0.45	1 (0%) 85 64	41, 54, 119, 181	0
49	BX	93/96 (96%)	0.13	4 (4%) 39 16	47, 74, 145, 179	0
49	DX	93/96 (96%)	0.04	6 (6%) 22 8	52, 76, 146, 179	0
50	BY	101/110 (91%)	0.93	16 (15%) 3 1	57, 107, 184, 192	0
50	DY	101/110 (91%)	0.83	18 (17%) 2 1	60, 108, 183, 193	0
51	BZ	177/206 (85%)	0.18	10 (5%) 28 11	68, 113, 158, 169	0
51	DZ	177/206 (85%)	0.54	23 (12%) 5 2	74, 117, 161, 168	0
All	All	20062/20922 (95%)	0.47	2309 (11%) 6 2	29, 99, 187, 194	0

The worst 5 of 2309 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	DA	2802	G	20.2
42	DQ	141	GLN	20.2
42	BQ	140	ALA	19.3
42	BQ	141	GLN	18.1
35	DF	208	GLY	16.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
52	MG	BA	3039	1/1	0.96	0.74	42.78	60,60,60,60	0
52	MG	DA	3103	1/1	0.95	0.82	42.34	70,70,70,70	0
52	MG	BA	3087	1/1	0.91	0.41	40.15	58,58,58,58	0
52	MG	BA	3001	1/1	0.94	0.36	37.54	49,49,49,49	0
52	MG	DA	3070	1/1	0.86	0.62	36.29	74,74,74,74	0
52	MG	DA	3154	1/1	0.96	0.69	32.09	62,62,62,62	0
52	MG	BA	3221	1/1	0.94	0.48	31.07	40,40,40,40	0
52	MG	BA	3195	1/1	0.92	0.63	30.37	58,58,58,58	0
52	MG	BA	3200	1/1	0.85	0.86	29.78	59,59,59,59	0
52	MG	DA	3264	1/1	0.82	0.82	28.10	80,80,80,80	0
52	MG	BA	3276	1/1	0.99	0.44	26.57	55,55,55,55	0
52	MG	DA	3115	1/1	0.88	0.40	26.30	72,72,72,72	0
52	MG	BA	3093	1/1	0.97	0.59	25.89	43,43,43,43	0
52	MG	BA	3049	1/1	0.93	0.58	25.55	41,41,41,41	0
52	MG	BA	3071	1/1	0.92	0.48	25.27	47,47,47,47	0
52	MG	CA	1641	1/1	0.95	0.80	24.76	87,87,87,87	0
52	MG	CA	1644	1/1	0.88	0.47	24.51	74,74,74,74	0
52	MG	BA	3209	1/1	0.95	0.56	24.34	56,56,56,56	0
52	MG	DA	3203	1/1	0.78	0.65	24.09	67,67,67,67	0
52	MG	BA	3176	1/1	0.96	0.51	23.81	48,48,48,48	0
52	MG	DA	3166	1/1	0.96	0.40	23.63	46,46,46,46	0
52	MG	DA	3053	1/1	0.96	0.60	23.57	51,51,51,51	0
54	K	DA	3310	1/1	0.78	0.48	23.50	106,106,106,106	0
52	MG	CA	1625	1/1	0.95	0.70	23.24	74,74,74,74	0
52	MG	DA	3088	1/1	0.97	0.52	22.80	34,34,34,34	0
52	MG	BA	3038	1/1	0.97	0.47	22.50	25,25,25,25	0
52	MG	DA	3095	1/1	0.98	0.52	21.97	53,53,53,53	0
52	MG	BA	3095	1/1	0.99	0.51	21.87	38,38,38,38	0
52	MG	CA	1623	1/1	0.83	0.51	21.59	67,67,67,67	0
52	MG	DA	3106	1/1	0.86	0.52	21.37	76,76,76,76	0
52	MG	CA	1643	1/1	0.96	0.75	20.76	62,62,62,62	0
52	MG	DA	3077	1/1	0.99	0.68	20.04	49,49,49,49	0
52	MG	DA	3285	1/1	0.95	0.55	19.87	66,66,66,66	0
52	MG	BA	3108	1/1	0.96	0.39	19.62	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3223	1/1	0.90	0.59	19.53	36,36,36,36	0
52	MG	BA	3331	1/1	0.91	0.46	19.27	46,46,46,46	0
52	MG	DA	3087	1/1	0.94	0.30	18.96	55,55,55,55	0
52	MG	DA	3009	1/1	0.99	0.49	18.91	54,54,54,54	0
52	MG	AA	1629	1/1	0.94	0.56	18.63	67,67,67,67	0
52	MG	BA	3315	1/1	0.90	0.36	18.42	69,69,69,69	0
52	MG	BA	3040	1/1	0.92	0.73	18.17	51,51,51,51	0
52	MG	DA	3089	1/1	0.98	0.60	18.11	47,47,47,47	0
52	MG	DA	3030	1/1	0.98	0.40	17.94	42,42,42,42	0
52	MG	BA	3153	1/1	0.99	0.48	17.76	25,25,25,25	0
52	MG	BA	3229	1/1	0.76	0.29	17.62	50,50,50,50	0
52	MG	DA	3217	1/1	0.92	0.64	17.40	62,62,62,62	0
52	MG	BA	3057	1/1	0.98	0.36	17.24	44,44,44,44	0
52	MG	BA	3285	1/1	0.94	0.52	17.21	57,57,57,57	0
52	MG	DA	3091	1/1	0.99	0.53	17.09	41,41,41,41	0
52	MG	DA	3022	1/1	0.96	0.39	16.61	47,47,47,47	0
52	MG	DA	3197	1/1	0.92	0.46	16.54	75,75,75,75	0
52	MG	BA	3161	1/1	0.97	0.35	16.45	42,42,42,42	0
52	MG	AA	1649	1/1	0.96	0.47	15.83	86,86,86,86	0
52	MG	DA	3110	1/1	0.93	0.39	15.23	73,73,73,73	0
52	MG	DA	3067	1/1	0.80	0.37	14.82	81,81,81,81	0
52	MG	BA	3047	1/1	0.99	0.45	14.56	21,21,21,21	0
52	MG	DA	3042	1/1	0.98	0.38	14.44	47,47,47,47	0
52	MG	BA	3313	1/1	0.95	0.42	14.42	54,54,54,54	0
52	MG	DA	3116	1/1	0.98	0.58	14.03	41,41,41,41	0
52	MG	CA	1618	1/1	0.92	0.40	13.96	62,62,62,62	0
52	MG	BA	3146	1/1	0.97	0.51	13.95	42,42,42,42	0
52	MG	BA	3074	1/1	0.92	0.46	13.78	36,36,36,36	0
52	MG	DA	3047	1/1	0.96	0.51	13.74	45,45,45,45	0
52	MG	DA	3111	1/1	0.98	0.49	13.35	71,71,71,71	0
52	MG	BA	3126	1/1	0.95	0.54	13.24	50,50,50,50	0
52	MG	DA	3133	1/1	0.94	0.58	13.01	53,53,53,53	0
52	MG	AA	1627	1/1	0.93	0.38	12.97	66,66,66,66	0
52	MG	DA	3032	1/1	0.98	0.40	12.92	69,69,69,69	0
52	MG	BA	3010	1/1	0.99	0.43	12.81	38,38,38,38	0
52	MG	DA	3266	1/1	0.93	0.28	12.71	75,75,75,75	0
52	MG	AA	1622	1/1	0.93	0.54	12.31	75,75,75,75	0
52	MG	DA	3159	1/1	0.97	0.47	12.05	61,61,61,61	0
52	MG	BA	3142	1/1	0.97	0.62	11.82	39,39,39,39	0
52	MG	DA	3059	1/1	0.73	0.39	11.70	53,53,53,53	0
52	MG	AA	1648	1/1	0.89	0.77	11.63	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3123	1/1	0.97	0.45	11.60	22,22,22,22	0
52	MG	DA	3072	1/1	0.93	0.37	11.58	46,46,46,46	0
52	MG	BA	3017	1/1	0.98	0.35	11.55	32,32,32,32	0
52	MG	BA	3008	1/1	0.97	0.49	11.46	34,34,34,34	0
52	MG	BA	3217	1/1	0.96	0.43	11.44	50,50,50,50	0
52	MG	BA	3121	1/1	0.96	0.40	11.40	57,57,57,57	0
54	K	BA	3350	1/1	0.54	0.46	11.33	95,95,95,95	0
52	MG	BA	3044	1/1	0.98	0.38	11.04	26,26,26,26	0
52	MG	DA	3137	1/1	0.98	0.41	10.97	38,38,38,38	0
52	MG	DA	3016	1/1	0.94	0.45	10.97	56,56,56,56	0
52	MG	BA	3023	1/1	0.98	0.35	10.81	34,34,34,34	0
52	MG	BA	3158	1/1	0.95	0.41	10.66	49,49,49,49	0
52	MG	DA	3015	1/1	0.95	0.36	10.64	23,23,23,23	0
52	MG	DA	3039	1/1	0.99	0.32	10.48	43,43,43,43	0
52	MG	DA	3045	1/1	0.96	0.48	10.29	39,39,39,39	0
52	MG	DA	3208	1/1	0.88	0.68	10.28	62,62,62,62	0
52	MG	BA	3032	1/1	0.99	0.32	10.16	15,15,15,15	0
52	MG	DA	3007	1/1	0.98	0.36	10.02	39,39,39,39	0
52	MG	DA	3304	1/1	0.92	0.36	9.98	52,52,52,52	0
52	MG	CA	1617	1/1	0.86	0.32	9.94	61,61,61,61	0
52	MG	BA	3037	1/1	0.98	0.32	9.93	14,14,14,14	0
52	MG	DA	3173	1/1	0.96	0.41	9.74	65,65,65,65	0
52	MG	DA	3283	1/1	0.98	0.44	9.74	72,72,72,72	0
52	MG	DA	3227	1/1	0.94	0.26	9.68	74,74,74,74	0
52	MG	DA	3094	1/1	0.91	0.41	9.68	56,56,56,56	0
52	MG	BA	3034	1/1	0.97	0.34	9.62	62,62,62,62	0
52	MG	BA	3169	1/1	0.98	0.36	9.32	46,46,46,46	0
52	MG	AA	1621	1/1	0.97	0.37	9.27	46,46,46,46	0
52	MG	CA	1605	1/1	0.86	0.55	9.25	61,61,61,61	0
52	MG	DA	3105	1/1	0.94	0.39	9.08	47,47,47,47	0
52	MG	DA	3055	1/1	0.99	0.37	9.03	42,42,42,42	0
52	MG	DA	3097	1/1	0.98	0.33	8.94	44,44,44,44	0
52	MG	BA	3051	1/1	0.99	0.31	8.86	14,14,14,14	0
52	MG	BA	3012	1/1	0.95	0.30	8.85	22,22,22,22	0
52	MG	DA	3054	1/1	0.95	0.30	8.73	36,36,36,36	0
52	MG	DA	3068	1/1	0.97	0.41	8.68	49,49,49,49	0
52	MG	DA	3049	1/1	0.94	0.35	8.65	35,35,35,35	0
52	MG	DA	3064	1/1	0.96	0.35	8.55	68,68,68,68	0
52	MG	DA	3036	1/1	0.98	0.48	8.52	39,39,39,39	0
52	MG	BA	3345	1/1	0.90	0.30	8.48	60,60,60,60	0
52	MG	DA	3006	1/1	0.98	0.44	8.35	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3298	1/1	0.78	0.33	8.33	61,61,61,61	0
52	MG	DA	3056	1/1	0.97	0.32	8.25	60,60,60,60	0
52	MG	BA	3252	1/1	0.98	0.31	8.25	50,50,50,50	0
52	MG	BA	3028	1/1	0.97	0.35	8.06	28,28,28,28	0
52	MG	DA	3011	1/1	0.90	0.54	7.97	50,50,50,50	0
52	MG	BA	3185	1/1	0.98	0.30	7.86	14,14,14,14	0
52	MG	BA	3303	1/1	0.85	0.43	7.69	68,68,68,68	0
52	MG	AA	1647	1/1	0.90	0.34	7.61	66,66,66,66	0
52	MG	BA	3268	1/1	0.91	0.26	7.57	40,40,40,40	0
52	MG	DA	3002	1/1	0.96	0.40	7.55	38,38,38,38	0
52	MG	DA	3044	1/1	0.96	0.41	7.46	46,46,46,46	0
52	MG	DA	3149	1/1	0.91	0.21	7.42	55,55,55,55	0
52	MG	BA	3041	1/1	0.96	0.33	7.40	29,29,29,29	0
52	MG	BA	3060	1/1	0.97	0.38	7.26	40,40,40,40	0
52	MG	BA	3020	1/1	0.97	0.44	7.16	38,38,38,38	0
52	MG	BA	3062	1/1	0.97	0.39	7.15	44,44,44,44	0
52	MG	D5	101	1/1	0.95	0.44	7.13	47,47,47,47	0
52	MG	BA	3271	1/1	0.98	0.30	6.80	46,46,46,46	0
52	MG	BA	3189	1/1	0.88	0.41	6.61	45,45,45,45	0
52	MG	BA	3021	1/1	0.99	0.31	6.54	16,16,16,16	0
52	MG	DA	3270	1/1	0.86	0.67	6.50	65,65,65,65	0
52	MG	BA	3073	1/1	0.96	0.34	6.49	53,53,53,53	0
52	MG	BA	3099	1/1	0.98	0.25	6.34	26,26,26,26	0
52	MG	DA	3241	1/1	0.93	0.29	6.30	60,60,60,60	0
52	MG	BA	3079	1/1	0.99	0.34	6.16	0,0,0,0	0
52	MG	AA	1612	1/1	0.94	0.30	6.14	66,66,66,66	0
52	MG	BA	3139	1/1	0.98	0.28	6.12	24,24,24,24	0
52	MG	BA	3091	1/1	0.99	0.30	6.04	9,9,9,9	0
52	MG	DA	3146	1/1	0.93	0.34	5.99	69,69,69,69	0
52	MG	BA	3302	1/1	0.83	0.27	5.86	72,72,72,72	0
52	MG	BA	3006	1/1	0.94	0.39	5.77	29,29,29,29	0
52	MG	DA	3135	1/1	0.96	0.22	5.64	71,71,71,71	0
52	MG	DA	3213	1/1	0.99	0.46	5.63	36,36,36,36	0
52	MG	DA	3142	1/1	0.95	0.45	5.58	41,41,41,41	0
52	MG	BA	3148	1/1	0.69	0.35	5.29	58,58,58,58	0
52	MG	DA	3138	1/1	0.94	0.33	5.20	50,50,50,50	0
52	MG	BA	3065	1/1	0.96	0.31	5.13	32,32,32,32	0
52	MG	BA	3275	1/1	0.96	0.23	5.12	47,47,47,47	0
52	MG	CA	1642	1/1	0.94	0.27	5.08	62,62,62,62	0
52	MG	BA	3016	1/1	0.98	0.26	4.89	21,21,21,21	0
52	MG	BA	3110	1/1	0.97	0.45	4.82	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3173	1/1	0.97	0.37	4.81	24,24,24,24	0
52	MG	BA	3059	1/1	0.98	0.30	4.79	39,39,39,39	0
52	MG	DA	3294	1/1	0.71	0.34	4.77	67,67,67,67	0
52	MG	BA	3069	1/1	0.98	0.27	4.72	18,18,18,18	0
52	MG	BA	3009	1/1	0.93	0.38	4.64	38,38,38,38	0
52	MG	DA	3026	1/1	0.98	0.28	4.62	43,43,43,43	0
52	MG	DA	3019	1/1	0.97	0.34	4.61	42,42,42,42	0
52	MG	CA	1606	1/1	0.90	0.38	4.57	72,72,72,72	0
52	MG	DA	3189	1/1	0.95	0.51	4.53	63,63,63,63	0
52	MG	BA	3115	1/1	0.96	0.24	4.50	49,49,49,49	0
52	MG	DA	3114	1/1	0.96	0.35	4.47	65,65,65,65	0
52	MG	BA	3100	1/1	0.98	0.27	4.46	21,21,21,21	0
52	MG	BA	3241	1/1	0.71	0.61	4.41	79,79,79,79	0
52	MG	DA	3112	1/1	0.93	0.33	4.40	68,68,68,68	0
52	MG	D7	101	1/1	0.83	0.35	4.30	62,62,62,62	0
52	MG	DA	3063	1/1	0.98	0.24	4.10	47,47,47,47	0
52	MG	BA	3052	1/1	0.97	0.29	4.10	15,15,15,15	0
52	MG	DA	3156	1/1	0.97	0.42	4.07	44,44,44,44	0
52	MG	BA	3347	1/1	0.96	0.26	4.02	66,66,66,66	0
52	MG	AA	1623	1/1	0.97	0.42	4.01	54,54,54,54	0
55	ZIT	DA	3311	52/52	0.92	0.31	3.98	100,100,100,100	0
52	MG	CA	1645	1/1	0.96	0.46	3.89	97,97,97,97	0
52	MG	CA	1647	1/1	0.91	0.21	3.74	84,84,84,84	0
52	MG	BA	3230	1/1	0.90	0.50	3.65	38,38,38,38	0
52	MG	BA	3190	1/1	0.81	0.30	3.60	53,53,53,53	0
52	MG	BA	3055	1/1	0.99	0.28	3.58	19,19,19,19	0
55	ZIT	BA	3351	52/52	0.91	0.32	3.51	100,100,100,100	0
52	MG	DA	3147	1/1	0.88	0.28	3.46	63,63,63,63	0
52	MG	BA	3193	1/1	0.97	0.28	3.40	28,28,28,28	0
52	MG	AA	1609	1/1	0.94	0.27	3.38	51,51,51,51	0
52	MG	BA	3311	1/1	0.89	0.35	3.33	46,46,46,46	0
52	MG	AA	1606	1/1	0.94	0.73	3.28	73,73,73,73	0
52	MG	D1	101	1/1	0.98	0.25	3.26	50,50,50,50	0
52	MG	DA	3171	1/1	0.92	0.34	3.17	43,43,43,43	0
52	MG	DA	3130	1/1	0.97	0.33	3.14	43,43,43,43	0
52	MG	CA	1619	1/1	0.93	0.35	3.13	75,75,75,75	0
52	MG	CA	1610	1/1	0.90	0.29	3.04	61,61,61,61	0
52	MG	BA	3254	1/1	0.97	0.21	3.02	53,53,53,53	0
52	MG	DA	3008	1/1	0.98	0.39	2.95	52,52,52,52	0
52	MG	DA	3214	1/1	0.94	0.38	2.92	65,65,65,65	0
52	MG	DA	3187	1/1	0.98	0.20	2.87	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3085	1/1	0.96	0.22	2.79	40,40,40,40	0
52	MG	DA	3246	1/1	0.79	0.26	2.79	87,87,87,87	0
52	MG	DA	3188	1/1	0.89	0.22	2.74	48,48,48,48	0
52	MG	CA	1609	1/1	0.89	0.22	2.72	94,94,94,94	0
52	MG	DA	3248	1/1	0.79	0.33	2.66	74,74,74,74	0
52	MG	BQ	202	1/1	0.90	0.29	2.64	59,59,59,59	0
52	MG	BA	3046	1/1	0.97	0.25	2.50	37,37,37,37	0
52	MG	BA	3002	1/1	0.98	0.24	2.44	20,20,20,20	0
52	MG	DA	3061	1/1	0.94	0.30	2.42	57,57,57,57	0
52	MG	AA	1651	1/1	0.92	0.26	2.37	75,75,75,75	0
52	MG	DA	3140	1/1	0.95	0.21	2.34	49,49,49,49	0
52	MG	BA	3326	1/1	0.91	0.22	2.20	54,54,54,54	0
52	MG	BU	201	1/1	0.98	0.33	2.18	26,26,26,26	0
52	MG	BA	3255	1/1	0.93	0.33	2.16	45,45,45,45	0
52	MG	DA	3279	1/1	0.88	0.24	1.87	64,64,64,64	0
52	MG	BA	3338	1/1	0.93	0.28	1.68	73,73,73,73	0
52	MG	BA	3141	1/1	0.97	0.43	1.51	27,27,27,27	0
52	MG	DA	3230	1/1	0.92	0.25	1.48	56,56,56,56	0
52	MG	DA	3245	1/1	0.71	0.19	1.46	78,78,78,78	0
52	MG	DA	3132	1/1	0.97	0.42	1.46	43,43,43,43	0
52	MG	DF	301	1/1	0.88	0.38	1.37	92,92,92,92	0
52	MG	DX	101	1/1	0.86	0.30	1.33	77,77,77,77	0
52	MG	DU	201	1/1	0.95	0.26	1.25	60,60,60,60	0
52	MG	BX	101	1/1	0.93	0.26	1.23	61,61,61,61	0
52	MG	BB	205	1/1	0.96	0.26	1.04	78,78,78,78	0
52	MG	DA	3058	1/1	0.93	0.21	1.00	58,58,58,58	0
52	MG	BA	3125	1/1	0.92	0.18	0.95	46,46,46,46	0
52	MG	AA	1607	1/1	0.91	0.29	0.94	74,74,74,74	0
52	MG	BA	3127	1/1	0.98	0.14	0.93	50,50,50,50	0
52	MG	BA	3018	1/1	0.97	0.20	0.89	26,26,26,26	0
52	MG	B1	101	1/1	0.98	0.25	0.87	39,39,39,39	0
52	MG	BA	3207	1/1	0.96	0.19	0.69	23,23,23,23	0
52	MG	DA	3244	1/1	0.78	0.28	0.60	86,86,86,86	0
52	MG	DA	3118	1/1	0.95	0.16	0.56	66,66,66,66	0
52	MG	BA	3119	1/1	0.96	0.24	0.53	52,52,52,52	0
52	MG	BA	3278	1/1	0.92	0.22	0.47	41,41,41,41	0
52	MG	BA	3086	1/1	0.96	0.19	0.39	18,18,18,18	0
52	MG	BA	3293	1/1	0.93	0.26	0.24	55,55,55,55	0
52	MG	DA	3263	1/1	0.91	0.27	0.14	67,67,67,67	0
52	MG	CA	1648	1/1	0.97	0.17	0.11	79,79,79,79	0
52	MG	DA	3084	1/1	0.94	0.18	0.06	54,54,54,54	0
52	MG	CA	1621	1/1	0.98	0.18	0.02	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3242	1/1	0.98	0.20	0.01	48,48,48,48	0
52	MG	DA	3281	1/1	0.94	0.16	-0.01	30,30,30,30	0
52	MG	BP	201	1/1	0.95	0.26	-0.06	13,13,13,13	0
52	MG	DA	3220	1/1	0.91	0.18	-0.06	62,62,62,62	0
52	MG	DA	3041	1/1	0.91	0.17	-0.23	37,37,37,37	0
52	MG	AA	1605	1/1	0.98	0.27	-0.24	75,75,75,75	0
52	MG	BA	3097	1/1	0.88	0.17	-0.27	70,70,70,70	0
52	MG	BA	3310	1/1	0.96	0.19	-0.36	47,47,47,47	0
53	ZN	AD	301	1/1	0.99	0.30	-0.40	108,108,108,108	0
53	ZN	CD	301	1/1	0.99	0.26	-0.51	93,93,93,93	0
52	MG	BA	3253	1/1	0.93	0.15	-0.57	51,51,51,51	0
52	MG	DA	3295	1/1	0.88	0.17	-0.75	88,88,88,88	0
52	MG	DA	3158	1/1	0.93	0.12	-0.76	61,61,61,61	0
53	ZN	AN	101	1/1	0.92	0.15	-0.81	159,159,159,159	0
53	ZN	CN	101	1/1	0.89	0.18	-0.81	157,157,157,157	0
52	MG	DA	3223	1/1	0.73	0.12	-0.81	65,65,65,65	0
52	MG	AA	1625	1/1	0.94	0.17	-0.82	73,73,73,73	0
52	MG	DA	3258	1/1	0.85	0.14	-0.82	61,61,61,61	0
52	MG	BA	3124	1/1	0.96	0.16	-0.83	42,42,42,42	0
52	MG	DA	3229	1/1	0.88	0.12	-0.89	45,45,45,45	0
52	MG	AA	1614	1/1	0.92	0.12	-1.00	77,77,77,77	0
52	MG	BA	3061	1/1	0.99	0.15	-1.01	23,23,23,23	0
52	MG	BA	3149	1/1	0.87	0.11	-1.03	51,51,51,51	0
52	MG	BA	3116	1/1	0.90	0.16	-1.12	51,51,51,51	0
52	MG	CA	1629	1/1	0.89	0.13	-1.13	82,82,82,82	0
52	MG	DA	3060	1/1	0.99	0.10	-1.22	34,34,34,34	0
52	MG	BF	301	1/1	0.88	0.17	-1.27	62,62,62,62	0
52	MG	BA	3283	1/1	0.90	0.12	-1.50	53,53,53,53	0
52	MG	AA	1613	1/1	0.88	0.14	-1.56	70,70,70,70	0
52	MG	BA	3112	1/1	0.92	0.14	-1.57	43,43,43,43	0
52	MG	BA	3043	1/1	0.98	0.15	-1.64	36,36,36,36	0
52	MG	DA	3117	1/1	0.94	0.10	-1.70	59,59,59,59	0
52	MG	DA	3119	1/1	0.86	0.07	-1.75	64,64,64,64	0
52	MG	BA	3056	1/1	0.98	0.17	-1.81	20,20,20,20	0
52	MG	BA	3090	1/1	0.97	0.16	-1.92	38,38,38,38	0
52	MG	DA	3228	1/1	0.87	0.11	-2.08	60,60,60,60	0
52	MG	BA	3147	1/1	0.96	0.13	-2.19	12,12,12,12	0
52	MG	B7	101	1/1	0.96	0.12	-2.29	37,37,37,37	0
52	MG	AA	1633	1/1	0.82	0.10	-2.48	81,81,81,81	0
52	MG	AA	1643	1/1	0.96	0.09	-2.77	78,78,78,78	0
52	MG	BA	3286	1/1	0.97	0.06	-2.80	45,45,45,45	0
52	MG	BA	3243	1/1	0.94	0.10	-3.22	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3175	1/1	0.97	0.08	-3.44	49,49,49,49	0
52	MG	BA	3227	1/1	0.92	0.13	-3.62	39,39,39,39	0
52	MG	BA	3111	1/1	0.92	0.13	-3.92	19,19,19,19	0
52	MG	DA	3212	1/1	0.97	0.10	-4.72	68,68,68,68	0
52	MG	DA	3206	1/1	0.95	0.10	-5.37	48,48,48,48	0
52	MG	BA	3247	1/1	0.98	0.06	-6.56	40,40,40,40	0
52	MG	BA	3208	1/1	0.91	0.11	-6.86	23,23,23,23	0
52	MG	CA	1627	1/1	0.96	0.09	-	66,66,66,66	0
52	MG	BA	3136	1/1	0.94	0.52	-	32,32,32,32	0
52	MG	BA	3321	1/1	0.95	0.50	-	75,75,75,75	0
52	MG	DA	3134	1/1	0.97	0.55	-	47,47,47,47	0
52	MG	BA	3029	1/1	0.99	0.23	-	26,26,26,26	0
52	MG	DA	3076	1/1	0.99	0.33	-	55,55,55,55	0
52	MG	BA	3019	1/1	0.96	0.42	-	24,24,24,24	0
52	MG	DA	3151	1/1	0.94	0.41	-	72,72,72,72	0
52	MG	DA	3275	1/1	0.89	0.45	-	62,62,62,62	0
52	MG	BB	203	1/1	0.98	0.35	-	41,41,41,41	0
52	MG	BA	3118	1/1	0.94	0.31	-	59,59,59,59	0
52	MG	AA	1646	1/1	0.90	0.76	-	82,82,82,82	0
52	MG	BA	3068	1/1	0.91	0.34	-	54,54,54,54	0
52	MG	BQ	201	1/1	0.98	0.17	-	32,32,32,32	0
52	MG	BA	3198	1/1	0.96	0.48	-	44,44,44,44	0
52	MG	BA	3180	1/1	0.92	0.57	-	64,64,64,64	0
52	MG	BA	3264	1/1	0.97	0.22	-	35,35,35,35	0
52	MG	DA	3293	1/1	0.98	0.14	-	53,53,53,53	0
52	MG	BA	3237	1/1	0.84	0.32	-	61,61,61,61	0
52	MG	BA	3151	1/1	0.92	0.30	-	74,74,74,74	0
52	MG	BE	301	1/1	0.98	0.46	-	29,29,29,29	0
52	MG	DA	3126	1/1	0.77	0.22	-	73,73,73,73	0
52	MG	DA	3075	1/1	0.98	0.54	-	55,55,55,55	0
52	MG	DA	3178	1/1	0.97	0.41	-	65,65,65,65	0
52	MG	DA	3024	1/1	0.92	0.45	-	61,61,61,61	0
52	MG	CA	1601	1/1	0.94	0.23	-	83,83,83,83	0
52	MG	BA	3160	1/1	0.97	0.36	-	39,39,39,39	0
52	MG	BA	3143	1/1	0.98	0.38	-	30,30,30,30	0
52	MG	AA	1635	1/1	0.92	0.65	-	63,63,63,63	0
52	MG	DA	3259	1/1	0.92	0.63	-	74,74,74,74	0
52	MG	DB	201	1/1	0.92	0.39	-	52,52,52,52	0
52	MG	BA	3182	1/1	0.93	0.51	-	68,68,68,68	0
52	MG	BA	3267	1/1	0.98	0.35	-	38,38,38,38	0
52	MG	DB	203	1/1	0.93	0.46	-	56,56,56,56	0
52	MG	BA	3081	1/1	0.89	0.23	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	CA	1631	1/1	0.96	0.86	-	70,70,70,70	0
52	MG	DA	3195	1/1	0.82	0.51	-	56,56,56,56	0
52	MG	DA	3232	1/1	0.98	0.29	-	72,72,72,72	0
52	MG	BA	3342	1/1	0.98	0.22	-	49,49,49,49	0
52	MG	DA	3267	1/1	0.69	0.59	-	72,72,72,72	0
52	MG	BA	3159	1/1	0.94	0.47	-	45,45,45,45	0
52	MG	BA	3107	1/1	0.97	0.11	-	34,34,34,34	0
52	MG	DA	3012	1/1	0.97	0.35	-	23,23,23,23	0
52	MG	DA	3144	1/1	0.96	0.39	-	47,47,47,47	0
52	MG	BA	3024	1/1	0.99	0.20	-	2,2,2,2	0
52	MG	BA	3007	1/1	0.94	0.54	-	48,48,48,48	0
52	MG	CA	1646	1/1	0.77	0.52	-	80,80,80,80	0
52	MG	BA	3026	1/1	0.96	0.14	-	49,49,49,49	0
52	MG	BA	3334	1/1	0.85	0.32	-	53,53,53,53	0
52	MG	BA	3033	1/1	0.99	0.17	-	20,20,20,20	0
52	MG	BA	3196	1/1	0.67	0.21	-	65,65,65,65	0
52	MG	DA	3287	1/1	0.99	0.16	-	51,51,51,51	0
52	MG	DA	3104	1/1	0.98	0.58	-	48,48,48,48	0
52	MG	BA	3280	1/1	0.88	0.35	-	75,75,75,75	0
52	MG	DA	3057	1/1	0.97	0.48	-	40,40,40,40	0
52	MG	DA	3291	1/1	0.61	1.08	-	86,86,86,86	0
52	MG	DA	3096	1/1	0.92	0.35	-	45,45,45,45	0
52	MG	BR	201	1/1	0.99	0.34	-	20,20,20,20	0
52	MG	BA	3232	1/1	0.86	0.38	-	70,70,70,70	0
52	MG	BA	3248	1/1	0.97	0.16	-	47,47,47,47	0
52	MG	BA	3053	1/1	0.98	0.38	-	15,15,15,15	0
52	MG	BA	3183	1/1	0.93	0.16	-	72,72,72,72	0
52	MG	DA	3242	1/1	0.91	0.19	-	69,69,69,69	0
52	MG	D0	101	1/1	0.89	0.15	-	62,62,62,62	0
52	MG	BA	3206	1/1	0.99	0.51	-	29,29,29,29	0
52	MG	DA	3001	1/1	0.91	0.41	-	76,76,76,76	0
52	MG	DA	3233	1/1	0.90	0.50	-	68,68,68,68	0
52	MG	DA	3033	1/1	0.99	0.41	-	44,44,44,44	0
52	MG	DA	3204	1/1	0.96	0.45	-	45,45,45,45	0
52	MG	DA	3305	1/1	0.63	0.34	-	76,76,76,76	0
52	MG	AA	1610	1/1	0.96	0.62	-	65,65,65,65	0
52	MG	DA	3141	1/1	0.98	0.49	-	61,61,61,61	0
52	MG	BA	3162	1/1	0.88	0.16	-	47,47,47,47	0
52	MG	BA	3299	1/1	0.96	0.46	-	58,58,58,58	0
52	MG	DA	3082	1/1	0.89	0.18	-	17,17,17,17	0
52	MG	DA	3243	1/1	0.78	0.48	-	70,70,70,70	0
52	MG	BA	3157	1/1	0.87	0.76	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3286	1/1	0.95	0.50	-	58,58,58,58	0
52	MG	DA	3169	1/1	0.97	0.79	-	51,51,51,51	0
52	MG	BA	3015	1/1	0.97	0.33	-	48,48,48,48	0
52	MG	DA	3069	1/1	0.92	0.52	-	51,51,51,51	0
52	MG	BA	3291	1/1	0.99	0.60	-	54,54,54,54	0
52	MG	DA	3017	1/1	0.87	0.32	-	47,47,47,47	0
52	MG	DA	3191	1/1	0.73	0.25	-	91,91,91,91	0
52	MG	DA	3048	1/1	0.97	0.25	-	40,40,40,40	0
52	MG	CA	1622	1/1	0.67	0.28	-	78,78,78,78	0
52	MG	BA	3273	1/1	0.96	0.51	-	58,58,58,58	0
52	MG	DA	3192	1/1	0.93	0.54	-	55,55,55,55	0
52	MG	BA	3234	1/1	0.97	0.42	-	45,45,45,45	0
52	MG	BA	3104	1/1	0.95	0.42	-	37,37,37,37	0
52	MG	BA	3274	1/1	0.87	0.16	-	81,81,81,81	0
52	MG	DA	3300	1/1	0.98	0.05	-	75,75,75,75	0
52	MG	DA	3037	1/1	0.90	0.63	-	74,74,74,74	0
52	MG	DA	3074	1/1	0.96	0.23	-	53,53,53,53	0
52	MG	AA	1632	1/1	0.89	0.65	-	72,72,72,72	0
52	MG	DA	3185	1/1	0.97	0.38	-	61,61,61,61	0
52	MG	BA	3094	1/1	0.95	0.39	-	52,52,52,52	0
52	MG	BA	3249	1/1	0.87	0.26	-	40,40,40,40	0
52	MG	DA	3066	1/1	0.98	0.51	-	60,60,60,60	0
52	MG	DA	3129	1/1	0.85	0.12	-	87,87,87,87	0
52	MG	DA	3065	1/1	0.97	0.23	-	49,49,49,49	0
52	MG	DA	3290	1/1	0.92	0.37	-	52,52,52,52	0
52	MG	BA	3080	1/1	0.97	0.52	-	34,34,34,34	0
52	MG	BA	3067	1/1	0.97	0.58	-	37,37,37,37	0
52	MG	BA	3083	1/1	0.99	0.21	-	5,5,5,5	0
52	MG	BA	3224	1/1	0.94	0.12	-	40,40,40,40	0
52	MG	DA	3256	1/1	0.93	0.19	-	57,57,57,57	0
52	MG	DA	3207	1/1	0.80	0.80	-	78,78,78,78	0
52	MG	DA	3078	1/1	0.97	0.65	-	46,46,46,46	0
52	MG	BA	3170	1/1	0.91	0.31	-	69,69,69,69	0
52	MG	DA	3239	1/1	0.96	0.22	-	59,59,59,59	0
52	MG	CA	1630	1/1	0.94	0.36	-	77,77,77,77	0
52	MG	DA	3199	1/1	0.95	0.21	-	47,47,47,47	0
52	MG	DA	3218	1/1	0.88	0.25	-	78,78,78,78	0
52	MG	DA	3276	1/1	0.96	0.13	-	70,70,70,70	0
52	MG	B0	101	1/1	0.96	0.16	-	34,34,34,34	0
52	MG	BA	3220	1/1	0.99	0.46	-	27,27,27,27	0
52	MG	CA	1636	1/1	0.91	0.50	-	79,79,79,79	0
52	MG	DA	3107	1/1	0.98	0.44	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	AA	1616	1/1	0.97	0.19	-	77,77,77,77	0
52	MG	DA	3215	1/1	0.97	0.42	-	59,59,59,59	0
52	MG	DA	3021	1/1	0.98	0.38	-	47,47,47,47	0
52	MG	DA	3306	1/1	0.72	0.37	-	87,87,87,87	0
52	MG	BB	201	1/1	0.84	0.45	-	42,42,42,42	0
52	MG	BA	3167	1/1	0.95	0.59	-	52,52,52,52	0
52	MG	BA	3166	1/1	0.95	0.61	-	39,39,39,39	0
52	MG	BA	3014	1/1	0.97	0.41	-	32,32,32,32	0
52	MG	DA	3255	1/1	0.64	0.44	-	75,75,75,75	0
52	MG	DA	3160	1/1	0.96	0.29	-	59,59,59,59	0
52	MG	BA	3004	1/1	0.98	0.23	-	23,23,23,23	0
52	MG	DA	3174	1/1	0.95	0.56	-	63,63,63,63	0
52	MG	B5	101	1/1	0.96	0.23	-	27,27,27,27	0
52	MG	BA	3084	1/1	0.96	0.09	-	14,14,14,14	0
52	MG	BA	3165	1/1	0.96	0.56	-	50,50,50,50	0
52	MG	AA	1637	1/1	0.85	0.29	-	69,69,69,69	0
52	MG	BA	3213	1/1	0.98	0.55	-	32,32,32,32	0
52	MG	CA	1624	1/1	0.92	0.41	-	65,65,65,65	0
52	MG	BA	3152	1/1	0.88	0.32	-	61,61,61,61	0
52	MG	BA	3027	1/1	0.94	0.47	-	42,42,42,42	0
52	MG	BA	3219	1/1	0.86	0.11	-	38,38,38,38	0
52	MG	DA	3161	1/1	0.92	0.70	-	72,72,72,72	0
52	MG	BA	3078	1/1	0.97	0.21	-	34,34,34,34	0
52	MG	BA	3292	1/1	0.97	0.78	-	60,60,60,60	0
52	MG	BA	3239	1/1	0.94	0.25	-	48,48,48,48	0
52	MG	BA	3228	1/1	0.93	0.65	-	69,69,69,69	0
52	MG	DB	202	1/1	0.93	0.36	-	63,63,63,63	0
52	MG	BA	3246	1/1	0.55	0.45	-	75,75,75,75	0
52	MG	DA	3163	1/1	0.94	0.58	-	68,68,68,68	0
52	MG	BA	3256	1/1	0.96	0.37	-	63,63,63,63	0
52	MG	BA	3088	1/1	0.93	0.25	-	10,10,10,10	0
52	MG	DA	3184	1/1	0.98	0.42	-	63,63,63,63	0
52	MG	DA	3253	1/1	0.98	0.39	-	50,50,50,50	0
52	MG	BA	3011	1/1	0.98	0.31	-	7,7,7,7	0
52	MG	BA	3333	1/1	0.90	0.17	-	80,80,80,80	0
52	MG	DA	3102	1/1	0.83	0.28	-	80,80,80,80	0
52	MG	BA	3211	1/1	0.97	0.17	-	39,39,39,39	0
52	MG	BA	3204	1/1	0.97	0.26	-	46,46,46,46	0
52	MG	BA	3137	1/1	0.94	0.26	-	61,61,61,61	0
52	MG	DA	3219	1/1	0.69	0.36	-	75,75,75,75	0
52	MG	BA	3048	1/1	0.98	0.48	-	30,30,30,30	0
52	MG	BA	3075	1/1	0.98	0.19	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3150	1/1	0.85	0.55	-	77,77,77,77	0
52	MG	DA	3073	1/1	0.98	0.23	-	42,42,42,42	0
52	MG	BA	3117	1/1	0.95	0.40	-	39,39,39,39	0
52	MG	AA	1644	1/1	0.66	1.25	-	99,99,99,99	0
52	MG	AA	1604	1/1	0.84	0.46	-	95,95,95,95	0
52	MG	BA	3072	1/1	0.99	0.30	-	24,24,24,24	0
52	MG	BA	3307	1/1	0.86	0.44	-	76,76,76,76	0
52	MG	DP	201	1/1	0.96	0.19	-	50,50,50,50	0
52	MG	DA	3289	1/1	0.94	0.34	-	92,92,92,92	0
52	MG	DA	3210	1/1	0.89	0.37	-	63,63,63,63	0
52	MG	BA	3128	1/1	0.92	0.28	-	54,54,54,54	0
52	MG	BA	3301	1/1	0.97	0.16	-	57,57,57,57	0
52	MG	DA	3027	1/1	0.97	0.41	-	61,61,61,61	0
52	MG	BA	3154	1/1	0.97	0.25	-	32,32,32,32	0
52	MG	DA	3029	1/1	0.91	0.21	-	87,87,87,87	0
52	MG	DD	301	1/1	0.95	0.14	-	35,35,35,35	0
52	MG	BA	3261	1/1	0.98	0.34	-	38,38,38,38	0
52	MG	CA	1616	1/1	0.99	0.52	-	73,73,73,73	0
52	MG	DA	3209	1/1	0.95	0.56	-	59,59,59,59	0
52	MG	BA	3076	1/1	0.97	0.28	-	43,43,43,43	0
52	MG	BA	3287	1/1	0.90	0.46	-	58,58,58,58	0
52	MG	BA	3251	1/1	0.96	0.16	-	35,35,35,35	0
52	MG	AA	1619	1/1	0.82	0.36	-	56,56,56,56	0
52	MG	DA	3303	1/1	0.92	0.59	-	49,49,49,49	0
52	MG	DA	3109	1/1	0.94	0.40	-	71,71,71,71	0
52	MG	BA	3332	1/1	0.88	0.29	-	61,61,61,61	0
52	MG	BA	3192	1/1	0.83	0.34	-	58,58,58,58	0
52	MG	DA	3205	1/1	0.95	0.51	-	54,54,54,54	0
52	MG	BA	3013	1/1	0.98	0.35	-	21,21,21,21	0
52	MG	DA	3224	1/1	0.90	0.09	-	68,68,68,68	0
52	MG	DA	3080	1/1	0.96	0.46	-	40,40,40,40	0
52	MG	AA	1631	1/1	0.97	0.12	-	60,60,60,60	0
52	MG	CA	1611	1/1	0.79	0.61	-	81,81,81,81	0
52	MG	DA	3271	1/1	0.97	0.16	-	46,46,46,46	0
52	MG	DA	3086	1/1	0.94	0.48	-	38,38,38,38	0
52	MG	BA	3005	1/1	0.98	0.39	-	47,47,47,47	0
52	MG	BA	3205	1/1	0.91	0.33	-	55,55,55,55	0
52	MG	BA	3324	1/1	0.95	0.41	-	59,59,59,59	0
52	MG	BA	3235	1/1	0.93	0.41	-	72,72,72,72	0
52	MG	DA	3268	1/1	0.82	1.51	-	81,81,81,81	0
52	MG	BA	3330	1/1	0.92	0.83	-	71,71,71,71	0
52	MG	AA	1650	1/1	0.78	0.53	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3258	1/1	0.98	0.33	-	61,61,61,61	0
52	MG	AA	1638	1/1	0.91	0.45	-	82,82,82,82	0
52	MG	CA	1637	1/1	0.95	0.91	-	80,80,80,80	0
52	MG	BA	3172	1/1	0.95	0.20	-	64,64,64,64	0
52	MG	DE	301	1/1	0.92	0.35	-	40,40,40,40	0
52	MG	DA	3182	1/1	0.87	0.28	-	55,55,55,55	0
52	MG	BA	3156	1/1	0.92	0.46	-	53,53,53,53	0
52	MG	BA	3030	1/1	0.98	0.25	-	17,17,17,17	0
52	MG	DA	3254	1/1	0.92	0.19	-	65,65,65,65	0
52	MG	DA	3235	1/1	0.94	0.28	-	79,79,79,79	0
52	MG	DA	3225	1/1	0.91	0.21	-	54,54,54,54	0
52	MG	CA	1639	1/1	0.97	0.20	-	64,64,64,64	0
52	MG	DA	3249	1/1	0.92	0.83	-	79,79,79,79	0
52	MG	CA	1607	1/1	0.93	0.48	-	82,82,82,82	0
52	MG	DA	3155	1/1	0.90	0.19	-	62,62,62,62	0
52	MG	AA	1626	1/1	0.92	0.49	-	76,76,76,76	0
52	MG	DA	3005	1/1	0.90	0.28	-	73,73,73,73	0
52	MG	DA	3157	1/1	0.83	0.50	-	65,65,65,65	0
52	MG	BA	3179	1/1	0.97	0.18	-	59,59,59,59	0
52	MG	BA	3348	1/1	0.88	0.12	-	61,61,61,61	0
52	MG	DA	3131	1/1	0.97	0.59	-	47,47,47,47	0
52	MG	DA	3222	1/1	0.75	0.84	-	67,67,67,67	0
52	MG	CA	1614	1/1	0.94	0.57	-	76,76,76,76	0
52	MG	DA	3272	1/1	0.91	0.27	-	74,74,74,74	0
52	MG	DA	3081	1/1	0.97	0.40	-	43,43,43,43	0
52	MG	BA	3236	1/1	0.91	0.34	-	70,70,70,70	0
52	MG	DA	3035	1/1	0.97	0.80	-	54,54,54,54	0
52	MG	BA	3131	1/1	0.96	0.21	-	45,45,45,45	0
52	MG	AA	1603	1/1	0.96	0.38	-	62,62,62,62	0
52	MG	BA	3309	1/1	0.79	0.97	-	61,61,61,61	0
52	MG	BA	3092	1/1	0.96	0.65	-	52,52,52,52	0
52	MG	BA	3343	1/1	0.87	0.45	-	58,58,58,58	0
52	MG	BA	3316	1/1	0.97	0.16	-	56,56,56,56	0
52	MG	DA	3200	1/1	0.92	0.36	-	50,50,50,50	0
52	MG	BP	202	1/1	0.93	0.32	-	58,58,58,58	0
52	MG	DA	3170	1/1	0.92	0.50	-	53,53,53,53	0
52	MG	DA	3240	1/1	0.98	0.46	-	89,89,89,89	0
52	MG	DA	3298	1/1	0.88	0.65	-	71,71,71,71	0
52	MG	AA	1640	1/1	0.80	0.62	-	83,83,83,83	0
52	MG	AA	1645	1/1	0.91	0.33	-	81,81,81,81	0
52	MG	DQ	201	1/1	0.69	0.39	-	78,78,78,78	0
52	MG	BA	3050	1/1	0.98	0.28	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3257	1/1	0.98	0.33	-	48,48,48,48	0
52	MG	BA	3270	1/1	0.96	0.23	-	50,50,50,50	0
52	MG	AA	1628	1/1	0.93	0.51	-	66,66,66,66	0
52	MG	BA	3064	1/1	0.96	0.23	-	28,28,28,28	0
52	MG	DA	3136	1/1	0.98	0.51	-	59,59,59,59	0
52	MG	BA	3282	1/1	0.95	0.14	-	67,67,67,67	0
52	MG	DA	3010	1/1	0.99	0.39	-	31,31,31,31	0
52	MG	DA	3101	1/1	0.97	0.35	-	43,43,43,43	0
52	MG	BA	3168	1/1	0.99	0.09	-	43,43,43,43	0
52	MG	BA	3294	1/1	0.87	0.54	-	65,65,65,65	0
52	MG	DA	3309	1/1	0.86	0.14	-	84,84,84,84	0
52	MG	DA	3127	1/1	0.98	0.42	-	35,35,35,35	0
52	MG	BA	3305	1/1	0.91	0.28	-	54,54,54,54	0
52	MG	BA	3297	1/1	0.93	0.29	-	61,61,61,61	0
52	MG	BA	3130	1/1	0.98	0.24	-	26,26,26,26	0
52	MG	DA	3098	1/1	0.95	0.17	-	49,49,49,49	0
52	MG	BA	3089	1/1	0.96	0.43	-	26,26,26,26	0
52	MG	DA	3100	1/1	0.81	0.71	-	50,50,50,50	0
52	MG	BA	3194	1/1	0.98	0.50	-	44,44,44,44	0
52	MG	DA	3301	1/1	0.95	0.28	-	57,57,57,57	0
52	MG	BA	3031	1/1	0.97	0.33	-	77,77,77,77	0
52	MG	AA	1611	1/1	0.91	0.16	-	75,75,75,75	0
52	MG	DA	3121	1/1	0.94	0.17	-	37,37,37,37	0
52	MG	DA	3179	1/1	0.88	0.85	-	77,77,77,77	0
52	MG	BA	3042	1/1	0.96	0.27	-	15,15,15,15	0
52	MG	DA	3262	1/1	0.86	0.87	-	77,77,77,77	0
52	MG	DA	3196	1/1	0.90	0.29	-	51,51,51,51	0
52	MG	DA	3296	1/1	0.98	0.08	-	60,60,60,60	0
52	MG	BA	3216	1/1	0.97	0.41	-	43,43,43,43	0
52	MG	CA	1628	1/1	0.75	0.45	-	75,75,75,75	0
52	MG	DA	3108	1/1	0.84	0.33	-	48,48,48,48	0
52	MG	DA	3164	1/1	0.91	0.11	-	71,71,71,71	0
52	MG	BA	3323	1/1	0.91	0.26	-	64,64,64,64	0
52	MG	DA	3181	1/1	0.98	0.34	-	50,50,50,50	0
52	MG	BA	3337	1/1	0.91	0.31	-	58,58,58,58	0
52	MG	DA	3237	1/1	0.96	0.17	-	53,53,53,53	0
52	MG	AA	1639	1/1	0.82	0.21	-	95,95,95,95	0
52	MG	AA	1630	1/1	0.97	0.54	-	59,59,59,59	0
52	MG	BA	3133	1/1	0.95	0.49	-	35,35,35,35	0
52	MG	DA	3092	1/1	0.89	0.28	-	61,61,61,61	0
52	MG	BA	3288	1/1	0.93	0.45	-	72,72,72,72	0
52	MG	DA	3288	1/1	0.88	0.20	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3225	1/1	0.99	0.30	-	33,33,33,33	0
52	MG	BA	3284	1/1	0.95	0.32	-	71,71,71,71	0
52	MG	DA	3168	1/1	0.89	0.28	-	53,53,53,53	0
52	MG	D5	102	1/1	0.81	0.64	-	79,79,79,79	0
52	MG	CA	1613	1/1	0.96	0.19	-	80,80,80,80	0
52	MG	DA	3265	1/1	0.87	1.11	-	79,79,79,79	0
52	MG	DA	3252	1/1	0.90	0.55	-	66,66,66,66	0
52	MG	CA	1633	1/1	0.86	1.26	-	87,87,87,87	0
52	MG	BA	3295	1/1	0.71	0.23	-	70,70,70,70	0
52	MG	BA	3025	1/1	0.97	0.33	-	54,54,54,54	0
52	MG	CA	1602	1/1	0.92	0.47	-	70,70,70,70	0
52	MG	BP	203	1/1	0.97	0.11	-	0,0,0,0	0
52	MG	DA	3062	1/1	0.96	0.60	-	65,65,65,65	0
52	MG	AA	1602	1/1	0.98	0.47	-	37,37,37,37	0
52	MG	BA	3197	1/1	0.91	0.30	-	52,52,52,52	0
52	MG	DA	3176	1/1	0.98	0.20	-	78,78,78,78	0
52	MG	BA	3214	1/1	0.91	0.47	-	66,66,66,66	0
52	MG	DA	3221	1/1	0.96	0.44	-	53,53,53,53	0
52	MG	BA	3203	1/1	0.99	0.39	-	35,35,35,35	0
52	MG	DA	3085	1/1	0.92	0.40	-	54,54,54,54	0
52	MG	BA	3266	1/1	0.99	0.38	-	35,35,35,35	0
52	MG	BA	3306	1/1	0.84	0.26	-	56,56,56,56	0
52	MG	BA	3174	1/1	0.94	0.64	-	57,57,57,57	0
52	MG	CA	1632	1/1	0.83	0.25	-	79,79,79,79	0
52	MG	BA	3259	1/1	0.94	0.51	-	46,46,46,46	0
52	MG	AA	1634	1/1	0.96	0.33	-	58,58,58,58	0
52	MG	DA	3216	1/1	0.69	0.61	-	85,85,85,85	0
52	MG	DA	3028	1/1	0.97	0.25	-	39,39,39,39	0
52	MG	BA	3240	1/1	0.82	0.46	-	60,60,60,60	0
52	MG	DA	3148	1/1	0.98	0.35	-	48,48,48,48	0
52	MG	DA	3050	1/1	0.98	0.34	-	42,42,42,42	0
52	MG	DA	3090	1/1	0.95	0.41	-	76,76,76,76	0
52	MG	DA	3183	1/1	0.94	0.37	-	44,44,44,44	0
52	MG	DA	3273	1/1	0.94	0.71	-	75,75,75,75	0
52	MG	DA	3236	1/1	0.98	0.42	-	67,67,67,67	0
52	MG	BA	3135	1/1	0.99	0.29	-	8,8,8,8	0
52	MG	DA	3299	1/1	0.97	0.30	-	66,66,66,66	0
52	MG	BA	3105	1/1	0.96	0.48	-	46,46,46,46	0
52	MG	BA	3341	1/1	0.65	0.71	-	63,63,63,63	0
52	MG	BA	3077	1/1	0.97	0.41	-	28,28,28,28	0
52	MG	B5	102	1/1	0.97	0.42	-	56,56,56,56	0
52	MG	DA	3120	1/1	0.79	0.31	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3211	1/1	0.91	0.15	-	79,79,79,79	0
52	MG	BB	204	1/1	0.96	0.54	-	56,56,56,56	0
52	MG	BA	3058	1/1	0.97	0.39	-	39,39,39,39	0
52	MG	BA	3129	1/1	0.89	0.13	-	18,18,18,18	0
52	MG	BA	3070	1/1	0.97	0.34	-	35,35,35,35	0
52	MG	BA	3322	1/1	0.99	0.22	-	20,20,20,20	0
52	MG	DA	3031	1/1	0.97	0.34	-	47,47,47,47	0
52	MG	BA	3318	1/1	0.86	0.53	-	60,60,60,60	0
52	MG	BA	3191	1/1	0.92	0.68	-	64,64,64,64	0
52	MG	DA	3280	1/1	0.85	0.55	-	77,77,77,77	0
52	MG	DA	3113	1/1	0.92	0.49	-	62,62,62,62	0
52	MG	BA	3187	1/1	0.99	0.50	-	42,42,42,42	0
52	MG	BA	3054	1/1	0.98	0.19	-	68,68,68,68	0
52	MG	DA	3180	1/1	0.95	0.49	-	52,52,52,52	0
52	MG	DA	3020	1/1	0.89	0.43	-	64,64,64,64	0
52	MG	AA	1636	1/1	0.97	0.19	-	63,63,63,63	0
52	MG	CA	1620	1/1	0.94	0.36	-	66,66,66,66	0
52	MG	BA	3120	1/1	0.95	0.46	-	52,52,52,52	0
52	MG	DA	3308	1/1	0.92	0.12	-	81,81,81,81	0
52	MG	BA	3222	1/1	0.98	0.24	-	23,23,23,23	0
52	MG	BA	3063	1/1	0.95	0.43	-	48,48,48,48	0
52	MG	BA	3272	1/1	0.95	0.31	-	51,51,51,51	0
52	MG	CA	1634	1/1	0.85	0.52	-	87,87,87,87	0
52	MG	BA	3262	1/1	0.95	0.15	-	75,75,75,75	0
52	MG	BA	3289	1/1	0.88	0.27	-	55,55,55,55	0
52	MG	BA	3144	1/1	0.81	0.27	-	53,53,53,53	0
52	MG	BA	3186	1/1	0.95	0.49	-	66,66,66,66	0
52	MG	CA	1608	1/1	0.95	0.25	-	51,51,51,51	0
52	MG	DA	3123	1/1	0.95	0.13	-	61,61,61,61	0
52	MG	AA	1624	1/1	0.94	0.38	-	56,56,56,56	0
52	MG	DA	3172	1/1	0.98	0.56	-	64,64,64,64	0
52	MG	DA	3231	1/1	0.87	0.36	-	79,79,79,79	0
52	MG	DA	3046	1/1	0.96	0.34	-	28,28,28,28	0
52	MG	BA	3150	1/1	0.98	0.44	-	50,50,50,50	0
52	MG	CA	1635	1/1	0.92	0.20	-	86,86,86,86	0
52	MG	DA	3023	1/1	0.98	0.25	-	47,47,47,47	0
52	MG	DA	3162	1/1	0.91	0.28	-	69,69,69,69	0
52	MG	BA	3296	1/1	0.77	0.72	-	67,67,67,67	0
52	MG	BA	3231	1/1	0.96	0.65	-	52,52,52,52	0
52	MG	BA	3177	1/1	0.99	0.42	-	52,52,52,52	0
52	MG	BA	3226	1/1	0.94	0.15	-	32,32,32,32	0
52	MG	BA	3098	1/1	0.97	0.26	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3171	1/1	0.97	0.33	-	62,62,62,62	0
52	MG	CA	1603	1/1	0.95	0.51	-	63,63,63,63	0
52	MG	BA	3045	1/1	0.98	0.34	-	26,26,26,26	0
52	MG	BA	3245	1/1	0.90	0.58	-	45,45,45,45	0
52	MG	DA	3260	1/1	0.71	0.81	-	73,73,73,73	0
52	MG	BA	3279	1/1	0.87	0.44	-	50,50,50,50	0
52	MG	DA	3297	1/1	0.95	0.36	-	74,74,74,74	0
52	MG	DA	3193	1/1	0.97	0.49	-	50,50,50,50	0
52	MG	BA	3113	1/1	0.96	0.35	-	26,26,26,26	0
52	MG	BA	3103	1/1	0.97	0.21	-	42,42,42,42	0
52	MG	AA	1601	1/1	0.94	0.19	-	58,58,58,58	0
52	MG	BA	3244	1/1	0.98	0.34	-	40,40,40,40	0
52	MG	BA	3349	1/1	0.88	0.09	-	61,61,61,61	0
52	MG	DA	3251	1/1	0.96	0.40	-	63,63,63,63	0
52	MG	DR	201	1/1	0.92	0.34	-	43,43,43,43	0
52	MG	BA	3188	1/1	0.86	0.67	-	62,62,62,62	0
52	MG	DA	3165	1/1	0.93	0.32	-	52,52,52,52	0
52	MG	CA	1612	1/1	0.88	0.10	-	77,77,77,77	0
52	MG	DA	3175	1/1	0.84	0.69	-	67,67,67,67	0
52	MG	BA	3250	1/1	0.96	0.29	-	54,54,54,54	0
52	MG	BA	3022	1/1	0.89	0.39	-	49,49,49,49	0
52	MG	BA	3314	1/1	0.96	0.27	-	56,56,56,56	0
52	MG	BA	3233	1/1	0.98	0.13	-	63,63,63,63	0
52	MG	DA	3257	1/1	0.87	0.91	-	63,63,63,63	0
52	MG	DA	3143	1/1	0.92	0.50	-	57,57,57,57	0
52	MG	BA	3329	1/1	0.89	0.65	-	68,68,68,68	0
52	MG	BA	3106	1/1	0.98	0.16	-	12,12,12,12	0
52	MG	DA	3284	1/1	0.82	0.71	-	65,65,65,65	0
52	MG	BA	3003	1/1	0.94	0.42	-	43,43,43,43	0
52	MG	DA	3122	1/1	0.96	0.23	-	61,61,61,61	0
52	MG	DA	3145	1/1	0.84	0.91	-	88,88,88,88	0
52	MG	DA	3177	1/1	0.93	0.31	-	61,61,61,61	0
52	MG	DA	3167	1/1	0.91	0.41	-	48,48,48,48	0
52	MG	CA	1626	1/1	0.71	0.54	-	78,78,78,78	0
52	MG	DA	3282	1/1	0.88	0.33	-	62,62,62,62	0
52	MG	DA	3083	1/1	0.90	0.23	-	47,47,47,47	0
52	MG	BA	3164	1/1	0.96	0.27	-	47,47,47,47	0
52	MG	DA	3071	1/1	0.98	0.36	-	40,40,40,40	0
52	MG	BA	3281	1/1	0.96	0.35	-	46,46,46,46	0
52	MG	BA	3138	1/1	0.87	0.12	-	74,74,74,74	0
52	MG	BA	3114	1/1	0.86	0.44	-	56,56,56,56	0
52	MG	DA	3139	1/1	0.96	0.38	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3302	1/1	0.85	0.68	-	86,86,86,86	0
52	MG	DA	3152	1/1	0.93	0.54	-	43,43,43,43	0
52	MG	DA	3052	1/1	0.97	0.39	-	63,63,63,63	0
52	MG	BA	3201	1/1	0.99	0.34	-	29,29,29,29	0
52	MG	DA	3128	1/1	0.97	0.65	-	51,51,51,51	0
52	MG	BA	3304	1/1	0.83	1.20	-	86,86,86,86	0
52	MG	AA	1617	1/1	0.97	0.40	-	64,64,64,64	0
52	MG	BA	3317	1/1	0.95	0.17	-	41,41,41,41	0
52	MG	BA	3109	1/1	0.97	0.42	-	34,34,34,34	0
52	MG	BA	3263	1/1	0.95	0.58	-	62,62,62,62	0
52	MG	DA	3261	1/1	0.66	0.52	-	95,95,95,95	0
52	MG	BA	3260	1/1	0.98	0.42	-	42,42,42,42	0
52	MG	DA	3099	1/1	0.99	0.58	-	46,46,46,46	0
52	MG	DA	3043	1/1	0.98	0.40	-	35,35,35,35	0
52	MG	DA	3093	1/1	0.96	0.31	-	64,64,64,64	0
52	MG	CA	1615	1/1	0.95	0.61	-	67,67,67,67	0
52	MG	DA	3247	1/1	0.86	0.70	-	87,87,87,87	0
52	MG	DA	3274	1/1	0.99	0.27	-	63,63,63,63	0
52	MG	BA	3132	1/1	0.96	0.22	-	55,55,55,55	0
52	MG	DA	3278	1/1	0.58	0.54	-	68,68,68,68	0
52	MG	AA	1618	1/1	0.94	0.60	-	72,72,72,72	0
52	MG	DA	3014	1/1	0.99	0.40	-	68,68,68,68	0
52	MG	BA	3155	1/1	0.97	0.41	-	41,41,41,41	0
52	MG	BA	3269	1/1	0.96	0.14	-	55,55,55,55	0
52	MG	BA	3320	1/1	0.95	0.35	-	54,54,54,54	0
52	MG	BA	3300	1/1	0.97	0.50	-	59,59,59,59	0
52	MG	BA	3082	1/1	0.90	0.53	-	49,49,49,49	0
52	MG	BA	3202	1/1	0.92	0.31	-	41,41,41,41	0
52	MG	DA	3018	1/1	0.98	0.55	-	32,32,32,32	0
52	MG	DA	3292	1/1	0.91	0.58	-	75,75,75,75	0
52	MG	BA	3340	1/1	0.93	0.46	-	62,62,62,62	0
52	MG	BB	202	1/1	0.97	0.28	-	30,30,30,30	0
52	MG	BA	3215	1/1	0.96	0.42	-	36,36,36,36	0
52	MG	DA	3238	1/1	0.90	0.38	-	73,73,73,73	0
52	MG	BD	301	1/1	0.94	0.20	-	43,43,43,43	0
52	MG	CA	1640	1/1	0.95	0.25	-	68,68,68,68	0
52	MG	DA	3194	1/1	0.86	0.30	-	60,60,60,60	0
52	MG	DA	3186	1/1	0.95	0.53	-	63,63,63,63	0
52	MG	DA	3013	1/1	0.88	0.49	-	77,77,77,77	0
52	MG	DA	3038	1/1	0.84	0.60	-	48,48,48,48	0
52	MG	BA	3140	1/1	0.92	0.62	-	40,40,40,40	0
52	MG	BA	3102	1/1	0.92	0.29	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3307	1/1	0.88	0.31	-	80,80,80,80	0
52	MG	BA	3346	1/1	0.95	0.44	-	80,80,80,80	0
52	MG	BA	3134	1/1	0.99	0.17	-	46,46,46,46	0
52	MG	DA	3004	1/1	0.95	0.25	-	49,49,49,49	0
52	MG	DA	3277	1/1	0.90	0.50	-	68,68,68,68	0
52	MG	BA	3312	1/1	0.62	0.66	-	87,87,87,87	0
52	MG	AA	1620	1/1	0.95	0.42	-	73,73,73,73	0
52	MG	BA	3336	1/1	0.79	0.48	-	65,65,65,65	0
52	MG	BA	3066	1/1	0.94	0.47	-	43,43,43,43	0
52	MG	BA	3122	1/1	0.95	0.30	-	40,40,40,40	0
52	MG	CA	1604	1/1	0.92	0.29	-	86,86,86,86	0
52	MG	AA	1608	1/1	0.93	0.33	-	54,54,54,54	0
52	MG	DA	3198	1/1	0.76	0.79	-	70,70,70,70	0
52	MG	BA	3328	1/1	0.91	0.17	-	65,65,65,65	0
52	MG	BA	3036	1/1	0.96	0.21	-	0,0,0,0	0
52	MG	BA	3035	1/1	0.98	0.26	-	21,21,21,21	0
52	MG	BA	3290	1/1	0.95	0.33	-	47,47,47,47	0
52	MG	BA	3319	1/1	0.91	0.49	-	40,40,40,40	0
52	MG	DA	3034	1/1	0.98	0.49	-	39,39,39,39	0
52	MG	BA	3265	1/1	0.98	0.36	-	63,63,63,63	0
52	MG	DA	3051	1/1	0.97	0.38	-	26,26,26,26	0
52	MG	AA	1615	1/1	0.95	0.51	-	76,76,76,76	0
52	MG	DA	3079	1/1	0.92	0.33	-	59,59,59,59	0
52	MG	DA	3125	1/1	0.95	0.63	-	58,58,58,58	0
52	MG	DA	3234	1/1	0.97	0.62	-	60,60,60,60	0
52	MG	BA	3199	1/1	0.98	0.57	-	49,49,49,49	0
52	MG	DA	3025	1/1	0.94	0.57	-	50,50,50,50	0
52	MG	DA	3269	1/1	0.91	0.16	-	61,61,61,61	0
52	MG	BA	3210	1/1	0.98	0.31	-	37,37,37,37	0
52	MG	BA	3325	1/1	0.94	0.41	-	43,43,43,43	0
52	MG	BA	3335	1/1	0.92	0.19	-	52,52,52,52	0
52	MG	BA	3163	1/1	0.93	0.41	-	47,47,47,47	0
52	MG	DA	3190	1/1	0.96	0.39	-	63,63,63,63	0
52	MG	BA	3238	1/1	0.83	0.47	-	49,49,49,49	0
52	MG	BA	3145	1/1	0.93	0.55	-	40,40,40,40	0
52	MG	AA	1641	1/1	0.87	0.15	-	69,69,69,69	0
52	MG	BA	3212	1/1	0.99	0.45	-	30,30,30,30	0
52	MG	BA	3101	1/1	0.94	0.42	-	39,39,39,39	0
52	MG	BA	3339	1/1	0.95	0.16	-	41,41,41,41	0
52	MG	DA	3226	1/1	0.71	0.35	-	64,64,64,64	0
52	MG	BA	3327	1/1	0.95	0.29	-	47,47,47,47	0
52	MG	BA	3344	1/1	0.94	0.74	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3250	1/1	0.95	0.17	-	75,75,75,75	0
52	MG	DA	3201	1/1	0.87	0.30	-	59,59,59,59	0
52	MG	DA	3003	1/1	0.96	0.70	-	56,56,56,56	0
52	MG	BA	3181	1/1	0.96	0.38	-	51,51,51,51	0
52	MG	CA	1638	1/1	0.94	0.30	-	71,71,71,71	0
52	MG	DA	3040	1/1	0.96	0.24	-	43,43,43,43	0
52	MG	BA	3096	1/1	0.85	0.33	-	55,55,55,55	0
52	MG	BA	3218	1/1	0.98	0.48	-	33,33,33,33	0
52	MG	DA	3153	1/1	0.94	0.53	-	59,59,59,59	0
52	MG	DA	3202	1/1	0.92	0.21	-	40,40,40,40	0
52	MG	DA	3124	1/1	0.97	0.31	-	83,83,83,83	0
52	MG	BA	3308	1/1	0.94	0.46	-	64,64,64,64	0
52	MG	AA	1642	1/1	0.96	0.32	-	51,51,51,51	0
52	MG	BA	3178	1/1	0.81	0.53	-	78,78,78,78	0
52	MG	BA	3277	1/1	0.92	0.47	-	62,62,62,62	0
52	MG	BA	3184	1/1	0.95	0.45	-	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.