



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:12 PM GMT

PDB ID : 4V97
Title : Crystal structure of the bacterial ribosome ram mutation G299A.
Authors : Fagan, C.E.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2012-04-06
Resolution : 3.52 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

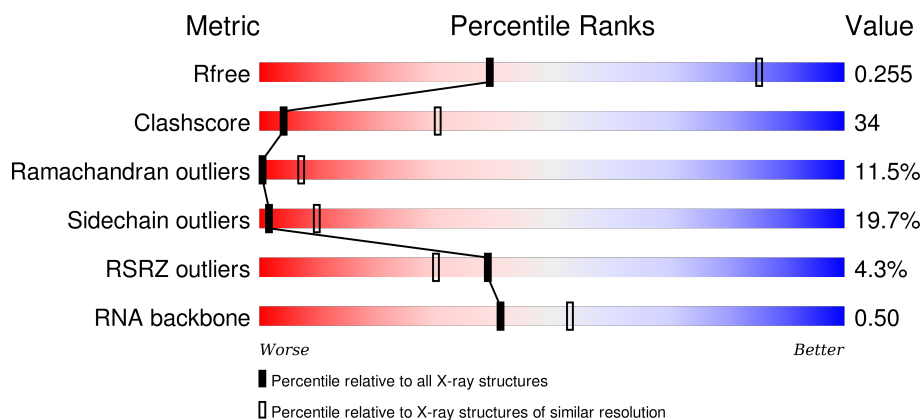
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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.



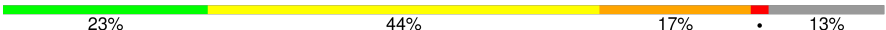
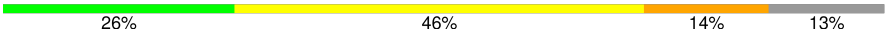
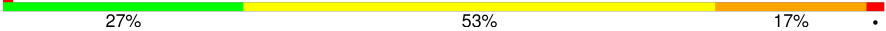


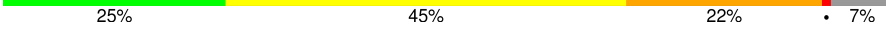





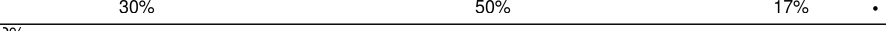

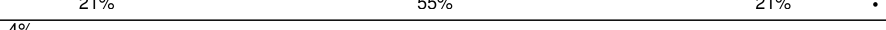




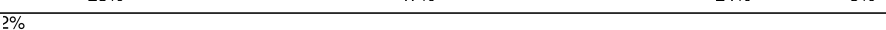
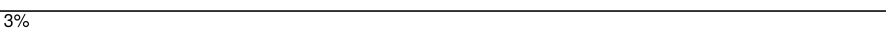

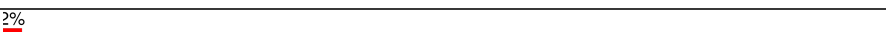
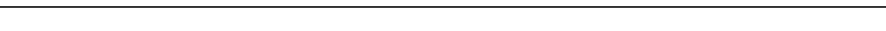


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1089 (3.64-3.40)
Clashscore	102246	1197 (3.64-3.40)
Ramachandran outliers	100387	1159 (3.64-3.40)
Sidechain outliers	100360	1160 (3.64-3.40)
RSRZ outliers	91569	1096 (3.64-3.40)
RNA backbone	2183	1051 (4.22-2.80)

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>3%</div> <div>49% 35% 15%</div> </div>
1	CA	1522	<div> <div>4%</div> <div>49% 33% 16%</div> </div>
2	AB	256	<div> <div>2%</div> <div>21% 50% 19% 8%</div> </div>
2	CB	256	<div> <div>4%</div> <div>18% 50% 22% 8%</div> </div>



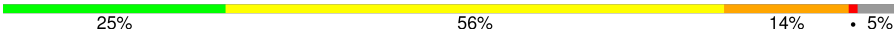
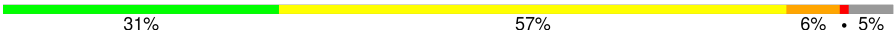
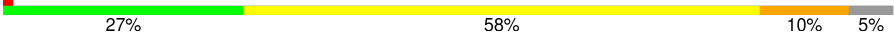
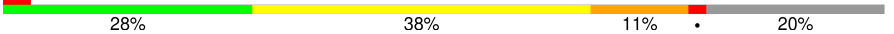
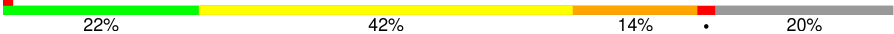
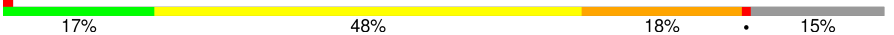
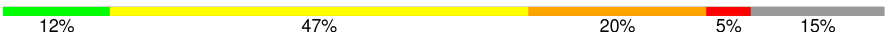
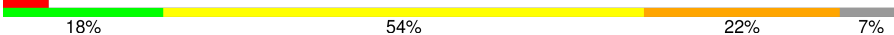
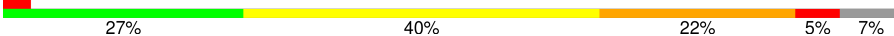
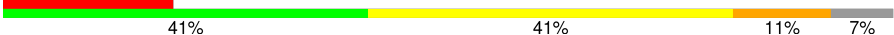
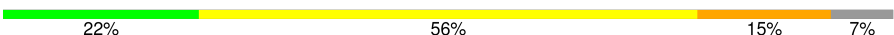
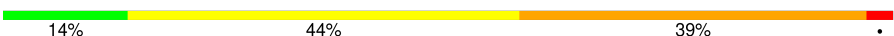



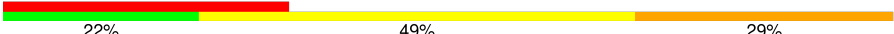







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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	CV	77	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	24	
24	CX	24	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	

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Mol	Chain	Length	Quality of chain
27	BC	229	
27	DC	229	
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	

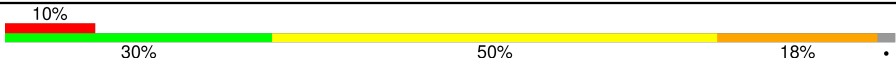
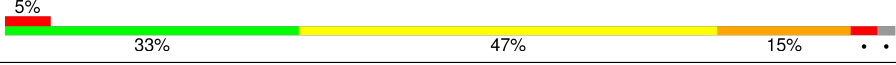
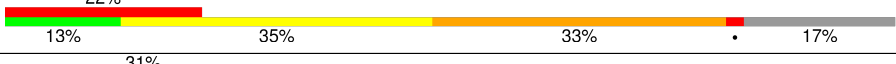
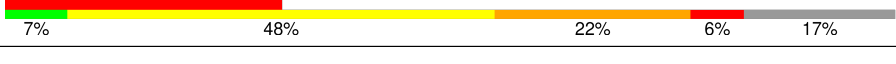
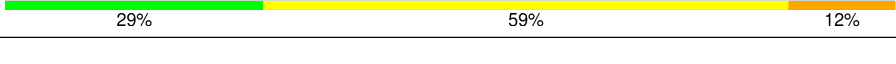
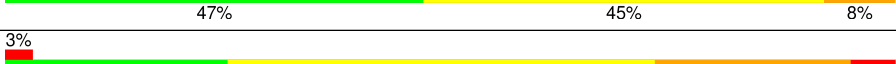
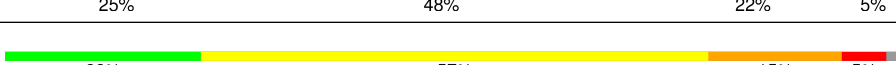
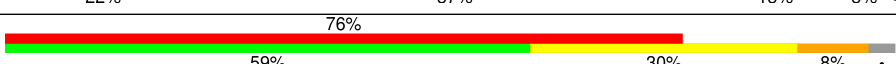


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Mol	Chain	Length	Quality of chain
39	DS	112	
40	BT	146	
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	7006	-	-	-	X
57	MG	AA	7008	-	-	-	X
57	MG	AA	7011	-	-	-	X
57	MG	AA	7013	-	-	-	X
57	MG	AA	7016	-	-	-	X
57	MG	AA	7018	-	-	-	X
57	MG	AA	7019	-	-	-	X
57	MG	AA	7021	-	-	-	X
57	MG	AA	7026	-	-	-	X
57	MG	AA	7034	-	-	-	X
57	MG	AA	7037	-	-	-	X
57	MG	AA	7043	-	-	-	X
57	MG	AA	7044	-	-	-	X
57	MG	AA	7051	-	-	-	X
57	MG	AA	7053	-	-	-	X
57	MG	AA	7054	-	-	-	X
57	MG	AA	7056	-	-	-	X
57	MG	AA	7058	-	-	-	X
57	MG	AA	7059	-	-	-	X
57	MG	AA	7061	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	7064	-	-	-	X
57	MG	AA	7066	-	-	-	X
57	MG	AA	7067	-	-	-	X
57	MG	AA	7071	-	-	-	X
57	MG	AA	7075	-	-	-	X
57	MG	AA	7090	-	-	-	X
57	MG	AA	7091	-	-	-	X
57	MG	AA	7094	-	-	-	X
57	MG	AA	7110	-	-	-	X
57	MG	B7	101	-	-	-	X
57	MG	BA	3004	-	-	-	X
57	MG	BA	3007	-	-	-	X
57	MG	BA	3008	-	-	-	X
57	MG	BA	3020	-	-	-	X
57	MG	BA	3027	-	-	-	X
57	MG	BA	3028	-	-	-	X
57	MG	BA	3030	-	-	-	X
57	MG	BA	3041	-	-	-	X
57	MG	BA	3044	-	-	-	X
57	MG	BA	3045	-	-	-	X
57	MG	BA	3046	-	-	-	X
57	MG	BA	3047	-	-	-	X
57	MG	BA	3051	-	-	-	X
57	MG	BA	3054	-	-	-	X
57	MG	BA	3065	-	-	-	X
57	MG	BA	3066	-	-	-	X
57	MG	BA	3069	-	-	-	X
57	MG	BA	3073	-	-	-	X
57	MG	BA	3081	-	-	-	X
57	MG	BA	3084	-	-	-	X
57	MG	BA	3086	-	-	-	X
57	MG	BA	3090	-	-	-	X
57	MG	BA	3098	-	-	-	X
57	MG	BA	3099	-	-	-	X
57	MG	BA	3111	-	-	-	X
57	MG	BA	3116	-	-	-	X
57	MG	BA	3119	-	-	-	X
57	MG	BA	3120	-	-	-	X
57	MG	BA	3125	-	-	-	X
57	MG	BA	3136	-	-	-	X
57	MG	BA	3142	-	-	-	X
57	MG	BA	3144	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3145	-	-	-	X
57	MG	BA	3146	-	-	-	X
57	MG	BA	3153	-	-	-	X
57	MG	BA	3159	-	-	-	X
57	MG	BA	3160	-	-	-	X
57	MG	BA	3182	-	-	-	X
57	MG	BA	3187	-	-	-	X
57	MG	BA	3188	-	-	-	X
57	MG	BA	3191	-	-	-	X
57	MG	BA	3193	-	-	-	X
57	MG	BA	3196	-	-	-	X
57	MG	BA	3198	-	-	-	X
57	MG	BA	3201	-	-	-	X
57	MG	BA	3203	-	-	-	X
57	MG	BA	3204	-	-	-	X
57	MG	BA	3205	-	-	-	X
57	MG	BA	3210	-	-	-	X
57	MG	BA	3218	-	-	-	X
57	MG	BA	3220	-	-	-	X
57	MG	BA	3222	-	-	-	X
57	MG	BA	3225	-	-	-	X
57	MG	BA	3227	-	-	-	X
57	MG	BA	3229	-	-	-	X
57	MG	BA	3234	-	-	-	X
57	MG	BA	3235	-	-	-	X
57	MG	BA	3238	-	-	-	X
57	MG	BA	3241	-	-	-	X
57	MG	BA	3243	-	-	-	X
57	MG	BA	3248	-	-	-	X
57	MG	BA	3249	-	-	-	X
57	MG	BA	3251	-	-	-	X
57	MG	BA	3252	-	-	-	X
57	MG	BA	3255	-	-	-	X
57	MG	BA	3264	-	-	-	X
57	MG	BA	3265	-	-	-	X
57	MG	BA	3270	-	-	-	X
57	MG	BA	3272	-	-	-	X
57	MG	BA	3276	-	-	-	X
57	MG	BA	3279	-	-	-	X
57	MG	BA	3281	-	-	-	X
57	MG	BA	3297	-	-	-	X
57	MG	BA	3300	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3306	-	-	-	X
57	MG	BA	3307	-	-	-	X
57	MG	BA	3308	-	-	-	X
57	MG	BA	3309	-	-	-	X
57	MG	BA	3310	-	-	-	X
57	MG	BD	301	-	-	-	X
57	MG	BE	302	-	-	-	X
57	MG	CA	1607	-	-	-	X
57	MG	CA	1610	-	-	-	X
57	MG	CA	1617	-	-	-	X
57	MG	CA	1624	-	-	-	X
57	MG	CA	1626	-	-	-	X
57	MG	CA	1629	-	-	-	X
57	MG	CA	1630	-	-	-	X
57	MG	CA	1631	-	-	-	X
57	MG	CA	1640	-	-	-	X
57	MG	CA	1645	-	-	-	X
57	MG	CA	1651	-	-	-	X
57	MG	CA	1652	-	-	-	X
57	MG	CA	1653	-	-	-	X
57	MG	CA	1665	-	-	-	X
57	MG	CA	1667	-	-	-	X
57	MG	CA	1668	-	-	-	X
57	MG	CA	1670	-	-	-	X
57	MG	CA	1674	-	-	-	X
57	MG	CA	1683	-	-	-	X
57	MG	CA	1685	-	-	-	X
57	MG	CA	1699	-	-	-	X
57	MG	CA	1705	-	-	-	X
57	MG	CA	1709	-	-	-	X
57	MG	CA	1710	-	-	-	X
57	MG	CA	1720	-	-	-	X
57	MG	CA	1727	-	-	-	X
57	MG	CA	1737	-	-	-	X
57	MG	D0	101	-	-	-	X
57	MG	DA	9305	-	-	-	X
57	MG	DA	9308	-	-	-	X
57	MG	DA	9310	-	-	-	X
57	MG	DA	9312	-	-	-	X
57	MG	DA	9319	-	-	-	X
57	MG	DA	9324	-	-	-	X
57	MG	DA	9335	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	9340	-	-	-	X
57	MG	DA	9347	-	-	-	X
57	MG	DA	9349	-	-	-	X
57	MG	DA	9355	-	-	-	X
57	MG	DA	9356	-	-	-	X
57	MG	DA	9358	-	-	-	X
57	MG	DA	9359	-	-	-	X
57	MG	DA	9360	-	-	-	X
57	MG	DA	9363	-	-	-	X
57	MG	DA	9364	-	-	-	X
57	MG	DA	9365	-	-	-	X
57	MG	DA	9366	-	-	-	X
57	MG	DA	9369	-	-	-	X
57	MG	DA	9370	-	-	-	X
57	MG	DA	9381	-	-	-	X
57	MG	DA	9382	-	-	-	X
57	MG	DA	9383	-	-	-	X
57	MG	DA	9392	-	-	-	X
57	MG	DA	9398	-	-	-	X
57	MG	DA	9399	-	-	-	X
57	MG	DA	9402	-	-	-	X
57	MG	DA	9404	-	-	-	X
57	MG	DA	9408	-	-	-	X
57	MG	DA	9409	-	-	-	X
57	MG	DA	9417	-	-	-	X
57	MG	DA	9418	-	-	-	X
57	MG	DA	9421	-	-	-	X
57	MG	DA	9425	-	-	-	X
57	MG	DA	9428	-	-	-	X
57	MG	DA	9430	-	-	-	X
57	MG	DA	9435	-	-	-	X
57	MG	DA	9436	-	-	-	X
57	MG	DA	9437	-	-	-	X
57	MG	DA	9438	-	-	-	X
57	MG	DA	9439	-	-	-	X
57	MG	DA	9441	-	-	-	X
57	MG	DA	9443	-	-	-	X
57	MG	DA	9445	-	-	-	X
57	MG	DA	9454	-	-	-	X
57	MG	DA	9458	-	-	-	X
57	MG	DA	9459	-	-	-	X
57	MG	DA	9460	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	9461	-	-	-	X
57	MG	DA	9472	-	-	-	X
57	MG	DA	9473	-	-	-	X
57	MG	DA	9479	-	-	-	X
57	MG	DA	9483	-	-	-	X
57	MG	DA	9484	-	-	-	X
57	MG	DA	9489	-	-	-	X
57	MG	DA	9491	-	-	-	X
57	MG	DA	9493	-	-	-	X
57	MG	DA	9497	-	-	-	X
57	MG	DA	9498	-	-	-	X
57	MG	DA	9503	-	-	-	X
57	MG	DA	9508	-	-	-	X
57	MG	DA	9512	-	-	-	X
57	MG	DA	9514	-	-	-	X
57	MG	DA	9515	-	-	-	X
57	MG	DA	9516	-	-	-	X
57	MG	DA	9517	-	-	-	X
57	MG	DA	9518	-	-	-	X
57	MG	DA	9521	-	-	-	X
57	MG	DA	9523	-	-	-	X
57	MG	DA	9526	-	-	-	X
57	MG	DA	9527	-	-	-	X
57	MG	DA	9528	-	-	-	X
57	MG	DA	9529	-	-	-	X
57	MG	DA	9530	-	-	-	X
57	MG	DA	9533	-	-	-	X
57	MG	DA	9536	-	-	-	X
57	MG	DA	9537	-	-	-	X
57	MG	DA	9539	-	-	-	X
57	MG	DA	9544	-	-	-	X
57	MG	DA	9545	-	-	-	X
57	MG	DA	9546	-	-	-	X
57	MG	DA	9549	-	-	-	X
57	MG	DA	9553	-	-	-	X
57	MG	DA	9554	-	-	-	X
57	MG	DA	9557	-	-	-	X
57	MG	DA	9570	-	-	-	X
57	MG	DA	9581	-	-	-	X
57	MG	DA	9584	-	-	-	X
57	MG	DA	9587	-	-	-	X
57	MG	DA	9590	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	9597	-	-	-	X
57	MG	DA	9600	-	-	-	X
57	MG	DA	9605	-	-	-	X
57	MG	DA	9613	-	-	-	X
57	MG	DA	9614	-	-	-	X
57	MG	DA	9618	-	-	-	X
57	MG	DA	9621	-	-	-	X
57	MG	DA	9623	-	-	-	X
57	MG	DA	9647	-	-	-	X
57	MG	DA	9649	-	-	-	X
57	MG	DA	9653	-	-	-	X
57	MG	DA	9655	-	-	-	X
57	MG	DA	9672	-	-	-	X
57	MG	DA	9673	-	-	-	X
57	MG	DA	9675	-	-	-	X
57	MG	DA	9681	-	-	-	X
57	MG	DA	9696	-	-	-	X
57	MG	DD	7101	-	-	-	X
57	MG	DD	7103	-	-	-	X
57	MG	DQ	201	-	-	-	X
58	PAR	AA	7111	-	-	-	X
58	PAR	CA	1741	-	-	-	X
59	ZN	CN	101	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293977 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
			32328	14390	5992	10443	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32328	14390	5992	10443	1503			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	299	A	G	ENGINEERED MUTATION	GB AP008226.1
CA	299	A	G	ENGINEERED MUTATION	GB AP008226.1

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			1010	639	197	174			
9	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called P-SITE tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	CV	77	Total	C	N	O	P	0	0	0
			1643	732	297	537	77			

- Molecule 23 is a RNA chain called E-SITE TRNA PHE OR A-SITE tRNA Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	AY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
23	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	CY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	12	Total	C	N	O	P	0	0	0
			255	115	46	82	12			
24	CX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2810	Total	C	N	O	P	0	0	0
			60527	26937	11326	19455	2809			
25	DA	2824	Total	C	N	O	P	0	0	0
			60827	27071	11381	19552	2823			

- Molecule 26 is a RNA chain called 5S rRNA.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	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
30	DF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
32	DH	168	Total	C	N	O	S	0	0	0
			1290	820	240	229	1			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
33	DI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
36	DP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
37	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
38	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
39	DS	111	Total	C	N	O		0	0	0
			882	556	176	150				

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
41	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
45	DY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	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
46	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
51	D4	40	Total	C	N	O	S	0	0	1
			298	189	50	54	5			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

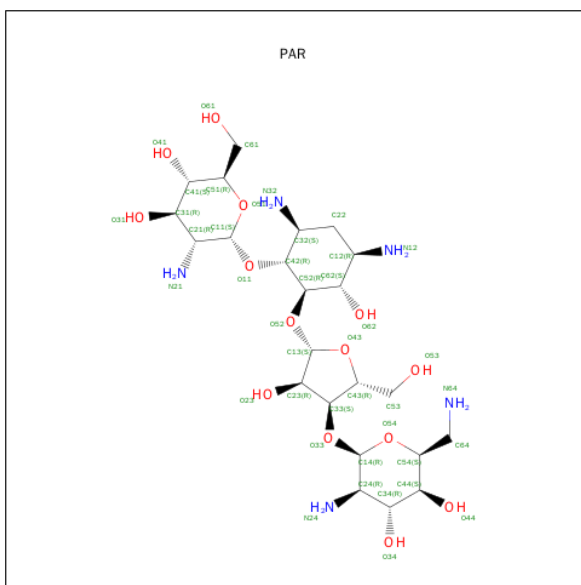
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BA	323	Total Mg 323 323	0	0
57	CA	141	Total Mg 141 141	0	0
57	DQ	1	Total Mg 1 1	0	0
57	DF	1	Total Mg 1 1	0	0
57	CV	5	Total Mg 5 5	0	0
57	D2	1	Total Mg 1 1	0	0
57	BE	3	Total Mg 3 3	0	0
57	DU	3	Total Mg 3 3	0	0
57	BP	1	Total Mg 1 1	0	0
57	AX	1	Total Mg 1 1	0	0
57	CY	1	Total Mg 1 1	0	0
57	DD	3	Total Mg 3 3	0	0
57	B5	1	Total Mg 1 1	0	0
57	BB	5	Total Mg 5 5	0	0
57	AE	1	Total Mg 1 1	0	0
57	BF	1	Total Mg 1 1	0	0
57	AV	5	Total Mg 5 5	0	0
57	D8	1	Total Mg 1 1	0	0
57	AA	110	Total Mg 110 110	0	0
57	CX	1	Total Mg 1 1	0	0
57	BU	1	Total Mg 1 1	0	0
57	BN	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	D0	2	Total 2	Mg 2	0	0
57	DE	2	Total 2	Mg 2	0	0
57	DX	1	Total 1	Mg 1	0	0
57	DA	397	Total 397	Mg 397	0	0
57	DW	1	Total 1	Mg 1	0	0
57	B7	1	Total 1	Mg 1	0	0
57	BO	1	Total 1	Mg 1	0	0
57	D1	2	Total 2	Mg 2	0	0
57	DP	3	Total 3	Mg 3	0	0
57	CW	1	Total 1	Mg 1	0	0
57	D5	2	Total 2	Mg 2	0	0
57	BD	2	Total 2	Mg 2	0	0
57	CE	2	Total 2	Mg 2	0	0
57	DB	5	Total 5	Mg 5	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	AA	1	Total 42	C 23	N 5	O 14	0	0
58	CA	1	Total 42	C 23	N 5	O 14	0	0

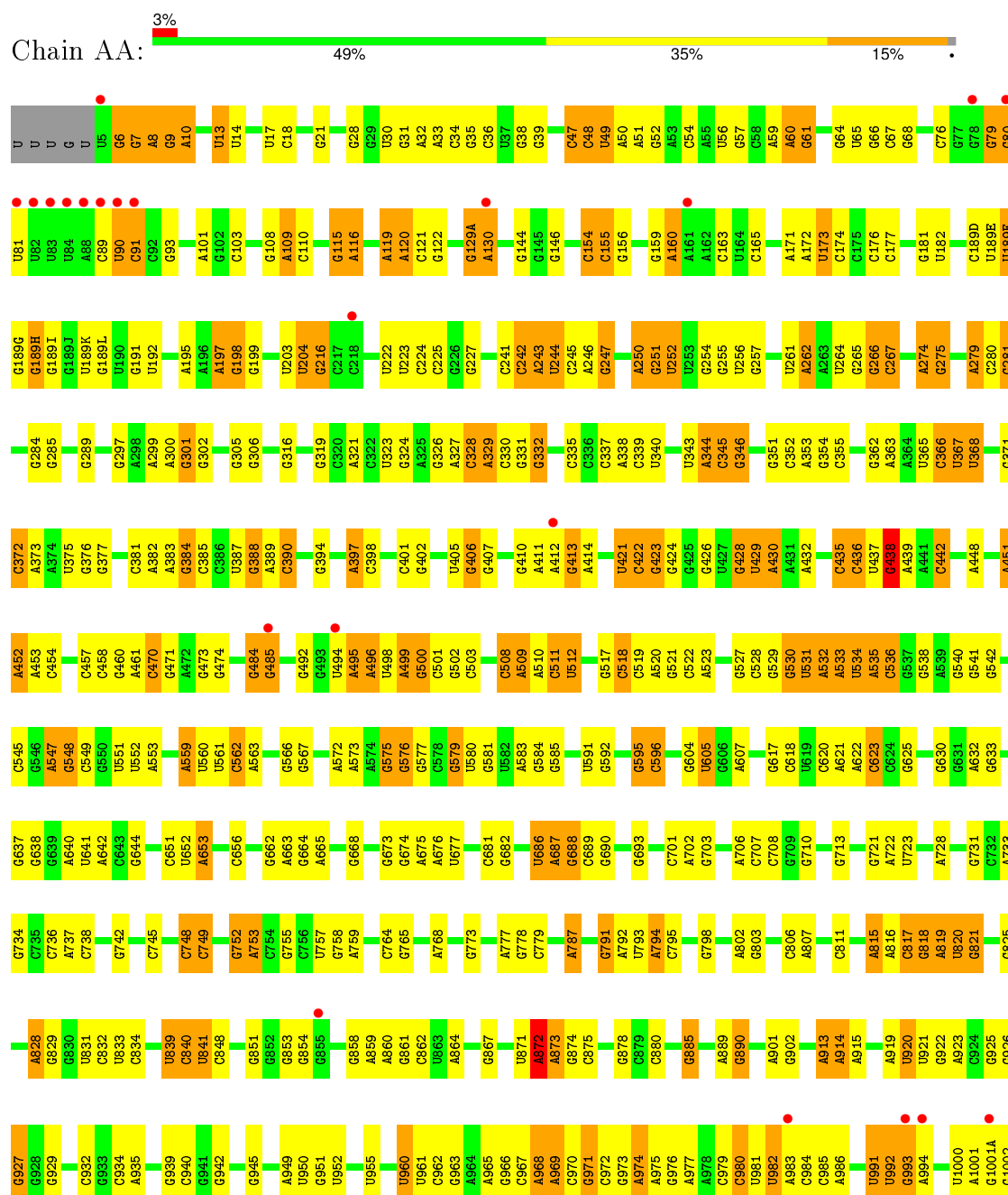
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

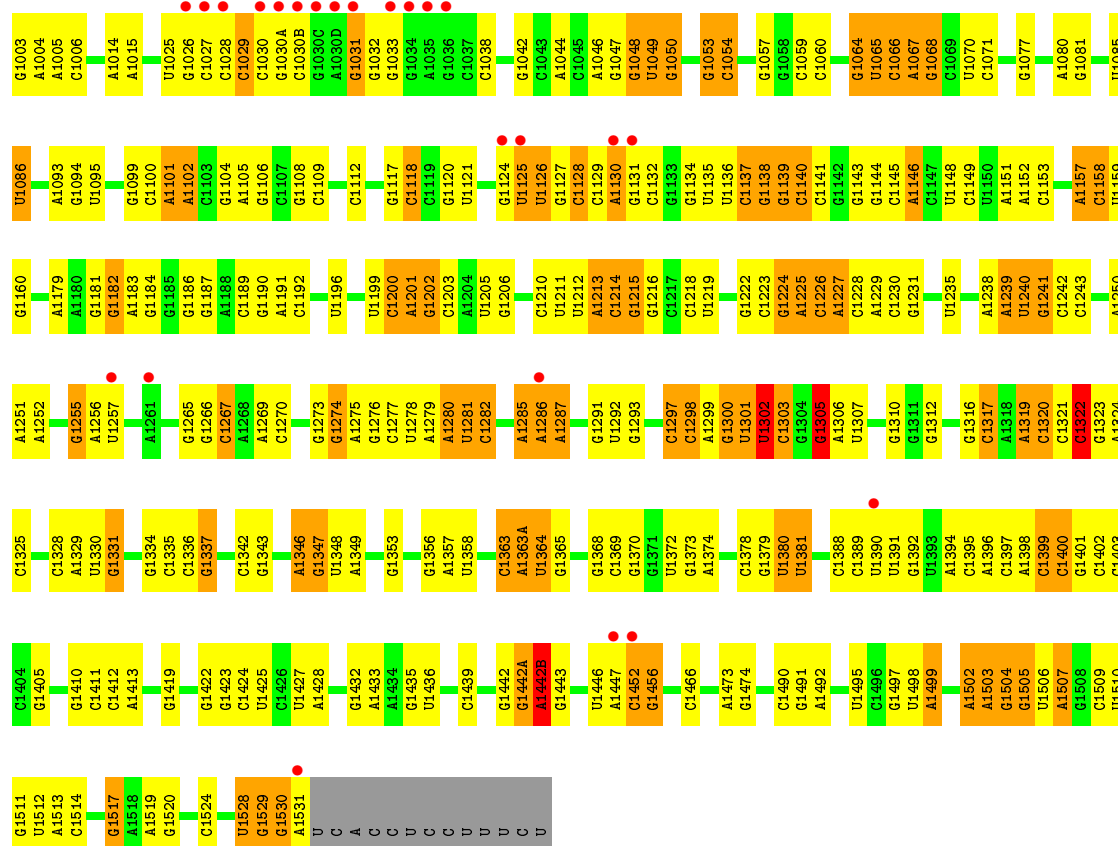
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	CN	1	Total Zn 1 1	0	0
59	AD	1	Total Zn 1 1	0	0
59	CD	1	Total Zn 1 1	0	0
59	AN	1	Total Zn 1 1	0	0

3 Residue-property plots

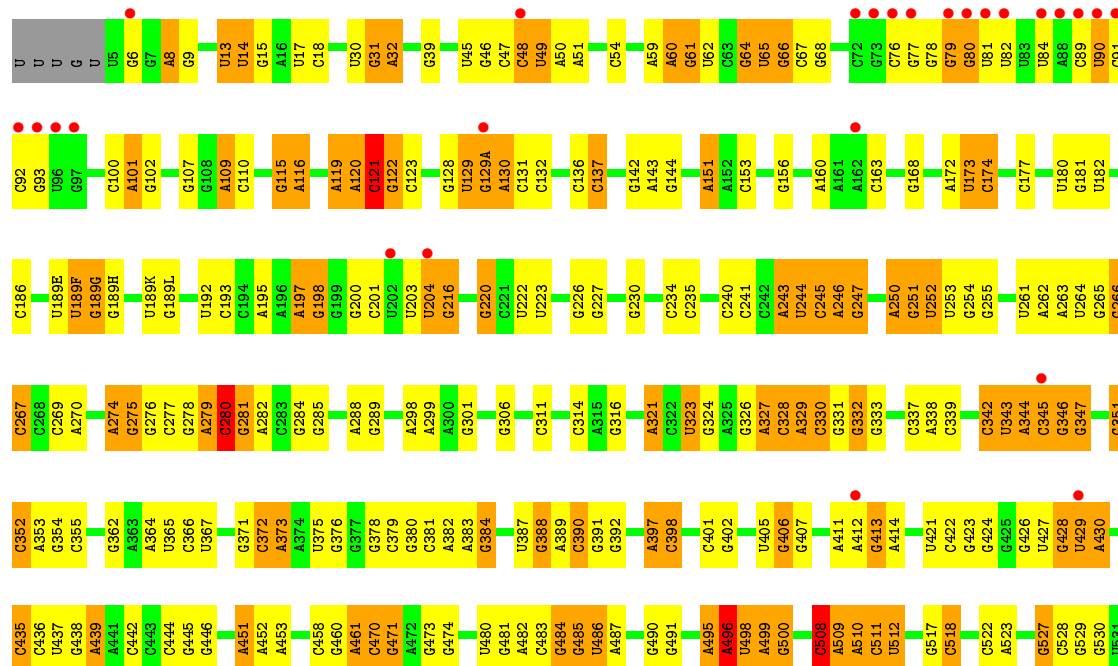
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA





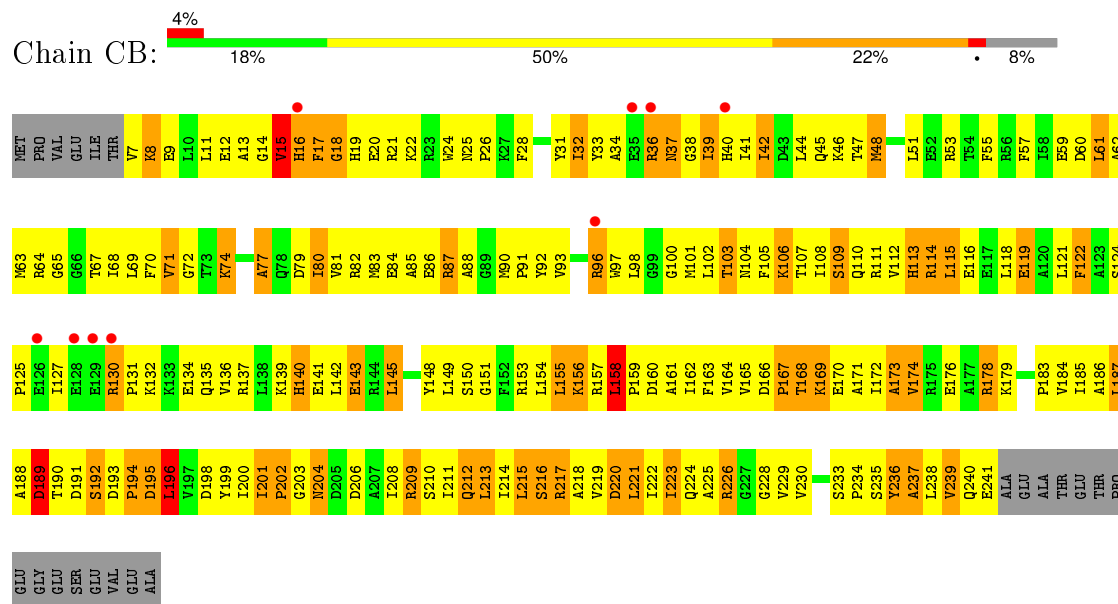
• Molecule 1: 16S rRNA



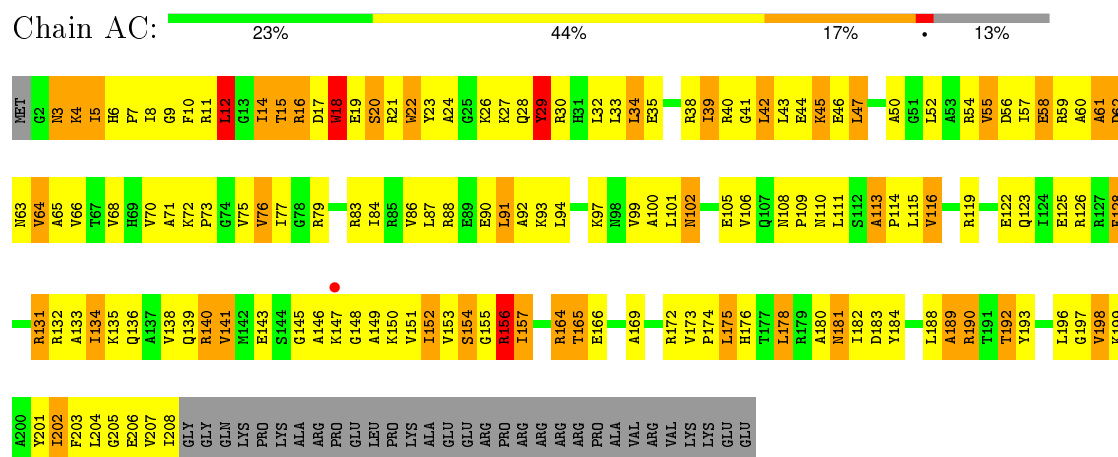




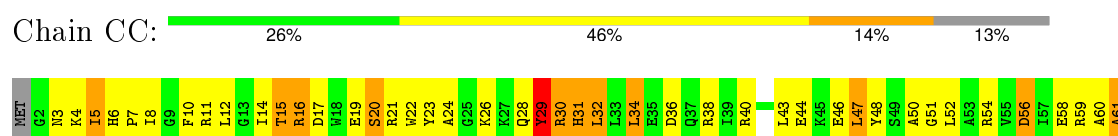
• Molecule 2: 30S ribosomal protein S2

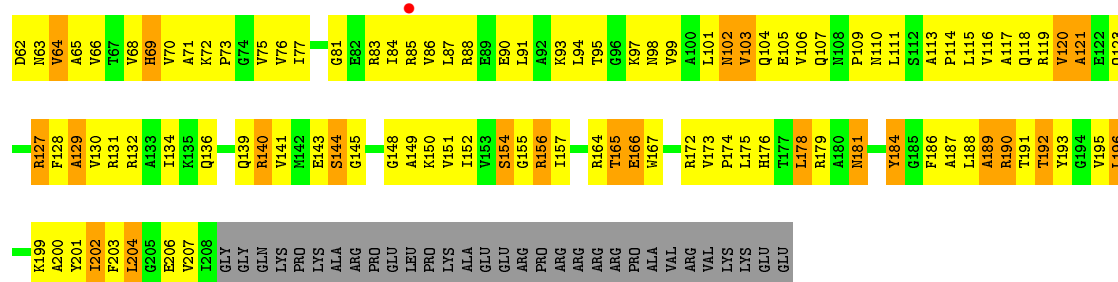


• Molecule 3: 30S ribosomal protein S3

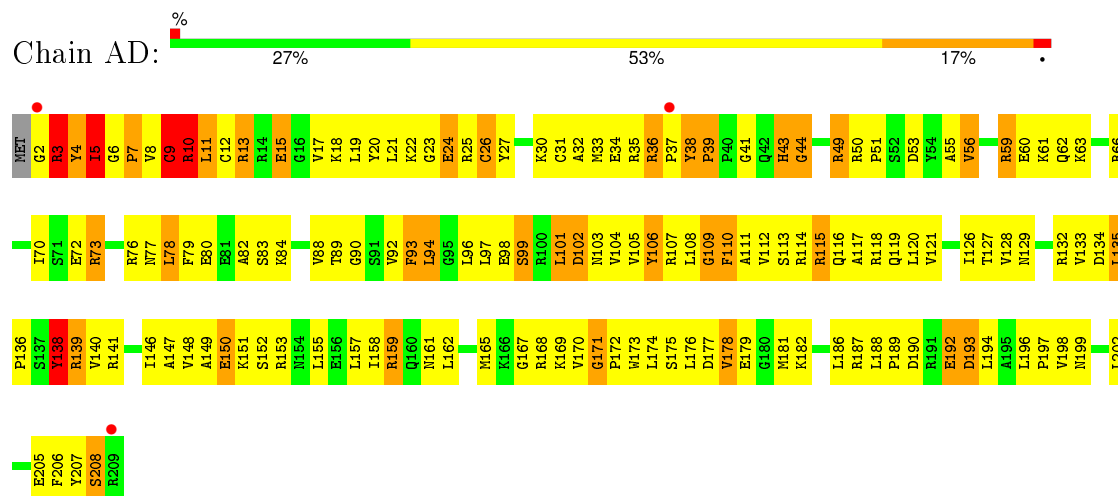


• Molecule 3: 30S ribosomal protein S3

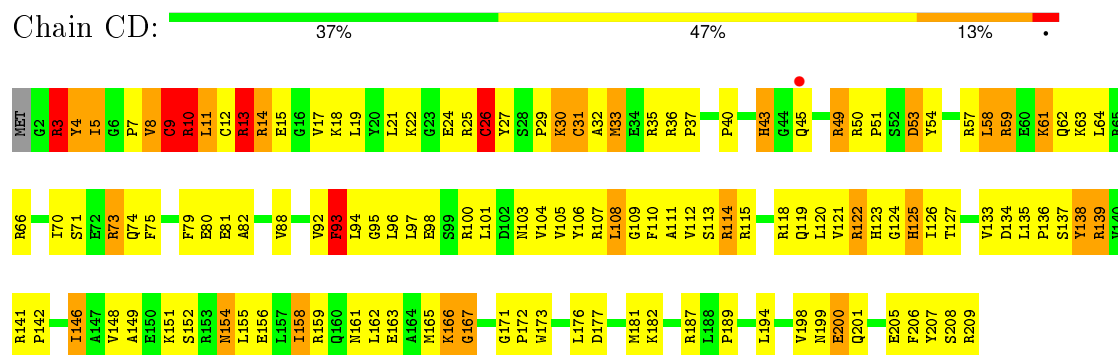




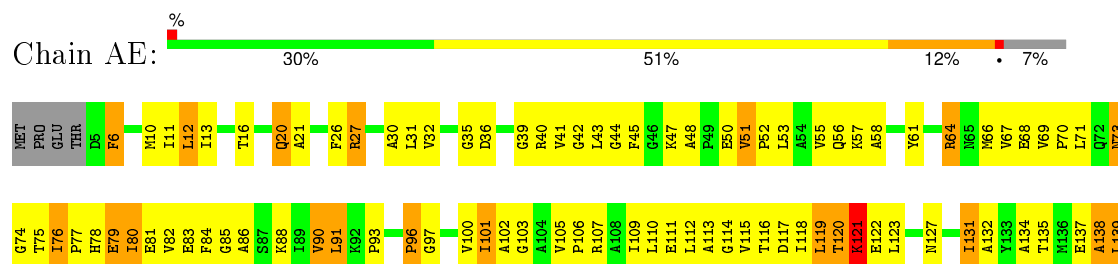
• Molecule 4: 30S ribosomal protein S4

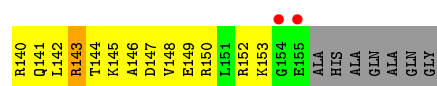


• Molecule 4: 30S ribosomal protein S4

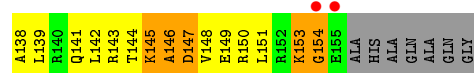


• Molecule 5: 30S ribosomal protein S5





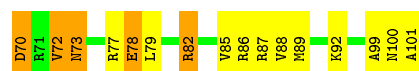
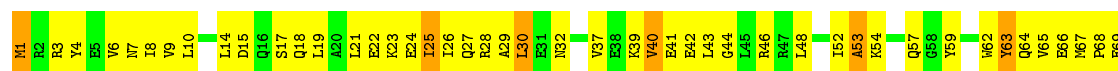
• Molecule 5: 30S ribosomal protein S5



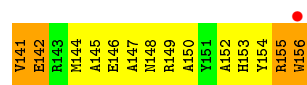
• Molecule 6: 30S ribosomal protein S6



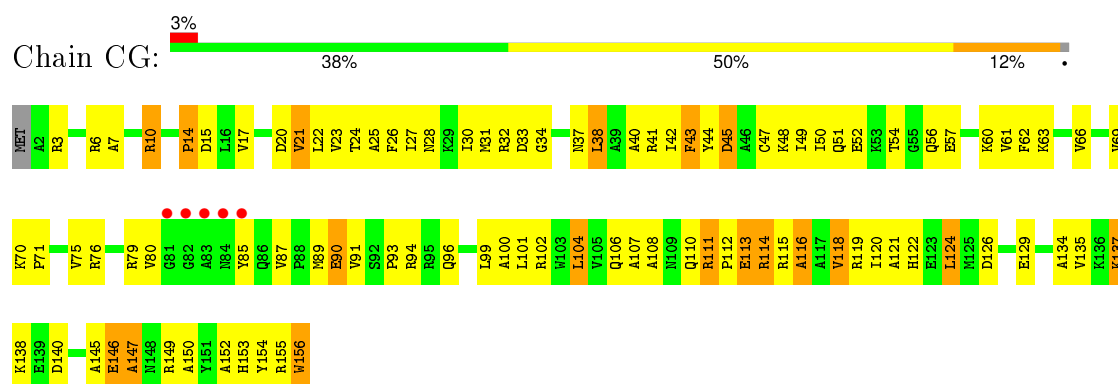
• Molecule 6: 30S ribosomal protein S6



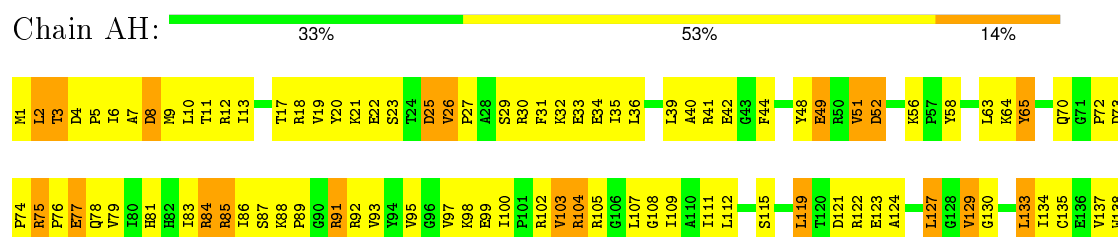
• Molecule 7: 30S ribosomal protein S7



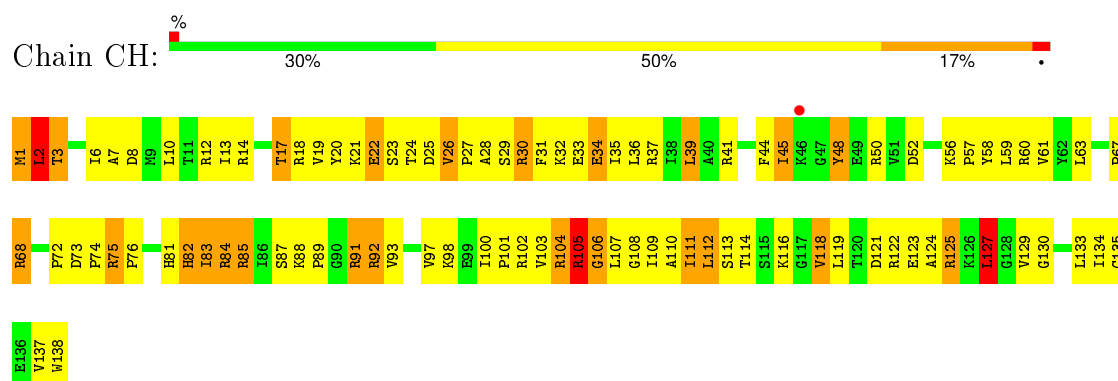
• Molecule 7: 30S ribosomal protein S7



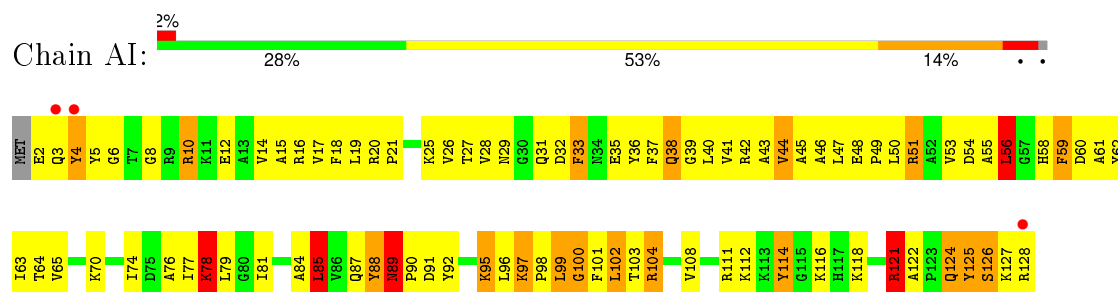
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

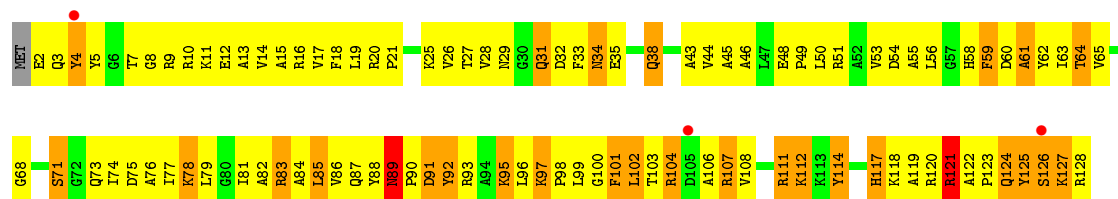


• Molecule 9: 30S ribosomal protein S9

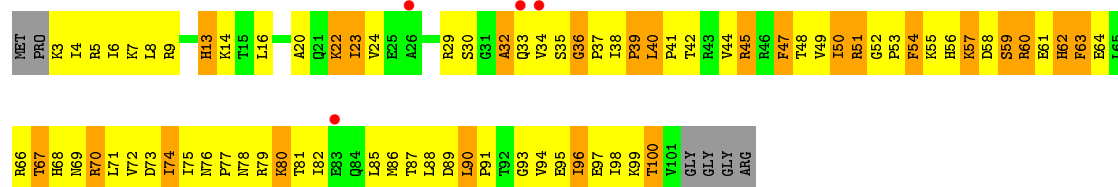
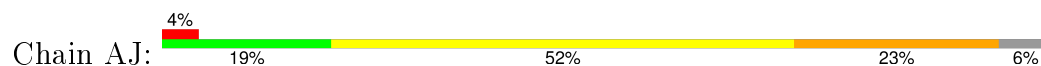


• Molecule 9: 30S ribosomal protein S9

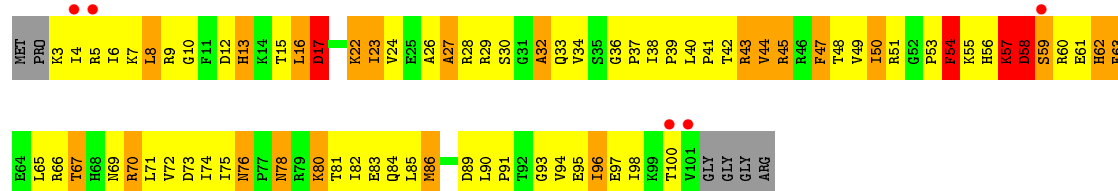
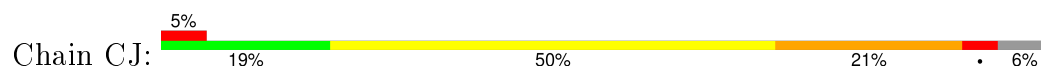




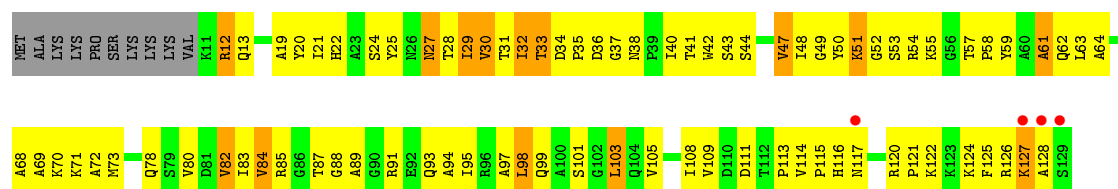
• Molecule 10: 30S ribosomal protein S10



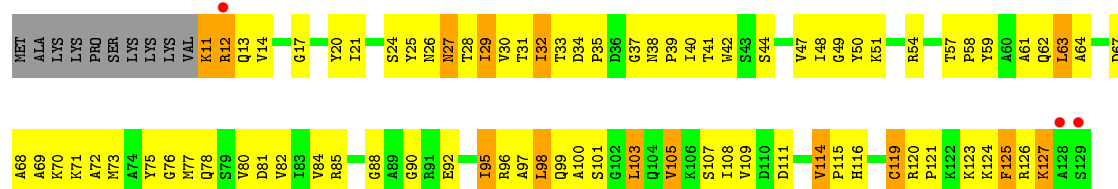
• Molecule 10: 30S ribosomal protein S10



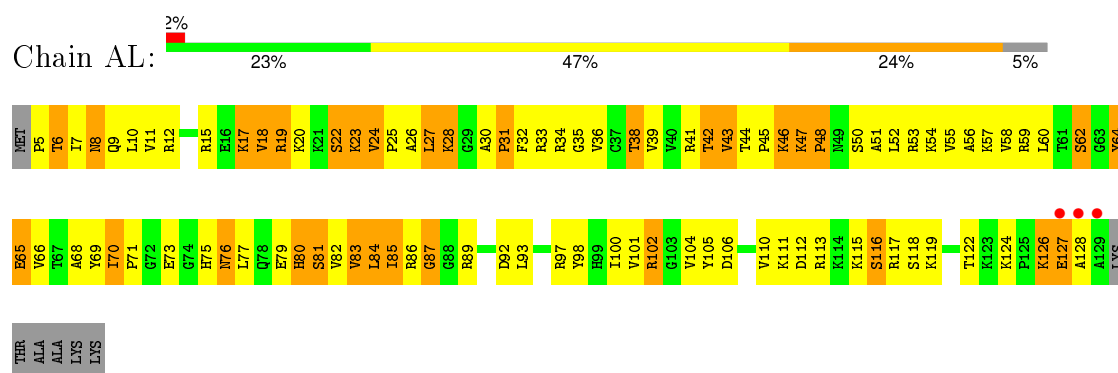
• Molecule 11: 30S ribosomal protein S11



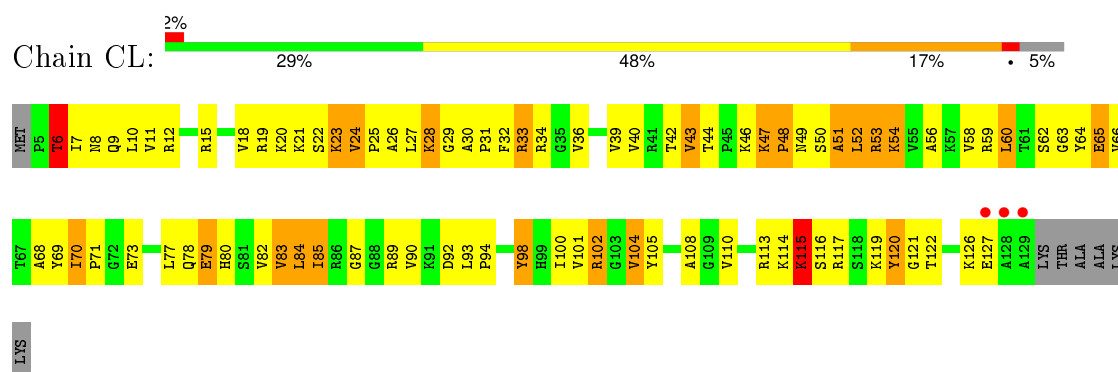
• Molecule 11: 30S ribosomal protein S11



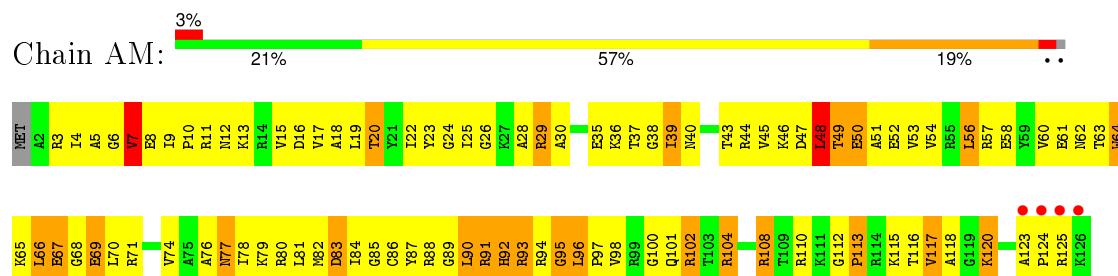
• Molecule 12: 30S ribosomal protein S12



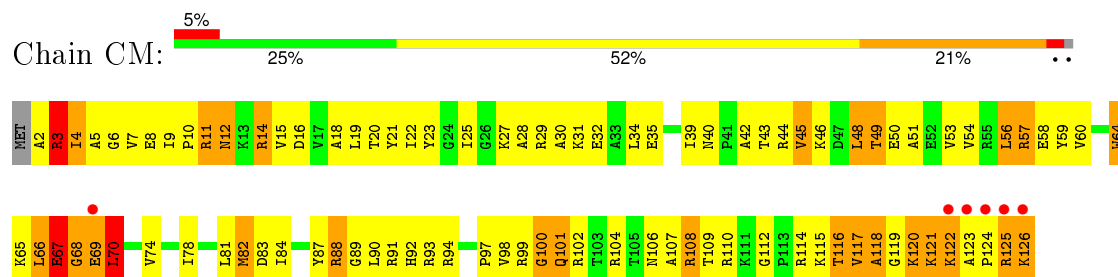
- Molecule 12: 30S ribosomal protein S12



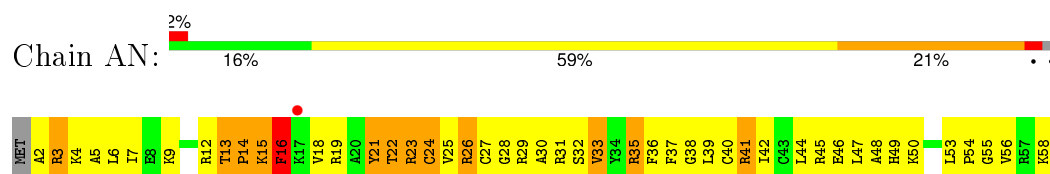
- Molecule 13: 30S ribosomal protein S13



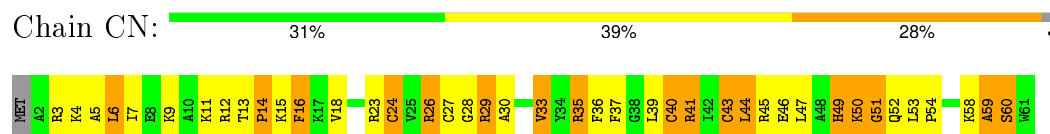
- Molecule 13: 30S ribosomal protein S13



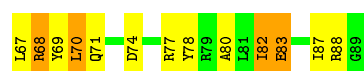
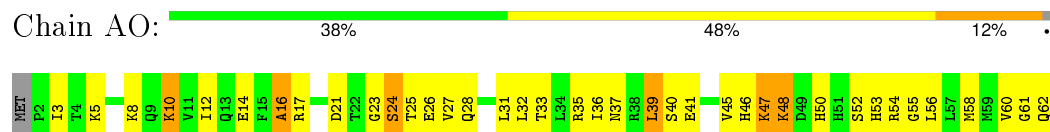
- Molecule 14: 30S ribosomal protein S14 type Z



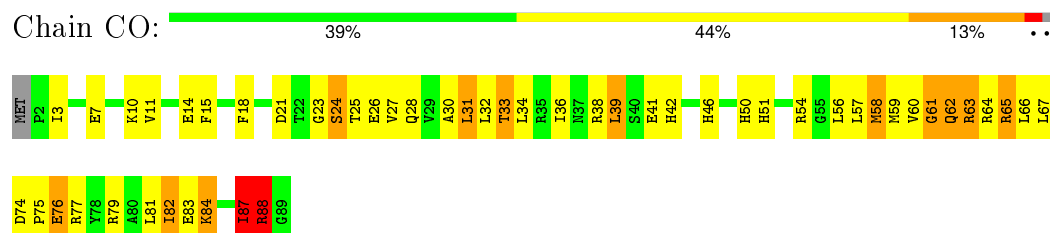
- Molecule 14: 30S ribosomal protein S14 type Z



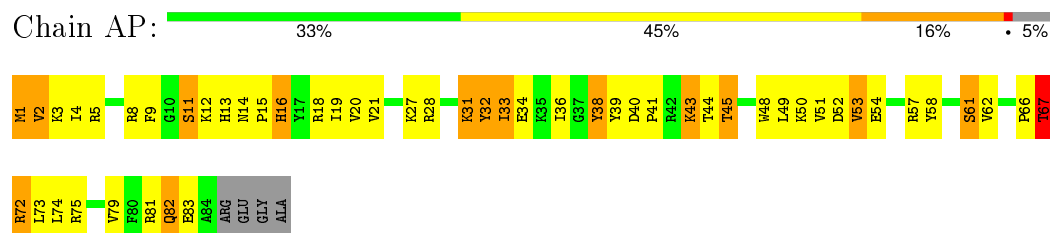
- Molecule 15: 30S ribosomal protein S15



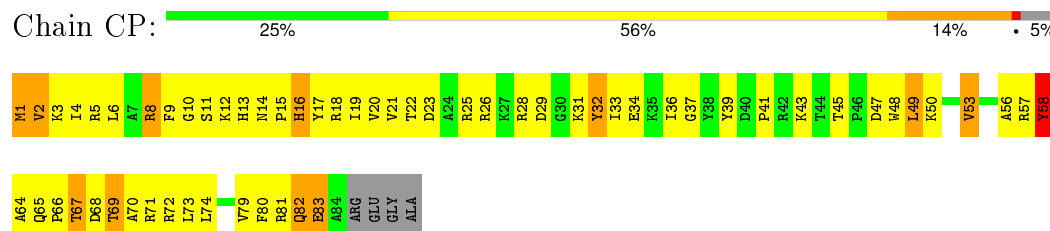
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

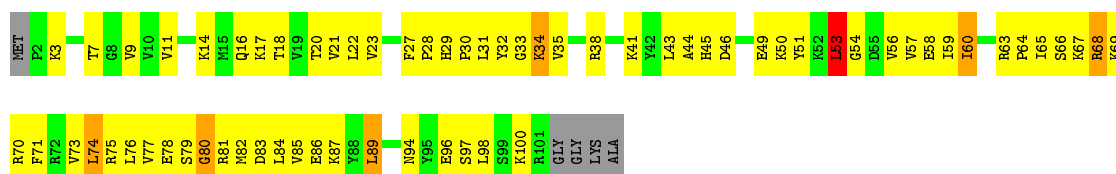


- Molecule 16: 30S ribosomal protein S16

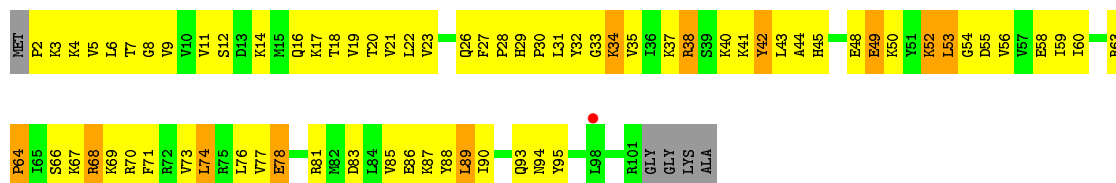


- Molecule 17: 30S ribosomal protein S17

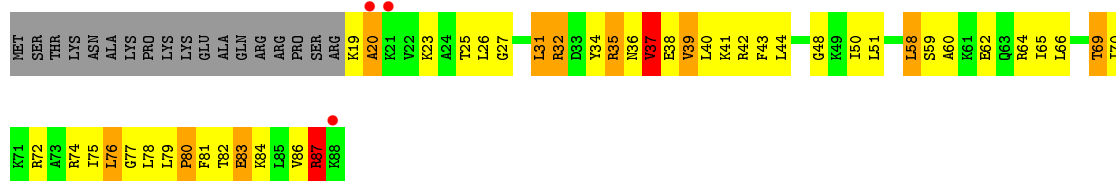




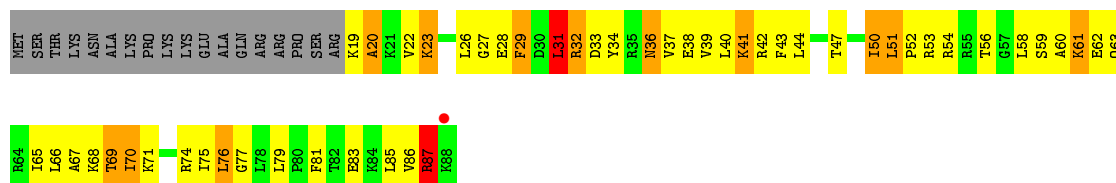
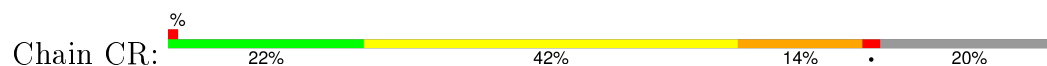
- Molecule 17: 30S ribosomal protein S17



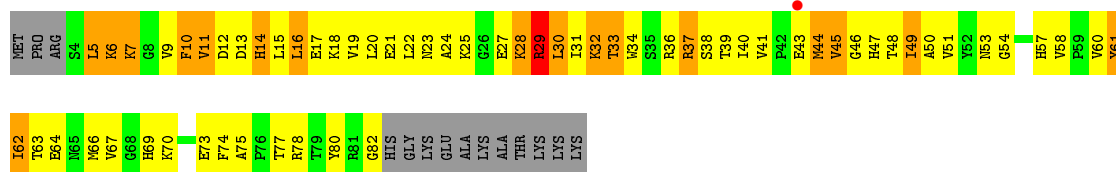
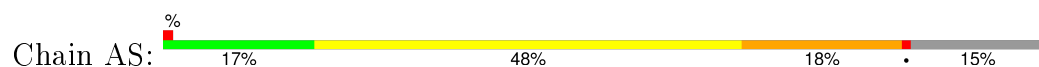
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

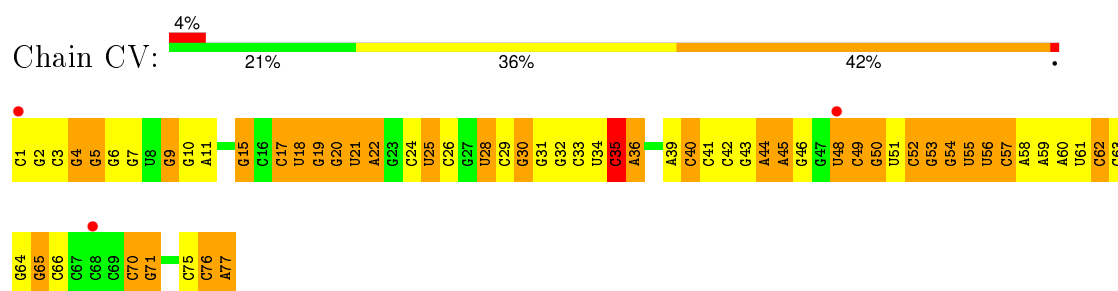


- Molecule 19: 30S ribosomal protein S19

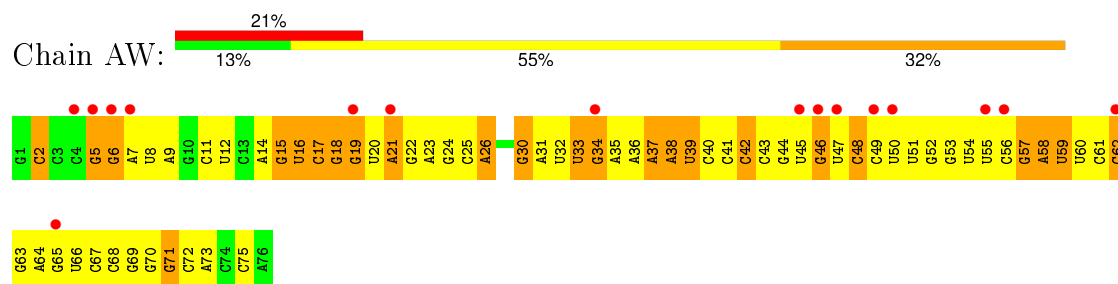


- Molecule 19: 30S ribosomal protein S19

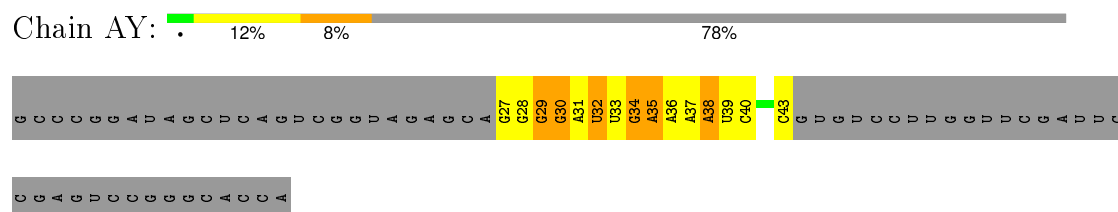




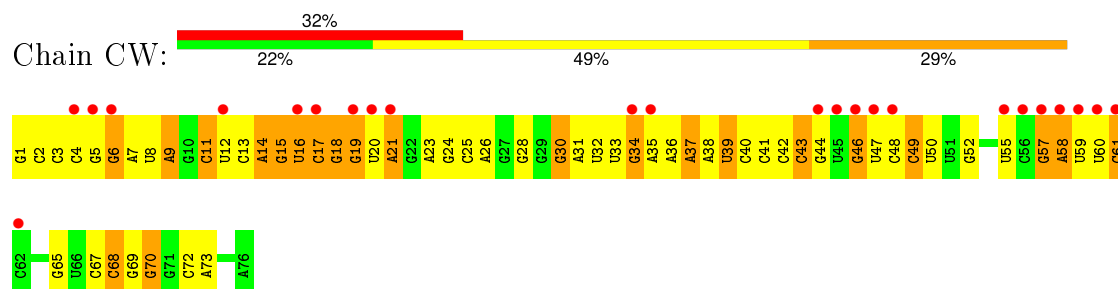
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe



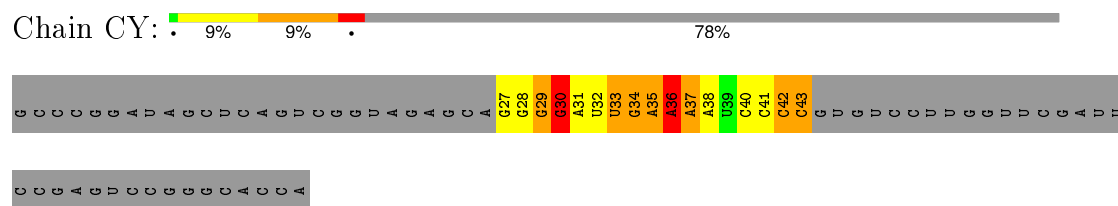
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe



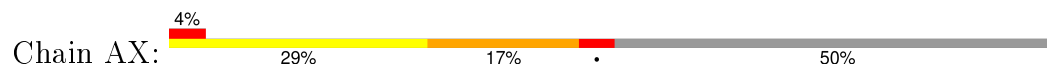
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

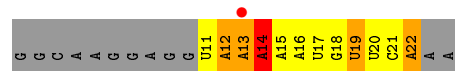


- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

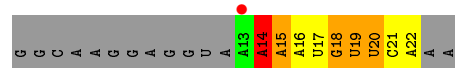


- Molecule 24: mRNA

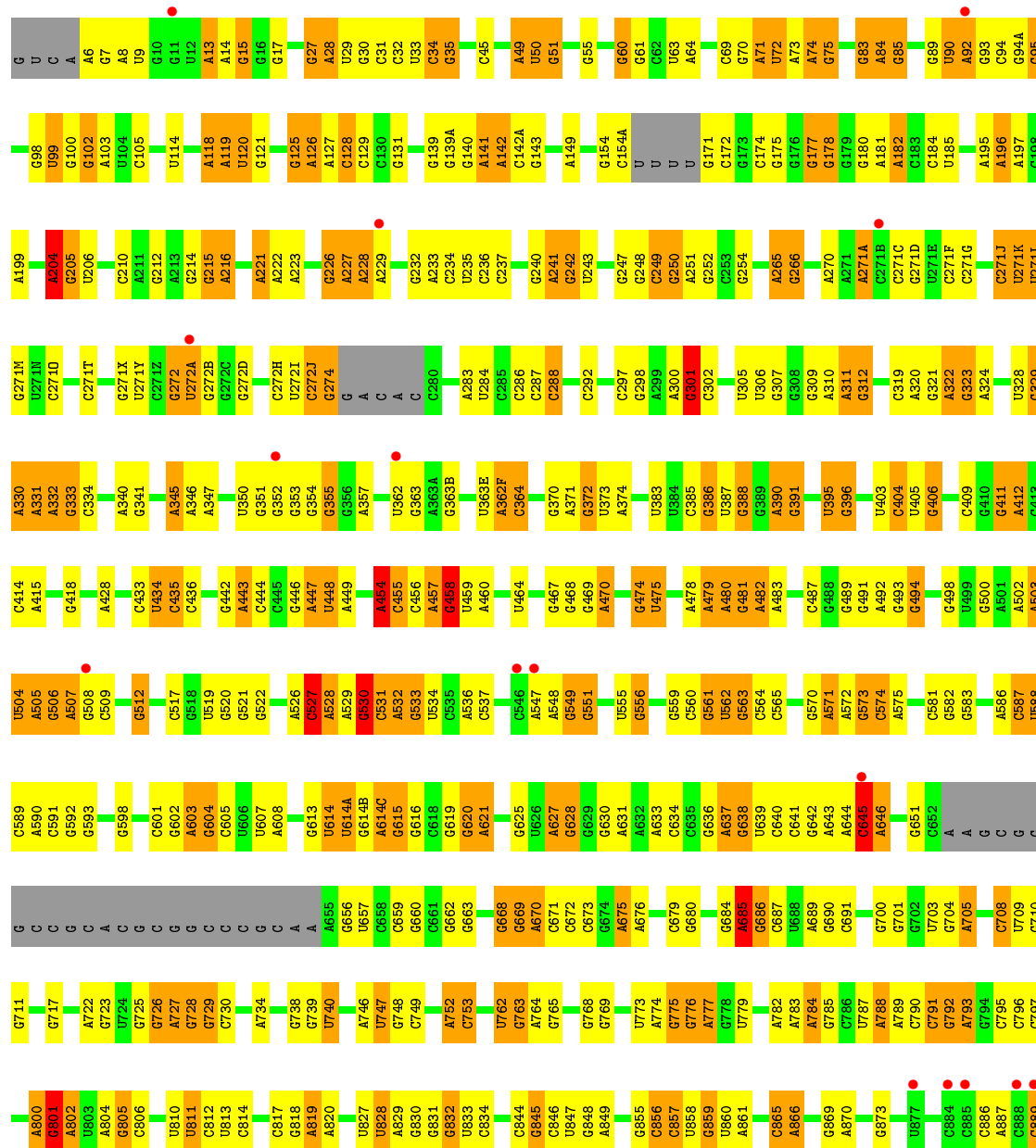




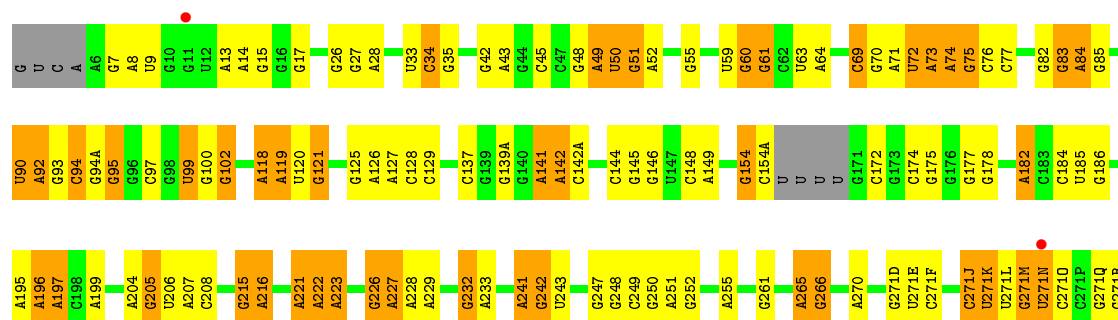
• Molecule 24: mRNA



• Molecule 25: 23S rRNA

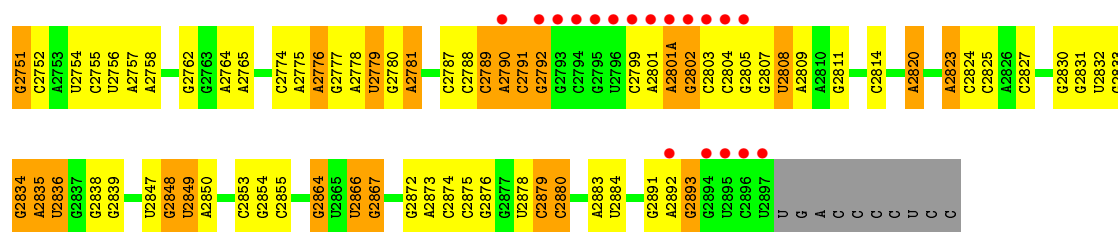


A2060	G1989	C1795	G1696	A1803	G1520	A1445	A1360	G1285	G1186	C1109	G975A	A890
G2061	G1990	U1796	G1697	C1607	G1523	C1445A	C1363	A1286	G1187	G1110	C976	G892
A2062	G1991	C1797	A1688	A1608	G1524	G1446	G1447	U1287	A1188	A1111	C976	C893
C2063	U1991	U1798	G1699	A1609	G1525	G1448	A1365	U1288	G1112	A980	A980	A896
C2065	U1992	C1799	A1700	A1610	G1526	A1449	A1365	C1289	G1195	U1113	A983	C897
C2066	U1993	G1801	U1706	C1611	G1527	A1450	G1368	C1290	G1114	A983	A983	A896
G2067	C1996	A1802	G1707	C1615	A1528	C1450A	G1450	C1291	G1115	A987	A987	A900
U2068	G1997	A1803	G1707	A1616	C1532	C1451	A1378	U1292	A1204	G987	G987	A901
G2069	G2000	A1809	G1718	C1617	U1533	A1452	G1379	C1297	U1205	A988	A988	C904
A2071	A2001	A1810	G1719	A1618	A1534	U1453	G1380	C1298	G1117	A990	A990	U907
G2072	G2002	A1812	U1720	A1619	C1543	A1455	A1384	U1299	G1122	C994	C994	U907
C2073	A1913	G1813	G1721	G1619	A1544	A1456	G1385	U1300	G1125	C995	C995	A910
U2074	C1914	A1814	A1722	G1620	C1547	A1457	G1386	A1301	A1126	C996	C996	A911
U2075	G2004	A1815	C1743	G1626	G1537	C1458	C1387	A1302	A1127	A996	A996	C912
G2076	U1917	G1816	G1740	C1626	G1541	A1460	G1387	G1303	A1128	G997	G997	U913
A2077	G1918	G1817	A1741	A1634	G1542	A1461	U1390	C1304	A1129	A1000	A1000	C914
C2078	A1919	U1818	G1742	G1635	C1543	U1391	U1391	C1305	U1130	A1005	A1005	A917
U2079	C1920	A1819	C1744	C1636	A1544	C1464	A1392	C1306	G1131	C1006	C1006	A918
G2080	A1821	U1820	G1747A	A1637	C1547	G1465	U1394	G1310	U1133	A918	A918	G919
U2086	G1929	C1836	G1747A	C1638	C1548	G1466	A1395	U1312	A1136	C1007	C1007	G920
G2087	G1930	U1837	A1748	U1639	C1549	C1467	U1396	U1313	G1136	C1008	C1008	G921
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U2089	A1936	G1645	G1750	C1645	C1550	G1470	U1397	C1314	A1241	A1010	A1010	C914
U2092	A1937	C1646	G1751	C1646	A1554	A1471	C1403	G1319	C1140	G1011	G1011	A926
G2093	C1938	G1647	C1754	G1647	G1555	A1472	U1406	C1320	U1141	C1012	C1012	A926
G2094	U1939	C1648	A1755	C1648	C1558	G1473	U1407	A1321	U1142	A1013	A1013	U930
G2095	U1940	G1651	G1756	C1651	A1558	G1478	A1322	A1322	U1142A	U1014	U1014	G931
U2096	C1941	A1652	U1757	G1652	G1559	G1478	C1408	U1323	A1143	G1015	G1015	G932
U2099	C1942	A1653	G1758	A1652	G1560	U1481	C1409	G1324	G1144	G1016	G1016	A933
U2103	U1943	C1654	G1759	C1654	C1566	G1482	C1410	U1325	G1149	C1017	C1017	A941
G2104	U1944	A1657	A1762	A1657	A1566	G1483	U1412	U1326	C1150	G1018	G1018	A942
C2107	G1945	C1658	G1763	C1658	A1567	G1484	G1413	G1327	A1020	A1021	A1021	U943
G2110	A1952	G1666	G1764	C1666	G1568	A1485	G1414	G1328	G1153	G1022	G1022	G944
C2111	A1953	G1667	G1765	G1667	A1569	A1486	U1415	U1329	A1155	U1023	U1023	A945
G2112	G1954	G1668	G1766	C1668	A1570	G1487	U1416	C1330	G1156	G1024	G1024	G946
U2113	U1955	A1669	G1767	A1669	A1571	U1488	G1417	G1332	G1157	U1025	U1025	G952
G2114	C1956	C1670	U1776	C1670	U1578	G1489	A1419	C1333	G1161	A1026	A1026	A953
A2115	U1957	U1673	U1777	U1673	A1580	G1490	U1420	C1336	G1162	A1027	A1027	G954
G2116	G1958	U1674	U1778	U1674	G1581	A1491	G1421	G1337	U1032	A1028	A1028	C955
A2117	U1959	G1675	U1779	G1675	C1584	A1495	G1422	G1338	U1033	A1032	A1032	G956
U2118	C1960	C1676	A1780	C1676	A1586	A1496	G1426	U1339	G1171	A1033	A1033	A957
A2119	C1961	A1677	C1782	A1677	A1587	U1497	A1427	U1340	G1173	A1034	A1034	U958
G2120	C1962	G1678	G1783	G1678	C1588	C1498	C1428	A1342	A1174	G1037	G1037	A959
U2121	G1963	U1679	A1784	U1679	C1589	C1502	G1429	G1343	U1175	C1038	C1038	A960
C2122	U1964	U1680	A1785	U1680	G1593	U1503	C1432	G1344	G1176	G1039	G1039	C961
G2123	A1965	G1681	A1786	G1681	C1594	U1498	U1433	A1275	A1177	C1040	C1040	G962
U2124	C1966	G1682	A1787	G1682	G1595	C1505	A1434	A1276	C1178	G1041	G1041	C965
G2125	C1967	C1679	G1788	C1679	C1598	C1509	C1437	G1345	C1179	C1042	C1042	C966
U2126	G1968	U1683	A1789	U1683	C1599	C1509	C1437	A1278	C1181	G1043	G1043	U969
G2127	A1969	A1689	C1790	A1689	G1599	A1509A	G1442	A1278	A1182	C1044	C1044	C973
C2128	G1970	C1694	G1792	C1694	C1600	U1512	G1442	U1352	G1183	A1045	A1045	A974
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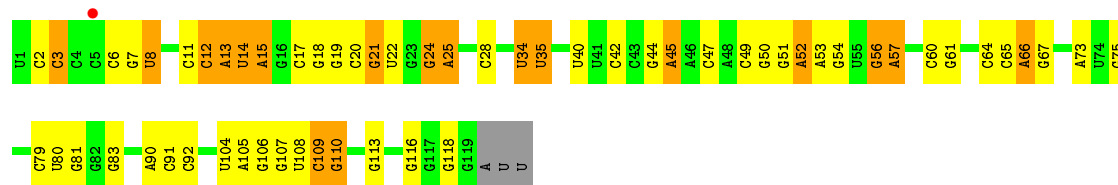


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U1405	A1321	G1225	G1136	A990	G991	G818	C749	C	U606	G518	C414		G9271
U1406	G1227	G1227	G1137	C992	C904	A819	A750	A	U607	U525	A428	U339	G9272
C1407	G1324	C1230	G1139	G993	A910	U827	A751	A655	A608	A526	U9274	A340	U9274
C1408	G1325	G1231	C1140	C994	A911	U828	A752	G656	G613	C527	C433	G341	C9275
C1409	G1232	G1232	U1141	C995	C912	A829	C753	U657	U614	A528	U433	G342	G272
A1412	U1329	G1236	U1142	A996	U913	G830	C754	C658	U614A	A529	C435	C343	U272A
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G1416	G1332	G1238	A1143	A1000	G915	C838	C756	C661	A614C	C531	A443	A345	G272C
G1417	C1333	G1239	A1144	A1001	G916	U839		G662	G615	A532	C444	A346	G272D
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A1419	G1339	U1240	C1150	C1005	G919	A841	A764	G	A621	U534	C446		C272H
G1421	U1340	A1241	G1151	U	U	G842	G765	G668	G625	C545	A447	G353	U272I
A1427	U1341	G1247	C1152	C1008	A926	G845	G766	G669	U626	A547	U448	U358	C272J
C1428	U1342	U1248	A1153	A1009	G927	C846	G767	A670	A627			A359	G274
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		A1253	G1162	U1014	G932	C850	A774	A675	A631	G556	A455	A	A
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C145A	A1354	G1264	G1171	C1018	U943	U858	G778	G686	C634	C560	U459	A362F	A284
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A1450	G1356	A1268	G1176	A1020	U946	U860	G780	U688	G636	U562	U464	C365	C285
G1451	U1357	U1269	U1177	A1021	G946	A861	A781	A689	A637	G563	U465	C366	C286
A1452	G1358	C1270	A1178	G1022	G946	G862	A782		G638	C564	A466	G370	C287
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G1454	U1360	U1272	G1180	G1024	G954	U864	A784	G704	C641	U568	A470	U373	A289
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A1457	U1371	G1281	G1195	A1046	U963	G869	A788	G707	C645	A572	G476	U383	A300
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G1465	U1374	U1288	U1198	C1049	G972	G882	G791	G710	G652	A575	A480	U387	G307
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C1467	U1379	U1297	U1205	A1050	A973	C884	G792	A716	G	C580	A482	C389	A311
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G1473	C1386	G1303	U1211	A105A	C976	C888	C806	A727	G	C584	A502	U395	C319
G1474	U1391	U1212	G1212	U105A	G978	C889	U807	G728	C	C585	A503	G396	A320
U1481	G1310	G1310	C1218	G	A	C890	U811	G729	A	A586	U504	G400	G321
G1482	U1311	U1311	A1127	U	U	C891	C812	C806	C	C587	G506	C403	A322
G1484	U1313	U1313	A1128	G	U	C892	U813	U907	C	U588	A507	U403	G323
			U1130	C	C	C893	U814	C730	C	C589	C509	U405	A324
						C894		C730	C	G593	G512	G406	U328
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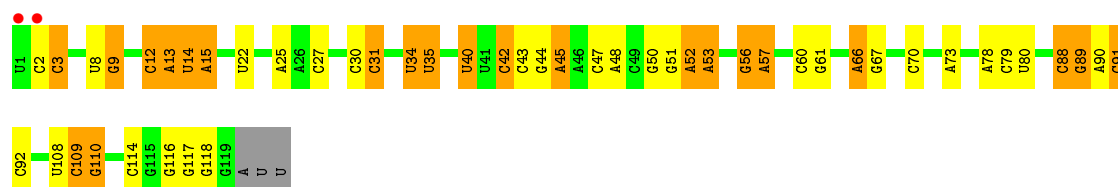
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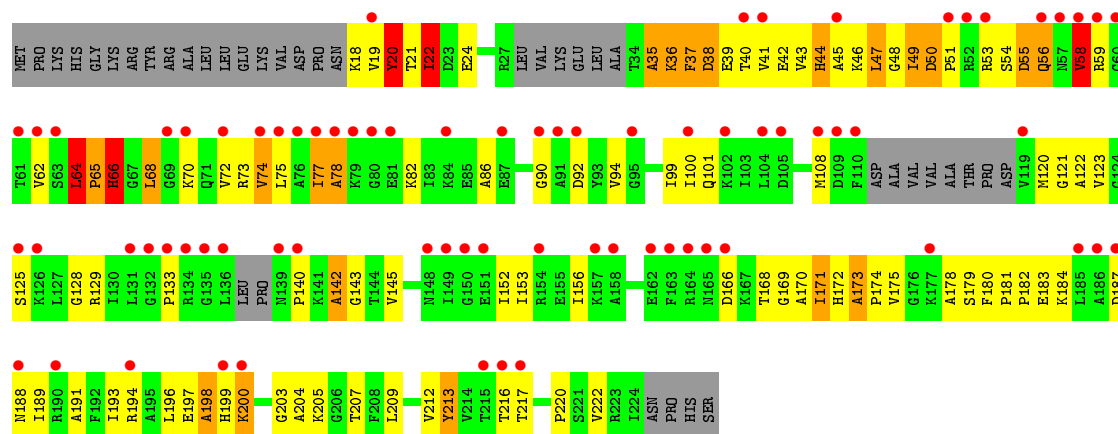
• Molecule 26: 5S rRNA



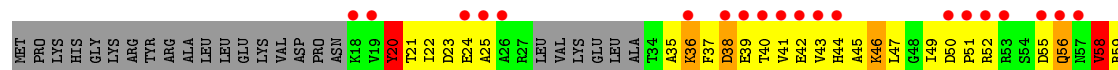
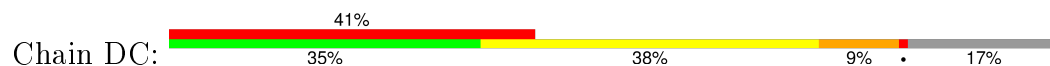
• Molecule 26: 5S rRNA

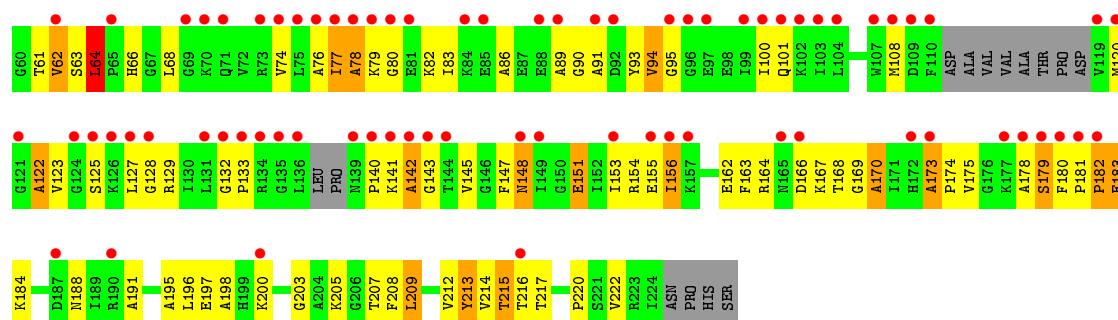


• Molecule 27: 50S RIBOSOMAL PROTEIN L1



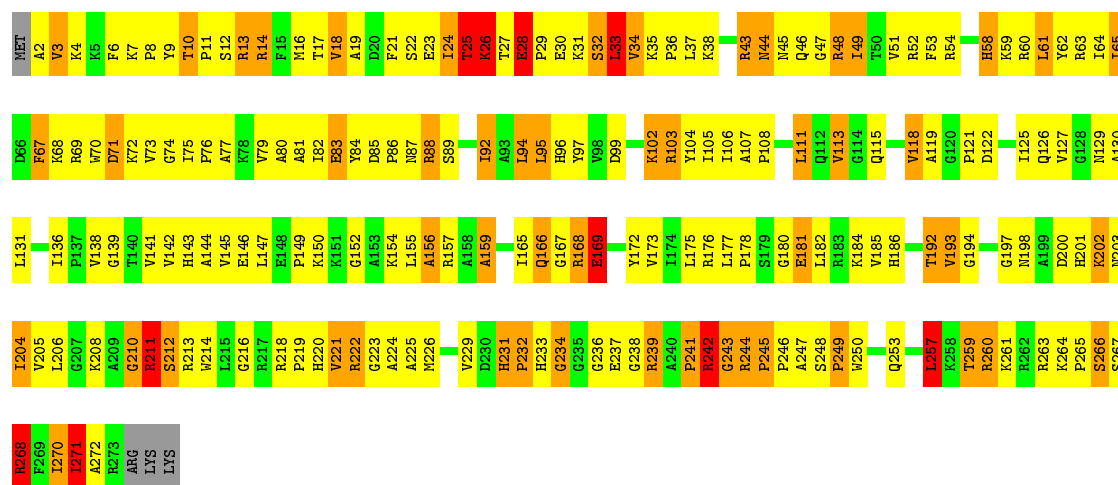
• Molecule 27: 50S RIBOSOMAL PROTEIN L1





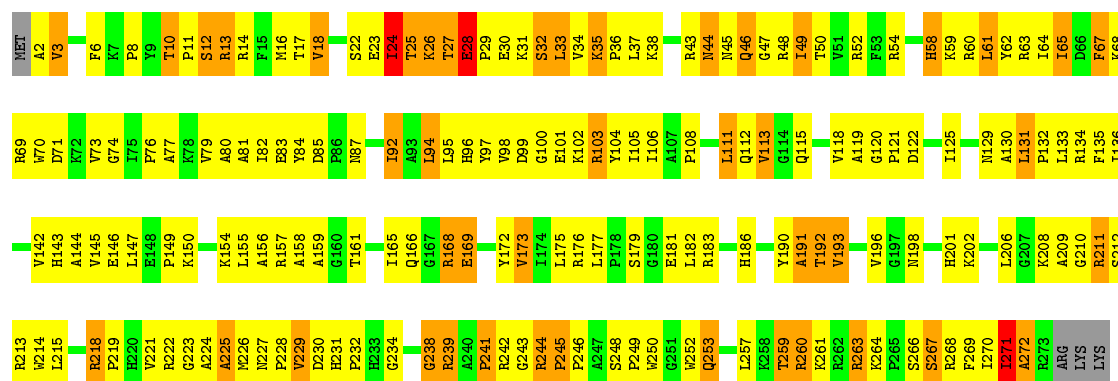
• Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain BD: 27% 49% 19% . .



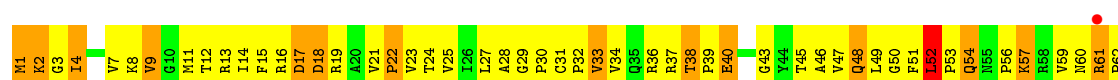
• Molecule 28: 50S RIBOSOMAL PROTEIN L2

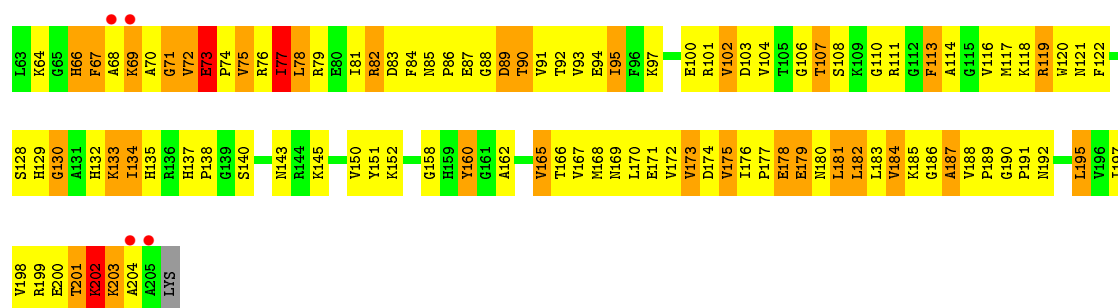
Chain DD: 32% 49% 16% . .



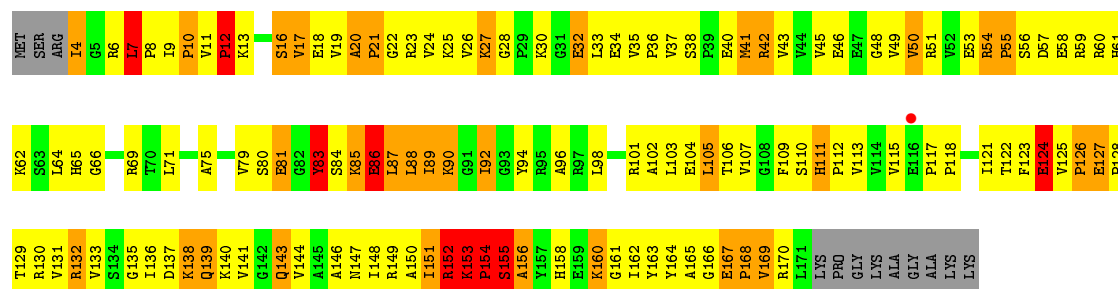
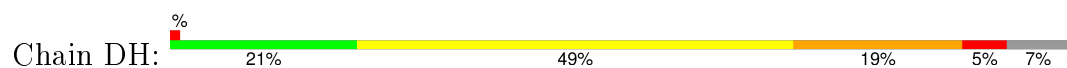
• Molecule 29: 50S RIBOSOMAL PROTEIN L3

Chain BE: 2% 24% 52% 22% .

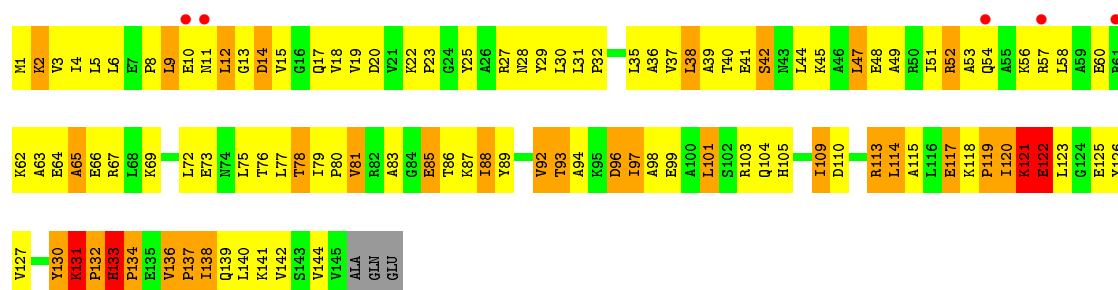




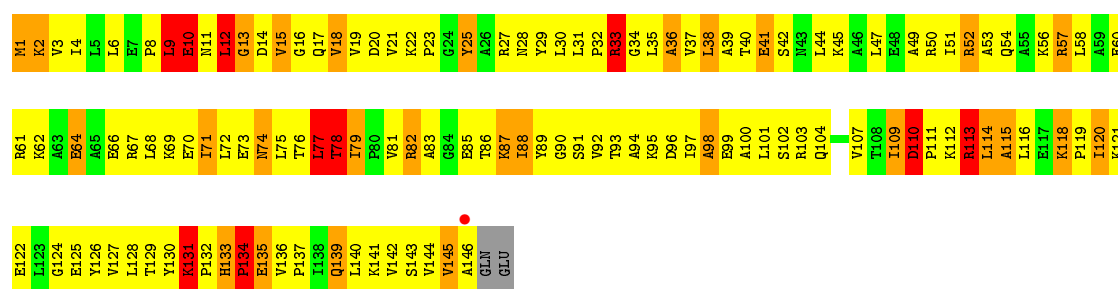
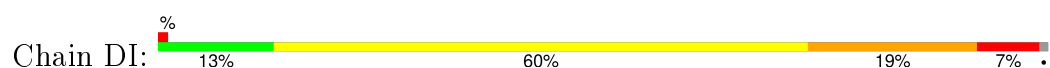
• Molecule 32: 50S RIBOSOMAL PROTEIN L6



• Molecule 33: 50S RIBOSOMAL PROTEIN L9

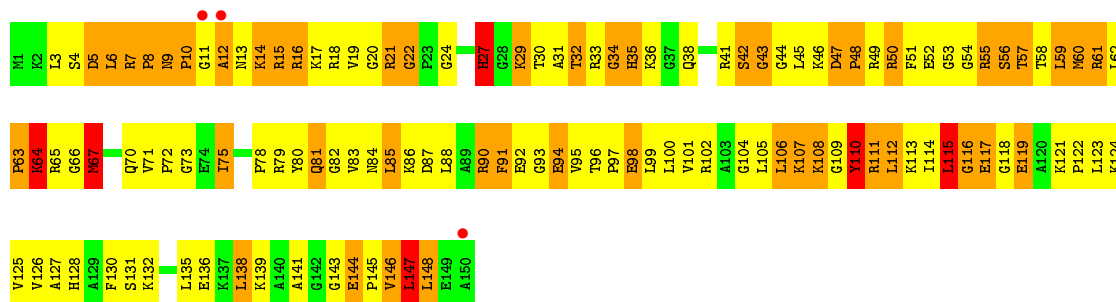


• Molecule 33: 50S RIBOSOMAL PROTEIN L9

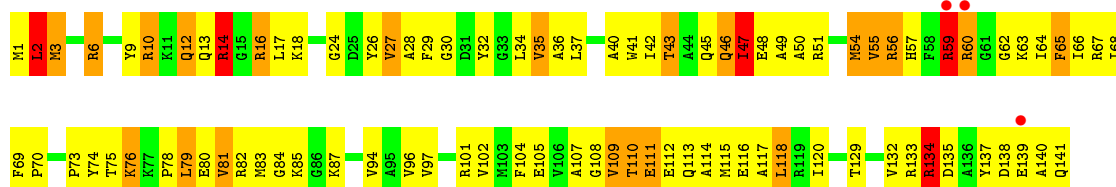


• Molecule 34: 50S RIBOSOMAL PROTEIN L13

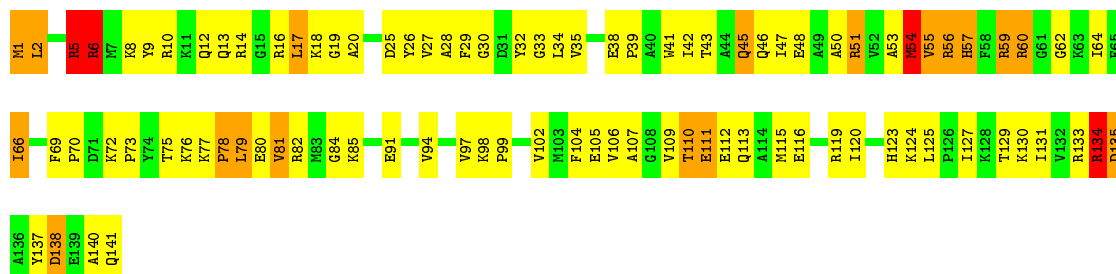




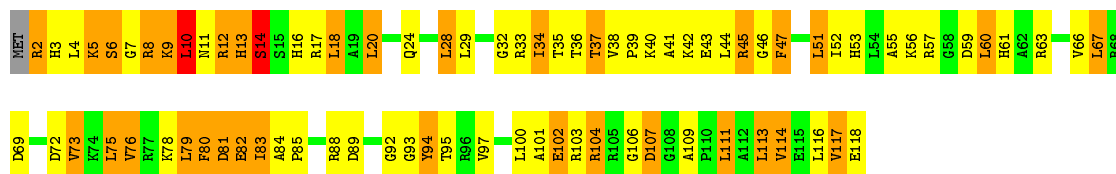
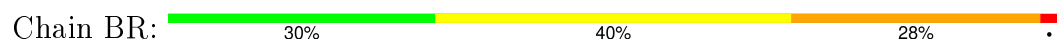
• Molecule 37: 50S RIBOSOMAL PROTEIN L16



• Molecule 37: 50S RIBOSOMAL PROTEIN L16



• Molecule 38: 50S RIBOSOMAL PROTEIN L17

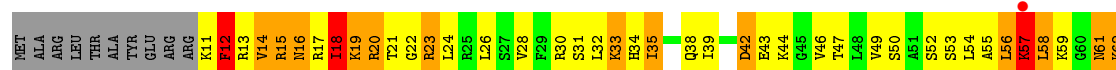
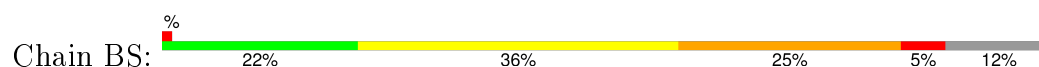


• Molecule 38: 50S RIBOSOMAL PROTEIN L17

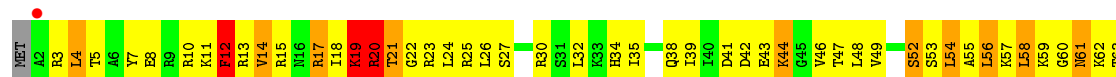




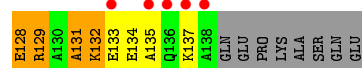
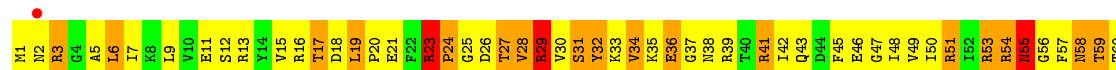
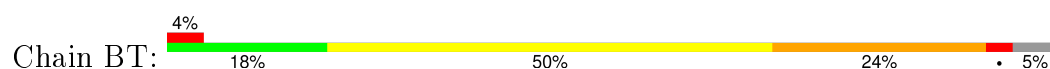
• Molecule 39: 50S RIBOSOMAL PROTEIN L18



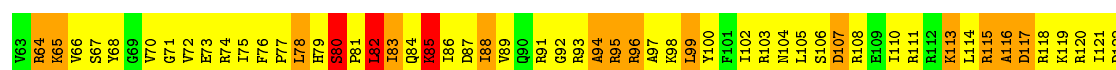
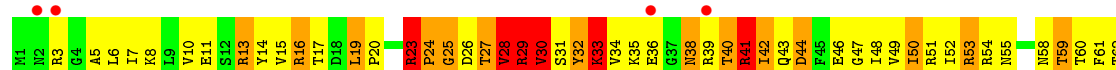
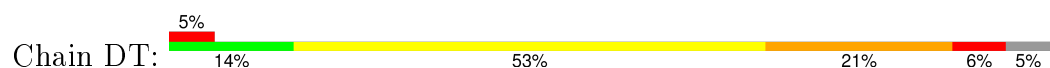
• Molecule 39: 50S RIBOSOMAL PROTEIN L18



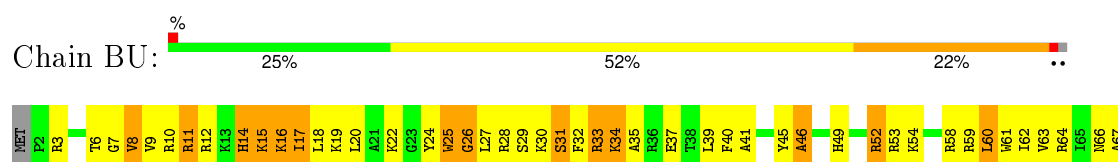
• Molecule 40: 50S RIBOSOMAL PROTEIN L19



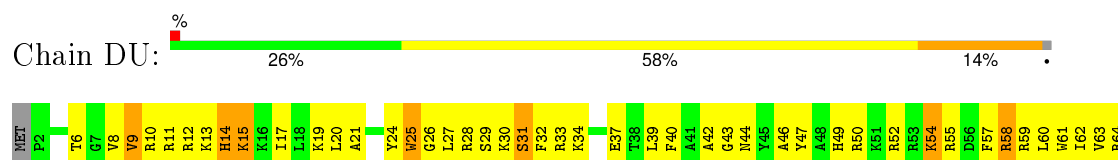
• Molecule 40: 50S RIBOSOMAL PROTEIN L19



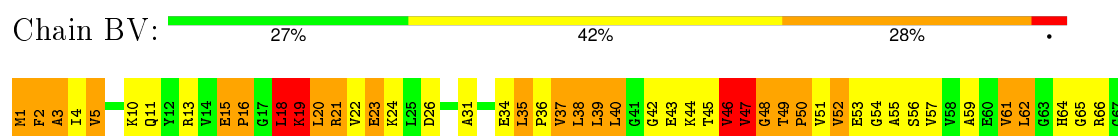
• Molecule 41: 50S RIBOSOMAL PROTEIN L20



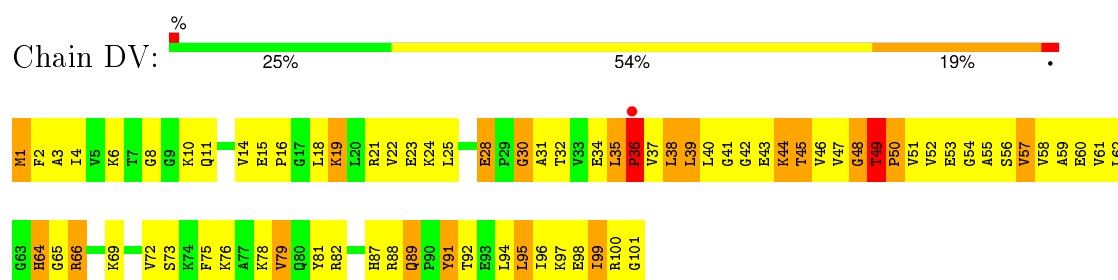
• Molecule 41: 50S RIBOSOMAL PROTEIN L20



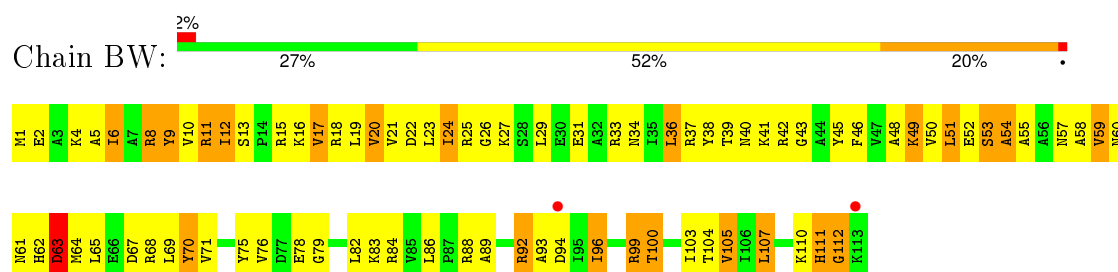
• Molecule 42: 50S RIBOSOMAL PROTEIN L21



• Molecule 42: 50S RIBOSOMAL PROTEIN L21

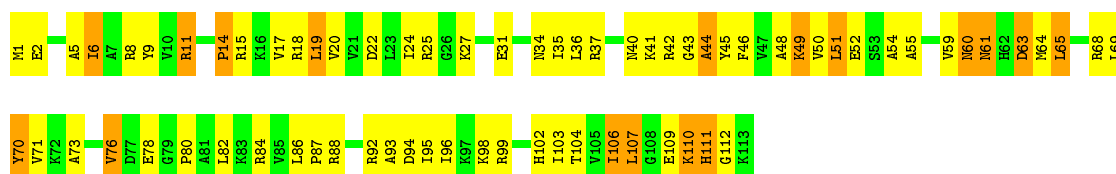


• Molecule 43: 50S RIBOSOMAL PROTEIN L22



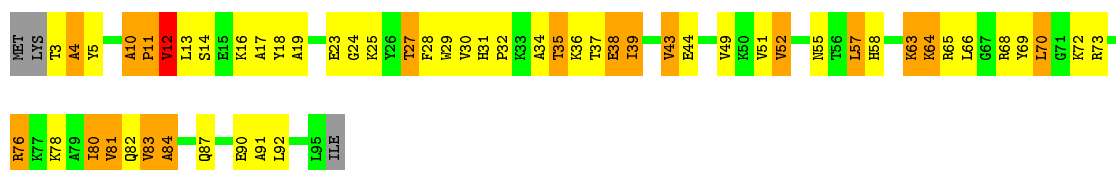
• Molecule 43: 50S RIBOSOMAL PROTEIN L22





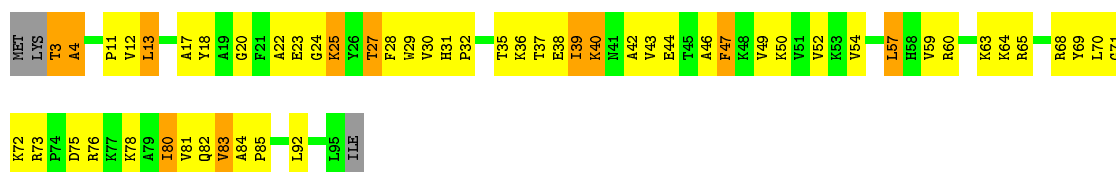
• Molecule 44: 50S RIBOSOMAL PROTEIN L23

Chain BX: 40% 38% 19% . .



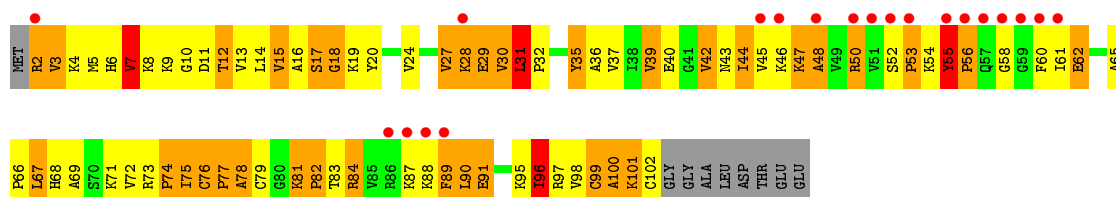
• Molecule 44: 50S RIBOSOMAL PROTEIN L23

Chain DX: 40% 46% 11% .



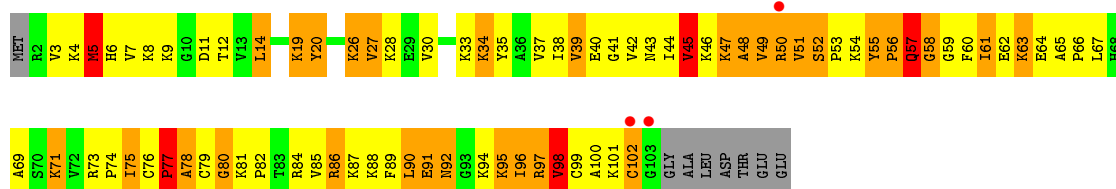
• Molecule 45: 50S RIBOSOMAL PROTEIN L24

Chain BY: 18% 20% 36% 32% . 8%



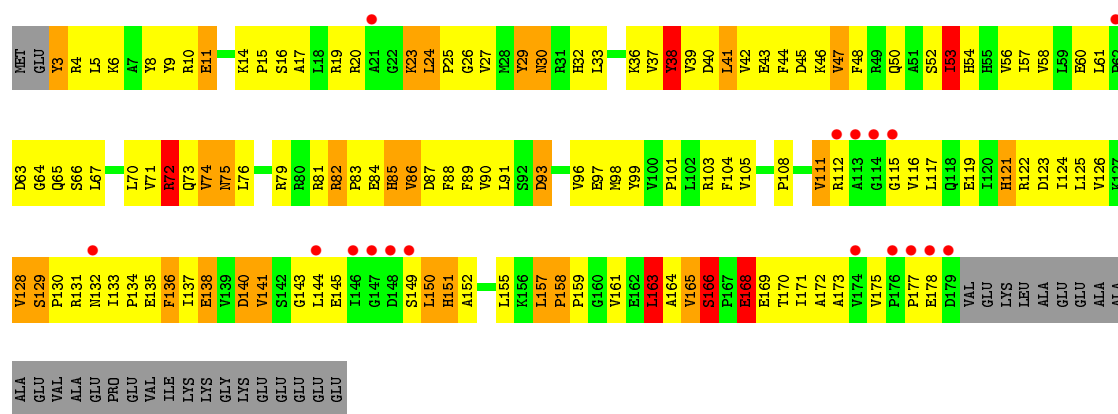
• Molecule 45: 50S RIBOSOMAL PROTEIN L24

Chain DY: 3% 20% 41% 27% 5% 7%

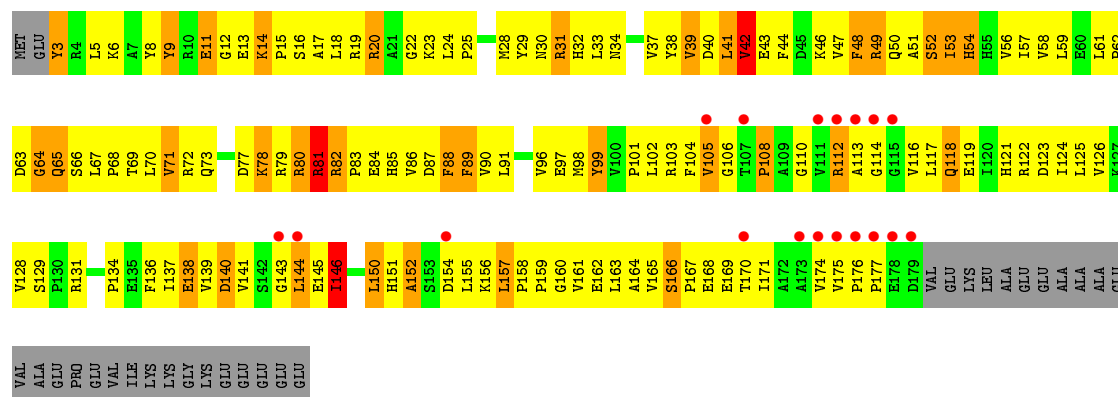
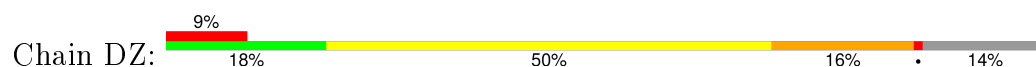


• Molecule 46: 50S RIBOSOMAL PROTEIN L25

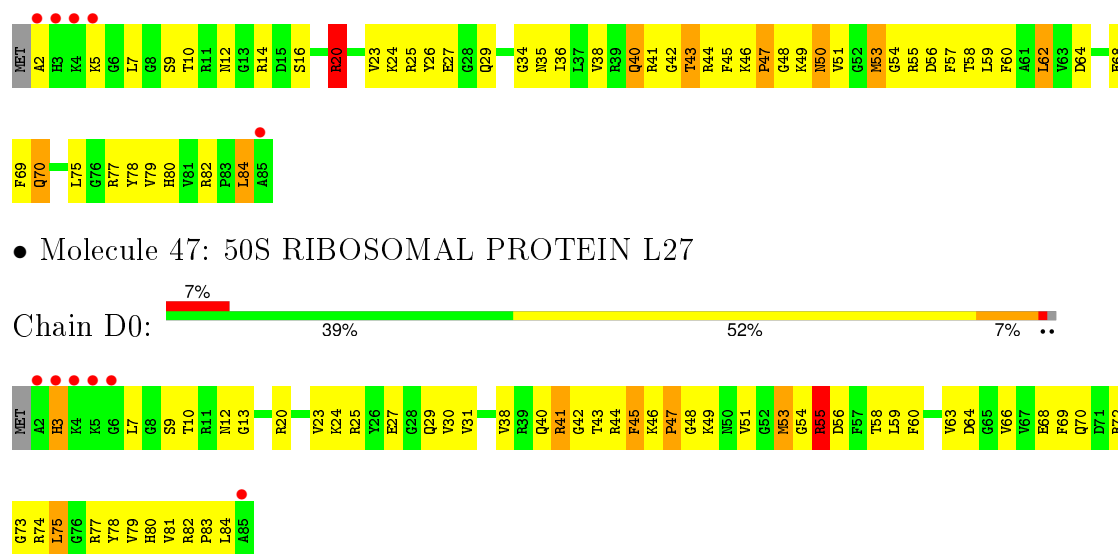
Chain BZ: 8% 23% 47% 13% . 14%



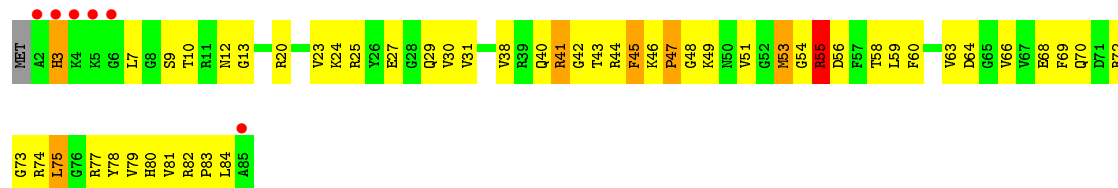
• Molecule 46: 50S RIBOSOMAL PROTEIN L25



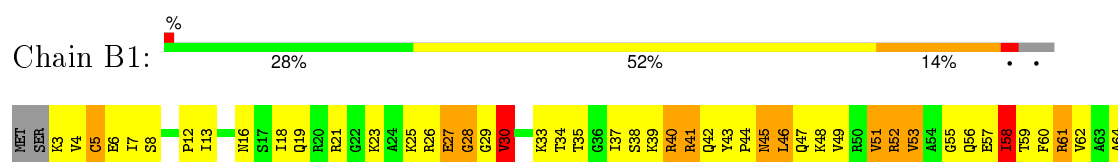
• Molecule 47: 50S RIBOSOMAL PROTEIN L27



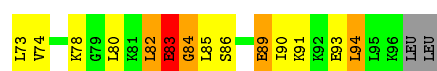
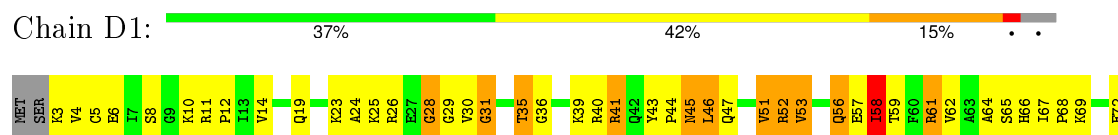
• Molecule 47: 50S RIBOSOMAL PROTEIN L27



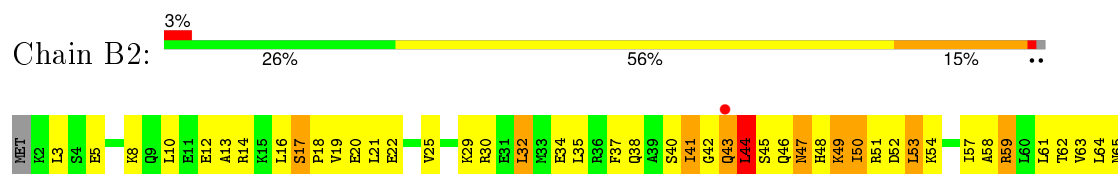
• Molecule 48: 50S RIBOSOMAL PROTEIN L28



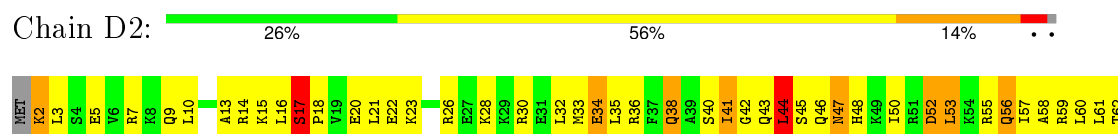
• Molecule 48: 50S RIBOSOMAL PROTEIN L28



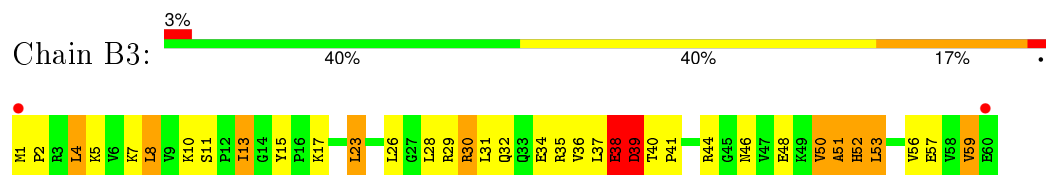
• Molecule 49: 50S RIBOSOMAL PROTEIN L29



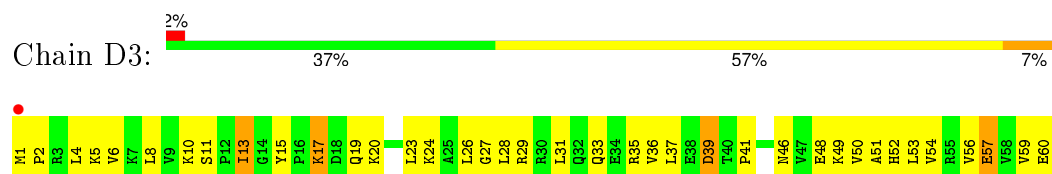
• Molecule 49: 50S RIBOSOMAL PROTEIN L29



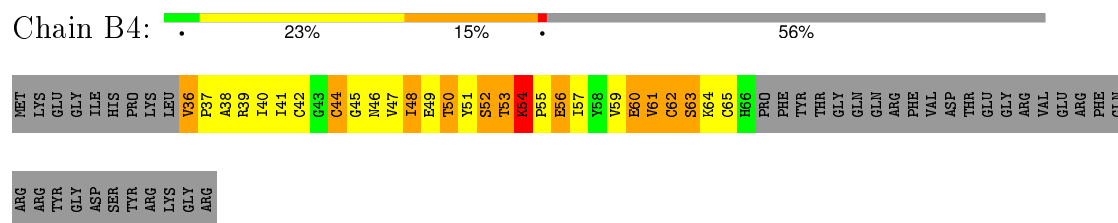
• Molecule 50: 50S RIBOSOMAL PROTEIN L30



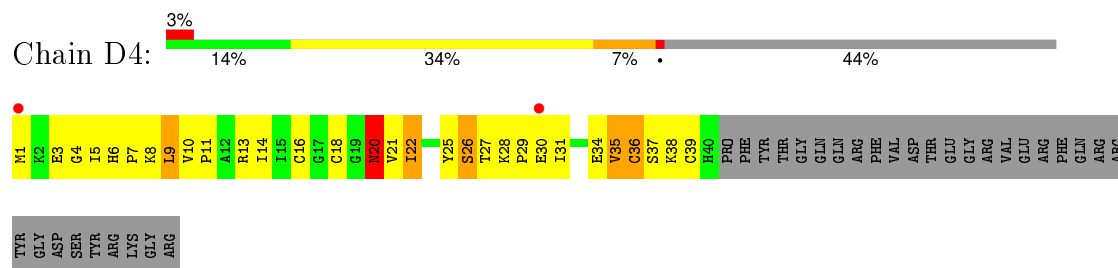
• Molecule 50: 50S RIBOSOMAL PROTEIN L30



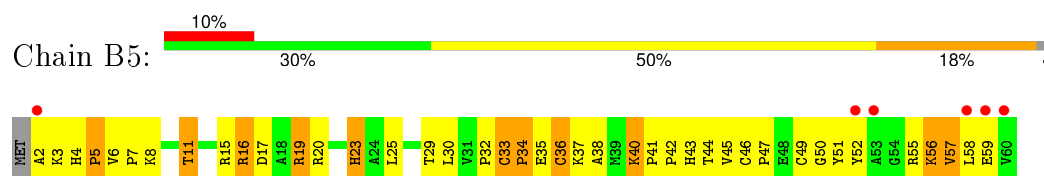
- Molecule 51: 50S RIBOSOMAL PROTEIN L31



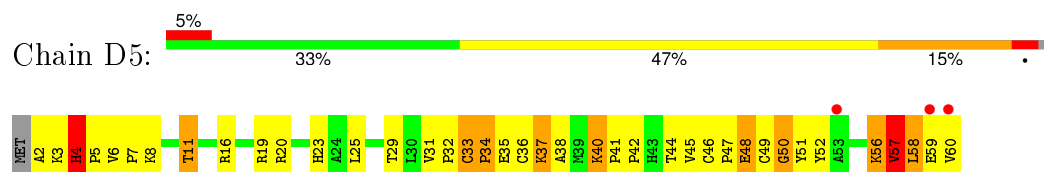
- Molecule 51: 50S RIBOSOMAL PROTEIN L31



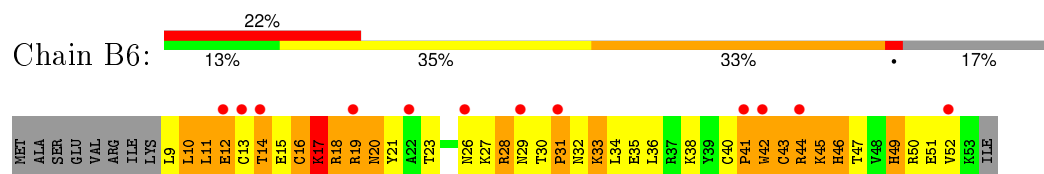
- Molecule 52: 50S RIBOSOMAL PROTEIN L32



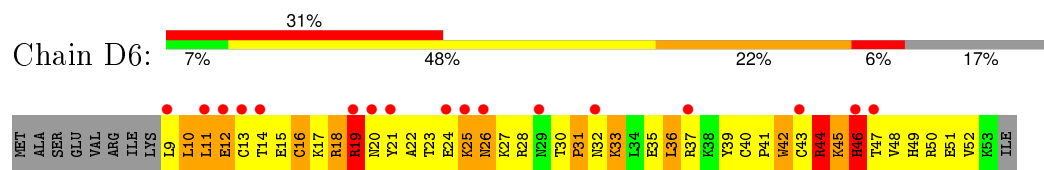
- Molecule 52: 50S RIBOSOMAL PROTEIN L32



- Molecule 53: 50S RIBOSOMAL PROTEIN L33



- Molecule 53: 50S RIBOSOMAL PROTEIN L33



- Molecule 54: 50S RIBOSOMAL PROTEIN L34

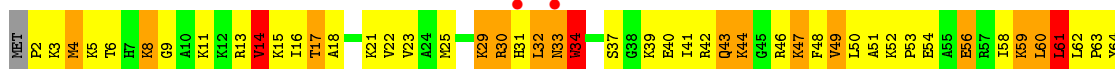




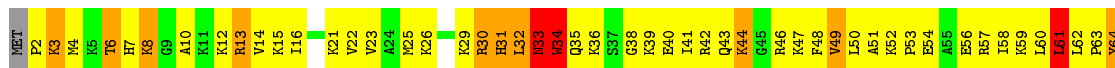
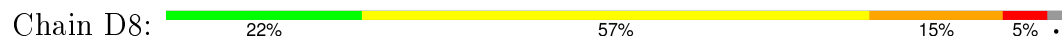
• Molecule 54: 50S RIBOSOMAL PROTEIN L34



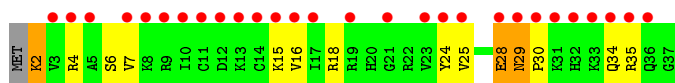
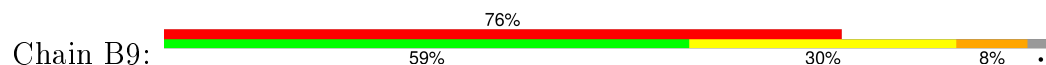
• Molecule 55: 50S RIBOSOMAL PROTEIN L35



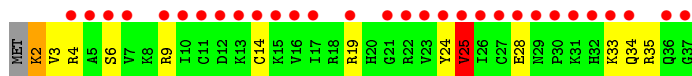
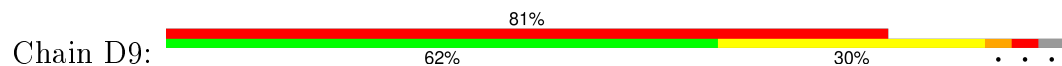
• Molecule 55: 50S RIBOSOMAL PROTEIN L35



• Molecule 56: 50S RIBOSOMAL PROTEIN L36



• Molecule 56: 50S RIBOSOMAL PROTEIN L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.46Å 447.34Å 622.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.07 – 3.52 35.07 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.07-3.52) 99.9 (35.07-3.52)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	0.46	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.47Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.210 , 0.249 0.216 , 0.255	Depositor DCC
R_{free} test set	32826 reflections (4.78%)	DCC
Wilson B-factor (Å ²)	91.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 80.9	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 720017 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	293977	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: ZN, MG, PAR

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	0.28	0/36189	0.82	11/56484 (0.0%)
1	CA	0.29	0/36189	0.82	14/56484 (0.0%)
2	AB	0.59	0/1936	0.68	0/2611
2	CB	0.67	0/1936	0.77	0/2611
3	AC	0.70	0/1637	0.76	0/2207
3	CC	0.73	0/1637	0.82	0/2207
4	AD	0.69	0/1733	0.80	0/2318
4	CD	0.77	1/1733 (0.1%)	0.85	0/2318
5	AE	0.71	0/1163	0.88	0/1566
5	CE	0.74	0/1163	0.84	0/1566
6	AF	0.73	0/856	0.89	0/1154
6	CF	0.79	0/856	0.82	0/1154
7	AG	0.72	0/1276	0.79	0/1709
7	CG	0.71	0/1276	0.77	0/1709
8	AH	0.69	1/1136 (0.1%)	0.78	0/1527
8	CH	0.73	0/1136	0.80	1/1527 (0.1%)
9	AI	0.71	0/1029	0.80	0/1379
9	CI	0.70	0/1029	0.81	1/1379 (0.1%)
10	AJ	0.70	0/808	0.79	0/1087
10	CJ	0.65	0/808	0.77	0/1087
11	AK	0.67	0/900	0.81	0/1213
11	CK	0.70	0/900	0.82	0/1213
12	AL	0.86	0/987	0.95	0/1322
12	CL	0.92	1/987 (0.1%)	1.01	0/1322
13	AM	0.67	0/999	0.82	0/1338
13	CM	0.48	1/1008 (0.1%)	0.75	1/1347 (0.1%)
14	AN	0.73	0/501	0.83	1/664 (0.2%)
14	CN	0.77	0/501	0.95	0/664
15	AO	0.72	0/745	0.79	0/992
15	CO	0.71	0/745	0.81	0/992
16	AP	0.72	0/717	0.86	0/965
16	CP	0.79	0/717	0.84	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.69	0/837	0.79	0/1119
17	CQ	0.73	0/837	0.81	0/1119
18	AR	0.69	0/579	0.83	0/768
18	CR	0.76	0/579	0.98	0/768
19	AS	0.66	0/643	0.76	0/867
19	CS	0.80	1/643 (0.2%)	0.86	0/867
20	AT	0.73	0/765	0.77	0/1007
20	CT	0.61	0/765	0.63	0/1007
21	AU	0.73	0/213	0.83	0/279
21	CU	0.75	0/213	0.78	0/279
22	AV	1.13	5/1836 (0.3%)	1.33	13/2859 (0.5%)
22	CV	1.02	0/1835	1.20	13/2859 (0.5%)
23	AW	0.93	3/1809 (0.2%)	1.07	4/2819 (0.1%)
23	AY	1.07	1/408 (0.2%)	1.39	4/634 (0.6%)
23	CW	0.90	0/1809	1.01	0/2819
23	CY	1.15	0/408	1.42	4/634 (0.6%)
24	AX	1.10	1/285 (0.4%)	0.91	2/441 (0.5%)
24	CX	0.96	0/235	1.27	3/364 (0.8%)
25	BA	0.34	1/67788 (0.0%)	0.87	42/105819 (0.0%)
25	DA	0.35	0/68124	0.88	36/106343 (0.0%)
26	BB	0.26	0/2853	0.78	0/4451
26	DB	0.28	0/2853	0.80	0/4451
27	BC	0.65	1/1145 (0.1%)	0.67	0/1556
27	DC	0.24	0/1145	0.46	0/1556
28	BD	0.85	0/2155	0.95	1/2907 (0.0%)
28	DD	0.54	0/2155	0.74	0/2907
29	BE	0.75	0/1597	0.89	0/2155
29	DE	0.49	1/1597 (0.1%)	0.72	0/2155
30	BF	0.80	0/1659	0.87	1/2246 (0.0%)
30	DF	0.49	0/1620	0.76	1/2194 (0.0%)
31	BG	0.70	0/1499	0.78	1/2016 (0.0%)
31	DG	0.42	1/1499 (0.1%)	0.68	1/2016 (0.0%)
32	BH	0.63	0/1246	0.69	0/1684
32	DH	0.40	0/1315	0.79	1/1780 (0.1%)
33	BI	0.67	0/1146	0.81	0/1551
33	DI	0.36	0/1151	0.74	1/1558 (0.1%)
34	BN	0.76	0/1132	0.83	0/1527
34	DN	0.43	0/1132	0.69	0/1527
35	BO	0.76	0/943	0.87	0/1269
35	DO	0.46	0/943	0.68	0/1269
36	BP	0.40	1/1162 (0.1%)	0.78	2/1544 (0.1%)
36	DP	0.39	0/1162	0.76	1/1544 (0.1%)
37	BQ	0.75	0/1143	0.87	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DQ	0.48	0/1143	0.65	0/1527
38	BR	0.80	0/974	0.90	1/1302 (0.1%)
38	DR	0.57	1/982 (0.1%)	0.79	2/1312 (0.2%)
39	BS	0.77	0/779	0.90	0/1038
39	DS	0.40	0/892	0.81	1/1187 (0.1%)
40	BT	0.71	0/1156	0.90	1/1544 (0.1%)
40	DT	0.56	1/1156 (0.1%)	0.84	6/1544 (0.4%)
41	BU	0.81	0/982	0.91	1/1306 (0.1%)
41	DU	0.51	0/975	0.75	0/1297
42	BV	0.72	0/790	0.90	1/1057 (0.1%)
42	DV	0.53	1/790 (0.1%)	0.82	0/1057
43	BW	0.81	0/907	0.89	1/1216 (0.1%)
43	DW	0.48	0/907	0.69	1/1216 (0.1%)
44	BX	0.75	0/740	0.89	1/995 (0.1%)
44	DX	0.52	0/740	0.68	0/995
45	BY	0.74	0/789	0.95	2/1053 (0.2%)
45	DY	0.55	2/798 (0.3%)	0.78	0/1064
46	BZ	0.72	0/1436	0.74	1/1951 (0.1%)
46	DZ	0.35	0/1436	0.57	0/1951
47	B0	0.79	1/671 (0.1%)	0.84	0/892
47	D0	0.44	0/671	0.64	0/892
48	B1	0.87	0/739	0.94	0/983
48	D1	0.48	0/739	0.73	0/983
49	B2	0.72	0/600	0.83	0/793
49	D2	0.54	0/600	0.71	0/793
50	B3	0.73	0/473	0.83	0/636
50	D3	0.43	0/473	0.71	0/636
51	B4	0.72	0/229	0.76	0/311
51	D4	0.40	0/303	0.70	0/409
52	B5	0.82	1/473 (0.2%)	0.83	0/639
52	D5	0.44	0/473	0.65	0/639
53	B6	0.67	0/388	0.92	0/520
53	D6	0.30	0/388	0.58	0/520
54	B7	0.88	0/427	0.99	0/563
54	D7	0.54	0/427	0.75	1/563 (0.2%)
55	B8	0.76	0/516	0.91	0/681
55	D8	0.51	0/516	0.82	0/681
56	B9	0.64	0/302	0.59	0/397
56	D9	0.26	0/302	0.46	0/397
All	All	0.48	27/318178 (0.0%)	0.85	180/475682 (0.0%)

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
28	BD	0	1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1453	U	O3'-P	29.98	1.97	1.61
24	AX	14	A	O3'-P	-13.06	1.45	1.61
38	DR	12	ARG	C-N	11.33	1.60	1.34
40	DT	28	VAL	C-N	10.90	1.59	1.34
22	AV	1	C	OP3-P	-9.31	1.50	1.61

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1453	U	P-O3'-C3'	-10.66	106.91	119.70
38	DR	12	ARG	O-C-N	9.52	137.93	122.70
36	BP	1	MET	CG-SD-CE	9.44	115.30	100.20
40	DT	28	VAL	O-C-N	8.73	136.67	122.70
40	DT	28	VAL	CA-C-N	-7.49	100.72	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	BD	222	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	32328	0	16317	795	0
1	CA	32328	0	16317	871	1
2	AB	1901	0	1951	245	0
2	CB	1901	0	1951	232	0
3	AC	1613	0	1677	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CC	1613	0	1677	148	0
4	AD	1703	0	1765	191	0
4	CD	1703	0	1764	174	0
5	AE	1147	0	1207	148	0
5	CE	1147	0	1207	159	0
6	AF	843	0	857	87	0
6	CF	843	0	857	63	0
7	AG	1257	0	1296	123	0
7	CG	1257	0	1296	102	0
8	AH	1116	0	1177	111	0
8	CH	1116	0	1177	111	0
9	AI	1010	0	1037	133	0
9	CI	1010	0	1037	144	0
10	AJ	795	0	840	127	0
10	CJ	795	0	840	135	0
11	AK	885	0	904	97	0
11	CK	885	0	904	109	0
12	AL	971	0	1057	126	0
12	CL	971	0	1057	123	0
13	AM	988	0	1059	151	0
13	CM	997	0	1072	164	0
14	AN	492	0	529	87	0
14	CN	492	0	531	69	0
15	AO	734	0	771	61	0
15	CO	734	0	771	51	0
16	AP	701	0	720	62	0
16	CP	701	0	720	101	0
17	AQ	824	0	891	68	0
17	CQ	824	0	891	85	0
18	AR	574	0	644	62	0
18	CR	574	0	644	68	0
19	AS	630	0	652	117	0
19	CS	630	0	652	106	0
20	AT	763	0	861	132	0
20	CT	763	0	861	166	0
21	AU	209	0	221	12	0
21	CU	209	0	221	22	0
22	AV	1644	0	836	110	0
22	CV	1643	0	836	143	0
23	AW	1619	0	822	122	0
23	AY	365	0	185	29	0
23	CW	1619	0	822	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	CY	365	0	185	37	0
24	AX	255	0	129	49	0
24	CX	210	0	109	23	0
25	BA	60527	0	30515	1623	1
25	DA	60827	0	30663	1373	0
26	BB	2551	0	1295	57	1
26	DB	2551	0	1295	55	0
27	BC	1142	0	865	78	0
27	DC	1142	0	865	70	0
28	BD	2105	0	2182	310	0
28	DD	2105	0	2182	277	0
29	BE	1564	0	1629	216	0
29	DE	1564	0	1629	206	0
30	BF	1624	0	1677	246	0
30	DF	1585	0	1632	188	0
31	BG	1474	0	1535	264	0
31	DG	1474	0	1535	209	0
32	BH	1223	0	1282	136	1
32	DH	1290	0	1364	238	0
33	BI	1131	0	1218	152	0
33	DI	1136	0	1223	229	0
34	BN	1105	0	1180	188	0
34	DN	1105	0	1180	140	0
35	BO	933	0	996	117	0
35	DO	933	0	996	90	0
36	BP	1145	0	1228	279	0
36	DP	1145	0	1228	283	3
37	BQ	1122	0	1179	129	0
37	DQ	1122	0	1179	123	0
38	BR	960	0	1021	146	0
38	DR	968	0	1033	109	0
39	BS	771	0	832	127	0
39	DS	882	0	943	149	0
40	BT	1142	0	1202	240	0
40	DT	1142	0	1202	269	0
41	BU	964	0	1022	160	0
41	DU	958	0	1014	198	0
42	BV	779	0	852	135	0
42	DV	779	0	852	150	3
43	BW	896	0	953	104	0
43	DW	896	0	953	89	0
44	BX	726	0	778	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DX	726	0	778	67	0
45	BY	776	0	870	172	0
45	DY	785	0	878	176	0
46	BZ	1404	0	1432	148	0
46	DZ	1404	0	1432	214	0
47	B0	662	0	688	60	0
47	D0	662	0	688	60	0
48	B1	732	0	808	78	0
48	D1	732	0	808	66	0
49	B2	598	0	653	64	0
49	D2	598	0	653	53	0
50	B3	468	0	523	40	3
50	D3	468	0	523	50	0
51	B4	226	0	229	39	0
51	D4	298	0	312	43	0
52	B5	459	0	480	50	0
52	D5	459	0	480	53	3
53	B6	381	0	391	51	0
53	D6	381	0	391	99	0
54	B7	419	0	467	35	0
54	D7	419	0	467	33	0
55	B8	508	0	576	115	0
55	D8	508	0	576	85	0
56	B9	299	0	326	13	0
56	D9	299	0	326	14	0
57	AA	110	0	0	0	0
57	AE	1	0	0	0	0
57	AV	5	0	0	0	0
57	AX	1	0	0	0	0
57	B5	1	0	0	0	0
57	B7	1	0	0	0	0
57	BA	323	0	0	0	0
57	BB	5	0	0	0	0
57	BD	2	0	0	0	0
57	BE	3	0	0	0	0
57	BF	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BP	1	0	0	0	0
57	BU	1	0	0	0	0
57	CA	141	0	0	0	0
57	CE	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CV	5	0	0	0	0
57	CW	1	0	0	0	0
57	CX	1	0	0	0	0
57	CY	1	0	0	0	0
57	D0	2	0	0	0	0
57	D1	2	0	0	0	0
57	D2	1	0	0	0	0
57	D5	2	0	0	0	0
57	D8	1	0	0	0	0
57	DA	397	0	0	0	0
57	DB	5	0	0	0	0
57	DD	3	0	0	0	0
57	DE	2	0	0	0	0
57	DF	1	0	0	0	0
57	DP	3	0	0	0	0
57	DQ	1	0	0	0	0
57	DU	3	0	0	0	0
57	DW	1	0	0	0	0
57	DX	1	0	0	0	0
58	AA	42	0	45	3	0
58	CA	42	0	45	2	0
59	AD	1	0	0	0	0
59	AN	1	0	0	1	0
59	CD	1	0	0	0	0
59	CN	1	0	0	3	0
All	All	293977	0	199058	16442	8

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 34.

The worst 5 of 16442 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)
39:BS:34:HIS:CE1	39:BS:54:LEU:HB2	1.32	1.58
42:DV:1:MET:SD	42:DV:1:MET:CG	2.01	1.47
40:BT:28:VAL:CG1	40:BT:46:GLU:HA	1.42	1.44
1:CA:748:C:H1'	1:CA:749:C:C5	1.53	1.44
34:BN:62:VAL:HG22	34:BN:66:LYS:CD	1.49	1.42

The worst 5 of 8 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)
50:B3:1:MET:N	36:DP:122:PRO:CG[3_455]	1.46	0.74
50:B3:1:MET:N	36:DP:122:PRO:CD[3_455]	1.64	0.56
42:DV:50:PRO:CG	52:D5:58:LEU:O[4_445]	1.80	0.40
42:DV:48:GLY:O	52:D5:58:LEU:CD1[4_445]	1.84	0.36
25:BA:1593:G:O2'	26:BB:54:G:OP1[1_655]	2.09	0.11

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%)	159 (68%)	53 (23%)	21 (9%)	1	11
2	CB	233/256 (91%)	158 (68%)	45 (19%)	30 (13%)	0	6
3	AC	205/239 (86%)	129 (63%)	54 (26%)	22 (11%)	0	8
3	CC	205/239 (86%)	135 (66%)	52 (25%)	18 (9%)	1	11
4	AD	206/209 (99%)	142 (69%)	43 (21%)	21 (10%)	1	9
4	CD	206/209 (99%)	141 (68%)	47 (23%)	18 (9%)	1	12
5	AE	149/162 (92%)	117 (78%)	20 (13%)	12 (8%)	1	13
5	CE	149/162 (92%)	113 (76%)	22 (15%)	14 (9%)	1	10
6	AF	99/101 (98%)	63 (64%)	29 (29%)	7 (7%)	1	17
6	CF	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	2	26
7	AG	153/156 (98%)	116 (76%)	26 (17%)	11 (7%)	1	16
7	CG	153/156 (98%)	117 (76%)	29 (19%)	7 (5%)	3	29
8	AH	136/138 (99%)	96 (71%)	35 (26%)	5 (4%)	4	36
8	CH	136/138 (99%)	102 (75%)	28 (21%)	6 (4%)	3	30
9	AI	125/128 (98%)	84 (67%)	32 (26%)	9 (7%)	1	16
9	CI	125/128 (98%)	87 (70%)	23 (18%)	15 (12%)	0	6
10	AJ	97/105 (92%)	59 (61%)	31 (32%)	7 (7%)	1	16
10	CJ	97/105 (92%)	60 (62%)	25 (26%)	12 (12%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	117/129 (91%)	92 (79%)	19 (16%)	6 (5%)	2	26
11	CK	117/129 (91%)	92 (79%)	23 (20%)	2 (2%)	11	53
12	AL	123/132 (93%)	78 (63%)	25 (20%)	20 (16%)	0	3
12	CL	123/132 (93%)	91 (74%)	20 (16%)	12 (10%)	1	10
13	AM	123/126 (98%)	82 (67%)	23 (19%)	18 (15%)	0	4
13	CM	123/126 (98%)	78 (63%)	22 (18%)	23 (19%)	0	2
14	AN	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	0	6
14	CN	58/61 (95%)	37 (64%)	14 (24%)	7 (12%)	0	6
15	AO	86/89 (97%)	65 (76%)	20 (23%)	1 (1%)	16	61
15	CO	86/89 (97%)	55 (64%)	25 (29%)	6 (7%)	1	17
16	AP	82/88 (93%)	53 (65%)	25 (30%)	4 (5%)	3	27
16	CP	82/88 (93%)	66 (80%)	13 (16%)	3 (4%)	4	36
17	AQ	98/105 (93%)	79 (81%)	13 (13%)	6 (6%)	2	21
17	CQ	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	2	21
18	AR	68/88 (77%)	49 (72%)	12 (18%)	7 (10%)	1	9
18	CR	68/88 (77%)	49 (72%)	11 (16%)	8 (12%)	0	7
19	AS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1	14
19	CS	77/93 (83%)	47 (61%)	17 (22%)	13 (17%)	0	3
20	AT	97/106 (92%)	68 (70%)	22 (23%)	7 (7%)	1	16
20	CT	97/106 (92%)	67 (69%)	18 (19%)	12 (12%)	0	6
21	AU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	12
27	BC	183/229 (80%)	85 (46%)	52 (28%)	46 (25%)	0	1
27	DC	183/229 (80%)	87 (48%)	45 (25%)	51 (28%)	0	0
28	BD	270/276 (98%)	200 (74%)	38 (14%)	32 (12%)	0	7
28	DD	270/276 (98%)	202 (75%)	44 (16%)	24 (9%)	1	11
29	BE	203/206 (98%)	145 (71%)	36 (18%)	22 (11%)	0	8
29	DE	203/206 (98%)	134 (66%)	36 (18%)	33 (16%)	0	3
30	BF	206/210 (98%)	142 (69%)	44 (21%)	20 (10%)	1	10
30	DF	200/210 (95%)	160 (80%)	29 (14%)	11 (6%)	2	24
31	BG	179/182 (98%)	121 (68%)	36 (20%)	22 (12%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DG	179/182 (98%)	124 (69%)	30 (17%)	25 (14%)	0	4
32	BH	158/180 (88%)	96 (61%)	37 (23%)	25 (16%)	0	3
32	DH	166/180 (92%)	96 (58%)	42 (25%)	28 (17%)	0	3
33	BI	143/148 (97%)	101 (71%)	26 (18%)	16 (11%)	0	7
33	DI	144/148 (97%)	78 (54%)	39 (27%)	27 (19%)	0	2
34	BN	137/140 (98%)	91 (66%)	24 (18%)	22 (16%)	0	3
34	DN	137/140 (98%)	86 (63%)	39 (28%)	12 (9%)	1	11
35	BO	120/122 (98%)	95 (79%)	17 (14%)	8 (7%)	1	19
35	DO	120/122 (98%)	97 (81%)	18 (15%)	5 (4%)	3	31
36	BP	148/150 (99%)	86 (58%)	26 (18%)	36 (24%)	0	1
36	DP	148/150 (99%)	86 (58%)	23 (16%)	39 (26%)	0	0
37	BQ	139/141 (99%)	104 (75%)	24 (17%)	11 (8%)	1	14
37	DQ	139/141 (99%)	109 (78%)	18 (13%)	12 (9%)	1	12
38	BR	115/118 (98%)	78 (68%)	25 (22%)	12 (10%)	1	9
38	DR	116/118 (98%)	86 (74%)	20 (17%)	10 (9%)	1	12
39	BS	97/112 (87%)	53 (55%)	16 (16%)	28 (29%)	0	0
39	DS	109/112 (97%)	71 (65%)	21 (19%)	17 (16%)	0	3
40	BT	136/146 (93%)	90 (66%)	28 (21%)	18 (13%)	0	5
40	DT	136/146 (93%)	95 (70%)	19 (14%)	22 (16%)	0	3
41	BU	115/118 (98%)	73 (64%)	30 (26%)	12 (10%)	1	9
41	DU	115/118 (98%)	75 (65%)	30 (26%)	10 (9%)	1	12
42	BV	99/101 (98%)	75 (76%)	9 (9%)	15 (15%)	0	3
42	DV	99/101 (98%)	80 (81%)	9 (9%)	10 (10%)	1	9
43	BW	111/113 (98%)	81 (73%)	22 (20%)	8 (7%)	1	16
43	DW	111/113 (98%)	82 (74%)	19 (17%)	10 (9%)	1	11
44	BX	91/96 (95%)	69 (76%)	16 (18%)	6 (7%)	1	19
44	DX	91/96 (95%)	76 (84%)	11 (12%)	4 (4%)	3	30
45	BY	99/110 (90%)	50 (50%)	22 (22%)	27 (27%)	0	0
45	DY	100/110 (91%)	64 (64%)	11 (11%)	25 (25%)	0	1
46	BZ	175/206 (85%)	114 (65%)	40 (23%)	21 (12%)	0	6
46	DZ	175/206 (85%)	101 (58%)	46 (26%)	28 (16%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	B0	82/85 (96%)	64 (78%)	13 (16%)	5 (6%)	2	21
47	D0	82/85 (96%)	67 (82%)	8 (10%)	7 (8%)	1	13
48	B1	92/98 (94%)	68 (74%)	13 (14%)	11 (12%)	0	6
48	D1	92/98 (94%)	69 (75%)	12 (13%)	11 (12%)	0	6
49	B2	69/72 (96%)	49 (71%)	15 (22%)	5 (7%)	1	16
49	D2	69/72 (96%)	57 (83%)	5 (7%)	7 (10%)	1	9
50	B3	58/60 (97%)	48 (83%)	3 (5%)	7 (12%)	0	6
50	D3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	12
51	B4	29/71 (41%)	17 (59%)	8 (28%)	4 (14%)	0	4
51	D4	38/71 (54%)	21 (55%)	12 (32%)	5 (13%)	0	5
52	B5	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	11
52	D5	57/60 (95%)	46 (81%)	5 (9%)	6 (10%)	1	8
53	B6	43/54 (80%)	17 (40%)	14 (33%)	12 (28%)	0	0
53	D6	43/54 (80%)	18 (42%)	15 (35%)	10 (23%)	0	1
54	B7	47/49 (96%)	38 (81%)	5 (11%)	4 (8%)	1	13
54	D7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	9	49
55	B8	62/65 (95%)	42 (68%)	14 (23%)	6 (10%)	1	10
55	D8	62/65 (95%)	41 (66%)	14 (23%)	7 (11%)	0	7
56	B9	34/37 (92%)	23 (68%)	10 (29%)	1 (3%)	6	42
56	D9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	6	42
All	All	11730/12586 (93%)	8097 (69%)	2283 (20%)	1350 (12%)	0	7

5 of 1350 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	195	ASP
2	AB	238	LEU
3	AC	18	TRP
3	AC	20	SER

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%)	161 (80%)	41 (20%)	1	9
2	CB	202/220 (92%)	155 (77%)	47 (23%)	1	5
3	AC	160/188 (85%)	127 (79%)	33 (21%)	1	9
3	CC	160/188 (85%)	130 (81%)	30 (19%)	2	11
4	AD	180/181 (99%)	149 (83%)	31 (17%)	2	15
4	CD	180/181 (99%)	151 (84%)	29 (16%)	3	18
5	AE	115/123 (94%)	97 (84%)	18 (16%)	3	20
5	CE	115/123 (94%)	87 (76%)	28 (24%)	1	5
6	AF	90/90 (100%)	76 (84%)	14 (16%)	3	20
6	CF	90/90 (100%)	79 (88%)	11 (12%)	6	30
7	AG	126/127 (99%)	103 (82%)	23 (18%)	2	12
7	CG	126/127 (99%)	106 (84%)	20 (16%)	3	19
8	AH	119/119 (100%)	101 (85%)	18 (15%)	3	21
8	CH	119/119 (100%)	87 (73%)	32 (27%)	0	4
9	AI	98/99 (99%)	77 (79%)	21 (21%)	1	8
9	CI	98/99 (99%)	72 (74%)	26 (26%)	0	4
10	AJ	88/92 (96%)	66 (75%)	22 (25%)	1	4
10	CJ	88/92 (96%)	66 (75%)	22 (25%)	1	4
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	13
11	CK	90/99 (91%)	72 (80%)	18 (20%)	1	9
12	AL	104/109 (95%)	85 (82%)	19 (18%)	2	12
12	CL	104/109 (95%)	84 (81%)	20 (19%)	2	10
13	AM	99/101 (98%)	82 (83%)	17 (17%)	2	15
13	CM	100/101 (99%)	83 (83%)	17 (17%)	2	15
14	AN	49/50 (98%)	37 (76%)	12 (24%)	1	5
14	CN	49/50 (98%)	38 (78%)	11 (22%)	1	6
15	AO	79/80 (99%)	64 (81%)	15 (19%)	2	11
15	CO	79/80 (99%)	66 (84%)	13 (16%)	3	17
16	AP	72/74 (97%)	58 (81%)	14 (19%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CP	72/74 (97%)	58 (81%)	14 (19%)	2	10
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	13	49
17	CQ	94/97 (97%)	82 (87%)	12 (13%)	5	28
18	AR	61/77 (79%)	51 (84%)	10 (16%)	3	17
18	CR	61/77 (79%)	50 (82%)	11 (18%)	2	13
19	AS	69/80 (86%)	51 (74%)	18 (26%)	0	4
19	CS	69/80 (86%)	49 (71%)	20 (29%)	0	3
20	AT	76/82 (93%)	56 (74%)	20 (26%)	0	4
20	CT	76/82 (93%)	53 (70%)	23 (30%)	0	3
21	AU	19/22 (86%)	18 (95%)	1 (5%)	28	67
21	CU	19/22 (86%)	14 (74%)	5 (26%)	0	4
27	BC	61/181 (34%)	49 (80%)	12 (20%)	1	10
27	DC	61/181 (34%)	53 (87%)	8 (13%)	5	27
28	BD	213/218 (98%)	164 (77%)	49 (23%)	1	6
28	DD	213/218 (98%)	178 (84%)	35 (16%)	3	17
29	BE	165/166 (99%)	125 (76%)	40 (24%)	1	5
29	DE	165/166 (99%)	141 (86%)	24 (14%)	4	23
30	BF	165/166 (99%)	127 (77%)	38 (23%)	1	6
30	DF	161/166 (97%)	136 (84%)	25 (16%)	3	20
31	BG	155/156 (99%)	118 (76%)	37 (24%)	1	5
31	DG	155/156 (99%)	135 (87%)	20 (13%)	5	28
32	BH	132/148 (89%)	114 (86%)	18 (14%)	5	26
32	DH	140/148 (95%)	114 (81%)	26 (19%)	2	11
33	BI	122/124 (98%)	95 (78%)	27 (22%)	1	7
33	DI	122/124 (98%)	92 (75%)	30 (25%)	1	5
34	BN	117/119 (98%)	88 (75%)	29 (25%)	1	5
34	DN	117/119 (98%)	96 (82%)	21 (18%)	2	13
35	BO	100/100 (100%)	77 (77%)	23 (23%)	1	6
35	DO	100/100 (100%)	90 (90%)	10 (10%)	9	41
36	BP	116/116 (100%)	86 (74%)	30 (26%)	0	4
36	DP	116/116 (100%)	89 (77%)	27 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BQ	111/111 (100%)	81 (73%)	30 (27%)	0	4
37	DQ	111/111 (100%)	92 (83%)	19 (17%)	2	15
38	BR	100/101 (99%)	68 (68%)	32 (32%)	0	2
38	DR	101/101 (100%)	86 (85%)	15 (15%)	4	22
39	BS	77/88 (88%)	56 (73%)	21 (27%)	0	4
39	DS	87/88 (99%)	75 (86%)	12 (14%)	4	25
40	BT	120/127 (94%)	90 (75%)	30 (25%)	1	4
40	DT	120/127 (94%)	91 (76%)	29 (24%)	1	5
41	BU	93/94 (99%)	70 (75%)	23 (25%)	1	5
41	DU	92/94 (98%)	80 (87%)	12 (13%)	5	28
42	BV	82/82 (100%)	55 (67%)	27 (33%)	0	2
42	DV	82/82 (100%)	64 (78%)	18 (22%)	1	7
43	BW	91/92 (99%)	69 (76%)	22 (24%)	1	5
43	DW	91/92 (99%)	83 (91%)	8 (9%)	12	48
44	BX	74/78 (95%)	58 (78%)	16 (22%)	1	7
44	DX	74/78 (95%)	61 (82%)	13 (18%)	2	14
45	BY	84/91 (92%)	67 (80%)	17 (20%)	1	9
45	DY	85/91 (93%)	66 (78%)	19 (22%)	1	6
46	BZ	155/179 (87%)	124 (80%)	31 (20%)	1	9
46	DZ	155/179 (87%)	136 (88%)	19 (12%)	6	29
47	B0	66/67 (98%)	57 (86%)	9 (14%)	5	26
47	D0	66/67 (98%)	57 (86%)	9 (14%)	5	26
48	B1	78/83 (94%)	61 (78%)	17 (22%)	1	7
48	D1	78/83 (94%)	61 (78%)	17 (22%)	1	7
49	B2	66/67 (98%)	53 (80%)	13 (20%)	1	10
49	D2	66/67 (98%)	53 (80%)	13 (20%)	1	10
50	B3	51/52 (98%)	40 (78%)	11 (22%)	1	7
50	D3	51/52 (98%)	49 (96%)	2 (4%)	39	76
51	B4	27/63 (43%)	17 (63%)	10 (37%)	0	1
51	D4	35/63 (56%)	31 (89%)	4 (11%)	7	33
52	B5	51/52 (98%)	42 (82%)	9 (18%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	D5	51/52 (98%)	43 (84%)	8 (16%)	3	20
53	B6	43/52 (83%)	31 (72%)	12 (28%)	0	3
53	D6	43/52 (83%)	33 (77%)	10 (23%)	1	5
54	B7	41/42 (98%)	35 (85%)	6 (15%)	4	23
54	D7	41/42 (98%)	37 (90%)	4 (10%)	10	42
55	B8	53/55 (96%)	38 (72%)	15 (28%)	0	3
55	D8	53/55 (96%)	41 (77%)	12 (23%)	1	6
56	B9	33/34 (97%)	29 (88%)	4 (12%)	6	30
56	D9	33/34 (97%)	29 (88%)	4 (12%)	6	30
All	All	9688/10428 (93%)	7777 (80%)	1911 (20%)	1	10

5 of 1911 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	BX	43	VAL
2	CB	196	LEU
42	DV	91	TYR
45	BY	89	PHE
50	B3	53	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
2	CB	204	ASN
12	CL	9	GLN
48	D1	45	ASN
5	CE	78	HIS
9	CI	38	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	366 (24%)	109 (7%)
1	CA	1503/1522 (98%)	359 (23%)	115 (7%)
22	AV	76/77 (98%)	26 (34%)	3 (3%)
22	CV	76/77 (98%)	30 (39%)	4 (5%)
23	AW	75/76 (98%)	22 (29%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	AY	16/76 (21%)	5 (31%)	0
23	CW	75/76 (98%)	26 (34%)	0
23	CY	16/76 (21%)	8 (50%)	0
24	AX	11/24 (45%)	4 (36%)	0
24	CX	9/24 (37%)	4 (44%)	1 (11%)
25	BA	2804/2915 (96%)	803 (28%)	260 (9%)
25	DA	2818/2915 (96%)	804 (28%)	264 (9%)
26	BB	118/122 (96%)	25 (21%)	5 (4%)
26	DB	118/122 (96%)	24 (20%)	7 (5%)
All	All	9218/9624 (95%)	2506 (27%)	768 (8%)

5 of 2506 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	10	A
1	AA	13	U

5 of 768 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2602	A
1	CA	575	G
25	DA	2238	G
25	BA	2750	A
1	CA	129(A)	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1039 ligands modelled in this entry, 1037 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	$\# Z > 2$
58	PAR	AA	7111	-	45,45,45	1.45	8 (17%)	59,67,67	1.19	5 (8%)
58	PAR	CA	1741	-	45,45,45	1.45	8 (17%)	59,67,67	1.20	5 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	AA	7111	-	-	0/18/94/94	0/4/4/4
58	PAR	CA	1741	-	-	0/18/94/94	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	CA	1741	PAR	O54-C54	2.03	1.49	1.44
58	AA	7111	PAR	O54-C54	2.04	1.49	1.44
58	CA	1741	PAR	O43-C13	2.11	1.45	1.41
58	AA	7111	PAR	C64-C54	2.12	1.57	1.52
58	CA	1741	PAR	C64-C54	2.14	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AA	7111	PAR	O52-C13-C23	2.01	111.93	107.75
58	CA	1741	PAR	C11-O51-C51	2.05	117.72	113.75
58	AA	7111	PAR	O23-C23-C33	2.33	117.88	111.16
58	CA	1741	PAR	O23-C23-C33	2.34	117.93	111.16
58	CA	1741	PAR	O54-C54-C64	3.01	111.99	106.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AA	7111	PAR	3	0
58	CA	1741	PAR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1453:U	O3'	1455:G	P	1.97

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%)	0.22	46 (3%) 52 43	31, 78, 168, 331	0
1	CA	1504/1522 (98%)	0.25	58 (3%) 43 34	24, 68, 165, 363	0
2	AB	235/256 (91%)	-0.05	4 (1%) 73 64	67, 121, 201, 279	0
2	CB	235/256 (91%)	-0.08	9 (3%) 44 36	44, 109, 202, 287	0
3	AC	207/239 (86%)	-0.10	1 (0%) 91 88	44, 104, 173, 240	0
3	CC	207/239 (86%)	-0.19	1 (0%) 91 88	38, 90, 151, 227	0
4	AD	208/209 (99%)	-0.26	3 (1%) 78 69	37, 89, 153, 217	0
4	CD	208/209 (99%)	-0.28	1 (0%) 91 88	30, 77, 129, 209	0
5	AE	151/162 (93%)	-0.21	2 (1%) 79 70	44, 87, 151, 240	0
5	CE	151/162 (93%)	-0.21	2 (1%) 79 70	22, 71, 131, 266	0
6	AF	101/101 (100%)	-0.17	0 100 100	29, 74, 120, 178	0
6	CF	101/101 (100%)	-0.26	0 100 100	25, 68, 134, 192	0
7	AG	155/156 (99%)	-0.12	7 (4%) 37 29	50, 93, 149, 256	0
7	CG	155/156 (99%)	-0.11	5 (3%) 51 42	32, 87, 151, 269	0
8	AH	138/138 (100%)	-0.26	0 100 100	41, 85, 129, 183	0
8	CH	138/138 (100%)	-0.31	1 (0%) 89 83	38, 75, 123, 181	0
9	AI	127/128 (99%)	0.04	3 (2%) 62 52	55, 113, 161, 319	0
9	CI	127/128 (99%)	-0.04	3 (2%) 62 52	45, 97, 170, 245	0
10	AJ	99/105 (94%)	0.32	4 (4%) 42 33	58, 124, 197, 302	0
10	CJ	99/105 (94%)	0.28	5 (5%) 32 24	38, 115, 191, 204	0
11	AK	119/129 (92%)	-0.09	4 (3%) 49 39	41, 77, 147, 249	0
11	CK	119/129 (92%)	-0.03	3 (2%) 61 50	29, 73, 139, 188	0
12	AL	125/132 (94%)	-0.12	3 (2%) 62 52	31, 64, 129, 300	0
12	CL	125/132 (94%)	-0.27	3 (2%) 62 52	9, 47, 127, 252	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.06	4 (3%) 51 42	29, 94, 148, 314	0
13	CM	125/126 (99%)	0.11	6 (4%) 34 27	39, 87, 174, 274	0
14	AN	60/61 (98%)	-0.04	1 (1%) 73 64	53, 92, 138, 207	0
14	CN	60/61 (98%)	-0.09	0 100 100	34, 71, 111, 194	0
15	AO	88/89 (98%)	-0.26	0 100 100	35, 80, 132, 142	0
15	CO	88/89 (98%)	-0.30	0 100 100	23, 69, 122, 147	0
16	AP	84/88 (95%)	-0.40	0 100 100	48, 74, 122, 182	0
16	CP	84/88 (95%)	-0.27	0 100 100	44, 76, 139, 200	0
17	AQ	100/105 (95%)	-0.19	0 100 100	50, 91, 141, 174	0
17	CQ	100/105 (95%)	-0.15	1 (1%) 84 76	38, 87, 144, 192	0
18	AR	70/88 (79%)	-0.18	3 (4%) 39 30	35, 77, 126, 183	0
18	CR	70/88 (79%)	-0.33	1 (1%) 78 69	36, 70, 122, 205	0
19	AS	79/93 (84%)	0.15	1 (1%) 79 70	46, 104, 202, 268	0
19	CS	79/93 (84%)	0.10	0 100 100	27, 82, 153, 206	0
20	AT	99/106 (93%)	0.08	5 (5%) 32 24	42, 90, 173, 211	0
20	CT	99/106 (93%)	0.16	3 (3%) 54 43	40, 97, 192, 295	0
21	AU	25/27 (92%)	0.73	5 (20%) 1 2	36, 92, 165, 229	0
21	CU	25/27 (92%)	-0.01	0 100 100	50, 78, 107, 150	0
22	AV	77/77 (100%)	0.14	0 100 100	45, 82, 163, 276	0
22	CV	77/77 (100%)	0.23	3 (3%) 43 34	32, 72, 133, 253	0
23	AW	76/76 (100%)	1.28	16 (21%) 1 1	48, 175, 249, 317	0
23	AY	17/76 (22%)	0.44	0 100 100	64, 94, 167, 176	0
23	CW	76/76 (100%)	1.64	24 (31%) 1 1	34, 184, 271, 295	0
23	CY	17/76 (22%)	0.72	0 100 100	44, 75, 149, 186	0
24	AX	12/24 (50%)	0.76	1 (8%) 14 12	49, 74, 217, 234	0
24	CX	10/24 (41%)	0.58	1 (10%) 9 9	42, 58, 144, 213	0
25	BA	2810/2915 (96%)	0.22	114 (4%) 41 32	17, 58, 187, 375	0
25	DA	2824/2915 (96%)	0.15	105 (3%) 45 36	6, 42, 178, 370	0
26	BB	119/122 (97%)	0.21	1 (0%) 87 80	59, 94, 132, 182	0
26	DB	119/122 (97%)	0.16	2 (1%) 73 64	38, 68, 113, 174	0
27	BC	191/229 (83%)	1.89	74 (38%) 0 0	89, 200, 319, 378	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DC	191/229 (83%)	2.28	93 (48%) 0 0	64, 208, 290, 334	0
28	BD	272/276 (98%)	-0.37	0 100 100	9, 45, 89, 166	0
28	DD	272/276 (98%)	-0.46	0 100 100	3, 33, 80, 197	0
29	BE	205/206 (99%)	-0.20	5 (2%) 62 52	17, 66, 128, 289	0
29	DE	205/206 (99%)	-0.20	4 (1%) 68 59	11, 55, 160, 338	0
30	BF	208/210 (99%)	-0.33	4 (1%) 70 61	14, 64, 164, 286	0
30	DF	202/210 (96%)	-0.29	2 (0%) 84 76	5, 51, 127, 208	0
31	BG	181/182 (99%)	-0.16	6 (3%) 50 41	40, 95, 175, 268	0
31	DG	181/182 (99%)	-0.15	4 (2%) 65 55	25, 76, 143, 219	0
32	BH	160/180 (88%)	0.91	30 (18%) 2 2	85, 179, 331, 429	0
32	DH	168/180 (93%)	0.04	1 (0%) 90 85	29, 81, 155, 234	0
33	BI	145/148 (97%)	-0.11	5 (3%) 49 39	33, 96, 156, 185	0
33	DI	146/148 (98%)	-0.05	1 (0%) 89 83	15, 104, 166, 207	0
34	BN	139/140 (99%)	-0.28	1 (0%) 89 83	36, 79, 147, 305	0
34	DN	139/140 (99%)	-0.31	0 100 100	7, 61, 137, 185	0
35	BO	122/122 (100%)	-0.47	0 100 100	32, 65, 97, 124	0
35	DO	122/122 (100%)	-0.58	0 100 100	10, 41, 84, 112	0
36	BP	150/150 (100%)	0.32	5 (3%) 50 41	27, 87, 179, 250	0
36	DP	150/150 (100%)	0.10	3 (2%) 68 59	23, 71, 151, 264	0
37	BQ	141/141 (100%)	-0.21	3 (2%) 67 58	36, 74, 126, 421	0
37	DQ	141/141 (100%)	-0.37	0 100 100	12, 52, 108, 281	0
38	BR	117/118 (99%)	-0.39	0 100 100	21, 57, 107, 148	0
38	DR	118/118 (100%)	-0.44	0 100 100	15, 50, 92, 126	0
39	BS	99/112 (88%)	-0.14	1 (1%) 84 76	38, 100, 171, 347	0
39	DS	111/112 (99%)	-0.10	2 (1%) 71 63	33, 73, 147, 197	0
40	BT	138/146 (94%)	-0.01	6 (4%) 39 30	29, 80, 225, 351	0
40	DT	138/146 (94%)	-0.02	8 (5%) 26 21	20, 71, 212, 304	0
41	BU	117/118 (99%)	-0.37	1 (0%) 85 78	29, 64, 131, 281	0
41	DU	117/118 (99%)	-0.48	1 (0%) 85 78	17, 52, 114, 180	0
42	BV	101/101 (100%)	-0.25	0 100 100	23, 90, 149, 344	0
42	DV	101/101 (100%)	-0.09	1 (0%) 84 76	9, 70, 131, 303	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BW	113/113 (100%)	-0.20	2 (1%) 71 63	19, 49, 113, 319	0
43	DW	113/113 (100%)	-0.29	0 100 100	14, 42, 128, 204	0
44	BX	93/96 (96%)	-0.31	0 100 100	30, 63, 99, 149	0
44	DX	93/96 (96%)	-0.30	0 100 100	12, 42, 87, 144	0
45	BY	101/110 (91%)	0.89	20 (19%) 1 2	42, 92, 253, 363	0
45	DY	102/110 (92%)	0.09	3 (2%) 55 45	28, 82, 182, 226	0
46	BZ	177/206 (85%)	0.43	17 (9%) 10 9	45, 125, 202, 316	0
46	DZ	177/206 (85%)	0.55	18 (10%) 9 8	29, 116, 254, 322	0
47	B0	84/85 (98%)	-0.00	5 (5%) 25 19	31, 69, 170, 242	0
47	D0	84/85 (98%)	-0.06	6 (7%) 19 15	18, 52, 136, 286	0
48	B1	94/98 (95%)	-0.15	1 (1%) 82 74	17, 53, 113, 219	0
48	D1	94/98 (95%)	-0.28	0 100 100	7, 44, 122, 237	0
49	B2	71/72 (98%)	-0.21	2 (2%) 56 46	35, 77, 128, 195	0
49	D2	71/72 (98%)	-0.20	0 100 100	14, 54, 137, 267	0
50	B3	60/60 (100%)	-0.00	2 (3%) 50 41	35, 75, 125, 382	0
50	D3	60/60 (100%)	-0.22	1 (1%) 73 64	20, 65, 142, 236	0
51	B4	31/71 (43%)	-0.13	0 100 100	67, 121, 152, 204	0
51	D4	40/71 (56%)	0.10	2 (5%) 32 25	55, 116, 173, 266	0
52	B5	59/60 (98%)	0.18	6 (10%) 9 8	17, 72, 180, 340	0
52	D5	59/60 (98%)	0.19	3 (5%) 32 24	12, 63, 214, 299	0
53	B6	45/54 (83%)	1.24	12 (26%) 1 1	44, 138, 207, 343	0
53	D6	45/54 (83%)	1.85	17 (37%) 0 0	59, 139, 235, 285	0
54	B7	49/49 (100%)	-0.38	0 100 100	11, 41, 123, 149	0
54	D7	49/49 (100%)	-0.56	0 100 100	1, 23, 101, 204	0
55	B8	64/65 (98%)	-0.03	2 (3%) 52 43	20, 60, 129, 325	0
55	D8	64/65 (98%)	-0.34	0 100 100	12, 51, 115, 172	0
56	B9	36/37 (97%)	3.55	28 (77%) 0 0	120, 197, 269, 389	0
56	D9	36/37 (97%)	3.46	30 (83%) 0 0	115, 172, 217, 282	0
All	All	21184/22210 (95%)	0.09	903 (4%) 39 30	1, 71, 192, 429	0

The worst 5 of 903 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	DA	2802	G	15.1
1	AA	81	U	13.2
25	BA	2802	G	13.2
27	DC	179	SER	12.7
23	CW	20	U	12.4

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
57	MG	DA	9364	1/1	0.98	0.82	64.20	1,1,1,1	0
57	MG	AA	7054	1/1	0.87	0.99	61.19	29,29,29,29	0
57	MG	DA	9435	1/1	0.92	0.98	50.74	30,30,30,30	0
57	MG	BA	3144	1/1	0.89	0.71	49.63	41,41,41,41	0
57	MG	DA	9523	1/1	0.97	0.77	37.34	9,9,9,9	0
57	MG	BA	3281	1/1	0.90	0.62	33.32	53,53,53,53	0
57	MG	DA	9312	1/1	0.98	0.67	32.76	4,4,4,4	0
57	MG	BA	3081	1/1	0.86	0.76	30.64	24,24,24,24	1
57	MG	DA	9549	1/1	0.94	0.74	27.03	44,44,44,44	0
57	MG	CA	1737	1/1	0.89	0.64	26.38	28,28,28,28	0
57	MG	DA	9514	1/1	0.94	0.82	25.36	19,19,19,19	0
57	MG	AA	7034	1/1	0.83	0.75	25.21	43,43,43,43	0
57	MG	AA	7090	1/1	0.89	1.01	24.68	69,69,69,69	0
57	MG	DA	9399	1/1	0.74	0.78	23.48	52,52,52,52	0
57	MG	DA	9655	1/1	0.37	0.92	23.17	35,35,35,35	0
57	MG	DA	9545	1/1	0.96	0.43	22.28	1,1,1,1	0
57	MG	DA	9369	1/1	0.99	0.59	22.14	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9392	1/1	0.98	0.70	21.90	12,12,12,12	0
57	MG	BA	3306	1/1	0.66	0.47	20.98	48,48,48,48	0
57	MG	CA	1631	1/1	0.95	0.89	20.77	22,22,22,22	0
57	MG	DA	9530	1/1	0.84	0.86	20.45	41,41,41,41	0
57	MG	DA	9498	1/1	0.96	0.50	20.31	2,2,2,2	0
57	MG	DA	9696	1/1	0.96	0.43	20.27	34,34,34,34	0
57	MG	DA	9436	1/1	0.94	0.54	20.19	3,3,3,3	0
57	MG	CA	1651	1/1	0.64	0.44	20.04	39,39,39,39	0
57	MG	CA	1640	1/1	0.94	0.84	20.01	49,49,49,49	0
57	MG	BA	3073	1/1	0.98	0.67	19.93	8,8,8,8	0
57	MG	BA	3297	1/1	0.79	0.93	19.85	46,46,46,46	0
57	MG	BA	3045	1/1	0.92	0.59	19.47	2,2,2,2	0
57	MG	DA	9324	1/1	0.98	0.48	19.37	2,2,2,2	0
57	MG	DA	9570	1/1	0.79	0.31	18.79	61,61,61,61	0
57	MG	DA	9618	1/1	0.92	0.79	18.75	28,28,28,28	1
57	MG	BA	3264	1/1	0.82	0.65	18.63	36,36,36,36	0
57	MG	BA	3007	1/1	0.95	0.66	18.59	4,4,4,4	0
57	MG	CA	1720	1/1	0.92	0.41	17.98	2,2,2,2	0
57	MG	CA	1699	1/1	0.61	0.39	17.78	45,45,45,45	1
57	MG	DA	9355	1/1	0.98	0.67	17.63	0,0,0,0	0
57	MG	BA	3028	1/1	0.67	0.55	17.54	44,44,44,44	0
57	MG	DA	9479	1/1	0.98	0.63	17.35	0,0,0,0	0
57	MG	DA	9359	1/1	0.98	0.38	17.15	0,0,0,0	0
57	MG	AA	7066	1/1	0.92	0.54	16.97	36,36,36,36	0
57	MG	BA	3198	1/1	0.96	0.34	16.87	0,0,0,0	0
57	MG	DA	9438	1/1	0.78	0.38	16.85	21,21,21,21	0
57	MG	DA	9319	1/1	0.90	0.80	16.78	30,30,30,30	0
57	MG	DA	9473	1/1	0.94	0.64	16.75	0,0,0,0	0
57	MG	DA	9398	1/1	0.99	0.44	16.61	0,0,0,0	0
57	MG	DA	9528	1/1	0.94	0.36	16.23	6,6,6,6	0
57	MG	BA	3309	1/1	0.95	0.79	16.20	25,25,25,25	0
57	MG	BA	3187	1/1	0.90	0.60	15.99	24,24,24,24	0
57	MG	DA	9521	1/1	0.96	0.57	15.28	2,2,2,2	0
57	MG	DA	9472	1/1	0.98	0.41	15.20	16,16,16,16	0
57	MG	BA	3220	1/1	0.85	0.77	15.07	56,56,56,56	0
57	MG	DA	9366	1/1	0.95	0.46	14.98	1,1,1,1	0
57	MG	BA	3065	1/1	0.97	0.66	14.95	2,2,2,2	0
57	MG	CA	1670	1/1	0.94	0.36	14.77	2,2,2,2	0
57	MG	BA	3227	1/1	0.58	0.71	14.67	40,40,40,40	0
57	MG	BA	3205	1/1	0.91	0.54	14.62	0,0,0,0	0
57	MG	BA	3044	1/1	0.93	0.58	14.61	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3116	1/1	0.85	0.27	14.54	38,38,38,38	0
57	MG	DA	9516	1/1	0.96	0.46	14.46	1,1,1,1	0
57	MG	BA	3153	1/1	0.93	0.55	14.46	0,0,0,0	0
57	MG	DA	9383	1/1	0.81	0.41	14.38	18,18,18,18	0
57	MG	BA	3234	1/1	0.98	0.56	14.35	10,10,10,10	0
57	MG	DA	9402	1/1	0.88	0.38	13.99	25,25,25,25	0
57	MG	DA	9459	1/1	0.95	0.52	13.92	3,3,3,3	0
57	MG	BA	3265	1/1	0.95	0.51	13.69	43,43,43,43	0
57	MG	BA	3276	1/1	0.88	0.56	13.59	31,31,31,31	0
57	MG	DA	9647	1/1	0.95	0.61	13.23	1,1,1,1	0
57	MG	DA	9445	1/1	0.84	0.44	13.21	22,22,22,22	0
57	MG	BA	3210	1/1	0.98	0.74	13.20	11,11,11,11	0
57	MG	DA	9358	1/1	0.93	0.47	13.18	5,5,5,5	0
57	MG	BA	3307	1/1	0.96	0.54	12.93	25,25,25,25	0
57	MG	AA	7026	1/1	0.89	0.40	12.83	30,30,30,30	0
57	MG	DA	9381	1/1	0.85	0.26	12.54	12,12,12,12	0
57	MG	BA	3193	1/1	0.86	0.44	12.46	12,12,12,12	0
57	MG	AA	7053	1/1	0.92	0.49	12.45	32,32,32,32	0
57	MG	DA	9305	1/1	0.96	0.46	12.38	0,0,0,0	0
57	MG	BA	3008	1/1	0.98	0.46	12.24	2,2,2,2	0
57	MG	BA	3203	1/1	0.67	0.45	12.24	37,37,37,37	0
57	MG	DA	9349	1/1	0.96	0.61	12.21	3,3,3,3	0
57	MG	DA	9518	1/1	0.99	0.36	12.11	0,0,0,0	0
57	MG	BA	3146	1/1	0.96	0.71	11.86	0,0,0,0	0
57	MG	DA	9681	1/1	0.80	0.35	11.79	13,13,13,13	0
57	MG	BA	3120	1/1	0.68	0.65	11.73	24,24,24,24	0
57	MG	BA	3030	1/1	0.93	0.55	11.27	22,22,22,22	0
57	MG	BA	3196	1/1	0.75	0.76	11.26	30,30,30,30	0
57	MG	BA	3041	1/1	0.96	0.50	11.23	7,7,7,7	0
57	MG	DA	9370	1/1	0.89	0.39	11.22	0,0,0,0	0
57	MG	AA	7008	1/1	0.80	0.85	11.18	35,35,35,35	0
57	MG	DA	9529	1/1	0.96	0.29	11.16	0,0,0,0	0
57	MG	AA	7094	1/1	0.93	0.54	11.12	8,8,8,8	0
57	MG	BA	3249	1/1	0.83	0.41	11.11	25,25,25,25	0
57	MG	AA	7018	1/1	0.92	0.56	10.96	27,27,27,27	0
57	MG	DA	9536	1/1	0.96	0.44	10.86	0,0,0,0	0
57	MG	AA	7075	1/1	0.82	0.49	10.84	53,53,53,53	0
57	MG	BA	3204	1/1	0.95	0.32	10.68	3,3,3,3	0
57	MG	DA	9425	1/1	0.90	0.41	10.66	37,37,37,37	0
57	MG	DA	9441	1/1	0.79	0.58	10.42	31,31,31,31	1
57	MG	CA	1645	1/1	0.98	0.34	10.30	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3159	1/1	0.94	0.53	10.18	9,9,9,9	0
57	MG	DA	9587	1/1	0.97	0.28	10.11	2,2,2,2	0
57	MG	DA	9673	1/1	0.87	0.42	10.06	8,8,8,8	0
57	MG	AA	7037	1/1	0.98	0.32	10.05	7,7,7,7	0
57	MG	BA	3248	1/1	0.63	0.70	10.01	49,49,49,49	0
57	MG	DA	9340	1/1	0.94	0.33	10.00	1,1,1,1	0
57	MG	BA	3020	1/1	0.97	0.48	9.95	1,1,1,1	0
57	MG	DA	9483	1/1	0.90	0.48	9.68	0,0,0,0	0
57	MG	CA	1626	1/1	0.95	0.55	9.33	28,28,28,28	0
57	MG	AA	7051	1/1	0.93	0.45	9.30	22,22,22,22	0
57	MG	AA	7059	1/1	0.93	0.51	9.26	96,96,96,96	0
57	MG	BA	3188	1/1	0.96	0.35	9.14	0,0,0,0	0
57	MG	DA	9360	1/1	0.98	0.36	8.84	7,7,7,7	0
57	MG	CA	1610	1/1	0.79	0.63	8.83	58,58,58,58	0
57	MG	DA	9653	1/1	0.94	0.41	8.75	5,5,5,5	0
57	MG	DD	7101	1/1	0.97	0.48	8.70	3,3,3,3	0
57	MG	DA	9430	1/1	0.98	0.39	8.67	0,0,0,0	0
57	MG	DA	9546	1/1	0.97	0.34	8.55	2,2,2,2	0
57	MG	BA	3051	1/1	0.98	0.41	8.51	6,6,6,6	0
57	MG	BD	301	1/1	0.97	0.57	8.45	7,7,7,7	0
57	MG	DA	9356	1/1	0.95	0.32	8.42	1,1,1,1	0
57	MG	AA	7019	1/1	0.99	0.56	8.41	16,16,16,16	0
57	MG	CA	1653	1/1	0.89	0.53	8.36	29,29,29,29	0
57	MG	BA	3272	1/1	0.92	0.37	8.36	10,10,10,10	0
57	MG	DA	9526	1/1	0.89	0.50	8.27	12,12,12,12	0
57	MG	AA	7071	1/1	0.70	0.53	8.14	38,38,38,38	0
57	MG	DA	9310	1/1	0.98	0.28	8.09	0,0,0,0	0
57	MG	CA	1629	1/1	0.96	0.34	7.83	37,37,37,37	0
57	MG	BA	3255	1/1	0.97	0.44	7.81	45,45,45,45	0
57	MG	DA	9491	1/1	0.96	0.45	7.80	11,11,11,11	0
57	MG	DA	9421	1/1	0.82	0.36	7.59	28,28,28,28	0
57	MG	CA	1652	1/1	0.97	0.60	7.54	6,6,6,6	0
57	MG	DA	9527	1/1	0.91	0.38	7.42	1,1,1,1	0
57	MG	CA	1710	1/1	0.88	0.50	7.41	19,19,19,19	0
57	MG	DA	9335	1/1	0.82	0.33	7.41	21,21,21,21	0
57	MG	B7	101	1/1	0.94	0.39	7.40	13,13,13,13	0
57	MG	DA	9515	1/1	0.97	0.32	7.20	10,10,10,10	0
57	MG	BA	3270	1/1	0.97	0.50	7.17	0,0,0,0	1
57	MG	BA	3182	1/1	0.98	0.57	7.12	2,2,2,2	0
57	MG	BA	3027	1/1	0.98	0.34	7.11	4,4,4,4	0
57	MG	DA	9308	1/1	0.98	0.44	7.10	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9544	1/1	0.84	0.41	7.08	10,10,10,10	0
57	MG	BA	3136	1/1	0.83	0.44	7.05	46,46,46,46	1
57	MG	BA	3243	1/1	0.97	0.45	6.96	5,5,5,5	0
57	MG	CA	1607	1/1	0.93	0.50	6.92	32,32,32,32	0
57	MG	DA	9489	1/1	0.92	0.41	6.86	37,37,37,37	0
57	MG	DA	9533	1/1	0.93	0.30	6.77	0,0,0,0	0
57	MG	BA	3046	1/1	0.98	0.64	6.76	1,1,1,1	0
57	MG	CA	1685	1/1	0.93	0.34	6.71	41,41,41,41	0
57	MG	CA	1674	1/1	0.72	0.40	6.44	89,89,89,89	0
57	MG	CA	1709	1/1	0.83	0.49	6.43	68,68,68,68	0
57	MG	DA	9621	1/1	0.97	0.59	6.35	0,0,0,0	1
57	MG	BA	3111	1/1	0.89	0.32	6.19	35,35,35,35	0
57	MG	DA	9512	1/1	0.93	0.43	6.16	2,2,2,2	0
57	MG	BA	3252	1/1	0.97	0.47	6.11	56,56,56,56	0
57	MG	DA	9581	1/1	0.94	0.42	6.10	4,4,4,4	0
57	MG	DA	9649	1/1	0.97	0.43	6.06	1,1,1,1	0
57	MG	DA	9458	1/1	0.79	0.41	6.05	22,22,22,22	0
57	MG	DA	9418	1/1	0.82	0.28	6.01	61,61,61,61	0
57	MG	BA	3160	1/1	0.93	0.39	5.99	22,22,22,22	0
57	MG	BA	3191	1/1	0.96	0.41	5.90	2,2,2,2	0
57	MG	BA	3004	1/1	0.96	0.59	5.90	1,1,1,1	0
57	MG	AA	7013	1/1	0.91	0.37	5.81	27,27,27,27	0
57	MG	DA	9590	1/1	0.97	0.49	5.76	1,1,1,1	0
57	MG	BA	3235	1/1	0.92	0.36	5.67	25,25,25,25	0
57	MG	DA	9584	1/1	0.98	0.35	5.61	0,0,0,0	0
57	MG	BA	3300	1/1	0.93	0.45	5.60	1,1,1,1	0
57	MG	DA	9623	1/1	0.97	0.37	5.59	13,13,13,13	0
57	MG	BA	3142	1/1	0.98	0.44	5.58	10,10,10,10	0
57	MG	DA	9553	1/1	0.95	0.35	5.54	20,20,20,20	0
57	MG	DA	9417	1/1	0.93	0.29	5.50	20,20,20,20	0
57	MG	BA	3222	1/1	0.96	0.39	5.48	5,5,5,5	0
57	MG	AA	7061	1/1	0.89	0.25	5.48	19,19,19,19	0
57	MG	DA	9408	1/1	0.98	0.25	5.47	3,3,3,3	0
57	MG	DA	9409	1/1	0.90	0.31	5.45	4,4,4,4	0
57	MG	AA	7006	1/1	0.99	0.37	5.40	20,20,20,20	0
57	MG	DA	9503	1/1	0.88	0.31	5.37	66,66,66,66	0
57	MG	DA	9347	1/1	0.82	0.29	5.24	22,22,22,22	0
57	MG	DA	9454	1/1	0.94	0.44	5.15	34,34,34,34	0
57	MG	DA	9428	1/1	0.94	0.41	5.09	15,15,15,15	0
57	MG	DA	9484	1/1	0.92	0.40	5.05	5,5,5,5	0
57	MG	BA	3119	1/1	0.73	0.32	5.03	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3098	1/1	0.93	0.29	4.91	36,36,36,36	0
57	MG	BA	3125	1/1	0.98	0.29	4.75	20,20,20,20	0
57	MG	BA	3241	1/1	0.94	0.45	4.71	4,4,4,4	0
57	MG	CA	1668	1/1	0.94	0.34	4.68	56,56,56,56	0
57	MG	BA	3084	1/1	0.99	0.50	4.66	1,1,1,1	0
57	MG	CA	1683	1/1	0.65	0.26	4.65	29,29,29,29	0
57	MG	AA	7064	1/1	0.94	0.28	4.53	50,50,50,50	0
57	MG	DA	9404	1/1	0.97	0.31	4.47	12,12,12,12	0
57	MG	BA	3310	1/1	0.84	0.40	4.45	35,35,35,35	0
57	MG	DA	9382	1/1	0.90	0.45	4.43	0,0,0,0	0
57	MG	BA	3069	1/1	0.95	0.32	4.41	5,5,5,5	0
57	MG	DA	9672	1/1	0.98	0.37	4.25	5,5,5,5	0
58	PAR	CA	1741	42/42	0.89	0.32	4.25	55,55,55,55	0
57	MG	DA	9517	1/1	0.97	0.29	4.22	0,0,0,0	0
57	MG	DA	9537	1/1	0.98	0.38	4.21	0,0,0,0	0
57	MG	DA	9614	1/1	0.84	0.25	4.15	12,12,12,12	0
57	MG	AA	7043	1/1	0.91	0.35	4.13	16,16,16,16	0
57	MG	BA	3086	1/1	0.96	0.23	4.01	1,1,1,1	0
57	MG	CA	1665	1/1	0.95	0.40	3.98	16,16,16,16	0
57	MG	BA	3047	1/1	0.97	0.29	3.92	0,0,0,0	0
57	MG	AA	7011	1/1	0.83	0.40	3.89	43,43,43,43	0
57	MG	AA	7044	1/1	0.95	0.35	3.82	21,21,21,21	0
57	MG	DA	9613	1/1	0.96	0.22	3.75	5,5,5,5	0
57	MG	AA	7110	1/1	0.96	0.33	3.72	31,31,31,31	0
57	MG	AA	7021	1/1	0.95	0.31	3.70	25,25,25,25	0
57	MG	AA	7091	1/1	0.96	0.23	3.62	22,22,22,22	0
57	MG	DA	9554	1/1	0.98	0.27	3.53	10,10,10,10	0
57	MG	BA	3201	1/1	0.91	0.32	3.49	6,6,6,6	0
57	MG	BA	3218	1/1	0.98	0.30	3.34	24,24,24,24	0
57	MG	DA	9365	1/1	0.90	0.28	3.25	1,1,1,1	0
57	MG	AA	7058	1/1	0.95	0.27	3.24	13,13,13,13	0
57	MG	CA	1667	1/1	0.96	0.28	3.22	12,12,12,12	0
57	MG	BA	3308	1/1	0.90	0.40	3.19	37,37,37,37	0
57	MG	BA	3066	1/1	0.87	0.27	3.15	48,48,48,48	0
57	MG	DA	9439	1/1	0.83	0.23	3.11	32,32,32,32	0
57	MG	BA	3251	1/1	0.86	0.22	3.06	34,34,34,34	0
57	MG	BA	3054	1/1	0.96	0.32	3.00	14,14,14,14	0
57	MG	CA	1705	1/1	0.93	0.27	2.98	15,15,15,15	0
57	MG	CA	1617	1/1	0.92	0.42	2.95	16,16,16,16	0
57	MG	DA	9497	1/1	0.95	0.36	2.93	29,29,29,29	0
57	MG	AA	7056	1/1	0.97	0.34	2.85	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9539	1/1	0.91	0.26	2.81	35,35,35,35	0
57	MG	DA	9675	1/1	0.96	0.29	2.79	11,11,11,11	0
57	MG	BA	3229	1/1	0.93	0.19	2.74	19,19,19,19	0
57	MG	BA	3145	1/1	0.92	0.28	2.72	22,22,22,22	0
57	MG	DQ	201	1/1	0.92	0.31	2.72	36,36,36,36	0
57	MG	DA	9461	1/1	0.83	0.34	2.60	13,13,13,13	0
57	MG	DA	9557	1/1	0.81	0.31	2.56	25,25,25,25	0
57	MG	DA	9460	1/1	0.89	0.25	2.52	40,40,40,40	0
57	MG	DA	9493	1/1	0.98	0.27	2.47	1,1,1,1	0
57	MG	DA	9600	1/1	0.79	0.34	2.47	55,55,55,55	0
57	MG	DA	9508	1/1	0.96	0.25	2.38	0,0,0,0	0
57	MG	BA	3225	1/1	0.94	0.29	2.35	2,2,2,2	0
57	MG	DA	9363	1/1	0.96	0.23	2.31	1,1,1,1	0
57	MG	BA	3090	1/1	0.94	0.41	2.28	2,2,2,2	0
57	MG	DD	7103	1/1	0.97	0.42	2.25	0,0,0,0	0
57	MG	DA	9437	1/1	0.98	0.19	2.23	14,14,14,14	0
57	MG	CA	1630	1/1	0.91	0.23	2.23	34,34,34,34	0
57	MG	CA	1727	1/1	0.92	0.34	2.22	27,27,27,27	0
57	MG	BA	3099	1/1	0.93	0.23	2.20	30,30,30,30	0
57	MG	DA	9597	1/1	0.93	0.23	2.15	12,12,12,12	0
57	MG	BE	302	1/1	0.89	0.28	2.12	74,74,74,74	0
57	MG	DA	9443	1/1	0.89	0.24	2.10	37,37,37,37	0
57	MG	BA	3279	1/1	0.98	0.25	2.10	31,31,31,31	0
57	MG	CA	1624	1/1	0.97	0.33	2.08	18,18,18,18	0
57	MG	AA	7016	1/1	0.94	0.32	2.07	45,45,45,45	0
57	MG	DA	9605	1/1	0.91	0.20	2.06	19,19,19,19	0
57	MG	BA	3238	1/1	0.98	0.33	2.03	9,9,9,9	0
58	PAR	AA	7111	42/42	0.92	0.26	2.02	58,58,58,58	0
57	MG	BA	3071	1/1	0.96	0.31	2.00	0,0,0,0	0
57	MG	BA	3022	1/1	0.89	0.23	1.96	40,40,40,40	0
57	MG	BA	3149	1/1	0.47	0.34	1.96	27,27,27,27	0
57	MG	AA	7067	1/1	0.86	0.45	1.94	28,28,28,28	0
57	MG	BA	3178	1/1	0.95	0.24	1.93	28,28,28,28	0
57	MG	BA	3058	1/1	0.91	0.33	1.87	1,1,1,1	0
57	MG	BU	201	1/1	0.94	0.30	1.82	170,170,170,170	1
57	MG	BA	3108	1/1	0.80	0.25	1.80	27,27,27,27	0
57	MG	DA	9431	1/1	0.83	0.30	1.80	12,12,12,12	0
57	MG	CA	1633	1/1	0.88	0.27	1.72	9,9,9,9	0
57	MG	BA	3076	1/1	0.70	0.22	1.70	18,18,18,18	0
57	MG	BA	3053	1/1	0.89	0.29	1.64	17,17,17,17	0
57	MG	BA	3185	1/1	0.94	0.26	1.60	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1666	1/1	0.77	0.36	1.58	66,66,66,66	0
57	MG	BA	3056	1/1	0.96	0.24	1.55	5,5,5,5	0
57	MG	CA	1719	1/1	0.95	0.35	1.40	10,10,10,10	0
57	MG	BA	3109	1/1	0.90	0.22	1.37	66,66,66,66	0
57	MG	DA	9561	1/1	0.93	0.27	1.34	10,10,10,10	0
57	MG	BA	3043	1/1	0.95	0.21	1.21	8,8,8,8	0
57	MG	BA	3085	1/1	0.97	0.26	1.18	29,29,29,29	0
57	MG	DA	9410	1/1	0.94	0.25	1.15	4,4,4,4	0
57	MG	DA	9388	1/1	0.72	0.18	1.06	28,28,28,28	0
57	MG	DA	9316	1/1	0.97	0.23	1.02	0,0,0,0	0
57	MG	BA	3208	1/1	0.92	0.22	1.01	8,8,8,8	0
57	MG	DB	202	1/1	0.83	0.22	1.01	28,28,28,28	0
57	MG	AA	7029	1/1	0.90	0.27	1.00	41,41,41,41	0
57	MG	DU	201	1/1	0.95	0.34	0.98	30,30,30,30	1
57	MG	DA	9433	1/1	0.93	0.22	0.95	13,13,13,13	0
57	MG	CA	1726	1/1	0.92	0.21	0.91	38,38,38,38	0
57	MG	BA	3061	1/1	0.92	0.25	0.87	32,32,32,32	0
57	MG	D0	101	1/1	0.95	0.45	0.86	27,27,27,27	0
57	MG	BA	3161	1/1	0.95	0.26	0.84	11,11,11,11	0
57	MG	DD	7102	1/1	0.94	0.28	0.82	0,0,0,0	0
57	MG	BA	3015	1/1	0.98	0.20	0.82	3,3,3,3	0
57	MG	DA	9506	1/1	0.96	0.23	0.77	0,0,0,0	0
57	MG	DA	9395	1/1	0.70	0.24	0.76	29,29,29,29	0
57	MG	DA	9482	1/1	0.93	0.21	0.66	12,12,12,12	0
57	MG	CA	1679	1/1	0.96	0.28	0.59	9,9,9,9	0
57	MG	DA	9339	1/1	0.90	0.20	0.55	13,13,13,13	0
57	MG	AA	7030	1/1	0.95	0.23	0.48	2,2,2,2	0
57	MG	BD	302	1/1	0.96	0.27	0.47	4,4,4,4	0
57	MG	BA	3031	1/1	0.88	0.23	0.47	44,44,44,44	0
57	MG	CA	1677	1/1	0.90	0.18	0.45	22,22,22,22	0
59	ZN	AD	301	1/1	0.93	0.32	0.41	41,41,41,41	0
57	MG	DA	9586	1/1	0.97	0.20	0.40	3,3,3,3	0
57	MG	DP	203	1/1	0.90	0.24	0.40	11,11,11,11	0
57	MG	DA	9697	1/1	0.97	0.23	0.39	41,41,41,41	0
59	ZN	CD	301	1/1	0.98	0.32	0.39	44,44,44,44	0
57	MG	BA	3115	1/1	0.84	0.24	0.33	33,33,33,33	0
57	MG	BA	3089	1/1	0.97	0.23	0.23	18,18,18,18	0
57	MG	DA	9487	1/1	0.93	0.25	0.19	71,71,71,71	0
57	MG	CA	1678	1/1	0.92	0.22	0.16	17,17,17,17	0
57	MG	CA	1671	1/1	0.89	0.23	0.15	38,38,38,38	0
57	MG	BA	3237	1/1	0.98	0.24	0.08	43,43,43,43	0
57	MG	BN	201	1/1	0.91	0.30	0.05	125,125,125,125	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3033	1/1	0.84	0.19	0.04	6,6,6,6	0
57	MG	DA	9302	1/1	0.87	0.18	-0.10	34,34,34,34	0
57	MG	DA	9547	1/1	0.96	0.21	-0.12	3,3,3,3	0
57	MG	DA	9499	1/1	0.96	0.15	-0.26	29,29,29,29	0
57	MG	CA	1656	1/1	0.91	0.21	-0.31	22,22,22,22	0
57	MG	BA	3293	1/1	0.95	0.21	-0.51	1,1,1,1	0
57	MG	CA	1605	1/1	0.87	0.21	-0.59	32,32,32,32	0
57	MG	CV	102	1/1	0.92	0.21	-0.60	1,1,1,1	0
59	ZN	CN	101	1/1	0.79	0.19	-0.61	171,171,171,171	0
57	MG	AA	7040	1/1	0.92	0.17	-0.64	36,36,36,36	0
57	MG	DA	9592	1/1	0.96	0.17	-0.64	36,36,36,36	0
57	MG	BA	3091	1/1	0.98	0.19	-0.66	0,0,0,0	0
57	MG	BA	3072	1/1	0.98	0.17	-0.68	25,25,25,25	0
57	MG	AA	7057	1/1	0.96	0.18	-0.68	44,44,44,44	0
57	MG	BA	3167	1/1	0.96	0.17	-0.70	30,30,30,30	0
57	MG	BA	3174	1/1	0.93	0.14	-0.73	31,31,31,31	0
57	MG	DA	9678	1/1	0.97	0.19	-0.75	33,33,33,33	0
57	MG	DA	9583	1/1	0.94	0.18	-0.76	1,1,1,1	0
57	MG	BF	301	1/1	0.86	0.22	-0.77	39,39,39,39	0
57	MG	BA	3224	1/1	0.99	0.17	-0.78	5,5,5,5	0
57	MG	BA	3256	1/1	0.92	0.15	-0.79	13,13,13,13	0
57	MG	DA	9629	1/1	0.93	0.15	-0.83	52,52,52,52	0
59	ZN	AN	101	1/1	0.97	0.10	-0.90	147,147,147,147	0
57	MG	BE	303	1/1	0.99	0.15	-1.03	1,1,1,1	0
57	MG	DA	9619	1/1	0.98	0.15	-1.08	0,0,0,0	0
57	MG	DA	9464	1/1	0.91	0.14	-1.13	25,25,25,25	0
57	MG	CA	1711	1/1	0.95	0.12	-1.19	26,26,26,26	0
57	MG	DA	9504	1/1	0.84	0.15	-1.23	27,27,27,27	0
57	MG	DU	202	1/1	0.98	0.14	-1.26	6,6,6,6	0
57	MG	AV	101	1/1	0.96	0.14	-1.35	2,2,2,2	0
57	MG	AA	7062	1/1	0.94	0.11	-1.37	31,31,31,31	0
57	MG	BP	201	1/1	0.75	0.20	-1.40	166,166,166,166	0
57	MG	DA	9558	1/1	0.99	0.15	-1.49	6,6,6,6	0
57	MG	DB	205	1/1	0.81	0.17	-1.52	6,6,6,6	1
57	MG	BA	3092	1/1	0.96	0.17	-1.53	1,1,1,1	0
57	MG	CA	1662	1/1	0.92	0.17	-1.56	29,29,29,29	0
57	MG	CA	1649	1/1	0.96	0.10	-1.61	33,33,33,33	0
57	MG	DA	9389	1/1	0.92	0.15	-1.73	11,11,11,11	0
57	MG	CA	1602	1/1	0.96	0.17	-1.77	14,14,14,14	0
57	MG	AA	7007	1/1	0.97	0.13	-1.77	1,1,1,1	0
57	MG	DA	9575	1/1	0.96	0.12	-1.79	35,35,35,35	0
57	MG	DA	9342	1/1	0.96	0.10	-1.80	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3029	1/1	0.93	0.15	-1.80	24,24,24,24	0
57	MG	DA	9373	1/1	0.88	0.16	-1.81	0,0,0,0	0
57	MG	BA	3038	1/1	0.83	0.16	-1.83	31,31,31,31	0
57	MG	AA	7087	1/1	0.96	0.13	-1.90	24,24,24,24	0
57	MG	BA	3059	1/1	0.86	0.16	-1.92	0,0,0,0	0
57	MG	BB	202	1/1	0.88	0.17	-1.95	62,62,62,62	0
57	MG	DA	9391	1/1	0.96	0.17	-1.99	1,1,1,1	0
57	MG	AA	7092	1/1	0.74	0.13	-2.07	37,37,37,37	0
57	MG	BA	3062	1/1	0.92	0.14	-2.20	27,27,27,27	0
57	MG	AA	7104	1/1	0.93	0.13	-2.22	33,33,33,33	0
57	MG	DU	203	1/1	0.99	0.14	-2.43	0,0,0,0	1
57	MG	DA	9377	1/1	0.85	0.19	-2.54	19,19,19,19	0
57	MG	CA	1632	1/1	0.93	0.15	-2.62	18,18,18,18	0
57	MG	BB	205	1/1	0.61	0.11	-3.12	19,19,19,19	1
57	MG	DA	9690	1/1	0.88	0.11	-3.16	5,5,5,5	0
57	MG	BA	3240	1/1	0.97	0.13	-3.19	21,21,21,21	0
57	MG	DF	301	1/1	0.87	0.14	-3.23	20,20,20,20	0
57	MG	DA	9446	1/1	0.93	0.08	-3.50	13,13,13,13	0
57	MG	CA	1622	1/1	0.97	0.09	-4.22	37,37,37,37	0
57	MG	BA	3068	1/1	0.95	0.11	-4.57	11,11,11,11	0
57	MG	AA	7042	1/1	0.97	0.08	-5.18	31,31,31,31	0
57	MG	AA	7095	1/1	0.95	0.08	-5.77	17,17,17,17	0
57	MG	AA	7003	1/1	0.97	0.10	-5.81	27,27,27,27	0
57	MG	DA	9481	1/1	0.98	0.09	-8.28	0,0,0,0	0
57	MG	AA	7027	1/1	0.79	0.41	-	28,28,28,28	0
57	MG	BA	3275	1/1	0.97	0.27	-	1,1,1,1	1
57	MG	DA	9563	1/1	0.76	0.26	-	3,3,3,3	0
57	MG	BA	3282	1/1	0.84	0.47	-	24,24,24,24	0
57	MG	BA	3133	1/1	0.92	0.21	-	43,43,43,43	0
57	MG	BA	3287	1/1	0.91	0.36	-	30,30,30,30	0
57	MG	AA	7068	1/1	0.97	0.09	-	34,34,34,34	0
57	MG	BA	3127	1/1	0.95	0.39	-	8,8,8,8	0
57	MG	BA	3312	1/1	0.95	0.30	-	45,45,45,45	0
57	MG	DA	9303	1/1	0.92	0.31	-	42,42,42,42	0
57	MG	DA	9434	1/1	0.70	0.45	-	4,4,4,4	0
57	MG	BA	3164	1/1	0.78	0.44	-	39,39,39,39	0
57	MG	AA	7085	1/1	0.94	0.17	-	15,15,15,15	0
57	MG	BA	3034	1/1	0.98	0.22	-	7,7,7,7	0
57	MG	DA	9354	1/1	0.99	0.49	-	2,2,2,2	0
57	MG	BA	3173	1/1	0.73	0.62	-	27,27,27,27	0
57	MG	DA	9593	1/1	0.84	0.62	-	25,25,25,25	0
57	MG	DA	9679	1/1	0.90	0.31	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	7014	1/1	0.83	0.96	-	20,20,20,20	0
57	MG	BA	3050	1/1	0.91	0.58	-	4,4,4,4	0
57	MG	BA	3253	1/1	0.94	0.60	-	34,34,34,34	0
57	MG	BA	3039	1/1	0.69	0.39	-	30,30,30,30	0
57	MG	DA	9680	1/1	0.89	0.39	-	24,24,24,24	0
57	MG	D2	101	1/1	0.90	0.24	-	34,34,34,34	0
57	MG	DB	203	1/1	0.89	0.90	-	1,1,1,1	1
57	MG	AA	7035	1/1	0.98	0.11	-	42,42,42,42	0
57	MG	DA	9574	1/1	0.82	0.38	-	14,14,14,14	1
57	MG	CA	1707	1/1	0.96	0.83	-	1,1,1,1	1
57	MG	BA	3102	1/1	0.87	0.48	-	1,1,1,1	0
57	MG	CA	1614	1/1	0.81	1.22	-	38,38,38,38	0
57	MG	CA	1738	1/1	0.88	0.42	-	49,49,49,49	0
57	MG	BA	3088	1/1	0.92	0.39	-	43,43,43,43	0
57	MG	BA	3131	1/1	0.85	0.40	-	38,38,38,38	0
57	MG	DA	9486	1/1	0.92	0.34	-	21,21,21,21	0
57	MG	DA	9659	1/1	0.83	0.27	-	52,52,52,52	0
57	MG	BA	3126	1/1	0.49	0.61	-	44,44,44,44	0
57	MG	CA	1657	1/1	0.85	0.26	-	30,30,30,30	0
57	MG	BA	3083	1/1	0.95	0.32	-	27,27,27,27	1
57	MG	AV	104	1/1	0.81	0.41	-	16,16,16,16	0
57	MG	CA	1730	1/1	0.93	0.15	-	49,49,49,49	0
57	MG	BA	3319	1/1	0.87	0.29	-	27,27,27,27	0
57	MG	CA	1606	1/1	0.94	0.20	-	8,8,8,8	0
57	MG	CA	1643	1/1	0.92	0.58	-	40,40,40,40	1
57	MG	BA	3158	1/1	0.90	0.37	-	29,29,29,29	0
57	MG	DA	9329	1/1	0.72	0.50	-	21,21,21,21	0
57	MG	DA	9644	1/1	0.97	0.16	-	25,25,25,25	0
57	MG	DA	9551	1/1	0.90	0.21	-	48,48,48,48	0
57	MG	DA	9684	1/1	0.93	0.21	-	8,8,8,8	0
57	MG	BA	3245	1/1	0.71	0.72	-	45,45,45,45	0
57	MG	CA	1639	1/1	0.59	0.69	-	55,55,55,55	0
57	MG	CA	1619	1/1	0.98	0.52	-	11,11,11,11	0
57	MG	DA	9307	1/1	0.97	0.37	-	12,12,12,12	0
57	MG	DA	9452	1/1	0.95	0.37	-	10,10,10,10	0
57	MG	DA	9555	1/1	0.93	0.32	-	39,39,39,39	0
57	MG	DA	9683	1/1	0.92	0.52	-	19,19,19,19	0
57	MG	DA	9610	1/1	0.95	0.64	-	19,19,19,19	0
57	MG	BA	3005	1/1	0.95	0.26	-	22,22,22,22	0
57	MG	BA	3097	1/1	0.86	0.26	-	43,43,43,43	0
57	MG	AA	7096	1/1	0.80	0.55	-	31,31,31,31	0
57	MG	BA	3316	1/1	0.98	0.42	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3087	1/1	0.89	0.24	-	21,21,21,21	0
57	MG	CE	201	1/1	0.95	0.67	-	16,16,16,16	0
57	MG	CA	1713	1/1	0.73	0.54	-	31,31,31,31	0
57	MG	AX	101	1/1	0.80	0.28	-	43,43,43,43	0
57	MG	BA	3016	1/1	0.96	0.35	-	8,8,8,8	0
57	MG	CA	1694	1/1	0.79	0.73	-	51,51,51,51	0
57	MG	BA	3244	1/1	0.96	0.20	-	1,1,1,1	0
57	MG	AA	7041	1/1	0.91	0.58	-	20,20,20,20	0
57	MG	BA	3217	1/1	0.84	0.16	-	28,28,28,28	0
57	MG	BA	3166	1/1	0.93	0.63	-	40,40,40,40	0
57	MG	BA	3018	1/1	0.95	0.17	-	37,37,37,37	0
57	MG	DA	9652	1/1	0.93	0.23	-	44,44,44,44	0
57	MG	CA	1655	1/1	0.82	0.47	-	24,24,24,24	0
57	MG	BA	3219	1/1	0.96	0.18	-	19,19,19,19	0
57	MG	DA	9320	1/1	0.93	0.25	-	10,10,10,10	0
57	MG	BA	3055	1/1	0.97	0.21	-	11,11,11,11	0
57	MG	DA	9687	1/1	0.68	0.28	-	12,12,12,12	0
57	MG	DA	9313	1/1	0.93	0.22	-	18,18,18,18	0
57	MG	BA	3094	1/1	0.87	0.35	-	7,7,7,7	0
57	MG	CA	1611	1/1	0.97	0.55	-	0,0,0,0	0
57	MG	AA	7023	1/1	0.90	0.26	-	56,56,56,56	0
57	MG	BA	3154	1/1	0.92	0.43	-	17,17,17,17	0
57	MG	DA	9641	1/1	0.98	0.07	-	11,11,11,11	0
57	MG	DA	9416	1/1	0.71	0.33	-	38,38,38,38	0
57	MG	BA	3157	1/1	0.89	0.22	-	6,6,6,6	0
57	MG	CA	1697	1/1	0.91	0.18	-	49,49,49,49	0
57	MG	BA	3323	1/1	0.91	0.48	-	26,26,26,26	0
57	MG	DA	9560	1/1	0.96	0.26	-	4,4,4,4	0
57	MG	BA	3048	1/1	0.97	0.29	-	17,17,17,17	0
57	MG	CA	1708	1/1	0.70	0.67	-	34,34,34,34	0
57	MG	AA	7069	1/1	0.77	0.76	-	11,11,11,11	1
57	MG	AA	7052	1/1	0.91	0.19	-	74,74,74,74	0
57	MG	DA	9361	1/1	0.86	0.34	-	5,5,5,5	0
57	MG	CA	1701	1/1	0.91	0.51	-	1,1,1,1	0
57	MG	DA	9676	1/1	0.79	0.23	-	13,13,13,13	0
57	MG	DA	9585	1/1	0.91	0.18	-	18,18,18,18	0
57	MG	DA	9379	1/1	0.80	0.32	-	41,41,41,41	0
57	MG	DA	9405	1/1	0.71	0.29	-	5,5,5,5	0
57	MG	BA	3318	1/1	0.74	0.41	-	37,37,37,37	0
57	MG	DA	9631	1/1	0.92	0.32	-	21,21,21,21	0
57	MG	DA	9668	1/1	0.97	0.51	-	4,4,4,4	0
57	MG	CA	1693	1/1	0.96	0.39	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9566	1/1	0.97	0.29	-	18,18,18,18	0
57	MG	DA	9427	1/1	0.97	0.20	-	91,91,91,91	0
57	MG	CA	1654	1/1	0.90	0.35	-	31,31,31,31	0
57	MG	BA	3194	1/1	0.96	0.28	-	1,1,1,1	0
57	MG	DA	9674	1/1	0.74	0.81	-	17,17,17,17	0
57	MG	BA	3180	1/1	0.97	0.60	-	2,2,2,2	0
57	MG	CA	1716	1/1	0.72	0.46	-	26,26,26,26	0
57	MG	DA	9390	1/1	0.98	0.28	-	0,0,0,0	0
57	MG	DA	9559	1/1	0.71	0.55	-	58,58,58,58	0
57	MG	DA	9686	1/1	0.88	0.20	-	11,11,11,11	0
57	MG	BA	3283	1/1	0.93	0.20	-	22,22,22,22	0
57	MG	BA	3063	1/1	0.63	0.47	-	55,55,55,55	0
57	MG	DA	9346	1/1	0.98	0.30	-	0,0,0,0	0
57	MG	BA	3280	1/1	0.97	0.28	-	19,19,19,19	1
57	MG	DA	9625	1/1	0.93	0.36	-	26,26,26,26	0
57	MG	CA	1660	1/1	0.85	0.37	-	9,9,9,9	0
57	MG	BA	3215	1/1	0.97	0.41	-	1,1,1,1	0
57	MG	DA	9456	1/1	0.88	0.62	-	19,19,19,19	0
57	MG	DA	9304	1/1	0.94	0.45	-	27,27,27,27	0
57	MG	AA	7070	1/1	0.93	0.15	-	61,61,61,61	0
57	MG	DA	9376	1/1	0.89	0.27	-	26,26,26,26	0
57	MG	DA	9323	1/1	0.94	0.56	-	33,33,33,33	0
57	MG	BA	3231	1/1	0.82	0.38	-	90,90,90,90	0
57	MG	CA	1736	1/1	0.92	0.31	-	6,6,6,6	0
57	MG	CA	1689	1/1	0.90	0.25	-	15,15,15,15	0
57	MG	BA	3132	1/1	0.92	0.32	-	51,51,51,51	0
57	MG	DA	9371	1/1	0.87	0.38	-	29,29,29,29	0
57	MG	DA	9415	1/1	0.93	0.49	-	0,0,0,0	0
57	MG	BA	3269	1/1	0.90	0.50	-	20,20,20,20	0
57	MG	DA	9509	1/1	0.97	0.44	-	17,17,17,17	0
57	MG	DA	9401	1/1	0.96	0.55	-	21,21,21,21	1
57	MG	AV	102	1/1	0.84	0.43	-	25,25,25,25	1
57	MG	BA	3095	1/1	0.77	1.01	-	35,35,35,35	0
57	MG	DA	9396	1/1	0.90	0.24	-	26,26,26,26	0
57	MG	DA	9535	1/1	0.88	0.42	-	14,14,14,14	0
57	MG	DA	9689	1/1	0.93	0.81	-	25,25,25,25	0
57	MG	CA	1733	1/1	0.98	0.46	-	11,11,11,11	0
57	MG	DA	9397	1/1	0.90	0.41	-	25,25,25,25	1
57	MG	BA	3320	1/1	0.76	0.42	-	54,54,54,54	0
57	MG	BA	3295	1/1	0.79	0.37	-	27,27,27,27	0
57	MG	DA	9608	1/1	0.90	0.46	-	19,19,19,19	0
57	MG	DA	9467	1/1	0.74	0.40	-	53,53,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CV	103	1/1	0.77	0.33	-	43,43,43,43	1
57	MG	CA	1729	1/1	0.98	0.43	-	35,35,35,35	0
57	MG	BA	3321	1/1	0.83	0.35	-	35,35,35,35	0
57	MG	BA	3021	1/1	0.80	0.48	-	49,49,49,49	0
57	MG	BA	3003	1/1	0.77	0.33	-	33,33,33,33	0
57	MG	DA	9630	1/1	0.91	0.27	-	16,16,16,16	1
57	MG	DA	9496	1/1	0.92	0.35	-	26,26,26,26	0
57	MG	BA	3035	1/1	0.95	0.39	-	0,0,0,0	0
57	MG	BA	3143	1/1	0.91	0.20	-	7,7,7,7	0
57	MG	CA	1650	1/1	0.93	0.52	-	34,34,34,34	0
57	MG	DA	9429	1/1	0.60	0.97	-	51,51,51,51	0
57	MG	CA	1625	1/1	0.94	0.43	-	26,26,26,26	0
57	MG	BA	3301	1/1	0.79	0.28	-	20,20,20,20	0
57	MG	AA	7074	1/1	0.75	0.76	-	26,26,26,26	0
57	MG	BA	3103	1/1	0.80	0.19	-	31,31,31,31	0
57	MG	DA	9400	1/1	0.98	0.41	-	0,0,0,0	0
57	MG	CA	1608	1/1	0.91	0.39	-	16,16,16,16	0
57	MG	CA	1703	1/1	0.94	0.46	-	9,9,9,9	0
57	MG	DA	9318	1/1	0.96	0.40	-	2,2,2,2	0
57	MG	DA	9353	1/1	0.96	0.55	-	24,24,24,24	0
57	MG	BA	3200	1/1	0.97	0.51	-	5,5,5,5	0
57	MG	D1	101	1/1	0.66	0.60	-	55,55,55,55	0
57	MG	AA	7073	1/1	0.90	0.23	-	29,29,29,29	0
57	MG	BA	3074	1/1	0.71	0.63	-	34,34,34,34	0
57	MG	BA	3246	1/1	0.74	0.65	-	33,33,33,33	0
57	MG	BA	3278	1/1	0.71	0.40	-	22,22,22,22	0
57	MG	BA	3226	1/1	0.91	0.65	-	36,36,36,36	0
57	MG	CA	1635	1/1	0.88	0.24	-	4,4,4,4	0
57	MG	CA	1682	1/1	0.76	0.27	-	60,60,60,60	0
57	MG	DA	9519	1/1	0.93	0.43	-	1,1,1,1	0
57	MG	AA	7098	1/1	0.93	0.34	-	28,28,28,28	0
57	MG	AA	7080	1/1	0.72	0.43	-	8,8,8,8	1
57	MG	DA	9651	1/1	0.89	0.14	-	81,81,81,81	0
57	MG	CA	1628	1/1	0.79	0.22	-	9,9,9,9	0
57	MG	BA	3209	1/1	0.89	0.34	-	1,1,1,1	0
57	MG	BA	3114	1/1	0.95	0.32	-	41,41,41,41	0
57	MG	BA	3186	1/1	0.92	0.36	-	2,2,2,2	0
57	MG	CA	1680	1/1	0.88	0.15	-	49,49,49,49	0
57	MG	CA	1641	1/1	0.86	0.21	-	40,40,40,40	0
57	MG	BA	3117	1/1	0.79	0.68	-	11,11,11,11	1
57	MG	DA	9643	1/1	0.76	0.72	-	34,34,34,34	1
57	MG	DA	9471	1/1	0.94	0.56	-	50,50,50,50	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	D8	101	1/1	0.95	0.23	-	3,3,3,3	0
57	MG	DA	9341	1/1	0.92	0.56	-	11,11,11,11	0
57	MG	DA	9685	1/1	0.65	0.64	-	22,22,22,22	0
57	MG	CA	1658	1/1	0.68	0.34	-	44,44,44,44	0
57	MG	BA	3267	1/1	0.88	0.39	-	41,41,41,41	0
57	MG	BA	3019	1/1	0.87	0.35	-	44,44,44,44	0
57	MG	DA	9543	1/1	0.96	0.30	-	5,5,5,5	0
57	MG	BA	3129	1/1	0.94	0.53	-	1,1,1,1	0
57	MG	AA	7086	1/1	0.56	1.00	-	30,30,30,30	0
57	MG	BA	3314	1/1	0.93	0.04	-	42,42,42,42	0
57	MG	DA	9495	1/1	0.97	0.74	-	3,3,3,3	0
57	MG	BA	3213	1/1	0.94	0.40	-	8,8,8,8	0
57	MG	AA	7022	1/1	0.92	0.26	-	32,32,32,32	0
57	MG	BA	3260	1/1	0.98	0.57	-	8,8,8,8	0
57	MG	DA	9576	1/1	0.88	0.42	-	22,22,22,22	0
57	MG	CA	1725	1/1	0.84	0.29	-	29,29,29,29	0
57	MG	CA	1698	1/1	0.96	0.14	-	1,1,1,1	1
57	MG	CA	1715	1/1	0.96	0.51	-	12,12,12,12	0
57	MG	BA	3172	1/1	0.97	0.28	-	58,58,58,58	0
57	MG	BA	3296	1/1	0.94	0.38	-	0,0,0,0	1
57	MG	DA	9656	1/1	0.89	0.29	-	58,58,58,58	0
57	MG	DA	9606	1/1	0.93	0.94	-	4,4,4,4	0
57	MG	BA	3292	1/1	0.83	0.29	-	28,28,28,28	0
57	MG	AA	7063	1/1	0.90	0.26	-	31,31,31,31	0
57	MG	DA	9591	1/1	0.92	0.25	-	52,52,52,52	0
57	MG	AA	7032	1/1	0.94	0.47	-	24,24,24,24	0
57	MG	CX	101	1/1	0.82	0.23	-	25,25,25,25	0
57	MG	DA	9474	1/1	0.96	0.30	-	28,28,28,28	0
57	MG	CA	1742	1/1	0.96	0.45	-	10,10,10,10	0
57	MG	DA	9594	1/1	0.91	0.78	-	19,19,19,19	0
57	MG	DA	9494	1/1	0.95	0.38	-	39,39,39,39	0
57	MG	DA	9635	1/1	0.81	0.59	-	24,24,24,24	0
57	MG	DA	9351	1/1	0.89	0.45	-	2,2,2,2	0
57	MG	BA	3266	1/1	0.79	0.39	-	33,33,33,33	0
57	MG	BA	3100	1/1	0.97	0.15	-	21,21,21,21	0
57	MG	DA	9598	1/1	0.92	0.50	-	14,14,14,14	0
57	MG	DA	9599	1/1	0.96	0.34	-	20,20,20,20	0
57	MG	BA	3163	1/1	0.93	0.32	-	28,28,28,28	0
57	MG	BA	3257	1/1	0.77	0.31	-	21,21,21,21	0
57	MG	DA	9660	1/1	0.79	0.27	-	176,176,176,176	0
57	MG	BA	3012	1/1	0.90	0.60	-	29,29,29,29	0
57	MG	BA	3118	1/1	0.93	0.61	-	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9322	1/1	0.97	0.25	-	8,8,8,8	0
57	MG	AA	7082	1/1	0.80	0.28	-	24,24,24,24	0
57	MG	BA	3273	1/1	0.63	0.26	-	71,71,71,71	0
57	MG	BA	3112	1/1	0.91	0.57	-	14,14,14,14	0
57	MG	DA	9548	1/1	0.95	0.72	-	26,26,26,26	0
57	MG	DA	9321	1/1	0.94	0.50	-	35,35,35,35	0
57	MG	D1	102	1/1	0.95	0.18	-	9,9,9,9	1
57	MG	DA	9432	1/1	0.74	0.63	-	38,38,38,38	0
57	MG	DA	9449	1/1	0.98	0.43	-	0,0,0,0	0
57	MG	BA	3305	1/1	0.96	0.25	-	24,24,24,24	0
57	MG	CA	1691	1/1	0.71	0.70	-	91,91,91,91	0
57	MG	DA	9542	1/1	0.98	0.35	-	6,6,6,6	0
57	MG	BA	3170	1/1	0.94	0.79	-	1,1,1,1	0
57	MG	DA	9567	1/1	0.93	0.43	-	31,31,31,31	0
57	MG	BA	3184	1/1	0.92	0.95	-	22,22,22,22	0
57	MG	BA	3223	1/1	0.95	0.19	-	9,9,9,9	0
57	MG	DA	9588	1/1	0.92	0.14	-	16,16,16,16	0
57	MG	CA	1681	1/1	0.84	0.86	-	18,18,18,18	1
57	MG	CA	1704	1/1	0.67	0.99	-	28,28,28,28	0
57	MG	DA	9637	1/1	0.97	0.37	-	18,18,18,18	0
57	MG	DA	9457	1/1	0.90	0.59	-	13,13,13,13	0
57	MG	BA	3002	1/1	0.92	0.27	-	53,53,53,53	0
57	MG	BA	3148	1/1	0.94	0.38	-	16,16,16,16	0
57	MG	CA	1603	1/1	0.96	0.17	-	0,0,0,0	0
57	MG	DA	9615	1/1	0.77	0.70	-	45,45,45,45	0
57	MG	DA	9344	1/1	0.97	0.44	-	33,33,33,33	0
57	MG	DA	9552	1/1	0.79	0.53	-	58,58,58,58	0
57	MG	BA	3075	1/1	0.93	0.70	-	12,12,12,12	0
57	MG	CA	1637	1/1	0.72	0.35	-	57,57,57,57	0
57	MG	DA	9667	1/1	0.85	0.36	-	10,10,10,10	0
57	MG	AA	7097	1/1	0.71	0.46	-	20,20,20,20	0
57	MG	BA	3151	1/1	0.97	0.13	-	12,12,12,12	0
57	MG	BA	3040	1/1	0.97	0.27	-	0,0,0,0	0
57	MG	AA	7106	1/1	0.95	0.25	-	12,12,12,12	0
57	MG	DA	9669	1/1	0.94	0.23	-	5,5,5,5	0
57	MG	CA	1723	1/1	0.68	0.34	-	15,15,15,15	0
57	MG	BA	3290	1/1	0.76	0.76	-	19,19,19,19	1
57	MG	BO	201	1/1	0.87	0.42	-	45,45,45,45	0
57	MG	D0	102	1/1	0.93	0.54	-	15,15,15,15	0
57	MG	BA	3070	1/1	0.82	0.43	-	34,34,34,34	0
57	MG	DA	9387	1/1	0.96	0.76	-	1,1,1,1	0
57	MG	CA	1673	1/1	0.86	0.24	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9465	1/1	0.89	0.39	-	34,34,34,34	0
57	MG	BA	3288	1/1	0.98	0.14	-	18,18,18,18	0
57	MG	BA	3214	1/1	0.85	0.31	-	39,39,39,39	0
57	MG	CA	1627	1/1	0.95	0.62	-	22,22,22,22	0
57	MG	DA	9573	1/1	0.77	0.40	-	45,45,45,45	0
57	MG	BA	3171	1/1	0.91	0.45	-	7,7,7,7	0
57	MG	AA	7031	1/1	0.81	0.20	-	44,44,44,44	0
57	MG	BA	3134	1/1	0.84	0.48	-	21,21,21,21	0
57	MG	DA	9357	1/1	0.96	0.37	-	0,0,0,0	0
57	MG	DA	9478	1/1	0.96	0.40	-	13,13,13,13	0
57	MG	AA	7048	1/1	0.91	0.27	-	27,27,27,27	0
57	MG	BA	3299	1/1	0.99	0.47	-	10,10,10,10	0
57	MG	BA	3271	1/1	0.57	0.72	-	52,52,52,52	0
57	MG	CA	1717	1/1	0.89	0.30	-	11,11,11,11	0
57	MG	CA	1687	1/1	0.52	0.36	-	47,47,47,47	0
57	MG	BA	3285	1/1	0.85	1.73	-	32,32,32,32	1
57	MG	BA	3011	1/1	0.97	0.52	-	36,36,36,36	0
57	MG	DA	9492	1/1	0.96	0.11	-	76,76,76,76	0
57	MG	BA	3211	1/1	0.96	0.17	-	2,2,2,2	0
57	MG	BA	3274	1/1	0.80	0.26	-	8,8,8,8	1
57	MG	DA	9330	1/1	0.95	0.35	-	0,0,0,0	0
57	MG	AA	7033	1/1	0.97	0.18	-	35,35,35,35	0
57	MG	DA	9677	1/1	0.77	0.50	-	27,27,27,27	0
57	MG	BA	3026	1/1	0.78	0.50	-	29,29,29,29	0
57	MG	AA	7105	1/1	0.84	0.74	-	42,42,42,42	0
57	MG	DA	9520	1/1	0.97	0.47	-	2,2,2,2	0
57	MG	BB	203	1/1	0.66	0.70	-	16,16,16,16	1
57	MG	DA	9477	1/1	0.90	0.56	-	36,36,36,36	0
57	MG	AA	7089	1/1	0.94	0.24	-	21,21,21,21	0
57	MG	DA	9695	1/1	0.83	0.39	-	63,63,63,63	0
57	MG	BA	3032	1/1	0.93	0.20	-	18,18,18,18	0
57	MG	AA	7025	1/1	0.97	0.21	-	1,1,1,1	0
57	MG	DA	9315	1/1	0.97	0.10	-	26,26,26,26	0
57	MG	DA	9607	1/1	0.91	0.34	-	49,49,49,49	0
57	MG	BA	3189	1/1	0.96	0.46	-	1,1,1,1	0
57	MG	B5	101	1/1	0.92	0.30	-	2,2,2,2	0
57	MG	AA	7107	1/1	0.87	0.45	-	24,24,24,24	0
57	MG	DA	9534	1/1	0.97	0.51	-	1,1,1,1	0
57	MG	BA	3199	1/1	0.92	0.48	-	1,1,1,1	0
57	MG	DA	9577	1/1	0.90	0.91	-	102,102,102,102	0
57	MG	DA	9476	1/1	0.94	0.47	-	2,2,2,2	0
57	MG	DA	9617	1/1	0.97	0.29	-	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3138	1/1	0.95	0.32	-	15,15,15,15	0
57	MG	AV	103	1/1	0.89	0.26	-	7,7,7,7	1
57	MG	CA	1621	1/1	0.66	0.39	-	52,52,52,52	0
57	MG	BA	3277	1/1	0.65	0.56	-	2,2,2,2	1
57	MG	AA	7039	1/1	0.93	0.34	-	11,11,11,11	0
57	MG	DA	9350	1/1	0.44	0.18	-	48,48,48,48	1
57	MG	BA	3197	1/1	0.98	0.22	-	1,1,1,1	0
57	MG	DA	9424	1/1	0.95	0.52	-	5,5,5,5	0
57	MG	BA	3302	1/1	0.94	0.48	-	8,8,8,8	0
57	MG	AA	7102	1/1	0.95	0.48	-	38,38,38,38	0
57	MG	CV	104	1/1	0.92	0.28	-	22,22,22,22	1
57	MG	DA	9507	1/1	0.95	0.55	-	2,2,2,2	0
57	MG	CA	1732	1/1	0.88	0.53	-	27,27,27,27	0
57	MG	BA	3124	1/1	0.98	0.20	-	17,17,17,17	0
57	MG	DA	9326	1/1	0.95	0.24	-	1,1,1,1	0
57	MG	BA	3181	1/1	0.95	0.49	-	1,1,1,1	0
57	MG	AA	7093	1/1	0.93	0.34	-	30,30,30,30	0
57	MG	CA	1672	1/1	0.75	0.39	-	62,62,62,62	0
57	MG	BA	3049	1/1	0.92	0.51	-	30,30,30,30	0
57	MG	DA	9616	1/1	0.87	0.54	-	54,54,54,54	0
57	MG	BA	3023	1/1	0.94	0.28	-	4,4,4,4	0
57	MG	DA	9501	1/1	0.90	0.48	-	42,42,42,42	0
57	MG	BA	3232	1/1	0.93	0.18	-	44,44,44,44	0
57	MG	BA	3303	1/1	0.96	0.29	-	19,19,19,19	0
57	MG	DA	9485	1/1	0.95	0.41	-	15,15,15,15	0
57	MG	BA	3155	1/1	0.76	0.56	-	33,33,33,33	0
57	MG	CA	1731	1/1	0.70	0.15	-	30,30,30,30	0
57	MG	BA	3104	1/1	0.90	0.24	-	16,16,16,16	0
57	MG	BA	3152	1/1	0.96	0.32	-	18,18,18,18	0
57	MG	DA	9654	1/1	0.95	0.29	-	15,15,15,15	0
57	MG	BA	3284	1/1	0.86	0.33	-	21,21,21,21	0
57	MG	BA	3101	1/1	0.87	1.28	-	27,27,27,27	1
57	MG	AA	7109	1/1	0.95	0.36	-	33,33,33,33	0
57	MG	CA	1706	1/1	0.79	0.36	-	32,32,32,32	0
57	MG	BA	3230	1/1	0.93	0.61	-	22,22,22,22	0
57	MG	CA	1663	1/1	0.90	0.66	-	11,11,11,11	0
57	MG	DA	9306	1/1	0.93	0.35	-	4,4,4,4	0
57	MG	CA	1675	1/1	0.87	0.42	-	55,55,55,55	0
57	MG	DA	9657	1/1	0.69	0.32	-	29,29,29,29	0
57	MG	DA	9693	1/1	0.83	0.97	-	47,47,47,47	0
57	MG	DA	9531	1/1	0.94	0.37	-	1,1,1,1	0
57	MG	CA	1616	1/1	0.91	0.41	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	7072	1/1	0.93	0.15	-	23,23,23,23	0
57	MG	DA	9571	1/1	0.97	0.44	-	0,0,0,0	0
57	MG	DA	9671	1/1	0.77	0.19	-	45,45,45,45	0
57	MG	DA	9627	1/1	0.98	0.30	-	0,0,0,0	1
57	MG	AA	7049	1/1	0.82	0.25	-	41,41,41,41	0
57	MG	BA	3014	1/1	0.93	0.25	-	33,33,33,33	0
57	MG	BA	3216	1/1	0.66	0.50	-	48,48,48,48	0
57	MG	CA	1601	1/1	0.88	0.39	-	39,39,39,39	0
57	MG	CA	1690	1/1	0.89	0.54	-	17,17,17,17	0
57	MG	BA	3258	1/1	0.87	1.06	-	19,19,19,19	0
57	MG	CA	1636	1/1	0.94	0.32	-	19,19,19,19	0
57	MG	DA	9568	1/1	0.89	0.37	-	3,3,3,3	0
57	MG	BA	3147	1/1	0.95	0.59	-	48,48,48,48	0
57	MG	BA	3042	1/1	0.94	0.67	-	8,8,8,8	0
57	MG	BA	3289	1/1	0.95	0.51	-	21,21,21,21	0
57	MG	CA	1721	1/1	0.94	0.20	-	1,1,1,1	0
57	MG	DA	9604	1/1	0.91	0.33	-	21,21,21,21	0
57	MG	BA	3141	1/1	0.91	0.26	-	18,18,18,18	0
57	MG	CA	1612	1/1	0.73	0.30	-	31,31,31,31	0
57	MG	DA	9311	1/1	0.95	0.47	-	29,29,29,29	0
57	MG	CA	1647	1/1	0.97	0.36	-	6,6,6,6	0
57	MG	BA	3082	1/1	0.78	0.32	-	23,23,23,23	0
57	MG	BA	3162	1/1	0.81	0.73	-	4,4,4,4	0
57	MG	DA	9336	1/1	0.79	0.33	-	52,52,52,52	0
57	MG	DA	9569	1/1	0.73	0.81	-	54,54,54,54	0
57	MG	CV	105	1/1	0.94	0.15	-	69,69,69,69	0
57	MG	DA	9692	1/1	0.83	0.42	-	30,30,30,30	0
57	MG	BB	204	1/1	0.95	0.30	-	23,23,23,23	0
57	MG	DA	9510	1/1	0.95	0.51	-	1,1,1,1	0
57	MG	BA	3202	1/1	0.89	0.50	-	7,7,7,7	0
57	MG	DE	302	1/1	0.90	0.22	-	35,35,35,35	0
57	MG	DE	301	1/1	0.95	0.32	-	1,1,1,1	0
57	MG	DA	9469	1/1	0.92	0.58	-	17,17,17,17	0
57	MG	DA	9579	1/1	0.82	0.67	-	38,38,38,38	0
57	MG	AA	7045	1/1	0.87	0.75	-	38,38,38,38	0
57	MG	AA	7065	1/1	0.76	0.38	-	23,23,23,23	0
57	MG	BA	3179	1/1	0.98	0.31	-	10,10,10,10	0
57	MG	CA	1642	1/1	0.78	0.37	-	54,54,54,54	0
57	MG	DA	9691	1/1	0.92	0.41	-	12,12,12,12	0
57	MG	DA	9648	1/1	0.74	0.31	-	34,34,34,34	0
57	MG	CA	1684	1/1	0.89	0.21	-	41,41,41,41	0
57	MG	DA	9375	1/1	0.95	0.54	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9622	1/1	0.70	0.56	-	36,36,36,36	0
57	MG	AA	7084	1/1	0.88	0.12	-	49,49,49,49	0
57	MG	DA	9448	1/1	0.94	0.38	-	18,18,18,18	0
57	MG	DA	9343	1/1	0.97	0.27	-	2,2,2,2	0
57	MG	DA	9620	1/1	0.79	0.41	-	26,26,26,26	0
57	MG	DA	9511	1/1	0.94	0.80	-	7,7,7,7	0
57	MG	DA	9378	1/1	0.78	0.34	-	29,29,29,29	0
57	MG	DA	9642	1/1	0.96	0.30	-	1,1,1,1	0
57	MG	DA	9661	1/1	0.57	0.38	-	57,57,57,57	0
57	MG	DA	9601	1/1	0.97	0.35	-	31,31,31,31	0
57	MG	DA	9420	1/1	0.91	0.52	-	6,6,6,6	0
57	MG	BA	3291	1/1	0.93	0.16	-	22,22,22,22	0
57	MG	DA	9386	1/1	0.98	0.47	-	2,2,2,2	0
57	MG	DA	9463	1/1	0.95	0.26	-	12,12,12,12	0
57	MG	DA	9480	1/1	0.90	0.28	-	30,30,30,30	0
57	MG	DA	9524	1/1	0.98	0.36	-	2,2,2,2	0
57	MG	AA	7004	1/1	0.88	0.29	-	30,30,30,30	0
57	MG	BA	3206	1/1	0.98	0.45	-	29,29,29,29	0
57	MG	DA	9406	1/1	0.98	0.19	-	32,32,32,32	0
57	MG	DA	9645	1/1	0.77	0.72	-	4,4,4,4	0
57	MG	CA	1648	1/1	0.96	0.42	-	23,23,23,23	0
57	MG	CA	1734	1/1	0.93	0.24	-	22,22,22,22	0
57	MG	DA	9500	1/1	0.97	0.22	-	1,1,1,1	0
57	MG	DP	202	1/1	0.87	0.26	-	173,173,173,173	0
57	MG	AA	7083	1/1	0.85	0.55	-	18,18,18,18	0
57	MG	DB	201	1/1	0.95	0.41	-	22,22,22,22	0
57	MG	BA	3268	1/1	0.84	0.33	-	13,13,13,13	1
57	MG	AA	7028	1/1	0.96	0.85	-	30,30,30,30	0
57	MG	DA	9367	1/1	0.89	0.41	-	35,35,35,35	0
57	MG	DA	9462	1/1	0.85	0.40	-	30,30,30,30	0
57	MG	BA	3036	1/1	0.47	0.19	-	78,78,78,78	1
57	MG	AA	7050	1/1	0.92	1.06	-	29,29,29,29	0
57	MG	BA	3052	1/1	0.70	0.45	-	40,40,40,40	0
57	MG	DA	9380	1/1	0.87	1.56	-	23,23,23,23	1
57	MG	BA	3192	1/1	0.93	0.38	-	2,2,2,2	0
57	MG	BA	3001	1/1	0.90	0.38	-	38,38,38,38	0
57	MG	BA	3123	1/1	0.92	0.20	-	14,14,14,14	0
57	MG	AA	7077	1/1	0.98	0.16	-	22,22,22,22	0
57	MG	DA	9532	1/1	0.94	0.43	-	9,9,9,9	0
57	MG	DA	9301	1/1	0.83	0.36	-	32,32,32,32	0
57	MG	AA	7024	1/1	0.95	0.50	-	27,27,27,27	0
57	MG	BA	3113	1/1	0.83	0.87	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9411	1/1	0.97	0.27	-	2,2,2,2	0
57	MG	DA	9646	1/1	0.96	0.22	-	31,31,31,31	0
57	MG	DA	9440	1/1	0.68	0.49	-	25,25,25,25	0
57	MG	AA	7002	1/1	0.64	0.48	-	35,35,35,35	0
57	MG	DA	9670	1/1	0.88	0.47	-	11,11,11,11	0
57	MG	DA	9314	1/1	0.93	0.32	-	1,1,1,1	0
57	MG	DA	9325	1/1	0.82	0.48	-	32,32,32,32	0
57	MG	CA	1735	1/1	0.87	0.47	-	29,29,29,29	0
57	MG	DA	9423	1/1	0.88	0.29	-	1,1,1,1	0
57	MG	BA	3169	1/1	0.95	0.51	-	3,3,3,3	0
57	MG	BA	3298	1/1	0.87	0.80	-	18,18,18,18	0
57	MG	AE	201	1/1	0.84	0.40	-	45,45,45,45	0
57	MG	DA	9550	1/1	0.73	0.44	-	55,55,55,55	0
57	MG	DA	9419	1/1	0.80	0.95	-	10,10,10,10	1
57	MG	BA	3122	1/1	0.55	0.30	-	13,13,13,13	0
57	MG	CA	1613	1/1	0.97	0.95	-	31,31,31,31	0
57	MG	DA	9468	1/1	0.88	0.72	-	2,2,2,2	1
57	MG	BA	3263	1/1	0.92	0.64	-	16,16,16,16	1
57	MG	BA	3259	1/1	0.99	0.32	-	18,18,18,18	0
57	MG	BA	3177	1/1	0.89	0.20	-	0,0,0,0	0
57	MG	BA	3107	1/1	0.78	0.45	-	36,36,36,36	0
57	MG	CA	1686	1/1	0.93	0.22	-	77,77,77,77	0
57	MG	BA	3137	1/1	0.86	0.61	-	1,1,1,1	1
57	MG	DA	9345	1/1	0.95	0.52	-	19,19,19,19	0
57	MG	DB	204	1/1	0.91	0.70	-	0,0,0,0	1
57	MG	AA	7079	1/1	0.90	0.41	-	35,35,35,35	0
57	MG	AA	7015	1/1	0.95	0.29	-	4,4,4,4	0
57	MG	DA	9538	1/1	0.96	0.46	-	1,1,1,1	0
57	MG	DA	9562	1/1	0.97	0.60	-	2,2,2,2	0
57	MG	BA	3080	1/1	0.97	0.56	-	0,0,0,0	0
57	MG	DA	9374	1/1	0.82	0.40	-	28,28,28,28	0
57	MG	AA	7012	1/1	0.89	0.78	-	12,12,12,12	0
57	MG	CA	1739	1/1	0.75	0.66	-	36,36,36,36	0
57	MG	DA	9407	1/1	0.91	0.22	-	2,2,2,2	0
57	MG	BA	3261	1/1	0.96	0.32	-	10,10,10,10	0
57	MG	DA	9662	1/1	0.93	0.54	-	2,2,2,2	0
57	MG	DW	201	1/1	0.84	0.47	-	27,27,27,27	0
57	MG	BA	3221	1/1	0.85	0.69	-	17,17,17,17	0
57	MG	BA	3006	1/1	0.91	0.33	-	38,38,38,38	0
57	MG	DA	9332	1/1	0.91	0.37	-	34,34,34,34	0
57	MG	CA	1700	1/1	0.91	0.28	-	20,20,20,20	0
57	MG	BA	3078	1/1	0.98	0.43	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	7046	1/1	0.69	0.42	-	35,35,35,35	0
57	MG	BA	3195	1/1	0.85	0.32	-	3,3,3,3	0
57	MG	AA	7020	1/1	0.90	0.36	-	33,33,33,33	0
57	MG	DA	9475	1/1	0.86	0.65	-	26,26,26,26	0
57	MG	DA	9596	1/1	0.95	0.14	-	27,27,27,27	0
57	MG	CW	101	1/1	0.82	0.47	-	29,29,29,29	1
57	MG	DA	9513	1/1	0.90	0.48	-	22,22,22,22	0
57	MG	DA	9694	1/1	0.74	0.85	-	25,25,25,25	0
57	MG	CY	101	1/1	0.90	0.58	-	33,33,33,33	0
57	MG	CA	1618	1/1	0.94	0.22	-	31,31,31,31	0
57	MG	BA	3017	1/1	0.92	0.55	-	22,22,22,22	0
57	MG	BA	3313	1/1	0.69	0.26	-	42,42,42,42	0
57	MG	DA	9633	1/1	0.91	0.73	-	30,30,30,30	0
57	MG	DA	9666	1/1	0.91	0.36	-	7,7,7,7	0
57	MG	BA	3037	1/1	0.49	0.27	-	83,83,83,83	0
57	MG	D5	102	1/1	0.95	0.33	-	32,32,32,32	1
57	MG	DA	9611	1/1	0.89	0.46	-	8,8,8,8	0
57	MG	DA	9522	1/1	0.97	0.48	-	2,2,2,2	0
57	MG	BA	3079	1/1	0.94	0.34	-	29,29,29,29	1
57	MG	DA	9639	1/1	0.88	0.49	-	57,57,57,57	0
57	MG	DA	9455	1/1	0.95	0.45	-	0,0,0,0	0
57	MG	BA	3139	1/1	0.96	0.46	-	0,0,0,0	0
57	MG	DA	9578	1/1	0.81	0.43	-	44,44,44,44	0
57	MG	BA	3156	1/1	0.96	0.33	-	19,19,19,19	0
57	MG	AA	7038	1/1	0.96	0.64	-	10,10,10,10	0
57	MG	BA	3067	1/1	0.92	0.80	-	2,2,2,2	0
57	MG	DA	9609	1/1	0.87	0.45	-	2,2,2,2	0
57	MG	BA	3150	1/1	0.88	0.30	-	1,1,1,1	0
57	MG	BA	3247	1/1	0.97	0.80	-	55,55,55,55	0
57	MG	DA	9540	1/1	0.95	0.34	-	0,0,0,0	0
57	MG	BA	3207	1/1	0.97	0.38	-	1,1,1,1	0
57	MG	BA	3212	1/1	0.94	0.24	-	8,8,8,8	0
57	MG	BA	3236	1/1	0.91	0.56	-	17,17,17,17	0
57	MG	BA	3250	1/1	0.97	0.31	-	18,18,18,18	0
57	MG	DA	9580	1/1	0.95	0.46	-	0,0,0,0	0
57	MG	CA	1714	1/1	0.74	0.45	-	53,53,53,53	0
57	MG	BA	3025	1/1	0.96	0.16	-	37,37,37,37	0
57	MG	BA	3009	1/1	0.98	0.15	-	2,2,2,2	0
57	MG	CA	1718	1/1	0.98	0.27	-	27,27,27,27	0
57	MG	BA	3239	1/1	0.99	0.35	-	1,1,1,1	0
57	MG	DA	9502	1/1	0.87	0.41	-	3,3,3,3	0
57	MG	AA	7017	1/1	0.96	0.08	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CE	202	1/1	0.90	0.38	-	34,34,34,34	0
57	MG	BA	3228	1/1	0.95	0.61	-	13,13,13,13	0
57	MG	DA	9682	1/1	0.95	0.42	-	20,20,20,20	0
57	MG	BA	3190	1/1	0.97	0.47	-	8,8,8,8	0
57	MG	DA	9368	1/1	0.94	0.19	-	1,1,1,1	0
57	MG	CA	1695	1/1	0.93	0.37	-	15,15,15,15	0
57	MG	BA	3121	1/1	0.97	0.60	-	1,1,1,1	0
57	MG	DA	9470	1/1	0.93	0.27	-	0,0,0,0	0
57	MG	DA	9664	1/1	0.96	0.54	-	1,1,1,1	0
57	MG	DA	9556	1/1	0.90	0.23	-	23,23,23,23	0
57	MG	AA	7088	1/1	0.90	0.13	-	60,60,60,60	0
57	MG	DA	9688	1/1	0.83	0.40	-	78,78,78,78	0
57	MG	CA	1692	1/1	0.80	0.37	-	28,28,28,28	0
57	MG	DP	201	1/1	0.96	0.12	-	7,7,7,7	0
57	MG	AA	7009	1/1	0.91	0.27	-	18,18,18,18	0
57	MG	DA	9442	1/1	0.94	0.54	-	36,36,36,36	0
57	MG	CA	1615	1/1	0.98	0.27	-	0,0,0,0	0
57	MG	DA	9422	1/1	0.88	0.96	-	56,56,56,56	0
57	MG	AA	7036	1/1	0.88	0.38	-	42,42,42,42	0
57	MG	AA	7108	1/1	0.87	0.42	-	27,27,27,27	0
57	MG	CA	1634	1/1	0.92	0.32	-	43,43,43,43	0
57	MG	AA	7100	1/1	0.84	0.82	-	21,21,21,21	0
57	MG	CA	1609	1/1	0.67	0.42	-	30,30,30,30	0
57	MG	BA	3254	1/1	0.84	0.90	-	54,54,54,54	0
57	MG	AA	7103	1/1	0.94	0.53	-	13,13,13,13	0
57	MG	DA	9334	1/1	0.92	0.44	-	27,27,27,27	0
57	MG	DA	9603	1/1	0.78	0.88	-	33,33,33,33	0
57	MG	CA	1644	1/1	0.94	0.14	-	45,45,45,45	0
57	MG	AA	7001	1/1	0.93	0.28	-	26,26,26,26	0
57	MG	DA	9393	1/1	0.91	0.30	-	24,24,24,24	0
57	MG	BB	201	1/1	0.84	0.15	-	34,34,34,34	0
57	MG	DA	9348	1/1	0.81	0.72	-	47,47,47,47	0
57	MG	CA	1712	1/1	0.95	0.21	-	34,34,34,34	1
57	MG	CA	1646	1/1	0.91	0.42	-	7,7,7,7	0
57	MG	AA	7078	1/1	0.93	0.25	-	30,30,30,30	0
57	MG	CA	1638	1/1	0.83	0.42	-	24,24,24,24	0
57	MG	CA	1604	1/1	0.96	0.43	-	15,15,15,15	0
57	MG	BA	3183	1/1	0.91	0.65	-	56,56,56,56	0
57	MG	DA	9333	1/1	0.90	0.11	-	31,31,31,31	0
57	MG	DA	9663	1/1	0.91	0.59	-	7,7,7,7	0
57	MG	CA	1620	1/1	0.98	0.27	-	1,1,1,1	0
57	MG	D5	101	1/1	0.96	0.36	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3057	1/1	0.93	0.54	-	2,2,2,2	0
57	MG	DA	9412	1/1	0.75	0.34	-	27,27,27,27	0
57	MG	DA	9384	1/1	0.95	0.29	-	16,16,16,16	0
57	MG	BA	3013	1/1	0.99	0.30	-	16,16,16,16	0
57	MG	BA	3315	1/1	0.17	0.44	-	84,84,84,84	0
57	MG	CA	1676	1/1	0.83	0.60	-	88,88,88,88	0
57	MG	DA	9327	1/1	0.86	0.17	-	20,20,20,20	0
57	MG	DA	9394	1/1	0.92	0.47	-	16,16,16,16	0
57	MG	DA	9450	1/1	0.79	0.54	-	2,2,2,2	1
57	MG	DA	9403	1/1	0.94	0.26	-	0,0,0,0	0
57	MG	DA	9650	1/1	0.97	0.26	-	7,7,7,7	0
57	MG	DA	9372	1/1	0.88	0.43	-	8,8,8,8	0
57	MG	CA	1669	1/1	0.94	0.10	-	10,10,10,10	0
57	MG	DA	9309	1/1	0.98	0.35	-	6,6,6,6	0
57	MG	DA	9352	1/1	0.85	0.22	-	89,89,89,89	0
57	MG	DA	9612	1/1	0.96	0.70	-	1,1,1,1	1
57	MG	BA	3168	1/1	0.92	0.71	-	36,36,36,36	0
57	MG	BA	3294	1/1	0.87	0.50	-	15,15,15,15	1
57	MG	DA	9640	1/1	0.85	0.41	-	42,42,42,42	0
57	MG	AA	7101	1/1	0.88	0.65	-	22,22,22,22	0
57	MG	DA	9466	1/1	0.87	0.45	-	36,36,36,36	0
57	MG	DA	9602	1/1	0.77	0.52	-	37,37,37,37	0
57	MG	AA	7060	1/1	0.95	0.13	-	8,8,8,8	0
57	MG	AA	7047	1/1	0.86	0.35	-	41,41,41,41	0
57	MG	BA	3311	1/1	0.95	0.43	-	13,13,13,13	0
57	MG	DA	9632	1/1	0.94	0.48	-	12,12,12,12	1
57	MG	DA	9636	1/1	0.92	0.28	-	16,16,16,16	0
57	MG	DA	9634	1/1	0.85	0.41	-	44,44,44,44	0
57	MG	BA	3024	1/1	0.93	0.61	-	22,22,22,22	0
57	MG	DA	9490	1/1	0.88	0.22	-	39,39,39,39	0
57	MG	CA	1659	1/1	0.95	0.28	-	28,28,28,28	0
57	MG	BA	3304	1/1	0.94	0.43	-	13,13,13,13	0
57	MG	DA	9338	1/1	0.91	0.56	-	58,58,58,58	0
57	MG	DA	9624	1/1	0.70	0.23	-	18,18,18,18	1
57	MG	BA	3093	1/1	0.87	0.29	-	49,49,49,49	0
57	MG	AA	7099	1/1	0.97	0.36	-	6,6,6,6	0
57	MG	DX	101	1/1	0.86	0.35	-	6,6,6,6	0
57	MG	BA	3060	1/1	0.98	0.57	-	1,1,1,1	0
57	MG	CA	1661	1/1	0.86	0.35	-	50,50,50,50	0
57	MG	CV	101	1/1	0.87	0.37	-	12,12,12,12	1
57	MG	AA	7081	1/1	0.94	0.46	-	44,44,44,44	0
57	MG	DA	9595	1/1	0.68	0.58	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1623	1/1	0.97	0.27	-	19,19,19,19	0
57	MG	DA	9328	1/1	0.89	0.33	-	1,1,1,1	0
57	MG	DA	9628	1/1	0.75	0.28	-	35,35,35,35	1
57	MG	CA	1728	1/1	0.78	0.35	-	59,59,59,59	0
57	MG	DA	9337	1/1	0.86	0.61	-	45,45,45,45	0
57	MG	DA	9658	1/1	0.74	0.19	-	36,36,36,36	0
57	MG	BA	3077	1/1	0.86	0.43	-	21,21,21,21	0
57	MG	BA	3242	1/1	0.74	0.59	-	44,44,44,44	0
57	MG	AV	105	1/1	0.90	0.34	-	54,54,54,54	0
57	MG	DA	9331	1/1	0.80	0.21	-	8,8,8,8	0
57	MG	DA	9444	1/1	0.88	0.51	-	42,42,42,42	0
57	MG	BA	3322	1/1	0.81	0.35	-	54,54,54,54	0
57	MG	AA	7055	1/1	0.68	0.46	-	29,29,29,29	0
57	MG	DA	9414	1/1	0.97	0.81	-	16,16,16,16	0
57	MG	AA	7010	1/1	0.73	0.26	-	30,30,30,30	0
57	MG	BA	3286	1/1	0.78	0.25	-	22,22,22,22	0
57	MG	BA	3010	1/1	0.96	0.89	-	28,28,28,28	0
57	MG	DA	9385	1/1	0.83	0.24	-	5,5,5,5	0
57	MG	AA	7076	1/1	0.66	0.57	-	60,60,60,60	0
57	MG	AA	7005	1/1	0.91	0.28	-	45,45,45,45	0
57	MG	DA	9317	1/1	0.90	0.26	-	18,18,18,18	0
57	MG	DA	9572	1/1	0.83	0.42	-	4,4,4,4	0
57	MG	CA	1722	1/1	0.79	0.34	-	27,27,27,27	0
57	MG	BA	3140	1/1	0.92	0.24	-	40,40,40,40	0
57	MG	DA	9488	1/1	0.98	0.56	-	0,0,0,0	0
57	MG	DA	9451	1/1	0.92	0.56	-	35,35,35,35	0
57	MG	BA	3175	1/1	0.96	0.28	-	4,4,4,4	0
57	MG	DA	9541	1/1	0.89	0.39	-	2,2,2,2	0
57	MG	BA	3176	1/1	0.98	0.33	-	0,0,0,0	0
57	MG	BA	3105	1/1	0.98	0.69	-	26,26,26,26	0
57	MG	DA	9426	1/1	0.95	0.43	-	9,9,9,9	1
57	MG	BA	3128	1/1	0.94	0.26	-	57,57,57,57	0
57	MG	DA	9626	1/1	0.57	0.19	-	8,8,8,8	1
57	MG	DA	9362	1/1	0.98	0.34	-	5,5,5,5	0
57	MG	CA	1740	1/1	0.87	0.61	-	48,48,48,48	0
57	MG	DA	9564	1/1	0.98	0.58	-	17,17,17,17	0
57	MG	DA	9525	1/1	0.93	0.30	-	4,4,4,4	0
57	MG	BA	3262	1/1	0.71	0.63	-	39,39,39,39	0
57	MG	DA	9413	1/1	0.91	0.38	-	3,3,3,3	0
57	MG	BA	3064	1/1	0.95	0.25	-	29,29,29,29	1
57	MG	DA	9665	1/1	0.70	0.99	-	9,9,9,9	0
57	MG	CA	1724	1/1	0.95	0.44	-	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9453	1/1	0.91	0.44	-	4,4,4,4	1
57	MG	DA	9565	1/1	0.86	0.38	-	11,11,11,11	0
57	MG	DA	9589	1/1	0.88	0.18	-	32,32,32,32	0
57	MG	CA	1688	1/1	0.90	0.15	-	16,16,16,16	0
57	MG	BA	3165	1/1	0.97	0.57	-	0,0,0,0	0
57	MG	BA	3130	1/1	0.86	0.19	-	3,3,3,3	0
57	MG	BA	3096	1/1	0.94	0.42	-	12,12,12,12	0
57	MG	DA	9582	1/1	0.94	0.88	-	21,21,21,21	0
57	MG	CA	1664	1/1	0.93	0.45	-	24,24,24,24	0
57	MG	BA	3233	1/1	0.91	0.45	-	19,19,19,19	0
57	MG	BA	3317	1/1	0.79	0.73	-	21,21,21,21	0
57	MG	DA	9505	1/1	0.95	0.29	-	0,0,0,0	0
57	MG	BE	301	1/1	0.82	0.24	-	0,0,0,0	0
57	MG	CA	1702	1/1	0.61	0.14	-	49,49,49,49	0
57	MG	BA	3110	1/1	0.73	0.59	-	23,23,23,23	1
57	MG	DA	9638	1/1	0.95	0.27	-	8,8,8,8	1
57	MG	BA	3106	1/1	0.83	0.49	-	34,34,34,34	0
57	MG	CA	1696	1/1	0.95	0.34	-	49,49,49,49	0
57	MG	DA	9447	1/1	0.95	0.23	-	68,68,68,68	0
57	MG	BA	3135	1/1	0.93	0.58	-	43,43,43,43	0

6.5 Other polymers

There are no such residues in this entry.