



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:54 PM GMT

PDB ID : 4V6A
Title : Structure of EF-P bound to the 70S ribosome.
Authors : Stanley, R.E.; Blaha, G.
Deposited on : 2009-06-15
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

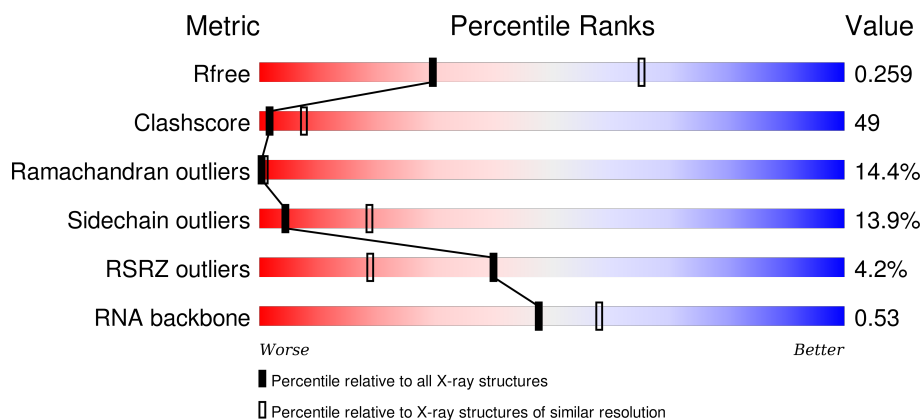
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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	1509	<div> <div>3%</div> <div>17%</div> <div>67%</div> <div>14%</div> <div>..</div> </div>
1	CA	1509	<div> <div>2%</div> <div>21%</div> <div>65%</div> <div>13%</div> <div>.</div> </div>
2	AB	256	<div> <div>7%</div> <div>13%</div> <div>59%</div> <div>19%</div> <div>8%</div> </div>
2	CB	256	<div> <div>7%</div> <div>15%</div> <div>56%</div> <div>19%</div> <div>8%</div> </div>

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

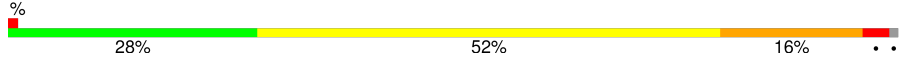
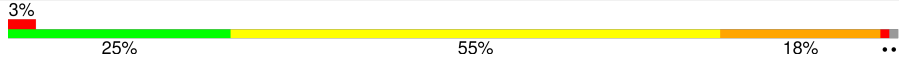
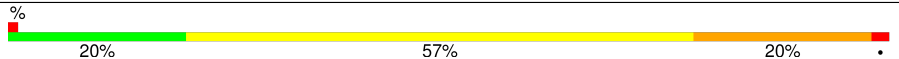
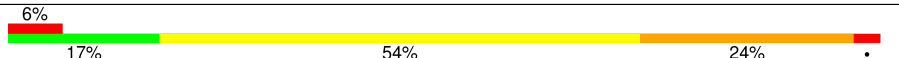
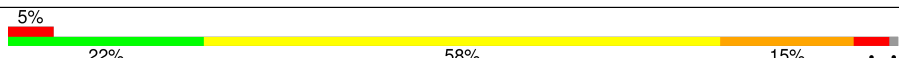
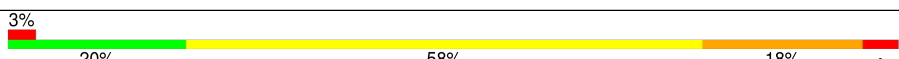
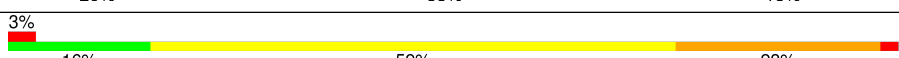
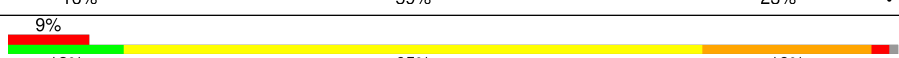
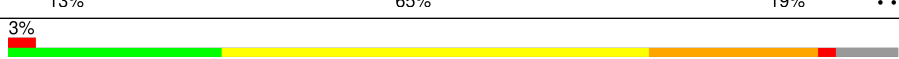
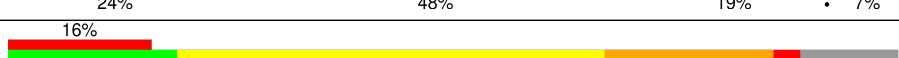
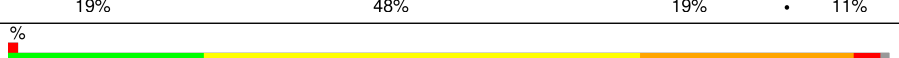
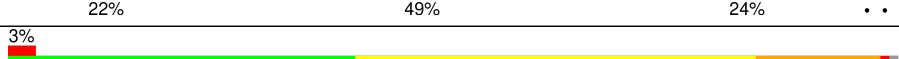
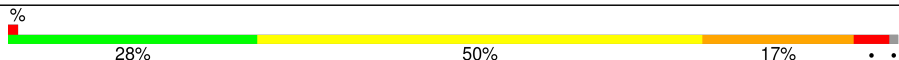
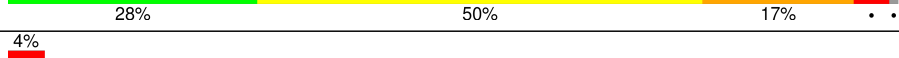
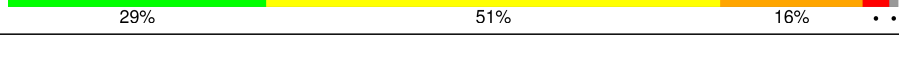
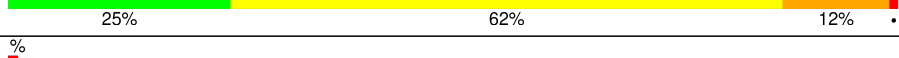
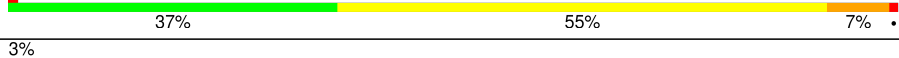
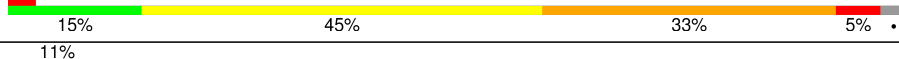
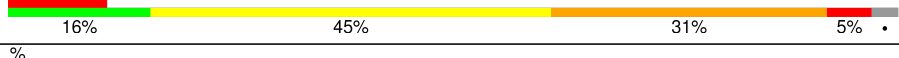
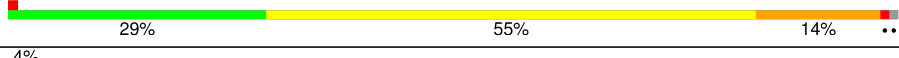

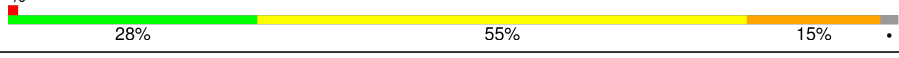
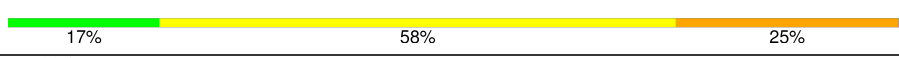


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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	184	
22	CV	184	
23	AW	77	
23	CW	77	
24	AX	5	
24	CX	5	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	
27	BC	229	
27	DC	229	

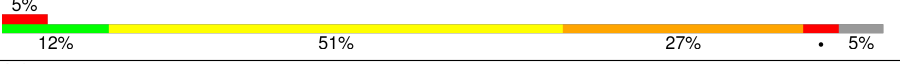
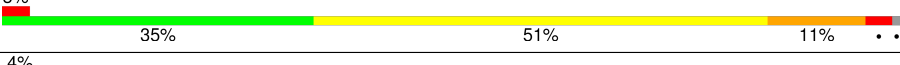
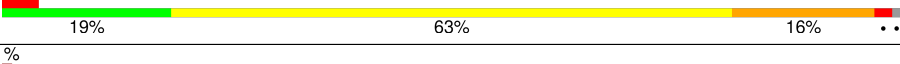
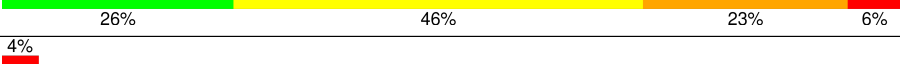
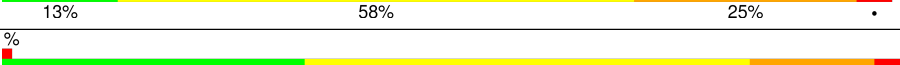
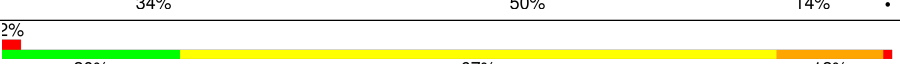
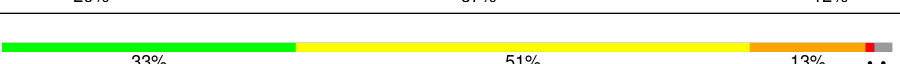
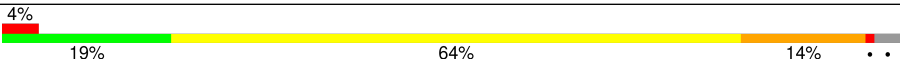

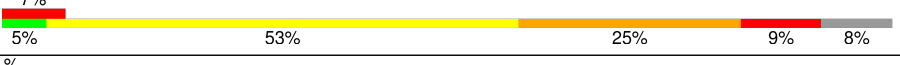
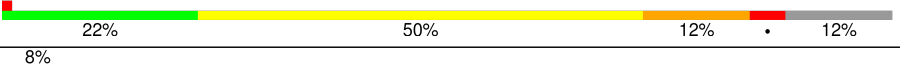
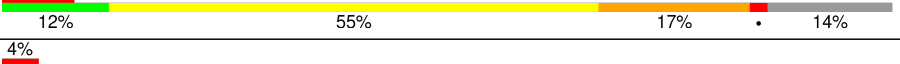
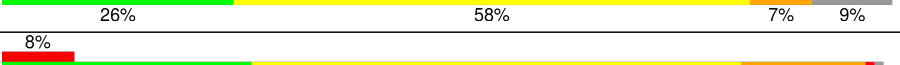
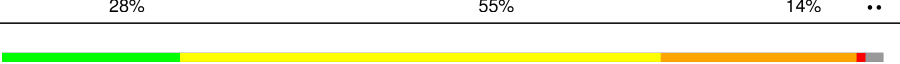
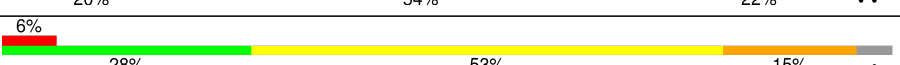
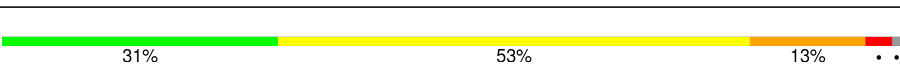
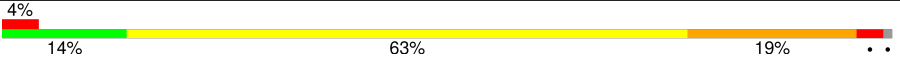
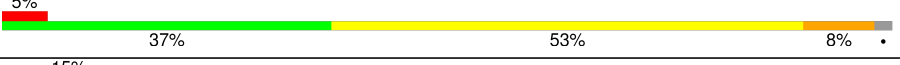
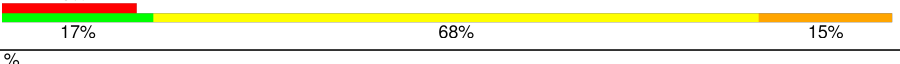


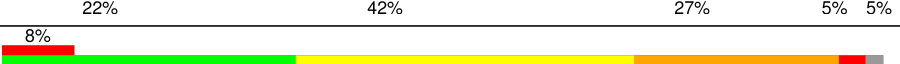
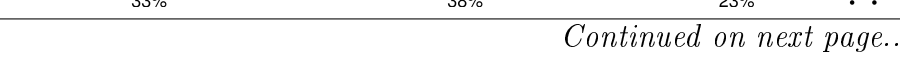


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Mol	Chain	Length	Quality of chain
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	
39	DS	112	
40	BT	146	

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Mol	Chain	Length	Quality of chain
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	
52	B5	60	
52	D5	60	

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Mol	Chain	Length	Quality of chain
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	1609	-	-	-	X
57	MG	AA	1616	-	-	-	X
57	MG	AA	1619	-	-	-	X
57	MG	AA	1622	-	-	-	X
57	MG	AA	1624	-	-	-	X
57	MG	AA	1628	-	-	-	X
57	MG	AA	1630	-	-	-	X
57	MG	AA	1635	-	-	-	X
57	MG	AA	1670	-	-	-	X
57	MG	AA	1676	-	-	-	X
57	MG	AA	1679	-	-	-	X
57	MG	AA	1698	-	-	-	X
57	MG	AA	1711	-	-	-	X
57	MG	AL	201	-	-	-	X
57	MG	BA	3004	-	-	-	X
57	MG	BA	3006	-	-	-	X
57	MG	BA	3008	-	-	-	X
57	MG	BA	3012	-	-	-	X
57	MG	BA	3015	-	-	-	X
57	MG	BA	3018	-	-	-	X
57	MG	BA	3020	-	-	-	X
57	MG	BA	3022	-	-	-	X
57	MG	BA	3023	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3024	-	-	-	X
57	MG	BA	3025	-	-	-	X
57	MG	BA	3030	-	-	-	X
57	MG	BA	3032	-	-	-	X
57	MG	BA	3034	-	-	-	X
57	MG	BA	3035	-	-	-	X
57	MG	BA	3040	-	-	-	X
57	MG	BA	3041	-	-	-	X
57	MG	BA	3042	-	-	-	X
57	MG	BA	3044	-	-	-	X
57	MG	BA	3046	-	-	-	X
57	MG	BA	3047	-	-	-	X
57	MG	BA	3048	-	-	-	X
57	MG	BA	3050	-	-	-	X
57	MG	BA	3052	-	-	-	X
57	MG	BA	3054	-	-	-	X
57	MG	BA	3056	-	-	-	X
57	MG	BA	3057	-	-	-	X
57	MG	BA	3061	-	-	-	X
57	MG	BA	3064	-	-	-	X
57	MG	BA	3071	-	-	-	X
57	MG	BA	3076	-	-	-	X
57	MG	BA	3077	-	-	-	X
57	MG	BA	3080	-	-	-	X
57	MG	BA	3081	-	-	-	X
57	MG	BA	3086	-	-	-	X
57	MG	BA	3088	-	-	-	X
57	MG	BA	3094	-	-	-	X
57	MG	BA	3095	-	-	-	X
57	MG	BA	3096	-	-	-	X
57	MG	BA	3097	-	-	-	X
57	MG	BA	3098	-	-	-	X
57	MG	BA	3099	-	-	-	X
57	MG	BA	3102	-	-	-	X
57	MG	BA	3106	-	-	-	X
57	MG	BA	3109	-	-	-	X
57	MG	BA	3117	-	-	-	X
57	MG	BA	3119	-	-	-	X
57	MG	BA	3123	-	-	-	X
57	MG	BA	3125	-	-	-	X
57	MG	BA	3133	-	-	-	X
57	MG	BA	3139	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3150	-	-	-	X
57	MG	BA	3151	-	-	-	X
57	MG	BA	3154	-	-	-	X
57	MG	BA	3155	-	-	-	X
57	MG	BA	3159	-	-	-	X
57	MG	BA	3177	-	-	-	X
57	MG	BA	3178	-	-	-	X
57	MG	BA	3180	-	-	-	X
57	MG	BA	3181	-	-	-	X
57	MG	BA	3186	-	-	-	X
57	MG	BA	3187	-	-	-	X
57	MG	BA	3188	-	-	-	X
57	MG	BA	3197	-	-	-	X
57	MG	BA	3206	-	-	-	X
57	MG	BA	3210	-	-	-	X
57	MG	BA	3211	-	-	-	X
57	MG	BA	3220	-	-	-	X
57	MG	BA	3240	-	-	-	X
57	MG	BA	3262	-	-	-	X
57	MG	BA	3275	-	-	-	X
57	MG	BA	3286	-	-	-	X
57	MG	BA	3294	-	-	-	X
57	MG	BA	3303	-	-	-	X
57	MG	BA	3307	-	-	-	X
57	MG	BA	3312	-	-	-	X
57	MG	BA	3313	-	-	-	X
57	MG	BA	3333	-	-	-	X
57	MG	BA	3337	-	-	-	X
57	MG	BA	3339	-	-	-	X
57	MG	BA	3345	-	-	-	X
57	MG	BA	3348	-	-	-	X
57	MG	BA	3352	-	-	-	X
57	MG	BA	3374	-	-	-	X
57	MG	BA	3387	-	-	-	X
57	MG	BA	3397	-	-	-	X
57	MG	BA	3399	-	-	-	X
57	MG	BA	3419	-	-	-	X
57	MG	BA	3436	-	-	-	X
57	MG	BA	3441	-	-	-	X
57	MG	BA	3449	-	-	-	X
57	MG	BB	204	-	-	-	X
57	MG	BR	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BU	201	-	-	-	X
57	MG	CA	1606	-	-	-	X
57	MG	CA	1608	-	-	-	X
57	MG	CA	1613	-	-	-	X
57	MG	CA	1620	-	-	-	X
57	MG	CA	1622	-	-	-	X
57	MG	CA	1635	-	-	-	X
57	MG	CA	1638	-	-	-	X
57	MG	CA	1644	-	-	-	X
57	MG	CA	1660	-	-	-	X
57	MG	CA	1661	-	-	-	X
57	MG	CA	1662	-	-	-	X
57	MG	CA	1664	-	-	-	X
57	MG	CA	1675	-	-	-	X
57	MG	CA	1684	-	-	-	X
57	MG	CA	1690	-	-	-	X
57	MG	CA	1695	-	-	-	X
57	MG	CW	104	-	-	-	X
57	MG	DA	3002	-	-	-	X
57	MG	DA	3005	-	-	-	X
57	MG	DA	3007	-	-	-	X
57	MG	DA	3012	-	-	-	X
57	MG	DA	3016	-	-	-	X
57	MG	DA	3017	-	-	-	X
57	MG	DA	3018	-	-	-	X
57	MG	DA	3019	-	-	-	X
57	MG	DA	3020	-	-	-	X
57	MG	DA	3033	-	-	-	X
57	MG	DA	3036	-	-	-	X
57	MG	DA	3037	-	-	-	X
57	MG	DA	3038	-	-	-	X
57	MG	DA	3039	-	-	-	X
57	MG	DA	3044	-	-	-	X
57	MG	DA	3050	-	-	-	X
57	MG	DA	3052	-	-	-	X
57	MG	DA	3053	-	-	-	X
57	MG	DA	3056	-	-	-	X
57	MG	DA	3060	-	-	-	X
57	MG	DA	3064	-	-	-	X
57	MG	DA	3068	-	-	-	X
57	MG	DA	3069	-	-	-	X
57	MG	DA	3072	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3073	-	-	-	X
57	MG	DA	3077	-	-	-	X
57	MG	DA	3085	-	-	-	X
57	MG	DA	3086	-	-	-	X
57	MG	DA	3100	-	-	-	X
57	MG	DA	3103	-	-	-	X
57	MG	DA	3105	-	-	-	X
57	MG	DA	3107	-	-	-	X
57	MG	DA	3127	-	-	-	X
57	MG	DA	3132	-	-	-	X
57	MG	DA	3144	-	-	-	X
57	MG	DA	3147	-	-	-	X
57	MG	DA	3149	-	-	-	X
57	MG	DA	3151	-	-	-	X
57	MG	DA	3152	-	-	-	X
57	MG	DA	3156	-	-	-	X
57	MG	DA	3157	-	-	-	X
57	MG	DA	3159	-	-	-	X
57	MG	DA	3169	-	-	-	X
57	MG	DA	3174	-	-	-	X
57	MG	DA	3179	-	-	-	X
57	MG	DA	3181	-	-	-	X
57	MG	DA	3184	-	-	-	X
57	MG	DA	3187	-	-	-	X
57	MG	DA	3192	-	-	-	X
57	MG	DA	3193	-	-	-	X
57	MG	DA	3211	-	-	-	X
57	MG	DA	3216	-	-	-	X
57	MG	DA	3225	-	-	-	X
57	MG	DA	3227	-	-	-	X
57	MG	DA	3231	-	-	-	X
57	MG	DA	3234	-	-	-	X
57	MG	DA	3248	-	-	-	X
57	MG	DA	3279	-	-	-	X
57	MG	DA	3288	-	-	-	X
57	MG	DA	3290	-	-	-	X
57	MG	DA	3294	-	-	-	X
57	MG	DA	3302	-	-	-	X
58	ZN	AD	301	-	-	-	X
58	ZN	D9	101	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 290405 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1495	Total	C	N	O	P	0	0	0
			32144	14306	5964	10379	1495			
1	CA	1504	Total	C	N	O	P	0	0	0
			32332	14390	5992	10446	1504			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1004	635	195	174			
9	CI	127	Total	C	N	O	0	0	0
			1004	635	195	174			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	120	Total	C	N	O	S	0	0	1
			947	585	196	164	2			
13	CM	120	Total	C	N	O	S	0	0	1
			947	585	196	164	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	80	Total	C	N	O	S	0	0	1
			613	392	110	109	2			
19	CS	78	Total	C	N	O	S	0	0	1
			619	397	111	109	2			

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

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

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

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

- Molecule 22 is a protein called Elongation factor P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	176	Total	C	N	O	S	0	0	0
			1367	870	223	267	7			
22	CV	176	Total	C	N	O	S	0	0	0
			1367	870	223	267	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
23	CW	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 24 is a RNA chain called RNA (5'-R(P*AP*AP*AP*UP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	5	Total	C	N	O	P	0	0	0
			110	49	22	34	5			
24	CX	5	Total	C	N	O	P	0	0	0
			110	49	22	34	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2767	Total	C	N	O	P	0	0	0
			59596	26524	11148	19158	2766			
25	DA	2777	Total	C	N	O	P	0	0	0
			59809	26619	11186	19228	2776			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	224	Total	C	N	O	S	2	0	0
			1702	1075	309	315	3			
27	DC	220	Total	C	N	O	S	1	0	0
			1640	1033	297	307	3			

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	274	Total	C	N	O	S	0	0	1
			2127	1341	425	358	3			
28	DD	274	Total	C	N	O	S	0	0	1
			2115	1335	419	358	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			
30	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- 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	168	Total	C	N	O	S	0	0	1
			1231	780	228	222	1			
32	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	146	Total	C	N	O	S	0	0	1
			1043	661	185	196	1			
33	DI	146	Total	C	N	O	S	0	0	1
			871	543	162	165	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	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
36	DP	146	Total	C	N	O	S	0	0	0
			1079	672	216	189	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	139	Total	C	N	O	S	0	0	1
			1099	702	209	181	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	116	Total	C	N	O		0	0	0
			923	575	191	157				
38	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	101	Total	C	N	O		0	0	1
			777	489	156	132				
39	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- 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
			958	604	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	94	Total	C	N	O	S	0	0	1
			735	477	134	124				
44	DX	93	Total	C	N	O	S	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
			757	486	144	123	4			
45	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	182	Total	C	N	O	S	0	0	1
			1438	917	258	261	2			
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	77	Total	C	N	O	S	0	0	0
			613	379	129	104	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	96	Total	C	N	O	S	0	0	0
			757	478	149	129	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	59	Total	C	N	O	S	0	0	1
			460	293	90	77				
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	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	57	Total	C	N	O	S	0	0	1
			435	272	88	70	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	49	Total	C	N	O	S	0	0	1
			401	247	82	68	4			
53	D6	48	Total	C	N	O	S	0	0	0
			322	199	62	57	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	63	Total	C	N	O	S	0	0	1
			496	317	101	76	2			
55	D8	62	Total	C	N	O	S	0	0	1
			467	299	95	71	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
			294	179	66	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	459	Total	Mg	0	0
			459	459		
57	CA	109	Total	Mg	0	0
			109	109		
57	DF	1	Total	Mg	0	0
			1	1		
57	BE	1	Total	Mg	0	0
			1	1		
57	AW	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B1	1	Total 1	Mg 1	0	0
57	BP	3	Total 3	Mg 3	0	0
57	DR	1	Total 1	Mg 1	0	0
57	B5	4	Total 4	Mg 4	0	0
57	BB	9	Total 9	Mg 9	0	0
57	BT	1	Total 1	Mg 1	0	0
57	BF	1	Total 1	Mg 1	0	0
57	BX	1	Total 1	Mg 1	0	0
57	AA	117	Total 117	Mg 117	0	0
57	BQ	3	Total 3	Mg 3	0	0
57	D6	2	Total 2	Mg 2	0	0
57	CX	1	Total 1	Mg 1	0	0
57	BU	1	Total 1	Mg 1	0	0
57	DD	1	Total 1	Mg 1	0	0
57	BR	1	Total 1	Mg 1	0	0
57	DA	305	Total 305	Mg 305	0	0
57	B7	1	Total 1	Mg 1	0	0
57	AL	1	Total 1	Mg 1	0	0
57	DP	1	Total 1	Mg 1	0	0
57	CW	5	Total 5	Mg 5	0	0
57	D5	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BD	1	Total 1	Mg 1	0	0
57	AT	1	Total 1	Mg 1	0	0
57	B0	2	Total 2	Mg 2	0	0
57	CE	1	Total 1	Mg 1	0	0
57	DB	10	Total 10	Mg 10	0	0
57	BH	1	Total 1	Mg 1	0	0

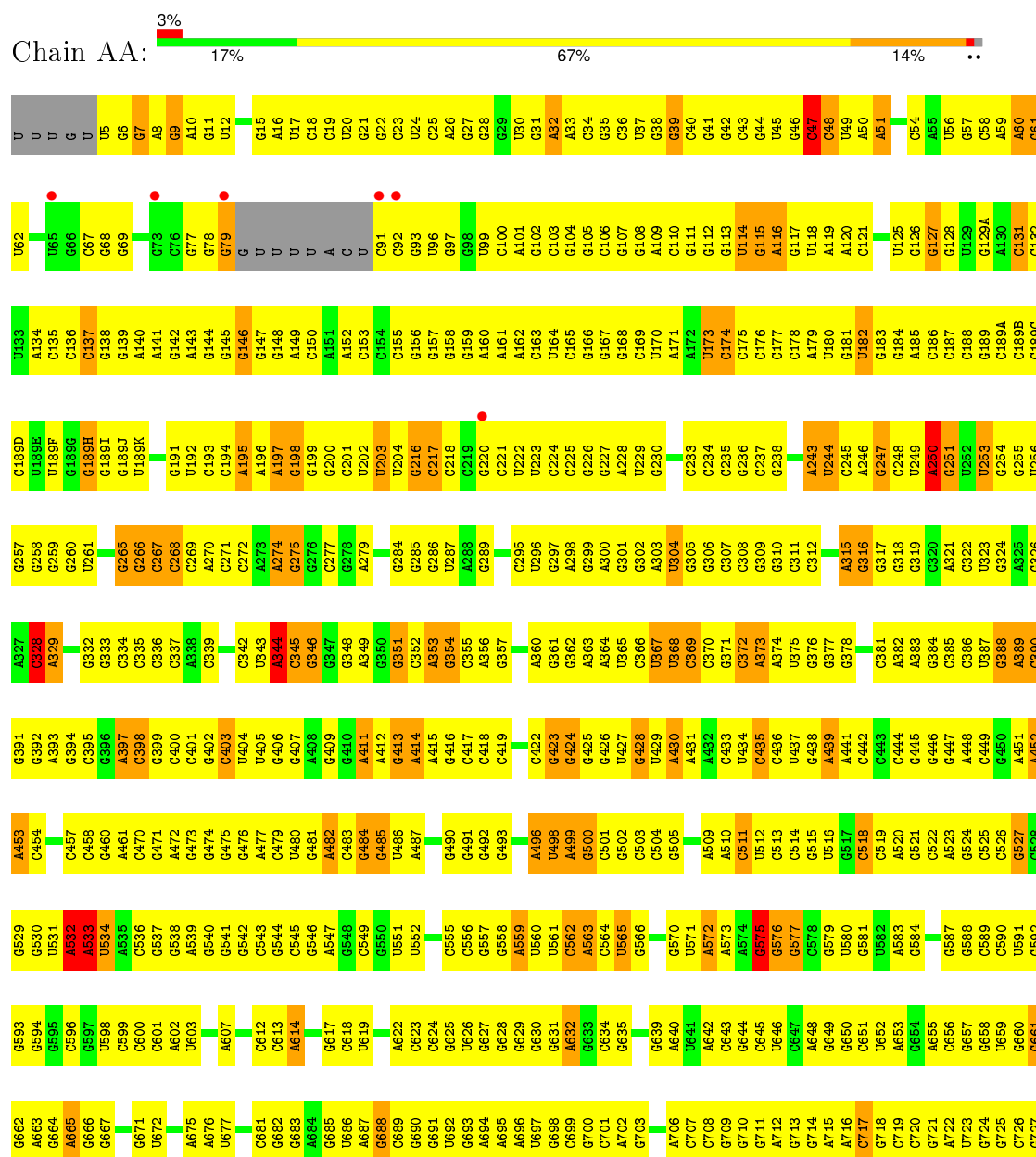
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

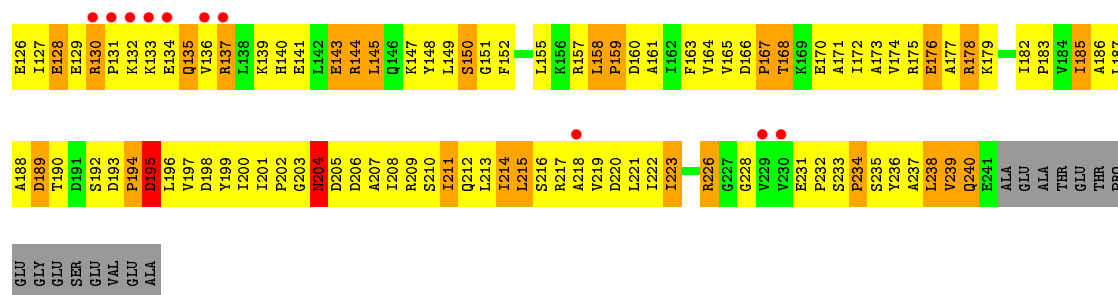
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S ribosomal RNA

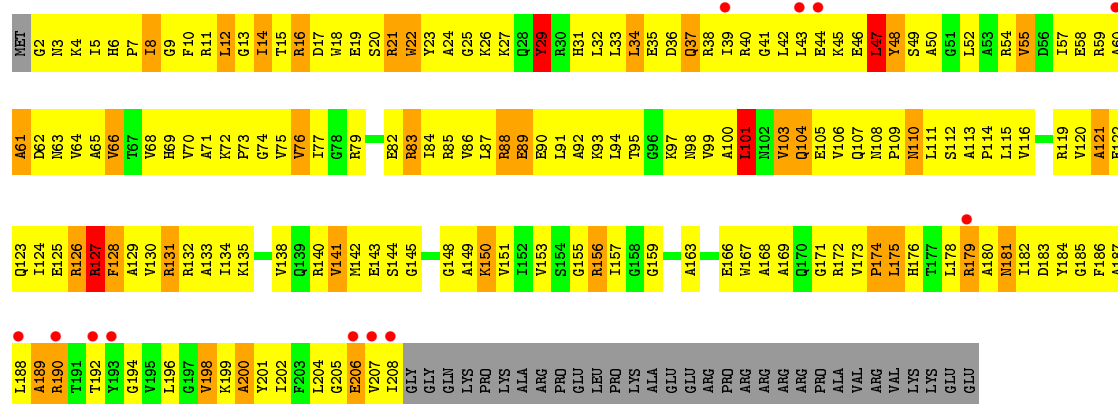
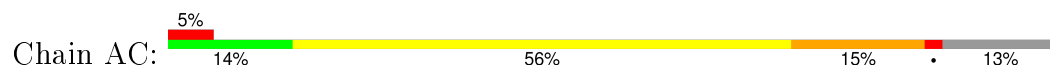




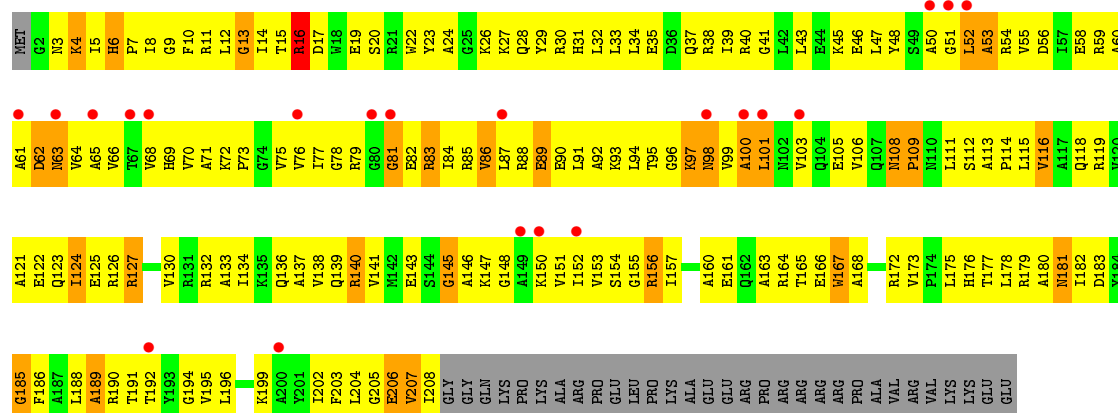
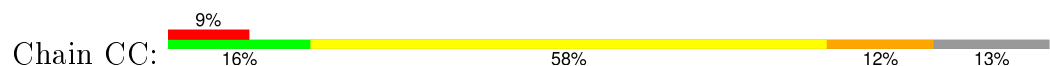
U1083	G1026	A892	C817	U740	G671	G606	G541	A472	G396	G332	C266	G191	G138	C63
G1084	C1027	A892	G818	G741	U672	A607	G542	G473	A397	G333	C267	U192	G139	G64
U1085	C1028	G898	A819	G742	G673	A608	G543	G474	A398	C336	C268	C193	G140	U85
U1086	C1029	G899	U820		G674	A609	G544		G399		C269	C194	A141	G66
U1087	G1030	A900	G821	G745	A675	A610	G545	A477	G402	A337	A270	A195	G147	C67
G1088	G1030A	A901	G822	A746	A676	A611	G546	A478	G403	A338	C271	A196	G148	G68
U1089	C1030B	G902	G823	G747	U677	G612	A547	U480	C403	A339	C272	A197	G149	G69
U1090	G1030C		G824	C748	U678	G613	G548	G481	U404	G340	A273	G198	G150	G70
U1091	A1030D	A909	G825	C749	G679	A614	G549	A482	U405	G341	A274	G199	C150	C71
A1092	G1031	C910	G826	G750	G680	A615	G550	G483	G406	G342	G275	G200	A151	C72
A1093	G1032	U911	U827	U751	C681	G616	G551	G484	G407	U343	G276	C201	A152	G73
U1094	G1033	C912	A828	G752	G682		U552	G485	A412	A344	C277	U202	C153	G74
U1095	G1034	A913	G829	A753	G683	A621		U486	G413	G345	C278	U203	C154	G75
A1096	A1035	A914	G830	C754	A684	A622	C555	A487	G414	G346	A279	U204	C155	G76
C1097	G1036		U831	G755	G685	A623	G556	A488	A415	G347	A282	G216	G156	G77
C1098	C1037		G832	G756	U686	G624	G557	G489	A416	G348		G217	G157	G78
U1099	C1038	A918	U833	U757	A687	G625	G558	G490	G417	A349	U287	C221	G158	U81
G1100	C1039	A919	U834	G758	G688	U626	G559	G491	C418	G350	A288	U222	A160	U82
A1101	U1040	U920	U835	A759	C689	G627	U560	G492	C419	G351	A289	U223	A161	U83
A1102	A1041	U921	G836	G760	U692	G628	U561	G493		C352	G289	U224	A162	U84
G1103	G1042	G922	G837	A766	G693	G629	C562	U494	C422	A353	C290	U225	C163	U88
G1104	C1043	A923	U838	A767	A694	G630	A563	A495	G423	G354	C291	C224	U164	C89
A1105	A1044		G839	G768	G695	G631	C564	A496	C424	C355	G292	C225	G165	U90
G1106	C1045	G926	G840	A768	G699	A632	U565	U498	G425	A356	G293	G226	G166	C91
C1107	A1046	G927	U841	G769	G700	G633	G566	G499	G426	G357	U294	G227	G167	C92
G1108	G1047	G928	C848	C770		G634	G567	G500		U358	C295	A288	G168	G93
			C849		G703	G635	G568	G501	U427	C359	U296	U229	G169	U96
C1112	U1048	C930	G853	G775		G636	C569	G502	G428	A360	G297	G230	C170	G97
C1113	U1049	C931	G854	A776	A706	G637	G570	C503	G429	A361	A298	G231	U170	G98
C1114	C1050	C932	G854	A777	G707	G638	U571		C430	G362	G299	G232	A171	U99
C1115	U1052	G933	G854	G778	C708	G639	A572	C507	A431	A363	A300	C233	U172	C100
C1116	G1053	C934	C857	C779	G709	A640	A573	C508	A432	A364	G301	C234	U173	A101
G1117	A1054	A935	G858	A780	G710	U641	A574	A509	C433	U365	G302	C235	C174	A102
C1118	A1055	C936	A859	A781	G711	A642	G575	A510	U434	G366	A303	G236	C175	C103
C1119	U1056	A937	G860	A782	G712	G643	G576	U512	C436	U370	G305	C241	G177	G107
C1120	G1057	A938	G861	G783	A713	G644	G577	C513	C437	G371	G309	C242	G178	G108
U1121	U1058	G939	C862	C784	G714	G645	G578	C514	G438	C372	G310	A243	A179	A109
U1122	C1059	C940	U863	G785	G715	U646	G579	C515	A439	A373	C311	U244	U180	G112
A1123	U1060	G941	A864	G786	A716	C647	U580	G515	A441	A374	C312	C245	U181	G113
G1124	G1061	G942	A865	A787		A648	G581		C442	U375	A313	A246	G182	U114
U1125	U1062		G868	A790	G721	G650	U582	C518	C443	G376	C314	A247	G183	G115
U1126	C1063	G945	G869	G791	U722	C651		A520	C444	G377	A315	C248	G184	A116
G1127	U1064	A946	U870	A792	U723	U652	G588	A521	G445	G378	G316	U249	A185	G117
C1128	C1065	C947	U871	U793	G724	A653	C589	C522	G446	C379	G317	A250	C186	U118
C1129	U1066	A948		G795	G725	G654	U591	A523		G380	G318	G251	C187	U119
A1130	A1067	U950	C875	C796	G726	G655	G592	C525	G450	C381	C319	U253	G188	A120
G1131	G1010	A949	G876	G797	G727	C656	G593	C526	A451	A382	G320	U254	G189	C121
C1132	U1012	G951	C877	C798	U728	G657	G594	G527	A452	A383	C322	G255	C189A	U125
G1133	G1013	U952	G878	G799	A729	U658			A453	G384	U323	G256	C189B	G126
G1134	A1014	G953	G879		G730	U659	C596		A454	C385	G324	U257	C189C	
U1135	U1070	C954	C880	A802	G731	G660	G597	A532	C455	C386	A325	U258	U189D	
U1136	G1071	U955	G881	G803	G732	U661	U598	A533	C456	U387	G326	G260	G189H	C131
C1137	C1075	U956	G882	U904	A733	G662	C599	U534	C457	U388	A327	U261	G189I	C132
G1138	G1018	U957	C882	C905	G734	A663	C600	A535	C458	G389	G328	A262	G189J	
G1139	U1077	A958	G885	C906	C735	G664	C601	A536	G460	C390	A329	A263	U189K	C135
C1140	G1078	A959	G886	A807	C736	A665	A602	G537	A461	G394	C330	U264	G189L	
C1141	U1079	U960	G887	C811	G738	G666	U603	G538	G471	C395	G331	G265	U190	
G1142	A1080	U961												
G1143	G1081	C962												
G1144	G1082	G963												



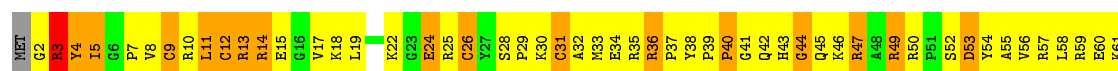
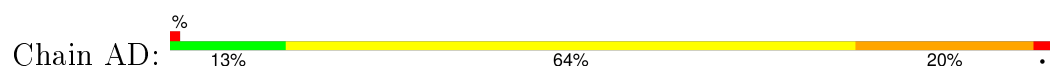
• Molecule 3: 30S ribosomal protein S3

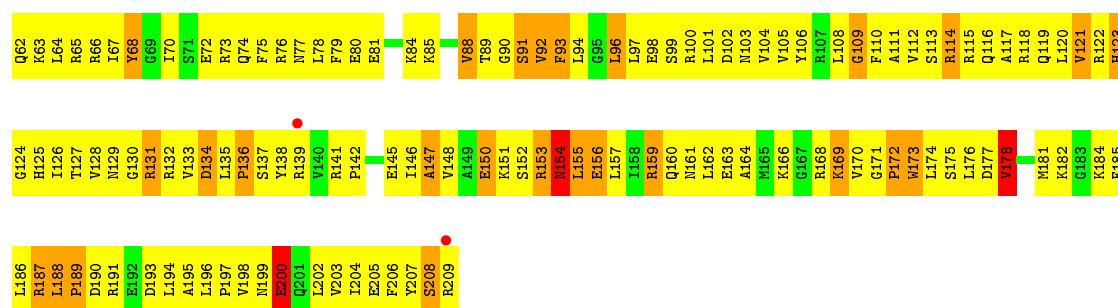


• Molecule 3: 30S ribosomal protein S3

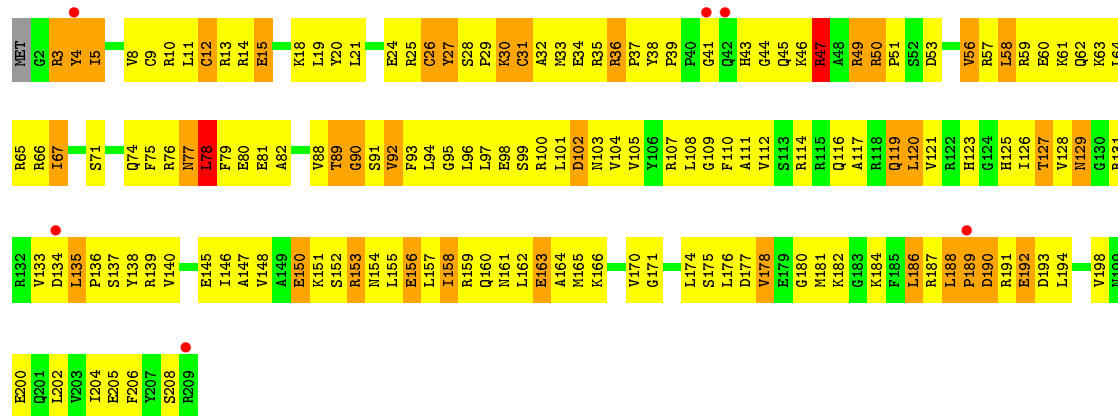


• Molecule 4: 30S ribosomal protein S4

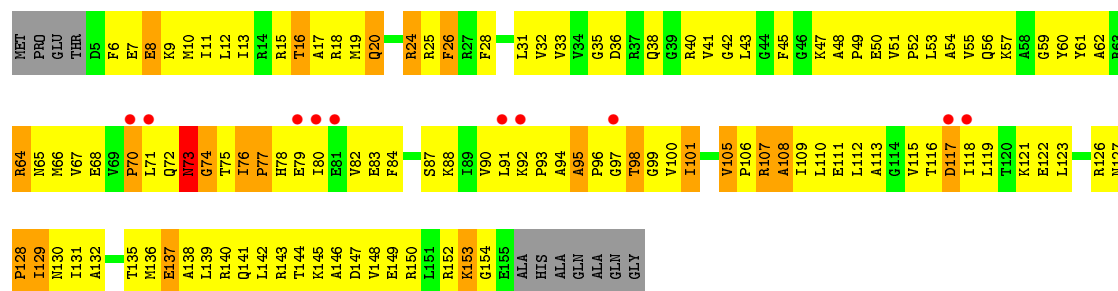




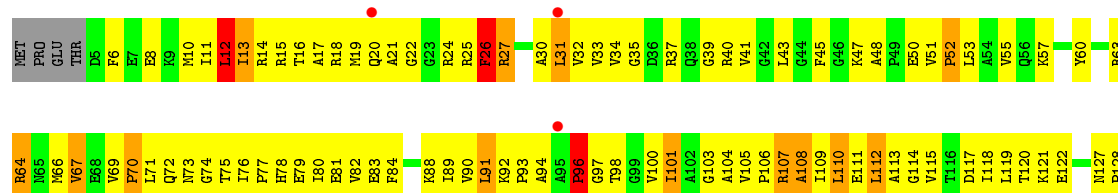
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5



- Chain CI:
-
- 23%
19% 62% 14% 5%
- | Category | Value |
|----------|-------|
| NET | 5% |
| E2 | 19% |
| E3 | 23% |
| T3 | 62% |
| Y4 | 14% |
| Y5 | 14% |
| G6 | 14% |
| T7 | 14% |
| G8 | 14% |
| R9 | 14% |
| R10 | 14% |
| K11 | 14% |
| E12 | 14% |
| A13 | 14% |
| V14 | 14% |
| A15 | 14% |
| R16 | 14% |
| V17 | 14% |
| F18 | 14% |
| L19 | 14% |
| R20 | 14% |
| G21 | 14% |
| P22 | 14% |
| G23 | 14% |
| I23 | 14% |
| G24 | 14% |
| K25 | 14% |
| V26 | 14% |
| T27 | 14% |
| V28 | 14% |
| I29 | 14% |
| D32 | 14% |
| F33 | 14% |
| A34 | 14% |
| E35 | 14% |
| V36 | 14% |
| F37 | 14% |
| Q38 | 14% |
| G39 | 14% |
| L40 | 14% |
| V41 | 14% |
| R42 | 14% |
| A43 | 14% |
| V44 | 14% |
| A45 | 14% |
| A46 | 14% |
| V47 | 14% |
| F48 | 14% |
| P49 | 14% |
| L50 | 14% |
| R51 | 14% |
| A52 | 14% |
| V53 | 14% |
| G54 | 14% |
| A55 | 14% |
| L56 | 14% |
| R57 | 14% |
| H58 | 14% |
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| E64 | 14% |
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| E121 | 14% |
| T122 | 14% |
| E123 | 14% |
| T124 | 14% |
| E125 | 14% |
| T126 | 14% |
| E127 | 14% |
| T128 | 14% |
| E129 | 14% |
| T130 | 14% |

Q124
Y125
S126
K127
R128

• Molecule 10: 30S ribosomal protein S10

Chain AJ: 15% 14% 60% 18% 6%

MET PRO K3 I4 R5 I6 K7 R9 F11 G10 D73 F12 H13 K14 T15 L16 D17 A20 Q21 K22 I23 V24 E25 A26 A27 R28 R29 S30 G31 A32 Q33 V34 S35 G36 P37 I38 P39 L40 P41 R45 R46 F47 T48 V49 I50 R51 G52 P53 F54 K55 H56 K57 D58 S59 R60 E61 H62 F63

B64 L65 R66 T67 H68 N69 R70 L71 V72 I74 I75 H76 F77 H78 R79 R80 T81 R82 E83 Q84 L85 K86 T87 L88 D89 L90 P91 T92 G93 I96 E97 R98 K99 T100 V101 GLY GLY ARG

• Molecule 10: 30S ribosomal protein S10

Chain CJ: 46% 15% 62% 17% 6%

MET PRO K3 I4 R5 I6 K7 R9 F11 G10 D73 F12 H13 K14 T15 L16 D17 A18 A19 Q20 Q21 K22 I23 V24 E25 A26 A27 R28 R29 S30 G31 A32 Q33 V34 S35 G36 P37 I38 P39 L40 P41 R45 R46 F47 T48 V49 I50 R51 G52 P53 F54 K55 H56 K57 D58 S59 R60 E61 H62

F63 B64 L65 R66 T67 H68 N69 R70 L71 V72 I74 I75 H76 F77 H78 R79 R80 T81 R82 E83 Q84 L85 K86 T87 L88 D89 L90 P91 T92 G93 I96 E97 R98 K99 T100 V101 GLY GLY ARG

• Molecule 11: 30S ribosomal protein S11

Chain AK: 9% 26% 59% 6% 8%

MET ALA L63 LYS PRO SER LYS LYS VAL K11 R12 Q13 Q14 A15 S16 G17 R18 A19 Y20 I21 H22 A23 A24 S24 Y25 Y26 I27 T28 T29 V30 T31 T32 L33 Q34 P35 N38 P39 T40 T41 W42 S43 S44 G45 G46 V47 I48 G49 Y50 K51 G52 S53 R54 K55 K56 G57 T57 P58 A60 A61

Q62 L63 A64 D67 A68 A69 R70 K71 LYS A72 Y75 G76 H77 Q78 S79 V80 D81 R82 I83 H84 R85 G88 A89 G90 A91 T92 S93 E94 Q95 I96 L97 A98 Q99 S101 G102 L103 Q104 V105 S107 T108 V109 D110 D111 H116 N117 R120 P121 K122 K123 K124 P125 F126 A127 A128 S129

• Molecule 11: 30S ribosomal protein S11

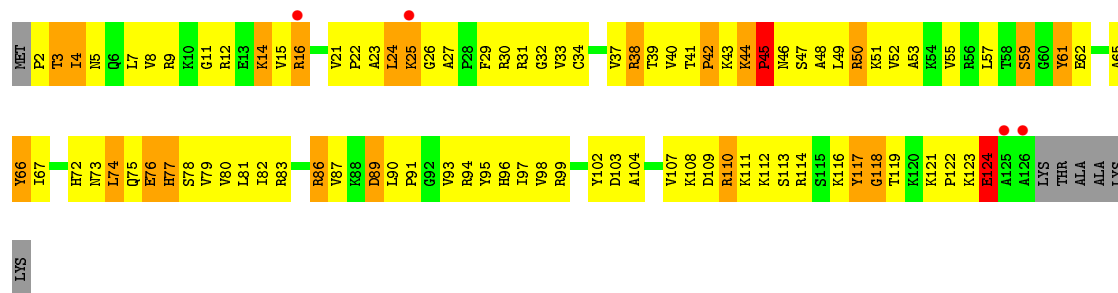
Chain CK: 3% 29% 53% 11% 8%

MET ALA L63 LYS PRO SER LYS LYS VAL K11 R12 Q13 Q14 A15 S16 G17 R18 A19 Y20 I21 H22 A23 A24 S24 Y25 Y26 I27 T28 T29 V30 T31 T32 L33 Q34 P35 N38 P39 T40 T41 W42 S43 S44 G45 G46 V47 I48 G49 Y50 K51 G52 S53 R54 K55 K56 G57 T57 P58 A60 A61

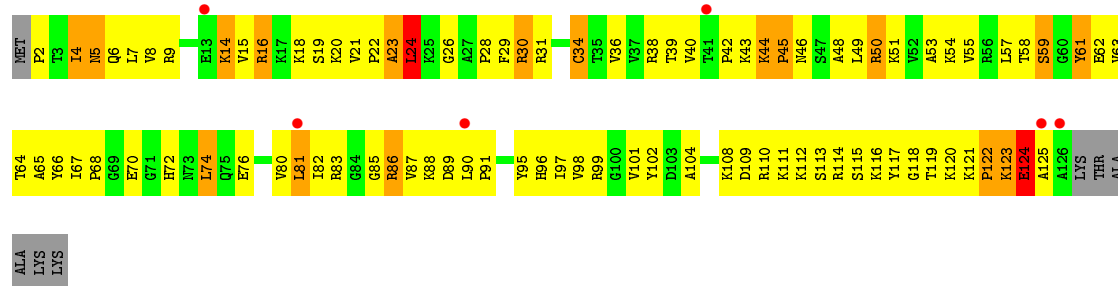
A65 L66 D67 A68 K71 A72 M73 A74 M77 Q78 S79 V80 D81 R82 I83 H84 R85 G86 G88 A89 G90 A91 T92 S93 E94 Q95 I96 L97 A98 Q99 S101 G102 L103 Q104 V105 S107 T108 V109 D110 D111 H116 N117 R120 P121 K122 K123 K124 P125 F126 A127 A128 S129

• Molecule 12: 30S ribosomal protein S12

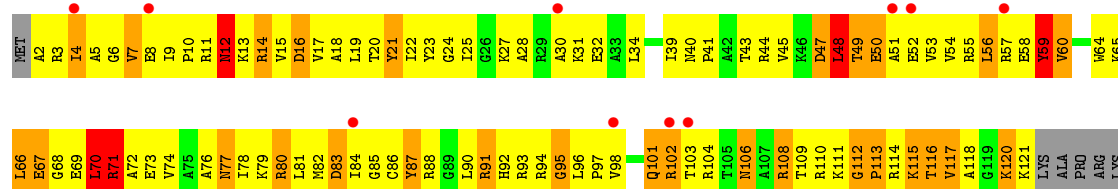
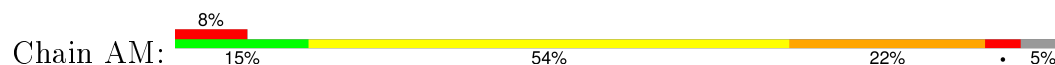
Chain AL: 3% 24% 53% 16% 5%



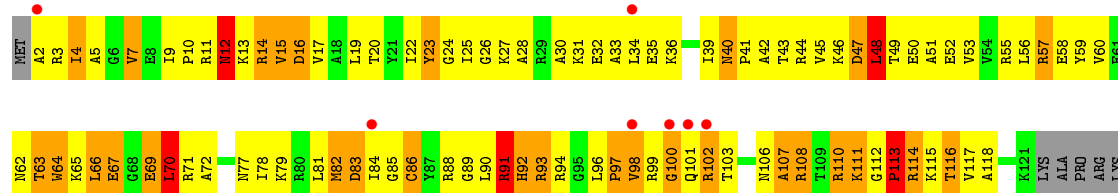
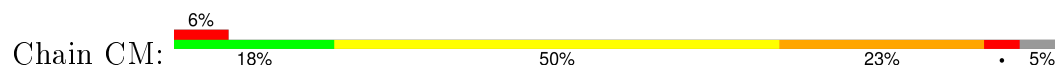
- Molecule 12: 30S ribosomal protein S12



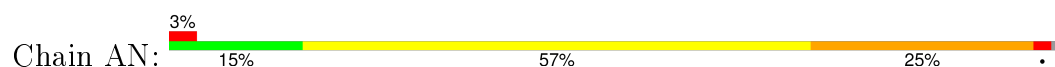
- Molecule 13: 30S ribosomal protein S13



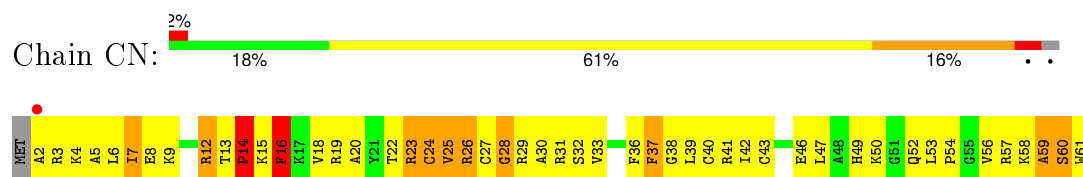
- Molecule 13: 30S ribosomal protein S13



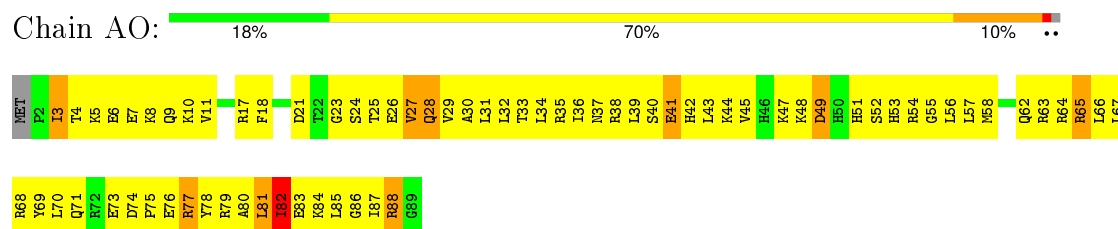
- Molecule 14: 30S ribosomal protein S14



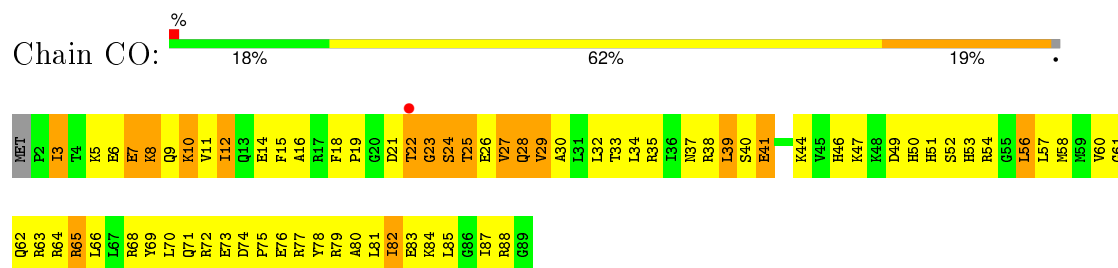
- Molecule 14: 30S ribosomal protein S14



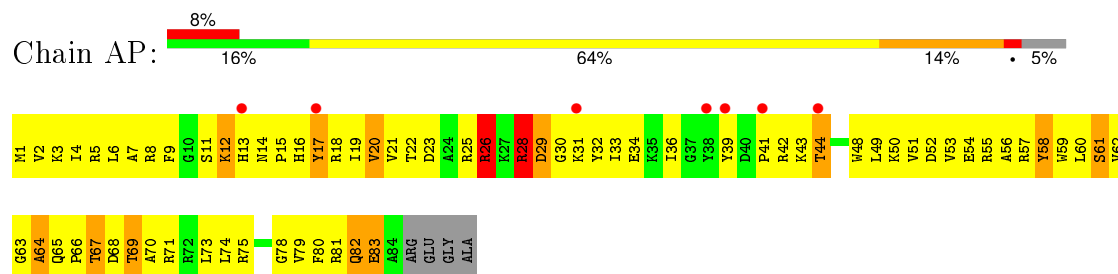
- Molecule 15: 30S ribosomal protein S15



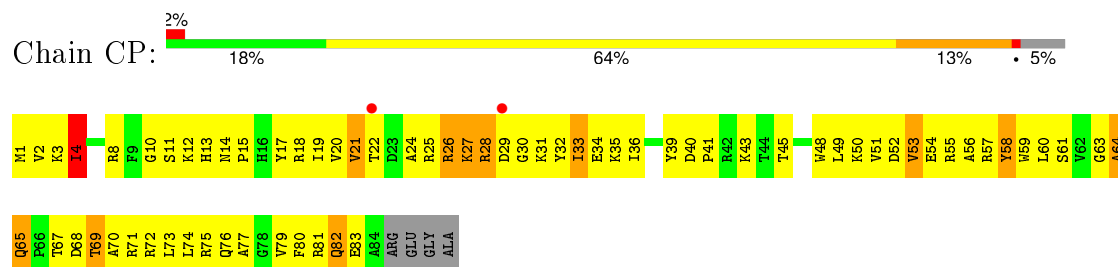
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

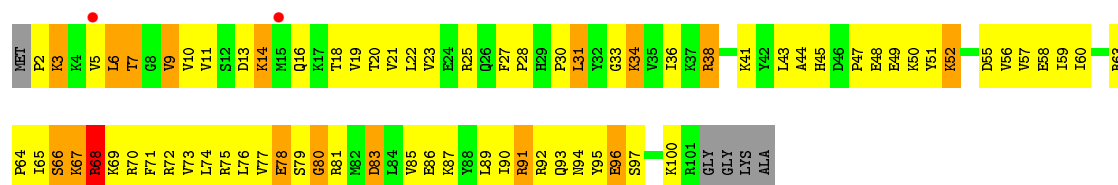


- Molecule 16: 30S ribosomal protein S16

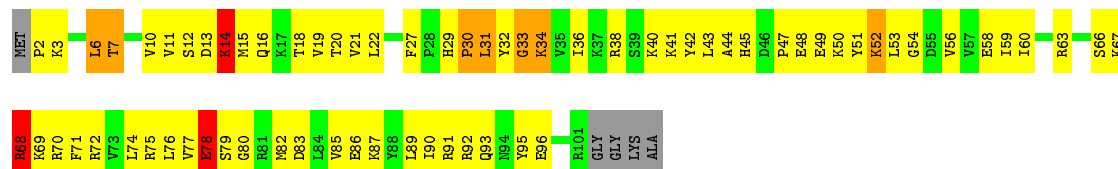


- Molecule 17: 30S ribosomal protein S17

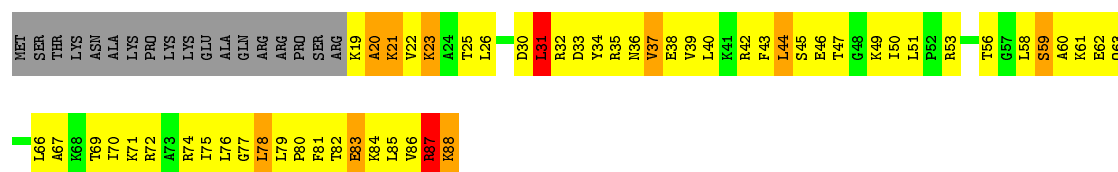
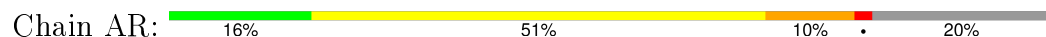




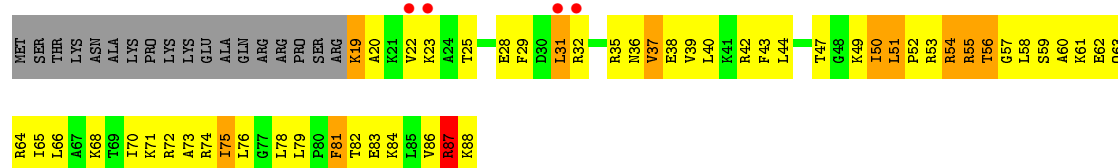
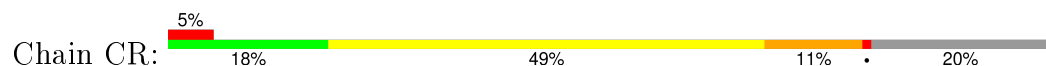
• Molecule 17: 30S ribosomal protein S17



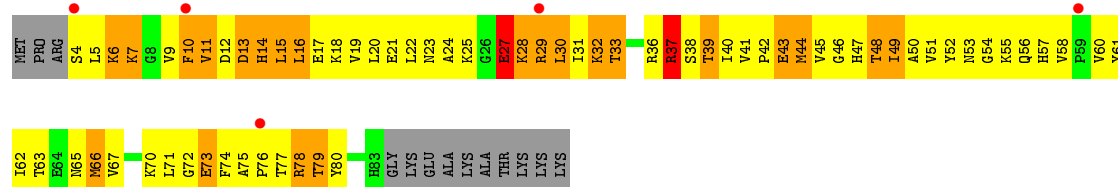
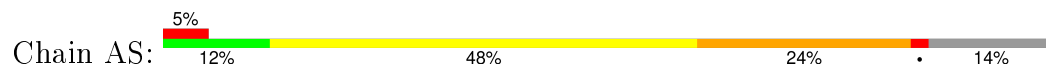
• Molecule 18: 30S ribosomal protein S18



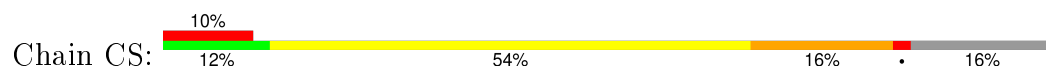
• Molecule 18: 30S ribosomal protein S18

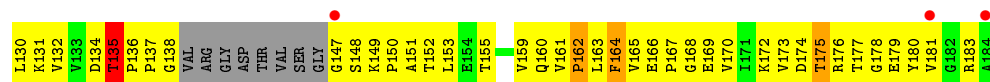


• Molecule 19: 30S ribosomal protein S19

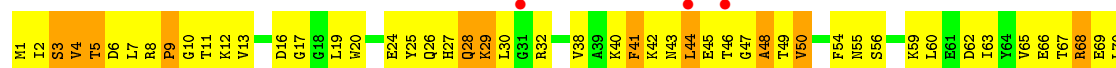


• Molecule 19: 30S ribosomal protein S19

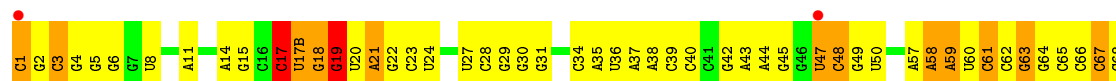




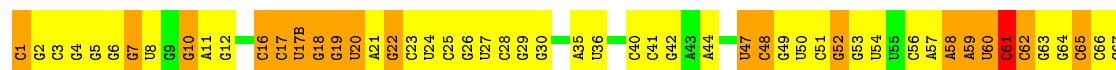
• Molecule 22: Elongation factor P



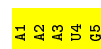
• Molecule 23: tRNA-Met



• Molecule 23: tRNA-Met



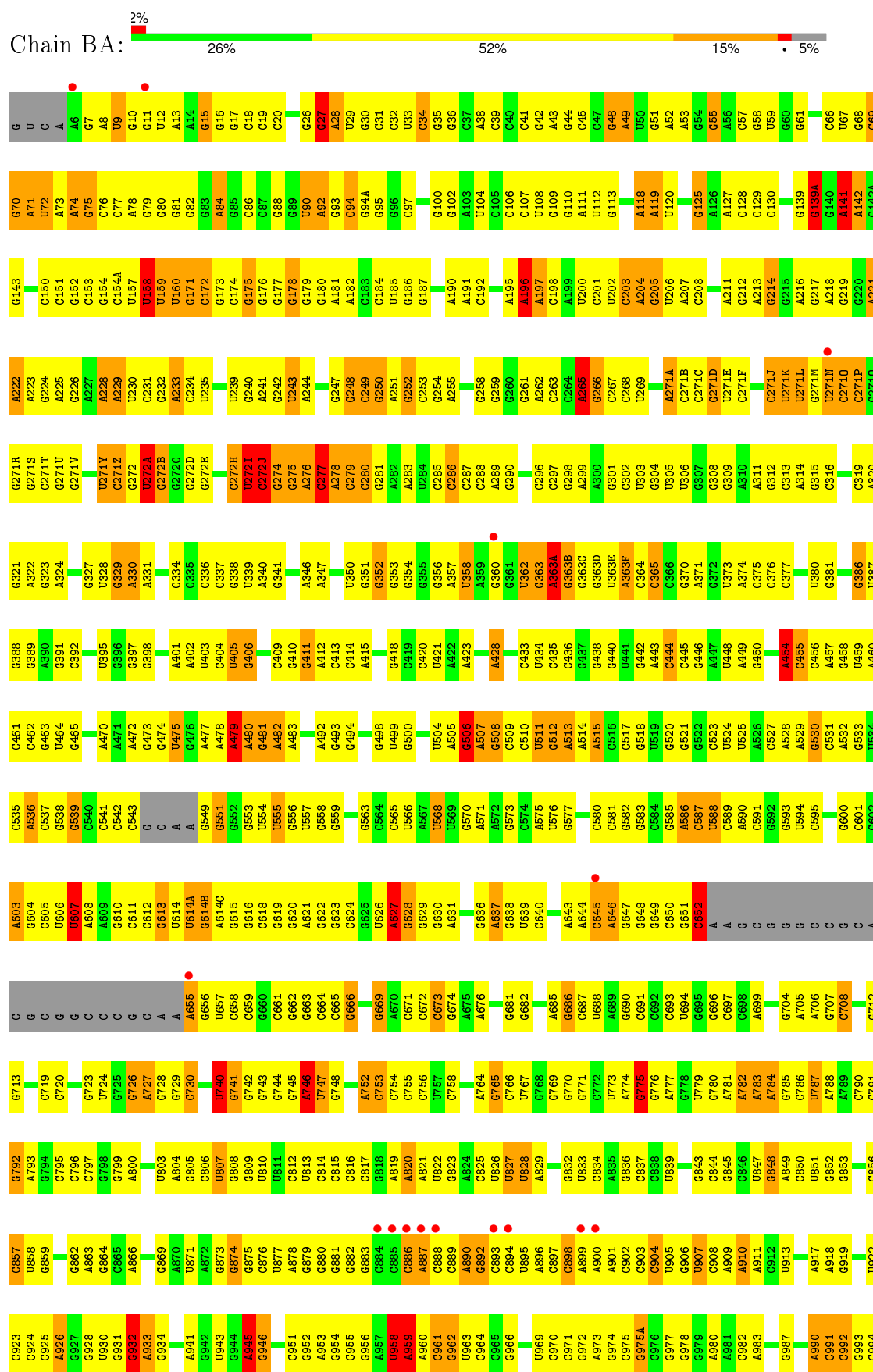
• Molecule 24: RNA (5'-R(P*AP*AP*AP*UP*G)-3')



• Molecule 24: RNA (5'-R(P*AP*AP*AP*UP*G)-3')



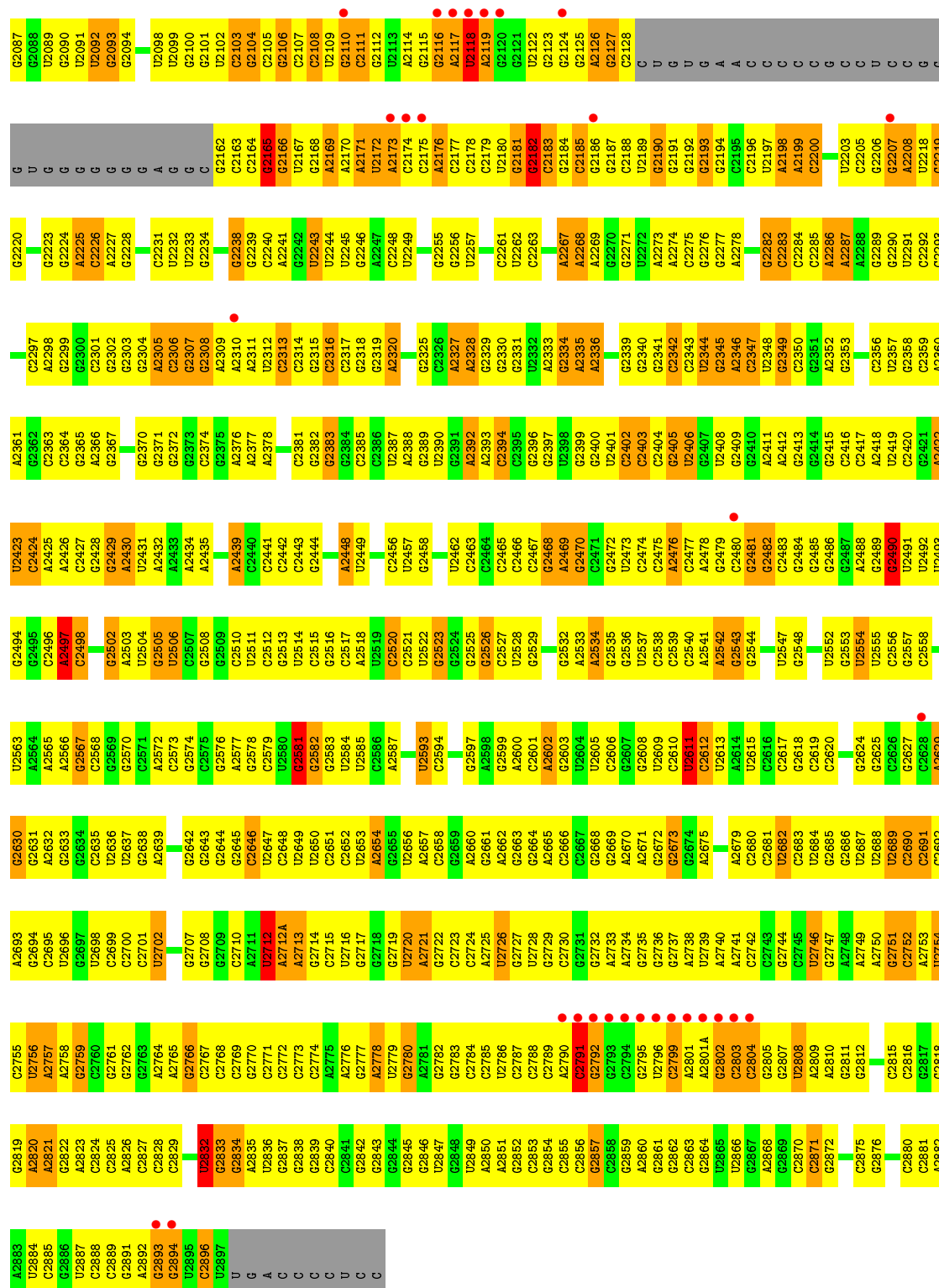
• Molecule 25: 23S ribosomal RNA

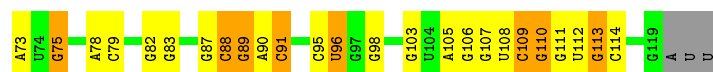




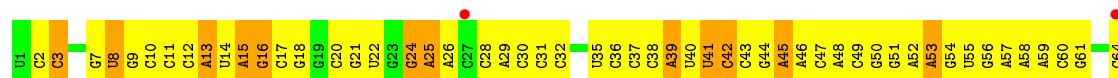


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G2023	A1953	G1883	A1802	G1647	U1577	A1509B	C1446	A1378	C1314	G1245	G1184	C1119	U
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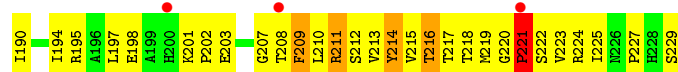
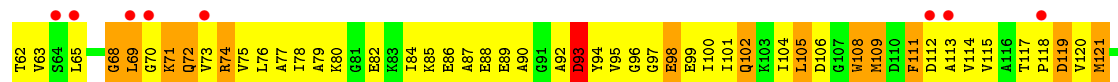
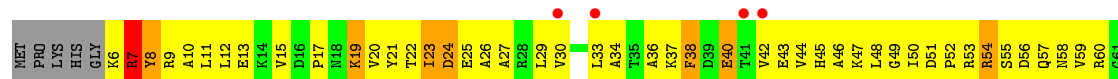




• Molecule 26: 5S ribosomal RNA



• Molecule 27: 50S ribosomal protein L1

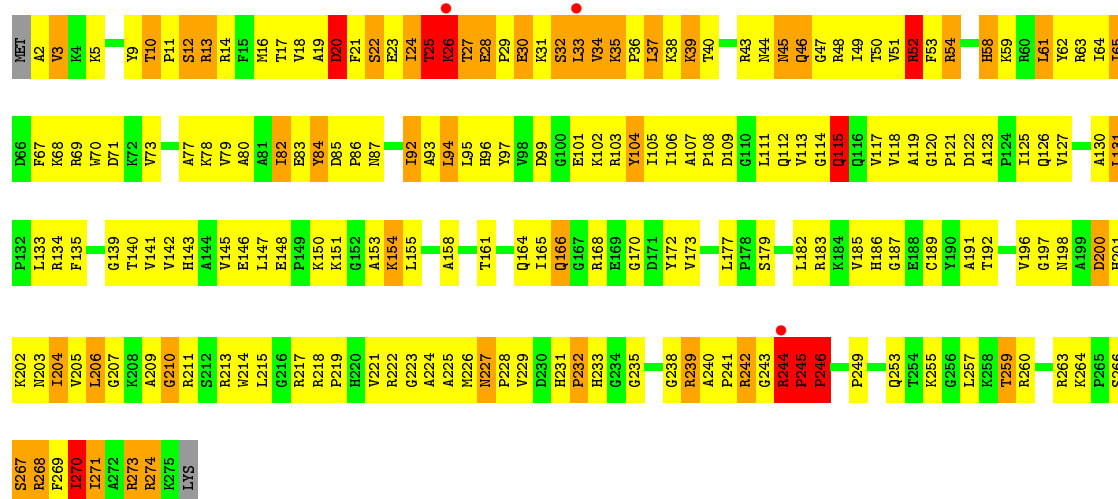


• Molecule 27: 50S ribosomal protein L1

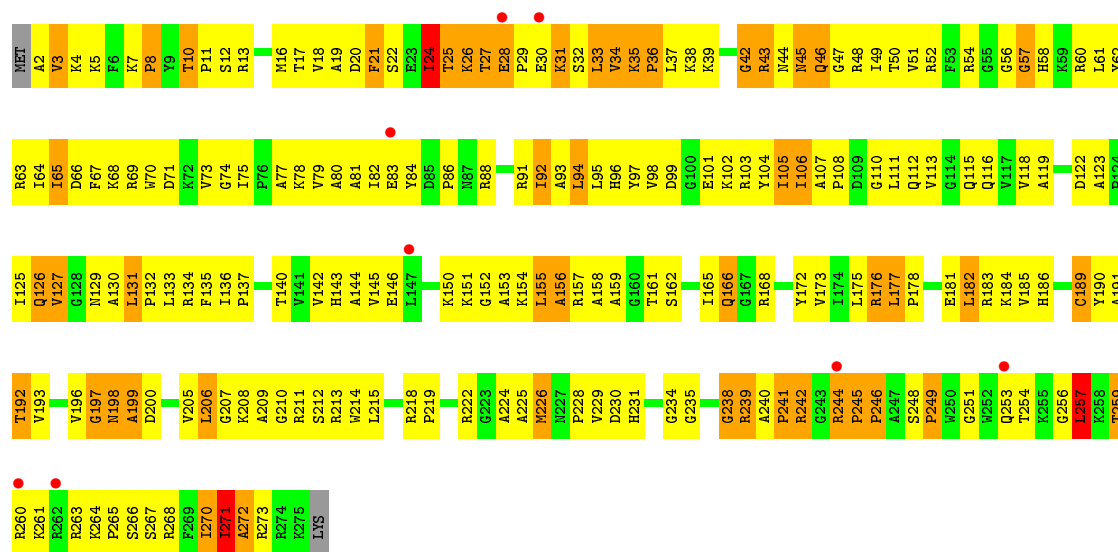


• Molecule 28: 50S ribosomal protein L2

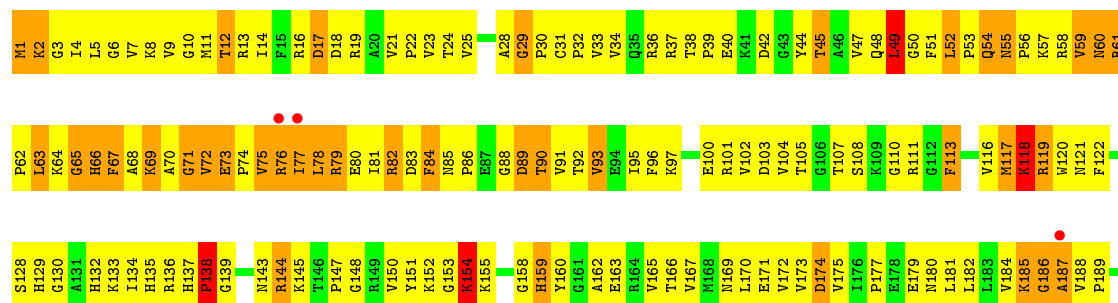




• Molecule 28: 50S ribosomal protein L2

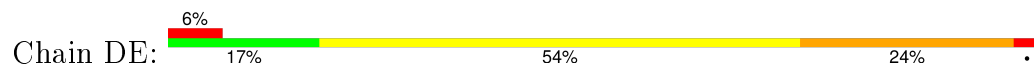


• Molecule 29: 50S ribosomal protein L3

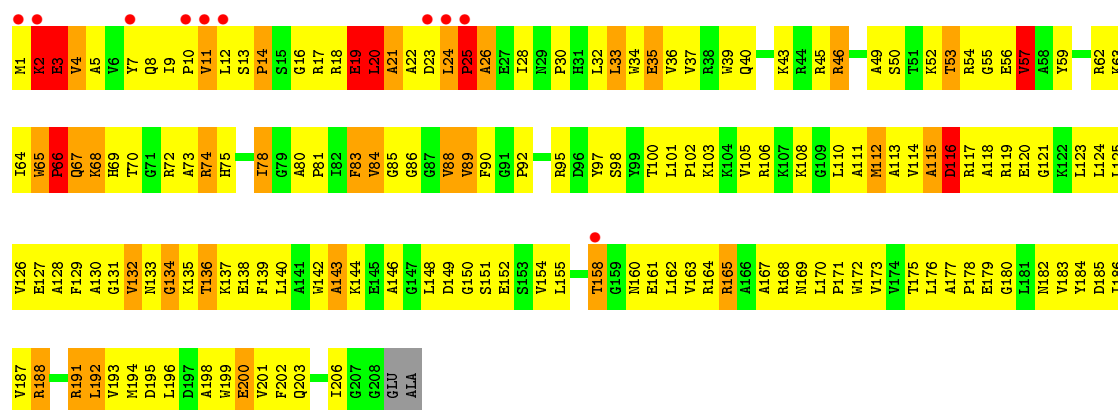




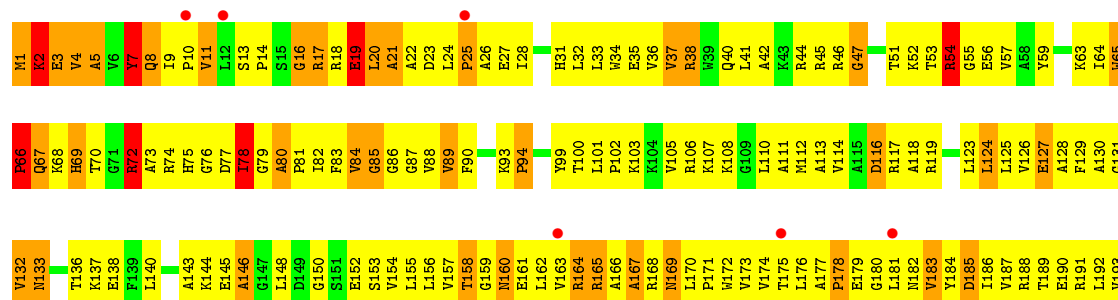
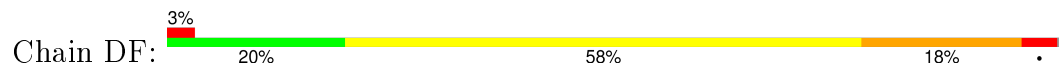
• Molecule 29: 50S ribosomal protein L3



• Molecule 30: 50S ribosomal protein L4

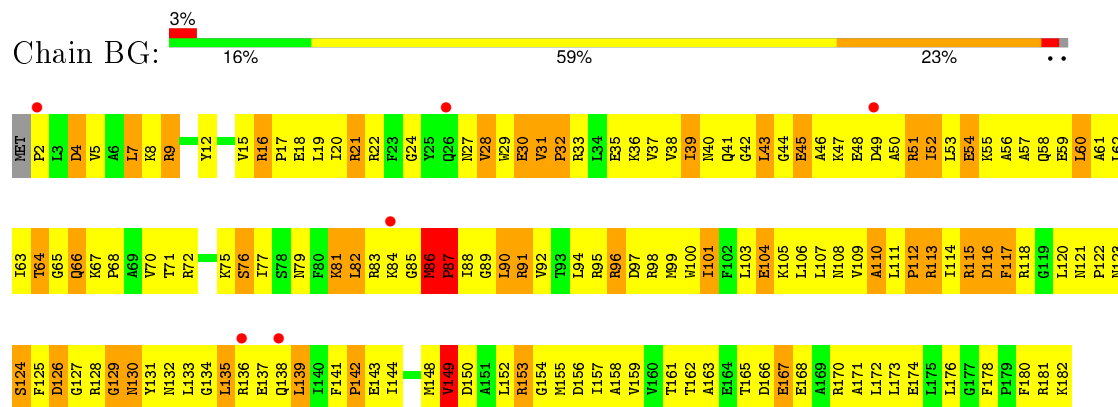


• Molecule 30: 50S ribosomal protein L4

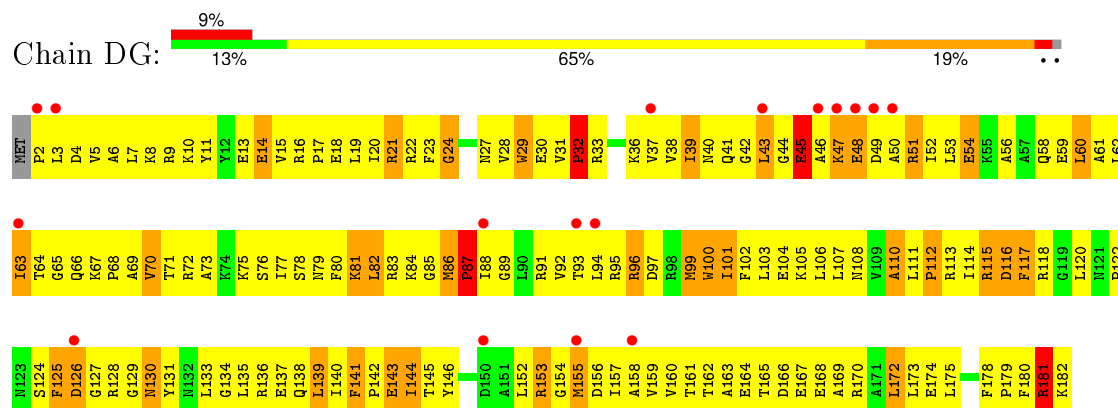




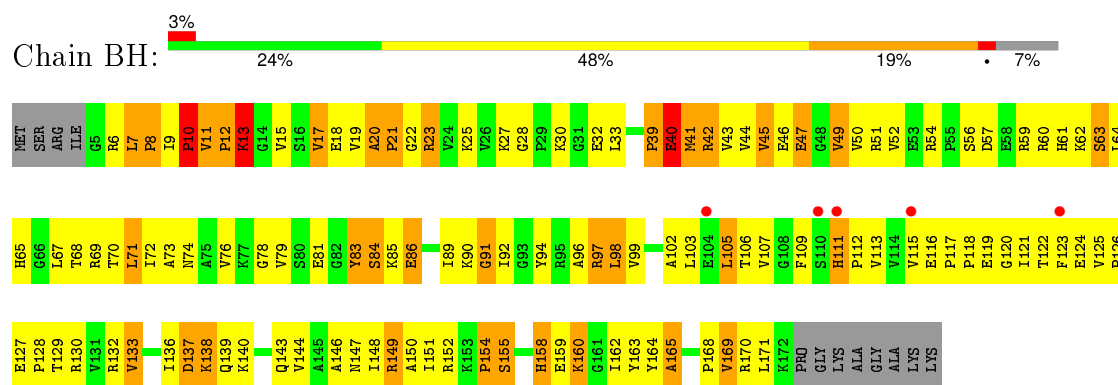
• Molecule 31: 50S ribosomal protein L5



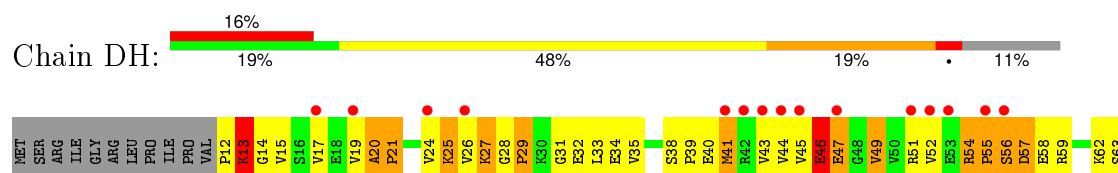
• Molecule 31: 50S ribosomal protein L5

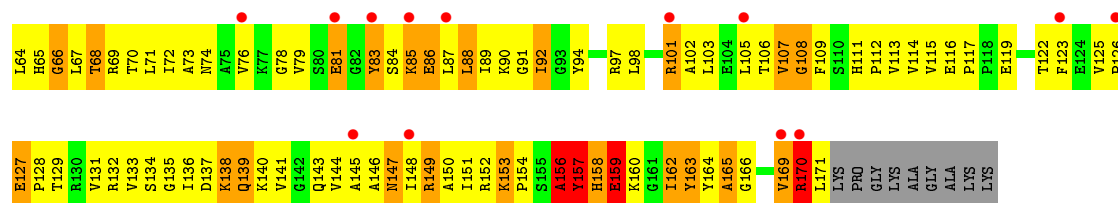


• Molecule 32: 50S ribosomal protein L6

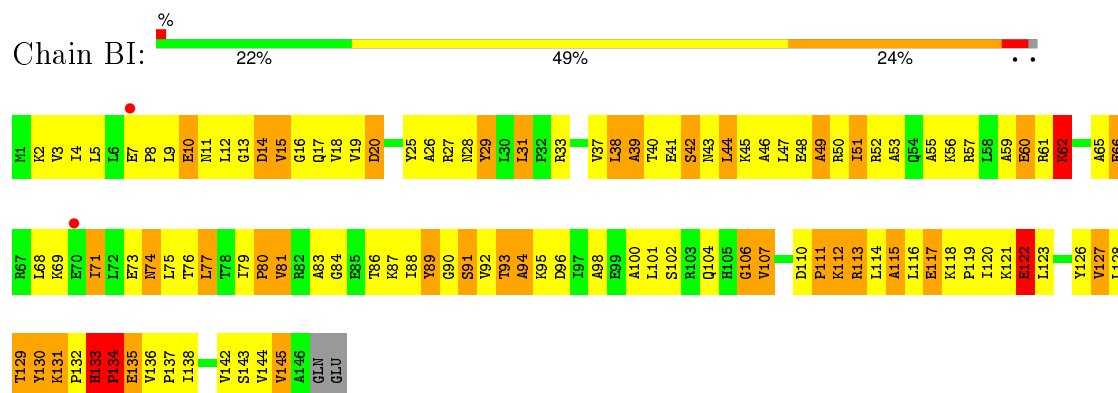


• Molecule 32: 50S ribosomal protein L6

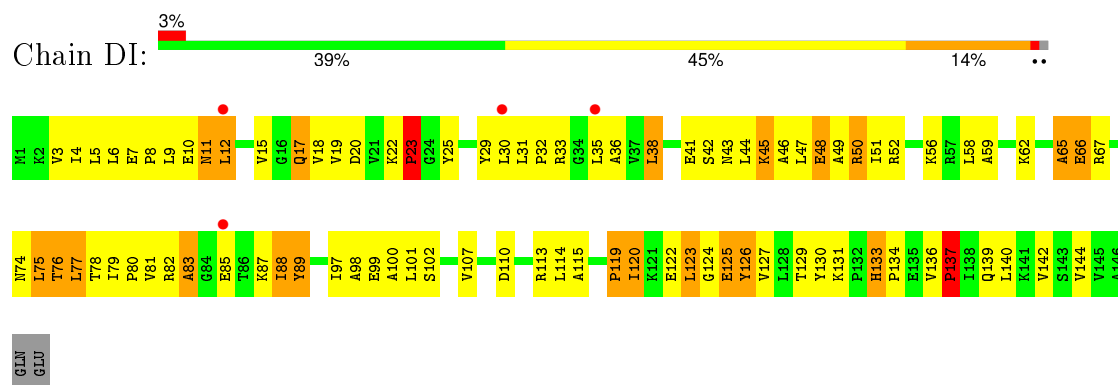




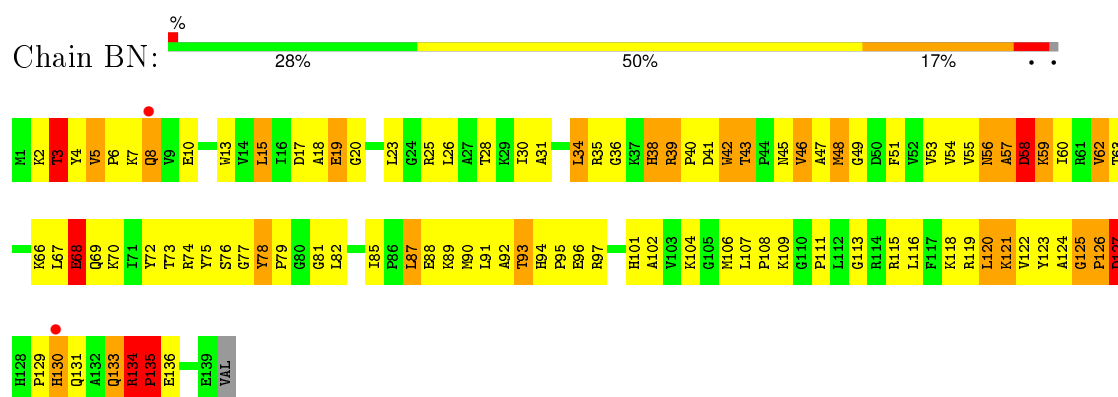
• Molecule 33: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L9

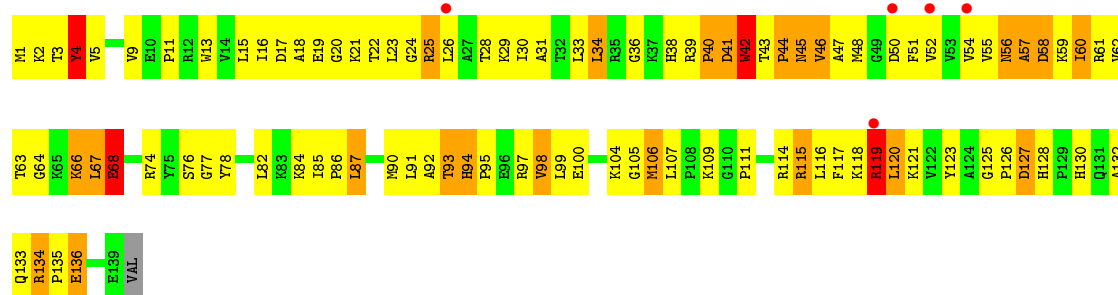


• Molecule 34: 50S ribosomal protein L13



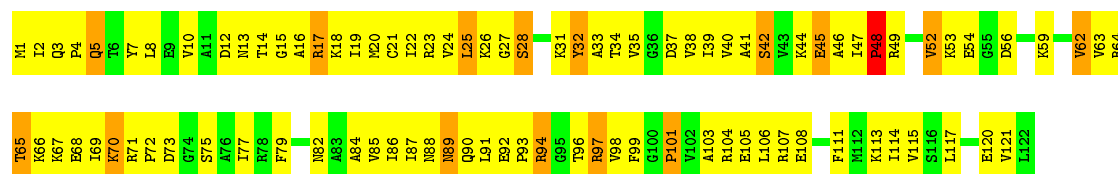
• Molecule 34: 50S ribosomal protein L13





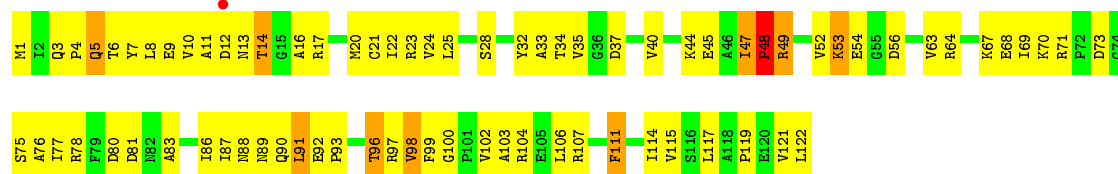
- Molecule 35: 50S ribosomal protein L14

Chain BO: 25% 62% 12%



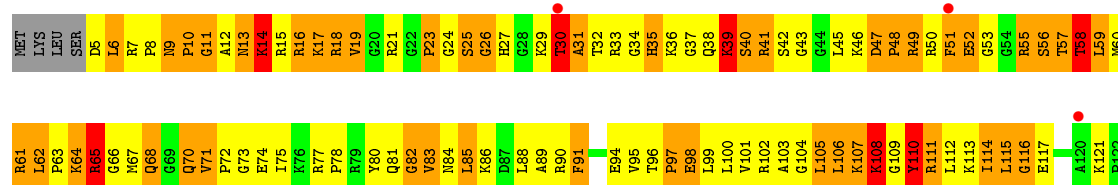
- Molecule 35: 50S ribosomal protein L14

Chain DO: 37% 55% 7%



- Molecule 36: 50S ribosomal protein L15

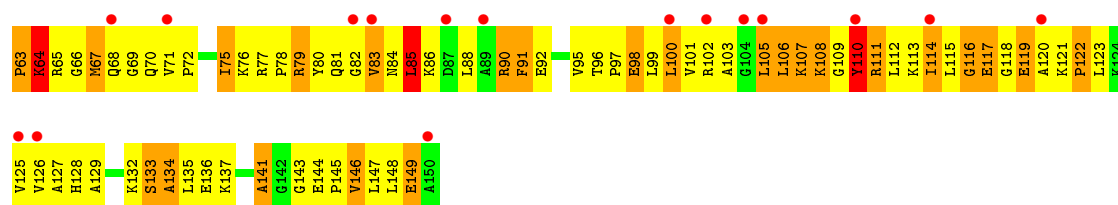
Chain BP: 15% 45% 33% 5%



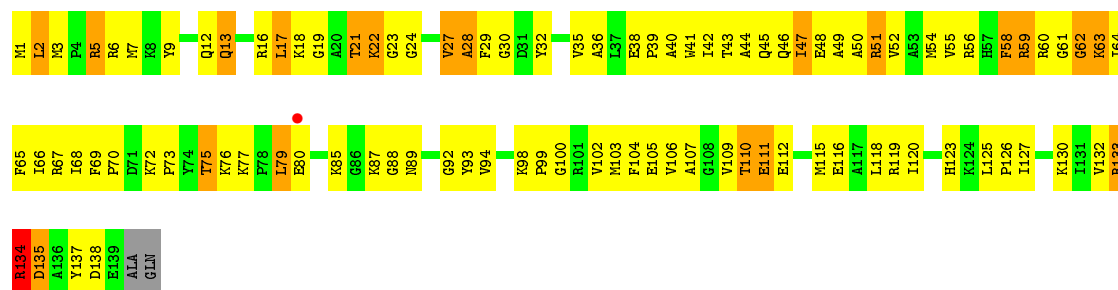
- Molecule 36: 50S ribosomal protein L15

Chain DP: 16% 45% 31% 5%

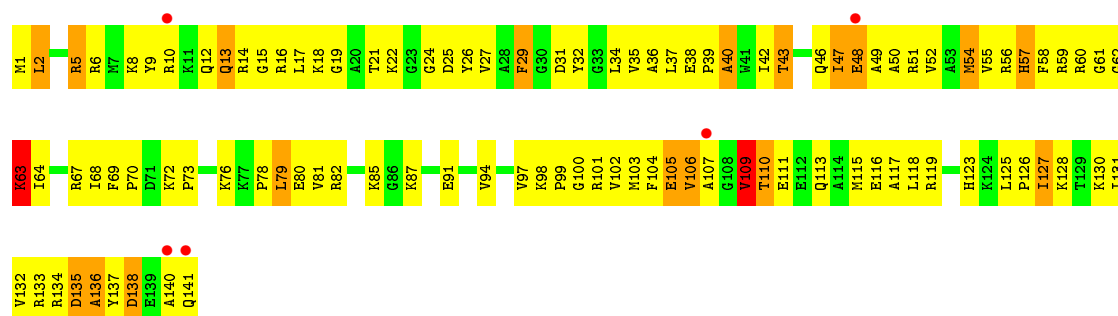
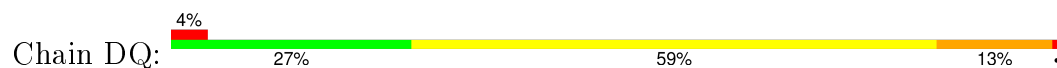




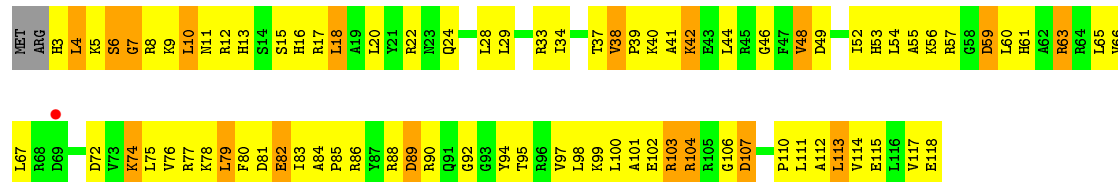
• Molecule 37: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L16

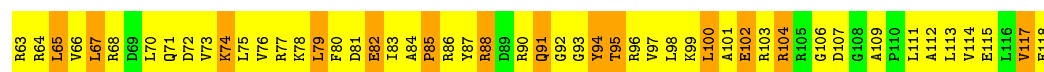


• Molecule 38: 50S ribosomal protein L17

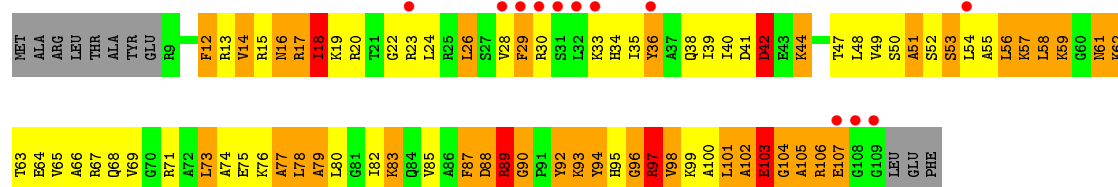
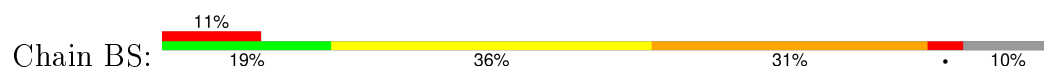


• Molecule 38: 50S ribosomal protein L17

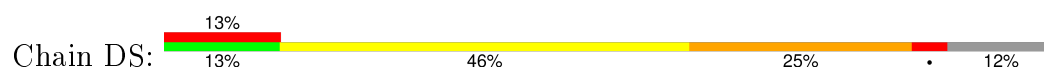




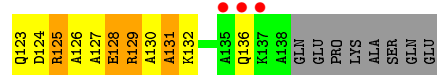
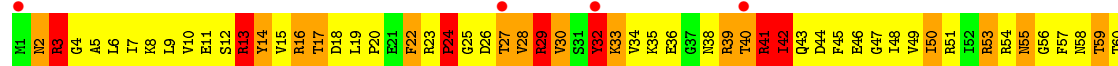
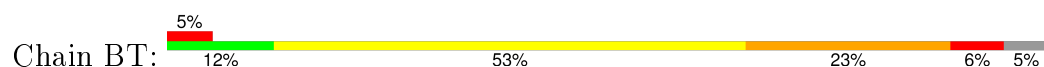
• Molecule 39: 50S ribosomal protein L18



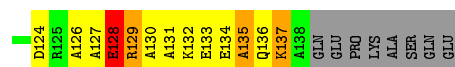
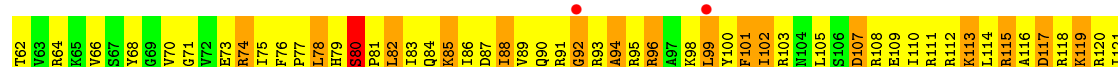
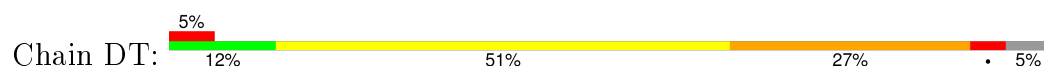
• Molecule 39: 50S ribosomal protein L18



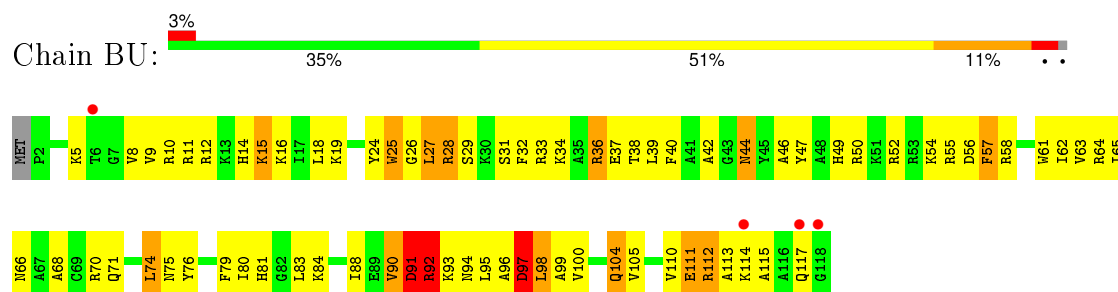
• Molecule 40: 50S ribosomal protein L19



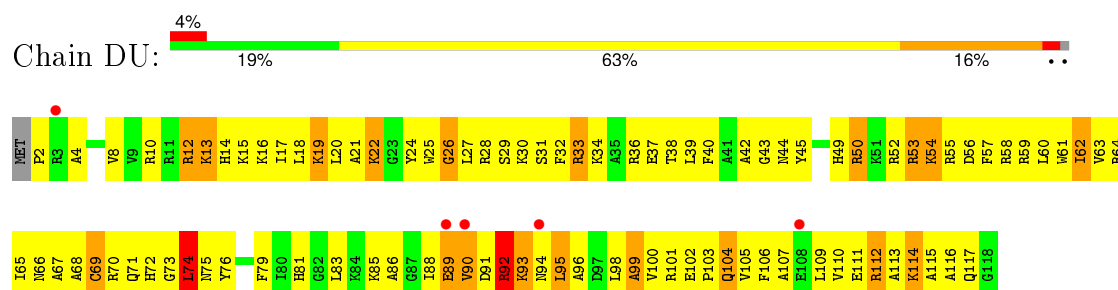
• Molecule 40: 50S ribosomal protein L19



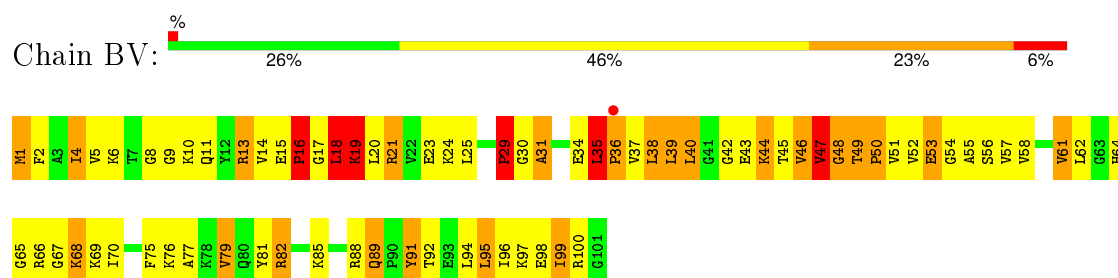
- Molecule 41: 50S ribosomal protein L20



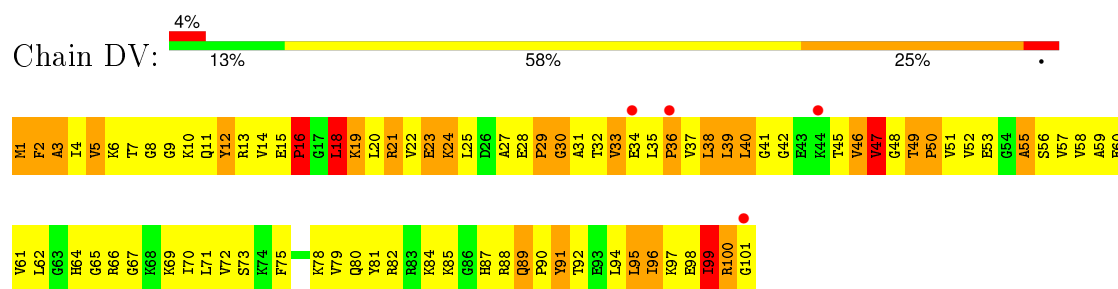
- Molecule 41: 50S ribosomal protein L20



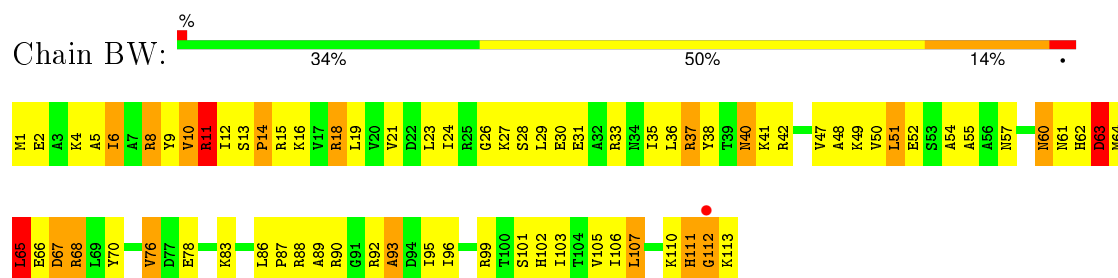
- Molecule 42: 50S ribosomal protein L21



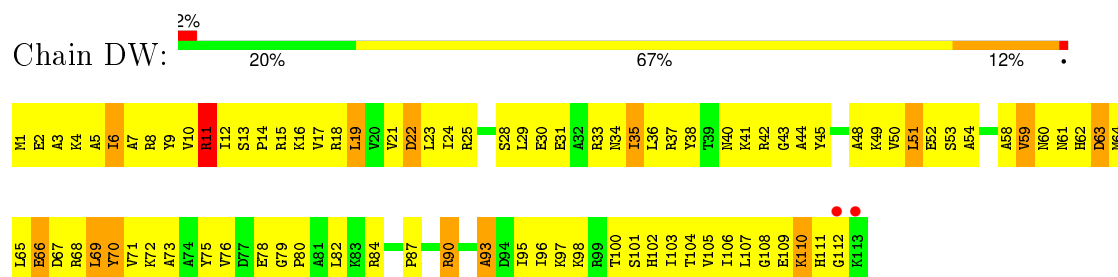
- Molecule 42: 50S ribosomal protein L21



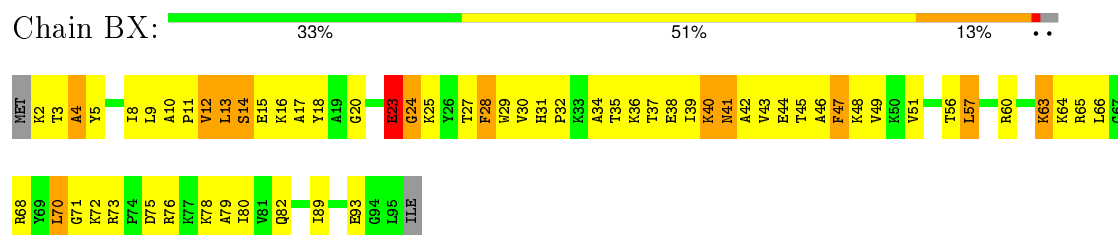
- Molecule 43: 50S ribosomal protein L22



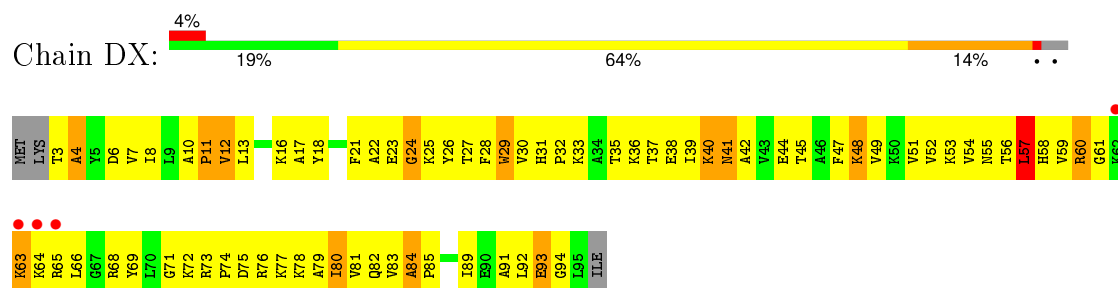
- Molecule 43: 50S ribosomal protein L22



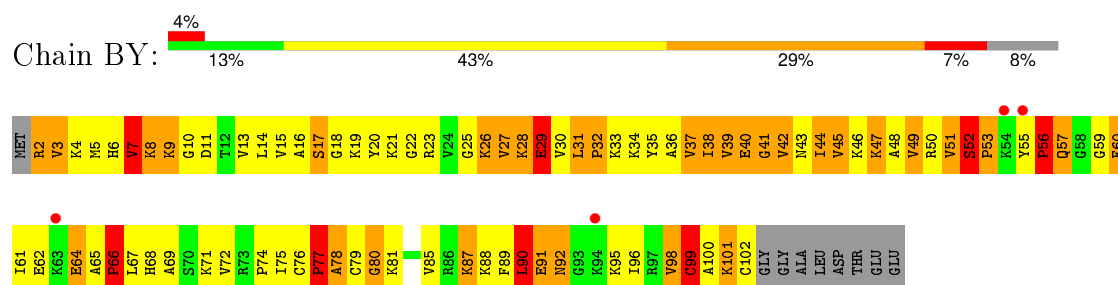
- Molecule 44: 50S ribosomal protein L23



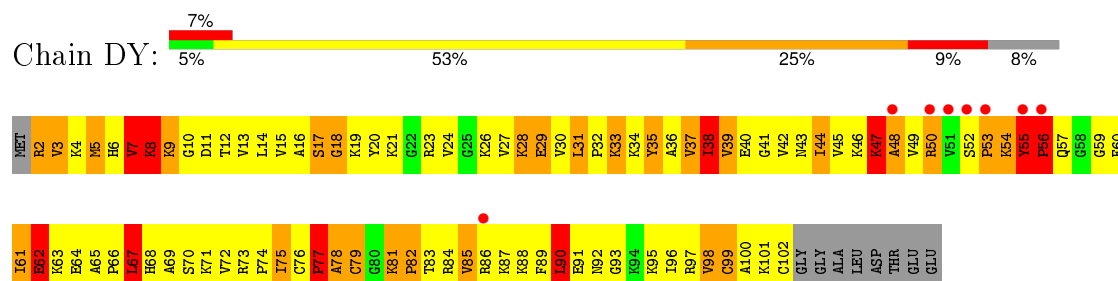
- Molecule 44: 50S ribosomal protein L23



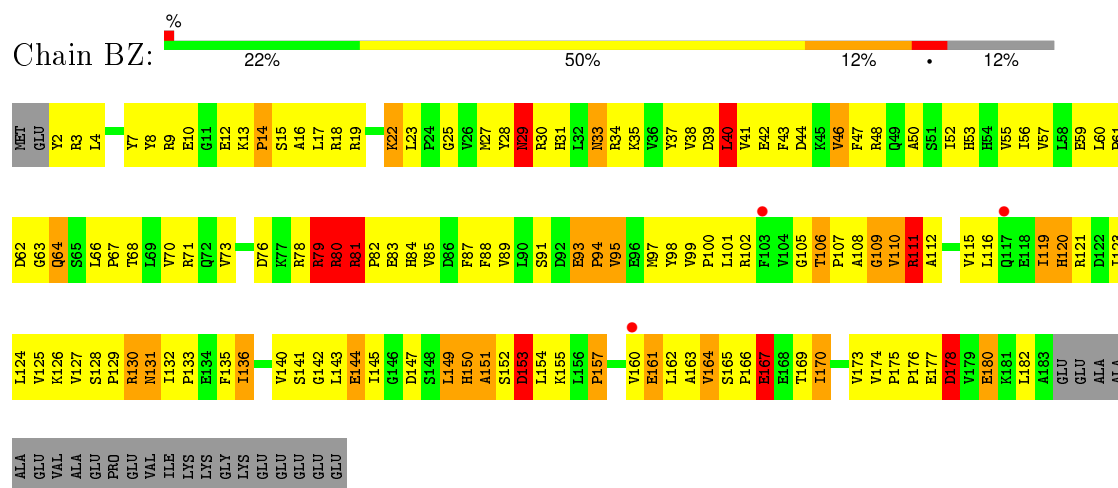
- Molecule 45: 50S ribosomal protein L24



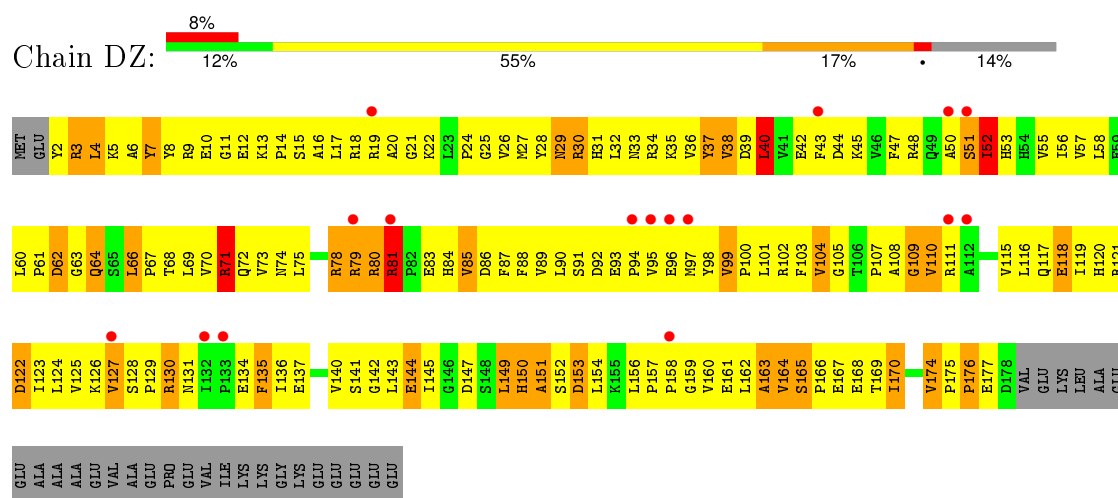
- Molecule 45: 50S ribosomal protein L24



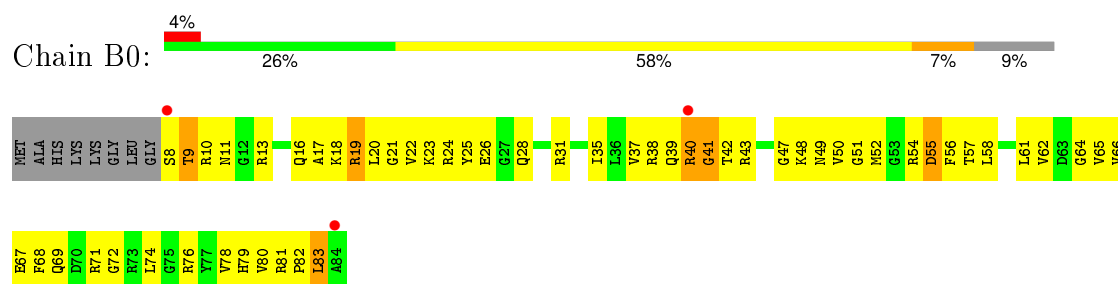
- Molecule 46: 50S ribosomal protein L25



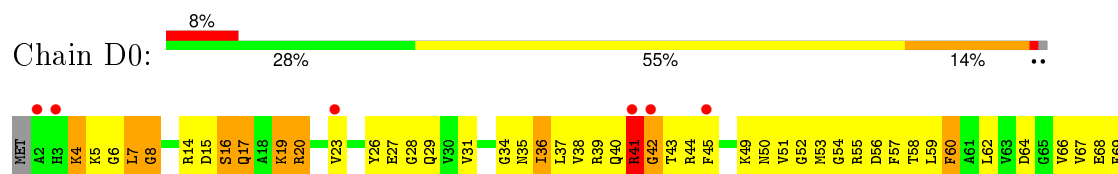
- Molecule 46: 50S ribosomal protein L25



- Molecule 47: 50S ribosomal protein L27



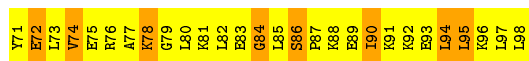
- Molecule 47: 50S ribosomal protein L27





- Molecule 48: 50S ribosomal protein L28

Chain B1: 20% 54% 22% ..



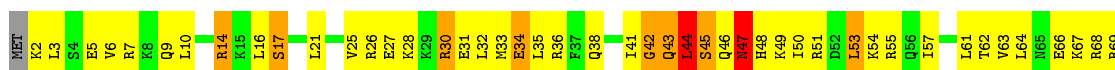
- Molecule 48: 50S ribosomal protein L28

Chain D1: 6% 28% 53% 15% .



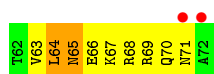
- Molecule 49: 50S ribosomal protein L29

Chain B2: 31% 53% 13% ..



- Molecule 49: 50S ribosomal protein L29

Chain D2: 4% 14% 63% 19% ..

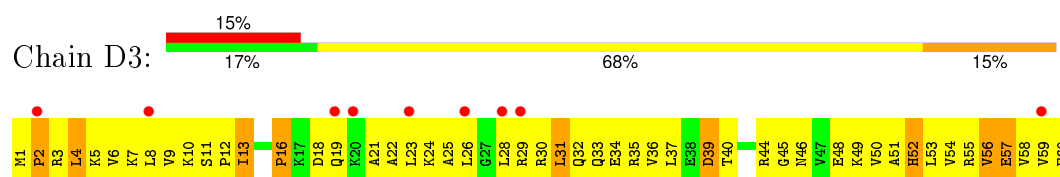


- Molecule 50: 50S ribosomal protein L30

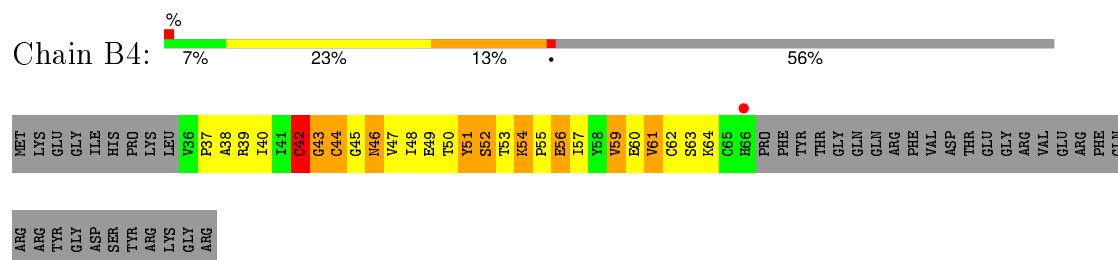
Chain B3: 5% 37% 53% 8% .



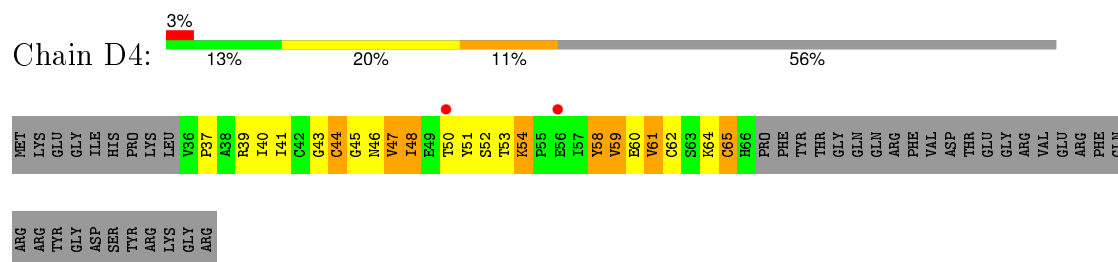
- Molecule 50: 50S ribosomal protein L30



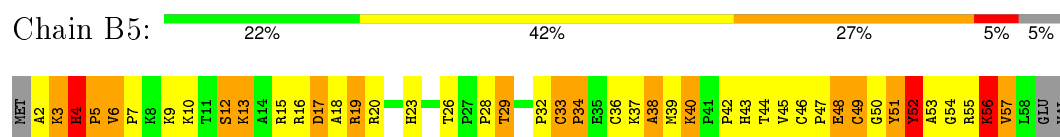
- Molecule 51: 50S ribosomal protein L31



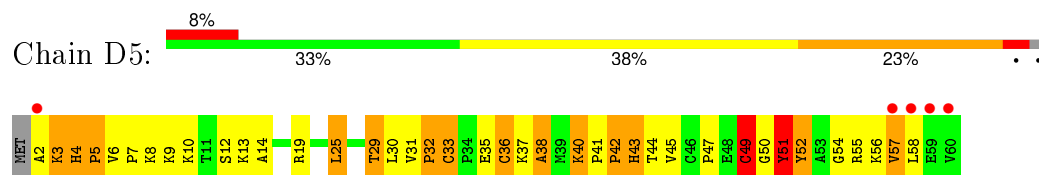
- Molecule 51: 50S ribosomal protein L31



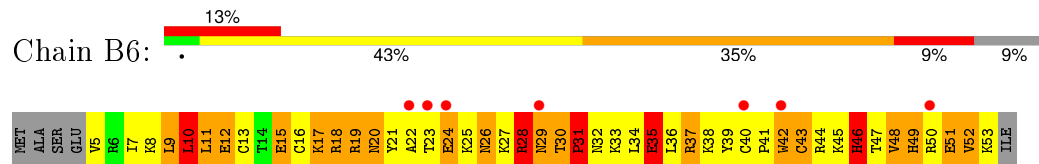
- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32

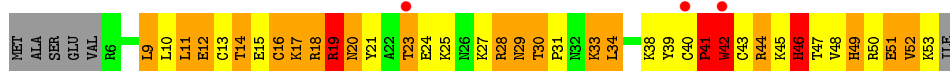


- Molecule 53: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L33

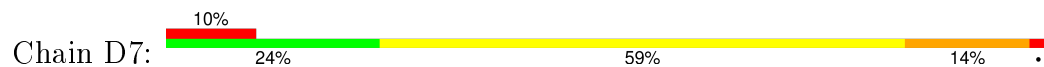




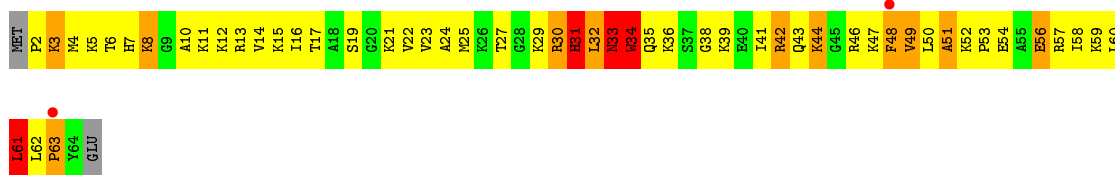
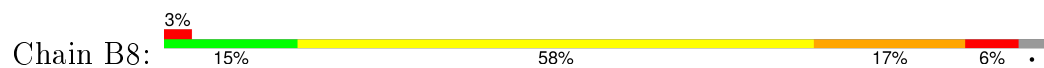
- Molecule 54: 50S ribosomal protein L34



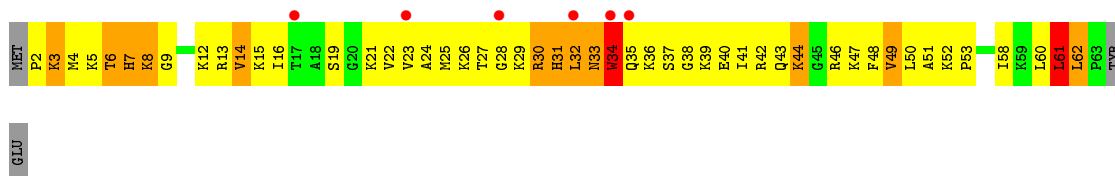
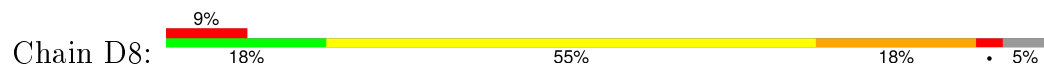
- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35

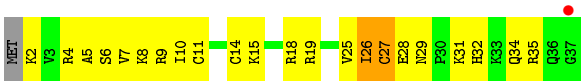


- Molecule 56: 50S ribosomal protein L36



- 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	209.53Å 447.03Å 622.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.10 49.65 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10) 94.7 (49.65-3.10)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.302 0.262 , 0.259	Depositor DCC
R_{free} test set	49631 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 989777 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	290405	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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

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	0.82	6/35982 (0.0%)	0.78	24/56156 (0.0%)
1	CA	0.47	0/36193	0.72	9/56490 (0.0%)
2	AB	0.41	0/1936	0.69	0/2611
2	CB	0.43	0/1936	0.73	1/2611 (0.0%)
3	AC	0.41	0/1637	0.66	0/2207
3	CC	0.40	0/1637	0.66	0/2207
4	AD	0.41	0/1733	0.69	0/2318
4	CD	0.42	0/1733	0.72	1/2318 (0.0%)
5	AE	0.42	0/1163	0.68	0/1566
5	CE	0.40	0/1163	0.69	0/1566
6	AF	0.44	0/856	0.71	0/1154
6	CF	0.40	0/856	0.70	0/1154
7	AG	0.42	0/1276	0.67	0/1709
7	CG	0.42	0/1276	0.67	0/1709
8	AH	0.41	0/1136	0.72	0/1527
8	CH	0.39	0/1136	0.67	0/1527
9	AI	0.46	0/1022	0.69	0/1369
9	CI	0.43	0/1022	0.70	0/1369
10	AJ	0.43	0/808	0.71	0/1087
10	CJ	0.45	0/808	0.72	0/1087
11	AK	0.41	0/900	0.72	1/1213 (0.1%)
11	CK	0.39	0/900	0.67	0/1213
12	AL	0.41	0/987	0.78	0/1322
12	CL	0.41	0/987	0.77	1/1322 (0.1%)
13	AM	0.41	0/957	0.78	1/1283 (0.1%)
13	CM	0.39	0/957	0.76	1/1283 (0.1%)
14	AN	0.43	0/501	0.69	0/664
14	CN	0.45	0/501	0.66	0/664
15	AO	0.42	0/745	0.66	0/992
15	CO	0.39	0/745	0.67	1/992 (0.1%)
16	AP	0.42	0/717	0.71	1/965 (0.1%)
16	CP	0.42	0/717	0.73	1/965 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.44	0/837	0.67	0/1119
17	CQ	0.40	0/837	0.70	0/1119
18	AR	0.40	0/579	0.73	0/768
18	CR	0.45	0/579	0.75	0/768
19	AS	0.42	0/625	0.74	0/844
19	CS	0.45	0/632	0.76	0/853
20	AT	0.37	0/765	0.74	0/1007
20	CT	0.38	0/765	0.73	0/1007
21	AU	0.52	0/213	0.58	0/279
21	CU	0.48	0/213	0.61	0/279
22	AV	0.47	0/1393	0.68	0/1883
22	CV	0.46	0/1393	0.67	0/1883
23	AW	0.61	3/1836 (0.2%)	0.90	6/2859 (0.2%)
23	CW	0.50	1/1836 (0.1%)	0.72	1/2859 (0.0%)
24	AX	0.99	1/123 (0.8%)	0.68	0/188
24	CX	0.89	1/123 (0.8%)	0.67	0/188
25	BA	0.68	8/66745 (0.0%)	0.78	54/104189 (0.1%)
25	DA	0.56	10/66983 (0.0%)	0.76	54/104560 (0.1%)
26	BB	0.50	0/2853	0.79	3/4451 (0.1%)
26	DB	0.47	0/2853	0.72	2/4451 (0.0%)
27	BC	0.41	0/1732	0.69	0/2335
27	DC	0.87	1/1668 (0.1%)	0.65	0/2251
28	BD	0.56	0/2177	0.88	4/2935 (0.1%)
28	DD	0.48	0/2165	0.83	0/2921
29	BE	0.52	0/1597	0.84	2/2155 (0.1%)
29	DE	0.49	0/1597	0.84	1/2155 (0.0%)
30	BF	0.54	0/1659	0.82	1/2246 (0.0%)
30	DF	0.44	0/1659	0.74	0/2246
31	BG	0.45	0/1499	0.75	1/2016 (0.0%)
31	DG	0.43	0/1499	0.77	2/2016 (0.1%)
32	BH	0.55	0/1254	0.83	0/1703
32	DH	0.43	0/1246	0.75	2/1684 (0.1%)
33	BI	0.41	0/1056	0.75	0/1443
33	DI	0.37	0/881	0.73	0/1219
34	BN	0.52	0/1132	0.82	2/1527 (0.1%)
34	DN	0.41	0/1132	0.75	0/1527
35	BO	0.52	0/943	0.79	0/1269
35	DO	0.47	0/943	0.72	0/1269
36	BP	0.54	0/1131	1.08	7/1504 (0.5%)
36	DP	0.45	0/1095	0.90	4/1460 (0.3%)
37	BQ	0.46	0/1120	0.70	0/1498
37	DQ	0.45	0/1143	0.71	0/1527
38	BR	0.49	0/936	0.80	1/1256 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.42	0/974	0.78	0/1302
39	BS	0.47	0/785	0.85	2/1048 (0.2%)
39	DS	0.47	0/779	0.83	1/1038 (0.1%)
40	BT	0.49	0/1156	0.87	3/1544 (0.2%)
40	DT	0.46	0/1156	0.85	1/1544 (0.1%)
41	BU	0.53	0/975	0.79	0/1297
41	DU	0.42	0/975	0.71	0/1297
42	BV	0.54	0/790	0.88	0/1057
42	DV	0.42	0/790	0.77	0/1057
43	BW	0.52	0/907	0.77	0/1216
43	DW	0.42	0/907	0.71	0/1216
44	BX	0.56	0/749	0.81	1/1006 (0.1%)
44	DX	0.47	0/740	0.72	0/995
45	BY	0.58	0/770	0.93	1/1031 (0.1%)
45	DY	0.49	0/789	0.88	1/1053 (0.1%)
46	BZ	0.44	0/1470	0.72	1/1998 (0.1%)
46	DZ	0.42	0/1436	0.70	0/1951
47	B0	0.54	0/621	0.76	0/827
47	D0	0.45	0/671	0.68	0/892
48	B1	0.51	0/764	0.78	0/1014
48	D1	0.41	0/739	0.72	0/983
49	B2	0.45	0/600	0.69	0/793
49	D2	0.42	0/600	0.69	0/793
50	B3	0.47	0/465	0.73	0/625
50	D3	0.36	0/473	0.70	0/636
51	B4	0.57	0/229	0.83	0/311
51	D4	0.46	0/229	0.73	0/311
52	B5	0.58	0/449	0.86	0/608
52	D5	0.51	0/473	0.73	0/639
53	B6	0.68	1/408 (0.2%)	0.95	2/548 (0.4%)
53	D6	0.47	0/328	0.96	1/450 (0.2%)
54	B7	0.59	0/427	0.83	1/563 (0.2%)
54	D7	0.47	0/427	0.74	0/563
55	B8	0.55	0/503	0.94	3/663 (0.5%)
55	D8	0.49	0/473	0.82	0/626
56	B9	0.49	0/297	0.74	0/391
56	D9	0.43	0/302	0.70	0/397
All	All	0.59	32/313996 (0.0%)	0.76	207/468619 (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
1	AA	0	38
1	CA	0	17
23	AW	0	2
23	CW	0	2
25	BA	3	106
25	DA	1	76
26	BB	0	2
26	DB	0	1
28	BD	0	1
52	B5	0	1
52	D5	0	1
All	All	4	247

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1223	C	C4'-C3'	85.69	2.47	1.53
1	AA	1223	C	C3'-C2'	69.16	2.29	1.52
1	AA	1223	C	C3'-O3'	-41.26	0.84	1.42
27	DC	180	SER	CB-OG	31.26	1.82	1.42
1	AA	1223	C	N3-C4	27.30	1.53	1.33

The worst 5 of 207 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1223	C	C4'-C3'-C2'	-42.89	59.71	102.60
1	AA	1223	C	C3'-C2'-C1'	32.11	127.19	101.50
1	AA	1223	C	P-O3'-C3'	-30.31	83.33	119.70
1	AA	1223	C	O4'-C4'-C3'	20.77	124.77	104.00
1	AA	1223	C	N3-C4-C5	-18.18	114.63	121.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	BA	454	A	C3'
25	BA	775	G	C3'
25	BA	1992	G	C3'
25	DA	1992	G	C3'

5 of 247 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	114	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	127	G	Sidechain
1	AA	250	A	Sidechain
1	AA	253	U	Sidechain
1	AA	47	C	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	32144	0	16225	1841	0
1	CA	32332	0	16317	1680	0
2	AB	1901	0	1951	360	0
2	CB	1901	0	1951	361	0
3	AC	1613	0	1677	329	0
3	CC	1613	0	1677	275	0
4	AD	1703	0	1763	325	0
4	CD	1703	0	1763	212	0
5	AE	1147	0	1207	168	0
5	CE	1147	0	1207	177	0
6	AF	843	0	857	111	0
6	CF	843	0	857	137	0
7	AG	1257	0	1296	192	0
7	CG	1257	0	1296	213	0
8	AH	1116	0	1177	183	0
8	CH	1116	0	1177	170	0
9	AI	1004	0	1031	187	0
9	CI	1004	0	1031	200	0
10	AJ	795	0	840	215	0
10	CJ	795	0	840	192	0
11	AK	885	0	904	130	0
11	CK	885	0	904	111	0
12	AL	971	0	1057	168	0
12	CL	971	0	1057	133	0
13	AM	947	0	1008	191	0
13	CM	947	0	1008	135	0
14	AN	492	0	533	111	0
14	CN	492	0	533	95	0
15	AO	734	0	771	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	111	0
16	AP	701	0	720	122	0
16	CP	701	0	720	98	0
17	AQ	824	0	891	108	0
17	CQ	824	0	891	88	0
18	AR	574	0	644	108	0
18	CR	574	0	644	102	0
19	AS	613	0	621	132	0
19	CS	619	0	639	120	0
20	AT	763	0	861	142	0
20	CT	763	0	861	138	0
21	AU	209	0	221	15	0
21	CU	209	0	221	31	0
22	AV	1367	0	1364	182	0
22	CV	1367	0	1364	199	0
23	AW	1644	0	834	67	0
23	CW	1644	0	836	75	0
24	AX	110	0	55	4	0
24	CX	110	0	55	3	0
25	BA	59596	0	30049	2582	0
25	DA	59809	0	30157	2949	0
26	BB	2551	0	1295	92	0
26	DB	2551	0	1295	145	0
27	BC	1702	0	1747	274	0
27	DC	1640	0	1651	242	0
28	BD	2127	0	2208	330	0
28	DD	2115	0	2186	338	0
29	BE	1564	0	1629	252	0
29	DE	1564	0	1629	273	0
30	BF	1624	0	1677	280	0
30	DF	1624	0	1677	300	0
31	BG	1474	0	1535	285	0
31	DG	1474	0	1535	269	0
32	BH	1231	0	1260	198	0
32	DH	1223	0	1282	234	0
33	BI	1043	0	1019	181	0
33	DI	871	0	680	103	0
34	BN	1105	0	1180	132	0
34	DN	1105	0	1180	175	0
35	BO	933	0	996	158	0
35	DO	933	0	996	112	0
36	BP	1114	0	1187	332	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DP	1079	0	1117	265	0
37	BQ	1099	0	1160	144	0
37	DQ	1122	0	1179	190	0
38	BR	923	0	949	105	0
38	DR	960	0	1021	156	0
39	BS	777	0	825	180	0
39	DS	771	0	832	159	0
40	BT	1142	0	1202	274	0
40	DT	1142	0	1202	231	0
41	BU	958	0	1015	150	0
41	DU	958	0	1015	224	0
42	BV	779	0	852	167	0
42	DV	779	0	852	217	0
43	BW	896	0	953	91	0
43	DW	896	0	953	126	0
44	BX	735	0	791	85	0
44	DX	726	0	778	122	0
45	BY	757	0	821	198	0
45	DY	776	0	870	199	0
46	BZ	1438	0	1455	202	0
46	DZ	1404	0	1432	302	0
47	B0	613	0	633	88	0
47	D0	662	0	688	109	0
48	B1	757	0	843	108	0
48	D1	732	0	808	99	0
49	B2	598	0	653	56	0
49	D2	598	0	653	101	0
50	B3	460	0	512	46	0
50	D3	468	0	523	91	0
51	B4	226	0	229	46	0
51	D4	226	0	229	39	0
52	B5	435	0	452	58	0
52	D5	459	0	477	64	0
53	B6	401	0	399	118	0
53	D6	322	0	250	85	0
54	B7	419	0	467	27	0
54	D7	419	0	467	49	0
55	B8	496	0	567	113	0
55	D8	467	0	519	114	0
56	B9	294	0	311	43	0
56	D9	299	0	325	31	0
57	AA	117	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AL	1	0	0	0	0
57	AT	1	0	0	0	0
57	AW	2	0	0	0	0
57	B0	2	0	0	0	0
57	B1	1	0	0	0	0
57	B5	4	0	0	0	0
57	B7	1	0	0	0	0
57	BA	459	0	0	1	0
57	BB	9	0	0	0	0
57	BD	1	0	0	0	0
57	BE	1	0	0	0	0
57	BF	1	0	0	0	0
57	BH	1	0	0	0	0
57	BP	3	0	0	0	0
57	BQ	3	0	0	0	0
57	BR	1	0	0	0	0
57	BT	1	0	0	0	0
57	BU	1	0	0	0	0
57	BX	1	0	0	0	0
57	CA	109	0	0	0	0
57	CE	1	0	0	0	0
57	CW	5	0	0	0	0
57	CX	1	0	0	0	0
57	D5	2	0	0	0	0
57	D6	2	0	0	0	0
57	DA	305	0	0	0	0
57	DB	10	0	0	0	0
57	DD	1	0	0	0	0
57	DF	1	0	0	0	0
57	DP	1	0	0	0	0
57	DR	1	0	0	0	0
58	AD	1	0	0	0	0
58	B5	1	0	0	0	0
58	B9	1	0	0	0	0
58	CD	1	0	0	0	0
58	D5	1	0	0	1	0
58	D9	1	0	0	2	0
All	All	290405	0	198457	23826	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

The worst 5 of 23826 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)
52:D5:49:CYS:SG	58:D5:103:ZN:ZN	0.84	1.63
56:D9:14:CYS:SG	58:D9:101:ZN:ZN	1.23	1.27
27:DC:180:SER:CB	27:DC:180:SER:OG	1.82	1.25
36:BP:59:LEU:HA	36:BP:61:ARG:NH1	1.53	1.21
39:BS:97:ARG:NH2	39:BS:98:VAL:HA	1.55	1.20

There are no symmetry-related clashes.

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%)	128 (55%)	72 (31%)	33 (14%)	0	1
2	CB	233/256 (91%)	138 (59%)	54 (23%)	41 (18%)	0	0
3	AC	205/239 (86%)	106 (52%)	68 (33%)	31 (15%)	0	0
3	CC	205/239 (86%)	134 (65%)	45 (22%)	26 (13%)	0	1
4	AD	206/209 (99%)	124 (60%)	52 (25%)	30 (15%)	0	1
4	CD	206/209 (99%)	132 (64%)	46 (22%)	28 (14%)	0	1
5	AE	149/162 (92%)	107 (72%)	26 (17%)	16 (11%)	0	3
5	CE	149/162 (92%)	98 (66%)	37 (25%)	14 (9%)	1	4
6	AF	99/101 (98%)	63 (64%)	27 (27%)	9 (9%)	1	5
6	CF	99/101 (98%)	61 (62%)	19 (19%)	19 (19%)	0	0
7	AG	153/156 (98%)	98 (64%)	39 (26%)	16 (10%)	1	3
7	CG	153/156 (98%)	95 (62%)	34 (22%)	24 (16%)	0	0
8	AH	136/138 (99%)	96 (71%)	28 (21%)	12 (9%)	1	5
8	CH	136/138 (99%)	93 (68%)	26 (19%)	17 (12%)	0	1
9	AI	125/128 (98%)	82 (66%)	27 (22%)	16 (13%)	0	1
9	CI	125/128 (98%)	80 (64%)	32 (26%)	13 (10%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	97/105 (92%)	58 (60%)	29 (30%)	10 (10%)	1	4
10	CJ	97/105 (92%)	59 (61%)	26 (27%)	12 (12%)	0	1
11	AK	117/129 (91%)	88 (75%)	23 (20%)	6 (5%)	2	15
11	CK	117/129 (91%)	86 (74%)	25 (21%)	6 (5%)	2	15
12	AL	123/132 (93%)	84 (68%)	23 (19%)	16 (13%)	0	1
12	CL	123/132 (93%)	86 (70%)	21 (17%)	16 (13%)	0	1
13	AM	118/126 (94%)	72 (61%)	24 (20%)	22 (19%)	0	0
13	CM	118/126 (94%)	72 (61%)	22 (19%)	24 (20%)	0	0
14	AN	58/61 (95%)	34 (59%)	14 (24%)	10 (17%)	0	0
14	CN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	0
15	AO	86/89 (97%)	58 (67%)	20 (23%)	8 (9%)	1	4
15	CO	86/89 (97%)	55 (64%)	19 (22%)	12 (14%)	0	1
16	AP	82/88 (93%)	46 (56%)	26 (32%)	10 (12%)	0	2
16	CP	82/88 (93%)	46 (56%)	26 (32%)	10 (12%)	0	2
17	AQ	98/105 (93%)	73 (74%)	14 (14%)	11 (11%)	0	3
17	CQ	98/105 (93%)	71 (72%)	19 (19%)	8 (8%)	1	6
18	AR	68/88 (77%)	39 (57%)	17 (25%)	12 (18%)	0	0
18	CR	68/88 (77%)	37 (54%)	26 (38%)	5 (7%)	1	7
19	AS	78/93 (84%)	47 (60%)	16 (20%)	15 (19%)	0	0
19	CS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	1
20	AT	97/106 (92%)	66 (68%)	18 (19%)	13 (13%)	0	1
20	CT	97/106 (92%)	57 (59%)	27 (28%)	13 (13%)	0	1
21	AU	23/27 (85%)	12 (52%)	7 (30%)	4 (17%)	0	0
21	CU	23/27 (85%)	13 (56%)	7 (30%)	3 (13%)	0	1
22	AV	172/184 (94%)	124 (72%)	31 (18%)	17 (10%)	1	4
22	CV	172/184 (94%)	126 (73%)	28 (16%)	18 (10%)	1	3
27	BC	222/229 (97%)	165 (74%)	33 (15%)	24 (11%)	0	3
27	DC	216/229 (94%)	141 (65%)	62 (29%)	13 (6%)	2	11
28	BD	272/276 (99%)	194 (71%)	47 (17%)	31 (11%)	0	2
28	DD	272/276 (99%)	187 (69%)	47 (17%)	38 (14%)	0	1
29	BE	203/206 (98%)	130 (64%)	37 (18%)	36 (18%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DE	203/206 (98%)	122 (60%)	35 (17%)	46 (23%)	0	0
30	BF	206/210 (98%)	136 (66%)	46 (22%)	24 (12%)	0	2
30	DF	206/210 (98%)	123 (60%)	48 (23%)	35 (17%)	0	0
31	BG	179/182 (98%)	118 (66%)	43 (24%)	18 (10%)	1	4
31	DG	179/182 (98%)	109 (61%)	44 (25%)	26 (14%)	0	1
32	BH	166/180 (92%)	98 (59%)	33 (20%)	35 (21%)	0	0
32	DH	158/180 (88%)	80 (51%)	49 (31%)	29 (18%)	0	0
33	BI	144/148 (97%)	84 (58%)	32 (22%)	28 (19%)	0	0
33	DI	144/148 (97%)	74 (51%)	41 (28%)	29 (20%)	0	0
34	BN	137/140 (98%)	104 (76%)	14 (10%)	19 (14%)	0	1
34	DN	137/140 (98%)	79 (58%)	38 (28%)	20 (15%)	0	1
35	BO	120/122 (98%)	91 (76%)	17 (14%)	12 (10%)	1	4
35	DO	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	3	19
36	BP	144/150 (96%)	71 (49%)	34 (24%)	39 (27%)	0	0
36	DP	144/150 (96%)	69 (48%)	34 (24%)	41 (28%)	0	0
37	BQ	137/141 (97%)	102 (74%)	23 (17%)	12 (9%)	1	5
37	DQ	139/141 (99%)	91 (66%)	35 (25%)	13 (9%)	1	4
38	BR	114/118 (97%)	82 (72%)	21 (18%)	11 (10%)	1	4
38	DR	115/118 (98%)	81 (70%)	17 (15%)	17 (15%)	0	1
39	BS	99/112 (88%)	44 (44%)	25 (25%)	30 (30%)	0	0
39	DS	97/112 (87%)	48 (50%)	25 (26%)	24 (25%)	0	0
40	BT	136/146 (93%)	86 (63%)	21 (15%)	29 (21%)	0	0
40	DT	136/146 (93%)	72 (53%)	33 (24%)	31 (23%)	0	0
41	BU	115/118 (98%)	74 (64%)	31 (27%)	10 (9%)	1	5
41	DU	115/118 (98%)	75 (65%)	25 (22%)	15 (13%)	0	1
42	BV	99/101 (98%)	68 (69%)	13 (13%)	18 (18%)	0	0
42	DV	99/101 (98%)	57 (58%)	20 (20%)	22 (22%)	0	0
43	BW	111/113 (98%)	75 (68%)	24 (22%)	12 (11%)	0	3
43	DW	111/113 (98%)	82 (74%)	18 (16%)	11 (10%)	1	4
44	BX	92/96 (96%)	64 (70%)	21 (23%)	7 (8%)	1	7
44	DX	91/96 (95%)	64 (70%)	16 (18%)	11 (12%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BY	99/110 (90%)	38 (38%)	23 (23%)	38 (38%)	0	0
45	DY	99/110 (90%)	39 (39%)	26 (26%)	34 (34%)	0	0
46	BZ	180/206 (87%)	114 (63%)	41 (23%)	25 (14%)	0	1
46	DZ	175/206 (85%)	103 (59%)	46 (26%)	26 (15%)	0	1
47	B0	75/85 (88%)	60 (80%)	13 (17%)	2 (3%)	6	31
47	D0	82/85 (96%)	60 (73%)	15 (18%)	7 (8%)	1	5
48	B1	94/98 (96%)	65 (69%)	15 (16%)	14 (15%)	0	1
48	D1	92/98 (94%)	65 (71%)	17 (18%)	10 (11%)	0	3
49	B2	69/72 (96%)	53 (77%)	9 (13%)	7 (10%)	1	4
49	D2	69/72 (96%)	41 (59%)	17 (25%)	11 (16%)	0	0
50	B3	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	11	42
50	D3	58/60 (97%)	38 (66%)	13 (22%)	7 (12%)	0	2
51	B4	29/71 (41%)	13 (45%)	9 (31%)	7 (24%)	0	0
51	D4	29/71 (41%)	13 (45%)	9 (31%)	7 (24%)	0	0
52	B5	55/60 (92%)	31 (56%)	10 (18%)	14 (26%)	0	0
52	D5	57/60 (95%)	35 (61%)	11 (19%)	11 (19%)	0	0
53	B6	47/54 (87%)	19 (40%)	13 (28%)	15 (32%)	0	0
53	D6	46/54 (85%)	19 (41%)	11 (24%)	16 (35%)	0	0
54	B7	47/49 (96%)	40 (85%)	7 (15%)	0	100	100
54	D7	47/49 (96%)	37 (79%)	6 (13%)	4 (8%)	1	5
55	B8	61/65 (94%)	36 (59%)	16 (26%)	9 (15%)	0	1
55	D8	60/65 (92%)	37 (62%)	14 (23%)	9 (15%)	0	0
56	B9	34/37 (92%)	24 (71%)	9 (26%)	1 (3%)	6	29
56	D9	34/37 (92%)	31 (91%)	3 (9%)	0	100	100
All	All	12117/12954 (94%)	7729 (64%)	2646 (22%)	1742 (14%)	0	1

5 of 1742 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	23	ARG
2	AB	26	PRO
2	AB	75	LYS
2	AB	128	GLU

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%)	173 (86%)	29 (14%)	4	17
2	CB	202/220 (92%)	179 (89%)	23 (11%)	7	28
3	AC	160/188 (85%)	142 (89%)	18 (11%)	7	28
3	CC	160/188 (85%)	146 (91%)	14 (9%)	12	43
4	AD	180/181 (99%)	157 (87%)	23 (13%)	5	21
4	CD	180/181 (99%)	158 (88%)	22 (12%)	6	24
5	AE	115/123 (94%)	102 (89%)	13 (11%)	7	28
5	CE	115/123 (94%)	104 (90%)	11 (10%)	10	37
6	AF	90/90 (100%)	77 (86%)	13 (14%)	4	17
6	CF	90/90 (100%)	81 (90%)	9 (10%)	9	34
7	AG	126/127 (99%)	112 (89%)	14 (11%)	8	29
7	CG	126/127 (99%)	110 (87%)	16 (13%)	5	22
8	AH	119/119 (100%)	109 (92%)	10 (8%)	14	46
8	CH	119/119 (100%)	108 (91%)	11 (9%)	11	40
9	AI	97/99 (98%)	80 (82%)	17 (18%)	2	10
9	CI	97/99 (98%)	78 (80%)	19 (20%)	1	7
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	4	16
10	CJ	88/92 (96%)	79 (90%)	9 (10%)	9	33
11	AK	90/99 (91%)	85 (94%)	5 (6%)	26	62
11	CK	90/99 (91%)	81 (90%)	9 (10%)	9	34
12	AL	104/109 (95%)	94 (90%)	10 (10%)	10	37
12	CL	104/109 (95%)	92 (88%)	12 (12%)	7	27
13	AM	95/101 (94%)	74 (78%)	21 (22%)	1	5
13	CM	95/101 (94%)	79 (83%)	16 (17%)	2	11
14	AN	49/50 (98%)	40 (82%)	9 (18%)	2	9
14	CN	49/50 (98%)	44 (90%)	5 (10%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	79/80 (99%)	73 (92%)	6 (8%)	16	51
15	CO	79/80 (99%)	73 (92%)	6 (8%)	16	51
16	AP	72/74 (97%)	64 (89%)	8 (11%)	8	29
16	CP	72/74 (97%)	65 (90%)	7 (10%)	10	36
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	13	45
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	13	45
18	AR	61/77 (79%)	57 (93%)	4 (7%)	21	56
18	CR	61/77 (79%)	54 (88%)	7 (12%)	7	27
19	AS	65/80 (81%)	52 (80%)	13 (20%)	1	7
19	CS	68/80 (85%)	56 (82%)	12 (18%)	2	10
20	AT	76/82 (93%)	67 (88%)	9 (12%)	6	25
20	CT	76/82 (93%)	66 (87%)	10 (13%)	5	20
21	AU	19/22 (86%)	17 (90%)	2 (10%)	8	31
21	CU	19/22 (86%)	18 (95%)	1 (5%)	28	64
22	AV	148/154 (96%)	136 (92%)	12 (8%)	15	47
22	CV	148/154 (96%)	129 (87%)	19 (13%)	5	21
27	BC	175/181 (97%)	148 (85%)	27 (15%)	3	14
27	DC	165/181 (91%)	146 (88%)	19 (12%)	7	27
28	BD	215/218 (99%)	179 (83%)	36 (17%)	3	11
28	DD	213/218 (98%)	184 (86%)	29 (14%)	5	19
29	BE	165/166 (99%)	144 (87%)	21 (13%)	5	22
29	DE	165/166 (99%)	140 (85%)	25 (15%)	3	14
30	BF	165/166 (99%)	137 (83%)	28 (17%)	2	11
30	DF	165/166 (99%)	143 (87%)	22 (13%)	5	20
31	BG	155/156 (99%)	126 (81%)	29 (19%)	2	8
31	DG	155/156 (99%)	132 (85%)	23 (15%)	4	16
32	BH	127/148 (86%)	115 (91%)	12 (9%)	11	39
32	DH	132/148 (89%)	111 (84%)	21 (16%)	3	13
33	BI	97/124 (78%)	78 (80%)	19 (20%)	1	7
33	DI	49/124 (40%)	41 (84%)	8 (16%)	3	12
34	BN	117/119 (98%)	95 (81%)	22 (19%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DN	117/119 (98%)	100 (86%)	17 (14%)	4	16
35	BO	100/100 (100%)	90 (90%)	10 (10%)	9	34
35	DO	100/100 (100%)	91 (91%)	9 (9%)	12	41
36	BP	112/116 (97%)	88 (79%)	24 (21%)	1	5
36	DP	103/116 (89%)	81 (79%)	22 (21%)	1	5
37	BQ	109/111 (98%)	95 (87%)	14 (13%)	5	21
37	DQ	111/111 (100%)	100 (90%)	11 (10%)	10	34
38	BR	92/101 (91%)	80 (87%)	12 (13%)	5	21
38	DR	100/101 (99%)	83 (83%)	17 (17%)	2	11
39	BS	76/88 (86%)	61 (80%)	15 (20%)	1	7
39	DS	77/88 (88%)	60 (78%)	17 (22%)	1	5
40	BT	120/127 (94%)	94 (78%)	26 (22%)	1	5
40	DT	120/127 (94%)	97 (81%)	23 (19%)	2	8
41	BU	92/94 (98%)	77 (84%)	15 (16%)	3	12
41	DU	92/94 (98%)	82 (89%)	10 (11%)	8	30
42	BV	82/82 (100%)	63 (77%)	19 (23%)	1	4
42	DV	82/82 (100%)	66 (80%)	16 (20%)	2	7
43	BW	91/92 (99%)	77 (85%)	14 (15%)	3	14
43	DW	91/92 (99%)	84 (92%)	7 (8%)	16	50
44	BX	75/78 (96%)	64 (85%)	11 (15%)	4	16
44	DX	74/78 (95%)	66 (89%)	8 (11%)	8	30
45	BY	79/91 (87%)	64 (81%)	15 (19%)	2	8
45	DY	84/91 (92%)	69 (82%)	15 (18%)	2	10
46	BZ	158/179 (88%)	136 (86%)	22 (14%)	4	19
46	DZ	155/179 (87%)	131 (84%)	24 (16%)	3	14
47	B0	62/67 (92%)	56 (90%)	6 (10%)	10	36
47	D0	66/67 (98%)	56 (85%)	10 (15%)	3	14
48	B1	81/83 (98%)	66 (82%)	15 (18%)	2	9
48	D1	78/83 (94%)	69 (88%)	9 (12%)	7	27
49	B2	66/67 (98%)	57 (86%)	9 (14%)	5	19
49	D2	66/67 (98%)	57 (86%)	9 (14%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B3	50/52 (96%)	43 (86%)	7 (14%)	4	18
50	D3	51/52 (98%)	48 (94%)	3 (6%)	24	60
51	B4	27/63 (43%)	23 (85%)	4 (15%)	4	16
51	D4	27/63 (43%)	25 (93%)	2 (7%)	17	51
52	B5	48/52 (92%)	36 (75%)	12 (25%)	1	2
52	D5	51/52 (98%)	44 (86%)	7 (14%)	4	19
53	B6	43/52 (83%)	32 (74%)	11 (26%)	0	2
53	D6	24/52 (46%)	14 (58%)	10 (42%)	0	0
54	B7	41/42 (98%)	38 (93%)	3 (7%)	17	52
54	D7	41/42 (98%)	32 (78%)	9 (22%)	1	5
55	B8	52/55 (94%)	44 (85%)	8 (15%)	3	14
55	D8	46/55 (84%)	36 (78%)	10 (22%)	1	5
56	B9	32/34 (94%)	26 (81%)	6 (19%)	2	8
56	D9	33/34 (97%)	28 (85%)	5 (15%)	3	14
All	All	9998/10736 (93%)	8606 (86%)	1392 (14%)	4	19

5 of 1392 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	BZ	79	ARG
4	CD	127	THR
45	DY	55	TYR
47	B0	9	THR
53	B6	24	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 340 such sidechains are listed below:

Mol	Chain	Res	Type
50	B3	46	ASN
6	CF	64	GLN
46	DZ	64	GLN
54	B7	8	ASN
3	CC	31	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1492/1509 (98%)	236 (15%)	40 (2%)
1	CA	1503/1509 (99%)	227 (15%)	33 (2%)
23	AW	76/77 (98%)	18 (23%)	2 (2%)
23	CW	76/77 (98%)	19 (25%)	6 (7%)
24	AX	4/5 (80%)	0	0
24	CX	4/5 (80%)	0	0
25	BA	2761/2915 (94%)	508 (18%)	77 (2%)
25	DA	2771/2915 (95%)	546 (19%)	84 (3%)
26	BB	118/122 (96%)	19 (16%)	2 (1%)
26	DB	118/122 (96%)	20 (16%)	2 (1%)
All	All	8923/9256 (96%)	1593 (17%)	246 (2%)

5 of 1593 RNA backbone outliers are listed below:

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

5 of 246 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2610	C
1	CA	484	G
25	DA	2422	A
25	BA	2750	A
1	CA	79	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1056 ligands modelled in this entry, 1056 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	1495/1509 (99%)	0.11	41 (2%) 58 34	43, 73, 89, 96	1 (0%)
1	CA	1504/1509 (99%)	0.18	35 (2%) 64 40	47, 71, 88, 97	1 (0%)
2	AB	235/256 (91%)	0.22	17 (7%) 18 7	65, 75, 82, 88	0
2	CB	235/256 (91%)	0.38	19 (8%) 15 5	66, 76, 82, 85	0
3	AC	207/239 (86%)	0.35	12 (5%) 26 11	67, 75, 82, 86	0
3	CC	207/239 (86%)	0.39	21 (10%) 9 3	67, 75, 81, 84	0
4	AD	208/209 (99%)	-0.06	2 (0%) 84 69	61, 72, 79, 85	0
4	CD	208/209 (99%)	0.00	6 (2%) 55 31	55, 68, 75, 83	0
5	AE	151/162 (93%)	0.27	10 (6%) 22 8	60, 69, 76, 83	0
5	CE	151/162 (93%)	0.22	5 (3%) 50 26	60, 69, 77, 90	0
6	AF	101/101 (100%)	-0.33	1 (0%) 84 69	56, 67, 76, 81	0
6	CF	101/101 (100%)	0.00	2 (1%) 68 46	61, 70, 78, 83	0
7	AG	155/156 (99%)	0.13	8 (5%) 31 13	63, 74, 80, 83	0
7	CG	155/156 (99%)	0.48	14 (9%) 12 4	67, 74, 81, 84	0
8	AH	138/138 (100%)	-0.02	2 (1%) 78 60	56, 69, 74, 79	0
8	CH	138/138 (100%)	0.03	4 (2%) 55 31	57, 70, 76, 82	0
9	AI	127/128 (99%)	0.58	11 (8%) 13 4	66, 77, 83, 87	0
9	CI	127/128 (99%)	1.08	30 (23%) 1 0	70, 77, 83, 86	0
10	AJ	99/105 (94%)	0.88	16 (16%) 3 1	66, 79, 84, 88	0
10	CJ	99/105 (94%)	2.02	48 (48%) 0 0	66, 79, 84, 87	0
11	AK	119/129 (92%)	0.64	11 (9%) 11 4	58, 68, 78, 82	0
11	CK	119/129 (92%)	0.10	4 (3%) 49 24	64, 72, 78, 84	0
12	AL	125/132 (94%)	-0.09	4 (3%) 51 27	53, 67, 76, 85	0
12	CL	125/132 (94%)	0.31	6 (4%) 34 15	56, 65, 74, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	120/126 (95%)	0.36	10 (8%) 14 5	66, 75, 81, 83	0
13	CM	120/126 (95%)	0.29	7 (5%) 26 11	65, 75, 81, 84	0
14	AN	60/61 (98%)	0.13	2 (3%) 50 26	65, 74, 80, 82	0
14	CN	60/61 (98%)	0.12	1 (1%) 73 52	62, 74, 78, 82	0
15	AO	88/89 (98%)	-0.02	0 100 100	52, 66, 74, 79	0
15	CO	88/89 (98%)	-0.02	1 (1%) 82 66	59, 68, 76, 78	0
16	AP	84/88 (95%)	0.25	7 (8%) 14 5	62, 69, 77, 80	0
16	CP	84/88 (95%)	0.42	2 (2%) 62 39	59, 66, 75, 83	0
17	AQ	100/105 (95%)	0.20	2 (2%) 68 46	59, 68, 75, 76	0
17	CQ	100/105 (95%)	-0.03	0 100 100	58, 68, 76, 78	0
18	AR	70/88 (79%)	0.08	0 100 100	58, 69, 78, 85	0
18	CR	70/88 (79%)	0.53	4 (5%) 27 11	63, 69, 77, 82	0
19	AS	80/93 (86%)	0.43	5 (6%) 23 9	66, 76, 83, 86	0
19	CS	78/93 (83%)	0.61	9 (11%) 6 2	70, 76, 82, 84	0
20	AT	99/106 (93%)	0.31	6 (6%) 25 10	62, 71, 79, 83	0
20	CT	99/106 (93%)	0.33	6 (6%) 25 10	63, 69, 77, 83	0
21	AU	25/27 (92%)	1.21	7 (28%) 1 0	67, 74, 81, 83	0
21	CU	25/27 (92%)	1.70	6 (24%) 1 0	68, 77, 83, 85	0
22	AV	176/184 (95%)	-0.01	5 (2%) 56 32	51, 71, 79, 83	0
22	CV	176/184 (95%)	0.34	10 (5%) 27 11	58, 72, 80, 84	0
23	AW	77/77 (100%)	0.26	2 (2%) 59 35	45, 69, 81, 92	0
23	CW	77/77 (100%)	-0.14	0 100 100	58, 72, 83, 87	0
24	AX	5/5 (100%)	0.77	0 100 100	65, 65, 83, 88	0
24	CX	5/5 (100%)	0.71	1 (20%) 1 0	68, 70, 82, 88	0
25	BA	2767/2915 (94%)	0.09	52 (1%) 70 48	25, 53, 82, 97	0
25	DA	2777/2915 (95%)	0.15	66 (2%) 62 39	38, 65, 85, 97	0
26	BB	119/122 (97%)	-0.17	0 100 100	53, 67, 77, 86	0
26	DB	119/122 (97%)	0.22	3 (2%) 61 37	68, 77, 83, 92	0
27	BC	224/229 (97%)	0.56	18 (8%) 15 5	67, 76, 81, 86	1 (0%)
27	DC	220/229 (96%)	0.58	27 (12%) 5 2	66, 76, 82, 87	1 (0%)
28	BD	274/276 (99%)	-0.04	3 (1%) 82 66	38, 53, 65, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	274/276 (99%)	0.11	8 (2%) 55 31	42, 59, 70, 77	0
29	BE	205/206 (99%)	-0.02	3 (1%) 76 58	38, 58, 73, 77	0
29	DE	205/206 (99%)	0.18	12 (5%) 26 11	46, 65, 78, 82	0
30	BF	208/210 (99%)	0.23	10 (4%) 34 15	35, 58, 78, 88	0
30	DF	208/210 (99%)	0.17	6 (2%) 55 31	52, 69, 78, 90	0
31	BG	181/182 (99%)	0.06	6 (3%) 50 26	60, 71, 79, 86	0
31	DG	181/182 (99%)	0.43	17 (9%) 11 4	65, 73, 81, 85	0
32	BH	168/180 (93%)	0.12	5 (2%) 54 29	25, 66, 75, 82	0
32	DH	160/180 (88%)	0.77	28 (17%) 2 1	66, 76, 82, 87	0
33	BI	146/148 (98%)	-0.14	2 (1%) 78 60	55, 71, 77, 84	0
33	DI	146/148 (98%)	0.06	4 (2%) 58 34	60, 73, 80, 83	0
34	BN	139/140 (99%)	-0.13	2 (1%) 78 60	46, 59, 72, 77	0
34	DN	139/140 (99%)	0.27	5 (3%) 46 23	60, 70, 77, 82	0
35	BO	122/122 (100%)	-0.16	0 100 100	44, 59, 70, 73	0
35	DO	122/122 (100%)	0.16	1 (0%) 87 75	50, 63, 71, 75	0
36	BP	146/150 (97%)	0.37	5 (3%) 49 24	40, 65, 76, 81	0
36	DP	146/150 (97%)	0.71	17 (11%) 6 2	52, 70, 78, 82	0
37	BQ	139/141 (98%)	-0.11	1 (0%) 89 78	45, 61, 71, 80	0
37	DQ	141/141 (100%)	0.19	5 (3%) 48 23	54, 69, 77, 83	0
38	BR	116/118 (98%)	0.03	1 (0%) 85 72	39, 57, 69, 74	0
38	DR	117/118 (99%)	0.13	0 100 100	50, 63, 73, 78	0
39	BS	101/112 (90%)	0.66	12 (11%) 6 2	49, 69, 74, 80	0
39	DS	99/112 (88%)	0.61	14 (14%) 4 2	63, 72, 79, 86	0
40	BT	138/146 (94%)	0.17	8 (5%) 26 11	52, 65, 79, 83	0
40	DT	138/146 (94%)	0.18	7 (5%) 32 13	56, 67, 81, 84	0
41	BU	117/118 (99%)	0.09	4 (3%) 49 24	41, 54, 68, 78	0
41	DU	117/118 (99%)	0.14	5 (4%) 39 18	55, 67, 76, 81	0
42	BV	101/101 (100%)	-0.13	1 (0%) 84 69	41, 60, 71, 75	0
42	DV	101/101 (100%)	0.43	4 (3%) 42 20	58, 74, 79, 85	0
43	BW	113/113 (100%)	0.01	1 (0%) 85 72	44, 53, 70, 86	0
43	DW	113/113 (100%)	0.01	2 (1%) 71 50	56, 64, 78, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	94/96 (97%)	0.03	0 100 100	42, 57, 69, 79	0
44	DX	93/96 (96%)	0.14	4 (4%) 39 18	53, 67, 73, 81	0
45	BY	101/110 (91%)	0.08	4 (3%) 42 20	51, 64, 77, 81	0
45	DY	101/110 (91%)	0.49	8 (7%) 15 5	63, 74, 82, 85	0
46	BZ	182/206 (88%)	-0.00	3 (1%) 74 55	56, 70, 78, 83	0
46	DZ	177/206 (85%)	0.51	16 (9%) 12 4	68, 76, 83, 87	0
47	B0	77/85 (90%)	0.17	3 (3%) 43 21	49, 59, 72, 81	0
47	D0	84/85 (98%)	0.47	7 (8%) 14 5	59, 68, 78, 84	0
48	B1	96/98 (97%)	-0.07	0 100 100	42, 60, 72, 77	0
48	D1	94/98 (95%)	0.37	6 (6%) 23 9	50, 64, 75, 78	0
49	B2	71/72 (98%)	-0.16	0 100 100	50, 61, 75, 80	0
49	D2	71/72 (98%)	-0.21	3 (4%) 40 19	60, 71, 79, 87	0
50	B3	59/60 (98%)	0.16	3 (5%) 32 13	45, 59, 71, 74	0
50	D3	60/60 (100%)	0.97	9 (15%) 3 1	62, 72, 82, 85	0
51	B4	31/71 (43%)	0.01	1 (3%) 51 27	69, 75, 80, 86	0
51	D4	31/71 (43%)	0.25	2 (6%) 22 8	67, 74, 81, 84	0
52	B5	57/60 (95%)	-0.20	0 100 100	40, 55, 71, 73	0
52	D5	59/60 (98%)	0.33	5 (8%) 13 4	55, 68, 78, 86	0
53	B6	49/54 (90%)	0.56	7 (14%) 4 2	39, 65, 75, 75	0
53	D6	48/54 (88%)	0.10	3 (6%) 23 9	54, 66, 73, 78	0
54	B7	49/49 (100%)	0.04	0 100 100	35, 46, 69, 76	0
54	D7	49/49 (100%)	0.81	5 (10%) 9 3	47, 58, 77, 83	0
55	B8	63/65 (96%)	0.15	2 (3%) 51 27	43, 56, 69, 75	0
55	D8	62/65 (95%)	0.39	6 (9%) 10 3	54, 62, 68, 76	0
56	B9	36/37 (97%)	0.50	5 (13%) 4 2	52, 59, 69, 71	0
56	D9	36/37 (97%)	0.32	1 (2%) 56 32	60, 69, 76, 82	0
All	All	21272/22210 (95%)	0.19	890 (4%) 40 19	25, 68, 82, 97	4 (0%)

The worst 5 of 890 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CA	82	U	10.8
1	CA	83	U	9.4

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Mol	Chain	Res	Type	RSRZ
25	DA	2802	G	8.8
45	DY	51	VAL	8.4
1	CA	81	U	8.3

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(Å ²)	Q<0.9
57	MG	BA	3086	1/1	0.75	1.91	120.67	130,130,130,130	0
57	MG	BA	3022	1/1	0.18	2.23	103.30	205,205,205,205	0
57	MG	BA	3139	1/1	0.43	0.88	42.54	72,72,72,72	0
57	MG	BA	3117	1/1	0.93	0.60	34.00	42,42,42,42	0
57	MG	BA	3077	1/1	0.90	0.82	33.46	63,63,63,63	0
57	MG	DA	3036	1/1	0.98	0.49	32.84	27,27,27,27	0
57	MG	DA	3007	1/1	0.96	0.43	29.74	54,54,54,54	0
57	MG	DA	3159	1/1	0.98	0.48	28.18	38,38,38,38	0
57	MG	BA	3419	1/1	0.94	0.40	28.11	44,44,44,44	0
57	MG	BA	3061	1/1	0.94	0.39	27.45	25,25,25,25	0
57	MG	BA	3188	1/1	0.68	0.85	26.54	87,87,87,87	0
57	MG	BA	3041	1/1	0.95	0.47	23.46	44,44,44,44	0
57	MG	BA	3057	1/1	0.92	0.41	22.89	39,39,39,39	0
57	MG	BA	3081	1/1	0.93	0.48	22.78	16,16,16,16	0
57	MG	BA	3052	1/1	0.69	0.45	22.70	30,30,30,30	0
57	MG	DA	3002	1/1	0.98	0.66	22.20	37,37,37,37	0
57	MG	BA	3159	1/1	0.96	0.49	21.84	29,29,29,29	0
57	MG	DA	3156	1/1	0.96	0.83	21.75	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3099	1/1	0.96	0.48	21.08	29,29,29,29	0
57	MG	AA	1635	1/1	0.93	0.43	20.17	31,31,31,31	0
57	MG	DA	3012	1/1	0.97	0.49	19.85	28,28,28,28	0
57	MG	BA	3186	1/1	0.97	0.54	19.61	24,24,24,24	0
57	MG	BA	3054	1/1	0.94	0.47	19.38	33,33,33,33	0
57	MG	DA	3033	1/1	0.70	0.59	19.19	59,59,59,59	0
57	MG	BA	3210	1/1	0.95	0.31	18.81	24,24,24,24	0
57	MG	BA	3333	1/1	0.94	0.61	18.40	77,77,77,77	0
57	MG	BA	3030	1/1	0.93	0.42	17.83	37,37,37,37	0
57	MG	DA	3072	1/1	0.48	0.51	17.67	72,72,72,72	0
57	MG	DA	3290	1/1	0.90	0.54	17.66	50,50,50,50	0
57	MG	DA	3017	1/1	0.93	0.41	16.55	21,21,21,21	0
57	MG	BA	3004	1/1	0.98	0.57	16.49	61,61,61,61	0
57	MG	BA	3133	1/1	0.75	0.37	16.47	60,60,60,60	0
57	MG	DA	3107	1/1	0.68	0.42	16.45	64,64,64,64	0
57	MG	DA	3149	1/1	0.84	0.49	15.98	38,38,38,38	0
57	MG	CA	1608	1/1	0.69	0.70	15.92	52,52,52,52	0
57	MG	DA	3184	1/1	0.67	0.36	15.65	54,54,54,54	0
57	MG	BA	3102	1/1	0.98	0.55	15.55	33,33,33,33	0
57	MG	BA	3181	1/1	0.93	0.56	15.33	19,19,19,19	0
57	MG	DA	3018	1/1	0.97	0.44	15.01	21,21,21,21	0
57	MG	AA	1628	1/1	0.96	0.47	14.88	43,43,43,43	0
57	MG	DA	3187	1/1	0.90	0.33	14.86	48,48,48,48	0
57	MG	BA	3125	1/1	0.74	0.35	14.55	60,60,60,60	0
57	MG	DA	3044	1/1	0.87	0.42	14.50	69,69,69,69	0
57	MG	BA	3097	1/1	0.90	0.41	14.40	34,34,34,34	0
57	MG	BA	3096	1/1	0.97	0.45	13.82	24,24,24,24	0
57	MG	BA	3025	1/1	0.90	0.36	13.68	31,31,31,31	0
57	MG	DA	3038	1/1	0.89	0.48	13.43	49,49,49,49	0
57	MG	BA	3155	1/1	0.92	0.55	13.34	37,37,37,37	0
57	MG	BA	3020	1/1	0.96	0.34	13.27	19,19,19,19	0
57	MG	DA	3085	1/1	0.93	0.46	13.27	49,49,49,49	0
57	MG	CW	104	1/1	0.90	0.39	12.72	52,52,52,52	0
57	MG	CA	1675	1/1	0.92	0.48	12.68	33,33,33,33	0
57	MG	DA	3053	1/1	0.93	0.37	12.62	21,21,21,21	0
57	MG	BA	3307	1/1	0.97	0.46	12.60	24,24,24,24	0
58	ZN	AD	301	1/1	0.78	0.59	12.48	192,192,192,192	0
57	MG	DA	3216	1/1	0.94	0.41	12.44	23,23,23,23	0
57	MG	BA	3012	1/1	0.96	0.38	12.44	22,22,22,22	0
57	MG	CA	1613	1/1	0.90	0.43	12.20	42,42,42,42	0
57	MG	DA	3060	1/1	0.94	0.28	11.52	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3147	1/1	0.93	0.50	11.39	18,18,18,18	0
57	MG	DA	3037	1/1	0.91	0.41	11.31	45,45,45,45	0
57	MG	BA	3294	1/1	0.90	0.34	11.29	29,29,29,29	0
57	MG	BA	3018	1/1	0.98	0.52	11.27	21,21,21,21	0
57	MG	DA	3073	1/1	0.87	0.45	11.20	49,49,49,49	0
57	MG	DA	3016	1/1	0.88	0.44	11.18	24,24,24,24	0
57	MG	BA	3056	1/1	0.97	0.42	11.17	26,26,26,26	0
57	MG	BA	3286	1/1	0.95	0.35	10.84	24,24,24,24	0
57	MG	DA	3069	1/1	0.85	0.48	10.18	30,30,30,30	0
57	MG	DA	3019	1/1	0.96	0.43	10.15	35,35,35,35	0
57	MG	BB	204	1/1	0.97	0.39	10.11	54,54,54,54	0
57	MG	BA	3262	1/1	0.86	0.52	9.95	32,32,32,32	0
57	MG	BA	3046	1/1	0.94	0.32	9.90	32,32,32,32	0
57	MG	BA	3071	1/1	0.92	0.34	9.73	25,25,25,25	0
57	MG	BA	3050	1/1	0.94	0.32	9.73	24,24,24,24	0
57	MG	BA	3313	1/1	0.91	0.37	9.68	26,26,26,26	0
57	MG	BA	3008	1/1	0.93	0.41	9.64	16,16,16,16	0
57	MG	DA	3050	1/1	0.89	0.40	9.60	46,46,46,46	0
57	MG	DA	3151	1/1	0.63	0.30	9.59	43,43,43,43	0
57	MG	BA	3023	1/1	0.95	0.42	9.43	45,45,45,45	0
57	MG	CA	1660	1/1	0.89	0.42	9.31	22,22,22,22	0
57	MG	BA	3119	1/1	0.97	0.42	9.30	23,23,23,23	0
57	MG	BA	3048	1/1	0.97	0.39	9.28	27,27,27,27	0
57	MG	CA	1644	1/1	0.89	0.39	9.06	30,30,30,30	0
57	MG	BA	3042	1/1	0.94	0.32	8.74	10,10,10,10	0
57	MG	BA	3015	1/1	0.81	0.45	8.70	21,21,21,21	0
57	MG	BA	3076	1/1	0.96	0.34	8.64	24,24,24,24	0
57	MG	AA	1698	1/1	0.95	0.36	8.44	37,37,37,37	0
57	MG	BA	3150	1/1	0.94	0.45	8.41	29,29,29,29	0
57	MG	BA	3024	1/1	0.92	0.34	8.39	20,20,20,20	0
57	MG	BA	3035	1/1	0.98	0.41	8.27	25,25,25,25	0
57	MG	BA	3047	1/1	0.98	0.39	8.14	62,62,62,62	0
57	MG	CA	1662	1/1	0.93	0.43	8.11	26,26,26,26	0
57	MG	DA	3077	1/1	0.95	0.40	7.93	22,22,22,22	0
57	MG	BA	3064	1/1	0.91	0.41	7.89	44,44,44,44	0
57	MG	BA	3187	1/1	0.92	0.42	7.79	45,45,45,45	0
57	MG	CA	1620	1/1	0.86	0.52	7.74	29,29,29,29	0
57	MG	BA	3080	1/1	0.95	0.31	7.62	32,32,32,32	0
57	MG	DA	3100	1/1	0.96	0.33	7.45	21,21,21,21	0
57	MG	DA	3211	1/1	0.63	0.35	7.42	55,55,55,55	0
57	MG	DA	3103	1/1	0.94	0.54	7.26	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1684	1/1	0.93	0.23	7.23	42,42,42,42	0
57	MG	DA	3169	1/1	0.85	0.40	7.10	18,18,18,18	0
57	MG	AA	1679	1/1	0.88	0.26	7.05	56,56,56,56	0
57	MG	BA	3348	1/1	0.93	0.36	7.04	55,55,55,55	0
57	MG	DA	3105	1/1	0.94	0.38	7.02	30,30,30,30	0
57	MG	DA	3302	1/1	0.86	0.35	6.86	36,36,36,36	0
57	MG	DA	3144	1/1	0.74	0.47	6.85	44,44,44,44	0
57	MG	BA	3211	1/1	0.84	0.27	6.81	38,38,38,38	0
57	MG	CA	1638	1/1	0.87	0.39	6.79	35,35,35,35	0
57	MG	BA	3275	1/1	0.96	0.28	6.70	27,27,27,27	0
57	MG	BA	3441	1/1	0.97	0.40	6.62	37,37,37,37	0
57	MG	BA	3106	1/1	0.96	0.34	6.53	23,23,23,23	0
57	MG	BA	3303	1/1	0.97	0.34	6.47	26,26,26,26	0
57	MG	DA	3039	1/1	0.97	0.31	6.43	18,18,18,18	0
57	MG	DA	3227	1/1	0.86	0.36	6.41	37,37,37,37	0
57	MG	BA	3178	1/1	0.85	0.28	6.36	22,22,22,22	0
57	MG	DA	3132	1/1	0.87	0.39	6.27	32,32,32,32	0
57	MG	BA	3094	1/1	0.98	0.30	6.12	34,34,34,34	0
57	MG	BA	3154	1/1	0.98	0.30	6.10	38,38,38,38	0
57	MG	BA	3345	1/1	0.91	0.32	6.06	34,34,34,34	0
57	MG	BU	201	1/1	0.87	0.34	5.98	21,21,21,21	0
57	MG	DA	3052	1/1	0.94	0.28	5.64	21,21,21,21	0
57	MG	CA	1690	1/1	0.92	0.27	5.63	44,44,44,44	0
57	MG	DA	3174	1/1	0.91	0.54	5.62	23,23,23,23	0
57	MG	BA	3436	1/1	0.94	0.29	5.58	48,48,48,48	0
57	MG	BA	3399	1/1	0.69	0.28	5.56	38,38,38,38	0
57	MG	BA	3151	1/1	0.87	0.40	5.55	24,24,24,24	0
57	MG	CA	1606	1/1	0.96	0.37	5.45	50,50,50,50	0
57	MG	BA	3339	1/1	0.93	0.29	5.27	29,29,29,29	0
57	MG	BA	3123	1/1	0.90	0.26	5.26	43,43,43,43	0
57	MG	DA	3005	1/1	0.96	0.48	5.25	45,45,45,45	0
57	MG	BA	3044	1/1	0.92	0.30	4.96	22,22,22,22	0
57	MG	BA	3387	1/1	0.90	0.27	4.94	46,46,46,46	0
57	MG	DA	3288	1/1	0.86	0.27	4.90	60,60,60,60	0
57	MG	AA	1711	1/1	0.83	0.24	4.71	58,58,58,58	0
57	MG	DA	3086	1/1	0.94	0.34	4.67	25,25,25,25	0
57	MG	AA	1676	1/1	0.97	0.30	4.65	30,30,30,30	0
57	MG	CA	1695	1/1	0.77	0.26	4.64	38,38,38,38	0
57	MG	DA	3294	1/1	0.97	0.41	4.52	19,19,19,19	0
57	MG	DA	3225	1/1	0.92	0.32	4.35	44,44,44,44	0
57	MG	DA	3231	1/1	0.91	0.38	4.31	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3179	1/1	0.95	0.33	4.27	30,30,30,30	0
57	MG	DA	3279	1/1	0.89	0.26	4.22	43,43,43,43	0
57	MG	DA	3152	1/1	0.80	0.33	4.22	61,61,61,61	0
57	MG	DA	3127	1/1	0.98	0.33	4.21	34,34,34,34	0
57	MG	AA	1619	1/1	0.78	0.47	4.17	66,66,66,66	0
57	MG	BA	3177	1/1	0.96	0.31	4.13	21,21,21,21	0
57	MG	DA	3020	1/1	0.85	0.34	4.07	23,23,23,23	0
57	MG	AL	201	1/1	0.90	0.38	4.03	29,29,29,29	0
57	MG	AA	1630	1/1	0.97	0.29	3.97	41,41,41,41	0
57	MG	BA	3312	1/1	0.96	0.31	3.89	22,22,22,22	0
57	MG	AA	1609	1/1	0.88	0.21	3.85	48,48,48,48	0
57	MG	BA	3240	1/1	0.93	0.22	3.79	23,23,23,23	0
57	MG	CA	1622	1/1	0.93	0.31	3.69	24,24,24,24	0
57	MG	BA	3374	1/1	0.80	0.24	3.55	51,51,51,51	0
57	MG	BA	3109	1/1	0.97	0.29	3.46	21,21,21,21	0
57	MG	BR	201	1/1	0.90	0.43	3.46	35,35,35,35	0
57	MG	BA	3337	1/1	0.96	0.25	3.44	37,37,37,37	0
57	MG	CA	1635	1/1	0.88	0.25	3.33	22,22,22,22	0
57	MG	DA	3234	1/1	0.92	0.30	3.32	33,33,33,33	0
57	MG	DA	3193	1/1	0.98	0.32	3.27	27,27,27,27	0
57	MG	BA	3095	1/1	0.82	0.26	3.25	45,45,45,45	0
57	MG	AA	1670	1/1	0.97	0.24	3.22	30,30,30,30	0
57	MG	CA	1664	1/1	0.91	0.28	3.16	42,42,42,42	0
57	MG	BA	3034	1/1	0.96	0.21	3.15	19,19,19,19	0
57	MG	BA	3088	1/1	0.91	0.28	3.14	24,24,24,24	0
57	MG	DA	3248	1/1	0.83	0.21	3.07	36,36,36,36	0
57	MG	DA	3181	1/1	0.96	0.30	3.04	36,36,36,36	0
57	MG	DA	3064	1/1	0.96	0.27	3.02	19,19,19,19	0
57	MG	AA	1624	1/1	0.95	0.34	2.98	33,33,33,33	0
57	MG	DA	3056	1/1	0.97	0.23	2.88	30,30,30,30	0
57	MG	CA	1661	1/1	0.90	0.26	2.87	26,26,26,26	0
57	MG	BA	3220	1/1	0.94	0.23	2.80	30,30,30,30	0
57	MG	BA	3040	1/1	0.98	0.22	2.78	24,24,24,24	0
57	MG	BA	3180	1/1	0.83	0.31	2.76	21,21,21,21	0
57	MG	BA	3206	1/1	0.95	0.24	2.69	22,22,22,22	0
57	MG	AA	1622	1/1	0.76	0.22	2.64	36,36,36,36	0
57	MG	BA	3197	1/1	0.91	0.34	2.53	20,20,20,20	0
57	MG	AA	1616	1/1	0.92	0.26	2.48	30,30,30,30	0
57	MG	BA	3098	1/1	0.97	0.23	2.47	25,25,25,25	0
57	MG	BA	3352	1/1	0.92	0.28	2.46	22,22,22,22	0
57	MG	BA	3032	1/1	0.94	0.25	2.35	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3006	1/1	0.93	0.24	2.33	27,27,27,27	0
57	MG	DA	3157	1/1	0.91	0.26	2.32	30,30,30,30	0
57	MG	DA	3192	1/1	0.79	0.26	2.17	43,43,43,43	0
57	MG	BA	3397	1/1	0.95	0.23	2.12	44,44,44,44	0
57	MG	BA	3449	1/1	0.76	0.20	2.10	53,53,53,53	0
57	MG	DA	3068	1/1	0.96	0.22	2.07	19,19,19,19	0
57	MG	BA	3289	1/1	0.92	0.32	1.95	38,38,38,38	0
57	MG	AA	1621	1/1	0.78	0.19	1.92	48,48,48,48	0
57	MG	AA	1655	1/1	0.99	0.22	1.90	6,6,6,6	0
57	MG	DA	3093	1/1	0.94	0.26	1.90	19,19,19,19	0
57	MG	DA	3097	1/1	0.98	0.26	1.81	21,21,21,21	0
57	MG	DA	3045	1/1	0.83	0.26	1.77	59,59,59,59	0
57	MG	DA	3150	1/1	0.85	0.27	1.73	21,21,21,21	0
57	MG	BA	3152	1/1	0.92	0.22	1.68	23,23,23,23	0
57	MG	DA	3055	1/1	0.94	0.26	1.64	24,24,24,24	0
57	MG	DA	3043	1/1	0.88	0.24	1.62	39,39,39,39	0
57	MG	DA	3129	1/1	0.84	0.23	1.48	47,47,47,47	0
57	MG	BA	3115	1/1	0.95	0.25	1.44	19,19,19,19	0
57	MG	BA	3365	1/1	0.93	0.35	1.43	23,23,23,23	0
57	MG	DA	3031	1/1	0.88	0.26	1.41	24,24,24,24	0
57	MG	BA	3063	1/1	0.95	0.24	1.41	17,17,17,17	0
57	MG	AA	1700	1/1	0.95	0.19	1.33	44,44,44,44	0
58	ZN	CD	301	1/1	0.97	0.33	1.32	81,81,81,81	0
57	MG	DA	3123	1/1	0.78	0.24	1.32	25,25,25,25	0
57	MG	DA	3061	1/1	0.91	0.25	1.31	22,22,22,22	0
57	MG	DA	3048	1/1	0.92	0.24	1.28	6,6,6,6	0
57	MG	DA	3008	1/1	0.94	0.26	1.20	6,6,6,6	0
57	MG	BA	3073	1/1	0.98	0.21	1.19	23,23,23,23	0
57	MG	CA	1649	1/1	0.79	0.31	1.17	65,65,65,65	0
57	MG	DA	3057	1/1	0.96	0.23	1.17	22,22,22,22	0
57	MG	BA	3184	1/1	0.91	0.25	1.16	53,53,53,53	0
57	MG	BA	3260	1/1	0.94	0.22	1.12	24,24,24,24	0
57	MG	DA	3203	1/1	0.86	0.20	1.08	52,52,52,52	0
57	MG	AA	1606	1/1	0.97	0.24	1.07	42,42,42,42	0
57	MG	BA	3144	1/1	0.96	0.20	1.06	24,24,24,24	0
57	MG	AA	1625	1/1	0.92	0.20	1.04	37,37,37,37	0
57	MG	BA	3036	1/1	0.91	0.20	1.01	30,30,30,30	0
57	MG	CA	1665	1/1	0.89	0.24	1.00	30,30,30,30	0
57	MG	BA	3110	1/1	0.96	0.23	1.00	32,32,32,32	0
57	MG	DA	3067	1/1	0.78	0.20	0.96	56,56,56,56	0
57	MG	BF	301	1/1	0.90	0.25	0.93	62,62,62,62	0
57	MG	BA	3229	1/1	0.97	0.25	0.93	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3251	1/1	0.86	0.27	0.92	23,23,23,23	0
57	MG	DA	3090	1/1	0.93	0.23	0.92	31,31,31,31	0
57	MG	AA	1696	1/1	0.96	0.23	0.91	26,26,26,26	0
57	MG	CA	1678	1/1	0.88	0.22	0.87	25,25,25,25	0
57	MG	AA	1663	1/1	0.97	0.16	0.77	27,27,27,27	0
57	MG	AA	1643	1/1	0.96	0.15	0.74	23,23,23,23	0
57	MG	DA	3194	1/1	0.89	0.23	0.68	61,61,61,61	0
57	MG	BA	3241	1/1	0.93	0.19	0.66	50,50,50,50	0
57	MG	CW	101	1/1	0.92	0.24	0.62	22,22,22,22	0
57	MG	BA	3011	1/1	0.95	0.22	0.58	6,6,6,6	0
57	MG	BA	3170	1/1	0.92	0.18	0.58	40,40,40,40	0
57	MG	DA	3009	1/1	0.97	0.22	0.55	18,18,18,18	0
57	MG	BA	3259	1/1	0.95	0.19	0.52	37,37,37,37	0
57	MG	DA	3198	1/1	0.83	0.23	0.52	31,31,31,31	0
57	MG	DA	3133	1/1	0.91	0.16	0.50	31,31,31,31	0
58	ZN	B5	105	1/1	0.97	0.17	0.45	90,90,90,90	0
57	MG	DA	3146	1/1	0.98	0.25	0.28	60,60,60,60	0
57	MG	DA	3119	1/1	0.90	0.23	0.27	42,42,42,42	0
57	MG	DB	203	1/1	0.81	0.21	0.25	66,66,66,66	0
57	MG	AA	1712	1/1	0.94	0.18	0.21	56,56,56,56	0
57	MG	DA	3022	1/1	0.94	0.21	0.19	21,21,21,21	0
57	MG	CA	1698	1/1	0.91	0.18	0.19	33,33,33,33	0
57	MG	AT	201	1/1	0.94	0.21	0.12	22,22,22,22	0
57	MG	BA	3383	1/1	0.82	0.20	0.10	48,48,48,48	0
57	MG	CA	1676	1/1	0.95	0.20	0.05	48,48,48,48	0
57	MG	DA	3190	1/1	0.86	0.23	-0.01	44,44,44,44	0
57	MG	DA	3104	1/1	0.92	0.23	-0.03	21,21,21,21	0
58	ZN	D5	103	1/1	0.93	0.16	-0.05	30,30,30,30	0
57	MG	BA	3341	1/1	0.97	0.18	-0.05	28,28,28,28	0
57	MG	B0	102	1/1	0.90	0.23	-0.05	33,33,33,33	0
57	MG	DA	3079	1/1	0.96	0.21	-0.07	45,45,45,45	0
57	MG	BD	301	1/1	0.96	0.25	-0.08	34,34,34,34	0
57	MG	BA	3332	1/1	0.57	0.17	-0.15	61,61,61,61	0
57	MG	DA	3058	1/1	0.97	0.20	-0.18	27,27,27,27	0
57	MG	AA	1659	1/1	0.81	0.20	-0.18	58,58,58,58	0
57	MG	DA	3206	1/1	0.93	0.17	-0.19	49,49,49,49	0
57	MG	DA	3126	1/1	0.94	0.20	-0.23	6,6,6,6	0
57	MG	CA	1621	1/1	0.93	0.18	-0.25	22,22,22,22	0
57	MG	BA	3160	1/1	0.97	0.15	-0.31	30,30,30,30	0
57	MG	AW	101	1/1	0.92	0.19	-0.32	6,6,6,6	0
57	MG	DA	3162	1/1	0.94	0.19	-0.32	24,24,24,24	0
57	MG	AA	1669	1/1	0.91	0.22	-0.33	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	B5	103	1/1	0.90	0.19	-0.35	20,20,20,20	0
57	MG	CA	1663	1/1	0.89	0.18	-0.36	33,33,33,33	0
57	MG	BA	3257	1/1	0.86	0.24	-0.37	41,41,41,41	0
57	MG	BA	3455	1/1	0.98	0.21	-0.37	46,46,46,46	0
57	MG	BA	3067	1/1	0.97	0.18	-0.38	30,30,30,30	0
57	MG	DA	3141	1/1	0.93	0.20	-0.46	25,25,25,25	0
57	MG	BT	201	1/1	0.93	0.21	-0.49	32,32,32,32	0
57	MG	BA	3298	1/1	0.94	0.15	-0.53	20,20,20,20	0
57	MG	CA	1627	1/1	0.85	0.18	-0.55	24,24,24,24	0
57	MG	CA	1653	1/1	0.94	0.19	-0.61	36,36,36,36	0
57	MG	BA	3066	1/1	0.92	0.20	-0.62	14,14,14,14	0
57	MG	CA	1692	1/1	0.92	0.17	-0.64	48,48,48,48	0
57	MG	DA	3243	1/1	0.95	0.13	-0.66	44,44,44,44	0
57	MG	BA	3221	1/1	0.95	0.21	-0.74	22,22,22,22	0
57	MG	BA	3459	1/1	0.83	0.18	-0.79	35,35,35,35	0
57	MG	BA	3104	1/1	0.95	0.17	-0.82	37,37,37,37	0
57	MG	AA	1668	1/1	0.98	0.13	-0.82	40,40,40,40	0
57	MG	BA	3398	1/1	0.96	0.17	-0.84	34,34,34,34	0
57	MG	DA	3166	1/1	0.74	0.17	-0.85	22,22,22,22	0
57	MG	D6	102	1/1	0.97	0.18	-0.87	23,23,23,23	0
57	MG	AA	1688	1/1	0.92	0.16	-0.88	56,56,56,56	0
57	MG	CA	1687	1/1	0.87	0.17	-0.93	37,37,37,37	0
57	MG	BA	3169	1/1	0.81	0.17	-0.98	21,21,21,21	0
57	MG	CA	1667	1/1	0.97	0.18	-0.99	23,23,23,23	0
57	MG	BA	3029	1/1	0.78	0.15	-1.01	40,40,40,40	0
57	MG	BA	3256	1/1	0.94	0.18	-1.02	25,25,25,25	0
57	MG	BA	3153	1/1	0.82	0.14	-1.03	42,42,42,42	0
57	MG	DD	301	1/1	0.94	0.19	-1.04	18,18,18,18	0
58	ZN	D9	101	1/1	0.99	0.15	-1.04	30,30,30,30	0
57	MG	BA	3330	1/1	0.95	0.18	-1.04	21,21,21,21	0
58	ZN	B9	101	1/1	0.99	0.12	-1.06	75,75,75,75	0
57	MG	CA	1642	1/1	0.93	0.13	-1.11	37,37,37,37	0
57	MG	CA	1616	1/1	0.92	0.16	-1.21	20,20,20,20	0
57	MG	BA	3315	1/1	0.89	0.16	-1.32	17,17,17,17	0
57	MG	CA	1636	1/1	0.98	0.17	-1.33	28,28,28,28	0
57	MG	BA	3121	1/1	0.94	0.18	-1.39	20,20,20,20	0
57	MG	BA	3202	1/1	0.97	0.17	-1.40	19,19,19,19	0
57	MG	DB	202	1/1	0.73	0.12	-1.46	61,61,61,61	0
57	MG	DA	3004	1/1	0.94	0.16	-1.49	21,21,21,21	0
57	MG	CA	1637	1/1	0.93	0.14	-1.58	26,26,26,26	0
57	MG	AA	1629	1/1	0.93	0.15	-1.59	56,56,56,56	0
57	MG	AA	1666	1/1	0.95	0.14	-1.61	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	BA	3070	1/1	0.96	0.15	-1.63	23,23,23,23	0
57	MG	DA	3063	1/1	0.95	0.17	-1.69	29,29,29,29	0
57	MG	DA	3172	1/1	0.91	0.16	-1.70	30,30,30,30	0
57	MG	CA	1685	1/1	0.92	0.12	-1.72	33,33,33,33	0
57	MG	BA	3138	1/1	0.95	0.14	-1.74	39,39,39,39	0
57	MG	AA	1693	1/1	0.95	0.12	-1.81	45,45,45,45	0
57	MG	BA	3157	1/1	0.90	0.16	-1.82	38,38,38,38	0
57	MG	BA	3237	1/1	0.98	0.13	-1.91	21,21,21,21	0
57	MG	BA	3105	1/1	0.93	0.16	-1.97	15,15,15,15	0
57	MG	AA	1690	1/1	0.94	0.09	-2.07	26,26,26,26	0
57	MG	BA	3093	1/1	0.89	0.17	-2.09	23,23,23,23	0
57	MG	DA	3155	1/1	0.89	0.06	-2.11	60,60,60,60	0
57	MG	DA	3263	1/1	0.95	0.18	-2.21	28,28,28,28	0
57	MG	BA	3420	1/1	0.98	0.17	-2.28	45,45,45,45	0
57	MG	DA	3041	1/1	0.97	0.15	-2.33	19,19,19,19	0
57	MG	DA	3289	1/1	0.97	0.17	-2.36	27,27,27,27	0
57	MG	CA	1641	1/1	0.96	0.06	-2.45	18,18,18,18	0
57	MG	BP	202	1/1	0.98	0.14	-2.48	22,22,22,22	0
57	MG	DA	3280	1/1	0.80	0.13	-2.49	44,44,44,44	0
57	MG	BA	3405	1/1	0.94	0.08	-2.53	25,25,25,25	0
57	MG	AA	1651	1/1	0.93	0.11	-2.66	49,49,49,49	0
57	MG	DA	3236	1/1	0.94	0.10	-2.67	30,30,30,30	0
57	MG	AA	1658	1/1	0.94	0.14	-2.69	23,23,23,23	0
57	MG	DA	3026	1/1	0.87	0.09	-2.69	33,33,33,33	0
57	MG	CA	1630	1/1	0.97	0.10	-2.72	29,29,29,29	0
57	MG	DA	3188	1/1	0.95	0.13	-3.07	27,27,27,27	0
57	MG	AA	1639	1/1	0.97	0.14	-3.11	27,27,27,27	0
57	MG	BA	3183	1/1	0.94	0.12	-3.11	22,22,22,22	0
57	MG	DA	3247	1/1	0.94	0.15	-3.15	23,23,23,23	0
57	MG	DR	201	1/1	0.96	0.15	-3.19	22,22,22,22	0
57	MG	CA	1697	1/1	0.95	0.08	-3.20	39,39,39,39	0
57	MG	DA	3027	1/1	0.96	0.14	-3.22	33,33,33,33	0
57	MG	AA	1691	1/1	0.91	0.12	-3.37	39,39,39,39	0
57	MG	BA	3205	1/1	0.91	0.10	-3.56	45,45,45,45	0
57	MG	AA	1662	1/1	0.94	0.13	-3.58	22,22,22,22	0
57	MG	BA	3435	1/1	0.98	0.05	-3.62	30,30,30,30	0
57	MG	B7	101	1/1	0.94	0.14	-3.70	12,12,12,12	0
57	MG	BA	3003	1/1	0.97	0.12	-3.87	25,25,25,25	0
57	MG	AA	1678	1/1	0.91	0.10	-4.07	33,33,33,33	0
57	MG	BA	3156	1/1	0.93	0.09	-4.26	26,26,26,26	0
57	MG	BA	3164	1/1	0.97	0.16	-4.32	35,35,35,35	0
57	MG	DA	3235	1/1	0.92	0.15	-4.37	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	BA	3111	1/1	0.90	0.15	-4.38	20,20,20,20	0
57	MG	BA	3189	1/1	0.94	0.10	-4.69	14,14,14,14	0
57	MG	BA	3338	1/1	0.95	0.10	-4.73	18,18,18,18	0
57	MG	CA	1679	1/1	0.95	0.13	-4.78	29,29,29,29	0
57	MG	DA	3304	1/1	0.91	0.12	-5.05	35,35,35,35	0
57	MG	BA	3309	1/1	0.94	0.08	-5.47	20,20,20,20	0
57	MG	DA	3260	1/1	0.94	0.12	-5.72	31,31,31,31	0
57	MG	DA	3178	1/1	0.90	0.09	-5.94	30,30,30,30	0
57	MG	DA	3089	1/1	0.96	0.13	-6.05	19,19,19,19	0
57	MG	BA	3234	1/1	0.95	0.05	-6.58	38,38,38,38	0
57	MG	AA	1677	1/1	0.97	0.12	-6.94	48,48,48,48	0
57	MG	BA	3062	1/1	0.88	0.11	-6.97	19,19,19,19	0
57	MG	DA	3083	1/1	0.97	0.09	-7.82	30,30,30,30	0
57	MG	BA	3394	1/1	0.92	0.11	-8.22	28,28,28,28	0
57	MG	BA	3101	1/1	0.97	0.10	-8.74	21,21,21,21	0
57	MG	DA	3084	1/1	0.96	0.12	-9.12	21,21,21,21	0
57	MG	DA	3109	1/1	0.92	0.11	-14.78	33,33,33,33	0
57	MG	BQ	202	1/1	0.95	0.28	-	30,30,30,30	0
57	MG	BA	3053	1/1	0.91	0.47	-	63,63,63,63	0
57	MG	CA	1694	1/1	0.91	0.73	-	51,51,51,51	0
57	MG	BA	3254	1/1	0.80	0.27	-	37,37,37,37	0
57	MG	AA	1699	1/1	0.97	0.27	-	29,29,29,29	0
57	MG	CA	1614	1/1	0.98	0.15	-	30,30,30,30	0
57	MG	DA	3186	1/1	0.96	0.08	-	29,29,29,29	0
57	MG	BA	3281	1/1	0.90	0.25	-	29,29,29,29	0
57	MG	DA	3094	1/1	0.79	0.43	-	71,71,71,71	0
57	MG	AA	1638	1/1	0.93	0.14	-	55,55,55,55	0
57	MG	BA	3198	1/1	0.89	0.16	-	34,34,34,34	0
57	MG	DA	3164	1/1	0.50	0.62	-	83,83,83,83	0
57	MG	CA	1701	1/1	0.94	0.22	-	25,25,25,25	0
57	MG	DA	3025	1/1	0.86	0.18	-	38,38,38,38	0
57	MG	AA	1631	1/1	0.93	0.16	-	29,29,29,29	0
57	MG	CW	105	1/1	0.85	0.32	-	61,61,61,61	0
57	MG	BA	3089	1/1	0.97	0.36	-	24,24,24,24	0
57	MG	BA	3049	1/1	0.98	0.43	-	24,24,24,24	0
57	MG	BA	3432	1/1	0.74	0.58	-	70,70,70,70	0
57	MG	DA	3125	1/1	0.88	0.27	-	26,26,26,26	0
57	MG	BA	3363	1/1	0.93	0.21	-	23,23,23,23	0
57	MG	BA	3415	1/1	0.95	0.24	-	36,36,36,36	0
57	MG	BA	3347	1/1	0.90	0.14	-	28,28,28,28	0
57	MG	BA	3425	1/1	0.81	0.18	-	55,55,55,55	0
57	MG	AA	1615	1/1	0.93	0.17	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3026	1/1	0.94	0.24	-	31,31,31,31	0
57	MG	BA	3411	1/1	0.94	0.38	-	53,53,53,53	0
57	MG	BA	3078	1/1	0.96	0.38	-	29,29,29,29	0
57	MG	BA	3253	1/1	0.88	0.53	-	41,41,41,41	0
57	MG	DA	3032	1/1	0.92	0.23	-	20,20,20,20	0
57	MG	DA	3267	1/1	0.69	0.49	-	73,73,73,73	0
57	MG	BA	3005	1/1	0.93	0.19	-	23,23,23,23	0
57	MG	AA	1704	1/1	0.81	0.16	-	64,64,64,64	0
57	MG	DA	3163	1/1	0.97	0.25	-	32,32,32,32	0
57	MG	CA	1657	1/1	0.91	0.11	-	37,37,37,37	0
57	MG	BA	3122	1/1	0.96	0.38	-	41,41,41,41	0
57	MG	BA	3168	1/1	0.97	0.14	-	33,33,33,33	0
57	MG	DA	3140	1/1	0.92	0.24	-	36,36,36,36	0
57	MG	CA	1673	1/1	0.97	0.17	-	26,26,26,26	0
57	MG	DA	3207	1/1	0.91	0.13	-	26,26,26,26	0
57	MG	BA	3428	1/1	0.81	0.20	-	24,24,24,24	0
57	MG	BA	3146	1/1	0.94	0.26	-	22,22,22,22	0
57	MG	DA	3212	1/1	0.95	0.19	-	18,18,18,18	0
57	MG	DA	3081	1/1	0.88	0.27	-	37,37,37,37	0
57	MG	BA	3403	1/1	0.86	0.24	-	48,48,48,48	0
57	MG	DA	3286	1/1	0.88	0.24	-	52,52,52,52	0
57	MG	BA	3118	1/1	0.64	2.54	-	205,205,205,205	0
57	MG	AA	1607	1/1	0.91	0.26	-	51,51,51,51	0
57	MG	BA	3207	1/1	0.61	0.26	-	74,74,74,74	0
57	MG	BA	3390	1/1	0.87	0.20	-	48,48,48,48	0
57	MG	BA	3193	1/1	0.92	0.11	-	47,47,47,47	0
57	MG	AA	1694	1/1	0.96	0.19	-	23,23,23,23	0
57	MG	BA	3447	1/1	0.93	0.42	-	27,27,27,27	0
57	MG	BA	3212	1/1	0.89	0.42	-	30,30,30,30	0
57	MG	DA	3196	1/1	0.92	0.29	-	26,26,26,26	0
57	MG	DA	3170	1/1	0.97	0.27	-	22,22,22,22	0
57	MG	BA	3427	1/1	0.85	0.17	-	40,40,40,40	0
57	MG	BA	3329	1/1	0.90	0.07	-	26,26,26,26	0
57	MG	DA	3112	1/1	0.90	0.28	-	27,27,27,27	0
57	MG	BA	3185	1/1	0.96	0.25	-	17,17,17,17	0
57	MG	BA	3308	1/1	0.93	0.31	-	22,22,22,22	0
57	MG	BB	202	1/1	0.96	0.31	-	21,21,21,21	0
57	MG	BA	3242	1/1	0.91	0.28	-	24,24,24,24	0
57	MG	CA	1689	1/1	0.92	0.17	-	39,39,39,39	0
57	MG	BA	3059	1/1	0.96	0.34	-	28,28,28,28	0
57	MG	BA	3137	1/1	0.94	0.41	-	46,46,46,46	0
57	MG	BA	3021	1/1	0.91	1.62	-	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3203	1/1	0.96	0.34	-	29,29,29,29	0
57	MG	AA	1604	1/1	0.68	0.40	-	38,38,38,38	0
57	MG	BA	3079	1/1	0.92	0.34	-	25,25,25,25	0
57	MG	BA	3113	1/1	0.92	0.39	-	32,32,32,32	0
57	MG	BA	3400	1/1	0.97	0.08	-	32,32,32,32	0
57	MG	BA	3368	1/1	0.89	0.42	-	49,49,49,49	0
57	MG	BA	3392	1/1	0.98	0.14	-	52,52,52,52	0
57	MG	BA	3335	1/1	0.97	0.11	-	47,47,47,47	0
57	MG	DB	209	1/1	0.79	0.22	-	41,41,41,41	0
57	MG	DB	210	1/1	0.75	0.23	-	41,41,41,41	0
57	MG	DA	3117	1/1	0.80	0.18	-	42,42,42,42	0
57	MG	DA	3246	1/1	0.76	0.34	-	43,43,43,43	0
57	MG	BA	3437	1/1	0.91	0.10	-	27,27,27,27	0
57	MG	BA	3282	1/1	0.95	0.41	-	22,22,22,22	0
57	MG	DA	3291	1/1	0.89	0.23	-	31,31,31,31	0
57	MG	BA	3167	1/1	0.91	0.32	-	65,65,65,65	0
57	MG	DF	301	1/1	0.81	0.59	-	49,49,49,49	0
57	MG	DA	3226	1/1	0.90	0.35	-	32,32,32,32	0
57	MG	BA	3230	1/1	0.89	0.28	-	34,34,34,34	0
57	MG	BA	3404	1/1	0.93	0.05	-	53,53,53,53	0
57	MG	BA	3361	1/1	0.82	0.24	-	31,31,31,31	0
57	MG	DA	3013	1/1	0.95	0.34	-	20,20,20,20	0
57	MG	DA	3051	1/1	0.98	0.18	-	6,6,6,6	0
57	MG	DA	3205	1/1	0.87	0.31	-	55,55,55,55	0
57	MG	BA	3418	1/1	0.88	0.22	-	31,31,31,31	0
57	MG	CA	1688	1/1	0.96	0.12	-	35,35,35,35	0
57	MG	DA	3113	1/1	0.96	0.42	-	26,26,26,26	0
57	MG	DA	3014	1/1	0.89	0.24	-	44,44,44,44	0
57	MG	CA	1666	1/1	0.98	0.41	-	18,18,18,18	0
57	MG	DA	3292	1/1	0.93	0.14	-	17,17,17,17	0
57	MG	BA	3140	1/1	0.92	0.14	-	33,33,33,33	0
57	MG	BA	3107	1/1	0.92	0.13	-	40,40,40,40	0
57	MG	AA	1647	1/1	0.79	0.22	-	45,45,45,45	0
57	MG	BA	3031	1/1	0.97	0.19	-	21,21,21,21	0
57	MG	DA	3010	1/1	0.85	0.41	-	66,66,66,66	0
57	MG	BA	3430	1/1	0.89	0.36	-	58,58,58,58	0
57	MG	BA	3068	1/1	0.96	0.23	-	30,30,30,30	0
57	MG	DA	3221	1/1	0.94	0.35	-	38,38,38,38	0
57	MG	BA	3391	1/1	0.94	0.23	-	44,44,44,44	0
57	MG	BA	3410	1/1	0.94	0.14	-	30,30,30,30	0
57	MG	BA	3045	1/1	0.97	0.22	-	6,6,6,6	0
57	MG	DA	3240	1/1	0.92	0.14	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3357	1/1	0.91	0.18	-	38,38,38,38	0
57	MG	AA	1602	1/1	0.80	0.30	-	77,77,77,77	0
57	MG	DA	3160	1/1	0.91	0.30	-	38,38,38,38	0
57	MG	BA	3231	1/1	0.92	0.39	-	54,54,54,54	0
57	MG	CA	1617	1/1	0.97	0.25	-	35,35,35,35	0
57	MG	DA	3204	1/1	0.82	0.13	-	41,41,41,41	0
57	MG	BA	3009	1/1	0.92	0.20	-	16,16,16,16	0
57	MG	BA	3350	1/1	0.92	0.19	-	37,37,37,37	0
57	MG	DA	3006	1/1	0.98	0.34	-	28,28,28,28	0
57	MG	DA	3021	1/1	0.87	0.26	-	34,34,34,34	0
57	MG	AA	1702	1/1	0.92	0.12	-	26,26,26,26	0
57	MG	BA	3364	1/1	0.99	0.17	-	32,32,32,32	0
57	MG	BA	3112	1/1	0.95	0.22	-	23,23,23,23	0
57	MG	BA	3297	1/1	0.92	0.23	-	21,21,21,21	0
57	MG	BA	3358	1/1	0.90	0.15	-	38,38,38,38	0
57	MG	BA	3422	1/1	0.90	0.45	-	20,20,20,20	0
57	MG	BA	3252	1/1	0.92	0.14	-	25,25,25,25	0
57	MG	CA	1705	1/1	0.96	0.24	-	48,48,48,48	0
57	MG	BA	3369	1/1	0.92	0.13	-	63,63,63,63	0
57	MG	CX	101	1/1	0.93	0.19	-	22,22,22,22	0
57	MG	BB	203	1/1	0.88	0.30	-	21,21,21,21	0
57	MG	BA	3124	1/1	0.88	0.21	-	41,41,41,41	0
57	MG	DA	3111	1/1	0.75	0.46	-	76,76,76,76	0
57	MG	BA	3412	1/1	0.87	0.28	-	35,35,35,35	0
57	MG	AA	1623	1/1	0.97	0.32	-	18,18,18,18	0
57	MG	BA	3401	1/1	0.94	0.13	-	46,46,46,46	0
57	MG	CA	1708	1/1	0.69	0.74	-	76,76,76,76	0
57	MG	DA	3078	1/1	0.94	0.31	-	44,44,44,44	0
57	MG	BA	3385	1/1	0.83	0.13	-	54,54,54,54	0
57	MG	AA	1620	1/1	0.96	0.19	-	27,27,27,27	0
57	MG	BA	3134	1/1	0.97	0.19	-	22,22,22,22	0
57	MG	DA	3232	1/1	0.89	0.29	-	40,40,40,40	0
57	MG	BA	3438	1/1	0.90	0.23	-	67,67,67,67	0
57	MG	AA	1664	1/1	0.66	0.53	-	77,77,77,77	0
57	MG	DA	3030	1/1	0.91	0.15	-	46,46,46,46	0
57	MG	DA	3214	1/1	0.91	0.35	-	29,29,29,29	0
57	MG	BA	3258	1/1	0.78	0.27	-	39,39,39,39	0
57	MG	CA	1700	1/1	0.91	0.30	-	56,56,56,56	0
57	MG	BA	3142	1/1	0.97	0.30	-	25,25,25,25	0
57	MG	AA	1633	1/1	0.86	0.11	-	36,36,36,36	0
57	MG	BA	3194	1/1	0.82	0.08	-	72,72,72,72	0
57	MG	BA	3179	1/1	0.95	0.47	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3145	1/1	0.97	0.73	-	57,57,57,57	0
57	MG	CA	1707	1/1	0.90	0.63	-	62,62,62,62	0
57	MG	DA	3265	1/1	0.94	0.40	-	54,54,54,54	0
57	MG	BB	205	1/1	0.94	0.25	-	19,19,19,19	0
57	MG	BA	3149	1/1	0.93	0.26	-	27,27,27,27	0
57	MG	BA	3218	1/1	0.89	0.40	-	23,23,23,23	0
57	MG	DA	3080	1/1	0.91	0.30	-	24,24,24,24	0
57	MG	BA	3007	1/1	0.95	0.38	-	19,19,19,19	0
57	MG	BA	3431	1/1	0.77	0.36	-	53,53,53,53	0
57	MG	CA	1602	1/1	0.85	0.19	-	35,35,35,35	0
57	MG	BA	3409	1/1	0.98	0.11	-	24,24,24,24	0
57	MG	AA	1626	1/1	0.90	0.24	-	35,35,35,35	0
57	MG	BA	3014	1/1	0.86	0.38	-	24,24,24,24	0
57	MG	BB	201	1/1	0.94	0.30	-	59,59,59,59	0
57	MG	BA	3416	1/1	0.96	0.13	-	42,42,42,42	0
57	MG	DA	3298	1/1	0.83	0.15	-	33,33,33,33	0
57	MG	CA	1677	1/1	0.94	0.34	-	27,27,27,27	0
57	MG	AA	1675	1/1	0.89	0.18	-	50,50,50,50	0
57	MG	DA	3297	1/1	0.84	0.17	-	48,48,48,48	0
57	MG	AA	1708	1/1	0.97	0.12	-	46,46,46,46	0
57	MG	DA	3142	1/1	0.78	0.26	-	51,51,51,51	0
57	MG	BA	3204	1/1	0.86	0.46	-	52,52,52,52	0
57	MG	BB	206	1/1	0.95	0.32	-	31,31,31,31	0
57	MG	AA	1667	1/1	0.94	0.21	-	62,62,62,62	0
57	MG	BA	3233	1/1	0.90	0.71	-	53,53,53,53	0
57	MG	BA	3103	1/1	0.95	0.32	-	21,21,21,21	0
57	MG	BA	3366	1/1	0.88	0.32	-	49,49,49,49	0
57	MG	CW	102	1/1	0.46	0.47	-	93,93,93,93	0
57	MG	DA	3296	1/1	0.94	0.34	-	40,40,40,40	0
57	MG	DA	3237	1/1	0.88	0.24	-	33,33,33,33	0
57	MG	AA	1617	1/1	0.86	0.28	-	43,43,43,43	0
57	MG	BA	3434	1/1	0.83	0.30	-	28,28,28,28	0
57	MG	DA	3213	1/1	0.87	0.18	-	28,28,28,28	0
57	MG	BA	3299	1/1	0.97	0.21	-	22,22,22,22	0
57	MG	DA	3071	1/1	0.95	0.31	-	20,20,20,20	0
57	MG	CA	1680	1/1	0.88	0.18	-	31,31,31,31	0
57	MG	CA	1643	1/1	0.80	0.18	-	44,44,44,44	0
57	MG	DA	3254	1/1	0.83	0.41	-	60,60,60,60	0
57	MG	BA	3075	1/1	0.93	0.22	-	24,24,24,24	0
57	MG	DA	3275	1/1	0.94	0.26	-	48,48,48,48	0
57	MG	BA	3292	1/1	0.83	0.42	-	24,24,24,24	0
57	MG	DA	3270	1/1	0.73	0.30	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1637	1/1	0.78	0.36	-	45,45,45,45	0
57	MG	BA	3388	1/1	0.76	0.40	-	37,37,37,37	0
57	MG	CA	1631	1/1	0.94	0.30	-	34,34,34,34	0
57	MG	BA	3376	1/1	0.91	0.17	-	33,33,33,33	0
57	MG	AA	1689	1/1	0.68	0.17	-	55,55,55,55	0
57	MG	BA	3166	1/1	0.90	0.56	-	38,38,38,38	0
57	MG	DA	3199	1/1	0.90	0.23	-	67,67,67,67	0
57	MG	BA	3344	1/1	0.77	0.21	-	24,24,24,24	0
57	MG	CA	1671	1/1	0.93	0.10	-	54,54,54,54	0
57	MG	B5	101	1/1	0.95	0.39	-	78,78,78,78	0
57	MG	CA	1601	1/1	0.71	0.22	-	39,39,39,39	0
57	MG	BA	3219	1/1	0.98	0.12	-	28,28,28,28	0
57	MG	AA	1717	1/1	0.90	0.25	-	25,25,25,25	0
57	MG	AA	1650	1/1	0.91	0.17	-	28,28,28,28	0
57	MG	BA	3200	1/1	0.94	0.33	-	20,20,20,20	0
57	MG	AA	1707	1/1	0.96	0.23	-	20,20,20,20	0
57	MG	DA	3040	1/1	0.91	0.36	-	26,26,26,26	0
57	MG	BA	3069	1/1	0.92	0.28	-	30,30,30,30	0
57	MG	DA	3098	1/1	0.90	0.40	-	32,32,32,32	0
57	MG	CA	1625	1/1	0.91	0.32	-	31,31,31,31	0
57	MG	CA	1611	1/1	0.96	0.10	-	25,25,25,25	0
57	MG	BA	3172	1/1	0.94	0.52	-	22,22,22,22	0
57	MG	DB	205	1/1	0.93	0.33	-	42,42,42,42	0
57	MG	BA	3120	1/1	0.95	0.31	-	35,35,35,35	0
57	MG	DA	3118	1/1	0.94	0.17	-	33,33,33,33	0
57	MG	BA	3371	1/1	0.94	0.15	-	48,48,48,48	0
57	MG	BA	3271	1/1	0.94	0.22	-	40,40,40,40	0
57	MG	CA	1603	1/1	0.89	0.21	-	49,49,49,49	0
57	MG	AA	1680	1/1	0.94	0.33	-	49,49,49,49	0
57	MG	DA	3269	1/1	0.83	0.27	-	47,47,47,47	0
57	MG	DA	3239	1/1	0.92	0.23	-	32,32,32,32	0
57	MG	DA	3301	1/1	0.91	0.11	-	33,33,33,33	0
57	MG	BB	207	1/1	0.90	0.16	-	44,44,44,44	0
57	MG	BA	3087	1/1	0.92	0.36	-	23,23,23,23	0
57	MG	DA	3271	1/1	0.93	0.20	-	42,42,42,42	0
57	MG	BA	3284	1/1	0.88	0.17	-	15,15,15,15	0
57	MG	BA	3163	1/1	0.89	0.18	-	21,21,21,21	0
57	MG	CA	1674	1/1	0.95	0.26	-	41,41,41,41	0
57	MG	BA	3147	1/1	0.96	0.32	-	24,24,24,24	0
57	MG	BA	3448	1/1	0.56	0.42	-	54,54,54,54	0
57	MG	CA	1655	1/1	0.77	0.19	-	34,34,34,34	0
57	MG	DA	3230	1/1	0.96	0.32	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1654	1/1	0.92	0.13	-	17,17,17,17	0
57	MG	BA	3245	1/1	0.98	0.19	-	27,27,27,27	0
57	MG	DA	3099	1/1	0.92	0.42	-	23,23,23,23	0
57	MG	DA	3120	1/1	0.96	0.21	-	25,25,25,25	0
57	MG	BA	3217	1/1	0.91	0.24	-	34,34,34,34	0
57	MG	CA	1709	1/1	0.95	0.34	-	28,28,28,28	0
57	MG	AA	1672	1/1	0.94	0.19	-	33,33,33,33	0
57	MG	AA	1710	1/1	0.93	0.10	-	30,30,30,30	0
57	MG	BA	3285	1/1	0.98	0.13	-	6,6,6,6	0
57	MG	AA	1618	1/1	0.82	0.20	-	64,64,64,64	0
57	MG	DA	3076	1/1	0.96	0.12	-	19,19,19,19	0
57	MG	DA	3091	1/1	0.96	0.13	-	26,26,26,26	0
57	MG	DA	3114	1/1	0.94	0.29	-	30,30,30,30	0
57	MG	BA	3301	1/1	0.89	0.23	-	33,33,33,33	0
57	MG	AA	1653	1/1	0.91	0.24	-	28,28,28,28	0
57	MG	BA	3208	1/1	0.96	0.05	-	56,56,56,56	0
57	MG	BA	3293	1/1	0.98	0.25	-	23,23,23,23	0
57	MG	DA	3029	1/1	0.94	0.14	-	22,22,22,22	0
57	MG	DA	3175	1/1	0.66	0.51	-	56,56,56,56	0
57	MG	BA	3300	1/1	0.80	0.52	-	67,67,67,67	0
57	MG	DA	3259	1/1	0.92	0.20	-	47,47,47,47	0
57	MG	AA	1714	1/1	0.95	0.25	-	42,42,42,42	0
57	MG	BA	3017	1/1	0.92	0.27	-	20,20,20,20	0
57	MG	DB	201	1/1	0.85	0.22	-	53,53,53,53	0
57	MG	DA	3059	1/1	0.92	0.23	-	26,26,26,26	0
57	MG	DA	3224	1/1	0.95	0.41	-	14,14,14,14	0
57	MG	BA	3306	1/1	0.92	0.31	-	47,47,47,47	0
57	MG	DA	3274	1/1	0.89	0.25	-	36,36,36,36	0
57	MG	BA	3362	1/1	0.93	0.31	-	30,30,30,30	0
57	MG	DA	3095	1/1	0.95	0.29	-	62,62,62,62	0
57	MG	DA	3255	1/1	0.55	0.31	-	46,46,46,46	0
57	MG	B5	102	1/1	0.92	0.38	-	40,40,40,40	0
57	MG	BA	3378	1/1	0.80	0.22	-	55,55,55,55	0
57	MG	DA	3261	1/1	0.87	0.21	-	58,58,58,58	0
57	MG	BA	3243	1/1	0.87	0.28	-	51,51,51,51	0
57	MG	BA	3451	1/1	0.94	0.18	-	23,23,23,23	0
57	MG	BP	201	1/1	0.65	1.35	-	205,205,205,205	0
57	MG	BA	3236	1/1	0.82	0.26	-	62,62,62,62	0
57	MG	DA	3202	1/1	0.96	0.58	-	38,38,38,38	0
57	MG	DA	3046	1/1	0.93	0.41	-	26,26,26,26	0
57	MG	BA	3244	1/1	0.96	0.26	-	47,47,47,47	0
57	MG	BA	3065	1/1	0.99	0.30	-	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	3122	1/1	0.71	0.20	-	48,48,48,48	0
57	MG	BA	3091	1/1	0.88	0.44	-	21,21,21,21	0
57	MG	BA	3201	1/1	0.94	0.12	-	24,24,24,24	0
57	MG	BA	3238	1/1	0.83	0.43	-	20,20,20,20	0
57	MG	BA	3216	1/1	0.97	0.44	-	20,20,20,20	0
57	MG	AA	1687	1/1	0.84	0.28	-	44,44,44,44	0
57	MG	DA	3137	1/1	0.90	0.20	-	30,30,30,30	0
57	MG	BA	3126	1/1	0.91	0.29	-	66,66,66,66	0
57	MG	BA	3116	1/1	0.89	0.11	-	23,23,23,23	0
57	MG	BA	3288	1/1	0.92	0.20	-	18,18,18,18	0
57	MG	CA	1706	1/1	0.92	0.22	-	59,59,59,59	0
57	MG	BE	301	1/1	0.96	0.30	-	43,43,43,43	0
57	MG	BA	3090	1/1	0.99	0.25	-	17,17,17,17	0
57	MG	BA	3158	1/1	0.92	0.31	-	37,37,37,37	0
57	MG	DA	3277	1/1	0.56	0.26	-	57,57,57,57	0
57	MG	DA	3135	1/1	0.91	0.26	-	42,42,42,42	0
57	MG	DA	3176	1/1	0.89	0.32	-	24,24,24,24	0
57	MG	BA	3323	1/1	0.59	1.28	-	205,205,205,205	0
57	MG	DA	3278	1/1	0.86	0.27	-	59,59,59,59	0
57	MG	CA	1629	1/1	0.79	0.24	-	25,25,25,25	0
57	MG	D5	101	1/1	0.86	0.19	-	38,38,38,38	0
57	MG	DA	3299	1/1	0.90	0.16	-	42,42,42,42	0
57	MG	CA	1610	1/1	0.98	0.33	-	30,30,30,30	0
57	MG	DA	3191	1/1	0.94	0.21	-	18,18,18,18	0
57	MG	BA	3213	1/1	0.97	0.29	-	43,43,43,43	0
57	MG	DA	3065	1/1	0.90	0.35	-	29,29,29,29	0
57	MG	BA	3038	1/1	0.78	1.44	-	163,163,163,163	0
57	MG	CA	1686	1/1	0.71	0.28	-	44,44,44,44	0
57	MG	BA	3135	1/1	0.95	0.16	-	23,23,23,23	0
57	MG	DA	3218	1/1	0.88	0.19	-	35,35,35,35	0
57	MG	CA	1626	1/1	0.90	0.53	-	67,67,67,67	0
57	MG	BA	3037	1/1	0.92	0.23	-	9,9,9,9	0
57	MG	DA	3281	1/1	0.90	0.10	-	49,49,49,49	0
57	MG	BA	3377	1/1	0.95	0.11	-	23,23,23,23	0
57	MG	BA	3354	1/1	0.80	0.39	-	25,25,25,25	0
57	MG	BA	3336	1/1	0.93	0.16	-	29,29,29,29	0
57	MG	BA	3382	1/1	0.90	0.23	-	26,26,26,26	0
57	MG	AA	1649	1/1	0.92	0.30	-	50,50,50,50	0
57	MG	DA	3220	1/1	0.84	0.36	-	31,31,31,31	0
57	MG	BA	3246	1/1	0.96	0.10	-	11,11,11,11	0
57	MG	DA	3054	1/1	0.96	0.58	-	27,27,27,27	0
57	MG	DA	3130	1/1	0.93	0.37	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3283	1/1	0.88	0.20	-	62,62,62,62	0
57	MG	AA	1640	1/1	0.94	0.24	-	19,19,19,19	0
57	MG	BA	3433	1/1	0.91	0.50	-	52,52,52,52	0
57	MG	BA	3272	1/1	0.97	0.47	-	23,23,23,23	0
57	MG	BA	3453	1/1	0.92	0.20	-	41,41,41,41	0
57	MG	AA	1686	1/1	0.85	0.16	-	42,42,42,42	0
57	MG	BA	3261	1/1	0.94	0.41	-	28,28,28,28	0
57	MG	DA	3200	1/1	0.80	0.29	-	66,66,66,66	0
57	MG	BA	3396	1/1	0.97	0.11	-	26,26,26,26	0
57	MG	BA	3321	1/1	0.95	0.37	-	22,22,22,22	0
57	MG	BA	3423	1/1	0.97	0.07	-	25,25,25,25	0
57	MG	BB	209	1/1	0.89	0.12	-	37,37,37,37	0
57	MG	DA	3300	1/1	0.70	0.20	-	38,38,38,38	0
57	MG	BA	3304	1/1	0.96	0.10	-	49,49,49,49	0
57	MG	BA	3092	1/1	0.87	0.32	-	36,36,36,36	0
57	MG	BA	3214	1/1	0.96	0.11	-	29,29,29,29	0
57	MG	AA	1706	1/1	0.88	0.12	-	47,47,47,47	0
57	MG	BA	3173	1/1	0.94	0.14	-	40,40,40,40	0
57	MG	BA	3273	1/1	0.96	0.23	-	40,40,40,40	0
57	MG	CA	1704	1/1	0.93	0.17	-	26,26,26,26	0
57	MG	DA	3229	1/1	0.96	0.17	-	19,19,19,19	0
57	MG	DA	3096	1/1	0.93	0.19	-	34,34,34,34	0
57	MG	DA	3042	1/1	0.80	0.33	-	28,28,28,28	0
57	MG	BA	3196	1/1	0.90	0.16	-	27,27,27,27	0
57	MG	BA	3458	1/1	0.86	0.46	-	47,47,47,47	0
57	MG	DA	3185	1/1	0.86	0.38	-	37,37,37,37	0
57	MG	BA	3346	1/1	0.86	0.49	-	50,50,50,50	0
57	MG	DA	3276	1/1	0.84	0.21	-	51,51,51,51	0
57	MG	AA	1603	1/1	0.82	0.11	-	18,18,18,18	0
57	MG	DA	3249	1/1	0.91	0.14	-	33,33,33,33	0
57	MG	BA	3055	1/1	0.95	0.27	-	24,24,24,24	0
57	MG	DA	3070	1/1	0.72	0.40	-	46,46,46,46	0
57	MG	CA	1628	1/1	0.96	0.12	-	26,26,26,26	0
57	MG	BA	3002	1/1	0.92	0.19	-	39,39,39,39	0
57	MG	D5	102	1/1	0.94	0.43	-	44,44,44,44	0
57	MG	BA	3269	1/1	0.92	0.26	-	27,27,27,27	0
57	MG	BA	3265	1/1	0.91	0.11	-	67,67,67,67	0
57	MG	BA	3443	1/1	0.97	0.22	-	24,24,24,24	0
57	MG	DA	3272	1/1	0.90	0.20	-	40,40,40,40	0
57	MG	DA	3092	1/1	0.96	0.37	-	25,25,25,25	0
57	MG	BA	3222	1/1	0.96	0.30	-	31,31,31,31	0
57	MG	DA	3285	1/1	0.95	0.23	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1632	1/1	0.88	0.42	-	18,18,18,18	0
57	MG	BA	3248	1/1	0.89	0.32	-	34,34,34,34	0
57	MG	CA	1693	1/1	0.93	0.21	-	36,36,36,36	0
57	MG	DA	3024	1/1	0.91	0.14	-	33,33,33,33	0
57	MG	BA	3161	1/1	0.94	0.21	-	25,25,25,25	0
57	MG	AA	1715	1/1	0.90	0.16	-	62,62,62,62	0
57	MG	BA	3367	1/1	0.95	0.40	-	33,33,33,33	0
57	MG	AA	1716	1/1	0.92	0.13	-	31,31,31,31	0
57	MG	DA	3047	1/1	0.96	0.34	-	26,26,26,26	0
57	MG	DA	3266	1/1	0.76	0.36	-	46,46,46,46	0
57	MG	BA	3033	1/1	0.95	0.23	-	34,34,34,34	0
57	MG	BA	3010	1/1	0.98	0.25	-	23,23,23,23	0
57	MG	BA	3291	1/1	0.90	0.36	-	24,24,24,24	0
57	MG	DA	3139	1/1	0.92	0.18	-	58,58,58,58	0
57	MG	BA	3268	1/1	0.78	0.62	-	46,46,46,46	0
57	MG	DA	3168	1/1	0.96	0.24	-	35,35,35,35	0
57	MG	CA	1652	1/1	0.77	0.46	-	59,59,59,59	0
57	MG	DA	3251	1/1	0.89	0.31	-	53,53,53,53	0
57	MG	DA	3082	1/1	0.96	0.29	-	21,21,21,21	0
57	MG	DA	3180	1/1	0.92	0.30	-	49,49,49,49	0
57	MG	DA	3303	1/1	0.91	0.22	-	54,54,54,54	0
57	MG	BA	3426	1/1	0.92	0.12	-	26,26,26,26	0
57	MG	BA	3224	1/1	0.88	0.30	-	31,31,31,31	0
57	MG	AA	1644	1/1	0.93	0.27	-	40,40,40,40	0
57	MG	BA	3274	1/1	0.97	0.35	-	27,27,27,27	0
57	MG	AA	1611	1/1	0.47	0.88	-	58,58,58,58	0
57	MG	BA	3228	1/1	0.96	0.38	-	36,36,36,36	0
57	MG	BA	3136	1/1	0.87	0.92	-	76,76,76,76	0
57	MG	DA	3161	1/1	0.83	0.78	-	50,50,50,50	0
57	MG	BH	201	1/1	0.94	0.20	-	21,21,21,21	0
57	MG	AA	1654	1/1	0.86	0.27	-	29,29,29,29	0
57	MG	BA	3445	1/1	0.89	0.14	-	36,36,36,36	0
57	MG	AA	1646	1/1	0.87	0.15	-	49,49,49,49	0
57	MG	BA	3141	1/1	0.90	0.31	-	45,45,45,45	0
57	MG	BA	3227	1/1	0.93	0.29	-	21,21,21,21	0
57	MG	BA	3232	1/1	0.88	0.44	-	38,38,38,38	0
57	MG	CA	1623	1/1	0.90	0.33	-	59,59,59,59	0
57	MG	DA	3258	1/1	0.96	0.21	-	64,64,64,64	0
57	MG	AA	1614	1/1	0.95	0.37	-	29,29,29,29	0
57	MG	DA	3250	1/1	0.92	0.37	-	26,26,26,26	0
57	MG	BA	3424	1/1	0.76	0.16	-	26,26,26,26	0
57	MG	DA	3074	1/1	0.98	0.26	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DB	204	1/1	0.72	0.18	-	43,43,43,43	0
57	MG	CA	1605	1/1	0.89	0.41	-	62,62,62,62	0
57	MG	BA	3314	1/1	0.96	0.07	-	22,22,22,22	0
57	MG	AA	1613	1/1	0.73	0.34	-	75,75,75,75	0
57	MG	BA	3072	1/1	0.97	0.44	-	23,23,23,23	0
57	MG	DA	3217	1/1	0.91	0.57	-	54,54,54,54	0
57	MG	BA	3360	1/1	0.96	0.15	-	27,27,27,27	0
57	MG	BA	3429	1/1	0.98	0.05	-	33,33,33,33	0
57	MG	BA	3145	1/1	0.95	0.35	-	29,29,29,29	0
57	MG	DA	3154	1/1	0.74	0.14	-	61,61,61,61	0
57	MG	DA	3245	1/1	0.85	0.28	-	52,52,52,52	0
57	MG	AA	1681	1/1	0.88	0.29	-	63,63,63,63	0
57	MG	BA	3381	1/1	0.86	0.43	-	66,66,66,66	0
57	MG	BA	3191	1/1	0.83	0.12	-	40,40,40,40	0
57	MG	AA	1642	1/1	0.66	0.35	-	67,67,67,67	0
57	MG	AA	1656	1/1	0.94	0.12	-	28,28,28,28	0
57	MG	CA	1703	1/1	0.91	0.41	-	34,34,34,34	0
57	MG	BA	3343	1/1	0.92	0.20	-	22,22,22,22	0
57	MG	AA	1627	1/1	0.96	0.16	-	21,21,21,21	0
57	MG	DA	3049	1/1	0.87	0.25	-	15,15,15,15	0
57	MG	CA	1699	1/1	0.98	0.24	-	32,32,32,32	0
57	MG	AW	102	1/1	0.93	0.09	-	26,26,26,26	0
57	MG	BA	3277	1/1	0.92	0.24	-	29,29,29,29	0
57	MG	DA	3208	1/1	0.87	0.09	-	59,59,59,59	0
57	MG	BA	3279	1/1	0.95	0.07	-	26,26,26,26	0
57	MG	DA	3264	1/1	0.94	0.11	-	25,25,25,25	0
57	MG	CA	1691	1/1	0.93	0.59	-	67,67,67,67	0
57	MG	DA	3210	1/1	0.94	0.26	-	41,41,41,41	0
57	MG	DA	3088	1/1	0.87	0.20	-	20,20,20,20	0
57	MG	CA	1624	1/1	0.93	0.60	-	39,39,39,39	0
57	MG	BQ	203	1/1	0.87	0.21	-	27,27,27,27	0
57	MG	BA	3379	1/1	0.75	0.21	-	40,40,40,40	0
57	MG	CA	1634	1/1	0.89	0.10	-	37,37,37,37	0
57	MG	CA	1672	1/1	0.86	0.24	-	29,29,29,29	0
57	MG	AA	1697	1/1	0.94	0.16	-	27,27,27,27	0
57	MG	BB	208	1/1	0.94	0.32	-	36,36,36,36	0
57	MG	BA	3380	1/1	0.88	0.30	-	37,37,37,37	0
57	MG	AA	1648	1/1	0.93	0.14	-	40,40,40,40	0
57	MG	BA	3408	1/1	0.85	0.45	-	57,57,57,57	0
57	MG	BA	3016	1/1	0.91	0.48	-	20,20,20,20	0
57	MG	BA	3384	1/1	0.89	0.25	-	42,42,42,42	0
57	MG	CW	103	1/1	0.89	0.34	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3242	1/1	0.96	0.08	-	32,32,32,32	0
57	MG	CA	1651	1/1	0.90	0.20	-	28,28,28,28	0
57	MG	BA	3215	1/1	0.92	0.21	-	35,35,35,35	0
57	MG	BA	3440	1/1	0.88	0.45	-	64,64,64,64	0
57	MG	BA	3305	1/1	0.93	0.35	-	41,41,41,41	0
57	MG	DA	3173	1/1	0.96	0.20	-	33,33,33,33	0
57	MG	AA	1701	1/1	0.90	0.32	-	33,33,33,33	0
57	MG	BA	3266	1/1	0.98	0.46	-	26,26,26,26	0
57	MG	CA	1640	1/1	0.82	0.62	-	61,61,61,61	0
57	MG	BA	3393	1/1	0.92	0.10	-	61,61,61,61	0
57	MG	BA	3356	1/1	0.93	0.17	-	21,21,21,21	0
57	MG	CA	1648	1/1	0.93	0.10	-	28,28,28,28	0
57	MG	DA	3256	1/1	0.82	0.28	-	62,62,62,62	0
57	MG	BA	3372	1/1	0.86	0.25	-	59,59,59,59	0
57	MG	DA	3215	1/1	0.89	0.34	-	37,37,37,37	0
57	MG	B5	104	1/1	0.93	0.24	-	33,33,33,33	0
57	MG	AA	1645	1/1	0.81	0.36	-	52,52,52,52	0
57	MG	AA	1652	1/1	0.96	0.16	-	44,44,44,44	0
57	MG	BA	3226	1/1	0.83	0.38	-	31,31,31,31	0
57	MG	DA	3233	1/1	0.92	0.17	-	17,17,17,17	0
57	MG	CA	1670	1/1	0.81	0.40	-	43,43,43,43	0
57	MG	AA	1703	1/1	0.89	0.17	-	51,51,51,51	0
57	MG	DA	3305	1/1	0.93	0.38	-	35,35,35,35	0
57	MG	CA	1659	1/1	0.94	0.36	-	32,32,32,32	0
57	MG	BA	3280	1/1	0.93	0.17	-	19,19,19,19	0
57	MG	B0	101	1/1	0.86	0.36	-	30,30,30,30	0
57	MG	DA	3282	1/1	0.84	0.24	-	65,65,65,65	0
57	MG	DA	3035	1/1	0.96	0.51	-	22,22,22,22	0
57	MG	DA	3241	1/1	0.92	0.10	-	26,26,26,26	0
57	MG	BA	3283	1/1	0.97	0.34	-	20,20,20,20	0
57	MG	CA	1645	1/1	0.91	0.28	-	41,41,41,41	0
57	MG	BA	3322	1/1	0.91	0.34	-	29,29,29,29	0
57	MG	DA	3124	1/1	0.94	0.17	-	26,26,26,26	0
57	MG	BA	3085	1/1	0.96	0.18	-	17,17,17,17	0
57	MG	D6	101	1/1	0.88	0.26	-	57,57,57,57	0
57	MG	DA	3257	1/1	0.98	0.14	-	35,35,35,35	0
57	MG	CA	1633	1/1	0.94	0.44	-	45,45,45,45	0
57	MG	AA	1683	1/1	0.95	0.29	-	31,31,31,31	0
57	MG	BX	101	1/1	0.93	0.15	-	36,36,36,36	0
57	MG	BA	3454	1/1	0.95	0.14	-	25,25,25,25	0
57	MG	DA	3222	1/1	0.89	0.31	-	26,26,26,26	0
57	MG	BA	3355	1/1	0.74	0.53	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3325	1/1	0.97	0.34	-	22,22,22,22	0
57	MG	DB	208	1/1	0.78	0.47	-	48,48,48,48	0
57	MG	BA	3114	1/1	0.95	0.37	-	24,24,24,24	0
57	MG	CA	1682	1/1	0.97	0.27	-	40,40,40,40	0
57	MG	BA	3255	1/1	0.96	0.44	-	31,31,31,31	0
57	MG	DA	3171	1/1	0.91	0.47	-	27,27,27,27	0
57	MG	DA	3138	1/1	0.94	0.26	-	17,17,17,17	0
57	MG	DA	3219	1/1	0.97	0.45	-	34,34,34,34	0
57	MG	AA	1674	1/1	0.80	0.22	-	49,49,49,49	0
57	MG	CA	1702	1/1	0.92	0.31	-	29,29,29,29	0
57	MG	BA	3143	1/1	0.79	0.31	-	31,31,31,31	0
57	MG	BA	3349	1/1	0.82	0.23	-	38,38,38,38	0
57	MG	BA	3131	1/1	0.94	0.33	-	26,26,26,26	0
57	MG	DA	3197	1/1	0.97	0.27	-	27,27,27,27	0
57	MG	BA	3083	1/1	0.95	0.14	-	22,22,22,22	0
57	MG	DA	3011	1/1	0.99	0.35	-	20,20,20,20	0
57	MG	DA	3252	1/1	0.93	0.50	-	27,27,27,27	0
57	MG	AA	1684	1/1	0.92	0.13	-	31,31,31,31	0
57	MG	DA	3268	1/1	0.91	0.18	-	43,43,43,43	0
57	MG	BA	3176	1/1	0.72	0.19	-	44,44,44,44	0
57	MG	DA	3177	1/1	0.88	0.46	-	52,52,52,52	0
57	MG	AA	1608	1/1	0.94	0.17	-	65,65,65,65	0
57	MG	BA	3452	1/1	0.99	0.15	-	16,16,16,16	0
57	MG	AA	1657	1/1	0.83	0.15	-	54,54,54,54	0
57	MG	BA	3132	1/1	0.94	0.29	-	28,28,28,28	0
57	MG	BA	3290	1/1	0.88	0.22	-	22,22,22,22	0
57	MG	BA	3195	1/1	0.84	0.20	-	47,47,47,47	0
57	MG	BA	3175	1/1	0.77	0.23	-	71,71,71,71	0
57	MG	BA	3414	1/1	0.91	0.35	-	36,36,36,36	0
57	MG	AA	1705	1/1	0.76	0.28	-	66,66,66,66	0
57	MG	BA	3370	1/1	0.90	0.10	-	48,48,48,48	0
57	MG	BA	3421	1/1	0.89	0.16	-	32,32,32,32	0
57	MG	DA	3134	1/1	0.96	0.17	-	24,24,24,24	0
57	MG	BA	3247	1/1	0.96	0.06	-	33,33,33,33	0
57	MG	BA	3328	1/1	0.91	0.24	-	32,32,32,32	0
57	MG	DA	3165	1/1	0.87	0.14	-	43,43,43,43	0
57	MG	DA	3287	1/1	0.88	0.28	-	48,48,48,48	0
57	MG	DA	3015	1/1	0.96	0.23	-	36,36,36,36	0
57	MG	DB	206	1/1	0.96	0.16	-	19,19,19,19	0
57	MG	DA	3106	1/1	0.95	0.50	-	25,25,25,25	0
57	MG	B1	101	1/1	0.94	0.42	-	63,63,63,63	0
57	MG	DA	3131	1/1	0.90	0.32	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3171	1/1	0.89	0.44	-	41,41,41,41	0
57	MG	BA	3013	1/1	0.89	0.18	-	56,56,56,56	0
57	MG	BA	3334	1/1	0.95	0.19	-	24,24,24,24	0
57	MG	CA	1658	1/1	0.90	0.17	-	21,21,21,21	0
57	MG	BA	3148	1/1	0.91	0.22	-	64,64,64,64	0
57	MG	DA	3189	1/1	0.92	0.20	-	34,34,34,34	0
57	MG	BA	3001	1/1	0.84	0.17	-	50,50,50,50	0
57	MG	DA	3244	1/1	0.93	0.31	-	26,26,26,26	0
57	MG	AA	1695	1/1	0.96	0.20	-	26,26,26,26	0
57	MG	BA	3413	1/1	0.98	0.26	-	24,24,24,24	0
57	MG	BQ	201	1/1	0.95	0.20	-	24,24,24,24	0
57	MG	BA	3446	1/1	0.85	0.69	-	60,60,60,60	0
57	MG	CA	1607	1/1	0.94	0.12	-	37,37,37,37	0
57	MG	CA	1681	1/1	0.85	0.18	-	44,44,44,44	0
57	MG	AA	1661	1/1	0.86	0.21	-	67,67,67,67	0
57	MG	BA	3318	1/1	0.90	0.38	-	41,41,41,41	0
57	MG	BA	3296	1/1	0.87	0.18	-	25,25,25,25	0
57	MG	BA	3386	1/1	0.94	0.29	-	68,68,68,68	0
57	MG	CA	1647	1/1	0.92	0.26	-	61,61,61,61	0
57	MG	BA	3267	1/1	0.98	0.16	-	19,19,19,19	0
57	MG	AA	1632	1/1	0.89	0.43	-	57,57,57,57	0
57	MG	AA	1605	1/1	0.85	0.17	-	51,51,51,51	0
57	MG	CA	1656	1/1	0.95	0.44	-	43,43,43,43	0
57	MG	BA	3127	1/1	0.92	0.23	-	30,30,30,30	0
57	MG	CA	1696	1/1	0.93	0.30	-	54,54,54,54	0
57	MG	AA	1709	1/1	0.78	0.20	-	66,66,66,66	0
57	MG	DA	3143	1/1	0.86	0.22	-	23,23,23,23	0
57	MG	BA	3340	1/1	0.97	0.23	-	29,29,29,29	0
57	MG	DA	3253	1/1	0.98	0.19	-	20,20,20,20	0
57	MG	DA	3262	1/1	0.93	0.28	-	29,29,29,29	0
57	MG	DA	3153	1/1	0.92	0.15	-	41,41,41,41	0
57	MG	DA	3273	1/1	0.87	0.31	-	55,55,55,55	0
57	MG	AA	1612	1/1	0.94	0.39	-	25,25,25,25	0
57	MG	CA	1683	1/1	0.95	0.15	-	36,36,36,36	0
57	MG	AA	1665	1/1	0.87	0.38	-	63,63,63,63	0
57	MG	BA	3108	1/1	0.97	0.23	-	35,35,35,35	0
57	MG	AA	1685	1/1	0.87	0.29	-	42,42,42,42	0
57	MG	BA	3327	1/1	0.97	0.20	-	28,28,28,28	0
57	MG	DA	3148	1/1	0.98	0.32	-	24,24,24,24	0
57	MG	BA	3287	1/1	0.99	0.17	-	20,20,20,20	0
57	MG	DA	3167	1/1	0.91	0.43	-	38,38,38,38	0
57	MG	BA	3351	1/1	0.97	0.15	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3316	1/1	0.95	0.19	-	28,28,28,28	0
57	MG	AA	1713	1/1	0.90	0.14	-	43,43,43,43	0
57	MG	AA	1641	1/1	0.96	0.16	-	30,30,30,30	0
57	MG	BA	3389	1/1	0.98	0.24	-	21,21,21,21	0
57	MG	BA	3084	1/1	0.95	0.69	-	61,61,61,61	0
57	MG	DA	3136	1/1	0.89	0.17	-	22,22,22,22	0
57	MG	BA	3250	1/1	0.99	0.50	-	22,22,22,22	0
57	MG	BA	3019	1/1	0.97	0.34	-	25,25,25,25	0
57	MG	DA	3121	1/1	0.80	0.30	-	57,57,57,57	0
57	MG	DA	3293	1/1	0.90	0.24	-	39,39,39,39	0
57	MG	BA	3235	1/1	0.92	0.25	-	51,51,51,51	0
57	MG	DA	3066	1/1	0.97	0.30	-	22,22,22,22	0
57	MG	AA	1636	1/1	0.85	0.17	-	62,62,62,62	0
57	MG	BA	3270	1/1	0.87	0.32	-	43,43,43,43	0
57	MG	BA	3302	1/1	0.96	0.11	-	37,37,37,37	0
57	MG	AA	1601	1/1	0.75	0.22	-	47,47,47,47	0
57	MG	BA	3331	1/1	0.91	0.27	-	28,28,28,28	0
57	MG	DA	3075	1/1	0.94	0.32	-	27,27,27,27	0
57	MG	DA	3062	1/1	0.93	0.16	-	33,33,33,33	0
57	MG	CA	1669	1/1	0.96	0.19	-	21,21,21,21	0
57	MG	BA	3027	1/1	0.93	0.20	-	26,26,26,26	0
57	MG	BA	3375	1/1	0.94	0.41	-	36,36,36,36	0
57	MG	BA	3199	1/1	0.87	0.33	-	23,23,23,23	0
57	MG	BP	203	1/1	0.95	0.22	-	27,27,27,27	0
57	MG	DA	3003	1/1	0.91	0.18	-	30,30,30,30	0
57	MG	BA	3130	1/1	0.96	0.39	-	35,35,35,35	0
57	MG	DA	3116	1/1	0.93	0.34	-	33,33,33,33	0
57	MG	DA	3028	1/1	0.86	0.14	-	34,34,34,34	0
57	MG	BA	3417	1/1	0.89	0.25	-	62,62,62,62	0
57	MG	CA	1604	1/1	0.70	0.25	-	38,38,38,38	0
57	MG	BA	3395	1/1	0.93	0.46	-	39,39,39,39	0
57	MG	DA	3087	1/1	0.92	0.40	-	26,26,26,26	0
57	MG	AA	1671	1/1	0.95	0.23	-	42,42,42,42	0
57	MG	DA	3183	1/1	0.93	0.22	-	54,54,54,54	0
57	MG	AA	1673	1/1	0.92	0.12	-	40,40,40,40	0
57	MG	AA	1682	1/1	0.96	0.21	-	18,18,18,18	0
57	MG	DA	3102	1/1	0.95	0.40	-	32,32,32,32	0
57	MG	BA	3320	1/1	0.88	0.28	-	25,25,25,25	0
57	MG	BA	3319	1/1	0.93	0.07	-	28,28,28,28	0
57	MG	DA	3201	1/1	0.90	0.45	-	32,32,32,32	0
57	MG	DA	3182	1/1	0.90	0.15	-	37,37,37,37	0
57	MG	BA	3192	1/1	0.94	0.26	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3225	1/1	0.94	0.16	-	16,16,16,16	0
57	MG	BA	3190	1/1	0.84	0.21	-	34,34,34,34	0
57	MG	BA	3456	1/1	0.88	0.26	-	43,43,43,43	0
57	MG	DA	3228	1/1	0.92	0.23	-	25,25,25,25	0
57	MG	CA	1612	1/1	0.90	0.37	-	55,55,55,55	0
57	MG	BA	3407	1/1	0.75	0.33	-	66,66,66,66	0
57	MG	DA	3115	1/1	0.94	0.08	-	36,36,36,36	0
57	MG	CA	1609	1/1	0.91	0.30	-	27,27,27,27	0
57	MG	DA	3101	1/1	0.90	0.23	-	35,35,35,35	0
57	MG	BA	3439	1/1	0.92	0.17	-	32,32,32,32	0
57	MG	DA	3023	1/1	0.92	0.23	-	42,42,42,42	0
57	MG	BA	3162	1/1	0.92	0.10	-	21,21,21,21	0
57	MG	BA	3174	1/1	0.93	0.17	-	53,53,53,53	0
57	MG	DA	3295	1/1	0.96	0.27	-	40,40,40,40	0
57	MG	BA	3295	1/1	0.95	0.27	-	20,20,20,20	0
57	MG	BA	3100	1/1	0.88	0.55	-	28,28,28,28	0
57	MG	BA	3249	1/1	0.73	0.26	-	46,46,46,46	0
57	MG	DA	3238	1/1	0.90	0.23	-	33,33,33,33	0
57	MG	BA	3317	1/1	0.70	0.37	-	27,27,27,27	0
57	MG	CA	1650	1/1	0.97	0.12	-	28,28,28,28	0
57	MG	BA	3263	1/1	0.93	0.09	-	36,36,36,36	0
57	MG	CE	201	1/1	0.67	0.36	-	42,42,42,42	0
57	MG	DB	207	1/1	0.97	0.18	-	27,27,27,27	0
57	MG	BA	3039	1/1	0.97	0.73	-	39,39,39,39	0
57	MG	BA	3311	1/1	0.89	0.18	-	31,31,31,31	0
57	MG	BA	3060	1/1	0.91	0.38	-	47,47,47,47	0
57	MG	BA	3209	1/1	0.94	0.25	-	23,23,23,23	0
57	MG	BA	3074	1/1	0.89	0.36	-	31,31,31,31	0
57	MG	BA	3276	1/1	0.96	0.39	-	21,21,21,21	0
57	MG	BA	3239	1/1	0.83	0.24	-	46,46,46,46	0
57	MG	BA	3028	1/1	0.90	0.22	-	29,29,29,29	0
57	MG	BA	3342	1/1	0.86	0.13	-	22,22,22,22	0
57	MG	DA	3158	1/1	0.88	0.35	-	44,44,44,44	0
57	MG	CA	1646	1/1	0.81	0.20	-	59,59,59,59	0
57	MG	DA	3001	1/1	0.89	0.30	-	61,61,61,61	0
57	MG	CA	1668	1/1	0.94	0.22	-	27,27,27,27	0
57	MG	BA	3326	1/1	0.92	0.17	-	21,21,21,21	0
57	MG	BA	3442	1/1	0.39	3.28	-	205,205,205,205	0
57	MG	BA	3182	1/1	0.93	0.45	-	27,27,27,27	0
57	MG	DA	3034	1/1	0.94	0.25	-	57,57,57,57	0
57	MG	DA	3223	1/1	0.87	0.24	-	32,32,32,32	0
57	MG	CA	1619	1/1	0.92	0.15	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	BA	3444	1/1	0.79	0.96	-	101,101,101,101	0
57	MG	AA	1610	1/1	0.97	0.45	-	21,21,21,21	0
57	MG	BA	3310	1/1	0.92	0.19	-	30,30,30,30	0
57	MG	BA	3373	1/1	0.87	0.20	-	31,31,31,31	0
57	MG	CA	1615	1/1	0.92	0.37	-	63,63,63,63	0
57	MG	BA	3450	1/1	0.91	0.41	-	44,44,44,44	0
57	MG	BA	3128	1/1	0.98	0.40	-	33,33,33,33	0
57	MG	DA	3195	1/1	0.69	0.86	-	73,73,73,73	0
57	MG	DP	201	1/1	0.90	0.16	-	38,38,38,38	0
57	MG	CA	1618	1/1	0.64	0.25	-	39,39,39,39	0
57	MG	BA	3082	1/1	0.94	0.32	-	24,24,24,24	0
57	MG	BA	3264	1/1	0.80	0.29	-	34,34,34,34	0
57	MG	BA	3278	1/1	0.96	0.17	-	33,33,33,33	0
57	MG	BA	3165	1/1	0.95	0.19	-	25,25,25,25	0
57	MG	DA	3209	1/1	0.93	0.26	-	33,33,33,33	0
57	MG	BA	3457	1/1	0.96	0.18	-	35,35,35,35	0
57	MG	DA	3128	1/1	0.96	0.26	-	24,24,24,24	0
57	MG	BA	3402	1/1	0.94	0.12	-	24,24,24,24	0
57	MG	BA	3223	1/1	0.82	0.24	-	49,49,49,49	0
57	MG	AA	1692	1/1	0.96	0.23	-	51,51,51,51	0
57	MG	BA	3324	1/1	0.97	0.17	-	25,25,25,25	0
57	MG	DA	3110	1/1	0.90	0.33	-	38,38,38,38	0
57	MG	BA	3353	1/1	0.92	0.38	-	36,36,36,36	0
57	MG	BA	3406	1/1	0.89	0.16	-	50,50,50,50	0
57	MG	AA	1634	1/1	0.96	0.41	-	41,41,41,41	0
57	MG	AA	1660	1/1	0.92	0.22	-	31,31,31,31	0
57	MG	BA	3129	1/1	0.85	0.18	-	25,25,25,25	0
57	MG	CA	1639	1/1	0.93	0.11	-	22,22,22,22	0
57	MG	BA	3359	1/1	0.90	0.28	-	44,44,44,44	0
57	MG	DA	3284	1/1	0.96	0.13	-	51,51,51,51	0
57	MG	BA	3051	1/1	0.91	0.45	-	51,51,51,51	0
57	MG	BA	3043	1/1	0.98	0.34	-	25,25,25,25	0
57	MG	DA	3108	1/1	0.71	0.59	-	47,47,47,47	0
57	MG	BA	3058	1/1	0.94	0.47	-	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.