wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:59 PM GMT

PDB ID	:	4W2E
Title	:	Crystal structure of Elongation Factor 4 (EF4/LepA) bound to the Thermus thermophilus 70S ribosome
Authors	:	Gagnon, M.G.; Lin, J.; Steitz, T.A.
Deposited on	:	2014-06-04
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

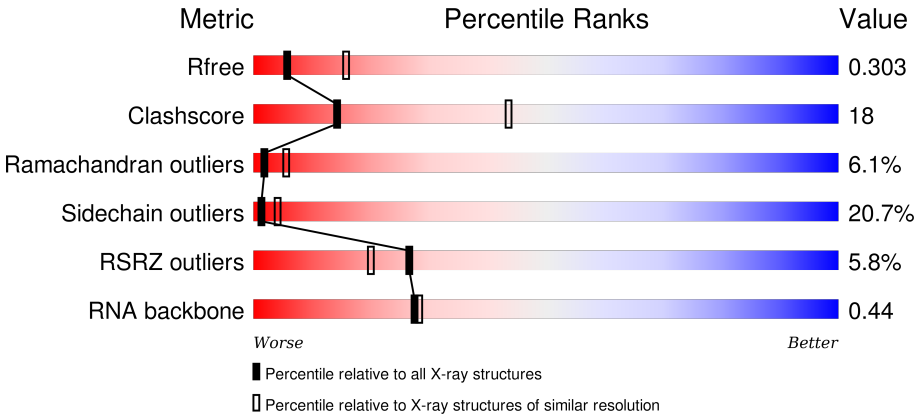
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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 <=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	A	2915	3% 34% 42% 20%
2	B	122	52% 39% 5%
3	D	276	% 37% 49% 12%
4	E	206	2% 50% 38% 9%

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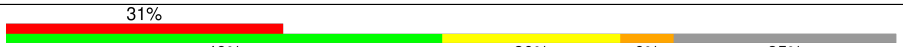
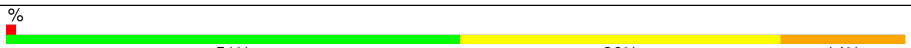
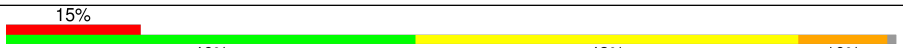
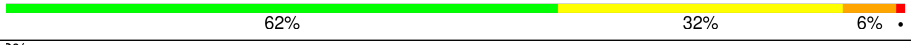
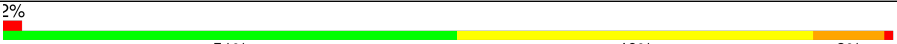
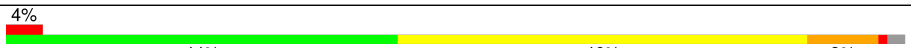
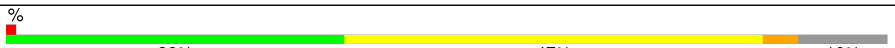
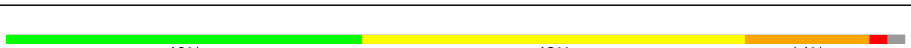
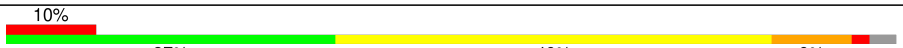
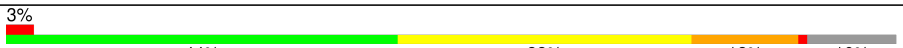
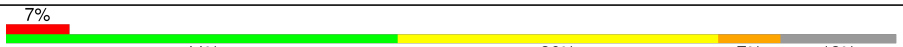
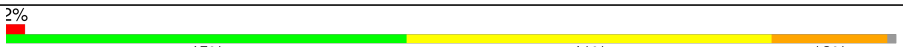
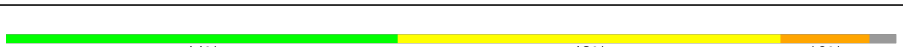
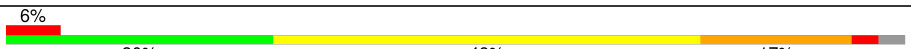
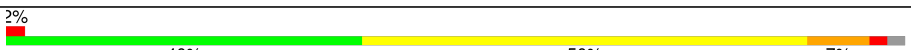
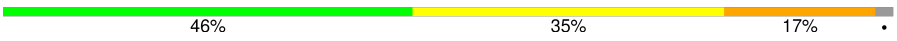
Mol	Chain	Length	Quality of chain
5	F	205	
6	G	182	
7	H	180	
8	J	173	
9	K	147	
10	N	140	
11	O	122	
12	P	150	
13	Q	141	
14	R	118	
15	S	112	
16	T	146	
17	U	118	
18	V	101	
19	W	113	
20	X	96	
21	Y	110	
22	Z	206	
23	0	85	
24	1	98	
25	2	72	
26	3	60	
27	4	71	
28	5	60	
29	6	54	

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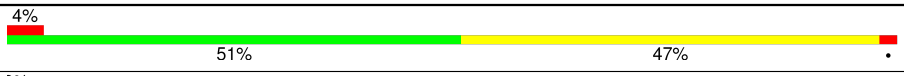
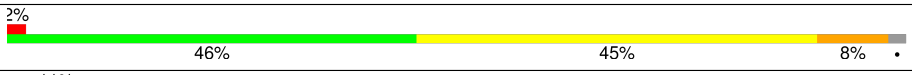
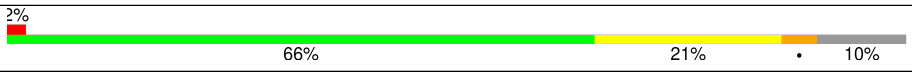
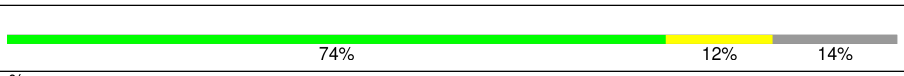
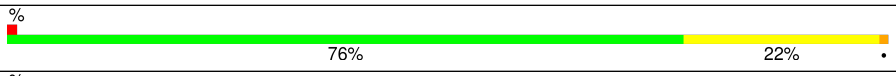
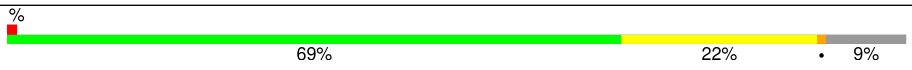
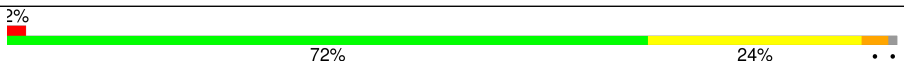
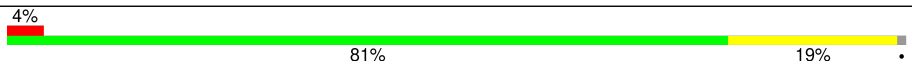
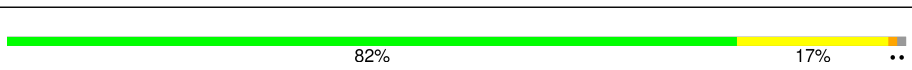
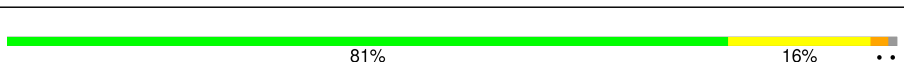
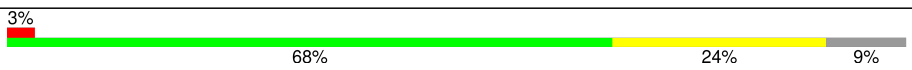
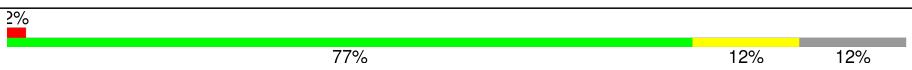
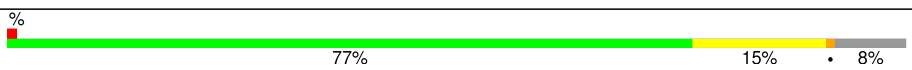
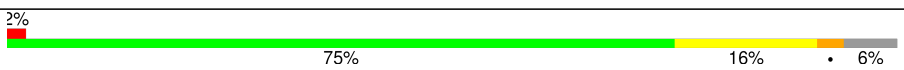
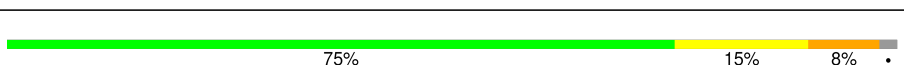
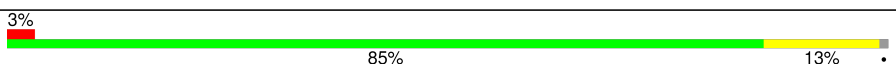
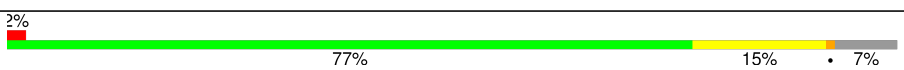
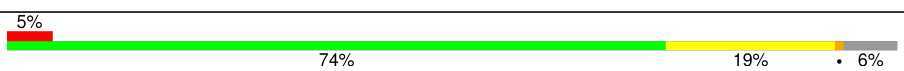
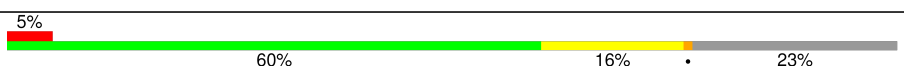
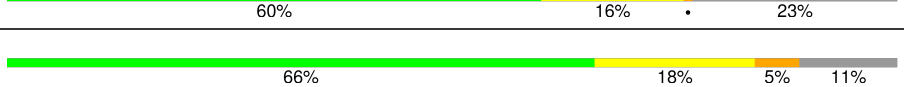
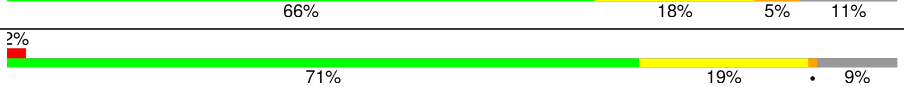
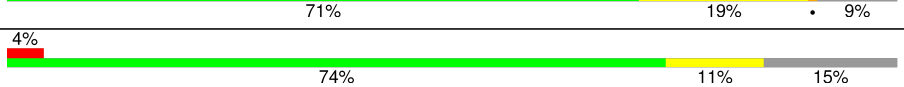
Mol	Chain	Length	Quality of chain
30	7	49	
31	8	65	
32	9	37	
33	x	76	
34	a	1521	
35	b	256	
36	c	239	
37	d	209	
38	e	162	
39	f	101	
40	g	156	
41	h	138	
42	i	128	
43	j	105	
44	k	129	
45	l	132	
46	m	126	
47	n	61	
48	o	89	
49	p	88	
50	q	105	
51	r	88	
52	s	93	
53	t	106	
54	u	27	

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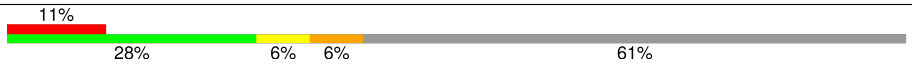
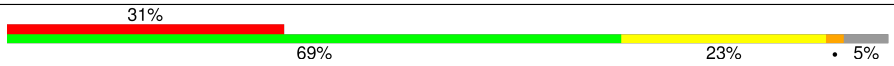
Mol	Chain	Length	Quality of chain
55	w	76	
56	v	18	
57	y	679	

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
58	MG	6	101	-	-	-	X
58	MG	7	101	-	-	-	X
58	MG	7	102	-	-	-	X
58	MG	A	3002	-	-	-	X
58	MG	A	3004	-	-	-	X
58	MG	A	3005	-	-	-	X
58	MG	A	3006	-	-	-	X
58	MG	A	3008	-	-	-	X
58	MG	A	3011	-	-	-	X
58	MG	A	3021	-	-	-	X
58	MG	A	3022	-	-	-	X
58	MG	A	3023	-	-	-	X
58	MG	A	3027	-	-	-	X
58	MG	A	3032	-	-	-	X
58	MG	A	3033	-	-	-	X
58	MG	A	3034	-	-	-	X
58	MG	A	3039	-	-	-	X
58	MG	A	3041	-	-	-	X
58	MG	A	3045	-	-	-	X
58	MG	A	3047	-	-	-	X
58	MG	A	3048	-	-	-	X
58	MG	A	3056	-	-	-	X
58	MG	A	3059	-	-	-	X
58	MG	A	3072	-	-	-	X
58	MG	A	3079	-	-	-	X
58	MG	A	3080	-	-	-	X
58	MG	A	3086	-	-	-	X
58	MG	A	3093	-	-	-	X
58	MG	A	3095	-	-	-	X
58	MG	A	3107	-	-	-	X
58	MG	A	3109	-	-	-	X
58	MG	A	3114	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	A	3117	-	-	-	X
58	MG	A	3118	-	-	-	X
58	MG	A	3119	-	-	-	X
58	MG	A	3120	-	-	-	X
58	MG	A	3125	-	-	-	X
58	MG	A	3141	-	-	-	X
58	MG	A	3143	-	-	-	X
58	MG	A	3144	-	-	-	X
58	MG	A	3147	-	-	-	X
58	MG	A	3155	-	-	-	X
58	MG	A	3157	-	-	-	X
58	MG	A	3164	-	-	-	X
58	MG	A	3165	-	-	-	X
58	MG	A	3166	-	-	-	X
58	MG	A	3167	-	-	-	X
58	MG	A	3170	-	-	-	X
58	MG	A	3171	-	-	-	X
58	MG	A	3174	-	-	-	X
58	MG	A	3184	-	-	-	X
58	MG	A	3187	-	-	-	X
58	MG	A	3188	-	-	-	X
58	MG	A	3189	-	-	-	X
58	MG	A	3190	-	-	-	X
58	MG	A	3191	-	-	-	X
58	MG	A	3192	-	-	-	X
58	MG	A	3200	-	-	-	X
58	MG	A	3201	-	-	-	X
58	MG	A	3207	-	-	-	X
58	MG	A	3208	-	-	-	X
58	MG	A	3209	-	-	-	X
58	MG	A	3214	-	-	-	X
58	MG	A	3222	-	-	-	X
58	MG	A	3223	-	-	-	X
58	MG	A	3225	-	-	-	X
58	MG	A	3230	-	-	-	X
58	MG	A	3231	-	-	-	X
58	MG	A	3234	-	-	-	X
58	MG	A	3239	-	-	-	X
58	MG	A	3244	-	-	-	X
58	MG	A	3252	-	-	-	X
58	MG	A	3274	-	-	-	X
58	MG	A	3293	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	A	3295	-	-	-	X
58	MG	A	3297	-	-	-	X
58	MG	A	3311	-	-	-	X
58	MG	A	3313	-	-	-	X
58	MG	A	3316	-	-	-	X
58	MG	A	3319	-	-	-	X
58	MG	A	3324	-	-	-	X
58	MG	A	3341	-	-	-	X
58	MG	A	3352	-	-	-	X
58	MG	A	3363	-	-	-	X
58	MG	A	3380	-	-	-	X
58	MG	A	3382	-	-	-	X
58	MG	A	3396	-	-	-	X
58	MG	A	3399	-	-	-	X
58	MG	A	3410	-	-	-	X
58	MG	A	3414	-	-	-	X
58	MG	A	3417	-	-	-	X
58	MG	A	3420	-	-	-	X
58	MG	A	3423	-	-	-	X
58	MG	A	3437	-	-	-	X
58	MG	A	3446	-	-	-	X
58	MG	A	3455	-	-	-	X
58	MG	A	3476	-	-	-	X
58	MG	A	3486	-	-	-	X
58	MG	A	3487	-	-	-	X
58	MG	A	3490	-	-	-	X
58	MG	A	3493	-	-	-	X
58	MG	A	3498	-	-	-	X
58	MG	A	3500	-	-	-	X
58	MG	A	3501	-	-	-	X
58	MG	A	3513	-	-	-	X
58	MG	A	3516	-	-	-	X
58	MG	A	3520	-	-	-	X
58	MG	A	3523	-	-	-	X
58	MG	A	3529	-	-	-	X
58	MG	A	3530	-	-	-	X
58	MG	A	3540	-	-	-	X
58	MG	A	3541	-	-	-	X
58	MG	A	3557	-	-	-	X
58	MG	A	3564	-	-	-	X
58	MG	A	3568	-	-	-	X
58	MG	A	3601	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	A	3616	-	-	-	X
58	MG	B	210	-	-	-	X
58	MG	D	301	-	-	-	X
58	MG	D	303	-	-	-	X
58	MG	E	301	-	-	-	X
58	MG	F	302	-	-	-	X
58	MG	F	304	-	-	-	X
58	MG	N	201	-	-	-	X
58	MG	P	201	-	-	-	X
58	MG	Q	201	-	-	-	X
58	MG	Q	202	-	-	-	X
58	MG	Q	204	-	-	-	X
58	MG	R	201	-	-	-	X
58	MG	U	201	-	-	-	X
58	MG	V	202	-	-	-	X
58	MG	a	3306	-	-	-	X
58	MG	a	3309	-	-	-	X
58	MG	a	3313	-	-	-	X
58	MG	a	3318	-	-	-	X
58	MG	a	3323	-	-	-	X
58	MG	a	3330	-	-	-	X
58	MG	a	3331	-	-	-	X
58	MG	a	3351	-	-	-	X
58	MG	a	3355	-	-	-	X
58	MG	a	3368	-	-	-	X
58	MG	a	3376	-	-	-	X
58	MG	a	3378	-	-	-	X
58	MG	a	3382	-	-	-	X
58	MG	a	3395	-	-	-	X
58	MG	a	3397	-	-	-	X
58	MG	a	3401	-	-	-	X
58	MG	a	3406	-	-	-	X
58	MG	a	3422	-	-	-	X
58	MG	a	3435	-	-	-	X
58	MG	a	3439	-	-	-	X
58	MG	a	3447	-	-	-	X
58	MG	a	3466	-	-	-	X
58	MG	a	3471	-	-	-	X
58	MG	a	3487	-	-	-	X
58	MG	l	202	-	-	-	X
58	MG	n	101	-	-	-	X
58	MG	x	3002	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 152111 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	2873	61879	27541	11577	19890	2871	0	0	0

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	120	2573	1146	476	832	119	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	275	2136	1349	423	361	3	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	204	1559	985	298	270	6	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	203	1584	1009	298	275	2	0	0	1

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	G	181	1425	914	256	251	4	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	130	Total	C	N	O	0	0	0
			641	381	130	130			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	139	Total	C	N	O	S	0	0	0
			1025	653	181	186	5			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	S	110	Total	C	N	O	0	0	0
			877	553	175	149			

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Z	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	0	74	Total	C	N	O	S	0	0	0
			591	366	126	98	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	4	69	Total	C	N	O	S	0	0	0
			557	350	101	101	5			

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 33 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
33	x	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	a	1496	Total	C	N	O	P	0	0	0
			32163	14314	5963	10390	1496			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	b	231	Total	C	N	O	S	0	0	0
			1850	1181	331	333	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	c	206	Total	C	N	O	S	0	0	0
			1550	974	302	273	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	f	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	g	155	Total	C	N	O	S	0	0	0
			1227	764	242	215	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	i	127	Total 983	C 623	N 193	O 167	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	j	96	Total 698	C 434	N 134	O 130	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	k	114	Total 829	C 516	N 155	O 155	S 3	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	l	122	Total 930	C 585	N 185	O 159	S 1	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	m	119	Total 924	C 570	N 192	O 160	S 2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	n	60	Total 492	C 312	N 104	O 72	S 4	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	o	88	Total 728	C 456	N 144	O 126	S 2	0	0	0

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	s	83	Total	C	N	O	S	0	0	0
			650	415	120	113	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	t	96	Total	C	N	O	S	0	0	0
			724	443	155	124	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	w	76	Total	C	N	O	P	S	0	0	0
			1643	740	291	534	76	2			

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	v	7	Total	C	N	O	P	0	0	0
			148	67	27	47	7			

- Molecule 57 is a protein called 50S ribosomal protein L9, Elongation factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	y	644	Total	C	N	O	S	0	0	0
			4000	2438	760	799	3			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	P	2	Total	Mg	0	0
			2	2		
58	B	18	Total	Mg	0	0
			18	18		
58	6	1	Total	Mg	0	0
			1	1		
58	W	1	Total	Mg	0	0
			1	1		
58	N	1	Total	Mg	0	0
			1	1		
58	X	1	Total	Mg	0	0
			1	1		
58	y	2	Total	Mg	0	0
			2	2		
58	f	1	Total	Mg	0	0
			1	1		
58	E	4	Total	Mg	0	0
			4	4		
58	V	2	Total	Mg	0	0
			2	2		
58	w	6	Total	Mg	0	0
			6	6		
58	A	635	Total	Mg	0	0
			635	635		
58	n	1	Total	Mg	0	0
			1	1		
58	5	1	Total	Mg	0	0
			1	1		
58	x	3	Total	Mg	0	0
			3	3		
58	R	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	D	5	Total Mg 5 5	0	0
58	e	1	Total Mg 1 1	0	0
58	v	1	Total Mg 1 1	0	0
58	Z	1	Total Mg 1 1	0	0
58	a	187	Total Mg 187 187	0	0
58	U	4	Total Mg 4 4	0	0
58	9	1	Total Mg 1 1	0	0
58	m	1	Total Mg 1 1	0	0
58	0	3	Total Mg 3 3	0	0
58	G	3	Total Mg 3 3	0	0
58	Q	5	Total Mg 5 5	0	0
58	7	3	Total Mg 3 3	0	0
58	8	1	Total Mg 1 1	0	0
58	O	1	Total Mg 1 1	0	0
58	l	2	Total Mg 2 2	0	0
58	F	5	Total Mg 5 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	Y	1	Total Zn 1 1	0	0
59	6	1	Total Zn 1 1	0	0
59	4	1	Total Zn 1 1	0	0

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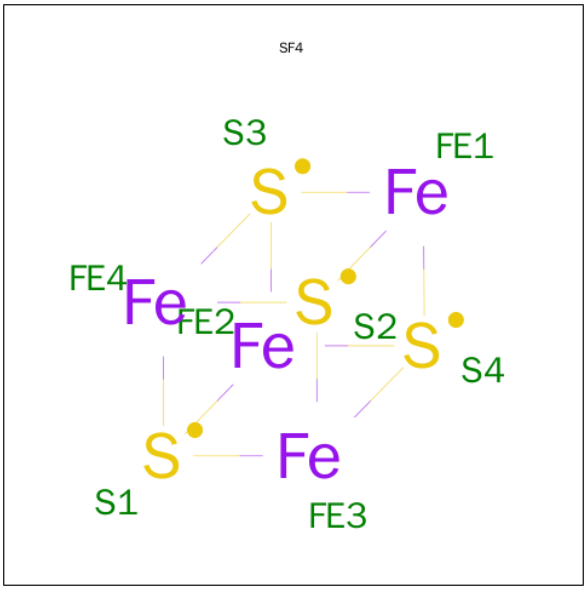
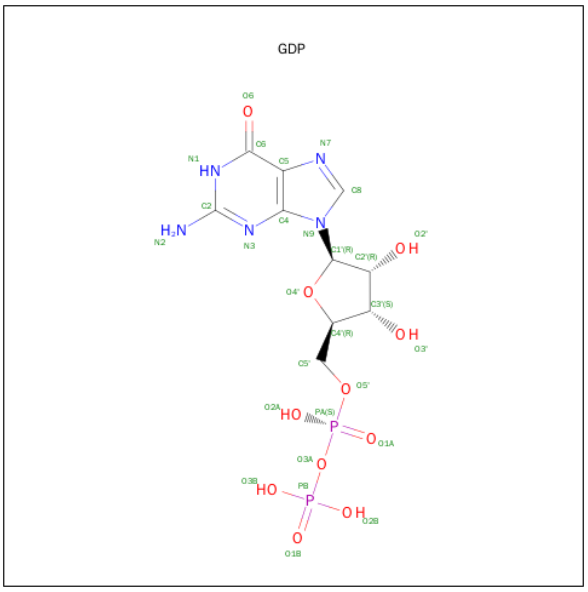
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	n	1	Total Zn 1 1	0	0
59	5	1	Total Zn 1 1	0	0
59	9	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	d	1	Total Fe S 8 4 4	0	0

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	y	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	A	710	Total	O	0	2
			710	710		
62	B	34	Total	O	0	0
			34	34		
62	D	4	Total	O	0	0
			4	4		
62	E	7	Total	O	0	0
			7	7		
62	F	5	Total	O	0	0
			5	5		
62	G	1	Total	O	0	0
			1	1		
62	H	1	Total	O	0	0
			1	1		
62	N	1	Total	O	0	0
			1	1		
62	O	3	Total	O	0	0
			3	3		
62	P	3	Total	O	0	0
			3	3		
62	Q	4	Total	O	0	0
			4	4		

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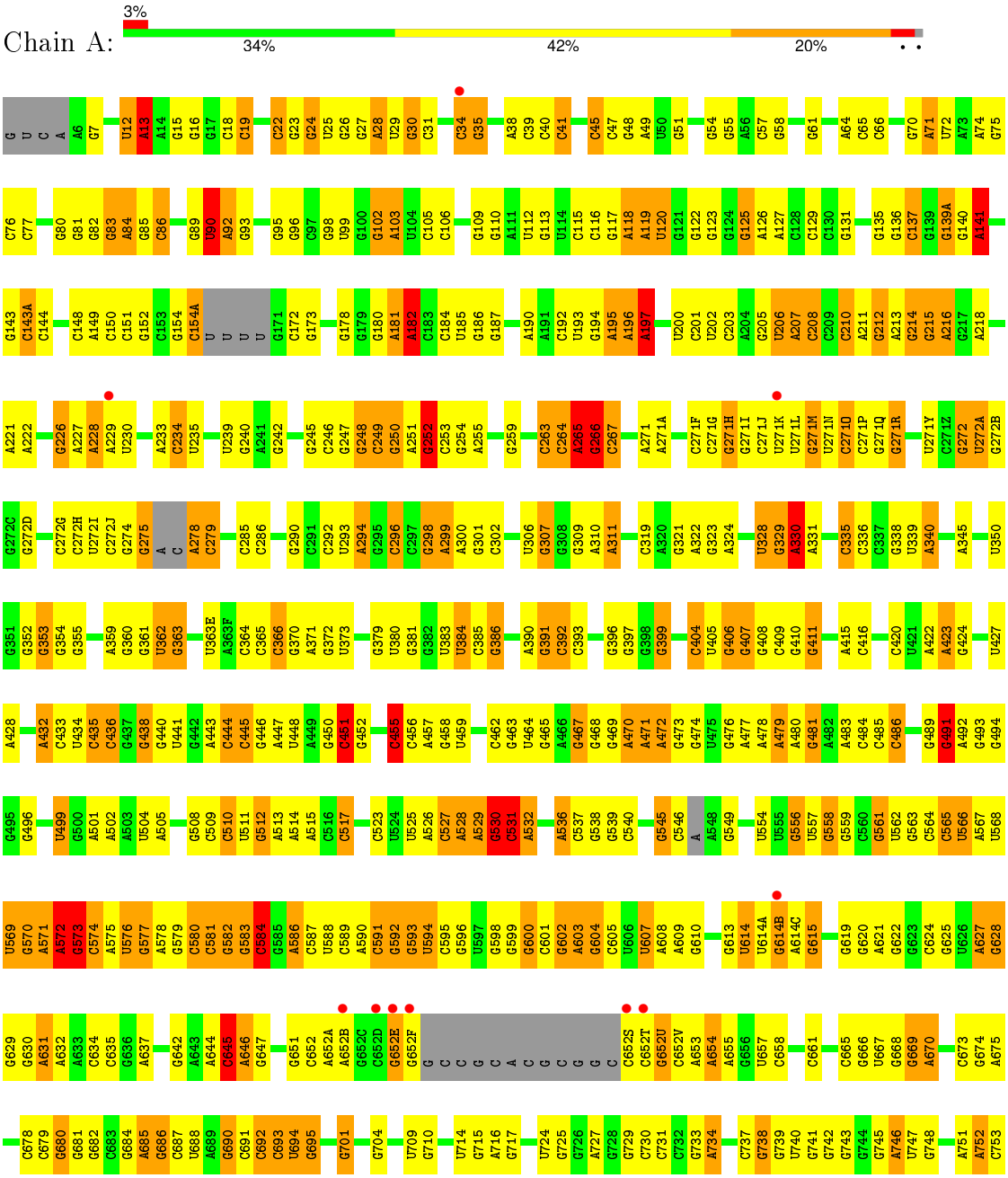
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	R	3	Total O 3 3	0	0
62	U	2	Total O 2 2	0	0
62	V	1	Total O 1 1	0	0
62	W	2	Total O 2 2	0	0
62	Y	1	Total O 1 1	0	0
62	0	4	Total O 4 4	0	0
62	1	2	Total O 2 2	0	0
62	3	1	Total O 1 1	0	0
62	5	1	Total O 1 1	0	0
62	7	2	Total O 2 2	0	0
62	8	4	Total O 4 4	0	0
62	9	1	Total O 1 1	0	0
62	x	1	Total O 1 1	0	0
62	a	167	Total O 167 167	0	0
62	l	1	Total O 1 1	0	0
62	v	3	Total O 3 3	0	0

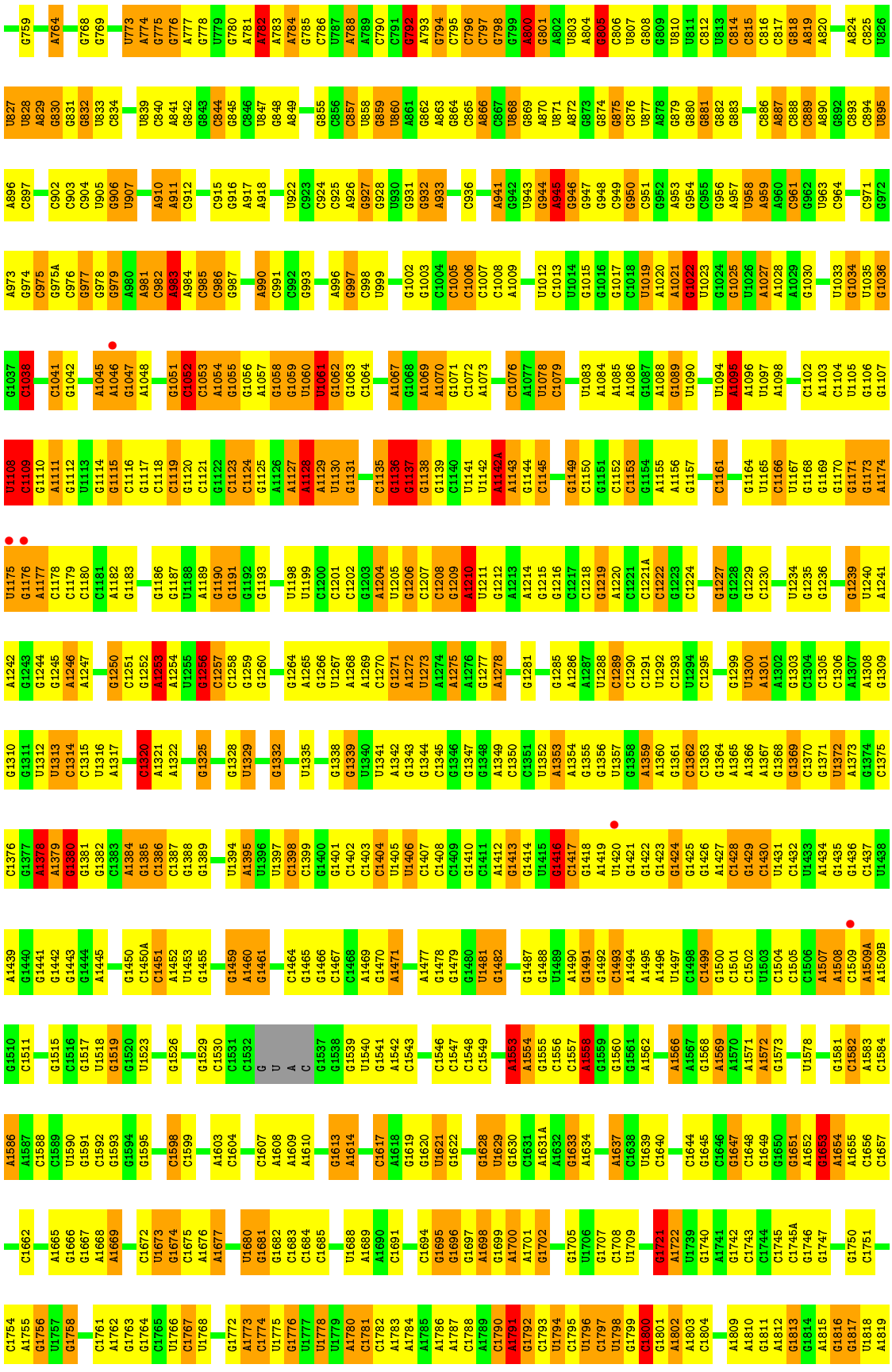
3 Residue-property plots (i)

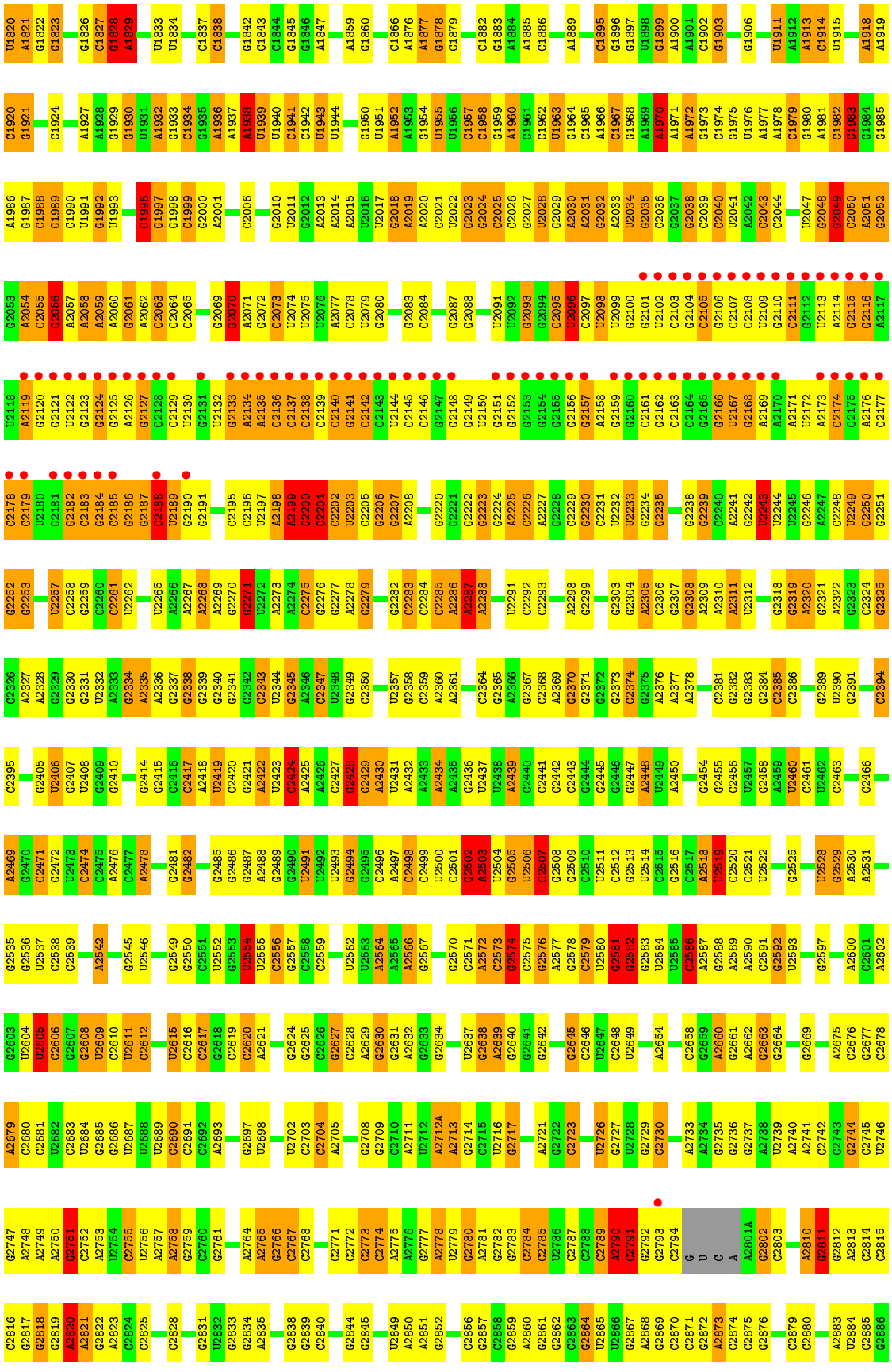
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

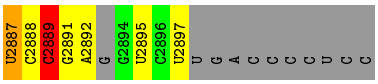
- Molecule 1: 23S Ribosomal RNA

Chain A:



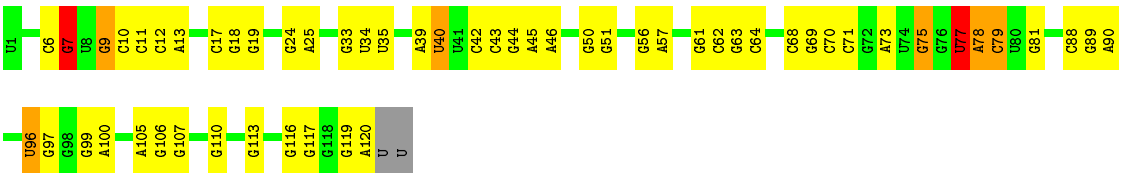






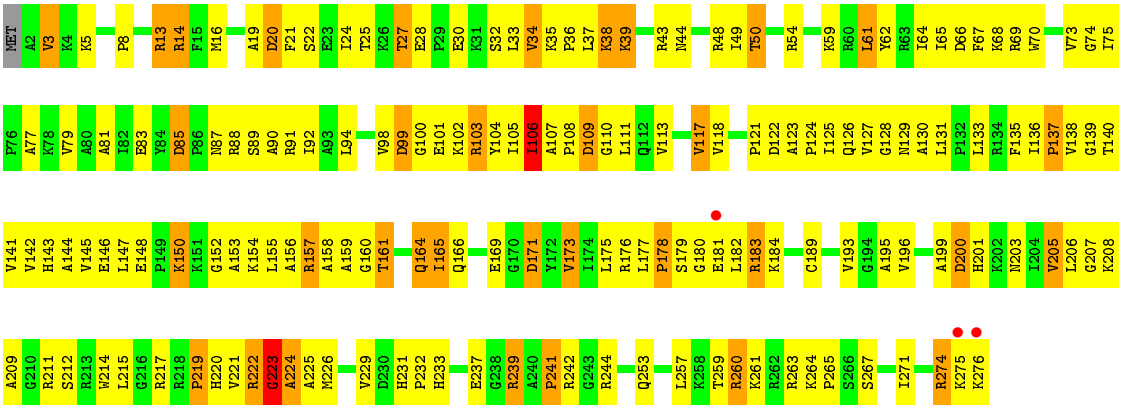
- Molecule 2: 5S Ribosomal RNA

Chain B:



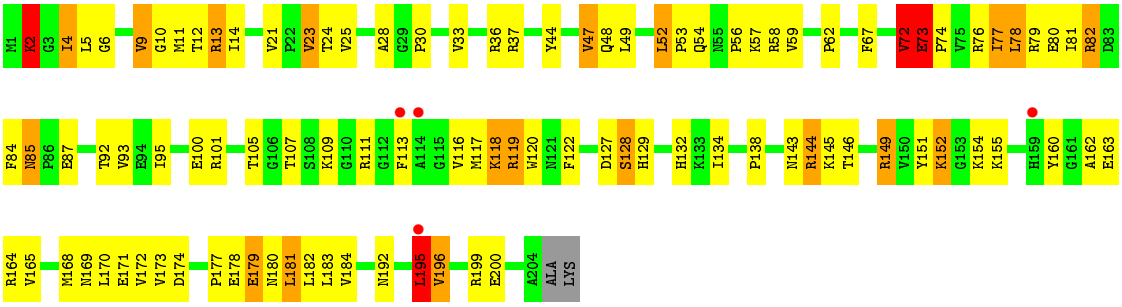
- Molecule 3: 50S ribosomal protein L2

Chain D:



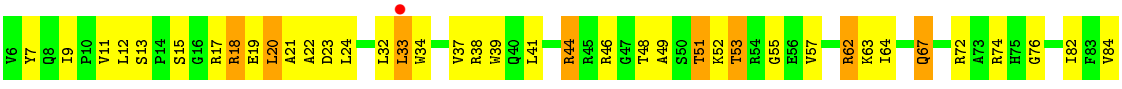
- Molecule 4: 50S ribosomal protein L3

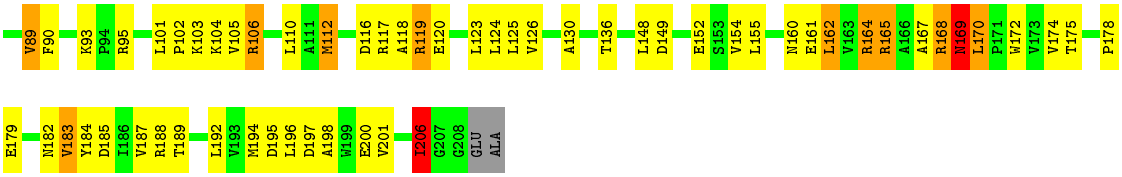
Chain E:



- Molecule 5: 50S ribosomal protein L4

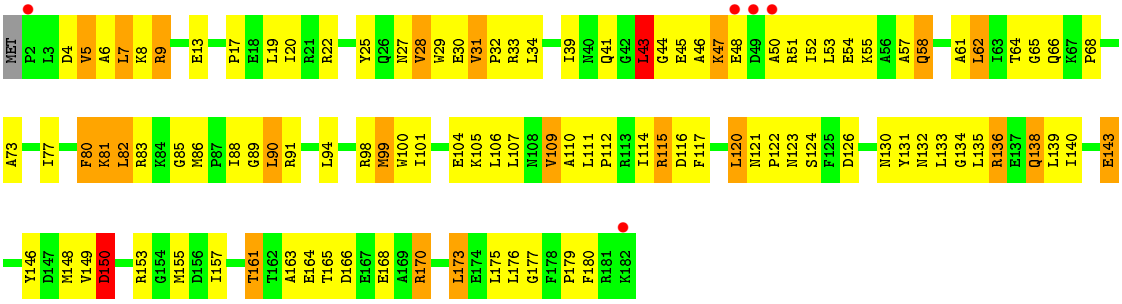
Chain F:





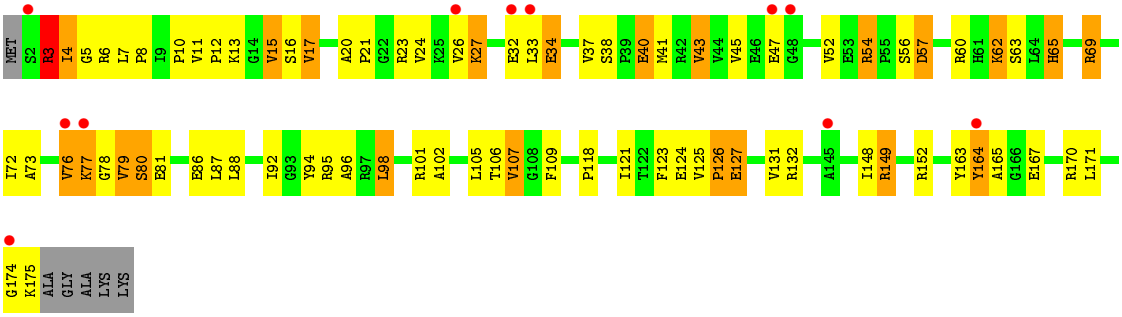
• Molecule 6: 50S ribosomal protein L5

Chain G:



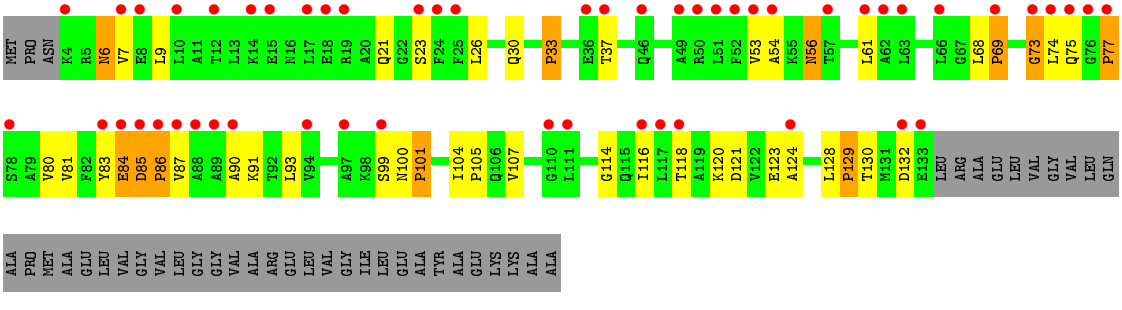
• Molecule 7: 50S ribosomal protein L6

Chain H:



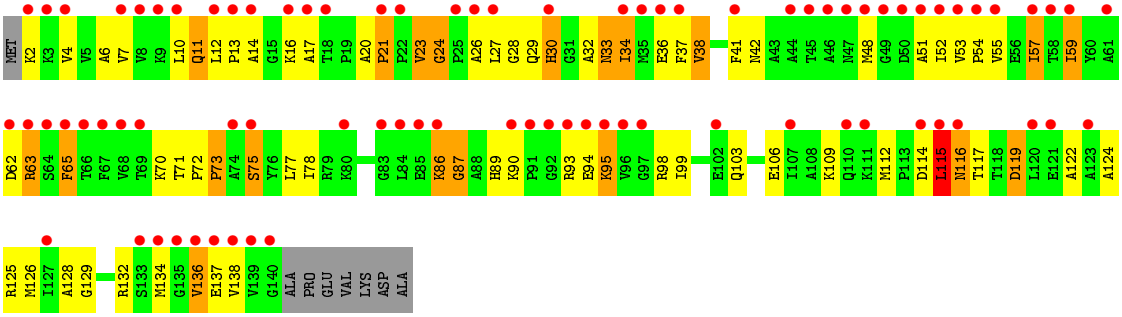
• Molecule 8: 50S ribosomal protein L10

Chain J:



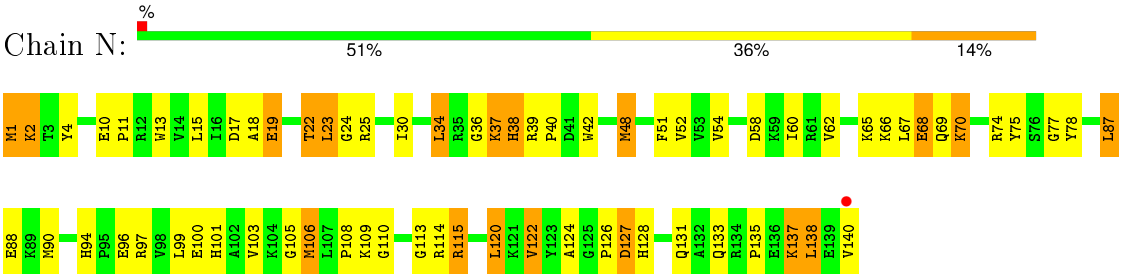
• Molecule 9: 50S ribosomal protein L11

Chain K:



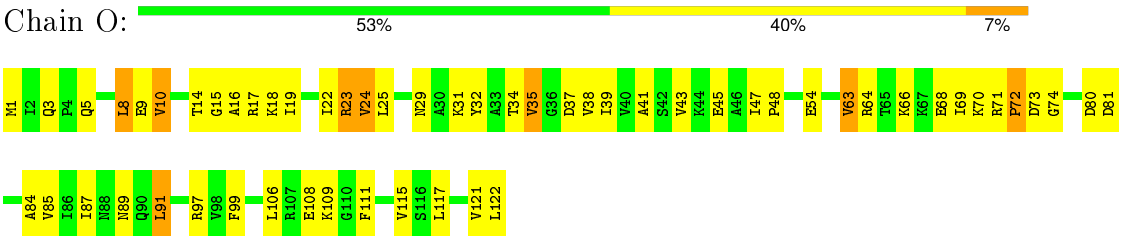
- Molecule 10: 50S ribosomal protein L13

Chain N:



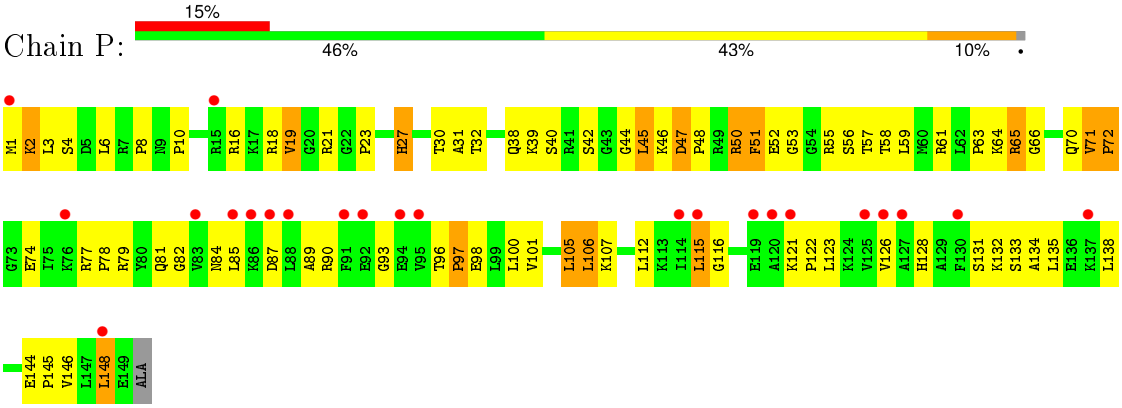
- Molecule 11: 50S ribosomal protein L14

Chain O:



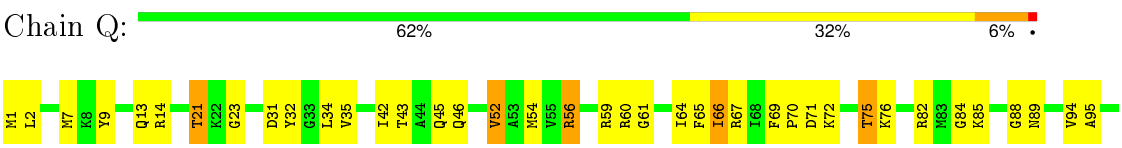
- Molecule 12: 50S ribosomal protein L15

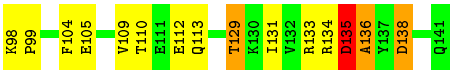
Chain P:



- Molecule 13: 50S ribosomal protein L16

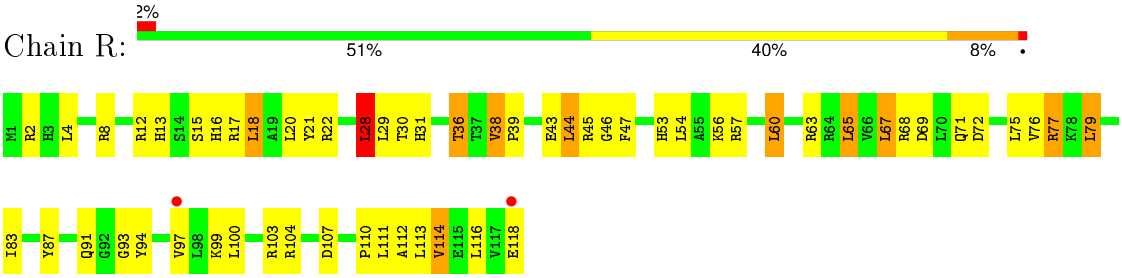
Chain Q:





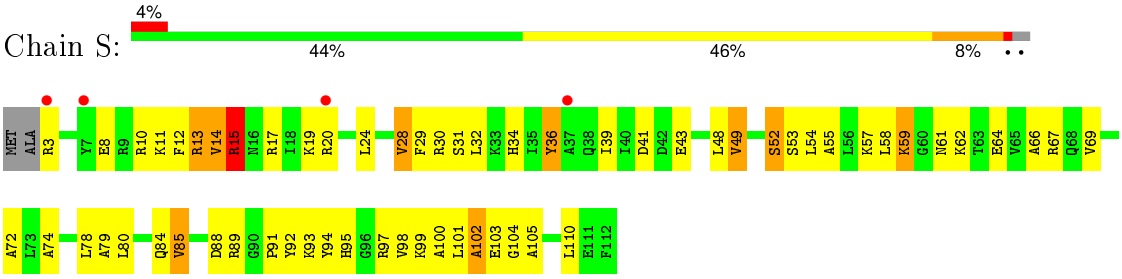
• Molecule 14: 50S ribosomal protein L17

Chain R:



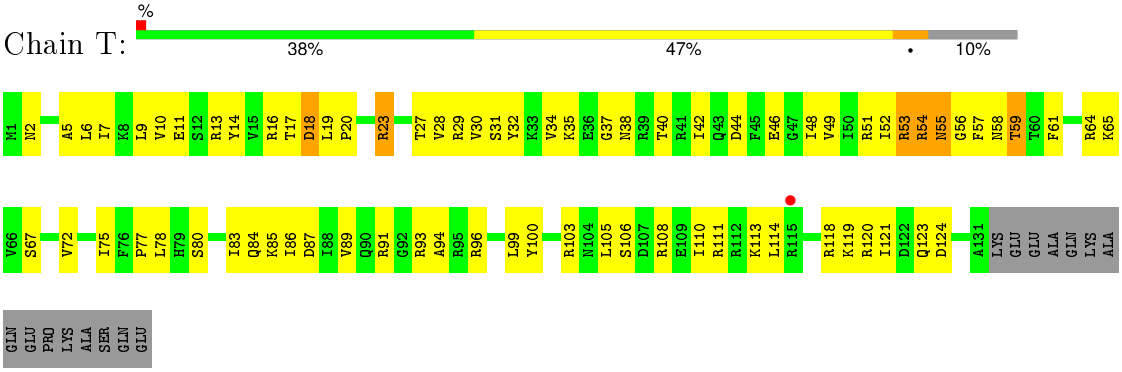
• Molecule 15: 50S ribosomal protein L18

Chain S:



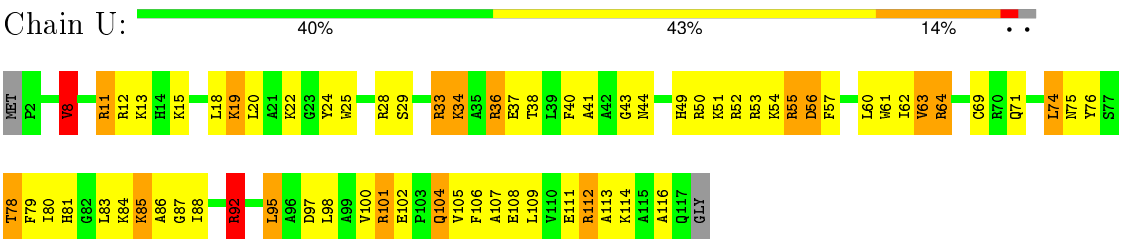
• Molecule 16: 50S ribosomal protein L19

Chain T:



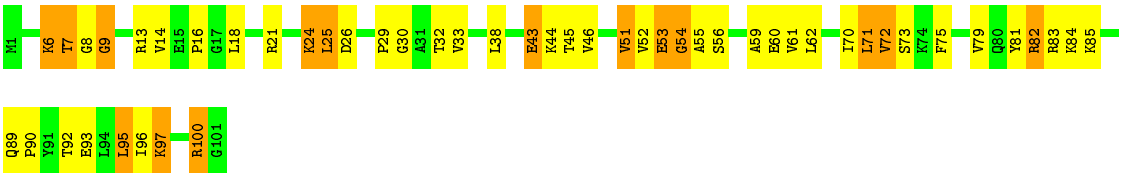
• Molecule 17: 50S ribosomal protein L20

Chain U:



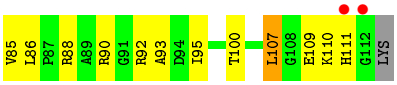
• Molecule 18: 50S ribosomal protein L21

Chain V:



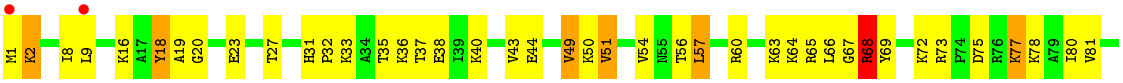
• Molecule 19: 50S ribosomal protein L22

Chain W:



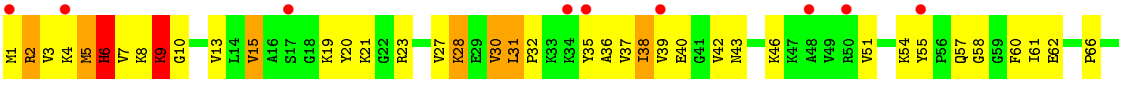
• Molecule 20: 50S ribosomal protein L23

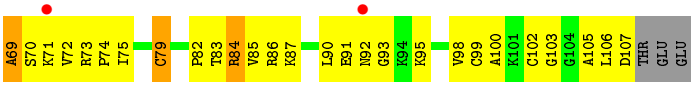
Chain X:



• Molecule 21: 50S ribosomal protein L24

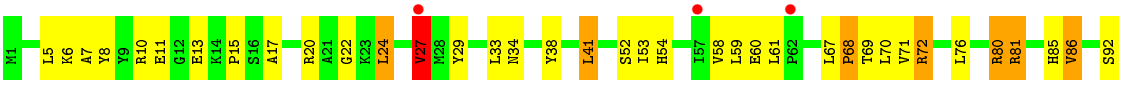
Chain Y:

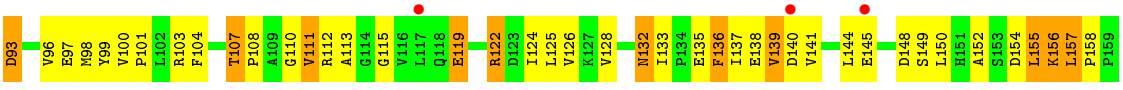


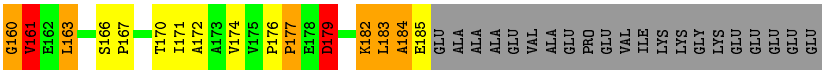


• Molecule 22: 50S ribosomal protein L25

Chain Z:

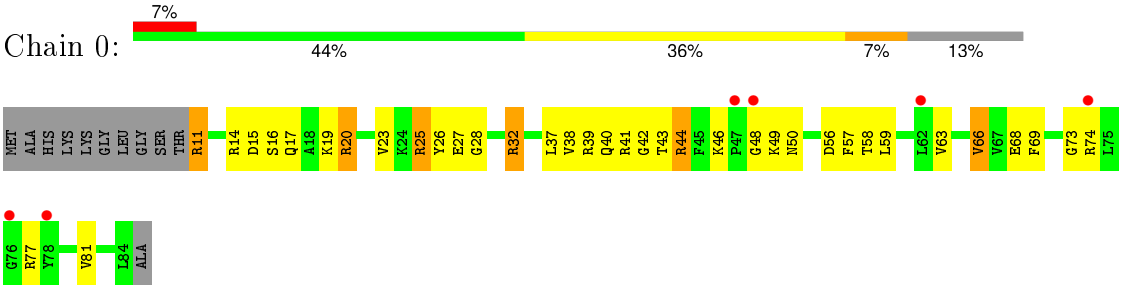






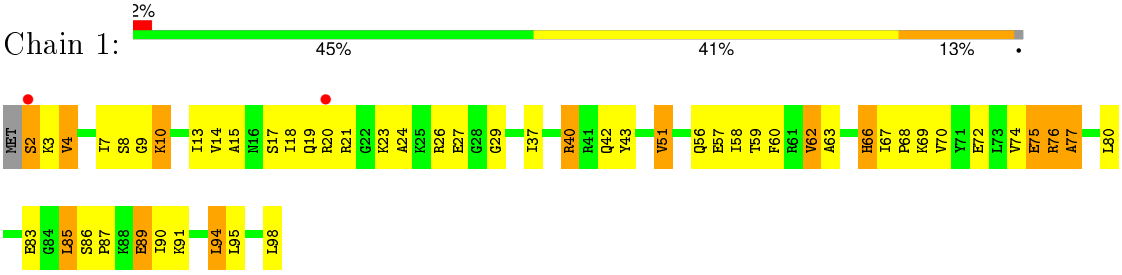
- Molecule 23: 50S ribosomal protein L27

Chain 0:



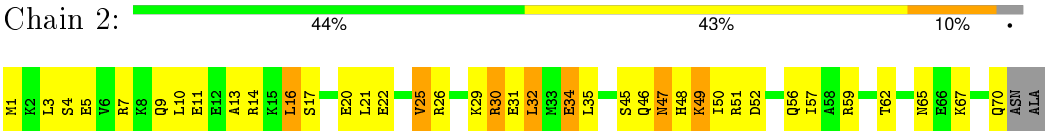
- Molecule 24: 50S ribosomal protein L28

Chain 1:



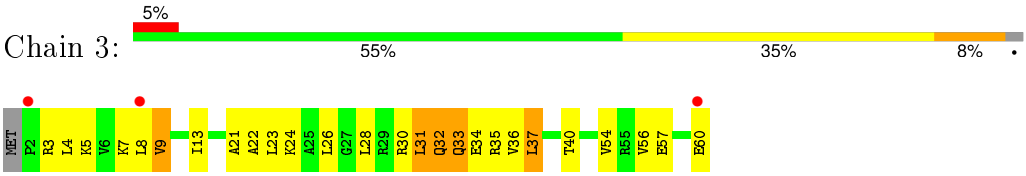
- Molecule 25: 50S ribosomal protein L29

Chain 2:



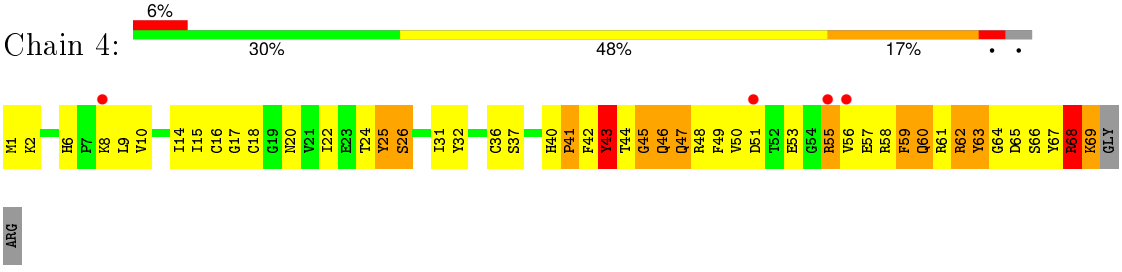
- Molecule 26: 50S ribosomal protein L30

Chain 3:



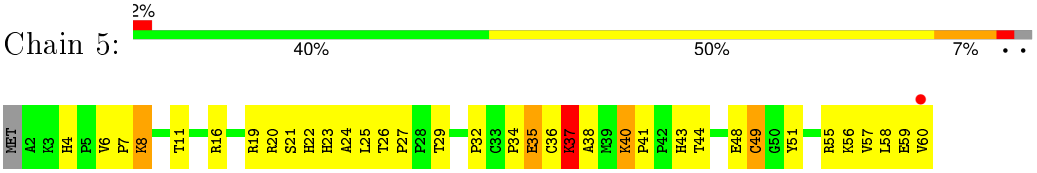
- Molecule 27: 50S ribosomal protein L31

Chain 4:



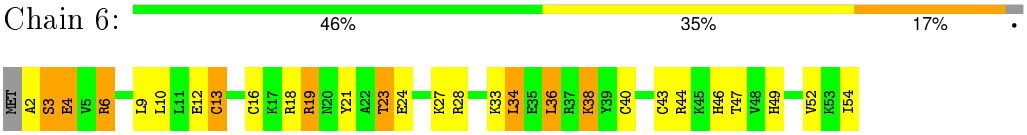
- Molecule 28: 50S ribosomal protein L32

Chain 5:



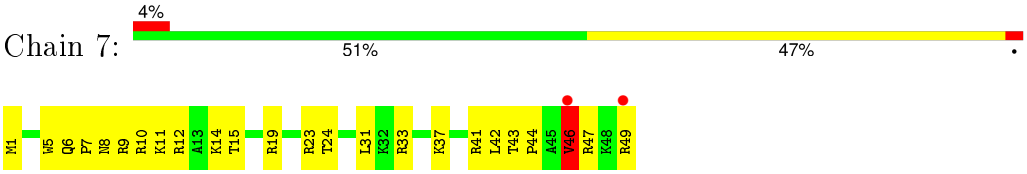
- Molecule 29: 50S ribosomal protein L33

Chain 6:



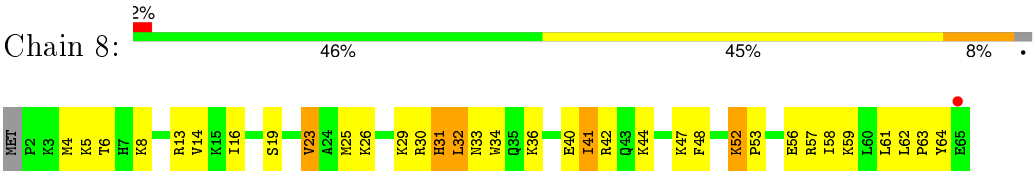
- Molecule 30: 50S ribosomal protein L34

Chain 7:



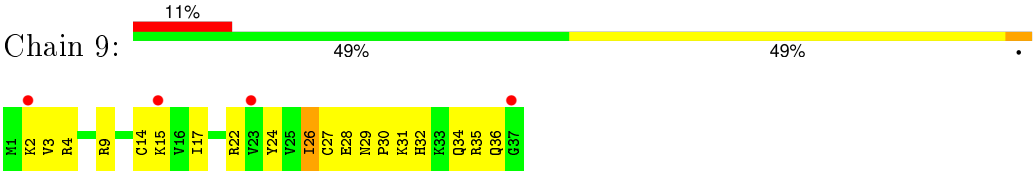
- Molecule 31: 50S ribosomal protein L35

Chain 8:



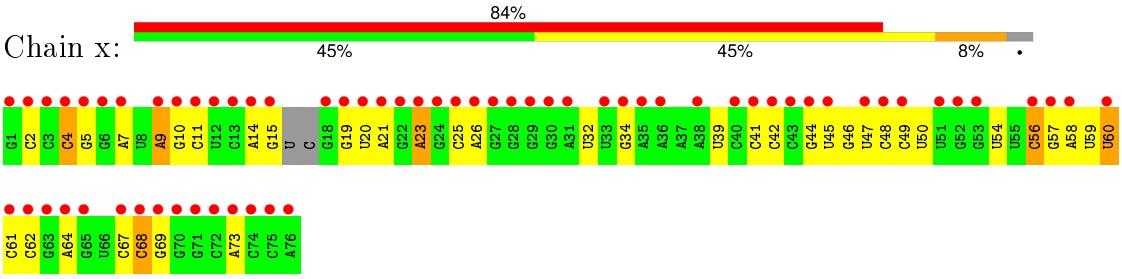
- Molecule 32: 50S ribosomal protein L36

Chain 9:



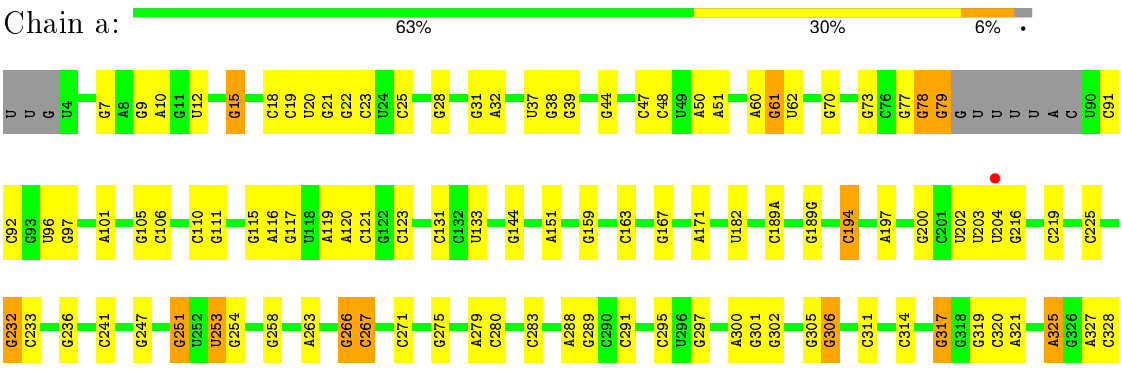
- Molecule 33: E-site tRNA

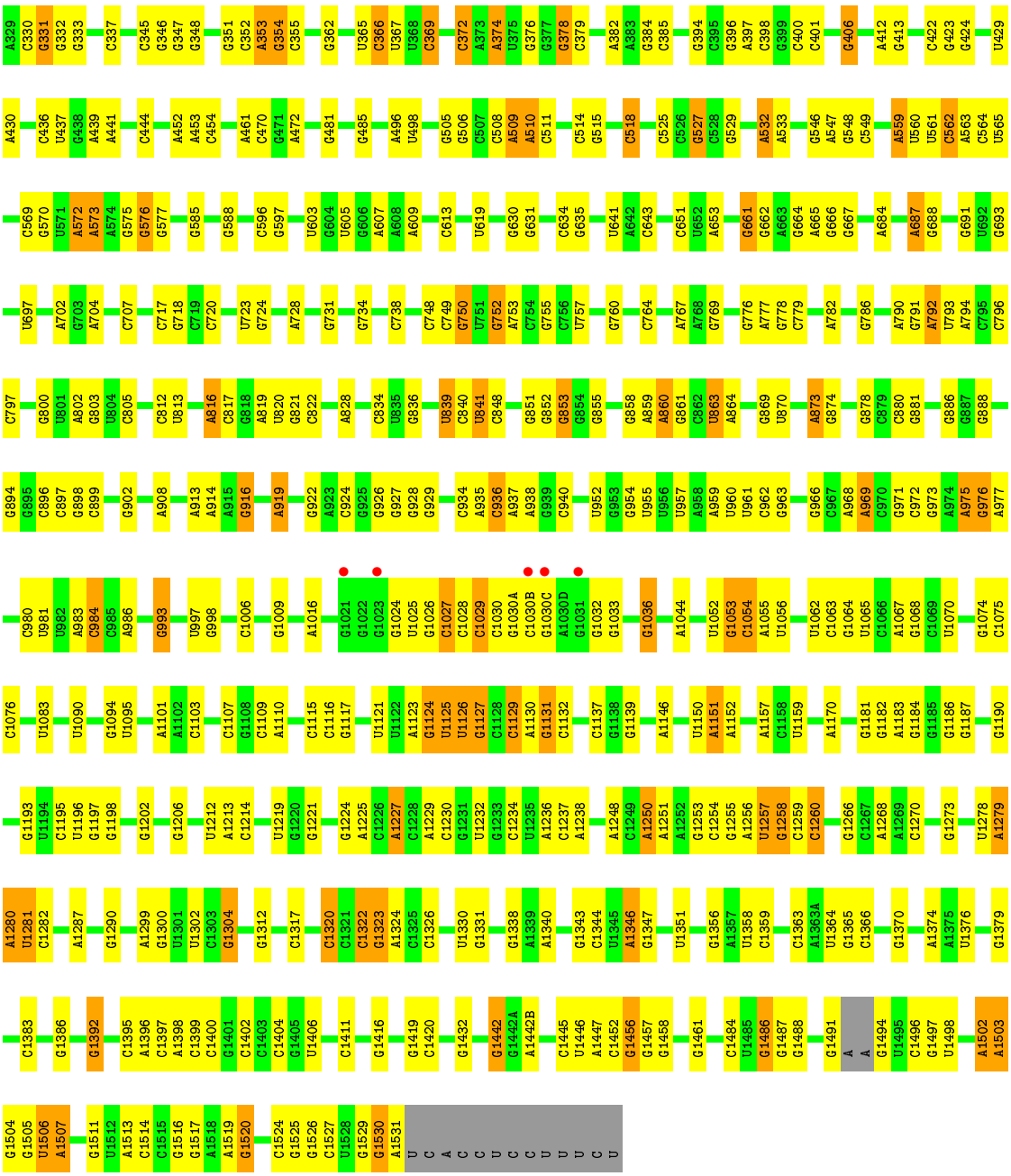
Chain x:



- Molecule 34: 16S Ribosomal RNA

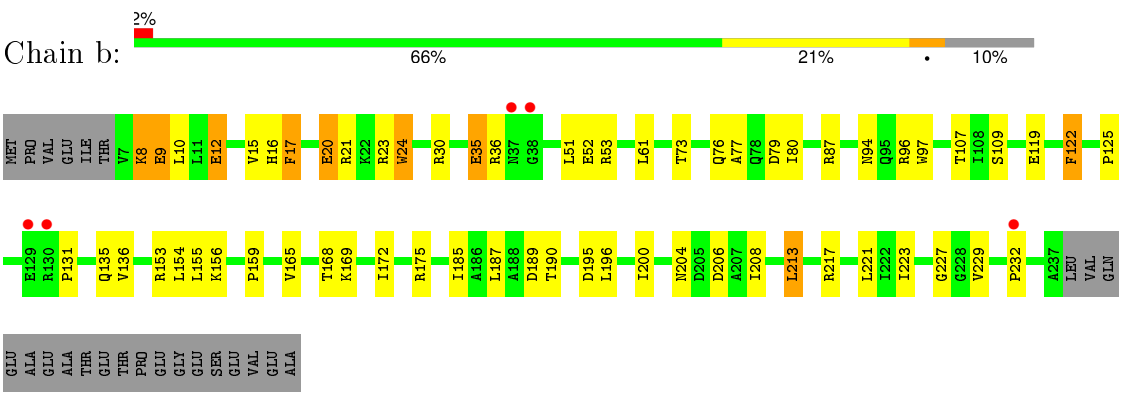
Chain a:





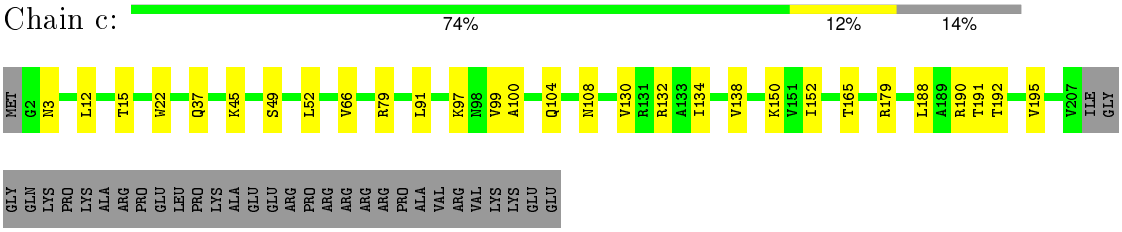
• Molecule 35: 30S ribosomal protein S2

Chain b:



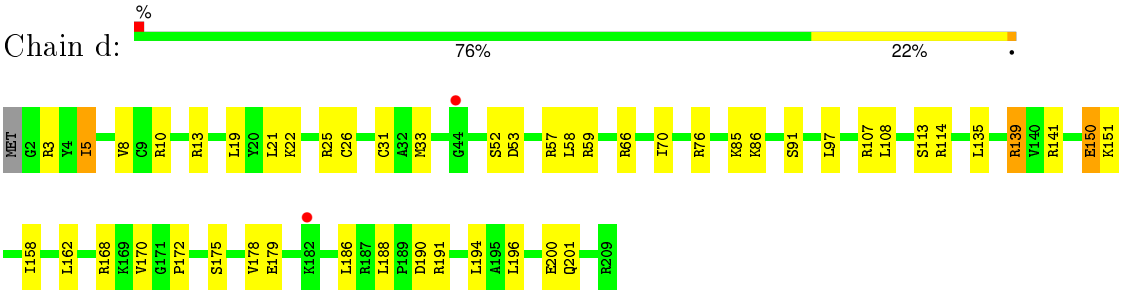
- Molecule 36: 30S ribosomal protein S3

Chain c:



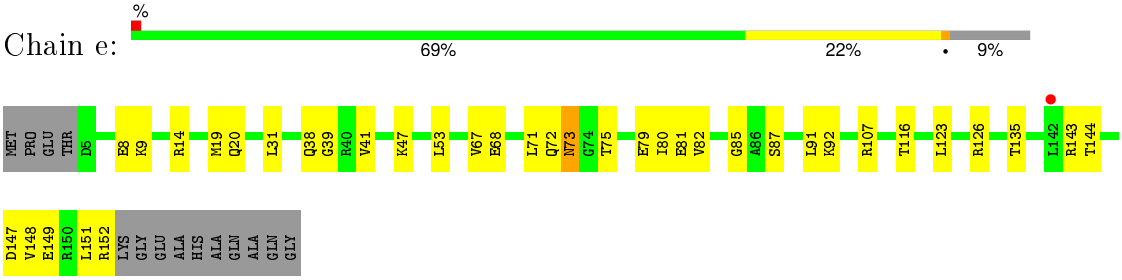
- Molecule 37: 30S ribosomal protein S4

Chain d:



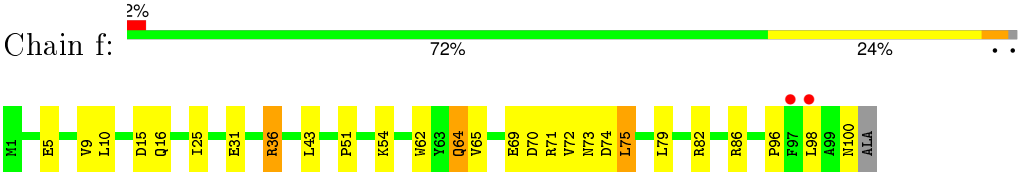
- Molecule 38: 30S ribosomal protein S5

Chain e:



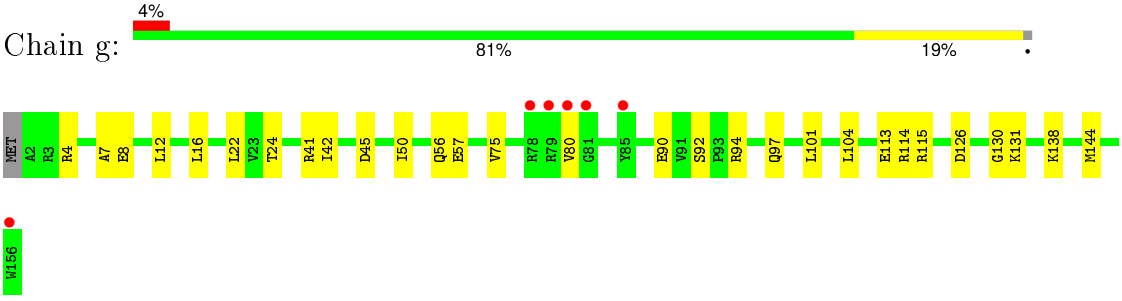
- Molecule 39: 30S ribosomal protein S6

Chain f:



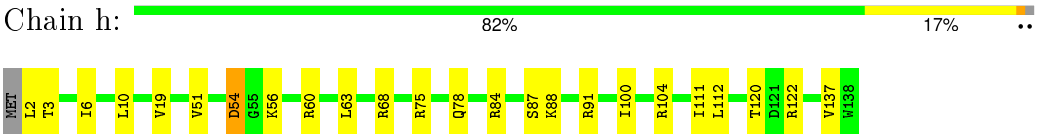
- Molecule 40: 30S ribosomal protein S7

Chain g:



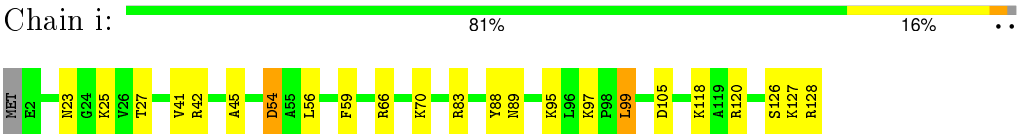
- Molecule 41: 30S ribosomal protein S8

Chain h:



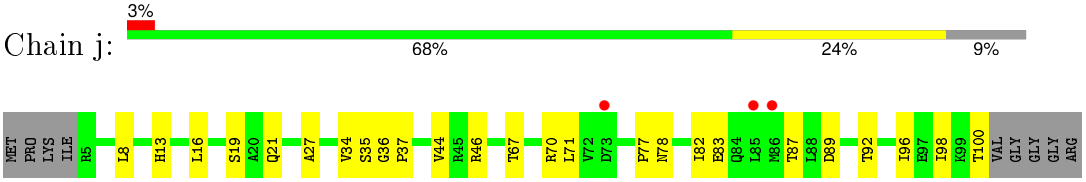
• Molecule 42: 30S ribosomal protein S9

Chain i:



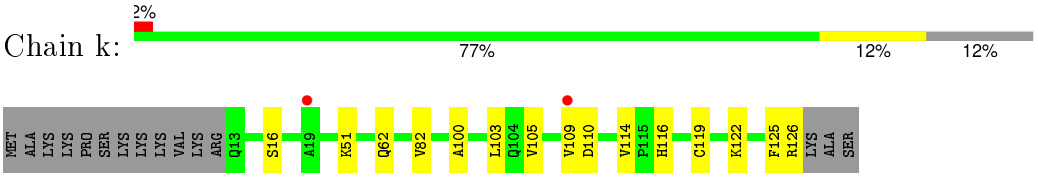
• Molecule 43: 30S ribosomal protein S10

Chain j:



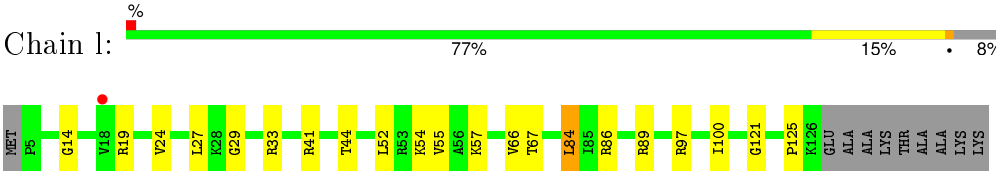
• Molecule 44: 30S ribosomal protein S11

Chain k:



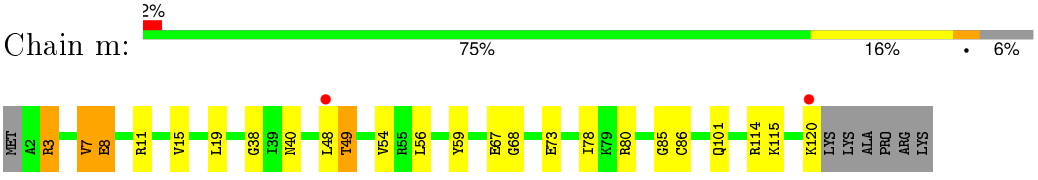
• Molecule 45: 30S ribosomal protein S12

Chain l:



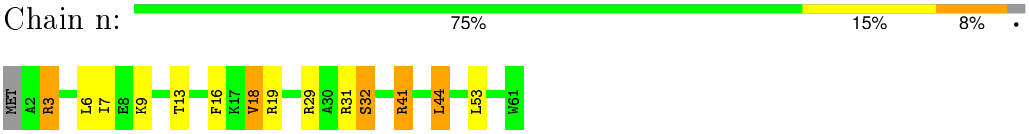
• Molecule 46: 30S ribosomal protein S13

Chain m:



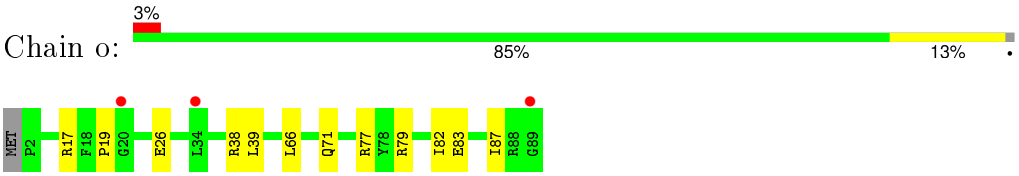
• Molecule 47: 30S ribosomal protein S14 type Z

Chain n:



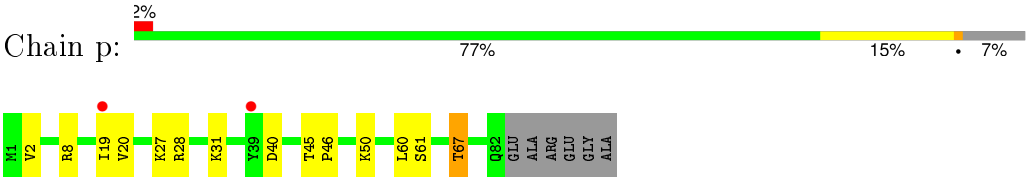
• Molecule 48: 30S ribosomal protein S15

Chain o:



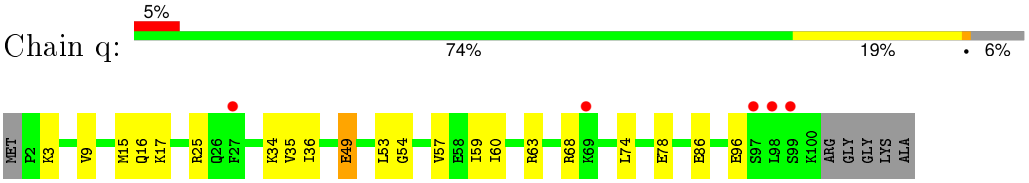
• Molecule 49: 30S ribosomal protein S16

Chain p:



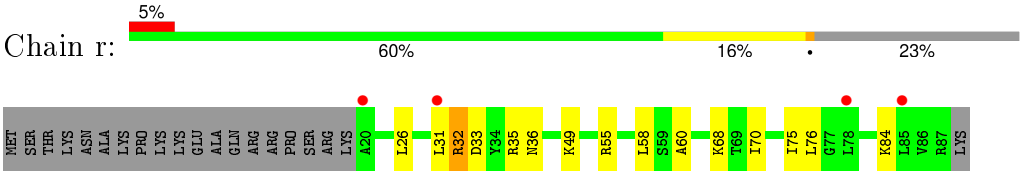
• Molecule 50: 30S ribosomal protein S17

Chain q:



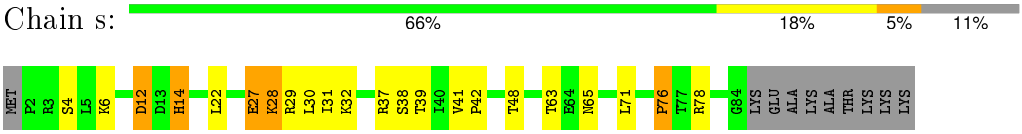
• Molecule 51: 30S ribosomal protein S18

Chain r:



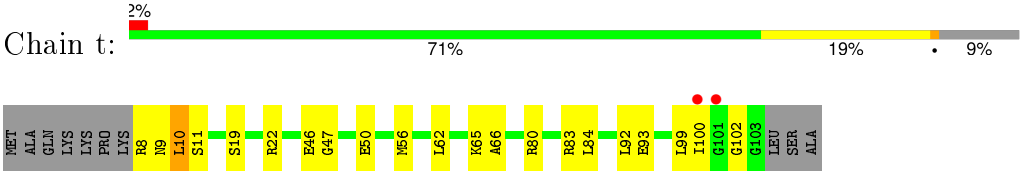
• Molecule 52: 30S ribosomal protein S19

Chain s:



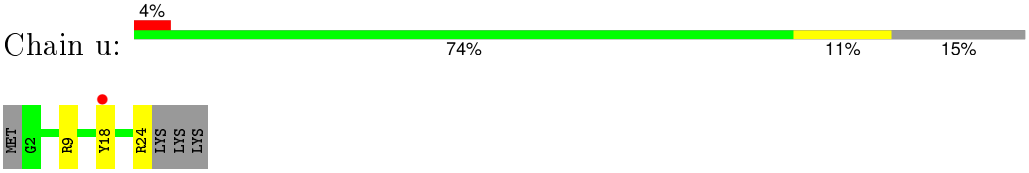
• Molecule 53: 30S ribosomal protein S20

Chain t:



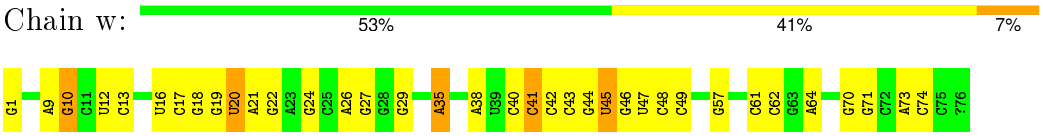
• Molecule 54: 30S ribosomal protein Thx

Chain u:



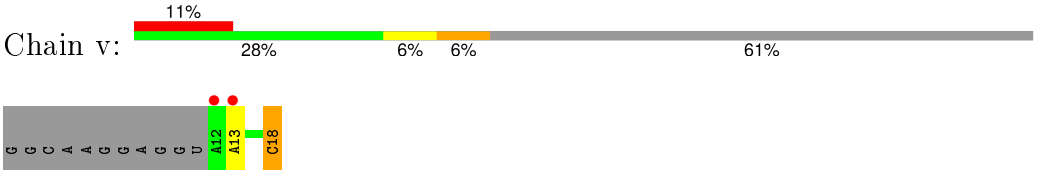
• Molecule 55: P-site tRNA

Chain w:



• Molecule 56: mRNA

Chain v:



• Molecule 57: 50S ribosomal protein L9, Elongation factor 4

Chain y:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	239.29Å 272.85Å 431.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 2.90 49.76 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.8 (49.76-2.90) 93.1 (49.76-2.89)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.238 , 0.304 0.241 , 0.303	Depositor DCC
R_{free} test set	29228 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	62.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 67.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 581414 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	152111	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 5MU, GDP, ZN, MIA, SF4, MG, F3O, 4SU, 7MG, PSU

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	A	0.86	29/69298 (0.0%)	1.53	1145/108168 (1.1%)
2	B	0.61	0/2878	1.24	15/4490 (0.3%)
3	D	0.66	1/2186 (0.0%)	0.84	0/2944
4	E	0.64	0/1592	0.87	2/2149 (0.1%)
5	F	0.60	0/1619	0.80	2/2193 (0.1%)
6	G	0.45	0/1450	0.73	0/1959
7	H	0.47	0/1356	0.72	1/1834 (0.1%)
8	J	0.42	0/640	0.86	7/889 (0.8%)
9	K	0.30	0/1044	0.56	0/1416
10	N	0.58	0/1144	0.75	0/1543
11	O	0.75	0/943	0.88	1/1269 (0.1%)
12	P	0.53	0/1152	0.85	1/1533 (0.1%)
13	Q	0.62	0/1143	0.72	0/1527
14	R	0.51	0/982	0.74	0/1312
15	S	0.45	0/887	0.73	0/1180
16	T	0.62	0/1105	0.79	0/1477
17	U	0.63	0/977	0.78	1/1301 (0.1%)
18	V	0.56	0/782	0.78	0/1049
19	W	0.61	0/897	0.84	0/1205
20	X	0.56	0/764	0.76	0/1025
21	Y	0.54	0/819	0.78	1/1095 (0.1%)
22	Z	0.53	0/1483	0.71	0/2017
23	0	0.53	0/599	0.73	0/798
24	1	0.61	0/762	0.79	0/1014
25	2	0.50	0/590	0.70	0/781
26	3	0.57	0/474	0.81	1/635 (0.2%)
27	4	0.52	0/570	0.82	0/768
28	5	0.57	0/473	0.74	0/639
29	6	0.56	0/460	0.73	0/613
30	7	0.64	0/438	0.82	0/575
31	8	0.59	0/519	0.66	0/684
32	9	0.61	0/310	0.77	0/407

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	x	0.60	0/1602	1.35	18/2493 (0.7%)
34	a	0.87	14/36002 (0.0%)	1.53	589/56188 (1.0%)
35	b	0.54	0/1885	0.82	1/2547 (0.0%)
36	c	0.58	0/1574	0.71	0/2127
37	d	0.59	0/1685	0.81	2/2262 (0.1%)
38	e	0.69	0/1145	0.83	0/1543
39	f	0.47	0/819	0.69	1/1111 (0.1%)
40	g	0.55	0/1246	0.70	0/1674
41	h	0.58	0/1108	0.75	0/1494
42	i	0.56	0/1002	0.78	0/1346
43	j	0.54	0/711	0.77	0/968
44	k	0.53	0/844	0.69	0/1145
45	l	0.65	0/946	0.87	2/1274 (0.2%)
46	m	0.58	0/934	0.84	0/1256
47	n	0.66	0/501	0.91	3/664 (0.5%)
48	o	0.54	0/739	0.74	0/985
49	p	0.65	0/697	0.80	0/939
50	q	0.66	0/836	0.81	0/1117
51	r	0.49	0/560	0.66	0/746
52	s	0.62	0/665	0.84	0/897
53	t	0.51	0/726	0.79	0/961
54	u	0.51	0/203	0.76	0/266
55	w	0.88	2/1626 (0.1%)	1.58	40/2530 (1.6%)
56	v	0.82	0/165	1.41	3/254 (1.2%)
57	y	0.78	13/4067 (0.3%)	1.12	30/5503 (0.5%)
All	All	0.78	59/162624 (0.0%)	1.36	1866/242779 (0.8%)

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
3	D	0	1
8	J	0	1
42	i	0	1
46	m	0	2
52	s	0	1
53	t	0	1
57	y	0	23
All	All	0	30

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	1	G	OP3-P	-10.81	1.48	1.61
34	a	1125	U	P-O5'	7.89	1.67	1.59
1	A	945	A	N9-C4	-7.33	1.33	1.37
1	A	945	A	N3-C4	-7.19	1.30	1.34
1	A	2790	A	N9-C4	7.08	1.42	1.37

The worst 5 of 1866 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2096	U	O5'-P-OP1	-18.05	89.04	110.70
34	a	1281	U	N3-C2-O2	-14.81	111.83	122.20
1	A	1021	A	C2-N3-C4	-13.57	103.82	110.60
1	A	945	A	N1-C6-N6	13.26	126.56	118.60
1	A	1190	G	N1-C6-O6	13.08	127.75	119.90

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	223	GLY	Peptide
8	J	6	ASN	Peptide
42	i	45	ALA	Peptide
46	m	7	VAL	Peptide
46	m	8	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61879	0	31203	1311	0
2	B	2573	0	1306	33	0
3	D	2136	0	2217	141	0
4	E	1559	0	1618	76	0
5	F	1584	0	1625	73	0
6	G	1425	0	1443	67	0
7	H	1330	0	1407	56	0
8	J	641	0	309	12	0
9	K	1025	0	1066	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	N	1117	0	1184	55	0
11	O	933	0	996	37	0
12	P	1135	0	1212	70	0
13	Q	1122	0	1179	40	0
14	R	968	0	1033	39	0
15	S	877	0	938	39	0
16	T	1091	0	1151	53	0
17	U	959	0	1019	60	0
18	V	771	0	830	29	0
19	W	886	0	940	36	0
20	X	750	0	814	41	0
21	Y	806	0	881	35	0
22	Z	1451	0	1457	73	0
23	0	591	0	607	34	0
24	1	755	0	826	38	0
25	2	588	0	643	22	0
26	3	469	0	518	15	0
27	4	557	0	537	42	0
28	5	459	0	476	29	0
29	6	453	0	473	17	0
30	7	430	0	480	17	0
31	8	511	0	571	31	0
32	9	307	0	335	12	0
33	x	1581	0	805	0	0
34	a	32163	0	16234	0	0
35	b	1850	0	1871	0	0
36	c	1550	0	1539	0	0
37	d	1655	0	1673	0	0
38	e	1129	0	1185	0	0
39	f	806	0	793	0	0
40	g	1227	0	1232	0	0
41	h	1088	0	1126	0	0
42	i	983	0	986	0	0
43	j	698	0	637	0	0
44	k	829	0	825	0	0
45	l	930	0	980	0	0
46	m	924	0	960	0	0
47	n	492	0	528	0	0
48	o	728	0	760	0	0
49	p	681	0	697	0	0
50	q	823	0	891	0	0
51	r	555	0	618	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	s	650	0	655	0	0
53	t	724	0	787	0	0
54	u	199	0	208	0	0
55	w	1643	0	849	0	0
56	v	148	0	76	0	0
57	y	4000	0	3218	0	0
58	0	3	0	0	0	0
58	5	1	0	0	0	0
58	6	1	0	0	0	0
58	7	3	0	0	0	0
58	8	1	0	0	0	0
58	9	1	0	0	0	0
58	A	635	0	0	0	0
58	B	18	0	0	0	0
58	D	5	0	0	0	0
58	E	4	0	0	0	0
58	F	5	0	0	0	0
58	G	3	0	0	0	0
58	N	1	0	0	0	0
58	O	1	0	0	0	0
58	P	2	0	0	0	0
58	Q	5	0	0	0	0
58	R	3	0	0	0	0
58	U	4	0	0	0	0
58	V	2	0	0	0	0
58	W	1	0	0	0	0
58	X	1	0	0	0	0
58	Z	1	0	0	0	0
58	a	187	0	0	0	0
58	e	1	0	0	0	0
58	f	1	0	0	0	0
58	l	2	0	0	0	0
58	m	1	0	0	0	0
58	n	1	0	0	0	0
58	v	1	0	0	0	0
58	w	6	0	0	0	0
58	x	3	0	0	0	0
58	y	2	0	0	0	0
59	4	1	0	0	0	0
59	5	1	0	0	0	0
59	6	1	0	0	0	0
59	9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	Y	1	0	0	0	0
59	n	1	0	0	0	0
60	d	8	0	0	0	0
61	y	28	0	12	0	0
62	0	4	0	0	0	0
62	1	2	0	0	0	0
62	3	1	0	0	0	0
62	5	1	0	0	0	0
62	7	2	0	0	0	0
62	8	4	0	0	0	0
62	9	1	0	0	0	0
62	A	710	0	0	110	0
62	B	34	0	0	2	0
62	D	4	0	0	1	0
62	E	7	0	0	1	0
62	F	5	0	0	0	0
62	G	1	0	0	0	0
62	H	1	0	0	0	0
62	N	1	0	0	0	0
62	O	3	0	0	0	0
62	P	3	0	0	0	0
62	Q	4	0	0	1	0
62	R	3	0	0	0	0
62	U	2	0	0	1	0
62	V	1	0	0	1	0
62	W	2	0	0	0	0
62	Y	1	0	0	0	0
62	a	167	0	0	0	0
62	l	1	0	0	0	0
62	v	3	0	0	0	0
62	x	1	0	0	0	0
All	All	152111	0	101439	2398	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 18.

The worst 5 of 2398 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:G:H1	1:A:893:C:N4	1.56	1.02
1:A:1019:U:HO2'	1:A:1021:A:H2	1.08	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2106:G:H1	1:A:2183:C:H42	0.98	0.96
12:P:100:LEU:HD12	12:P:112:LEU:HD11	1.48	0.96
1:A:143:G:H1'	20:X:37:THR:HG21	1.49	0.94

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
3	D	273/276 (99%)	233 (85%)	26 (10%)	14 (5%)	2 9
4	E	202/206 (98%)	165 (82%)	27 (13%)	10 (5%)	3 9
5	F	201/205 (98%)	152 (76%)	37 (18%)	12 (6%)	2 6
6	G	179/182 (98%)	143 (80%)	25 (14%)	11 (6%)	2 5
7	H	172/180 (96%)	128 (74%)	34 (20%)	10 (6%)	2 6
8	J	128/173 (74%)	69 (54%)	31 (24%)	28 (22%)	0 0
9	K	137/147 (93%)	94 (69%)	33 (24%)	10 (7%)	1 3
10	N	138/140 (99%)	106 (77%)	24 (17%)	8 (6%)	2 6
11	O	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	5 20
12	P	147/150 (98%)	108 (74%)	29 (20%)	10 (7%)	1 4
13	Q	139/141 (99%)	122 (88%)	12 (9%)	5 (4%)	4 18
14	R	116/118 (98%)	92 (79%)	21 (18%)	3 (3%)	7 26
15	S	108/112 (96%)	77 (71%)	20 (18%)	11 (10%)	1 2
16	T	129/146 (88%)	113 (88%)	15 (12%)	1 (1%)	24 60
17	U	114/118 (97%)	92 (81%)	16 (14%)	6 (5%)	2 8
18	V	99/101 (98%)	72 (73%)	18 (18%)	9 (9%)	1 2
19	W	110/113 (97%)	86 (78%)	14 (13%)	10 (9%)	1 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	X	93/96 (97%)	73 (78%)	12 (13%)	8 (9%)	1 2
21	Y	105/110 (96%)	82 (78%)	12 (11%)	11 (10%)	1 1
22	Z	183/206 (89%)	145 (79%)	24 (13%)	14 (8%)	1 3
23	0	72/85 (85%)	65 (90%)	6 (8%)	1 (1%)	14 44
24	1	95/98 (97%)	76 (80%)	13 (14%)	6 (6%)	2 5
25	2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	13 42
26	3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	4 18
27	4	67/71 (94%)	42 (63%)	14 (21%)	11 (16%)	0 0
28	5	57/60 (95%)	47 (82%)	5 (9%)	5 (9%)	1 2
29	6	51/54 (94%)	43 (84%)	6 (12%)	2 (4%)	4 15
30	7	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	9 32
31	8	62/65 (95%)	57 (92%)	5 (8%)	0	100 100
32	9	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	6 23
35	b	229/256 (90%)	167 (73%)	41 (18%)	21 (9%)	1 2
36	c	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	4 15
37	d	206/209 (99%)	163 (79%)	33 (16%)	10 (5%)	3 10
38	e	146/162 (90%)	108 (74%)	30 (20%)	8 (6%)	2 7
39	f	98/101 (97%)	70 (71%)	20 (20%)	8 (8%)	1 2
40	g	153/156 (98%)	123 (80%)	26 (17%)	4 (3%)	7 26
41	h	135/138 (98%)	115 (85%)	18 (13%)	2 (2%)	13 42
42	i	125/128 (98%)	98 (78%)	17 (14%)	10 (8%)	1 3
43	j	94/105 (90%)	73 (78%)	12 (13%)	9 (10%)	1 2
44	k	112/129 (87%)	88 (79%)	20 (18%)	4 (4%)	4 18
45	l	120/132 (91%)	106 (88%)	9 (8%)	5 (4%)	3 13
46	m	117/126 (93%)	91 (78%)	16 (14%)	10 (8%)	1 2
47	n	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2 8
48	o	86/89 (97%)	69 (80%)	15 (17%)	2 (2%)	8 30
49	p	80/88 (91%)	61 (76%)	17 (21%)	2 (2%)	7 27
50	q	97/105 (92%)	78 (80%)	13 (13%)	6 (6%)	2 5
51	r	66/88 (75%)	57 (86%)	6 (9%)	3 (4%)	3 12
52	s	81/93 (87%)	64 (79%)	9 (11%)	8 (10%)	1 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	t	94/106 (89%)	74 (79%)	10 (11%)	10 (11%)	0 1
54	u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
57	y	640/679 (94%)	534 (83%)	67 (10%)	39 (6%)	2 5
All	All	6466/6910 (94%)	5145 (80%)	924 (14%)	397 (6%)	2 5

5 of 397 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	14	ARG
3	D	224	ALA
4	E	195	LEU
5	F	89	VAL
5	F	130	ALA

5.3.2 Protein sidechains (i)

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
3	D	215/218 (99%)	163 (76%)	52 (24%)	1 2
4	E	164/166 (99%)	134 (82%)	30 (18%)	2 6
5	F	160/162 (99%)	133 (83%)	27 (17%)	2 8
6	G	143/156 (92%)	103 (72%)	40 (28%)	0 1
7	H	144/148 (97%)	115 (80%)	29 (20%)	1 5
9	K	104/111 (94%)	84 (81%)	20 (19%)	2 5
10	N	118/119 (99%)	93 (79%)	25 (21%)	1 4
11	O	100/100 (100%)	89 (89%)	11 (11%)	8 23
12	P	115/116 (99%)	93 (81%)	22 (19%)	2 5
13	Q	111/111 (100%)	93 (84%)	18 (16%)	3 9
14	R	101/101 (100%)	83 (82%)	18 (18%)	2 6
15	S	87/88 (99%)	74 (85%)	13 (15%)	4 11
16	T	115/127 (91%)	95 (83%)	20 (17%)	2 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	U	93/94 (99%)	72 (77%)	21 (23%)	1 3
18	V	80/82 (98%)	63 (79%)	17 (21%)	1 4
19	W	90/92 (98%)	74 (82%)	16 (18%)	2 6
20	X	77/78 (99%)	65 (84%)	12 (16%)	3 10
21	Y	85/91 (93%)	66 (78%)	19 (22%)	1 3
22	Z	156/179 (87%)	127 (81%)	29 (19%)	2 6
23	0	59/67 (88%)	50 (85%)	9 (15%)	3 10
24	1	80/83 (96%)	62 (78%)	18 (22%)	1 3
25	2	65/67 (97%)	50 (77%)	15 (23%)	1 3
26	3	51/52 (98%)	42 (82%)	9 (18%)	2 7
27	4	60/63 (95%)	46 (77%)	14 (23%)	1 3
28	5	51/52 (98%)	39 (76%)	12 (24%)	1 2
29	6	51/52 (98%)	38 (74%)	13 (26%)	1 2
30	7	42/42 (100%)	33 (79%)	9 (21%)	1 4
31	8	53/55 (96%)	44 (83%)	9 (17%)	2 7
32	9	34/34 (100%)	30 (88%)	4 (12%)	6 19
35	b	193/220 (88%)	144 (75%)	49 (25%)	1 2
36	c	142/188 (76%)	121 (85%)	21 (15%)	4 11
37	d	169/181 (93%)	129 (76%)	40 (24%)	1 2
38	e	113/123 (92%)	83 (74%)	30 (26%)	0 2
39	f	83/90 (92%)	62 (75%)	21 (25%)	1 2
40	g	118/127 (93%)	93 (79%)	25 (21%)	1 4
41	h	114/119 (96%)	91 (80%)	23 (20%)	1 4
42	i	90/99 (91%)	76 (84%)	14 (16%)	3 10
43	j	65/92 (71%)	49 (75%)	16 (25%)	1 2
44	k	82/99 (83%)	71 (87%)	11 (13%)	5 13
45	l	97/109 (89%)	82 (84%)	15 (16%)	3 10
46	m	89/101 (88%)	73 (82%)	16 (18%)	2 6
47	n	49/50 (98%)	36 (74%)	13 (26%)	0 2
48	o	78/80 (98%)	68 (87%)	10 (13%)	5 16
49	p	69/74 (93%)	56 (81%)	13 (19%)	2 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	q	94/97 (97%)	78 (83%)	16 (17%)	2 7
51	r	59/77 (77%)	46 (78%)	13 (22%)	1 3
52	s	68/80 (85%)	50 (74%)	18 (26%)	0 2
53	t	69/82 (84%)	58 (84%)	11 (16%)	3 9
54	u	18/22 (82%)	15 (83%)	3 (17%)	3 8
57	y	289/560 (52%)	193 (67%)	96 (33%)	0 1
All	All	4952/5576 (89%)	3927 (79%)	1025 (21%)	1 4

5 of 1025 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	1	89	GLU
35	b	107	THR
57	y	4	GLU
25	2	52	ASP
29	6	19	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
29	6	29	ASN
36	c	136	GLN
53	t	16	HIS
31	8	35	GLN
35	b	94	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2865/2915 (98%)	639 (22%)	38 (1%)
2	B	119/122 (97%)	18 (15%)	0
33	x	71/76 (93%)	37 (52%)	0
34	a	1493/1521 (98%)	311 (20%)	0
55	w	73/76 (96%)	21 (28%)	0
56	v	6/18 (33%)	1 (16%)	0
All	All	4627/4728 (97%)	1027 (22%)	38 (0%)

5 of 1027 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	15	G
1	A	22	C
1	A	23	G
1	A	28	A

5 of 38 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1145	C
1	A	1300	U
1	A	2611	U
1	A	1176	G
1	A	1379	A

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	PSU	w	32	55	13,21,22	1.29	1 (7%)	18,30,33	3.68	6 (33%)
55	MIA	w	37	55	21,31,32	2.37	4 (19%)	26,44,47	3.74	5 (19%)
55	PSU	w	39	55	13,21,22	1.16	1 (7%)	18,30,33	2.95	6 (33%)
55	7MG	w	46	55	19,26,27	0.87	1 (5%)	24,39,42	2.80	7 (29%)
55	5MU	w	54	55	12,22,23	0.40	0	14,32,35	2.42	2 (14%)
55	PSU	w	55	55	13,21,22	1.25	1 (7%)	18,30,33	3.08	6 (33%)
55	F3O	w	76	55,58	26,36,37	1.07	1 (3%)	31,51,54	2.15	6 (19%)
55	4SU	w	8	55	11,21,22	1.13	1 (9%)	13,30,33	1.27	1 (7%)
33	PSU	x	32	33	13,21,22	1.03	1 (7%)	18,30,33	3.37	5 (27%)
33	MIA	x	37	33	15,24,32	1.24	2 (13%)	16,35,47	2.00	2 (12%)
33	PSU	x	39	33	13,21,22	1.23	1 (7%)	18,30,33	3.46	6 (33%)
33	7MG	x	46	33	19,26,27	1.13	2 (10%)	24,39,42	3.51	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	5MU	x	54	33	12,22,23	0.34	0	14,32,35	2.52	2 (14%)
33	PSU	x	55	33	13,21,22	1.41	1 (7%)	18,30,33	3.17	5 (27%)
33	4SU	x	8	33	11,21,22	1.25	1 (9%)	13,30,33	1.18	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	w	32	55	-	0/7/25/26	0/2/2/2
55	MIA	w	37	55	-	0/11/33/34	0/3/3/3
55	PSU	w	39	55	-	0/7/25/26	0/2/2/2
55	7MG	w	46	55	-	0/7/37/38	0/3/3/3
55	5MU	w	54	55	-	0/3/25/26	0/2/2/2
55	PSU	w	55	55	-	0/7/25/26	0/2/2/2
55	F3O	w	76	55,58	-	0/15/37/38	0/4/4/4
55	4SU	w	8	55	-	0/3/25/26	0/2/2/2
33	PSU	x	32	33	-	0/7/25/26	0/2/2/2
33	MIA	x	37	33	-	0/3/25/34	0/3/3/3
33	PSU	x	39	33	-	0/7/25/26	0/2/2/2
33	7MG	x	46	33	-	0/7/37/38	0/3/3/3
33	5MU	x	54	33	-	0/3/25/26	0/2/2/2
33	PSU	x	55	33	-	0/7/25/26	0/2/2/2
33	4SU	x	8	33	-	0/3/25/26	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	37	MIA	C2-S10	-9.23	1.67	1.75
33	x	55	PSU	C5-C1'	-4.64	1.48	1.52
55	w	55	PSU	C5-C1'	-4.08	1.48	1.52
33	x	39	PSU	C5-C1'	-3.86	1.48	1.52
33	x	8	4SU	C4-S4	-3.84	1.60	1.67

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	w	37	MIA	C11-S10-C2	-17.61	90.96	102.26
55	w	32	PSU	N1-C2-N3	-11.79	120.81	128.33
33	x	39	PSU	N1-C2-N3	-10.91	121.37	128.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	x	46	7MG	C5-C4-N3	-10.88	116.21	126.82
33	x	32	PSU	N1-C2-N3	-10.75	121.47	128.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 914 ligands modelled in this entry, 912 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	SF4	d	501	37	0,12,12	0.00	-	0,24,24	0.00	-
61	GDP	y	703	58	23,30,30	1.30	2 (8%)	30,47,47	1.71	8 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	d	501	37	-	0/0/48/48	0/6/5/5
61	GDP	y	703	58	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	y	703	GDP	C5-C4	3.27	1.47	1.40
61	y	703	GDP	C6-C5	4.15	1.49	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	y	703	GDP	C5-C6-N1	-3.98	118.15	123.59
61	y	703	GDP	C4-C5-N7	-3.89	105.90	109.48
61	y	703	GDP	N3-C2-N1	-2.61	123.47	127.44
61	y	703	GDP	PA-O3A-PB	-2.41	124.59	132.67
61	y	703	GDP	C2'-C1'-N9	-2.33	110.73	114.29

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	A	2873/2915 (98%)	-0.02	94 (3%) 50 42	35, 61, 175, 394	0
2	B	120/122 (98%)	-0.07	0 100 100	65, 93, 121, 133	0
3	D	275/276 (99%)	-0.00	3 (1%) 82 80	35, 56, 75, 108	0
4	E	204/206 (99%)	-0.13	4 (1%) 68 64	34, 57, 77, 101	0
5	F	203/205 (99%)	0.04	1 (0%) 91 90	38, 70, 108, 135	0
6	G	181/182 (99%)	-0.04	5 (2%) 56 50	68, 84, 106, 128	0
7	H	174/180 (96%)	0.43	11 (6%) 23 17	62, 96, 131, 154	0
8	J	130/173 (75%)	2.12	53 (40%) 0 0	129, 161, 183, 197	0
9	K	139/147 (94%)	2.88	82 (58%) 0 0	192, 218, 229, 234	0
10	N	140/140 (100%)	0.00	1 (0%) 89 88	47, 64, 93, 110	0
11	O	122/122 (100%)	0.00	0 100 100	37, 52, 68, 75	0
12	P	149/150 (99%)	0.70	23 (15%) 3 1	42, 81, 109, 116	0
13	Q	141/141 (100%)	0.00	0 100 100	44, 64, 80, 97	0
14	R	118/118 (100%)	0.35	2 (1%) 73 70	46, 66, 86, 102	0
15	S	110/112 (98%)	0.27	4 (3%) 46 38	75, 90, 102, 113	0
16	T	131/146 (89%)	-0.04	1 (0%) 87 86	49, 61, 94, 113	0
17	U	116/118 (98%)	-0.09	0 100 100	42, 56, 75, 83	0
18	V	101/101 (100%)	0.05	0 100 100	41, 73, 93, 104	0
19	W	112/113 (99%)	0.29	4 (3%) 46 38	46, 62, 89, 128	0
20	X	95/96 (98%)	0.19	2 (2%) 67 62	56, 74, 95, 116	0
21	Y	107/110 (97%)	0.66	11 (10%) 9 5	66, 79, 116, 137	0
22	Z	185/206 (89%)	0.30	6 (3%) 51 43	68, 90, 114, 135	0
23	0	74/85 (87%)	0.51	6 (8%) 15 9	50, 67, 85, 105	0
24	1	97/98 (98%)	0.37	2 (2%) 67 62	48, 68, 104, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	2	70/72 (97%)	0.16	0 100 100	69, 86, 100, 109	0
26	3	59/60 (98%)	0.43	3 (5%) 32 25	52, 68, 101, 116	0
27	4	69/71 (97%)	0.15	4 (5%) 26 20	80, 107, 150, 158	0
28	5	59/60 (98%)	-0.24	1 (1%) 73 70	41, 63, 81, 100	0
29	6	53/54 (98%)	0.06	0 100 100	62, 71, 85, 87	0
30	7	49/49 (100%)	0.10	2 (4%) 41 34	40, 49, 73, 96	0
31	8	64/65 (98%)	0.11	1 (1%) 74 72	51, 59, 65, 86	0
32	9	37/37 (100%)	0.77	4 (10%) 8 4	52, 63, 78, 88	0
33	x	67/76 (88%)	4.83	64 (95%) 0 0	94, 267, 283, 306	0
34	a	1496/1521 (98%)	-0.21	6 (0%) 93 92	37, 60, 119, 295	0
35	b	231/256 (90%)	-0.10	5 (2%) 65 60	53, 84, 134, 165	0
36	c	206/239 (86%)	-0.36	0 100 100	50, 65, 88, 99	0
37	d	208/209 (99%)	0.04	2 (0%) 84 82	52, 68, 95, 109	0
38	e	148/162 (91%)	-0.25	1 (0%) 89 88	40, 55, 72, 107	0
39	f	100/101 (99%)	0.24	2 (2%) 68 64	74, 106, 138, 146	0
40	g	155/156 (99%)	0.01	6 (3%) 43 36	54, 73, 124, 156	0
41	h	137/138 (99%)	0.05	0 100 100	47, 59, 72, 90	0
42	i	127/128 (99%)	0.08	0 100 100	45, 70, 91, 102	0
43	j	96/105 (91%)	-0.00	3 (3%) 52 45	42, 70, 119, 133	0
44	k	114/129 (88%)	0.06	2 (1%) 71 68	49, 77, 96, 104	0
45	l	122/132 (92%)	-0.16	1 (0%) 87 86	39, 53, 68, 80	0
46	m	119/126 (94%)	-0.02	2 (1%) 73 70	43, 72, 99, 111	0
47	n	60/61 (98%)	-0.26	0 100 100	42, 51, 66, 69	0
48	o	88/89 (98%)	0.21	3 (3%) 49 41	57, 74, 98, 107	0
49	p	82/88 (93%)	0.20	2 (2%) 62 57	45, 57, 69, 85	0
50	q	99/105 (94%)	0.13	5 (5%) 32 25	50, 62, 80, 93	0
51	r	68/88 (77%)	0.53	4 (5%) 26 19	67, 85, 107, 116	0
52	s	83/93 (89%)	-0.19	0 100 100	45, 57, 76, 89	0
53	t	96/106 (90%)	0.18	2 (2%) 67 62	51, 65, 88, 96	0
54	u	23/27 (85%)	0.44	1 (4%) 39 32	54, 62, 69, 79	0
55	w	68/76 (89%)	-0.27	0 100 100	43, 75, 96, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
56	v	7/18 (38%)	1.31	2 (28%) 1 0	49, 50, 130, 149	0
57	y	644/679 (94%)	1.57	211 (32%) 0 0	69, 151, 188, 213	0
All	All	11201/11638 (96%)	0.19	654 (5%) 26 20	34, 68, 168, 394	0

The worst 5 of 654 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	J	51	LEU	23.2
9	K	52	ILE	17.0
1	A	2178	C	16.6
1	A	2145	C	13.7
1	A	2165	G	13.1

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
55	4SU	w	8	20/21	0.95	0.14	-	56,58,64,64	0
33	MIA	x	37	22/30	0.51	0.78	-	204,221,237,241	0
33	PSU	x	55	20/21	0.32	0.84	-	274,285,289,293	0
55	5MU	w	54	21/22	0.96	0.14	-	67,77,82,84	0
33	5MU	x	54	21/22	0.20	0.66	-	275,282,283,285	0
33	PSU	x	32	20/21	0.41	0.64	-	188,202,216,216	0
55	PSU	w	32	20/21	0.97	0.12	-	40,46,49,51	0
55	PSU	w	39	20/21	0.96	0.14	-	41,50,55,56	0
55	MIA	w	37	29/30	0.95	0.17	-	46,55,61,64	0
55	PSU	w	55	20/21	0.93	0.16	-	75,83,85,86	0
55	F3O	w	76	33/34	0.92	0.26	-	50,60,79,81	0
33	4SU	x	8	20/21	0.33	0.42	-	263,275,277,277	0
33	PSU	x	39	20/21	0.73	0.33	-	175,193,200,201	0
33	7MG	x	46	24/25	0.35	0.36	-	275,282,285,287	0
55	7MG	w	46	24/25	0.92	0.18	-	59,76,103,118	0

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, 95^{th} 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
58	MG	A	3114	1/1	0.84	1.01	81.38	57,57,57,57	0
58	MG	A	3165	1/1	0.68	1.02	66.51	60,60,60,60	0
58	MG	A	3117	1/1	0.83	1.11	66.27	50,50,50,50	0
58	MG	A	3120	1/1	0.82	0.76	28.68	52,52,52,52	0
58	MG	a	3306	1/1	0.87	0.69	28.63	55,55,55,55	0
58	MG	a	3309	1/1	0.96	0.80	28.16	37,37,37,37	0
58	MG	A	3118	1/1	0.89	0.88	27.84	52,52,52,52	0
58	MG	7	102	1/1	0.83	1.36	27.62	66,66,66,66	0
58	MG	a	3397	1/1	0.97	0.39	25.06	27,27,27,27	0
58	MG	a	3323	1/1	0.62	0.51	23.90	69,69,69,69	0
58	MG	A	3072	1/1	0.87	0.32	23.23	43,43,43,43	0
58	MG	A	3274	1/1	0.95	0.47	22.68	45,45,45,45	0
58	MG	E	301	1/1	0.90	0.81	19.90	56,56,56,56	0
58	MG	D	303	1/1	0.89	0.92	19.54	49,49,49,49	0
58	MG	A	3032	1/1	0.79	0.32	19.47	50,50,50,50	0
58	MG	A	3039	1/1	0.85	0.84	18.59	59,59,59,59	0
58	MG	A	3093	1/1	0.66	0.31	18.50	81,81,81,81	0
58	MG	A	3500	1/1	0.96	0.29	18.31	40,40,40,40	0
58	MG	A	3056	1/1	0.58	0.42	18.18	68,68,68,68	0
58	MG	A	3191	1/1	0.98	0.36	17.61	33,33,33,33	0
58	MG	A	3107	1/1	0.91	1.42	17.34	75,75,75,75	0
58	MG	a	3447	1/1	0.98	0.41	16.48	36,36,36,36	0
58	MG	A	3231	1/1	0.76	0.39	16.36	48,48,48,48	0
58	MG	a	3401	1/1	0.93	0.38	16.12	44,44,44,44	0
58	MG	A	3316	1/1	0.94	0.31	15.98	47,47,47,47	0
58	MG	A	3095	1/1	0.78	0.40	15.30	63,63,63,63	0
58	MG	A	3023	1/1	0.89	0.31	15.20	48,48,48,48	0
58	MG	A	3234	1/1	0.96	0.36	14.55	48,48,48,48	0
58	MG	7	101	1/1	0.95	0.70	13.26	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3059	1/1	0.80	0.33	13.11	66,66,66,66	0
58	MG	A	3144	1/1	0.97	0.32	12.86	38,38,38,38	0
58	MG	A	3208	1/1	0.95	0.27	12.65	40,40,40,40	0
58	MG	A	3616	1/1	0.89	0.31	12.23	59,59,59,59	0
58	MG	V	202	1/1	0.88	0.75	12.19	51,51,51,51	0
58	MG	A	3446	1/1	0.94	0.29	12.02	39,39,39,39	0
58	MG	A	3557	1/1	0.96	0.33	11.95	60,60,60,60	0
58	MG	A	3011	1/1	0.59	0.46	11.78	79,79,79,79	0
58	MG	Q	202	1/1	0.90	0.95	11.56	51,51,51,51	0
58	MG	A	3541	1/1	0.96	0.26	11.54	56,56,56,56	0
58	MG	A	3005	1/1	0.89	0.37	11.44	40,40,40,40	0
58	MG	A	3174	1/1	0.81	0.32	11.36	59,59,59,59	0
58	MG	A	3423	1/1	0.89	0.22	11.35	59,59,59,59	0
58	MG	A	3414	1/1	0.91	0.28	11.25	31,31,31,31	0
58	MG	A	3187	1/1	0.96	0.44	11.04	47,47,47,47	0
58	MG	F	302	1/1	0.92	0.81	11.04	52,52,52,52	0
58	MG	A	3006	1/1	0.92	0.59	10.70	57,57,57,57	0
58	MG	A	3189	1/1	0.95	0.31	10.68	37,37,37,37	0
58	MG	A	3192	1/1	0.99	0.28	10.63	39,39,39,39	0
58	MG	A	3167	1/1	0.93	0.55	10.50	65,65,65,65	0
58	MG	A	3190	1/1	0.96	0.30	10.40	38,38,38,38	0
58	MG	A	3396	1/1	0.97	0.25	10.16	38,38,38,38	0
58	MG	A	3399	1/1	0.98	0.28	9.82	29,29,29,29	0
58	MG	A	3252	1/1	0.89	0.27	9.79	58,58,58,58	0
58	MG	A	3487	1/1	0.92	0.22	9.79	60,60,60,60	0
58	MG	P	201	1/1	0.79	0.54	9.54	54,54,54,54	0
58	MG	A	3529	1/1	0.94	0.24	9.50	56,56,56,56	0
58	MG	A	3184	1/1	0.98	0.39	9.46	40,40,40,40	0
58	MG	a	3330	1/1	0.89	0.55	9.00	63,63,63,63	0
58	MG	A	3493	1/1	0.90	0.37	8.73	33,33,33,33	0
58	MG	A	3080	1/1	0.93	0.30	8.46	54,54,54,54	0
58	MG	A	3501	1/1	0.96	0.25	8.41	46,46,46,46	0
58	MG	x	3002	1/1	0.78	1.22	8.37	101,101,101,101	0
58	MG	A	3297	1/1	0.79	0.24	8.34	67,67,67,67	0
58	MG	Q	204	1/1	0.91	0.63	8.34	56,56,56,56	0
58	MG	B	210	1/1	0.76	0.22	8.33	68,68,68,68	0
58	MG	A	3155	1/1	0.96	0.27	8.17	44,44,44,44	0
58	MG	A	3513	1/1	0.99	0.29	8.07	41,41,41,41	0
58	MG	A	3476	1/1	0.94	0.30	8.01	50,50,50,50	0
58	MG	A	3417	1/1	0.96	0.20	7.96	30,30,30,30	0
58	MG	A	3341	1/1	0.93	0.33	7.93	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3520	1/1	0.86	0.21	7.90	80,80,80,80	0
58	MG	A	3239	1/1	0.85	0.32	7.58	56,56,56,56	0
58	MG	A	3141	1/1	0.86	0.23	7.52	55,55,55,55	0
58	MG	A	3109	1/1	0.87	0.26	7.45	52,52,52,52	0
58	MG	a	3331	1/1	0.93	0.24	7.38	55,55,55,55	0
58	MG	a	3406	1/1	0.99	0.21	7.34	52,52,52,52	0
58	MG	A	3170	1/1	0.98	0.23	7.29	43,43,43,43	0
58	MG	A	3352	1/1	0.82	0.31	7.25	47,47,47,47	0
58	MG	Q	201	1/1	0.94	0.51	7.07	51,51,51,51	0
58	MG	A	3041	1/1	0.94	0.24	7.06	42,42,42,42	0
58	MG	a	3395	1/1	0.98	0.30	6.91	32,32,32,32	0
58	MG	A	3079	1/1	0.90	0.45	6.86	63,63,63,63	0
58	MG	a	3422	1/1	0.94	0.32	6.80	50,50,50,50	0
58	MG	A	3188	1/1	0.98	0.32	6.79	44,44,44,44	0
58	MG	a	3471	1/1	0.97	0.27	6.69	49,49,49,49	0
58	MG	A	3295	1/1	0.94	0.27	6.63	30,30,30,30	0
58	MG	A	3568	1/1	0.81	0.20	6.39	83,83,83,83	0
58	MG	A	3293	1/1	0.80	0.33	6.34	51,51,51,51	0
58	MG	A	3319	1/1	0.70	0.23	6.05	31,31,31,31	0
58	MG	A	3143	1/1	0.90	0.26	6.05	60,60,60,60	0
58	MG	A	3008	1/1	0.89	0.99	6.01	80,80,80,80	0
58	MG	A	3125	1/1	0.94	0.29	5.98	31,31,31,31	0
58	MG	A	3225	1/1	0.97	0.25	5.94	36,36,36,36	0
58	MG	A	3119	1/1	0.87	0.26	5.49	50,50,50,50	0
58	MG	A	3311	1/1	0.94	0.28	5.44	52,52,52,52	0
58	MG	N	201	1/1	0.76	0.40	5.41	57,57,57,57	0
58	MG	a	3487	1/1	0.98	0.32	5.39	35,35,35,35	0
58	MG	a	3368	1/1	0.87	0.23	5.34	44,44,44,44	0
58	MG	n	101	1/1	0.98	0.25	5.32	42,42,42,42	0
58	MG	D	301	1/1	0.97	0.29	5.26	41,41,41,41	0
58	MG	A	3230	1/1	0.97	0.24	5.21	46,46,46,46	0
58	MG	A	3002	1/1	0.69	0.34	5.11	50,50,50,50	0
58	MG	6	101	1/1	0.80	0.32	5.08	64,64,64,64	0
58	MG	A	3363	1/1	0.94	0.18	5.04	30,30,30,30	0
58	MG	A	3045	1/1	0.85	0.21	4.98	68,68,68,68	0
58	MG	A	3455	1/1	0.95	0.22	4.92	73,73,73,73	0
58	MG	A	3516	1/1	0.88	0.21	4.84	55,55,55,55	0
58	MG	A	3420	1/1	0.96	0.20	4.83	31,31,31,31	0
58	MG	A	3022	1/1	0.93	0.28	4.73	33,33,33,33	0
58	MG	a	3439	1/1	0.97	0.21	4.63	48,48,48,48	0
58	MG	a	3378	1/1	0.96	0.24	4.62	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3564	1/1	0.79	0.21	4.51	75,75,75,75	0
58	MG	a	3355	1/1	0.97	0.20	4.38	39,39,39,39	0
58	MG	R	201	1/1	0.84	0.56	4.26	67,67,67,67	0
58	MG	a	3313	1/1	0.89	0.19	4.17	61,61,61,61	0
58	MG	a	3318	1/1	0.98	0.24	4.10	41,41,41,41	0
58	MG	a	3466	1/1	0.94	0.18	4.09	60,60,60,60	0
58	MG	A	3222	1/1	0.95	0.21	4.01	33,33,33,33	0
58	MG	A	3004	1/1	0.92	0.21	3.94	55,55,55,55	0
58	MG	l	202	1/1	0.95	0.33	3.93	61,61,61,61	0
58	MG	a	3435	1/1	0.93	0.19	3.91	57,57,57,57	0
58	MG	A	3157	1/1	0.34	0.24	3.84	118,118,118,118	0
58	MG	A	3530	1/1	0.99	0.25	3.82	38,38,38,38	0
58	MG	A	3601	1/1	0.85	0.19	3.80	45,45,45,45	0
58	MG	a	3376	1/1	0.91	0.20	3.65	46,46,46,46	0
58	MG	A	3490	1/1	0.87	0.25	3.58	47,47,47,47	0
58	MG	A	3200	1/1	0.95	0.18	3.42	44,44,44,44	0
58	MG	A	3209	1/1	0.79	0.18	3.38	71,71,71,71	0
58	MG	A	3086	1/1	0.88	0.19	3.30	50,50,50,50	0
58	MG	A	3540	1/1	0.96	0.22	3.15	55,55,55,55	0
58	MG	A	3164	1/1	0.95	0.19	3.03	51,51,51,51	0
58	MG	A	3171	1/1	0.82	0.18	3.00	37,37,37,37	0
58	MG	A	3027	1/1	0.93	0.25	2.97	44,44,44,44	0
58	MG	A	3437	1/1	0.97	0.20	2.91	28,28,28,28	0
58	MG	A	3380	1/1	0.94	0.19	2.90	52,52,52,52	0
58	MG	A	3207	1/1	0.90	0.17	2.83	40,40,40,40	0
58	MG	A	3047	1/1	0.94	0.19	2.79	39,39,39,39	0
58	MG	A	3382	1/1	0.94	0.24	2.78	36,36,36,36	0
58	MG	A	3021	1/1	0.98	0.18	2.72	34,34,34,34	0
58	MG	A	3147	1/1	0.94	0.23	2.72	64,64,64,64	0
58	MG	A	3048	1/1	0.91	0.20	2.64	43,43,43,43	0
58	MG	A	3523	1/1	0.98	0.23	2.63	36,36,36,36	0
58	MG	A	3214	1/1	0.92	0.41	2.58	52,52,52,52	0
58	MG	U	201	1/1	0.93	0.40	2.58	72,72,72,72	0
58	MG	F	304	1/1	0.91	0.27	2.56	60,60,60,60	0
58	MG	A	3033	1/1	0.94	0.19	2.47	39,39,39,39	0
58	MG	a	3351	1/1	0.94	0.19	2.42	36,36,36,36	0
58	MG	A	3244	1/1	0.85	0.20	2.42	59,59,59,59	0
58	MG	a	3382	1/1	0.97	0.22	2.34	31,31,31,31	0
58	MG	A	3034	1/1	0.83	0.20	2.29	71,71,71,71	0
58	MG	A	3498	1/1	0.86	0.18	2.29	76,76,76,76	0
58	MG	A	3223	1/1	0.88	0.31	2.28	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3166	1/1	0.96	0.30	2.25	57,57,57,57	0
58	MG	A	3486	1/1	0.94	0.23	2.23	40,40,40,40	0
58	MG	A	3313	1/1	0.93	0.17	2.13	44,44,44,44	0
58	MG	A	3410	1/1	0.75	0.20	2.07	51,51,51,51	0
58	MG	A	3324	1/1	0.96	0.22	2.02	43,43,43,43	0
58	MG	A	3201	1/1	0.92	0.20	2.00	63,63,63,63	0
58	MG	A	3067	1/1	0.81	0.16	1.93	70,70,70,70	0
58	MG	A	3442	1/1	0.93	0.17	1.88	56,56,56,56	0
58	MG	A	3485	1/1	0.97	0.22	1.86	38,38,38,38	0
58	MG	D	302	1/1	0.59	0.28	1.81	74,74,74,74	0
58	MG	A	3552	1/1	0.94	0.18	1.78	64,64,64,64	0
58	MG	A	3233	1/1	0.98	0.17	1.74	53,53,53,53	0
58	MG	A	3394	1/1	0.95	0.19	1.67	30,30,30,30	0
58	MG	A	3606	1/1	0.87	0.18	1.65	55,55,55,55	0
58	MG	A	3103	1/1	0.89	0.29	1.60	56,56,56,56	0
58	MG	A	3378	1/1	0.99	0.19	1.49	31,31,31,31	0
58	MG	A	3404	1/1	0.93	0.20	1.42	57,57,57,57	0
58	MG	A	3049	1/1	0.97	0.19	1.41	41,41,41,41	0
58	MG	A	3173	1/1	0.89	0.18	1.39	57,57,57,57	0
58	MG	A	3340	1/1	0.97	0.23	1.36	65,65,65,65	0
58	MG	A	3544	1/1	0.87	0.17	1.30	55,55,55,55	0
58	MG	G	202	1/1	0.69	0.24	1.29	67,67,67,67	0
58	MG	A	3007	1/1	0.93	0.27	1.24	46,46,46,46	0
58	MG	A	3509	1/1	0.97	0.24	1.24	51,51,51,51	0
58	MG	A	3323	1/1	0.91	0.15	1.18	42,42,42,42	0
58	MG	y	701	1/1	0.84	0.26	1.13	68,68,68,68	0
58	MG	A	3594	1/1	0.92	0.19	1.13	37,37,37,37	0
58	MG	A	3536	1/1	0.96	0.21	1.08	39,39,39,39	0
58	MG	A	3154	1/1	0.93	0.18	1.07	60,60,60,60	0
58	MG	A	3009	1/1	0.85	0.30	1.05	50,50,50,50	0
58	MG	a	3414	1/1	0.95	0.20	1.02	50,50,50,50	0
58	MG	A	3364	1/1	0.97	0.16	1.00	61,61,61,61	0
58	MG	A	3077	1/1	0.96	0.13	0.95	48,48,48,48	0
58	MG	A	3215	1/1	0.88	0.18	0.95	66,66,66,66	0
58	MG	a	3486	1/1	0.91	0.19	0.95	38,38,38,38	0
58	MG	A	3046	1/1	0.90	0.17	0.95	55,55,55,55	0
58	MG	A	3384	1/1	0.95	0.23	0.94	51,51,51,51	0
58	MG	a	3415	1/1	0.97	0.20	0.89	62,62,62,62	0
58	MG	A	3450	1/1	0.95	0.16	0.82	57,57,57,57	0
58	MG	A	3358	1/1	0.96	0.18	0.82	63,63,63,63	0
58	MG	A	3397	1/1	0.89	0.16	0.72	36,36,36,36	0
58	MG	a	3438	1/1	0.99	0.16	0.69	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3545	1/1	0.94	0.23	0.69	64,64,64,64	0
58	MG	A	3163	1/1	0.96	0.15	0.64	34,34,34,34	0
58	MG	A	3128	1/1	0.96	0.19	0.63	45,45,45,45	0
58	MG	A	3494	1/1	0.97	0.17	0.56	42,42,42,42	0
58	MG	A	3480	1/1	0.98	0.15	0.48	35,35,35,35	0
58	MG	A	3362	1/1	0.97	0.17	0.47	50,50,50,50	0
58	MG	A	3196	1/1	0.93	0.18	0.44	44,44,44,44	0
58	MG	a	3440	1/1	0.78	0.14	0.42	69,69,69,69	0
58	MG	a	3467	1/1	0.94	0.14	0.30	62,62,62,62	0
58	MG	A	3565	1/1	0.82	0.14	0.28	67,67,67,67	0
58	MG	A	3015	1/1	0.98	0.20	0.25	43,43,43,43	0
58	MG	A	3598	1/1	0.82	0.13	0.20	74,74,74,74	0
58	MG	Q	205	1/1	0.90	0.17	0.13	55,55,55,55	0
58	MG	A	3251	1/1	0.91	0.14	0.13	35,35,35,35	0
58	MG	E	304	1/1	0.89	0.21	0.13	55,55,55,55	0
58	MG	A	3123	1/1	0.95	0.16	0.08	51,51,51,51	0
58	MG	a	3420	1/1	0.92	0.17	0.05	62,62,62,62	0
58	MG	a	3343	1/1	0.98	0.16	0.04	29,29,29,29	0
58	MG	a	3403	1/1	0.85	0.15	0.03	61,61,61,61	0
58	MG	A	3626	1/1	0.97	0.13	0.01	51,51,51,51	0
58	MG	a	3456	1/1	0.95	0.18	-0.02	59,59,59,59	0
58	MG	A	3537	1/1	0.98	0.18	-0.13	32,32,32,32	0
58	MG	A	3097	1/1	0.87	0.13	-0.17	60,60,60,60	0
58	MG	A	3342	1/1	0.94	0.16	-0.17	61,61,61,61	0
58	MG	A	3301	1/1	0.93	0.17	-0.17	57,57,57,57	0
60	SF4	d	501	8/8	0.99	0.16	-0.28	48,60,64,65	0
58	MG	A	3100	1/1	0.97	0.13	-0.29	45,45,45,45	0
58	MG	A	3024	1/1	0.92	0.14	-0.35	63,63,63,63	0
58	MG	A	3043	1/1	0.91	0.16	-0.40	59,59,59,59	0
58	MG	E	302	1/1	0.94	0.13	-0.44	35,35,35,35	0
58	MG	A	3140	1/1	0.93	0.16	-0.47	57,57,57,57	0
59	ZN	n	102	1/1	0.98	0.14	-0.50	61,61,61,61	0
58	MG	B	204	1/1	0.94	0.15	-0.52	85,85,85,85	0
58	MG	A	3289	1/1	0.94	0.14	-0.64	43,43,43,43	0
58	MG	A	3403	1/1	0.91	0.15	-0.65	40,40,40,40	0
58	MG	a	3327	1/1	0.85	0.12	-0.67	62,62,62,62	0
58	MG	A	3070	1/1	0.96	0.11	-0.70	57,57,57,57	0
58	MG	A	3473	1/1	0.96	0.15	-0.70	46,46,46,46	0
58	MG	A	3159	1/1	0.92	0.13	-0.72	78,78,78,78	0
58	MG	a	3346	1/1	0.89	0.14	-0.77	50,50,50,50	0
58	MG	A	3428	1/1	0.93	0.15	-0.81	36,36,36,36	0
61	GDP	y	703	28/28	0.93	0.15	-0.82	91,120,142,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3199	1/1	0.90	0.15	-0.91	42,42,42,42	0
59	ZN	5	102	1/1	0.94	0.08	-1.02	70,70,70,70	0
58	MG	a	3384	1/1	0.94	0.14	-1.02	49,49,49,49	0
58	MG	A	3508	1/1	0.93	0.13	-1.04	46,46,46,46	0
58	MG	A	3331	1/1	0.94	0.12	-1.06	54,54,54,54	0
58	MG	a	3418	1/1	0.89	0.11	-1.07	67,67,67,67	0
58	MG	a	3357	1/1	0.90	0.12	-1.20	48,48,48,48	0
59	ZN	Y	501	1/1	0.97	0.08	-1.20	92,92,92,92	0
58	MG	B	213	1/1	0.66	0.11	-1.22	81,81,81,81	0
58	MG	A	3388	1/1	0.85	0.15	-1.27	47,47,47,47	0
58	MG	a	3385	1/1	0.89	0.12	-1.28	33,33,33,33	0
58	MG	A	3462	1/1	0.94	0.12	-1.35	53,53,53,53	0
58	MG	a	3307	1/1	0.97	0.14	-1.35	35,35,35,35	0
58	MG	a	3409	1/1	0.88	0.10	-1.44	74,74,74,74	0
59	ZN	6	102	1/1	0.97	0.09	-1.48	70,70,70,70	0
59	ZN	9	102	1/1	0.97	0.10	-1.52	72,72,72,72	0
58	MG	A	3395	1/1	0.99	0.12	-1.58	31,31,31,31	0
58	MG	A	3430	1/1	0.88	0.14	-1.63	44,44,44,44	0
58	MG	A	3468	1/1	0.96	0.13	-1.64	48,48,48,48	0
58	MG	a	3387	1/1	0.94	0.08	-1.68	55,55,55,55	0
58	MG	A	3609	1/1	0.97	0.13	-1.68	39,39,39,39	0
58	MG	a	3451	1/1	0.86	0.13	-1.72	49,49,49,49	0
58	MG	A	3321	1/1	0.96	0.09	-1.90	41,41,41,41	0
58	MG	A	3181	1/1	0.82	0.10	-2.25	35,35,35,35	0
58	MG	A	3375	1/1	0.81	0.12	-2.28	55,55,55,55	0
58	MG	A	3219	1/1	0.96	0.11	-2.41	61,61,61,61	0
58	MG	a	3389	1/1	0.95	0.11	-2.49	38,38,38,38	0
58	MG	A	3017	1/1	0.99	0.11	-2.49	63,63,63,63	0
58	MG	a	3429	1/1	0.93	0.15	-2.50	49,49,49,49	0
58	MG	A	3433	1/1	0.89	0.08	-2.80	64,64,64,64	0
58	MG	A	3514	1/1	0.85	0.14	-2.96	34,34,34,34	0
58	MG	A	3407	1/1	0.92	0.10	-2.98	38,38,38,38	0
59	ZN	4	501	1/1	0.95	0.06	-3.10	117,117,117,117	0
58	MG	A	3553	1/1	0.96	0.08	-3.56	40,40,40,40	0
58	MG	a	3433	1/1	0.91	0.12	-3.56	32,32,32,32	0
58	MG	A	3176	1/1	0.98	0.10	-3.62	35,35,35,35	0
58	MG	A	3583	1/1	0.97	0.10	-3.64	55,55,55,55	0
58	MG	A	3026	1/1	0.94	0.09	-3.84	55,55,55,55	0
58	MG	a	3396	1/1	0.86	0.11	-3.88	42,42,42,42	0
58	MG	a	3312	1/1	0.98	0.07	-4.06	26,26,26,26	0
58	MG	A	3083	1/1	0.95	0.07	-4.37	37,37,37,37	0
58	MG	a	3443	1/1	0.97	0.06	-4.42	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3205	1/1	0.95	0.12	-5.64	43,43,43,43	0
58	MG	A	3374	1/1	0.89	0.15	-	58,58,58,58	0
58	MG	A	3229	1/1	0.96	0.14	-	46,46,46,46	0
58	MG	B	207	1/1	0.82	0.26	-	103,103,103,103	0
58	MG	A	3250	1/1	0.89	0.22	-	58,58,58,58	0
58	MG	A	3133	1/1	0.95	0.50	-	44,44,44,44	0
58	MG	A	3560	1/1	0.67	0.26	-	79,79,79,79	0
58	MG	A	3126	1/1	0.88	0.21	-	60,60,60,60	0
58	MG	a	3448	1/1	0.97	0.07	-	42,42,42,42	0
58	MG	A	3559	1/1	0.95	0.23	-	46,46,46,46	0
58	MG	A	3198	1/1	0.89	0.21	-	55,55,55,55	0
58	MG	A	3591	1/1	0.92	0.13	-	66,66,66,66	0
58	MG	A	3127	1/1	0.98	0.14	-	73,73,73,73	0
58	MG	a	3400	1/1	0.86	0.30	-	61,61,61,61	0
58	MG	A	3454	1/1	0.93	0.49	-	51,51,51,51	0
58	MG	A	3438	1/1	0.96	0.12	-	53,53,53,53	0
58	MG	A	3092	1/1	0.87	0.38	-	67,67,67,67	0
58	MG	A	3116	1/1	0.95	0.34	-	50,50,50,50	0
58	MG	a	3402	1/1	0.99	0.19	-	43,43,43,43	0
58	MG	A	3634	1/1	0.95	0.14	-	56,56,56,56	0
58	MG	a	3390	1/1	0.44	0.44	-	45,45,45,45	0
58	MG	A	3172	1/1	0.93	0.32	-	31,31,31,31	0
58	MG	A	3593	1/1	0.97	0.30	-	41,41,41,41	0
58	MG	A	3412	1/1	0.96	0.22	-	45,45,45,45	0
58	MG	a	3310	1/1	0.90	0.10	-	52,52,52,52	0
58	MG	A	3294	1/1	0.80	0.37	-	44,44,44,44	0
58	MG	A	3546	1/1	0.91	0.32	-	53,53,53,53	0
58	MG	U	204	1/1	0.97	0.13	-	37,37,37,37	0
58	MG	A	3139	1/1	0.90	0.58	-	62,62,62,62	0
58	MG	A	3445	1/1	0.96	0.08	-	51,51,51,51	0
58	MG	A	3610	1/1	0.93	0.23	-	61,61,61,61	0
58	MG	A	3195	1/1	0.98	0.23	-	41,41,41,41	0
58	MG	A	3282	1/1	0.57	0.44	-	66,66,66,66	0
58	MG	A	3270	1/1	0.80	0.24	-	61,61,61,61	0
58	MG	A	3303	1/1	0.95	0.07	-	55,55,55,55	0
58	MG	A	3355	1/1	0.88	0.13	-	84,84,84,84	0
58	MG	y	702	1/1	0.98	0.18	-	75,75,75,75	0
58	MG	A	3193	1/1	0.99	0.22	-	38,38,38,38	0
58	MG	9	101	1/1	0.93	0.30	-	57,57,57,57	0
58	MG	A	3134	1/1	0.88	0.46	-	67,67,67,67	0
58	MG	A	3499	1/1	0.96	0.10	-	60,60,60,60	0
58	MG	A	3344	1/1	0.95	0.06	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	e	201	1/1	0.92	0.15	-	69,69,69,69	0
58	MG	a	3303	1/1	0.89	0.17	-	58,58,58,58	0
58	MG	a	3423	1/1	0.87	0.40	-	66,66,66,66	0
58	MG	A	3206	1/1	0.95	0.14	-	65,65,65,65	0
58	MG	A	3308	1/1	0.90	0.13	-	56,56,56,56	0
58	MG	A	3351	1/1	0.95	0.20	-	38,38,38,38	0
58	MG	A	3602	1/1	0.88	0.11	-	73,73,73,73	0
58	MG	A	3302	1/1	0.94	0.33	-	59,59,59,59	0
58	MG	a	3475	1/1	0.96	0.37	-	38,38,38,38	0
58	MG	A	3503	1/1	0.96	0.21	-	41,41,41,41	0
58	MG	A	3203	1/1	0.93	0.19	-	53,53,53,53	0
58	MG	A	3020	1/1	0.90	0.15	-	50,50,50,50	0
58	MG	a	3374	1/1	0.97	0.40	-	30,30,30,30	0
58	MG	a	3394	1/1	0.99	0.19	-	32,32,32,32	0
58	MG	A	3030	1/1	0.88	0.36	-	64,64,64,64	0
58	MG	a	3338	1/1	0.96	0.17	-	66,66,66,66	0
58	MG	A	3317	1/1	0.96	0.20	-	31,31,31,31	0
58	MG	A	3506	1/1	0.93	0.14	-	49,49,49,49	0
58	MG	A	3347	1/1	0.87	0.18	-	75,75,75,75	0
58	MG	a	3334	1/1	0.89	0.35	-	43,43,43,43	0
58	MG	A	3479	1/1	0.90	0.18	-	43,43,43,43	0
58	MG	A	3278	1/1	0.87	0.45	-	64,64,64,64	0
58	MG	w	106	1/1	0.95	0.18	-	45,45,45,45	0
58	MG	a	3446	1/1	0.94	0.18	-	68,68,68,68	0
58	MG	A	3469	1/1	0.92	0.13	-	54,54,54,54	0
58	MG	A	3607	1/1	0.80	0.17	-	90,90,90,90	0
58	MG	A	3246	1/1	0.84	0.24	-	49,49,49,49	0
58	MG	a	3358	1/1	0.87	0.35	-	70,70,70,70	0
58	MG	a	3308	1/1	0.91	0.21	-	41,41,41,41	0
58	MG	A	3475	1/1	0.95	0.07	-	55,55,55,55	0
58	MG	A	3492	1/1	0.96	0.10	-	62,62,62,62	0
58	MG	8	101	1/1	0.93	0.11	-	66,66,66,66	0
58	MG	A	3162	1/1	0.82	0.17	-	71,71,71,71	0
58	MG	a	3319	1/1	0.92	0.39	-	39,39,39,39	0
58	MG	A	3158	1/1	0.93	0.50	-	97,97,97,97	0
58	MG	v	101	1/1	0.84	0.51	-	89,89,89,89	0
58	MG	A	3018	1/1	0.85	0.23	-	49,49,49,49	0
58	MG	A	3633	1/1	0.97	0.31	-	64,64,64,64	0
58	MG	a	3477	1/1	0.94	0.13	-	68,68,68,68	0
58	MG	a	3454	1/1	0.91	0.24	-	39,39,39,39	0
58	MG	A	3052	1/1	0.79	0.38	-	59,59,59,59	0
58	MG	a	3349	1/1	0.93	0.38	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3400	1/1	0.97	0.09	-	35,35,35,35	0
58	MG	a	3391	1/1	0.69	0.15	-	72,72,72,72	0
58	MG	A	3447	1/1	0.97	0.22	-	67,67,67,67	0
58	MG	A	3150	1/1	0.90	0.14	-	74,74,74,74	0
58	MG	A	3221	1/1	0.93	0.48	-	58,58,58,58	0
58	MG	A	3054	1/1	0.71	0.27	-	71,71,71,71	0
58	MG	a	3360	1/1	0.86	0.35	-	40,40,40,40	0
58	MG	A	3526	1/1	0.97	0.11	-	41,41,41,41	0
58	MG	R	203	1/1	0.96	0.24	-	44,44,44,44	0
58	MG	V	201	1/1	0.81	0.14	-	53,53,53,53	0
58	MG	a	3393	1/1	0.83	0.52	-	69,69,69,69	0
58	MG	a	3311	1/1	0.95	0.20	-	51,51,51,51	0
58	MG	A	3019	1/1	0.92	0.27	-	49,49,49,49	0
58	MG	a	3302	1/1	0.94	0.26	-	58,58,58,58	0
58	MG	a	3381	1/1	0.97	0.18	-	55,55,55,55	0
58	MG	A	3010	1/1	0.89	0.20	-	41,41,41,41	0
58	MG	A	3413	1/1	0.98	0.25	-	51,51,51,51	0
58	MG	A	3515	1/1	0.91	0.29	-	48,48,48,48	0
58	MG	A	3149	1/1	0.94	0.18	-	53,53,53,53	0
58	MG	A	3550	1/1	0.95	0.13	-	58,58,58,58	0
58	MG	A	3481	1/1	0.82	0.32	-	65,65,65,65	0
58	MG	A	3071	1/1	0.96	0.21	-	41,41,41,41	0
58	MG	a	3459	1/1	0.90	0.26	-	91,91,91,91	0
58	MG	A	3087	1/1	0.76	0.29	-	58,58,58,58	0
58	MG	w	102	1/1	0.99	0.31	-	49,49,49,49	0
58	MG	A	3102	1/1	0.84	0.13	-	59,59,59,59	0
58	MG	a	3405	1/1	0.91	0.18	-	70,70,70,70	0
58	MG	A	3074	1/1	0.90	0.16	-	42,42,42,42	0
58	MG	A	3161	1/1	0.64	0.44	-	67,67,67,67	0
58	MG	A	3555	1/1	0.89	0.17	-	69,69,69,69	0
58	MG	a	3428	1/1	0.85	0.26	-	46,46,46,46	0
58	MG	a	3416	1/1	0.95	0.25	-	61,61,61,61	0
58	MG	A	3614	1/1	0.85	0.16	-	75,75,75,75	0
58	MG	A	3459	1/1	0.97	0.18	-	36,36,36,36	0
58	MG	R	202	1/1	0.94	0.28	-	53,53,53,53	0
58	MG	a	3412	1/1	0.97	0.11	-	48,48,48,48	0
58	MG	A	3580	1/1	0.91	0.23	-	67,67,67,67	0
58	MG	A	3240	1/1	0.80	0.23	-	79,79,79,79	0
58	MG	A	3415	1/1	0.92	0.27	-	42,42,42,42	0
58	MG	A	3393	1/1	0.93	0.32	-	57,57,57,57	0
58	MG	A	3217	1/1	0.92	0.38	-	50,50,50,50	0
58	MG	A	3551	1/1	0.87	0.20	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3470	1/1	0.97	0.18	-	43,43,43,43	0
58	MG	A	3532	1/1	0.86	0.42	-	66,66,66,66	0
58	MG	A	3366	1/1	0.89	0.11	-	58,58,58,58	0
58	MG	A	3474	1/1	0.95	0.12	-	51,51,51,51	0
58	MG	5	101	1/1	0.86	0.58	-	69,69,69,69	0
58	MG	a	3342	1/1	0.94	0.46	-	50,50,50,50	0
58	MG	A	3632	1/1	0.96	0.26	-	63,63,63,63	0
58	MG	A	3271	1/1	0.93	0.16	-	57,57,57,57	0
58	MG	a	3339	1/1	0.91	0.24	-	50,50,50,50	0
58	MG	A	3359	1/1	0.95	0.13	-	45,45,45,45	0
58	MG	A	3365	1/1	0.92	0.13	-	51,51,51,51	0
58	MG	x	3003	1/1	0.54	1.35	-	215,215,215,215	0
58	MG	A	3272	1/1	0.87	0.35	-	62,62,62,62	0
58	MG	a	3399	1/1	0.96	0.18	-	36,36,36,36	0
58	MG	A	3590	1/1	0.92	0.13	-	59,59,59,59	0
58	MG	A	3050	1/1	0.89	0.12	-	39,39,39,39	0
58	MG	a	3452	1/1	0.96	0.10	-	52,52,52,52	0
58	MG	A	3623	1/1	0.95	0.20	-	52,52,52,52	0
58	MG	a	3350	1/1	0.89	0.12	-	73,73,73,73	0
58	MG	A	3456	1/1	0.93	0.29	-	47,47,47,47	0
58	MG	a	3457	1/1	0.93	0.33	-	41,41,41,41	0
58	MG	A	3402	1/1	0.94	0.09	-	50,50,50,50	0
58	MG	A	3441	1/1	0.93	0.14	-	73,73,73,73	0
58	MG	A	3261	1/1	0.91	0.23	-	61,61,61,61	0
58	MG	F	301	1/1	0.90	0.30	-	71,71,71,71	0
58	MG	A	3135	1/1	0.85	0.45	-	54,54,54,54	0
58	MG	A	3082	1/1	0.93	0.62	-	53,53,53,53	0
58	MG	A	3275	1/1	0.86	0.16	-	63,63,63,63	0
58	MG	A	3372	1/1	0.97	0.17	-	59,59,59,59	0
58	MG	A	3248	1/1	0.92	0.61	-	57,57,57,57	0
58	MG	A	3058	1/1	0.76	0.51	-	57,57,57,57	0
58	MG	A	3581	1/1	0.92	0.14	-	55,55,55,55	0
58	MG	A	3467	1/1	0.89	0.35	-	52,52,52,52	0
58	MG	A	3573	1/1	0.83	0.22	-	70,70,70,70	0
58	MG	A	3263	1/1	0.78	0.33	-	55,55,55,55	0
58	MG	A	3346	1/1	0.89	0.23	-	68,68,68,68	0
58	MG	a	3335	1/1	0.89	0.37	-	37,37,37,37	0
58	MG	a	3427	1/1	0.94	0.26	-	50,50,50,50	0
58	MG	a	3419	1/1	0.86	0.23	-	72,72,72,72	0
58	MG	A	3512	1/1	0.90	0.15	-	51,51,51,51	0
58	MG	A	3183	1/1	0.98	0.19	-	54,54,54,54	0
58	MG	A	3279	1/1	0.94	0.14	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3348	1/1	0.95	0.19	-	71,71,71,71	0
58	MG	A	3078	1/1	0.90	0.35	-	47,47,47,47	0
58	MG	A	3185	1/1	0.82	0.35	-	63,63,63,63	0
58	MG	B	201	1/1	0.95	0.33	-	51,51,51,51	0
58	MG	x	3001	1/1	0.51	0.28	-	237,237,237,237	0
58	MG	A	3101	1/1	0.80	0.32	-	74,74,74,74	0
58	MG	B	215	1/1	0.61	0.13	-	114,114,114,114	0
58	MG	A	3060	1/1	0.89	0.26	-	81,81,81,81	0
58	MG	A	3304	1/1	0.90	0.18	-	39,39,39,39	0
58	MG	A	3548	1/1	0.96	0.14	-	40,40,40,40	0
58	MG	a	3372	1/1	0.94	0.30	-	47,47,47,47	0
58	MG	A	3349	1/1	0.96	0.27	-	39,39,39,39	0
58	MG	a	3324	1/1	0.90	0.47	-	40,40,40,40	0
58	MG	A	3029	1/1	0.83	0.19	-	52,52,52,52	0
58	MG	A	3549	1/1	0.85	0.46	-	75,75,75,75	0
58	MG	A	3106	1/1	0.90	0.40	-	57,57,57,57	0
58	MG	A	3025	1/1	0.77	0.20	-	60,60,60,60	0
58	MG	A	3452	1/1	0.91	0.27	-	53,53,53,53	0
58	MG	A	3111	1/1	0.93	0.51	-	61,61,61,61	0
58	MG	A	3408	1/1	0.72	0.12	-	98,98,98,98	0
58	MG	a	3449	1/1	0.97	0.21	-	50,50,50,50	0
58	MG	a	3345	1/1	0.94	0.22	-	47,47,47,47	0
58	MG	a	3383	1/1	0.90	0.21	-	56,56,56,56	0
58	MG	A	3620	1/1	0.95	0.32	-	49,49,49,49	0
58	MG	A	3411	1/1	0.91	0.24	-	47,47,47,47	0
58	MG	a	3437	1/1	0.94	0.15	-	54,54,54,54	0
58	MG	w	104	1/1	0.96	0.09	-	38,38,38,38	0
58	MG	a	3347	1/1	0.96	0.23	-	41,41,41,41	0
58	MG	A	3595	1/1	0.93	0.15	-	63,63,63,63	0
58	MG	A	3322	1/1	0.90	0.24	-	61,61,61,61	0
58	MG	A	3367	1/1	0.90	0.48	-	51,51,51,51	0
58	MG	B	212	1/1	0.95	0.17	-	75,75,75,75	0
58	MG	a	3314	1/1	0.89	0.19	-	60,60,60,60	0
58	MG	A	3376	1/1	0.84	0.12	-	67,67,67,67	0
58	MG	A	3298	1/1	0.86	0.17	-	58,58,58,58	0
58	MG	a	3369	1/1	0.75	0.24	-	60,60,60,60	0
58	MG	a	3305	1/1	0.99	0.20	-	46,46,46,46	0
58	MG	A	3619	1/1	0.76	0.28	-	78,78,78,78	0
58	MG	A	3306	1/1	0.97	0.18	-	50,50,50,50	0
58	MG	A	3260	1/1	0.89	0.11	-	68,68,68,68	0
58	MG	B	211	1/1	0.90	0.34	-	61,61,61,61	0
58	MG	A	3392	1/1	0.93	0.22	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3227	1/1	0.92	0.44	-	43,43,43,43	0
58	MG	A	3124	1/1	0.83	0.14	-	54,54,54,54	0
58	MG	a	3470	1/1	0.93	0.15	-	56,56,56,56	0
58	MG	a	3353	1/1	0.92	0.15	-	48,48,48,48	0
58	MG	A	3131	1/1	0.90	0.29	-	53,53,53,53	0
58	MG	a	3473	1/1	0.97	0.45	-	43,43,43,43	0
58	MG	A	3216	1/1	0.65	0.36	-	62,62,62,62	0
58	MG	A	3605	1/1	0.90	0.24	-	70,70,70,70	0
58	MG	a	3417	1/1	0.96	0.31	-	37,37,37,37	0
58	MG	A	3290	1/1	0.91	0.23	-	49,49,49,49	0
58	MG	a	3336	1/1	0.90	0.29	-	62,62,62,62	0
58	MG	A	3121	1/1	0.84	0.18	-	62,62,62,62	0
58	MG	a	3329	1/1	0.84	0.16	-	46,46,46,46	0
58	MG	A	3236	1/1	0.81	0.55	-	67,67,67,67	0
58	MG	A	3044	1/1	0.73	0.37	-	72,72,72,72	0
58	MG	A	3110	1/1	0.86	0.28	-	42,42,42,42	0
58	MG	A	3335	1/1	0.89	0.10	-	56,56,56,56	0
58	MG	A	3089	1/1	0.88	0.19	-	47,47,47,47	0
58	MG	A	3571	1/1	0.91	0.37	-	89,89,89,89	0
58	MG	A	3531	1/1	0.94	0.07	-	91,91,91,91	0
58	MG	A	3281	1/1	0.89	0.14	-	57,57,57,57	0
58	MG	A	3612	1/1	0.97	0.05	-	53,53,53,53	0
58	MG	A	3085	1/1	0.85	0.34	-	52,52,52,52	0
58	MG	A	3314	1/1	0.95	0.23	-	54,54,54,54	0
58	MG	A	3505	1/1	0.92	0.18	-	68,68,68,68	0
58	MG	A	3156	1/1	0.96	0.08	-	86,86,86,86	0
58	MG	0	103	1/1	0.93	0.19	-	61,61,61,61	0
58	MG	A	3371	1/1	0.94	0.11	-	53,53,53,53	0
58	MG	A	3057	1/1	0.82	0.25	-	56,56,56,56	0
58	MG	A	3320	1/1	0.97	0.12	-	49,49,49,49	0
58	MG	B	209	1/1	0.64	0.27	-	70,70,70,70	0
58	MG	a	3408	1/1	0.93	0.12	-	55,55,55,55	0
58	MG	0	102	1/1	0.85	0.10	-	61,61,61,61	0
58	MG	a	3434	1/1	0.85	0.24	-	54,54,54,54	0
58	MG	A	3224	1/1	0.89	0.44	-	51,51,51,51	0
58	MG	a	3301	1/1	0.92	0.23	-	49,49,49,49	0
58	MG	7	103	1/1	0.86	0.26	-	57,57,57,57	0
58	MG	a	3377	1/1	0.83	0.22	-	85,85,85,85	0
58	MG	A	3235	1/1	0.90	0.14	-	48,48,48,48	0
58	MG	l	201	1/1	0.90	0.47	-	61,61,61,61	0
58	MG	B	218	1/1	0.95	0.23	-	74,74,74,74	0
58	MG	A	3576	1/1	0.83	0.34	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3547	1/1	0.97	0.20	-	60,60,60,60	0
58	MG	A	3611	1/1	0.89	0.20	-	52,52,52,52	0
58	MG	a	3352	1/1	0.79	0.25	-	59,59,59,59	0
58	MG	A	3377	1/1	0.98	0.16	-	44,44,44,44	0
58	MG	A	3073	1/1	0.80	0.45	-	56,56,56,56	0
58	MG	Q	203	1/1	0.86	0.21	-	45,45,45,45	0
58	MG	A	3247	1/1	0.82	0.42	-	66,66,66,66	0
58	MG	U	202	1/1	0.94	0.37	-	62,62,62,62	0
58	MG	A	3339	1/1	0.80	0.17	-	68,68,68,68	0
58	MG	A	3152	1/1	0.74	0.44	-	68,68,68,68	0
58	MG	A	3031	1/1	0.91	0.17	-	70,70,70,70	0
58	MG	A	3204	1/1	0.93	0.24	-	43,43,43,43	0
58	MG	A	3115	1/1	0.96	0.12	-	48,48,48,48	0
58	MG	A	3332	1/1	0.98	0.20	-	39,39,39,39	0
58	MG	A	3112	1/1	0.83	0.36	-	66,66,66,66	0
58	MG	A	3325	1/1	0.93	0.28	-	52,52,52,52	0
58	MG	A	3495	1/1	0.98	0.25	-	40,40,40,40	0
58	MG	A	3461	1/1	0.86	0.50	-	59,59,59,59	0
58	MG	a	3442	1/1	0.93	0.08	-	45,45,45,45	0
58	MG	a	3365	1/1	0.95	0.73	-	45,45,45,45	0
58	MG	A	3588	1/1	0.98	0.17	-	40,40,40,40	0
58	MG	A	3266	1/1	0.91	0.38	-	61,61,61,61	0
58	MG	a	3304	1/1	0.94	0.09	-	55,55,55,55	0
58	MG	A	3567	1/1	0.92	0.17	-	47,47,47,47	0
58	MG	A	3066	1/1	0.78	0.19	-	56,56,56,56	0
58	MG	a	3375	1/1	0.96	0.56	-	41,41,41,41	0
58	MG	A	3562	1/1	0.88	0.19	-	59,59,59,59	0
58	MG	a	3481	1/1	0.93	0.27	-	46,46,46,46	0
58	MG	A	3586	1/1	0.86	0.28	-	55,55,55,55	0
58	MG	A	3525	1/1	0.89	0.15	-	54,54,54,54	0
58	MG	A	3558	1/1	0.94	0.14	-	73,73,73,73	0
58	MG	A	3603	1/1	0.75	0.34	-	82,82,82,82	0
58	MG	A	3466	1/1	0.93	0.08	-	67,67,67,67	0
58	MG	A	3630	1/1	0.97	0.18	-	43,43,43,43	0
58	MG	A	3449	1/1	0.93	0.23	-	51,51,51,51	0
58	MG	m	201	1/1	0.95	0.20	-	35,35,35,35	0
58	MG	A	3334	1/1	0.67	0.13	-	84,84,84,84	0
58	MG	A	3256	1/1	0.98	0.14	-	55,55,55,55	0
58	MG	A	3434	1/1	0.84	0.22	-	56,56,56,56	0
58	MG	A	3343	1/1	0.90	0.13	-	69,69,69,69	0
58	MG	A	3069	1/1	0.91	0.23	-	46,46,46,46	0
58	MG	a	3379	1/1	0.98	0.21	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	a	3348	1/1	0.82	0.50	-	53,53,53,53	0
58	MG	A	3472	1/1	0.94	0.17	-	53,53,53,53	0
58	MG	A	3277	1/1	0.90	0.53	-	71,71,71,71	0
58	MG	A	3604	1/1	0.95	0.35	-	64,64,64,64	0
58	MG	A	3238	1/1	0.98	0.26	-	45,45,45,45	0
58	MG	A	3130	1/1	0.93	0.46	-	43,43,43,43	0
58	MG	a	3476	1/1	0.94	0.09	-	50,50,50,50	0
58	MG	A	3286	1/1	0.88	0.16	-	62,62,62,62	0
58	MG	A	3137	1/1	0.93	0.46	-	59,59,59,59	0
58	MG	A	3618	1/1	0.95	0.29	-	45,45,45,45	0
58	MG	A	3091	1/1	0.93	0.21	-	63,63,63,63	0
58	MG	A	3182	1/1	0.79	0.30	-	53,53,53,53	0
58	MG	A	3463	1/1	0.90	0.25	-	46,46,46,46	0
58	MG	A	3197	1/1	0.87	0.28	-	40,40,40,40	0
58	MG	A	3312	1/1	0.91	0.23	-	59,59,59,59	0
58	MG	A	3444	1/1	0.92	0.34	-	48,48,48,48	0
58	MG	A	3001	1/1	0.85	0.33	-	70,70,70,70	0
58	MG	A	3051	1/1	0.90	0.24	-	43,43,43,43	0
58	MG	a	3364	1/1	0.92	0.43	-	56,56,56,56	0
58	MG	Z	301	1/1	0.88	0.18	-	66,66,66,66	0
58	MG	A	3213	1/1	0.70	0.45	-	67,67,67,67	0
58	MG	A	3253	1/1	0.63	0.29	-	66,66,66,66	0
58	MG	A	3084	1/1	0.71	0.21	-	57,57,57,57	0
58	MG	A	3108	1/1	0.77	0.35	-	54,54,54,54	0
58	MG	A	3291	1/1	0.90	0.12	-	60,60,60,60	0
58	MG	w	101	1/1	0.87	0.75	-	60,60,60,60	0
58	MG	A	3012	1/1	0.96	0.15	-	37,37,37,37	0
58	MG	A	3326	1/1	0.88	0.17	-	69,69,69,69	0
58	MG	A	3427	1/1	0.95	0.16	-	62,62,62,62	0
58	MG	A	3569	1/1	0.82	0.45	-	85,85,85,85	0
58	MG	A	3596	1/1	0.83	0.20	-	45,45,45,45	0
58	MG	B	216	1/1	0.63	0.12	-	86,86,86,86	0
58	MG	A	3418	1/1	0.98	0.37	-	32,32,32,32	0
58	MG	A	3076	1/1	0.92	0.19	-	41,41,41,41	0
58	MG	a	3337	1/1	0.95	0.26	-	50,50,50,50	0
58	MG	A	3220	1/1	0.77	0.21	-	49,49,49,49	0
58	MG	A	3517	1/1	0.90	0.25	-	51,51,51,51	0
58	MG	A	3287	1/1	0.81	0.25	-	54,54,54,54	0
58	MG	A	3534	1/1	0.96	0.36	-	45,45,45,45	0
58	MG	D	305	1/1	0.82	0.18	-	37,37,37,37	0
58	MG	A	3578	1/1	0.91	0.23	-	64,64,64,64	0
58	MG	A	3307	1/1	0.96	0.20	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	a	3468	1/1	0.88	0.18	-	69,69,69,69	0
58	MG	A	3390	1/1	0.95	0.24	-	46,46,46,46	0
58	MG	A	3406	1/1	0.91	0.14	-	56,56,56,56	0
58	MG	A	3042	1/1	0.87	0.16	-	92,92,92,92	0
58	MG	A	3296	1/1	0.97	0.36	-	52,52,52,52	0
58	MG	A	3431	1/1	0.90	0.35	-	69,69,69,69	0
58	MG	A	3460	1/1	0.98	0.19	-	44,44,44,44	0
58	MG	a	3411	1/1	0.93	0.16	-	53,53,53,53	0
58	MG	a	3483	1/1	0.99	0.17	-	39,39,39,39	0
58	MG	a	3321	1/1	0.88	0.18	-	48,48,48,48	0
58	MG	X	101	1/1	0.90	0.23	-	72,72,72,72	0
58	MG	A	3528	1/1	0.98	0.09	-	51,51,51,51	0
58	MG	A	3257	1/1	0.96	0.18	-	50,50,50,50	0
58	MG	A	3186	1/1	0.89	0.16	-	90,90,90,90	0
58	MG	A	3245	1/1	0.81	0.28	-	56,56,56,56	0
58	MG	A	3268	1/1	0.88	0.26	-	58,58,58,58	0
58	MG	A	3488	1/1	0.97	0.31	-	50,50,50,50	0
58	MG	A	3533	1/1	0.90	0.18	-	47,47,47,47	0
58	MG	A	3360	1/1	0.83	0.21	-	60,60,60,60	0
58	MG	a	3367	1/1	0.96	0.25	-	30,30,30,30	0
58	MG	a	3410	1/1	0.87	0.37	-	45,45,45,45	0
58	MG	A	3309	1/1	0.87	0.26	-	52,52,52,52	0
58	MG	A	3276	1/1	0.85	0.07	-	73,73,73,73	0
58	MG	A	3180	1/1	0.95	0.64	-	44,44,44,44	0
58	MG	a	3450	1/1	0.85	0.08	-	55,55,55,55	0
58	MG	A	3361	1/1	0.92	0.12	-	84,84,84,84	0
58	MG	A	3451	1/1	0.85	0.18	-	82,82,82,82	0
58	MG	a	3315	1/1	0.89	0.22	-	60,60,60,60	0
58	MG	A	3457	1/1	0.97	0.20	-	41,41,41,41	0
58	MG	A	3584	1/1	0.93	0.24	-	62,62,62,62	0
58	MG	a	3370	1/1	0.91	0.18	-	66,66,66,66	0
58	MG	A	3061	1/1	0.91	0.22	-	54,54,54,54	0
58	MG	a	3326	1/1	0.92	0.21	-	48,48,48,48	0
58	MG	A	3369	1/1	0.97	0.17	-	54,54,54,54	0
58	MG	A	3338	1/1	0.97	0.28	-	30,30,30,30	0
58	MG	A	3265	1/1	0.60	0.18	-	61,61,61,61	0
58	MG	A	3280	1/1	0.95	0.28	-	32,32,32,32	0
58	MG	A	3328	1/1	0.84	0.20	-	62,62,62,62	0
58	MG	A	3613	1/1	0.93	0.17	-	52,52,52,52	0
58	MG	a	3380	1/1	0.90	0.22	-	57,57,57,57	0
58	MG	a	3366	1/1	0.89	0.23	-	38,38,38,38	0
58	MG	A	3175	1/1	0.83	0.38	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	a	3432	1/1	0.96	0.09	-	46,46,46,46	0
58	MG	A	3249	1/1	0.98	0.11	-	31,31,31,31	0
58	MG	a	3472	1/1	0.76	0.17	-	61,61,61,61	0
58	MG	B	214	1/1	0.61	1.51	-	83,83,83,83	0
58	MG	A	3090	1/1	0.96	0.38	-	38,38,38,38	0
58	MG	A	3283	1/1	0.97	0.12	-	55,55,55,55	0
58	MG	a	3340	1/1	0.88	0.45	-	81,81,81,81	0
58	MG	A	3136	1/1	0.92	0.40	-	49,49,49,49	0
58	MG	a	3404	1/1	0.96	0.44	-	38,38,38,38	0
58	MG	A	3210	1/1	0.94	0.21	-	56,56,56,56	0
58	MG	A	3629	1/1	0.94	0.20	-	70,70,70,70	0
58	MG	A	3243	1/1	0.84	0.55	-	58,58,58,58	0
58	MG	A	3178	1/1	0.97	0.23	-	31,31,31,31	0
58	MG	A	3241	1/1	0.94	0.15	-	42,42,42,42	0
58	MG	A	3299	1/1	0.91	0.19	-	64,64,64,64	0
58	MG	A	3065	1/1	0.94	0.25	-	74,74,74,74	0
58	MG	A	3510	1/1	0.96	0.16	-	60,60,60,60	0
58	MG	A	3285	1/1	0.88	0.25	-	50,50,50,50	0
58	MG	A	3202	1/1	0.94	0.37	-	50,50,50,50	0
58	MG	B	203	1/1	0.96	0.07	-	56,56,56,56	0
58	MG	a	3317	1/1	0.97	0.31	-	26,26,26,26	0
58	MG	A	3096	1/1	0.94	0.23	-	58,58,58,58	0
58	MG	B	202	1/1	0.98	0.27	-	66,66,66,66	0
58	MG	A	3484	1/1	0.93	0.14	-	50,50,50,50	0
58	MG	A	3527	1/1	0.96	0.20	-	63,63,63,63	0
58	MG	A	3511	1/1	0.91	0.17	-	99,99,99,99	0
58	MG	a	3421	1/1	0.88	0.11	-	61,61,61,61	0
58	MG	A	3489	1/1	0.94	0.12	-	55,55,55,55	0
58	MG	a	3436	1/1	0.80	0.26	-	66,66,66,66	0
58	MG	A	3003	1/1	0.82	0.30	-	59,59,59,59	0
58	MG	A	3566	1/1	0.96	0.11	-	40,40,40,40	0
58	MG	A	3345	1/1	0.92	0.20	-	44,44,44,44	0
58	MG	A	3518	1/1	0.98	0.04	-	65,65,65,65	0
58	MG	A	3036	1/1	0.92	0.11	-	74,74,74,74	0
58	MG	A	3267	1/1	0.96	0.27	-	59,59,59,59	0
58	MG	A	3579	1/1	0.97	0.19	-	53,53,53,53	0
58	MG	A	3062	1/1	0.90	0.26	-	42,42,42,42	0
58	MG	A	3585	1/1	0.89	0.18	-	47,47,47,47	0
58	MG	A	3416	1/1	0.98	0.21	-	41,41,41,41	0
58	MG	a	3431	1/1	0.93	0.10	-	41,41,41,41	0
58	MG	A	3477	1/1	0.95	0.14	-	65,65,65,65	0
58	MG	a	3485	1/1	0.94	0.25	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3608	1/1	0.29	0.47	-	108,108,108,108	0
58	MG	A	3194	1/1	0.98	0.34	-	34,34,34,34	0
58	MG	A	3439	1/1	0.93	0.18	-	58,58,58,58	0
58	MG	A	3098	1/1	0.96	0.15	-	48,48,48,48	0
58	MG	A	3383	1/1	0.85	0.24	-	55,55,55,55	0
58	MG	A	3242	1/1	0.90	0.11	-	63,63,63,63	0
58	MG	A	3543	1/1	0.88	0.14	-	71,71,71,71	0
58	MG	A	3507	1/1	0.89	0.17	-	46,46,46,46	0
58	MG	A	3621	1/1	0.93	0.30	-	59,59,59,59	0
58	MG	a	3458	1/1	0.86	0.26	-	62,62,62,62	0
58	MG	a	3325	1/1	0.91	0.82	-	55,55,55,55	0
58	MG	a	3386	1/1	0.95	0.47	-	41,41,41,41	0
58	MG	A	3627	1/1	0.92	0.14	-	91,91,91,91	0
58	MG	E	303	1/1	0.92	0.19	-	41,41,41,41	0
58	MG	A	3563	1/1	0.83	0.19	-	73,73,73,73	0
58	MG	A	3356	1/1	0.92	0.24	-	57,57,57,57	0
58	MG	A	3168	1/1	0.91	0.41	-	48,48,48,48	0
58	MG	a	3453	1/1	0.97	0.07	-	41,41,41,41	0
58	MG	A	3016	1/1	0.93	0.14	-	49,49,49,49	0
58	MG	B	217	1/1	0.81	0.27	-	67,67,67,67	0
58	MG	A	3401	1/1	0.94	0.11	-	37,37,37,37	0
58	MG	A	3577	1/1	0.67	0.20	-	72,72,72,72	0
58	MG	A	3292	1/1	0.96	0.23	-	54,54,54,54	0
58	MG	a	3388	1/1	0.73	0.23	-	59,59,59,59	0
58	MG	f	201	1/1	0.83	0.25	-	92,92,92,92	0
58	MG	0	101	1/1	0.62	0.39	-	73,73,73,73	0
58	MG	A	3421	1/1	0.98	0.18	-	40,40,40,40	0
58	MG	A	3145	1/1	0.88	0.09	-	48,48,48,48	0
58	MG	a	3341	1/1	0.87	0.27	-	60,60,60,60	0
58	MG	a	3424	1/1	0.92	0.11	-	43,43,43,43	0
58	MG	A	3635	1/1	0.81	0.62	-	69,69,69,69	0
58	MG	a	3461	1/1	0.93	0.14	-	44,44,44,44	0
58	MG	A	3063	1/1	0.90	0.16	-	62,62,62,62	0
58	MG	A	3288	1/1	0.82	0.33	-	60,60,60,60	0
58	MG	a	3344	1/1	0.96	0.12	-	51,51,51,51	0
58	MG	A	3038	1/1	0.99	0.15	-	55,55,55,55	0
58	MG	a	3361	1/1	0.89	0.15	-	73,73,73,73	0
58	MG	A	3337	1/1	0.97	0.27	-	44,44,44,44	0
58	MG	a	3322	1/1	0.97	0.10	-	50,50,50,50	0
58	MG	A	3575	1/1	0.91	0.09	-	70,70,70,70	0
58	MG	A	3624	1/1	0.89	0.15	-	52,52,52,52	0
58	MG	A	3398	1/1	0.92	0.26	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3177	1/1	0.92	0.17	-	65,65,65,65	0
58	MG	A	3628	1/1	0.94	0.16	-	87,87,87,87	0
58	MG	F	303	1/1	0.93	0.11	-	36,36,36,36	0
58	MG	A	3478	1/1	0.88	0.11	-	65,65,65,65	0
58	MG	A	3353	1/1	0.86	0.17	-	79,79,79,79	0
58	MG	A	3122	1/1	0.83	0.19	-	35,35,35,35	0
58	MG	A	3254	1/1	0.74	0.37	-	67,67,67,67	0
58	MG	A	3497	1/1	0.92	0.25	-	50,50,50,50	0
58	MG	O	201	1/1	0.97	0.10	-	38,38,38,38	0
58	MG	A	3255	1/1	0.81	0.32	-	57,57,57,57	0
58	MG	A	3129	1/1	0.87	0.24	-	48,48,48,48	0
58	MG	a	3316	1/1	0.74	0.25	-	54,54,54,54	0
58	MG	A	3385	1/1	0.96	0.19	-	57,57,57,57	0
58	MG	a	3328	1/1	0.86	0.25	-	60,60,60,60	0
58	MG	a	3463	1/1	0.94	0.21	-	45,45,45,45	0
58	MG	A	3491	1/1	0.91	0.26	-	72,72,72,72	0
58	MG	A	3142	1/1	0.90	0.10	-	84,84,84,84	0
58	MG	B	206	1/1	0.82	0.17	-	75,75,75,75	0
58	MG	A	3453	1/1	0.95	0.16	-	44,44,44,44	0
58	MG	A	3064	1/1	0.89	0.37	-	50,50,50,50	0
58	MG	A	3284	1/1	0.76	0.28	-	67,67,67,67	0
58	MG	A	3422	1/1	0.96	0.18	-	52,52,52,52	0
58	MG	A	3535	1/1	0.97	0.21	-	49,49,49,49	0
58	MG	A	3381	1/1	0.96	0.24	-	43,43,43,43	0
58	MG	w	105	1/1	0.94	0.24	-	29,29,29,29	0
58	MG	A	3258	1/1	0.94	0.21	-	43,43,43,43	0
58	MG	a	3332	1/1	0.84	0.16	-	45,45,45,45	0
58	MG	A	3425	1/1	0.92	0.23	-	62,62,62,62	0
58	MG	A	3146	1/1	0.92	0.27	-	56,56,56,56	0
58	MG	A	3212	1/1	0.87	0.15	-	55,55,55,55	0
58	MG	A	3496	1/1	0.96	0.18	-	47,47,47,47	0
58	MG	a	3373	1/1	0.86	0.24	-	63,63,63,63	0
58	MG	A	3471	1/1	0.92	0.33	-	56,56,56,56	0
58	MG	A	3300	1/1	0.95	0.17	-	60,60,60,60	0
58	MG	a	3371	1/1	0.81	0.25	-	65,65,65,65	0
58	MG	A	3521	1/1	0.99	0.22	-	60,60,60,60	0
58	MG	A	3379	1/1	0.94	0.25	-	50,50,50,50	0
58	MG	a	3455	1/1	0.70	0.10	-	67,67,67,67	0
58	MG	A	3436	1/1	0.85	0.17	-	87,87,87,87	0
58	MG	A	3075	1/1	0.76	0.17	-	67,67,67,67	0
58	MG	A	3597	1/1	0.96	0.27	-	65,65,65,65	0
58	MG	A	3055	1/1	0.97	0.12	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3357	1/1	0.82	0.24	-	69,69,69,69	0
58	MG	A	3035	1/1	0.95	0.09	-	47,47,47,47	0
58	MG	D	304	1/1	0.91	0.36	-	74,74,74,74	0
58	MG	A	3625	1/1	0.92	0.19	-	84,84,84,84	0
58	MG	A	3305	1/1	0.81	0.28	-	70,70,70,70	0
58	MG	A	3429	1/1	0.98	0.25	-	30,30,30,30	0
58	MG	A	3409	1/1	0.97	0.25	-	60,60,60,60	0
58	MG	A	3600	1/1	0.86	0.25	-	64,64,64,64	0
58	MG	A	3539	1/1	0.96	0.13	-	52,52,52,52	0
58	MG	a	3398	1/1	0.97	0.39	-	27,27,27,27	0
58	MG	A	3315	1/1	0.94	0.26	-	56,56,56,56	0
58	MG	A	3572	1/1	0.68	0.38	-	70,70,70,70	0
58	MG	A	3104	1/1	0.87	0.21	-	64,64,64,64	0
58	MG	A	3519	1/1	0.97	0.30	-	30,30,30,30	0
58	MG	A	3556	1/1	0.96	0.16	-	55,55,55,55	0
58	MG	a	3359	1/1	0.88	0.14	-	65,65,65,65	0
58	MG	a	3462	1/1	0.92	0.13	-	74,74,74,74	0
58	MG	A	3617	1/1	0.81	0.19	-	65,65,65,65	0
58	MG	B	205	1/1	0.96	0.22	-	81,81,81,81	0
58	MG	A	3435	1/1	0.38	0.39	-	95,95,95,95	0
58	MG	A	3088	1/1	0.96	0.15	-	63,63,63,63	0
58	MG	a	3464	1/1	0.95	0.07	-	44,44,44,44	0
58	MG	A	3432	1/1	0.92	0.19	-	58,58,58,58	0
58	MG	A	3336	1/1	0.92	0.22	-	36,36,36,36	0
58	MG	a	3474	1/1	0.88	0.16	-	64,64,64,64	0
58	MG	A	3482	1/1	0.93	0.09	-	67,67,67,67	0
58	MG	A	3014	1/1	0.87	0.14	-	39,39,39,39	0
58	MG	A	3631	1/1	0.91	0.24	-	87,87,87,87	0
58	MG	a	3356	1/1	0.93	0.22	-	49,49,49,49	0
58	MG	A	3387	1/1	0.96	0.17	-	53,53,53,53	0
58	MG	A	3237	1/1	0.88	0.16	-	51,51,51,51	0
58	MG	a	3469	1/1	0.95	0.38	-	42,42,42,42	0
58	MG	A	3465	1/1	0.89	0.15	-	68,68,68,68	0
58	MG	a	3479	1/1	0.97	0.18	-	47,47,47,47	0
58	MG	A	3148	1/1	0.86	0.38	-	60,60,60,60	0
58	MG	A	3053	1/1	0.89	0.45	-	61,61,61,61	0
58	MG	a	3460	1/1	0.97	0.14	-	52,52,52,52	0
58	MG	a	3354	1/1	0.94	0.13	-	51,51,51,51	0
58	MG	G	201	1/1	0.89	0.16	-	71,71,71,71	0
58	MG	A	3599	1/1	0.96	0.21	-	57,57,57,57	0
58	MG	a	3425	1/1	0.84	0.25	-	47,47,47,47	0
58	MG	A	3424	1/1	0.97	0.27	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	B	208	1/1	0.73	0.11	-	74,74,74,74	0
58	MG	A	3262	1/1	0.91	0.08	-	63,63,63,63	0
58	MG	A	3592	1/1	0.98	0.08	-	67,67,67,67	0
58	MG	A	3113	1/1	0.76	0.31	-	63,63,63,63	0
58	MG	A	3504	1/1	0.92	0.37	-	38,38,38,38	0
58	MG	P	202	1/1	0.85	0.27	-	86,86,86,86	0
58	MG	A	3615	1/1	0.85	0.23	-	50,50,50,50	0
58	MG	A	3179	1/1	0.98	0.18	-	43,43,43,43	0
58	MG	a	3484	1/1	0.83	0.23	-	67,67,67,67	0
58	MG	A	3589	1/1	0.85	0.24	-	46,46,46,46	0
58	MG	A	3169	1/1	0.97	0.29	-	57,57,57,57	0
58	MG	a	3465	1/1	0.98	0.07	-	57,57,57,57	0
58	MG	A	3426	1/1	0.83	0.28	-	55,55,55,55	0
58	MG	A	3464	1/1	0.89	0.25	-	49,49,49,49	0
58	MG	A	3354	1/1	0.66	0.24	-	101,101,101,101	0
58	MG	A	3561	1/1	0.96	0.14	-	54,54,54,54	0
58	MG	A	3502	1/1	0.88	0.25	-	56,56,56,56	0
58	MG	a	3482	1/1	0.97	0.14	-	37,37,37,37	0
58	MG	A	3333	1/1	0.94	0.08	-	62,62,62,62	0
58	MG	w	103	1/1	0.94	0.18	-	38,38,38,38	0
58	MG	A	3524	1/1	0.94	0.11	-	53,53,53,53	0
58	MG	A	3160	1/1	0.66	0.48	-	61,61,61,61	0
58	MG	a	3445	1/1	0.93	0.20	-	66,66,66,66	0
58	MG	A	3582	1/1	0.95	0.15	-	63,63,63,63	0
58	MG	A	3226	1/1	0.72	0.43	-	68,68,68,68	0
58	MG	A	3132	1/1	0.70	0.77	-	48,48,48,48	0
58	MG	A	3228	1/1	0.95	0.19	-	62,62,62,62	0
58	MG	a	3320	1/1	0.94	0.14	-	39,39,39,39	0
58	MG	A	3105	1/1	0.94	0.12	-	35,35,35,35	0
58	MG	A	3522	1/1	0.96	0.17	-	51,51,51,51	0
58	MG	A	3264	1/1	0.88	0.33	-	65,65,65,65	0
58	MG	A	3542	1/1	0.93	0.65	-	60,60,60,60	0
58	MG	a	3426	1/1	0.85	0.13	-	69,69,69,69	0
58	MG	a	3480	1/1	0.78	0.27	-	77,77,77,77	0
58	MG	A	3318	1/1	0.96	0.32	-	60,60,60,60	0
58	MG	G	203	1/1	0.94	0.09	-	69,69,69,69	0
58	MG	A	3037	1/1	0.90	0.27	-	61,61,61,61	0
58	MG	A	3273	1/1	0.81	0.42	-	77,77,77,77	0
58	MG	A	3232	1/1	0.92	0.30	-	36,36,36,36	0
58	MG	A	3218	1/1	0.95	0.45	-	32,32,32,32	0
58	MG	a	3413	1/1	0.88	0.14	-	54,54,54,54	0
58	MG	A	3099	1/1	0.92	0.20	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3538	1/1	0.97	0.17	-	40,40,40,40	0
58	MG	A	3389	1/1	0.97	0.25	-	30,30,30,30	0
58	MG	a	3363	1/1	0.94	0.24	-	43,43,43,43	0
58	MG	A	3040	1/1	0.80	0.27	-	58,58,58,58	0
58	MG	A	3094	1/1	0.99	0.27	-	31,31,31,31	0
58	MG	a	3441	1/1	0.94	0.19	-	62,62,62,62	0
58	MG	A	3587	1/1	0.96	0.25	-	48,48,48,48	0
58	MG	A	3458	1/1	0.97	0.32	-	27,27,27,27	0
58	MG	A	3350	1/1	0.87	0.10	-	63,63,63,63	0
58	MG	A	3386	1/1	0.90	0.17	-	59,59,59,59	0
58	MG	A	3622	1/1	0.94	0.23	-	49,49,49,49	0
58	MG	A	3310	1/1	0.94	0.14	-	45,45,45,45	0
58	MG	a	3430	1/1	0.95	0.08	-	65,65,65,65	0
58	MG	A	3259	1/1	0.81	0.09	-	74,74,74,74	0
58	MG	a	3478	1/1	0.97	0.13	-	48,48,48,48	0
58	MG	A	3443	1/1	0.98	0.14	-	39,39,39,39	0
58	MG	A	3211	1/1	0.93	0.47	-	55,55,55,55	0
58	MG	a	3333	1/1	0.93	0.16	-	51,51,51,51	0
58	MG	A	3013	1/1	0.88	0.21	-	52,52,52,52	0
58	MG	F	305	1/1	0.85	0.25	-	59,59,59,59	0
58	MG	a	3362	1/1	0.87	0.16	-	73,73,73,73	0
58	MG	A	3028	1/1	0.94	0.27	-	66,66,66,66	0
58	MG	A	3327	1/1	0.93	0.14	-	49,49,49,49	0
58	MG	A	3574	1/1	0.87	0.16	-	57,57,57,57	0
58	MG	a	3407	1/1	0.92	0.34	-	82,82,82,82	0
58	MG	A	3368	1/1	0.95	0.23	-	47,47,47,47	0
58	MG	A	3370	1/1	0.87	0.16	-	64,64,64,64	0
58	MG	A	3405	1/1	0.83	0.15	-	61,61,61,61	0
58	MG	A	3138	1/1	0.92	0.22	-	77,77,77,77	0
58	MG	A	3330	1/1	0.89	0.34	-	55,55,55,55	0
58	MG	A	3373	1/1	0.87	0.08	-	64,64,64,64	0
58	MG	A	3570	1/1	0.81	0.17	-	57,57,57,57	0
58	MG	A	3153	1/1	0.93	0.22	-	82,82,82,82	0
58	MG	a	3444	1/1	0.95	0.16	-	53,53,53,53	0
58	MG	A	3419	1/1	0.89	0.13	-	74,74,74,74	0
58	MG	A	3440	1/1	0.96	0.20	-	74,74,74,74	0
58	MG	A	3269	1/1	0.89	0.23	-	54,54,54,54	0
58	MG	W	201	1/1	0.91	1.25	-	77,77,77,77	0
58	MG	A	3081	1/1	0.85	0.28	-	61,61,61,61	0
58	MG	A	3554	1/1	0.71	0.21	-	74,74,74,74	0
58	MG	A	3391	1/1	0.97	0.21	-	30,30,30,30	0
58	MG	a	3392	1/1	0.74	0.14	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
58	MG	A	3329	1/1	0.98	0.14	-	40,40,40,40	0
58	MG	A	3151	1/1	0.95	0.29	-	43,43,43,43	0
58	MG	U	203	1/1	0.54	0.46	-	67,67,67,67	0
58	MG	A	3483	1/1	0.98	0.17	-	55,55,55,55	0
58	MG	A	3448	1/1	0.91	0.44	-	48,48,48,48	0
58	MG	A	3068	1/1	0.66	0.28	-	56,56,56,56	0

6.5 Other polymers

There are no such residues in this entry.