



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2017 – 01:22 AM EDT

PDB ID : 5J8B
Title : Crystal structure of Elongation Factor 4 (EF-4/LepA) in complex with
GDP-CP bound to the Thermus thermophilus 70S ribosome
Authors : Gagnon, M.G.; Lin, J.; Steitz, T.A.
Deposited on : unknown
Resolution : 2.60 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

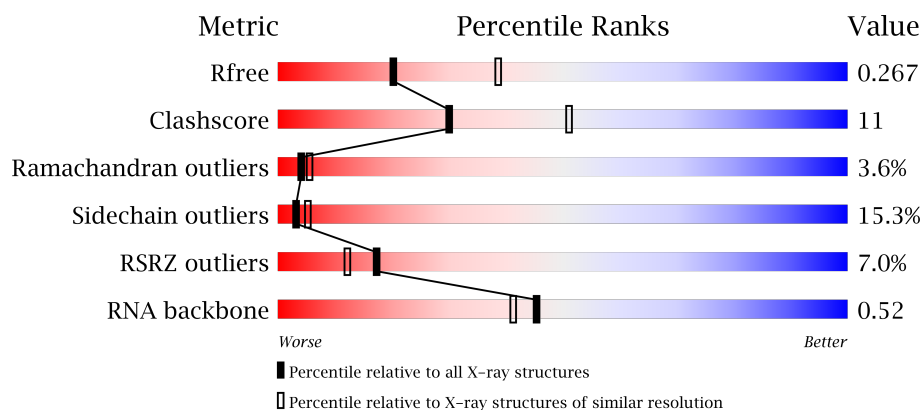
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)
RNA backbone	2435	1140 (3.00-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	2915	<div> <div>5%</div> <div> <div>56%</div> <div>32%</div> <div>9%</div> <div>..</div> </div> </div>
2	B	121	<div> <div>62%</div> <div>32%</div> <div>5%</div> <div>.</div> </div>
3	C	228	<div> <div>26%</div> <div>22%</div> <div>29%</div> <div>8%</div> <div>40%</div> </div>
4	D	276	<div> <div>68%</div> <div>25%</div> <div>7%</div> </div>

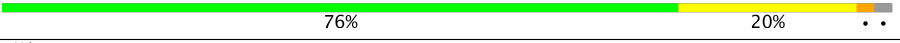










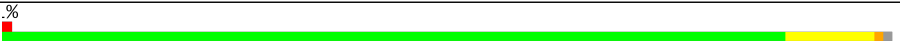




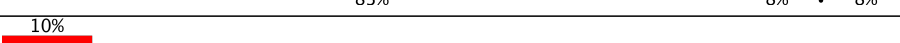
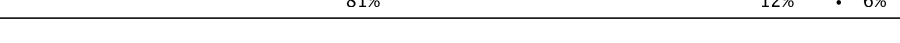



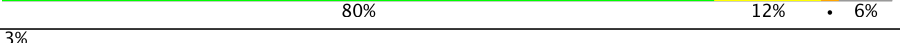



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Mol	Chain	Length	Quality of chain
5	E	206	
6	F	210	
7	G	182	
8	H	180	
9	J	173	
10	K	147	
11	N	140	
12	O	122	
13	P	150	
14	Q	141	
15	R	118	
16	S	112	
17	T	146	
18	U	118	
19	V	101	
20	W	113	
21	X	96	
22	Y	110	
23	Z	206	
24	0	85	
25	1	98	
26	2	72	
27	3	60	
28	4	71	
29	5	60	

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Mol	Chain	Length	Quality of chain
30	6	54	
31	7	49	
32	8	65	
33	9	37	
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	v	24	
56	w	76	
57	x	77	
58	y	76	
59	z	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
60	MG	0	102	-	-	-	X
60	MG	0	104	-	-	-	X
60	MG	5	101	-	-	-	X
60	MG	6	101	-	-	-	X
60	MG	A	3003	-	-	-	X
60	MG	A	3004	-	-	-	X
60	MG	A	3006	-	-	-	X
60	MG	A	3007	-	-	-	X
60	MG	A	3010	-	-	-	X
60	MG	A	3018	-	-	-	X
60	MG	A	3019	-	-	-	X
60	MG	A	3024	-	-	-	X
60	MG	A	3029	-	-	-	X
60	MG	A	3031	-	-	-	X
60	MG	A	3035	-	-	-	X
60	MG	A	3036	-	-	-	X
60	MG	A	3038	-	-	-	X
60	MG	A	3042	-	-	-	X
60	MG	A	3043	-	-	-	X
60	MG	A	3045	-	-	-	X
60	MG	A	3053	-	-	-	X
60	MG	A	3056	-	-	-	X
60	MG	A	3069	-	-	-	X
60	MG	A	3073	-	-	-	X
60	MG	A	3099	-	-	-	X
60	MG	A	3109	-	-	-	X
60	MG	A	3112	-	-	-	X
60	MG	A	3113	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	A	3114	-	-	-	X
60	MG	A	3115	-	-	-	X
60	MG	A	3120	-	-	-	X
60	MG	A	3136	-	-	-	X
60	MG	A	3137	-	-	-	X
60	MG	A	3147	-	-	-	X
60	MG	A	3157	-	-	-	X
60	MG	A	3158	-	-	-	X
60	MG	A	3162	-	-	-	X
60	MG	A	3165	-	-	-	X
60	MG	A	3168	-	-	-	X
60	MG	A	3169	-	-	-	X
60	MG	A	3174	-	-	-	X
60	MG	A	3177	-	-	-	X
60	MG	A	3180	-	-	-	X
60	MG	A	3181	-	-	-	X
60	MG	A	3182	-	-	-	X
60	MG	A	3183	-	-	-	X
60	MG	A	3185	-	-	-	X
60	MG	A	3189	-	-	-	X
60	MG	A	3193	-	-	-	X
60	MG	A	3199	-	-	-	X
60	MG	A	3201	-	-	-	X
60	MG	A	3211	-	-	-	X
60	MG	A	3214	-	-	-	X
60	MG	A	3216	-	-	-	X
60	MG	A	3217	-	-	-	X
60	MG	A	3221	-	-	-	X
60	MG	A	3224	-	-	-	X
60	MG	A	3225	-	-	-	X
60	MG	A	3228	-	-	-	X
60	MG	A	3230	-	-	-	X
60	MG	A	3235	-	-	-	X
60	MG	A	3238	-	-	-	X
60	MG	A	3241	-	-	-	X
60	MG	A	3246	-	-	-	X
60	MG	A	3256	-	-	-	X
60	MG	A	3258	-	-	-	X
60	MG	A	3264	-	-	-	X
60	MG	A	3279	-	-	-	X
60	MG	A	3283	-	-	-	X
60	MG	A	3284	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	A	3285	-	-	-	X
60	MG	A	3286	-	-	-	X
60	MG	A	3291	-	-	-	X
60	MG	A	3297	-	-	-	X
60	MG	A	3300	-	-	-	X
60	MG	A	3308	-	-	-	X
60	MG	A	3319	-	-	-	X
60	MG	A	3320	-	-	-	X
60	MG	A	3327	-	-	-	X
60	MG	A	3330	-	-	-	X
60	MG	A	3331	-	-	-	X
60	MG	A	3334	-	-	-	X
60	MG	A	3341	-	-	-	X
60	MG	A	3347	-	-	-	X
60	MG	A	3351	-	-	-	X
60	MG	A	3352	-	-	-	X
60	MG	A	3354	-	-	-	X
60	MG	A	3360	-	-	-	X
60	MG	A	3363	-	-	-	X
60	MG	A	3370	-	-	-	X
60	MG	A	3371	-	-	-	X
60	MG	A	3373	-	-	-	X
60	MG	A	3374	-	-	-	X
60	MG	A	3377	-	-	-	X
60	MG	A	3378	-	-	-	X
60	MG	A	3382	-	-	-	X
60	MG	A	3384	-	-	-	X
60	MG	A	3387	-	-	-	X
60	MG	A	3391	-	-	-	X
60	MG	A	3397	-	-	-	X
60	MG	A	3401	-	-	-	X
60	MG	A	3404	-	-	-	X
60	MG	A	3417	-	-	-	X
60	MG	A	3424	-	-	-	X
60	MG	A	3429	-	-	-	X
60	MG	A	3431	-	-	-	X
60	MG	A	3433	-	-	-	X
60	MG	A	3449	-	-	-	X
60	MG	A	3455	-	-	-	X
60	MG	A	3463	-	-	-	X
60	MG	A	3472	-	-	-	X
60	MG	A	3474	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	A	3477	-	-	-	X
60	MG	A	3480	-	-	-	X
60	MG	A	3488	-	-	-	X
60	MG	A	3496	-	-	-	X
60	MG	A	3506	-	-	-	X
60	MG	A	3515	-	-	-	X
60	MG	A	3523	-	-	-	X
60	MG	A	3525	-	-	-	X
60	MG	A	3530	-	-	-	X
60	MG	A	3531	-	-	-	X
60	MG	A	3553	-	-	-	X
60	MG	A	3580	-	-	-	X
60	MG	A	3585	-	-	-	X
60	MG	A	3595	-	-	-	X
60	MG	A	3596	-	-	-	X
60	MG	A	3602	-	-	-	X
60	MG	A	3608	-	-	-	X
60	MG	A	3626	-	-	-	X
60	MG	A	3627	-	-	-	X
60	MG	A	3628	-	-	-	X
60	MG	A	3630	-	-	-	X
60	MG	A	3631	-	-	-	X
60	MG	A	3632	-	-	-	X
60	MG	A	3633	-	-	-	X
60	MG	A	3635	-	-	-	X
60	MG	A	3636	-	-	-	X
60	MG	A	3638	-	-	-	X
60	MG	A	3639	-	-	-	X
60	MG	A	3642	-	-	-	X
60	MG	A	3643	-	-	-	X
60	MG	A	3644	-	-	-	X
60	MG	D	301	-	-	-	X
60	MG	D	303	-	-	-	X
60	MG	D	304	-	-	-	X
60	MG	E	303	-	-	-	X
60	MG	F	301	-	-	-	X
60	MG	F	302	-	-	-	X
60	MG	F	303	-	-	-	X
60	MG	F	304	-	-	-	X
60	MG	N	201	-	-	-	X
60	MG	Q	202	-	-	-	X
60	MG	U	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	a	1608	-	-	-	X
60	MG	a	1610	-	-	-	X
60	MG	a	1613	-	-	-	X
60	MG	a	1619	-	-	-	X
60	MG	a	1622	-	-	-	X
60	MG	a	1632	-	-	-	X
60	MG	a	1659	-	-	-	X
60	MG	a	1660	-	-	-	X
60	MG	a	1662	-	-	-	X
60	MG	a	1671	-	-	-	X
60	MG	a	1678	-	-	-	X
60	MG	a	1682	-	-	-	X
60	MG	a	1683	-	-	-	X
60	MG	a	1687	-	-	-	X
60	MG	a	1688	-	-	-	X
60	MG	a	1693	-	-	-	X
60	MG	a	1695	-	-	-	X
60	MG	a	1702	-	-	-	X
60	MG	a	1712	-	-	-	X
60	MG	a	1717	-	-	-	X
60	MG	a	1724	-	-	-	X
60	MG	a	1740	-	-	-	X
60	MG	a	1743	-	-	-	X
60	MG	a	1752	-	-	-	X
60	MG	a	1766	-	-	-	X
60	MG	a	1778	-	-	-	X
60	MG	a	1786	-	-	-	X
60	MG	n	102	-	-	-	X
60	MG	n	103	-	-	-	X
61	ZN	6	102	-	-	-	X

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155465 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
1	A	2874	Total	C	N	O	P	11	0	0
			61902	27550	11582	19897	2873			

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

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

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	136	Total	C	N	O	S	1	0	0
			1024	644	190	189	1			

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L10.

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

- Molecule 10 is a protein called 50S ribosomal protein L11.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

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

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

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

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	107	Total	C	N	O	S	1	0	0
			806	517	152	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	94	Total	C	N	O	S	0	0	0
			784	499	150	134	1			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	0	74	Total	C	N	O	S	0	0	0
			591	366	126	98	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	69	Total	C	N	O	S	0	0	0
			557	350	101	101	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	a	1498	Total	C	N	O	P	4	0	0
			32207	14334	5973	10402	1498			

- 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	C	N	O	0	0	0
			983	623	193	167			

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

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

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

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

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

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

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

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

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

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

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

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

- 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 mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 56 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	w	74	Total	C	N	O	P	S	1	0	0
			1586	713	285	513	73	2			

- Molecule 57 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	x	77	Total	C	N	O	P	S	3	0	0
			1645	734	297	536	77	1			

- Molecule 58 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
58	y	74	Total	C	N	O	P	S	0	0	0
			1580	706	285	515	73	1			

- Molecule 59 is a protein called GDPCP fused to the N-terminus of the ribosomal protein L9,Elongation factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	z	671	Total	C	N	O	S	0	0	0
			5200	3333	897	961	9			

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	P	3	Total	Mg	0	0
			3	3		
60	B	18	Total	Mg	0	0
			18	18		
60	6	2	Total	Mg	0	0
			2	2		
60	W	1	Total	Mg	0	0
			1	1		
60	N	1	Total	Mg	0	0
			1	1		
60	X	1	Total	Mg	0	0
			1	1		
60	f	1	Total	Mg	0	0
			1	1		
60	E	5	Total	Mg	0	0
			5	5		
60	V	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	A	644	Total 644	Mg 644	0	0
60	n	3	Total 3	Mg 3	0	0
60	5	2	Total 2	Mg 2	0	0
60	x	9	Total 9	Mg 9	0	0
60	R	2	Total 2	Mg 2	0	0
60	D	6	Total 6	Mg 6	0	0
60	e	1	Total 1	Mg 1	0	0
60	v	2	Total 2	Mg 2	0	0
60	Z	1	Total 1	Mg 1	0	0
60	a	188	Total 188	Mg 188	0	0
60	U	1	Total 1	Mg 1	0	0
60	9	1	Total 1	Mg 1	0	0
60	m	2	Total 2	Mg 2	0	0
60	0	4	Total 4	Mg 4	0	0
60	G	2	Total 2	Mg 2	0	0
60	Q	2	Total 2	Mg 2	0	0
60	d	1	Total 1	Mg 1	0	0
60	H	1	Total 1	Mg 1	0	0
60	7	1	Total 1	Mg 1	0	0
60	z	2	Total 2	Mg 2	0	0
60	8	1	Total 1	Mg 1	0	0

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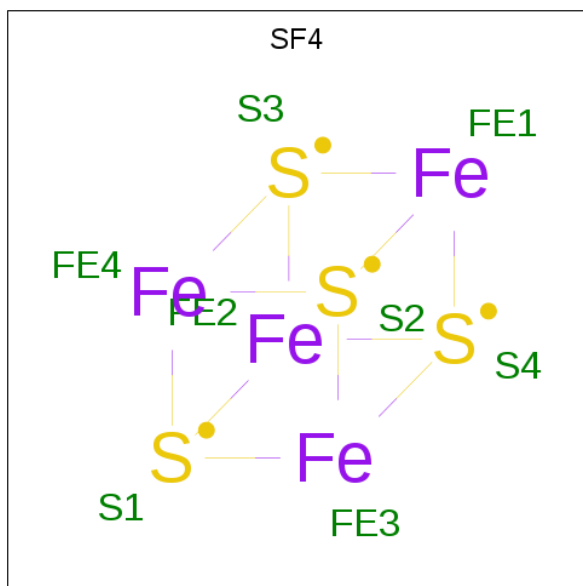
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	O	2	Total	Mg	0	0
			2	2		
60	l	1	Total	Mg	0	0
			1	1		
60	F	6	Total	Mg	0	0
			6	6		

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

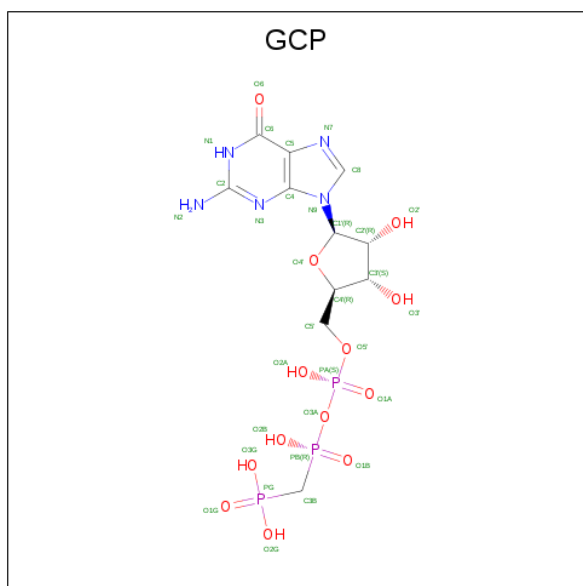
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	Y	1	Total	Zn	0	0
			1	1		
61	6	1	Total	Zn	0	0
			1	1		
61	4	1	Total	Zn	0	0
			1	1		
61	n	1	Total	Zn	0	0
			1	1		
61	5	1	Total	Zn	0	0
			1	1		
61	9	1	Total	Zn	0	0
			1	1		

- Molecule 62 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 63 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
63	z	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	A	715	Total	O	0	0
			715	715		
64	B	32	Total	O	0	0
			32	32		
64	D	4	Total	O	0	0
			4	4		
64	E	6	Total	O	0	0
			6	6		
64	F	5	Total	O	0	0
			5	5		
64	H	1	Total	O	0	0
			1	1		
64	N	1	Total	O	0	0
			1	1		

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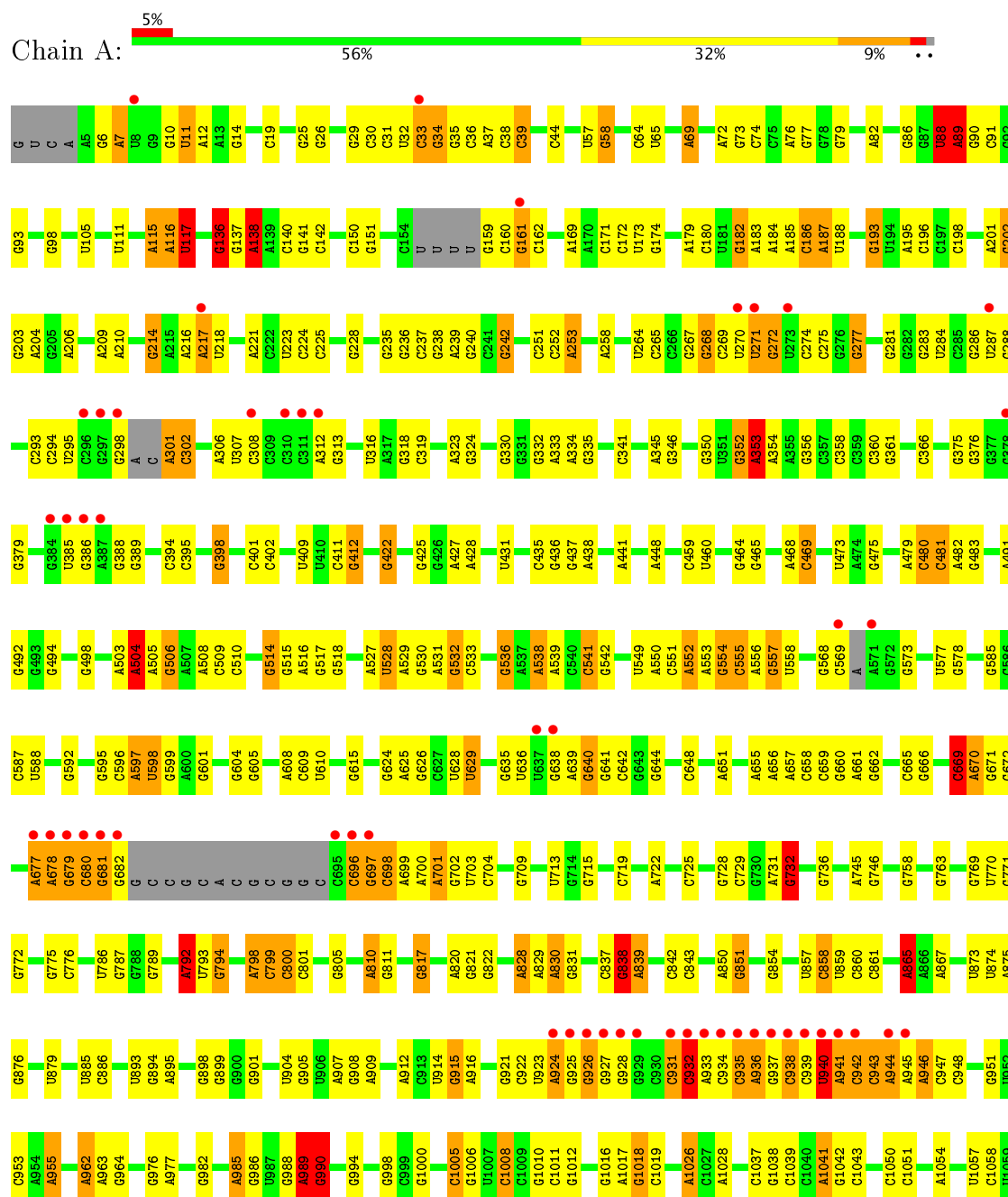
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	O	3	Total 3	O 3	0	0
64	P	8	Total 8	O 8	0	0
64	Q	3	Total 3	O 3	0	0
64	T	2	Total 2	O 2	0	0
64	U	3	Total 3	O 3	0	0
64	V	1	Total 1	O 1	0	0
64	0	3	Total 3	O 3	0	0
64	1	1	Total 1	O 1	0	0
64	3	1	Total 1	O 1	0	0
64	7	1	Total 1	O 1	0	0
64	8	4	Total 4	O 4	0	0
64	a	165	Total 165	O 165	0	0
64	l	1	Total 1	O 1	0	0
64	p	1	Total 1	O 1	0	0
64	v	3	Total 3	O 3	0	0
64	w	1	Total 1	O 1	0	0
64	z	1	Total 1	O 1	0	0

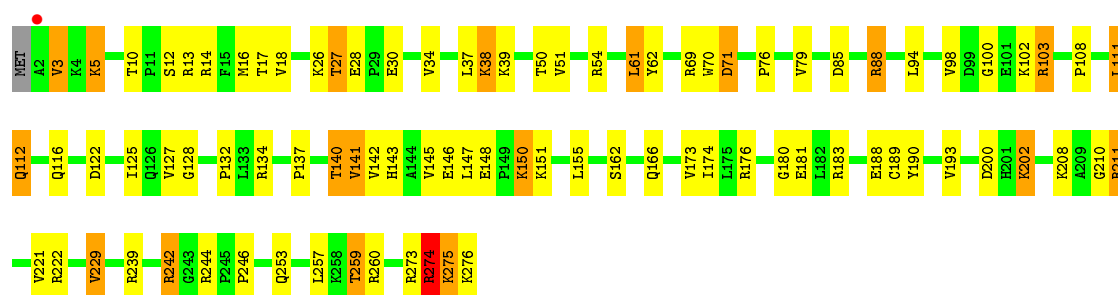
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

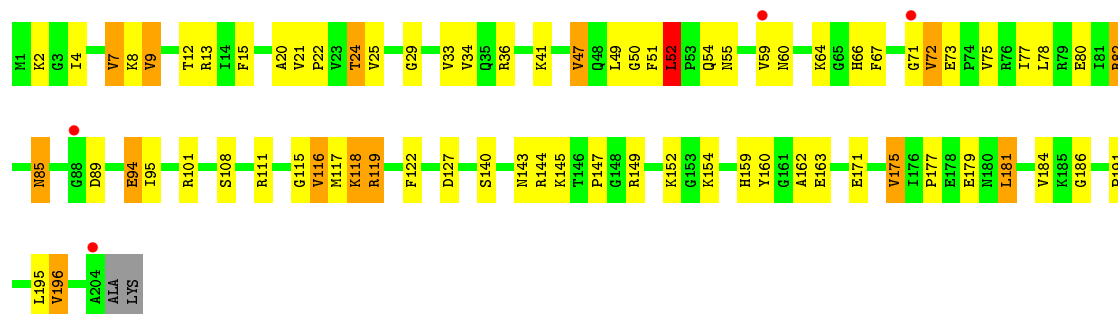
• Molecule 1: 23S Ribosomal RNA



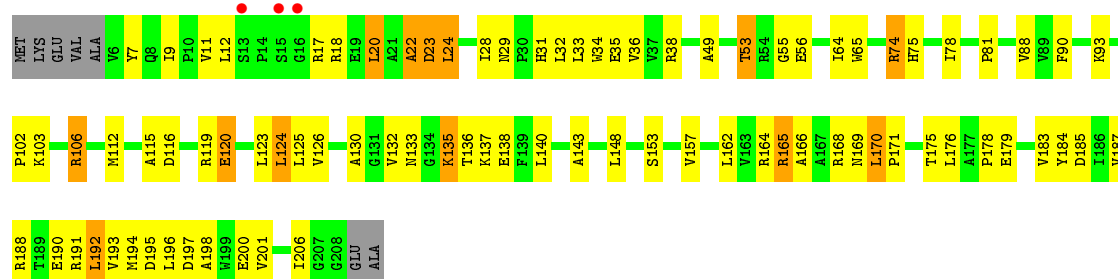
G2257	G2182	G2121	G1810	A1700	G1605	C1522	U1417	U1300	U1212	G1132	G1060
A2258	G2183	G2122	C1811	A1711	G1606	A1523	A1423	G1301	G1213	A1133	
G2261	C2124	C2123	A1812	G1712	A1612	G1524	A1424	C1302	G1214	U1064	
A2280	G2186	G2125	A1813	G1711	A1613	G1525	A1425	C1303	U1135	A1065	
G2281	G2187	G2126	A1814	G1720	G1614	G1528	G1429	G1304	G1216	A1066	
G2282	U2188	G2127	C1818	G1732	A1615	G1529	A1430	G1305	G1217	A1067	
U2283	G2189	C2128	A1819	G1733	A1616	G1530	G1431	G1306	G1218	U1068	
A2284	A2191	U2130	C1820	U1734	A1617	G1532	A1432	A1307	U1219	G1069	
A2285	A2192	A1906	A1821	A1735	C1621	U1622	G1445	U1310	U1220	G1070	
G2286	U2193	U2043	U1824	U1735	U1623	G1537	G1446	U1311	U1221	A1071	
G2287	G2132	G2044	C1825	U1739	U1624	U1538	G1447	U1312	U1222	A1072	
G2288	G2133	G2045	U1826	U1742	A1625	A1539	G1448	A1313	C1223	A1073	
G2289	C2136	C2046	C1827	G1743	A1626	A1540	G1449	G1316	G1228	G1076	
G2290	G2137	C2047	U1828	G1744	G1627	A1541	U1448	A1317	A1148	U1077	
C2294	C2200	U2049	C1829	G1745	G1628	G1545	U1450	U1318	U1150	G1084	
U2291	U2050	A1921	C1830	A1746	A1629	U1548	U1451	C1335	G1151		
G2292	G2051	A1927	C1831	A1748	A1630	U1549	G1452	C1336	U1152		
A2298	A2052	G1927	A1832	C1758	A1631	C1549	A1457	U1337	U1153	A1090	
C2204	G2053	C1945	U1833	U1759	C1632	C1550	G1458	C1338	U1154	A1091	
G2205	A2054	C1946	U1835	G1760	C1633	C1551	G1459	C1339	G1155	A1092	
C2206	U2055	C1946	A1839	G1762	U1635	A1552	U1460	C1343	A1156	A1093	
G2207	G2056	G1950	A1840	G1763	G1636	C1554	U1461	U1345	G1157		
G2208	A2063	U1951	G1844	U1764	G1637	A1555	G1462	A1346	G1160		
C2209	G2064	A1952	A1845	U1765	G1638	A1556	U1463	C1350	G1161		
U2210	C2064	A1953	C1846	A1766	G1639	G1557	G1464	U1351	G1162		
G2211	G2070	G1954	C1847	U1767	G1643	U1561	U1465	G1355	G1163		
G2212		C1955	U1848	G1768		G1567	G1466	G1356	G1170		
G2213	G2075	G1956	C1849	A1769	G1646	U1568	G1467	U1357			
G2214	A2075	A1957	U1850	G1770	U1647	G1569	G1468	C1359	A1173		
C2217	C2076	U1958	A1851	C1771	G1649	C1578	G1473	A1366	U1175		
U2218	G2077	A1959	C1852	G1772		G	G1474	U1369	G1179		
A2219	A2081	U1960	G1853	C1773	C1652	U	C1475	G1370	G1180		
C2220	G2082	G1961	C1856	U1774	A1653	A	C1482	U1381	G1181		
A2220	A2083	C1962	U1858	G1775	A1654	C	G1489	G1382	G1182		
G2221	C2084	U1965	C1859	U1776	A1655	G1584	A1490	U1385	G1183		
G2226	C2085	U1976	A1865	G1777	A1659	G1587	A1491	G1389	U1186		
G2227	C2086	A1981	C1868	U1778	C1682	A1588	G1501	U1399	G1187		
U2229	G2090	U1984	C1869	U1785	G1667	C1589	A1506	G1400	G1194		
G2230	U2100	G1985	C1873	U1788	G1670	C1593	G1507	U1401	G1195		
G2235	A2092	U1984	A1877	G1793	G1671	C1594	G1512	G1402	G1196		
A2236	G2093	G1985	C1883	U1794	C1682	C1596	C1513	U1403	G1197		
G2237	U2100	G1985	A1884	U1796	U1685	C1597	C1514	A1404	G1198		
U2244	U2103	C1988	C1885	G1799	C1686	A1599	G1516	A1405	G1199		
G2245	U2107	A1991	G1886	G1799	A1600	G1601	A1517	G1406	A1201		
G2246	G2108	A1992	C1887	A1803	G1602	C1603	A1518	A1410	G1202		
G2247	G2113	A1993	G1888	U1808	C1604	G1604	A1519	G1416	G1209		
G2248	U2113	G2001	C1889	U1809	G1699				U1210		
G2249	G2114	G2013	G1891						A1129		
G2250	G2118	U2014	G1892						C1211		
A2254	U2119	G2014	G1893								
G2255	U2119	G2014	G1894								
G2256	U2120	G2018	G1895								



• Molecule 5: 50S ribosomal protein L3



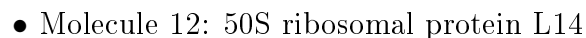
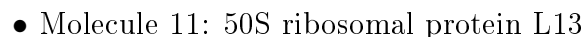
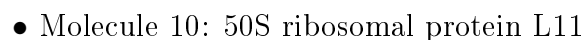
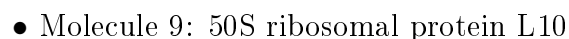
• Molecule 6: 50S ribosomal protein L4

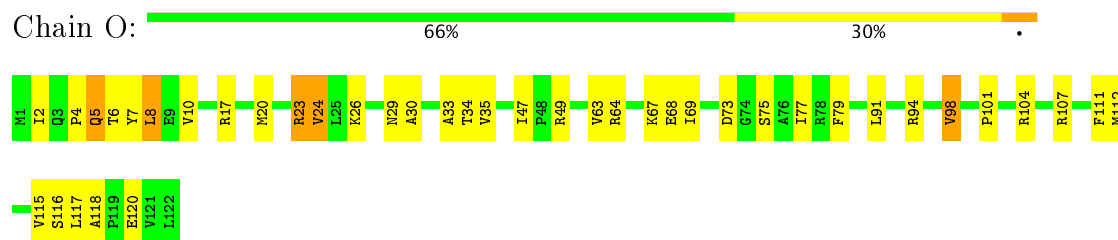


• Molecule 7: 50S ribosomal protein L5

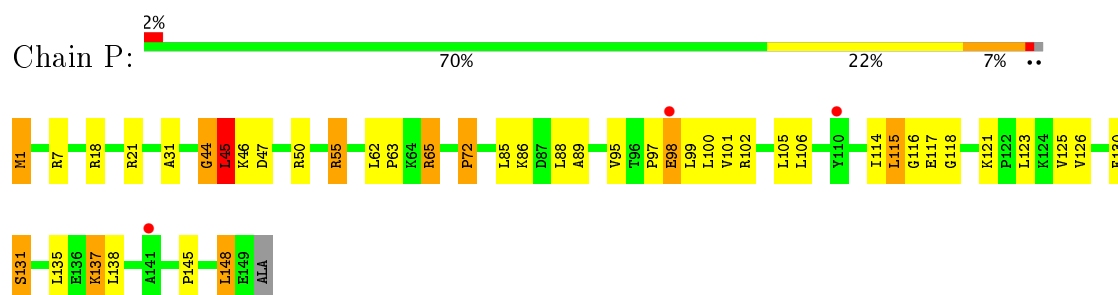


• Molecule 8: 50S ribosomal protein L6

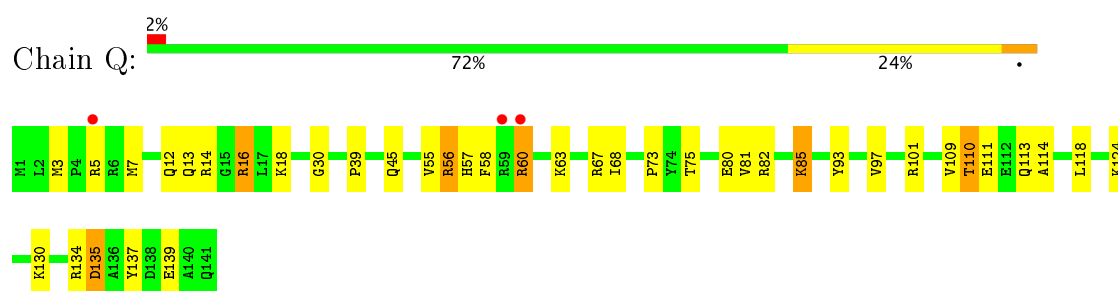




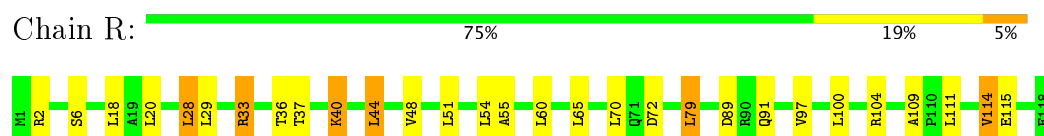
• Molecule 13: 50S ribosomal protein L15



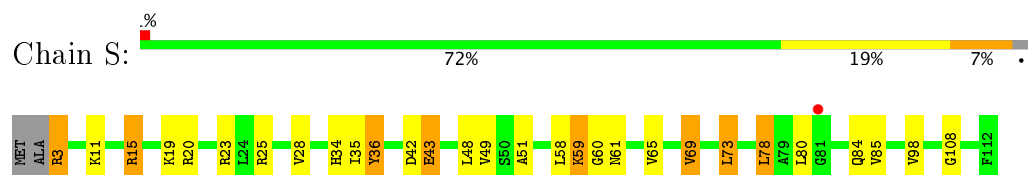
• Molecule 14: 50S ribosomal protein L16



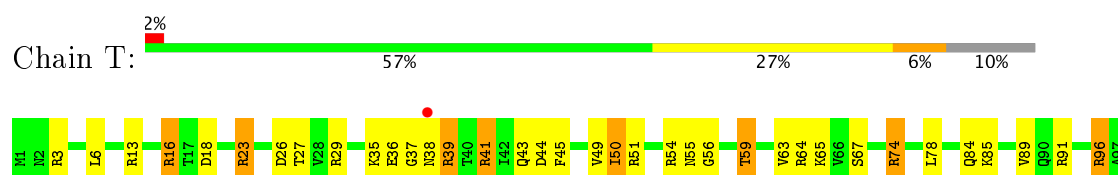
• Molecule 15: 50S ribosomal protein L17

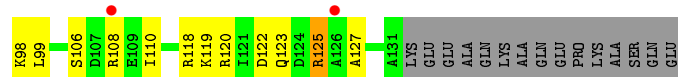


• Molecule 16: 50S ribosomal protein L18

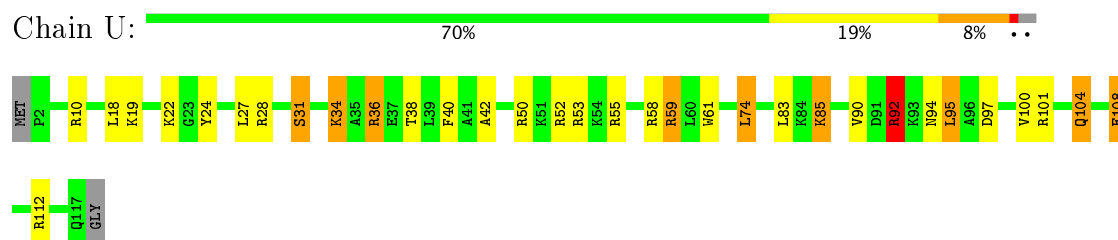


• Molecule 17: 50S ribosomal protein L19

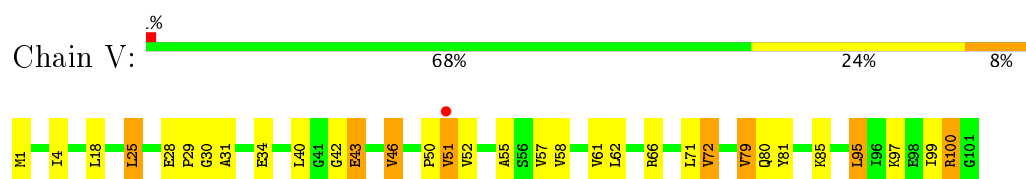




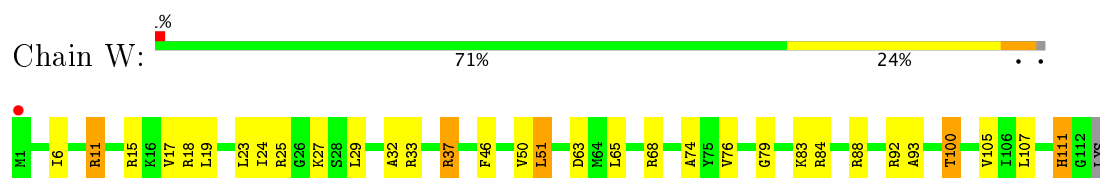
- Molecule 18: 50S ribosomal protein L20



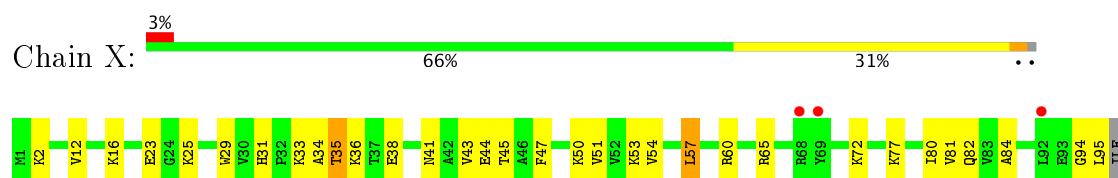
- Molecule 19: 50S ribosomal protein L21



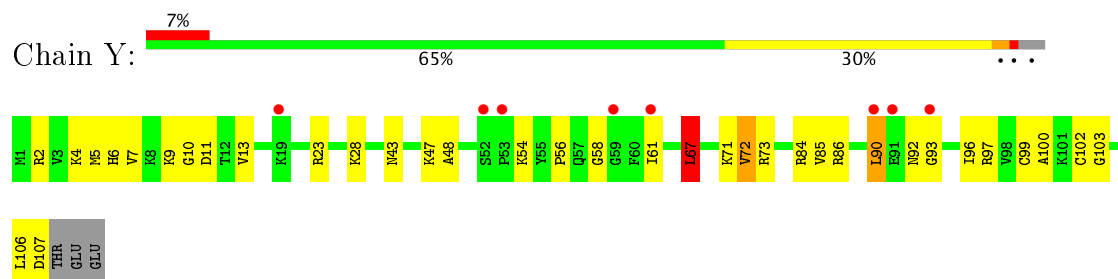
- Molecule 20: 50S ribosomal protein L22



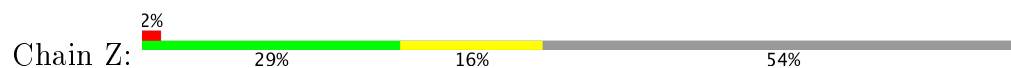
- Molecule 21: 50S ribosomal protein L23



- Molecule 22: 50S ribosomal protein L24



- Molecule 23: 50S ribosomal protein L25







- Molecule 30: 50S ribosomal protein L33

Chain 6: 76% 20% ..



- Molecule 31: 50S ribosomal protein L34

Chain 7: 4% 73% 18% 8%



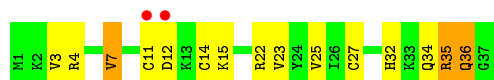
- Molecule 32: 50S ribosomal protein L35

Chain 8: 71% 26% ..



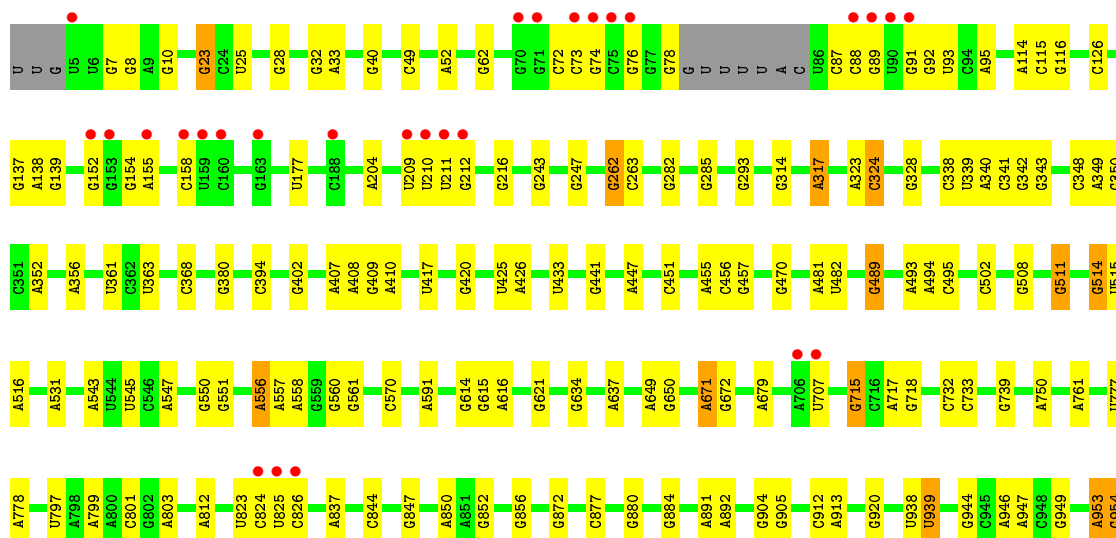
- Molecule 33: 50S ribosomal protein L36

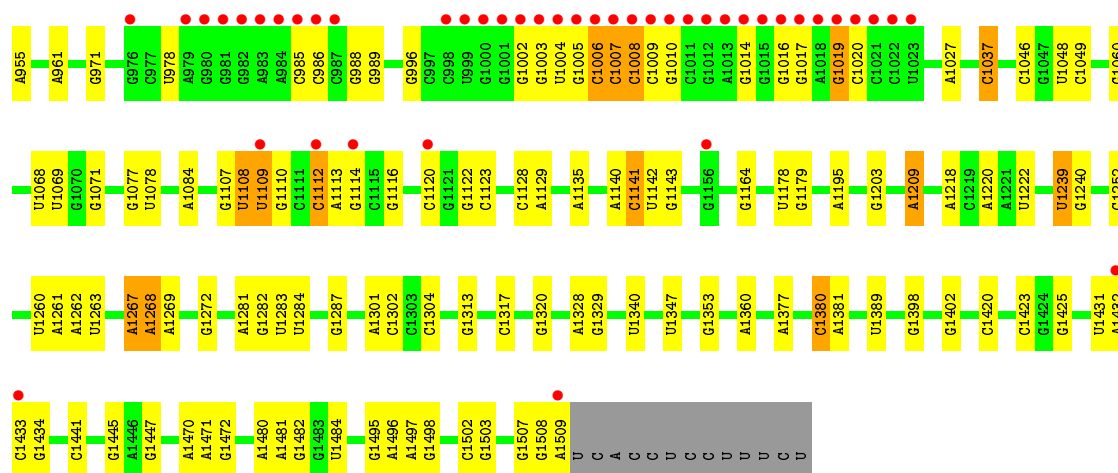
Chain 9: 5% 59% 32% 8%



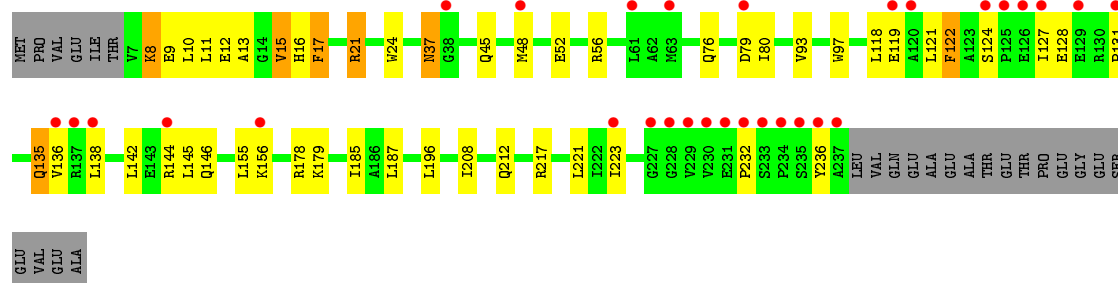
- Molecule 34: 16S Ribosomal RNA

Chain a: 5% 79% 17% ..

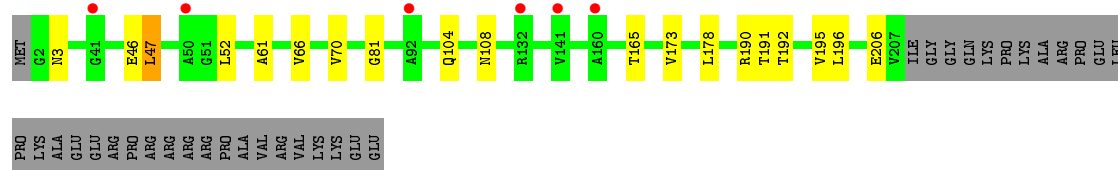
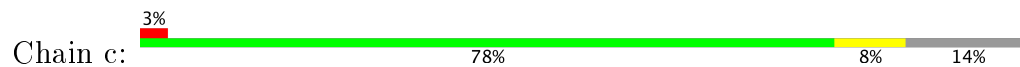




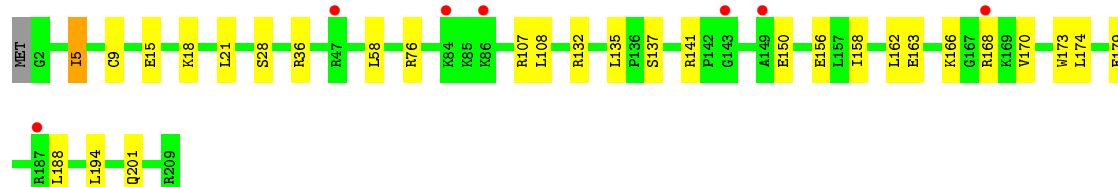
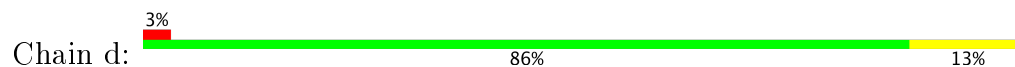
• Molecule 35: 30S ribosomal protein S2



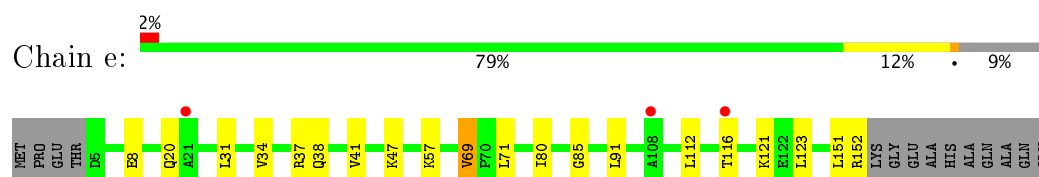
• Molecule 36: 30S ribosomal protein S3



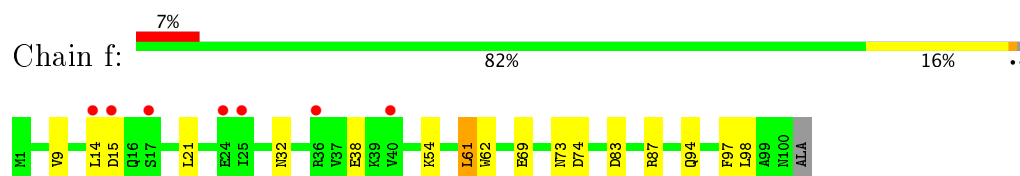
• Molecule 37: 30S ribosomal protein S4



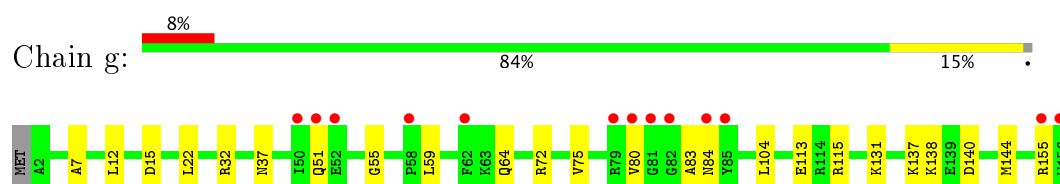
• Molecule 38: 30S ribosomal protein S5



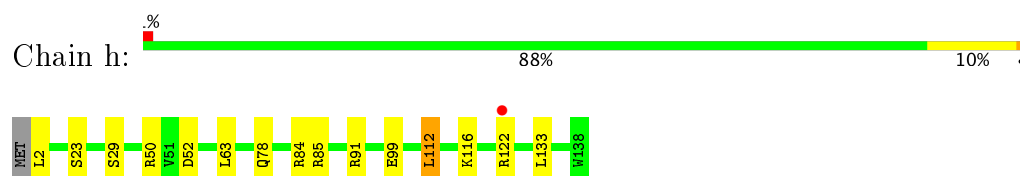
- Molecule 39: 30S ribosomal protein S6



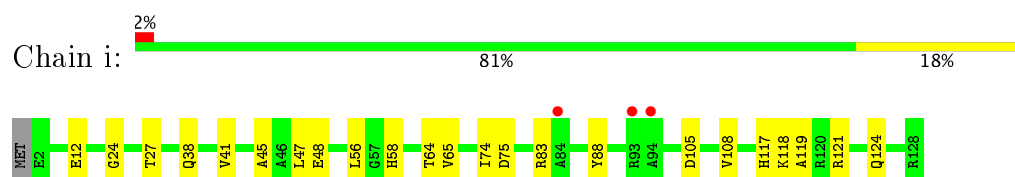
- Molecule 40: 30S ribosomal protein S7



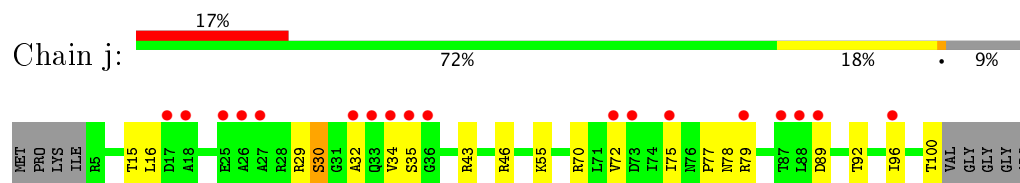
- Molecule 41: 30S ribosomal protein S8



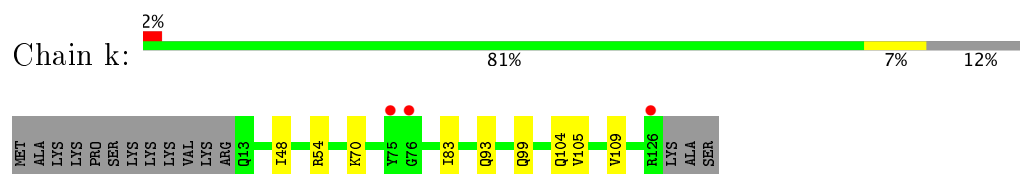
- Molecule 42: 30S ribosomal protein S9



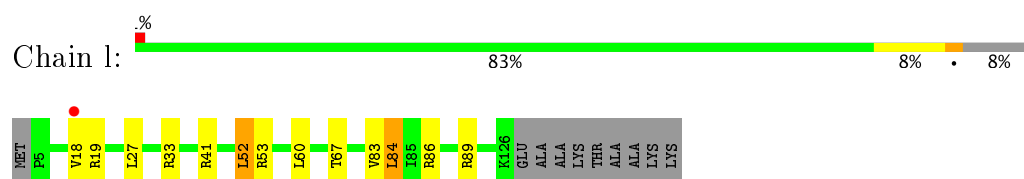
- Molecule 43: 30S ribosomal protein S10



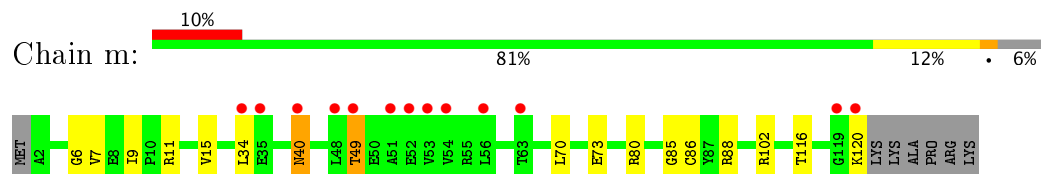
- Molecule 44: 30S ribosomal protein S11



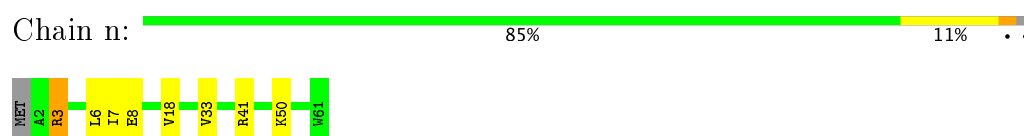
- Molecule 45: 30S ribosomal protein S12



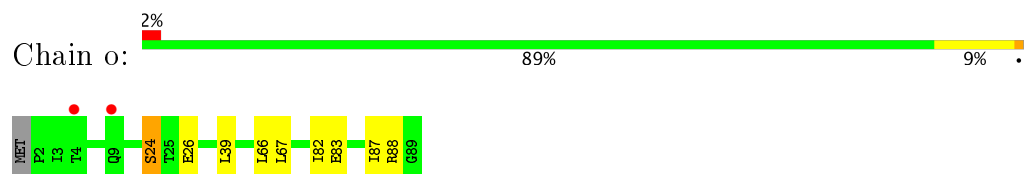
- Molecule 46: 30S ribosomal protein S13



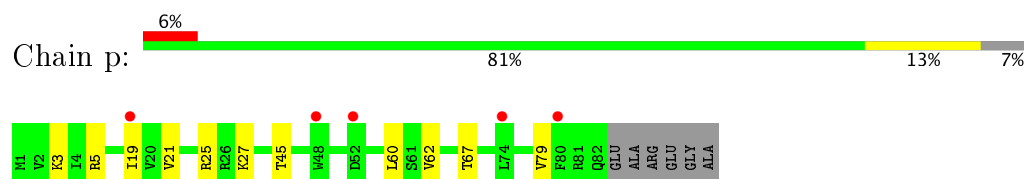
- Molecule 47: 30S ribosomal protein S14 type Z



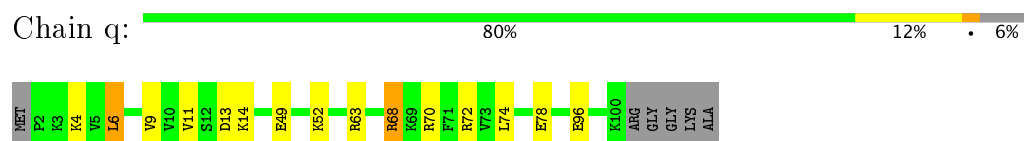
- Molecule 48: 30S ribosomal protein S15



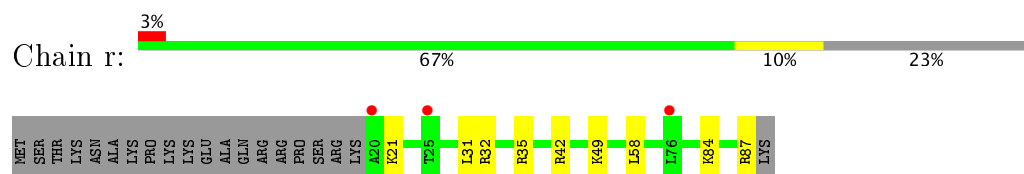
- Molecule 49: 30S ribosomal protein S16



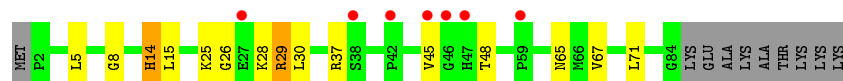
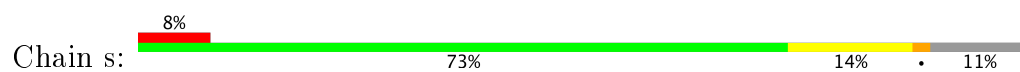
- Molecule 50: 30S ribosomal protein S17



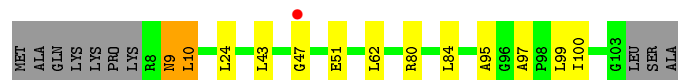
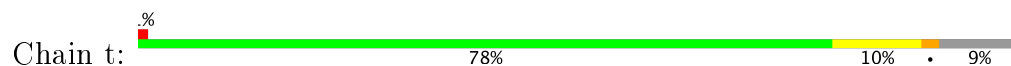
- Molecule 51: 30S ribosomal protein S18



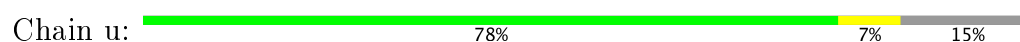
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



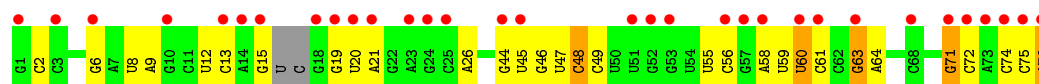
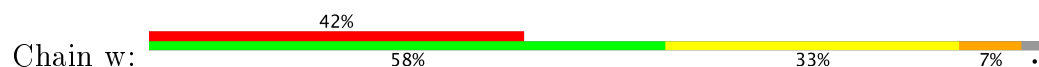
- Molecule 54: 30S ribosomal protein Thx



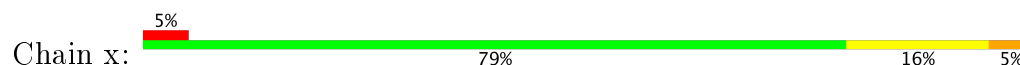
- Molecule 55: mRNA



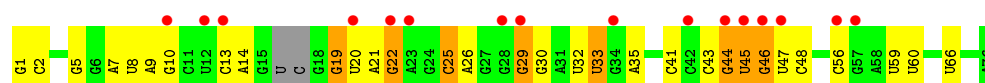
- Molecule 56: A-site tRNA



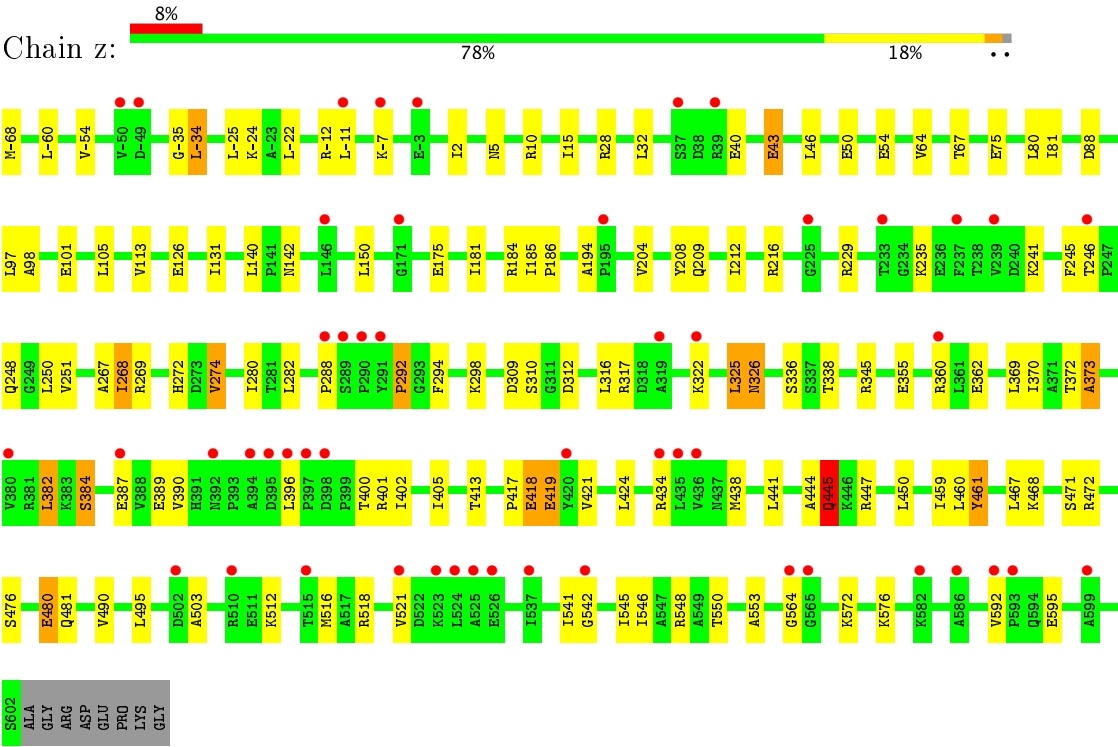
- Molecule 57: P-site tRNA



- Molecule 58: E-site tRNA



- Molecule 59: GDP CP fused to the N-terminus of the ribosomal protein L9, Elongation factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	213.12Å 271.72Å 436.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.60 49.52 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.52-2.60) 98.7 (49.52-2.59)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155	Depositor
R, R_{free}	0.192 , 0.261 0.203 , 0.267	Depositor DCC
R_{free} test set	38521 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	155465	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MIA, SF4, MG, GCP, 5MC, 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	0.69	11/69327 (0.0%)	1.23	339/108217 (0.3%)
2	B	0.51	0/2878	1.00	1/4490 (0.0%)
3	C	0.36	0/1044	0.66	1/1413 (0.1%)
4	D	0.50	0/2186	0.73	1/2944 (0.0%)
5	E	0.45	0/1592	0.69	0/2149
6	F	0.46	0/1619	0.62	0/2193
7	G	0.38	0/1450	0.64	1/1959 (0.1%)
8	H	0.42	0/1356	0.63	0/1834
9	J	0.32	0/640	0.55	0/889
10	K	0.43	0/1044	0.65	1/1416 (0.1%)
11	N	0.41	0/1144	0.63	0/1543
12	O	0.49	0/943	0.68	1/1269 (0.1%)
13	P	0.47	0/1152	0.74	1/1533 (0.1%)
14	Q	0.46	0/1143	0.58	0/1527
15	R	0.38	0/982	0.66	0/1312
16	S	0.40	0/887	0.63	0/1180
17	T	0.43	0/1105	0.65	0/1477
18	U	0.46	0/977	0.69	2/1301 (0.2%)
19	V	0.48	0/782	0.68	1/1049 (0.1%)
20	W	0.46	0/897	0.63	0/1205
21	X	0.43	0/764	0.65	1/1025 (0.1%)
22	Y	0.43	0/819	0.66	1/1095 (0.1%)
23	Z	0.38	0/801	0.59	0/1079
24	0	0.43	0/599	0.64	0/798
25	1	0.52	0/762	0.74	1/1014 (0.1%)
26	2	0.38	0/590	0.58	0/781
27	3	0.38	0/474	0.69	1/635 (0.2%)
28	4	0.40	0/570	0.64	0/768
29	5	0.44	0/473	0.71	0/639
30	6	0.46	0/460	0.64	0/613
31	7	0.46	0/438	0.71	0/575
32	8	0.47	0/519	0.67	0/684

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.49	0/310	0.73	0/407
34	a	0.62	2/36053 (0.0%)	1.14	114/56270 (0.2%)
35	b	0.37	0/1885	0.61	0/2547
36	c	0.41	1/1574 (0.1%)	0.58	0/2127
37	d	0.38	0/1685	0.58	0/2262
38	e	0.42	0/1145	0.65	0/1543
39	f	0.39	0/819	0.57	0/1111
40	g	0.37	0/1246	0.54	0/1674
41	h	0.39	0/1108	0.64	1/1494 (0.1%)
42	i	0.39	0/1002	0.61	0/1346
43	j	0.38	0/711	0.55	0/968
44	k	0.38	0/844	0.60	0/1145
45	l	0.48	0/946	0.76	2/1274 (0.2%)
46	m	0.38	0/934	0.70	0/1256
47	n	0.46	0/501	0.65	0/664
48	o	0.39	0/739	0.61	0/985
49	p	0.37	0/697	0.65	0/939
50	q	0.44	0/836	0.68	1/1117 (0.1%)
51	r	0.38	0/560	0.62	0/746
52	s	0.35	0/665	0.68	0/897
53	t	0.39	0/726	0.64	0/961
54	u	0.44	0/203	0.64	0/266
55	v	0.71	0/310	1.31	3/480 (0.6%)
56	w	0.67	3/1602 (0.2%)	1.69	31/2493 (1.2%)
57	x	0.76	4/1747 (0.2%)	1.48	32/2723 (1.2%)
58	y	0.62	0/1628	1.49	31/2534 (1.2%)
59	z	0.40	0/5296	0.65	4/7179 (0.1%)
All	All	0.60	21/166189 (0.0%)	1.08	572/248014 (0.2%)

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
10	K	0	1
19	V	0	1
26	2	0	1
28	4	0	1
37	d	0	1
39	f	0	1
42	i	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
52	s	0	2
53	t	0	1
59	z	0	6
All	All	0	17

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	71	G	C6-N1	-10.59	1.32	1.39
56	w	71	G	N1-C2	-10.38	1.29	1.37
57	x	14	A	N7-C5	-8.86	1.33	1.39
1	A	353	A	N9-C4	-7.12	1.33	1.37
1	A	1091	A	C5-C6	-7.12	1.34	1.41

The worst 5 of 572 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	71	G	N3-C2-N2	23.02	136.02	119.90
56	w	71	G	C5-C6-O6	22.98	142.39	128.60
56	w	2	C	N1-C2-O2	21.56	131.84	118.90
56	w	71	G	N1-C2-N2	-21.15	97.16	116.20
1	A	1091	A	N9-C4-C5	-17.30	98.88	105.80

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	2	44	LEU	Peptide
28	4	65	ASP	Peptide
10	K	70	LYS	Peptide
19	V	43	GLU	Peptide
37	d	179	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61902	0	31210	820	1
2	B	2573	0	1306	29	0
3	C	1024	0	1007	81	0
4	D	2136	0	2218	65	0
5	E	1559	0	1618	46	0
6	F	1584	0	1625	52	0
7	G	1425	0	1443	56	0
8	H	1330	0	1407	47	0
9	J	641	0	309	19	0
10	K	1025	0	1066	64	0
11	N	1117	0	1184	27	0
12	O	933	0	996	30	0
13	P	1135	0	1212	38	0
14	Q	1122	0	1179	23	0
15	R	968	0	1033	12	0
16	S	877	0	938	32	0
17	T	1091	0	1151	33	0
18	U	959	0	1019	26	0
19	V	771	0	830	19	0
20	W	886	0	940	23	1
21	X	750	0	814	19	0
22	Y	806	0	881	17	0
23	Z	784	0	796	18	0
24	0	591	0	607	15	0
25	1	755	0	826	22	0
26	2	588	0	643	15	0
27	3	469	0	518	8	0
28	4	557	0	535	28	0
29	5	459	0	476	13	0
30	6	453	0	473	7	0
31	7	430	0	480	8	0
32	8	511	0	571	16	0
33	9	307	0	335	13	0
34	a	32207	0	16255	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	529	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
52	s	650	0	655	0	0
53	t	724	0	787	0	0
54	u	199	0	208	0	0
55	v	277	0	140	0	0
56	w	1586	0	819	0	0
57	x	1645	0	839	0	0
58	y	1580	0	801	0	0
59	z	5200	0	5309	0	0
60	0	4	0	0	0	0
60	5	2	0	0	0	0
60	6	2	0	0	0	0
60	7	1	0	0	0	0
60	8	1	0	0	0	0
60	9	1	0	0	0	0
60	A	644	0	0	0	0
60	B	18	0	0	0	0
60	D	6	0	0	0	0
60	E	5	0	0	0	0
60	F	6	0	0	0	0
60	G	2	0	0	0	0
60	H	1	0	0	0	0
60	N	1	0	0	0	0
60	O	2	0	0	0	0
60	P	3	0	0	0	0
60	Q	2	0	0	0	0
60	R	2	0	0	0	0
60	U	1	0	0	0	0
60	V	2	0	0	0	0
60	W	1	0	0	0	0
60	X	1	0	0	0	0
60	Z	1	0	0	0	0
60	a	188	0	0	0	0
60	d	1	0	0	0	0
60	e	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	f	1	0	0	0	0
60	l	1	0	0	0	0
60	m	2	0	0	0	0
60	n	3	0	0	0	0
60	v	2	0	0	0	0
60	x	9	0	0	0	0
60	z	2	0	0	0	0
61	4	1	0	0	0	0
61	5	1	0	0	0	0
61	6	1	0	0	0	0
61	9	1	0	0	0	0
61	Y	1	0	0	0	0
61	n	1	0	0	0	0
62	d	8	0	0	0	0
63	z	32	0	14	0	0
64	0	3	0	0	0	0
64	1	1	0	0	0	0
64	3	1	0	0	0	0
64	7	1	0	0	0	0
64	8	4	0	0	0	0
64	A	715	0	0	37	0
64	B	32	0	0	0	0
64	D	4	0	0	0	0
64	E	6	0	0	1	0
64	F	5	0	0	0	0
64	H	1	0	0	0	0
64	N	1	0	0	0	0
64	O	3	0	0	0	0
64	P	8	0	0	0	0
64	Q	3	0	0	0	0
64	T	2	0	0	0	0
64	U	3	0	0	0	0
64	V	1	0	0	0	0
64	a	165	0	0	0	0
64	l	1	0	0	0	0
64	p	1	0	0	0	0
64	v	3	0	0	0	0
64	w	1	0	0	0	0
64	z	1	0	0	0	0
All	All	155465	0	104775	1518	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1518 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)
3:C:201:PRO:C	3:C:203:GLY:HA2	1.75	1.06
3:C:199:HIS:O	3:C:201:PRO:HD3	1.57	1.03
1:A:1091:A:N1	9:J:6:ASN:N	2.14	0.95
1:A:679:G:O6	1:A:698:C:N4	2.02	0.92
1:A:1649:C:OP2	64:A:3701:HOH:O	1.90	0.89

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1519:G:N2	20:W:111:HIS:O[4_557]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	130/228 (57%)	94 (72%)	25 (19%)	11 (8%)	1	1
4	D	273/276 (99%)	255 (93%)	15 (6%)	3 (1%)	17	35
5	E	202/206 (98%)	188 (93%)	11 (5%)	3 (2%)	12	24
6	F	201/210 (96%)	184 (92%)	12 (6%)	5 (2%)	6	11
7	G	179/182 (98%)	162 (90%)	10 (6%)	7 (4%)	3	4
8	H	172/180 (96%)	148 (86%)	17 (10%)	7 (4%)	3	4
9	J	128/173 (74%)	76 (59%)	22 (17%)	30 (23%)	0	0
10	K	137/147 (93%)	85 (62%)	31 (23%)	21 (15%)	0	0
11	N	138/140 (99%)	129 (94%)	5 (4%)	4 (3%)	5	8
12	O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	22	44
13	P	147/150 (98%)	129 (88%)	16 (11%)	2 (1%)	13	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	25	49
15	R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
16	S	108/112 (96%)	96 (89%)	10 (9%)	2 (2%)	9	18
17	T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	22	44
18	U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
19	V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	9	17
20	W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
21	X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	17	35
22	Y	105/110 (96%)	89 (85%)	12 (11%)	4 (4%)	4	5
23	Z	92/206 (45%)	84 (91%)	8 (9%)	0	100	100
24	0	72/85 (85%)	67 (93%)	3 (4%)	2 (3%)	6	9
25	1	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	5	7
26	2	68/72 (94%)	65 (96%)	2 (3%)	1 (2%)	12	24
27	3	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	4	67/71 (94%)	45 (67%)	15 (22%)	7 (10%)	0	0
29	5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
31	7	47/49 (96%)	44 (94%)	1 (2%)	2 (4%)	3	4
32	8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
33	9	35/37 (95%)	35 (100%)	0	0	100	100
35	b	229/256 (90%)	192 (84%)	23 (10%)	14 (6%)	2	2
36	c	204/239 (85%)	177 (87%)	20 (10%)	7 (3%)	4	6
37	d	206/209 (99%)	187 (91%)	16 (8%)	3 (2%)	12	24
38	e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	8	15
39	f	98/101 (97%)	84 (86%)	11 (11%)	3 (3%)	5	8
40	g	153/156 (98%)	135 (88%)	13 (8%)	5 (3%)	4	7
41	h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
42	i	125/128 (98%)	113 (90%)	5 (4%)	7 (6%)	2	2
43	j	94/105 (90%)	79 (84%)	6 (6%)	9 (10%)	1	0
44	k	112/129 (87%)	107 (96%)	4 (4%)	1 (1%)	20	40
45	l	120/132 (91%)	112 (93%)	7 (6%)	1 (1%)	22	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	m	117/126 (93%)	102 (87%)	9 (8%)	6 (5%)	2	3
47	n	58/61 (95%)	57 (98%)	0	1 (2%)	11	21
48	o	86/89 (97%)	78 (91%)	5 (6%)	3 (4%)	4	6
49	p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	14	29
50	q	97/105 (92%)	86 (89%)	8 (8%)	3 (3%)	5	8
51	r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
52	s	81/93 (87%)	72 (89%)	4 (5%)	5 (6%)	2	1
53	t	94/106 (89%)	84 (89%)	4 (4%)	6 (6%)	1	1
54	u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
59	z	669/679 (98%)	568 (85%)	62 (9%)	39 (6%)	2	2
All	All	6534/7143 (92%)	5800 (89%)	497 (8%)	237 (4%)	4	5

5 of 237 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	65	PRO
3	C	172	HIS
3	C	224	ILE
4	D	275	LYS
6	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	C	103/180 (57%)	79 (77%)	24 (23%)	1	1
4	D	215/218 (99%)	186 (86%)	29 (14%)	4	7
5	E	164/166 (99%)	138 (84%)	26 (16%)	3	5
6	F	160/166 (96%)	135 (84%)	25 (16%)	3	5
7	G	143/156 (92%)	116 (81%)	27 (19%)	2	2
8	H	144/148 (97%)	128 (89%)	16 (11%)	7	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	K	104/111 (94%)	71 (68%)	33 (32%)	0	0
11	N	118/119 (99%)	96 (81%)	22 (19%)	2	3
12	O	100/100 (100%)	91 (91%)	9 (9%)	11	21
13	P	115/116 (99%)	103 (90%)	12 (10%)	8	15
14	Q	111/111 (100%)	94 (85%)	17 (15%)	3	5
15	R	101/101 (100%)	84 (83%)	17 (17%)	2	4
16	S	87/88 (99%)	77 (88%)	10 (12%)	6	12
17	T	115/127 (91%)	100 (87%)	15 (13%)	5	8
18	U	93/94 (99%)	80 (86%)	13 (14%)	4	7
19	V	80/82 (98%)	67 (84%)	13 (16%)	3	4
20	W	90/92 (98%)	79 (88%)	11 (12%)	6	10
21	X	77/78 (99%)	69 (90%)	8 (10%)	8	15
22	Y	85/91 (93%)	75 (88%)	10 (12%)	6	11
23	Z	84/179 (47%)	73 (87%)	11 (13%)	5	8
24	0	59/67 (88%)	55 (93%)	4 (7%)	18	37
25	1	80/83 (96%)	69 (86%)	11 (14%)	4	7
26	2	65/67 (97%)	54 (83%)	11 (17%)	2	4
27	3	51/52 (98%)	44 (86%)	7 (14%)	4	7
28	4	60/63 (95%)	45 (75%)	15 (25%)	1	1
29	5	51/52 (98%)	45 (88%)	6 (12%)	6	11
30	6	51/52 (98%)	47 (92%)	4 (8%)	15	29
31	7	42/42 (100%)	34 (81%)	8 (19%)	2	2
32	8	53/55 (96%)	48 (91%)	5 (9%)	10	19
33	9	34/34 (100%)	29 (85%)	5 (15%)	3	6
35	b	193/220 (88%)	150 (78%)	43 (22%)	1	2
36	c	142/188 (76%)	130 (92%)	12 (8%)	12	24
37	d	169/181 (93%)	143 (85%)	26 (15%)	3	5
38	e	113/123 (92%)	95 (84%)	18 (16%)	3	5
39	f	83/90 (92%)	69 (83%)	14 (17%)	2	4
40	g	118/127 (93%)	99 (84%)	19 (16%)	3	4
41	h	114/119 (96%)	99 (87%)	15 (13%)	5	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	i	90/99 (91%)	76 (84%)	14 (16%)	3	5
43	j	65/92 (71%)	53 (82%)	12 (18%)	2	3
44	k	82/99 (83%)	74 (90%)	8 (10%)	9	17
45	l	97/109 (89%)	85 (88%)	12 (12%)	5	10
46	m	89/101 (88%)	76 (85%)	13 (15%)	3	6
47	n	49/50 (98%)	41 (84%)	8 (16%)	3	4
48	o	78/80 (98%)	71 (91%)	7 (9%)	11	21
49	p	69/74 (93%)	59 (86%)	10 (14%)	4	6
50	q	94/97 (97%)	81 (86%)	13 (14%)	4	7
51	r	59/77 (77%)	50 (85%)	9 (15%)	3	5
52	s	68/80 (85%)	58 (85%)	10 (15%)	3	6
53	t	69/82 (84%)	61 (88%)	8 (12%)	6	11
54	u	18/22 (82%)	16 (89%)	2 (11%)	7	13
59	z	542/560 (97%)	436 (80%)	106 (20%)	1	2
All	All	5236/5760 (91%)	4433 (85%)	803 (15%)	3	5

5 of 803 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	2	1	MET
35	b	136	VAL
59	z	250	LEU
26	2	70	GLN
31	7	14	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
36	c	6	HIS
37	d	123	HIS
59	z	275	GLN
36	c	37	GLN
36	c	162	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2868/2915 (98%)	464 (16%)	42 (1%)
2	B	119/121 (98%)	14 (11%)	0
34	a	1496/1521 (98%)	243 (16%)	0
55	v	12/24 (50%)	1 (8%)	0
56	w	71/76 (93%)	26 (36%)	0
57	x	76/77 (98%)	13 (17%)	0
58	y	71/76 (93%)	28 (39%)	0
All	All	4713/4810 (97%)	789 (16%)	42 (0%)

5 of 789 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	10	G
1	A	14	G
1	A	34	G
1	A	44	C

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1120	C
1	A	1238	A
1	A	2450	A
1	A	1132	G
1	A	1218	A

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

17 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	$\# Z > 2$
56	PSU	w	32	56	16,21,22	1.44	1 (6%)	20,30,33	3.64	7 (35%)
56	MIA	w	37	56	22,29,32	1.78	2 (9%)	24,41,47	1.99	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	w	39	56	16,21,22	1.55	1 (6%)	20,30,33	3.58	7 (35%)
56	7MG	w	46	56	20,26,27	1.78	2 (10%)	22,39,42	2.79	5 (22%)
56	5MU	w	54	56	14,22,23	0.67	0	16,32,35	2.60	2 (12%)
56	PSU	w	55	56	16,21,22	1.22	1 (6%)	20,30,33	3.57	6 (30%)
56	4SU	w	8	56	14,21,22	1.33	2 (14%)	15,30,33	1.63	2 (13%)
57	5MC	x	32	57	15,22,23	1.43	1 (6%)	17,32,35	1.05	2 (11%)
57	5MU	x	54	60,57	14,22,23	0.83	1 (7%)	16,32,35	2.36	3 (18%)
57	PSU	x	55	57	16,21,22	1.58	2 (12%)	20,30,33	3.64	7 (35%)
57	4SU	x	8	57	14,21,22	1.32	2 (14%)	15,30,33	3.84	2 (13%)
58	PSU	y	32	58	16,21,22	1.12	1 (6%)	20,30,33	3.55	6 (30%)
58	MIA	y	37	58,34	18,24,32	1.37	3 (16%)	17,35,47	1.88	2 (11%)
58	PSU	y	39	58	16,21,22	1.42	2 (12%)	20,30,33	3.72	7 (35%)
58	5MU	y	54	58	14,22,23	0.80	0	16,32,35	2.45	3 (18%)
58	PSU	y	55	58	16,21,22	1.26	1 (6%)	20,30,33	3.44	7 (35%)
58	4SU	y	8	58	14,21,22	3.26	5 (35%)	15,30,33	1.44	2 (13%)

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
56	PSU	w	32	56	-	0/7/25/26	0/2/2/2
56	MIA	w	37	56	-	0/10/31/34	0/3/3/3
56	PSU	w	39	56	-	0/7/25/26	0/2/2/2
56	7MG	w	46	56	-	0/7/37/38	0/3/3/3
56	5MU	w	54	56	-	0/3/25/26	0/2/2/2
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
56	4SU	w	8	56	-	0/3/25/26	0/2/2/2
57	5MC	x	32	57	-	0/3/25/26	0/2/2/2
57	5MU	x	54	60,57	-	0/3/25/26	0/2/2/2
57	PSU	x	55	57	-	0/7/25/26	0/2/2/2
57	4SU	x	8	57	-	0/3/25/26	0/2/2/2
58	PSU	y	32	58	-	0/7/25/26	0/2/2/2
58	MIA	y	37	58,34	-	0/3/25/34	0/3/3/3
58	PSU	y	39	58	-	0/7/25/26	0/2/2/2
58	5MU	y	54	58	-	0/3/25/26	0/2/2/2
58	PSU	y	55	58	-	0/7/25/26	0/2/2/2
58	4SU	y	8	58	-	0/3/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	w	37	MIA	C2-S10	-7.32	1.69	1.75
56	w	39	PSU	C5-C1'	-4.98	1.47	1.52
57	x	55	PSU	C5-C1'	-4.74	1.48	1.52
56	w	32	PSU	C5-C1'	-4.48	1.48	1.52
58	y	39	PSU	C5-C1'	-4.31	1.48	1.52

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	w	55	PSU	N1-C2-N3	-10.16	121.09	128.40
56	w	39	PSU	N1-C2-N3	-9.46	121.59	128.40
58	y	55	PSU	N1-C2-N3	-9.38	121.65	128.40
58	y	32	PSU	N1-C2-N3	-9.36	121.67	128.40
58	y	39	PSU	N1-C2-N3	-9.24	121.75	128.40

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 927 ligands modelled in this entry, 925 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	$\# Z > 2$
62	SF4	d	302	37	0,12,12	0.00	-	0,24,24	0.00	-
63	GCP	z	703	60	25,34,34	3.44	9 (36%)	28,54,54	1.42	4 (14%)

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
62	SF4	d	302	37	-	0/0/48/48	0/6/5/5
63	GCP	z	703	60	-	0/18/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	703	GCP	C4-N9	-12.62	1.30	1.47
63	z	703	GCP	PB-O2B	-6.13	1.41	1.56
63	z	703	GCP	C8-N9	-4.95	1.31	1.46
63	z	703	GCP	PG-O3G	-4.18	1.45	1.54
63	z	703	GCP	C5-C6	-3.84	1.46	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	703	GCP	O3'-C3'-C2'	-2.82	102.79	111.83
63	z	703	GCP	C2'-C1'-N9	-2.73	106.29	113.34
63	z	703	GCP	O2G-PG-O1G	-2.18	106.47	112.32
63	z	703	GCP	O3G-PG-O2G	2.42	115.24	108.14

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2874/2915 (98%)	0.19	149 (5%) 28 21	22, 39, 92, 112	465 (16%)
2	B	120/121 (99%)	0.15	0 100 100	36, 57, 73, 93	18 (15%)
3	C	136/228 (59%)	2.04	60 (44%) 0 0	72, 89, 95, 97	104 (76%)
4	D	275/276 (99%)	-0.01	1 (0%) 92 91	18, 37, 49, 69	42 (15%)
5	E	204/206 (99%)	0.18	4 (1%) 65 59	20, 41, 63, 76	38 (18%)
6	F	203/210 (96%)	0.09	3 (1%) 74 69	22, 50, 75, 90	31 (15%)
7	G	181/182 (99%)	0.35	10 (5%) 26 19	42, 58, 78, 84	38 (20%)
8	H	174/180 (96%)	0.29	8 (4%) 33 26	39, 54, 70, 73	30 (17%)
9	J	130/173 (75%)	3.73	88 (67%) 0 0	84, 138, 186, 214	10 (7%)
10	K	139/147 (94%)	4.74	113 (81%) 0 0	93, 102, 107, 110	115 (82%)
11	N	140/140 (100%)	0.07	2 (1%) 75 71	26, 43, 65, 83	27 (19%)
12	O	122/122 (100%)	-0.06	0 100 100	27, 39, 50, 65	7 (5%)
13	P	149/150 (99%)	0.20	3 (2%) 65 59	21, 49, 65, 83	38 (25%)
14	Q	141/141 (100%)	-0.03	3 (2%) 64 58	27, 42, 59, 87	36 (25%)
15	R	118/118 (100%)	0.09	0 100 100	26, 43, 55, 69	16 (13%)
16	S	110/112 (98%)	0.28	1 (0%) 84 81	40, 52, 65, 75	24 (21%)
17	T	131/146 (89%)	0.23	3 (2%) 61 54	34, 45, 72, 92	22 (16%)
18	U	116/118 (98%)	0.13	0 100 100	26, 40, 49, 53	23 (19%)
19	V	101/101 (100%)	0.07	1 (0%) 82 79	28, 48, 59, 66	12 (11%)
20	W	112/113 (99%)	0.15	1 (0%) 84 81	28, 41, 63, 79	24 (21%)
21	X	95/96 (98%)	0.24	3 (3%) 48 40	39, 50, 72, 84	14 (14%)
22	Y	107/110 (97%)	0.44	8 (7%) 15 10	44, 54, 81, 87	24 (22%)
23	Z	94/206 (45%)	0.47	5 (5%) 27 20	42, 59, 74, 97	15 (15%)
24	0	74/85 (87%)	-0.01	0 100 100	26, 39, 52, 65	16 (21%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	1	97/98 (98%)	0.29	5 (5%) 28 21	24, 39, 70, 81	21 (21%)
26	2	70/72 (97%)	0.51	2 (2%) 52 45	44, 57, 67, 79	13 (18%)
27	3	59/60 (98%)	0.52	4 (6%) 18 13	29, 43, 66, 78	12 (20%)
28	4	69/71 (97%)	1.16	16 (23%) 1 0	52, 73, 94, 99	26 (37%)
29	5	59/60 (98%)	0.04	0 100 100	22, 43, 62, 71	8 (13%)
30	6	53/54 (98%)	0.17	0 100 100	35, 41, 52, 58	11 (20%)
31	7	49/49 (100%)	0.05	2 (4%) 38 30	25, 30, 54, 70	9 (18%)
32	8	64/65 (98%)	0.00	0 100 100	26, 34, 40, 51	7 (10%)
33	9	37/37 (100%)	0.33	2 (5%) 26 20	32, 39, 51, 58	11 (29%)
34	a	1498/1521 (98%)	0.22	72 (4%) 31 24	28, 45, 92, 113	228 (15%)
35	b	231/256 (90%)	0.81	30 (12%) 4 2	51, 71, 92, 100	56 (24%)
36	c	206/239 (86%)	0.24	6 (2%) 52 45	40, 58, 73, 83	19 (9%)
37	d	208/209 (99%)	0.40	7 (3%) 46 38	47, 59, 79, 86	49 (23%)
38	e	148/162 (91%)	0.06	3 (2%) 65 59	33, 48, 60, 78	23 (15%)
39	f	100/101 (99%)	0.39	7 (7%) 17 12	48, 66, 76, 86	17 (17%)
40	g	155/156 (99%)	0.57	13 (8%) 12 8	41, 58, 89, 98	40 (25%)
41	h	137/138 (99%)	0.16	1 (0%) 87 85	39, 48, 57, 65	14 (10%)
42	i	127/128 (99%)	0.36	3 (2%) 59 52	35, 61, 77, 83	15 (11%)
43	j	96/105 (91%)	1.00	18 (18%) 1 1	34, 65, 87, 94	27 (28%)
44	k	114/129 (88%)	0.25	3 (2%) 56 49	32, 54, 67, 72	16 (14%)
45	l	122/132 (92%)	-0.03	1 (0%) 86 83	28, 40, 55, 65	23 (18%)
46	m	119/126 (94%)	0.63	13 (10%) 6 4	32, 57, 77, 82	24 (20%)
47	n	60/61 (98%)	0.22	0 100 100	33, 44, 54, 63	4 (6%)
48	o	88/89 (98%)	0.41	2 (2%) 61 54	37, 50, 65, 74	21 (23%)
49	p	82/88 (93%)	0.59	5 (6%) 22 16	43, 55, 69, 76	14 (17%)
50	q	99/105 (94%)	0.10	0 100 100	41, 49, 61, 65	18 (18%)
51	r	68/88 (77%)	0.56	3 (4%) 35 27	48, 59, 78, 86	14 (20%)
52	s	83/93 (89%)	0.47	7 (8%) 12 8	39, 55, 75, 80	13 (15%)
53	t	96/106 (90%)	0.36	1 (1%) 82 79	40, 49, 59, 71	16 (16%)
54	u	23/27 (85%)	0.44	0 100 100	38, 45, 50, 51	4 (17%)
55	v	13/24 (54%)	0.58	1 (7%) 14 10	36, 48, 70, 81	4 (30%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	w	67/76 (88%)	2.15	32 (47%) 0 0	47, 92, 104, 107	54 (80%)
57	x	73/77 (94%)	0.33	4 (5%) 26 19	27, 49, 72, 88	13 (17%)
58	y	68/76 (89%)	1.34	16 (23%) 1 0	29, 84, 103, 108	39 (57%)
59	z	671/679 (98%)	0.52	51 (7%) 15 10	32, 66, 85, 99	164 (24%)
All	All	11355/11953 (94%)	0.40	796 (7%) 17 12	18, 49, 93, 214	2236 (19%)

The worst 5 of 796 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	K	92	GLY	14.9
1	A	934	C	14.7
10	K	122	ALA	14.7
10	K	135	GLY	13.9
10	K	139	VAL	12.4

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	PSU	w	39	20/21	0.94	0.27	-	54,63,69,70	7
56	PSU	w	32	20/21	0.93	0.15	-	54,61,66,72	2
58	PSU	y	32	20/21	0.82	0.20	-	92,98,106,108	11
57	5MU	x	54	21/22	0.94	0.20	-	40,51,55,61	10
58	MIA	y	37	22/30	0.83	0.18	-	75,84,87,89	8
57	4SU	x	8	20/21	0.96	0.16	-	41,49,54,54	7
58	5MU	y	54	21/22	0.87	0.24	-	67,72,82,83	11
56	4SU	w	8	20/21	0.83	0.24	-	86,92,95,95	12
56	5MU	w	54	21/22	0.68	0.48	-	94,99,101,104	14
58	4SU	y	8	20/21	0.83	0.20	-	78,95,101,102	10
56	7MG	w	46	24/25	0.79	0.23	-	91,97,102,104	13
56	MIA	w	37	27/30	0.94	0.24	-	42,47,52,52	8
57	5MC	x	32	21/22	0.96	0.18	-	33,40,44,46	4
58	PSU	y	39	20/21	0.79	0.23	-	85,93,96,96	8
56	PSU	w	55	20/21	0.67	0.31	-	96,105,110,111	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	PSU	x	55	20/21	0.95	0.18	-	39,51,54,57	7
58	PSU	y	55	20/21	0.82	0.21	-	68,75,84,88	11

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3472	1/1	0.96	0.47	70.73	25,25,25,25	0
60	MG	A	3463	1/1	0.93	0.68	56.23	48,48,48,48	0
60	MG	A	3165	1/1	0.91	0.34	52.04	42,42,42,42	0
60	MG	A	3157	1/1	0.76	0.55	43.76	40,40,40,40	1
60	MG	A	3114	1/1	0.90	0.39	40.47	42,42,42,42	0
60	MG	A	3169	1/1	0.60	0.45	39.52	44,44,44,44	1
60	MG	A	3258	1/1	0.86	0.41	34.18	41,41,41,41	0
60	MG	a	1717	1/1	0.90	0.63	30.36	54,54,54,54	0
60	MG	a	1702	1/1	0.97	0.48	27.43	42,42,42,42	0
60	MG	A	3283	1/1	0.53	0.53	25.65	41,41,41,41	0
60	MG	A	3530	1/1	0.86	0.42	24.94	38,38,38,38	1
60	MG	A	3391	1/1	0.78	0.41	22.37	56,56,56,56	0
60	MG	A	3201	1/1	0.89	0.48	21.25	45,45,45,45	0
60	MG	A	3004	1/1	0.79	0.41	21.20	40,40,40,40	1
60	MG	A	3217	1/1	0.76	0.56	20.57	56,56,56,56	1
60	MG	F	304	1/1	0.88	0.70	20.48	28,28,28,28	1
60	MG	A	3580	1/1	0.87	0.35	20.25	43,43,43,43	0
60	MG	A	3279	1/1	0.95	0.29	20.23	30,30,30,30	1
60	MG	A	3264	1/1	0.85	0.29	19.00	23,23,23,23	1
60	MG	A	3401	1/1	0.98	0.37	17.62	36,36,36,36	0
60	MG	A	3285	1/1	0.93	0.31	17.24	31,31,31,31	0
60	MG	a	1610	1/1	0.98	0.29	17.12	32,32,32,32	1
60	MG	A	3480	1/1	0.90	0.34	16.90	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3181	1/1	0.89	0.40	16.87	49,49,49,49	0
60	MG	A	3230	1/1	0.96	0.26	16.80	40,40,40,40	0
60	MG	A	3010	1/1	0.90	0.36	16.37	32,32,32,32	1
60	MG	a	1687	1/1	0.91	0.29	15.90	29,29,29,29	0
60	MG	a	1695	1/1	0.92	0.41	15.72	40,40,40,40	0
60	MG	A	3180	1/1	0.81	0.35	15.35	44,44,44,44	0
60	MG	A	3330	1/1	0.96	0.34	15.20	37,37,37,37	1
60	MG	A	3174	1/1	0.95	0.26	15.20	25,25,25,25	0
60	MG	A	3631	1/1	0.92	0.43	15.06	24,24,24,24	1
60	MG	A	3045	1/1	0.91	0.35	15.00	20,20,20,20	0
60	MG	A	3216	1/1	0.97	0.38	14.87	31,31,31,31	0
60	MG	A	3351	1/1	0.88	0.37	14.50	33,33,33,33	0
60	MG	a	1632	1/1	0.87	0.36	14.46	42,42,42,42	0
60	MG	A	3417	1/1	0.95	0.28	14.44	43,43,43,43	0
60	MG	A	3035	1/1	0.91	0.41	14.41	30,30,30,30	1
60	MG	A	3225	1/1	0.85	0.29	14.34	54,54,54,54	0
60	MG	a	1724	1/1	0.98	0.34	14.22	42,42,42,42	0
60	MG	A	3214	1/1	0.94	0.52	13.91	44,44,44,44	1
60	MG	A	3137	1/1	0.84	0.28	13.75	35,35,35,35	0
60	MG	a	1786	1/1	0.81	0.78	13.57	38,38,38,38	1
60	MG	A	3112	1/1	0.89	0.27	13.50	44,44,44,44	0
60	MG	A	3284	1/1	0.82	0.28	12.99	39,39,39,39	1
60	MG	A	3352	1/1	0.94	0.36	12.96	39,39,39,39	0
60	MG	A	3120	1/1	0.97	0.33	12.93	26,26,26,26	0
60	MG	a	1660	1/1	0.75	0.36	12.88	53,53,53,53	0
60	MG	A	3291	1/1	0.87	0.40	12.66	55,55,55,55	0
60	MG	A	3370	1/1	0.91	0.38	12.63	39,39,39,39	0
60	MG	A	3042	1/1	0.90	0.38	12.48	40,40,40,40	0
60	MG	6	101	1/1	0.81	0.35	12.46	42,42,42,42	1
60	MG	A	3531	1/1	0.85	0.41	12.37	55,55,55,55	0
60	MG	A	3515	1/1	0.95	0.28	11.82	47,47,47,47	0
60	MG	A	3256	1/1	0.91	0.50	11.80	62,62,62,62	0
60	MG	A	3221	1/1	0.88	0.31	11.74	49,49,49,49	0
60	MG	A	3238	1/1	0.98	0.31	11.67	38,38,38,38	0
60	MG	A	3334	1/1	0.91	0.37	11.65	57,57,57,57	0
60	MG	A	3474	1/1	0.89	0.34	11.50	44,44,44,44	0
60	MG	A	3029	1/1	0.82	0.30	11.50	48,48,48,48	0
60	MG	A	3431	1/1	0.93	0.31	11.42	52,52,52,52	0
60	MG	A	3053	1/1	0.94	0.27	11.13	35,35,35,35	0
60	MG	A	3189	1/1	0.93	0.31	11.00	50,50,50,50	0
60	MG	A	3602	1/1	0.72	0.34	10.79	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3158	1/1	0.83	0.35	10.51	38,38,38,38	1
60	MG	A	3182	1/1	0.87	0.40	10.27	43,43,43,43	0
60	MG	A	3109	1/1	0.89	0.30	10.20	25,25,25,25	1
60	MG	a	1671	1/1	0.92	0.22	10.19	48,48,48,48	0
60	MG	0	104	1/1	0.95	0.40	10.04	36,36,36,36	1
60	MG	A	3632	1/1	0.92	0.26	10.04	35,35,35,35	1
60	MG	A	3626	1/1	0.92	0.27	9.75	30,30,30,30	1
60	MG	a	1743	1/1	0.96	0.31	9.52	45,45,45,45	0
60	MG	a	1683	1/1	0.90	0.40	9.49	58,58,58,58	0
60	MG	A	3183	1/1	0.85	0.25	9.40	21,21,21,21	0
60	MG	A	3378	1/1	0.97	0.31	9.34	41,41,41,41	0
60	MG	A	3246	1/1	0.88	0.29	9.14	66,66,66,66	0
60	MG	A	3136	1/1	0.92	0.27	8.99	32,32,32,32	0
60	MG	A	3115	1/1	0.92	0.33	8.80	27,27,27,27	1
60	MG	A	3630	1/1	0.75	0.38	8.52	34,34,34,34	1
60	MG	A	3371	1/1	0.75	0.24	8.49	40,40,40,40	0
60	MG	A	3354	1/1	0.87	0.30	8.33	53,53,53,53	0
60	MG	n	102	1/1	0.91	0.32	8.28	28,28,28,28	0
60	MG	A	3297	1/1	0.88	0.28	8.22	35,35,35,35	1
60	MG	a	1613	1/1	0.94	0.26	8.20	29,29,29,29	0
60	MG	A	3043	1/1	0.86	0.24	8.01	39,39,39,39	0
60	MG	A	3449	1/1	0.77	0.31	8.01	29,29,29,29	1
60	MG	A	3429	1/1	0.86	0.29	7.77	45,45,45,45	0
60	MG	A	3424	1/1	0.98	0.33	7.66	20,20,20,20	0
60	MG	A	3177	1/1	0.97	0.37	7.64	39,39,39,39	0
60	MG	A	3308	1/1	0.98	0.23	7.56	14,14,14,14	0
60	MG	A	3211	1/1	0.93	0.23	7.39	50,50,50,50	0
60	MG	a	1752	1/1	0.86	0.35	7.26	43,43,43,43	0
60	MG	A	3404	1/1	0.86	0.27	7.26	35,35,35,35	0
60	MG	A	3635	1/1	0.92	0.35	7.23	29,29,29,29	1
60	MG	A	3235	1/1	0.78	0.20	7.12	43,43,43,43	0
60	MG	A	3638	1/1	0.90	0.23	7.06	38,38,38,38	0
60	MG	A	3099	1/1	0.74	0.28	6.95	51,51,51,51	0
60	MG	A	3397	1/1	0.95	0.26	6.91	38,38,38,38	0
60	MG	A	3525	1/1	0.64	0.24	6.89	37,37,37,37	0
60	MG	A	3384	1/1	0.86	0.23	6.84	39,39,39,39	0
60	MG	A	3286	1/1	0.94	0.49	6.72	48,48,48,48	0
60	MG	A	3069	1/1	0.95	0.24	6.69	30,30,30,30	0
60	MG	F	302	1/1	0.87	0.27	6.65	32,32,32,32	1
60	MG	n	103	1/1	0.94	0.31	6.50	55,55,55,55	0
60	MG	A	3488	1/1	0.93	0.24	6.44	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	D	304	1/1	0.86	0.32	6.42	36,36,36,36	1
60	MG	A	3347	1/1	0.93	0.27	6.37	37,37,37,37	1
60	MG	A	3595	1/1	0.95	0.27	6.23	27,27,27,27	0
60	MG	A	3185	1/1	0.94	0.22	6.22	32,32,32,32	0
60	MG	a	1778	1/1	0.93	0.26	6.21	53,53,53,53	0
60	MG	A	3596	1/1	0.93	0.25	6.18	44,44,44,44	1
60	MG	F	301	1/1	0.90	0.20	6.14	44,44,44,44	0
60	MG	A	3382	1/1	0.88	0.27	6.08	30,30,30,30	0
60	MG	A	3300	1/1	0.92	0.28	6.04	42,42,42,42	0
60	MG	A	3018	1/1	0.98	0.25	6.00	27,27,27,27	0
60	MG	A	3585	1/1	0.67	0.25	5.87	46,46,46,46	0
60	MG	Q	202	1/1	0.91	0.21	5.84	33,33,33,33	0
60	MG	A	3036	1/1	0.98	0.25	5.80	25,25,25,25	1
60	MG	A	3455	1/1	0.93	0.27	5.76	28,28,28,28	0
60	MG	A	3377	1/1	0.92	0.29	5.73	26,26,26,26	0
60	MG	a	1712	1/1	0.91	0.25	5.62	54,54,54,54	0
60	MG	A	3523	1/1	0.94	0.28	5.61	31,31,31,31	0
60	MG	a	1619	1/1	0.93	0.27	5.56	32,32,32,32	0
60	MG	E	303	1/1	0.91	0.31	5.40	32,32,32,32	1
60	MG	A	3168	1/1	0.95	0.22	5.29	23,23,23,23	0
60	MG	A	3019	1/1	0.93	0.31	5.26	20,20,20,20	0
60	MG	a	1608	1/1	0.99	0.29	5.26	23,23,23,23	0
60	MG	A	3199	1/1	0.68	0.24	5.24	45,45,45,45	0
60	MG	A	3506	1/1	0.96	0.32	5.24	41,41,41,41	0
60	MG	A	3608	1/1	0.94	0.22	5.14	32,32,32,32	0
60	MG	A	3147	1/1	0.90	0.24	5.11	50,50,50,50	0
60	MG	A	3162	1/1	0.96	0.19	5.02	29,29,29,29	0
60	MG	A	3636	1/1	0.89	0.32	4.93	37,37,37,37	1
60	MG	a	1622	1/1	0.91	0.21	4.92	36,36,36,36	0
60	MG	5	101	1/1	0.93	0.30	4.90	44,44,44,44	1
60	MG	A	3643	1/1	0.94	0.29	4.87	34,34,34,34	0
60	MG	U	201	1/1	0.87	0.34	4.86	30,30,30,30	1
60	MG	A	3644	1/1	0.80	0.23	4.85	42,42,42,42	0
60	MG	A	3038	1/1	0.88	0.21	4.79	29,29,29,29	0
60	MG	A	3241	1/1	0.94	0.22	4.72	20,20,20,20	0
60	MG	A	3642	1/1	0.87	0.21	4.55	38,38,38,38	1
60	MG	A	3628	1/1	0.95	0.30	4.48	35,35,35,35	0
60	MG	A	3496	1/1	0.88	0.31	4.45	33,33,33,33	1
60	MG	F	303	1/1	0.88	0.21	4.26	53,53,53,53	0
60	MG	A	3228	1/1	0.74	0.31	4.13	49,49,49,49	0
60	MG	A	3341	1/1	0.83	0.27	4.12	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3633	1/1	0.86	0.31	4.10	30,30,30,30	0
60	MG	a	1662	1/1	0.64	0.33	4.10	53,53,53,53	0
60	MG	a	1740	1/1	0.91	0.24	4.03	58,58,58,58	0
60	MG	a	1693	1/1	0.85	0.32	3.97	39,39,39,39	0
60	MG	a	1659	1/1	0.89	0.27	3.90	55,55,55,55	0
60	MG	A	3006	1/1	0.62	0.38	3.88	52,52,52,52	1
60	MG	A	3639	1/1	0.82	0.29	3.85	36,36,36,36	0
60	MG	A	3553	1/1	0.93	0.25	3.77	51,51,51,51	1
60	MG	A	3224	1/1	0.88	0.20	3.74	34,34,34,34	0
60	MG	0	102	1/1	0.75	0.26	3.68	47,47,47,47	0
60	MG	A	3024	1/1	0.86	0.28	3.67	40,40,40,40	0
60	MG	A	3477	1/1	0.97	0.22	3.58	21,21,21,21	0
60	MG	A	3373	1/1	0.96	0.25	3.50	34,34,34,34	0
60	MG	A	3363	1/1	0.94	0.20	3.47	35,35,35,35	0
60	MG	a	1682	1/1	0.91	0.20	3.45	45,45,45,45	0
60	MG	A	3007	1/1	0.93	0.21	3.32	35,35,35,35	0
60	MG	A	3331	1/1	0.94	0.21	3.31	31,31,31,31	0
60	MG	A	3387	1/1	0.83	0.24	3.20	26,26,26,26	0
60	MG	A	3193	1/1	0.93	0.22	3.10	27,27,27,27	0
60	MG	A	3056	1/1	0.83	0.24	3.07	39,39,39,39	0
60	MG	a	1678	1/1	0.92	0.23	3.06	36,36,36,36	0
60	MG	A	3627	1/1	0.83	0.22	3.04	25,25,25,25	0
60	MG	A	3113	1/1	0.96	0.25	3.00	29,29,29,29	1
60	MG	a	1688	1/1	0.98	0.22	2.96	32,32,32,32	0
60	MG	a	1766	1/1	0.94	0.24	2.85	49,49,49,49	0
60	MG	A	3031	1/1	0.97	0.20	2.82	33,33,33,33	0
60	MG	A	3374	1/1	0.89	0.22	2.61	54,54,54,54	0
60	MG	A	3003	1/1	0.90	0.24	2.39	32,32,32,32	0
60	MG	A	3319	1/1	0.89	0.21	2.33	43,43,43,43	0
61	ZN	6	102	1/1	0.95	0.25	2.25	72,72,72,72	0
60	MG	A	3327	1/1	0.94	0.23	2.24	30,30,30,30	0
60	MG	D	303	1/1	0.89	0.24	2.23	24,24,24,24	1
60	MG	D	301	1/1	0.97	0.26	2.20	21,21,21,21	0
60	MG	A	3433	1/1	0.85	0.20	2.12	27,27,27,27	1
60	MG	N	201	1/1	0.91	0.24	2.10	42,42,42,42	0
60	MG	A	3360	1/1	0.96	0.19	2.06	54,54,54,54	0
60	MG	A	3073	1/1	0.87	0.21	2.01	32,32,32,32	0
60	MG	A	3320	1/1	0.87	0.21	2.01	62,62,62,62	0
60	MG	A	3483	1/1	0.98	0.21	1.86	31,31,31,31	0
60	MG	a	1667	1/1	0.85	0.21	1.70	55,55,55,55	0
60	MG	a	1731	1/1	0.83	0.20	1.61	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	z	701	1/1	0.83	0.28	1.55	59,59,59,59	0
60	MG	B	204	1/1	0.62	0.24	1.50	63,63,63,63	0
60	MG	D	302	1/1	0.92	0.19	1.50	43,43,43,43	0
60	MG	A	3140	1/1	0.94	0.19	1.43	48,48,48,48	0
60	MG	A	3313	1/1	0.93	0.17	1.42	29,29,29,29	0
60	MG	A	3287	1/1	0.94	0.19	1.38	35,35,35,35	0
60	MG	A	3079	1/1	0.91	0.17	1.30	18,18,18,18	0
60	MG	A	3368	1/1	0.95	0.21	1.22	36,36,36,36	0
60	MG	A	3156	1/1	0.93	0.19	1.22	26,26,26,26	0
60	MG	A	3200	1/1	0.81	0.19	1.21	39,39,39,39	0
60	MG	A	3494	1/1	0.93	0.20	1.20	35,35,35,35	0
60	MG	A	3245	1/1	0.91	0.18	1.12	45,45,45,45	0
60	MG	A	3021	1/1	0.92	0.19	1.07	34,34,34,34	0
60	MG	a	1661	1/1	0.56	0.19	1.07	69,69,69,69	0
60	MG	A	3522	1/1	0.95	0.21	1.04	28,28,28,28	0
60	MG	A	3067	1/1	0.86	0.18	1.04	34,34,34,34	0
60	MG	m	201	1/1	0.96	0.22	1.01	38,38,38,38	1
60	MG	A	3312	1/1	0.91	0.18	1.00	40,40,40,40	0
60	MG	A	3037	1/1	0.79	0.18	0.99	44,44,44,44	0
60	MG	A	3030	1/1	0.96	0.18	0.96	33,33,33,33	0
60	MG	A	3457	1/1	0.93	0.18	0.94	24,24,24,24	0
60	MG	a	1668	1/1	0.95	0.18	0.81	30,30,30,30	0
60	MG	A	3008	1/1	0.83	0.18	0.61	42,42,42,42	0
60	MG	A	3134	1/1	0.93	0.19	0.48	25,25,25,25	0
60	MG	A	3582	1/1	0.97	0.19	0.38	21,21,21,21	1
60	MG	A	3150	1/1	0.82	0.17	0.38	54,54,54,54	0
60	MG	8	101	1/1	0.91	0.21	0.34	35,35,35,35	0
60	MG	A	3303	1/1	0.93	0.17	0.27	57,57,57,57	0
60	MG	a	1739	1/1	0.94	0.17	0.26	42,42,42,42	0
60	MG	A	3500	1/1	0.93	0.20	0.26	30,30,30,30	0
60	MG	A	3166	1/1	0.92	0.17	0.22	40,40,40,40	0
60	MG	6	103	1/1	0.94	0.17	0.12	41,41,41,41	0
60	MG	A	3159	1/1	0.90	0.18	0.12	45,45,45,45	1
60	MG	A	3023	1/1	0.96	0.17	0.11	34,34,34,34	0
60	MG	A	3396	1/1	0.99	0.18	0.11	26,26,26,26	0
60	MG	E	304	1/1	0.90	0.20	0.08	35,35,35,35	0
60	MG	A	3519	1/1	0.82	0.17	0.04	48,48,48,48	0
60	MG	A	3058	1/1	0.91	0.21	0.04	59,59,59,59	0
60	MG	G	201	1/1	0.93	0.20	-0.09	48,48,48,48	0
60	MG	A	3407	1/1	0.98	0.17	-0.13	30,30,30,30	0
60	MG	a	1701	1/1	0.58	0.18	-0.17	66,66,66,66	0
60	MG	A	3151	1/1	0.69	0.18	-0.40	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3516	1/1	0.94	0.19	-0.43	25,25,25,25	1
60	MG	A	3641	1/1	0.93	0.17	-0.54	32,32,32,32	1
60	MG	A	3629	1/1	0.95	0.17	-0.57	21,21,21,21	0
60	MG	A	3074	1/1	0.95	0.15	-0.57	29,29,29,29	0
60	MG	a	1685	1/1	0.91	0.16	-0.60	46,46,46,46	0
60	MG	A	3539	1/1	0.93	0.17	-0.61	21,21,21,21	0
60	MG	E	301	1/1	0.91	0.17	-0.62	33,33,33,33	0
60	MG	A	3104	1/1	0.92	0.17	-0.66	25,25,25,25	0
61	ZN	9	102	1/1	0.97	0.19	-0.67	49,49,49,49	1
60	MG	B	213	1/1	0.96	0.17	-0.69	52,52,52,52	0
63	GCP	z	703	32/32	0.96	0.15	-0.69	47,57,62,63	13
60	MG	a	1644	1/1	0.85	0.17	-0.76	46,46,46,46	0
60	MG	a	1694	1/1	0.87	0.15	-0.77	41,41,41,41	0
60	MG	E	305	1/1	0.99	0.16	-0.82	23,23,23,23	1
60	MG	a	1707	1/1	0.94	0.16	-0.87	34,34,34,34	0
60	MG	a	1762	1/1	0.91	0.15	-1.04	52,52,52,52	0
60	MG	A	3310	1/1	0.88	0.16	-1.10	37,37,37,37	0
60	MG	a	1773	1/1	0.92	0.14	-1.11	58,58,58,58	0
60	MG	A	3584	1/1	0.94	0.13	-1.28	39,39,39,39	0
61	ZN	n	104	1/1	0.99	0.15	-1.31	44,44,44,44	0
60	MG	A	3046	1/1	0.96	0.16	-1.35	29,29,29,29	0
60	MG	a	1735	1/1	0.96	0.15	-1.37	37,37,37,37	0
60	MG	A	3385	1/1	0.91	0.16	-1.38	35,35,35,35	0
60	MG	A	3005	1/1	0.96	0.17	-1.38	31,31,31,31	1
60	MG	F	305	1/1	0.80	0.14	-1.43	46,46,46,46	0
60	MG	A	3302	1/1	0.97	0.15	-1.46	22,22,22,22	0
60	MG	a	1624	1/1	0.94	0.14	-1.60	39,39,39,39	0
60	MG	a	1690	1/1	0.85	0.14	-1.62	69,69,69,69	0
60	MG	D	306	1/1	0.93	0.16	-1.73	25,25,25,25	0
60	MG	A	3640	1/1	0.96	0.14	-1.75	30,30,30,30	1
60	MG	a	1744	1/1	0.97	0.16	-1.76	46,46,46,46	0
60	MG	A	3501	1/1	0.98	0.15	-1.87	24,24,24,24	0
60	MG	A	3507	1/1	0.93	0.13	-1.87	42,42,42,42	0
60	MG	a	1728	1/1	0.97	0.13	-1.95	33,33,33,33	0
60	MG	A	3481	1/1	0.95	0.13	-2.03	46,46,46,46	0
60	MG	A	3222	1/1	0.92	0.15	-2.11	39,39,39,39	0
60	MG	B	210	1/1	0.97	0.13	-2.15	44,44,44,44	0
60	MG	A	3367	1/1	0.92	0.15	-2.15	40,40,40,40	0
61	ZN	4	501	1/1	0.95	0.06	-2.39	79,79,79,79	0
60	MG	x	103	1/1	0.80	0.10	-2.48	62,62,62,62	0
60	MG	A	3096	1/1	0.98	0.14	-2.48	27,27,27,27	0
61	ZN	5	103	1/1	0.97	0.08	-2.64	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	a	1684	1/1	0.95	0.14	-2.65	31,31,31,31	0
60	MG	A	3064	1/1	0.77	0.14	-2.70	58,58,58,58	0
60	MG	A	3473	1/1	0.95	0.18	-2.74	27,27,27,27	0
60	MG	A	3194	1/1	0.92	0.12	-2.83	63,63,63,63	0
60	MG	A	3615	1/1	0.99	0.14	-2.98	34,34,34,34	0
60	MG	A	3343	1/1	0.87	0.09	-3.00	64,64,64,64	0
60	MG	x	105	1/1	0.94	0.12	-3.11	51,51,51,51	0
60	MG	A	3420	1/1	0.79	0.16	-3.13	55,55,55,55	0
60	MG	A	3383	1/1	0.97	0.10	-3.25	28,28,28,28	0
60	MG	a	1708	1/1	0.98	0.11	-3.30	40,40,40,40	0
60	MG	z	702	1/1	0.82	0.08	-3.33	57,57,57,57	0
62	SF4	d	302	8/8	0.95	0.05	-3.34	60,65,70,71	2
60	MG	a	1706	1/1	0.91	0.11	-3.40	48,48,48,48	0
60	MG	A	3389	1/1	0.95	0.10	-3.44	33,33,33,33	0
60	MG	A	3028	1/1	0.92	0.11	-3.49	57,57,57,57	0
60	MG	A	3589	1/1	0.90	0.14	-3.51	42,42,42,42	0
60	MG	a	1647	1/1	0.91	0.10	-4.01	35,35,35,35	0
60	MG	a	1788	1/1	0.98	0.10	-4.04	43,43,43,43	1
60	MG	a	1658	1/1	0.93	0.12	-4.35	30,30,30,30	0
60	MG	A	3202	1/1	0.90	0.09	-4.82	36,36,36,36	0
61	ZN	Y	501	1/1	0.96	0.05	-4.82	63,63,63,63	0
60	MG	A	3490	1/1	0.96	0.12	-4.94	40,40,40,40	0
60	MG	A	3152	1/1	0.88	0.10	-5.11	48,48,48,48	0
60	MG	A	3376	1/1	0.97	0.14	-5.53	31,31,31,31	0
60	MG	A	3460	1/1	0.91	0.13	-5.96	41,41,41,41	0
60	MG	A	3415	1/1	0.97	0.11	-5.99	34,34,34,34	0
60	MG	a	1734	1/1	0.98	0.09	-6.21	33,33,33,33	0
60	MG	a	1747	1/1	0.91	0.11	-7.51	38,38,38,38	0
60	MG	a	1736	1/1	0.91	0.07	-7.95	46,46,46,46	0
60	MG	A	3213	1/1	0.98	0.10	-8.28	34,34,34,34	1
60	MG	B	217	1/1	0.97	0.13	-	40,40,40,40	0
60	MG	a	1634	1/1	0.94	0.35	-	53,53,53,53	0
60	MG	A	3117	1/1	0.62	0.30	-	48,48,48,48	0
60	MG	a	1730	1/1	0.91	0.45	-	53,53,53,53	0
60	MG	A	3357	1/1	0.95	0.48	-	36,36,36,36	0
60	MG	A	3055	1/1	0.68	0.22	-	47,47,47,47	0
60	MG	A	3268	1/1	0.89	0.27	-	52,52,52,52	0
60	MG	A	3590	1/1	0.97	0.29	-	63,63,63,63	0
60	MG	a	1692	1/1	0.96	0.25	-	41,41,41,41	0
60	MG	a	1782	1/1	0.82	0.59	-	62,62,62,62	0
60	MG	A	3197	1/1	0.71	0.33	-	48,48,48,48	1
60	MG	A	3440	1/1	0.97	0.13	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3063	1/1	0.86	0.30	-	49,49,49,49	0
60	MG	a	1612	1/1	0.84	0.13	-	57,57,57,57	0
60	MG	a	1764	1/1	0.98	0.49	-	37,37,37,37	0
60	MG	A	3243	1/1	0.71	0.22	-	52,52,52,52	0
60	MG	A	3271	1/1	0.85	0.48	-	71,71,71,71	0
60	MG	A	3478	1/1	0.94	0.34	-	50,50,50,50	0
60	MG	A	3060	1/1	0.78	0.13	-	54,54,54,54	0
60	MG	A	3237	1/1	0.69	0.42	-	43,43,43,43	1
60	MG	A	3438	1/1	0.81	0.13	-	77,77,77,77	0
60	MG	A	3195	1/1	0.93	0.47	-	55,55,55,55	0
60	MG	A	3524	1/1	0.91	0.20	-	49,49,49,49	1
60	MG	a	1781	1/1	0.97	0.23	-	46,46,46,46	0
60	MG	A	3349	1/1	0.93	0.18	-	42,42,42,42	0
60	MG	a	1722	1/1	0.96	0.15	-	51,51,51,51	0
60	MG	A	3609	1/1	0.90	0.21	-	31,31,31,31	0
60	MG	A	3476	1/1	0.93	0.09	-	58,58,58,58	0
60	MG	A	3309	1/1	0.98	0.20	-	49,49,49,49	0
60	MG	A	3444	1/1	0.98	0.31	-	39,39,39,39	0
60	MG	A	3533	1/1	0.94	0.41	-	52,52,52,52	0
60	MG	A	3125	1/1	0.92	0.30	-	22,22,22,22	1
60	MG	A	3561	1/1	0.93	0.20	-	60,60,60,60	0
60	MG	A	3206	1/1	0.84	0.31	-	50,50,50,50	0
60	MG	a	1646	1/1	0.95	0.20	-	52,52,52,52	0
60	MG	a	1753	1/1	0.93	0.32	-	46,46,46,46	0
60	MG	A	3344	1/1	0.79	0.11	-	70,70,70,70	0
60	MG	x	108	1/1	0.75	0.26	-	55,55,55,55	0
60	MG	a	1759	1/1	0.88	0.13	-	53,53,53,53	0
60	MG	A	3273	1/1	0.99	0.33	-	37,37,37,37	1
60	MG	A	3227	1/1	0.74	0.35	-	63,63,63,63	0
60	MG	A	3255	1/1	0.71	0.38	-	94,94,94,94	0
60	MG	A	3485	1/1	0.95	0.16	-	59,59,59,59	0
60	MG	A	3637	1/1	0.94	0.44	-	37,37,37,37	0
60	MG	l	201	1/1	0.95	0.22	-	31,31,31,31	0
60	MG	A	3203	1/1	0.91	0.26	-	52,52,52,52	0
60	MG	A	3592	1/1	0.88	0.48	-	41,41,41,41	1
60	MG	A	3121	1/1	0.79	0.34	-	38,38,38,38	1
60	MG	D	305	1/1	0.95	0.43	-	43,43,43,43	0
60	MG	A	3419	1/1	0.96	0.26	-	30,30,30,30	1
60	MG	x	106	1/1	0.72	0.45	-	56,56,56,56	1
60	MG	a	1749	1/1	0.95	0.33	-	54,54,54,54	0
60	MG	A	3599	1/1	0.78	0.20	-	45,45,45,45	0
60	MG	A	3298	1/1	0.96	0.20	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3179	1/1	0.72	0.25	-	61,61,61,61	0
60	MG	a	1648	1/1	0.80	0.28	-	58,58,58,58	0
60	MG	m	202	1/1	0.97	0.31	-	56,56,56,56	0
60	MG	A	3406	1/1	0.91	0.06	-	74,74,74,74	0
60	MG	A	3402	1/1	0.77	0.35	-	36,36,36,36	0
60	MG	A	3015	1/1	0.81	0.18	-	45,45,45,45	0
60	MG	A	3622	1/1	0.94	0.35	-	57,57,57,57	0
60	MG	A	3155	1/1	0.51	0.28	-	65,65,65,65	0
60	MG	A	3498	1/1	0.94	0.15	-	68,68,68,68	0
60	MG	A	3578	1/1	0.91	0.19	-	60,60,60,60	0
60	MG	a	1763	1/1	0.85	0.27	-	34,34,34,34	1
60	MG	A	3130	1/1	0.80	0.29	-	55,55,55,55	0
60	MG	A	3332	1/1	0.90	0.13	-	53,53,53,53	0
60	MG	A	3316	1/1	0.80	0.37	-	63,63,63,63	0
60	MG	A	3461	1/1	0.91	0.22	-	40,40,40,40	0
60	MG	Q	201	1/1	0.96	0.45	-	47,47,47,47	0
60	MG	A	3426	1/1	0.95	0.15	-	36,36,36,36	0
60	MG	A	3612	1/1	0.87	0.10	-	62,62,62,62	0
60	MG	V	202	1/1	0.50	0.55	-	73,73,73,73	0
60	MG	A	3281	1/1	0.83	0.23	-	43,43,43,43	0
60	MG	R	202	1/1	0.70	0.19	-	62,62,62,62	0
60	MG	A	3339	1/1	0.88	0.12	-	54,54,54,54	0
60	MG	v	102	1/1	0.94	0.30	-	42,42,42,42	0
60	MG	A	3581	1/1	0.80	0.10	-	63,63,63,63	0
60	MG	A	3487	1/1	0.97	0.21	-	35,35,35,35	0
60	MG	A	3129	1/1	0.88	0.19	-	35,35,35,35	1
60	MG	a	1689	1/1	0.62	0.24	-	74,74,74,74	0
60	MG	A	3097	1/1	0.75	0.29	-	56,56,56,56	0
60	MG	a	1614	1/1	0.29	0.67	-	75,75,75,75	0
60	MG	a	1704	1/1	0.81	0.22	-	52,52,52,52	0
60	MG	A	3450	1/1	0.87	0.33	-	58,58,58,58	0
60	MG	a	1698	1/1	0.72	0.22	-	49,49,49,49	0
60	MG	A	3364	1/1	0.94	0.10	-	45,45,45,45	0
60	MG	A	3572	1/1	0.84	0.21	-	58,58,58,58	0
60	MG	A	3607	1/1	0.74	0.14	-	54,54,54,54	0
60	MG	O	201	1/1	0.81	0.23	-	55,55,55,55	0
60	MG	a	1626	1/1	0.90	0.42	-	52,52,52,52	0
60	MG	A	3393	1/1	0.94	0.28	-	41,41,41,41	0
60	MG	A	3226	1/1	0.89	0.28	-	45,45,45,45	0
60	MG	a	1737	1/1	0.94	0.35	-	46,46,46,46	0
60	MG	A	3260	1/1	0.83	0.32	-	44,44,44,44	1
60	MG	A	3379	1/1	0.92	0.15	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	a	1681	1/1	0.86	0.16	-	55,55,55,55	0
60	MG	A	3022	1/1	0.72	0.29	-	59,59,59,59	0
60	MG	A	3611	1/1	0.80	0.20	-	46,46,46,46	0
60	MG	A	3388	1/1	0.92	0.19	-	31,31,31,31	0
60	MG	a	1785	1/1	0.80	0.47	-	53,53,53,53	0
60	MG	a	1672	1/1	0.87	0.23	-	41,41,41,41	0
60	MG	A	3430	1/1	0.98	0.22	-	43,43,43,43	0
60	MG	A	3282	1/1	0.76	0.29	-	68,68,68,68	0
60	MG	a	1606	1/1	0.76	0.12	-	48,48,48,48	0
60	MG	A	3084	1/1	0.85	0.11	-	56,56,56,56	0
60	MG	A	3328	1/1	0.88	0.17	-	62,62,62,62	0
60	MG	A	3265	1/1	0.69	0.24	-	64,64,64,64	0
60	MG	A	3306	1/1	0.92	0.28	-	33,33,33,33	0
60	MG	A	3634	1/1	0.92	0.15	-	42,42,42,42	1
60	MG	A	3535	1/1	0.90	0.26	-	55,55,55,55	0
60	MG	W	201	1/1	0.85	0.29	-	59,59,59,59	0
60	MG	a	1677	1/1	0.89	0.20	-	63,63,63,63	0
60	MG	A	3459	1/1	0.96	0.24	-	33,33,33,33	0
60	MG	A	3163	1/1	0.90	0.11	-	26,26,26,26	0
60	MG	A	3597	1/1	0.82	0.34	-	47,47,47,47	0
60	MG	a	1754	1/1	0.93	0.12	-	42,42,42,42	0
60	MG	A	3223	1/1	0.74	0.42	-	52,52,52,52	0
60	MG	A	3085	1/1	0.79	0.24	-	70,70,70,70	0
60	MG	A	3132	1/1	0.82	0.42	-	43,43,43,43	1
60	MG	A	3252	1/1	0.49	0.18	-	76,76,76,76	0
60	MG	A	3280	1/1	0.85	0.33	-	46,46,46,46	0
60	MG	F	306	1/1	0.84	0.33	-	46,46,46,46	0
60	MG	A	3212	1/1	0.82	0.13	-	46,46,46,46	0
60	MG	A	3092	1/1	0.65	0.26	-	58,58,58,58	0
60	MG	A	3441	1/1	0.86	0.56	-	52,52,52,52	0
60	MG	A	3050	1/1	0.70	0.41	-	60,60,60,60	0
60	MG	A	3445	1/1	0.97	0.26	-	42,42,42,42	1
60	MG	A	3123	1/1	0.95	0.22	-	30,30,30,30	1
60	MG	a	1611	1/1	0.80	0.18	-	58,58,58,58	0
60	MG	A	3294	1/1	0.95	0.18	-	25,25,25,25	1
60	MG	A	3446	1/1	0.97	0.24	-	26,26,26,26	0
60	MG	A	3567	1/1	0.95	0.15	-	38,38,38,38	1
60	MG	a	1657	1/1	0.88	0.14	-	57,57,57,57	0
60	MG	A	3090	1/1	0.90	0.21	-	43,43,43,43	0
60	MG	B	203	1/1	0.96	0.07	-	56,56,56,56	0
60	MG	A	3510	1/1	0.81	0.33	-	48,48,48,48	0
60	MG	A	3198	1/1	0.97	0.10	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3131	1/1	0.94	0.20	-	57,57,57,57	0
60	MG	A	3605	1/1	0.94	0.36	-	50,50,50,50	0
60	MG	A	3276	1/1	0.88	0.20	-	51,51,51,51	1
60	MG	A	3275	1/1	0.83	0.29	-	55,55,55,55	1
60	MG	A	3514	1/1	0.88	0.14	-	69,69,69,69	0
60	MG	a	1641	1/1	0.73	0.34	-	68,68,68,68	0
60	MG	A	3563	1/1	0.75	0.26	-	46,46,46,46	0
60	MG	a	1609	1/1	0.85	0.55	-	51,51,51,51	0
60	MG	A	3142	1/1	0.79	0.23	-	57,57,57,57	0
60	MG	A	3538	1/1	0.92	0.27	-	39,39,39,39	0
60	MG	a	1705	1/1	0.39	0.38	-	72,72,72,72	0
60	MG	A	3583	1/1	0.93	0.21	-	46,46,46,46	0
60	MG	a	1602	1/1	0.87	0.28	-	57,57,57,57	0
60	MG	A	3293	1/1	0.92	0.26	-	48,48,48,48	0
60	MG	A	3527	1/1	0.74	0.29	-	45,45,45,45	0
60	MG	A	3542	1/1	0.84	0.25	-	63,63,63,63	0
60	MG	A	3540	1/1	0.86	0.10	-	57,57,57,57	0
60	MG	A	3321	1/1	0.91	0.17	-	49,49,49,49	0
60	MG	a	1725	1/1	0.81	0.30	-	51,51,51,51	0
60	MG	a	1654	1/1	0.88	0.16	-	50,50,50,50	0
60	MG	A	3250	1/1	0.85	0.28	-	64,64,64,64	0
60	MG	a	1755	1/1	0.93	0.08	-	40,40,40,40	0
60	MG	A	3381	1/1	0.93	0.16	-	56,56,56,56	0
60	MG	A	3267	1/1	0.59	0.45	-	64,64,64,64	0
60	MG	A	3139	1/1	0.94	0.30	-	37,37,37,37	0
60	MG	A	3138	1/1	0.94	0.12	-	31,31,31,31	0
60	MG	A	3170	1/1	0.82	0.25	-	33,33,33,33	0
60	MG	A	3188	1/1	0.84	0.29	-	39,39,39,39	0
60	MG	A	3248	1/1	0.92	0.34	-	48,48,48,48	1
60	MG	A	3345	1/1	0.94	0.25	-	48,48,48,48	0
60	MG	A	3088	1/1	0.81	0.32	-	53,53,53,53	0
60	MG	a	1710	1/1	0.94	0.34	-	53,53,53,53	1
60	MG	A	3324	1/1	0.97	0.11	-	38,38,38,38	0
60	MG	a	1636	1/1	0.71	0.42	-	59,59,59,59	0
60	MG	A	3333	1/1	0.79	0.24	-	61,61,61,61	1
60	MG	A	3205	1/1	0.94	0.17	-	53,53,53,53	0
60	MG	A	3336	1/1	0.91	0.10	-	52,52,52,52	0
60	MG	A	3432	1/1	0.94	0.16	-	54,54,54,54	0
60	MG	O	202	1/1	0.96	0.16	-	50,50,50,50	0
60	MG	a	1627	1/1	0.86	0.28	-	47,47,47,47	0
60	MG	d	301	1/1	0.83	0.56	-	59,59,59,59	0
60	MG	A	3259	1/1	0.79	0.31	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	a	1697	1/1	0.90	0.22	-	34,34,34,34	0
60	MG	A	3072	1/1	0.85	0.17	-	46,46,46,46	0
60	MG	A	3560	1/1	0.89	0.20	-	58,58,58,58	0
60	MG	A	3558	1/1	0.96	0.24	-	53,53,53,53	0
60	MG	A	3075	1/1	0.87	0.14	-	60,60,60,60	1
60	MG	A	3577	1/1	0.73	0.42	-	60,60,60,60	0
60	MG	A	3048	1/1	0.93	0.15	-	35,35,35,35	0
60	MG	A	3234	1/1	0.42	0.54	-	61,61,61,61	0
60	MG	B	216	1/1	0.86	0.11	-	53,53,53,53	0
60	MG	a	1720	1/1	0.98	0.22	-	48,48,48,48	0
60	MG	a	1723	1/1	0.96	0.27	-	48,48,48,48	0
60	MG	a	1709	1/1	0.87	0.12	-	36,36,36,36	0
60	MG	A	3594	1/1	0.97	0.34	-	85,85,85,85	0
60	MG	a	1665	1/1	0.76	0.52	-	47,47,47,47	1
60	MG	A	3012	1/1	0.88	0.30	-	60,60,60,60	0
60	MG	a	1635	1/1	0.84	0.26	-	55,55,55,55	0
60	MG	A	3044	1/1	0.84	0.30	-	25,25,25,25	1
60	MG	v	101	1/1	0.91	0.36	-	35,35,35,35	1
60	MG	A	3451	1/1	0.97	0.29	-	45,45,45,45	0
60	MG	A	3491	1/1	0.97	0.34	-	39,39,39,39	0
60	MG	B	205	1/1	0.91	0.15	-	52,52,52,52	0
60	MG	A	3210	1/1	0.93	0.56	-	30,30,30,30	0
60	MG	x	102	1/1	0.94	0.07	-	77,77,77,77	0
60	MG	A	3172	1/1	0.79	0.39	-	49,49,49,49	0
60	MG	a	1623	1/1	0.93	0.22	-	46,46,46,46	1
60	MG	A	3146	1/1	0.89	0.09	-	72,72,72,72	0
60	MG	n	101	1/1	0.83	0.66	-	64,64,64,64	0
60	MG	A	3369	1/1	0.98	0.14	-	31,31,31,31	0
60	MG	A	3437	1/1	0.91	0.21	-	30,30,30,30	1
60	MG	A	3503	1/1	0.98	0.21	-	53,53,53,53	0
60	MG	a	1700	1/1	0.96	0.25	-	50,50,50,50	0
60	MG	A	3362	1/1	0.83	0.28	-	47,47,47,47	0
60	MG	a	1772	1/1	0.77	0.35	-	62,62,62,62	0
60	MG	a	1703	1/1	0.73	0.24	-	57,57,57,57	1
60	MG	B	208	1/1	0.95	0.08	-	64,64,64,64	0
60	MG	A	3009	1/1	0.92	0.14	-	52,52,52,52	0
60	MG	A	3413	1/1	0.97	0.13	-	35,35,35,35	0
60	MG	A	3311	1/1	0.91	0.20	-	41,41,41,41	0
60	MG	A	3623	1/1	0.92	0.35	-	57,57,57,57	0
60	MG	a	1675	1/1	0.81	0.60	-	61,61,61,61	0
60	MG	a	1716	1/1	0.96	0.16	-	36,36,36,36	0
60	MG	A	3435	1/1	0.91	0.33	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	Z	301	1/1	0.80	0.16	-	61,61,61,61	0
60	MG	A	3559	1/1	0.87	0.27	-	38,38,38,38	1
60	MG	A	3619	1/1	0.96	0.30	-	16,16,16,16	0
60	MG	a	1640	1/1	0.86	0.62	-	68,68,68,68	0
60	MG	a	1676	1/1	0.46	0.24	-	58,58,58,58	0
60	MG	a	1670	1/1	0.92	0.10	-	57,57,57,57	0
60	MG	a	1669	1/1	0.85	0.27	-	60,60,60,60	0
60	MG	A	3586	1/1	0.55	0.52	-	75,75,75,75	0
60	MG	A	3521	1/1	0.77	0.23	-	35,35,35,35	1
60	MG	A	3049	1/1	0.73	0.32	-	68,68,68,68	0
60	MG	a	1607	1/1	0.99	0.35	-	42,42,42,42	1
60	MG	A	3464	1/1	0.93	0.13	-	56,56,56,56	0
60	MG	A	3261	1/1	0.97	0.19	-	46,46,46,46	0
60	MG	a	1750	1/1	0.95	0.22	-	41,41,41,41	0
60	MG	A	3016	1/1	0.89	0.38	-	59,59,59,59	0
60	MG	A	3105	1/1	0.95	0.25	-	28,28,28,28	1
60	MG	A	3244	1/1	0.81	0.19	-	53,53,53,53	0
60	MG	A	3475	1/1	0.97	0.15	-	41,41,41,41	0
60	MG	A	3191	1/1	0.89	0.22	-	51,51,51,51	0
60	MG	a	1630	1/1	0.91	0.31	-	44,44,44,44	0
60	MG	A	3548	1/1	0.88	0.38	-	65,65,65,65	0
60	MG	A	3469	1/1	0.94	0.12	-	48,48,48,48	0
60	MG	A	3366	1/1	0.96	0.15	-	19,19,19,19	1
60	MG	A	3141	1/1	0.81	0.32	-	42,42,42,42	1
60	MG	A	3570	1/1	0.95	0.17	-	54,54,54,54	0
60	MG	A	3528	1/1	0.85	0.51	-	51,51,51,51	0
60	MG	A	3218	1/1	0.91	0.65	-	52,52,52,52	0
60	MG	A	3410	1/1	0.95	0.23	-	44,44,44,44	0
60	MG	A	3232	1/1	0.89	0.20	-	35,35,35,35	0
60	MG	A	3409	1/1	0.93	0.16	-	35,35,35,35	0
60	MG	A	3325	1/1	0.93	0.14	-	23,23,23,23	0
60	MG	a	1625	1/1	0.81	0.30	-	60,60,60,60	0
60	MG	A	3618	1/1	0.88	0.17	-	57,57,57,57	0
60	MG	A	3098	1/1	0.60	0.24	-	61,61,61,61	0
60	MG	a	1663	1/1	0.74	0.29	-	60,60,60,60	0
60	MG	a	1615	1/1	0.71	0.41	-	54,54,54,54	0
60	MG	A	3532	1/1	0.88	0.20	-	41,41,41,41	0
60	MG	a	1616	1/1	0.82	0.21	-	54,54,54,54	0
60	MG	0	103	1/1	0.94	0.08	-	53,53,53,53	0
60	MG	a	1732	1/1	0.89	0.17	-	54,54,54,54	0
60	MG	a	1645	1/1	0.96	0.20	-	42,42,42,42	0
60	MG	A	3061	1/1	0.95	0.28	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	a	1714	1/1	0.92	0.44	-	54,54,54,54	0
60	MG	A	3307	1/1	0.92	0.17	-	60,60,60,60	0
60	MG	A	3102	1/1	0.89	0.31	-	55,55,55,55	0
60	MG	A	3145	1/1	0.97	0.41	-	61,61,61,61	0
60	MG	A	3322	1/1	0.97	0.18	-	42,42,42,42	1
60	MG	A	3499	1/1	0.91	0.19	-	36,36,36,36	0
60	MG	A	3400	1/1	0.91	0.35	-	42,42,42,42	0
60	MG	A	3556	1/1	0.82	0.29	-	35,35,35,35	1
60	MG	A	3184	1/1	0.99	0.42	-	30,30,30,30	0
60	MG	0	101	1/1	0.90	0.23	-	39,39,39,39	0
60	MG	A	3278	1/1	0.65	0.24	-	56,56,56,56	0
60	MG	A	3513	1/1	0.95	0.18	-	58,58,58,58	0
60	MG	H	201	1/1	0.89	0.18	-	62,62,62,62	0
60	MG	A	3295	1/1	0.62	0.36	-	58,58,58,58	0
60	MG	a	1691	1/1	0.76	0.29	-	53,53,53,53	0
60	MG	A	3571	1/1	0.87	0.29	-	38,38,38,38	1
60	MG	B	202	1/1	0.97	0.14	-	52,52,52,52	0
60	MG	a	1679	1/1	0.80	0.21	-	39,39,39,39	0
60	MG	A	3541	1/1	0.84	0.08	-	63,63,63,63	0
60	MG	A	3508	1/1	0.93	0.11	-	68,68,68,68	0
60	MG	A	3624	1/1	0.68	0.60	-	63,63,63,63	0
60	MG	A	3249	1/1	0.82	0.41	-	72,72,72,72	0
60	MG	a	1649	1/1	0.93	0.43	-	67,67,67,67	0
60	MG	A	3579	1/1	0.78	0.24	-	50,50,50,50	0
60	MG	A	3251	1/1	0.89	0.15	-	46,46,46,46	0
60	MG	A	3083	1/1	0.89	0.18	-	51,51,51,51	0
60	MG	a	1741	1/1	0.83	0.18	-	63,63,63,63	0
60	MG	a	1768	1/1	0.93	0.36	-	43,43,43,43	0
60	MG	A	3039	1/1	0.80	0.16	-	63,63,63,63	0
60	MG	A	3453	1/1	0.80	0.14	-	57,57,57,57	0
60	MG	A	3292	1/1	0.92	0.42	-	47,47,47,47	0
60	MG	A	3403	1/1	0.91	0.20	-	37,37,37,37	0
60	MG	a	1721	1/1	0.86	0.08	-	41,41,41,41	0
60	MG	A	3229	1/1	0.88	0.26	-	39,39,39,39	0
60	MG	A	3443	1/1	0.86	0.28	-	41,41,41,41	0
60	MG	A	3133	1/1	0.87	0.26	-	36,36,36,36	1
60	MG	A	3340	1/1	0.96	0.24	-	45,45,45,45	0
60	MG	a	1765	1/1	0.89	0.13	-	55,55,55,55	0
60	MG	a	1686	1/1	0.74	0.24	-	61,61,61,61	0
60	MG	A	3220	1/1	0.90	0.29	-	45,45,45,45	0
60	MG	A	3591	1/1	0.74	0.34	-	39,39,39,39	1
60	MG	a	1779	1/1	0.69	0.33	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3550	1/1	0.89	0.39	-	65,65,65,65	0
60	MG	A	3081	1/1	0.85	0.35	-	56,56,56,56	0
60	MG	a	1746	1/1	0.96	0.09	-	49,49,49,49	0
60	MG	A	3270	1/1	0.82	0.19	-	51,51,51,51	0
60	MG	A	3011	1/1	0.80	0.70	-	53,53,53,53	0
60	MG	a	1719	1/1	0.92	0.20	-	48,48,48,48	0
60	MG	A	3566	1/1	0.93	0.44	-	55,55,55,55	0
60	MG	P	201	1/1	0.80	0.36	-	59,59,59,59	0
60	MG	A	3338	1/1	0.90	0.29	-	20,20,20,20	0
60	MG	A	3416	1/1	0.95	0.17	-	31,31,31,31	0
60	MG	a	1745	1/1	0.94	0.21	-	40,40,40,40	0
60	MG	A	3355	1/1	0.97	0.17	-	61,61,61,61	0
60	MG	A	3484	1/1	0.98	0.40	-	41,41,41,41	0
60	MG	a	1742	1/1	0.88	0.18	-	58,58,58,58	0
60	MG	A	3116	1/1	0.96	0.24	-	47,47,47,47	0
60	MG	A	3465	1/1	0.75	0.10	-	59,59,59,59	0
60	MG	A	3545	1/1	0.89	0.42	-	42,42,42,42	0
60	MG	A	3489	1/1	0.96	0.26	-	27,27,27,27	0
60	MG	A	3414	1/1	0.92	0.09	-	47,47,47,47	0
60	MG	a	1715	1/1	0.83	0.31	-	58,58,58,58	0
60	MG	A	3167	1/1	0.82	0.37	-	51,51,51,51	0
60	MG	G	202	1/1	0.85	0.10	-	48,48,48,48	0
60	MG	A	3154	1/1	0.70	0.33	-	67,67,67,67	0
60	MG	A	3301	1/1	0.95	0.29	-	54,54,54,54	0
60	MG	A	3318	1/1	0.98	0.17	-	42,42,42,42	1
60	MG	A	3392	1/1	0.91	0.17	-	42,42,42,42	0
60	MG	a	1639	1/1	0.92	0.14	-	48,48,48,48	0
60	MG	A	3160	1/1	0.89	0.46	-	57,57,57,57	0
60	MG	A	3537	1/1	0.89	0.16	-	45,45,45,45	0
60	MG	B	214	1/1	0.96	0.08	-	59,59,59,59	0
60	MG	A	3427	1/1	0.93	0.20	-	49,49,49,49	0
60	MG	A	3428	1/1	0.93	0.19	-	56,56,56,56	0
60	MG	A	3148	1/1	0.85	0.30	-	47,47,47,47	0
60	MG	A	3026	1/1	0.85	0.25	-	43,43,43,43	0
60	MG	A	3093	1/1	0.93	0.29	-	50,50,50,50	0
60	MG	A	3262	1/1	0.83	0.12	-	50,50,50,50	1
60	MG	A	3588	1/1	0.84	0.29	-	60,60,60,60	0
60	MG	a	1605	1/1	0.92	0.27	-	54,54,54,54	0
60	MG	A	3462	1/1	0.84	0.13	-	58,58,58,58	0
60	MG	A	3266	1/1	0.83	0.54	-	67,67,67,67	0
60	MG	A	3574	1/1	0.85	0.18	-	39,39,39,39	0
60	MG	A	3314	1/1	0.98	0.09	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	a	1601	1/1	0.85	0.52	-	68,68,68,68	0
60	MG	A	3394	1/1	0.59	0.31	-	81,81,81,81	0
60	MG	A	3442	1/1	0.92	0.44	-	60,60,60,60	0
60	MG	A	3439	1/1	0.97	0.25	-	50,50,50,50	0
60	MG	a	1775	1/1	0.87	0.18	-	53,53,53,53	1
60	MG	7	101	1/1	0.87	0.14	-	63,63,63,63	0
60	MG	A	3032	1/1	0.97	0.26	-	50,50,50,50	0
60	MG	a	1642	1/1	0.83	0.38	-	70,70,70,70	0
60	MG	A	3614	1/1	0.92	0.19	-	39,39,39,39	0
60	MG	A	3062	1/1	0.98	0.16	-	41,41,41,41	0
60	MG	A	3094	1/1	0.62	0.54	-	55,55,55,55	0
60	MG	A	3482	1/1	0.93	0.25	-	38,38,38,38	0
60	MG	A	3593	1/1	0.89	0.08	-	70,70,70,70	0
60	MG	e	201	1/1	0.78	0.15	-	78,78,78,78	0
60	MG	A	3263	1/1	0.81	0.21	-	67,67,67,67	0
60	MG	A	3108	1/1	0.92	0.36	-	60,60,60,60	0
60	MG	B	211	1/1	0.71	0.28	-	69,69,69,69	0
60	MG	A	3118	1/1	0.85	0.23	-	64,64,64,64	0
60	MG	A	3549	1/1	0.84	0.09	-	47,47,47,47	0
60	MG	A	3425	1/1	0.98	0.28	-	54,54,54,54	0
60	MG	a	1633	1/1	0.96	0.21	-	32,32,32,32	0
60	MG	A	3405	1/1	0.95	0.29	-	32,32,32,32	0
60	MG	a	1652	1/1	0.95	0.18	-	20,20,20,20	0
60	MG	A	3454	1/1	0.95	0.42	-	44,44,44,44	0
60	MG	A	3086	1/1	0.98	0.31	-	21,21,21,21	0
60	MG	A	3569	1/1	0.92	0.17	-	41,41,41,41	0
60	MG	A	3346	1/1	0.91	0.21	-	57,57,57,57	0
60	MG	A	3242	1/1	0.73	0.41	-	61,61,61,61	0
60	MG	B	209	1/1	0.70	0.32	-	60,60,60,60	0
60	MG	a	1787	1/1	0.91	0.90	-	40,40,40,40	1
60	MG	A	3598	1/1	0.91	0.18	-	29,29,29,29	0
60	MG	a	1656	1/1	0.89	0.10	-	60,60,60,60	0
60	MG	a	1653	1/1	0.87	0.43	-	61,61,61,61	0
60	MG	A	3518	1/1	0.78	0.19	-	39,39,39,39	0
60	MG	a	1769	1/1	0.91	0.12	-	58,58,58,58	0
60	MG	A	3534	1/1	0.98	0.23	-	35,35,35,35	0
60	MG	A	3502	1/1	0.88	0.14	-	44,44,44,44	0
60	MG	a	1673	1/1	0.89	0.24	-	60,60,60,60	0
60	MG	A	3219	1/1	0.92	0.20	-	50,50,50,50	0
60	MG	5	102	1/1	0.90	0.39	-	58,58,58,58	0
60	MG	A	3207	1/1	0.93	0.31	-	61,61,61,61	0
60	MG	A	3353	1/1	0.85	0.22	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3236	1/1	0.64	0.64	-	47,47,47,47	1
60	MG	f	201	1/1	0.86	0.19	-	53,53,53,53	0
60	MG	A	3398	1/1	0.94	0.10	-	37,37,37,37	0
60	MG	A	3135	1/1	0.67	0.14	-	59,59,59,59	0
60	MG	a	1604	1/1	0.61	0.25	-	64,64,64,64	0
60	MG	A	3529	1/1	0.96	0.12	-	59,59,59,59	0
60	MG	A	3077	1/1	0.96	0.31	-	24,24,24,24	1
60	MG	A	3512	1/1	0.98	0.22	-	44,44,44,44	0
60	MG	A	3568	1/1	0.85	0.24	-	61,61,61,61	0
60	MG	A	3448	1/1	0.86	0.43	-	60,60,60,60	0
60	MG	A	3196	1/1	0.89	0.20	-	51,51,51,51	0
60	MG	A	3386	1/1	0.94	0.24	-	33,33,33,33	0
60	MG	A	3543	1/1	0.92	0.25	-	51,51,51,51	0
60	MG	B	215	1/1	0.64	0.28	-	75,75,75,75	1
60	MG	X	101	1/1	0.93	0.25	-	50,50,50,50	0
60	MG	A	3051	1/1	0.98	0.31	-	54,54,54,54	0
60	MG	A	3505	1/1	0.80	0.14	-	41,41,41,41	0
60	MG	A	3190	1/1	0.88	0.49	-	58,58,58,58	0
60	MG	a	1770	1/1	0.90	0.35	-	56,56,56,56	0
60	MG	A	3173	1/1	0.97	0.65	-	37,37,37,37	0
60	MG	V	201	1/1	0.89	0.40	-	55,55,55,55	0
60	MG	A	3153	1/1	0.87	0.23	-	45,45,45,45	0
60	MG	A	3509	1/1	0.98	0.36	-	45,45,45,45	0
60	MG	A	3546	1/1	0.85	0.13	-	53,53,53,53	0
60	MG	A	3041	1/1	0.89	0.26	-	38,38,38,38	0
60	MG	A	3504	1/1	0.92	0.21	-	25,25,25,25	0
60	MG	A	3337	1/1	0.96	0.29	-	48,48,48,48	0
60	MG	A	3192	1/1	0.94	0.18	-	26,26,26,26	0
60	MG	A	3555	1/1	0.81	0.15	-	63,63,63,63	0
60	MG	A	3411	1/1	0.97	0.15	-	39,39,39,39	0
60	MG	A	3126	1/1	0.95	0.28	-	28,28,28,28	1
60	MG	A	3013	1/1	0.98	0.23	-	24,24,24,24	0
60	MG	A	3621	1/1	0.94	0.31	-	48,48,48,48	0
60	MG	A	3412	1/1	0.96	0.21	-	44,44,44,44	0
60	MG	a	1638	1/1	0.54	0.42	-	53,53,53,53	0
60	MG	A	3536	1/1	0.77	0.31	-	57,57,57,57	0
60	MG	A	3466	1/1	0.93	0.22	-	49,49,49,49	0
60	MG	A	3603	1/1	0.83	0.37	-	50,50,50,50	0
60	MG	A	3080	1/1	0.83	0.43	-	48,48,48,48	0
60	MG	A	3617	1/1	0.88	0.16	-	45,45,45,45	0
60	MG	A	3040	1/1	0.83	0.36	-	31,31,31,31	1
60	MG	A	3434	1/1	0.95	0.23	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3375	1/1	0.87	0.20	-	35,35,35,35	0
60	MG	A	3329	1/1	0.92	0.21	-	33,33,33,33	1
60	MG	B	201	1/1	0.76	0.47	-	53,53,53,53	1
60	MG	x	109	1/1	0.62	0.17	-	77,77,77,77	0
60	MG	x	104	1/1	0.98	0.30	-	43,43,43,43	0
60	MG	A	3033	1/1	0.95	0.27	-	59,59,59,59	1
60	MG	A	3418	1/1	0.84	0.34	-	48,48,48,48	0
60	MG	a	1784	1/1	0.83	0.41	-	52,52,52,52	0
60	MG	A	3575	1/1	0.93	0.29	-	39,39,39,39	1
60	MG	A	3164	1/1	0.88	0.32	-	31,31,31,31	0
60	MG	A	3025	1/1	0.88	0.28	-	51,51,51,51	1
60	MG	A	3076	1/1	0.92	0.27	-	33,33,33,33	1
60	MG	A	3107	1/1	0.90	0.21	-	55,55,55,55	0
60	MG	a	1777	1/1	0.93	0.28	-	32,32,32,32	1
60	MG	A	3471	1/1	0.90	0.13	-	65,65,65,65	0
60	MG	A	3587	1/1	0.98	0.28	-	23,23,23,23	1
60	MG	a	1729	1/1	0.96	0.35	-	50,50,50,50	0
60	MG	A	3272	1/1	0.84	0.31	-	55,55,55,55	0
60	MG	A	3573	1/1	0.79	0.69	-	34,34,34,34	1
60	MG	a	1618	1/1	0.94	0.54	-	54,54,54,54	0
60	MG	A	3066	1/1	0.67	0.33	-	58,58,58,58	0
60	MG	A	3014	1/1	0.70	0.31	-	37,37,37,37	0
60	MG	A	3613	1/1	0.90	0.31	-	67,67,67,67	0
60	MG	A	3059	1/1	0.85	0.22	-	37,37,37,37	1
60	MG	A	3601	1/1	0.95	0.24	-	33,33,33,33	0
60	MG	a	1726	1/1	0.97	0.10	-	43,43,43,43	0
60	MG	A	3304	1/1	0.94	0.13	-	53,53,53,53	0
60	MG	A	3052	1/1	0.74	0.26	-	51,51,51,51	1
60	MG	a	1631	1/1	0.86	0.43	-	42,42,42,42	0
60	MG	E	302	1/1	0.96	0.29	-	32,32,32,32	0
60	MG	a	1776	1/1	0.97	0.25	-	52,52,52,52	0
60	MG	a	1756	1/1	0.96	0.15	-	52,52,52,52	0
60	MG	a	1783	1/1	0.91	0.39	-	60,60,60,60	0
60	MG	A	3089	1/1	0.84	0.15	-	58,58,58,58	0
60	MG	A	3372	1/1	0.94	0.20	-	41,41,41,41	0
60	MG	a	1727	1/1	0.98	0.13	-	49,49,49,49	0
60	MG	A	3034	1/1	0.92	0.43	-	59,59,59,59	0
60	MG	a	1757	1/1	0.95	0.24	-	46,46,46,46	0
60	MG	A	3054	1/1	0.71	0.27	-	48,48,48,48	0
60	MG	A	3470	1/1	0.96	0.22	-	51,51,51,51	0
60	MG	A	3186	1/1	0.95	0.13	-	33,33,33,33	0
60	MG	A	3240	1/1	0.90	0.08	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3078	1/1	0.94	0.33	-	27,27,27,27	1
60	MG	a	1674	1/1	0.85	0.44	-	50,50,50,50	0
60	MG	A	3350	1/1	0.86	0.12	-	59,59,59,59	0
60	MG	a	1733	1/1	0.97	0.28	-	51,51,51,51	0
60	MG	x	107	1/1	0.93	0.09	-	69,69,69,69	0
60	MG	A	3511	1/1	0.81	0.34	-	50,50,50,50	0
60	MG	9	101	1/1	0.91	0.31	-	50,50,50,50	0
60	MG	A	3493	1/1	0.91	0.25	-	48,48,48,48	1
60	MG	B	212	1/1	0.85	0.18	-	52,52,52,52	0
60	MG	A	3068	1/1	0.81	0.38	-	69,69,69,69	0
60	MG	A	3288	1/1	0.92	0.24	-	45,45,45,45	0
60	MG	a	1748	1/1	0.97	0.07	-	46,46,46,46	0
60	MG	A	3257	1/1	0.81	0.16	-	52,52,52,52	0
60	MG	a	1761	1/1	0.78	0.25	-	55,55,55,55	1
60	MG	A	3495	1/1	0.96	0.16	-	35,35,35,35	0
60	MG	A	3365	1/1	0.91	0.16	-	35,35,35,35	0
60	MG	A	3458	1/1	0.85	0.24	-	38,38,38,38	0
60	MG	A	3149	1/1	0.93	0.08	-	54,54,54,54	0
60	MG	A	3436	1/1	0.87	0.21	-	43,43,43,43	0
60	MG	A	3087	1/1	0.79	0.14	-	41,41,41,41	0
60	MG	A	3421	1/1	0.97	0.14	-	57,57,57,57	0
60	MG	A	3110	1/1	0.87	0.27	-	25,25,25,25	1
60	MG	a	1696	1/1	0.93	0.49	-	52,52,52,52	0
60	MG	A	3127	1/1	0.72	0.33	-	24,24,24,24	1
60	MG	a	1621	1/1	0.96	0.10	-	64,64,64,64	0
60	MG	a	1713	1/1	0.88	0.46	-	43,43,43,43	0
60	MG	A	3358	1/1	0.76	0.32	-	46,46,46,46	1
60	MG	a	1780	1/1	0.96	0.23	-	54,54,54,54	0
60	MG	a	1650	1/1	0.90	0.47	-	47,47,47,47	0
60	MG	A	3486	1/1	0.98	0.17	-	44,44,44,44	0
60	MG	a	1774	1/1	0.94	0.13	-	29,29,29,29	0
60	MG	A	3253	1/1	0.78	0.14	-	67,67,67,67	0
60	MG	A	3562	1/1	0.91	0.16	-	67,67,67,67	0
60	MG	B	207	1/1	0.80	0.16	-	76,76,76,76	0
60	MG	A	3520	1/1	0.85	0.36	-	55,55,55,55	0
60	MG	A	3204	1/1	0.92	0.36	-	39,39,39,39	0
60	MG	A	3001	1/1	0.88	0.20	-	51,51,51,51	0
60	MG	A	3616	1/1	0.95	0.17	-	45,45,45,45	0
60	MG	A	3305	1/1	0.81	0.39	-	38,38,38,38	0
60	MG	A	3526	1/1	0.94	0.20	-	29,29,29,29	0
60	MG	A	3277	1/1	0.72	0.41	-	47,47,47,47	1
60	MG	A	3175	1/1	0.94	0.18	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3408	1/1	0.95	0.27	-	33,33,33,33	0
60	MG	A	3468	1/1	0.90	0.18	-	37,37,37,37	1
60	MG	A	3215	1/1	0.95	0.42	-	44,44,44,44	0
60	MG	A	3604	1/1	0.82	0.17	-	64,64,64,64	0
60	MG	A	3380	1/1	0.97	0.19	-	45,45,45,45	0
60	MG	a	1666	1/1	0.69	0.44	-	68,68,68,68	0
60	MG	A	3209	1/1	0.81	0.30	-	72,72,72,72	0
60	MG	A	3106	1/1	0.83	0.28	-	46,46,46,46	1
60	MG	a	1680	1/1	0.91	0.33	-	60,60,60,60	0
60	MG	A	3095	1/1	0.92	0.10	-	32,32,32,32	0
60	MG	A	3017	1/1	0.96	0.28	-	41,41,41,41	0
60	MG	A	3492	1/1	0.73	0.37	-	64,64,64,64	1
60	MG	A	3551	1/1	0.81	0.17	-	71,71,71,71	0
60	MG	A	3423	1/1	0.85	0.20	-	73,73,73,73	0
60	MG	A	3456	1/1	0.77	0.28	-	46,46,46,46	1
60	MG	a	1651	1/1	0.90	0.13	-	64,64,64,64	0
60	MG	A	3620	1/1	0.88	0.18	-	29,29,29,29	0
60	MG	R	201	1/1	0.90	0.45	-	50,50,50,50	0
60	MG	A	3317	1/1	0.92	0.09	-	52,52,52,52	0
60	MG	A	3065	1/1	0.89	0.29	-	64,64,64,64	0
60	MG	B	218	1/1	0.95	0.27	-	49,49,49,49	0
60	MG	A	3554	1/1	0.90	0.16	-	67,67,67,67	0
60	MG	A	3269	1/1	0.89	0.20	-	64,64,64,64	0
60	MG	A	3452	1/1	0.93	0.07	-	69,69,69,69	0
60	MG	A	3565	1/1	0.98	0.12	-	35,35,35,35	0
60	MG	A	3517	1/1	0.78	0.21	-	85,85,85,85	0
60	MG	A	3422	1/1	0.96	0.21	-	52,52,52,52	0
60	MG	A	3323	1/1	0.95	0.16	-	72,72,72,72	0
60	MG	a	1751	1/1	0.91	0.14	-	59,59,59,59	0
60	MG	A	3552	1/1	0.85	0.12	-	48,48,48,48	0
60	MG	A	3020	1/1	0.93	0.18	-	26,26,26,26	0
60	MG	a	1603	1/1	0.81	0.29	-	67,67,67,67	0
60	MG	A	3399	1/1	0.99	0.28	-	44,44,44,44	0
60	MG	a	1637	1/1	0.92	0.41	-	54,54,54,54	0
60	MG	A	3290	1/1	0.89	0.21	-	56,56,56,56	0
60	MG	A	3124	1/1	0.80	0.25	-	32,32,32,32	1
60	MG	a	1620	1/1	0.80	0.50	-	47,47,47,47	0
60	MG	A	3299	1/1	0.88	0.32	-	35,35,35,35	0
60	MG	a	1699	1/1	0.98	0.26	-	56,56,56,56	0
60	MG	a	1643	1/1	0.74	0.46	-	58,58,58,58	0
60	MG	A	3479	1/1	0.96	0.10	-	41,41,41,41	0
60	MG	a	1664	1/1	0.80	0.26	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3497	1/1	0.98	0.25	-	38,38,38,38	1
60	MG	A	3342	1/1	0.75	0.30	-	58,58,58,58	0
60	MG	A	3128	1/1	0.94	0.26	-	37,37,37,37	0
60	MG	A	3326	1/1	0.92	0.18	-	32,32,32,32	0
60	MG	A	3335	1/1	0.70	0.35	-	59,59,59,59	1
60	MG	A	3576	1/1	0.87	0.12	-	59,59,59,59	0
60	MG	A	3467	1/1	0.95	0.21	-	37,37,37,37	0
60	MG	A	3254	1/1	0.88	0.30	-	62,62,62,62	0
60	MG	A	3002	1/1	0.84	0.09	-	58,58,58,58	0
60	MG	a	1758	1/1	0.89	0.49	-	72,72,72,72	0
60	MG	P	202	1/1	0.75	0.40	-	59,59,59,59	0
60	MG	A	3547	1/1	0.94	0.10	-	41,41,41,41	0
60	MG	A	3082	1/1	0.85	0.31	-	43,43,43,43	1
60	MG	A	3103	1/1	0.92	0.17	-	44,44,44,44	0
60	MG	A	3557	1/1	0.66	0.28	-	70,70,70,70	0
60	MG	A	3390	1/1	0.92	0.13	-	36,36,36,36	0
60	MG	a	1718	1/1	0.80	0.41	-	55,55,55,55	1
60	MG	A	3208	1/1	0.49	0.33	-	60,60,60,60	0
60	MG	a	1771	1/1	0.95	0.13	-	67,67,67,67	0
60	MG	A	3233	1/1	0.92	0.12	-	56,56,56,56	0
60	MG	A	3071	1/1	0.89	0.15	-	61,61,61,61	0
60	MG	a	1628	1/1	0.91	0.20	-	45,45,45,45	0
60	MG	A	3610	1/1	0.75	0.24	-	62,62,62,62	0
60	MG	A	3315	1/1	0.91	0.16	-	37,37,37,37	0
60	MG	A	3057	1/1	0.54	0.38	-	72,72,72,72	0
60	MG	A	3111	1/1	0.86	0.23	-	46,46,46,46	0
60	MG	B	206	1/1	0.39	0.38	-	86,86,86,86	0
60	MG	A	3600	1/1	0.97	0.08	-	53,53,53,53	0
60	MG	A	3447	1/1	0.97	0.20	-	47,47,47,47	0
60	MG	A	3176	1/1	0.91	0.13	-	37,37,37,37	0
60	MG	a	1738	1/1	0.97	0.17	-	35,35,35,35	0
60	MG	a	1711	1/1	0.94	0.18	-	48,48,48,48	0
60	MG	a	1655	1/1	0.95	0.40	-	47,47,47,47	0
60	MG	a	1760	1/1	0.95	0.17	-	38,38,38,38	0
60	MG	A	3564	1/1	0.94	0.13	-	52,52,52,52	0
60	MG	A	3070	1/1	0.98	0.26	-	10,10,10,10	0
60	MG	A	3171	1/1	0.98	0.18	-	31,31,31,31	0
60	MG	a	1629	1/1	0.81	0.15	-	44,44,44,44	0
60	MG	x	101	1/1	0.93	0.33	-	29,29,29,29	1
60	MG	A	3101	1/1	0.89	0.22	-	47,47,47,47	0
60	MG	A	3625	1/1	0.89	0.11	-	45,45,45,45	0
60	MG	A	3047	1/1	0.90	0.18	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	A	3348	1/1	0.98	0.23	-	30,30,30,30	0
60	MG	A	3100	1/1	0.73	0.50	-	66,66,66,66	0
60	MG	A	3143	1/1	0.84	0.22	-	55,55,55,55	0
60	MG	A	3187	1/1	0.95	0.40	-	31,31,31,31	0
60	MG	A	3027	1/1	0.95	0.14	-	62,62,62,62	0
60	MG	A	3296	1/1	0.89	0.20	-	31,31,31,31	0
60	MG	A	3231	1/1	0.88	0.24	-	68,68,68,68	0
60	MG	A	3395	1/1	0.96	0.29	-	51,51,51,51	0
60	MG	A	3289	1/1	0.89	0.19	-	59,59,59,59	0
60	MG	A	3274	1/1	0.59	0.23	-	66,66,66,66	0
60	MG	A	3239	1/1	0.88	0.49	-	51,51,51,51	0
60	MG	A	3544	1/1	0.88	0.34	-	53,53,53,53	0
60	MG	A	3359	1/1	0.92	0.16	-	63,63,63,63	0
60	MG	a	1767	1/1	0.85	0.12	-	45,45,45,45	0
60	MG	A	3161	1/1	0.85	0.29	-	34,34,34,34	1
60	MG	A	3178	1/1	0.97	0.40	-	56,56,56,56	0
60	MG	A	3119	1/1	0.90	0.18	-	68,68,68,68	0
60	MG	P	203	1/1	0.97	0.28	-	45,45,45,45	1
60	MG	A	3247	1/1	0.86	0.24	-	46,46,46,46	1
60	MG	A	3361	1/1	0.79	0.18	-	64,64,64,64	0
60	MG	A	3144	1/1	0.75	0.42	-	51,51,51,51	0
60	MG	a	1617	1/1	0.93	0.38	-	47,47,47,47	0
60	MG	A	3091	1/1	0.91	0.21	-	49,49,49,49	0
60	MG	A	3122	1/1	0.80	0.31	-	51,51,51,51	1
60	MG	A	3606	1/1	0.66	0.26	-	56,56,56,56	0
60	MG	A	3356	1/1	0.86	0.40	-	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.