wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 06:01 PM EST

PDB ID	:	6N9E
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with a short substrate mimic CC-Pmn and bound to mRNA and P-site tRNA at 3.7A resolution
Authors	:	Melnikov, S.V.; Khabibullina, N.F.; Mairhofer, E.; Vargas-Rodriguez, O.; Reynolds, N.M.; Micura, R.; Soll, D.; Polikanov, Y.S.
Deposited on	:	2018-12-03
Resolution	:	3.70 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

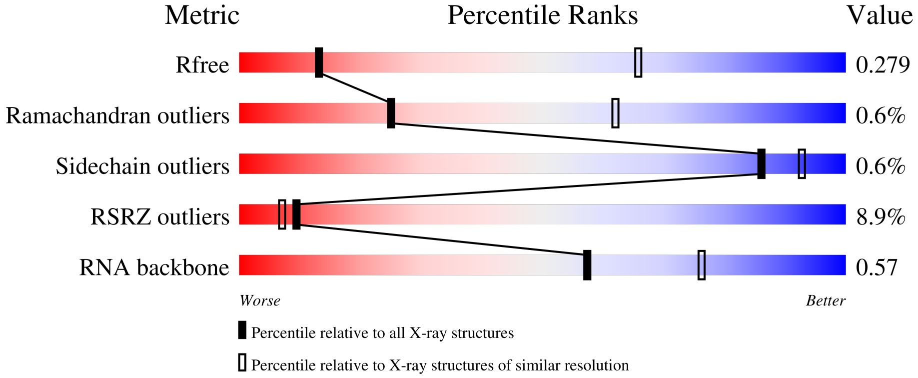
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

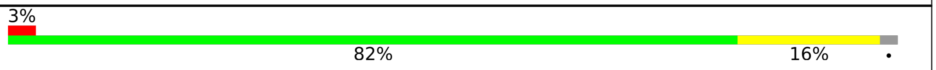
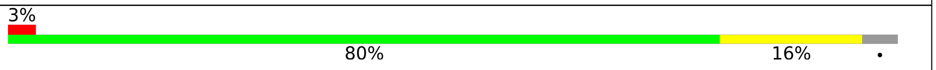
The reported resolution of this entry is 3.70 Å.

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}	130704	1049 (3.88-3.52)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	
1	2A	2915	
2	1B	121	
2	2B	121	

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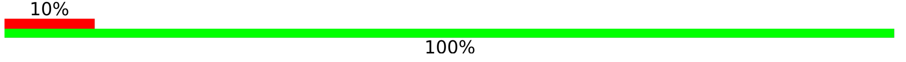
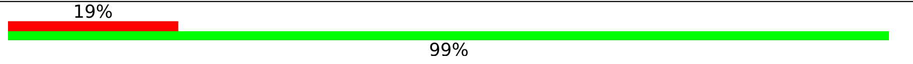
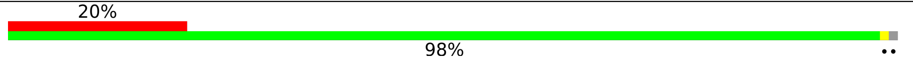
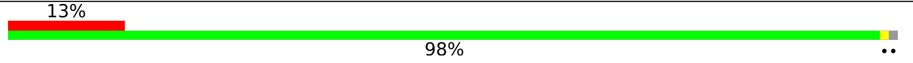
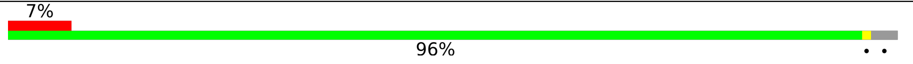
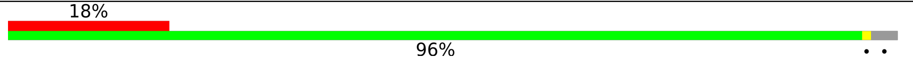
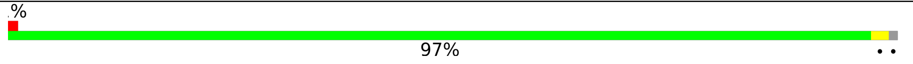
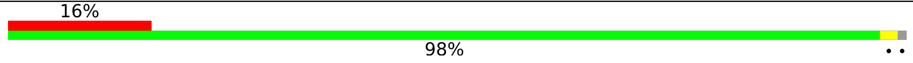
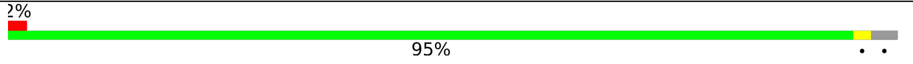
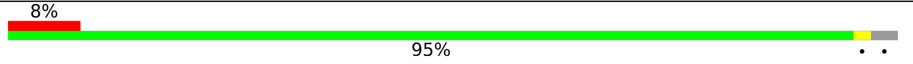
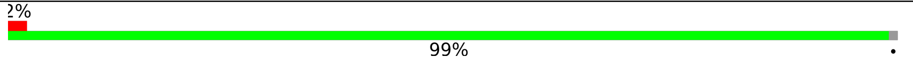
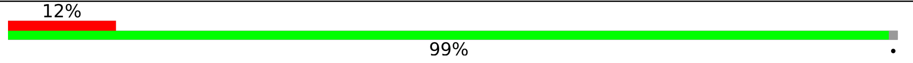
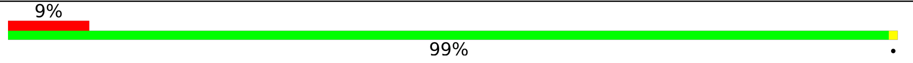
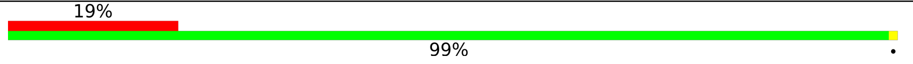
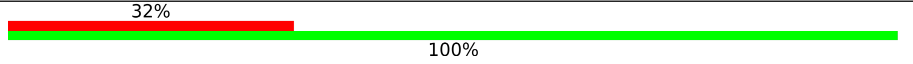
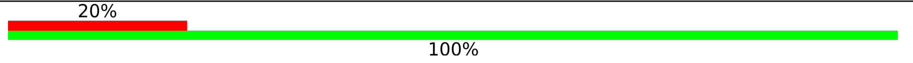
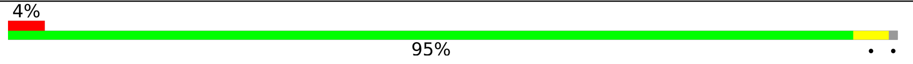
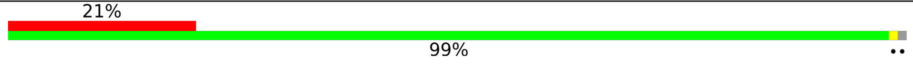
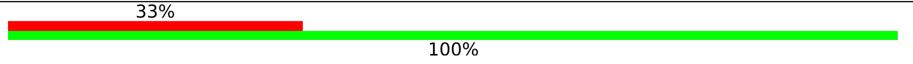
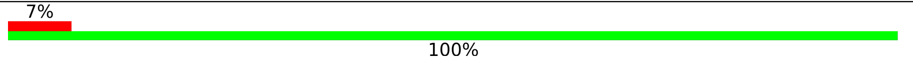
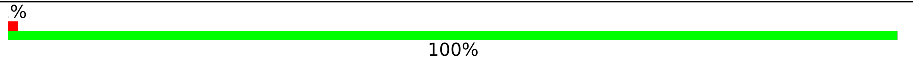
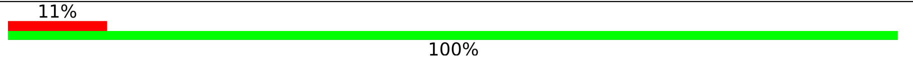
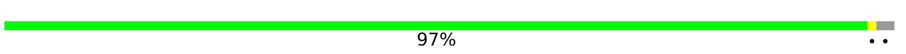
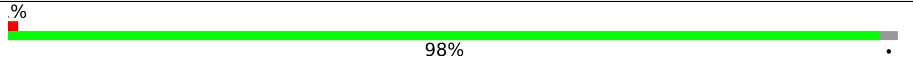
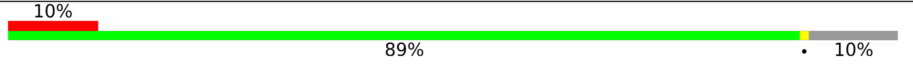
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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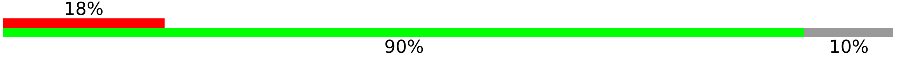
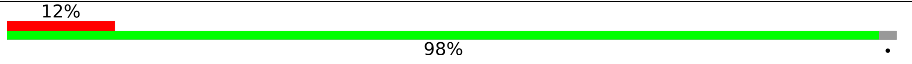
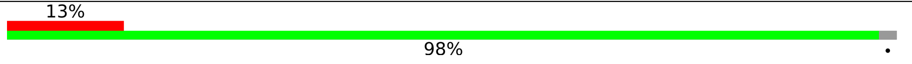
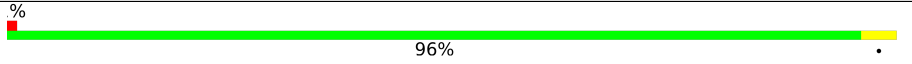
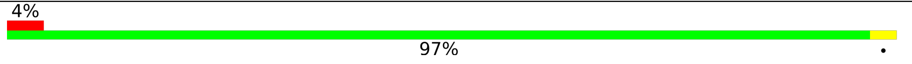
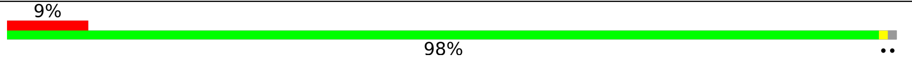
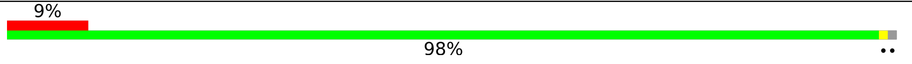
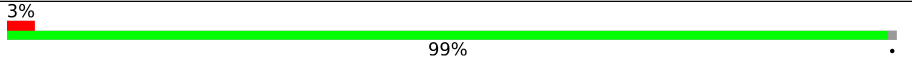
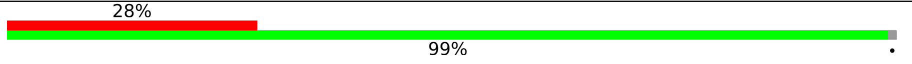
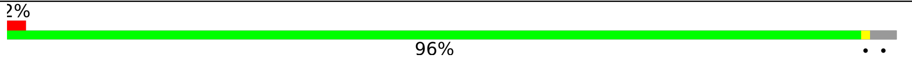
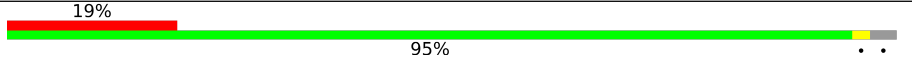
Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
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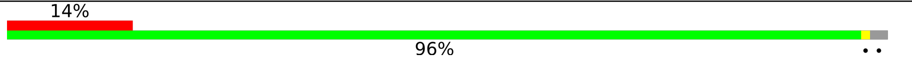
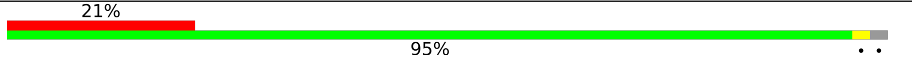
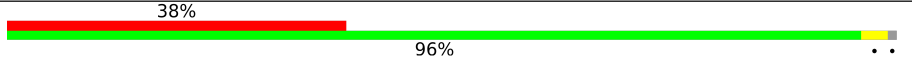
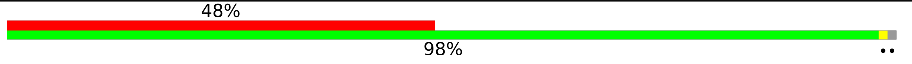
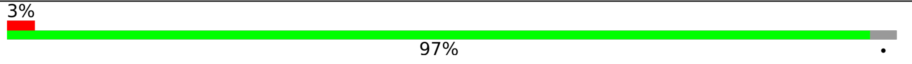
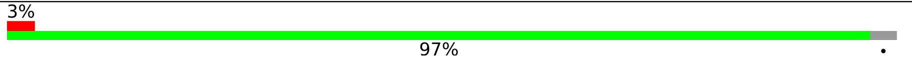
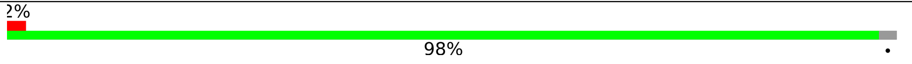
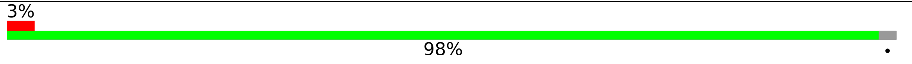
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
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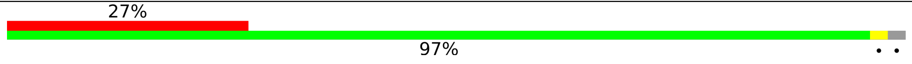
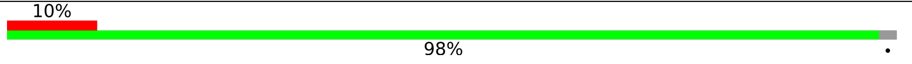
26	24	71	
27	15	60	
27	25	60	

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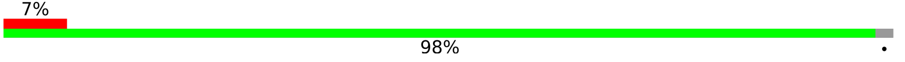
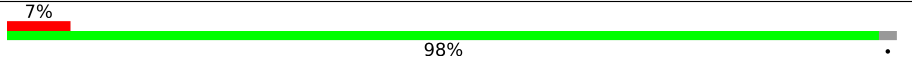
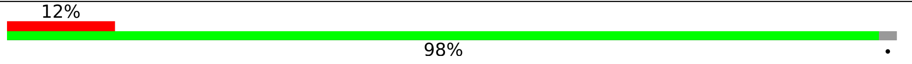
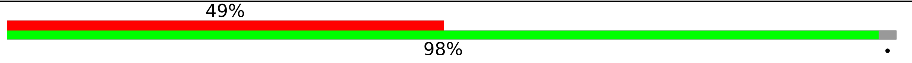
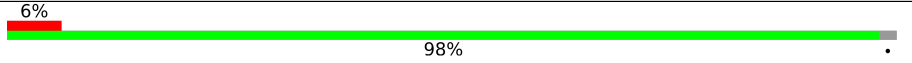
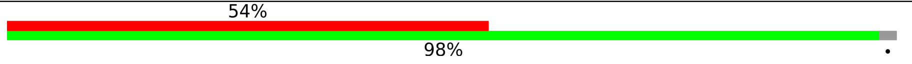
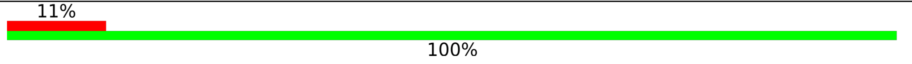
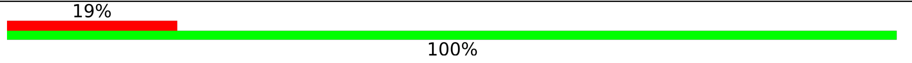
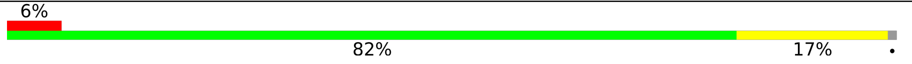
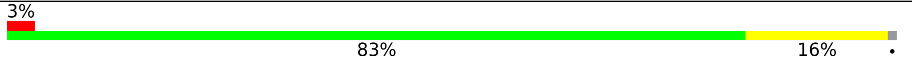
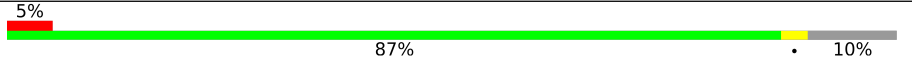
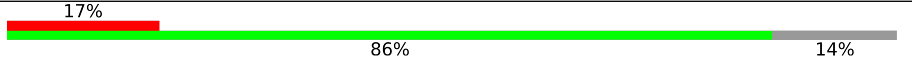
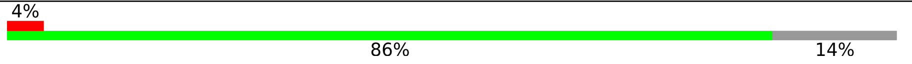
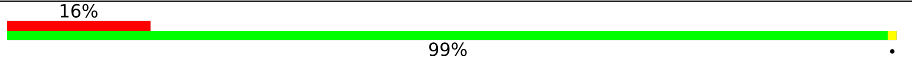
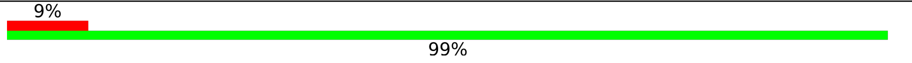
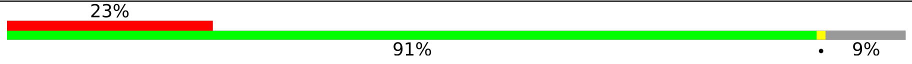
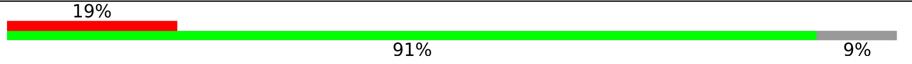
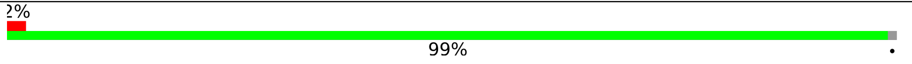
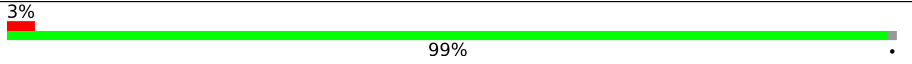
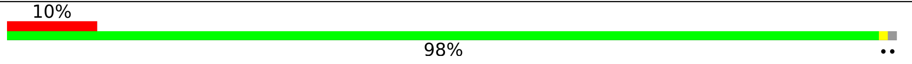
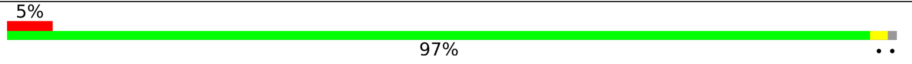
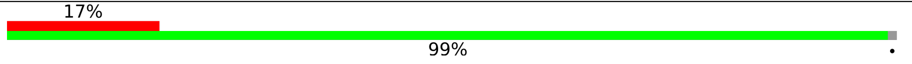
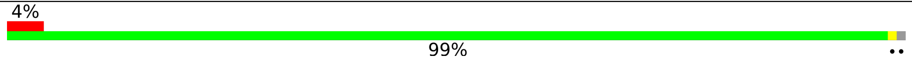
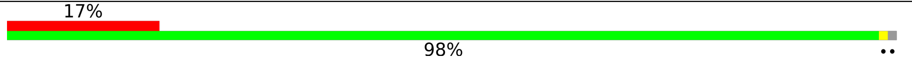
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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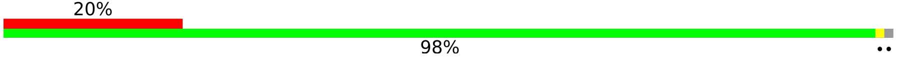
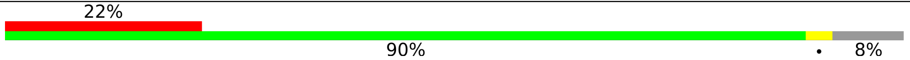
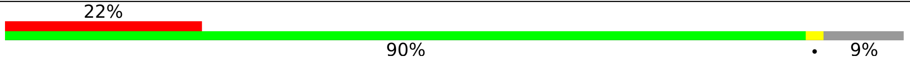
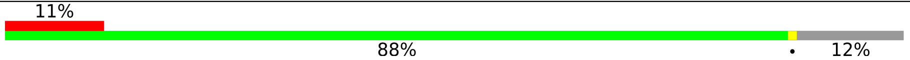
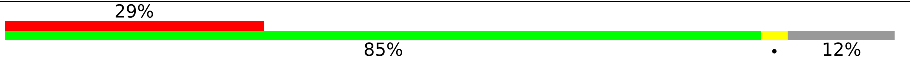
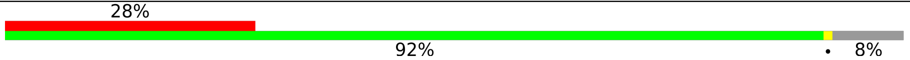
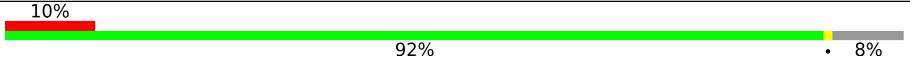
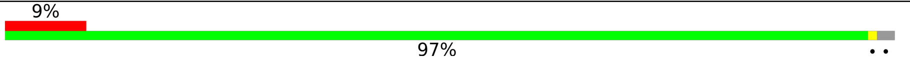
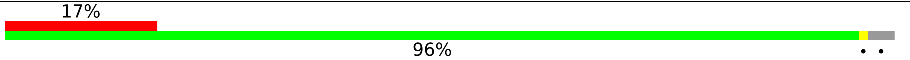
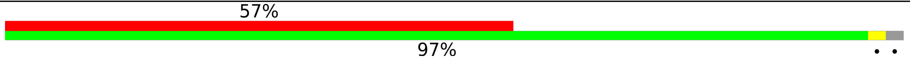
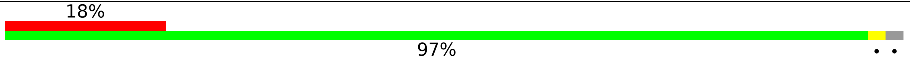
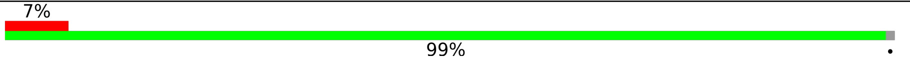
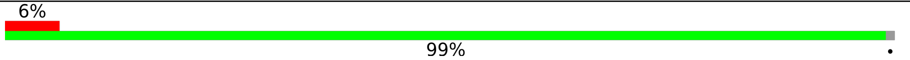
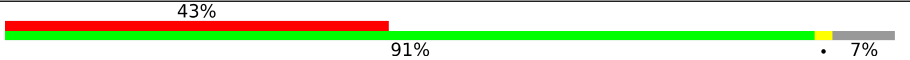
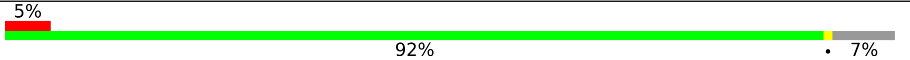
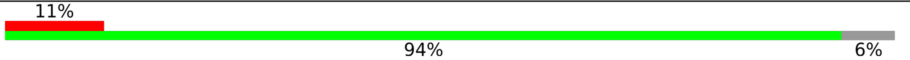
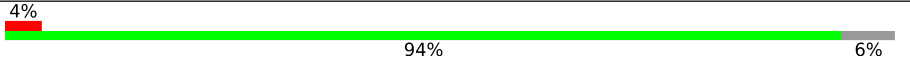
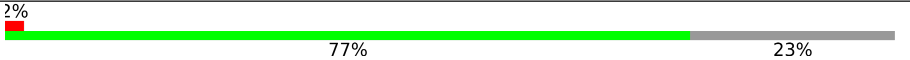
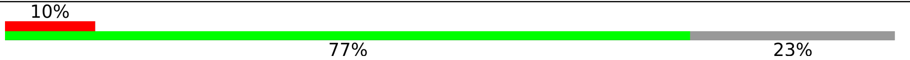
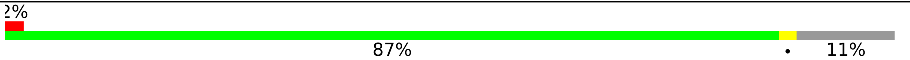
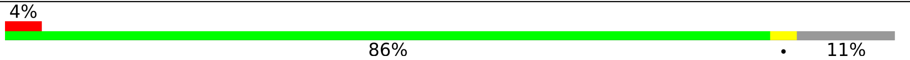
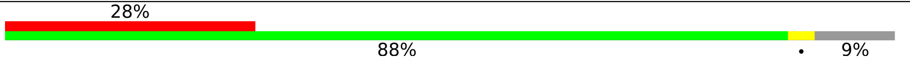
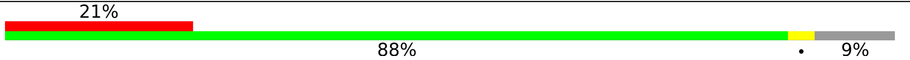
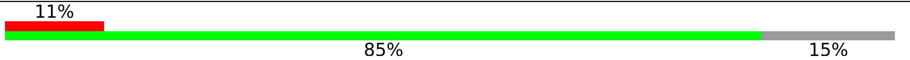
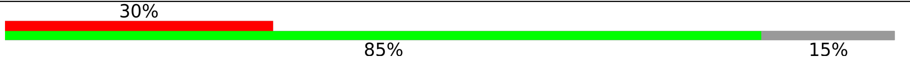
Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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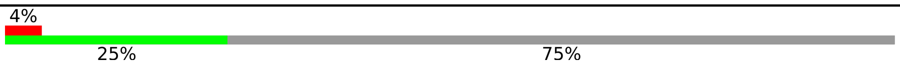
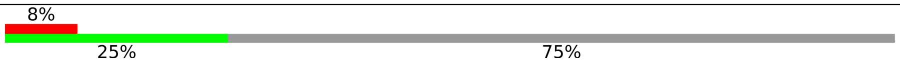
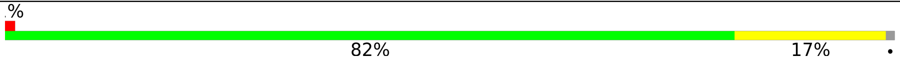
Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	3	
54	2w	3	
55	1x	77	
55	2x	77	

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
56	MG	10	103	-	-	-	X
56	MG	1A	3014	-	-	-	X
56	MG	1A	3026	-	-	-	X
56	MG	1A	3034	-	-	-	X
56	MG	1A	3039	-	-	-	X
56	MG	1A	3040	-	-	-	X
56	MG	1A	3051	-	-	-	X
56	MG	1A	3054	-	-	-	X
56	MG	1A	3067	-	-	-	X
56	MG	1A	3068	-	-	-	X
56	MG	1A	3070	-	-	-	X
56	MG	1A	3075	-	-	-	X
56	MG	1A	3078	-	-	-	X
56	MG	1A	3082	-	-	-	X
56	MG	1A	3104	-	-	-	X
56	MG	1A	3115	-	-	-	X
56	MG	1A	3124	-	-	-	X
56	MG	1A	3142	-	-	-	X
56	MG	1A	3144	-	-	-	X
56	MG	1A	3146	-	-	-	X
56	MG	1A	3148	-	-	-	X
56	MG	1A	3154	-	-	-	X
56	MG	1A	3159	-	-	-	X
56	MG	1A	3165	-	-	-	X
56	MG	1A	3172	-	-	-	X
56	MG	1A	3173	-	-	-	X
56	MG	1A	3177	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3187	-	-	-	X
56	MG	1A	3192	-	-	-	X
56	MG	1A	3197	-	-	-	X
56	MG	1A	3202	-	-	-	X
56	MG	1A	3217	-	-	-	X
56	MG	1A	3221	-	-	-	X
56	MG	1A	3224	-	-	-	X
56	MG	1A	3232	-	-	-	X
56	MG	1A	3237	-	-	-	X
56	MG	1A	3239	-	-	-	X
56	MG	1A	3245	-	-	-	X
56	MG	1A	3250	-	-	-	X
56	MG	1A	3252	-	-	-	X
56	MG	1A	3254	-	-	-	X
56	MG	1A	3255	-	-	-	X
56	MG	1A	3257	-	-	-	X
56	MG	1A	3258	-	-	-	X
56	MG	1A	3262	-	-	-	X
56	MG	1A	3264	-	-	-	X
56	MG	1A	3293	-	-	-	X
56	MG	1A	3299	-	-	-	X
56	MG	1A	3308	-	-	-	X
56	MG	1A	3312	-	-	-	X
56	MG	1A	3322	-	-	-	X
56	MG	1A	3327	-	-	-	X
56	MG	1A	3340	-	-	-	X
56	MG	1A	3341	-	-	-	X
56	MG	1A	3349	-	-	-	X
56	MG	1A	3358	-	-	-	X
56	MG	1A	3360	-	-	-	X
56	MG	1A	3402	-	-	-	X
56	MG	1A	3420	-	-	-	X
56	MG	1A	3437	-	-	-	X
56	MG	1A	3440	-	-	-	X
56	MG	1A	3445	-	-	-	X
56	MG	1A	3471	-	-	-	X
56	MG	1A	3479	-	-	-	X
56	MG	1B	201	-	-	-	X
56	MG	1B	202	-	-	-	X
56	MG	1E	304	-	-	-	X
56	MG	1Q	201	-	-	-	X
56	MG	1a	1603	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	1645	-	-	-	X
56	MG	1a	1687	-	-	-	X
56	MG	1l	201	-	-	-	X
56	MG	1x	102	-	-	-	X
56	MG	20	101	-	-	-	X
56	MG	27	101	-	-	-	X
56	MG	2A	3002	-	-	-	X
56	MG	2A	3011	-	-	-	X
56	MG	2A	3014	-	-	-	X
56	MG	2A	3015	-	-	-	X
56	MG	2A	3024	-	-	-	X
56	MG	2A	3027	-	-	-	X
56	MG	2A	3030	-	-	-	X
56	MG	2A	3039	-	-	-	X
56	MG	2A	3049	-	-	-	X
56	MG	2A	3059	-	-	-	X
56	MG	2A	3061	-	-	-	X
56	MG	2A	3113	-	-	-	X
56	MG	2A	3122	-	-	-	X
56	MG	2A	3157	-	-	-	X
56	MG	2A	3162	-	-	-	X
56	MG	2A	3183	-	-	-	X
56	MG	2A	3187	-	-	-	X
56	MG	2A	3209	-	-	-	X
56	MG	2A	3220	-	-	-	X
56	MG	2A	3253	-	-	-	X
56	MG	2A	3258	-	-	-	X
56	MG	2A	3263	-	-	-	X
56	MG	2A	3266	-	-	-	X
56	MG	2A	3276	-	-	-	X
56	MG	2A	3285	-	-	-	X
56	MG	2A	3323	-	-	-	X
56	MG	2A	3326	-	-	-	X
56	MG	2A	3327	-	-	-	X
56	MG	2A	3332	-	-	-	X
56	MG	2A	3337	-	-	-	X
56	MG	2A	3349	-	-	-	X
56	MG	2B	201	-	-	-	X
56	MG	2B	202	-	-	-	X
56	MG	2E	302	-	-	-	X
56	MG	2O	201	-	-	-	X
56	MG	2T	202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2a	3068	-	-	-	X
56	MG	2a	3069	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 287828 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2871	61852	27531	11572	19878	2871	0	0	0
1	2A	2800	60322	26848	11284	19390	2800	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	2577	1146	476	835	120	0	0	0
2	2B	120	2575	1146	476	833	120	0	0	0

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	2136	1349	423	361	3	0	0	0
3	2D	275	2136	1349	423	361	3	0	0	0

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	1E	204	1559	985	298	270	6	0	0	0
4	2E	204	1559	985	298	270	6	0	0	0

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	1F	203	Total C N O S 1584 1009 298 275 2	0	0	1
5	2F	203	Total C N O S 1580 1007 297 274 2	0	0	1

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	1G	181	Total C N O S 1423 913 253 253 4	0	0	0
6	2G	181	Total C N O S 1428 913 258 253 4	0	0	0

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	1H	174	Total C N O S 1330 845 248 236 1	0	0	0
7	2H	174	Total C N O S 1330 845 248 236 1	0	0	0

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	1I	146	Total C N O S 1097 701 191 204 1	0	0	0
8	2I	146	Total C N O S 1064 681 186 196 1	0	0	0

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	1N	140	Total C N O S 1117 719 207 187 4	0	0	0
9	2N	140	Total C N O S 1117 719 207 187 4	0	0	0

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	1O	122	Total C N O S 933 588 171 170 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	24	69	532	339	97	91	5	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	15	59	455	285	89	76	5	0	0	0
27	25	59	455	285	89	76	5	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	16	53	453	281	91	77	4	0	0	0
28	26	53	449	279	91	75	4	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	17	48	418	257	104	55	2	0	0	0
29	27	48	418	257	104	55	2	0	0	0

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	18	64	517	331	102	82	2	0	0	0
30	28	64	517	331	102	82	2	0	0	0

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	19	37	307	188	68	47	4	0	0	0
31	29	37	307	188	68	47	4	0	0	0

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
32	1a	1500	32246	14358	5975	10413	1500	0	0	0
32	2a	1503	32327	14396	5990	10438	1503	0	0	0

- Molecule 33 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	1b	231	1846	1179	331	331	5	0	0	0
33	2b	231	1825	1167	326	327	5	0	0	0

- Molecule 34 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	1c	206	1548	973	301	273	1	0	0	0
34	2c	206	1542	968	300	273	1	0	0	0

- Molecule 35 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	1d	208	1655	1038	326	284	7	0	0	0
35	2d	208	1674	1050	333	284	7	0	0	0

- Molecule 36 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	1e	148	1129	714	213	198	4	0	0	0
36	2e	148	1133	716	214	199	4	0	0	0

- Molecule 37 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 39 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	2k	114	Total C N O S 833 519 156 155 3	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
43	1l	122	Total C N O S 932 586 185 159 2	0	0	0
43	2l	122	Total C N O S 932 586 185 159 2	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
44	1m	123	Total C N O S 958 592 198 166 2	0	0	0
44	2m	122	Total C N O S 950 586 197 165 2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	1n	60	Total C N O S 492 312 104 72 4	0	0	0
45	2n	60	Total C N O S 492 312 104 72 4	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
46	1o	88	Total C N O S 728 456 144 126 2	0	0	0
46	2o	88	Total C N O S 728 456 144 126 2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	1p	82	Total C N O S 681 433 134 113 1	0	0	0
47	2p	82	Total C N O S 677 430 133 113 1	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
49	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 50 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 51 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	6	Total 113	C 49	N 22	O 36	P 6	0	0	0
53	2v	6	Total 113	C 49	N 22	O 36	P 6	0	0	0

- Molecule 54 is a RNA chain called CC-Pmn.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	3	Total 74	C 40	N 13	O 19	P 2	0	0	0
54	2w	3	Total 74	C 40	N 13	O 19	P 2	0	0	0

- Molecule 55 is a RNA chain called P-site tRNA, Deacylated Initiator Methionyl-tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total 1625	C 725	N 294	O 529	P 76	S 1	0	0	0
55	2x	76	Total 1625	C 725	N 294	O 529	P 76	S 1	0	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	498	Total 498	Mg 498	0	0
56	1B	12	Total 12	Mg 12	0	0
56	1D	1	Total 1	Mg 1	0	0
56	1E	6	Total 6	Mg 6	0	0
56	1F	1	Total 1	Mg 1	0	0
56	1Q	1	Total 1	Mg 1	0	0
56	1S	1	Total 1	Mg 1	0	0
56	1U	1	Total 1	Mg 1	0	0
56	1V	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1W	1	Total Mg 1 1	0	0
56	10	3	Total Mg 3 3	0	0
56	13	1	Total Mg 1 1	0	0
56	15	1	Total Mg 1 1	0	0
56	16	1	Total Mg 1 1	0	0
56	17	2	Total Mg 2 2	0	0
56	18	1	Total Mg 1 1	0	0
56	1a	93	Total Mg 93 93	0	0
56	1d	1	Total Mg 1 1	0	0
56	1l	1	Total Mg 1 1	0	0
56	1r	1	Total Mg 1 1	0	0
56	1x	2	Total Mg 2 2	0	0
56	2A	385	Total Mg 385 385	0	0
56	2B	9	Total Mg 9 9	0	0
56	2D	1	Total Mg 1 1	0	0
56	2E	6	Total Mg 6 6	0	0
56	2O	1	Total Mg 1 1	0	0
56	2Q	2	Total Mg 2 2	0	0
56	2R	2	Total Mg 2 2	0	0
56	2T	2	Total Mg 2 2	0	0
56	2Y	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	20	2	Total Mg 2 2	0	0
56	21	1	Total Mg 1 1	0	0
56	23	1	Total Mg 1 1	0	0
56	25	1	Total Mg 1 1	0	0
56	27	1	Total Mg 1 1	0	0
56	28	2	Total Mg 2 2	0	0
56	2a	103	Total Mg 103 103	0	0
56	2d	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	2l	1	Total Mg 1 1	0	0
56	2r	1	Total Mg 1 1	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1Y	1	Total Zn 1 1	0	0
57	14	1	Total Zn 1 1	0	0
57	15	1	Total Zn 1 1	0	0
57	16	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0

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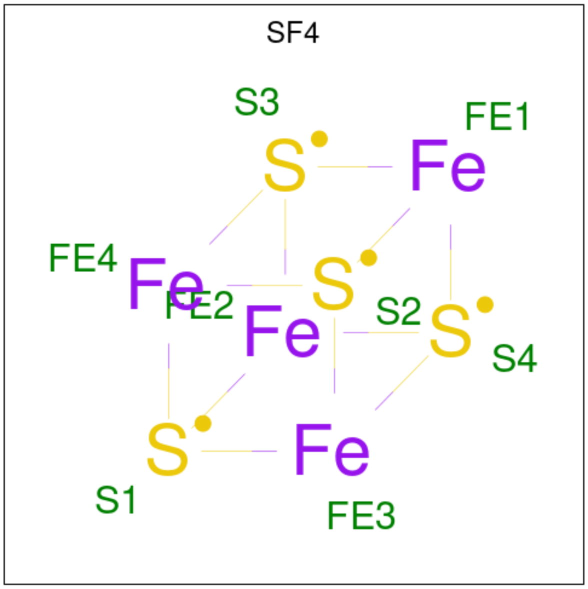
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	25	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0
57	29	1	Total Zn 1 1	0	0
57	2n	1	Total Zn 1 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1d	1	Total Fe S 8 4 4	0	0
58	2d	1	Total Fe S 8 4 4	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	53	Total O 53 53	0	0
59	1D	3	Total O 3 3	0	0
59	1a	15	Total O 15 15	0	0

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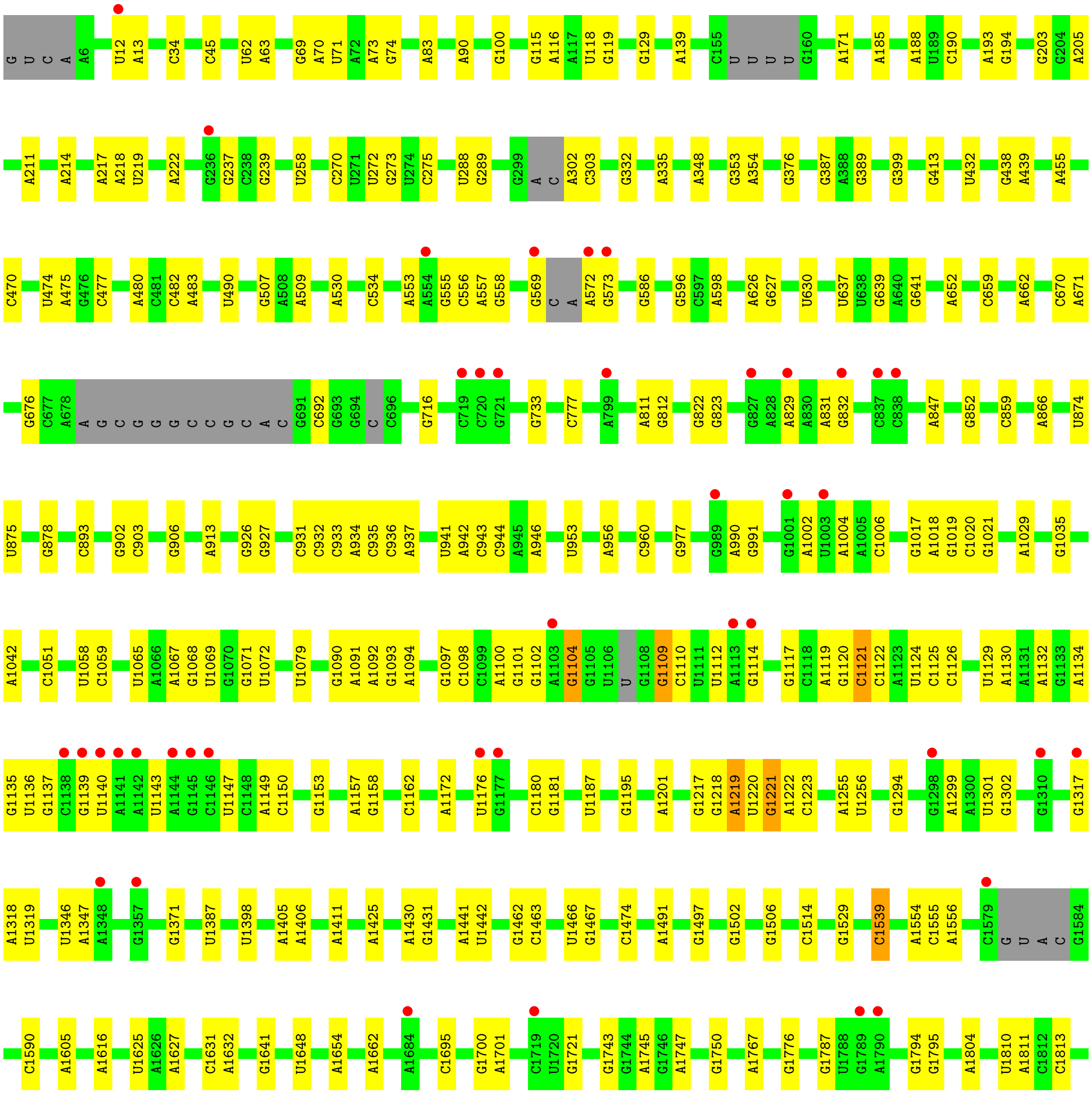
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1x	2	Total O 2 2	0	0
59	2A	32	Total O 32 32	0	0
59	2B	1	Total O 1 1	0	0
59	2a	19	Total O 19 19	0	0

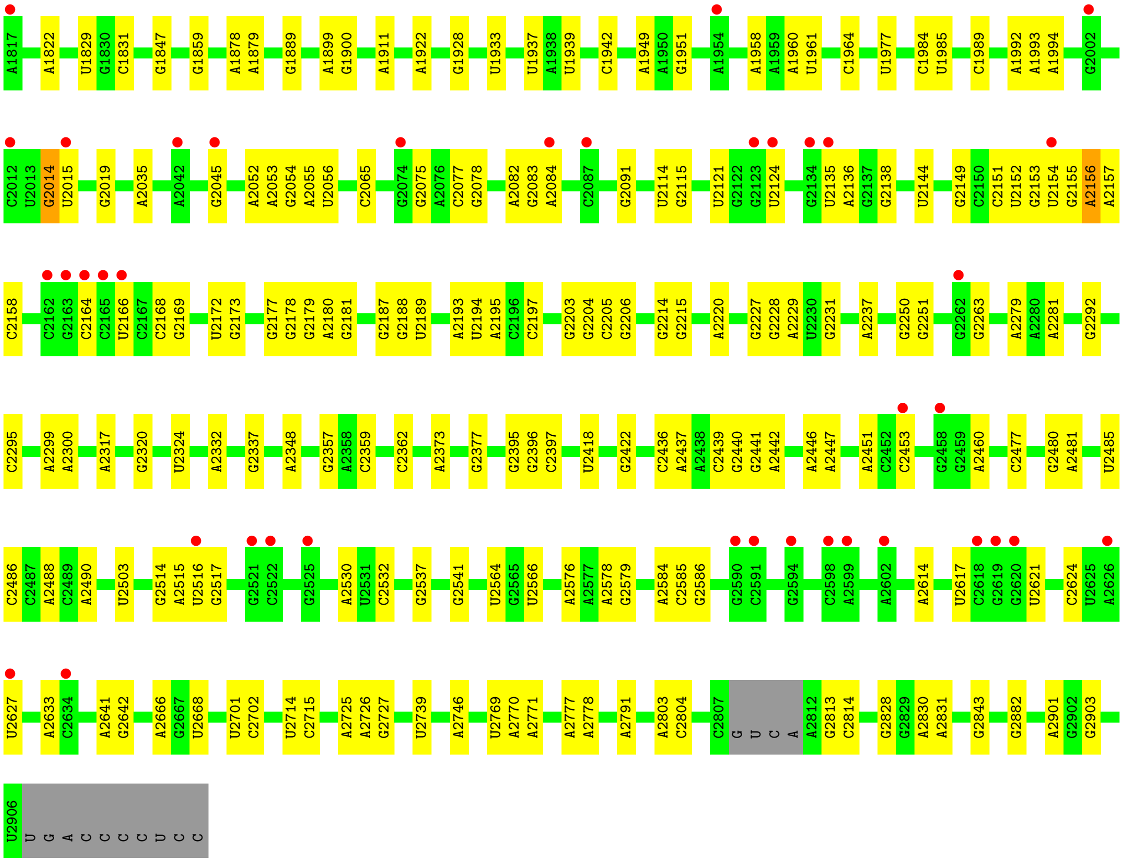
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

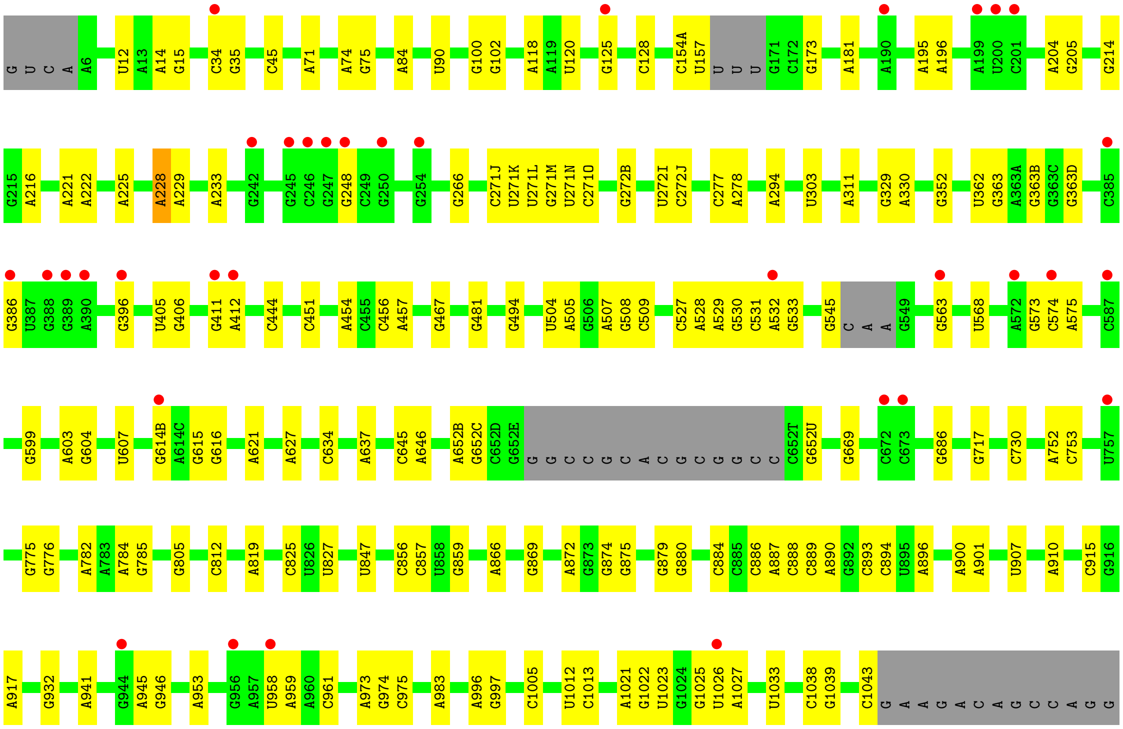
Chain 1A:

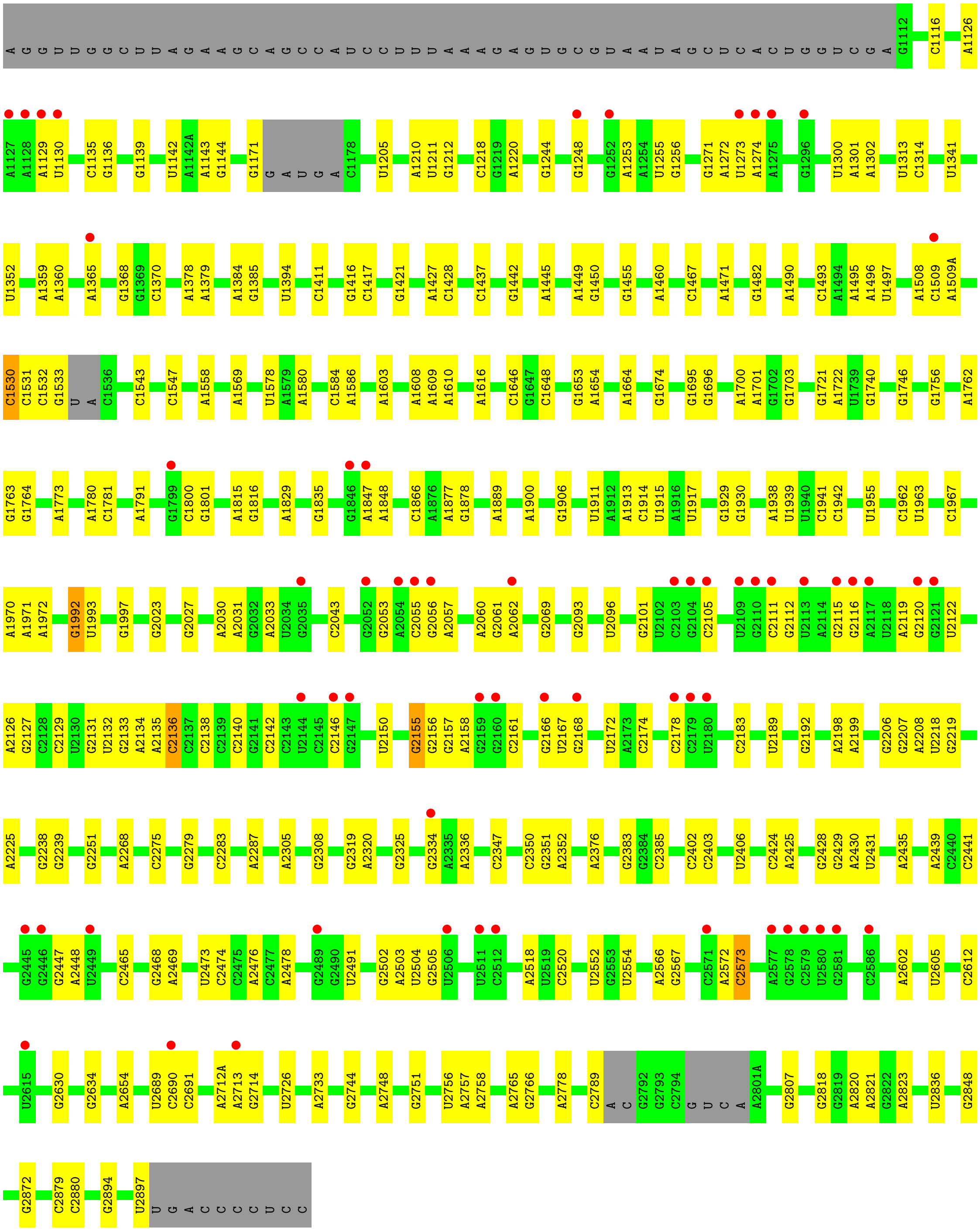




• Molecule 1: 23S Ribosomal RNA

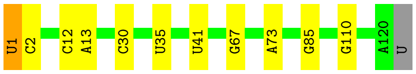
Chain 2A:





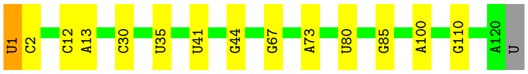
- Molecule 2: 5S Ribosomal RNA

Chain 1B:



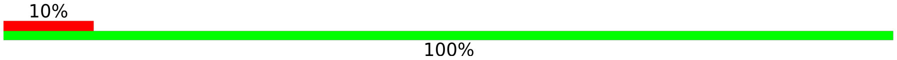
- Molecule 2: 5S Ribosomal RNA

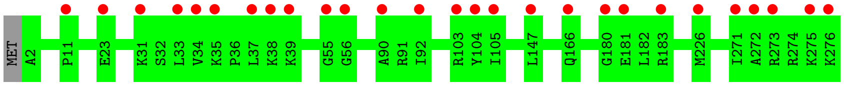
Chain 2B:



- Molecule 3: 50S Ribosomal Protein L2

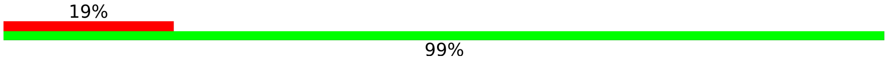
Chain 1D:

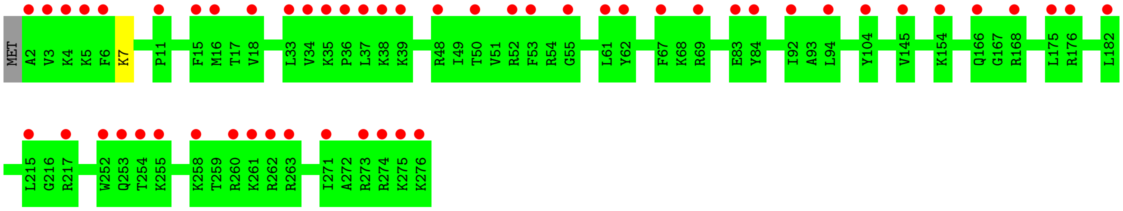




- Molecule 3: 50S Ribosomal Protein L2

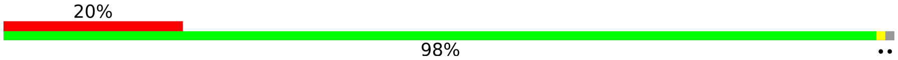
Chain 2D:

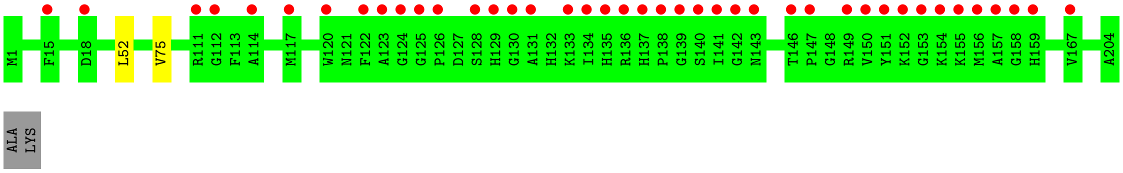




- Molecule 4: 50S Ribosomal Protein L3

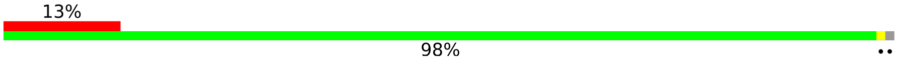
Chain 1E:

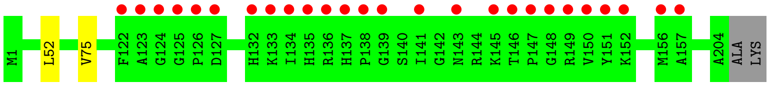




- Molecule 4: 50S Ribosomal Protein L3

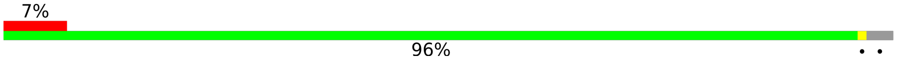
Chain 2E:

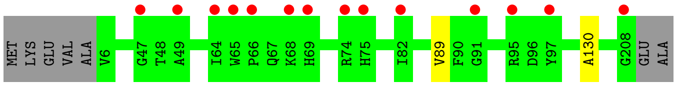




- Molecule 5: 50S Ribosomal Protein L4

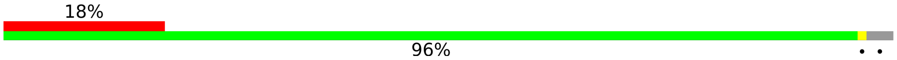
Chain 1F:

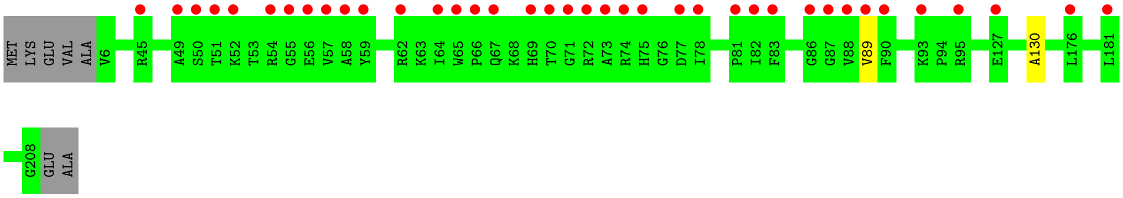




- Molecule 5: 50S Ribosomal Protein L4

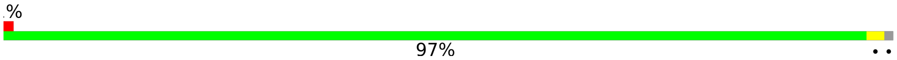
Chain 2F:

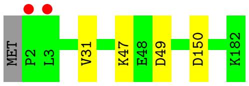




- Molecule 6: 50S Ribosomal Protein L5

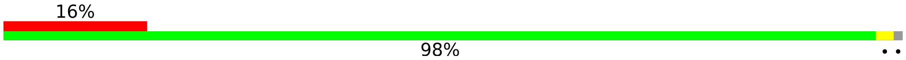
Chain 1G:

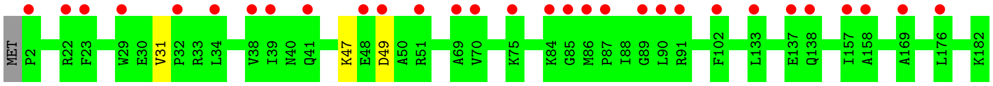




- Molecule 6: 50S Ribosomal Protein L5

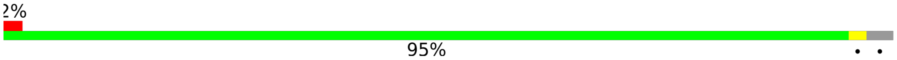
Chain 2G:

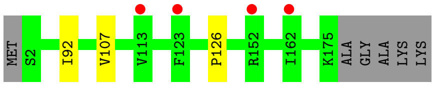




- Molecule 7: 50S Ribosomal Protein L6

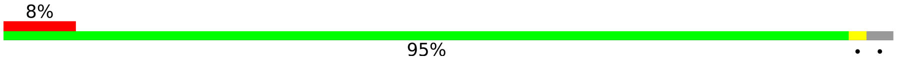
Chain 1H:

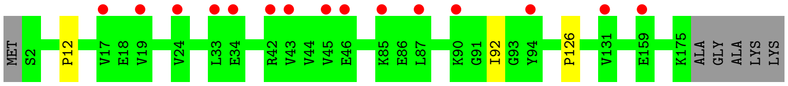




- Molecule 7: 50S Ribosomal Protein L6

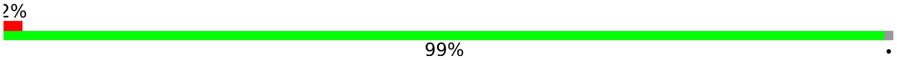
Chain 2H:

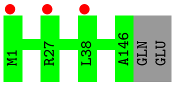




- Molecule 8: 50S Ribosomal Protein L9

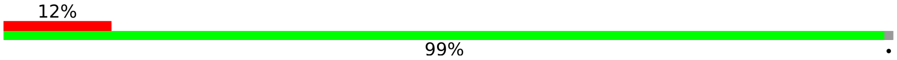
Chain 1I:

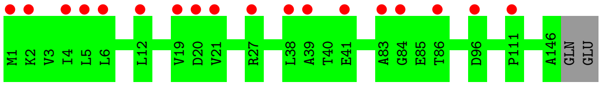




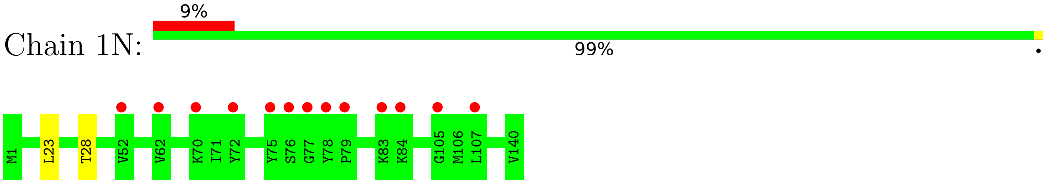
- Molecule 8: 50S Ribosomal Protein L9

Chain 2I:

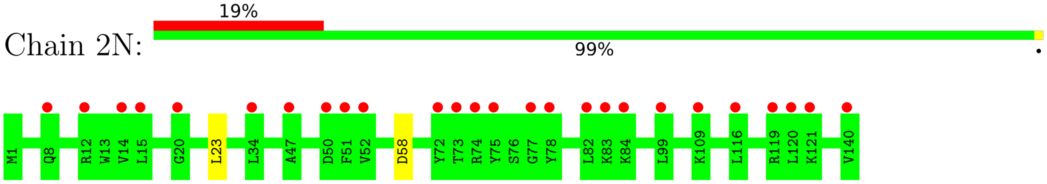




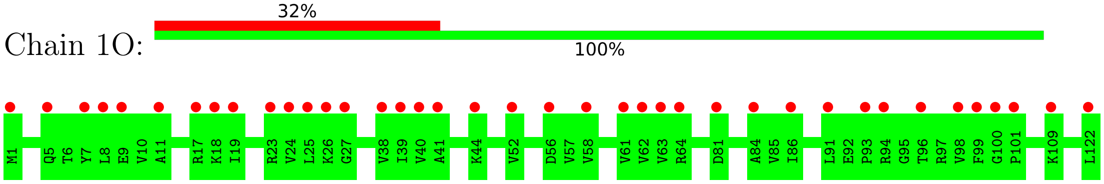
- Molecule 9: 50S Ribosomal Protein L13



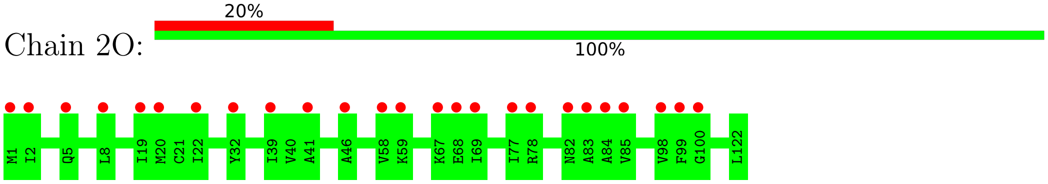
- Molecule 9: 50S Ribosomal Protein L13



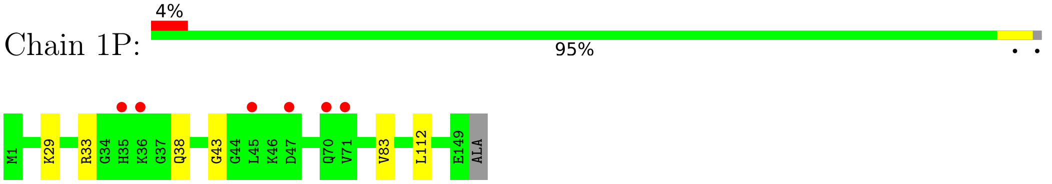
- Molecule 10: 50S Ribosomal Protein L14



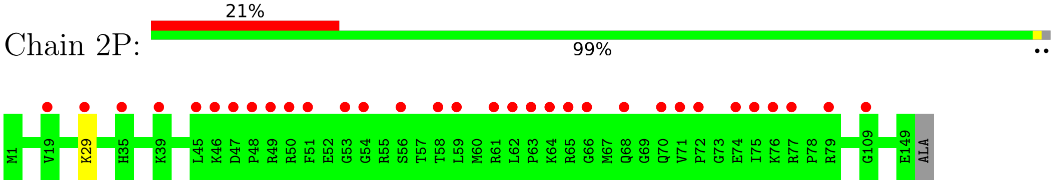
- Molecule 10: 50S Ribosomal Protein L14



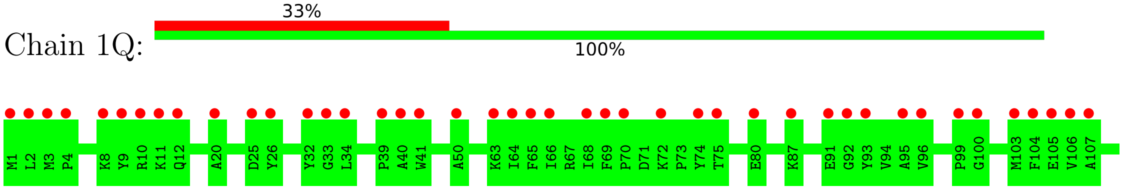
- Molecule 11: 50S Ribosomal Protein L15

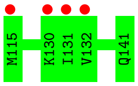


- Molecule 11: 50S Ribosomal Protein L15



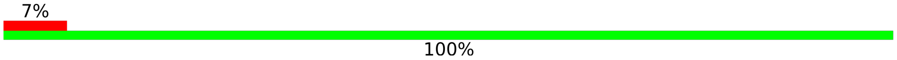
- Molecule 12: 50S Ribosomal Protein L16

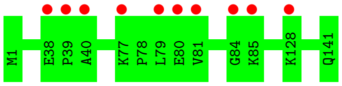




- Molecule 12: 50S Ribosomal Protein L16

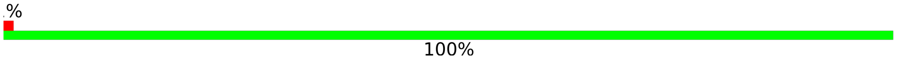
Chain 2Q:

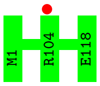




- Molecule 13: 50S Ribosomal Protein L17

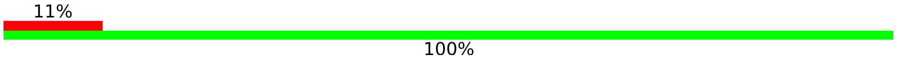
Chain 1R:

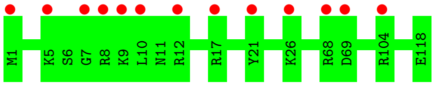




- Molecule 13: 50S Ribosomal Protein L17

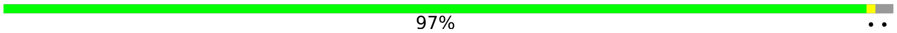
Chain 2R:

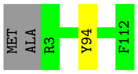




- Molecule 14: 50S Ribosomal Protein L18

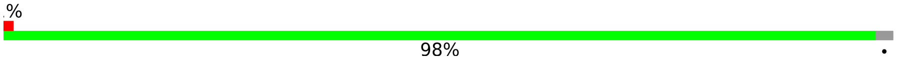
Chain 1S:

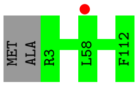




- Molecule 14: 50S Ribosomal Protein L18

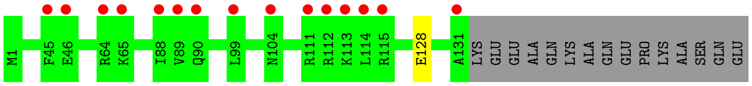
Chain 2S:





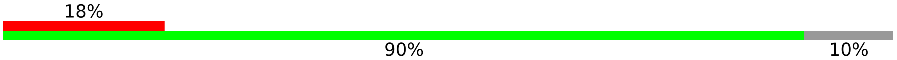
- Molecule 15: 50S Ribosomal Protein L19

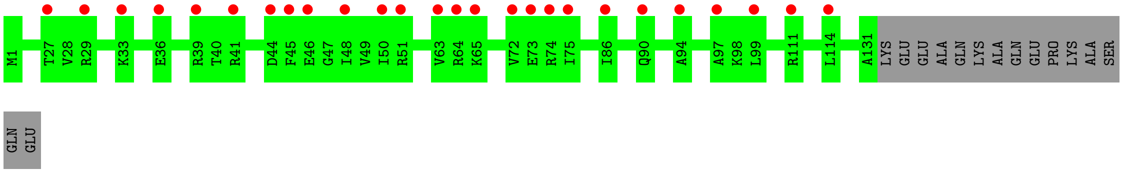
Chain 1T:



- Molecule 15: 50S Ribosomal Protein L19

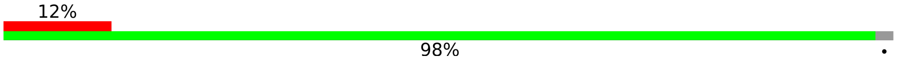
Chain 2T:

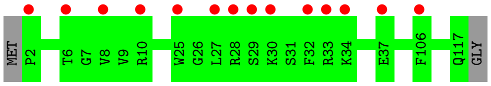




- Molecule 16: 50S Ribosomal Protein L20

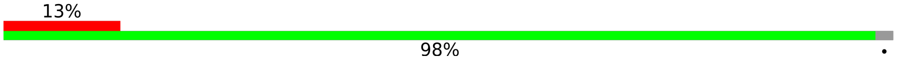
Chain 1U:

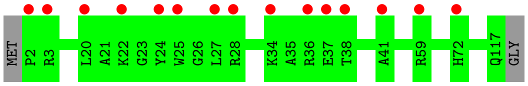




- Molecule 16: 50S Ribosomal Protein L20

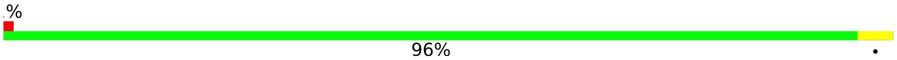
Chain 2U:

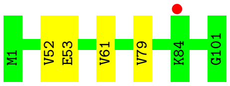




- Molecule 17: 50S Ribosomal Protein L21

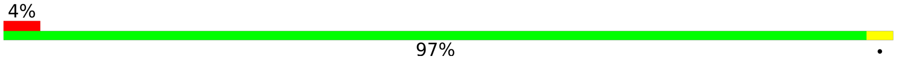
Chain 1V:

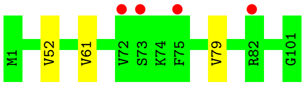




- Molecule 17: 50S Ribosomal Protein L21

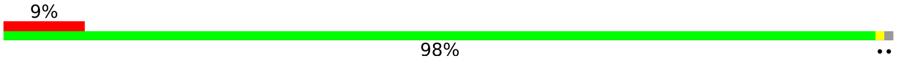
Chain 2V:

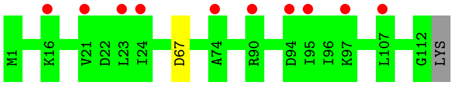




- Molecule 18: 50S Ribosomal Protein L22

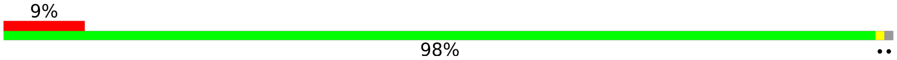
Chain 1W:

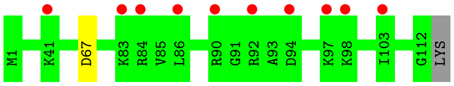




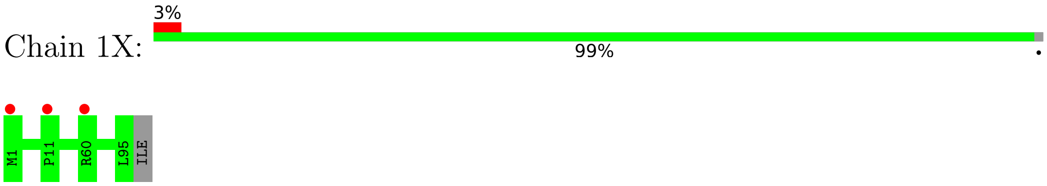
- Molecule 18: 50S Ribosomal Protein L22

Chain 2W:

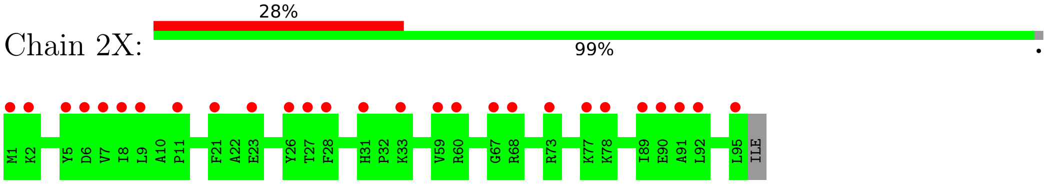




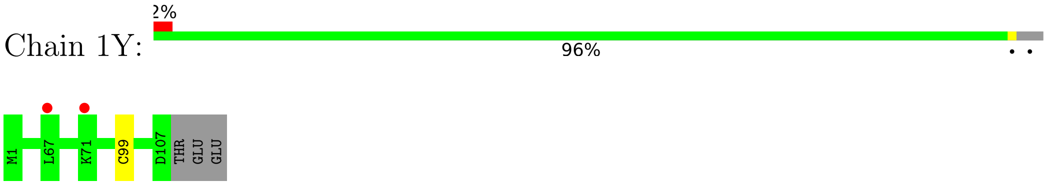
- Molecule 19: 50S Ribosomal Protein L23



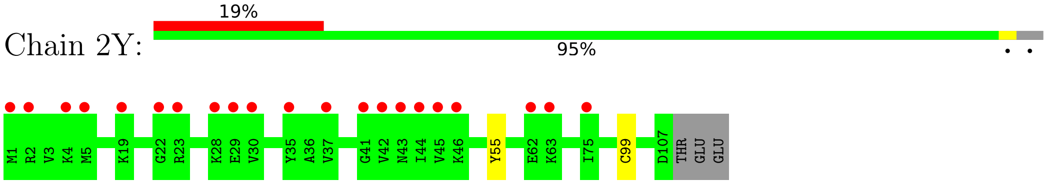
- Molecule 19: 50S Ribosomal Protein L23



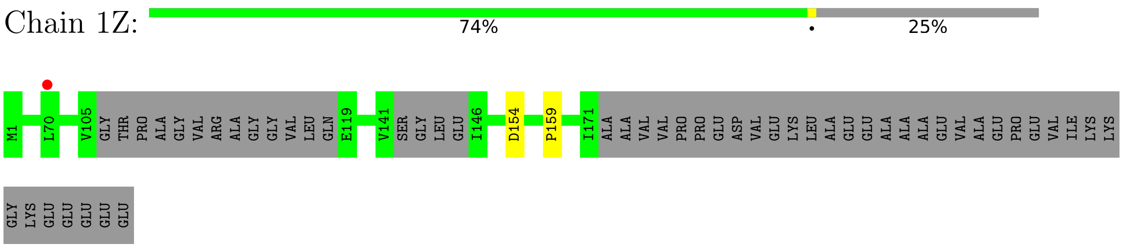
- Molecule 20: 50S ribosomal protein L24



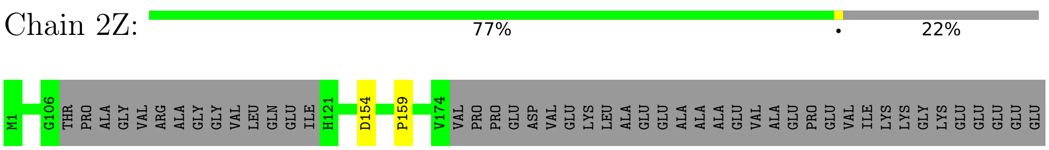
- Molecule 20: 50S ribosomal protein L24



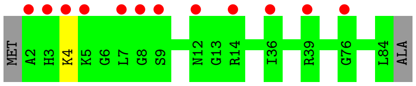
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25

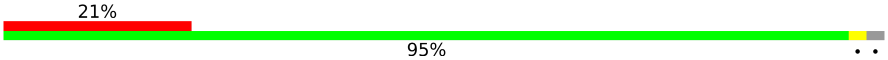


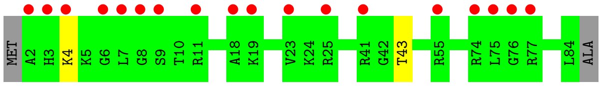
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27

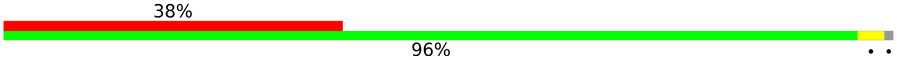
Chain 20:

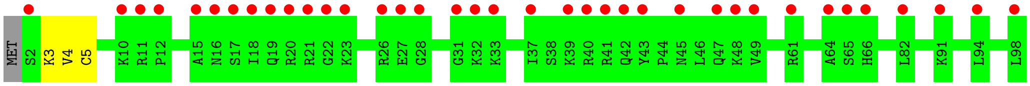




- Molecule 23: 50S ribosomal protein L28

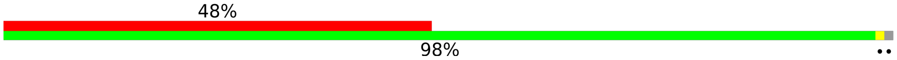
Chain 11:

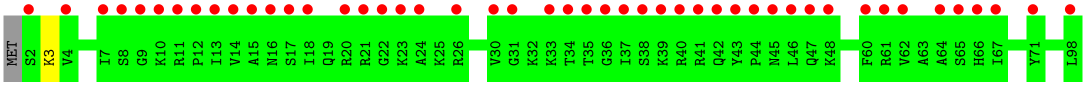




- Molecule 23: 50S ribosomal protein L28

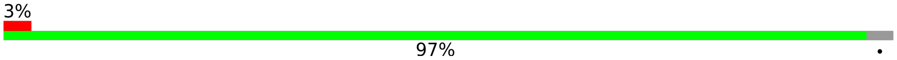
Chain 21:

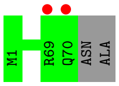




- Molecule 24: 50S ribosomal protein L29

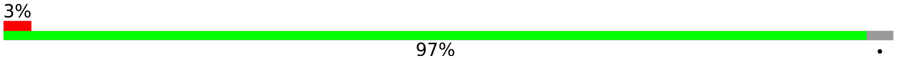
Chain 12:

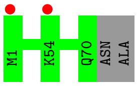




- Molecule 24: 50S ribosomal protein L29

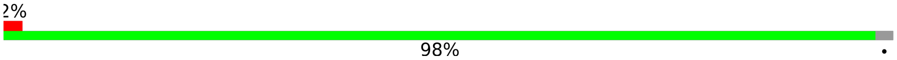
Chain 22:

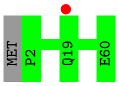




- Molecule 25: 50S ribosomal protein L30

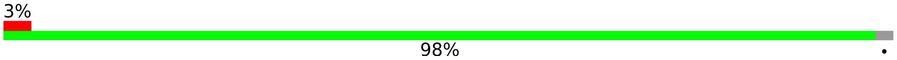
Chain 13:

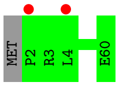




- Molecule 25: 50S ribosomal protein L30

Chain 23:



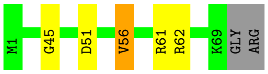


- Molecule 26: 50S ribosomal protein L31

Chain 14:

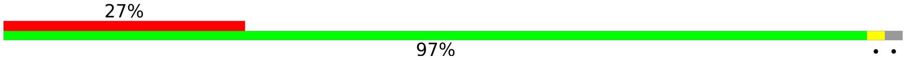
- Molecule 26: 50S ribosomal protein L31

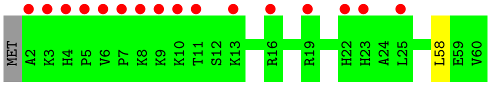
Chain 24:



- Molecule 27: 50S ribosomal protein L32

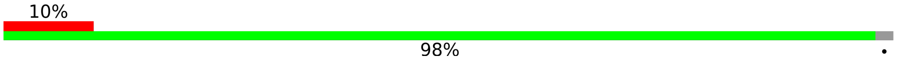
Chain 15:

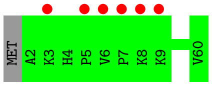




- Molecule 27: 50S ribosomal protein L32

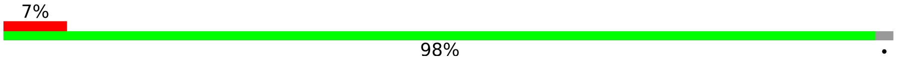
Chain 25:

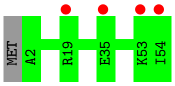




- Molecule 28: 50S ribosomal protein L33

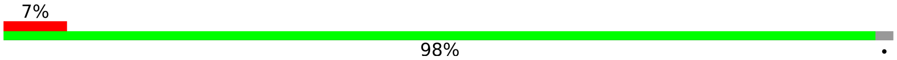
Chain 16:

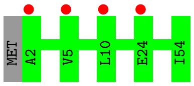




- Molecule 28: 50S ribosomal protein L33

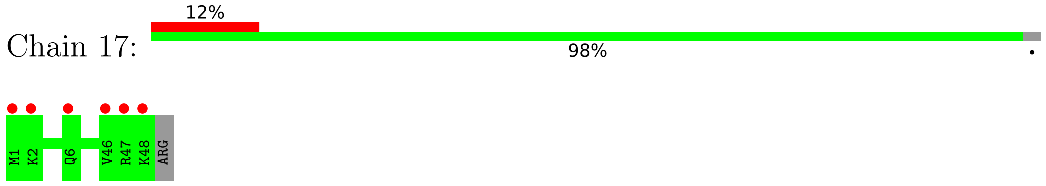
Chain 26:





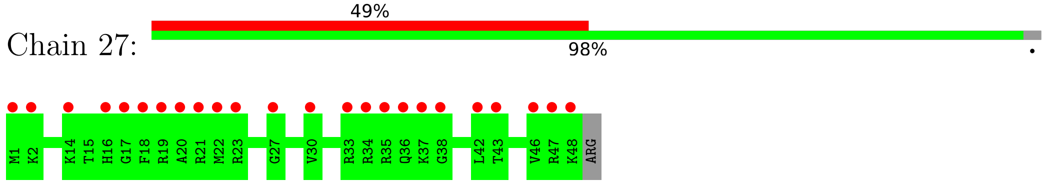
- Molecule 29: 50S ribosomal protein L34

Chain 17:



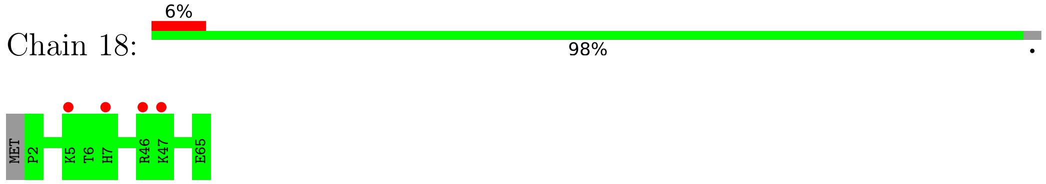
- Molecule 29: 50S ribosomal protein L34

Chain 27:



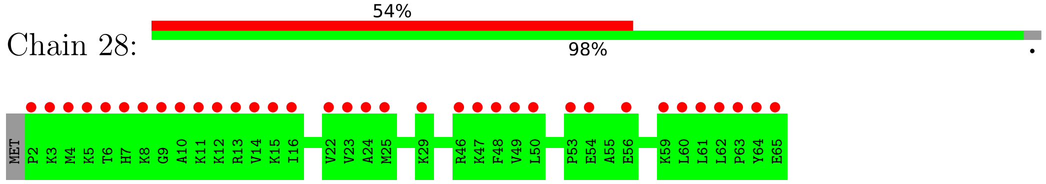
- Molecule 30: 50S Ribosomal Protein L35

Chain 18:



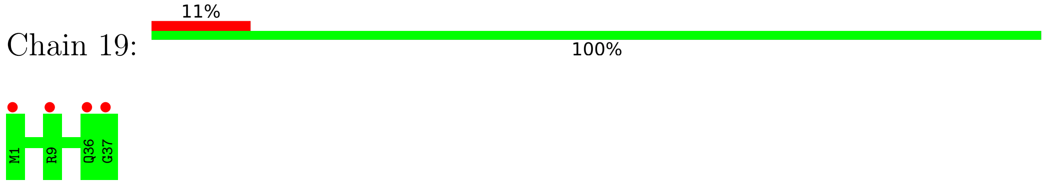
- Molecule 30: 50S Ribosomal Protein L35

Chain 28:



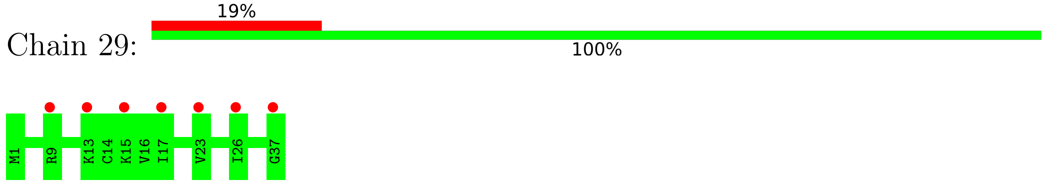
- Molecule 31: 50S Ribosomal Protein L36

Chain 19:



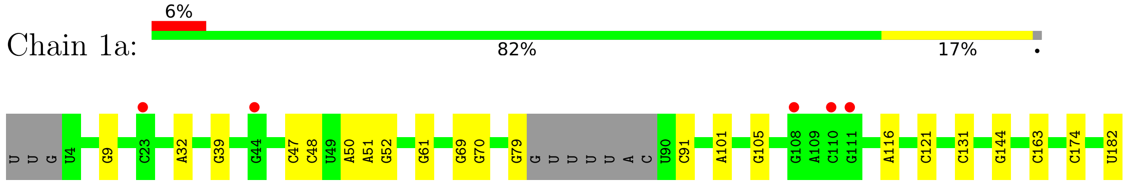
- Molecule 31: 50S Ribosomal Protein L36

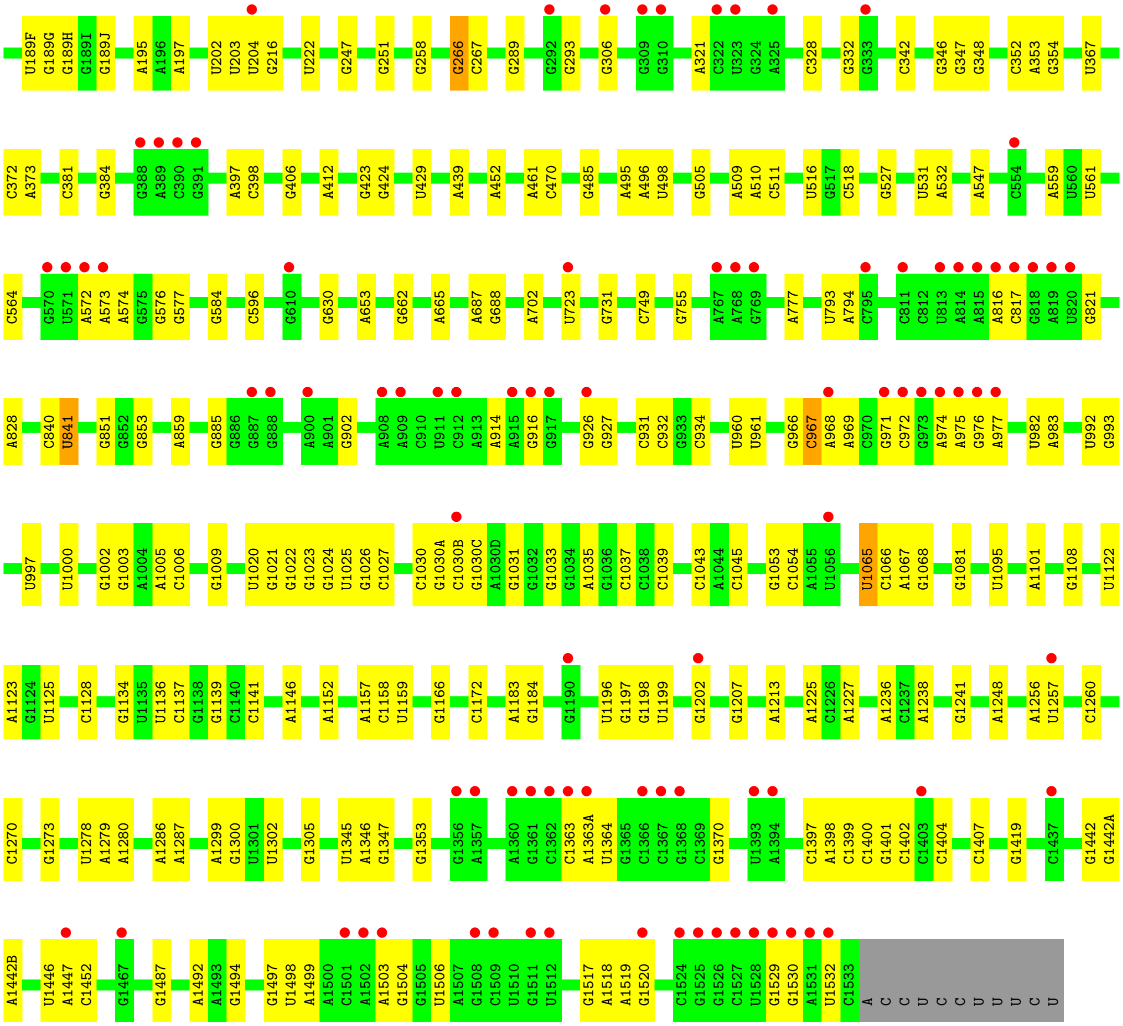
Chain 29:



- Molecule 32: 16S Ribosomal RNA

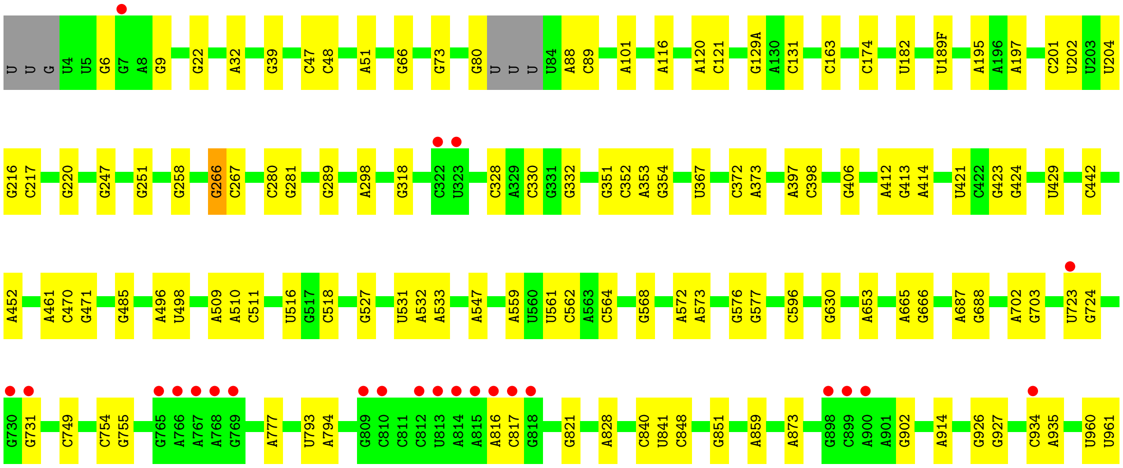
Chain 1a:

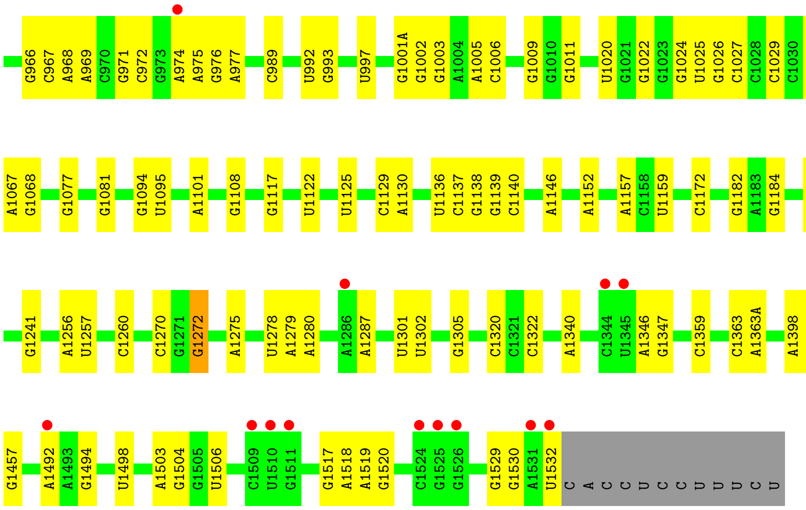




- Molecule 32: 16S Ribosomal RNA

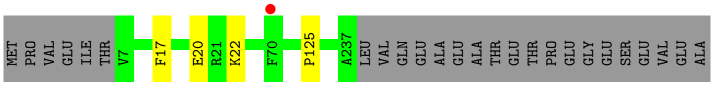
Chain 2a:





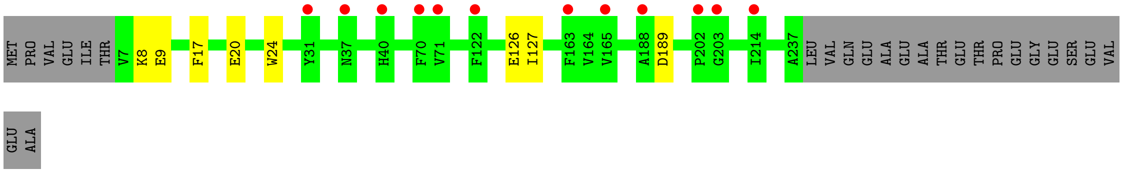
- Molecule 33: 30S Ribosomal Protein S2

Chain 1b:



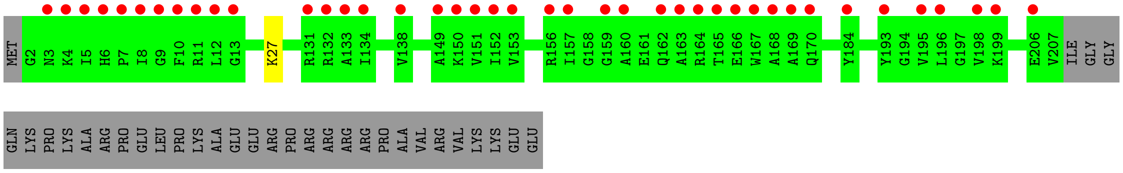
- Molecule 33: 30S Ribosomal Protein S2

Chain 2b:



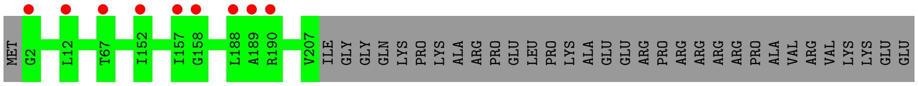
- Molecule 34: 30S Ribosomal Protein S3

Chain 1c:



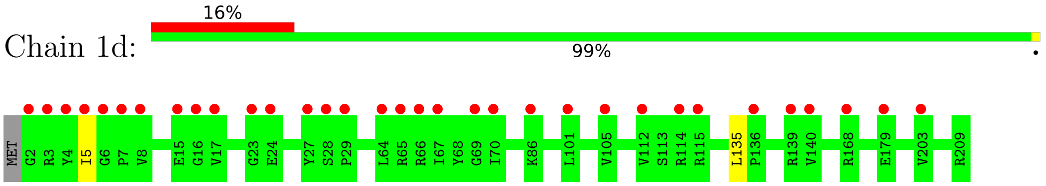
- Molecule 34: 30S Ribosomal Protein S3

Chain 2c:



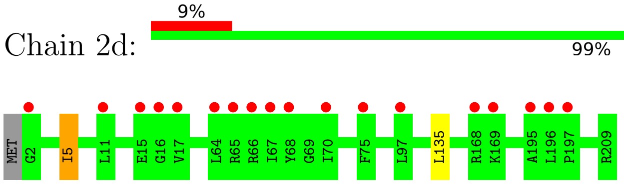
- Molecule 35: 30S Ribosomal Protein S4

Chain 1d:



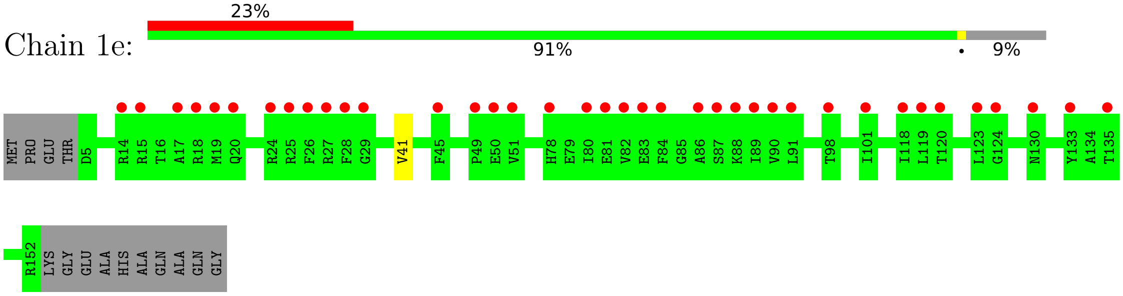
- Molecule 35: 30S Ribosomal Protein S4

Chain 2d:



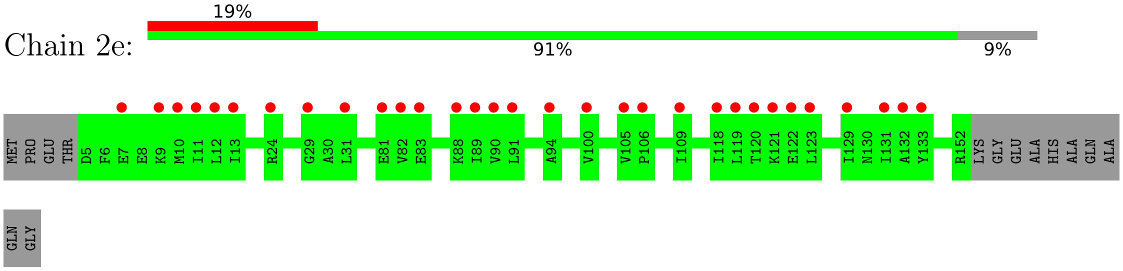
- Molecule 36: 30S Ribosomal Protein S5

Chain 1e:



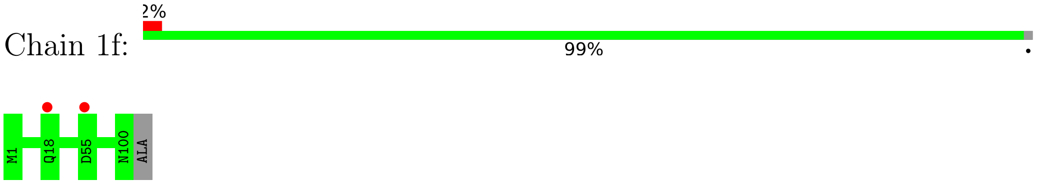
- Molecule 36: 30S Ribosomal Protein S5

Chain 2e:



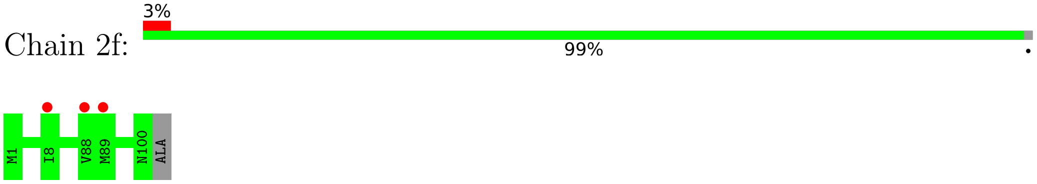
- Molecule 37: 30S Ribosomal Protein S6

Chain 1f:



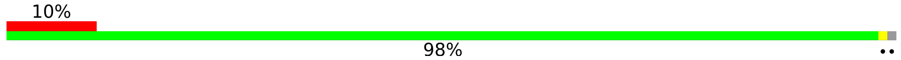
- Molecule 37: 30S Ribosomal Protein S6

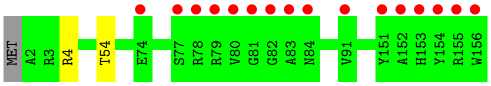
Chain 2f:



- Molecule 38: 30S Ribosomal Protein S7

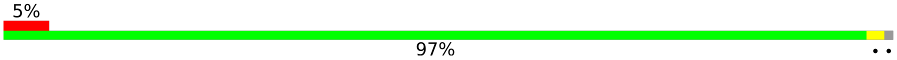
Chain 1g:

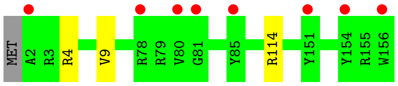




- Molecule 38: 30S Ribosomal Protein S7

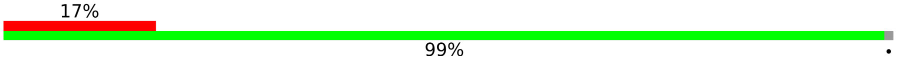
Chain 2g:

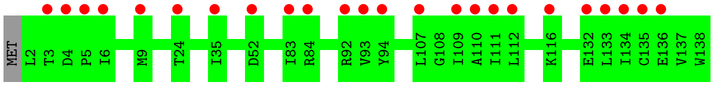




- Molecule 39: 30S Ribosomal Protein S8

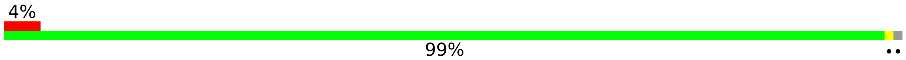
Chain 1h:

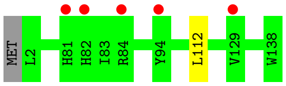




- Molecule 39: 30S Ribosomal Protein S8

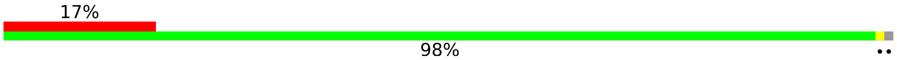
Chain 2h:

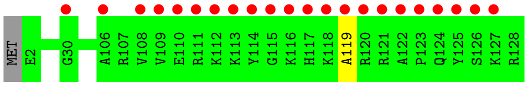




- Molecule 40: 30S ribosomal protein S9

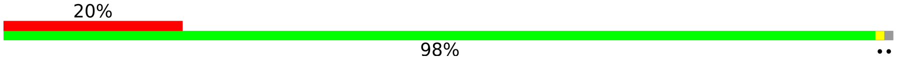
Chain 1i:

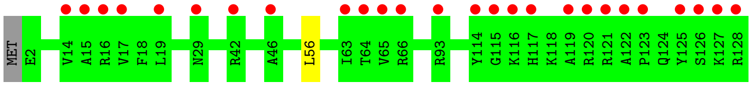




- Molecule 40: 30S ribosomal protein S9

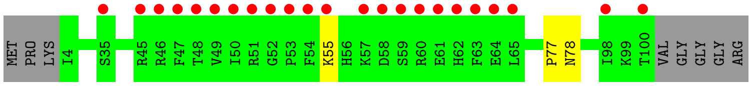
Chain 2i:



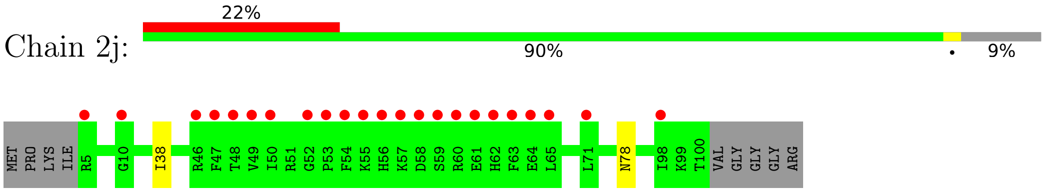


- Molecule 41: 30S ribosomal protein S10

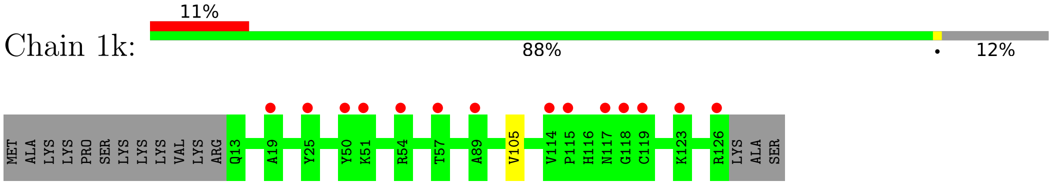
Chain 1j:



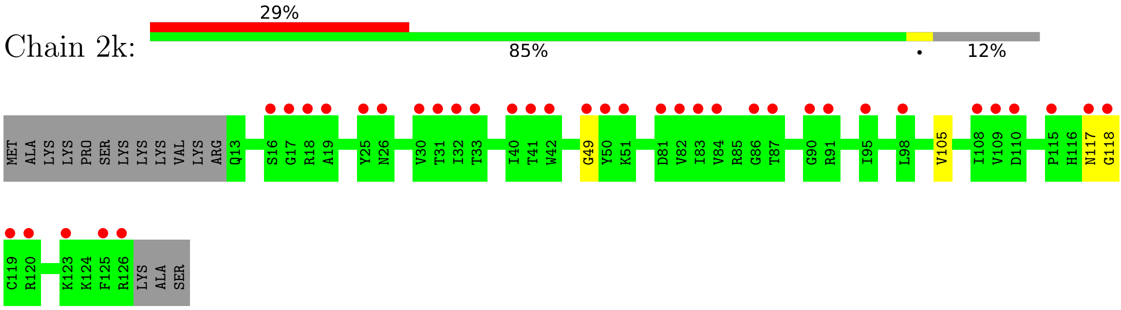
- Molecule 41: 30S ribosomal protein S10



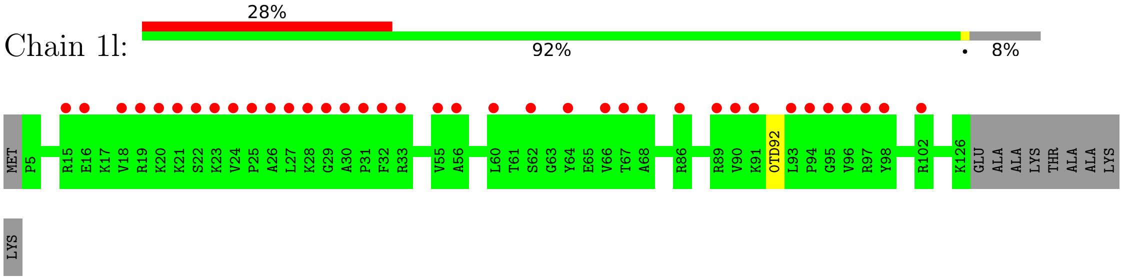
- Molecule 42: 30S ribosomal protein S11



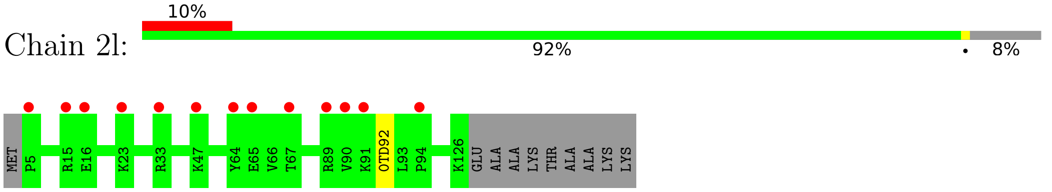
- Molecule 42: 30S ribosomal protein S11



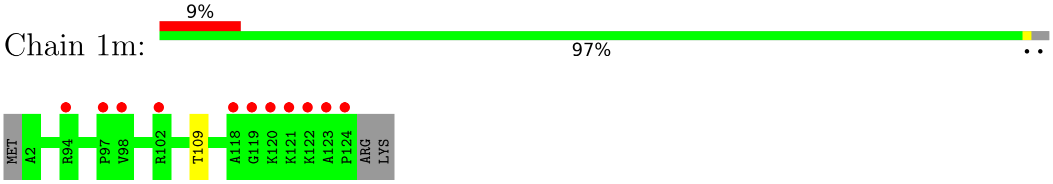
- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12

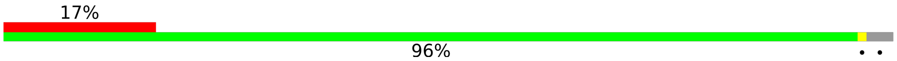


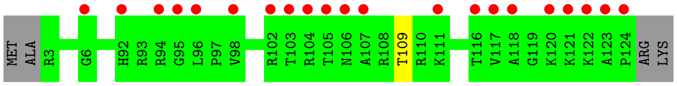
- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13

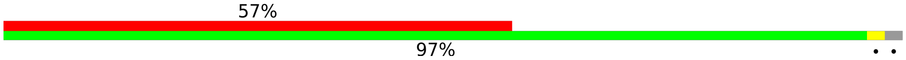
Chain 2m:

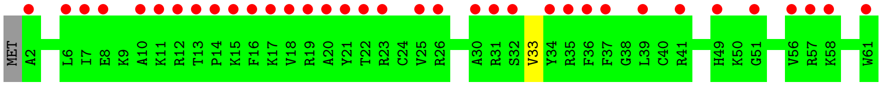




- Molecule 45: 30S ribosomal protein S14 type Z

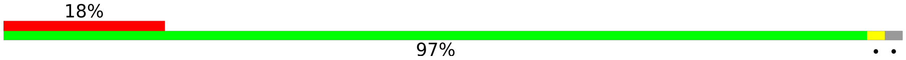
Chain 1n:

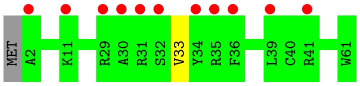




- Molecule 45: 30S ribosomal protein S14 type Z

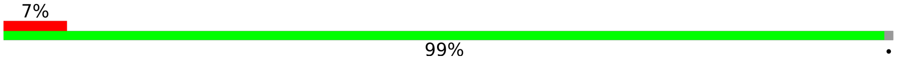
Chain 2n:

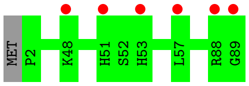




- Molecule 46: 30S ribosomal protein S15

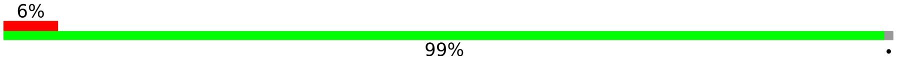
Chain 1o:

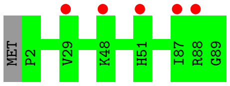




- Molecule 46: 30S ribosomal protein S15

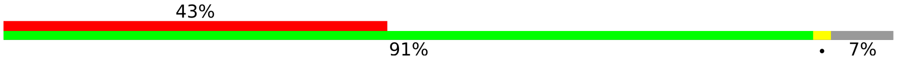
Chain 2o:

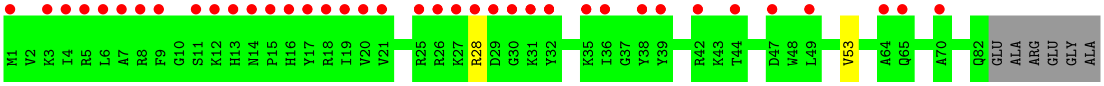




- Molecule 47: 30S ribosomal protein S16

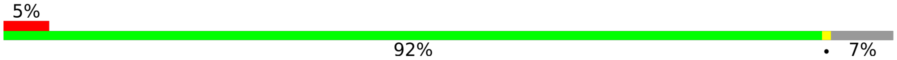
Chain 1p:

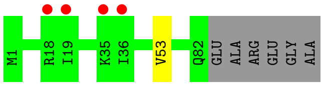




- Molecule 47: 30S ribosomal protein S16

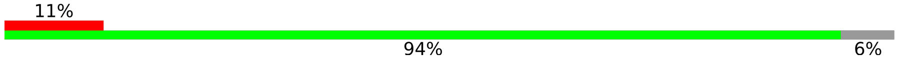
Chain 2p:

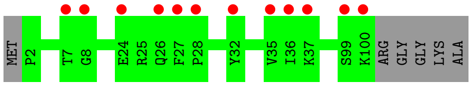




- Molecule 48: 30S ribosomal protein S17

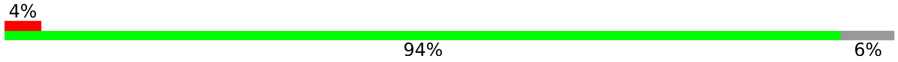
Chain 1q:

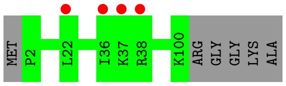




- Molecule 48: 30S ribosomal protein S17

Chain 2q:



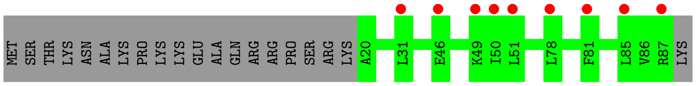


- Molecule 49: 30S ribosomal protein S18

Chain 1r:

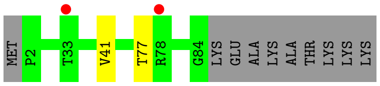
- Molecule 49: 30S ribosomal protein S18

Chain 2r:



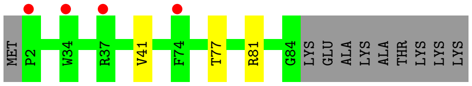
- Molecule 50: 30S Ribosomal Protein S19

Chain 1s:



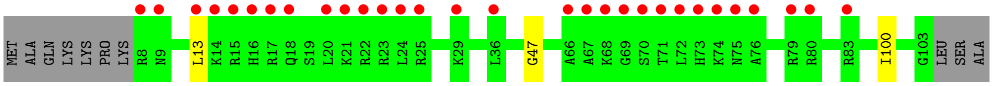
- Molecule 50: 30S Ribosomal Protein S19

Chain 2s:



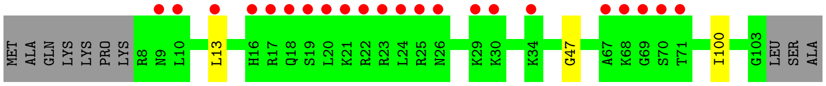
- Molecule 51: 30S Ribosomal Protein S20

Chain 1t:



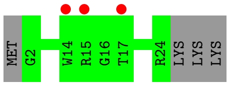
- Molecule 51: 30S Ribosomal Protein S20

Chain 2t:



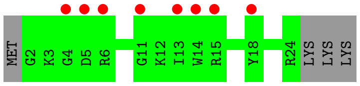
- Molecule 52: 30S ribosomal protein Thx

Chain 1u:



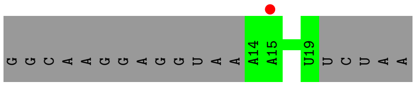
- Molecule 52: 30S ribosomal protein Thx

Chain 2u:



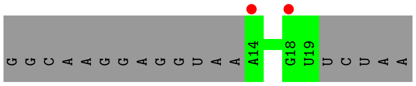
- Molecule 53: mRNA

Chain 1v:



- Molecule 53: mRNA

Chain 2v:



- Molecule 54: CC-Pmn

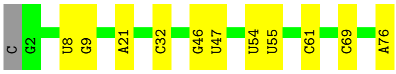
Chain 1w:

- Molecule 54: CC-Pmn

Chain 2w:

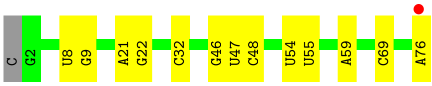
- Molecule 55: P-site tRNA, Deacylated Initiator Methionyl-tRNA

Chain 1x:



- Molecule 55: P-site tRNA, Deacylated Initiator Methionyl-tRNA

Chain 2x:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	212.24Å 452.84Å 620.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.71 – 3.70 212.69 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (146.71-3.70) 99.1 (212.69-3.70)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.68Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.237 , 0.278 0.237 , 0.279	Depositor DCC
R_{free} test set	31415 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	135.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	287828	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 7MG, 4OC, 2MG, 5MU, M2G, 2MA, 2MU, OMG, MA6, SF4, 0TD, PPU, 5MC, ZN, 4SU, UR3, PSU, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	1A	0.37	0/69009	0.82	20/107712 (0.0%)
1	2A	0.33	0/67293	0.80	13/105034 (0.0%)
2	1B	0.33	1/2882 (0.0%)	0.76	0/4494
2	2B	0.33	1/2879 (0.0%)	0.78	1/4487 (0.0%)
3	1D	0.33	0/2186	0.48	0/2944
3	2D	0.35	1/2186 (0.0%)	0.48	0/2944
4	1E	0.29	0/1592	0.48	0/2149
4	2E	0.28	0/1592	0.46	0/2149
5	1F	0.30	0/1619	0.46	0/2193
5	2F	0.28	0/1615	0.44	0/2188
6	1G	0.27	0/1448	0.47	0/1957
6	2G	0.27	0/1453	0.46	0/1963
7	1H	0.27	0/1356	0.43	0/1834
7	2H	0.28	0/1356	0.43	0/1834
8	1I	0.26	0/1112	0.44	0/1514
8	2I	0.27	0/1079	0.45	0/1475
9	1N	0.31	0/1144	0.47	0/1543
9	2N	0.28	0/1144	0.46	0/1543
10	1O	0.31	0/943	0.47	0/1269
10	2O	0.30	0/943	0.47	0/1269
11	1P	0.28	0/1152	0.52	1/1533 (0.1%)
11	2P	0.29	0/1152	0.52	0/1533
12	1Q	0.30	0/1143	0.47	0/1527
12	2Q	0.27	0/1143	0.45	0/1527
13	1R	0.26	0/982	0.46	0/1312
13	2R	0.26	0/982	0.44	0/1312
14	1S	0.27	0/883	0.43	0/1176
14	2S	0.28	0/880	0.42	0/1172
15	1T	0.28	0/1105	0.45	0/1477
15	2T	0.28	0/1097	0.44	0/1468
16	1U	0.28	0/977	0.41	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\lvert Z\rvert >5$	RMSZ	$\#\lvert Z\rvert >5$
16	2U	0.27	0/977	0.40	0/1301
17	1V	0.29	0/782	0.48	0/1049
17	2V	0.28	0/782	0.50	0/1049
18	1W	0.28	0/897	0.44	0/1205
18	2W	0.29	0/897	0.46	0/1205
19	1X	0.30	0/764	0.47	0/1025
19	2X	0.27	0/764	0.46	0/1025
20	1Y	0.31	0/819	0.46	0/1095
20	2Y	0.30	0/819	0.46	0/1095
21	1Z	0.27	0/1267	0.48	0/1717
21	2Z	0.27	0/1299	0.46	0/1763
22	10	0.28	0/662	0.47	0/881
22	20	0.28	0/662	0.46	0/881
23	11	0.30	0/762	0.46	0/1014
23	21	0.30	0/762	0.46	0/1014
24	12	0.27	0/590	0.39	0/781
24	22	0.27	0/590	0.37	0/781
25	13	0.29	0/474	0.43	0/635
25	23	0.26	0/469	0.43	0/630
26	14	0.30	0/565	0.56	0/761
26	24	0.35	0/545	0.50	0/737
27	15	0.33	0/469	0.48	0/635
27	25	0.32	0/469	0.47	0/635
28	16	0.27	0/460	0.47	0/613
28	26	0.26	0/456	0.46	0/608
29	17	0.29	0/426	0.43	0/561
29	27	0.26	0/426	0.44	0/561
30	18	0.28	0/525	0.45	0/691
30	28	0.27	0/525	0.45	0/691
31	19	0.33	0/310	0.50	0/407
31	29	0.30	0/310	0.48	0/407
32	1a	0.31	0/35795	0.83	19/55864 (0.0%)
32	2a	0.31	2/35886 (0.0%)	0.83	11/56005 (0.0%)
33	1b	0.28	0/1881	0.46	0/2542
33	2b	0.28	0/1860	0.45	0/2518
34	1c	0.28	0/1572	0.45	0/2126
34	2c	0.27	0/1566	0.44	0/2119
35	1d	0.29	0/1685	0.44	0/2262
35	2d	0.28	0/1704	0.44	0/2284
36	1e	0.27	0/1145	0.46	0/1543
36	2e	0.28	0/1149	0.48	0/1548
37	1f	0.27	0/823	0.46	0/1115
37	2f	0.27	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.27	0/1250	0.42	0/1679
38	2g	0.28	0/1254	0.41	0/1683
39	1h	0.26	0/1108	0.44	0/1494
39	2h	0.28	0/1108	0.44	0/1494
40	1i	0.29	0/1002	0.46	0/1346
40	2i	0.30	0/997	0.46	0/1343
41	1j	0.26	0/722	0.46	0/982
41	2j	0.26	0/727	0.46	0/988
42	1k	0.27	0/844	0.44	0/1145
42	2k	0.26	0/848	0.43	0/1149
43	1l	0.28	0/937	0.49	0/1260
43	2l	0.28	0/937	0.48	0/1260
44	1m	0.26	0/969	0.43	0/1302
44	2m	0.26	0/961	0.46	0/1291
45	1n	0.28	0/501	0.44	0/664
45	2n	0.28	0/501	0.45	0/664
46	1o	0.26	0/739	0.40	0/985
46	2o	0.25	0/739	0.40	0/985
47	1p	0.26	0/697	0.47	0/939
47	2p	0.27	0/693	0.45	0/935
48	1q	0.27	0/836	0.43	0/1117
48	2q	0.27	0/836	0.42	0/1117
49	1r	0.26	0/560	0.42	0/746
49	2r	0.27	0/560	0.44	0/746
50	1s	0.26	0/667	0.47	0/900
50	2s	0.25	0/661	0.48	0/893
51	1t	0.31	0/730	0.41	0/965
51	2t	0.25	0/729	0.39	0/965
52	1u	0.23	0/203	0.44	0/266
52	2u	0.24	0/203	0.43	0/266
53	1v	0.35	0/126	0.86	0/195
53	2v	0.33	0/126	0.81	0/195
54	1w	0.46	0/40	0.95	0/60
54	2w	0.35	0/40	1.05	0/60
55	1x	0.38	0/1725	0.97	1/2689 (0.0%)
55	2x	0.37	0/1725	0.96	3/2689 (0.1%)
All	All	0.32	5/310047 (0.0%)	0.74	69/463792 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	1Z	0	1
21	2Z	0	1
33	2b	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1B	1	U	OP3-P	-10.34	1.48	1.61
2	2B	1	U	OP3-P	-10.27	1.48	1.61
3	2D	7	LYS	C-N	-8.87	1.17	1.34
32	2a	1272	G	C6-N1	-6.71	1.34	1.39
32	2a	1272	G	N1-C2	-5.10	1.33	1.37

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1272	G	C5-C6-O6	13.95	136.97	128.60
32	2a	1272	G	N1-C6-O6	-11.59	112.94	119.90
32	2a	1272	G	N3-C2-N2	11.37	127.86	119.90
32	2a	1272	G	N1-C2-N2	-10.97	106.33	116.20
1	1A	1109	G	C5-C6-O6	9.10	134.06	128.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	1Z	159	PRO	Peptide
21	2Z	159	PRO	Peptide
33	2b	9	GLU	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1D	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	29	66
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	66
5	1F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	15	51
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	15	51
6	1G	179/182 (98%)	168 (94%)	9 (5%)	2 (1%)	14	50
6	2G	179/182 (98%)	170 (95%)	7 (4%)	2 (1%)	14	50
7	1H	172/180 (96%)	162 (94%)	8 (5%)	2 (1%)	13	48
7	2H	172/180 (96%)	165 (96%)	4 (2%)	3 (2%)	9	42
8	1I	144/148 (97%)	135 (94%)	9 (6%)	0	100	100
8	2I	144/148 (97%)	132 (92%)	12 (8%)	0	100	100
9	1N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	22	59
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	22	59
10	1O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	136 (92%)	8 (5%)	3 (2%)	7	39
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	22	59
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	54
14	2S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	19	56
15	2T	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	2V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
18	1W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
19	2X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	1Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	130 (88%)	18 (12%)	0	100	100
21	2Z	156/206 (76%)	142 (91%)	14 (9%)	0	100	100
22	10	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	48
22	20	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	48
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	14	50
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	50
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	57 (100%)	0	0	100	100
25	23	57/60 (95%)	57 (100%)	0	0	100	100
26	14	67/71 (94%)	51 (76%)	9 (13%)	7 (10%)	0	7
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	13
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	201 (88%)	24 (10%)	4 (2%)	9	42
33	2b	229/256 (90%)	203 (89%)	23 (10%)	3 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	29	66
34	2c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
35	1d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29	66
35	2d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	29	66
36	1e	146/162 (90%)	132 (90%)	14 (10%)	0	100	100
36	2e	146/162 (90%)	138 (94%)	8 (6%)	0	100	100
37	1f	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	12	47
38	2g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	12	47
39	1h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
39	2h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
40	1i	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	19	56
40	2i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	19	56
41	1j	95/105 (90%)	88 (93%)	4 (4%)	3 (3%)	4	31
41	2j	94/105 (90%)	86 (92%)	7 (7%)	1 (1%)	14	50
42	1k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	54
42	2k	112/129 (87%)	104 (93%)	4 (4%)	4 (4%)	3	29
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
43	2l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
44	1m	121/126 (96%)	115 (95%)	6 (5%)	0	100	100
44	2m	120/126 (95%)	114 (95%)	6 (5%)	0	100	100
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	1p	80/88 (91%)	74 (92%)	4 (5%)	2 (2%)	5	35
47	2p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	12	47
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	66 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	2r	66/88 (75%)	66 (100%)	0	0	100	100
50	1s	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
50	2s	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	13	48
51	1t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	7	38
51	2t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	7	38
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11370/12128 (94%)	10706 (94%)	591 (5%)	73 (1%)	25	62

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1H	92	ILE
26	14	46	GLN
26	14	51	ASP
26	14	57	GLU
33	1b	22	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	215 (100%)	0	100	100
3	2D	215/218 (99%)	215 (100%)	0	100	100
4	1E	164/166 (99%)	163 (99%)	1 (1%)	86	93
4	2E	164/166 (99%)	163 (99%)	1 (1%)	86	93
5	1F	160/166 (96%)	160 (100%)	0	100	100
5	2F	159/166 (96%)	159 (100%)	0	100	100
6	1G	143/156 (92%)	141 (99%)	2 (1%)	67	82
6	2G	143/156 (92%)	142 (99%)	1 (1%)	84	91
7	1H	144/148 (97%)	143 (99%)	1 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	2H	144/148 (97%)	144 (100%)	0	100	100
8	1I	113/124 (91%)	113 (100%)	0	100	100
8	2I	105/124 (85%)	105 (100%)	0	100	100
9	1N	118/119 (99%)	117 (99%)	1 (1%)	81	89
9	2N	118/119 (99%)	117 (99%)	1 (1%)	81	89
10	1O	100/100 (100%)	100 (100%)	0	100	100
10	2O	100/100 (100%)	100 (100%)	0	100	100
11	1P	115/116 (99%)	113 (98%)	2 (2%)	60	79
11	2P	115/116 (99%)	115 (100%)	0	100	100
12	1Q	111/111 (100%)	111 (100%)	0	100	100
12	2Q	111/111 (100%)	111 (100%)	0	100	100
13	1R	101/101 (100%)	101 (100%)	0	100	100
13	2R	101/101 (100%)	101 (100%)	0	100	100
14	1S	86/88 (98%)	86 (100%)	0	100	100
14	2S	85/88 (97%)	85 (100%)	0	100	100
15	1T	115/127 (91%)	115 (100%)	0	100	100
15	2T	113/127 (89%)	113 (100%)	0	100	100
16	1U	93/94 (99%)	93 (100%)	0	100	100
16	2U	93/94 (99%)	93 (100%)	0	100	100
17	1V	80/82 (98%)	77 (96%)	3 (4%)	33	61
17	2V	80/82 (98%)	77 (96%)	3 (4%)	33	61
18	1W	90/92 (98%)	89 (99%)	1 (1%)	73	85
18	2W	90/92 (98%)	89 (99%)	1 (1%)	73	85
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	77 (100%)	0	100	100
20	1Y	85/91 (93%)	84 (99%)	1 (1%)	71	84
20	2Y	85/91 (93%)	83 (98%)	2 (2%)	49	71
21	1Z	135/179 (75%)	134 (99%)	1 (1%)	84	91
21	2Z	137/179 (76%)	136 (99%)	1 (1%)	84	91
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	64 (98%)	1 (2%)	65	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	11	80/83 (96%)	78 (98%)	2 (2%)	47	70
23	21	80/83 (96%)	80 (100%)	0	100	100
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	51 (100%)	0	100	100
25	23	50/52 (96%)	50 (100%)	0	100	100
26	14	59/63 (94%)	56 (95%)	3 (5%)	24	55
26	24	53/63 (84%)	52 (98%)	1 (2%)	57	76
27	15	50/52 (96%)	49 (98%)	1 (2%)	55	74
27	25	50/52 (96%)	50 (100%)	0	100	100
28	16	51/52 (98%)	51 (100%)	0	100	100
28	26	50/52 (96%)	50 (100%)	0	100	100
29	17	41/42 (98%)	41 (100%)	0	100	100
29	27	41/42 (98%)	41 (100%)	0	100	100
30	18	54/55 (98%)	54 (100%)	0	100	100
30	28	54/55 (98%)	54 (100%)	0	100	100
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	192 (100%)	0	100	100
33	2b	187/220 (85%)	183 (98%)	4 (2%)	53	74
34	1c	142/188 (76%)	142 (100%)	0	100	100
34	2c	140/188 (74%)	140 (100%)	0	100	100
35	1d	169/181 (93%)	168 (99%)	1 (1%)	86	93
35	2d	173/181 (96%)	171 (99%)	2 (1%)	71	84
36	1e	113/123 (92%)	112 (99%)	1 (1%)	78	88
36	2e	114/123 (93%)	114 (100%)	0	100	100
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	85 (100%)	0	100	100
38	1g	119/127 (94%)	119 (100%)	0	100	100
38	2g	120/127 (94%)	119 (99%)	1 (1%)	81	89
39	1h	114/119 (96%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	2h	114/119 (96%)	113 (99%)	1 (1%)	78	88
40	1i	90/99 (91%)	90 (100%)	0	100	100
40	2i	89/99 (90%)	89 (100%)	0	100	100
41	1j	66/92 (72%)	66 (100%)	0	100	100
41	2j	69/92 (75%)	68 (99%)	1 (1%)	67	82
42	1k	82/99 (83%)	82 (100%)	0	100	100
42	2k	83/99 (84%)	83 (100%)	0	100	100
43	1l	96/108 (89%)	96 (100%)	0	100	100
43	2l	96/108 (89%)	96 (100%)	0	100	100
44	1m	93/101 (92%)	92 (99%)	1 (1%)	73	85
44	2m	92/101 (91%)	91 (99%)	1 (1%)	73	85
45	1n	49/50 (98%)	48 (98%)	1 (2%)	55	74
45	2n	49/50 (98%)	48 (98%)	1 (2%)	55	74
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	78 (100%)	0	100	100
47	1p	69/74 (93%)	69 (100%)	0	100	100
47	2p	68/74 (92%)	68 (100%)	0	100	100
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	94 (100%)	0	100	100
49	1r	59/77 (77%)	59 (100%)	0	100	100
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	67 (97%)	2 (3%)	42	66
50	2s	67/80 (84%)	65 (97%)	2 (3%)	41	66
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67	82
51	2t	70/82 (85%)	69 (99%)	1 (1%)	67	82
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	9251 (99%)	52 (1%)	86	93

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	2N	58	ASP

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Mol	Chain	Res	Type
21	2Z	154	ASP
50	2s	41	VAL
17	2V	52	VAL
18	2W	67	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
50	1s	83	HIS
40	2i	58	HIS
8	2I	11	ASN
38	2g	122	HIS
50	2s	57	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	438 (15%)	28 (0%)
1	2A	2788/2915 (95%)	443 (15%)	21 (0%)
2	1B	120/121 (99%)	10 (8%)	1 (0%)
2	2B	119/121 (98%)	12 (10%)	1 (0%)
32	1a	1494/1521 (98%)	243 (16%)	0
32	2a	1498/1521 (98%)	231 (15%)	0
53	1v	4/24 (16%)	0	0
53	2v	4/24 (16%)	0	0
54	1w	1/3 (33%)	1 (100%)	0
54	2w	1/3 (33%)	1 (100%)	0
55	1x	75/77 (97%)	6 (8%)	0
55	2x	75/77 (97%)	7 (9%)	0
All	All	9040/9322 (96%)	1392 (15%)	51 (0%)

5 of 1392 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	62	U

5 of 51 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1B	1	U
1	2A	752	A
1	2A	2756	U
1	2A	195	A
1	2A	271(M)	G

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

58 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	$\#\|Z\| > 2$
1	4OC	1A	1942	1	19,22,24	0.81	0	26,31,35	0.95	1 (3%)
32	5MC	2a	967	32	18,22,23	1.00	2 (11%)	26,32,35	1.06	2 (7%)
32	2MG	1a	1207	32	18,26,27	0.88	1 (5%)	16,38,41	1.11	2 (12%)
32	4OC	1a	1402	32	20,23,24	0.76	0	26,32,35	0.83	1 (3%)
1	2MA	2A	2503	1,56	17,25,26	1.03	1 (5%)	17,37,40	0.97	2 (11%)
43	0TD	1l	92	43	7,9,10	4.60	1 (14%)	6,11,13	7.50	2 (33%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	22,30,33	1.96	3 (13%)
32	5MC	2a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.09	2 (7%)
1	PSU	1A	2617	1	18,21,22	1.38	2 (11%)	22,30,33	1.88	3 (13%)
1	PSU	2A	2605	1	18,21,22	1.33	3 (16%)	22,30,33	1.79	4 (18%)
32	M2G	2a	966	32	20,27,28	1.47	3 (15%)	22,40,43	0.88	1 (4%)
55	5MC	1x	32	55	18,22,23	0.99	2 (11%)	26,32,35	1.22	3 (11%)
1	PSU	1A	1933	1	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
32	UR3	1a	1498	32	19,22,23	1.03	2 (10%)	26,32,35	1.44	2 (7%)
32	7MG	1a	527	32	22,26,27	1.36	3 (13%)	29,39,42	2.43	5 (17%)
32	MA6	2a	1519	32	19,26,27	1.01	1 (5%)	18,38,41	1.75	5 (27%)
1	2MA	1A	2515	1,56	17,25,26	1.02	2 (11%)	17,37,40	1.00	2 (11%)
1	5MC	2A	1942	1	18,22,23	0.97	2 (11%)	26,32,35	1.17	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	5MC	2x	32	55	18,22,23	0.97	2 (11%)	26,32,35	1.17	3 (11%)
1	5MU	1A	1937	1	19,22,23	1.46	4 (21%)	28,32,35	1.99	6 (21%)
1	PSU	2A	1917	1	18,21,22	1.41	3 (16%)	22,30,33	1.90	4 (18%)
1	5MC	1A	1964	1	18,22,23	0.97	2 (11%)	26,32,35	1.07	3 (11%)
32	M2G	1a	966	32	20,27,28	1.45	3 (15%)	22,40,43	0.99	2 (9%)
32	5MC	2a	1407	32	18,22,23	1.00	2 (11%)	26,32,35	1.17	2 (7%)
32	PSU	2a	516	32	18,21,22	1.34	2 (11%)	22,30,33	1.81	4 (18%)
32	5MC	1a	1400	32	18,22,23	0.95	2 (11%)	26,32,35	1.12	1 (3%)
32	MA6	2a	1518	32	19,26,27	0.97	1 (5%)	18,38,41	1.77	6 (33%)
1	5MU	2A	1939	1	19,22,23	1.34	4 (21%)	28,32,35	2.15	6 (21%)
1	2MU	2A	2552	1	19,22,24	1.26	2 (10%)	26,31,36	1.80	5 (19%)
54	PPU	1w	76	54,1	32,40,41	0.92	1 (3%)	33,57,60	1.67	8 (24%)
32	PSU	1a	516	32,56	18,21,22	1.38	2 (11%)	22,30,33	1.79	4 (18%)
55	PSU	1x	55	55	18,21,22	1.34	2 (11%)	22,30,33	1.91	5 (22%)
32	5MC	1a	967	32	18,22,23	1.00	1 (5%)	26,32,35	1.11	3 (11%)
1	5MC	1A	1984	1	18,22,23	0.98	2 (11%)	26,32,35	1.31	5 (19%)
1	5MC	2A	1962	1	18,22,23	0.95	2 (11%)	26,32,35	1.26	4 (15%)
1	2MU	1A	2564	1	19,22,24	1.27	3 (15%)	26,31,36	1.68	5 (19%)
32	5MC	2a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.10	3 (11%)
32	MA6	1a	1519	32	19,26,27	0.97	1 (5%)	18,38,41	1.69	6 (33%)
32	UR3	2a	1498	32	19,22,23	1.00	2 (10%)	26,32,35	1.42	2 (7%)
43	0TD	2l	92	43	7,9,10	4.64	1 (14%)	6,11,13	7.95	2 (33%)
1	OMG	1A	2263	55,1	18,26,27	1.02	1 (5%)	19,38,41	1.02	2 (10%)
54	PPU	2w	76	54,1,56	32,40,41	0.90	1 (3%)	33,57,60	1.60	8 (24%)
1	5MU	2A	1915	1	19,22,23	1.38	5 (26%)	28,32,35	2.04	6 (21%)
1	PSU	1A	1939	1	18,21,22	1.38	2 (11%)	22,30,33	1.83	3 (13%)
32	7MG	2a	527	32	22,26,27	1.37	3 (13%)	29,39,42	2.53	8 (27%)
55	5MU	1x	54	55	19,22,23	1.43	6 (31%)	28,32,35	1.88	6 (21%)
55	4SU	1x	8	55	18,21,22	1.86	4 (22%)	26,30,33	1.81	6 (23%)
32	MA6	1a	1518	32	19,26,27	0.94	1 (5%)	18,38,41	1.65	4 (22%)
32	4OC	2a	1402	32	20,23,24	0.79	0	26,32,35	0.92	1 (3%)
1	4OC	2A	1920	1	19,22,24	0.83	0	26,31,35	0.84	0
1	5MU	1A	1961	1	19,22,23	1.41	5 (26%)	28,32,35	2.30	6 (21%)
1	OMG	2A	2251	55,1	18,26,27	1.01	1 (5%)	19,38,41	1.00	2 (10%)
32	2MG	2a	1207	32	18,26,27	0.83	0	16,38,41	1.21	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
32	5MC	1a	1407	32	18,22,23	1.00	1 (5%)	26,32,35	1.20	3 (11%)
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	28,32,35	2.04	6 (21%)
32	5MC	1a	1404	32	18,22,23	0.95	2 (11%)	26,32,35	1.12	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
55	4SU	2x	8	55	18,21,22	1.97	5 (27%)	26,30,33	1.61	5 (19%)

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
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	4/7/29/30	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	0/7/37/38	0/3/3/3
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
1	2MA	1A	2515	1,56	-	1/3/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MU	2A	2552	1	-	0/9/27/28	0/2/2/2
54	PPU	1w	76	54,1	-	5/21/43/44	0/4/4/4
32	PSU	1a	516	32,56	-	2/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2564	1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
1	OMG	1A	2263	55,1	-	0/5/27/28	0/3/3/3
54	PPU	2w	76	54,1,56	-	5/21/43/44	0/4/4/4
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	0/7/37/38	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.00	1.70	1.82
43	1l	92	0TD	CB-SB	-11.86	1.70	1.82
32	1a	966	M2G	C2-N3	4.70	1.36	1.30
32	2a	966	M2G	C2-N3	4.68	1.36	1.30
55	1x	8	4SU	C4-S4	-4.56	1.59	1.68

The worst 5 of 209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-19.14	67.82	102.44
43	1l	92	0TD	CSB-SB-CB	-18.05	69.78	102.44
32	2a	527	7MG	N9-C4-N3	8.76	138.56	125.47
32	1a	527	7MG	N9-C4-N3	8.55	138.25	125.47
55	2x	55	PSU	N1-C2-N3	6.24	122.20	115.13

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	O-C-CA-CB
32	1a	516	PSU	C2'-C1'-C5-C4
32	1a	516	PSU	C2'-C1'-C5-C6
32	2a	966	M2G	N1-C2-N2-CM2
32	2a	966	M2G	N3-C2-N2-CM1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1170 ligands modelled in this entry, 1168 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	SF4	1d	302	35	0,12,12	-	-	-		
58	SF4	2d	302	35	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	1d	302	35	-	-	0/6/5/5
58	SF4	2d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	2D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2D	7:LYS	C	8:PRO	N	1.17

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	1A	2860/2915 (98%)	0.24	80 (2%)	53	40	82, 102, 143, 157	0
1	2A	2789/2915 (95%)	0.12	95 (3%)	45	34	88, 107, 136, 157	0
2	1B	120/121 (99%)	-0.38	0	100	100	104, 121, 132, 134	0
2	2B	120/121 (99%)	-0.57	0	100	100	111, 125, 135, 152	0
3	1D	275/276 (99%)	0.88	27 (9%)	7	6	84, 95, 108, 127	0
3	2D	275/276 (99%)	1.15	53 (19%)	1	1	88, 104, 114, 123	0
4	1E	204/206 (99%)	0.63	41 (20%)	1	0	86, 108, 122, 131	0
4	2E	204/206 (99%)	0.31	26 (12%)	3	4	88, 105, 119, 129	0
5	1F	203/210 (96%)	0.23	14 (6%)	16	11	79, 102, 120, 137	0
5	2F	203/210 (96%)	0.64	38 (18%)	1	1	90, 108, 122, 130	0
6	1G	181/182 (99%)	-0.27	2 (1%)	80	71	112, 122, 131, 139	0
6	2G	181/182 (99%)	0.72	30 (16%)	1	1	113, 126, 136, 149	0
7	1H	174/180 (96%)	0.20	4 (2%)	60	48	96, 113, 124, 131	0
7	2H	174/180 (96%)	0.49	15 (8%)	10	8	105, 125, 134, 142	0
8	1I	146/148 (98%)	-0.32	3 (2%)	63	52	102, 115, 124, 134	0
8	2I	146/148 (98%)	0.30	18 (12%)	4	4	109, 124, 138, 143	0
9	1N	140/140 (100%)	0.72	13 (9%)	8	6	93, 106, 119, 122	0
9	2N	140/140 (100%)	1.08	26 (18%)	1	1	97, 111, 122, 135	0
10	1O	122/122 (100%)	1.55	39 (31%)	0	0	90, 108, 122, 128	0
10	2O	122/122 (100%)	1.19	25 (20%)	1	0	87, 102, 113, 118	0
11	1P	149/150 (99%)	0.40	6 (4%)	38	28	85, 109, 124, 130	0
11	2P	149/150 (99%)	0.83	32 (21%)	0	0	90, 115, 126, 134	0
12	1Q	141/141 (100%)	1.58	47 (33%)	0	0	89, 108, 119, 127	0
12	2Q	141/141 (100%)	0.22	10 (7%)	16	11	96, 110, 122, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.35	1 (0%) 86 78	94, 104, 116, 125	0
13	2R	118/118 (100%)	0.63	13 (11%) 5 4	89, 103, 111, 118	0
14	1S	110/112 (98%)	-0.42	0 100 100	106, 116, 125, 131	0
14	2S	110/112 (98%)	-0.16	1 (0%) 84 76	106, 119, 127, 130	0
15	1T	131/146 (89%)	0.46	15 (11%) 4 4	95, 110, 123, 138	0
15	2T	131/146 (89%)	0.86	26 (19%) 1 0	92, 106, 121, 129	0
16	1U	116/118 (98%)	0.55	14 (12%) 4 4	86, 105, 119, 134	0
16	2U	116/118 (98%)	0.81	15 (12%) 3 3	94, 109, 121, 125	0
17	1V	101/101 (100%)	0.02	1 (0%) 82 73	88, 106, 120, 127	0
17	2V	101/101 (100%)	0.21	4 (3%) 38 28	93, 114, 127, 136	0
18	1W	112/113 (99%)	0.84	10 (8%) 9 7	88, 101, 120, 131	0
18	2W	112/113 (99%)	0.47	10 (8%) 9 7	87, 101, 113, 129	0
19	1X	95/96 (98%)	0.44	3 (3%) 47 35	87, 98, 116, 125	0
19	2X	95/96 (98%)	1.41	27 (28%) 0 0	98, 107, 127, 132	0
20	1Y	107/110 (97%)	0.15	2 (1%) 66 55	86, 108, 121, 126	0
20	2Y	107/110 (97%)	0.96	21 (19%) 1 1	91, 113, 126, 133	0
21	1Z	154/206 (74%)	-0.28	1 (0%) 89 83	109, 120, 132, 138	0
21	2Z	160/206 (77%)	-0.57	0 100 100	111, 123, 131, 135	0
22	10	83/85 (97%)	0.75	12 (14%) 2 2	94, 108, 116, 124	0
22	20	83/85 (97%)	1.13	18 (21%) 0 0	101, 114, 122, 125	0
23	11	97/98 (98%)	1.52	37 (38%) 0 0	87, 101, 121, 131	0
23	21	97/98 (98%)	1.94	47 (48%) 0 0	92, 110, 124, 130	0
24	12	70/72 (97%)	0.03	2 (2%) 51 39	87, 101, 111, 128	0
24	22	70/72 (97%)	0.49	2 (2%) 51 39	106, 116, 126, 129	0
25	13	59/60 (98%)	0.08	1 (1%) 70 59	86, 107, 121, 139	0
25	23	59/60 (98%)	0.65	2 (3%) 45 34	99, 108, 131, 143	0
26	14	69/71 (97%)	-0.75	0 100 100	121, 130, 141, 147	0
26	24	69/71 (97%)	-0.29	0 100 100	117, 128, 137, 144	0
27	15	59/60 (98%)	1.11	16 (27%) 0 0	89, 103, 117, 122	0
27	25	59/60 (98%)	0.20	6 (10%) 6 5	90, 103, 117, 125	0
28	16	53/54 (98%)	0.57	4 (7%) 14 10	95, 108, 120, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.50	4 (7%) 14 10	105, 114, 124, 134	0
29	17	48/49 (97%)	0.93	6 (12%) 3 4	82, 90, 107, 119	0
29	27	48/49 (97%)	2.11	24 (50%) 0 0	86, 99, 116, 124	0
30	18	64/65 (98%)	0.94	4 (6%) 20 13	89, 100, 111, 120	0
30	28	64/65 (98%)	2.17	35 (54%) 0 0	98, 106, 114, 120	0
31	19	37/37 (100%)	0.77	4 (10%) 5 4	99, 108, 113, 117	0
31	29	37/37 (100%)	1.09	7 (18%) 1 1	105, 116, 127, 130	0
32	1a	1488/1521 (97%)	0.03	95 (6%) 19 13	92, 123, 141, 160	0
32	2a	1491/1521 (98%)	-0.14	41 (2%) 54 42	97, 119, 138, 155	0
33	1b	231/256 (90%)	-0.20	1 (0%) 92 88	113, 127, 135, 144	0
33	2b	231/256 (90%)	-0.04	12 (5%) 27 20	105, 126, 137, 143	0
34	1c	206/239 (86%)	0.74	41 (19%) 1 0	113, 129, 137, 141	0
34	2c	206/239 (86%)	-0.23	9 (4%) 34 25	115, 124, 132, 141	0
35	1d	208/209 (99%)	0.78	33 (15%) 1 1	104, 121, 131, 137	0
35	2d	208/209 (99%)	0.52	18 (8%) 10 7	104, 117, 128, 136	0
36	1e	148/162 (91%)	0.99	38 (25%) 0 0	103, 119, 127, 133	0
36	2e	148/162 (91%)	0.88	31 (20%) 1 0	107, 117, 128, 136	0
37	1f	100/101 (99%)	-0.18	2 (2%) 65 53	101, 117, 126, 133	0
37	2f	100/101 (99%)	-0.12	3 (3%) 50 37	105, 118, 127, 132	0
38	1g	155/156 (99%)	0.23	16 (10%) 6 5	111, 125, 135, 141	0
38	2g	155/156 (99%)	-0.05	8 (5%) 27 20	112, 124, 135, 145	0
39	1h	137/138 (99%)	0.82	24 (17%) 1 1	108, 122, 129, 134	0
39	2h	137/138 (99%)	-0.06	5 (3%) 42 32	103, 118, 127, 135	0
40	1i	127/128 (99%)	0.38	22 (17%) 1 1	114, 128, 135, 139	0
40	2i	127/128 (99%)	0.81	26 (20%) 1 0	115, 127, 135, 144	0
41	1j	97/105 (92%)	0.87	23 (23%) 0 0	121, 131, 138, 143	0
41	2j	96/105 (91%)	0.72	23 (23%) 0 0	118, 129, 137, 142	0
42	1k	114/129 (88%)	0.72	14 (12%) 4 4	103, 117, 126, 130	0
42	2k	114/129 (88%)	1.33	37 (32%) 0 0	107, 120, 129, 137	0
43	1l	121/132 (91%)	1.45	37 (30%) 0 0	103, 117, 124, 136	0
43	2l	121/132 (91%)	0.43	13 (10%) 6 5	100, 112, 122, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	-0.11	11 (8%) 9 7	113, 125, 133, 139	0
44	2m	122/126 (96%)	0.47	21 (17%) 1 1	111, 125, 137, 147	0
45	1n	60/61 (98%)	2.21	35 (58%) 0 0	118, 128, 137, 144	0
45	2n	60/61 (98%)	0.54	11 (18%) 1 1	114, 124, 130, 134	0
46	1o	88/89 (98%)	0.23	6 (6%) 17 12	101, 116, 122, 124	0
46	2o	88/89 (98%)	0.42	5 (5%) 23 16	101, 119, 127, 132	0
47	1p	82/88 (93%)	1.81	38 (46%) 0 0	115, 124, 131, 137	0
47	2p	82/88 (93%)	0.23	4 (4%) 29 22	99, 111, 118, 123	0
48	1q	99/105 (94%)	0.43	12 (12%) 4 4	103, 118, 125, 131	0
48	2q	99/105 (94%)	0.24	4 (4%) 38 28	102, 113, 122, 126	0
49	1r	68/88 (77%)	0.22	2 (2%) 51 39	109, 116, 125, 130	0
49	2r	68/88 (77%)	0.58	9 (13%) 3 3	109, 119, 126, 131	0
50	1s	83/93 (89%)	-0.25	2 (2%) 59 47	117, 128, 136, 143	0
50	2s	83/93 (89%)	0.11	4 (4%) 30 22	116, 126, 135, 137	0
51	1t	96/106 (90%)	1.16	30 (31%) 0 0	111, 122, 128, 132	0
51	2t	96/106 (90%)	0.89	22 (22%) 0 0	101, 116, 126, 129	0
52	1u	23/27 (85%)	0.55	3 (13%) 3 3	119, 126, 129, 131	0
52	2u	23/27 (85%)	1.51	8 (34%) 0 0	123, 127, 131, 133	0
53	1v	6/24 (25%)	0.93	1 (16%) 1 1	110, 116, 131, 136	0
53	2v	6/24 (25%)	1.69	2 (33%) 0 0	113, 116, 131, 147	0
54	1w	2/3 (66%)	0.44	0 100 100	88, 88, 88, 89	0
54	2w	2/3 (66%)	0.79	0 100 100	103, 103, 103, 106	0
55	1x	72/77 (93%)	-0.41	0 100 100	90, 118, 130, 140	0
55	2x	72/77 (93%)	-0.26	1 (1%) 75 64	96, 123, 134, 144	0
All	All	20600/21450 (96%)	0.33	1842 (8%) 9 7	79, 114, 134, 160	0

The worst 5 of 1842 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	10.7
41	1j	61	GLU	10.0
44	1m	124	PRO	8.6
3	2D	276	LYS	8.5
38	1g	82	GLY	8.4

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	PSU	2x	55	20/21	0.84	0.23	114,125,136,143	0
55	4SU	2x	8	20/21	0.86	0.13	120,133,139,140	0
1	5MU	1A	1937	21/22	0.86	0.13	115,126,133,144	0
32	PSU	2a	516	20/21	0.87	0.14	117,122,126,128	0
32	PSU	1a	516	20/21	0.89	0.12	113,120,128,129	0
32	7MG	1a	527	24/25	0.89	0.25	101,115,123,126	0
32	2MG	2a	1207	24/25	0.90	0.14	114,124,129,137	0
32	4OC	1a	1402	22/23	0.90	0.31	104,112,120,123	0
32	4OC	2a	1402	22/23	0.90	0.26	104,109,115,116	0
32	7MG	2a	527	24/25	0.90	0.22	99,117,123,125	0
32	5MC	2a	967	21/22	0.90	0.25	102,116,124,125	0
55	4SU	1x	8	20/21	0.91	0.14	111,122,128,128	0
1	5MU	2A	1915	21/22	0.91	0.13	114,120,131,143	0
1	4OC	1A	1942	21/23	0.91	0.19	96,108,120,123	0
55	PSU	1x	55	20/21	0.92	0.11	109,117,129,133	0
54	PPU	2w	76	37/38	0.92	0.45	86,100,107,111	0
32	5MC	2a	1404	21/22	0.93	0.28	101,111,116,121	0
32	UR3	1a	1498	21/22	0.93	0.24	96,107,111,114	0
32	5MC	1a	967	21/22	0.93	0.33	104,115,127,130	0
1	PSU	2A	1911	20/21	0.93	0.14	96,105,117,118	0
1	PSU	1A	2617	20/21	0.93	0.31	81,90,100,100	0
55	5MU	2x	54	21/22	0.93	0.21	108,120,136,142	0
1	PSU	2A	1917	20/21	0.93	0.15	106,110,120,127	0
32	M2G	2a	966	25/26	0.93	0.29	107,119,123,126	0
1	PSU	2A	2605	20/21	0.94	0.24	81,91,98,102	0
32	5MC	1a	1407	21/22	0.94	0.17	100,110,116,121	0
32	5MC	2a	1407	21/22	0.94	0.24	90,106,116,118	0
1	4OC	2A	1920	21/23	0.94	0.19	94,114,119,120	0
32	UR3	2a	1498	21/22	0.94	0.40	95,105,114,115	0
32	MA6	1a	1518	24/25	0.94	0.21	103,109,113,116	0
1	5MU	2A	1939	21/22	0.94	0.23	89,98,104,114	0
32	2MG	1a	1207	24/25	0.94	0.15	114,124,132,136	0
1	5MC	1A	1964	21/22	0.94	0.18	82,93,104,111	0
55	5MC	1x	32	21/22	0.94	0.18	99,116,123,128	0
55	5MC	2x	32	21/22	0.94	0.27	110,118,124,126	0
55	5MU	1x	54	21/22	0.94	0.12	111,118,130,131	0
32	5MC	1a	1400	21/22	0.94	0.21	106,115,124,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
43	0TD	1l	92	10/11	0.94	0.46	110,119,124,142	0
32	M2G	1a	966	25/26	0.94	0.26	104,110,120,121	0
32	MA6	2a	1518	24/25	0.95	0.26	100,109,116,117	0
54	PPU	1w	76	37/38	0.95	0.40	84,91,103,108	0
32	5MC	2a	1400	21/22	0.95	0.20	101,114,128,132	0
1	2MA	2A	2503	23/24	0.95	0.31	81,92,103,114	0
1	2MU	1A	2564	21/23	0.95	0.37	85,95,105,109	0
1	2MU	2A	2552	21/23	0.95	0.20	84,90,101,104	0
1	PSU	1A	1939	20/21	0.95	0.13	95,110,117,117	0
1	PSU	1A	1933	20/21	0.95	0.14	90,105,108,109	0
43	0TD	2l	92	10/11	0.95	0.48	117,123,129,141	0
1	5MC	2A	1942	21/22	0.95	0.16	88,97,104,108	0
1	5MC	1A	1984	21/22	0.95	0.18	87,96,104,106	0
1	5MU	1A	1961	21/22	0.96	0.28	85,92,100,103	0
32	MA6	2a	1519	24/25	0.96	0.33	93,107,112,116	0
1	5MC	2A	1962	21/22	0.96	0.19	79,100,106,110	0
1	OMG	1A	2263	24/25	0.96	0.33	70,88,102,105	0
32	5MC	1a	1404	21/22	0.96	0.34	95,106,113,115	0
1	2MA	1A	2515	23/24	0.96	0.28	76,84,97,103	0
32	MA6	1a	1519	24/25	0.97	0.32	93,107,119,119	0
1	OMG	2A	2251	24/25	0.97	0.29	85,96,109,111	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors($Å^2$)	Q<0.9
56	MG	1a	1669	1/1	0.14	0.34	102,102,102,102	0
56	MG	1A	3124	1/1	0.30	0.42	75,75,75,75	0
56	MG	2A	3157	1/1	0.31	0.44	88,88,88,88	0
56	MG	1x	102	1/1	0.33	0.52	85,85,85,85	0
56	MG	1A	3115	1/1	0.33	0.51	89,89,89,89	0
56	MG	2a	3088	1/1	0.36	0.35	83,83,83,83	0
56	MG	2d	301	1/1	0.38	0.32	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3176	1/1	0.39	0.36	79,79,79,79	0
56	MG	2A	3105	1/1	0.40	0.35	74,74,74,74	0
56	MG	2A	3194	1/1	0.42	0.40	79,79,79,79	0
56	MG	2A	3125	1/1	0.44	0.32	82,82,82,82	0
56	MG	1A	3220	1/1	0.45	0.37	85,85,85,85	0
56	MG	2A	3301	1/1	0.47	0.29	77,77,77,77	0
56	MG	1A	3308	1/1	0.49	0.63	76,76,76,76	0
56	MG	1A	3086	1/1	0.50	0.31	90,90,90,90	0
56	MG	1A	3217	1/1	0.50	0.53	65,65,65,65	0
56	MG	2A	3311	1/1	0.51	0.17	79,79,79,79	0
56	MG	2O	201	1/1	0.51	1.98	73,73,73,73	0
56	MG	1A	3358	1/1	0.51	0.65	75,75,75,75	0
56	MG	2A	3015	1/1	0.51	0.47	76,76,76,76	0
56	MG	1A	3471	1/1	0.52	0.46	75,75,75,75	0
56	MG	1A	3299	1/1	0.52	0.50	83,83,83,83	0
56	MG	2a	3098	1/1	0.54	0.31	85,85,85,85	0
56	MG	1A	3341	1/1	0.54	0.45	77,77,77,77	0
56	MG	2A	3088	1/1	0.55	0.26	76,76,76,76	0
56	MG	2A	3187	1/1	0.55	0.81	74,74,74,74	0
56	MG	1A	3070	1/1	0.55	0.54	87,87,87,87	0
56	MG	2a	3069	1/1	0.56	0.52	104,104,104,104	0
56	MG	1a	1684	1/1	0.56	0.32	74,74,74,74	0
56	MG	2A	3052	1/1	0.56	0.24	86,86,86,86	0
56	MG	1A	3438	1/1	0.56	0.36	84,84,84,84	0
56	MG	2A	3141	1/1	0.57	0.35	81,81,81,81	0
56	MG	2A	3114	1/1	0.57	0.18	75,75,75,75	0
56	MG	2A	3010	1/1	0.57	0.28	87,87,87,87	0
56	MG	1A	3154	1/1	0.58	0.42	77,77,77,77	0
56	MG	1A	3226	1/1	0.58	0.28	79,79,79,79	0
56	MG	1A	3268	1/1	0.59	0.23	68,68,68,68	0
56	MG	2a	3051	1/1	0.59	0.27	79,79,79,79	0
56	MG	2A	3101	1/1	0.59	0.27	80,80,80,80	0
56	MG	1A	3054	1/1	0.60	1.02	75,75,75,75	0
56	MG	1A	3349	1/1	0.60	0.68	80,80,80,80	0
56	MG	2a	3067	1/1	0.60	0.12	96,96,96,96	0
56	MG	1A	3114	1/1	0.60	0.33	82,82,82,82	0
56	MG	2A	3205	1/1	0.60	0.26	81,81,81,81	0
56	MG	1a	1687	1/1	0.60	0.46	100,100,100,100	0
56	MG	1A	3264	1/1	0.60	0.60	83,83,83,83	0
56	MG	1a	1642	1/1	0.61	0.29	81,81,81,81	0
56	MG	1A	3258	1/1	0.61	0.72	98,98,98,98	0
56	MG	2a	3093	1/1	0.61	0.34	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3088	1/1	0.61	0.28	74,74,74,74	0
56	MG	1a	1603	1/1	0.61	0.94	94,94,94,94	0
56	MG	1a	1641	1/1	0.62	0.27	82,82,82,82	0
56	MG	10	103	1/1	0.62	0.52	69,69,69,69	0
56	MG	2a	3026	1/1	0.62	0.22	76,76,76,76	0
56	MG	2A	3290	1/1	0.62	0.33	72,72,72,72	0
56	MG	1A	3327	1/1	0.62	0.46	83,83,83,83	0
56	MG	2A	3061	1/1	0.63	0.43	69,69,69,69	0
56	MG	1A	3187	1/1	0.63	0.66	83,83,83,83	0
56	MG	1A	3240	1/1	0.63	0.36	66,66,66,66	0
56	MG	2A	3276	1/1	0.64	0.46	74,74,74,74	0
56	MG	1A	3239	1/1	0.64	1.06	90,90,90,90	0
56	MG	1A	3034	1/1	0.64	0.42	91,91,91,91	0
56	MG	1a	1689	1/1	0.64	0.36	78,78,78,78	0
56	MG	1l	201	1/1	0.64	1.89	80,80,80,80	0
56	MG	1A	3165	1/1	0.64	1.11	84,84,84,84	0
56	MG	2a	3040	1/1	0.64	0.21	78,78,78,78	0
56	MG	1A	3051	1/1	0.65	0.50	89,89,89,89	0
56	MG	2A	3327	1/1	0.65	0.40	70,70,70,70	0
56	MG	1A	3082	1/1	0.65	0.65	74,74,74,74	0
56	MG	1A	3221	1/1	0.65	0.56	86,86,86,86	0
56	MG	2A	3160	1/1	0.66	0.16	75,75,75,75	0
56	MG	1A	3312	1/1	0.66	0.48	65,65,65,65	0
56	MG	1a	1611	1/1	0.66	0.13	93,93,93,93	0
56	MG	1a	1671	1/1	0.66	0.37	99,99,99,99	0
56	MG	1a	1681	1/1	0.66	0.36	79,79,79,79	0
56	MG	2A	3266	1/1	0.66	0.45	69,69,69,69	0
56	MG	1A	3202	1/1	0.66	0.63	85,85,85,85	0
56	MG	2A	3345	1/1	0.67	0.29	62,62,62,62	0
56	MG	1a	1686	1/1	0.67	0.36	76,76,76,76	0
56	MG	2T	201	1/1	0.67	0.38	63,63,63,63	0
56	MG	2A	3306	1/1	0.67	0.21	80,80,80,80	0
56	MG	2A	3352	1/1	0.68	0.40	107,107,107,107	0
56	MG	1a	1675	1/1	0.68	0.17	110,110,110,110	0
56	MG	1A	3008	1/1	0.68	0.34	109,109,109,109	0
56	MG	27	101	1/1	0.68	0.41	69,69,69,69	0
56	MG	1A	3245	1/1	0.68	0.59	81,81,81,81	0
56	MG	1B	201	1/1	0.68	0.59	82,82,82,82	0
56	MG	2A	3026	1/1	0.68	0.20	76,76,76,76	0
56	MG	2A	3030	1/1	0.68	0.40	91,91,91,91	0
56	MG	1A	3232	1/1	0.68	0.45	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3056	1/1	0.68	0.27	79,79,79,79	0
56	MG	1A	3197	1/1	0.68	0.43	71,71,71,71	0
56	MG	2A	3335	1/1	0.68	0.26	68,68,68,68	0
56	MG	2A	3078	1/1	0.68	0.17	79,79,79,79	0
56	MG	2A	3254	1/1	0.69	0.30	82,82,82,82	0
56	MG	2A	3337	1/1	0.69	0.76	87,87,87,87	0
56	MG	2a	3003	1/1	0.69	0.26	90,90,90,90	0
56	MG	1a	1629	1/1	0.69	0.15	94,94,94,94	0
56	MG	1A	3252	1/1	0.69	0.53	80,80,80,80	0
56	MG	1A	3322	1/1	0.69	0.77	94,94,94,94	0
56	MG	2A	3113	1/1	0.70	0.52	70,70,70,70	0
56	MG	1Q	201	1/1	0.70	0.84	75,75,75,75	0
56	MG	1a	1678	1/1	0.70	0.35	89,89,89,89	0
56	MG	2A	3100	1/1	0.70	0.34	74,74,74,74	0
56	MG	2A	3332	1/1	0.70	0.47	80,80,80,80	0
56	MG	2A	3253	1/1	0.70	0.45	62,62,62,62	0
56	MG	1A	3255	1/1	0.70	0.62	77,77,77,77	0
56	MG	1A	3321	1/1	0.70	0.36	67,67,67,67	0
56	MG	2A	3161	1/1	0.70	0.27	72,72,72,72	0
56	MG	2A	3175	1/1	0.70	0.25	107,107,107,107	0
56	MG	2A	3297	1/1	0.70	0.37	77,77,77,77	0
56	MG	1A	3180	1/1	0.71	0.36	61,61,61,61	0
56	MG	1A	3224	1/1	0.71	0.47	76,76,76,76	0
56	MG	1A	3083	1/1	0.71	0.38	83,83,83,83	0
56	MG	2A	3102	1/1	0.71	0.33	73,73,73,73	0
56	MG	1A	3173	1/1	0.71	0.50	87,87,87,87	0
56	MG	2a	3061	1/1	0.71	0.39	72,72,72,72	0
56	MG	2A	3014	1/1	0.71	0.78	90,90,90,90	0
56	MG	1B	202	1/1	0.71	0.52	80,80,80,80	0
56	MG	2a	3076	1/1	0.71	0.26	82,82,82,82	0
56	MG	2A	3122	1/1	0.71	0.63	85,85,85,85	0
56	MG	2B	201	1/1	0.71	0.47	80,80,80,80	0
56	MG	2A	3189	1/1	0.71	0.40	75,75,75,75	0
56	MG	2A	3305	1/1	0.71	0.19	83,83,83,83	0
56	MG	20	101	1/1	0.72	0.64	75,75,75,75	0
56	MG	1a	1640	1/1	0.72	0.18	91,91,91,91	0
56	MG	1A	3177	1/1	0.72	0.50	62,62,62,62	0
56	MG	1A	3172	1/1	0.72	0.65	96,96,96,96	0
56	MG	2A	3239	1/1	0.72	0.23	68,68,68,68	0
56	MG	2a	3046	1/1	0.72	0.30	99,99,99,99	0
56	MG	2A	3248	1/1	0.72	0.31	78,78,78,78	0
56	MG	1a	1649	1/1	0.72	0.11	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3181	1/1	0.72	0.36	73,73,73,73	0
56	MG	2A	3257	1/1	0.72	0.38	84,84,84,84	0
56	MG	1A	3480	1/1	0.72	0.37	69,69,69,69	0
56	MG	1A	3494	1/1	0.72	0.14	85,85,85,85	0
56	MG	2A	3183	1/1	0.72	0.51	81,81,81,81	0
56	MG	2A	3293	1/1	0.72	0.13	77,77,77,77	0
56	MG	1A	3142	1/1	0.72	0.46	71,71,71,71	0
56	MG	1A	3237	1/1	0.73	0.50	79,79,79,79	0
56	MG	1A	3078	1/1	0.73	0.81	80,80,80,80	0
56	MG	2A	3057	1/1	0.73	0.28	91,91,91,91	0
56	MG	2A	3209	1/1	0.73	0.43	77,77,77,77	0
56	MG	1A	3040	1/1	0.73	0.40	79,79,79,79	0
56	MG	2A	3155	1/1	0.73	0.22	92,92,92,92	0
56	MG	1a	1630	1/1	0.73	0.17	80,80,80,80	0
56	MG	2A	3012	1/1	0.73	0.35	66,66,66,66	0
56	MG	1A	3140	1/1	0.73	0.20	73,73,73,73	0
56	MG	2A	3166	1/1	0.73	0.27	94,94,94,94	0
56	MG	2a	3080	1/1	0.73	0.26	74,74,74,74	0
56	MG	1E	304	1/1	0.73	0.54	78,78,78,78	0
56	MG	2A	3024	1/1	0.73	0.50	73,73,73,73	0
56	MG	1A	3440	1/1	0.73	0.47	70,70,70,70	0
56	MG	1A	3192	1/1	0.73	0.43	61,61,61,61	0
56	MG	2A	3147	1/1	0.74	0.26	75,75,75,75	0
56	MG	1A	3437	1/1	0.74	0.57	99,99,99,99	0
56	MG	2A	3011	1/1	0.74	0.48	82,82,82,82	0
56	MG	1A	3075	1/1	0.74	0.45	72,72,72,72	0
56	MG	2A	3315	1/1	0.74	0.33	68,68,68,68	0
56	MG	2E	303	1/1	0.74	0.28	81,81,81,81	0
56	MG	1A	3113	1/1	0.74	0.34	77,77,77,77	0
56	MG	2A	3042	1/1	0.74	0.16	75,75,75,75	0
56	MG	2E	302	1/1	0.75	0.47	80,80,80,80	0
56	MG	2A	3326	1/1	0.75	0.60	74,74,74,74	0
56	MG	1A	3148	1/1	0.75	0.80	79,79,79,79	0
56	MG	2a	3068	1/1	0.75	0.54	81,81,81,81	0
56	MG	1d	301	1/1	0.75	0.18	91,91,91,91	0
56	MG	1A	3104	1/1	0.75	1.08	69,69,69,69	0
56	MG	1A	3159	1/1	0.75	0.50	81,81,81,81	0
56	MG	2A	3139	1/1	0.75	0.34	64,64,64,64	0
56	MG	2A	3002	1/1	0.75	0.56	70,70,70,70	0
56	MG	2A	3374	1/1	0.75	0.24	62,62,62,62	0
56	MG	1A	3254	1/1	0.75	0.66	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	2A	3006	1/1	0.76	0.24	76,76,76,76	0
56	MG	2a	3011	1/1	0.76	0.26	94,94,94,94	0
56	MG	2a	3014	1/1	0.76	0.27	81,81,81,81	0
56	MG	1a	1609	1/1	0.76	0.17	103,103,103,103	0
56	MG	2a	3035	1/1	0.76	0.32	73,73,73,73	0
56	MG	1A	3144	1/1	0.76	0.43	87,87,87,87	0
56	MG	1A	3146	1/1	0.76	1.17	64,64,64,64	0
56	MG	1A	3360	1/1	0.76	0.52	82,82,82,82	0
56	MG	1a	1631	1/1	0.76	0.20	97,97,97,97	0
56	MG	2A	3285	1/1	0.76	0.44	73,73,73,73	0
56	MG	1A	3118	1/1	0.76	0.40	75,75,75,75	0
56	MG	1A	3291	1/1	0.76	0.28	77,77,77,77	0
56	MG	1A	3293	1/1	0.76	0.54	84,84,84,84	0
56	MG	1a	1645	1/1	0.76	0.44	90,90,90,90	0
56	MG	2A	3049	1/1	0.76	0.47	73,73,73,73	0
56	MG	1A	3071	1/1	0.76	0.35	75,75,75,75	0
56	MG	1a	1651	1/1	0.76	0.20	71,71,71,71	0
56	MG	1A	3479	1/1	0.76	0.53	72,72,72,72	0
56	MG	1A	3402	1/1	0.77	0.45	62,62,62,62	0
56	MG	2A	3059	1/1	0.77	0.41	82,82,82,82	0
56	MG	1A	3432	1/1	0.77	0.27	68,68,68,68	0
56	MG	2A	3027	1/1	0.77	0.56	83,83,83,83	0
56	MG	1A	3194	1/1	0.77	0.30	92,92,92,92	0
56	MG	1A	3250	1/1	0.77	0.51	71,71,71,71	0
56	MG	1A	3251	1/1	0.77	0.39	82,82,82,82	0
56	MG	2a	3086	1/1	0.77	0.36	74,74,74,74	0
56	MG	2A	3377	1/1	0.77	0.25	92,92,92,92	0
56	MG	2A	3263	1/1	0.77	0.48	70,70,70,70	0
56	MG	1a	1644	1/1	0.77	0.20	76,76,76,76	0
56	MG	1A	3364	1/1	0.77	0.35	81,81,81,81	0
57	ZN	2Y	202	1/1	0.77	0.09	176,176,176,176	0
56	MG	2A	3300	1/1	0.78	0.26	74,74,74,74	0
56	MG	2A	3110	1/1	0.78	0.32	88,88,88,88	0
56	MG	1A	3007	1/1	0.78	0.27	74,74,74,74	0
56	MG	1A	3257	1/1	0.78	0.82	82,82,82,82	0
56	MG	2A	3119	1/1	0.78	0.39	63,63,63,63	0
56	MG	2a	3023	1/1	0.78	0.38	72,72,72,72	0
56	MG	1A	3072	1/1	0.78	0.29	79,79,79,79	0
56	MG	1A	3134	1/1	0.78	0.38	80,80,80,80	0
56	MG	2A	3127	1/1	0.78	0.27	93,93,93,93	0
56	MG	2A	3129	1/1	0.78	0.26	61,61,61,61	0
56	MG	2A	3016	1/1	0.78	0.36	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3056	1/1	0.78	0.15	85,85,85,85	0
56	MG	1A	3288	1/1	0.78	0.30	78,78,78,78	0
56	MG	2A	3349	1/1	0.78	0.65	76,76,76,76	0
56	MG	2A	3258	1/1	0.78	0.46	80,80,80,80	0
56	MG	2A	3085	1/1	0.78	0.27	71,71,71,71	0
56	MG	1A	3253	1/1	0.78	0.40	79,79,79,79	0
56	MG	2A	3094	1/1	0.78	0.23	83,83,83,83	0
56	MG	2B	202	1/1	0.78	0.62	87,87,87,87	0
56	MG	2a	3090	1/1	0.78	0.24	73,73,73,73	0
56	MG	1A	3342	1/1	0.78	0.37	62,62,62,62	0
56	MG	2A	3039	1/1	0.78	0.59	93,93,93,93	0
56	MG	2A	3041	1/1	0.78	0.35	91,91,91,91	0
56	MG	1A	3039	1/1	0.78	0.48	71,71,71,71	0
56	MG	2A	3120	1/1	0.79	0.23	78,78,78,78	0
56	MG	1A	3067	1/1	0.79	0.50	64,64,64,64	0
56	MG	1A	3420	1/1	0.79	0.58	70,70,70,70	0
56	MG	2A	3208	1/1	0.79	0.13	82,82,82,82	0
56	MG	1a	1636	1/1	0.79	0.29	93,93,93,93	0
56	MG	2A	3323	1/1	0.79	0.47	64,64,64,64	0
56	MG	2A	3229	1/1	0.79	0.36	72,72,72,72	0
56	MG	2A	3071	1/1	0.79	0.33	61,61,61,61	0
56	MG	1A	3340	1/1	0.79	0.43	61,61,61,61	0
56	MG	1A	3093	1/1	0.79	0.36	76,76,76,76	0
56	MG	1A	3068	1/1	0.79	0.44	75,75,75,75	0
56	MG	1A	3262	1/1	0.79	0.42	82,82,82,82	0
56	MG	2a	3065	1/1	0.79	0.38	75,75,75,75	0
56	MG	1A	3445	1/1	0.79	0.70	78,78,78,78	0
56	MG	2A	3031	1/1	0.79	0.13	89,89,89,89	0
56	MG	1A	3026	1/1	0.79	0.80	75,75,75,75	0
56	MG	2A	3162	1/1	0.79	0.46	90,90,90,90	0
56	MG	2A	3277	1/1	0.79	0.37	70,70,70,70	0
56	MG	1A	3001	1/1	0.79	0.18	80,80,80,80	0
56	MG	1a	1665	1/1	0.79	0.35	74,74,74,74	0
56	MG	1a	1667	1/1	0.79	0.15	78,78,78,78	0
56	MG	2E	305	1/1	0.79	0.24	67,67,67,67	0
56	MG	1a	1614	1/1	0.79	0.26	76,76,76,76	0
56	MG	1A	3047	1/1	0.79	0.36	67,67,67,67	0
56	MG	2T	202	1/1	0.79	0.75	82,82,82,82	0
56	MG	20	102	1/1	0.80	0.23	75,75,75,75	0
56	MG	2A	3097	1/1	0.80	0.22	93,93,93,93	0
56	MG	1A	3139	1/1	0.80	0.29	70,70,70,70	0
56	MG	1A	3418	1/1	0.80	0.34	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3099	1/1	0.80	0.69	98,98,98,98	0
56	MG	2A	3159	1/1	0.80	0.28	83,83,83,83	0
56	MG	2A	3334	1/1	0.80	0.28	77,77,77,77	0
56	MG	1A	3014	1/1	0.80	0.49	86,86,86,86	0
56	MG	1A	3171	1/1	0.80	0.30	76,76,76,76	0
56	MG	1V	203	1/1	0.80	0.81	81,81,81,81	0
56	MG	1A	3121	1/1	0.80	0.26	79,79,79,79	0
56	MG	1A	3062	1/1	0.80	0.23	89,89,89,89	0
56	MG	2A	3369	1/1	0.80	0.35	70,70,70,70	0
56	MG	1A	3065	1/1	0.80	0.84	88,88,88,88	0
56	MG	2A	3180	1/1	0.80	0.51	76,76,76,76	0
56	MG	1A	3270	1/1	0.80	0.22	62,62,62,62	0
56	MG	2A	3291	1/1	0.80	0.35	78,78,78,78	0
56	MG	2E	301	1/1	0.80	0.26	87,87,87,87	0
56	MG	2A	3079	1/1	0.80	0.37	79,79,79,79	0
56	MG	1a	1655	1/1	0.80	0.21	84,84,84,84	0
56	MG	1A	3377	1/1	0.80	0.52	77,77,77,77	0
56	MG	2A	3131	1/1	0.80	0.24	63,63,63,63	0
56	MG	2A	3137	1/1	0.80	0.26	62,62,62,62	0
56	MG	1A	3379	1/1	0.80	0.39	80,80,80,80	0
56	MG	2A	3220	1/1	0.80	0.40	64,64,64,64	0
56	MG	2R	201	1/1	0.81	0.67	64,64,64,64	0
56	MG	2A	3118	1/1	0.81	0.31	71,71,71,71	0
56	MG	1A	3087	1/1	0.81	0.31	82,82,82,82	0
56	MG	1W	201	1/1	0.81	0.81	65,65,65,65	0
56	MG	2A	3058	1/1	0.81	0.32	82,82,82,82	0
56	MG	1A	3236	1/1	0.81	0.34	102,102,102,102	0
56	MG	1a	1664	1/1	0.81	0.90	67,67,67,67	0
56	MG	2a	3004	1/1	0.81	0.32	91,91,91,91	0
56	MG	17	101	1/1	0.81	0.47	66,66,66,66	0
56	MG	2A	3331	1/1	0.81	0.46	73,73,73,73	0
56	MG	1A	3156	1/1	0.81	0.35	78,78,78,78	0
56	MG	1A	3373	1/1	0.81	0.49	61,61,61,61	0
56	MG	2A	3081	1/1	0.81	0.56	76,76,76,76	0
56	MG	1A	3020	1/1	0.81	0.30	84,84,84,84	0
56	MG	1A	3162	1/1	0.81	0.43	65,65,65,65	0
56	MG	2A	3091	1/1	0.81	0.17	75,75,75,75	0
56	MG	1A	3491	1/1	0.81	0.20	91,91,91,91	0
56	MG	2A	3355	1/1	0.81	0.13	86,86,86,86	0
56	MG	1A	3211	1/1	0.81	0.57	93,93,93,93	0
56	MG	1A	3497	1/1	0.81	0.33	65,65,65,65	0
56	MG	2A	3375	1/1	0.81	0.30	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	1A	3249	1/1	0.81	0.54	90,90,90,90	0
56	MG	1A	3228	1/1	0.81	0.34	77,77,77,77	0
56	MG	1B	204	1/1	0.81	0.51	66,66,66,66	0
56	MG	2a	3087	1/1	0.81	0.26	61,61,61,61	0
56	MG	2A	3109	1/1	0.81	0.35	63,63,63,63	0
56	MG	1A	3351	1/1	0.81	0.36	64,64,64,64	0
56	MG	2A	3112	1/1	0.81	0.49	68,68,68,68	0
56	MG	1E	306	1/1	0.81	0.27	72,72,72,72	0
56	MG	1A	3357	1/1	0.81	1.32	68,68,68,68	0
56	MG	2Q	202	1/1	0.81	0.39	69,69,69,69	0
56	MG	28	102	1/1	0.82	0.36	61,61,61,61	0
56	MG	2A	3142	1/1	0.82	0.29	73,73,73,73	0
56	MG	1B	209	1/1	0.82	0.60	122,122,122,122	0
56	MG	2a	3009	1/1	0.82	0.19	79,79,79,79	0
56	MG	2A	3152	1/1	0.82	0.31	81,81,81,81	0
56	MG	1A	3409	1/1	0.82	0.20	82,82,82,82	0
56	MG	2A	3048	1/1	0.82	0.35	82,82,82,82	0
56	MG	1A	3025	1/1	0.82	0.41	77,77,77,77	0
56	MG	2A	3050	1/1	0.82	0.16	76,76,76,76	0
56	MG	2A	3008	1/1	0.82	1.02	69,69,69,69	0
56	MG	1F	301	1/1	0.82	0.22	72,72,72,72	0
56	MG	1a	1635	1/1	0.82	0.26	84,84,84,84	0
56	MG	1a	1674	1/1	0.82	0.24	92,92,92,92	0
56	MG	1A	3157	1/1	0.82	0.31	79,79,79,79	0
56	MG	1A	3028	1/1	0.82	0.42	107,107,107,107	0
56	MG	2A	3065	1/1	0.82	0.43	68,68,68,68	0
56	MG	1A	3235	1/1	0.82	0.59	77,77,77,77	0
56	MG	1A	3316	1/1	0.82	0.41	63,63,63,63	0
56	MG	1A	3498	1/1	0.82	0.79	74,74,74,74	0
56	MG	2a	3084	1/1	0.82	0.31	72,72,72,72	0
56	MG	2A	3310	1/1	0.82	0.49	67,67,67,67	0
56	MG	1A	3161	1/1	0.82	0.29	65,65,65,65	0
56	MG	2A	3029	1/1	0.82	0.35	70,70,70,70	0
56	MG	2A	3086	1/1	0.82	0.16	77,77,77,77	0
56	MG	1a	1607	1/1	0.82	0.13	100,100,100,100	0
56	MG	2A	3138	1/1	0.82	0.29	76,76,76,76	0
56	MG	1A	3443	1/1	0.82	0.81	91,91,91,91	0
56	MG	1A	3184	1/1	0.82	0.51	69,69,69,69	0
56	MG	2A	3178	1/1	0.83	1.27	75,75,75,75	0
56	MG	1A	3213	1/1	0.83	0.29	72,72,72,72	0
56	MG	2A	3098	1/1	0.83	0.09	97,97,97,97	0
56	MG	1A	3269	1/1	0.83	0.57	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	2A	3134	1/1	0.83	0.31	82,82,82,82	0
56	MG	2a	3039	1/1	0.83	0.21	79,79,79,79	0
56	MG	1A	3256	1/1	0.83	0.51	78,78,78,78	0
56	MG	2A	3197	1/1	0.83	0.47	61,61,61,61	0
56	MG	1A	3355	1/1	0.83	0.23	71,71,71,71	0
56	MG	1A	3473	1/1	0.83	0.43	61,61,61,61	0
56	MG	1A	3027	1/1	0.83	0.42	78,78,78,78	0
56	MG	1E	305	1/1	0.83	0.32	72,72,72,72	0
56	MG	1A	3105	1/1	0.83	0.36	108,108,108,108	0
56	MG	1a	1615	1/1	0.83	0.23	83,83,83,83	0
56	MG	1A	3178	1/1	0.83	0.53	65,65,65,65	0
56	MG	2A	3115	1/1	0.83	0.23	84,84,84,84	0
56	MG	2A	3117	1/1	0.83	0.27	74,74,74,74	0
56	MG	1A	3297	1/1	0.83	0.66	79,79,79,79	0
56	MG	1S	201	1/1	0.83	0.23	78,78,78,78	0
56	MG	1V	201	1/1	0.83	0.42	80,80,80,80	0
56	MG	1V	202	1/1	0.83	1.03	68,68,68,68	0
56	MG	2a	3092	1/1	0.83	0.29	82,82,82,82	0
56	MG	2A	3124	1/1	0.83	0.14	94,94,94,94	0
56	MG	1A	3100	1/1	0.83	0.25	86,86,86,86	0
56	MG	2a	3008	1/1	0.83	0.42	102,102,102,102	0
56	MG	2A	3280	1/1	0.83	0.34	61,61,61,61	0
57	ZN	24	501	1/1	0.83	0.05	182,182,182,182	0
56	MG	1A	3101	1/1	0.84	0.35	74,74,74,74	0
56	MG	2a	3024	1/1	0.84	0.24	83,83,83,83	0
56	MG	2A	3214	1/1	0.84	0.25	82,82,82,82	0
56	MG	1A	3203	1/1	0.84	0.40	72,72,72,72	0
56	MG	2a	3037	1/1	0.84	0.19	84,84,84,84	0
56	MG	1A	3320	1/1	0.84	0.51	74,74,74,74	0
56	MG	1A	3279	1/1	0.84	0.17	65,65,65,65	0
56	MG	1A	3043	1/1	0.84	0.21	76,76,76,76	0
56	MG	2a	3047	1/1	0.84	0.25	77,77,77,77	0
56	MG	1a	1620	1/1	0.84	0.18	81,81,81,81	0
56	MG	1A	3260	1/1	0.84	0.28	81,81,81,81	0
56	MG	1A	3074	1/1	0.84	0.48	77,77,77,77	0
56	MG	1A	3263	1/1	0.84	0.52	105,105,105,105	0
56	MG	1A	3045	1/1	0.84	0.42	74,74,74,74	0
56	MG	2R	202	1/1	0.84	0.40	67,67,67,67	0
56	MG	2a	3073	1/1	0.84	0.27	76,76,76,76	0
56	MG	2A	3053	1/1	0.84	0.29	74,74,74,74	0
56	MG	2A	3271	1/1	0.84	0.20	63,63,63,63	0
56	MG	1A	3462	1/1	0.84	0.56	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	208	1/1	0.84	0.55	81,81,81,81	0
56	MG	1A	3057	1/1	0.84	0.49	73,73,73,73	0
56	MG	2A	3347	1/1	0.84	0.42	61,61,61,61	0
56	MG	2a	3089	1/1	0.84	0.27	79,79,79,79	0
56	MG	17	102	1/1	0.84	0.74	83,83,83,83	0
56	MG	2A	3350	1/1	0.84	0.15	93,93,93,93	0
56	MG	1a	1643	1/1	0.84	0.21	71,71,71,71	0
56	MG	2a	3096	1/1	0.84	0.32	70,70,70,70	0
56	MG	2A	3062	1/1	0.84	0.36	72,72,72,72	0
56	MG	2a	3102	1/1	0.84	0.09	127,127,127,127	0
56	MG	2a	3010	1/1	0.84	0.30	70,70,70,70	0
56	MG	2l	201	1/1	0.84	1.15	80,80,80,80	0
56	MG	1B	212	1/1	0.84	0.43	83,83,83,83	0
56	MG	2A	3066	1/1	0.84	0.32	85,85,85,85	0
56	MG	2A	3145	1/1	0.85	0.48	79,79,79,79	0
56	MG	1A	3010	1/1	0.85	0.39	72,72,72,72	0
56	MG	2A	3151	1/1	0.85	0.15	109,109,109,109	0
56	MG	2A	3348	1/1	0.85	0.46	77,77,77,77	0
56	MG	2a	3032	1/1	0.85	0.14	75,75,75,75	0
56	MG	1A	3189	1/1	0.85	0.32	82,82,82,82	0
56	MG	2A	3259	1/1	0.85	0.38	72,72,72,72	0
56	MG	2A	3262	1/1	0.85	0.26	80,80,80,80	0
56	MG	2A	3107	1/1	0.85	0.24	81,81,81,81	0
56	MG	1A	3123	1/1	0.85	0.31	81,81,81,81	0
56	MG	2A	3268	1/1	0.85	0.53	68,68,68,68	0
56	MG	1A	3424	1/1	0.85	0.27	61,61,61,61	0
56	MG	1A	3428	1/1	0.85	0.61	61,61,61,61	0
56	MG	1A	3193	1/1	0.85	0.29	71,71,71,71	0
56	MG	1a	1648	1/1	0.85	0.40	100,100,100,100	0
56	MG	1A	3044	1/1	0.85	0.40	83,83,83,83	0
56	MG	18	101	1/1	0.85	0.30	65,65,65,65	0
56	MG	1B	203	1/1	0.85	0.60	106,106,106,106	0
56	MG	1A	3247	1/1	0.85	0.32	69,69,69,69	0
56	MG	2a	3077	1/1	0.85	0.30	95,95,95,95	0
56	MG	1A	3439	1/1	0.85	0.36	67,67,67,67	0
56	MG	1A	3222	1/1	0.85	0.35	71,71,71,71	0
56	MG	1B	211	1/1	0.85	0.36	72,72,72,72	0
56	MG	1A	3170	1/1	0.85	0.29	79,79,79,79	0
56	MG	2A	3126	1/1	0.85	0.22	76,76,76,76	0
56	MG	1a	1672	1/1	0.85	0.17	104,104,104,104	0
56	MG	1A	3198	1/1	0.85	0.34	64,64,64,64	0
56	MG	1a	1623	1/1	0.85	0.17	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	1A	3126	1/1	0.85	0.30	80,80,80,80	0
56	MG	1A	3470	1/1	0.85	1.17	68,68,68,68	0
56	MG	2a	3097	1/1	0.85	0.54	74,74,74,74	0
56	MG	1A	3009	1/1	0.85	0.41	84,84,84,84	0
56	MG	1A	3275	1/1	0.85	0.42	63,63,63,63	0
56	MG	2A	3237	1/1	0.85	0.21	82,82,82,82	0
56	MG	1A	3205	1/1	0.85	0.49	74,74,74,74	0
56	MG	1a	1688	1/1	0.85	0.48	80,80,80,80	0
56	MG	2A	3336	1/1	0.85	0.53	91,91,91,91	0
56	MG	1A	3234	1/1	0.86	0.17	85,85,85,85	0
56	MG	1A	3378	1/1	0.86	0.63	77,77,77,77	0
56	MG	1A	3449	1/1	0.86	0.96	83,83,83,83	0
56	MG	1E	302	1/1	0.86	0.35	76,76,76,76	0
56	MG	2a	3033	1/1	0.86	0.21	72,72,72,72	0
56	MG	2A	3359	1/1	0.86	0.28	74,74,74,74	0
56	MG	1A	3167	1/1	0.86	0.26	80,80,80,80	0
56	MG	2A	3023	1/1	0.86	0.29	73,73,73,73	0
56	MG	1A	3463	1/1	0.86	0.49	72,72,72,72	0
56	MG	2A	3080	1/1	0.86	0.52	69,69,69,69	0
56	MG	2A	3382	1/1	0.86	0.17	124,124,124,124	0
56	MG	1A	3149	1/1	0.86	0.34	72,72,72,72	0
56	MG	2a	3056	1/1	0.86	0.55	82,82,82,82	0
56	MG	1a	1676	1/1	0.86	0.12	77,77,77,77	0
56	MG	2B	207	1/1	0.86	0.53	84,84,84,84	0
56	MG	1A	3150	1/1	0.86	0.65	90,90,90,90	0
56	MG	2A	3128	1/1	0.86	0.43	61,61,61,61	0
56	MG	1A	3410	1/1	0.86	0.32	83,83,83,83	0
56	MG	1A	3478	1/1	0.86	0.21	76,76,76,76	0
56	MG	1A	3415	1/1	0.86	0.23	80,80,80,80	0
56	MG	1A	3011	1/1	0.86	0.34	72,72,72,72	0
56	MG	2A	3210	1/1	0.86	0.23	68,68,68,68	0
56	MG	1A	3081	1/1	0.86	0.83	65,65,65,65	0
56	MG	1A	3098	1/1	0.86	0.24	81,81,81,81	0
56	MG	1A	3117	1/1	0.86	0.36	63,63,63,63	0
56	MG	2Y	201	1/1	0.86	0.35	71,71,71,71	0
56	MG	1A	3145	1/1	0.86	0.22	79,79,79,79	0
56	MG	2A	3143	1/1	0.86	0.38	69,69,69,69	0
56	MG	1A	3434	1/1	0.86	0.24	72,72,72,72	0
56	MG	2A	3251	1/1	0.86	0.30	75,75,75,75	0
56	MG	2a	3094	1/1	0.86	0.26	66,66,66,66	0
56	MG	2A	3001	1/1	0.86	0.32	80,80,80,80	0
56	MG	2A	3108	1/1	0.86	0.34	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3256	1/1	0.86	0.43	66,66,66,66	0
56	MG	1A	3227	1/1	0.86	0.26	71,71,71,71	0
56	MG	1A	3266	1/1	0.86	0.26	77,77,77,77	0
56	MG	1A	3129	1/1	0.86	0.46	77,77,77,77	0
57	ZN	1Y	501	1/1	0.86	0.15	156,156,156,156	0
56	MG	1A	3073	1/1	0.86	0.28	86,86,86,86	0
56	MG	2a	3021	1/1	0.86	0.24	82,82,82,82	0
56	MG	2a	3034	1/1	0.87	0.20	78,78,78,78	0
56	MG	1A	3356	1/1	0.87	0.24	61,61,61,61	0
56	MG	1a	1650	1/1	0.87	0.22	82,82,82,82	0
56	MG	2B	203	1/1	0.87	0.41	75,75,75,75	0
56	MG	2B	205	1/1	0.87	0.24	89,89,89,89	0
56	MG	1A	3208	1/1	0.87	0.46	62,62,62,62	0
56	MG	1A	3243	1/1	0.87	0.39	71,71,71,71	0
56	MG	2A	3309	1/1	0.87	0.29	61,61,61,61	0
56	MG	2A	3055	1/1	0.87	0.31	82,82,82,82	0
56	MG	1A	3425	1/1	0.87	0.58	67,67,67,67	0
56	MG	1A	3128	1/1	0.87	0.54	77,77,77,77	0
56	MG	1a	1617	1/1	0.87	0.14	91,91,91,91	0
56	MG	2A	3154	1/1	0.87	0.22	68,68,68,68	0
56	MG	1a	1668	1/1	0.87	0.49	78,78,78,78	0
56	MG	1A	3168	1/1	0.87	0.69	71,71,71,71	0
56	MG	1a	1670	1/1	0.87	0.17	97,97,97,97	0
56	MG	1A	3214	1/1	0.87	1.15	69,69,69,69	0
56	MG	1A	3290	1/1	0.87	0.29	80,80,80,80	0
56	MG	1A	3037	1/1	0.87	0.80	68,68,68,68	0
56	MG	1A	3292	1/1	0.87	0.97	75,75,75,75	0
56	MG	1A	3397	1/1	0.87	0.25	84,84,84,84	0
56	MG	1A	3400	1/1	0.87	0.32	87,87,87,87	0
56	MG	2A	3177	1/1	0.87	0.26	63,63,63,63	0
56	MG	1A	3160	1/1	0.87	0.70	67,67,67,67	0
56	MG	15	101	1/1	0.87	0.20	70,70,70,70	0
56	MG	1A	3038	1/1	0.87	0.45	61,61,61,61	0
56	MG	2A	3032	1/1	0.87	0.29	85,85,85,85	0
56	MG	1A	3136	1/1	0.87	0.23	76,76,76,76	0
56	MG	2A	3366	1/1	0.87	0.34	63,63,63,63	0
56	MG	2A	3287	1/1	0.87	0.29	66,66,66,66	0
56	MG	1A	3059	1/1	0.87	0.32	92,92,92,92	0
56	MG	1A	3469	1/1	0.87	0.58	88,88,88,88	0
56	MG	2a	3029	1/1	0.87	0.15	104,104,104,104	0
56	MG	2r	101	1/1	0.87	0.23	77,77,77,77	0
56	MG	2a	3030	1/1	0.87	0.51	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	2A	3044	1/1	0.87	0.47	81,81,81,81	0
56	MG	1a	1604	1/1	0.87	0.18	107,107,107,107	0
56	MG	1A	3206	1/1	0.88	0.53	76,76,76,76	0
56	MG	2a	3015	1/1	0.88	0.15	80,80,80,80	0
56	MG	1a	1634	1/1	0.88	0.11	102,102,102,102	0
56	MG	2a	3022	1/1	0.88	0.40	81,81,81,81	0
56	MG	1A	3063	1/1	0.88	0.56	77,77,77,77	0
56	MG	1A	3436	1/1	0.88	0.52	61,61,61,61	0
56	MG	1A	3210	1/1	0.88	0.63	81,81,81,81	0
56	MG	2A	3144	1/1	0.88	0.32	83,83,83,83	0
56	MG	2A	3255	1/1	0.88	0.32	71,71,71,71	0
56	MG	2A	3037	1/1	0.88	0.33	90,90,90,90	0
56	MG	1A	3069	1/1	0.88	0.78	81,81,81,81	0
56	MG	1A	3383	1/1	0.88	0.24	73,73,73,73	0
56	MG	2A	3363	1/1	0.88	0.37	65,65,65,65	0
56	MG	1A	3345	1/1	0.88	0.29	72,72,72,72	0
56	MG	1A	3298	1/1	0.88	0.39	71,71,71,71	0
56	MG	2A	3103	1/1	0.88	0.49	78,78,78,78	0
56	MG	2A	3047	1/1	0.88	0.40	81,81,81,81	0
56	MG	2A	3376	1/1	0.88	0.35	72,72,72,72	0
56	MG	1a	1690	1/1	0.88	0.18	84,84,84,84	0
56	MG	2A	3380	1/1	0.88	0.18	85,85,85,85	0
56	MG	1A	3444	1/1	0.88	0.16	109,109,109,109	0
56	MG	2a	3064	1/1	0.88	0.43	67,67,67,67	0
56	MG	1a	1647	1/1	0.88	1.09	106,106,106,106	0
56	MG	2A	3051	1/1	0.88	1.39	79,79,79,79	0
56	MG	2A	3165	1/1	0.88	0.28	73,73,73,73	0
56	MG	1A	3241	1/1	0.88	0.58	61,61,61,61	0
56	MG	1A	3212	1/1	0.88	0.45	62,62,62,62	0
56	MG	2a	3074	1/1	0.88	0.29	76,76,76,76	0
56	MG	2A	3054	1/1	0.88	0.15	78,78,78,78	0
56	MG	1A	3274	1/1	0.88	0.36	74,74,74,74	0
56	MG	2a	3078	1/1	0.88	0.44	62,62,62,62	0
56	MG	2A	3292	1/1	0.88	0.34	64,64,64,64	0
56	MG	2A	3003	1/1	0.88	0.22	73,73,73,73	0
56	MG	1B	210	1/1	0.88	0.36	96,96,96,96	0
56	MG	2A	3181	1/1	0.88	0.30	101,101,101,101	0
56	MG	1A	3015	1/1	0.88	0.46	62,62,62,62	0
56	MG	2A	3185	1/1	0.88	0.27	72,72,72,72	0
56	MG	1A	3464	1/1	0.88	0.33	95,95,95,95	0
56	MG	1A	3191	1/1	0.88	0.27	70,70,70,70	0
56	MG	1E	303	1/1	0.88	0.35	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	2A	3013	1/1	0.88	0.32	73,73,73,73	0
56	MG	1A	3359	1/1	0.88	0.46	78,78,78,78	0
56	MG	2A	3320	1/1	0.88	0.40	74,74,74,74	0
56	MG	1A	3018	1/1	0.88	0.37	77,77,77,77	0
56	MG	1A	3472	1/1	0.88	0.41	67,67,67,67	0
56	MG	1a	1626	1/1	0.88	0.28	81,81,81,81	0
56	MG	2a	3007	1/1	0.88	0.24	73,73,73,73	0
56	MG	2A	3211	1/1	0.88	0.29	63,63,63,63	0
56	MG	1A	3362	1/1	0.88	0.52	62,62,62,62	0
56	MG	1A	3166	1/1	0.88	0.65	69,69,69,69	0
56	MG	2A	3084	1/1	0.88	0.25	79,79,79,79	0
56	MG	1A	3233	1/1	0.89	0.63	76,76,76,76	0
56	MG	1A	3079	1/1	0.89	0.58	78,78,78,78	0
56	MG	1A	3175	1/1	0.89	0.30	62,62,62,62	0
56	MG	1A	3204	1/1	0.89	0.69	72,72,72,72	0
56	MG	1A	3176	1/1	0.89	0.20	75,75,75,75	0
56	MG	2A	3302	1/1	0.89	0.27	82,82,82,82	0
56	MG	1A	3371	1/1	0.89	0.49	75,75,75,75	0
56	MG	1A	3475	1/1	0.89	0.68	65,65,65,65	0
56	MG	1A	3035	1/1	0.89	0.84	75,75,75,75	0
56	MG	2A	3038	1/1	0.89	0.18	77,77,77,77	0
56	MG	1a	1653	1/1	0.89	0.18	63,63,63,63	0
56	MG	2a	3019	1/1	0.89	0.24	77,77,77,77	0
56	MG	2A	3082	1/1	0.89	0.51	79,79,79,79	0
56	MG	1A	3375	1/1	0.89	0.45	95,95,95,95	0
56	MG	1A	3016	1/1	0.89	0.08	95,95,95,95	0
56	MG	1A	3060	1/1	0.89	0.24	79,79,79,79	0
56	MG	2A	3045	1/1	0.89	0.90	74,74,74,74	0
56	MG	1A	3004	1/1	0.89	0.19	89,89,89,89	0
56	MG	1A	3122	1/1	0.89	0.43	106,106,106,106	0
56	MG	1A	3347	1/1	0.89	0.27	90,90,90,90	0
56	MG	1a	1633	1/1	0.89	0.18	97,97,97,97	0
56	MG	1A	3261	1/1	0.89	0.63	77,77,77,77	0
56	MG	1A	3246	1/1	0.89	0.23	77,77,77,77	0
56	MG	1A	3230	1/1	0.89	0.33	79,79,79,79	0
56	MG	1A	3456	1/1	0.89	0.32	68,68,68,68	0
56	MG	1A	3248	1/1	0.89	0.51	68,68,68,68	0
56	MG	1a	1677	1/1	0.89	0.14	85,85,85,85	0
56	MG	2A	3021	1/1	0.89	0.16	90,90,90,90	0
56	MG	2A	3351	1/1	0.89	0.29	94,94,94,94	0
56	MG	2a	3052	1/1	0.89	0.52	68,68,68,68	0
56	MG	1A	3201	1/1	0.89	0.66	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	2A	3158	1/1	0.90	0.28	73,73,73,73	0
56	MG	1a	1601	1/1	0.90	0.15	72,72,72,72	0
56	MG	2A	3244	1/1	0.90	0.30	61,61,61,61	0
56	MG	2a	3045	1/1	0.90	0.46	79,79,79,79	0
56	MG	2A	3121	1/1	0.90	0.21	66,66,66,66	0
56	MG	2A	3321	1/1	0.90	0.19	81,81,81,81	0
56	MG	1A	3185	1/1	0.90	0.41	62,62,62,62	0
56	MG	2A	3092	1/1	0.90	0.28	75,75,75,75	0
56	MG	1A	3489	1/1	0.90	0.17	78,78,78,78	0
56	MG	1A	3186	1/1	0.90	0.34	84,84,84,84	0
56	MG	2A	3171	1/1	0.90	0.26	94,94,94,94	0
56	MG	1A	3024	1/1	0.90	0.22	85,85,85,85	0
56	MG	2A	3099	1/1	0.90	0.19	81,81,81,81	0
56	MG	1A	3158	1/1	0.90	0.30	75,75,75,75	0
56	MG	1A	3325	1/1	0.90	0.26	70,70,70,70	0
56	MG	1A	3431	1/1	0.90	0.28	62,62,62,62	0
56	MG	28	101	1/1	0.90	0.46	80,80,80,80	0
56	MG	1A	3127	1/1	0.90	0.44	69,69,69,69	0
56	MG	2a	3002	1/1	0.90	0.30	65,65,65,65	0
56	MG	2A	3182	1/1	0.90	0.29	76,76,76,76	0
56	MG	1A	3433	1/1	0.90	0.70	75,75,75,75	0
56	MG	2A	3184	1/1	0.90	0.29	70,70,70,70	0
56	MG	2A	3106	1/1	0.90	0.14	83,83,83,83	0
56	MG	1A	3218	1/1	0.90	0.29	66,66,66,66	0
56	MG	2A	3043	1/1	0.90	0.35	70,70,70,70	0
56	MG	1A	3106	1/1	0.90	0.21	73,73,73,73	0
56	MG	1A	3111	1/1	0.90	0.18	78,78,78,78	0
56	MG	2A	3364	1/1	0.90	0.19	80,80,80,80	0
56	MG	1A	3131	1/1	0.90	0.26	76,76,76,76	0
56	MG	2A	3146	1/1	0.90	0.15	79,79,79,79	0
56	MG	2a	3095	1/1	0.90	0.20	84,84,84,84	0
56	MG	1A	3365	1/1	0.90	0.30	69,69,69,69	0
56	MG	2A	3295	1/1	0.90	0.12	76,76,76,76	0
56	MG	1a	1661	1/1	0.90	0.32	72,72,72,72	0
56	MG	2A	3299	1/1	0.90	0.15	78,78,78,78	0
56	MG	2A	3083	1/1	0.90	0.43	77,77,77,77	0
56	MG	2A	3022	1/1	0.90	0.31	66,66,66,66	0
56	MG	1A	3411	1/1	0.90	0.44	75,75,75,75	0
56	MG	1A	3058	1/1	0.90	0.43	73,73,73,73	0
56	MG	2A	3230	1/1	0.90	0.42	62,62,62,62	0
56	MG	2A	3232	1/1	0.90	0.20	66,66,66,66	0
56	MG	1A	3350	1/1	0.91	0.61	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3046	1/1	0.91	0.81	78,78,78,78	0
56	MG	1A	3017	1/1	0.91	0.41	61,61,61,61	0
56	MG	2A	3338	1/1	0.91	1.37	75,75,75,75	0
56	MG	2A	3340	1/1	0.91	0.38	86,86,86,86	0
56	MG	2A	3342	1/1	0.91	0.29	85,85,85,85	0
56	MG	2A	3343	1/1	0.91	0.17	73,73,73,73	0
56	MG	1A	3238	1/1	0.91	0.27	75,75,75,75	0
56	MG	1A	3496	1/1	0.91	0.11	94,94,94,94	0
56	MG	1A	3151	1/1	0.91	0.23	76,76,76,76	0
56	MG	2a	3027	1/1	0.91	0.10	79,79,79,79	0
56	MG	2a	3028	1/1	0.91	0.34	83,83,83,83	0
56	MG	1A	3002	1/1	0.91	0.17	94,94,94,94	0
56	MG	1A	3219	1/1	0.91	0.29	90,90,90,90	0
56	MG	2A	3156	1/1	0.91	0.25	63,63,63,63	0
56	MG	1A	3052	1/1	0.91	0.31	85,85,85,85	0
56	MG	1A	3313	1/1	0.91	0.49	70,70,70,70	0
56	MG	1A	3363	1/1	0.91	0.47	77,77,77,77	0
56	MG	2A	3261	1/1	0.91	0.22	72,72,72,72	0
56	MG	1A	3103	1/1	0.91	0.66	64,64,64,64	0
56	MG	1A	3317	1/1	0.91	0.89	77,77,77,77	0
56	MG	1a	1628	1/1	0.91	0.51	61,61,61,61	0
56	MG	2A	3371	1/1	0.91	0.20	62,62,62,62	0
56	MG	1A	3369	1/1	0.91	0.35	76,76,76,76	0
56	MG	1A	3120	1/1	0.91	0.24	61,61,61,61	0
56	MG	1A	3077	1/1	0.91	0.86	81,81,81,81	0
56	MG	1a	1632	1/1	0.91	0.18	88,88,88,88	0
56	MG	1D	301	1/1	0.91	0.24	73,73,73,73	0
56	MG	1E	301	1/1	0.91	0.22	71,71,71,71	0
56	MG	1A	3031	1/1	0.91	0.23	69,69,69,69	0
56	MG	1A	3089	1/1	0.91	0.25	74,74,74,74	0
56	MG	1a	1637	1/1	0.91	0.20	89,89,89,89	0
56	MG	2B	204	1/1	0.91	0.62	80,80,80,80	0
56	MG	1A	3107	1/1	0.91	0.27	64,64,64,64	0
56	MG	2B	206	1/1	0.91	0.44	89,89,89,89	0
56	MG	1A	3450	1/1	0.91	0.21	75,75,75,75	0
56	MG	1A	3331	1/1	0.91	0.30	63,63,63,63	0
56	MG	1A	3339	1/1	0.91	0.24	73,73,73,73	0
56	MG	1A	3396	1/1	0.91	0.28	84,84,84,84	0
56	MG	1A	3163	1/1	0.91	0.48	78,78,78,78	0
56	MG	2A	3191	1/1	0.91	0.18	78,78,78,78	0
56	MG	1A	3164	1/1	0.91	0.27	69,69,69,69	0
56	MG	2A	3196	1/1	0.91	0.28	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	1A	3285	1/1	0.91	0.18	83,83,83,83	0
56	MG	2A	3199	1/1	0.91	0.23	83,83,83,83	0
56	MG	1A	3403	1/1	0.91	0.46	87,87,87,87	0
56	MG	1A	3109	1/1	0.91	0.12	92,92,92,92	0
56	MG	2A	3133	1/1	0.91	0.36	77,77,77,77	0
56	MG	2A	3019	1/1	0.91	0.37	69,69,69,69	0
56	MG	25	101	1/1	0.91	0.56	69,69,69,69	0
56	MG	1A	3346	1/1	0.91	0.49	65,65,65,65	0
56	MG	2A	3212	1/1	0.91	0.43	78,78,78,78	0
56	MG	2A	3325	1/1	0.91	0.27	67,67,67,67	0
56	MG	13	101	1/1	0.91	0.35	72,72,72,72	0
56	MG	1A	3147	1/1	0.91	0.34	76,76,76,76	0
56	MG	2A	3330	1/1	0.91	0.23	82,82,82,82	0
56	MG	16	101	1/1	0.91	0.27	75,75,75,75	0
56	MG	1A	3414	1/1	0.91	0.24	70,70,70,70	0
56	MG	1A	3006	1/1	0.91	0.22	72,72,72,72	0
56	MG	2A	3241	1/1	0.92	0.20	65,65,65,65	0
56	MG	1A	3419	1/1	0.92	0.27	72,72,72,72	0
56	MG	1A	3454	1/1	0.92	0.47	73,73,73,73	0
56	MG	2A	3322	1/1	0.92	0.17	89,89,89,89	0
56	MG	1A	3302	1/1	0.92	0.24	62,62,62,62	0
56	MG	2A	3132	1/1	0.92	0.21	71,71,71,71	0
56	MG	1A	3306	1/1	0.92	0.53	61,61,61,61	0
56	MG	2D	3100	1/1	0.92	0.19	83,83,83,83	0
56	MG	1A	3033	1/1	0.92	0.28	86,86,86,86	0
56	MG	2A	3328	1/1	0.92	0.21	68,68,68,68	0
56	MG	1B	205	1/1	0.92	0.42	68,68,68,68	0
56	MG	1B	207	1/1	0.92	0.39	106,106,106,106	0
56	MG	1A	3055	1/1	0.92	0.68	83,83,83,83	0
56	MG	2Q	201	1/1	0.92	0.12	93,93,93,93	0
56	MG	1A	3465	1/1	0.92	0.43	61,61,61,61	0
56	MG	1A	3429	1/1	0.92	0.95	79,79,79,79	0
56	MG	1A	3398	1/1	0.92	0.41	70,70,70,70	0
56	MG	2A	3188	1/1	0.92	0.30	74,74,74,74	0
56	MG	2A	3265	1/1	0.92	0.53	73,73,73,73	0
56	MG	1a	1602	1/1	0.92	0.32	74,74,74,74	0
56	MG	2a	3070	1/1	0.92	0.20	78,78,78,78	0
56	MG	1A	3090	1/1	0.92	0.21	75,75,75,75	0
56	MG	1A	3401	1/1	0.92	0.25	64,64,64,64	0
56	MG	23	101	1/1	0.92	0.31	68,68,68,68	0
56	MG	1A	3289	1/1	0.92	0.37	84,84,84,84	0
56	MG	1A	3066	1/1	0.92	0.17	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3406	1/1	0.92	0.47	76,76,76,76	0
56	MG	2a	3082	1/1	0.92	0.34	66,66,66,66	0
56	MG	2A	3202	1/1	0.92	0.27	70,70,70,70	0
56	MG	1A	3408	1/1	0.92	0.53	61,61,61,61	0
56	MG	1A	3096	1/1	0.92	0.23	76,76,76,76	0
56	MG	1A	3108	1/1	0.92	0.16	75,75,75,75	0
56	MG	1x	101	1/1	0.92	0.48	92,92,92,92	0
56	MG	1a	1652	1/1	0.92	0.17	74,74,74,74	0
56	MG	1A	3084	1/1	0.92	0.19	79,79,79,79	0
56	MG	1a	1621	1/1	0.92	0.27	73,73,73,73	0
56	MG	2A	3218	1/1	0.92	0.14	72,72,72,72	0
56	MG	2A	3368	1/1	0.92	0.53	62,62,62,62	0
56	MG	2A	3219	1/1	0.92	0.28	75,75,75,75	0
56	MG	1A	3085	1/1	0.92	0.84	79,79,79,79	0
56	MG	2A	3372	1/1	0.92	0.19	70,70,70,70	0
56	MG	1A	3012	1/1	0.92	0.82	75,75,75,75	0
56	MG	2A	3007	1/1	0.92	0.24	78,78,78,78	0
56	MG	1A	3053	1/1	0.92	0.63	77,77,77,77	0
56	MG	2A	3234	1/1	0.92	0.25	68,68,68,68	0
56	MG	2A	3167	1/1	0.92	0.46	72,72,72,72	0
57	ZN	14	501	1/1	0.92	0.07	166,166,166,166	0
56	MG	2A	3170	1/1	0.92	0.43	67,67,67,67	0
56	MG	2A	3384	1/1	0.92	0.10	91,91,91,91	0
57	ZN	25	102	1/1	0.92	0.19	104,104,104,104	0
56	MG	1A	3102	1/1	0.93	0.60	74,74,74,74	0
56	MG	1A	3455	1/1	0.93	0.46	63,63,63,63	0
56	MG	1A	3324	1/1	0.93	0.11	67,67,67,67	0
56	MG	1A	3461	1/1	0.93	0.59	83,83,83,83	0
56	MG	2A	3379	1/1	0.93	0.14	77,77,77,77	0
56	MG	1A	3265	1/1	0.93	0.50	72,72,72,72	0
56	MG	1A	3097	1/1	0.93	0.54	77,77,77,77	0
56	MG	1A	3209	1/1	0.93	0.51	61,61,61,61	0
56	MG	1A	3336	1/1	0.93	0.27	64,64,64,64	0
56	MG	1A	3338	1/1	0.93	0.41	61,61,61,61	0
56	MG	2A	3213	1/1	0.93	0.25	67,67,67,67	0
56	MG	2a	3041	1/1	0.93	0.29	80,80,80,80	0
56	MG	1A	3416	1/1	0.93	0.45	103,103,103,103	0
56	MG	1a	1680	1/1	0.93	0.95	73,73,73,73	0
56	MG	2A	3316	1/1	0.93	0.30	62,62,62,62	0
56	MG	2A	3148	1/1	0.93	0.27	72,72,72,72	0
56	MG	2A	3150	1/1	0.93	0.22	101,101,101,101	0
56	MG	1A	3022	1/1	0.93	0.51	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	1a	1682	1/1	0.93	0.14	96,96,96,96	0
56	MG	1A	3366	1/1	0.93	0.27	61,61,61,61	0
56	MG	1a	1685	1/1	0.93	0.10	76,76,76,76	0
56	MG	2E	306	1/1	0.93	0.17	64,64,64,64	0
56	MG	1A	3143	1/1	0.93	0.44	62,62,62,62	0
56	MG	2A	3104	1/1	0.93	0.54	80,80,80,80	0
56	MG	1A	3061	1/1	0.93	0.44	71,71,71,71	0
56	MG	2a	3071	1/1	0.93	0.21	75,75,75,75	0
56	MG	2a	3072	1/1	0.93	0.27	72,72,72,72	0
56	MG	1A	3095	1/1	0.93	0.35	69,69,69,69	0
56	MG	1A	3276	1/1	0.93	0.23	75,75,75,75	0
56	MG	1A	3376	1/1	0.93	0.28	61,61,61,61	0
56	MG	1a	1693	1/1	0.93	0.12	127,127,127,127	0
56	MG	2A	3163	1/1	0.93	0.24	62,62,62,62	0
56	MG	2a	3079	1/1	0.93	0.18	62,62,62,62	0
56	MG	1A	3481	1/1	0.93	0.40	68,68,68,68	0
56	MG	2A	3111	1/1	0.93	0.36	76,76,76,76	0
56	MG	2a	3083	1/1	0.93	0.29	61,61,61,61	0
56	MG	1A	3277	1/1	0.93	0.54	61,61,61,61	0
56	MG	1r	101	1/1	0.93	0.33	81,81,81,81	0
56	MG	1A	3169	1/1	0.93	0.33	62,62,62,62	0
56	MG	2A	3344	1/1	0.93	0.17	78,78,78,78	0
56	MG	1A	3348	1/1	0.93	0.36	79,79,79,79	0
56	MG	1A	3132	1/1	0.93	0.28	74,74,74,74	0
56	MG	2a	3091	1/1	0.93	0.55	79,79,79,79	0
56	MG	1A	3387	1/1	0.93	0.19	80,80,80,80	0
56	MG	1A	3395	1/1	0.93	0.24	67,67,67,67	0
56	MG	1A	3036	1/1	0.93	0.23	83,83,83,83	0
56	MG	1A	3319	1/1	0.93	0.22	61,61,61,61	0
56	MG	2A	3060	1/1	0.93	0.17	88,88,88,88	0
56	MG	1A	3352	1/1	0.93	0.30	101,101,101,101	0
56	MG	1A	3399	1/1	0.93	0.30	73,73,73,73	0
56	MG	2a	3099	1/1	0.93	0.58	79,79,79,79	0
56	MG	2a	3013	1/1	0.93	0.58	80,80,80,80	0
56	MG	1A	3353	1/1	0.93	0.34	62,62,62,62	0
56	MG	1a	1608	1/1	0.93	0.20	73,73,73,73	0
56	MG	1a	1656	1/1	0.93	0.23	82,82,82,82	0
56	MG	1A	3354	1/1	0.93	0.29	61,61,61,61	0
56	MG	1A	3135	1/1	0.93	0.36	80,80,80,80	0
56	MG	1a	1612	1/1	0.93	0.13	97,97,97,97	0
56	MG	1A	3116	1/1	0.93	0.51	68,68,68,68	0
56	MG	2A	3373	1/1	0.93	0.36	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3374	1/1	0.94	0.34	62,62,62,62	0
56	MG	1A	3259	1/1	0.94	0.22	73,73,73,73	0
56	MG	1A	3422	1/1	0.94	0.29	61,61,61,61	0
56	MG	2A	3228	1/1	0.94	0.15	67,67,67,67	0
56	MG	1A	3282	1/1	0.94	0.25	70,70,70,70	0
56	MG	10	101	1/1	0.94	0.25	65,65,65,65	0
56	MG	2A	3339	1/1	0.94	0.06	85,85,85,85	0
56	MG	10	102	1/1	0.94	0.37	73,73,73,73	0
56	MG	1A	3112	1/1	0.94	0.53	63,63,63,63	0
56	MG	1A	3476	1/1	0.94	0.42	62,62,62,62	0
56	MG	1A	3183	1/1	0.94	0.70	74,74,74,74	0
56	MG	2A	3089	1/1	0.94	0.17	87,87,87,87	0
56	MG	2A	3153	1/1	0.94	0.32	100,100,100,100	0
56	MG	1A	3199	1/1	0.94	0.43	84,84,84,84	0
56	MG	2A	3250	1/1	0.94	0.39	62,62,62,62	0
56	MG	1A	3430	1/1	0.94	0.30	68,68,68,68	0
56	MG	2A	3252	1/1	0.94	0.25	77,77,77,77	0
56	MG	2a	3031	1/1	0.94	0.11	76,76,76,76	0
56	MG	1a	1657	1/1	0.94	0.25	93,93,93,93	0
56	MG	2A	3353	1/1	0.94	0.42	70,70,70,70	0
56	MG	2A	3354	1/1	0.94	0.19	65,65,65,65	0
56	MG	1A	3019	1/1	0.94	0.37	80,80,80,80	0
56	MG	2a	3036	1/1	0.94	0.36	76,76,76,76	0
56	MG	2A	3357	1/1	0.94	0.20	69,69,69,69	0
56	MG	1a	1663	1/1	0.94	0.20	68,68,68,68	0
56	MG	2A	3025	1/1	0.94	0.30	89,89,89,89	0
56	MG	1A	3486	1/1	0.94	0.14	78,78,78,78	0
56	MG	2a	3042	1/1	0.94	0.13	91,91,91,91	0
56	MG	2a	3044	1/1	0.94	0.66	75,75,75,75	0
56	MG	1A	3386	1/1	0.94	0.27	77,77,77,77	0
56	MG	2A	3028	1/1	0.94	0.44	91,91,91,91	0
56	MG	1a	1666	1/1	0.94	0.27	94,94,94,94	0
56	MG	2A	3164	1/1	0.94	0.28	68,68,68,68	0
56	MG	1A	3323	1/1	0.94	0.39	62,62,62,62	0
56	MG	1A	3389	1/1	0.94	0.17	71,71,71,71	0
56	MG	2a	3058	1/1	0.94	0.86	73,73,73,73	0
56	MG	1A	3495	1/1	0.94	0.30	98,98,98,98	0
56	MG	2A	3169	1/1	0.94	0.60	69,69,69,69	0
56	MG	1a	1605	1/1	0.94	0.12	99,99,99,99	0
56	MG	2A	3275	1/1	0.94	0.24	62,62,62,62	0
56	MG	1A	3390	1/1	0.94	0.46	61,61,61,61	0
56	MG	1A	3216	1/1	0.94	0.37	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3041	1/1	0.94	0.59	69,69,69,69	0
56	MG	1A	3326	1/1	0.94	0.29	63,63,63,63	0
56	MG	2A	3385	1/1	0.94	0.13	76,76,76,76	0
56	MG	1A	3042	1/1	0.94	0.28	79,79,79,79	0
56	MG	2A	3288	1/1	0.94	0.19	66,66,66,66	0
56	MG	2a	3075	1/1	0.94	0.26	92,92,92,92	0
56	MG	1A	3441	1/1	0.94	0.25	76,76,76,76	0
56	MG	1A	3442	1/1	0.94	0.60	61,61,61,61	0
56	MG	1A	3294	1/1	0.94	0.33	75,75,75,75	0
56	MG	1a	1618	1/1	0.94	0.11	96,96,96,96	0
56	MG	1B	206	1/1	0.94	0.55	89,89,89,89	0
56	MG	2B	209	1/1	0.94	0.13	91,91,91,91	0
56	MG	1A	3335	1/1	0.94	0.46	85,85,85,85	0
56	MG	2A	3186	1/1	0.94	0.10	92,92,92,92	0
56	MG	2a	3085	1/1	0.94	0.21	92,92,92,92	0
56	MG	1A	3048	1/1	0.94	0.41	69,69,69,69	0
56	MG	1A	3141	1/1	0.94	0.32	83,83,83,83	0
56	MG	1A	3080	1/1	0.94	0.23	82,82,82,82	0
56	MG	1A	3451	1/1	0.94	0.15	77,77,77,77	0
56	MG	2A	3192	1/1	0.94	0.49	79,79,79,79	0
56	MG	2A	3307	1/1	0.94	0.25	77,77,77,77	0
56	MG	2A	3308	1/1	0.94	0.26	85,85,85,85	0
56	MG	1A	3271	1/1	0.94	0.17	75,75,75,75	0
56	MG	1A	3050	1/1	0.94	0.25	83,83,83,83	0
56	MG	1A	3023	1/1	0.94	0.21	73,73,73,73	0
56	MG	1A	3457	1/1	0.94	0.28	62,62,62,62	0
56	MG	1A	3460	1/1	0.94	0.47	67,67,67,67	0
56	MG	2A	3203	1/1	0.94	0.34	61,61,61,61	0
56	MG	1A	3367	1/1	0.94	0.23	61,61,61,61	0
56	MG	2a	3101	1/1	0.94	0.13	102,102,102,102	0
56	MG	2A	3207	1/1	0.94	0.10	89,89,89,89	0
56	MG	2a	3103	1/1	0.94	0.11	101,101,101,101	0
56	MG	1A	3368	1/1	0.94	0.37	77,77,77,77	0
56	MG	2A	3324	1/1	0.94	0.18	82,82,82,82	0
56	MG	1A	3344	1/1	0.94	0.36	73,73,73,73	0
56	MG	1A	3225	1/1	0.94	0.11	90,90,90,90	0
56	MG	1A	3372	1/1	0.94	0.37	72,72,72,72	0
56	MG	2A	3069	1/1	0.94	0.23	83,83,83,83	0
56	MG	1A	3003	1/1	0.94	0.26	68,68,68,68	0
56	MG	1U	201	1/1	0.94	0.37	67,67,67,67	0
56	MG	1A	3421	1/1	0.95	0.27	65,65,65,65	0
56	MG	1A	3315	1/1	0.95	0.26	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	2a	3025	1/1	0.95	0.22	81,81,81,81	0
56	MG	1A	3423	1/1	0.95	0.27	62,62,62,62	0
56	MG	2A	3260	1/1	0.95	0.23	70,70,70,70	0
56	MG	1A	3190	1/1	0.95	0.66	79,79,79,79	0
56	MG	2A	3179	1/1	0.95	0.22	93,93,93,93	0
56	MG	1A	3392	1/1	0.95	0.30	73,73,73,73	0
56	MG	1a	1606	1/1	0.95	0.14	69,69,69,69	0
56	MG	1A	3426	1/1	0.95	0.15	89,89,89,89	0
56	MG	2A	3123	1/1	0.95	0.24	78,78,78,78	0
56	MG	2A	3269	1/1	0.95	0.23	62,62,62,62	0
56	MG	1A	3223	1/1	0.95	0.20	64,64,64,64	0
56	MG	1A	3110	1/1	0.95	0.17	70,70,70,70	0
56	MG	1A	3013	1/1	0.95	0.26	83,83,83,83	0
56	MG	1A	3091	1/1	0.95	0.23	77,77,77,77	0
56	MG	2A	3370	1/1	0.95	0.16	75,75,75,75	0
56	MG	1a	1662	1/1	0.95	0.10	94,94,94,94	0
56	MG	2A	3281	1/1	0.95	0.33	73,73,73,73	0
56	MG	2a	3043	1/1	0.95	0.21	62,62,62,62	0
56	MG	1a	1613	1/1	0.95	0.09	87,87,87,87	0
56	MG	2A	3286	1/1	0.95	0.19	62,62,62,62	0
56	MG	2A	3190	1/1	0.95	0.18	82,82,82,82	0
56	MG	2A	3075	1/1	0.95	0.21	95,95,95,95	0
56	MG	2a	3049	1/1	0.95	0.26	80,80,80,80	0
56	MG	1A	3295	1/1	0.95	0.24	69,69,69,69	0
56	MG	2A	3193	1/1	0.95	0.20	87,87,87,87	0
56	MG	1A	3137	1/1	0.95	0.41	61,61,61,61	0
56	MG	1a	1616	1/1	0.95	0.77	69,69,69,69	0
56	MG	2A	3294	1/1	0.95	0.32	87,87,87,87	0
56	MG	2a	3063	1/1	0.95	0.47	61,61,61,61	0
56	MG	2A	3136	1/1	0.95	0.38	78,78,78,78	0
56	MG	1A	3370	1/1	0.95	0.47	88,88,88,88	0
56	MG	2a	3066	1/1	0.95	0.40	86,86,86,86	0
56	MG	2A	3298	1/1	0.95	0.21	69,69,69,69	0
56	MG	2A	3200	1/1	0.95	0.19	74,74,74,74	0
56	MG	1A	3138	1/1	0.95	0.39	108,108,108,108	0
56	MG	1a	1619	1/1	0.95	0.21	92,92,92,92	0
56	MG	2A	3204	1/1	0.95	0.16	68,68,68,68	0
56	MG	2A	3304	1/1	0.95	0.31	63,63,63,63	0
56	MG	1A	3474	1/1	0.95	0.35	70,70,70,70	0
56	MG	1A	3281	1/1	0.95	0.22	63,63,63,63	0
56	MG	1a	1622	1/1	0.95	0.26	66,66,66,66	0
56	MG	1A	3301	1/1	0.95	0.46	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3477	1/1	0.95	0.32	61,61,61,61	0
56	MG	1A	3407	1/1	0.95	0.20	94,94,94,94	0
56	MG	1A	3229	1/1	0.95	0.17	75,75,75,75	0
56	MG	2A	3314	1/1	0.95	0.44	78,78,78,78	0
56	MG	2A	3093	1/1	0.95	0.10	82,82,82,82	0
56	MG	1A	3330	1/1	0.95	0.13	69,69,69,69	0
56	MG	2A	3317	1/1	0.95	0.27	65,65,65,65	0
56	MG	2A	3095	1/1	0.95	0.26	81,81,81,81	0
56	MG	2A	3096	1/1	0.95	0.10	92,92,92,92	0
56	MG	2A	3034	1/1	0.95	0.28	94,94,94,94	0
56	MG	2A	3035	1/1	0.95	0.35	76,76,76,76	0
56	MG	2A	3036	1/1	0.95	0.24	77,77,77,77	0
56	MG	1A	3303	1/1	0.95	0.36	83,83,83,83	0
56	MG	1A	3284	1/1	0.95	0.24	76,76,76,76	0
56	MG	1A	3488	1/1	0.95	0.22	69,69,69,69	0
56	MG	2A	3235	1/1	0.95	0.23	75,75,75,75	0
56	MG	1A	3005	1/1	0.95	0.11	82,82,82,82	0
56	MG	2A	3238	1/1	0.95	0.18	67,67,67,67	0
56	MG	1A	3490	1/1	0.95	0.11	79,79,79,79	0
56	MG	1A	3310	1/1	0.95	0.32	62,62,62,62	0
56	MG	1A	3446	1/1	0.95	0.28	77,77,77,77	0
56	MG	2A	3246	1/1	0.95	0.13	79,79,79,79	0
56	MG	1a	1639	1/1	0.95	0.53	77,77,77,77	0
56	MG	2A	3249	1/1	0.95	0.23	74,74,74,74	0
56	MG	1A	3447	1/1	0.95	0.48	78,78,78,78	0
56	MG	1A	3188	1/1	0.95	0.42	62,62,62,62	0
56	MG	2A	3341	1/1	0.95	0.21	76,76,76,76	0
56	MG	1A	3384	1/1	0.95	0.29	71,71,71,71	0
56	MG	1A	3133	1/1	0.95	0.26	72,72,72,72	0
56	MG	2a	3017	1/1	0.95	0.18	87,87,87,87	0
56	MG	1A	3453	1/1	0.95	0.51	80,80,80,80	0
56	MG	1A	3361	1/1	0.95	0.48	94,94,94,94	0
56	MG	1a	1646	1/1	0.95	0.47	71,71,71,71	0
57	ZN	29	501	1/1	0.95	0.13	114,114,114,114	0
56	MG	2A	3195	1/1	0.96	0.24	66,66,66,66	0
56	MG	1A	3231	1/1	0.96	0.27	65,65,65,65	0
56	MG	1A	3094	1/1	0.96	0.09	84,84,84,84	0
56	MG	2A	3198	1/1	0.96	0.43	96,96,96,96	0
56	MG	2B	208	1/1	0.96	0.66	62,62,62,62	0
56	MG	1A	3296	1/1	0.96	0.23	73,73,73,73	0
56	MG	1A	3278	1/1	0.96	0.26	63,63,63,63	0
56	MG	2a	3048	1/1	0.96	0.15	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
56	MG	1A	3242	1/1	0.96	0.34	61,61,61,61	0
56	MG	2a	3050	1/1	0.96	0.19	88,88,88,88	0
56	MG	1A	3482	1/1	0.96	0.33	61,61,61,61	0
56	MG	1A	3485	1/1	0.96	0.12	72,72,72,72	0
56	MG	2A	3333	1/1	0.96	0.29	74,74,74,74	0
56	MG	2A	3009	1/1	0.96	0.24	110,110,110,110	0
56	MG	2a	3059	1/1	0.96	0.14	80,80,80,80	0
56	MG	2a	3060	1/1	0.96	0.05	120,120,120,120	0
56	MG	2A	3206	1/1	0.96	0.12	78,78,78,78	0
56	MG	2a	3062	1/1	0.96	0.54	68,68,68,68	0
56	MG	1A	3207	1/1	0.96	0.38	62,62,62,62	0
56	MG	2A	3046	1/1	0.96	0.16	65,65,65,65	0
56	MG	1A	3300	1/1	0.96	0.28	63,63,63,63	0
56	MG	2A	3090	1/1	0.96	0.05	110,110,110,110	0
56	MG	1A	3244	1/1	0.96	0.32	77,77,77,77	0
56	MG	1A	3283	1/1	0.96	0.30	61,61,61,61	0
56	MG	1A	3267	1/1	0.96	0.22	70,70,70,70	0
56	MG	2A	3282	1/1	0.96	0.30	74,74,74,74	0
56	MG	1A	3304	1/1	0.96	0.42	61,61,61,61	0
56	MG	21	101	1/1	0.96	0.35	63,63,63,63	0
56	MG	1A	3435	1/1	0.96	0.23	90,90,90,90	0
56	MG	2A	3173	1/1	0.96	0.22	78,78,78,78	0
56	MG	2A	3174	1/1	0.96	0.18	80,80,80,80	0
56	MG	2A	3221	1/1	0.96	0.29	80,80,80,80	0
56	MG	2A	3223	1/1	0.96	0.16	70,70,70,70	0
56	MG	2A	3225	1/1	0.96	0.16	62,62,62,62	0
56	MG	2A	3227	1/1	0.96	0.15	62,62,62,62	0
56	MG	1A	3200	1/1	0.96	0.11	69,69,69,69	0
56	MG	2a	3081	1/1	0.96	0.12	64,64,64,64	0
56	MG	1A	3332	1/1	0.96	0.31	74,74,74,74	0
56	MG	1A	3334	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	3466	1/1	0.96	0.18	61,61,61,61	0
56	MG	2A	3358	1/1	0.96	0.19	81,81,81,81	0
56	MG	1A	3467	1/1	0.96	0.21	66,66,66,66	0
56	MG	2A	3360	1/1	0.96	0.27	61,61,61,61	0
56	MG	1A	3179	1/1	0.96	0.21	64,64,64,64	0
56	MG	2A	3236	1/1	0.96	0.14	66,66,66,66	0
56	MG	2A	3365	1/1	0.96	0.22	67,67,67,67	0
56	MG	2A	3140	1/1	0.96	0.46	73,73,73,73	0
56	MG	2A	3303	1/1	0.96	0.15	76,76,76,76	0
56	MG	1a	1654	1/1	0.96	0.25	71,71,71,71	0
56	MG	1A	3152	1/1	0.96	0.35	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
56	MG	1A	3032	1/1	0.96	0.50	77,77,77,77	0
56	MG	2A	3242	1/1	0.96	0.32	61,61,61,61	0
56	MG	1a	1691	1/1	0.96	0.09	94,94,94,94	0
56	MG	2A	3245	1/1	0.96	0.45	64,64,64,64	0
56	MG	1A	3273	1/1	0.96	0.23	80,80,80,80	0
56	MG	1A	3314	1/1	0.96	0.17	71,71,71,71	0
56	MG	2A	3312	1/1	0.96	0.24	64,64,64,64	0
56	MG	2A	3378	1/1	0.96	0.16	83,83,83,83	0
56	MG	2A	3313	1/1	0.96	0.17	76,76,76,76	0
56	MG	2f	201	1/1	0.96	0.19	77,77,77,77	0
56	MG	2A	3068	1/1	0.96	0.26	90,90,90,90	0
56	MG	1A	3155	1/1	0.96	0.36	73,73,73,73	0
56	MG	2A	3149	1/1	0.96	0.10	82,82,82,82	0
56	MG	1A	3076	1/1	0.96	0.20	65,65,65,65	0
56	MG	2A	3073	1/1	0.96	0.38	73,73,73,73	0
56	MG	2a	3038	1/1	0.96	0.10	80,80,80,80	0
56	MG	1A	3343	1/1	0.96	0.37	80,80,80,80	0
56	MG	2A	3076	1/1	0.96	0.31	69,69,69,69	0
56	MG	2A	3270	1/1	0.97	0.09	80,80,80,80	0
56	MG	2A	3226	1/1	0.97	0.25	82,82,82,82	0
56	MG	2a	3005	1/1	0.97	0.11	87,87,87,87	0
56	MG	2A	3274	1/1	0.97	0.22	61,61,61,61	0
56	MG	1a	1659	1/1	0.97	0.28	67,67,67,67	0
56	MG	1a	1660	1/1	0.97	0.33	61,61,61,61	0
56	MG	2A	3087	1/1	0.97	0.20	68,68,68,68	0
56	MG	1A	3393	1/1	0.97	0.29	61,61,61,61	0
56	MG	2a	3012	1/1	0.97	0.15	104,104,104,104	0
56	MG	1A	3049	1/1	0.97	0.21	104,104,104,104	0
56	MG	1A	3153	1/1	0.97	0.20	72,72,72,72	0
56	MG	2A	3284	1/1	0.97	0.24	71,71,71,71	0
56	MG	1a	1692	1/1	0.97	0.10	114,114,114,114	0
56	MG	2a	3018	1/1	0.97	0.15	86,86,86,86	0
56	MG	1a	1638	1/1	0.97	0.16	75,75,75,75	0
56	MG	1A	3309	1/1	0.97	0.21	62,62,62,62	0
56	MG	1A	3458	1/1	0.97	0.25	79,79,79,79	0
56	MG	1A	3380	1/1	0.97	0.26	73,73,73,73	0
56	MG	1A	3381	1/1	0.97	0.30	63,63,63,63	0
56	MG	1A	3318	1/1	0.97	0.26	75,75,75,75	0
56	MG	1A	3329	1/1	0.97	0.23	74,74,74,74	0
56	MG	2A	3063	1/1	0.97	0.14	79,79,79,79	0
56	MG	2A	3201	1/1	0.97	0.12	75,75,75,75	0
56	MG	2A	3296	1/1	0.97	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3385	1/1	0.97	0.39	63,63,63,63	0
56	MG	1A	3487	1/1	0.97	0.18	74,74,74,74	0
56	MG	2A	3135	1/1	0.97	0.08	111,111,111,111	0
56	MG	2A	3004	1/1	0.97	0.07	88,88,88,88	0
56	MG	1A	3021	1/1	0.97	0.15	73,73,73,73	0
56	MG	2A	3172	1/1	0.97	0.07	87,87,87,87	0
56	MG	2E	304	1/1	0.97	0.11	63,63,63,63	0
56	MG	1A	3404	1/1	0.97	0.30	81,81,81,81	0
56	MG	1A	3311	1/1	0.97	0.29	62,62,62,62	0
56	MG	2A	3074	1/1	0.97	0.16	71,71,71,71	0
56	MG	1A	3388	1/1	0.97	0.23	71,71,71,71	0
56	MG	1A	3492	1/1	0.97	0.07	95,95,95,95	0
56	MG	1A	3493	1/1	0.97	0.09	97,97,97,97	0
56	MG	2A	3356	1/1	0.97	0.22	68,68,68,68	0
56	MG	1A	3130	1/1	0.97	0.22	84,84,84,84	0
56	MG	2a	3100	1/1	0.97	0.12	95,95,95,95	0
56	MG	1A	3182	1/1	0.97	0.18	69,69,69,69	0
56	MG	1A	3391	1/1	0.97	0.18	66,66,66,66	0
56	MG	1A	3030	1/1	0.97	0.16	76,76,76,76	0
56	MG	2A	3362	1/1	0.97	0.26	80,80,80,80	0
56	MG	2A	3264	1/1	0.97	0.23	70,70,70,70	0
56	MG	1A	3412	1/1	0.97	0.28	65,65,65,65	0
56	MG	2A	3222	1/1	0.97	0.32	75,75,75,75	0
56	MG	2A	3267	1/1	0.97	0.23	81,81,81,81	0
56	MG	2A	3367	1/1	0.97	0.20	62,62,62,62	0
57	ZN	16	102	1/1	0.97	0.16	102,102,102,102	0
57	ZN	1n	501	1/1	0.97	0.09	148,148,148,148	0
56	MG	2a	3057	1/1	0.97	0.24	101,101,101,101	0
56	MG	2A	3018	1/1	0.97	0.09	73,73,73,73	0
56	MG	2a	3001	1/1	0.97	0.11	80,80,80,80	0
56	MG	2A	3116	1/1	0.97	0.14	72,72,72,72	0
58	SF4	1d	302	8/8	0.97	0.14	111,128,150,164	0
56	MG	2a	3054	1/1	0.98	0.22	69,69,69,69	0
56	MG	2a	3055	1/1	0.98	0.24	79,79,79,79	0
56	MG	1A	3483	1/1	0.98	0.19	68,68,68,68	0
56	MG	2A	3243	1/1	0.98	0.21	64,64,64,64	0
56	MG	1a	1679	1/1	0.98	0.26	107,107,107,107	0
56	MG	1A	3484	1/1	0.98	0.31	67,67,67,67	0
56	MG	1a	1624	1/1	0.98	0.28	109,109,109,109	0
56	MG	2A	3247	1/1	0.98	0.27	81,81,81,81	0
56	MG	1a	1625	1/1	0.98	0.13	102,102,102,102	0
56	MG	1a	1683	1/1	0.98	0.23	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3017	1/1	0.98	0.44	69,69,69,69	0
56	MG	1A	3064	1/1	0.98	0.13	79,79,79,79	0
56	MG	1a	1627	1/1	0.98	0.09	80,80,80,80	0
56	MG	1A	3029	1/1	0.98	0.10	86,86,86,86	0
56	MG	1A	3287	1/1	0.98	0.33	63,63,63,63	0
56	MG	2a	3006	1/1	0.98	0.14	76,76,76,76	0
56	MG	2A	3168	1/1	0.98	0.16	68,68,68,68	0
56	MG	2A	3130	1/1	0.98	0.21	63,63,63,63	0
56	MG	1A	3405	1/1	0.98	0.32	93,93,93,93	0
56	MG	1a	1658	1/1	0.98	0.15	75,75,75,75	0
56	MG	1A	3333	1/1	0.98	0.34	68,68,68,68	0
56	MG	1A	3119	1/1	0.98	0.22	64,64,64,64	0
56	MG	1A	3196	1/1	0.98	0.18	65,65,65,65	0
56	MG	1A	3468	1/1	0.98	0.16	63,63,63,63	0
56	MG	2A	3215	1/1	0.98	0.16	61,61,61,61	0
56	MG	2a	3016	1/1	0.98	0.18	84,84,84,84	0
56	MG	2A	3216	1/1	0.98	0.18	62,62,62,62	0
56	MG	2A	3318	1/1	0.98	0.23	62,62,62,62	0
56	MG	2A	3319	1/1	0.98	0.21	64,64,64,64	0
56	MG	2a	3020	1/1	0.98	0.31	105,105,105,105	0
56	MG	2A	3217	1/1	0.98	0.18	78,78,78,78	0
56	MG	1A	3427	1/1	0.98	0.62	61,61,61,61	0
56	MG	1A	3215	1/1	0.98	0.19	67,67,67,67	0
56	MG	2A	3064	1/1	0.98	0.07	101,101,101,101	0
56	MG	2A	3381	1/1	0.98	0.09	76,76,76,76	0
56	MG	1A	3394	1/1	0.98	0.21	61,61,61,61	0
56	MG	1A	3337	1/1	0.98	0.28	79,79,79,79	0
56	MG	2A	3067	1/1	0.98	0.24	73,73,73,73	0
56	MG	2A	3272	1/1	0.98	0.16	62,62,62,62	0
56	MG	2A	3273	1/1	0.98	0.32	62,62,62,62	0
56	MG	2A	3329	1/1	0.98	0.23	82,82,82,82	0
56	MG	2A	3224	1/1	0.98	0.19	61,61,61,61	0
56	MG	2A	3033	1/1	0.98	0.18	82,82,82,82	0
56	MG	1A	3280	1/1	0.98	0.35	64,64,64,64	0
56	MG	2A	3070	1/1	0.98	0.16	81,81,81,81	0
56	MG	2A	3278	1/1	0.98	0.17	61,61,61,61	0
56	MG	1A	3452	1/1	0.98	0.22	76,76,76,76	0
56	MG	2A	3072	1/1	0.98	0.14	96,96,96,96	0
56	MG	1A	3413	1/1	0.98	0.17	68,68,68,68	0
56	MG	2A	3283	1/1	0.98	0.26	61,61,61,61	0
56	MG	2A	3231	1/1	0.98	0.19	74,74,74,74	0
56	MG	1A	3272	1/1	0.98	0.26	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3233	1/1	0.98	0.34	70,70,70,70	0
56	MG	1A	3092	1/1	0.98	0.21	71,71,71,71	0
56	MG	1A	3125	1/1	0.98	0.20	62,62,62,62	0
56	MG	2A	3289	1/1	0.98	0.14	77,77,77,77	0
57	ZN	15	102	1/1	0.98	0.21	106,106,106,106	0
56	MG	2A	3077	1/1	0.98	0.16	62,62,62,62	0
57	ZN	19	501	1/1	0.98	0.20	104,104,104,104	0
56	MG	2A	3346	1/1	0.98	0.27	86,86,86,86	0
56	MG	1A	3417	1/1	0.98	0.18	64,64,64,64	0
56	MG	1A	3328	1/1	0.98	0.32	61,61,61,61	0
56	MG	1A	3459	1/1	0.98	0.21	76,76,76,76	0
57	ZN	26	501	1/1	0.98	0.15	107,107,107,107	0
56	MG	1A	3305	1/1	0.98	0.35	61,61,61,61	0
57	ZN	2n	501	1/1	0.98	0.16	118,118,118,118	0
56	MG	2a	3053	1/1	0.98	0.12	74,74,74,74	0
56	MG	2A	3240	1/1	0.99	0.27	61,61,61,61	0
56	MG	2A	3040	1/1	0.99	0.20	95,95,95,95	0
56	MG	2A	3005	1/1	0.99	0.15	85,85,85,85	0
56	MG	1A	3286	1/1	0.99	0.40	76,76,76,76	0
56	MG	2A	3361	1/1	0.99	0.31	62,62,62,62	0
56	MG	1A	3174	1/1	0.99	0.67	73,73,73,73	0
56	MG	1A	3382	1/1	0.99	0.11	91,91,91,91	0
56	MG	2A	3279	1/1	0.99	0.14	80,80,80,80	0
56	MG	1A	3448	1/1	0.99	0.37	74,74,74,74	0
56	MG	1A	3195	1/1	0.99	0.20	71,71,71,71	0
56	MG	1a	1673	1/1	0.99	0.06	99,99,99,99	0
56	MG	2A	3020	1/1	0.99	0.27	88,88,88,88	0
56	MG	1A	3307	1/1	0.99	0.34	71,71,71,71	0
56	MG	2A	3383	1/1	0.99	0.18	76,76,76,76	0
58	SF4	2d	302	8/8	0.99	0.16	99,114,123,127	0
56	MG	1a	1610	1/1	1.00	0.16	104,104,104,104	0

6.5 Other polymers ⓘ

There are no such residues in this entry.