



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:18 AM UTC

PDB ID : 5E81 / pdb_00005e81
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA^{Lys} in the A-site with wobble pair
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-10-13
Resolution : 2.95 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

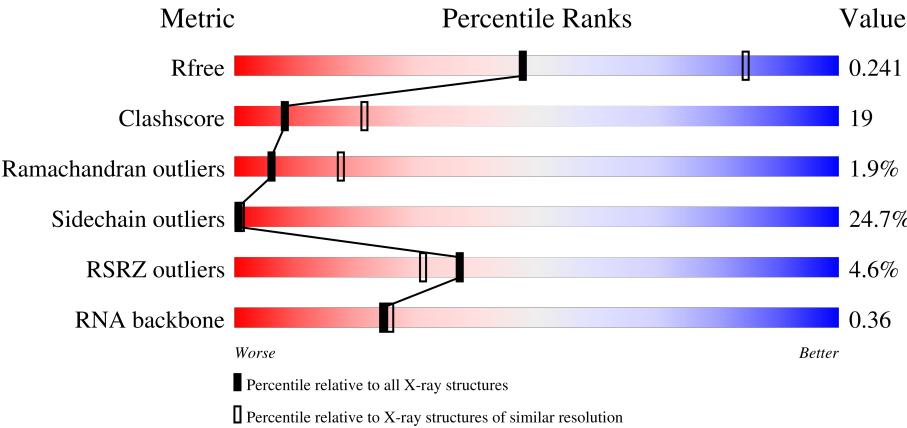
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)
RNA backbone	3983	1046 (3.16-2.76)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	13	1519	2% 35% 48% 14%
1	1G	1519	2% 40% 45% 14%
2	12	256	9% 32% 39% 9% 19%
2	1E	256	9% 34% 41% 13% 10%

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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	
15	6A	89	

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
22	1L	76	
23	2K	77	
23	2L	77	
24	3K	76	
24	3L	76	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	

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Mol	Chain	Length	Quality of chain
28	71	229	
28	79	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	

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Mol	Chain	Length	Quality of chain
40	A8	112	
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	

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Mol	Chain	Length	Quality of chain
53	N8	60	
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	

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	13	1655	-	-	-	X
56	MG	14	3028	-	-	-	X
56	MG	14	3149	-	-	-	X
56	MG	14	3212	-	-	-	X
56	MG	1G	1641	-	-	-	X
56	MG	1G	1656	-	-	-	X
56	MG	1H	3015	-	-	-	X
56	MG	1H	3258	-	-	-	X
57	SF4	32	302	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 297904 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1506	Total	C	N	O	P	0	0	0
			32371	14409	6001	10456	1505			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	207	Total	C	N	O	S	0	0	0
			1696	1083	306	303	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	195	Total	C	N	O	S	0	0	0
			1537	973	297	266	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1698	1064	338	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	149	Total	C	N	O	S	0	0	0
			1139	721	216	198	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	100	Total	C	N	O	S	0	0	0
			837	528	154	152	3			
6	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	140	Total	C	N	O	S	0	0	0
			1120	695	223	196	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
8	72	137	Total	C	N	O	S	0	0	0
			1107	700	214	191	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O		0	0	0
			1000	634	196	170				
9	82	121	Total	C	N	O		0	0	0
			953	605	186	162				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	95	Total	C	N	O	S	0	0	0
			754	471	148	134	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	1A	80	Total	C	N	O	0	0	0
			646	403	129	114			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	2I	111	Total	C	N	O	0	0	0
			823	512	154	154			
11	2A	113	Total	C	N	O	0	0	0
			835	520	156	156			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	0	0	0
			956	603	193	159			
12	3A	122	Total	C	N	O	0	0	0
			956	603	193	159			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	4I	119	Total	C	N	O	0	0	0
			942	582	194	164			
13	4A	111	Total	C	N	O	0	0	0
			893	552	183	156			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	0	0	0
			491	312	104	71			
14	5A	59	Total	C	N	O	0	0	0
			486	309	103	70			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	0	0	0
			729	457	146	124			
15	6A	87	Total	C	N	O	0	0	0
			729	457	146	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	8A	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	67	Total	C	N	O	0	0	0
			544	349	104	91			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			661	422	123	114	2			
19	AA	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	1B	22	Total	C	N	O	0	0	0
			188	116	44	28			

- Molecule 22 is a RNA chain called tRNA-Lys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	S	0	0	0
			1542	691	269	509	72	1			
22	1L	69	Total	C	N	O	P	S	0	0	0
			1477	662	257	488	69	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			

- Molecule 24 is a RNA chain called tRNA-Lys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1483	664	260	490	69			
24	3L	72	Total	C	N	O	P	0	0	0
			1528	684	270	503	71			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	21	Total	C	N	O	P	0	0	0
			464	208	99	136	21			
25	4L	19	Total	C	N	O	P	0	0	0
			419	188	89	123	19			

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2885	Total	C	N	O	P	0	3	0
			62204	27685	11631	20000	2888			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	2855	Total	C	N	O	P	0	0	0
			61505	27372	11512	19766	2855			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1058	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
27	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	133	Total	C	N	O	S	0	0	0
			1033	651	194	187	1			
28	79	57	Total	C	N	O		0	0	0
			456	283	91	82				

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
31	39	204	Total	C	N	O	S	0	0	0
			1602	1022	299	279	2			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	181	Total	C	N	O	S	0	0	0
			1468	937	268	259	4			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
33	59	70	Total	C	N	O	S	0	0	0
			543	341	110	92				

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
34	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	137	Total	C	N	O	S	0	0	0
			1096	706	205	181	4			
35	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
36	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
37	35	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1117	712	211	187	7			
38	45	139	Total	C	N	O	S	0	0	0
			1104	705	209	184	6			

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
39	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
40	65	110	Total	C	N	O	0	0	0
			876	553	175	148			

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	136	Total	C	N	O	S	0	0	0
			1124	700	231	192	1			
41	75	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	C8	115	Total	C	N	O	S	0	0	0
			950	603	199	147	1			
42	85	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			
43	95	100	Total	C	N	O	S	0	0	0
			770	496	140	133	1			

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			
44	A5	111	Total	C	N	O	S	0	0	0
			886	558	174	152	2			

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			743	482	134	126	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	B5	94	Total	C	N	O	0	0	0
			735	477	133	125			

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	103	Total	C	N	O	S	0	0	0
			783	504	148	126	5			
46	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	170	Total	C	N	O	S	0	0	0
			1365	870	246	246	3			
47	D5	133	Total	C	N	O	S	0	0	0
			1079	694	194	189	2			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			
48	E5	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			
49	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
50	G5	69	Total	C	N	O	S	0	0	0
			576	358	116	101	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	L8	58	Total	C	N	O	0	0	0
			459	293	89	77			
51	H5	58	Total	C	N	O	0	0	0
			459	293	89	77			

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	49	Total	C	N	O	S	0	0	0
			376	240	63	68	5			

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	48	Total	C	N	O	S	0	0	0
			369	229	75	60	5			
53	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	P8	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			
54	L5	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Q8	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			
55	M5	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	161	Total	Mg	0	0
			161	161		

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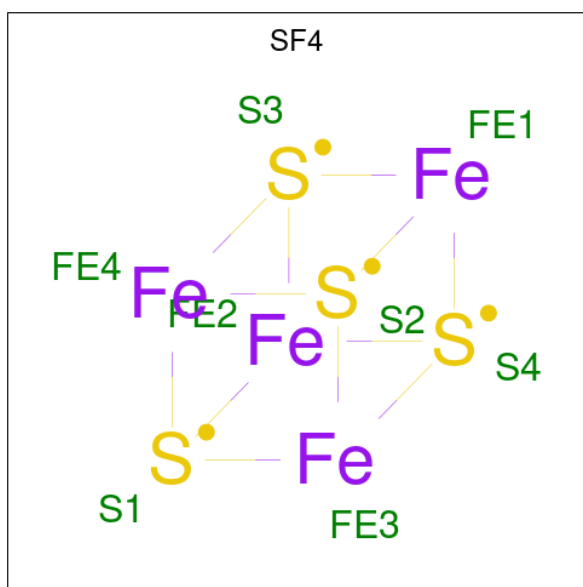
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	5E	1	Total 1	Mg 1	0	0
56	5I	1	Total 1	Mg 1	0	0
56	1K	1	Total 1	Mg 1	0	0
56	2K	3	Total 3	Mg 3	0	0
56	4K	1	Total 1	Mg 1	0	0
56	1H	572	Total 572	Mg 572	0	0
56	16	13	Total 13	Mg 13	0	0
56	11	3	Total 3	Mg 3	0	0
56	21	3	Total 3	Mg 3	0	0
56	41	2	Total 2	Mg 2	0	0
56	78	2	Total 2	Mg 2	0	0
56	88	3	Total 3	Mg 3	0	0
56	98	1	Total 1	Mg 1	0	0
56	F8	1	Total 1	Mg 1	0	0
56	I8	1	Total 1	Mg 1	0	0
56	L8	1	Total 1	Mg 1	0	0
56	P8	1	Total 1	Mg 1	0	0
56	Q8	1	Total 1	Mg 1	0	0
56	1G	126	Total 126	Mg 126	0	0
56	32	1	Total 1	Mg 1	0	0
56	42	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	52	1	Total 1	Mg 1	0	0
56	2A	1	Total 1	Mg 1	0	0
56	2L	3	Total 3	Mg 3	0	0
56	14	471	Total 471	Mg 471	0	0
56	1J	11	Total 11	Mg 11	0	0
56	29	1	Total 1	Mg 1	0	0
56	39	2	Total 2	Mg 2	0	0
56	25	2	Total 2	Mg 2	0	0
56	35	3	Total 3	Mg 3	0	0
56	45	2	Total 2	Mg 2	0	0
56	B5	1	Total 1	Mg 1	0	0
56	E5	3	Total 3	Mg 3	0	0
56	M5	1	Total 1	Mg 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	3E	1	Total	Fe	S	0	0
			8	4	4		
57	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	5I	1	Total	Zn	0	0
			1	1		
58	G8	1	Total	Zn	0	0
			1	1		
58	5A	1	Total	Zn	0	0
			1	1		
58	C5	1	Total	Zn	0	0
			1	1		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	13	389	Total	O	0	0
			389	389		
59	1E	1	Total	O	0	0
			1	1		
59	3E	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	4E	1	Total 1	O 1	0	0
59	8E	3	Total 3	O 3	0	0
59	1I	2	Total 2	O 2	0	0
59	3I	2	Total 2	O 2	0	0
59	4I	2	Total 2	O 2	0	0
59	5I	2	Total 2	O 2	0	0
59	6I	3	Total 3	O 3	0	0
59	7I	1	Total 1	O 1	0	0
59	1F	2	Total 2	O 2	0	0
59	1K	8	Total 8	O 8	0	0
59	2K	6	Total 6	O 6	0	0
59	3K	1	Total 1	O 1	0	0
59	4K	5	Total 5	O 5	0	0
59	1H	1539	Total 1539	O 1539	0	0
59	16	35	Total 35	O 35	0	0
59	11	16	Total 16	O 16	0	0
59	21	7	Total 7	O 7	0	0
59	31	6	Total 6	O 6	0	0
59	41	1	Total 1	O 1	0	0
59	58	2	Total 2	O 2	0	0
59	68	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	78	8	Total 8	O 8	0	0
59	88	8	Total 8	O 8	0	0
59	C8	4	Total 4	O 4	0	0
59	D8	2	Total 2	O 2	0	0
59	F8	2	Total 2	O 2	0	0
59	G8	1	Total 1	O 1	0	0
59	I8	7	Total 7	O 7	0	0
59	J8	2	Total 2	O 2	0	0
59	K8	1	Total 1	O 1	0	0
59	L8	3	Total 3	O 3	0	0
59	P8	1	Total 1	O 1	0	0
59	Q8	8	Total 8	O 8	0	0
59	1G	297	Total 297	O 297	0	0
59	32	2	Total 2	O 2	0	0
59	42	1	Total 1	O 1	0	0
59	52	4	Total 4	O 4	0	0
59	62	3	Total 3	O 3	0	0
59	2A	3	Total 3	O 3	0	0
59	3A	1	Total 1	O 1	0	0
59	6A	1	Total 1	O 1	0	0
59	7A	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	9A	2	Total 2	O 2	0	0
59	BA	5	Total 5	O 5	0	0
59	1L	1	Total 1	O 1	0	0
59	2L	6	Total 6	O 6	0	0
59	4L	5	Total 5	O 5	0	0
59	14	1225	Total 1225	O 1225	0	0
59	1J	12	Total 12	O 12	0	0
59	19	11	Total 11	O 11	0	0
59	29	5	Total 5	O 5	0	0
59	39	7	Total 7	O 7	0	0
59	25	6	Total 6	O 6	0	0
59	35	8	Total 8	O 8	0	0
59	45	4	Total 4	O 4	0	0
59	55	3	Total 3	O 3	0	0
59	85	1	Total 1	O 1	0	0
59	95	1	Total 1	O 1	0	0
59	A5	1	Total 1	O 1	0	0
59	B5	1	Total 1	O 1	0	0
59	C5	3	Total 3	O 3	0	0
59	F5	1	Total 1	O 1	0	0
59	H5	2	Total 2	O 2	0	0

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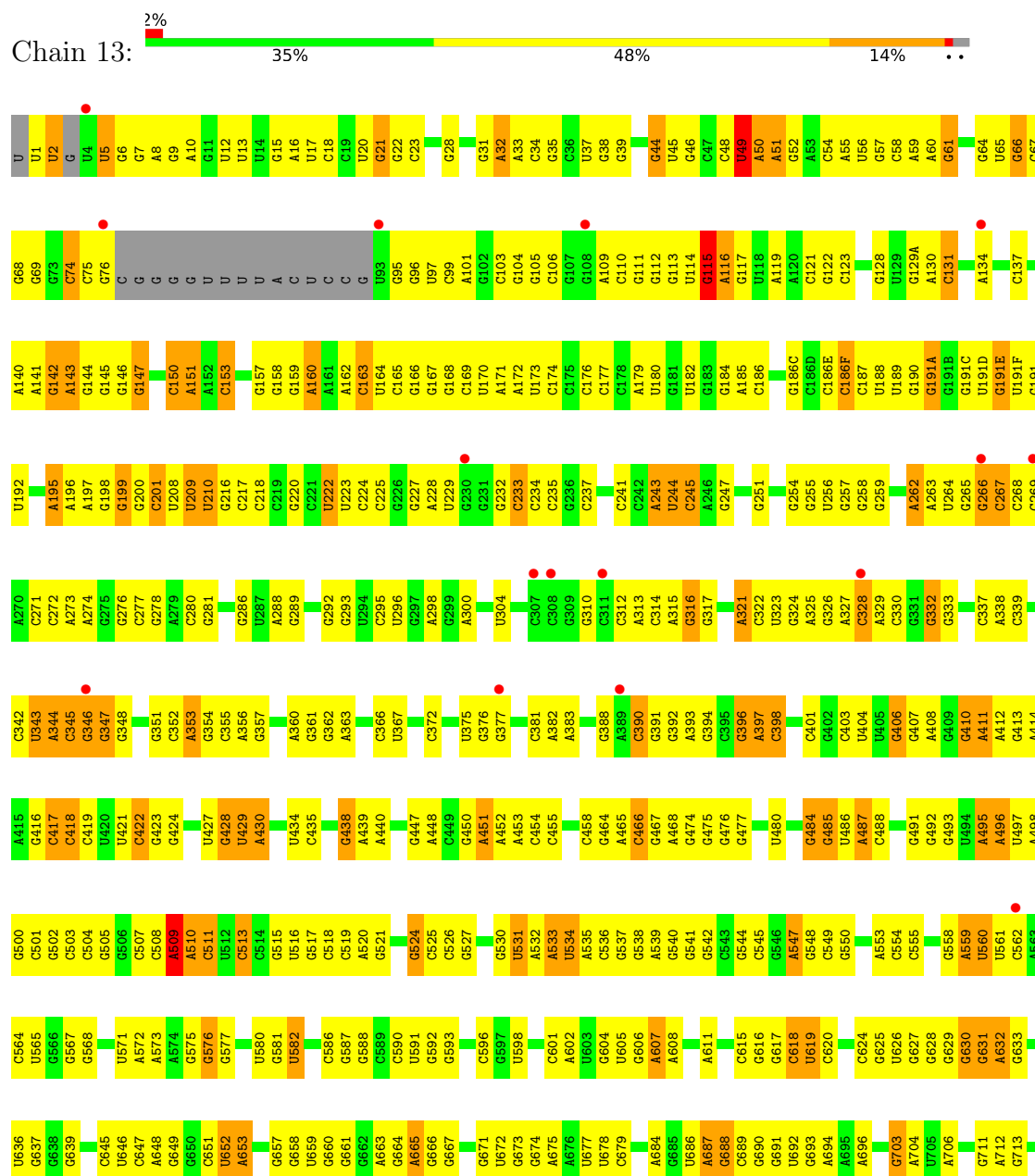
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	L5	3	Total	O	0	0
			3	3		
59	M5	6	Total	O	0	0
			6	6		

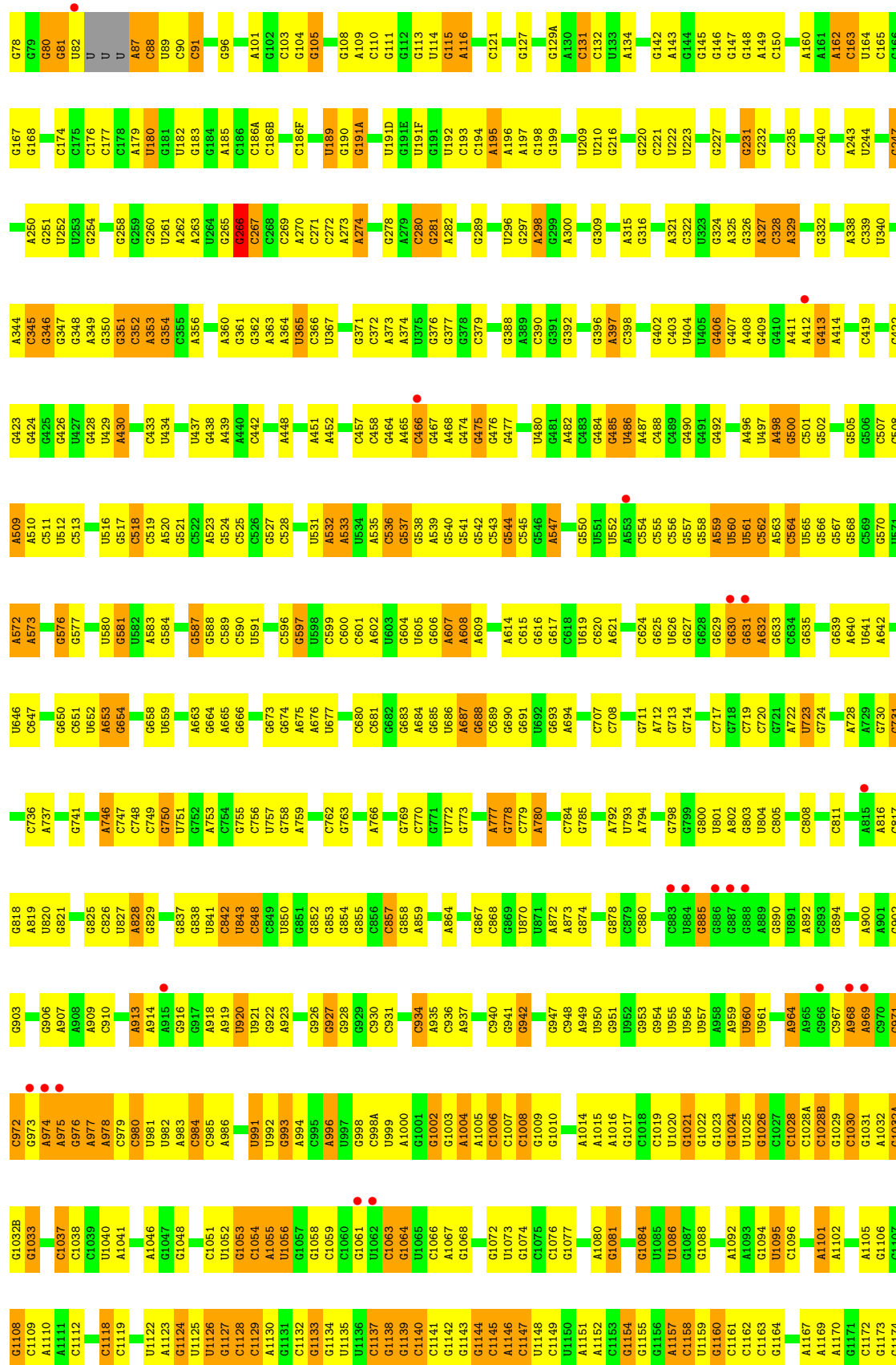
3 Residue-property plots

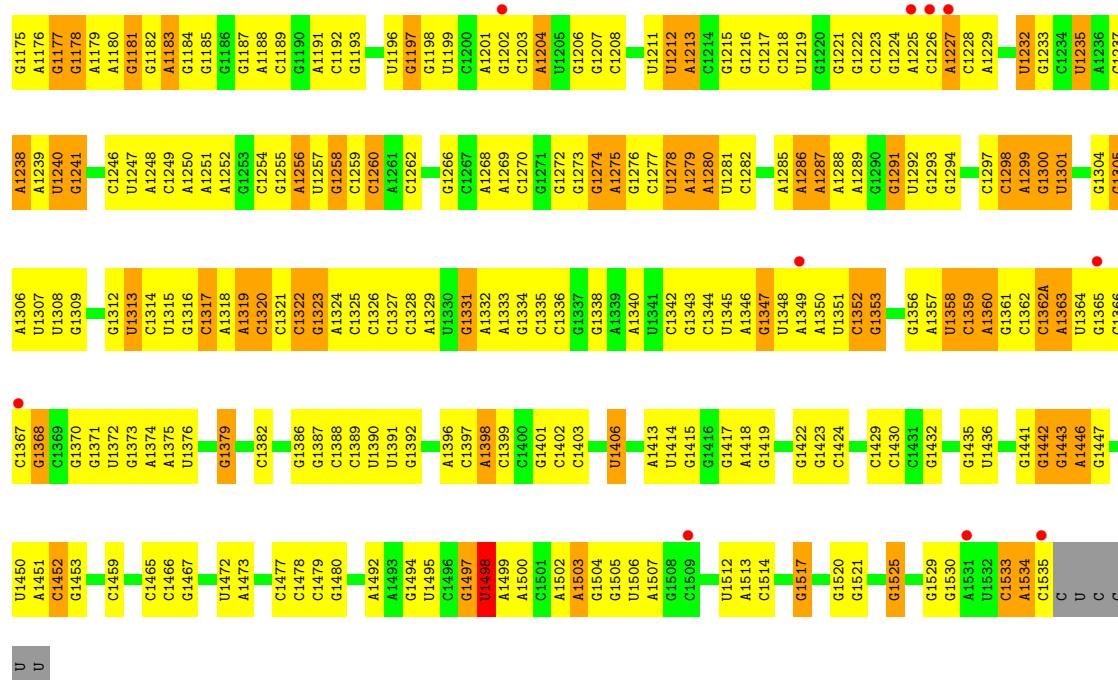
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 16S ribosomal RNA

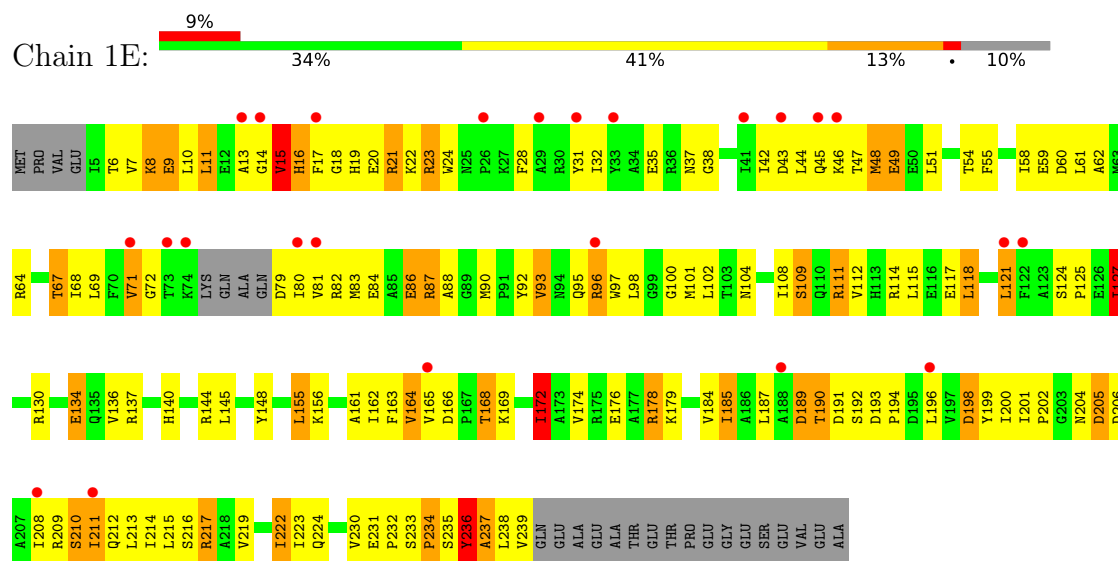




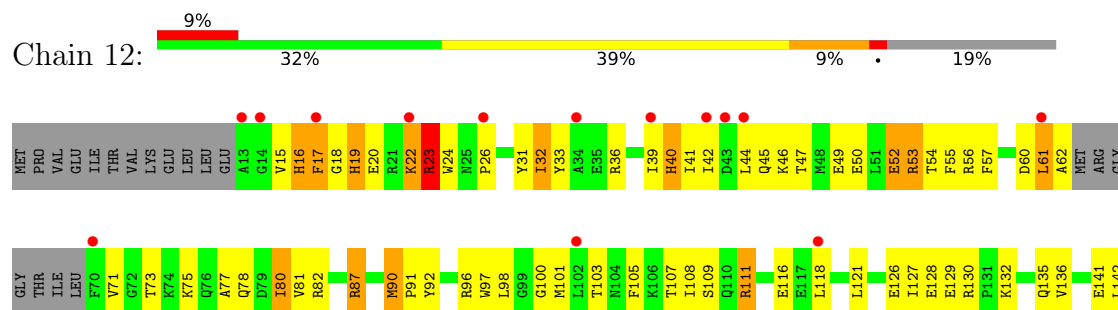


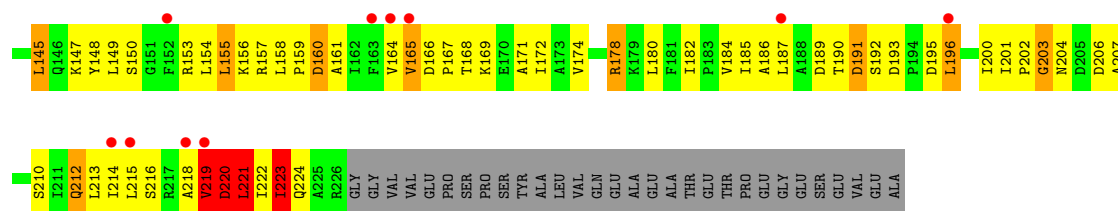


• Molecule 2: 30S ribosomal protein S2

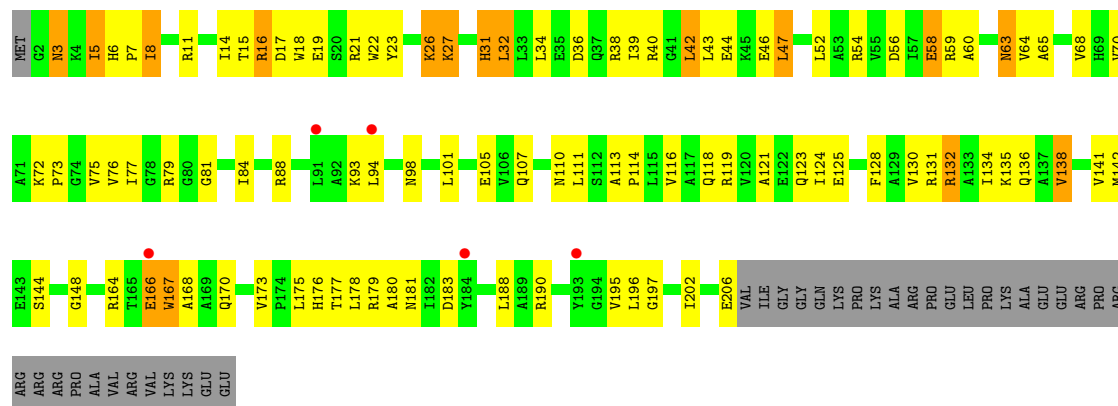
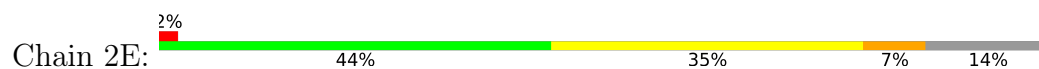


• Molecule 2: 30S ribosomal protein S2

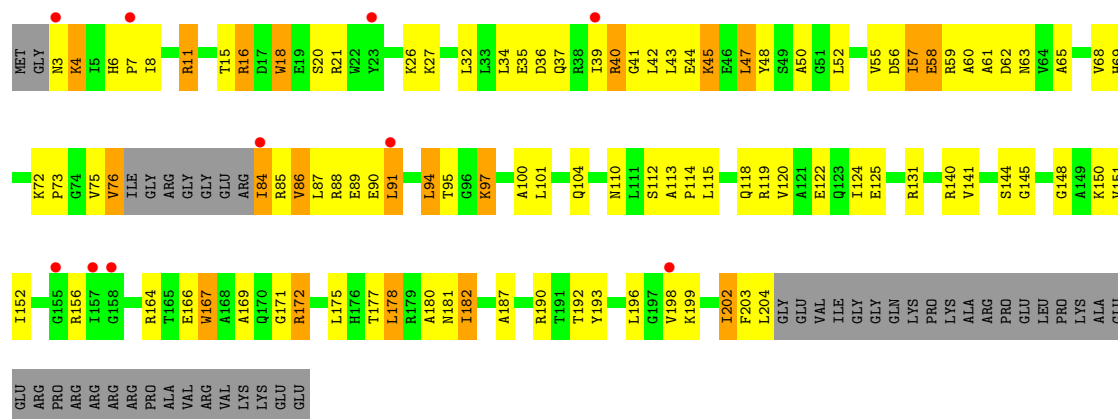




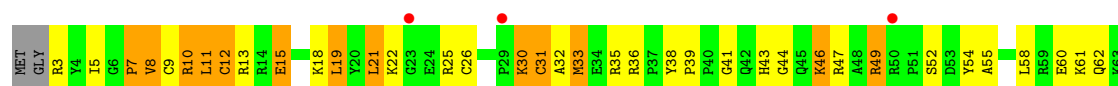
• Molecule 3: 30S ribosomal protein S3

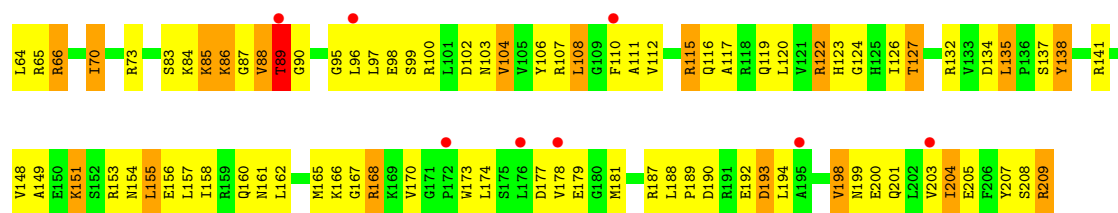


• Molecule 3: 30S ribosomal protein S3

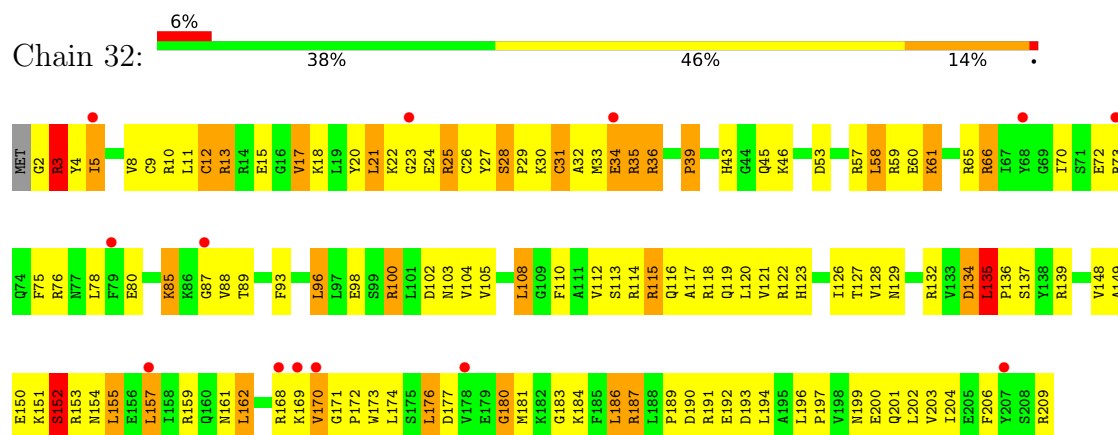


• Molecule 4: 30S ribosomal protein S4

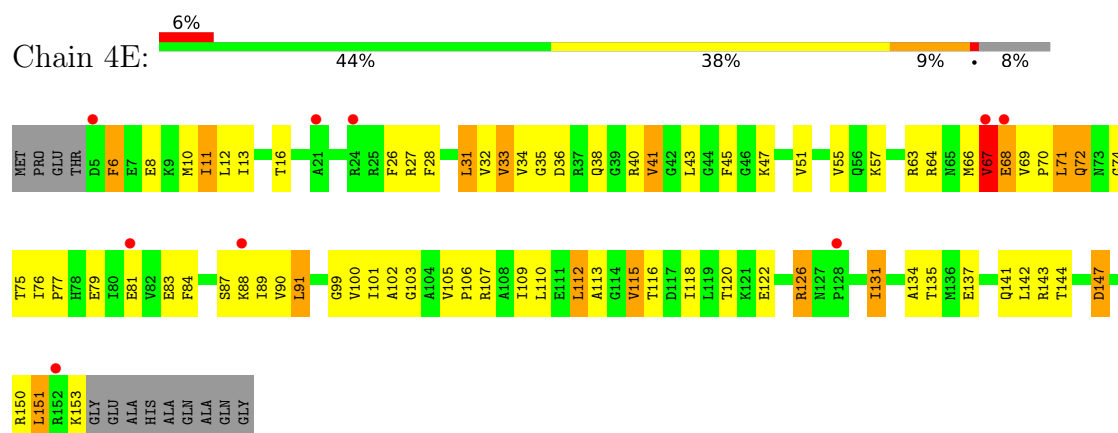




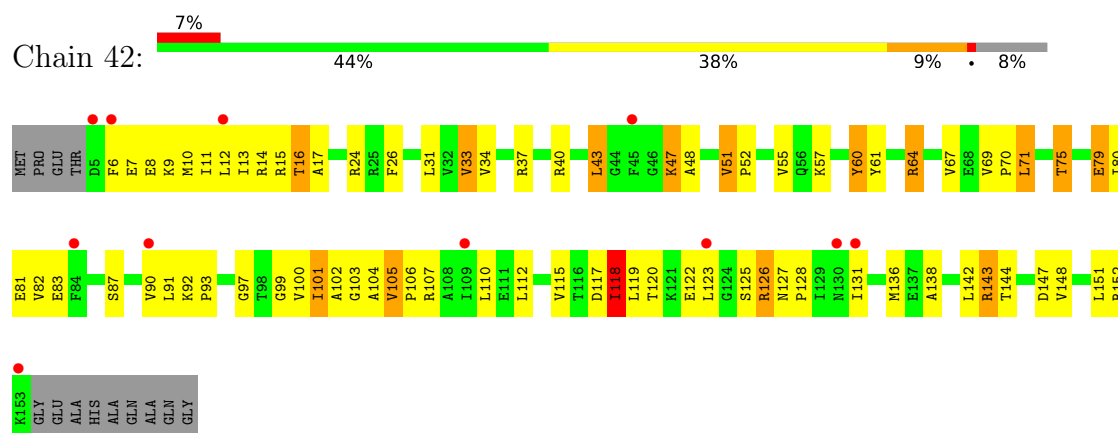
• Molecule 4: 30S ribosomal protein S4



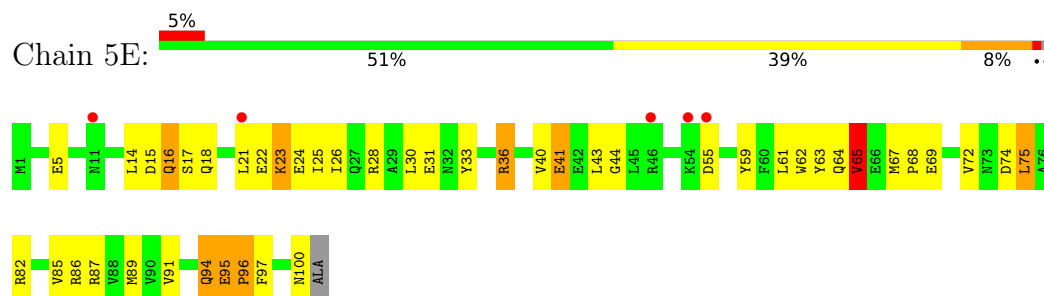
• Molecule 5: 30S ribosomal protein S5



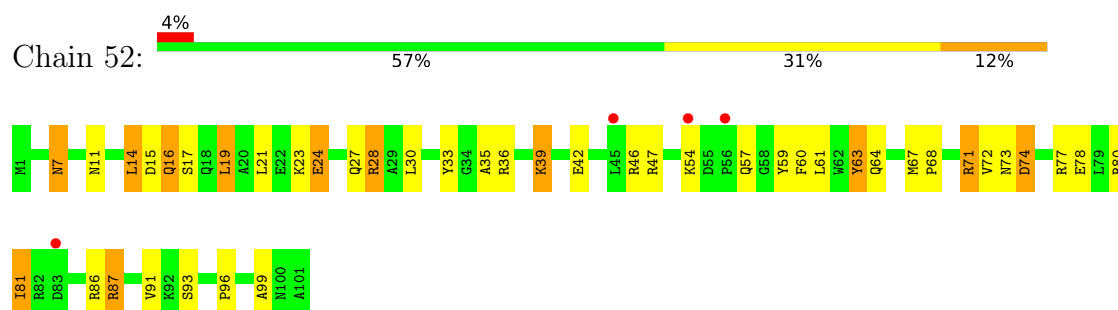
• Molecule 5: 30S ribosomal protein S5



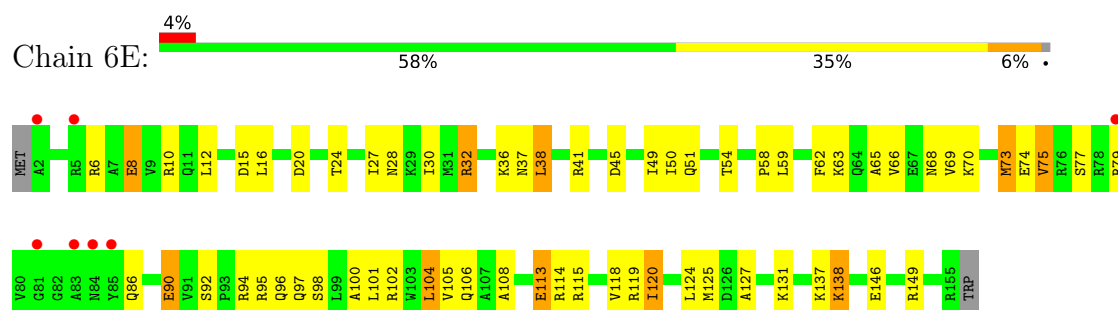
- Molecule 6: 30S ribosomal protein S6



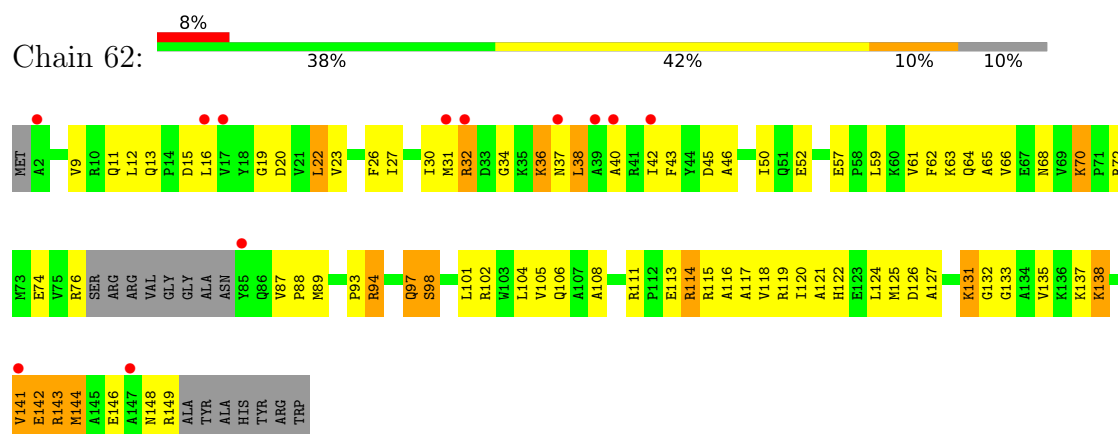
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

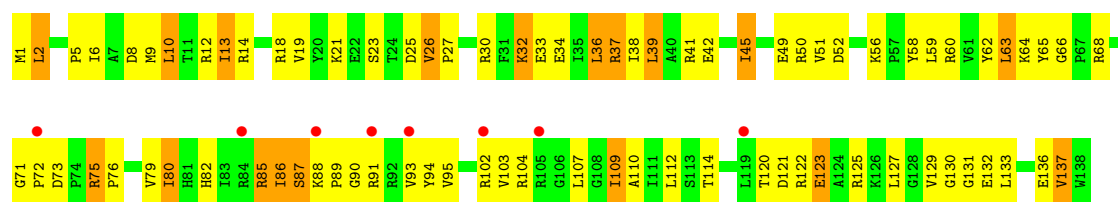


- Molecule 7: 30S ribosomal protein S7

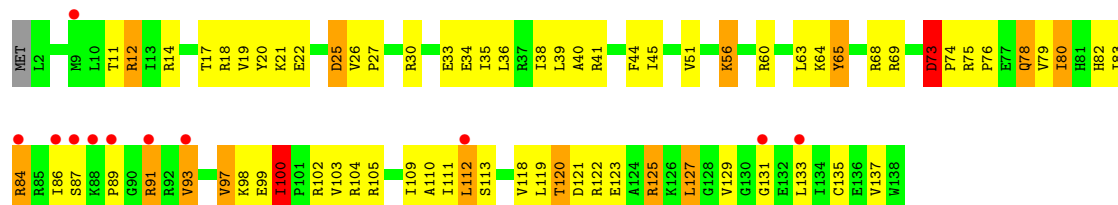


- Molecule 8: 30S ribosomal protein S8

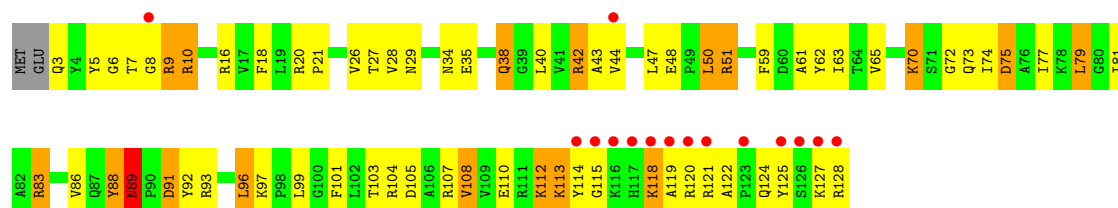




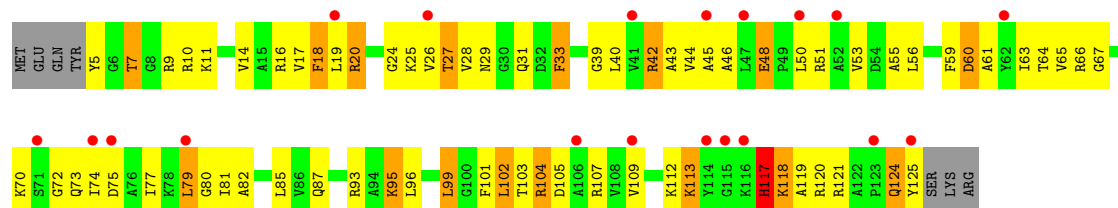
• Molecule 8: 30S ribosomal protein S8



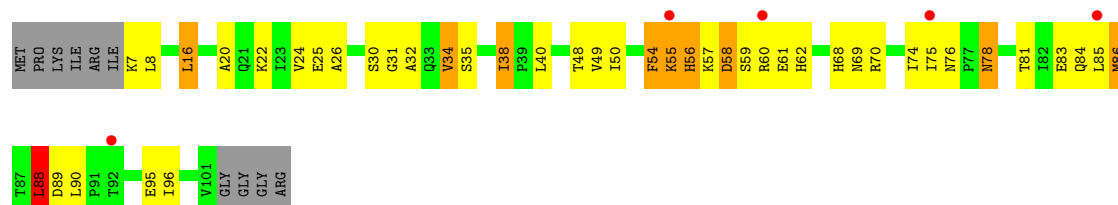
• Molecule 9: 30S ribosomal protein S9



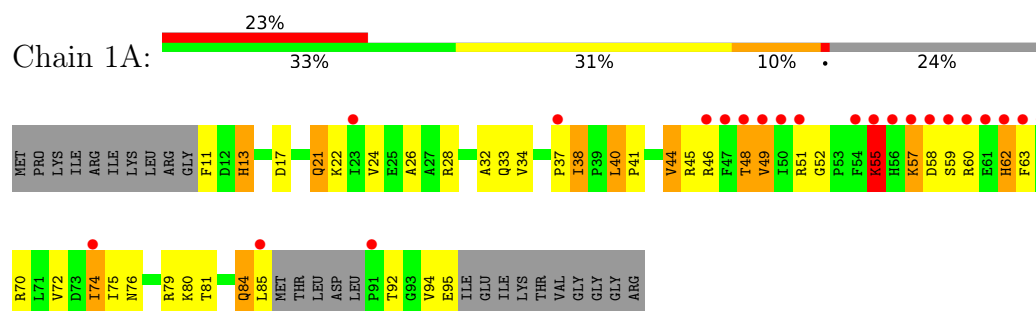
• Molecule 9: 30S ribosomal protein S9



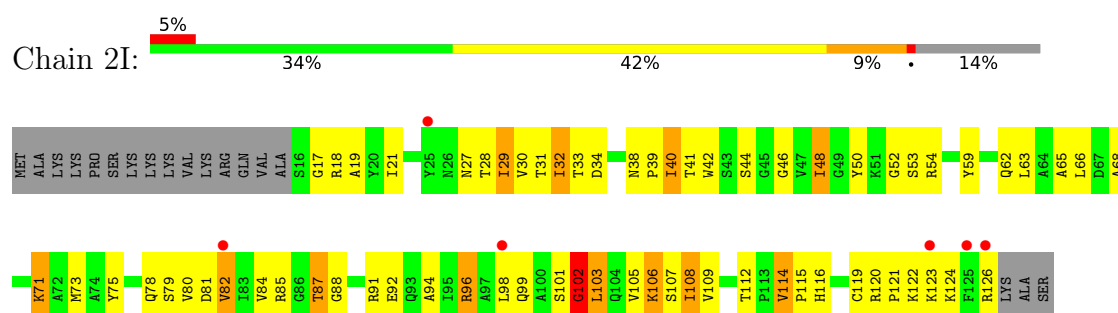
• Molecule 10: 30S ribosomal protein S10



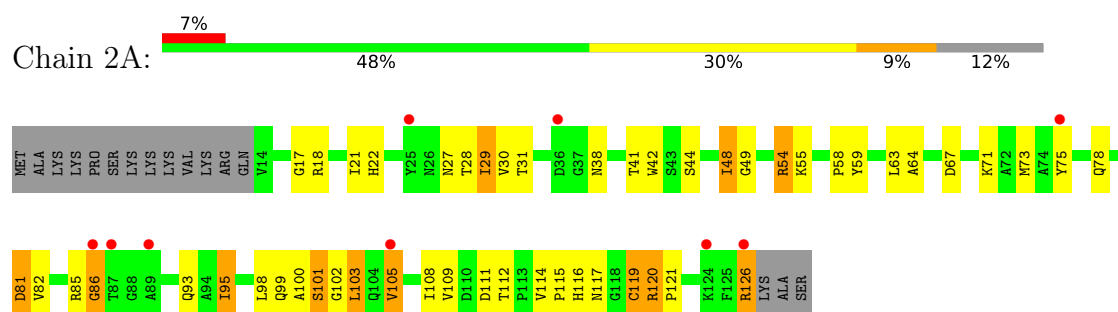
- Molecule 10: 30S ribosomal protein S10



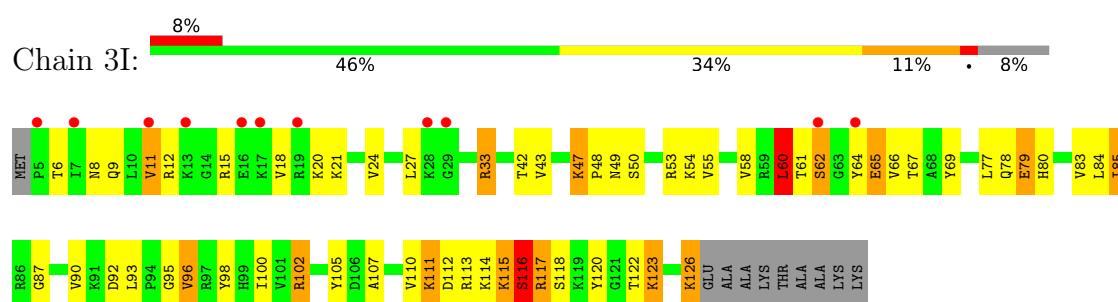
- Molecule 11: 30S ribosomal protein S11



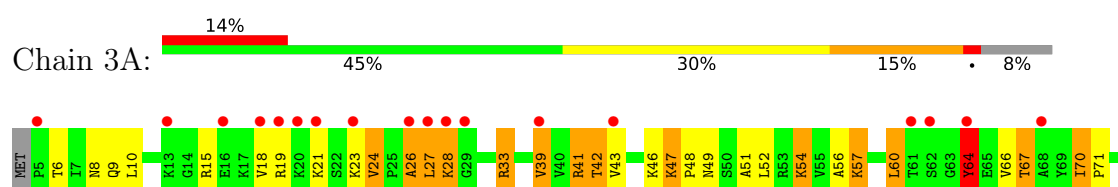
- Molecule 11: 30S ribosomal protein S11

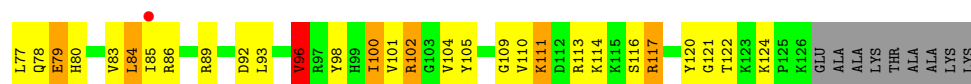


- Molecule 12: 30S ribosomal protein S12

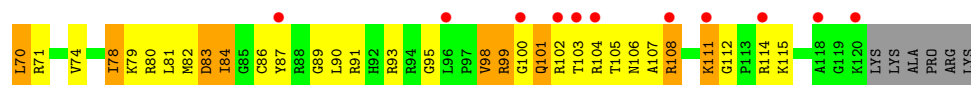
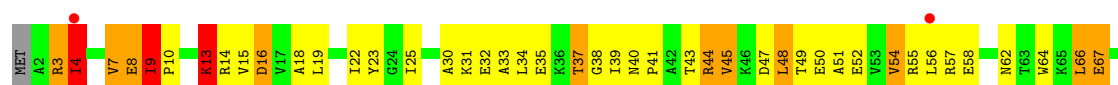


- Molecule 12: 30S ribosomal protein S12

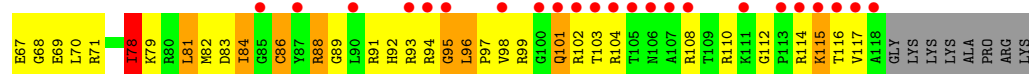




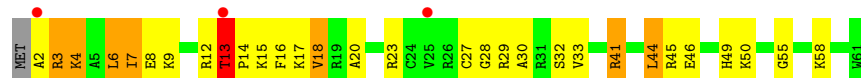
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



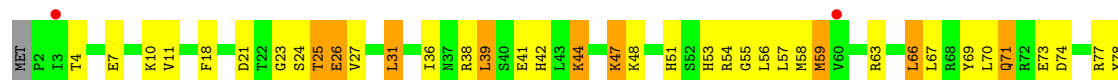
- Molecule 14: 30S ribosomal protein S14 type Z



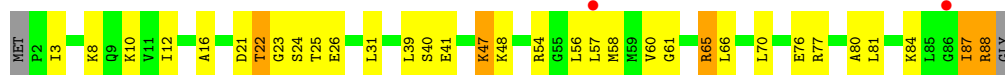
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15



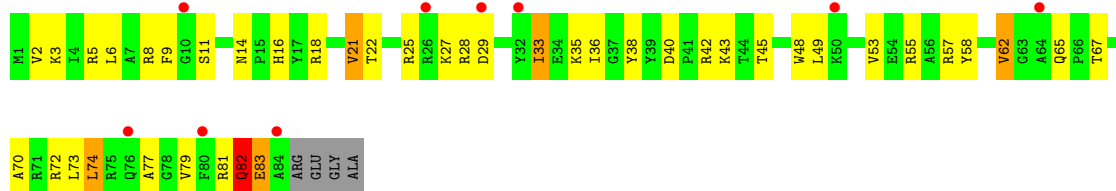
- Molecule 15: 30S ribosomal protein S15



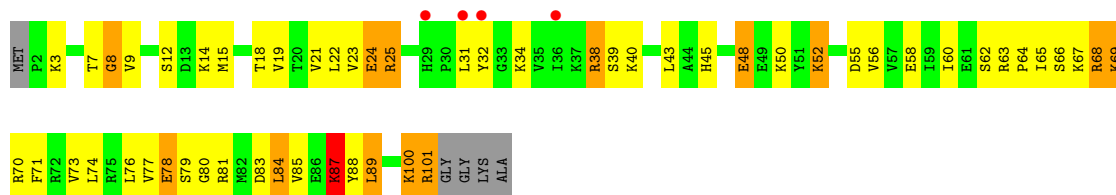
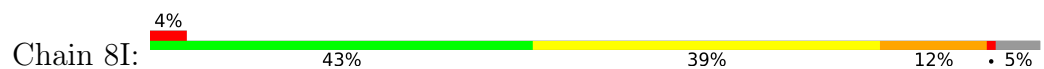
- Molecule 16: 30S ribosomal protein S16



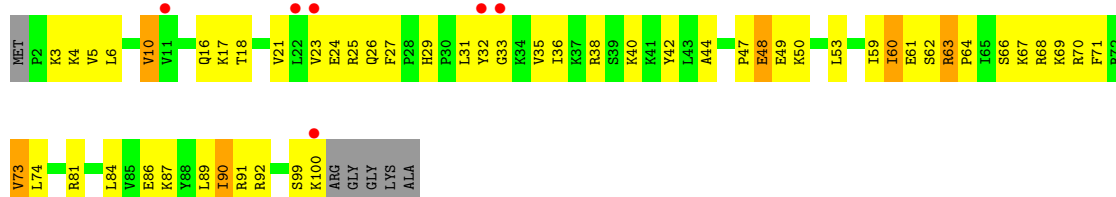
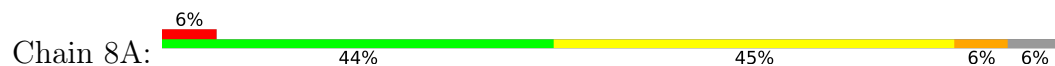
- Molecule 16: 30S ribosomal protein S16



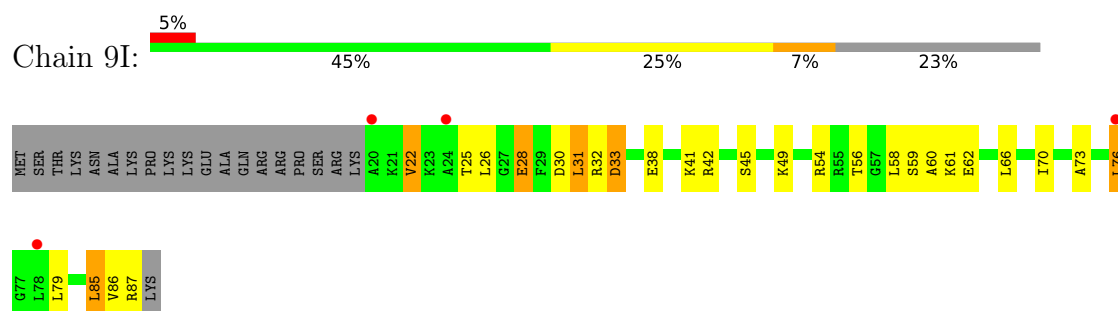
- Molecule 17: 30S ribosomal protein S17



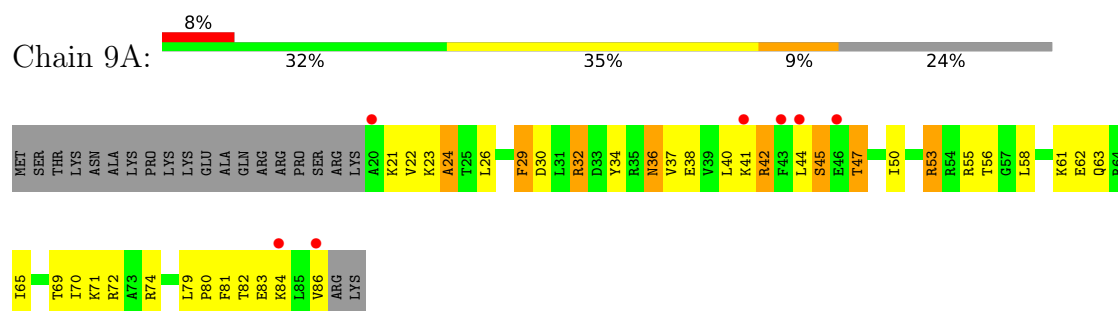
- Molecule 17: 30S ribosomal protein S17



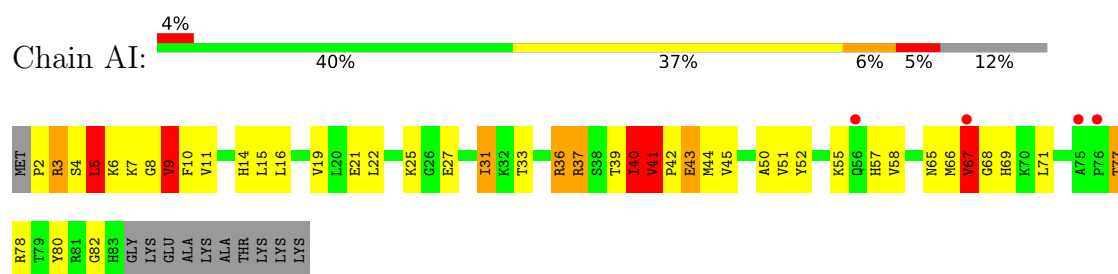
• Molecule 18: 30S ribosomal protein S18



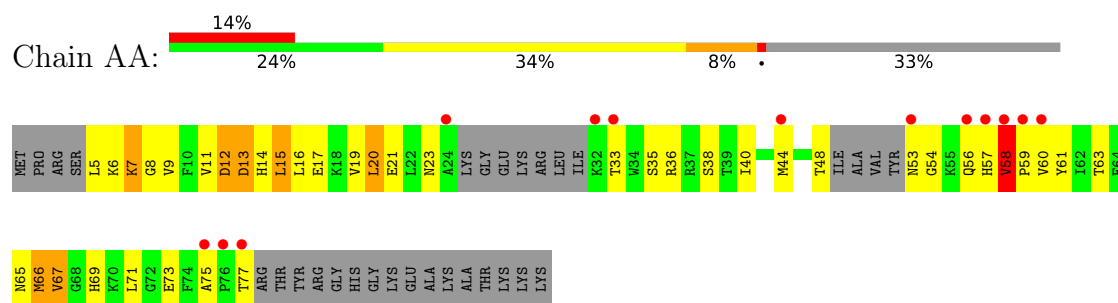
• Molecule 18: 30S ribosomal protein S18



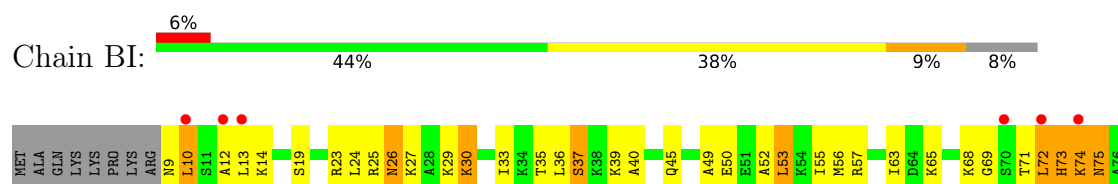
• Molecule 19: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S19

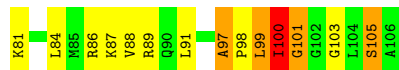


• Molecule 20: 30S ribosomal protein S20





- Molecule 20: 30S ribosomal protein S20



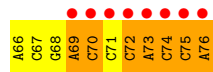
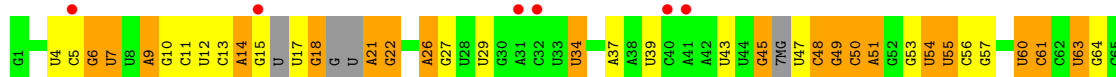
- Molecule 21: 30S ribosomal protein Thx



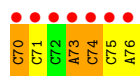
- Molecule 21: 30S ribosomal protein Thx



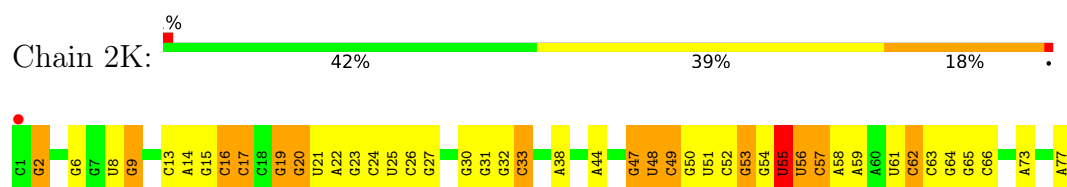
- Molecule 22: tRNA-Lys



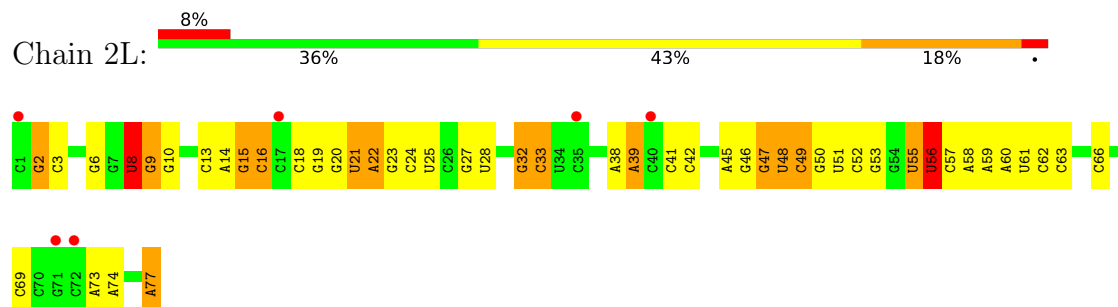
- Molecule 22: tRNA-Lys



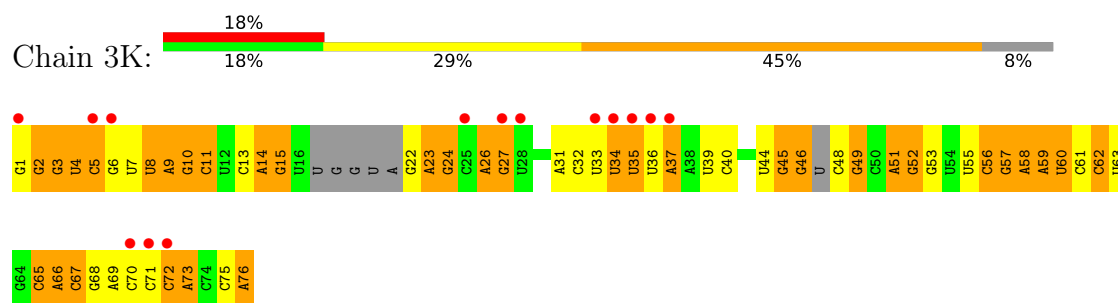
- Molecule 23: tRNA-fMet



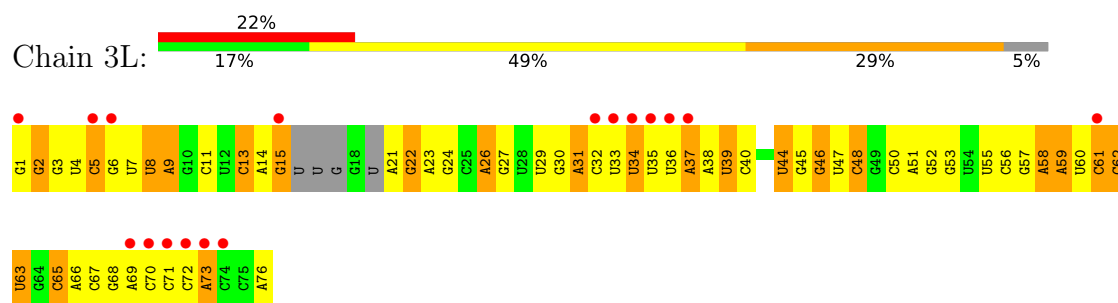
- Molecule 23: tRNA-fMet



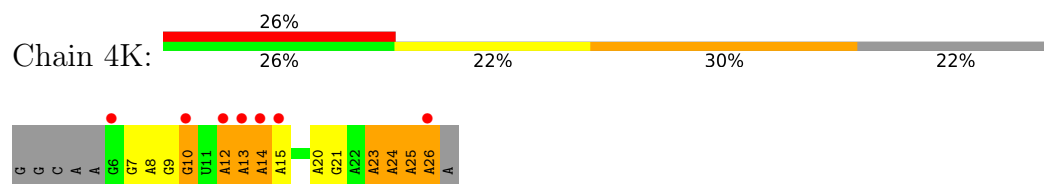
- Molecule 24: tRNA-Lys



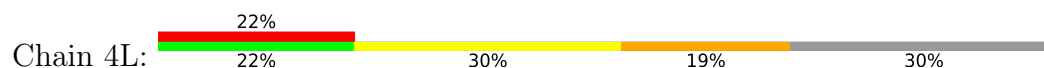
- Molecule 24: tRNA-Lys



- Molecule 25: mRNA



- Molecule 25: mRNA



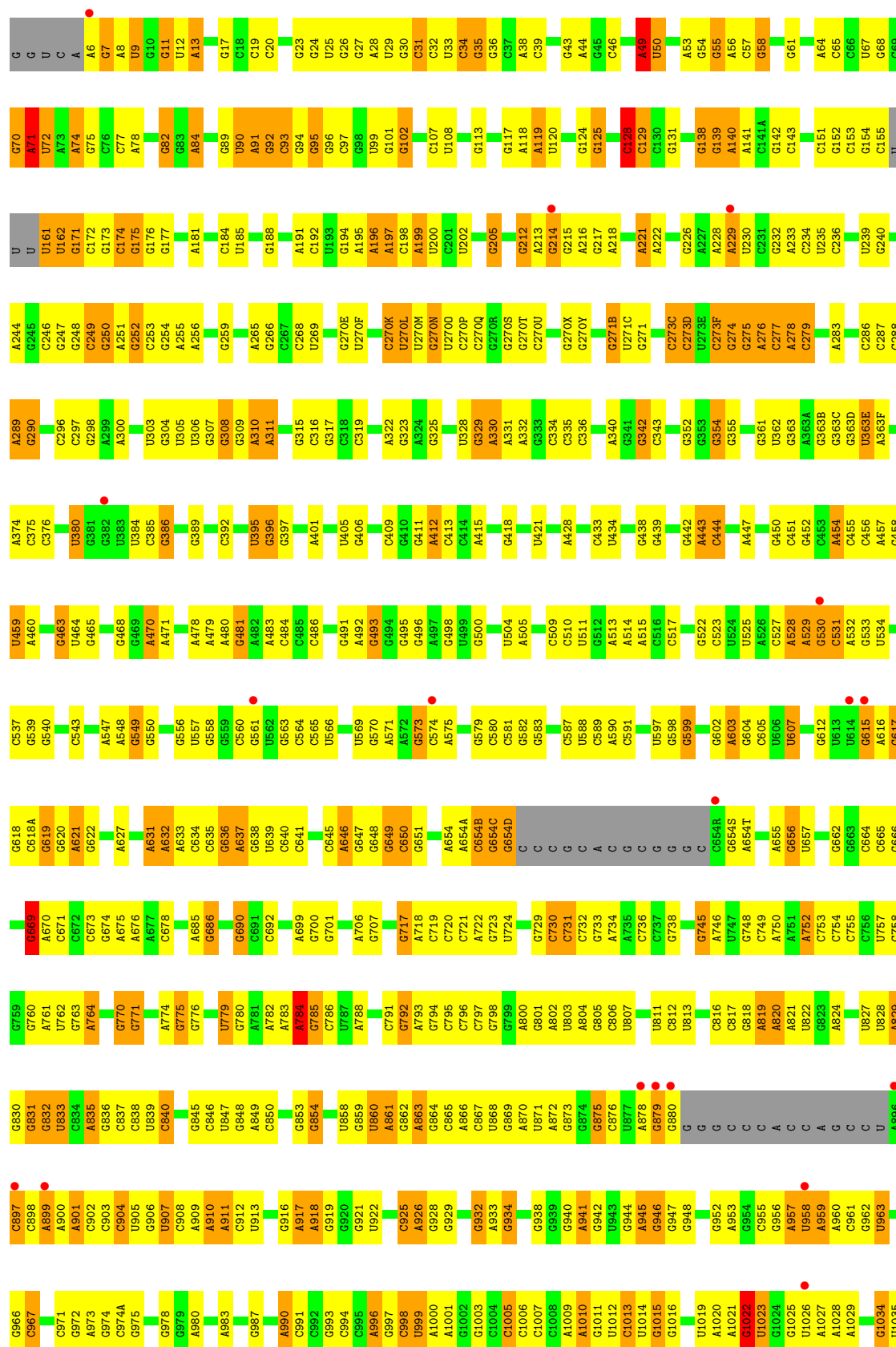


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• Molecule 26: 23S ribosomal RNA



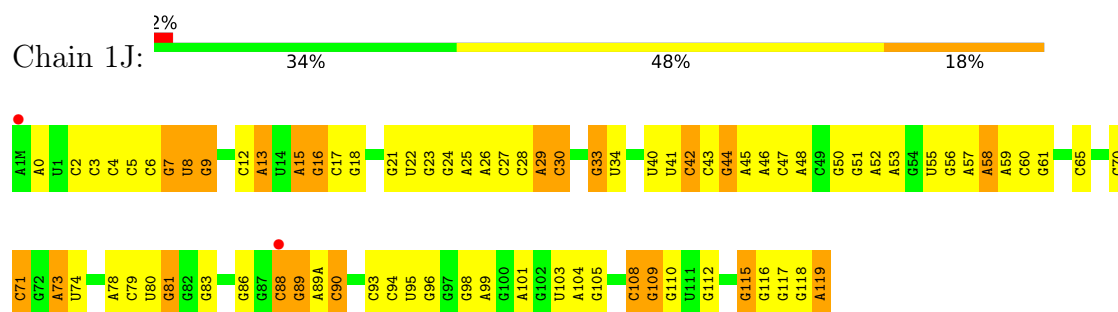


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U2068	G1826	G1759	G1759	G1654	G1582	A1496	G1421	A1354	G1279	G1202	G1136	C1072
G2069	G1827	G1760	G1760	G1655	G1583	G1497	G1422			G1137	G1137	A1073
C2070	G1828	G1761	G1761	G1656	A1584	G1498	G1423	U1357	A1287	A1204	G1138	G1074
G2001	G1829	G1762	G1762	G1657	A1585	G1500	G1424	G1358	U1288	G1205	G1139	C1075
A2002	G1830	G1763	G1763	G1658	A1586	G1501	G1425	A1359	C1289		C1140	C1076
G2003	G1831	G1764	G1764	G1659	A1587	C1505	G1426		C1290	A1210	U1141	A
U2074	G1832	G1765	G1765	G1660	A1588	C1506	A1427	G1364	C1291	U1211	U1142	U
U2075	G1833	G1766	G1766	G1661	A1589	C1507	C1428	A1365	U1292	G1212	A1142A	C
U2076	G1834	G1767	G1767	G1662	G1593	A1508	G1429	A1366	C1293	A1213	A1143	A
A2077	G1835	G1768	G1768	G1663	G1594	C1509	C1430	A1367		A1214	G1144	U
C2078	G1836	G1769	G1769	G1664	G1595	A1510	U1431	G1368	C1297	G1215	C1145	U
G2081	G1837	G1770	G1770	G1665	A1596	A1511		G1369		G1216		U
A2082	G1838	G1771	G1771	G1666	A1597	C1515	A1434	C1370	U1300	A1148	A1148	A
G2083	G1839	G1772	G1772	G1667	A1598	C1516	G1435	A1301	A1302	G1149	A1085	A1086
U2086	G1840	G1773	G1773	G1668	A1599	U1516	G1436	U1372	G1303	C1151	G1087	G1087
G2087	G1841	G1774	G1774	G1669	A1600	G1519	G1443	G1374		C1152	A1088	
U2088	G1842	G1775	G1775	G1670	A1601	U1520	G1444	C1375	C1306	C1153	G1089	
U2089	G1843	G1776	G1776	G1671	A1602	G1521	G1445			C1154	U1090	U1090
A2019	G1844	G1777	G1777	G1672	A1603	G1522	A1444A	A1379	G1309	A1155	G1091	G1091
A2020	G1845	G1778	G1778	G1673	A1604	U1523	C1445	G1380	G1229	A1156	G1092	G1092
C2021	G1846	G1779	G1779	G1674	A1605	G1524	G1448	G1381	U1312	G1157	G1093	G1093
U2022	G1847	G1780	G1780	G1675	A1606	U1525	G1449	G1382	U1313	C1158	U	
G2023	G1848	G1781	G1781	G1676	A1607	G1526	A1450	C1383	C1314	U1159	A	A
G2024	G1849	G1782	G1782	G1677	A1608	G1527	G1449A	G1384	G1315	G1239	G1160	G1160
C2025	G1850	G1783	G1783	G1678	A1609	U1528		G1385	U1316	U1240	U	U
G2029	G1851	G1784	G1784	G1679	A1610	G1529	G1450					
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A2031	G1853	G1786	G1786	G1681	A1612	G1531						
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	G1866	G1799	G1799	G1694	A1625	G1544						
	G1867	G1800	G1800	G1695	A1626	G1545						
	G1868	G1801	G1801	G1696	A1627	G1546						
	G1869	G1802	G1802	G1697	A1628	G1547						
	G1870	G1803	G1803	G1698	A1629	G1548						
	G1871	G1804	G1804	G1699	A1630	G1549						
	G1872	G1805	G1805	G1700	A1631	G1550						
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	G1890	G1823	G1823	G1718	A1649	G1568						
	G1891	G1824	G1824	G1719	A1650	G1569						
	G1892	G1825	G1825	G1720	A1651	G1570						
	G1893	G1826	G1826	G1721	A1652	G1571						
	G1894	G1827	G1827	G1722	A1653	G1572						
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	G1896	G1829	G1829	G1724	A1655	G1574						
	G1897	G1830	G1830	G1725	A1656	G1575						
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	G1899	G1832	G1832	G1727	A1658	G1577						
	G1900	G1833	G1833	G1728	A1659	G1578						
	G1901	G1834	G1834	G1729	A1660	G1579						
	G1902	G1835	G1835	G1730	A1661	G1580						
	G1903	G1836	G1836	G1731	A1662	G1581						
	G1904	G1837	G1837	G1732	A1663	G1582						
	G1905	G1838	G1838	G1733	A1664	G1583						
	G1906	G1839	G1839	G1734	A1665	G1584						
	G1907	G1840	G1840	G1735	A1666	G1585						
	G1908	G1841	G1841	G1736	A1667	G1586						
	G1909	G1842	G1842	G1737	A1668	G1587						
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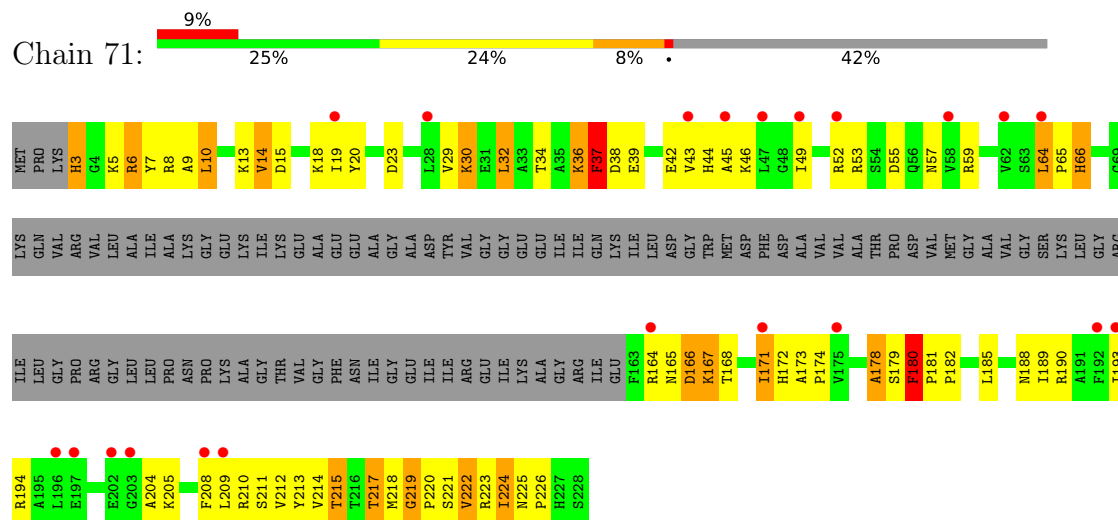


Response	Percentage
Yes, more action	36%
No, not more action	49%
Don't know	15%

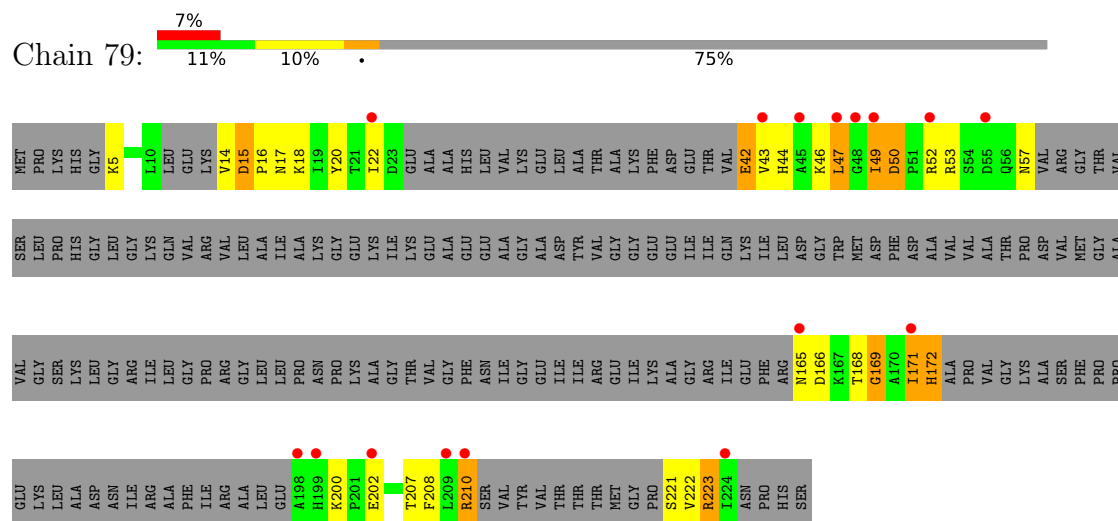




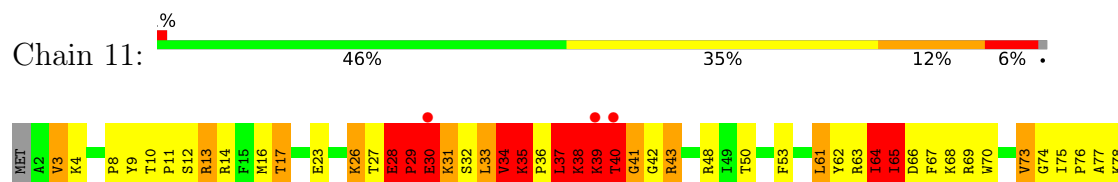
• Molecule 28: 50S ribosomal protein L1

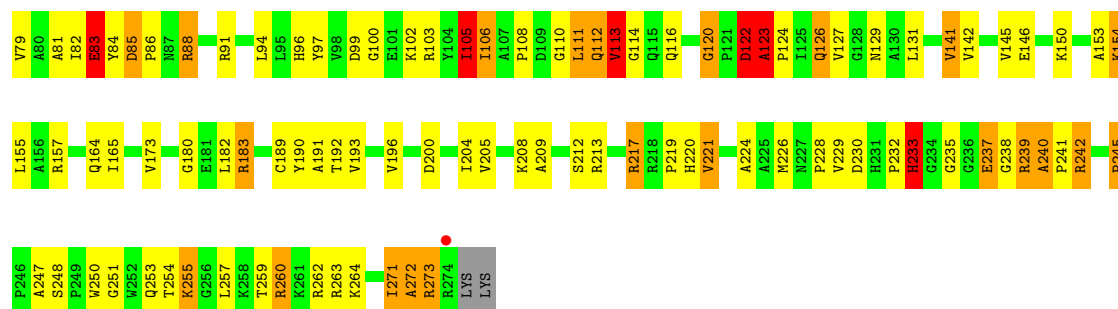


• Molecule 28: 50S ribosomal protein L1

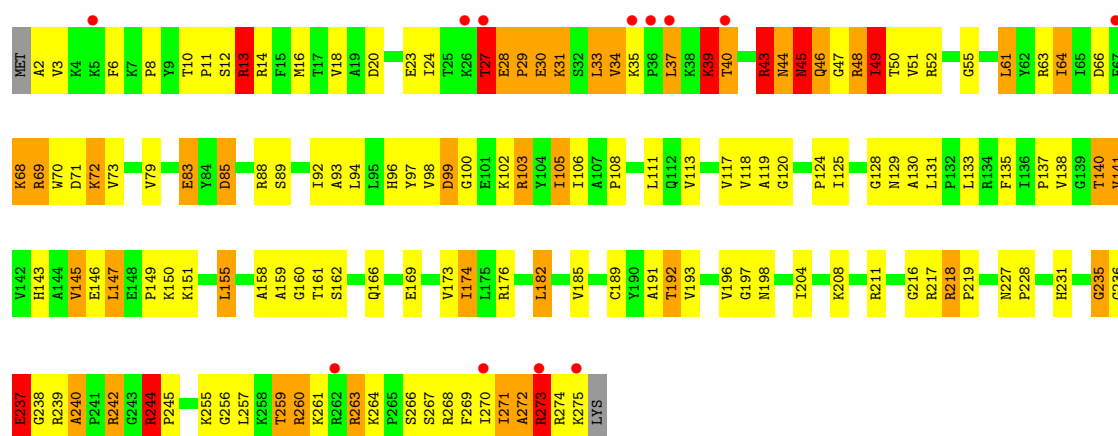


• Molecule 29: 50S ribosomal protein L2

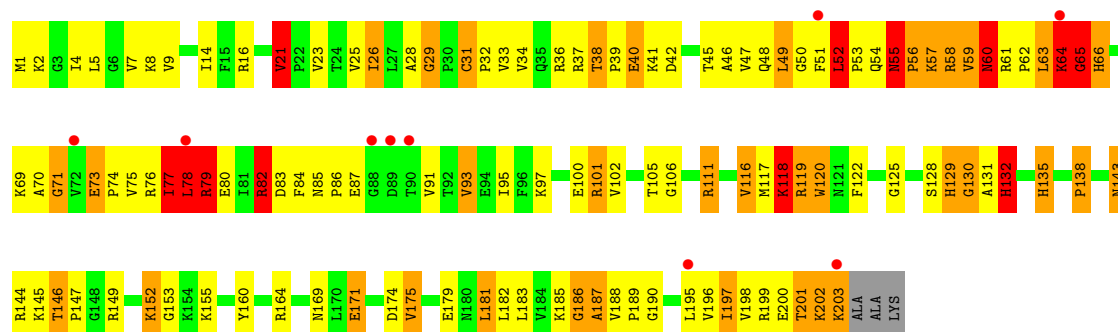




• Molecule 29: 50S ribosomal protein L2

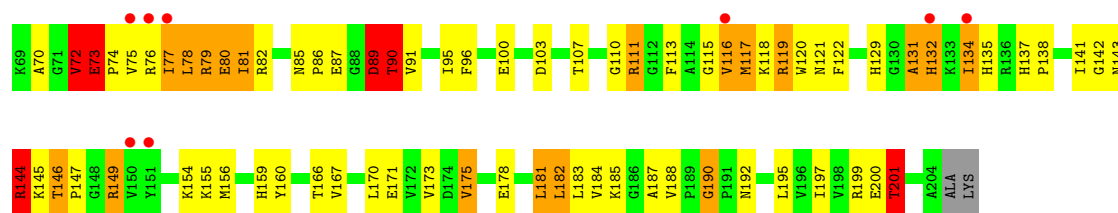


• Molecule 30: 50S ribosomal protein L3

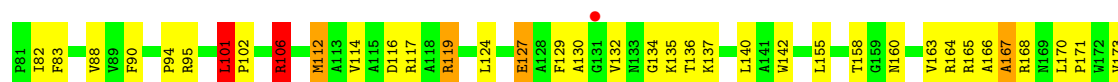


• Molecule 30: 50S ribosomal protein L3

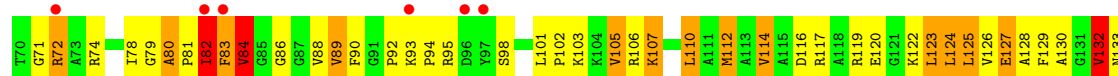
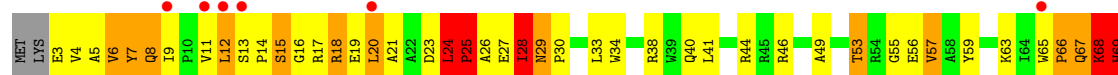




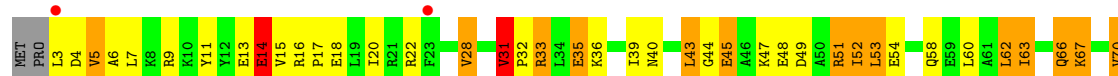
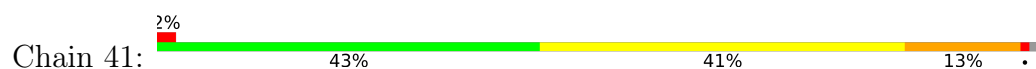
• Molecule 31: 50S ribosomal protein L4



• Molecule 31: 50S ribosomal protein L4

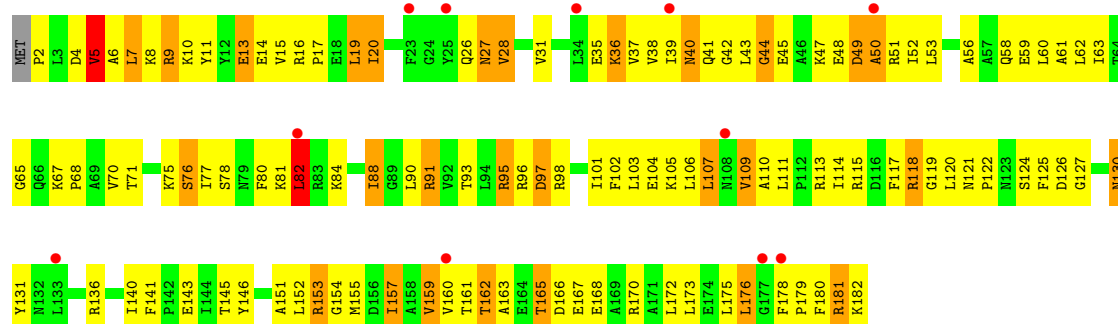


• Molecule 32: 50S ribosomal protein L5

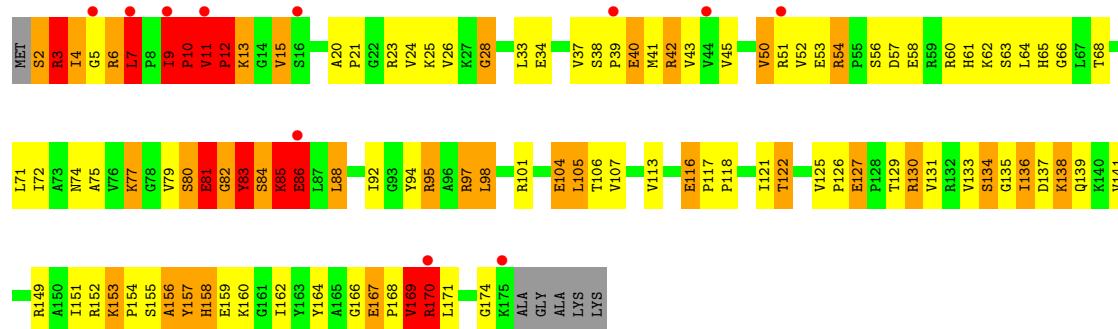




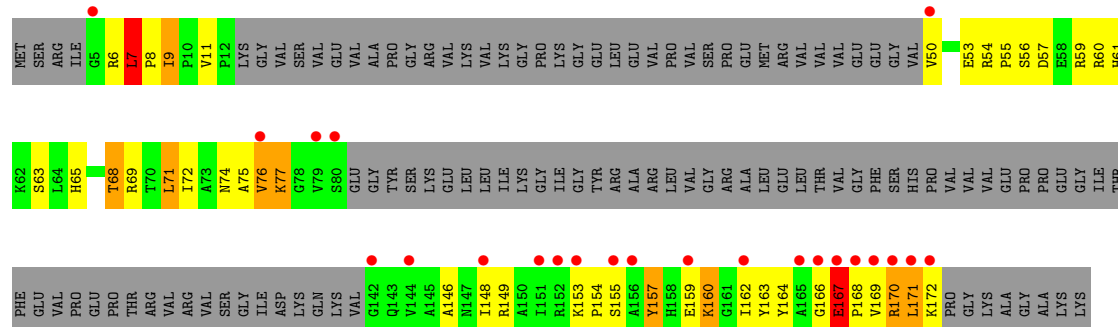
• Molecule 32: 50S ribosomal protein L5



• Molecule 33: 50S ribosomal protein L6

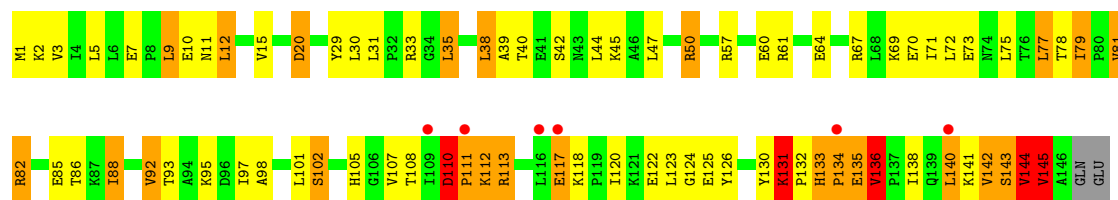


• Molecule 33: 50S ribosomal protein L6

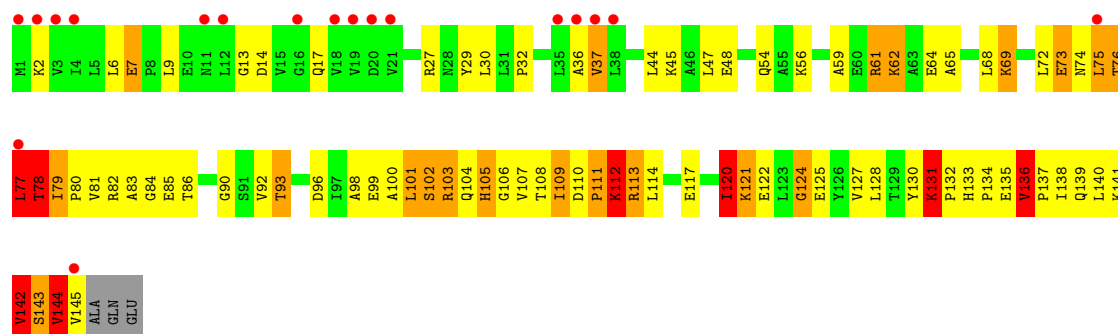
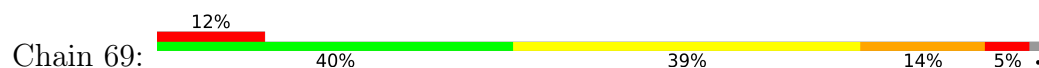


• Molecule 34: 50S ribosomal protein L9

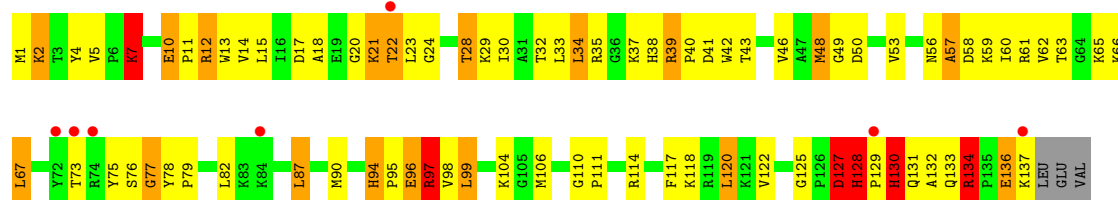




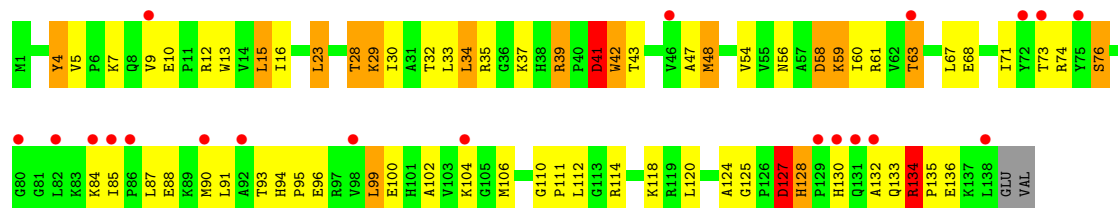
• Molecule 34: 50S ribosomal protein L9



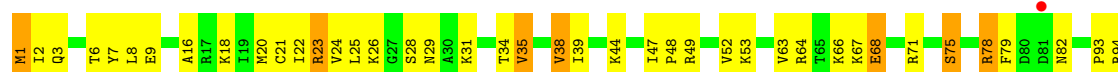
• Molecule 35: 50S ribosomal protein L13



• Molecule 35: 50S ribosomal protein L13

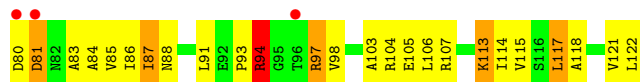


• Molecule 36: 50S ribosomal protein L14

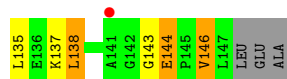
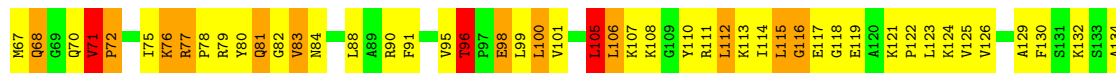
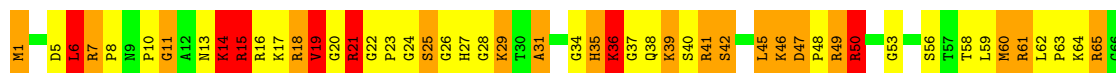




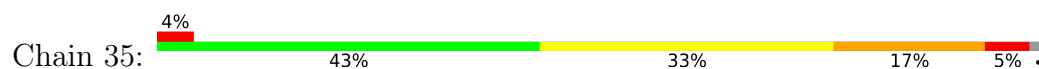
- Molecule 36: 50S ribosomal protein L14



- Molecule 37: 50S ribosomal protein L15



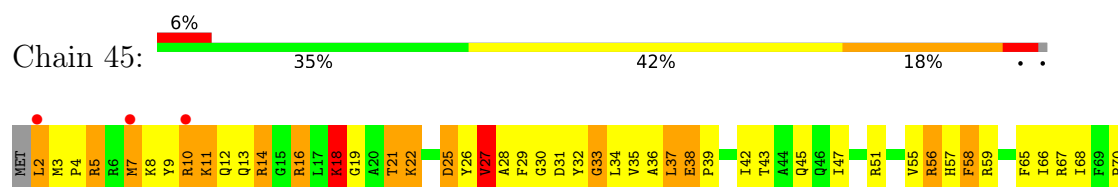
- Molecule 37: 50S ribosomal protein L15



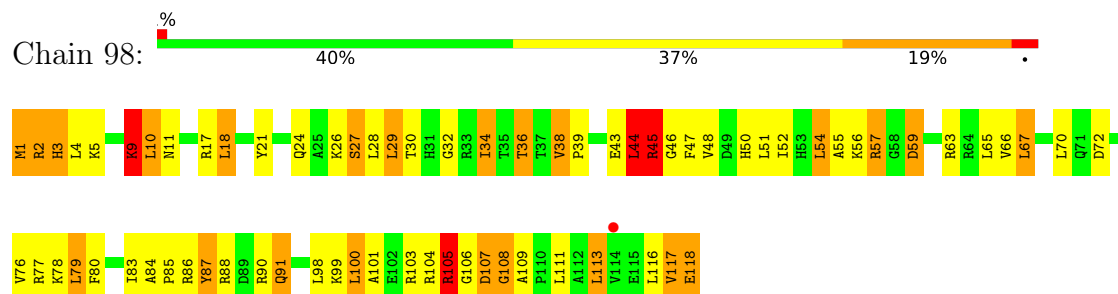
- Molecule 38: 50S ribosomal protein L16



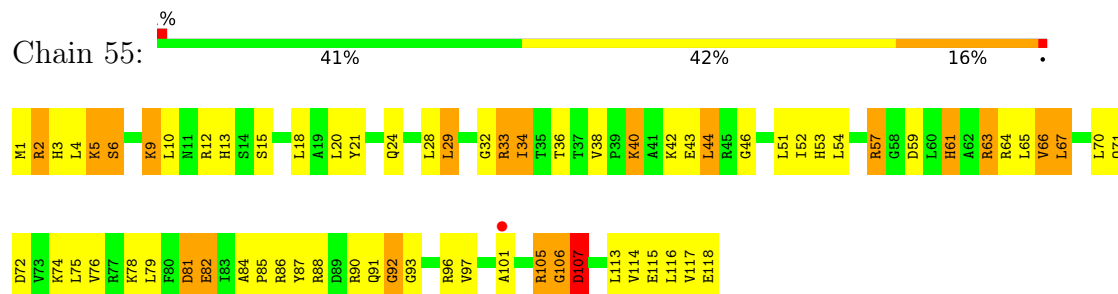
- Molecule 38: 50S ribosomal protein L16



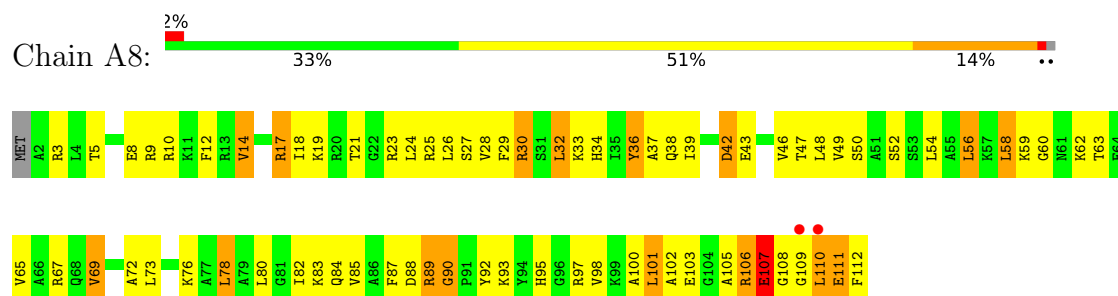
• Molecule 39: 50S ribosomal protein L17



• Molecule 39: 50S ribosomal protein L17

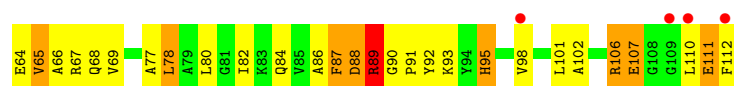


• Molecule 40: 50S ribosomal protein L18

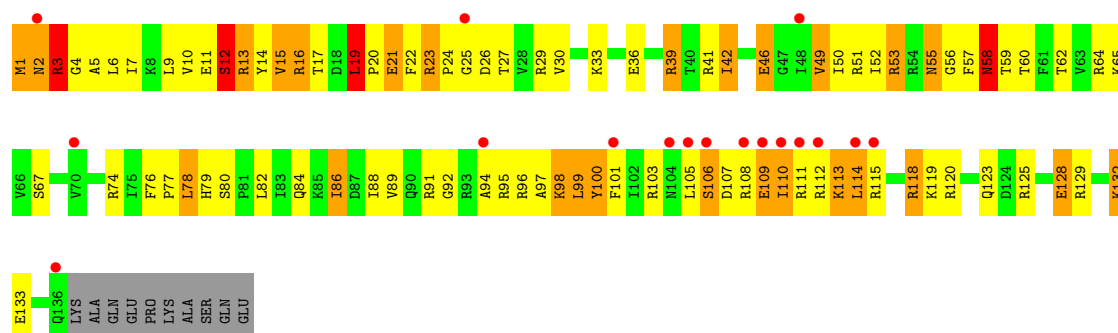


• Molecule 40: 50S ribosomal protein L18

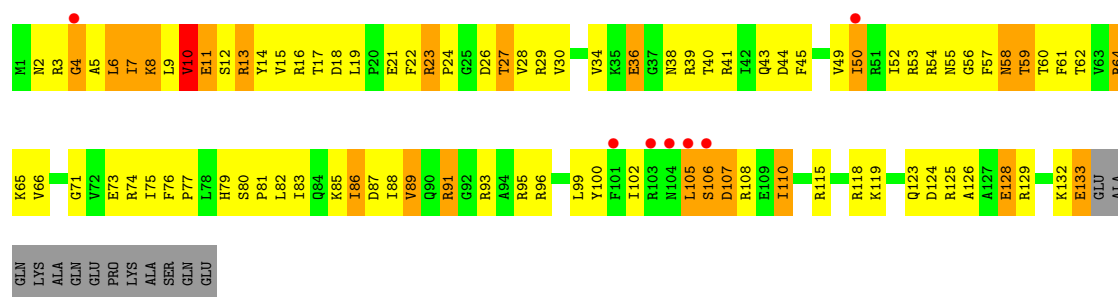




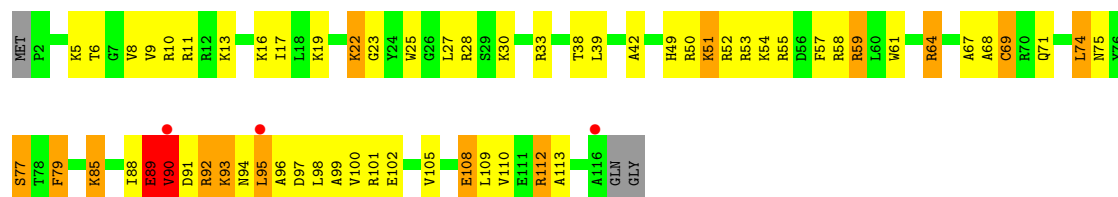
- Molecule 41: 50S ribosomal protein L19



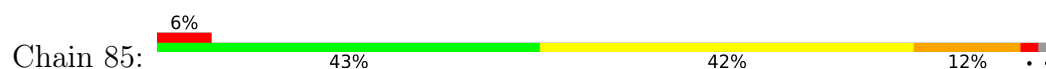
- Molecule 41: 50S ribosomal protein L19

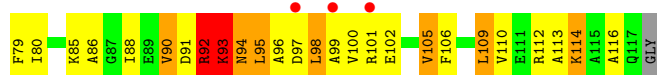


- Molecule 42: 50S ribosomal protein L20

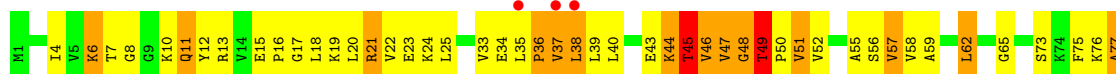
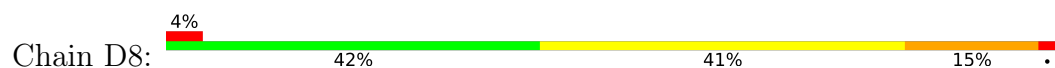


- Molecule 42: 50S ribosomal protein L20





- Molecule 43: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L21



- Molecule 44: 50S ribosomal protein L22

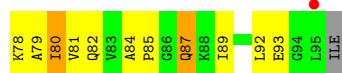


- Molecule 44: 50S ribosomal protein L22

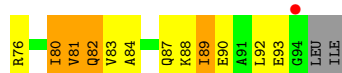
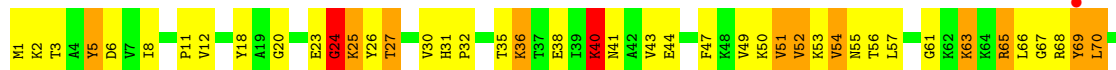
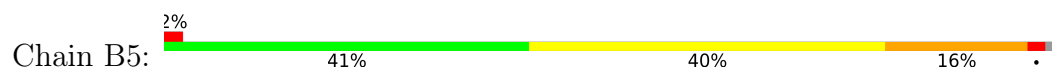


- Molecule 45: 50S ribosomal protein L23

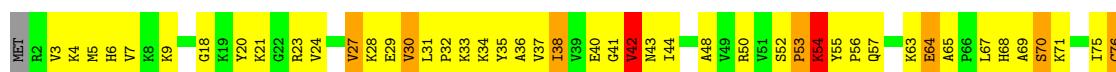




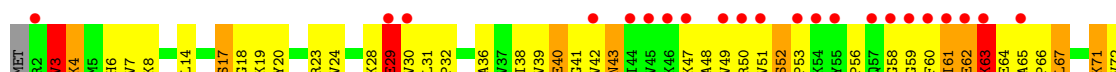
• Molecule 45: 50S ribosomal protein L23



• Molecule 46: 50S ribosomal protein L24

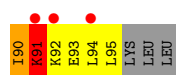


• Molecule 46: 50S ribosomal protein L24

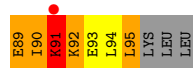


• Molecule 47: 50S ribosomal protein L25





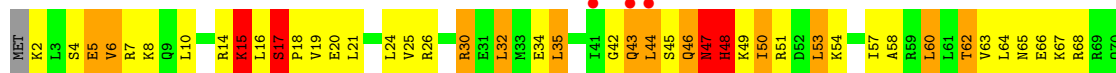
- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L29



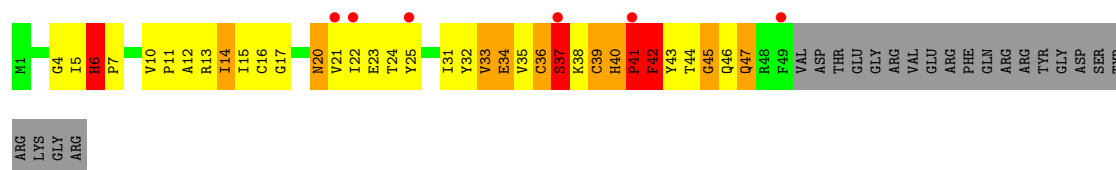
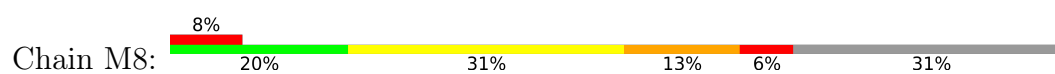
- Molecule 51: 50S ribosomal protein L30



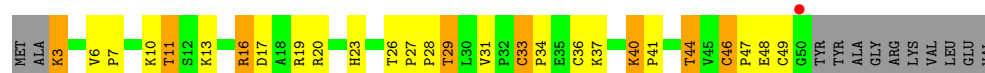
- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32



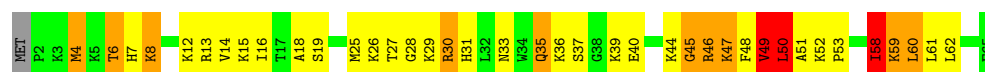
- Molecule 54: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.20Å 448.50Å 619.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.01 – 2.95 147.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (147.01-2.95) 91.6 (147.01-2.95)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.242 0.197 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	297904	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, ZN, G7M, 5MU, T6A, OMC, U8U, PSU, SF4, 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	13	0.51	0/35994	0.79	19/56171 (0.0%)
1	1G	0.43	0/36236	0.70	8/56555 (0.0%)
2	12	0.59	0/1727	1.17	12/2326 (0.5%)
2	1E	0.65	0/1908	1.22	20/2573 (0.8%)
3	22	0.58	0/1560	0.99	1/2104 (0.0%)
3	2E	0.75	0/1629	1.04	0/2195
4	32	0.67	0/1732	1.17	11/2318 (0.5%)
4	3E	0.74	0/1728	1.20	9/2313 (0.4%)
5	42	0.67	0/1155	1.07	5/1555 (0.3%)
5	4E	0.82	0/1158	1.16	6/1559 (0.4%)
6	52	0.76	0/855	1.02	2/1154 (0.2%)
6	5E	0.79	0/850	1.05	4/1147 (0.3%)
7	62	0.62	0/1132	1.08	7/1514 (0.5%)
7	6E	0.65	0/1259	0.97	1/1686 (0.1%)
8	72	0.59	0/1127	1.10	5/1517 (0.3%)
8	7E	0.74	0/1135	1.21	6/1527 (0.4%)
9	82	0.56	0/971	1.04	2/1304 (0.2%)
9	8E	0.65	0/1019	1.06	7/1367 (0.5%)
10	1A	0.61	0/658	1.18	4/885 (0.5%)
10	1I	0.84	1/767 (0.1%)	1.15	3/1034 (0.3%)
11	2A	0.69	0/850	1.10	8/1150 (0.7%)
11	2I	0.80	0/838	1.28	11/1133 (1.0%)
12	3A	0.86	0/972	1.22	7/1301 (0.5%)
12	3I	1.09	1/972 (0.1%)	1.40	7/1301 (0.5%)
13	4A	0.61	0/903	1.15	8/1211 (0.7%)
13	4I	0.81	0/952	1.22	8/1277 (0.6%)
14	5A	0.63	0/495	1.10	3/657 (0.5%)
14	5I	0.89	0/500	1.14	2/664 (0.3%)
15	6A	0.72	0/740	0.96	1/987 (0.1%)
15	6I	0.83	1/740 (0.1%)	1.05	2/987 (0.2%)
16	7A	0.80	0/721	1.20	5/970 (0.5%)
16	7I	0.75	0/716	1.13	2/963 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.68	0/836	1.07	2/1117 (0.2%)
17	8I	0.82	0/847	1.15	6/1131 (0.5%)
18	9A	0.75	0/549	1.10	1/732 (0.1%)
18	9I	0.76	0/554	1.17	1/739 (0.1%)
19	AA	0.60	0/490	1.14	5/662 (0.8%)
19	AI	0.85	2/676 (0.3%)	1.45	9/910 (1.0%)
20	BA	0.68	0/764	1.13	4/1007 (0.4%)
20	BI	0.61	0/748	1.12	1/986 (0.1%)
21	1B	0.62	0/192	1.20	0/252
21	1F	0.60	0/203	1.13	2/266 (0.8%)
22	1K	0.45	0/1589	0.63	0/2464
22	1L	0.35	0/1516	0.53	0/2350
23	2K	0.58	1/1721 (0.1%)	0.82	0/2682
23	2L	0.49	1/1721 (0.1%)	0.74	0/2682
24	3K	0.40	0/1654	0.62	0/2570
24	3L	0.37	0/1705	0.57	0/2650
25	4K	0.56	0/523	0.73	0/813
25	4L	0.42	0/473	0.76	0/737
26	14	0.61	0/68883	0.88	58/107521 (0.1%)
26	1H	0.70	1/69669 (0.0%)	0.97	113/108757 (0.1%)
27	16	0.58	0/2928	0.95	0/4568
27	1J	0.50	0/2928	0.82	0/4568
28	71	0.58	1/1055 (0.1%)	1.19	8/1425 (0.6%)
28	79	0.56	0/459	1.08	6/608 (1.0%)
29	11	1.33	12/2170 (0.6%)	1.70	56/2926 (1.9%)
29	19	1.17	9/2175 (0.4%)	1.54	32/2933 (1.1%)
30	21	1.10	3/1591 (0.2%)	1.66	36/2146 (1.7%)
30	29	1.06	3/1596 (0.2%)	1.53	34/2153 (1.6%)
31	31	1.11	1/1620 (0.1%)	1.43	15/2194 (0.7%)
31	39	0.97	1/1637 (0.1%)	1.50	19/2218 (0.9%)
32	41	0.85	1/1481 (0.1%)	1.25	9/1994 (0.5%)
32	49	0.66	0/1492	1.16	9/2008 (0.4%)
33	51	0.98	1/1354 (0.1%)	1.59	34/1833 (1.9%)
33	59	0.66	0/552	1.50	8/743 (1.1%)
34	61	0.79	0/1151	1.29	15/1558 (1.0%)
34	69	0.78	1/1146 (0.1%)	1.35	20/1551 (1.3%)
35	15	0.75	0/1131	1.22	12/1525 (0.8%)
35	58	0.90	1/1123 (0.1%)	1.37	10/1514 (0.7%)
36	25	0.92	1/942 (0.1%)	1.26	7/1269 (0.6%)
36	68	1.02	0/942	1.27	8/1269 (0.6%)
37	35	0.93	1/1139 (0.1%)	1.54	18/1514 (1.2%)
37	78	1.12	0/1139	1.75	31/1514 (2.0%)
38	45	0.96	1/1125 (0.1%)	1.36	11/1505 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	88	1.25	4/1138 (0.4%)	1.53	23/1523 (1.5%)
39	55	0.93	0/981	1.27	4/1312 (0.3%)
39	98	0.96	1/981 (0.1%)	1.30	7/1312 (0.5%)
40	65	0.80	0/886	1.33	5/1180 (0.4%)
40	A8	0.97	0/891	1.29	5/1187 (0.4%)
41	75	0.91	0/1123	1.28	6/1500 (0.4%)
41	B8	1.02	0/1138	1.49	22/1521 (1.4%)
42	85	0.92	0/977	1.24	6/1301 (0.5%)
42	C8	1.06	2/968 (0.2%)	1.25	5/1289 (0.4%)
43	95	0.86	1/781 (0.1%)	1.40	5/1048 (0.5%)
43	D8	0.91	1/785 (0.1%)	1.39	4/1052 (0.4%)
44	A5	1.08	3/897 (0.3%)	1.25	3/1204 (0.2%)
44	E8	1.04	0/886	1.29	4/1189 (0.3%)
45	B5	1.01	1/749 (0.1%)	1.27	6/1007 (0.6%)
45	F8	1.15	0/757	1.49	10/1017 (1.0%)
46	C5	0.94	1/807 (0.1%)	1.34	7/1076 (0.7%)
46	G8	1.14	1/796 (0.1%)	1.65	18/1062 (1.7%)
47	D5	0.71	0/1103	1.26	17/1494 (1.1%)
47	H8	0.81	2/1395 (0.1%)	1.22	8/1890 (0.4%)
48	E5	1.01	0/611	1.33	6/814 (0.7%)
48	I8	1.18	1/619 (0.2%)	1.63	10/825 (1.2%)
49	F5	1.03	1/744 (0.1%)	1.60	21/989 (2.1%)
49	J8	1.11	2/744 (0.3%)	1.42	6/989 (0.6%)
50	G5	0.82	0/578	1.33	4/766 (0.5%)
50	K8	1.09	1/577 (0.2%)	1.51	11/763 (1.4%)
51	H5	0.83	0/464	1.32	4/623 (0.6%)
51	L8	1.03	1/464 (0.2%)	1.41	7/623 (1.1%)
52	M8	0.91	0/385	1.64	9/521 (1.7%)
53	J5	1.05	0/448	1.37	6/606 (1.0%)
53	N8	1.07	1/381 (0.3%)	1.52	7/516 (1.4%)
54	L5	1.05	0/409	1.45	2/540 (0.4%)
54	P8	1.31	0/409	1.53	6/540 (1.1%)
55	M5	1.10	1/524 (0.2%)	1.42	7/691 (1.0%)
55	Q8	1.27	2/524 (0.4%)	1.77	13/691 (1.9%)
All	All	0.69	72/318108 (0.0%)	1.00	1080/476630 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	1
4	32	0	1
9	82	0	1
9	8E	0	1
10	1I	0	1
11	2A	0	1
11	2I	0	1
12	3I	0	3
13	4A	0	2
13	4I	0	3
14	5A	0	1
20	BA	0	3
28	71	0	3
29	11	0	6
29	19	0	5
30	21	0	9
30	29	0	5
31	39	0	10
32	41	0	1
32	49	0	3
33	51	0	5
33	59	0	3
34	61	0	3
34	69	0	5
35	15	0	2
35	58	0	2
37	35	0	3
37	78	0	5
38	45	0	3
38	88	0	2
39	55	0	1
39	98	0	1
40	65	0	1
41	75	0	1
41	B8	0	3
42	85	0	3
42	C8	0	2
43	95	0	1
43	D8	0	4
44	A5	0	1
45	B5	0	2
45	F8	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	C5	0	2
46	G8	0	6
47	D5	0	5
47	H8	0	3
49	F5	0	2
49	J8	0	3
50	G5	0	3
50	K8	0	4
52	M8	0	4
54	P8	0	1
55	M5	0	2
55	Q8	0	2
All	All	0	158

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	11	39	LYS	CA-C	9.43	1.65	1.52
48	I8	10	THR	CA-CB	9.28	1.69	1.53
29	11	123	ALA	CA-CB	-8.52	1.40	1.53
29	19	40	THR	CA-C	8.30	1.63	1.52
30	21	131	ALA	CA-CB	8.07	1.67	1.53

The worst 5 of 1080 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	88	140	ALA	N-CA-C	-19.86	85.65	108.49
43	95	49	THR	CA-C-N	-14.82	102.69	118.85
43	95	49	THR	C-N-CA	-14.82	102.69	118.85
29	19	272	ALA	N-CA-C	14.57	125.24	108.49
29	11	271	ILE	N-CA-C	14.22	126.95	111.88

There are no chirality outliers.

5 of 158 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
10	1I	88	LEU	Peptide
11	2I	102	GLY	Peptide
12	3I	47	LYS	Peptide
9	8E	110	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16234	832	0
1	1G	32371	0	16342	805	0
2	12	1696	0	1730	103	0
2	1E	1874	0	1926	117	0
3	22	1537	0	1603	78	0
3	2E	1605	0	1668	53	0
4	32	1702	0	1764	128	0
4	3E	1698	0	1759	103	0
5	42	1139	0	1202	51	0
5	4E	1142	0	1204	57	0
6	52	842	0	857	32	0
6	5E	837	0	852	35	0
7	62	1120	0	1167	57	0
7	6E	1242	0	1286	39	0
8	72	1107	0	1165	58	0
8	7E	1115	0	1177	60	0
9	82	953	0	983	82	0
9	8E	1000	0	1031	56	0
10	1A	646	0	662	36	0
10	1I	754	0	769	45	0
11	2A	835	0	847	33	0
11	2I	823	0	833	34	0
12	3A	956	0	1046	42	0
12	3I	956	0	1046	42	0
13	4A	893	0	946	59	0
13	4I	942	0	997	63	0
14	5A	486	0	525	38	0
14	5I	491	0	529	28	0
15	6A	729	0	768	17	0
15	6I	729	0	768	36	0
16	7A	705	0	725	23	0
16	7I	700	0	720	50	0
17	8A	823	0	891	31	0
17	8I	834	0	904	47	0
18	9A	544	0	605	32	0
18	9I	549	0	607	18	0
19	AA	481	0	468	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	661	0	683	64	0
20	BA	762	0	861	38	0
20	BI	746	0	843	44	0
21	1B	188	0	195	11	0
21	1F	199	0	208	14	0
22	1K	1542	0	790	46	0
22	1L	1477	0	758	27	0
23	2K	1646	0	844	24	0
23	2L	1646	0	844	36	0
24	3K	1483	0	756	63	0
24	3L	1528	0	778	49	0
25	4K	464	0	231	20	0
25	4L	419	0	208	11	0
26	14	61505	0	30997	1443	0
26	1H	62204	0	31336	1596	0
27	16	2617	0	1328	74	0
27	1J	2617	0	1328	69	0
28	71	1033	0	1048	73	0
28	79	456	0	460	25	0
29	11	2120	0	2197	138	0
29	19	2125	0	2199	132	0
30	21	1558	0	1624	108	0
30	29	1563	0	1629	103	0
31	31	1585	0	1632	80	0
31	39	1602	0	1649	115	0
32	41	1457	0	1514	93	0
32	49	1468	0	1520	85	0
33	51	1328	0	1396	102	0
33	59	543	0	566	30	0
34	61	1136	0	1223	54	0
34	69	1131	0	1218	57	0
35	15	1104	0	1180	40	0
35	58	1096	0	1169	75	0
36	25	932	0	996	49	0
36	68	932	0	996	32	0
37	35	1122	0	1206	69	0
37	78	1122	0	1206	95	0
38	45	1104	0	1159	94	0
38	88	1117	0	1168	54	0
39	55	967	0	1033	57	0
39	98	967	0	1033	52	0
40	65	876	0	938	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	A8	881	0	943	64	0
41	75	1109	0	1170	78	0
41	B8	1124	0	1179	76	0
42	85	959	0	1019	60	0
42	C8	950	0	1011	58	0
43	95	770	0	838	46	0
43	D8	774	0	849	39	0
44	A5	886	0	948	38	0
44	E8	876	0	941	27	0
45	B5	735	0	785	39	0
45	F8	743	0	794	35	0
46	C5	794	0	886	64	0
46	G8	783	0	869	58	0
47	D5	1079	0	1088	65	0
47	H8	1365	0	1391	78	0
48	E5	603	0	620	37	0
48	I8	611	0	631	33	0
49	F5	737	0	813	42	0
49	J8	737	0	813	43	0
50	G5	576	0	625	31	0
50	K8	575	0	634	49	0
51	H5	459	0	512	9	0
51	L8	459	0	512	12	0
52	M8	376	0	374	53	0
53	J5	434	0	454	21	0
53	N8	369	0	388	21	0
54	L5	401	0	436	15	0
54	P8	401	0	436	19	0
55	M5	516	0	581	28	0
55	Q8	516	0	582	44	0
56	11	3	0	0	0	0
56	13	161	0	0	0	0
56	14	471	0	0	0	0
56	16	13	0	0	0	0
56	1G	126	0	0	0	0
56	1H	572	0	0	0	0
56	1J	11	0	0	0	0
56	1K	1	0	0	0	0
56	21	3	0	0	0	0
56	25	2	0	0	0	0
56	29	1	0	0	0	0
56	2A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2K	3	0	0	0	0
56	2L	3	0	0	0	0
56	32	1	0	0	0	0
56	35	3	0	0	0	0
56	39	2	0	0	0	0
56	41	2	0	0	0	0
56	42	2	0	0	0	0
56	45	2	0	0	0	0
56	4K	1	0	0	0	0
56	52	1	0	0	0	0
56	5E	1	0	0	0	0
56	5I	1	0	0	0	0
56	78	2	0	0	0	0
56	88	3	0	0	0	0
56	98	1	0	0	0	0
56	B5	1	0	0	0	0
56	E5	3	0	0	0	0
56	F8	1	0	0	0	0
56	I8	1	0	0	0	0
56	L8	1	0	0	0	0
56	M5	1	0	0	0	0
56	P8	1	0	0	0	0
56	Q8	1	0	0	0	0
57	32	8	0	0	3	0
57	3E	8	0	0	0	0
58	5A	1	0	0	0	0
58	5I	1	0	0	0	0
58	C5	1	0	0	0	0
58	G8	1	0	0	0	0
59	11	16	0	0	6	0
59	13	389	0	0	54	0
59	14	1225	0	0	216	0
59	16	35	0	0	7	0
59	19	11	0	0	3	0
59	1E	1	0	0	0	0
59	1F	2	0	0	0	0
59	1G	297	0	0	46	0
59	1H	1539	0	0	288	0
59	1I	2	0	0	0	0
59	1J	12	0	0	2	0
59	1K	8	0	0	1	0
59	1L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	21	7	0	0	1	0
59	25	6	0	0	0	0
59	29	5	0	0	0	0
59	2A	3	0	0	0	0
59	2K	6	0	0	0	0
59	2L	6	0	0	0	0
59	31	6	0	0	0	0
59	32	2	0	0	1	0
59	35	8	0	0	1	0
59	39	7	0	0	0	0
59	3A	1	0	0	0	0
59	3E	2	0	0	0	0
59	3I	2	0	0	0	0
59	3K	1	0	0	0	0
59	41	1	0	0	0	0
59	42	1	0	0	0	0
59	45	4	0	0	0	0
59	4E	1	0	0	0	0
59	4I	2	0	0	0	0
59	4K	5	0	0	0	0
59	4L	5	0	0	0	0
59	52	4	0	0	0	0
59	55	3	0	0	4	0
59	58	2	0	0	0	0
59	5I	2	0	0	0	0
59	62	3	0	0	0	0
59	68	2	0	0	0	0
59	6A	1	0	0	0	0
59	6I	3	0	0	0	0
59	78	8	0	0	1	0
59	7A	6	0	0	0	0
59	7I	1	0	0	0	0
59	85	1	0	0	0	0
59	88	8	0	0	0	0
59	8E	3	0	0	0	0
59	95	1	0	0	0	0
59	9A	2	0	0	1	0
59	A5	1	0	0	0	0
59	B5	1	0	0	0	0
59	BA	5	0	0	1	0
59	C5	3	0	0	0	0
59	C8	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	D8	2	0	0	0	0
59	F5	1	0	0	0	0
59	F8	2	0	0	0	0
59	G8	1	0	0	0	0
59	H5	2	0	0	0	0
59	I8	7	0	0	1	0
59	J8	2	0	0	1	0
59	K8	1	0	0	0	0
59	L5	3	0	0	0	0
59	L8	3	0	0	0	0
59	M5	6	0	0	1	0
59	P8	1	0	0	0	0
59	Q8	8	0	0	1	0
All	All	297904	0	196675	9120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 9120 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:592:G:H21	55:Q8:4:MET:HE1	1.06	1.18
39:55:3:HIS:NE2	59:55:201:HOH:O	1.77	1.14
49:J8:93:GLU:HG3	49:J8:94:LEU:H	1.01	1.12
26:14:730:C:OP2	59:14:3501:HOH:O	1.68	1.11
19:AI:3:ARG:HE	19:AI:9:VAL:HG11	1.10	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	203/256 (79%)	165 (81%)	33 (16%)	5 (2%)	4	13
2	1E	227/256 (89%)	187 (82%)	39 (17%)	1 (0%)	30	53
3	22	191/239 (80%)	165 (86%)	25 (13%)	1 (0%)	24	49
3	2E	203/239 (85%)	183 (90%)	20 (10%)	0	100	100
4	32	206/209 (99%)	181 (88%)	23 (11%)	2 (1%)	12	32
4	3E	205/209 (98%)	191 (93%)	13 (6%)	1 (0%)	24	49
5	42	147/162 (91%)	138 (94%)	9 (6%)	0	100	100
5	4E	147/162 (91%)	138 (94%)	8 (5%)	1 (1%)	18	40
6	52	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	136/156 (87%)	123 (90%)	13 (10%)	0	100	100
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	123 (91%)	9 (7%)	3 (2%)	5	15
8	7E	136/138 (99%)	124 (91%)	10 (7%)	2 (2%)	8	23
9	82	119/128 (93%)	110 (92%)	8 (7%)	1 (1%)	16	37
9	8E	124/128 (97%)	106 (86%)	18 (14%)	0	100	100
10	1A	76/105 (72%)	72 (95%)	4 (5%)	0	100	100
10	1I	93/105 (89%)	84 (90%)	9 (10%)	0	100	100
11	2A	111/129 (86%)	101 (91%)	8 (7%)	2 (2%)	6	19
11	2I	109/129 (84%)	98 (90%)	9 (8%)	2 (2%)	6	19
12	3A	120/132 (91%)	102 (85%)	14 (12%)	4 (3%)	3	7
12	3I	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	16	37
13	4A	109/126 (86%)	91 (84%)	15 (14%)	3 (3%)	4	11
13	4I	117/126 (93%)	97 (83%)	20 (17%)	0	100	100
14	5A	57/61 (93%)	47 (82%)	9 (16%)	1 (2%)	6	19
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	7
15	6A	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
15	6I	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
16	7A	82/88 (93%)	74 (90%)	8 (10%)	0	100	100
16	7I	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	98/105 (93%)	92 (94%)	5 (5%)	1 (1%)	12	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	65/88 (74%)	64 (98%)	1 (2%)	0	100	100
18	9I	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	8	23
19	AA	56/93 (60%)	48 (86%)	6 (11%)	2 (4%)	2	6
19	AI	80/93 (86%)	68 (85%)	8 (10%)	4 (5%)	1	3
20	BA	97/106 (92%)	79 (81%)	15 (16%)	3 (3%)	3	8
20	BI	95/106 (90%)	84 (88%)	11 (12%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	129/229 (56%)	122 (95%)	7 (5%)	0	100	100
28	79	45/229 (20%)	43 (96%)	2 (4%)	0	100	100
29	11	271/276 (98%)	237 (88%)	25 (9%)	9 (3%)	3	7
29	19	272/276 (99%)	240 (88%)	25 (9%)	7 (3%)	4	12
30	21	201/206 (98%)	155 (77%)	37 (18%)	9 (4%)	2	4
30	29	202/206 (98%)	152 (75%)	37 (18%)	13 (6%)	1	2
31	31	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
31	39	202/210 (96%)	155 (77%)	40 (20%)	7 (4%)	3	7
32	41	177/182 (97%)	156 (88%)	19 (11%)	2 (1%)	11	29
32	49	179/182 (98%)	155 (87%)	22 (12%)	2 (1%)	11	29
33	51	172/180 (96%)	142 (83%)	20 (12%)	10 (6%)	1	2
33	59	64/180 (36%)	48 (75%)	13 (20%)	3 (5%)	2	4
34	61	144/148 (97%)	116 (81%)	25 (17%)	3 (2%)	5	16
34	69	143/148 (97%)	115 (80%)	24 (17%)	4 (3%)	4	11
35	15	136/140 (97%)	121 (89%)	14 (10%)	1 (1%)	18	40
35	58	135/140 (96%)	115 (85%)	15 (11%)	5 (4%)	2	6
36	25	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	37
36	68	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
37	35	145/150 (97%)	118 (81%)	26 (18%)	1 (1%)	18	40
37	78	145/150 (97%)	114 (79%)	21 (14%)	10 (7%)	1	1
38	45	137/141 (97%)	111 (81%)	23 (17%)	3 (2%)	5	15
38	88	139/141 (99%)	116 (84%)	16 (12%)	7 (5%)	1	3
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	98	116/118 (98%)	99 (85%)	15 (13%)	2 (2%)	7	20
40	65	108/112 (96%)	89 (82%)	16 (15%)	3 (3%)	4	11
40	A8	109/112 (97%)	89 (82%)	20 (18%)	0	100	100
41	75	131/146 (90%)	118 (90%)	11 (8%)	2 (2%)	8	23
41	B8	134/146 (92%)	119 (89%)	14 (10%)	1 (1%)	18	40
42	85	114/118 (97%)	102 (90%)	9 (8%)	3 (3%)	4	12
42	C8	113/118 (96%)	102 (90%)	8 (7%)	3 (3%)	4	11
43	95	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	3	8
43	D8	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	3	8
44	A5	109/113 (96%)	101 (93%)	7 (6%)	1 (1%)	14	34
44	E8	108/113 (96%)	100 (93%)	7 (6%)	1 (1%)	14	34
45	B5	92/96 (96%)	83 (90%)	6 (6%)	3 (3%)	3	7
45	F8	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
46	C5	102/110 (93%)	75 (74%)	20 (20%)	7 (7%)	1	1
46	G8	101/110 (92%)	82 (81%)	13 (13%)	6 (6%)	1	2
47	D5	127/206 (62%)	98 (77%)	26 (20%)	3 (2%)	4	13
47	H8	168/206 (82%)	136 (81%)	26 (16%)	6 (4%)	2	6
48	E5	74/85 (87%)	65 (88%)	7 (10%)	2 (3%)	4	11
48	I8	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	9	26
49	F5	92/98 (94%)	78 (85%)	12 (13%)	2 (2%)	5	15
49	J8	92/98 (94%)	86 (94%)	5 (5%)	1 (1%)	11	29
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	3	9
50	K8	66/72 (92%)	60 (91%)	3 (4%)	3 (4%)	2	4
51	H5	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
51	L8	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
52	M8	47/71 (66%)	28 (60%)	17 (36%)	2 (4%)	2	4
53	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
53	N8	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	40 (89%)	4 (9%)	1 (2%)	5	15
55	M5	62/65 (95%)	51 (82%)	10 (16%)	1 (2%)	7	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	Q8	62/65 (95%)	53 (86%)	6 (10%)	3 (5%)	2	3
All	All	10980/12333 (89%)	9564 (87%)	1210 (11%)	206 (2%)	6	17

5 of 206 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	3I	48	PRO
14	5I	13	THR
19	AI	9	VAL
19	AI	41	VAL
29	11	28	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	179/220 (81%)	148 (83%)	31 (17%)	2	5
2	1E	200/220 (91%)	151 (76%)	49 (24%)	1	1
3	22	154/188 (82%)	120 (78%)	34 (22%)	1	2
3	2E	159/188 (85%)	111 (70%)	48 (30%)	0	0
4	32	180/181 (99%)	139 (77%)	41 (23%)	1	2
4	3E	180/181 (99%)	139 (77%)	41 (23%)	1	2
5	42	114/123 (93%)	86 (75%)	28 (25%)	1	1
5	4E	115/123 (94%)	92 (80%)	23 (20%)	1	3
6	52	90/90 (100%)	68 (76%)	22 (24%)	1	1
6	5E	90/90 (100%)	71 (79%)	19 (21%)	1	2
7	62	114/127 (90%)	89 (78%)	25 (22%)	1	2
7	6E	125/127 (98%)	106 (85%)	19 (15%)	3	8
8	72	118/119 (99%)	92 (78%)	26 (22%)	1	2
8	7E	119/119 (100%)	89 (75%)	30 (25%)	0	1
9	82	92/99 (93%)	71 (77%)	21 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	8E	97/99 (98%)	74 (76%)	23 (24%)	1	1
10	1A	71/92 (77%)	52 (73%)	19 (27%)	0	0
10	1I	81/92 (88%)	65 (80%)	16 (20%)	1	3
11	2A	85/99 (86%)	69 (81%)	16 (19%)	1	4
11	2I	84/99 (85%)	65 (77%)	19 (23%)	1	2
12	3A	103/109 (94%)	76 (74%)	27 (26%)	0	1
12	3I	103/109 (94%)	82 (80%)	21 (20%)	1	3
13	4A	91/101 (90%)	62 (68%)	29 (32%)	0	0
13	4I	94/101 (93%)	69 (73%)	25 (27%)	0	1
14	5A	49/50 (98%)	39 (80%)	10 (20%)	1	3
14	5I	49/50 (98%)	39 (80%)	10 (20%)	1	3
15	6A	79/80 (99%)	65 (82%)	14 (18%)	2	4
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2	4
16	7A	72/74 (97%)	53 (74%)	19 (26%)	0	1
16	7I	72/74 (97%)	55 (76%)	17 (24%)	1	1
17	8A	94/97 (97%)	78 (83%)	16 (17%)	2	5
17	8I	95/97 (98%)	75 (79%)	20 (21%)	1	2
18	9A	58/77 (75%)	44 (76%)	14 (24%)	1	1
18	9I	58/77 (75%)	48 (83%)	10 (17%)	2	5
19	AA	52/80 (65%)	40 (77%)	12 (23%)	1	2
19	AI	72/80 (90%)	57 (79%)	15 (21%)	1	3
20	BA	76/82 (93%)	61 (80%)	15 (20%)	1	3
20	BI	75/82 (92%)	59 (79%)	16 (21%)	1	2
21	1B	17/22 (77%)	16 (94%)	1 (6%)	18	41
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	2
28	71	109/181 (60%)	85 (78%)	24 (22%)	1	2
28	79	48/181 (26%)	36 (75%)	12 (25%)	0	1
29	11	214/218 (98%)	162 (76%)	52 (24%)	1	1
29	19	214/218 (98%)	165 (77%)	49 (23%)	1	2
30	21	165/166 (99%)	122 (74%)	43 (26%)	0	1
30	29	165/166 (99%)	122 (74%)	43 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	31	161/166 (97%)	123 (76%)	38 (24%)	1	1
31	39	163/166 (98%)	120 (74%)	43 (26%)	0	1
32	41	153/156 (98%)	114 (74%)	39 (26%)	0	1
32	49	153/156 (98%)	118 (77%)	35 (23%)	1	2
33	51	143/148 (97%)	100 (70%)	43 (30%)	0	0
33	59	56/148 (38%)	44 (79%)	12 (21%)	1	2
34	61	122/124 (98%)	86 (70%)	36 (30%)	0	0
34	69	122/124 (98%)	89 (73%)	33 (27%)	0	0
35	15	117/119 (98%)	85 (73%)	32 (27%)	0	0
35	58	116/119 (98%)	87 (75%)	29 (25%)	0	1
36	25	100/100 (100%)	77 (77%)	23 (23%)	1	2
36	68	100/100 (100%)	79 (79%)	21 (21%)	1	2
37	35	114/116 (98%)	81 (71%)	33 (29%)	0	0
37	78	114/116 (98%)	69 (60%)	45 (40%)	0	0
38	45	109/111 (98%)	75 (69%)	34 (31%)	0	0
38	88	110/111 (99%)	84 (76%)	26 (24%)	1	1
39	55	101/101 (100%)	73 (72%)	28 (28%)	0	0
39	98	101/101 (100%)	72 (71%)	29 (29%)	0	0
40	65	87/88 (99%)	57 (66%)	30 (34%)	0	0
40	A8	87/88 (99%)	61 (70%)	26 (30%)	0	0
41	75	117/127 (92%)	83 (71%)	34 (29%)	0	0
41	B8	117/127 (92%)	83 (71%)	34 (29%)	0	0
42	85	93/94 (99%)	72 (77%)	21 (23%)	1	2
42	C8	92/94 (98%)	76 (83%)	16 (17%)	2	5
43	95	81/82 (99%)	55 (68%)	26 (32%)	0	0
43	D8	82/82 (100%)	55 (67%)	27 (33%)	0	0
44	A5	91/92 (99%)	68 (75%)	23 (25%)	0	1
44	E8	90/92 (98%)	71 (79%)	19 (21%)	1	2
45	B5	74/78 (95%)	55 (74%)	19 (26%)	0	1
45	F8	75/78 (96%)	55 (73%)	20 (27%)	0	0
46	C5	85/91 (93%)	57 (67%)	28 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	G8	84/91 (92%)	56 (67%)	28 (33%)	0	0
47	D5	118/179 (66%)	90 (76%)	28 (24%)	1	1
47	H8	151/179 (84%)	114 (76%)	37 (24%)	1	1
48	E5	61/67 (91%)	55 (90%)	6 (10%)	7	21
48	I8	62/67 (92%)	47 (76%)	15 (24%)	1	1
49	F5	79/83 (95%)	59 (75%)	20 (25%)	0	1
49	J8	79/83 (95%)	63 (80%)	16 (20%)	1	3
50	G5	63/67 (94%)	39 (62%)	24 (38%)	0	0
50	K8	64/67 (96%)	41 (64%)	23 (36%)	0	0
51	H5	50/52 (96%)	36 (72%)	14 (28%)	0	0
51	L8	50/52 (96%)	35 (70%)	15 (30%)	0	0
52	M8	42/63 (67%)	31 (74%)	11 (26%)	0	1
53	J5	48/52 (92%)	38 (79%)	10 (21%)	1	3
53	N8	43/52 (83%)	31 (72%)	12 (28%)	0	0
54	L5	38/42 (90%)	31 (82%)	7 (18%)	1	4
54	P8	38/42 (90%)	30 (79%)	8 (21%)	1	2
55	M5	54/55 (98%)	36 (67%)	18 (33%)	0	0
55	Q8	54/55 (98%)	44 (82%)	10 (18%)	1	4
All	All	9272/10193 (91%)	6986 (75%)	2286 (25%)	1	1

5 of 2286 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	15	90	MET
37	35	121	LYS
35	15	85	ILE
43	95	71	LEU
37	78	39	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
11	2A	99	GLN
33	59	74	ASN
15	6A	9	GLN

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Mol	Chain	Res	Type
29	19	96	HIS
36	25	5	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1519 (98%)	376 (25%)	38 (2%)
1	1G	1505/1519 (99%)	350 (23%)	37 (2%)
22	1K	69/76 (90%)	30 (43%)	5 (7%)
22	1L	65/76 (85%)	22 (33%)	4 (6%)
23	2K	76/77 (98%)	29 (38%)	1 (1%)
23	2L	76/77 (98%)	18 (23%)	2 (2%)
24	3K	67/76 (88%)	39 (58%)	4 (5%)
24	3L	69/76 (90%)	31 (44%)	2 (2%)
25	4K	20/27 (74%)	12 (60%)	2 (10%)
25	4L	18/27 (66%)	8 (44%)	2 (11%)
26	14	2847/2917 (97%)	770 (27%)	53 (1%)
26	1H	2878/2917 (98%)	715 (24%)	57 (1%)
27	16	121/122 (99%)	28 (23%)	2 (1%)
27	1J	121/122 (99%)	34 (28%)	2 (1%)
All	All	9425/9628 (97%)	2462 (26%)	211 (2%)

5 of 2462 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	9	G
1	13	15	G

5 of 211 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	251	G
1	1G	1442	G
26	14	2432	A
1	1G	412	A
1	1G	972	C

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

20 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$
23	G7M	2K	47	23	23,26,27	4.60	7 (30%)	34,39,42	3.23	14 (41%)
23	4SU	2L	8	23	18,21,22	2.01	3 (16%)	25,30,33	2.75	5 (20%)
23	PSU	2K	56	23	18,21,22	1.36	2 (11%)	21,30,33	2.37	6 (28%)
23	OMC	2L	33	23	19,22,23	1.58	3 (15%)	25,31,34	1.13	1 (4%)
23	OMC	2K	33	23	19,22,23	1.57	3 (15%)	25,31,34	1.07	3 (12%)
23	G7M	2L	47	23	23,26,27	4.71	8 (34%)	34,39,42	3.31	14 (41%)
22	PSU	1K	39	22	18,21,22	1.03	2 (11%)	21,30,33	1.61	4 (19%)
22	T6A	1K	37	22	31,34,35	2.04	9 (29%)	43,49,52	2.17	16 (37%)
22	PSU	1K	55	22	18,21,22	1.31	1 (5%)	21,30,33	1.77	4 (19%)
23	5MU	2K	55	23	19,22,23	3.97	5 (26%)	27,32,35	3.35	7 (25%)
22	PSU	1L	55	22	18,21,22	1.23	2 (11%)	21,30,33	1.61	4 (19%)
22	PSU	1L	39	22	18,21,22	1.12	1 (5%)	21,30,33	1.53	3 (14%)
23	PSU	2L	56	23	18,21,22	1.24	2 (11%)	21,30,33	1.65	2 (9%)
23	5MU	2L	55	23	19,22,23	3.88	5 (26%)	27,32,35	3.45	10 (37%)
22	5MU	1K	54	22	19,22,23	3.89	5 (26%)	27,32,35	2.80	8 (29%)
22	T6A	1L	37	22	31,34,35	1.95	7 (22%)	43,49,52	2.26	12 (27%)
22	U8U	1L	34	25,22	20,24,25	2.39	6 (30%)	22,34,37	1.10	3 (13%)
22	U8U	1K	34	25,22	20,24,25	2.20	6 (30%)	22,34,37	1.09	3 (13%)
23	4SU	2K	8	23	18,21,22	2.03	3 (16%)	25,30,33	2.69	5 (20%)
22	5MU	1L	54	22	19,22,23	3.98	5 (26%)	27,32,35	3.36	8 (29%)

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
23	G7M	2K	47	23	-	0/7/25/26	0/3/3/3
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	1/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/9/27/28	0/2/2/2
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2
23	G7M	2L	47	23	-	2/7/25/26	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	2/23/41/42	0/3/3/3
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
22	PSU	1L	55	22	-	1/7/25/26	0/2/2/2
22	PSU	1L	39	22	-	2/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
22	T6A	1L	37	22	-	1/23/41/42	0/3/3/3
22	U8U	1L	34	25,22	-	4/10/28/29	0/2/2/2
22	U8U	1K	34	25,22	-	1/10/28/29	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
22	5MU	1L	54	22	-	0/7/25/26	0/2/2/2

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	G7M	C8-N7	18.92	1.65	1.33
23	2K	47	G7M	C8-N7	18.47	1.64	1.33
22	1L	54	5MU	C2-N1	13.21	1.59	1.38
23	2K	55	5MU	C2-N1	13.03	1.58	1.38
22	1K	54	5MU	C2-N1	12.60	1.58	1.38

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	47	G7M	CN7-N7-C5	11.62	141.28	126.80
22	1L	54	5MU	C5-C4-N3	11.15	125.02	115.32
23	2K	47	G7M	CN7-N7-C5	10.77	140.23	126.80
23	2L	55	5MU	C5-C4-N3	10.60	124.54	115.32
23	2K	55	5MU	C5-C4-N3	10.27	124.25	115.32

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1L	37	T6A	C14-C12-N11-C10
22	1K	34	U8U	C5-C-N-CA
22	1L	34	U8U	N-C-C5-C4
22	1L	34	U8U	O4'-C4'-C5'-O5'
23	2K	33	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

15 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	47	G7M	1	0
23	2L	8	4SU	1	0
23	2K	56	PSU	1	0
23	2L	33	OMC	1	0
23	2K	33	OMC	1	0
23	2L	47	G7M	2	0
22	1K	55	PSU	2	0
23	2K	55	5MU	2	0
22	1L	55	PSU	1	0
22	1L	39	PSU	1	0
23	2L	56	PSU	2	0
23	2L	55	5MU	1	0
22	1K	54	5MU	1	0
22	1L	34	U8U	1	0
22	1K	34	U8U	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1409 ligands modelled in this entry, 1407 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	$\# Z > 2$
57	SF4	3E	301	4	0,12,12	-	-	-		
57	SF4	32	302	4	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
57	SF4	3E	301	4	-	-	0/6/5/5
57	SF4	32	302	4	-	-	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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	32	302	SF4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	4K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4K	25:A	O3'	26:A	P	3.07

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	13	1496/1519 (98%)	-0.12	32 (2%) 63 55	52, 95, 168, 235	0
1	1G	1506/1519 (99%)	-0.10	32 (2%) 63 55	67, 112, 176, 243	0
2	12	207/256 (80%)	0.85	24 (11%) 9 8	128, 159, 178, 183	0
2	1E	231/256 (90%)	0.85	24 (10%) 11 10	108, 138, 168, 172	0
3	22	195/239 (81%)	0.56	10 (5%) 33 28	119, 140, 163, 172	0
3	2E	205/239 (85%)	0.36	5 (2%) 59 51	82, 105, 135, 142	0
4	32	208/209 (99%)	0.63	13 (6%) 26 22	92, 113, 135, 140	0
4	3E	207/209 (99%)	0.58	11 (5%) 32 27	77, 104, 125, 136	0
5	42	149/162 (91%)	0.63	11 (7%) 20 18	97, 118, 134, 142	0
5	4E	149/162 (91%)	0.56	9 (6%) 27 23	76, 96, 115, 122	0
6	52	101/101 (100%)	0.54	4 (3%) 42 35	81, 99, 115, 130	0
6	5E	100/101 (99%)	0.50	5 (5%) 34 28	76, 97, 116, 122	0
7	62	140/156 (89%)	0.48	12 (8%) 16 14	108, 126, 138, 140	0
7	6E	154/156 (98%)	0.28	7 (4%) 38 31	96, 114, 144, 165	0
8	72	137/138 (99%)	0.65	11 (8%) 18 16	95, 123, 136, 143	0
8	7E	138/138 (100%)	0.56	8 (5%) 29 24	84, 104, 116, 127	0
9	82	121/128 (94%)	0.96	19 (15%) 5 5	109, 156, 170, 181	0
9	8E	126/128 (98%)	0.78	15 (11%) 9 8	80, 133, 153, 158	0
10	1A	80/105 (76%)	1.68	24 (30%) 1 1	114, 151, 163, 163	0
10	1I	95/105 (90%)	0.63	5 (5%) 32 27	76, 120, 160, 164	0
11	2A	113/129 (87%)	0.63	9 (7%) 18 16	78, 106, 120, 129	0
11	2I	111/129 (86%)	0.40	6 (5%) 31 26	69, 102, 117, 129	0
12	3A	122/132 (92%)	0.89	19 (15%) 5 5	80, 96, 120, 140	0
12	3I	122/132 (92%)	0.38	11 (9%) 15 13	61, 72, 100, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	0.91	24 (21%) 2 2	112, 142, 159, 167	0
13	4I	119/126 (94%)	0.59	13 (10%) 10 9	81, 108, 129, 137	0
14	5A	59/61 (96%)	0.94	9 (15%) 5 5	124, 137, 150, 154	0
14	5I	60/61 (98%)	0.39	3 (5%) 34 28	77, 93, 107, 120	0
15	6A	87/89 (97%)	-0.01	2 (2%) 61 53	78, 106, 118, 120	0
15	6I	87/89 (97%)	0.09	2 (2%) 61 53	73, 92, 109, 116	0
16	7A	84/88 (95%)	0.78	9 (10%) 11 10	88, 101, 121, 145	0
16	7I	83/88 (94%)	0.96	8 (9%) 13 12	93, 106, 134, 154	0
17	8A	99/105 (94%)	0.29	6 (6%) 27 22	90, 105, 120, 124	0
17	8I	100/105 (95%)	0.36	4 (4%) 42 35	85, 101, 110, 115	0
18	9A	67/88 (76%)	0.70	7 (10%) 11 10	89, 107, 126, 130	0
18	9I	68/88 (77%)	0.54	4 (5%) 28 23	83, 102, 124, 127	0
19	AA	62/93 (66%)	1.18	13 (20%) 2 2	132, 153, 166, 171	0
19	AI	82/93 (88%)	0.37	4 (4%) 35 29	83, 106, 127, 139	0
20	BA	99/106 (93%)	0.21	4 (4%) 42 35	84, 104, 131, 142	0
20	BI	97/106 (91%)	0.45	6 (6%) 26 22	98, 116, 141, 150	0
21	1B	22/27 (81%)	0.77	3 (13%) 7 6	118, 127, 133, 141	0
21	1F	23/27 (85%)	0.00	0 100 100	84, 95, 101, 111	0
22	1K	67/76 (88%)	1.46	14 (20%) 2 2	76, 147, 198, 203	0
22	1L	64/76 (84%)	2.05	21 (32%) 1 1	108, 196, 215, 219	0
23	2K	72/77 (93%)	0.10	1 (1%) 73 67	64, 86, 118, 128	0
23	2L	72/77 (93%)	0.55	6 (8%) 17 15	73, 105, 137, 148	0
24	3K	70/76 (92%)	1.38	14 (20%) 3 3	71, 198, 240, 244	0
24	3L	72/76 (94%)	1.29	17 (23%) 2 2	77, 194, 224, 230	0
25	4K	21/27 (77%)	1.12	7 (33%) 1 1	67, 124, 208, 209	0
25	4L	19/27 (70%)	1.12	6 (31%) 1 1	86, 143, 217, 218	0
26	14	2855/2917 (97%)	-0.32	39 (1%) 73 67	45, 78, 200, 265	0
26	1H	2885/2917 (98%)	-0.50	21 (0%) 84 80	31, 66, 193, 330	3 (0%)
27	16	122/122 (100%)	-0.63	0 100 100	57, 82, 103, 188	0
27	1J	122/122 (100%)	-0.09	2 (1%) 70 63	78, 110, 130, 191	0
28	71	133/229 (58%)	1.08	21 (15%) 5 4	146, 216, 237, 244	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	79	57/229 (24%)	1.67	16 (28%) 1 1	146, 199, 221, 227	0
29	11	273/276 (98%)	-0.01	4 (1%) 72 65	37, 59, 76, 92	0
29	19	274/276 (99%)	0.33	12 (4%) 39 32	46, 69, 87, 106	0
30	21	203/206 (98%)	0.39	9 (4%) 39 32	46, 80, 123, 134	0
30	29	204/206 (99%)	0.39	11 (5%) 31 26	53, 88, 124, 134	0
31	31	202/210 (96%)	-0.08	2 (0%) 79 74	43, 72, 107, 128	0
31	39	204/210 (97%)	0.34	12 (5%) 28 23	51, 98, 144, 167	0
32	41	179/182 (98%)	0.14	3 (1%) 69 62	72, 93, 130, 142	0
32	49	181/182 (99%)	0.53	11 (6%) 27 22	106, 125, 148, 166	0
33	51	174/180 (96%)	0.50	11 (6%) 26 22	75, 98, 112, 124	0
33	59	70/180 (38%)	1.84	23 (32%) 1 1	136, 156, 178, 182	0
34	61	146/148 (98%)	0.42	6 (4%) 41 34	73, 123, 144, 151	0
34	69	145/148 (97%)	0.68	18 (12%) 8 8	83, 118, 146, 155	0
35	15	138/140 (98%)	1.03	20 (14%) 6 5	73, 99, 128, 143	0
35	58	137/140 (97%)	0.54	7 (5%) 33 28	61, 83, 118, 132	0
36	25	122/122 (100%)	0.07	5 (4%) 41 34	64, 81, 99, 111	0
36	68	122/122 (100%)	-0.07	1 (0%) 82 78	53, 68, 85, 93	0
37	35	147/150 (98%)	0.36	6 (4%) 41 34	52, 95, 126, 140	0
37	78	147/150 (98%)	-0.13	1 (0%) 84 80	42, 74, 98, 107	0
38	45	139/141 (98%)	0.57	9 (6%) 25 21	64, 95, 114, 130	0
38	88	141/141 (100%)	-0.11	1 (0%) 84 80	49, 70, 92, 112	0
39	55	118/118 (100%)	-0.07	1 (0%) 82 78	59, 74, 88, 106	0
39	98	118/118 (100%)	0.07	1 (0%) 82 78	58, 76, 93, 107	0
40	65	110/112 (98%)	0.60	9 (8%) 17 15	82, 104, 124, 131	0
40	A8	111/112 (99%)	-0.05	2 (1%) 67 59	66, 82, 103, 110	0
41	75	133/146 (91%)	0.34	7 (5%) 32 27	77, 91, 124, 144	0
41	B8	136/146 (93%)	0.51	17 (12%) 8 7	64, 83, 122, 132	0
42	85	116/118 (98%)	0.61	7 (6%) 27 23	60, 87, 118, 120	0
42	C8	115/118 (97%)	0.29	3 (2%) 57 49	50, 73, 102, 109	0
43	95	100/101 (99%)	0.69	6 (6%) 27 23	58, 109, 127, 135	0
43	D8	100/101 (99%)	0.63	4 (4%) 42 35	52, 96, 116, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	A5	111/113 (98%)	0.11	3 (2%) 56 48	55, 70, 94, 135	0
44	E8	110/113 (97%)	-0.04	3 (2%) 56 48	51, 67, 91, 104	0
45	B5	94/96 (97%)	0.17	2 (2%) 63 55	62, 78, 98, 110	0
45	F8	95/96 (98%)	-0.03	1 (1%) 78 73	47, 63, 90, 97	0
46	C5	104/110 (94%)	1.41	28 (26%) 1 1	85, 113, 147, 155	0
46	G8	103/110 (93%)	0.81	10 (9%) 13 12	66, 88, 118, 129	0
47	D5	133/206 (64%)	0.51	7 (5%) 32 27	102, 130, 153, 163	0
47	H8	170/206 (82%)	0.19	4 (2%) 59 51	76, 111, 188, 193	0
48	E5	76/85 (89%)	0.24	2 (2%) 57 49	56, 83, 96, 104	0
48	I8	77/85 (90%)	-0.13	3 (3%) 43 35	45, 65, 78, 93	0
49	F5	94/98 (95%)	0.46	7 (7%) 20 18	59, 76, 106, 129	0
49	J8	94/98 (95%)	0.43	8 (8%) 16 15	46, 67, 110, 116	0
50	G5	69/72 (95%)	0.30	3 (4%) 40 32	77, 96, 116, 124	0
50	K8	68/72 (94%)	0.16	3 (4%) 39 32	54, 72, 92, 114	0
51	H5	58/60 (96%)	0.19	0 100 100	70, 90, 116, 124	0
51	L8	58/60 (96%)	-0.08	0 100 100	55, 74, 99, 111	0
52	M8	49/71 (69%)	0.84	6 (12%) 8 8	94, 136, 150, 166	0
53	J5	56/60 (93%)	0.27	1 (1%) 67 59	52, 77, 126, 137	0
53	N8	48/60 (80%)	-0.09	1 (2%) 63 55	44, 77, 124, 127	0
54	L5	47/49 (95%)	-0.37	1 (2%) 63 55	44, 55, 77, 97	0
54	P8	47/49 (95%)	-0.42	2 (4%) 40 32	40, 46, 68, 76	0
55	M5	64/65 (98%)	0.20	3 (4%) 36 30	62, 73, 88, 112	0
55	Q8	64/65 (98%)	-0.24	0 100 100	47, 60, 76, 88	0
All	All	20647/21961 (94%)	0.13	959 (4%) 37 31	31, 93, 171, 330	3 (0%)

The worst 5 of 959 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	1L	76	A	13.1
22	1K	76	A	9.5
43	D8	37	VAL	8.9
33	59	170	ARG	8.0
9	82	115	GLY	7.8

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, 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($\text{\AA}^2$)	Q<0.9
22	PSU	1L	55	20/21	0.78	0.09	113,126,140,141	0
22	5MU	1L	54	21/22	0.84	0.09	113,125,134,142	0
22	PSU	1K	55	20/21	0.84	0.10	95,109,120,124	0
22	U8U	1L	34	23/24	0.88	0.17	102,117,122,124	0
23	5MU	2L	55	21/22	0.88	0.09	99,108,115,124	0
23	PSU	2L	56	20/21	0.89	0.08	98,105,111,115	0
23	G7M	2L	47	24/25	0.90	0.11	110,117,123,127	0
23	5MU	2K	55	21/22	0.90	0.08	89,95,100,103	0
22	5MU	1K	54	21/22	0.90	0.08	93,106,119,128	0
23	4SU	2L	8	20/21	0.90	0.13	94,104,108,112	0
23	PSU	2K	56	20/21	0.91	0.07	86,90,100,104	0
23	G7M	2K	47	24/25	0.92	0.08	86,95,107,113	0
22	T6A	1L	37	32/33	0.92	0.17	91,110,116,118	0
22	PSU	1L	39	20/21	0.94	0.18	88,116,127,129	0
22	U8U	1K	34	23/24	0.94	0.11	76,81,86,100	0
23	OMC	2K	33	21/22	0.95	0.17	67,74,78,82	0
23	OMC	2L	33	21/22	0.95	0.11	88,93,99,103	0
23	4SU	2K	8	20/21	0.95	0.11	75,83,88,90	0
22	PSU	1K	39	20/21	0.95	0.15	74,91,100,100	0
22	T6A	1K	37	32/33	0.96	0.13	58,79,98,99	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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($\text{\AA}^2$)	Q<0.9
56	MG	1G	1661	1/1	0.44	0.39	92,92,92,92	0
56	MG	1H	3263	1/1	0.48	0.37	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3231	1/1	0.49	0.26	106,106,106,106	0
56	MG	1G	1631	1/1	0.53	0.34	99,99,99,99	0
56	MG	1H	3011	1/1	0.56	0.25	119,119,119,119	0
56	MG	1H	3208	1/1	0.57	0.22	141,141,141,141	0
56	MG	14	3151	1/1	0.58	0.34	107,107,107,107	0
56	MG	1H	3219	1/1	0.61	0.16	79,79,79,79	0
56	MG	1G	1632	1/1	0.61	0.35	92,92,92,92	0
56	MG	13	1640	1/1	0.62	0.33	99,99,99,99	0
56	MG	42	201	1/1	0.62	0.32	111,111,111,111	0
56	MG	1G	1635	1/1	0.62	0.22	101,101,101,101	0
56	MG	1G	1645	1/1	0.63	0.25	113,113,113,113	0
56	MG	2K	101	1/1	0.63	0.27	91,91,91,91	0
56	MG	1G	1643	1/1	0.64	0.29	106,106,106,106	0
56	MG	14	3178	1/1	0.64	0.30	114,114,114,114	0
56	MG	1H	3177	1/1	0.65	0.39	75,75,75,75	0
56	MG	1H	3015	1/1	0.65	0.41	82,82,82,82	0
56	MG	13	1628	1/1	0.66	0.27	89,89,89,89	0
56	MG	4K	101	1/1	0.66	0.36	96,96,96,96	0
56	MG	14	3209	1/1	0.66	0.30	90,90,90,90	0
56	MG	13	1658	1/1	0.67	0.13	116,116,116,116	0
56	MG	1H	3286	1/1	0.67	0.22	119,119,119,119	0
56	MG	1G	1637	1/1	0.68	0.35	89,89,89,89	0
56	MG	13	1653	1/1	0.68	0.34	80,80,80,80	0
56	MG	1J	207	1/1	0.68	0.16	88,88,88,88	0
56	MG	1H	3158	1/1	0.69	0.24	72,72,72,72	0
56	MG	1G	1656	1/1	0.70	0.43	89,89,89,89	0
56	MG	1H	3210	1/1	0.70	0.32	75,75,75,75	0
56	MG	1G	1668	1/1	0.70	0.28	96,96,96,96	0
56	MG	1H	3144	1/1	0.70	0.31	86,86,86,86	0
56	MG	1H	3455	1/1	0.70	0.12	76,76,76,76	0
56	MG	14	3166	1/1	0.70	0.31	85,85,85,85	0
56	MG	1G	1619	1/1	0.70	0.34	103,103,103,103	0
56	MG	13	1679	1/1	0.70	0.27	81,81,81,81	0
56	MG	14	3212	1/1	0.70	0.41	82,82,82,82	0
56	MG	1G	1655	1/1	0.70	0.27	106,106,106,106	0
56	MG	13	1668	1/1	0.71	0.26	105,105,105,105	0
56	MG	13	1662	1/1	0.71	0.25	114,114,114,114	0
56	MG	1H	3096	1/1	0.71	0.28	77,77,77,77	0
56	MG	14	3214	1/1	0.71	0.31	113,113,113,113	0
56	MG	1H	3143	1/1	0.71	0.37	84,84,84,84	0
56	MG	14	3180	1/1	0.72	0.31	74,74,74,74	0
56	MG	1H	3228	1/1	0.72	0.29	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1638	1/1	0.72	0.35	92,92,92,92	0
56	MG	1H	3207	1/1	0.72	0.22	119,119,119,119	0
56	MG	1H	3194	1/1	0.72	0.33	83,83,83,83	0
56	MG	1H	3169	1/1	0.73	0.26	111,111,111,111	0
56	MG	14	3158	1/1	0.73	0.37	91,91,91,91	0
56	MG	1H	3258	1/1	0.73	0.48	97,97,97,97	0
56	MG	1G	1604	1/1	0.73	0.30	102,102,102,102	0
56	MG	13	1655	1/1	0.73	0.43	99,99,99,99	0
56	MG	14	3192	1/1	0.73	0.26	81,81,81,81	0
56	MG	1G	1642	1/1	0.73	0.21	102,102,102,102	0
56	MG	1H	3276	1/1	0.73	0.26	78,78,78,78	0
56	MG	14	3118	1/1	0.73	0.30	89,89,89,89	0
56	MG	14	3148	1/1	0.73	0.20	78,78,78,78	0
56	MG	1H	3077	1/1	0.74	0.15	70,70,70,70	0
56	MG	14	3179	1/1	0.74	0.24	92,92,92,92	0
56	MG	13	1627	1/1	0.74	0.33	82,82,82,82	0
56	MG	14	3183	1/1	0.74	0.26	87,87,87,87	0
56	MG	1H	3270	1/1	0.74	0.34	78,78,78,78	0
56	MG	14	3205	1/1	0.74	0.29	87,87,87,87	0
56	MG	1G	1614	1/1	0.74	0.29	91,91,91,91	0
56	MG	1H	3256	1/1	0.74	0.30	100,100,100,100	0
56	MG	14	3161	1/1	0.74	0.34	86,86,86,86	0
56	MG	1G	1624	1/1	0.74	0.23	87,87,87,87	0
56	MG	39	302	1/1	0.74	0.14	73,73,73,73	0
56	MG	13	1676	1/1	0.75	0.15	92,92,92,92	0
56	MG	14	3124	1/1	0.75	0.12	62,62,62,62	0
56	MG	14	3190	1/1	0.75	0.17	81,81,81,81	0
56	MG	1H	3203	1/1	0.75	0.23	68,68,68,68	0
56	MG	13	1601	1/1	0.75	0.29	102,102,102,102	0
56	MG	1H	3153	1/1	0.75	0.33	88,88,88,88	0
56	MG	13	1685	1/1	0.75	0.31	100,100,100,100	0
56	MG	13	1688	1/1	0.75	0.24	92,92,92,92	0
56	MG	1J	202	1/1	0.75	0.20	91,91,91,91	0
56	MG	13	1661	1/1	0.75	0.31	73,73,73,73	0
56	MG	1H	3181	1/1	0.75	0.24	88,88,88,88	0
56	MG	14	3116	1/1	0.76	0.28	89,89,89,89	0
56	MG	13	1673	1/1	0.76	0.31	93,93,93,93	0
56	MG	1H	3195	1/1	0.76	0.15	69,69,69,69	0
56	MG	1H	3217	1/1	0.76	0.10	61,61,61,61	0
56	MG	1J	206	1/1	0.76	0.21	86,86,86,86	0
56	MG	14	3177	1/1	0.76	0.26	91,91,91,91	0
56	MG	14	3149	1/1	0.76	0.41	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3234	1/1	0.77	0.30	90,90,90,90	0
56	MG	13	1672	1/1	0.77	0.22	79,79,79,79	0
56	MG	1H	3161	1/1	0.77	0.18	82,82,82,82	0
56	MG	13	1687	1/1	0.77	0.26	82,82,82,82	0
56	MG	1H	3170	1/1	0.77	0.22	115,115,115,115	0
56	MG	13	1624	1/1	0.77	0.29	80,80,80,80	0
56	MG	13	1663	1/1	0.77	0.29	90,90,90,90	0
56	MG	42	202	1/1	0.77	0.22	110,110,110,110	0
56	MG	14	3081	1/1	0.77	0.30	89,89,89,89	0
56	MG	13	1677	1/1	0.77	0.21	77,77,77,77	0
56	MG	13	1643	1/1	0.77	0.31	69,69,69,69	0
56	MG	1G	1641	1/1	0.78	0.46	91,91,91,91	0
56	MG	1H	3230	1/1	0.78	0.31	89,89,89,89	0
56	MG	13	1667	1/1	0.78	0.17	105,105,105,105	0
56	MG	14	3027	1/1	0.78	0.23	86,86,86,86	0
56	MG	14	3028	1/1	0.78	0.43	83,83,83,83	0
56	MG	16	203	1/1	0.78	0.20	78,78,78,78	0
56	MG	14	3175	1/1	0.78	0.15	74,74,74,74	0
56	MG	1H	3264	1/1	0.78	0.20	80,80,80,80	0
56	MG	1H	3209	1/1	0.78	0.17	65,65,65,65	0
56	MG	1H	3079	1/1	0.78	0.32	88,88,88,88	0
56	MG	14	3141	1/1	0.78	0.32	86,86,86,86	0
56	MG	1G	1660	1/1	0.79	0.23	92,92,92,92	0
56	MG	13	1629	1/1	0.79	0.17	85,85,85,85	0
56	MG	14	3140	1/1	0.79	0.24	78,78,78,78	0
56	MG	1G	1667	1/1	0.79	0.28	97,97,97,97	0
56	MG	1G	1639	1/1	0.79	0.23	87,87,87,87	0
56	MG	1H	3204	1/1	0.79	0.32	74,74,74,74	0
56	MG	13	1602	1/1	0.79	0.27	61,61,61,61	0
56	MG	1H	3227	1/1	0.79	0.15	79,79,79,79	0
56	MG	16	202	1/1	0.79	0.16	66,66,66,66	0
56	MG	14	3049	1/1	0.79	0.34	79,79,79,79	0
56	MG	14	3050	1/1	0.79	0.28	76,76,76,76	0
56	MG	1H	3105	1/1	0.79	0.39	72,72,72,72	0
56	MG	1H	3156	1/1	0.79	0.08	55,55,55,55	0
56	MG	1H	3107	1/1	0.80	0.27	73,73,73,73	0
56	MG	1H	3180	1/1	0.80	0.28	87,87,87,87	0
56	MG	14	3186	1/1	0.80	0.29	80,80,80,80	0
56	MG	1H	3089	1/1	0.80	0.28	82,82,82,82	0
56	MG	13	1730	1/1	0.80	0.12	102,102,102,102	0
56	MG	14	3199	1/1	0.80	0.32	89,89,89,89	0
56	MG	1G	1607	1/1	0.80	0.18	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3145	1/1	0.80	0.32	82,82,82,82	0
56	MG	14	3163	1/1	0.80	0.31	76,76,76,76	0
56	MG	14	3213	1/1	0.80	0.33	78,78,78,78	0
56	MG	1H	3082	1/1	0.80	0.16	55,55,55,55	0
56	MG	14	3244	1/1	0.80	0.27	71,71,71,71	0
56	MG	1G	1620	1/1	0.80	0.28	85,85,85,85	0
56	MG	14	3129	1/1	0.80	0.16	62,62,62,62	0
56	MG	14	3131	1/1	0.80	0.17	62,62,62,62	0
56	MG	1J	209	1/1	0.80	0.22	93,93,93,93	0
56	MG	1H	3254	1/1	0.80	0.20	69,69,69,69	0
56	MG	16	201	1/1	0.81	0.27	84,84,84,84	0
56	MG	1G	1617	1/1	0.81	0.37	86,86,86,86	0
56	MG	14	3197	1/1	0.81	0.13	44,44,44,44	0
56	MG	1H	3186	1/1	0.81	0.28	76,76,76,76	0
56	MG	1H	3281	1/1	0.81	0.14	82,82,82,82	0
56	MG	88	201	1/1	0.81	0.30	73,73,73,73	0
56	MG	14	3127	1/1	0.81	0.16	85,85,85,85	0
56	MG	1G	1602	1/1	0.81	0.28	87,87,87,87	0
56	MG	14	3130	1/1	0.81	0.15	75,75,75,75	0
56	MG	14	3221	1/1	0.81	0.32	86,86,86,86	0
56	MG	1H	3213	1/1	0.81	0.30	96,96,96,96	0
56	MG	14	3432	1/1	0.81	0.16	92,92,92,92	0
56	MG	1G	1651	1/1	0.81	0.16	84,84,84,84	0
56	MG	1G	1654	1/1	0.81	0.25	99,99,99,99	0
56	MG	14	3143	1/1	0.81	0.33	86,86,86,86	0
56	MG	1J	208	1/1	0.81	0.25	90,90,90,90	0
56	MG	1H	3059	1/1	0.81	0.32	73,73,73,73	0
56	MG	14	3187	1/1	0.81	0.44	81,81,81,81	0
56	MG	13	1654	1/1	0.82	0.18	91,91,91,91	0
56	MG	14	3075	1/1	0.82	0.22	78,78,78,78	0
56	MG	5I	101	1/1	0.82	0.16	77,77,77,77	0
56	MG	16	206	1/1	0.82	0.19	81,81,81,81	0
56	MG	13	1678	1/1	0.82	0.36	83,83,83,83	0
56	MG	1H	3251	1/1	0.82	0.28	80,80,80,80	0
56	MG	1H	3157	1/1	0.82	0.15	96,96,96,96	0
56	MG	13	1671	1/1	0.82	0.22	79,79,79,79	0
56	MG	1G	1608	1/1	0.82	0.33	96,96,96,96	0
56	MG	1G	1613	1/1	0.82	0.16	85,85,85,85	0
56	MG	13	1644	1/1	0.82	0.23	94,94,94,94	0
56	MG	13	1657	1/1	0.82	0.27	89,89,89,89	0
56	MG	1H	3040	1/1	0.82	0.27	71,71,71,71	0
56	MG	1H	3211	1/1	0.82	0.16	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3128	1/1	0.82	0.28	76,76,76,76	0
56	MG	1G	1630	1/1	0.82	0.28	97,97,97,97	0
56	MG	14	3225	1/1	0.82	0.32	84,84,84,84	0
56	MG	14	3231	1/1	0.82	0.28	69,69,69,69	0
56	MG	14	3236	1/1	0.82	0.17	94,94,94,94	0
56	MG	14	3238	1/1	0.82	0.29	83,83,83,83	0
56	MG	14	3157	1/1	0.82	0.20	76,76,76,76	0
56	MG	1H	3132	1/1	0.82	0.19	58,58,58,58	0
56	MG	14	3019	1/1	0.82	0.19	48,48,48,48	0
56	MG	1J	204	1/1	0.82	0.29	90,90,90,90	0
56	MG	1H	3041	1/1	0.82	0.18	86,86,86,86	0
56	MG	13	1622	1/1	0.82	0.26	104,104,104,104	0
56	MG	14	3173	1/1	0.82	0.28	93,93,93,93	0
56	MG	14	3045	1/1	0.82	0.14	67,67,67,67	0
56	MG	1H	3193	1/1	0.82	0.19	78,78,78,78	0
56	MG	25	201	1/1	0.82	0.23	93,93,93,93	0
56	MG	14	3224	1/1	0.83	0.31	82,82,82,82	0
56	MG	14	3109	1/1	0.83	0.22	86,86,86,86	0
56	MG	1G	1644	1/1	0.83	0.22	92,92,92,92	0
56	MG	13	1681	1/1	0.83	0.21	83,83,83,83	0
56	MG	14	3152	1/1	0.83	0.20	85,85,85,85	0
56	MG	1G	1646	1/1	0.83	0.15	119,119,119,119	0
56	MG	1H	3094	1/1	0.83	0.24	61,61,61,61	0
56	MG	13	1617	1/1	0.83	0.11	53,53,53,53	0
56	MG	14	3058	1/1	0.83	0.23	93,93,93,93	0
56	MG	13	1674	1/1	0.83	0.24	67,67,67,67	0
56	MG	14	3137	1/1	0.83	0.25	61,61,61,61	0
56	MG	14	3138	1/1	0.83	0.15	71,71,71,71	0
56	MG	14	3079	1/1	0.83	0.20	75,75,75,75	0
56	MG	13	1648	1/1	0.83	0.17	105,105,105,105	0
56	MG	14	3103	1/1	0.83	0.23	81,81,81,81	0
56	MG	13	1631	1/1	0.84	0.22	89,89,89,89	0
56	MG	14	3215	1/1	0.84	0.10	79,79,79,79	0
56	MG	14	3048	1/1	0.84	0.15	68,68,68,68	0
56	MG	1H	3172	1/1	0.84	0.33	70,70,70,70	0
56	MG	2K	103	1/1	0.84	0.20	56,56,56,56	0
56	MG	1G	1659	1/1	0.84	0.24	85,85,85,85	0
56	MG	14	3234	1/1	0.84	0.20	71,71,71,71	0
56	MG	14	3064	1/1	0.84	0.26	62,62,62,62	0
56	MG	1H	3127	1/1	0.84	0.18	44,44,44,44	0
56	MG	14	3240	1/1	0.84	0.21	83,83,83,83	0
56	MG	13	1639	1/1	0.84	0.31	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3298	1/1	0.84	0.13	105,105,105,105	0
56	MG	14	3328	1/1	0.84	0.16	83,83,83,83	0
56	MG	1H	3050	1/1	0.84	0.13	49,49,49,49	0
56	MG	1H	3241	1/1	0.84	0.40	81,81,81,81	0
56	MG	1H	3247	1/1	0.84	0.27	62,62,62,62	0
56	MG	1J	205	1/1	0.84	0.25	90,90,90,90	0
56	MG	13	1626	1/1	0.84	0.18	60,60,60,60	0
56	MG	1H	3162	1/1	0.84	0.20	66,66,66,66	0
56	MG	1H	3215	1/1	0.84	0.27	83,83,83,83	0
56	MG	1H	3066	1/1	0.84	0.23	57,57,57,57	0
56	MG	14	3029	1/1	0.84	0.20	68,68,68,68	0
56	MG	14	3171	1/1	0.84	0.27	84,84,84,84	0
56	MG	1G	1664	1/1	0.85	0.17	126,126,126,126	0
56	MG	1H	3431	1/1	0.85	0.18	74,74,74,74	0
56	MG	14	3128	1/1	0.85	0.12	49,49,49,49	0
56	MG	14	3193	1/1	0.85	0.16	74,74,74,74	0
56	MG	1H	3115	1/1	0.85	0.28	59,59,59,59	0
56	MG	14	3198	1/1	0.85	0.37	84,84,84,84	0
56	MG	1H	3238	1/1	0.85	0.13	76,76,76,76	0
56	MG	14	3200	1/1	0.85	0.29	94,94,94,94	0
56	MG	13	1636	1/1	0.85	0.29	70,70,70,70	0
56	MG	14	3206	1/1	0.85	0.25	72,72,72,72	0
56	MG	14	3208	1/1	0.85	0.31	77,77,77,77	0
56	MG	14	3134	1/1	0.85	0.31	88,88,88,88	0
56	MG	14	3211	1/1	0.85	0.25	70,70,70,70	0
56	MG	14	3136	1/1	0.85	0.12	83,83,83,83	0
56	MG	14	3005	1/1	0.85	0.20	73,73,73,73	0
56	MG	1G	1636	1/1	0.85	0.20	91,91,91,91	0
56	MG	1H	3084	1/1	0.85	0.22	58,58,58,58	0
56	MG	14	3217	1/1	0.85	0.35	94,94,94,94	0
56	MG	13	1642	1/1	0.85	0.22	78,78,78,78	0
56	MG	1H	3212	1/1	0.85	0.21	90,90,90,90	0
56	MG	1H	3012	1/1	0.85	0.24	78,78,78,78	0
56	MG	1H	3164	1/1	0.85	0.08	53,53,53,53	0
56	MG	1H	3260	1/1	0.85	0.25	74,74,74,74	0
56	MG	1H	3013	1/1	0.85	0.25	69,69,69,69	0
56	MG	14	3154	1/1	0.85	0.13	60,60,60,60	0
56	MG	14	3239	1/1	0.85	0.36	82,82,82,82	0
56	MG	14	3056	1/1	0.85	0.47	69,69,69,69	0
56	MG	14	3241	1/1	0.85	0.15	77,77,77,77	0
56	MG	1G	1612	1/1	0.85	0.36	76,76,76,76	0
56	MG	14	3062	1/1	0.85	0.22	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3311	1/1	0.85	0.15	73,73,73,73	0
56	MG	1H	3201	1/1	0.85	0.39	82,82,82,82	0
56	MG	13	1633	1/1	0.85	0.10	80,80,80,80	0
56	MG	1H	3171	1/1	0.85	0.37	67,67,67,67	0
56	MG	1G	1618	1/1	0.85	0.27	88,88,88,88	0
56	MG	14	3095	1/1	0.85	0.30	76,76,76,76	0
56	MG	1H	3205	1/1	0.85	0.29	73,73,73,73	0
56	MG	13	1669	1/1	0.85	0.27	95,95,95,95	0
56	MG	14	3110	1/1	0.85	0.22	51,51,51,51	0
56	MG	14	3112	1/1	0.85	0.20	69,69,69,69	0
56	MG	1H	3287	1/1	0.85	0.20	121,121,121,121	0
56	MG	1G	1629	1/1	0.85	0.26	69,69,69,69	0
56	MG	14	3119	1/1	0.86	0.21	67,67,67,67	0
56	MG	14	3169	1/1	0.86	0.37	81,81,81,81	0
56	MG	14	3033	1/1	0.86	0.22	63,63,63,63	0
56	MG	1G	1648	1/1	0.86	0.16	94,94,94,94	0
56	MG	13	1646	1/1	0.86	0.18	89,89,89,89	0
56	MG	1H	3027	1/1	0.86	0.21	68,68,68,68	0
56	MG	1H	3199	1/1	0.86	0.22	74,74,74,74	0
56	MG	1H	3232	1/1	0.86	0.32	77,77,77,77	0
56	MG	14	3133	1/1	0.86	0.26	72,72,72,72	0
56	MG	16	205	1/1	0.86	0.20	83,83,83,83	0
56	MG	14	3184	1/1	0.86	0.17	70,70,70,70	0
56	MG	1H	3102	1/1	0.86	0.23	63,63,63,63	0
56	MG	1H	3014	1/1	0.86	0.23	75,75,75,75	0
56	MG	1H	3165	1/1	0.86	0.22	63,63,63,63	0
56	MG	14	3078	1/1	0.86	0.22	80,80,80,80	0
56	MG	1H	3278	1/1	0.86	0.24	76,76,76,76	0
56	MG	1H	3106	1/1	0.86	0.26	55,55,55,55	0
56	MG	14	3084	1/1	0.86	0.28	77,77,77,77	0
56	MG	1H	3284	1/1	0.86	0.29	44,44,44,44	0
56	MG	1H	3190	1/1	0.86	0.09	60,60,60,60	0
56	MG	1H	3252	1/1	0.86	0.37	75,75,75,75	0
56	MG	14	3153	1/1	0.86	0.38	74,74,74,74	0
56	MG	1H	3363	1/1	0.86	0.15	78,78,78,78	0
56	MG	14	3111	1/1	0.86	0.25	73,73,73,73	0
56	MG	1H	3407	1/1	0.86	0.14	89,89,89,89	0
56	MG	1H	3133	1/1	0.86	0.26	64,64,64,64	0
56	MG	1H	3444	1/1	0.86	0.14	82,82,82,82	0
56	MG	1H	3220	1/1	0.87	0.36	71,71,71,71	0
56	MG	14	3189	1/1	0.87	0.11	60,60,60,60	0
56	MG	1H	3479	1/1	0.87	0.13	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3495	1/1	0.87	0.08	100,100,100,100	0
56	MG	14	3004	1/1	0.87	0.28	58,58,58,58	0
56	MG	1H	3540	1/1	0.87	0.08	78,78,78,78	0
56	MG	14	3013	1/1	0.87	0.20	60,60,60,60	0
56	MG	14	3016	1/1	0.87	0.26	55,55,55,55	0
56	MG	1H	3257	1/1	0.87	0.22	83,83,83,83	0
56	MG	14	3201	1/1	0.87	0.08	84,84,84,84	0
56	MG	14	3024	1/1	0.87	0.21	65,65,65,65	0
56	MG	13	1686	1/1	0.87	0.14	98,98,98,98	0
56	MG	1H	3191	1/1	0.87	0.12	59,59,59,59	0
56	MG	1H	3137	1/1	0.87	0.20	70,70,70,70	0
56	MG	1H	3138	1/1	0.87	0.18	59,59,59,59	0
56	MG	1G	1640	1/1	0.87	0.20	95,95,95,95	0
56	MG	11	302	1/1	0.87	0.14	55,55,55,55	0
56	MG	1H	3160	1/1	0.87	0.21	70,70,70,70	0
56	MG	1H	3123	1/1	0.87	0.24	65,65,65,65	0
56	MG	14	3052	1/1	0.87	0.35	71,71,71,71	0
56	MG	14	3219	1/1	0.87	0.30	86,86,86,86	0
56	MG	14	3053	1/1	0.87	0.25	53,53,53,53	0
56	MG	1H	3236	1/1	0.87	0.29	78,78,78,78	0
56	MG	1G	1605	1/1	0.87	0.22	76,76,76,76	0
56	MG	1H	3019	1/1	0.87	0.22	39,39,39,39	0
56	MG	14	3063	1/1	0.87	0.21	82,82,82,82	0
56	MG	1H	3240	1/1	0.87	0.15	75,75,75,75	0
56	MG	14	3072	1/1	0.87	0.27	67,67,67,67	0
56	MG	14	3160	1/1	0.87	0.39	78,78,78,78	0
56	MG	1G	1650	1/1	0.87	0.15	89,89,89,89	0
56	MG	14	3076	1/1	0.87	0.27	68,68,68,68	0
56	MG	1H	3285	1/1	0.87	0.28	50,50,50,50	0
56	MG	14	3167	1/1	0.87	0.09	54,54,54,54	0
56	MG	1H	3214	1/1	0.87	0.37	83,83,83,83	0
56	MG	13	1635	1/1	0.87	0.18	72,72,72,72	0
56	MG	14	3400	1/1	0.87	0.12	90,90,90,90	0
56	MG	1H	3345	1/1	0.87	0.11	91,91,91,91	0
56	MG	14	3463	1/1	0.87	0.19	97,97,97,97	0
56	MG	14	3470	1/1	0.87	0.16	79,79,79,79	0
56	MG	14	3093	1/1	0.87	0.13	71,71,71,71	0
56	MG	1G	1658	1/1	0.87	0.17	79,79,79,79	0
56	MG	14	3097	1/1	0.87	0.25	70,70,70,70	0
56	MG	1H	3034	1/1	0.87	0.24	63,63,63,63	0
56	MG	1H	3218	1/1	0.87	0.19	65,65,65,65	0
56	MG	14	3181	1/1	0.87	0.23	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3253	1/1	0.87	0.16	62,62,62,62	0
56	MG	1H	3187	1/1	0.87	0.29	77,77,77,77	0
56	MG	1G	1627	1/1	0.87	0.09	139,139,139,139	0
56	MG	35	201	1/1	0.87	0.12	74,74,74,74	0
56	MG	E5	103	1/1	0.87	0.32	80,80,80,80	0
56	MG	13	1734	1/1	0.88	0.08	105,105,105,105	0
56	MG	13	1747	1/1	0.88	0.08	107,107,107,107	0
56	MG	98	201	1/1	0.88	0.31	67,67,67,67	0
56	MG	14	3185	1/1	0.88	0.24	71,71,71,71	0
56	MG	1H	3048	1/1	0.88	0.15	45,45,45,45	0
56	MG	14	3237	1/1	0.88	0.15	88,88,88,88	0
56	MG	13	1613	1/1	0.88	0.26	86,86,86,86	0
56	MG	1H	3147	1/1	0.88	0.13	43,43,43,43	0
56	MG	14	3150	1/1	0.88	0.39	84,84,84,84	0
56	MG	1H	3151	1/1	0.88	0.13	52,52,52,52	0
56	MG	1H	3245	1/1	0.88	0.10	58,58,58,58	0
56	MG	1H	3246	1/1	0.88	0.22	71,71,71,71	0
56	MG	14	3308	1/1	0.88	0.13	90,90,90,90	0
56	MG	13	1620	1/1	0.88	0.35	74,74,74,74	0
56	MG	1H	3065	1/1	0.88	0.18	61,61,61,61	0
56	MG	13	1614	1/1	0.88	0.31	73,73,73,73	0
56	MG	1H	3016	1/1	0.88	0.22	72,72,72,72	0
56	MG	14	3435	1/1	0.88	0.15	93,93,93,93	0
56	MG	13	1638	1/1	0.88	0.20	71,71,71,71	0
56	MG	1H	3473	1/1	0.88	0.15	88,88,88,88	0
56	MG	1H	3124	1/1	0.88	0.24	70,70,70,70	0
56	MG	1G	1625	1/1	0.88	0.17	81,81,81,81	0
56	MG	1H	3080	1/1	0.88	0.23	74,74,74,74	0
56	MG	1H	3005	1/1	0.88	0.32	83,83,83,83	0
56	MG	1H	3083	1/1	0.88	0.18	81,81,81,81	0
56	MG	1H	3229	1/1	0.88	0.10	59,59,59,59	0
56	MG	1H	3008	1/1	0.88	0.23	61,61,61,61	0
56	MG	1H	3087	1/1	0.88	0.20	66,66,66,66	0
56	MG	1G	1695	1/1	0.88	0.10	99,99,99,99	0
56	MG	14	3220	1/1	0.88	0.21	74,74,74,74	0
56	MG	1H	3271	1/1	0.88	0.18	63,63,63,63	0
56	MG	13	1607	1/1	0.89	0.09	74,74,74,74	0
56	MG	1H	3196	1/1	0.89	0.19	62,62,62,62	0
56	MG	14	3203	1/1	0.89	0.19	69,69,69,69	0
56	MG	1H	3267	1/1	0.89	0.39	90,90,90,90	0
56	MG	1H	3141	1/1	0.89	0.12	53,53,53,53	0
56	MG	14	3038	1/1	0.89	0.20	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3167	1/1	0.89	0.13	45,45,45,45	0
56	MG	1H	3275	1/1	0.89	0.20	68,68,68,68	0
56	MG	4I	202	1/1	0.89	0.17	75,75,75,75	0
56	MG	1H	3168	1/1	0.89	0.36	75,75,75,75	0
56	MG	1H	3277	1/1	0.89	0.34	81,81,81,81	0
56	MG	P8	101	1/1	0.89	0.24	66,66,66,66	0
56	MG	1H	3023	1/1	0.89	0.22	56,56,56,56	0
56	MG	1H	3279	1/1	0.89	0.11	67,67,67,67	0
56	MG	1H	3049	1/1	0.89	0.11	50,50,50,50	0
56	MG	1H	3009	1/1	0.89	0.23	74,74,74,74	0
56	MG	1G	1653	1/1	0.89	0.24	82,82,82,82	0
56	MG	14	3067	1/1	0.89	0.22	85,85,85,85	0
56	MG	1H	3146	1/1	0.89	0.39	90,90,90,90	0
56	MG	14	3232	1/1	0.89	0.15	88,88,88,88	0
56	MG	14	3074	1/1	0.89	0.26	76,76,76,76	0
56	MG	14	3235	1/1	0.89	0.23	83,83,83,83	0
56	MG	1H	3176	1/1	0.89	0.27	51,51,51,51	0
56	MG	1H	3118	1/1	0.89	0.26	52,52,52,52	0
56	MG	14	3164	1/1	0.89	0.32	64,64,64,64	0
56	MG	1H	3311	1/1	0.89	0.17	56,56,56,56	0
56	MG	1H	3032	1/1	0.89	0.28	68,68,68,68	0
56	MG	14	3168	1/1	0.89	0.21	52,52,52,52	0
56	MG	1H	3064	1/1	0.89	0.32	76,76,76,76	0
56	MG	1H	3369	1/1	0.89	0.11	57,57,57,57	0
56	MG	14	3087	1/1	0.89	0.20	73,73,73,73	0
56	MG	1H	3183	1/1	0.89	0.23	74,74,74,74	0
56	MG	14	3319	1/1	0.89	0.15	84,84,84,84	0
56	MG	1G	1665	1/1	0.89	0.10	104,104,104,104	0
56	MG	13	1649	1/1	0.89	0.33	87,87,87,87	0
56	MG	1H	3039	1/1	0.89	0.24	74,74,74,74	0
56	MG	1G	1626	1/1	0.89	0.18	78,78,78,78	0
56	MG	14	3447	1/1	0.89	0.11	116,116,116,116	0
56	MG	1G	1702	1/1	0.89	0.15	100,100,100,100	0
56	MG	1H	3068	1/1	0.89	0.19	50,50,50,50	0
56	MG	1G	1628	1/1	0.89	0.24	77,77,77,77	0
56	MG	2L	103	1/1	0.89	0.26	70,70,70,70	0
56	MG	14	3002	1/1	0.89	0.15	61,61,61,61	0
56	MG	13	1682	1/1	0.89	0.09	91,91,91,91	0
56	MG	14	3122	1/1	0.89	0.24	53,53,53,53	0
56	MG	1H	3192	1/1	0.89	0.31	61,61,61,61	0
56	MG	14	3125	1/1	0.89	0.25	76,76,76,76	0
56	MG	1H	3135	1/1	0.89	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3104	1/1	0.89	0.16	65,65,65,65	0
56	MG	1G	1634	1/1	0.89	0.16	91,91,91,91	0
56	MG	35	203	1/1	0.89	0.18	83,83,83,83	0
56	MG	1H	3551	1/1	0.89	0.11	105,105,105,105	0
56	MG	1H	3556	1/1	0.90	0.09	101,101,101,101	0
56	MG	1H	3557	1/1	0.90	0.10	84,84,84,84	0
56	MG	1H	3283	1/1	0.90	0.10	58,58,58,58	0
56	MG	1G	1621	1/1	0.90	0.20	76,76,76,76	0
56	MG	13	1659	1/1	0.90	0.24	57,57,57,57	0
56	MG	14	3018	1/1	0.90	0.23	75,75,75,75	0
56	MG	1H	3090	1/1	0.90	0.21	50,50,50,50	0
56	MG	14	3144	1/1	0.90	0.25	60,60,60,60	0
56	MG	14	3085	1/1	0.90	0.20	64,64,64,64	0
56	MG	14	3191	1/1	0.90	0.14	66,66,66,66	0
56	MG	14	3242	1/1	0.90	0.24	83,83,83,83	0
56	MG	1H	3018	1/1	0.90	0.29	51,51,51,51	0
56	MG	14	3245	1/1	0.90	0.12	61,61,61,61	0
56	MG	14	3089	1/1	0.90	0.12	53,53,53,53	0
56	MG	14	3025	1/1	0.90	0.19	59,59,59,59	0
56	MG	1H	3233	1/1	0.90	0.21	57,57,57,57	0
56	MG	14	3316	1/1	0.90	0.12	79,79,79,79	0
56	MG	1H	3173	1/1	0.90	0.16	67,67,67,67	0
56	MG	1H	3262	1/1	0.90	0.39	86,86,86,86	0
56	MG	14	3155	1/1	0.90	0.21	73,73,73,73	0
56	MG	14	3032	1/1	0.90	0.27	50,50,50,50	0
56	MG	1H	3159	1/1	0.90	0.08	69,69,69,69	0
56	MG	88	203	1/1	0.90	0.22	87,87,87,87	0
56	MG	13	1645	1/1	0.90	0.27	84,84,84,84	0
56	MG	1H	3239	1/1	0.90	0.34	69,69,69,69	0
56	MG	1H	3125	1/1	0.90	0.17	50,50,50,50	0
56	MG	1H	3020	1/1	0.90	0.19	56,56,56,56	0
56	MG	13	1612	1/1	0.90	0.13	78,78,78,78	0
56	MG	1H	3470	1/1	0.90	0.14	82,82,82,82	0
56	MG	1H	3047	1/1	0.90	0.30	76,76,76,76	0
56	MG	1H	3224	1/1	0.90	0.15	74,74,74,74	0
56	MG	1G	1726	1/1	0.90	0.20	92,92,92,92	0
56	MG	1H	3085	1/1	0.90	0.19	85,85,85,85	0
56	MG	13	1625	1/1	0.90	0.22	78,78,78,78	0
56	MG	14	3222	1/1	0.90	0.20	88,88,88,88	0
56	MG	2L	101	1/1	0.90	0.27	71,71,71,71	0
56	MG	45	201	1/1	0.90	0.19	87,87,87,87	0
56	MG	1H	3155	1/1	0.90	0.20	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3273	1/1	0.91	0.21	76,76,76,76	0
56	MG	1H	3108	1/1	0.91	0.20	34,34,34,34	0
56	MG	16	211	1/1	0.91	0.15	92,92,92,92	0
56	MG	14	3204	1/1	0.91	0.20	63,63,63,63	0
56	MG	1H	3112	1/1	0.91	0.10	53,53,53,53	0
56	MG	14	3037	1/1	0.91	0.22	61,61,61,61	0
56	MG	13	1632	1/1	0.91	0.17	69,69,69,69	0
56	MG	1H	3117	1/1	0.91	0.12	61,61,61,61	0
56	MG	1H	3081	1/1	0.91	0.36	76,76,76,76	0
56	MG	14	3139	1/1	0.91	0.28	75,75,75,75	0
56	MG	1H	3121	1/1	0.91	0.39	64,64,64,64	0
56	MG	13	1605	1/1	0.91	0.16	79,79,79,79	0
56	MG	13	1683	1/1	0.91	0.19	92,92,92,92	0
56	MG	14	3216	1/1	0.91	0.30	79,79,79,79	0
56	MG	1G	1652	1/1	0.91	0.29	76,76,76,76	0
56	MG	14	3145	1/1	0.91	0.20	75,75,75,75	0
56	MG	14	3146	1/1	0.91	0.21	72,72,72,72	0
56	MG	13	1684	1/1	0.91	0.23	71,71,71,71	0
56	MG	13	1650	1/1	0.91	0.15	121,121,121,121	0
56	MG	14	3059	1/1	0.91	0.16	53,53,53,53	0
56	MG	1H	3054	1/1	0.91	0.45	70,70,70,70	0
56	MG	14	3227	1/1	0.91	0.23	70,70,70,70	0
56	MG	1H	3001	1/1	0.91	0.12	61,61,61,61	0
56	MG	13	1675	1/1	0.91	0.11	65,65,65,65	0
56	MG	1H	3134	1/1	0.91	0.16	74,74,74,74	0
56	MG	13	1651	1/1	0.91	0.29	82,82,82,82	0
56	MG	1G	1615	1/1	0.91	0.12	93,93,93,93	0
56	MG	13	1652	1/1	0.91	0.34	91,91,91,91	0
56	MG	1H	3421	1/1	0.91	0.09	98,98,98,98	0
56	MG	1H	3100	1/1	0.91	0.25	59,59,59,59	0
56	MG	1H	3101	1/1	0.91	0.15	79,79,79,79	0
56	MG	1H	3142	1/1	0.91	0.11	74,74,74,74	0
56	MG	14	3083	1/1	0.91	0.15	74,74,74,74	0
56	MG	14	3243	1/1	0.91	0.29	60,60,60,60	0
56	MG	1G	1622	1/1	0.91	0.24	73,73,73,73	0
56	MG	13	1712	1/1	0.91	0.14	96,96,96,96	0
56	MG	14	3284	1/1	0.91	0.21	87,87,87,87	0
56	MG	1H	3471	1/1	0.91	0.08	91,91,91,91	0
56	MG	14	3170	1/1	0.91	0.10	63,63,63,63	0
56	MG	1H	3069	1/1	0.91	0.21	45,45,45,45	0
56	MG	14	3313	1/1	0.91	0.10	53,53,53,53	0
56	MG	14	3172	1/1	0.91	0.28	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3091	1/1	0.91	0.16	44,44,44,44	0
56	MG	1H	3178	1/1	0.91	0.32	69,69,69,69	0
56	MG	14	3176	1/1	0.91	0.22	72,72,72,72	0
56	MG	1H	3216	1/1	0.91	0.18	71,71,71,71	0
56	MG	1H	3498	1/1	0.91	0.12	85,85,85,85	0
56	MG	13	1670	1/1	0.91	0.27	80,80,80,80	0
56	MG	14	3455	1/1	0.91	0.20	87,87,87,87	0
56	MG	14	3462	1/1	0.91	0.12	99,99,99,99	0
56	MG	14	3106	1/1	0.91	0.31	75,75,75,75	0
56	MG	1H	3549	1/1	0.91	0.14	75,75,75,75	0
56	MG	14	3006	1/1	0.91	0.22	67,67,67,67	0
56	MG	1H	3078	1/1	0.91	0.24	70,70,70,70	0
56	MG	14	3015	1/1	0.91	0.18	80,80,80,80	0
56	MG	14	3113	1/1	0.91	0.10	67,67,67,67	0
56	MG	14	3115	1/1	0.91	0.23	64,64,64,64	0
56	MG	13	1606	1/1	0.91	0.19	71,71,71,71	0
56	MG	1H	3184	1/1	0.91	0.12	57,57,57,57	0
56	MG	1H	3222	1/1	0.91	0.13	72,72,72,72	0
56	MG	14	3020	1/1	0.91	0.21	73,73,73,73	0
56	MG	1H	3223	1/1	0.91	0.23	76,76,76,76	0
56	MG	1H	3149	1/1	0.91	0.13	54,54,54,54	0
56	MG	14	3026	1/1	0.91	0.24	70,70,70,70	0
56	MG	E5	101	1/1	0.91	0.36	74,74,74,74	0
56	MG	E5	102	1/1	0.91	0.34	72,72,72,72	0
56	MG	16	204	1/1	0.91	0.12	57,57,57,57	0
58	ZN	G8	201	1/1	0.91	0.16	143,143,143,143	0
56	MG	14	3223	1/1	0.92	0.20	78,78,78,78	0
56	MG	1H	3445	1/1	0.92	0.08	90,90,90,90	0
56	MG	1H	3221	1/1	0.92	0.12	65,65,65,65	0
56	MG	13	1758	1/1	0.92	0.09	137,137,137,137	0
56	MG	14	3230	1/1	0.92	0.17	74,74,74,74	0
56	MG	1H	3166	1/1	0.92	0.07	52,52,52,52	0
56	MG	13	1761	1/1	0.92	0.18	75,75,75,75	0
56	MG	1H	3225	1/1	0.92	0.11	60,60,60,60	0
56	MG	1H	3198	1/1	0.92	0.19	65,65,65,65	0
56	MG	14	3034	1/1	0.92	0.32	72,72,72,72	0
56	MG	14	3117	1/1	0.92	0.22	79,79,79,79	0
56	MG	13	1630	1/1	0.92	0.39	81,81,81,81	0
56	MG	1H	3504	1/1	0.92	0.07	86,86,86,86	0
56	MG	14	3120	1/1	0.92	0.14	72,72,72,72	0
56	MG	1H	3519	1/1	0.92	0.13	78,78,78,78	0
56	MG	1H	3530	1/1	0.92	0.24	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3533	1/1	0.92	0.15	86,86,86,86	0
56	MG	1G	1663	1/1	0.92	0.10	85,85,85,85	0
56	MG	1H	3200	1/1	0.92	0.27	70,70,70,70	0
56	MG	13	1615	1/1	0.92	0.16	94,94,94,94	0
56	MG	1H	3202	1/1	0.92	0.21	63,63,63,63	0
56	MG	14	3305	1/1	0.92	0.09	96,96,96,96	0
56	MG	13	1623	1/1	0.92	0.25	62,62,62,62	0
56	MG	1G	1694	1/1	0.92	0.12	103,103,103,103	0
56	MG	1H	3053	1/1	0.92	0.19	40,40,40,40	0
56	MG	13	1637	1/1	0.92	0.09	73,73,73,73	0
56	MG	1G	1723	1/1	0.92	0.10	106,106,106,106	0
56	MG	1H	3086	1/1	0.92	0.17	65,65,65,65	0
56	MG	14	3360	1/1	0.92	0.09	88,88,88,88	0
56	MG	14	3196	1/1	0.92	0.07	77,77,77,77	0
56	MG	14	3071	1/1	0.92	0.24	52,52,52,52	0
56	MG	13	1664	1/1	0.92	0.34	69,69,69,69	0
56	MG	14	3437	1/1	0.92	0.06	115,115,115,115	0
56	MG	1H	3122	1/1	0.92	0.17	58,58,58,58	0
56	MG	13	1665	1/1	0.92	0.31	76,76,76,76	0
56	MG	13	1666	1/1	0.92	0.29	79,79,79,79	0
56	MG	1H	3030	1/1	0.92	0.17	49,49,49,49	0
56	MG	14	3465	1/1	0.92	0.14	85,85,85,85	0
56	MG	14	3468	1/1	0.92	0.20	58,58,58,58	0
56	MG	1H	3095	1/1	0.92	0.23	66,66,66,66	0
56	MG	21	301	1/1	0.92	0.21	62,62,62,62	0
56	MG	13	1647	1/1	0.92	0.12	73,73,73,73	0
56	MG	14	3207	1/1	0.92	0.23	63,63,63,63	0
56	MG	14	3012	1/1	0.92	0.20	56,56,56,56	0
56	MG	1H	3129	1/1	0.92	0.20	66,66,66,66	0
56	MG	14	3086	1/1	0.92	0.14	61,61,61,61	0
56	MG	1H	3131	1/1	0.92	0.11	54,54,54,54	0
56	MG	39	301	1/1	0.92	0.15	92,92,92,92	0
56	MG	1H	3010	1/1	0.92	0.12	53,53,53,53	0
56	MG	14	3017	1/1	0.92	0.25	54,54,54,54	0
56	MG	1H	3070	1/1	0.92	0.27	54,54,54,54	0
56	MG	35	202	1/1	0.92	0.20	78,78,78,78	0
56	MG	14	3094	1/1	0.92	0.21	73,73,73,73	0
56	MG	14	3159	1/1	0.92	0.15	70,70,70,70	0
56	MG	1H	3255	1/1	0.92	0.09	75,75,75,75	0
56	MG	13	1750	1/1	0.92	0.12	101,101,101,101	0
56	MG	13	1752	1/1	0.92	0.08	108,108,108,108	0
56	MG	14	3104	1/1	0.92	0.45	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3033	1/1	0.93	0.24	67,67,67,67	0
56	MG	1H	3348	1/1	0.93	0.16	78,78,78,78	0
56	MG	1H	3002	1/1	0.93	0.15	59,59,59,59	0
56	MG	14	3080	1/1	0.93	0.15	53,53,53,53	0
56	MG	1G	1633	1/1	0.93	0.14	92,92,92,92	0
56	MG	14	3229	1/1	0.93	0.13	66,66,66,66	0
56	MG	1H	3057	1/1	0.93	0.21	63,63,63,63	0
56	MG	14	3003	1/1	0.93	0.15	43,43,43,43	0
56	MG	1H	3405	1/1	0.93	0.08	91,91,91,91	0
56	MG	14	3233	1/1	0.93	0.09	61,61,61,61	0
56	MG	16	210	1/1	0.93	0.10	89,89,89,89	0
56	MG	1H	3103	1/1	0.93	0.16	62,62,62,62	0
56	MG	14	3008	1/1	0.93	0.17	84,84,84,84	0
56	MG	14	3090	1/1	0.93	0.22	55,55,55,55	0
56	MG	1H	3419	1/1	0.93	0.08	78,78,78,78	0
56	MG	1H	3058	1/1	0.93	0.18	69,69,69,69	0
56	MG	21	302	1/1	0.93	0.25	75,75,75,75	0
56	MG	13	1723	1/1	0.93	0.11	75,75,75,75	0
56	MG	1H	3060	1/1	0.93	0.08	54,54,54,54	0
56	MG	14	3100	1/1	0.93	0.14	77,77,77,77	0
56	MG	14	3102	1/1	0.93	0.18	60,60,60,60	0
56	MG	88	202	1/1	0.93	0.22	67,67,67,67	0
56	MG	13	1689	1/1	0.93	0.08	65,65,65,65	0
56	MG	1H	3136	1/1	0.93	0.51	76,76,76,76	0
56	MG	14	3302	1/1	0.93	0.09	96,96,96,96	0
56	MG	14	3021	1/1	0.93	0.18	36,36,36,36	0
56	MG	F8	101	1/1	0.93	0.11	63,63,63,63	0
56	MG	1G	1647	1/1	0.93	0.14	82,82,82,82	0
56	MG	1H	3461	1/1	0.93	0.07	90,90,90,90	0
56	MG	1H	3163	1/1	0.93	0.38	83,83,83,83	0
56	MG	14	3114	1/1	0.93	0.17	68,68,68,68	0
56	MG	14	3327	1/1	0.93	0.09	60,60,60,60	0
56	MG	1H	3272	1/1	0.93	0.51	67,67,67,67	0
56	MG	14	3331	1/1	0.93	0.15	65,65,65,65	0
56	MG	14	3346	1/1	0.93	0.10	74,74,74,74	0
56	MG	1H	3026	1/1	0.93	0.18	71,71,71,71	0
56	MG	1H	3110	1/1	0.93	0.18	44,44,44,44	0
56	MG	1H	3482	1/1	0.93	0.09	85,85,85,85	0
56	MG	1H	3043	1/1	0.93	0.14	47,47,47,47	0
56	MG	14	3035	1/1	0.93	0.23	67,67,67,67	0
56	MG	13	1616	1/1	0.93	0.29	77,77,77,77	0
56	MG	14	3449	1/1	0.93	0.10	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3454	1/1	0.93	0.20	78,78,78,78	0
56	MG	1H	3088	1/1	0.93	0.37	74,74,74,74	0
56	MG	14	3457	1/1	0.93	0.07	92,92,92,92	0
56	MG	14	3459	1/1	0.93	0.06	97,97,97,97	0
56	MG	1H	3509	1/1	0.93	0.16	46,46,46,46	0
56	MG	13	1719	1/1	0.93	0.13	89,89,89,89	0
56	MG	1H	3524	1/1	0.93	0.08	96,96,96,96	0
56	MG	1G	1662	1/1	0.93	0.19	94,94,94,94	0
56	MG	1H	3280	1/1	0.93	0.21	76,76,76,76	0
56	MG	1H	3248	1/1	0.93	0.19	72,72,72,72	0
56	MG	14	3132	1/1	0.93	0.35	56,56,56,56	0
56	MG	14	3054	1/1	0.93	0.17	55,55,55,55	0
56	MG	1H	3249	1/1	0.93	0.33	67,67,67,67	0
56	MG	14	3057	1/1	0.93	0.21	61,61,61,61	0
56	MG	1H	3031	1/1	0.93	0.21	74,74,74,74	0
56	MG	1H	3092	1/1	0.93	0.23	55,55,55,55	0
56	MG	1G	1672	1/1	0.93	0.07	109,109,109,109	0
56	MG	1H	3554	1/1	0.93	0.13	100,100,100,100	0
56	MG	1H	3075	1/1	0.93	0.23	80,80,80,80	0
56	MG	14	3066	1/1	0.93	0.15	49,49,49,49	0
56	MG	1G	1700	1/1	0.93	0.08	87,87,87,87	0
56	MG	14	3068	1/1	0.93	0.18	59,59,59,59	0
56	MG	1H	3076	1/1	0.93	0.24	60,60,60,60	0
56	MG	1G	1713	1/1	0.93	0.07	112,112,112,112	0
56	MG	14	3073	1/1	0.93	0.25	65,65,65,65	0
56	MG	1H	3563	1/1	0.93	0.19	75,75,75,75	0
56	MG	5E	201	1/1	0.93	0.13	71,71,71,71	0
56	MG	14	3105	1/1	0.94	0.09	72,72,72,72	0
56	MG	1H	3061	1/1	0.94	0.20	41,41,41,41	0
56	MG	1H	3097	1/1	0.94	0.22	53,53,53,53	0
56	MG	1G	1616	1/1	0.94	0.26	71,71,71,71	0
56	MG	14	3036	1/1	0.94	0.18	39,39,39,39	0
56	MG	1H	3098	1/1	0.94	0.13	58,58,58,58	0
56	MG	13	1610	1/1	0.94	0.13	77,77,77,77	0
56	MG	14	3043	1/1	0.94	0.17	68,68,68,68	0
56	MG	13	1756	1/1	0.94	0.05	120,120,120,120	0
56	MG	14	3046	1/1	0.94	0.14	52,52,52,52	0
56	MG	1H	3226	1/1	0.94	0.19	78,78,78,78	0
56	MG	14	3254	1/1	0.94	0.07	92,92,92,92	0
56	MG	1H	3331	1/1	0.94	0.08	49,49,49,49	0
56	MG	14	3296	1/1	0.94	0.12	70,70,70,70	0
56	MG	13	1634	1/1	0.94	0.07	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3051	1/1	0.94	0.19	62,62,62,62	0
56	MG	1G	1623	1/1	0.94	0.12	77,77,77,77	0
56	MG	1H	3067	1/1	0.94	0.27	75,75,75,75	0
56	MG	1G	1691	1/1	0.94	0.07	110,110,110,110	0
56	MG	1H	3179	1/1	0.94	0.15	47,47,47,47	0
56	MG	13	1611	1/1	0.94	0.20	64,64,64,64	0
56	MG	1G	1697	1/1	0.94	0.11	94,94,94,94	0
56	MG	14	3324	1/1	0.94	0.12	70,70,70,70	0
56	MG	1H	3390	1/1	0.94	0.07	102,102,102,102	0
56	MG	1H	3401	1/1	0.94	0.10	46,46,46,46	0
56	MG	1H	3261	1/1	0.94	0.24	65,65,65,65	0
56	MG	14	3342	1/1	0.94	0.10	75,75,75,75	0
56	MG	1G	1719	1/1	0.94	0.07	100,100,100,100	0
56	MG	14	3349	1/1	0.94	0.10	65,65,65,65	0
56	MG	14	3357	1/1	0.94	0.10	79,79,79,79	0
56	MG	1H	3051	1/1	0.94	0.17	46,46,46,46	0
56	MG	14	3368	1/1	0.94	0.07	75,75,75,75	0
56	MG	14	3390	1/1	0.94	0.12	72,72,72,72	0
56	MG	14	3395	1/1	0.94	0.07	69,69,69,69	0
56	MG	14	3396	1/1	0.94	0.06	102,102,102,102	0
56	MG	1H	3411	1/1	0.94	0.11	65,65,65,65	0
56	MG	14	3405	1/1	0.94	0.05	106,106,106,106	0
56	MG	14	3417	1/1	0.94	0.09	116,116,116,116	0
56	MG	1H	3182	1/1	0.94	0.18	56,56,56,56	0
56	MG	14	3202	1/1	0.94	0.11	65,65,65,65	0
56	MG	1H	3037	1/1	0.94	0.32	63,63,63,63	0
56	MG	1H	3265	1/1	0.94	0.07	69,69,69,69	0
56	MG	1H	3438	1/1	0.94	0.07	71,71,71,71	0
56	MG	1H	3440	1/1	0.94	0.08	72,72,72,72	0
56	MG	14	3142	1/1	0.94	0.14	83,83,83,83	0
56	MG	1H	3074	1/1	0.94	0.05	52,52,52,52	0
56	MG	1H	3235	1/1	0.94	0.25	65,65,65,65	0
56	MG	14	3210	1/1	0.94	0.26	74,74,74,74	0
56	MG	78	201	1/1	0.94	0.20	70,70,70,70	0
56	MG	14	3464	1/1	0.94	0.09	105,105,105,105	0
56	MG	1H	3451	1/1	0.94	0.09	78,78,78,78	0
56	MG	1H	3452	1/1	0.94	0.07	72,72,72,72	0
56	MG	1H	3025	1/1	0.94	0.17	32,32,32,32	0
56	MG	13	1604	1/1	0.94	0.14	66,66,66,66	0
56	MG	1H	3111	1/1	0.94	0.17	57,57,57,57	0
56	MG	L8	101	1/1	0.94	0.19	80,80,80,80	0
56	MG	1H	3274	1/1	0.94	0.19	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3091	1/1	0.94	0.12	65,65,65,65	0
56	MG	13	1603	1/1	0.94	0.15	72,72,72,72	0
56	MG	1G	1649	1/1	0.94	0.11	83,83,83,83	0
56	MG	1H	3243	1/1	0.94	0.14	54,54,54,54	0
56	MG	14	3022	1/1	0.94	0.21	73,73,73,73	0
56	MG	1G	1606	1/1	0.94	0.09	80,80,80,80	0
56	MG	14	3226	1/1	0.94	0.12	51,51,51,51	0
56	MG	1H	3093	1/1	0.94	0.15	60,60,60,60	0
56	MG	13	1608	1/1	0.94	0.17	71,71,71,71	0
56	MG	1G	1611	1/1	0.94	0.13	84,84,84,84	0
56	MG	B5	101	1/1	0.94	0.08	76,76,76,76	0
56	MG	14	3101	1/1	0.94	0.18	70,70,70,70	0
56	MG	1H	3120	1/1	0.94	0.07	39,39,39,39	0
56	MG	1H	3046	1/1	0.94	0.15	59,59,59,59	0
56	MG	1G	1657	1/1	0.94	0.24	77,77,77,77	0
56	MG	1H	3435	1/1	0.95	0.06	55,55,55,55	0
56	MG	14	3253	1/1	0.95	0.06	57,57,57,57	0
56	MG	1H	3035	1/1	0.95	0.09	64,64,64,64	0
56	MG	14	3263	1/1	0.95	0.07	64,64,64,64	0
56	MG	14	3269	1/1	0.95	0.09	60,60,60,60	0
56	MG	1H	3439	1/1	0.95	0.07	55,55,55,55	0
56	MG	13	1744	1/1	0.95	0.06	111,111,111,111	0
56	MG	1H	3442	1/1	0.95	0.15	64,64,64,64	0
56	MG	13	1746	1/1	0.95	0.06	102,102,102,102	0
56	MG	1H	3126	1/1	0.95	0.16	64,64,64,64	0
56	MG	14	3188	1/1	0.95	0.09	61,61,61,61	0
56	MG	1G	1709	1/1	0.95	0.10	99,99,99,99	0
56	MG	1G	1710	1/1	0.95	0.06	95,95,95,95	0
56	MG	14	3314	1/1	0.95	0.10	46,46,46,46	0
56	MG	1H	3188	1/1	0.95	0.22	69,69,69,69	0
56	MG	11	301	1/1	0.95	0.08	77,77,77,77	0
56	MG	1G	1722	1/1	0.95	0.06	102,102,102,102	0
56	MG	14	3195	1/1	0.95	0.18	71,71,71,71	0
56	MG	13	1680	1/1	0.95	0.29	73,73,73,73	0
56	MG	1H	3454	1/1	0.95	0.17	67,67,67,67	0
56	MG	14	3335	1/1	0.95	0.12	78,78,78,78	0
56	MG	14	3341	1/1	0.95	0.10	76,76,76,76	0
56	MG	1H	3017	1/1	0.95	0.26	55,55,55,55	0
56	MG	14	3345	1/1	0.95	0.07	66,66,66,66	0
56	MG	1H	3148	1/1	0.95	0.08	56,56,56,56	0
56	MG	14	3065	1/1	0.95	0.16	58,58,58,58	0
56	MG	14	3354	1/1	0.95	0.07	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3468	1/1	0.95	0.09	68,68,68,68	0
56	MG	1H	3073	1/1	0.95	0.14	39,39,39,39	0
56	MG	14	3363	1/1	0.95	0.06	54,54,54,54	0
56	MG	1H	3150	1/1	0.95	0.18	51,51,51,51	0
56	MG	13	1618	1/1	0.95	0.10	45,45,45,45	0
56	MG	1H	3114	1/1	0.95	0.15	66,66,66,66	0
56	MG	1H	3341	1/1	0.95	0.09	43,43,43,43	0
56	MG	1H	3491	1/1	0.95	0.19	73,73,73,73	0
56	MG	1H	3154	1/1	0.95	0.21	60,60,60,60	0
56	MG	14	3407	1/1	0.95	0.12	79,79,79,79	0
56	MG	14	3010	1/1	0.95	0.18	50,50,50,50	0
56	MG	14	3077	1/1	0.95	0.19	45,45,45,45	0
56	MG	1H	3099	1/1	0.95	0.32	80,80,80,80	0
56	MG	1G	1603	1/1	0.95	0.13	85,85,85,85	0
56	MG	1H	3242	1/1	0.95	0.20	70,70,70,70	0
56	MG	1H	3268	1/1	0.95	0.16	78,78,78,78	0
56	MG	1H	3386	1/1	0.95	0.06	88,88,88,88	0
56	MG	1H	3520	1/1	0.95	0.16	98,98,98,98	0
56	MG	1H	3269	1/1	0.95	0.17	61,61,61,61	0
56	MG	14	3218	1/1	0.95	0.10	74,74,74,74	0
56	MG	1G	1609	1/1	0.95	0.13	70,70,70,70	0
56	MG	1H	3526	1/1	0.95	0.10	73,73,73,73	0
56	MG	1H	3044	1/1	0.95	0.14	39,39,39,39	0
56	MG	14	3156	1/1	0.95	0.40	86,86,86,86	0
56	MG	14	3467	1/1	0.95	0.20	71,71,71,71	0
56	MG	14	3023	1/1	0.95	0.14	69,69,69,69	0
56	MG	1H	3244	1/1	0.95	0.10	67,67,67,67	0
56	MG	14	3471	1/1	0.95	0.10	68,68,68,68	0
56	MG	1J	201	1/1	0.95	0.05	70,70,70,70	0
56	MG	13	1656	1/1	0.95	0.10	60,60,60,60	0
56	MG	1J	203	1/1	0.95	0.18	70,70,70,70	0
56	MG	1H	3546	1/1	0.95	0.07	93,93,93,93	0
56	MG	1H	3119	1/1	0.95	0.10	46,46,46,46	0
56	MG	14	3096	1/1	0.95	0.12	48,48,48,48	0
56	MG	1H	3415	1/1	0.95	0.13	73,73,73,73	0
56	MG	14	3165	1/1	0.95	0.18	67,67,67,67	0
56	MG	14	3098	1/1	0.95	0.17	68,68,68,68	0
56	MG	29	301	1/1	0.95	0.16	49,49,49,49	0
56	MG	1K	101	1/1	0.95	0.08	119,119,119,119	0
56	MG	14	3030	1/1	0.95	0.16	38,38,38,38	0
56	MG	1H	3021	1/1	0.95	0.17	43,43,43,43	0
56	MG	1H	3426	1/1	0.95	0.12	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3562	1/1	0.95	0.15	69,69,69,69	0
56	MG	1H	3022	1/1	0.95	0.16	45,45,45,45	0
56	MG	1G	1666	1/1	0.95	0.07	100,100,100,100	0
56	MG	1H	3568	1/1	0.95	0.14	94,94,94,94	0
56	MG	1H	3572	1/1	0.95	0.18	54,54,54,54	0
56	MG	14	3042	1/1	0.95	0.20	85,85,85,85	0
56	MG	1G	1669	1/1	0.95	0.08	81,81,81,81	0
56	MG	14	3044	1/1	0.95	0.30	78,78,78,78	0
56	MG	1H	3062	1/1	0.96	0.06	29,29,29,29	0
56	MG	13	1749	1/1	0.96	0.06	106,106,106,106	0
56	MG	1H	3522	1/1	0.96	0.05	98,98,98,98	0
56	MG	14	3174	1/1	0.96	0.16	64,64,64,64	0
56	MG	1H	3045	1/1	0.96	0.14	42,42,42,42	0
56	MG	1G	1610	1/1	0.96	0.08	70,70,70,70	0
56	MG	14	3299	1/1	0.96	0.05	99,99,99,99	0
56	MG	14	3301	1/1	0.96	0.10	111,111,111,111	0
56	MG	1H	3424	1/1	0.96	0.08	44,44,44,44	0
56	MG	1H	3028	1/1	0.96	0.11	49,49,49,49	0
56	MG	14	3031	1/1	0.96	0.20	48,48,48,48	0
56	MG	1H	3427	1/1	0.96	0.10	60,60,60,60	0
56	MG	1H	3534	1/1	0.96	0.06	85,85,85,85	0
56	MG	14	3107	1/1	0.96	0.08	61,61,61,61	0
56	MG	14	3315	1/1	0.96	0.07	56,56,56,56	0
56	MG	14	3108	1/1	0.96	0.04	67,67,67,67	0
56	MG	14	3318	1/1	0.96	0.06	65,65,65,65	0
56	MG	1H	3536	1/1	0.96	0.07	98,98,98,98	0
56	MG	14	3321	1/1	0.96	0.06	88,88,88,88	0
56	MG	14	3322	1/1	0.96	0.13	77,77,77,77	0
56	MG	1H	3538	1/1	0.96	0.20	78,78,78,78	0
56	MG	1H	3428	1/1	0.96	0.06	64,64,64,64	0
56	MG	1H	3029	1/1	0.96	0.10	48,48,48,48	0
56	MG	1H	3432	1/1	0.96	0.05	44,44,44,44	0
56	MG	14	3333	1/1	0.96	0.10	64,64,64,64	0
56	MG	14	3334	1/1	0.96	0.09	69,69,69,69	0
56	MG	14	3040	1/1	0.96	0.12	58,58,58,58	0
56	MG	1H	3282	1/1	0.96	0.14	66,66,66,66	0
56	MG	1G	1682	1/1	0.96	0.16	117,117,117,117	0
56	MG	1G	1688	1/1	0.96	0.08	81,81,81,81	0
56	MG	14	3194	1/1	0.96	0.31	79,79,79,79	0
56	MG	14	3347	1/1	0.96	0.10	74,74,74,74	0
56	MG	1H	3189	1/1	0.96	0.13	53,53,53,53	0
56	MG	1H	3555	1/1	0.96	0.21	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	13	1641	1/1	0.96	0.10	78,78,78,78	0
56	MG	14	3121	1/1	0.96	0.15	45,45,45,45	0
56	MG	1G	1696	1/1	0.96	0.07	107,107,107,107	0
56	MG	14	3123	1/1	0.96	0.08	60,60,60,60	0
56	MG	14	3376	1/1	0.96	0.11	91,91,91,91	0
56	MG	14	3383	1/1	0.96	0.05	102,102,102,102	0
56	MG	14	3384	1/1	0.96	0.09	79,79,79,79	0
56	MG	14	3385	1/1	0.96	0.07	80,80,80,80	0
56	MG	13	1733	1/1	0.96	0.10	102,102,102,102	0
56	MG	14	3392	1/1	0.96	0.06	85,85,85,85	0
56	MG	1G	1698	1/1	0.96	0.06	102,102,102,102	0
56	MG	1H	3560	1/1	0.96	0.11	85,85,85,85	0
56	MG	13	1754	1/1	0.96	0.07	80,80,80,80	0
56	MG	1G	1703	1/1	0.96	0.13	85,85,85,85	0
56	MG	14	3055	1/1	0.96	0.19	50,50,50,50	0
56	MG	14	3413	1/1	0.96	0.12	64,64,64,64	0
56	MG	1H	3071	1/1	0.96	0.10	57,57,57,57	0
56	MG	14	3424	1/1	0.96	0.05	81,81,81,81	0
56	MG	14	3429	1/1	0.96	0.10	68,68,68,68	0
56	MG	1H	3293	1/1	0.96	0.06	41,41,41,41	0
56	MG	1G	1712	1/1	0.96	0.05	122,122,122,122	0
56	MG	14	3436	1/1	0.96	0.08	98,98,98,98	0
56	MG	1H	3447	1/1	0.96	0.07	59,59,59,59	0
56	MG	14	3061	1/1	0.96	0.18	47,47,47,47	0
56	MG	1G	1717	1/1	0.96	0.06	118,118,118,118	0
56	MG	14	3451	1/1	0.96	0.07	88,88,88,88	0
56	MG	1H	3449	1/1	0.96	0.12	53,53,53,53	0
56	MG	1H	3130	1/1	0.96	0.09	54,54,54,54	0
56	MG	1H	3326	1/1	0.96	0.09	56,56,56,56	0
56	MG	13	1713	1/1	0.96	0.17	82,82,82,82	0
56	MG	14	3461	1/1	0.96	0.11	80,80,80,80	0
56	MG	1H	3266	1/1	0.96	0.11	61,61,61,61	0
56	MG	1H	3456	1/1	0.96	0.12	102,102,102,102	0
56	MG	52	201	1/1	0.96	0.05	109,109,109,109	0
56	MG	1H	3006	1/1	0.96	0.20	43,43,43,43	0
56	MG	14	3466	1/1	0.96	0.10	92,92,92,92	0
56	MG	1H	3463	1/1	0.96	0.07	78,78,78,78	0
56	MG	14	3147	1/1	0.96	0.11	66,66,66,66	0
56	MG	1H	3467	1/1	0.96	0.06	95,95,95,95	0
56	MG	1H	3197	1/1	0.96	0.13	69,69,69,69	0
56	MG	1H	3469	1/1	0.96	0.05	79,79,79,79	0
56	MG	1H	3174	1/1	0.96	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	13	1740	1/1	0.96	0.06	96,96,96,96	0
56	MG	1H	3372	1/1	0.96	0.06	54,54,54,54	0
56	MG	1H	3379	1/1	0.96	0.05	86,86,86,86	0
56	MG	14	3011	1/1	0.96	0.20	50,50,50,50	0
56	MG	14	3082	1/1	0.96	0.10	73,73,73,73	0
56	MG	1H	3055	1/1	0.96	0.14	43,43,43,43	0
56	MG	1H	3484	1/1	0.96	0.06	88,88,88,88	0
56	MG	1J	210	1/1	0.96	0.08	91,91,91,91	0
56	MG	13	1741	1/1	0.96	0.06	110,110,110,110	0
56	MG	13	1621	1/1	0.96	0.14	84,84,84,84	0
56	MG	13	1609	1/1	0.96	0.19	64,64,64,64	0
56	MG	14	3162	1/1	0.96	0.06	50,50,50,50	0
56	MG	14	3088	1/1	0.96	0.07	105,105,105,105	0
56	MG	1H	3501	1/1	0.96	0.06	76,76,76,76	0
56	MG	Q8	101	1/1	0.96	0.15	71,71,71,71	0
56	MG	13	1724	1/1	0.96	0.06	94,94,94,94	0
56	MG	14	3092	1/1	0.96	0.14	43,43,43,43	0
56	MG	1H	3505	1/1	0.96	0.18	82,82,82,82	0
56	MG	13	1748	1/1	0.96	0.12	102,102,102,102	0
56	MG	14	3252	1/1	0.96	0.06	52,52,52,52	0
56	MG	M5	101	1/1	0.96	0.14	81,81,81,81	0
56	MG	1H	3518	1/1	0.96	0.11	76,76,76,76	0
58	ZN	C5	201	1/1	0.96	0.05	156,156,156,156	0
56	MG	1H	3332	1/1	0.97	0.05	50,50,50,50	0
56	MG	14	3268	1/1	0.97	0.06	64,64,64,64	0
56	MG	1G	1675	1/1	0.97	0.09	101,101,101,101	0
56	MG	14	3270	1/1	0.97	0.05	80,80,80,80	0
56	MG	14	3272	1/1	0.97	0.05	68,68,68,68	0
56	MG	1G	1677	1/1	0.97	0.06	93,93,93,93	0
56	MG	14	3290	1/1	0.97	0.06	67,67,67,67	0
56	MG	14	3291	1/1	0.97	0.10	82,82,82,82	0
56	MG	1G	1678	1/1	0.97	0.10	93,93,93,93	0
56	MG	14	3297	1/1	0.97	0.06	91,91,91,91	0
56	MG	1G	1681	1/1	0.97	0.05	99,99,99,99	0
56	MG	1H	3340	1/1	0.97	0.10	65,65,65,65	0
56	MG	14	3300	1/1	0.97	0.04	76,76,76,76	0
56	MG	1G	1684	1/1	0.97	0.05	98,98,98,98	0
56	MG	1G	1687	1/1	0.97	0.06	75,75,75,75	0
56	MG	1H	3152	1/1	0.97	0.14	87,87,87,87	0
56	MG	1G	1689	1/1	0.97	0.06	79,79,79,79	0
56	MG	14	3310	1/1	0.97	0.08	98,98,98,98	0
56	MG	13	1736	1/1	0.97	0.12	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	13	1710	1/1	0.97	0.09	85,85,85,85	0
56	MG	1H	3477	1/1	0.97	0.04	91,91,91,91	0
56	MG	1G	1601	1/1	0.97	0.09	78,78,78,78	0
56	MG	1H	3353	1/1	0.97	0.05	68,68,68,68	0
56	MG	1H	3360	1/1	0.97	0.06	59,59,59,59	0
56	MG	1H	3362	1/1	0.97	0.06	55,55,55,55	0
56	MG	1H	3485	1/1	0.97	0.05	97,97,97,97	0
56	MG	1H	3488	1/1	0.97	0.07	85,85,85,85	0
56	MG	1G	1705	1/1	0.97	0.06	116,116,116,116	0
56	MG	14	3326	1/1	0.97	0.04	81,81,81,81	0
56	MG	1G	1708	1/1	0.97	0.10	84,84,84,84	0
56	MG	1H	3490	1/1	0.97	0.07	95,95,95,95	0
56	MG	14	3330	1/1	0.97	0.04	77,77,77,77	0
56	MG	13	1660	1/1	0.97	0.14	55,55,55,55	0
56	MG	1H	3366	1/1	0.97	0.12	67,67,67,67	0
56	MG	1H	3496	1/1	0.97	0.15	76,76,76,76	0
56	MG	1H	3497	1/1	0.97	0.07	75,75,75,75	0
56	MG	14	3336	1/1	0.97	0.06	75,75,75,75	0
56	MG	13	1742	1/1	0.97	0.05	105,105,105,105	0
56	MG	1G	1720	1/1	0.97	0.10	129,129,129,129	0
56	MG	14	3182	1/1	0.97	0.04	66,66,66,66	0
56	MG	1H	3499	1/1	0.97	0.17	82,82,82,82	0
56	MG	13	1743	1/1	0.97	0.06	102,102,102,102	0
56	MG	14	3348	1/1	0.97	0.05	51,51,51,51	0
56	MG	1G	1724	1/1	0.97	0.09	102,102,102,102	0
56	MG	14	3350	1/1	0.97	0.06	44,44,44,44	0
56	MG	14	3353	1/1	0.97	0.05	91,91,91,91	0
56	MG	1G	1725	1/1	0.97	0.06	95,95,95,95	0
56	MG	14	3356	1/1	0.97	0.05	60,60,60,60	0
56	MG	1H	3503	1/1	0.97	0.10	75,75,75,75	0
56	MG	1H	3375	1/1	0.97	0.06	85,85,85,85	0
56	MG	1H	3377	1/1	0.97	0.04	49,49,49,49	0
56	MG	13	1619	1/1	0.97	0.07	51,51,51,51	0
56	MG	14	3373	1/1	0.97	0.07	58,58,58,58	0
56	MG	1H	3513	1/1	0.97	0.15	64,64,64,64	0
56	MG	14	3379	1/1	0.97	0.04	94,94,94,94	0
56	MG	1H	3185	1/1	0.97	0.22	54,54,54,54	0
56	MG	1H	3388	1/1	0.97	0.05	97,97,97,97	0
56	MG	14	3099	1/1	0.97	0.21	51,51,51,51	0
56	MG	14	3387	1/1	0.97	0.05	87,87,87,87	0
56	MG	14	3388	1/1	0.97	0.04	90,90,90,90	0
56	MG	1H	3063	1/1	0.97	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3391	1/1	0.97	0.06	73,73,73,73	0
56	MG	1H	3397	1/1	0.97	0.06	46,46,46,46	0
56	MG	14	3393	1/1	0.97	0.05	98,98,98,98	0
56	MG	1H	3398	1/1	0.97	0.06	55,55,55,55	0
56	MG	1H	3042	1/1	0.97	0.06	43,43,43,43	0
56	MG	14	3398	1/1	0.97	0.06	84,84,84,84	0
56	MG	13	1716	1/1	0.97	0.04	108,108,108,108	0
56	MG	14	3009	1/1	0.97	0.10	41,41,41,41	0
56	MG	1H	3532	1/1	0.97	0.05	96,96,96,96	0
56	MG	14	3408	1/1	0.97	0.05	94,94,94,94	0
56	MG	14	3410	1/1	0.97	0.09	83,83,83,83	0
56	MG	14	3412	1/1	0.97	0.06	76,76,76,76	0
56	MG	13	1718	1/1	0.97	0.08	54,54,54,54	0
56	MG	1H	3409	1/1	0.97	0.09	65,65,65,65	0
56	MG	14	3422	1/1	0.97	0.14	70,70,70,70	0
56	MG	1H	3113	1/1	0.97	0.05	37,37,37,37	0
56	MG	14	3425	1/1	0.97	0.09	96,96,96,96	0
56	MG	1H	3537	1/1	0.97	0.08	79,79,79,79	0
56	MG	14	3431	1/1	0.97	0.06	84,84,84,84	0
56	MG	1H	3003	1/1	0.97	0.14	44,44,44,44	0
56	MG	14	3433	1/1	0.97	0.10	143,143,143,143	0
56	MG	1H	3417	1/1	0.97	0.07	71,71,71,71	0
56	MG	1H	3543	1/1	0.97	0.11	81,81,81,81	0
56	MG	1H	3544	1/1	0.97	0.07	81,81,81,81	0
56	MG	14	3438	1/1	0.97	0.05	115,115,115,115	0
56	MG	14	3440	1/1	0.97	0.05	95,95,95,95	0
56	MG	14	3442	1/1	0.97	0.07	96,96,96,96	0
56	MG	14	3443	1/1	0.97	0.06	91,91,91,91	0
56	MG	14	3444	1/1	0.97	0.09	90,90,90,90	0
56	MG	14	3446	1/1	0.97	0.07	98,98,98,98	0
56	MG	1H	3545	1/1	0.97	0.08	88,88,88,88	0
56	MG	1H	3418	1/1	0.97	0.16	68,68,68,68	0
56	MG	1H	3547	1/1	0.97	0.11	91,91,91,91	0
56	MG	1H	3140	1/1	0.97	0.16	50,50,50,50	0
56	MG	1H	3420	1/1	0.97	0.11	55,55,55,55	0
56	MG	13	1691	1/1	0.97	0.06	76,76,76,76	0
56	MG	1H	3250	1/1	0.97	0.13	64,64,64,64	0
56	MG	14	3460	1/1	0.97	0.09	93,93,93,93	0
56	MG	13	1695	1/1	0.97	0.07	78,78,78,78	0
56	MG	13	1701	1/1	0.97	0.08	100,100,100,100	0
56	MG	1H	3559	1/1	0.97	0.07	73,73,73,73	0
56	MG	13	1704	1/1	0.97	0.14	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3126	1/1	0.97	0.04	55,55,55,55	0
56	MG	13	1732	1/1	0.97	0.05	113,113,113,113	0
56	MG	13	1706	1/1	0.97	0.04	92,92,92,92	0
56	MG	1H	3565	1/1	0.97	0.14	60,60,60,60	0
56	MG	14	3469	1/1	0.97	0.05	55,55,55,55	0
56	MG	1H	3052	1/1	0.97	0.08	59,59,59,59	0
56	MG	1H	3570	1/1	0.97	0.07	48,48,48,48	0
56	MG	13	1707	1/1	0.97	0.05	63,63,63,63	0
56	MG	14	3228	1/1	0.97	0.20	63,63,63,63	0
56	MG	13	1759	1/1	0.97	0.04	118,118,118,118	0
56	MG	1H	3288	1/1	0.97	0.05	38,38,38,38	0
56	MG	14	3039	1/1	0.97	0.08	63,63,63,63	0
56	MG	1H	3292	1/1	0.97	0.05	38,38,38,38	0
56	MG	14	3041	1/1	0.97	0.11	44,44,44,44	0
56	MG	1H	3259	1/1	0.97	0.11	58,58,58,58	0
56	MG	1H	3294	1/1	0.97	0.06	43,43,43,43	0
56	MG	1H	3296	1/1	0.97	0.06	43,43,43,43	0
56	MG	16	208	1/1	0.97	0.18	80,80,80,80	0
56	MG	1H	3448	1/1	0.97	0.08	74,74,74,74	0
56	MG	14	3047	1/1	0.97	0.13	46,46,46,46	0
56	MG	1H	3305	1/1	0.97	0.05	48,48,48,48	0
56	MG	1H	3175	1/1	0.97	0.10	55,55,55,55	0
56	MG	1H	3312	1/1	0.97	0.09	49,49,49,49	0
56	MG	1H	3315	1/1	0.97	0.05	85,85,85,85	0
56	MG	1H	3316	1/1	0.97	0.06	60,60,60,60	0
56	MG	1H	3320	1/1	0.97	0.08	43,43,43,43	0
56	MG	14	3247	1/1	0.97	0.06	58,58,58,58	0
56	MG	14	3251	1/1	0.97	0.05	48,48,48,48	0
56	MG	13	1735	1/1	0.97	0.04	109,109,109,109	0
56	MG	1H	3327	1/1	0.97	0.09	68,68,68,68	0
56	MG	1H	3056	1/1	0.97	0.14	28,28,28,28	0
56	MG	14	3259	1/1	0.97	0.06	57,57,57,57	0
56	MG	13	1757	1/1	0.98	0.12	84,84,84,84	0
56	MG	14	3303	1/1	0.98	0.04	68,68,68,68	0
56	MG	1H	3465	1/1	0.98	0.04	58,58,58,58	0
56	MG	14	3306	1/1	0.98	0.17	76,76,76,76	0
56	MG	1H	3373	1/1	0.98	0.12	100,100,100,100	0
56	MG	14	3309	1/1	0.98	0.04	76,76,76,76	0
56	MG	13	1692	1/1	0.98	0.04	79,79,79,79	0
56	MG	1H	3376	1/1	0.98	0.05	50,50,50,50	0
56	MG	14	3312	1/1	0.98	0.08	47,47,47,47	0
56	MG	13	1726	1/1	0.98	0.04	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3378	1/1	0.98	0.06	83,83,83,83	0
56	MG	16	207	1/1	0.98	0.04	60,60,60,60	0
56	MG	1H	3472	1/1	0.98	0.04	82,82,82,82	0
56	MG	14	3317	1/1	0.98	0.11	119,119,119,119	0
56	MG	16	209	1/1	0.98	0.04	67,67,67,67	0
56	MG	1G	1671	1/1	0.98	0.05	82,82,82,82	0
56	MG	13	1760	1/1	0.98	0.04	113,113,113,113	0
56	MG	1G	1673	1/1	0.98	0.08	86,86,86,86	0
56	MG	14	3323	1/1	0.98	0.04	57,57,57,57	0
56	MG	1H	3291	1/1	0.98	0.06	44,44,44,44	0
56	MG	1G	1676	1/1	0.98	0.12	97,97,97,97	0
56	MG	14	3060	1/1	0.98	0.06	47,47,47,47	0
56	MG	16	212	1/1	0.98	0.07	68,68,68,68	0
56	MG	14	3329	1/1	0.98	0.07	54,54,54,54	0
56	MG	16	213	1/1	0.98	0.08	87,87,87,87	0
56	MG	1G	1679	1/1	0.98	0.04	70,70,70,70	0
56	MG	1H	3387	1/1	0.98	0.04	96,96,96,96	0
56	MG	1H	3206	1/1	0.98	0.07	53,53,53,53	0
56	MG	13	1727	1/1	0.98	0.07	87,87,87,87	0
56	MG	1G	1685	1/1	0.98	0.06	63,63,63,63	0
56	MG	14	3337	1/1	0.98	0.07	70,70,70,70	0
56	MG	1H	3391	1/1	0.98	0.04	56,56,56,56	0
56	MG	14	3070	1/1	0.98	0.10	49,49,49,49	0
56	MG	41	201	1/1	0.98	0.06	62,62,62,62	0
56	MG	1H	3486	1/1	0.98	0.09	95,95,95,95	0
56	MG	1H	3487	1/1	0.98	0.10	71,71,71,71	0
56	MG	1G	1693	1/1	0.98	0.05	114,114,114,114	0
56	MG	78	202	1/1	0.98	0.08	63,63,63,63	0
56	MG	1H	3395	1/1	0.98	0.04	47,47,47,47	0
56	MG	14	3352	1/1	0.98	0.04	66,66,66,66	0
56	MG	1H	3036	1/1	0.98	0.11	45,45,45,45	0
56	MG	1H	3295	1/1	0.98	0.05	55,55,55,55	0
56	MG	1H	3493	1/1	0.98	0.06	87,87,87,87	0
56	MG	1H	3400	1/1	0.98	0.06	48,48,48,48	0
56	MG	14	3359	1/1	0.98	0.09	57,57,57,57	0
56	MG	13	1729	1/1	0.98	0.10	88,88,88,88	0
56	MG	14	3362	1/1	0.98	0.08	65,65,65,65	0
56	MG	1H	3402	1/1	0.98	0.05	40,40,40,40	0
56	MG	14	3364	1/1	0.98	0.07	83,83,83,83	0
56	MG	14	3366	1/1	0.98	0.05	65,65,65,65	0
56	MG	1H	3303	1/1	0.98	0.11	57,57,57,57	0
56	MG	14	3372	1/1	0.98	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1707	1/1	0.98	0.08	114,114,114,114	0
56	MG	14	3374	1/1	0.98	0.04	68,68,68,68	0
56	MG	14	3375	1/1	0.98	0.07	87,87,87,87	0
56	MG	1H	3237	1/1	0.98	0.04	41,41,41,41	0
56	MG	14	3377	1/1	0.98	0.05	77,77,77,77	0
56	MG	14	3378	1/1	0.98	0.04	96,96,96,96	0
56	MG	1H	3500	1/1	0.98	0.04	103,103,103,103	0
56	MG	14	3381	1/1	0.98	0.06	101,101,101,101	0
56	MG	1H	3408	1/1	0.98	0.06	42,42,42,42	0
56	MG	1G	1711	1/1	0.98	0.04	102,102,102,102	0
56	MG	1H	3502	1/1	0.98	0.04	87,87,87,87	0
56	MG	1H	3310	1/1	0.98	0.05	43,43,43,43	0
56	MG	1G	1714	1/1	0.98	0.04	101,101,101,101	0
56	MG	1G	1715	1/1	0.98	0.05	116,116,116,116	0
56	MG	1H	3410	1/1	0.98	0.05	57,57,57,57	0
56	MG	1G	1718	1/1	0.98	0.05	89,89,89,89	0
56	MG	1H	3038	1/1	0.98	0.04	70,70,70,70	0
56	MG	1H	3508	1/1	0.98	0.06	37,37,37,37	0
56	MG	1G	1721	1/1	0.98	0.09	84,84,84,84	0
56	MG	14	3397	1/1	0.98	0.04	95,95,95,95	0
56	MG	1H	3412	1/1	0.98	0.05	39,39,39,39	0
56	MG	14	3399	1/1	0.98	0.04	82,82,82,82	0
56	MG	13	1703	1/1	0.98	0.04	75,75,75,75	0
56	MG	14	3401	1/1	0.98	0.04	75,75,75,75	0
56	MG	14	3402	1/1	0.98	0.04	94,94,94,94	0
56	MG	1H	3516	1/1	0.98	0.06	81,81,81,81	0
56	MG	14	3406	1/1	0.98	0.16	86,86,86,86	0
56	MG	1H	3517	1/1	0.98	0.07	84,84,84,84	0
56	MG	1H	3416	1/1	0.98	0.05	70,70,70,70	0
56	MG	32	301	1/1	0.98	0.06	112,112,112,112	0
56	MG	14	3411	1/1	0.98	0.05	101,101,101,101	0
56	MG	13	1745	1/1	0.98	0.03	99,99,99,99	0
56	MG	1H	3109	1/1	0.98	0.17	34,34,34,34	0
56	MG	14	3414	1/1	0.98	0.04	78,78,78,78	0
56	MG	1H	3317	1/1	0.98	0.07	63,63,63,63	0
56	MG	14	3419	1/1	0.98	0.07	97,97,97,97	0
56	MG	14	3420	1/1	0.98	0.08	66,66,66,66	0
56	MG	14	3421	1/1	0.98	0.04	84,84,84,84	0
56	MG	2A	201	1/1	0.98	0.09	103,103,103,103	0
56	MG	14	3423	1/1	0.98	0.06	52,52,52,52	0
56	MG	1H	3523	1/1	0.98	0.13	76,76,76,76	0
56	MG	2L	102	1/1	0.98	0.06	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3319	1/1	0.98	0.05	51,51,51,51	0
56	MG	14	3430	1/1	0.98	0.07	86,86,86,86	0
56	MG	14	3001	1/1	0.98	0.05	51,51,51,51	0
56	MG	1H	3525	1/1	0.98	0.16	71,71,71,71	0
56	MG	13	1731	1/1	0.98	0.08	83,83,83,83	0
56	MG	14	3434	1/1	0.98	0.05	77,77,77,77	0
56	MG	1H	3527	1/1	0.98	0.04	86,86,86,86	0
56	MG	1H	3529	1/1	0.98	0.04	102,102,102,102	0
56	MG	1H	3325	1/1	0.98	0.10	56,56,56,56	0
56	MG	14	3007	1/1	0.98	0.04	55,55,55,55	0
56	MG	2K	102	1/1	0.98	0.08	83,83,83,83	0
56	MG	14	3441	1/1	0.98	0.04	95,95,95,95	0
56	MG	13	1717	1/1	0.98	0.06	51,51,51,51	0
56	MG	13	1699	1/1	0.98	0.05	75,75,75,75	0
56	MG	1H	3430	1/1	0.98	0.04	46,46,46,46	0
56	MG	14	3445	1/1	0.98	0.09	89,89,89,89	0
56	MG	1H	3139	1/1	0.98	0.10	52,52,52,52	0
56	MG	1H	3333	1/1	0.98	0.05	53,53,53,53	0
56	MG	14	3448	1/1	0.98	0.17	72,72,72,72	0
56	MG	14	3014	1/1	0.98	0.11	64,64,64,64	0
56	MG	14	3450	1/1	0.98	0.04	100,100,100,100	0
56	MG	1H	3434	1/1	0.98	0.06	47,47,47,47	0
56	MG	14	3453	1/1	0.98	0.04	102,102,102,102	0
56	MG	1H	3541	1/1	0.98	0.04	85,85,85,85	0
56	MG	1H	3542	1/1	0.98	0.05	81,81,81,81	0
56	MG	14	3456	1/1	0.98	0.07	99,99,99,99	0
56	MG	1H	3334	1/1	0.98	0.06	59,59,59,59	0
56	MG	14	3458	1/1	0.98	0.12	91,91,91,91	0
56	MG	1H	3335	1/1	0.98	0.04	77,77,77,77	0
56	MG	1H	3336	1/1	0.98	0.08	86,86,86,86	0
56	MG	1H	3339	1/1	0.98	0.04	41,41,41,41	0
56	MG	1H	3441	1/1	0.98	0.08	76,76,76,76	0
56	MG	1H	3548	1/1	0.98	0.07	98,98,98,98	0
56	MG	13	1711	1/1	0.98	0.08	101,101,101,101	0
56	MG	14	3135	1/1	0.98	0.04	59,59,59,59	0
56	MG	14	3246	1/1	0.98	0.11	57,57,57,57	0
56	MG	1H	3550	1/1	0.98	0.14	125,125,125,125	0
56	MG	14	3249	1/1	0.98	0.04	64,64,64,64	0
56	MG	13	1722	1/1	0.98	0.04	78,78,78,78	0
56	MG	1H	3552	1/1	0.98	0.15	73,73,73,73	0
56	MG	1H	3116	1/1	0.98	0.03	64,64,64,64	0
56	MG	1H	3446	1/1	0.98	0.06	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3258	1/1	0.98	0.07	52,52,52,52	0
56	MG	13	1751	1/1	0.98	0.09	76,76,76,76	0
56	MG	14	3260	1/1	0.98	0.04	52,52,52,52	0
56	MG	14	3261	1/1	0.98	0.04	57,57,57,57	0
56	MG	13	1705	1/1	0.98	0.04	102,102,102,102	0
56	MG	14	3267	1/1	0.98	0.04	50,50,50,50	0
56	MG	1H	3558	1/1	0.98	0.03	99,99,99,99	0
56	MG	1H	3355	1/1	0.98	0.04	40,40,40,40	0
56	MG	1H	3356	1/1	0.98	0.09	64,64,64,64	0
56	MG	14	3271	1/1	0.98	0.05	60,60,60,60	0
56	MG	1H	3561	1/1	0.98	0.05	87,87,87,87	0
56	MG	14	3275	1/1	0.98	0.05	47,47,47,47	0
56	MG	14	3282	1/1	0.98	0.04	92,92,92,92	0
56	MG	25	202	1/1	0.98	0.05	108,108,108,108	0
56	MG	13	1737	1/1	0.98	0.04	83,83,83,83	0
56	MG	1H	3072	1/1	0.98	0.13	33,33,33,33	0
56	MG	1H	3564	1/1	0.98	0.04	95,95,95,95	0
56	MG	14	3293	1/1	0.98	0.07	94,94,94,94	0
56	MG	14	3294	1/1	0.98	0.05	59,59,59,59	0
56	MG	1H	3007	1/1	0.98	0.11	60,60,60,60	0
56	MG	1H	3566	1/1	0.98	0.04	105,105,105,105	0
56	MG	1H	3567	1/1	0.98	0.05	42,42,42,42	0
56	MG	13	1755	1/1	0.98	0.04	101,101,101,101	0
57	SF4	3E	301	8/8	0.98	0.03	75,82,92,93	0
56	MG	1H	3569	1/1	0.98	0.07	85,85,85,85	0
56	MG	13	1738	1/1	0.98	0.07	71,71,71,71	0
56	MG	14	3325	1/1	0.99	0.05	66,66,66,66	0
56	MG	1H	3462	1/1	0.99	0.03	66,66,66,66	0
56	MG	1H	3380	1/1	0.99	0.04	69,69,69,69	0
56	MG	1G	1674	1/1	0.99	0.05	97,97,97,97	0
56	MG	1H	3464	1/1	0.99	0.04	40,40,40,40	0
56	MG	1H	3381	1/1	0.99	0.02	74,74,74,74	0
56	MG	1H	3571	1/1	0.99	0.03	39,39,39,39	0
56	MG	14	3332	1/1	0.99	0.06	70,70,70,70	0
56	MG	1H	3466	1/1	0.99	0.08	74,74,74,74	0
56	MG	1H	3382	1/1	0.99	0.05	70,70,70,70	0
56	MG	1G	1680	1/1	0.99	0.07	68,68,68,68	0
56	MG	1H	3383	1/1	0.99	0.03	61,61,61,61	0
56	MG	1H	3384	1/1	0.99	0.05	77,77,77,77	0
56	MG	14	3338	1/1	0.99	0.05	83,83,83,83	0
56	MG	14	3339	1/1	0.99	0.04	73,73,73,73	0
56	MG	1G	1683	1/1	0.99	0.03	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3069	1/1	0.99	0.02	47,47,47,47	0
56	MG	14	3343	1/1	0.99	0.02	42,42,42,42	0
56	MG	14	3344	1/1	0.99	0.04	56,56,56,56	0
56	MG	1H	3385	1/1	0.99	0.03	74,74,74,74	0
56	MG	1H	3321	1/1	0.99	0.04	59,59,59,59	0
56	MG	1G	1686	1/1	0.99	0.03	90,90,90,90	0
56	MG	1H	3322	1/1	0.99	0.11	67,67,67,67	0
56	MG	1H	3324	1/1	0.99	0.04	70,70,70,70	0
56	MG	1H	3474	1/1	0.99	0.07	79,79,79,79	0
56	MG	14	3351	1/1	0.99	0.05	54,54,54,54	0
56	MG	1G	1690	1/1	0.99	0.03	90,90,90,90	0
56	MG	1H	3475	1/1	0.99	0.07	73,73,73,73	0
56	MG	1G	1692	1/1	0.99	0.03	106,106,106,106	0
56	MG	1H	3476	1/1	0.99	0.04	91,91,91,91	0
56	MG	1H	3389	1/1	0.99	0.06	46,46,46,46	0
56	MG	14	3358	1/1	0.99	0.05	76,76,76,76	0
56	MG	1H	3478	1/1	0.99	0.05	78,78,78,78	0
56	MG	13	1690	1/1	0.99	0.05	56,56,56,56	0
56	MG	14	3361	1/1	0.99	0.03	41,41,41,41	0
56	MG	1H	3480	1/1	0.99	0.07	66,66,66,66	0
56	MG	1H	3481	1/1	0.99	0.03	59,59,59,59	0
56	MG	1G	1699	1/1	0.99	0.04	86,86,86,86	0
56	MG	14	3365	1/1	0.99	0.03	44,44,44,44	0
56	MG	11	303	1/1	0.99	0.03	49,49,49,49	0
56	MG	14	3367	1/1	0.99	0.04	75,75,75,75	0
56	MG	1G	1701	1/1	0.99	0.06	106,106,106,106	0
56	MG	14	3369	1/1	0.99	0.05	93,93,93,93	0
56	MG	14	3370	1/1	0.99	0.09	83,83,83,83	0
56	MG	14	3371	1/1	0.99	0.09	75,75,75,75	0
56	MG	13	1753	1/1	0.99	0.05	64,64,64,64	0
56	MG	1H	3483	1/1	0.99	0.12	76,76,76,76	0
56	MG	1G	1704	1/1	0.99	0.06	99,99,99,99	0
56	MG	1H	3392	1/1	0.99	0.03	63,63,63,63	0
56	MG	1G	1706	1/1	0.99	0.07	82,82,82,82	0
56	MG	1H	3393	1/1	0.99	0.08	61,61,61,61	0
56	MG	1H	3394	1/1	0.99	0.04	40,40,40,40	0
56	MG	1H	3289	1/1	0.99	0.05	48,48,48,48	0
56	MG	14	3380	1/1	0.99	0.05	95,95,95,95	0
56	MG	1H	3396	1/1	0.99	0.03	41,41,41,41	0
56	MG	14	3382	1/1	0.99	0.04	47,47,47,47	0
56	MG	1H	3489	1/1	0.99	0.07	87,87,87,87	0
56	MG	1H	3328	1/1	0.99	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3329	1/1	0.99	0.03	41,41,41,41	0
56	MG	14	3386	1/1	0.99	0.07	81,81,81,81	0
56	MG	1H	3492	1/1	0.99	0.07	74,74,74,74	0
56	MG	I8	101	1/1	0.99	0.08	55,55,55,55	0
56	MG	14	3389	1/1	0.99	0.04	82,82,82,82	0
56	MG	1G	1716	1/1	0.99	0.06	88,88,88,88	0
56	MG	1H	3330	1/1	0.99	0.02	46,46,46,46	0
56	MG	1H	3494	1/1	0.99	0.03	53,53,53,53	0
56	MG	1H	3290	1/1	0.99	0.07	40,40,40,40	0
56	MG	14	3394	1/1	0.99	0.09	63,63,63,63	0
56	MG	13	1697	1/1	0.99	0.03	91,91,91,91	0
56	MG	1H	3403	1/1	0.99	0.04	71,71,71,71	0
56	MG	13	1739	1/1	0.99	0.04	79,79,79,79	0
56	MG	1H	3406	1/1	0.99	0.13	52,52,52,52	0
56	MG	1H	3004	1/1	0.99	0.07	46,46,46,46	0
56	MG	13	1725	1/1	0.99	0.10	65,65,65,65	0
56	MG	13	1698	1/1	0.99	0.08	98,98,98,98	0
56	MG	1H	3338	1/1	0.99	0.06	45,45,45,45	0
56	MG	14	3403	1/1	0.99	0.11	80,80,80,80	0
56	MG	14	3404	1/1	0.99	0.03	77,77,77,77	0
56	MG	1H	3024	1/1	0.99	0.06	47,47,47,47	0
56	MG	1H	3297	1/1	0.99	0.04	52,52,52,52	0
56	MG	1H	3506	1/1	0.99	0.02	58,58,58,58	0
56	MG	1H	3507	1/1	0.99	0.05	84,84,84,84	0
56	MG	1H	3413	1/1	0.99	0.03	59,59,59,59	0
56	MG	1H	3414	1/1	0.99	0.08	68,68,68,68	0
56	MG	1H	3510	1/1	0.99	0.06	92,92,92,92	0
56	MG	1H	3511	1/1	0.99	0.04	78,78,78,78	0
56	MG	1H	3512	1/1	0.99	0.04	60,60,60,60	0
56	MG	14	3415	1/1	0.99	0.03	78,78,78,78	0
56	MG	14	3416	1/1	0.99	0.05	80,80,80,80	0
56	MG	1H	3299	1/1	0.99	0.06	35,35,35,35	0
56	MG	14	3418	1/1	0.99	0.11	75,75,75,75	0
56	MG	1H	3514	1/1	0.99	0.04	69,69,69,69	0
56	MG	1H	3515	1/1	0.99	0.14	57,57,57,57	0
56	MG	1H	3343	1/1	0.99	0.07	39,39,39,39	0
56	MG	1H	3344	1/1	0.99	0.02	42,42,42,42	0
56	MG	14	3248	1/1	0.99	0.06	47,47,47,47	0
56	MG	1H	3301	1/1	0.99	0.03	42,42,42,42	0
56	MG	14	3250	1/1	0.99	0.04	55,55,55,55	0
56	MG	14	3427	1/1	0.99	0.12	69,69,69,69	0
56	MG	14	3428	1/1	0.99	0.11	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3347	1/1	0.99	0.05	72,72,72,72	0
56	MG	1H	3302	1/1	0.99	0.06	52,52,52,52	0
56	MG	1H	3350	1/1	0.99	0.02	43,43,43,43	0
56	MG	1H	3422	1/1	0.99	0.04	42,42,42,42	0
56	MG	14	3256	1/1	0.99	0.03	65,65,65,65	0
56	MG	14	3257	1/1	0.99	0.03	42,42,42,42	0
56	MG	1H	3423	1/1	0.99	0.07	33,33,33,33	0
56	MG	1H	3351	1/1	0.99	0.03	50,50,50,50	0
56	MG	1H	3425	1/1	0.99	0.03	39,39,39,39	0
56	MG	1H	3352	1/1	0.99	0.03	57,57,57,57	0
56	MG	14	3439	1/1	0.99	0.10	86,86,86,86	0
56	MG	14	3262	1/1	0.99	0.04	54,54,54,54	0
56	MG	1H	3528	1/1	0.99	0.09	72,72,72,72	0
56	MG	14	3264	1/1	0.99	0.04	59,59,59,59	0
56	MG	13	1714	1/1	0.99	0.03	59,59,59,59	0
56	MG	1H	3354	1/1	0.99	0.04	45,45,45,45	0
56	MG	1H	3531	1/1	0.99	0.14	56,56,56,56	0
56	MG	1H	3429	1/1	0.99	0.04	49,49,49,49	0
56	MG	13	1728	1/1	0.99	0.04	77,77,77,77	0
56	MG	1H	3306	1/1	0.99	0.03	38,38,38,38	0
56	MG	14	3273	1/1	0.99	0.06	55,55,55,55	0
56	MG	14	3274	1/1	0.99	0.06	50,50,50,50	0
56	MG	1H	3535	1/1	0.99	0.04	70,70,70,70	0
56	MG	14	3452	1/1	0.99	0.03	90,90,90,90	0
56	MG	14	3276	1/1	0.99	0.03	56,56,56,56	0
56	MG	14	3278	1/1	0.99	0.04	50,50,50,50	0
56	MG	14	3279	1/1	0.99	0.10	45,45,45,45	0
56	MG	14	3280	1/1	0.99	0.04	47,47,47,47	0
56	MG	1H	3357	1/1	0.99	0.02	66,66,66,66	0
56	MG	14	3283	1/1	0.99	0.05	79,79,79,79	0
56	MG	1H	3433	1/1	0.99	0.04	37,37,37,37	0
56	MG	14	3285	1/1	0.99	0.02	55,55,55,55	0
56	MG	14	3286	1/1	0.99	0.03	68,68,68,68	0
56	MG	14	3287	1/1	0.99	0.10	71,71,71,71	0
56	MG	14	3288	1/1	0.99	0.05	76,76,76,76	0
56	MG	14	3289	1/1	0.99	0.07	64,64,64,64	0
56	MG	1H	3359	1/1	0.99	0.06	59,59,59,59	0
56	MG	1H	3539	1/1	0.99	0.05	90,90,90,90	0
56	MG	14	3292	1/1	0.99	0.10	63,63,63,63	0
56	MG	1H	3307	1/1	0.99	0.03	50,50,50,50	0
56	MG	1H	3436	1/1	0.99	0.06	64,64,64,64	0
56	MG	14	3295	1/1	0.99	0.03	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3437	1/1	0.99	0.03	62,62,62,62	0
56	MG	1H	3308	1/1	0.99	0.08	49,49,49,49	0
56	MG	13	1715	1/1	0.99	0.04	94,94,94,94	0
56	MG	1H	3364	1/1	0.99	0.04	51,51,51,51	0
56	MG	1H	3365	1/1	0.99	0.07	50,50,50,50	0
56	MG	13	1693	1/1	0.99	0.02	80,80,80,80	0
56	MG	1H	3443	1/1	0.99	0.04	72,72,72,72	0
56	MG	1H	3368	1/1	0.99	0.03	49,49,49,49	0
56	MG	13	1700	1/1	0.99	0.04	64,64,64,64	0
56	MG	1H	3370	1/1	0.99	0.03	37,37,37,37	0
56	MG	14	3307	1/1	0.99	0.16	60,60,60,60	0
56	MG	1J	211	1/1	0.99	0.03	85,85,85,85	0
56	MG	1H	3371	1/1	0.99	0.07	64,64,64,64	0
56	MG	1H	3553	1/1	0.99	0.05	78,78,78,78	0
56	MG	1H	3314	1/1	0.99	0.06	74,74,74,74	0
56	MG	13	1708	1/1	0.99	0.04	80,80,80,80	0
56	MG	1H	3374	1/1	0.99	0.08	68,68,68,68	0
56	MG	13	1709	1/1	0.99	0.07	68,68,68,68	0
56	MG	1H	3453	1/1	0.99	0.05	81,81,81,81	0
56	MG	13	1720	1/1	0.99	0.08	66,66,66,66	0
56	MG	1H	3318	1/1	0.99	0.03	72,72,72,72	0
56	MG	45	202	1/1	0.99	0.11	66,66,66,66	0
56	MG	13	1721	1/1	0.99	0.02	82,82,82,82	0
56	MG	1H	3457	1/1	0.99	0.02	78,78,78,78	0
56	MG	1H	3458	1/1	0.99	0.06	56,56,56,56	0
56	MG	14	3320	1/1	0.99	0.06	79,79,79,79	0
56	MG	1H	3459	1/1	0.99	0.05	69,69,69,69	0
56	MG	1H	3460	1/1	0.99	0.07	75,75,75,75	0
57	SF4	32	302	8/8	0.99	0.04	99,104,114,118	0
58	ZN	5I	102	1/1	0.99	0.02	87,87,87,87	0
56	MG	1G	1670	1/1	0.99	0.06	71,71,71,71	0
58	ZN	5A	101	1/1	0.99	0.04	130,130,130,130	0
56	MG	13	1694	1/1	0.99	0.06	79,79,79,79	0
56	MG	1H	3337	1/1	1.00	0.03	41,41,41,41	0
56	MG	14	3304	1/1	1.00	0.04	64,64,64,64	0
56	MG	14	3255	1/1	1.00	0.03	42,42,42,42	0
56	MG	1H	3349	1/1	1.00	0.02	42,42,42,42	0
56	MG	14	3281	1/1	1.00	0.04	69,69,69,69	0
56	MG	1H	3298	1/1	1.00	0.03	46,46,46,46	0
56	MG	13	1702	1/1	1.00	0.04	64,64,64,64	0
56	MG	1H	3323	1/1	1.00	0.03	64,64,64,64	0
56	MG	1H	3367	1/1	1.00	0.03	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3521	1/1	1.00	0.07	79,79,79,79	0
56	MG	1H	3309	1/1	1.00	0.03	47,47,47,47	0
56	MG	14	3340	1/1	1.00	0.02	54,54,54,54	0
56	MG	14	3426	1/1	1.00	0.06	75,75,75,75	0
56	MG	1H	3450	1/1	1.00	0.08	45,45,45,45	0
56	MG	1H	3399	1/1	1.00	0.02	52,52,52,52	0
56	MG	14	3265	1/1	1.00	0.04	51,51,51,51	0
56	MG	14	3266	1/1	1.00	0.07	43,43,43,43	0
56	MG	1H	3342	1/1	1.00	0.01	44,44,44,44	0
56	MG	1H	3304	1/1	1.00	0.03	42,42,42,42	0
56	MG	1H	3300	1/1	1.00	0.03	41,41,41,41	0
56	MG	13	1696	1/1	1.00	0.07	72,72,72,72	0
56	MG	1H	3404	1/1	1.00	0.03	45,45,45,45	0
56	MG	1H	3358	1/1	1.00	0.06	78,78,78,78	0
56	MG	1H	3346	1/1	1.00	0.07	60,60,60,60	0
56	MG	1H	3313	1/1	1.00	0.10	58,58,58,58	0
56	MG	14	3409	1/1	1.00	0.03	73,73,73,73	0
56	MG	1H	3361	1/1	1.00	0.08	56,56,56,56	0
56	MG	21	303	1/1	1.00	0.02	42,42,42,42	0
56	MG	14	3355	1/1	1.00	0.07	52,52,52,52	0
56	MG	14	3277	1/1	1.00	0.02	57,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.