



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:24 AM UTC

PDB ID : 5IB8 / pdb_00005ib8
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet} and near-cognate tRNA^{Lys} with U-G mismatch in the A-site
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2016-02-22
Resolution : 3.13 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

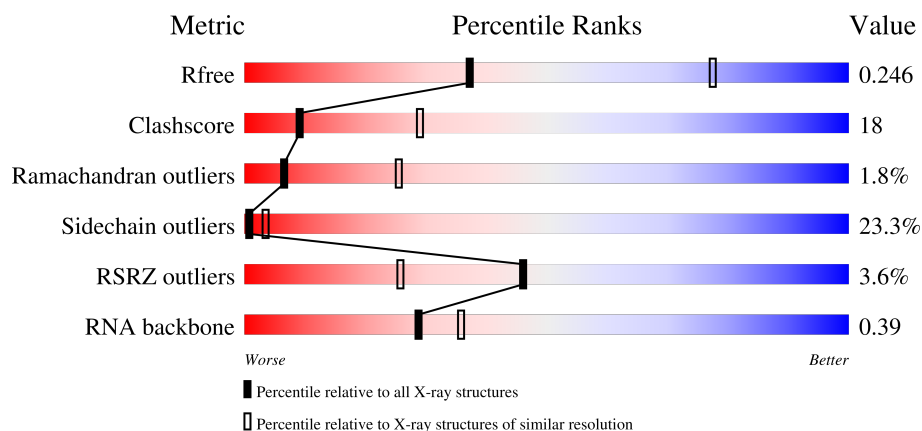
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)
RNA backbone	3983	1040 (3.38-2.90)

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	1522	3% 34% 50% 14% .
1	1G	1522	3% 35% 48% 16% .
2	12	256	3% 30% 39% 10% . 19%
2	1E	256	2% 38% 39% 14% 10%

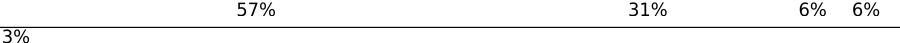
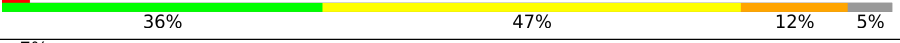
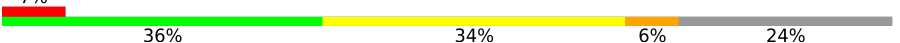
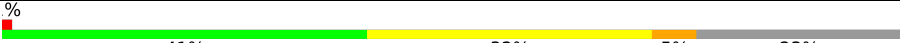
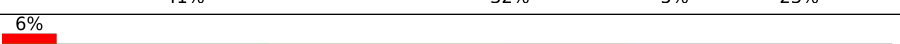
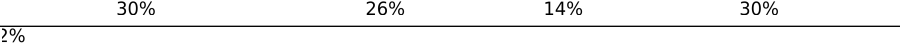
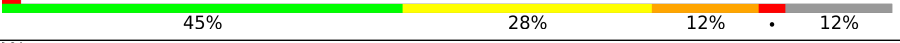
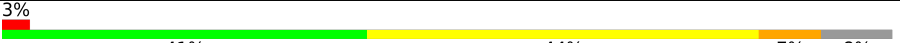
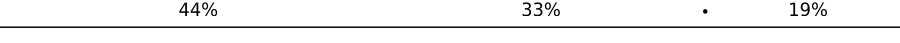
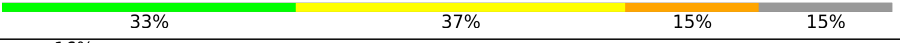
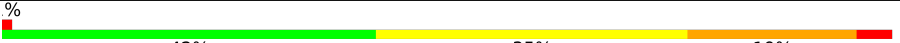
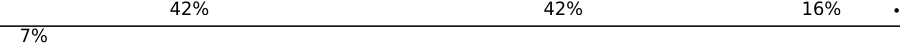
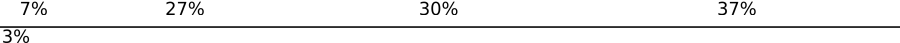
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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
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	
23	2K	77	
23	2L	77	
24	3K	76	
24	3L	76	
25	4K	30	
25	4L	30	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	7I	229	

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Mol	Chain	Length	Quality of chain
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	
40	A8	112	
41	75	146	

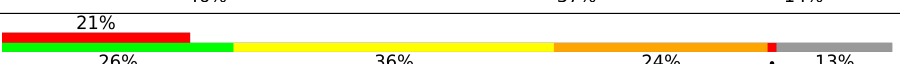
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Mol	Chain	Length	Quality of chain
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	
54	L5	49	

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Mol	Chain	Length	Quality of chain
54	P8	49	
55	M5	65	
55	Q8	65	
56	1L	76	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	13	1659	-	-	-	X
57	MG	13	1668	-	-	-	X
57	MG	14	3103	-	-	-	X
57	MG	14	3133	-	-	-	X
57	MG	14	3134	-	-	-	X
57	MG	14	3147	-	-	-	X
57	MG	1G	1621	-	-	-	X
57	MG	1G	1642	-	-	-	X
57	MG	1H	3130	-	-	-	X
57	MG	1H	3159	-	-	-	X
57	MG	1H	3167	-	-	-	X
57	MG	E5	101	-	-	-	X
58	SF4	32	302	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296999 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	1500	Total	C	N	O	P	0	0	0
			32246	14352	5978	10416	1500			
1	1G	1509	Total	C	N	O	P	0	0	0
			32437	14437	6010	10481	1509			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	U	conflict	GB 55771382
1G	1542	G	U	conflict	GB 55771382

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	150	Total	C	N	O	S	0	0	0
			1141	719	217	201	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	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	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	94	Total	C	N	O	S	0	0	0
			749	468	147	133	1			
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	S	0	0	0
			823	512	154	154	3			
11	2A	113	Total	C	N	O	S	0	0	0
			835	520	156	156	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	121	Total	C	N	O	S	0	0	0
			947	597	191	158	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
13	4A	109	Total	C	N	O	S	0	0	0
			879	544	181	152	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			
14	5A	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			
15	6A	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- 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	65	Total	C	N	O	S	0	0	0
			510	324	92	92	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

- 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	20	Total	C	N	O	P	0	0	0
			442	198	94	130	20			
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	2831	Total	C	N	O	P	0	0	0
			60991	27142	11416	19602	2831			
26	14	2825	Total	C	N	O	P	0	0	0
			60857	27083	11390	19559	2825			

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	132	Total	C	N	O	S	0	0	0
			1027	648	193	185	1			

- 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
			1546	978	295	267	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	180	Total	C	N	O	S	0	0	0
			1459	931	266	258	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	169	Total	C	N	O	S	0	0	0
			1295	823	241	230	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	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	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

- 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	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	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	135	Total	C	N	O	S	0	0	0
			1119	697	230	191	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
			750	488	135	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	177	Total	C	N	O	S	0	0	0
			1411	901	253	255	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	96	Total	C	N	O	S	0	0	0
			747	469	148	129	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	60	Total	C	N	O	S	0	0	0
			475	300	84	86	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 a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	66	Total	C	N	O	P	0	0	0
			1402	627	244	465	66			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

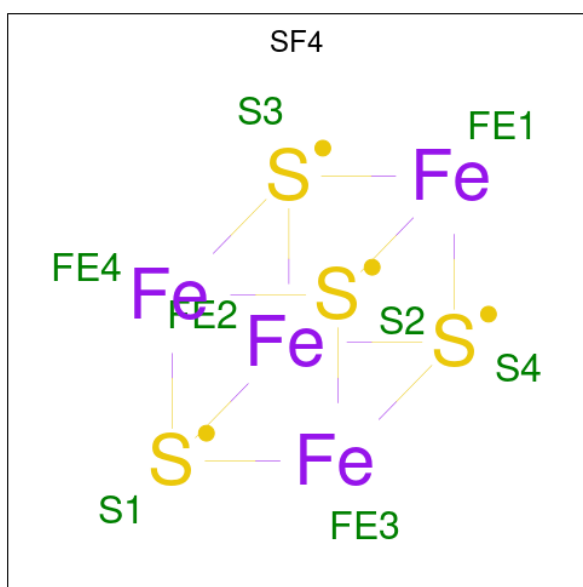
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	141	Total 141	Mg 141	0	0
57	2I	1	Total 1	Mg 1	0	0
57	3I	1	Total 1	Mg 1	0	0
57	2K	3	Total 3	Mg 3	0	0
57	1H	552	Total 552	Mg 552	0	0
57	16	12	Total 12	Mg 12	0	0
57	21	3	Total 3	Mg 3	0	0
57	31	1	Total 1	Mg 1	0	0
57	41	1	Total 1	Mg 1	0	0
57	88	3	Total 3	Mg 3	0	0
57	F8	1	Total 1	Mg 1	0	0
57	I8	2	Total 2	Mg 2	0	0
57	P8	1	Total 1	Mg 1	0	0
57	Q8	1	Total 1	Mg 1	0	0
57	1G	125	Total 125	Mg 125	0	0
57	32	1	Total 1	Mg 1	0	0
57	42	2	Total 2	Mg 2	0	0
57	52	1	Total 1	Mg 1	0	0
57	7A	1	Total 1	Mg 1	0	0
57	2L	2	Total 2	Mg 2	0	0
57	4L	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	14	460	Total 460	Mg 460	0	0
57	1J	10	Total 10	Mg 10	0	0
57	19	1	Total 1	Mg 1	0	0
57	29	1	Total 1	Mg 1	0	0
57	39	1	Total 1	Mg 1	0	0
57	25	1	Total 1	Mg 1	0	0
57	35	2	Total 2	Mg 2	0	0
57	45	1	Total 1	Mg 1	0	0
57	B5	1	Total 1	Mg 1	0	0
57	E5	2	Total 2	Mg 2	0	0
57	M5	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

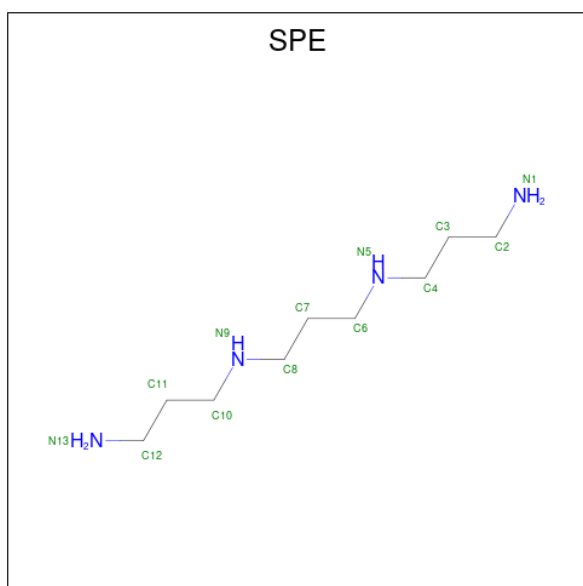


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	3E	1	Total	Fe	S	0	0
			8	4	4		
58	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	5I	1	Total	Zn	0	0
			1	1		
59	G8	1	Total	Zn	0	0
			1	1		
59	5A	1	Total	Zn	0	0
			1	1		
59	C5	1	Total	Zn	0	0
			1	1		

- Molecule 60 is THERMINE (CCD ID: SPE) (formula: C₉H₂₄N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1G	1	Total	C	N	0	0
			13	9	4		
60	14	1	Total	C	N	0	0
			13	9	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	354	Total 354	O 354	0	0
61	3E	2	Total 2	O 2	0	0
61	4E	3	Total 3	O 3	0	0
61	8E	2	Total 2	O 2	0	0
61	1I	2	Total 2	O 2	0	0
61	3I	2	Total 2	O 2	0	0
61	5I	1	Total 1	O 1	0	0
61	7I	2	Total 2	O 2	0	0
61	BI	3	Total 3	O 3	0	0
61	1K	1	Total 1	O 1	0	0
61	2K	8	Total 8	O 8	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	5	Total 5	O 5	0	0
61	1H	1720	Total 1720	O 1720	0	0
61	16	12	Total 12	O 12	0	0
61	11	10	Total 10	O 10	0	0
61	21	6	Total 6	O 6	0	0
61	31	6	Total 6	O 6	0	0
61	58	2	Total 2	O 2	0	0
61	68	2	Total 2	O 2	0	0
61	78	13	Total 13	O 13	0	0
61	98	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	B8	1	Total 1	O 1	0	0
61	C8	4	Total 4	O 4	0	0
61	E8	1	Total 1	O 1	0	0
61	F8	3	Total 3	O 3	0	0
61	G8	3	Total 3	O 3	0	0
61	I8	6	Total 6	O 6	0	0
61	J8	5	Total 5	O 5	0	0
61	L8	4	Total 4	O 4	0	0
61	N8	1	Total 1	O 1	0	0
61	Q8	5	Total 5	O 5	0	0
61	1G	364	Total 364	O 364	0	0
61	32	4	Total 4	O 4	0	0
61	42	1	Total 1	O 1	0	0
61	52	4	Total 4	O 4	0	0
61	1A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	4A	2	Total 2	O 2	0	0
61	6A	3	Total 3	O 3	0	0
61	7A	4	Total 4	O 4	0	0
61	9A	2	Total 2	O 2	0	0
61	BA	3	Total 3	O 3	0	0

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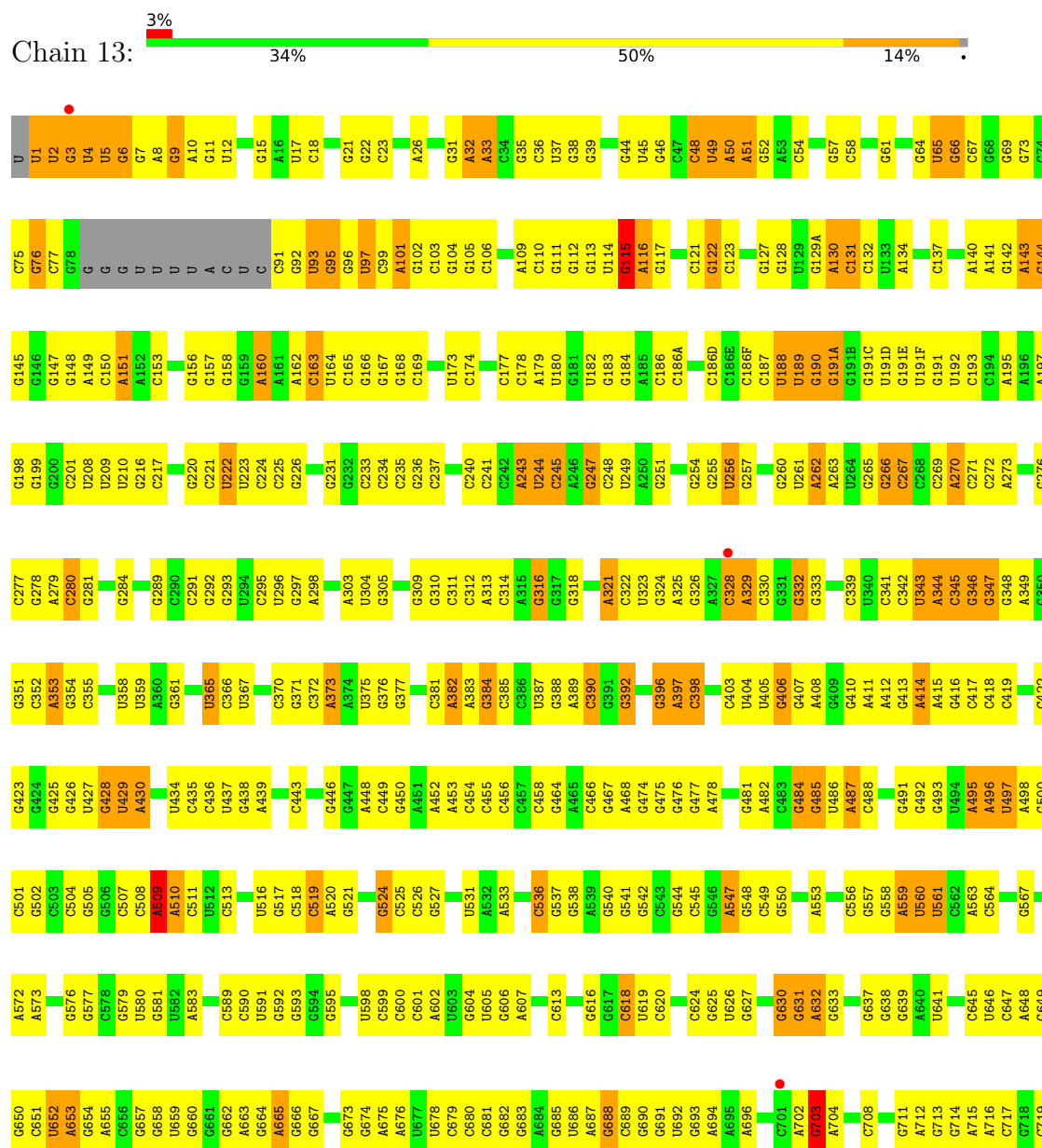
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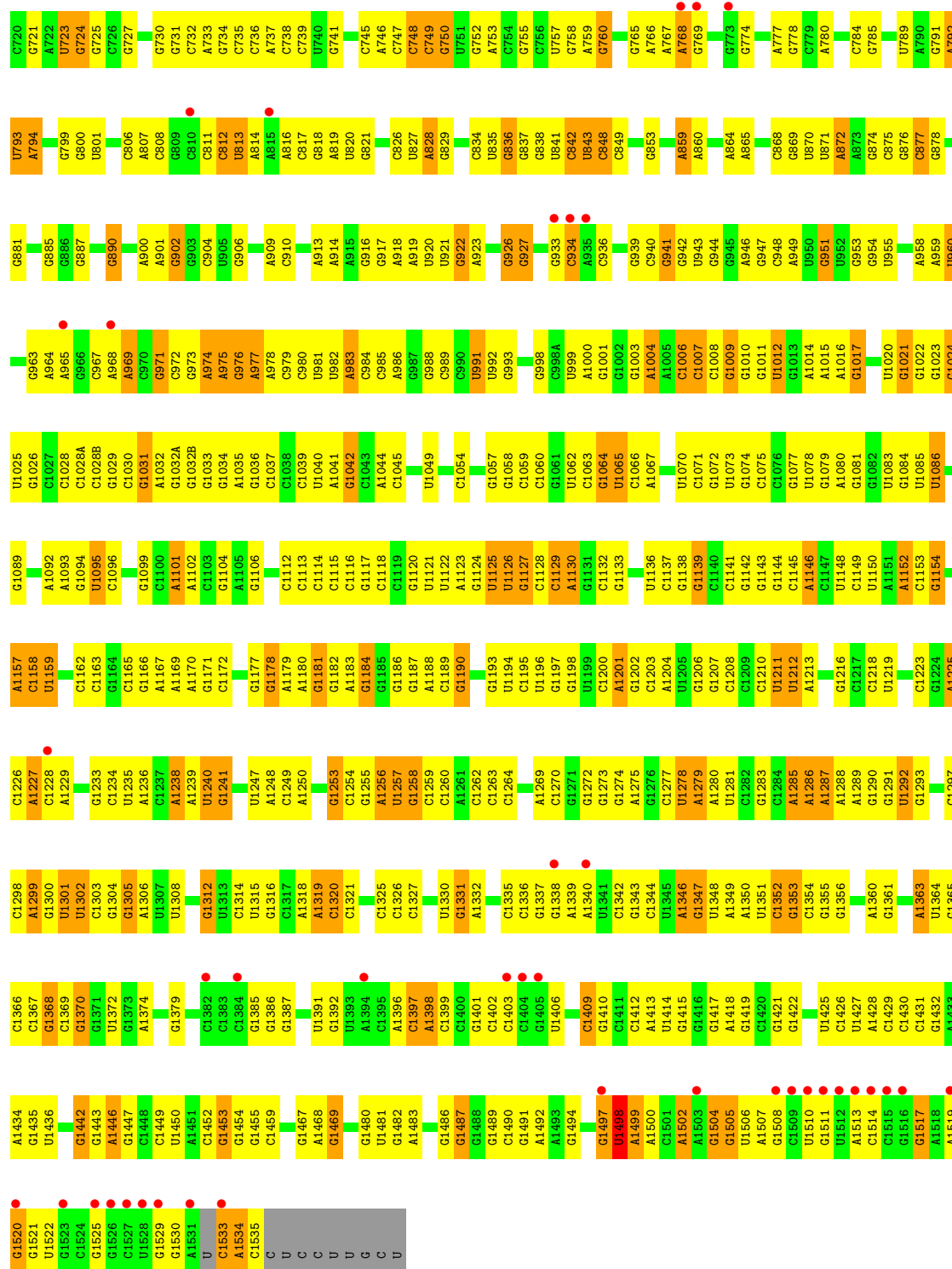
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2L	8	Total 8	O 8	0	0
61	4L	3	Total 3	O 3	0	0
61	14	1303	Total 1303	O 1303	0	0
61	1J	27	Total 27	O 27	0	0
61	19	14	Total 14	O 14	0	0
61	29	6	Total 6	O 6	0	0
61	39	8	Total 8	O 8	0	0
61	15	3	Total 3	O 3	0	0
61	25	8	Total 8	O 8	0	0
61	35	8	Total 8	O 8	0	0
61	55	1	Total 1	O 1	0	0
61	75	1	Total 1	O 1	0	0
61	85	1	Total 1	O 1	0	0
61	B5	1	Total 1	O 1	0	0
61	C5	3	Total 3	O 3	0	0
61	F5	1	Total 1	O 1	0	0
61	H5	1	Total 1	O 1	0	0
61	L5	1	Total 1	O 1	0	0
61	M5	8	Total 8	O 8	0	0

3 Residue-property plots

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

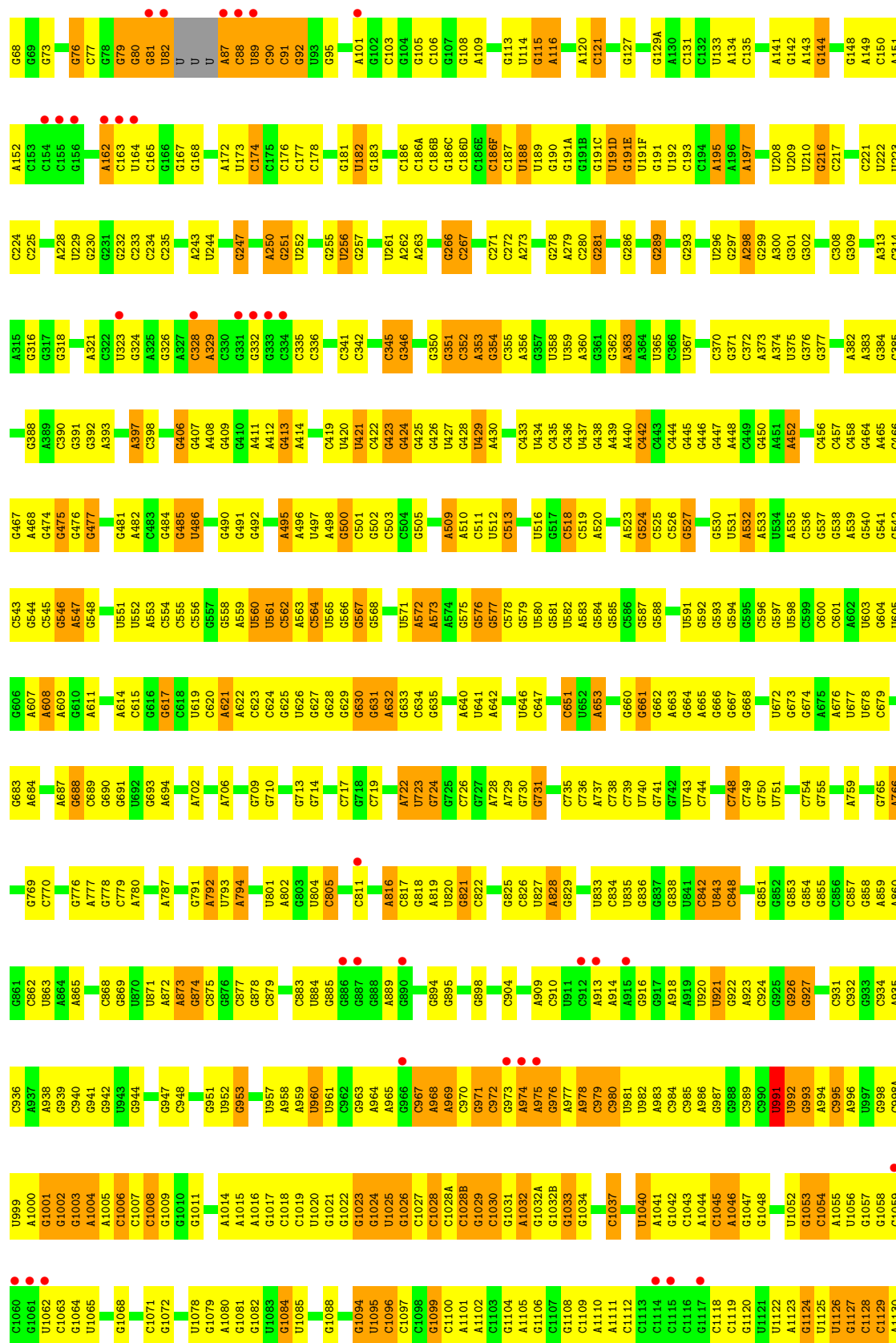
• Molecule 1: 16S ribosomal RNA

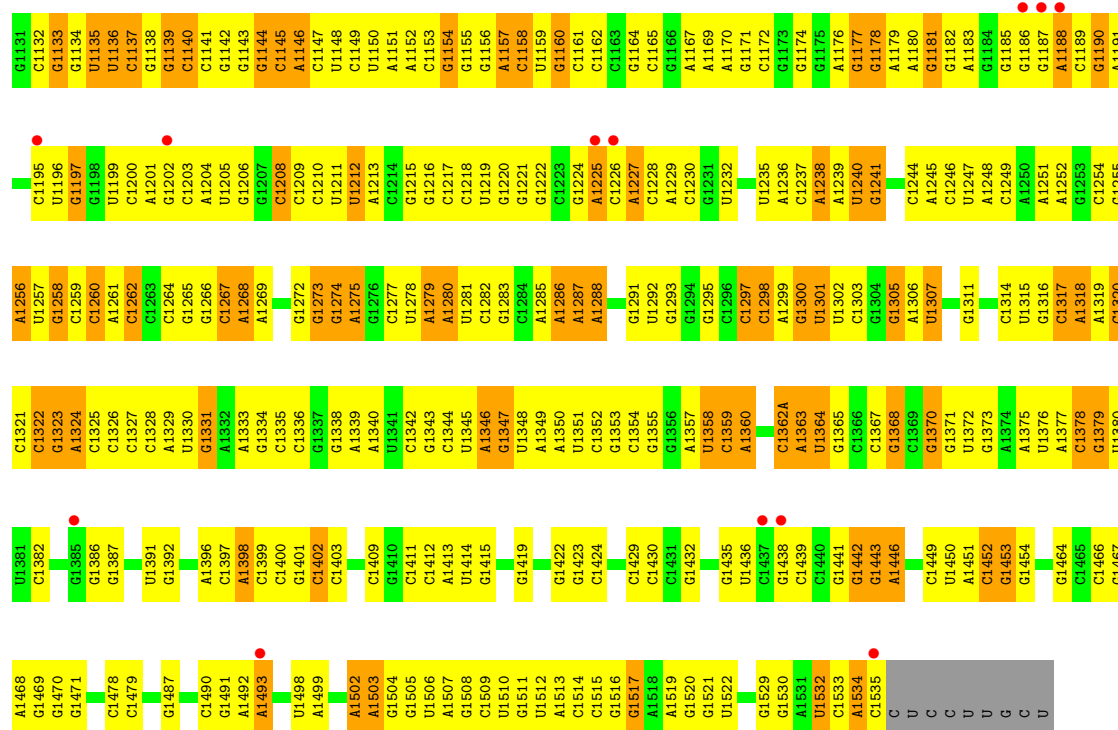




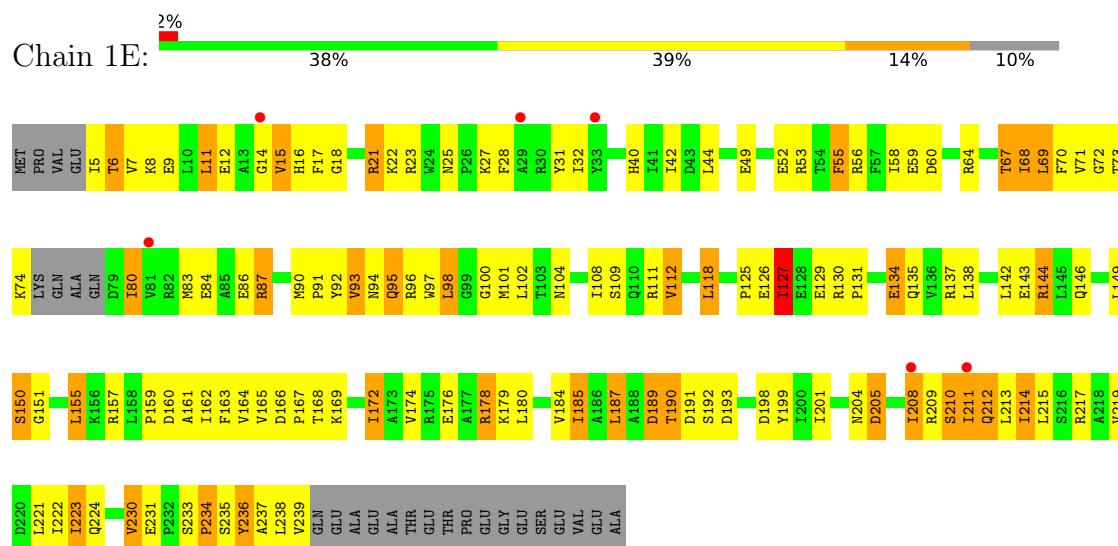
• Molecule 1: 16S ribosomal RNA



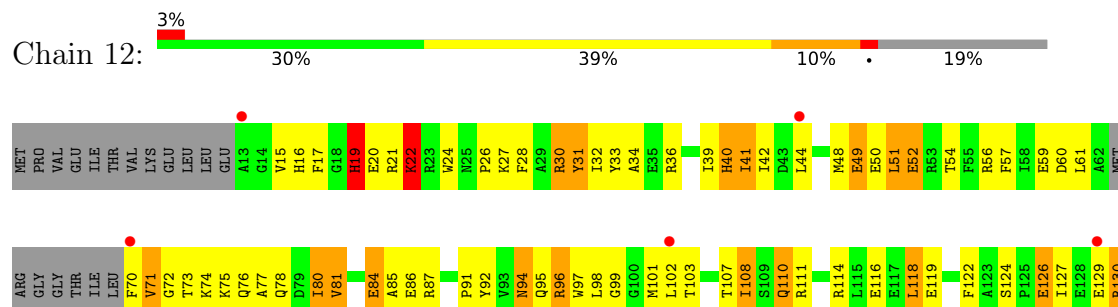


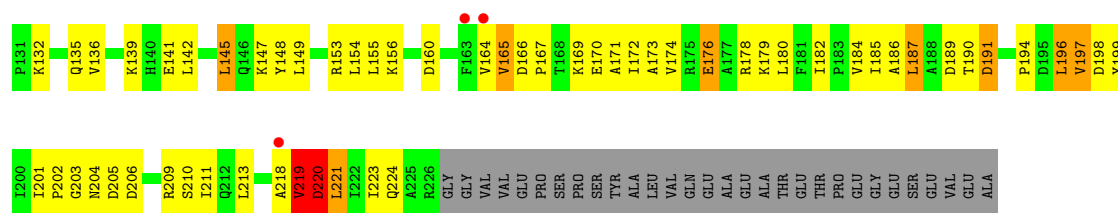


• Molecule 2: 30S ribosomal protein S2

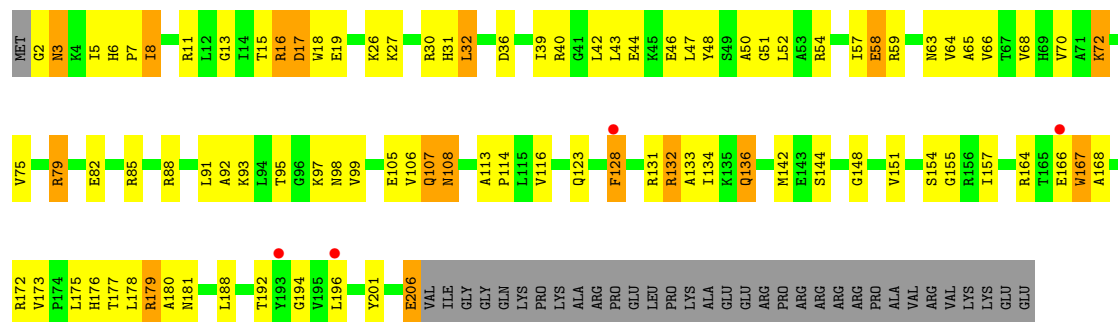


• Molecule 2: 30S ribosomal protein S2

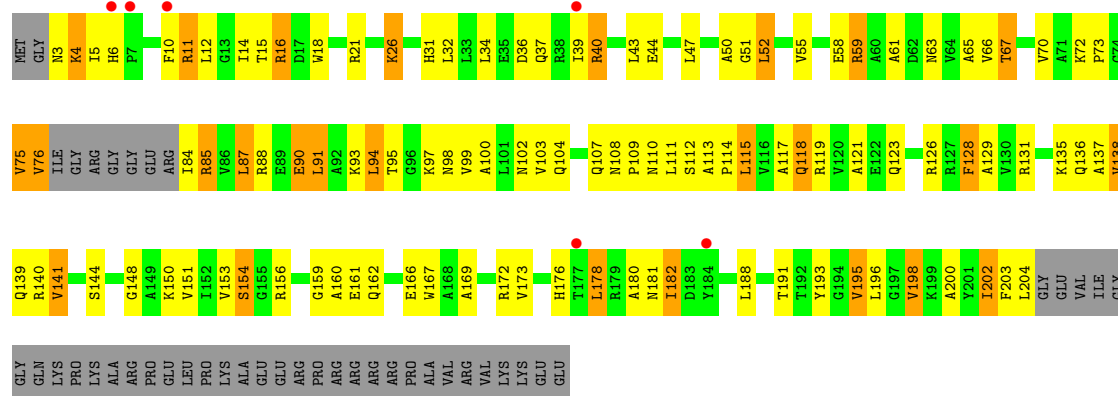




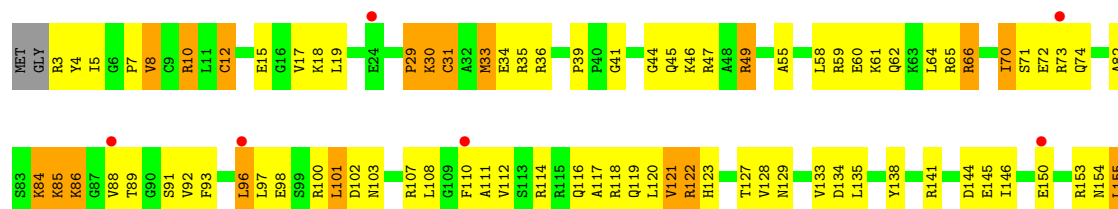
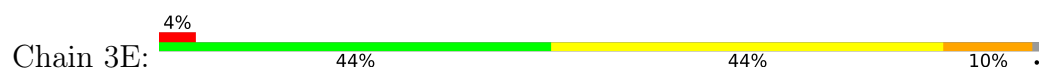
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

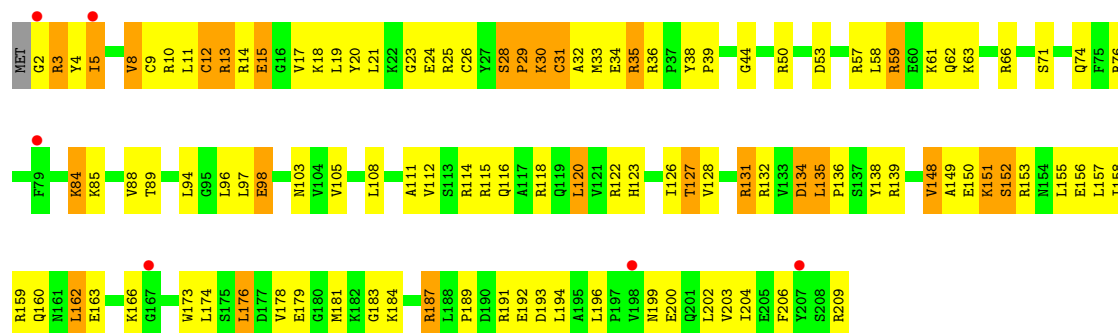


• Molecule 4: 30S ribosomal protein S4

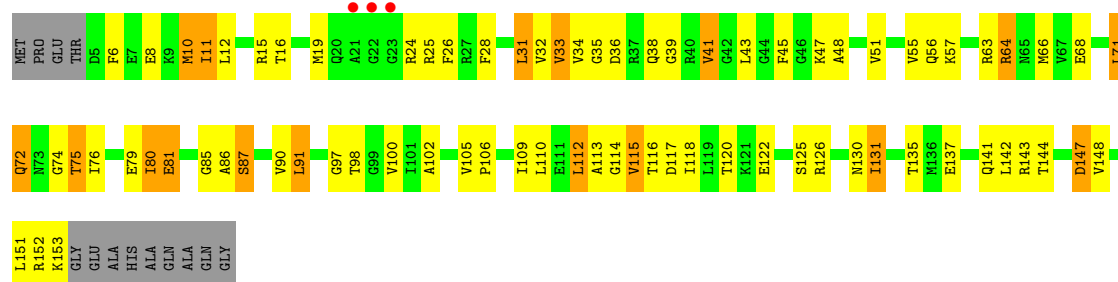
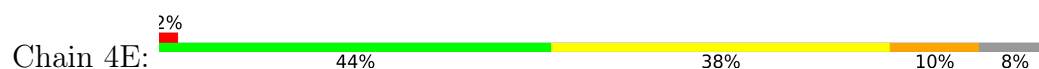




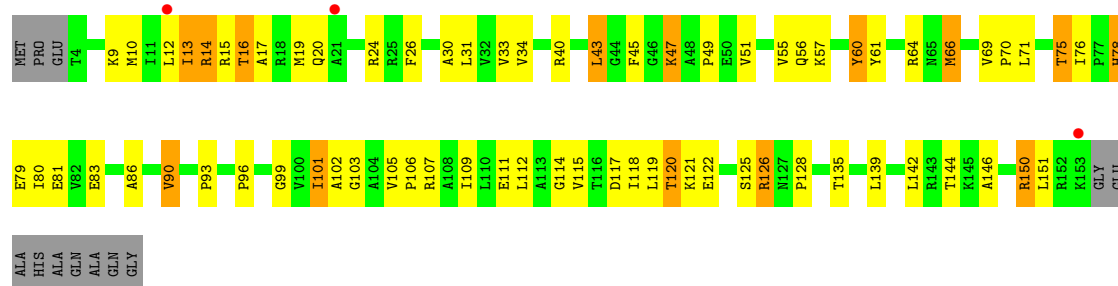
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

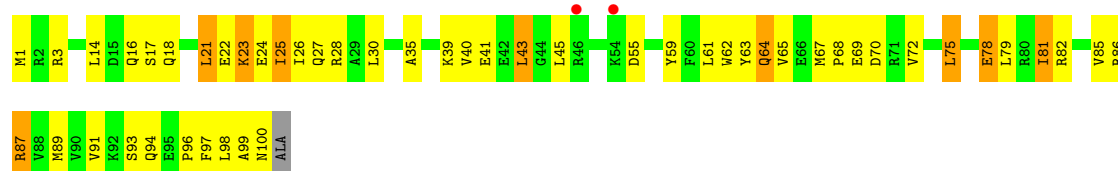


• Molecule 5: 30S ribosomal protein S5

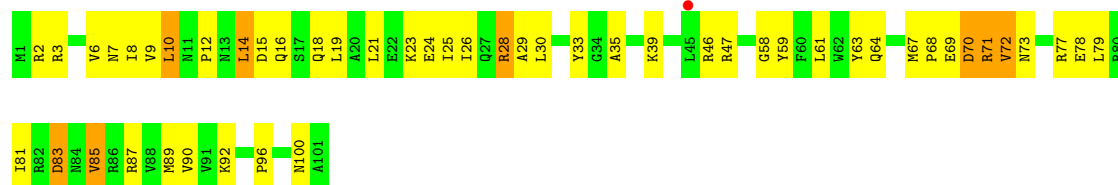


• Molecule 6: 30S ribosomal protein S6

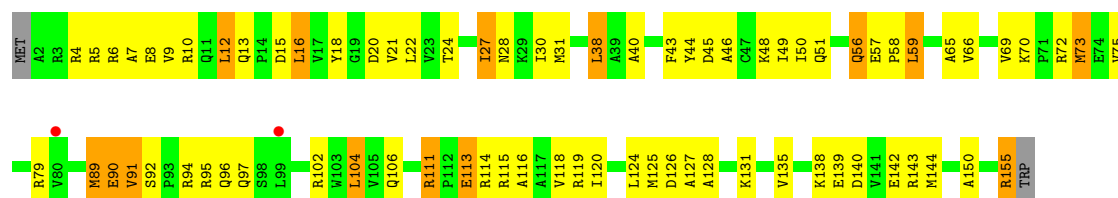




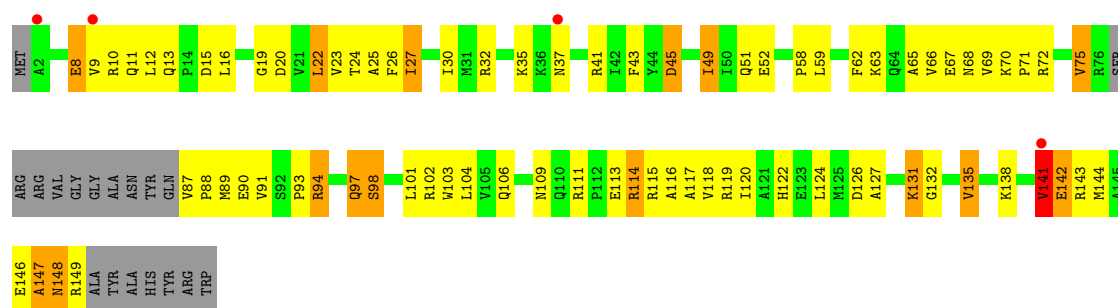
• Molecule 6: 30S ribosomal protein S6



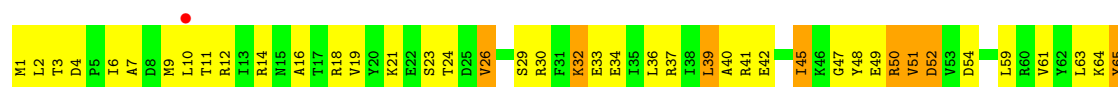
• Molecule 7: 30S ribosomal protein S7

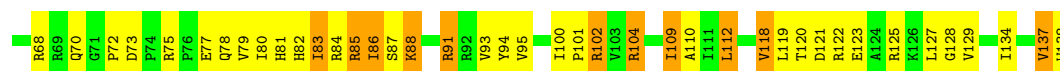


• Molecule 7: 30S ribosomal protein S7

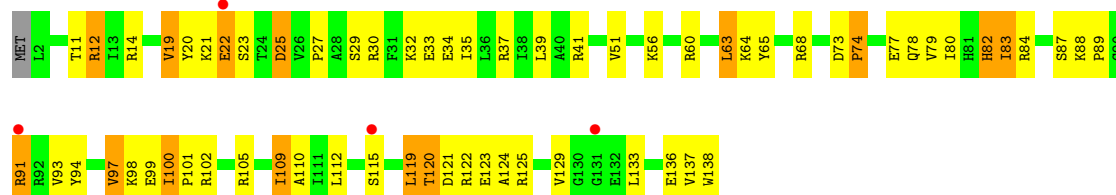


• Molecule 8: 30S ribosomal protein S8

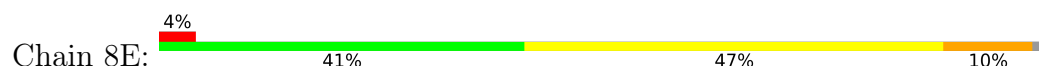




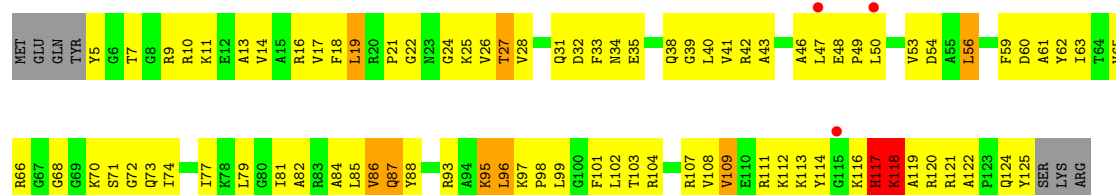
• Molecule 8: 30S ribosomal protein S8



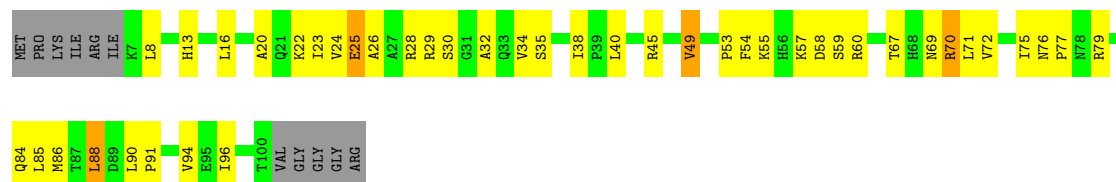
• Molecule 9: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S9

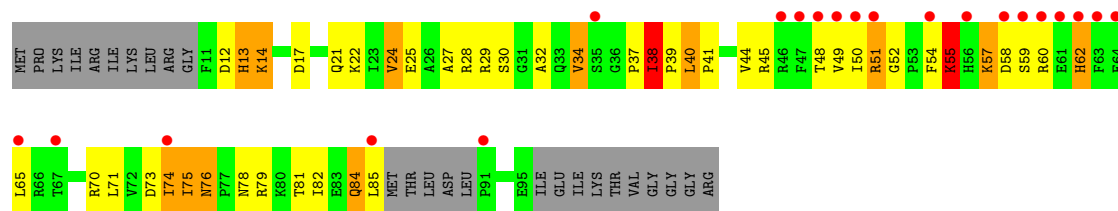


• Molecule 10: 30S ribosomal protein S10

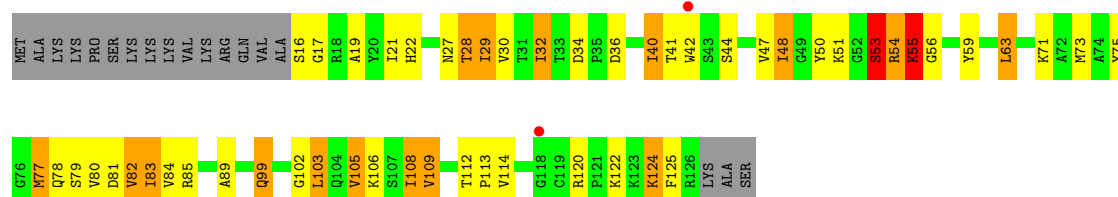


• Molecule 10: 30S ribosomal protein S10

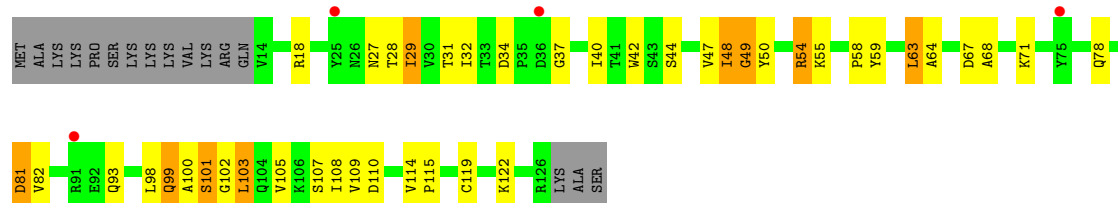




• Molecule 11: 30S ribosomal protein S11



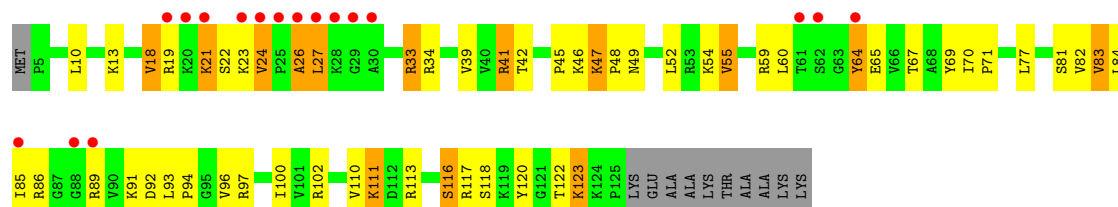
• Molecule 11: 30S ribosomal protein S11



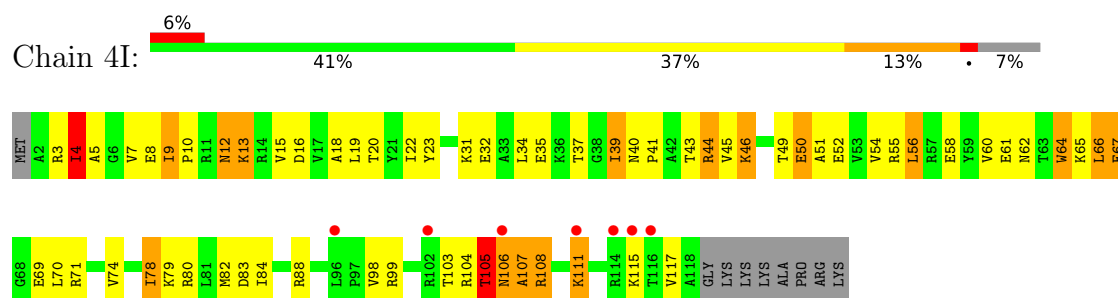
• Molecule 12: 30S ribosomal protein S12



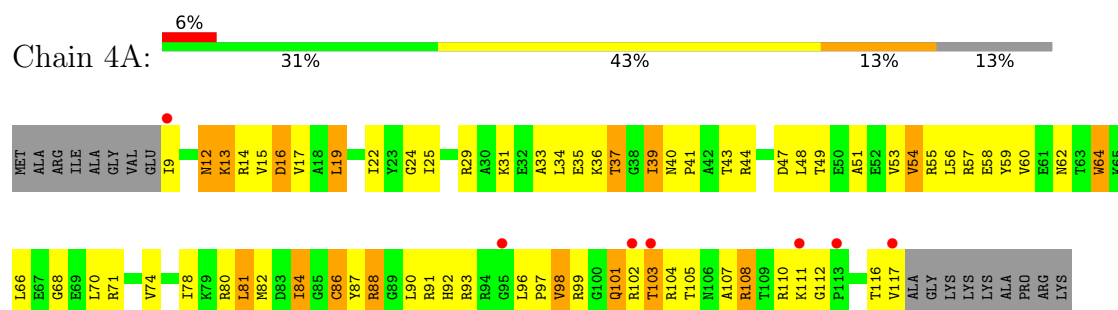
• Molecule 12: 30S ribosomal protein S12



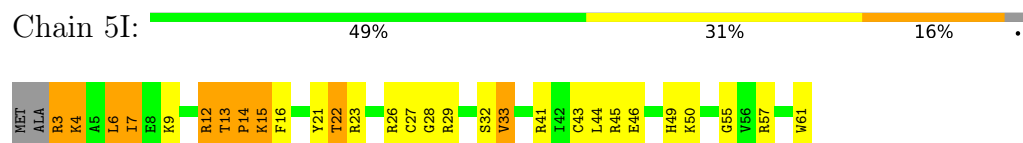
- Molecule 13: 30S ribosomal protein S13



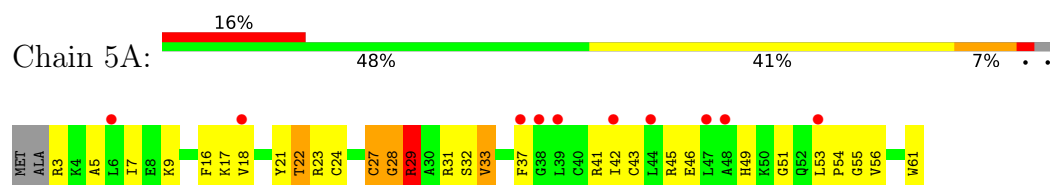
- Molecule 13: 30S ribosomal protein S13



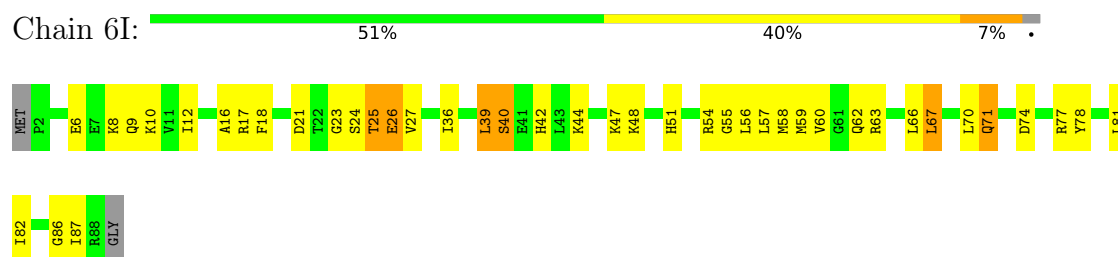
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

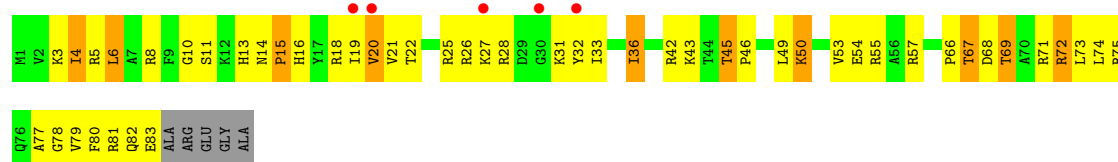


- Molecule 15: 30S ribosomal protein S15

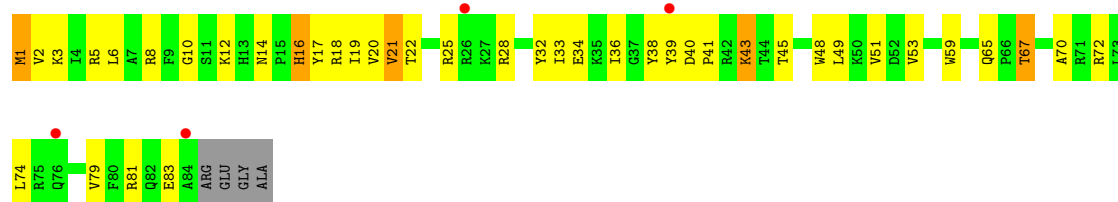




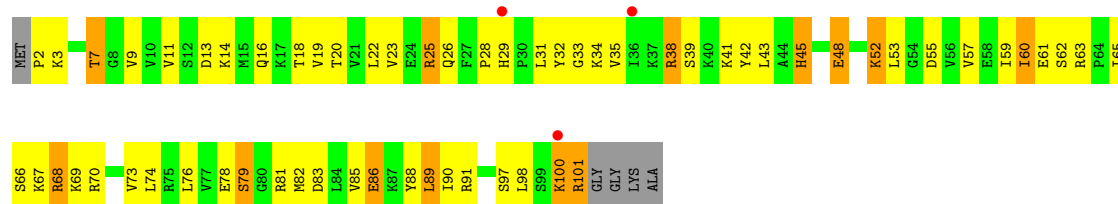
- Molecule 16: 30S ribosomal protein S16



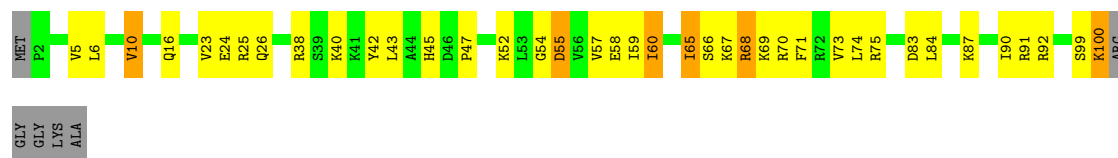
- Molecule 16: 30S ribosomal protein S16



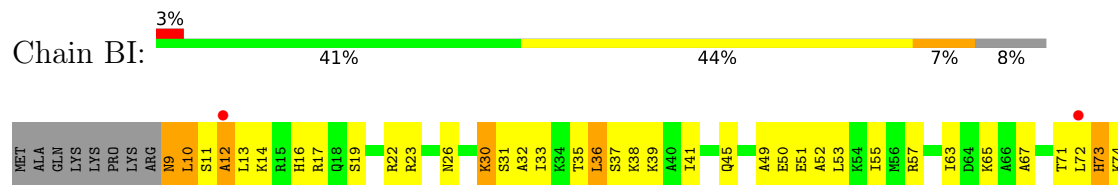
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

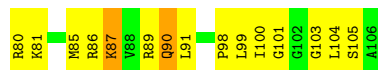


- Molecule 18: 30S ribosomal protein S18





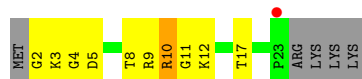
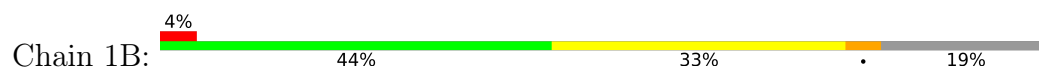
- Molecule 20: 30S ribosomal protein S20



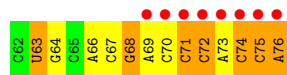
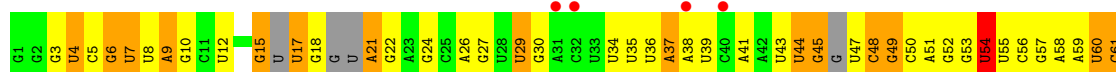
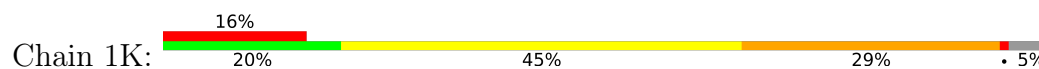
- Molecule 21: 30S ribosomal protein Thx



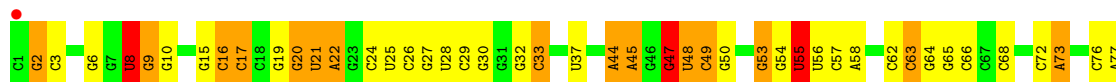
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA^{Lys}

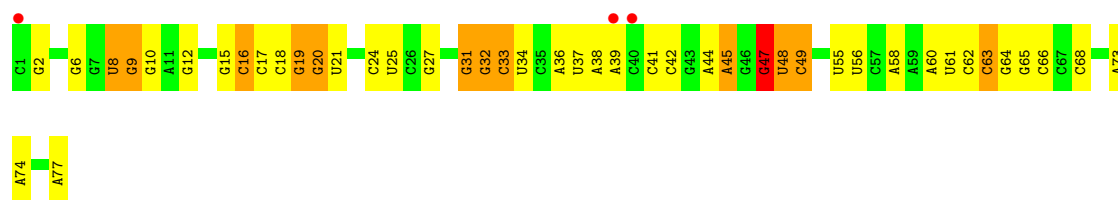


- Molecule 23: tRNA^{fMet}

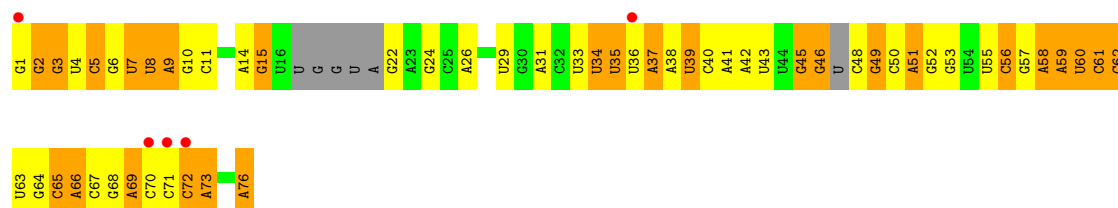
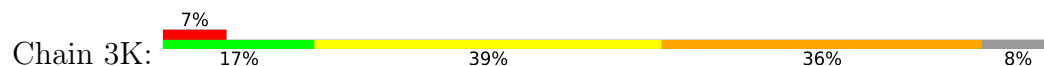


- Molecule 23: tRNA^{fMet}

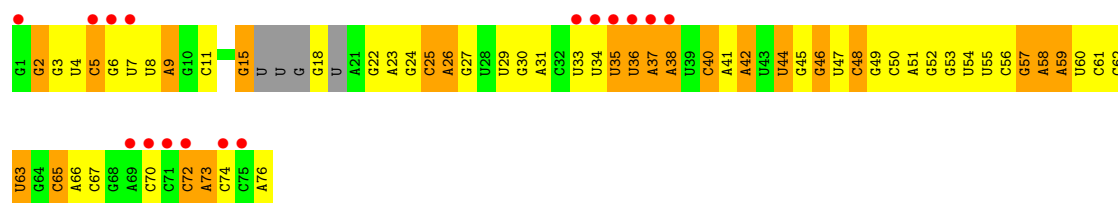
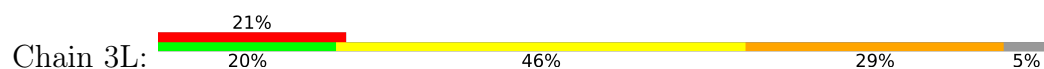




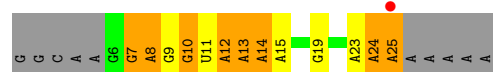
• Molecule 24: tRNA^{Lys}



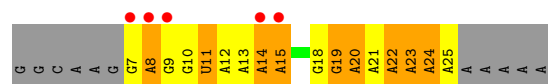
• Molecule 24: tRNA^{Lys}



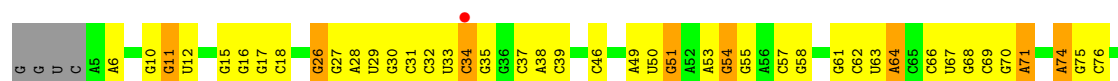
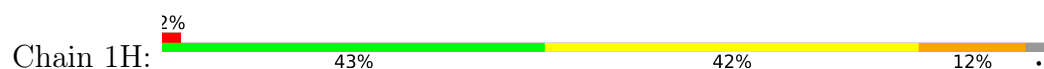
• Molecule 25: mRNA



• Molecule 25: mRNA



• Molecule 26: 23S ribosomal RNA



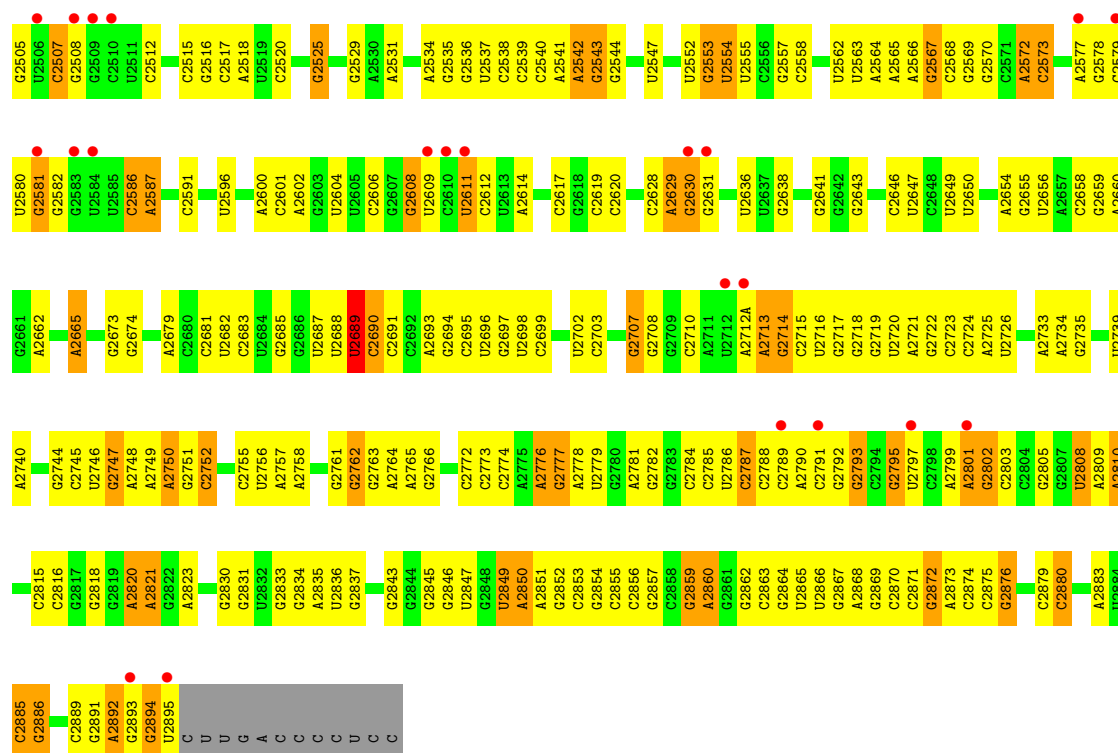


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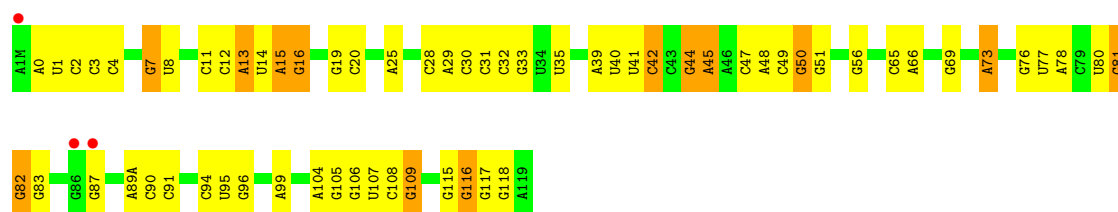


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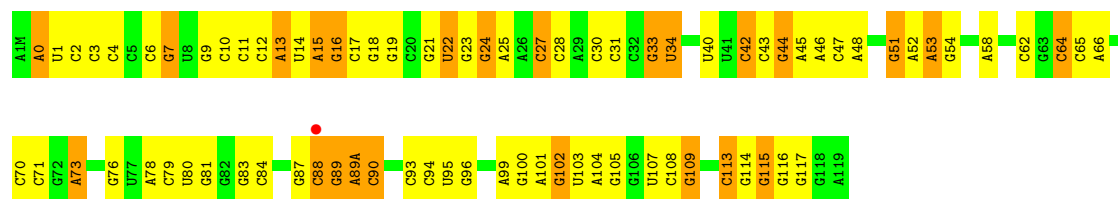
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C2063	C2064	C2065	C2066	G2067	G2068	G2069	G2070	A2071	U2074	U2075	U2076	A2077	G2080	C2081	A2082	G2083	C2084	C2085	G2086	G2087	C2095	U2096	U2099	G2100	G2101	U2102	G2103	G2104	G2105	G2106	C2107	C2108	U2109	C2110	C2111	C2112	C2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	C2128	C2129	U2130	G2131							
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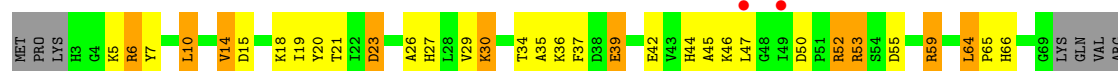
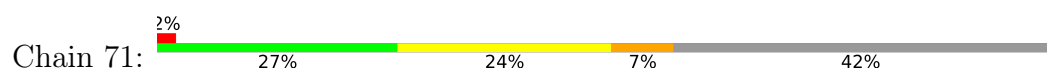
• Molecule 27: 5S ribosomal RNA

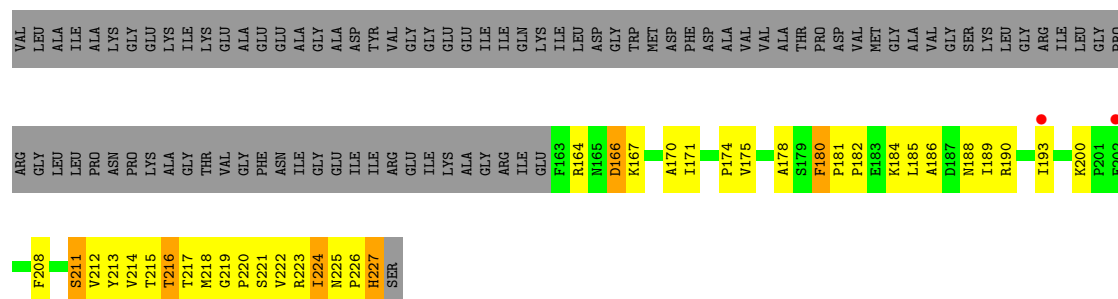


• Molecule 27: 5S ribosomal RNA

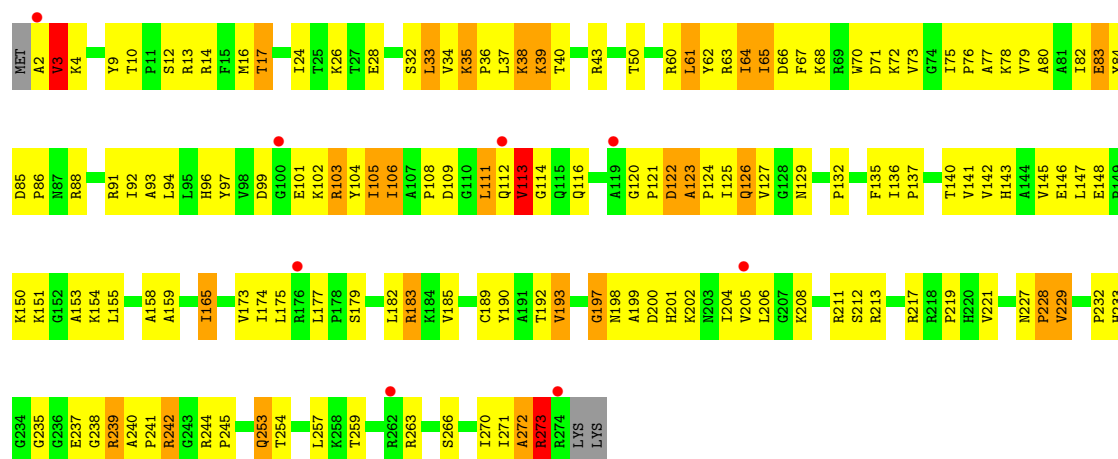


• Molecule 28: 50S ribosomal protein L1

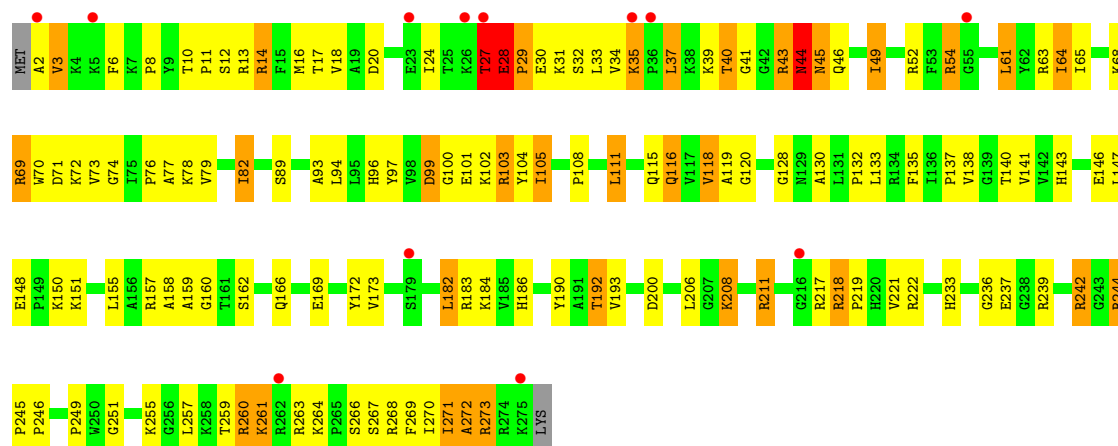




• Molecule 29: 50S ribosomal protein L2

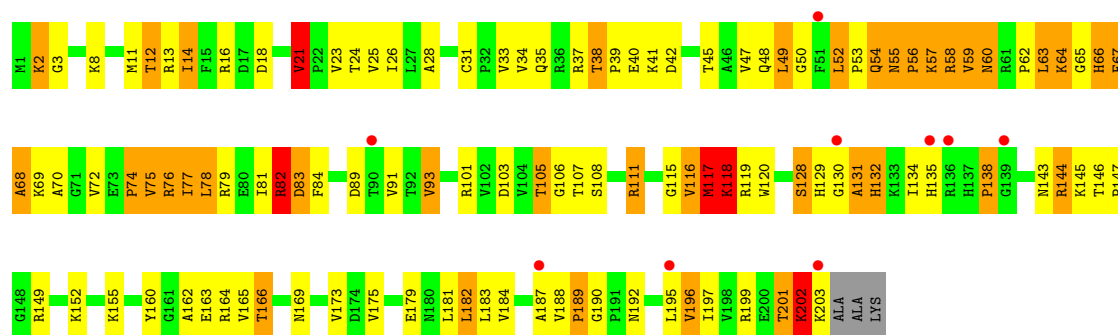


• Molecule 29: 50S ribosomal protein L2

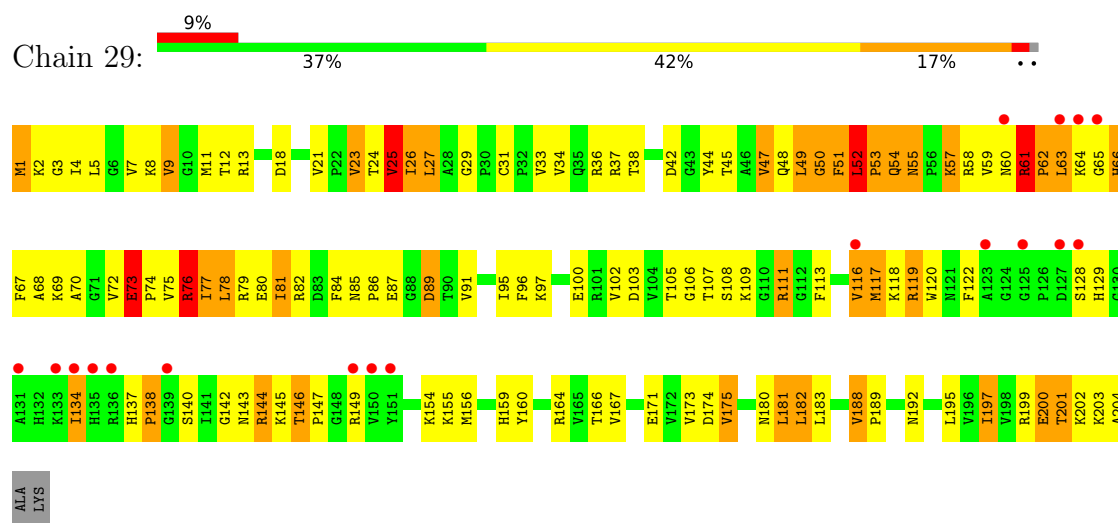


• Molecule 30: 50S ribosomal protein L3

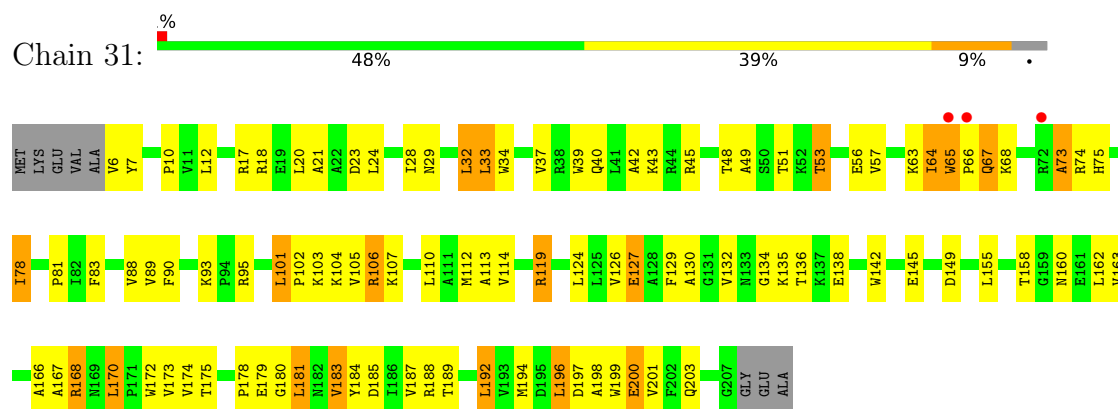




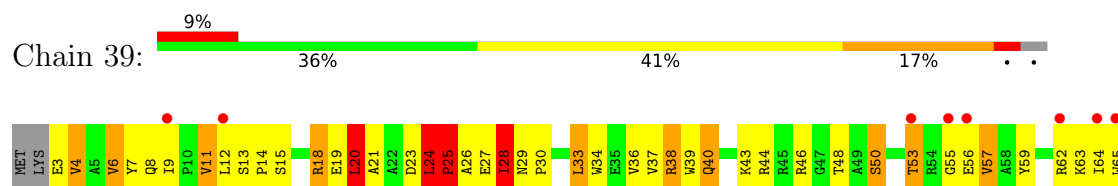
• Molecule 30: 50S ribosomal protein L3

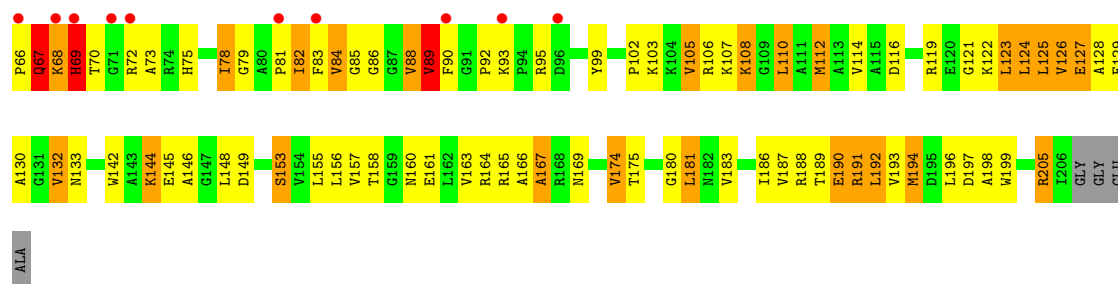


• Molecule 31: 50S ribosomal protein L4

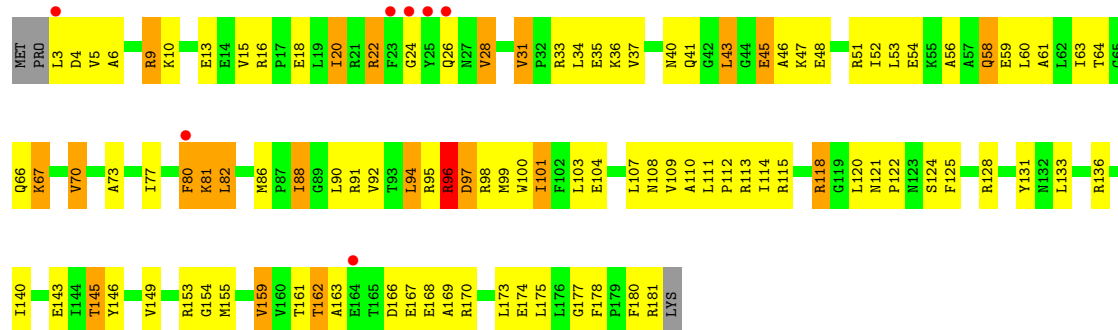


• Molecule 31: 50S ribosomal protein L4

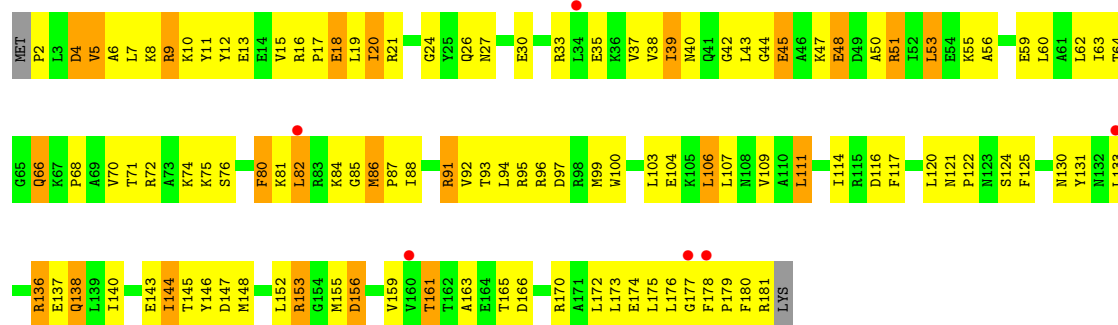




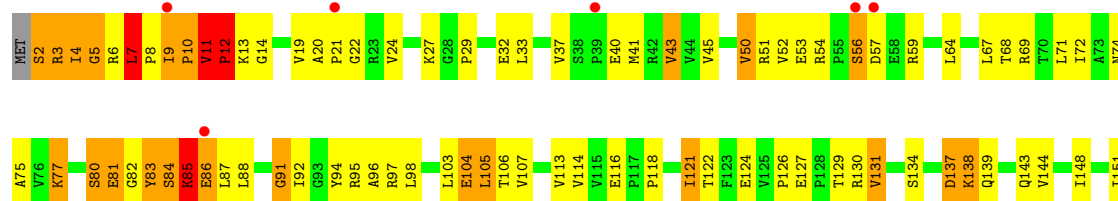
• Molecule 32: 50S ribosomal protein L5



• Molecule 32: 50S ribosomal protein L5

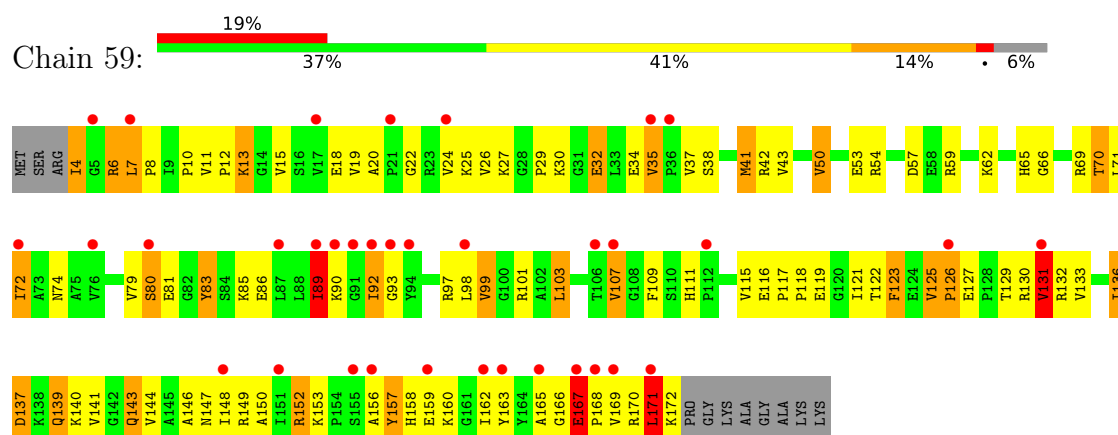


• Molecule 33: 50S ribosomal protein L6

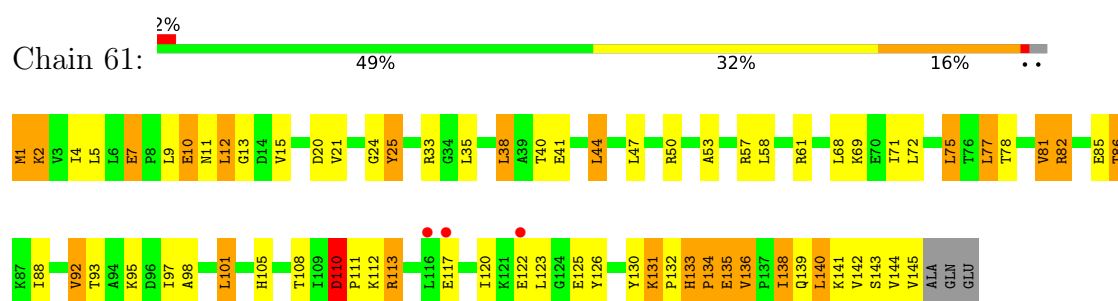




- Molecule 33: 50S ribosomal protein L6

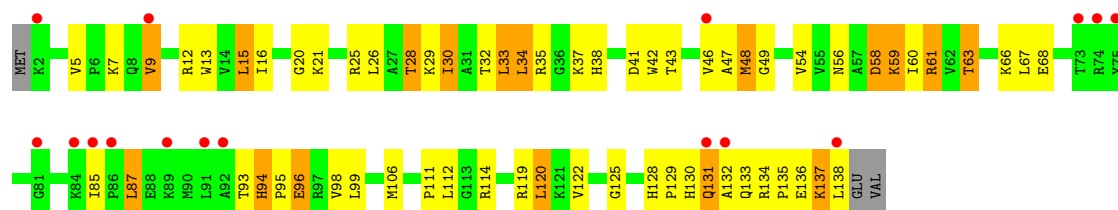


- Molecule 34: 50S ribosomal protein L9

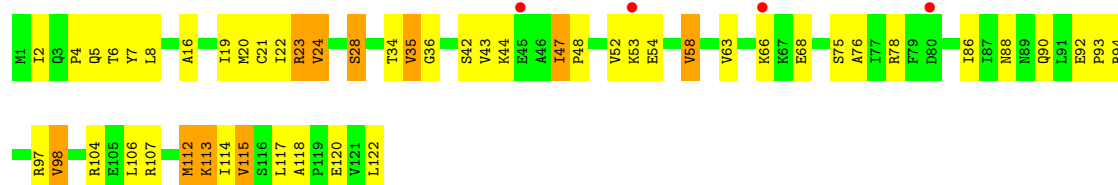




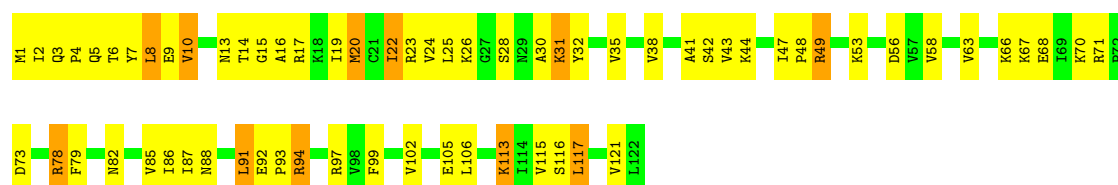
• Molecule 35: 50S ribosomal protein L13



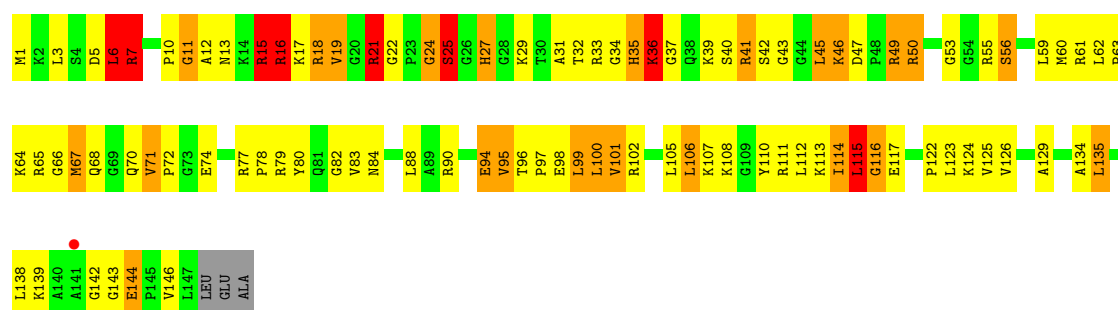
• Molecule 36: 50S ribosomal protein L14



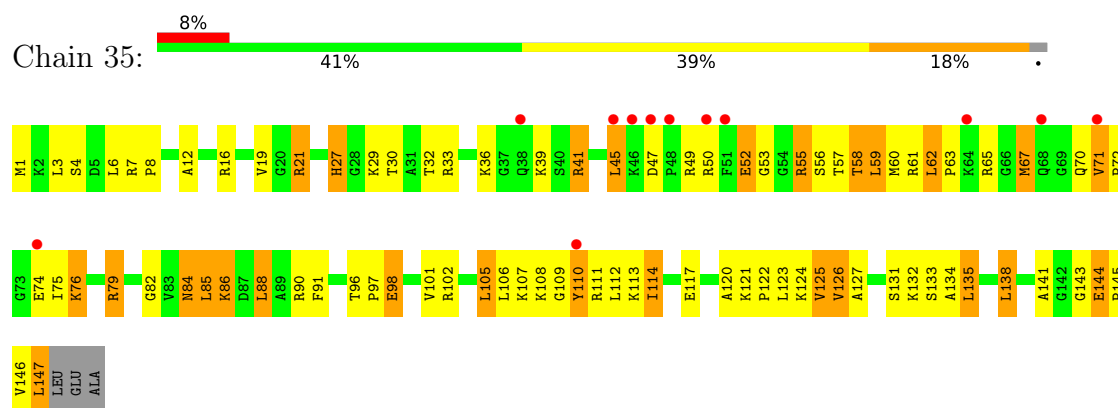
• Molecule 36: 50S ribosomal protein L14



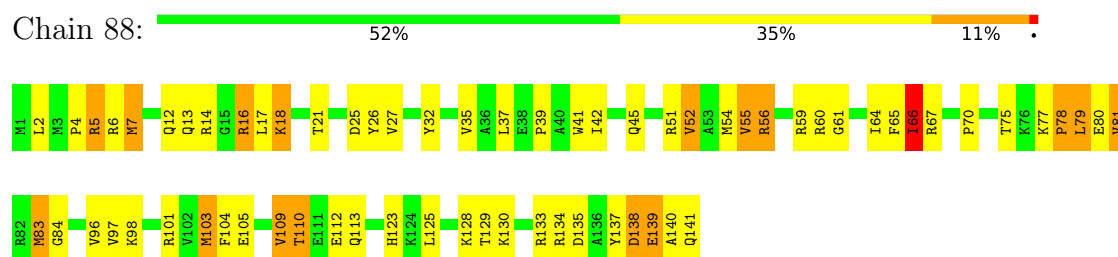
• Molecule 37: 50S ribosomal protein L15



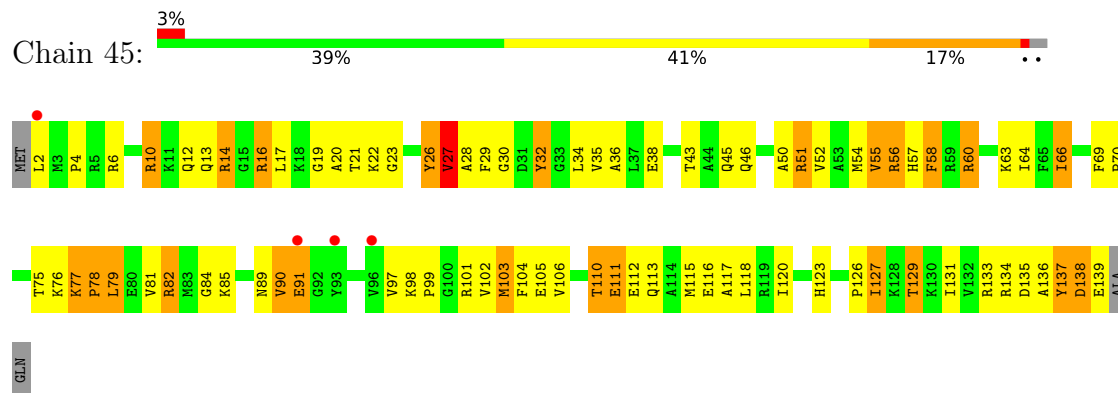
• Molecule 37: 50S ribosomal protein L15



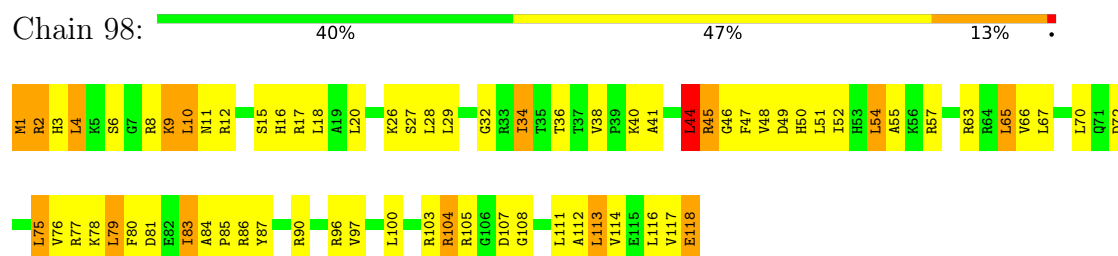
- Molecule 38: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L16

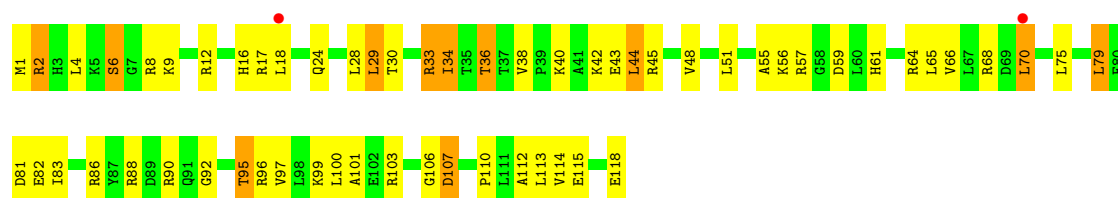


- Molecule 39: 50S ribosomal protein L17

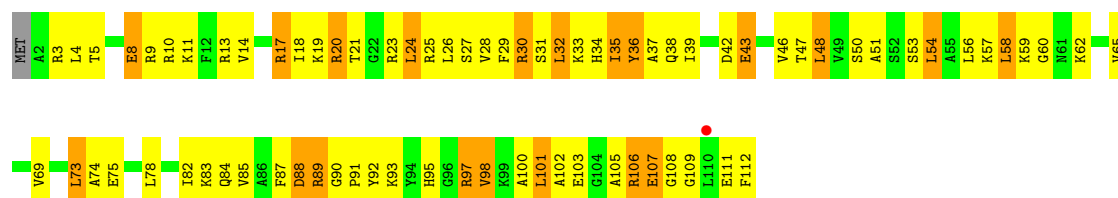


- Molecule 39: 50S ribosomal protein L17

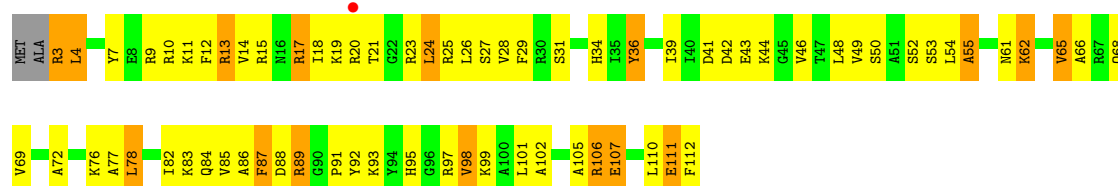




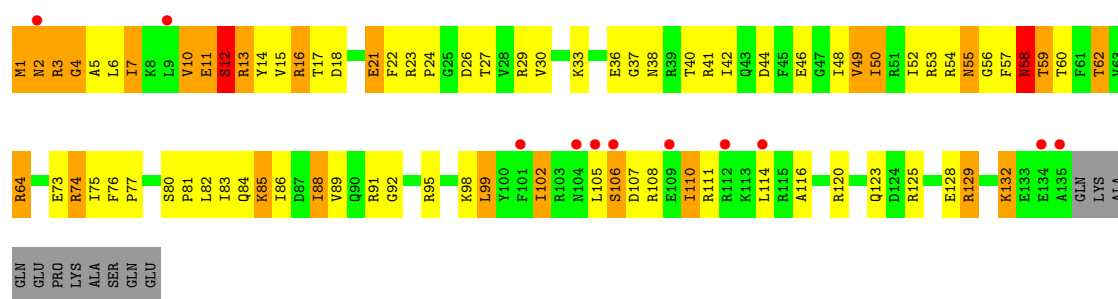
• Molecule 40: 50S ribosomal protein L18



• Molecule 40: 50S ribosomal protein L18

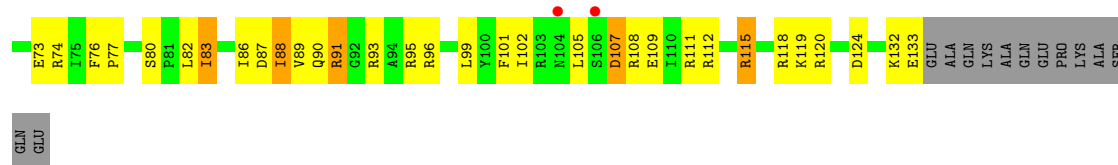


• Molecule 41: 50S ribosomal protein L19

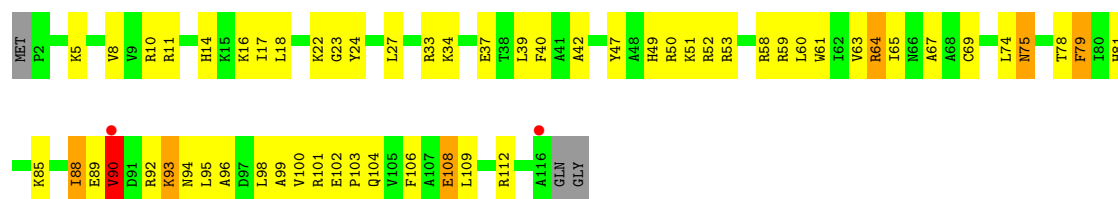


• Molecule 41: 50S ribosomal protein L19

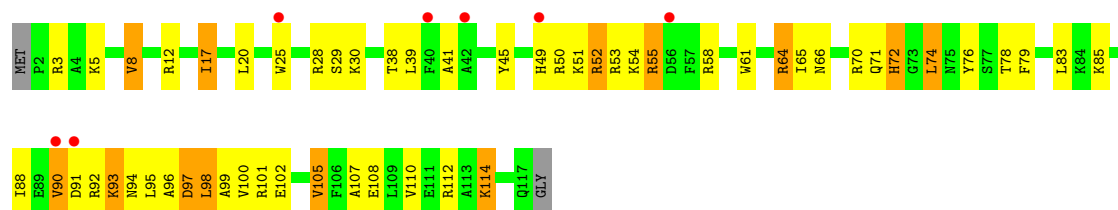




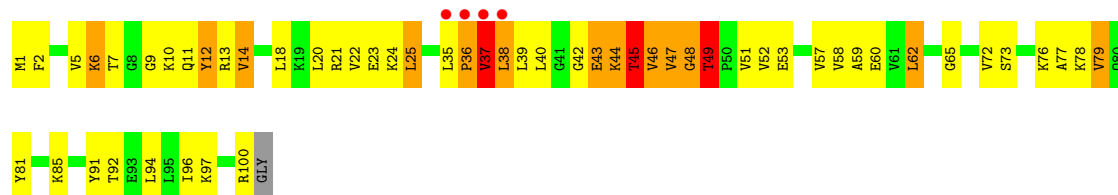
- Molecule 42: 50S ribosomal protein L20



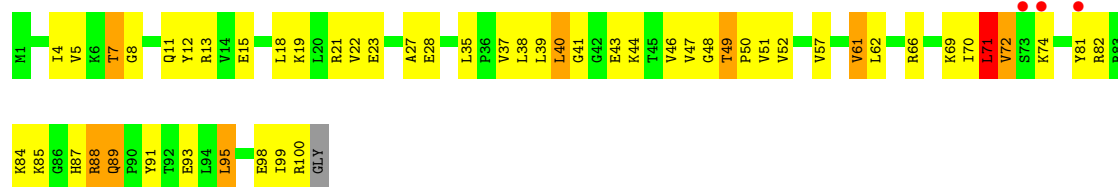
- Molecule 42: 50S ribosomal protein L20



- Molecule 43: 50S ribosomal protein L21



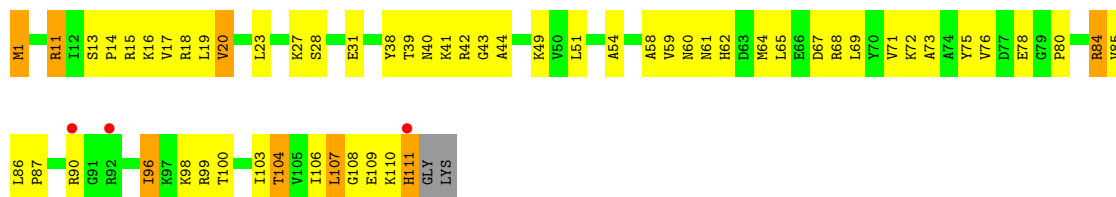
- Molecule 43: 50S ribosomal protein L21



- Molecule 44: 50S ribosomal protein L22



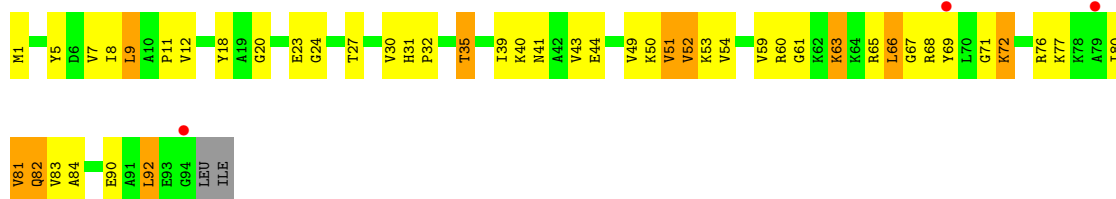
- Molecule 44: 50S ribosomal protein L22



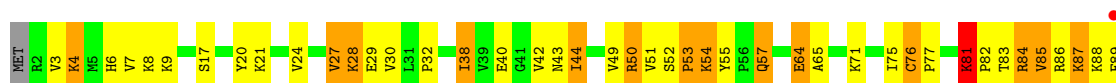
- Molecule 45: 50S ribosomal protein L23

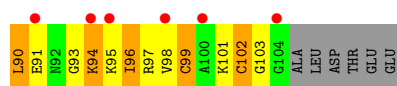


- Molecule 45: 50S ribosomal protein L23

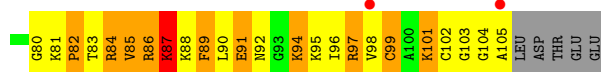
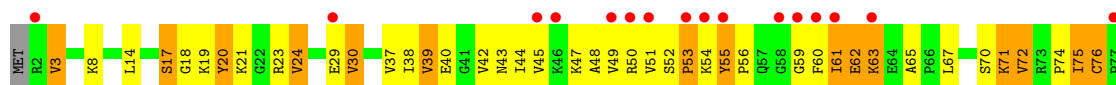


- Molecule 46: 50S ribosomal protein L24

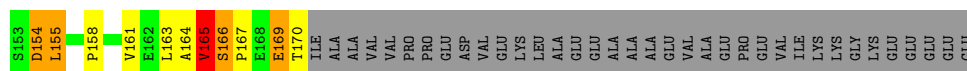
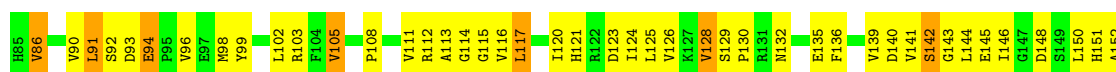
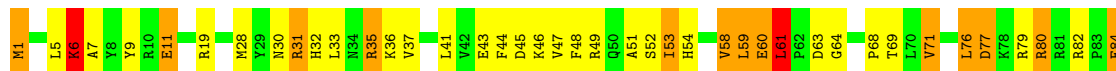
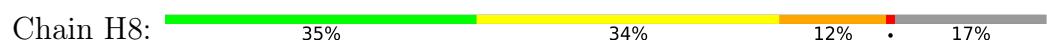




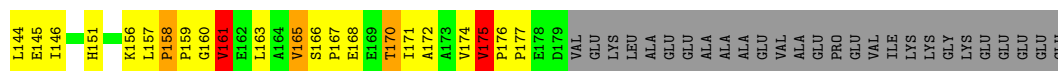
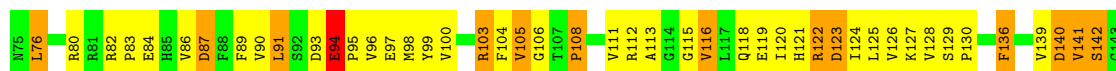
- Molecule 46: 50S ribosomal protein L24



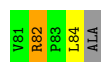
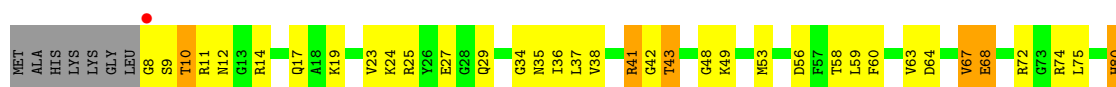
- Molecule 47: 50S ribosomal protein L25



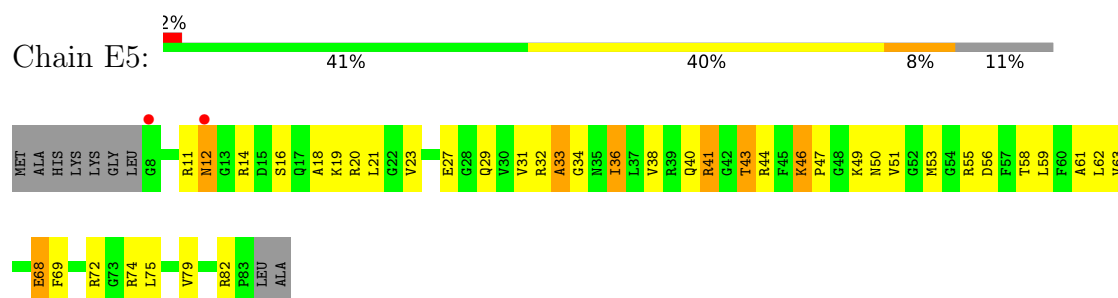
- Molecule 47: 50S ribosomal protein L25



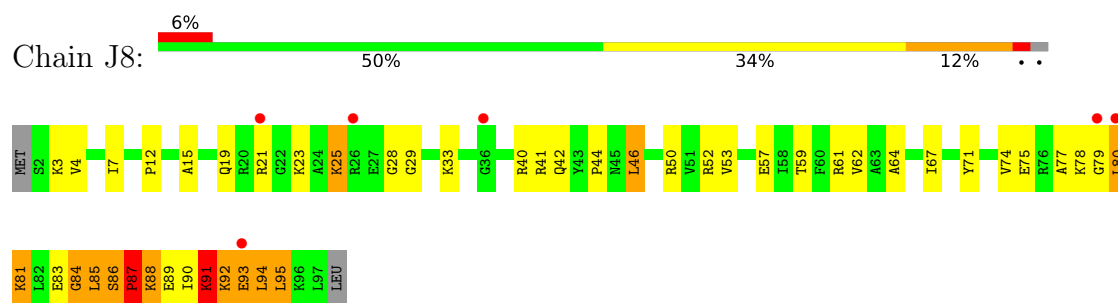
- Molecule 48: 50S ribosomal protein L27



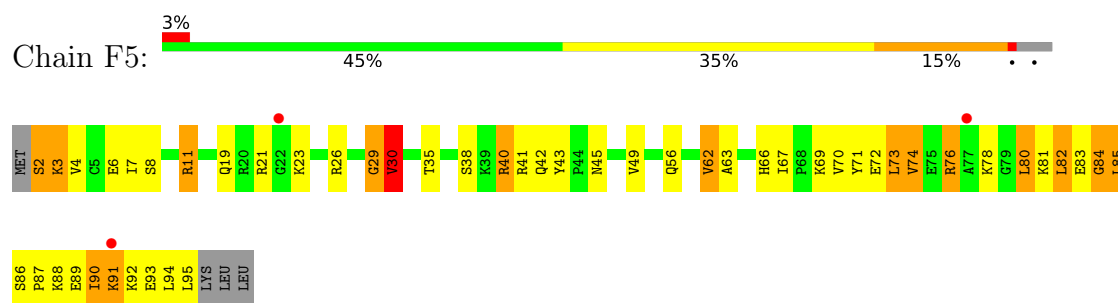
- Molecule 48: 50S ribosomal protein L27



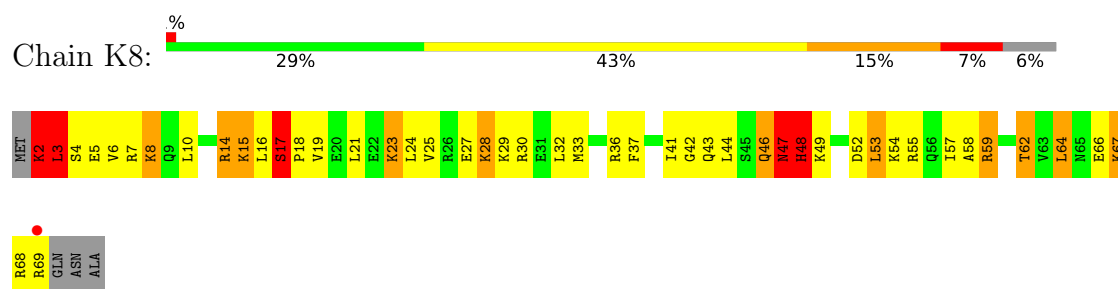
- Molecule 49: 50S ribosomal protein L28



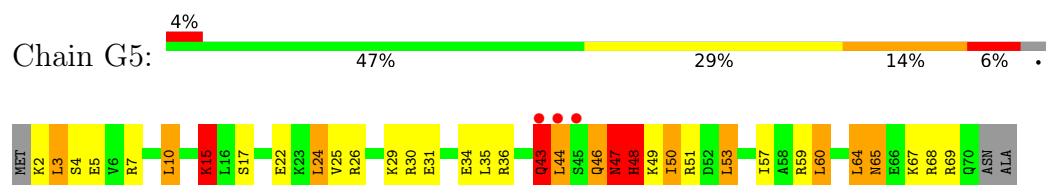
- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29

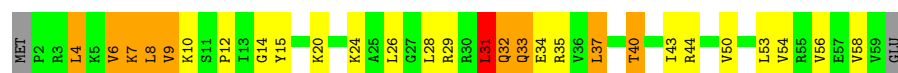


- Molecule 50: 50S ribosomal protein L29



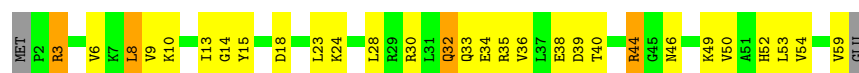
- Molecule 51: 50S ribosomal protein L30

Chain L8: 

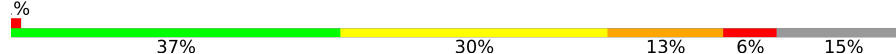


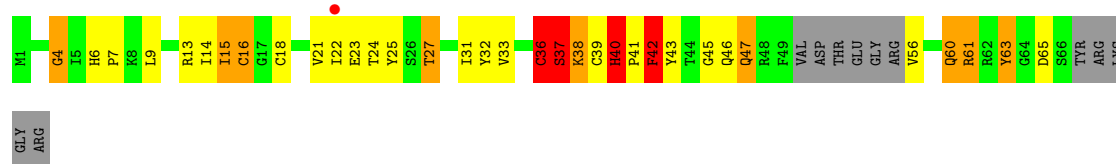
- Molecule 51: 50S ribosomal protein L30

Chain H5: 

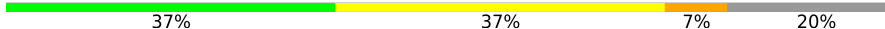


- Molecule 52: 50S ribosomal protein L31

Chain M8: 



- Molecule 53: 50S ribosomal protein L32

Chain N8: 



- Molecule 53: 50S ribosomal protein L32

Chain J5: 



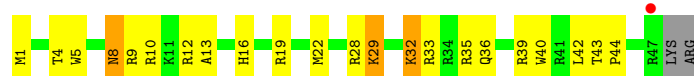
- Molecule 54: 50S ribosomal protein L34

Chain P8: 



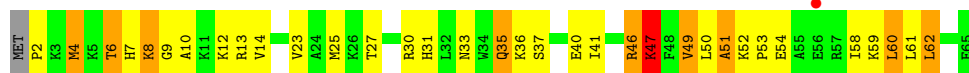
- Molecule 54: 50S ribosomal protein L34

Chain L5: 



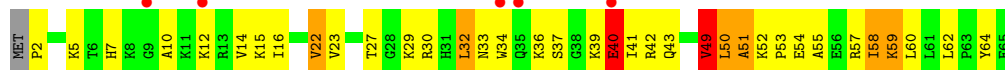
- Molecule 55: 50S ribosomal protein L35

Chain Q8:  2% 46% 37% 14% ..



- Molecule 55: 50S ribosomal protein L35

Chain M5:  8% 43% 43% 9% ..



- Molecule 56: tRNA^{Lys}

Chain 1L:  21% 26% 36% 24% • 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.15Å 448.16Å 617.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.45 – 3.13 154.45 – 3.13	Depositor EDS
% Data completeness (in resolution range)	100.0 (154.45-3.13) 90.9 (154.45-3.13)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.81 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.244 0.195 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 74.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	296999	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: MG, T6A, U8U, SF4, SPE, 7MG, OMC, PSU, H2U, 5MU, ZN, 4SU

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	0.38	0/36095	0.62	5/56332 (0.0%)
1	1G	0.34	0/36309	0.58	2/56668 (0.0%)
2	12	0.35	0/1727	0.69	3/2326 (0.1%)
2	1E	0.36	1/1908 (0.1%)	0.64	0/2573
3	22	0.40	1/1560 (0.1%)	0.56	0/2104
3	2E	0.39	1/1629 (0.1%)	0.57	0/2195
4	32	0.36	0/1732	0.65	0/2318
4	3E	0.42	1/1728 (0.1%)	0.65	0/2313
5	42	0.34	0/1156	0.59	0/1557
5	4E	0.36	0/1158	0.62	0/1559
6	52	0.37	0/855	0.57	0/1154
6	5E	0.40	0/850	0.60	0/1147
7	62	0.34	0/1122	0.63	3/1500 (0.2%)
7	6E	0.33	0/1259	0.51	0/1686
8	72	0.32	0/1127	0.59	0/1517
8	7E	0.35	0/1135	0.61	0/1527
9	82	0.31	0/971	0.63	0/1304
9	8E	0.33	0/1019	0.62	0/1367
10	1A	0.79	2/658 (0.3%)	0.61	0/885
10	1I	0.34	0/762	0.65	0/1027
11	2A	0.33	0/850	0.59	0/1150
11	2I	0.39	0/838	0.66	0/1133
12	3A	0.44	0/963	0.70	0/1290
12	3I	0.53	0/972	0.86	1/1301 (0.1%)
13	4A	0.30	0/889	0.61	0/1192
13	4I	0.41	0/943	0.68	0/1265
14	5A	0.35	0/495	0.75	2/657 (0.3%)
14	5I	0.40	0/495	0.80	2/657 (0.3%)
15	6A	0.34	0/740	0.59	0/987
15	6I	0.40	0/740	0.65	0/987
16	7A	0.36	0/721	0.66	0/970
16	7I	0.36	0/716	0.67	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.35	0/836	0.62	0/1117
17	8I	0.38	0/847	0.72	2/1131 (0.2%)
18	9A	0.40	0/549	0.63	0/732
18	9I	0.37	0/554	0.67	0/739
19	AA	0.39	0/520	0.77	2/700 (0.3%)
19	AI	0.36	0/676	0.85	6/910 (0.7%)
20	BA	0.34	0/764	0.75	3/1007 (0.3%)
20	BI	0.32	0/748	0.60	0/986
21	1B	0.30	0/192	0.60	0/252
21	1F	0.37	0/203	0.62	0/266
22	1K	0.33	0/1568	0.54	0/2434
23	2K	0.43	1/1721 (0.1%)	0.63	0/2682
23	2L	0.39	0/1721	0.58	0/2682
24	3K	0.31	0/1654	0.55	0/2570
24	3L	0.31	0/1705	0.51	0/2650
25	4K	0.43	0/499	0.66	0/778
25	4L	0.38	0/473	0.67	0/737
26	14	0.46	0/68159	0.68	15/106398 (0.0%)
26	1H	0.55	0/68309	0.74	8/106631 (0.0%)
27	16	0.42	0/2928	0.69	0/4568
27	1J	0.37	0/2928	0.63	0/4568
28	71	0.23	0/1049	0.53	0/1417
29	11	0.62	0/2170	0.97	5/2926 (0.2%)
29	19	0.57	0/2175	0.92	9/2933 (0.3%)
30	21	0.60	1/1579 (0.1%)	1.08	12/2131 (0.6%)
30	29	0.53	0/1596	0.93	4/2153 (0.2%)
31	31	0.56	0/1620	0.87	0/2194
31	39	0.49	0/1637	0.94	7/2218 (0.3%)
32	41	0.38	0/1481	0.71	0/1994
32	49	0.38	1/1483 (0.1%)	0.66	1/1997 (0.1%)
33	51	0.51	0/1354	1.04	15/1833 (0.8%)
33	59	0.38	0/1320	0.76	2/1787 (0.1%)
34	61	0.41	0/1146	0.75	4/1551 (0.3%)
34	69	0.42	1/1146 (0.1%)	0.77	4/1551 (0.3%)
35	15	0.39	0/1123	0.69	0/1515
35	58	0.47	0/1123	0.83	3/1514 (0.2%)
36	25	0.44	0/942	0.72	0/1269
36	68	0.52	0/942	0.74	0/1269
37	35	0.51	0/1139	0.87	0/1514
37	78	0.61	0/1139	1.08	5/1514 (0.3%)
38	45	0.57	1/1120 (0.1%)	0.94	0/1498
38	88	0.59	0/1138	0.98	0/1523
39	55	0.47	0/981	0.76	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	98	0.50	0/981	0.83	2/1312 (0.2%)
40	65	0.41	0/886	0.82	0/1180
40	A8	0.50	0/891	0.81	0/1187
41	75	0.47	0/1123	0.86	3/1500 (0.2%)
41	B8	0.52	0/1133	0.90	4/1514 (0.3%)
42	85	0.41	0/977	0.72	0/1301
42	C8	0.53	0/968	0.80	0/1289
43	95	0.43	0/781	0.85	2/1048 (0.2%)
43	D8	0.53	1/785 (0.1%)	0.86	2/1052 (0.2%)
44	A5	0.51	0/897	0.75	0/1204
44	E8	0.52	0/886	0.80	0/1189
45	B5	0.50	0/749	0.78	0/1007
45	F8	0.55	0/764	0.85	0/1025
46	C5	0.72	2/807 (0.2%)	1.00	2/1076 (0.2%)
46	G8	0.67	0/796	1.18	10/1062 (0.9%)
47	D5	0.60	1/1443 (0.1%)	0.69	1/1960 (0.1%)
47	H8	0.42	1/1395 (0.1%)	0.79	1/1890 (0.1%)
48	E5	0.46	0/611	0.81	0/814
48	I8	0.55	0/619	0.90	0/825
49	F5	0.48	0/744	0.96	3/989 (0.3%)
49	J8	0.60	0/754	1.02	1/1003 (0.1%)
50	G5	0.48	0/578	0.88	2/766 (0.3%)
50	K8	0.59	0/577	1.04	3/763 (0.4%)
51	H5	0.42	0/464	0.67	0/623
51	L8	0.47	0/464	0.74	1/623 (0.2%)
52	M8	0.45	0/485	1.10	5/652 (0.8%)
53	J5	0.44	0/448	0.74	0/606
53	N8	0.69	1/381 (0.3%)	0.85	0/516
54	L5	0.50	0/409	0.82	0/540
54	P8	0.67	0/409	0.93	0/540
55	M5	0.63	0/524	0.94	0/691
55	Q8	0.61	0/524	1.08	3/691 (0.4%)
56	1L	0.26	0/1516	0.45	0/2350
All	All	0.46	17/316848 (0.0%)	0.70	170/474550 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	5
4	3E	0	1
8	72	0	1
9	82	0	2
9	8E	0	2
10	1A	0	1
11	2A	0	1
12	3A	0	1
12	3I	0	3
13	4I	0	3
14	5A	0	1
16	7I	0	1
19	AA	0	1
19	AI	0	1
20	BA	0	3
20	BI	0	1
29	11	0	4
29	19	0	2
30	21	0	7
30	29	0	5
31	39	0	8
32	49	0	2
33	51	0	6
33	59	0	4
34	61	0	3
34	69	0	4
35	15	0	1
35	58	0	1
37	35	0	1
37	78	0	6
38	45	0	2
38	88	0	1
39	98	0	2
40	65	0	2
40	A8	0	1
41	75	0	3
41	B8	0	3
42	85	0	4
42	C8	0	3
43	D8	0	3
44	A5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	B5	0	2
46	C5	0	3
46	G8	0	3
47	D5	0	4
47	H8	0	5
49	F5	0	1
49	J8	0	3
50	G5	0	3
50	K8	0	3
52	M8	0	4
55	M5	0	4
55	Q8	0	2
All	All	0	151

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	D5	94	GLU	C-N	19.11	1.78	1.33
10	1A	38	ILE	C-N	15.95	1.71	1.33
3	22	173	VAL	C-N	10.60	1.58	1.33
53	N8	4	HIS	C-O	8.97	1.28	1.23
30	21	144	ARG	CA-C	8.23	1.56	1.52

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	M8	40	HIS	CA-C-N	9.59	131.82	119.84
52	M8	40	HIS	C-N-CA	9.59	131.82	119.84
30	21	202	LYS	N-CA-C	9.58	125.25	113.17
37	78	15	ARG	CA-C-N	9.40	139.50	121.54
37	78	15	ARG	C-N-CA	9.40	139.50	121.54

There are no chirality outliers.

5 of 151 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	234	PRO	Peptide
2	1E	236	TYR	Peptide
2	1E	9	GLU	Peptide
4	3E	29	PRO	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	32246	0	16276	867	0
1	1G	32437	0	16372	887	2
2	12	1696	0	1730	97	0
2	1E	1874	0	1926	103	0
3	22	1537	0	1603	88	0
3	2E	1605	0	1668	62	0
4	32	1702	0	1765	103	0
4	3E	1698	0	1761	86	0
5	42	1141	0	1198	45	0
5	4E	1142	0	1204	57	0
6	52	842	0	857	35	0
6	5E	837	0	852	36	0
7	62	1110	0	1163	66	0
7	6E	1242	0	1286	55	0
8	72	1107	0	1165	51	0
8	7E	1115	0	1177	69	0
9	82	953	0	983	75	0
9	8E	1000	0	1031	61	0
10	1A	646	0	662	43	0
10	1I	749	0	767	44	0
11	2A	835	0	847	29	0
11	2I	823	0	832	43	0
12	3A	947	0	1033	37	0
12	3I	956	0	1046	33	0
13	4A	879	0	935	69	0
13	4I	933	0	992	54	0
14	5A	486	0	525	34	0
14	5I	486	0	524	29	0
15	6A	729	0	768	28	0
15	6I	729	0	768	30	0
16	7A	705	0	725	29	0
16	7I	700	0	720	50	0
17	8A	823	0	891	32	0
17	8I	834	0	904	63	0
18	9A	544	0	605	25	0
18	9I	549	0	607	24	0
19	AA	510	0	507	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	661	0	683	38	0
20	BA	762	0	861	40	0
20	BI	746	0	843	46	0
21	1B	188	0	195	10	0
21	1F	199	0	208	14	0
22	1K	1542	0	790	42	0
23	2K	1646	0	843	34	0
23	2L	1646	0	845	32	0
24	3K	1483	0	756	67	0
24	3L	1528	0	778	48	0
25	4K	442	0	219	9	0
25	4L	419	0	208	23	0
26	14	60857	0	30679	1325	1
26	1H	60991	0	30744	1364	1
27	16	2617	0	1328	57	0
27	1J	2617	0	1328	83	0
28	71	1027	0	1043	66	0
29	11	2120	0	2197	124	0
29	19	2125	0	2199	112	0
30	21	1546	0	1602	99	0
30	29	1563	0	1629	113	0
31	31	1585	0	1632	94	0
31	39	1602	0	1649	99	0
32	41	1457	0	1514	80	0
32	49	1459	0	1507	76	0
33	51	1328	0	1396	79	0
33	59	1295	0	1366	76	0
34	61	1131	0	1218	44	0
34	69	1131	0	1218	57	0
35	15	1096	0	1168	57	0
35	58	1096	0	1169	68	0
36	25	932	0	996	52	0
36	68	932	0	996	40	0
37	35	1122	0	1206	76	0
37	78	1122	0	1206	100	0
38	45	1099	0	1154	78	0
38	88	1117	0	1168	56	0
39	55	967	0	1033	49	0
39	98	967	0	1033	53	0
40	65	876	0	938	56	0
40	A8	881	0	943	56	0
41	75	1109	0	1170	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	B8	1119	0	1177	73	0
42	85	959	0	1019	66	0
42	C8	950	0	1011	61	0
43	95	770	0	838	42	0
43	D8	774	0	849	41	0
44	A5	886	0	948	37	0
44	E8	876	0	941	27	0
45	B5	735	0	785	34	0
45	F8	750	0	814	34	0
46	C5	794	0	885	63	0
46	G8	783	0	869	49	0
47	D5	1411	0	1436	83	0
47	H8	1365	0	1391	67	0
48	E5	603	0	620	40	0
48	I8	611	0	631	34	0
49	F5	737	0	813	42	0
49	J8	747	0	817	37	0
50	G5	576	0	625	34	0
50	K8	575	0	634	45	0
51	H5	459	0	512	15	0
51	L8	459	0	512	22	0
52	M8	475	0	465	35	0
53	J5	434	0	454	23	0
53	N8	369	0	388	21	0
54	L5	401	0	436	21	0
54	P8	401	0	436	15	0
55	M5	516	0	582	28	0
55	Q8	516	0	582	34	0
56	1L	1402	0	715	32	0
57	13	141	0	0	0	0
57	14	460	0	0	0	0
57	16	12	0	0	0	0
57	19	1	0	0	0	0
57	1G	125	0	0	0	0
57	1H	552	0	0	0	0
57	1J	10	0	0	0	0
57	21	3	0	0	0	0
57	25	1	0	0	0	0
57	29	1	0	0	0	0
57	2I	1	0	0	0	0
57	2K	3	0	0	0	0
57	2L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	31	1	0	0	0	0
57	32	1	0	0	0	0
57	35	2	0	0	0	0
57	39	1	0	0	0	0
57	3I	1	0	0	0	0
57	41	1	0	0	0	0
57	42	2	0	0	0	0
57	45	1	0	0	0	0
57	4L	1	0	0	0	0
57	52	1	0	0	0	0
57	7A	1	0	0	0	0
57	88	3	0	0	0	0
57	B5	1	0	0	0	0
57	E5	2	0	0	0	0
57	F8	1	0	0	0	0
57	I8	2	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	32	8	0	0	2	0
58	3E	8	0	0	0	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	C5	1	0	0	0	0
59	G8	1	0	0	0	0
60	14	13	0	24	0	0
60	1G	13	0	22	3	0
61	11	10	0	0	6	0
61	13	354	0	0	20	0
61	14	1303	0	0	91	0
61	15	3	0	0	0	0
61	16	12	0	0	1	0
61	19	14	0	0	1	0
61	1A	2	0	0	0	0
61	1G	364	0	0	24	0
61	1H	1720	0	0	128	0
61	1I	2	0	0	0	0
61	1J	27	0	0	1	0
61	1K	1	0	0	0	0
61	21	6	0	0	1	0
61	25	8	0	0	0	0
61	29	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2A	1	0	0	0	0
61	2K	8	0	0	0	0
61	2L	8	0	0	0	0
61	31	6	0	0	0	0
61	32	4	0	0	0	0
61	35	8	0	0	0	0
61	39	8	0	0	0	0
61	3E	2	0	0	0	0
61	3I	2	0	0	0	0
61	3K	1	0	0	0	0
61	42	1	0	0	0	0
61	4A	2	0	0	0	0
61	4E	3	0	0	2	0
61	4K	5	0	0	0	0
61	4L	3	0	0	0	0
61	52	4	0	0	0	0
61	55	1	0	0	0	0
61	58	2	0	0	0	0
61	5I	1	0	0	0	0
61	68	2	0	0	0	0
61	6A	3	0	0	0	0
61	75	1	0	0	0	0
61	78	13	0	0	4	0
61	7A	4	0	0	0	0
61	7I	2	0	0	0	0
61	85	1	0	0	0	0
61	8E	2	0	0	0	0
61	98	1	0	0	2	0
61	9A	2	0	0	0	0
61	B5	1	0	0	0	0
61	B8	1	0	0	0	0
61	BA	3	0	0	0	0
61	BI	3	0	0	1	0
61	C5	3	0	0	0	0
61	C8	4	0	0	0	0
61	E8	1	0	0	0	0
61	F5	1	0	0	0	0
61	F8	3	0	0	1	0
61	G8	3	0	0	0	0
61	H5	1	0	0	2	0
61	I8	6	0	0	0	0
61	J8	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	L5	1	0	0	0	0
61	L8	4	0	0	0	0
61	M5	8	0	0	2	0
61	N8	1	0	0	0	0
61	Q8	5	0	0	1	0
All	All	296999	0	196564	8683	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 8683 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)
10:1A:38:ILE:C	10:1A:39:PRO:N	1.71	1.44
47:D5:94:GLU:C	47:D5:95:PRO:N	1.78	1.41
38:45:27:VAL:HB	38:45:28:ALA:HA	1.16	1.08
26:1H:1604:C:OP2	61:1H:3655:HOH:O	1.75	1.04
8:72:12:ARG:HH21	8:72:27:PRO:HD3	1.22	1.02

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	2.14	0.06
26:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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%)	173 (85%)	23 (11%)	7 (3%)	3 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1E	227/256 (89%)	186 (82%)	39 (17%)	2 (1%)	14	41
3	22	191/239 (80%)	172 (90%)	19 (10%)	0	100	100
3	2E	203/239 (85%)	186 (92%)	16 (8%)	1 (0%)	24	54
4	32	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	24	54
4	3E	205/209 (98%)	193 (94%)	11 (5%)	1 (0%)	24	54
5	42	148/162 (91%)	142 (96%)	5 (3%)	1 (1%)	18	47
5	4E	147/162 (91%)	136 (92%)	10 (7%)	1 (1%)	18	47
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	134/156 (86%)	125 (93%)	8 (6%)	1 (1%)	18	47
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	8	29
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	18	47
9	82	119/128 (93%)	109 (92%)	9 (8%)	1 (1%)	16	44
9	8E	124/128 (97%)	107 (86%)	17 (14%)	0	100	100
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	92/105 (88%)	83 (90%)	9 (10%)	0	100	100
11	2A	111/129 (86%)	99 (89%)	10 (9%)	2 (2%)	6	25
11	2I	109/129 (84%)	93 (85%)	11 (10%)	5 (5%)	2	10
12	3A	119/132 (90%)	101 (85%)	14 (12%)	4 (3%)	3	14
12	3I	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	16	44
13	4A	107/126 (85%)	89 (83%)	17 (16%)	1 (1%)	14	41
13	4I	115/126 (91%)	97 (84%)	17 (15%)	1 (1%)	14	41
14	5A	57/61 (93%)	49 (86%)	7 (12%)	1 (2%)	6	25
14	5I	57/61 (93%)	48 (84%)	7 (12%)	2 (4%)	3	14
15	6A	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
15	6I	85/89 (96%)	79 (93%)	6 (7%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	81/88 (92%)	76 (94%)	5 (6%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	93 (95%)	4 (4%)	1 (1%)	12	38

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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%)	63 (96%)	2 (3%)	1 (2%)	8	29
19	AA	59/93 (63%)	49 (83%)	7 (12%)	3 (5%)	1	9
19	AI	80/93 (86%)	69 (86%)	7 (9%)	4 (5%)	1	9
20	BA	97/106 (92%)	79 (81%)	16 (16%)	2 (2%)	5	22
20	BI	95/106 (90%)	83 (87%)	12 (13%)	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	7I	128/229 (56%)	121 (94%)	7 (6%)	0	100	100
29	11	271/276 (98%)	255 (94%)	10 (4%)	6 (2%)	5	21
29	19	272/276 (99%)	248 (91%)	21 (8%)	3 (1%)	11	36
30	21	201/206 (98%)	160 (80%)	28 (14%)	13 (6%)	1	5
30	29	202/206 (98%)	150 (74%)	40 (20%)	12 (6%)	1	7
31	31	200/210 (95%)	177 (88%)	22 (11%)	1 (0%)	24	54
31	39	202/210 (96%)	159 (79%)	36 (18%)	7 (4%)	3	14
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	7	27
32	49	178/182 (98%)	155 (87%)	22 (12%)	1 (1%)	21	50
33	51	172/180 (96%)	139 (81%)	23 (13%)	10 (6%)	1	7
33	59	167/180 (93%)	129 (77%)	32 (19%)	6 (4%)	2	13
34	61	143/148 (97%)	123 (86%)	18 (13%)	2 (1%)	9	31
34	69	143/148 (97%)	112 (78%)	28 (20%)	3 (2%)	5	22
35	15	135/140 (96%)	124 (92%)	11 (8%)	0	100	100
35	58	135/140 (96%)	114 (84%)	16 (12%)	5 (4%)	2	13
36	25	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
36	68	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
37	35	145/150 (97%)	120 (83%)	25 (17%)	0	100	100
37	78	145/150 (97%)	113 (78%)	21 (14%)	11 (8%)	1	4
38	45	136/141 (96%)	110 (81%)	23 (17%)	3 (2%)	5	21
38	88	139/141 (99%)	119 (86%)	14 (10%)	6 (4%)	2	10
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	41
39	98	116/118 (98%)	101 (87%)	15 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	65	108/112 (96%)	87 (81%)	19 (18%)	2 (2%)	6	24
40	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	14	41
41	75	131/146 (90%)	118 (90%)	11 (8%)	2 (2%)	8	29
41	B8	133/146 (91%)	118 (89%)	14 (10%)	1 (1%)	16	44
42	85	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
42	C8	113/118 (96%)	107 (95%)	2 (2%)	4 (4%)	3	14
43	95	98/101 (97%)	81 (83%)	14 (14%)	3 (3%)	3	16
43	D8	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	3	16
44	A5	109/113 (96%)	101 (93%)	8 (7%)	0	100	100
44	E8	108/113 (96%)	102 (94%)	6 (6%)	0	100	100
45	B5	92/96 (96%)	82 (89%)	8 (9%)	2 (2%)	5	21
45	F8	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
46	C5	102/110 (93%)	74 (72%)	22 (22%)	6 (6%)	1	7
46	G8	101/110 (92%)	83 (82%)	14 (14%)	4 (4%)	2	11
47	D5	175/206 (85%)	133 (76%)	32 (18%)	10 (6%)	1	7
47	H8	168/206 (82%)	136 (81%)	25 (15%)	7 (4%)	2	11
48	E5	74/85 (87%)	65 (88%)	8 (11%)	1 (1%)	9	31
48	I8	75/85 (88%)	67 (89%)	8 (11%)	0	100	100
49	F5	92/98 (94%)	81 (88%)	10 (11%)	1 (1%)	11	36
49	J8	94/98 (96%)	80 (85%)	9 (10%)	5 (5%)	1	8
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	3	16
50	K8	66/72 (92%)	59 (89%)	4 (6%)	3 (4%)	2	10
51	H5	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	M8	56/71 (79%)	39 (70%)	17 (30%)	0	100	100
53	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	4 (9%)	0	100	100
55	M5	62/65 (95%)	51 (82%)	11 (18%)	0	100	100
55	Q8	62/65 (95%)	51 (82%)	7 (11%)	4 (6%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11086/12104 (92%)	9718 (88%)	1167 (10%)	201 (2%)	6 25

5 of 201 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	2I	55	LYS
12	3I	48	PRO
18	9I	22	VAL
19	AI	41	VAL
29	11	239	ARG

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%)	139 (78%)	40 (22%)	1 4
2	1E	200/220 (91%)	154 (77%)	46 (23%)	1 4
3	22	154/188 (82%)	118 (77%)	36 (23%)	1 3
3	2E	159/188 (85%)	128 (80%)	31 (20%)	1 6
4	32	180/181 (99%)	144 (80%)	36 (20%)	1 5
4	3E	180/181 (99%)	146 (81%)	34 (19%)	1 7
5	42	114/123 (93%)	87 (76%)	27 (24%)	1 3
5	4E	115/123 (94%)	86 (75%)	29 (25%)	0 2
6	52	90/90 (100%)	77 (86%)	13 (14%)	3 13
6	5E	90/90 (100%)	72 (80%)	18 (20%)	1 5
7	62	114/127 (90%)	84 (74%)	30 (26%)	0 2
7	6E	125/127 (98%)	101 (81%)	24 (19%)	1 6
8	72	118/119 (99%)	95 (80%)	23 (20%)	1 6
8	7E	119/119 (100%)	86 (72%)	33 (28%)	0 1
9	82	92/99 (93%)	74 (80%)	18 (20%)	1 6
9	8E	97/99 (98%)	71 (73%)	26 (27%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1A	71/92 (77%)	46 (65%)	25 (35%)	0	0
10	1I	81/92 (88%)	72 (89%)	9 (11%)	6	21
11	2A	85/99 (86%)	73 (86%)	12 (14%)	3	13
11	2I	84/99 (85%)	63 (75%)	21 (25%)	0	2
12	3A	102/109 (94%)	78 (76%)	24 (24%)	1	3
12	3I	103/109 (94%)	78 (76%)	25 (24%)	1	3
13	4A	90/101 (89%)	69 (77%)	21 (23%)	1	3
13	4I	94/101 (93%)	68 (72%)	26 (28%)	0	1
14	5A	49/50 (98%)	41 (84%)	8 (16%)	2	10
14	5I	49/50 (98%)	40 (82%)	9 (18%)	1	7
15	6A	79/80 (99%)	66 (84%)	13 (16%)	2	9
15	6I	79/80 (99%)	66 (84%)	13 (16%)	2	9
16	7A	72/74 (97%)	60 (83%)	12 (17%)	2	9
16	7I	72/74 (97%)	57 (79%)	15 (21%)	1	5
17	8A	94/97 (97%)	78 (83%)	16 (17%)	2	9
17	8I	95/97 (98%)	76 (80%)	19 (20%)	1	5
18	9A	58/77 (75%)	47 (81%)	11 (19%)	1	7
18	9I	58/77 (75%)	49 (84%)	9 (16%)	2	11
19	AA	56/80 (70%)	42 (75%)	14 (25%)	0	2
19	AI	72/80 (90%)	56 (78%)	16 (22%)	1	4
20	BA	76/82 (93%)	67 (88%)	9 (12%)	5	19
20	BI	75/82 (92%)	65 (87%)	10 (13%)	4	15
21	1B	17/22 (77%)	16 (94%)	1 (6%)	18	44
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	4
28	7I	108/181 (60%)	88 (82%)	20 (18%)	1	7
29	11	214/218 (98%)	168 (78%)	46 (22%)	1	4
29	19	214/218 (98%)	160 (75%)	54 (25%)	0	2
30	21	162/166 (98%)	119 (74%)	43 (26%)	0	2
30	29	165/166 (99%)	123 (74%)	42 (26%)	0	2
31	31	161/166 (97%)	130 (81%)	31 (19%)	1	6
31	39	163/166 (98%)	113 (69%)	50 (31%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	41	153/156 (98%)	116 (76%)	37 (24%)	1	3
32	49	152/156 (97%)	112 (74%)	40 (26%)	0	2
33	51	143/148 (97%)	106 (74%)	37 (26%)	0	2
33	59	140/148 (95%)	99 (71%)	41 (29%)	0	1
34	61	122/124 (98%)	85 (70%)	37 (30%)	0	1
34	69	122/124 (98%)	84 (69%)	38 (31%)	0	0
35	15	116/119 (98%)	88 (76%)	28 (24%)	1	3
35	58	116/119 (98%)	88 (76%)	28 (24%)	1	3
36	25	100/100 (100%)	79 (79%)	21 (21%)	1	5
36	68	100/100 (100%)	84 (84%)	16 (16%)	2	10
37	35	114/116 (98%)	74 (65%)	40 (35%)	0	0
37	78	114/116 (98%)	76 (67%)	38 (33%)	0	0
38	45	109/111 (98%)	77 (71%)	32 (29%)	0	1
38	88	110/111 (99%)	88 (80%)	22 (20%)	1	5
39	55	101/101 (100%)	83 (82%)	18 (18%)	2	8
39	98	101/101 (100%)	77 (76%)	24 (24%)	1	3
40	65	87/88 (99%)	64 (74%)	23 (26%)	0	2
40	A8	87/88 (99%)	59 (68%)	28 (32%)	0	0
41	75	117/127 (92%)	83 (71%)	34 (29%)	0	1
41	B8	117/127 (92%)	83 (71%)	34 (29%)	0	1
42	85	93/94 (99%)	78 (84%)	15 (16%)	2	10
42	C8	92/94 (98%)	80 (87%)	12 (13%)	4	16
43	95	81/82 (99%)	63 (78%)	18 (22%)	1	4
43	D8	82/82 (100%)	54 (66%)	28 (34%)	0	0
44	A5	91/92 (99%)	69 (76%)	22 (24%)	1	3
44	E8	90/92 (98%)	69 (77%)	21 (23%)	1	3
45	B5	74/78 (95%)	56 (76%)	18 (24%)	1	3
45	F8	77/78 (99%)	56 (73%)	21 (27%)	0	1
46	C5	85/91 (93%)	57 (67%)	28 (33%)	0	0
46	G8	84/91 (92%)	61 (73%)	23 (27%)	0	1
47	D5	156/179 (87%)	116 (74%)	40 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	H8	151/179 (84%)	119 (79%)	32 (21%)	1	4
48	E5	61/67 (91%)	52 (85%)	9 (15%)	3	12
48	I8	62/67 (92%)	53 (86%)	9 (14%)	3	13
49	F5	79/83 (95%)	56 (71%)	23 (29%)	0	1
49	J8	79/83 (95%)	66 (84%)	13 (16%)	2	9
50	G5	63/67 (94%)	47 (75%)	16 (25%)	0	2
50	K8	64/67 (96%)	39 (61%)	25 (39%)	0	0
51	H5	50/52 (96%)	34 (68%)	16 (32%)	0	0
51	L8	50/52 (96%)	38 (76%)	12 (24%)	1	3
52	M8	52/63 (82%)	37 (71%)	15 (29%)	0	1
53	J5	48/52 (92%)	39 (81%)	9 (19%)	1	7
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1	5
54	L5	38/42 (90%)	31 (82%)	7 (18%)	1	7
54	P8	38/42 (90%)	30 (79%)	8 (21%)	1	5
55	M5	54/55 (98%)	41 (76%)	13 (24%)	1	3
55	Q8	54/55 (98%)	44 (82%)	10 (18%)	1	7
All	All	9354/10012 (93%)	7174 (77%)	2180 (23%)	1	3

5 of 2180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	45	60	ARG
40	65	89	ARG
38	45	55	VAL
47	D5	142	SER
39	98	10	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
54	P8	36	GLN
35	15	101	HIS
3	22	3	ASN
33	59	147	ASN
41	75	123	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1500/1522 (98%)	352 (23%)	39 (2%)
1	1G	1508/1522 (99%)	356 (23%)	40 (2%)
22	1K	70/76 (92%)	29 (41%)	5 (7%)
23	2K	76/77 (98%)	25 (32%)	2 (2%)
23	2L	76/77 (98%)	20 (26%)	1 (1%)
24	3K	67/76 (88%)	39 (58%)	2 (2%)
24	3L	69/76 (90%)	32 (46%)	2 (2%)
25	4K	19/30 (63%)	11 (57%)	2 (10%)
25	4L	18/30 (60%)	13 (72%)	1 (5%)
26	14	2820/2917 (96%)	668 (23%)	45 (1%)
26	1H	2824/2917 (96%)	604 (21%)	36 (1%)
27	16	121/122 (99%)	22 (18%)	3 (2%)
27	1J	121/122 (99%)	33 (27%)	2 (1%)
56	1L	63/76 (82%)	27 (42%)	4 (6%)
All	All	9352/9640 (97%)	2231 (23%)	184 (1%)

5 of 2231 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	3	G
1	13	4	U
1	13	5	U
1	13	6	G

5 of 184 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	991	U
26	14	278	A
1	1G	1157	A
56	1L	9	A
26	14	888	C

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

18 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	4SU	2K	8	23	18,21,22	1.64	3 (16%)	25,30,33	2.72	5 (20%)
22	PSU	1K	55	22	18,21,22	1.22	1 (5%)	21,30,33	1.84	4 (19%)
23	OMC	2K	33	23	19,22,23	1.70	3 (15%)	25,31,34	0.89	1 (4%)
22	5MU	1K	54	22	19,22,23	4.04	5 (26%)	27,32,35	3.02	9 (33%)
23	4SU	2L	8	23	18,21,22	2.00	3 (16%)	25,30,33	2.52	5 (20%)
56	PSU	1L	55	56	18,21,22	1.33	1 (5%)	21,30,33	1.75	4 (19%)
22	U8U	1K	34	25,22	20,24,25	2.35	6 (30%)	22,34,37	1.17	3 (13%)
23	5MU	2K	55	23	19,22,23	3.85	5 (26%)	27,32,35	3.28	11 (40%)
22	T6A	1K	37	22	31,34,35	2.07	8 (25%)	43,49,52	2.27	13 (30%)
23	OMC	2L	33	23	19,22,23	1.77	3 (15%)	25,31,34	0.84	0
22	H2U	1K	17	22	18,21,22	2.13	4 (22%)	19,30,33	1.74	4 (21%)
22	PSU	1K	39	22	18,21,22	1.25	2 (11%)	21,30,33	1.69	3 (14%)
23	7MG	2L	47	23	23,26,27	2.88	8 (34%)	27,39,42	3.07	9 (33%)
23	PSU	2K	56	23	18,21,22	1.23	2 (11%)	21,30,33	2.08	5 (23%)
23	PSU	2L	56	23	18,21,22	1.40	2 (11%)	21,30,33	1.86	5 (23%)
56	5MU	1L	54	56	19,22,23	4.04	5 (26%)	27,32,35	3.21	9 (33%)
23	5MU	2L	55	23	19,22,23	4.02	5 (26%)	27,32,35	3.20	9 (33%)
23	7MG	2K	47	23	23,26,27	3.30	7 (30%)	27,39,42	3.20	11 (40%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	T6A	1K	37	22	-	5/23/41/42	0/3/3/3
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
22	H2U	1K	17	22	-	0/7/38/39	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	7MG	2L	47	23	-	3/7/37/38	0/3/3/3
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	3/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	3/7/37/38	0/3/3/3

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	54	5MU	C2-N1	13.37	1.59	1.38
56	1L	54	5MU	C2-N1	13.33	1.59	1.38
23	2L	55	5MU	C2-N1	13.07	1.58	1.38
23	2K	55	5MU	C2-N1	12.37	1.57	1.38
23	2K	47	7MG	C5-N7	7.84	1.45	1.35

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1L	54	5MU	C5-C4-N3	10.23	124.21	115.32
23	2K	55	5MU	C5-C4-N3	10.06	124.06	115.32
23	2L	55	5MU	C5-C4-N3	9.90	123.93	115.32
22	1K	54	5MU	C5-C4-N3	9.67	123.72	115.32
23	2L	47	7MG	C4-C5-N7	8.75	115.72	105.38

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	34	U8U	C5-C-N-CA
22	1K	37	T6A	C14-C12-N11-C10
22	1K	37	T6A	N11-C12-C14-O14
22	1K	37	T6A	N11-C12-C14-C15
22	1K	37	T6A	C13-C12-C14-O14

There are no ring outliers.

9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	8	4SU	1	0
23	2K	33	OMC	1	0
22	1K	54	5MU	3	0
23	2K	55	5MU	4	0
22	1K	37	T6A	1	0
23	2L	33	OMC	3	0
23	2L	47	7MG	3	0
56	1L	54	5MU	2	0
23	2K	47	7MG	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1345 ligands modelled in this entry, 1341 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	SPE	14	3458	-	12,12,12	0.44	0	11,11,11	0.76	0
58	SF4	3E	301	4	0,12,12	-	-	-		
60	SPE	1G	1725	1	12,12,12	0.41	0	11,11,11	0.72	0
58	SF4	32	302	-	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
60	SPE	14	3458	-	-	5/10/10/10	-
58	SF4	3E	301	4	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SPE	1G	1725	1	-	5/10/10/10	-
58	SF4	32	302	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	1G	1725	SPE	C2-C3-C4-N5
60	14	3458	SPE	N9-C10-C11-C12
60	14	3458	SPE	C2-C3-C4-N5
60	14	3458	SPE	C6-C7-C8-N9
60	1G	1725	SPE	C11-C10-N9-C8

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1G	1725	SPE	3	0
58	32	302	SF4	2	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
56	1L	1
47	D5	1
10	1A	1
34	69	1
4	3E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1L	72:C	O3'	73:A	P	3.48
1	D5	94:GLU	C	95:PRO	N	1.78
1	1A	38:ILE	C	39:PRO	N	1.71
1	69	79:ILE	C	80:PRO	N	1.17
1	3E	36:ARG	C	37:PRO	N	1.15

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	1500/1522 (98%)	-0.13	43 (2%)	53	32	67, 111, 176, 243	0
1	1G	1509/1522 (99%)	-0.02	49 (3%)	50	29	76, 123, 193, 253	0
2	12	207/256 (80%)	0.42	8 (3%)	43	23	139, 165, 185, 196	0
2	1E	231/256 (90%)	0.34	6 (2%)	57	35	118, 145, 172, 180	0
3	22	195/239 (81%)	0.26	6 (3%)	51	30	123, 147, 164, 175	0
3	2E	205/239 (85%)	0.21	4 (1%)	65	43	97, 117, 144, 155	0
4	32	208/209 (99%)	0.37	6 (2%)	53	32	104, 123, 142, 149	0
4	3E	207/209 (99%)	0.50	8 (3%)	43	23	93, 118, 137, 144	0
5	42	150/162 (92%)	0.26	3 (2%)	65	43	106, 123, 139, 146	0
5	4E	149/162 (91%)	0.40	3 (2%)	65	43	87, 109, 128, 133	0
6	52	101/101 (100%)	0.17	1 (0%)	79	61	93, 110, 124, 135	0
6	5E	100/101 (99%)	0.20	2 (2%)	65	43	92, 111, 127, 135	0
7	62	138/156 (88%)	0.18	4 (2%)	53	32	122, 135, 145, 151	0
7	6E	154/156 (98%)	0.05	2 (1%)	75	55	111, 127, 155, 174	0
8	72	137/138 (99%)	0.35	4 (2%)	53	32	106, 129, 141, 149	0
8	7E	138/138 (100%)	0.16	1 (0%)	84	68	102, 117, 129, 139	0
9	82	121/128 (94%)	0.39	3 (2%)	58	36	118, 161, 171, 178	0
9	8E	126/128 (98%)	0.20	5 (3%)	42	22	96, 141, 159, 165	0
10	1A	80/105 (76%)	1.14	21 (26%)	1	1	122, 152, 167, 170	0
10	1I	94/105 (89%)	0.25	0	100	100	92, 136, 171, 178	0
11	2A	113/129 (87%)	0.41	4 (3%)	47	26	91, 116, 131, 138	0
11	2I	111/129 (86%)	0.24	2 (1%)	67	46	84, 113, 129, 138	0
12	3A	121/132 (91%)	0.74	17 (14%)	6	3	94, 109, 128, 144	0
12	3I	122/132 (92%)	0.35	11 (9%)	15	7	81, 89, 110, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	109/126 (86%)	0.32	7 (6%) 25 13	125, 152, 170, 187	0
13	4I	117/126 (92%)	0.18	7 (5%) 27 14	97, 125, 138, 145	0
14	5A	59/61 (96%)	0.95	10 (16%) 4 2	131, 146, 164, 167	0
14	5I	59/61 (96%)	-0.07	0 100 100	92, 106, 121, 129	0
15	6A	87/89 (97%)	-0.07	1 (1%) 78 59	93, 117, 133, 137	0
15	6I	87/89 (97%)	-0.11	0 100 100	89, 107, 126, 130	0
16	7A	84/88 (95%)	0.41	4 (4%) 35 18	100, 116, 137, 159	0
16	7I	83/88 (94%)	0.59	5 (6%) 27 14	107, 119, 145, 163	0
17	8A	99/105 (94%)	-0.06	0 100 100	100, 112, 125, 131	0
17	8I	100/105 (95%)	0.11	3 (3%) 52 31	95, 114, 124, 128	0
18	9A	67/88 (76%)	0.49	6 (8%) 15 7	101, 117, 135, 140	0
18	9I	68/88 (77%)	0.08	1 (1%) 72 51	97, 113, 133, 138	0
19	AA	65/93 (69%)	0.75	6 (9%) 14 7	130, 162, 174, 180	0
19	AI	82/93 (88%)	0.09	2 (2%) 59 38	108, 126, 146, 153	0
20	BA	99/106 (93%)	0.09	2 (2%) 65 43	94, 119, 140, 153	0
20	BI	97/106 (91%)	0.22	3 (3%) 51 30	113, 127, 150, 157	0
21	1B	22/27 (81%)	0.27	1 (4%) 38 20	122, 139, 143, 150	0
21	1F	23/27 (85%)	-0.40	0 100 100	103, 110, 116, 123	0
22	1K	66/76 (86%)	1.20	12 (18%) 3 1	104, 183, 206, 212	0
23	2K	72/77 (93%)	-0.07	1 (1%) 73 53	75, 100, 133, 145	0
23	2L	72/77 (93%)	0.25	3 (4%) 40 21	85, 120, 153, 162	0
24	3K	70/76 (92%)	0.81	5 (7%) 22 11	82, 225, 245, 249	0
24	3L	72/76 (94%)	1.41	16 (22%) 2 1	87, 206, 223, 228	0
25	4K	20/30 (66%)	0.57	1 (5%) 34 17	81, 145, 215, 216	0
25	4L	19/30 (63%)	1.22	5 (26%) 1 1	101, 162, 218, 218	0
26	14	2825/2917 (96%)	-0.20	89 (3%) 50 29	62, 91, 198, 251	0
26	1H	2831/2917 (97%)	-0.41	44 (1%) 70 49	51, 79, 176, 251	0
27	16	122/122 (100%)	-0.60	3 (2%) 58 36	76, 98, 118, 204	0
27	1J	122/122 (100%)	-0.19	1 (0%) 82 65	94, 133, 152, 210	0
28	7I	132/229 (57%)	0.33	4 (3%) 52 31	143, 206, 228, 235	0
29	11	273/276 (98%)	0.08	8 (2%) 53 32	48, 71, 88, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	19	274/276 (99%)	0.16	12 (4%) 39 20	56, 80, 94, 111	0
30	21	203/206 (98%)	0.35	9 (4%) 39 20	57, 90, 121, 133	0
30	29	204/206 (99%)	0.32	18 (8%) 15 8	66, 97, 133, 147	0
31	31	202/210 (96%)	-0.22	3 (1%) 72 51	51, 82, 114, 134	0
31	39	204/210 (97%)	0.27	18 (8%) 15 8	64, 105, 148, 175	0
32	41	179/182 (98%)	0.02	7 (3%) 43 23	90, 109, 139, 154	0
32	49	180/182 (98%)	0.28	6 (3%) 49 28	125, 147, 166, 179	0
33	51	174/180 (96%)	0.27	8 (4%) 37 19	82, 105, 123, 133	0
33	59	169/180 (93%)	1.20	35 (20%) 2 1	157, 203, 223, 233	0
34	61	145/148 (97%)	0.21	3 (2%) 63 42	82, 128, 147, 153	0
34	69	145/148 (97%)	0.20	8 (5%) 30 16	91, 129, 149, 154	0
35	15	137/140 (97%)	0.86	16 (11%) 9 4	82, 110, 140, 150	0
35	58	137/140 (97%)	0.13	2 (1%) 72 51	71, 90, 122, 138	0
36	25	122/122 (100%)	-0.18	0 100 100	74, 90, 108, 120	0
36	68	122/122 (100%)	0.17	4 (3%) 49 28	67, 82, 98, 106	0
37	35	147/150 (98%)	0.48	12 (8%) 17 9	64, 106, 141, 158	0
37	78	147/150 (98%)	-0.15	1 (0%) 84 68	58, 84, 106, 114	0
38	45	138/141 (97%)	0.31	4 (2%) 53 32	79, 106, 127, 138	0
38	88	141/141 (100%)	-0.16	0 100 100	62, 83, 104, 133	0
39	55	118/118 (100%)	-0.22	2 (1%) 69 48	68, 85, 100, 113	0
39	98	118/118 (100%)	-0.11	0 100 100	67, 86, 103, 117	0
40	65	110/112 (98%)	0.24	1 (0%) 81 63	99, 124, 141, 145	0
40	A8	111/112 (99%)	-0.15	1 (0%) 81 63	82, 95, 114, 127	0
41	75	133/146 (91%)	-0.07	3 (2%) 61 39	82, 97, 127, 145	0
41	B8	135/146 (92%)	0.48	11 (8%) 18 9	79, 96, 135, 151	0
42	85	116/118 (98%)	0.50	7 (6%) 27 14	72, 101, 129, 136	0
42	C8	115/118 (97%)	0.11	2 (1%) 69 48	60, 82, 108, 115	0
43	95	100/101 (99%)	0.51	3 (3%) 52 31	72, 120, 140, 147	0
43	D8	100/101 (99%)	0.16	4 (4%) 42 22	62, 100, 120, 130	0
44	A5	111/113 (98%)	0.17	3 (2%) 56 34	71, 81, 107, 139	0
44	E8	110/113 (97%)	0.07	5 (4%) 38 20	64, 77, 100, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
45	B5	94/96 (97%)	-0.10	3 (3%)	50	29	78, 90, 111, 121	0
45	F8	95/96 (98%)	-0.11	1 (1%)	78	59	59, 74, 98, 108	0
46	C5	104/110 (94%)	1.10	18 (17%)	4	2	92, 119, 152, 158	0
46	G8	103/110 (93%)	0.61	7 (6%)	23	12	76, 97, 124, 134	0
47	D5	177/206 (85%)	0.09	0	100	100	117, 159, 218, 223	0
47	H8	170/206 (82%)	-0.28	0	100	100	88, 121, 189, 196	0
48	E5	76/85 (89%)	0.15	2 (2%)	57	35	78, 97, 111, 120	0
48	I8	77/85 (90%)	-0.30	1 (1%)	75	55	64, 79, 96, 108	0
49	F5	94/98 (95%)	0.29	3 (3%)	50	29	69, 89, 125, 139	0
49	J8	96/98 (97%)	0.48	6 (6%)	26	13	61, 80, 117, 123	0
50	G5	69/72 (95%)	0.08	3 (4%)	40	21	90, 109, 132, 144	0
50	K8	68/72 (94%)	0.10	1 (1%)	72	51	68, 84, 105, 129	0
51	H5	58/60 (96%)	0.03	0	100	100	81, 101, 126, 136	0
51	L8	58/60 (96%)	-0.36	0	100	100	70, 84, 110, 122	0
52	M8	60/71 (84%)	0.32	1 (1%)	69	48	114, 150, 177, 181	0
53	J5	56/60 (93%)	0.27	2 (3%)	46	26	67, 90, 133, 143	0
53	N8	48/60 (80%)	-0.16	0	100	100	56, 85, 128, 135	0
54	L5	47/49 (95%)	-0.40	1 (2%)	63	42	61, 69, 91, 100	0
54	P8	47/49 (95%)	-0.46	0	100	100	54, 59, 77, 89	0
55	M5	64/65 (98%)	0.49	5 (7%)	19	9	76, 86, 101, 117	0
55	Q8	64/65 (98%)	-0.01	1 (1%)	70	49	61, 75, 88, 101	0
56	1L	64/76 (84%)	1.25	16 (25%)	2	1	140, 201, 221, 227	0
All	All	20656/21744 (94%)	0.04	742 (3%)	46	26	48, 105, 181, 253	0

The worst 5 of 742 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	1K	76	A	11.0
20	BA	9	ASN	9.1
43	D8	37	VAL	8.3
41	B8	104	ASN	8.1
26	14	229	A	7.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	H2U	1K	17	20/21	0.68	0.10	130,139,153,158	0
56	PSU	1L	55	20/21	0.72	0.10	121,135,144,145	0
22	PSU	1K	55	20/21	0.77	0.10	115,126,136,137	0
56	5MU	1L	54	21/22	0.82	0.09	125,136,146,154	0
22	5MU	1K	54	21/22	0.82	0.10	116,121,138,149	0
23	7MG	2K	47	24/25	0.84	0.12	99,108,119,120	0
23	PSU	2L	56	20/21	0.84	0.09	112,122,130,133	0
23	5MU	2L	55	21/22	0.86	0.09	115,126,133,135	0
23	PSU	2K	56	20/21	0.87	0.07	102,108,119,120	0
23	7MG	2L	47	24/25	0.88	0.11	124,131,143,146	0
23	4SU	2L	8	20/21	0.89	0.14	108,116,123,125	0
23	5MU	2K	55	21/22	0.91	0.07	105,112,118,128	0
23	4SU	2K	8	20/21	0.91	0.12	91,99,105,106	0
22	PSU	1K	39	20/21	0.92	0.14	100,119,123,124	0
22	T6A	1K	37	32/33	0.94	0.18	91,108,133,134	0
23	OMC	2K	33	21/22	0.94	0.15	85,89,90,91	0
22	U8U	1K	34	23/24	0.95	0.10	98,105,115,118	0
23	OMC	2L	33	21/22	0.95	0.10	100,107,110,117	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(Å ²)	Q<0.9
57	MG	1G	1638	1/1	0.32	0.30	119,119,119,119	0
57	MG	14	3019	1/1	0.35	0.28	131,131,131,131	0
57	MG	1G	1648	1/1	0.36	0.35	121,121,121,121	0
57	MG	1G	1621	1/1	0.36	0.43	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1629	1/1	0.41	0.26	129,129,129,129	0
57	MG	14	3163	1/1	0.49	0.34	104,104,104,104	0
57	MG	13	1669	1/1	0.51	0.31	111,111,111,111	0
57	MG	1J	205	1/1	0.51	0.16	101,101,101,101	0
57	MG	1H	3147	1/1	0.52	0.31	125,125,125,125	0
57	MG	13	1665	1/1	0.52	0.23	128,128,128,128	0
57	MG	16	202	1/1	0.53	0.28	103,103,103,103	0
57	MG	1H	3197	1/1	0.53	0.39	93,93,93,93	0
57	MG	1G	1623	1/1	0.53	0.24	109,109,109,109	0
57	MG	1H	3238	1/1	0.54	0.34	102,102,102,102	0
57	MG	14	3135	1/1	0.55	0.25	112,112,112,112	0
57	MG	13	1647	1/1	0.55	0.35	99,99,99,99	0
57	MG	1H	3117	1/1	0.55	0.35	96,96,96,96	0
57	MG	13	1648	1/1	0.56	0.30	117,117,117,117	0
57	MG	1H	3130	1/1	0.56	0.42	97,97,97,97	0
57	MG	14	3094	1/1	0.56	0.39	100,100,100,100	0
57	MG	13	1659	1/1	0.57	0.42	109,109,109,109	0
57	MG	14	3020	1/1	0.58	0.16	69,69,69,69	0
57	MG	13	1668	1/1	0.59	0.40	112,112,112,112	0
57	MG	1G	1602	1/1	0.59	0.33	105,105,105,105	0
57	MG	1G	1628	1/1	0.59	0.30	123,123,123,123	0
57	MG	14	3187	1/1	0.59	0.33	106,106,106,106	0
57	MG	1G	1605	1/1	0.59	0.30	109,109,109,109	0
57	MG	13	1656	1/1	0.60	0.28	107,107,107,107	0
57	MG	1H	3156	1/1	0.60	0.33	106,106,106,106	0
57	MG	14	3142	1/1	0.61	0.34	98,98,98,98	0
57	MG	1J	202	1/1	0.61	0.36	106,106,106,106	0
57	MG	13	1662	1/1	0.61	0.29	90,90,90,90	0
57	MG	14	3161	1/1	0.62	0.17	94,94,94,94	0
57	MG	1H	3235	1/1	0.62	0.17	96,96,96,96	0
57	MG	1G	1642	1/1	0.62	0.45	100,100,100,100	0
57	MG	13	1651	1/1	0.62	0.23	118,118,118,118	0
57	MG	1H	3222	1/1	0.62	0.34	86,86,86,86	0
57	MG	13	1645	1/1	0.63	0.38	117,117,117,117	0
57	MG	14	3102	1/1	0.63	0.26	94,94,94,94	0
57	MG	13	1627	1/1	0.63	0.30	94,94,94,94	0
57	MG	14	3175	1/1	0.64	0.37	100,100,100,100	0
57	MG	14	3103	1/1	0.66	0.46	80,80,80,80	0
57	MG	E5	101	1/1	0.66	0.42	99,99,99,99	0
57	MG	13	1638	1/1	0.67	0.29	103,103,103,103	0
57	MG	14	3064	1/1	0.67	0.26	99,99,99,99	0
57	MG	14	3157	1/1	0.68	0.33	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3125	1/1	0.68	0.28	79,79,79,79	0
57	MG	1H	3210	1/1	0.68	0.34	87,87,87,87	0
57	MG	13	1602	1/1	0.68	0.23	130,130,130,130	0
57	MG	1H	3176	1/1	0.68	0.34	102,102,102,102	0
57	MG	1H	3182	1/1	0.68	0.22	108,108,108,108	0
57	MG	1H	3530	1/1	0.68	0.26	99,99,99,99	0
57	MG	14	3147	1/1	0.68	0.41	86,86,86,86	0
57	MG	14	3107	1/1	0.69	0.34	94,94,94,94	0
57	MG	1H	3140	1/1	0.69	0.20	90,90,90,90	0
57	MG	14	3078	1/1	0.70	0.23	88,88,88,88	0
57	MG	14	3443	1/1	0.70	0.21	115,115,115,115	0
57	MG	1H	3493	1/1	0.70	0.20	106,106,106,106	0
57	MG	1H	3159	1/1	0.70	0.45	95,95,95,95	0
57	MG	1H	3074	1/1	0.70	0.26	75,75,75,75	0
57	MG	1H	3177	1/1	0.71	0.17	143,143,143,143	0
57	MG	1H	3131	1/1	0.71	0.32	101,101,101,101	0
57	MG	1G	1624	1/1	0.71	0.26	103,103,103,103	0
57	MG	1G	1712	1/1	0.71	0.14	110,110,110,110	0
57	MG	13	1629	1/1	0.71	0.27	100,100,100,100	0
57	MG	1H	3056	1/1	0.71	0.40	86,86,86,86	0
57	MG	1J	204	1/1	0.72	0.18	102,102,102,102	0
57	MG	1G	1650	1/1	0.72	0.22	111,111,111,111	0
57	MG	1G	1620	1/1	0.72	0.33	93,93,93,93	0
57	MG	13	1661	1/1	0.73	0.25	101,101,101,101	0
57	MG	14	3153	1/1	0.73	0.23	123,123,123,123	0
57	MG	13	1601	1/1	0.73	0.28	97,97,97,97	0
57	MG	14	3133	1/1	0.73	0.47	89,89,89,89	0
57	MG	1H	3124	1/1	0.73	0.24	90,90,90,90	0
57	MG	13	1641	1/1	0.73	0.34	79,79,79,79	0
57	MG	13	1612	1/1	0.74	0.21	111,111,111,111	0
57	MG	13	1666	1/1	0.74	0.31	98,98,98,98	0
57	MG	1H	3060	1/1	0.74	0.33	90,90,90,90	0
57	MG	13	1643	1/1	0.74	0.19	95,95,95,95	0
57	MG	1H	3532	1/1	0.74	0.27	79,79,79,79	0
57	MG	14	3176	1/1	0.74	0.28	90,90,90,90	0
57	MG	14	3109	1/1	0.74	0.35	94,94,94,94	0
57	MG	14	3017	1/1	0.74	0.26	74,74,74,74	0
57	MG	1H	3545	1/1	0.74	0.32	102,102,102,102	0
57	MG	14	3140	1/1	0.74	0.26	89,89,89,89	0
57	MG	1H	3550	1/1	0.74	0.27	111,111,111,111	0
57	MG	39	301	1/1	0.74	0.12	80,80,80,80	0
57	MG	1H	3077	1/1	0.74	0.31	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1647	1/1	0.75	0.27	99,99,99,99	0
57	MG	P8	101	1/1	0.75	0.26	76,76,76,76	0
57	MG	14	3180	1/1	0.75	0.31	86,86,86,86	0
57	MG	1H	3184	1/1	0.75	0.31	100,100,100,100	0
57	MG	1H	3143	1/1	0.75	0.22	79,79,79,79	0
57	MG	42	201	1/1	0.75	0.29	107,107,107,107	0
57	MG	1G	1612	1/1	0.75	0.18	103,103,103,103	0
57	MG	13	1673	1/1	0.75	0.19	110,110,110,110	0
57	MG	1H	3167	1/1	0.75	0.43	86,86,86,86	0
57	MG	14	3165	1/1	0.75	0.32	97,97,97,97	0
57	MG	14	3134	1/1	0.76	0.45	99,99,99,99	0
57	MG	1H	3120	1/1	0.76	0.32	69,69,69,69	0
57	MG	1G	1652	1/1	0.76	0.26	105,105,105,105	0
57	MG	1H	3085	1/1	0.76	0.27	79,79,79,79	0
57	MG	1H	3089	1/1	0.76	0.36	88,88,88,88	0
57	MG	14	3149	1/1	0.76	0.31	94,94,94,94	0
57	MG	35	201	1/1	0.76	0.24	81,81,81,81	0
57	MG	1H	3050	1/1	0.76	0.27	85,85,85,85	0
57	MG	14	3050	1/1	0.77	0.27	87,87,87,87	0
57	MG	13	1667	1/1	0.77	0.23	104,104,104,104	0
57	MG	1H	3497	1/1	0.77	0.24	96,96,96,96	0
57	MG	14	3088	1/1	0.77	0.32	82,82,82,82	0
57	MG	16	206	1/1	0.77	0.13	83,83,83,83	0
57	MG	1H	3227	1/1	0.77	0.21	90,90,90,90	0
57	MG	1H	3122	1/1	0.77	0.25	80,80,80,80	0
57	MG	13	1642	1/1	0.77	0.20	95,95,95,95	0
57	MG	14	3110	1/1	0.78	0.26	85,85,85,85	0
57	MG	1H	3014	1/1	0.78	0.28	86,86,86,86	0
57	MG	14	3030	1/1	0.78	0.20	90,90,90,90	0
57	MG	13	1634	1/1	0.78	0.28	91,91,91,91	0
57	MG	1G	1649	1/1	0.78	0.39	96,96,96,96	0
57	MG	14	3194	1/1	0.78	0.39	84,84,84,84	0
57	MG	1H	3172	1/1	0.78	0.14	64,64,64,64	0
57	MG	1H	3090	1/1	0.78	0.19	82,82,82,82	0
57	MG	13	1637	1/1	0.78	0.18	90,90,90,90	0
57	MG	1G	1637	1/1	0.78	0.30	106,106,106,106	0
57	MG	42	202	1/1	0.78	0.24	115,115,115,115	0
57	MG	1H	3233	1/1	0.78	0.29	94,94,94,94	0
57	MG	1H	3119	1/1	0.78	0.27	79,79,79,79	0
57	MG	1H	3200	1/1	0.79	0.20	82,82,82,82	0
57	MG	14	3179	1/1	0.79	0.12	103,103,103,103	0
57	MG	1H	3010	1/1	0.79	0.34	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3144	1/1	0.79	0.17	84,84,84,84	0
57	MG	14	3190	1/1	0.79	0.26	89,89,89,89	0
57	MG	1H	3211	1/1	0.79	0.27	69,69,69,69	0
57	MG	13	1692	1/1	0.79	0.13	110,110,110,110	0
57	MG	1H	3135	1/1	0.79	0.14	73,73,73,73	0
57	MG	1H	3139	1/1	0.79	0.33	90,90,90,90	0
57	MG	1H	3166	1/1	0.79	0.18	67,67,67,67	0
57	MG	1H	3096	1/1	0.79	0.34	83,83,83,83	0
57	MG	1H	3404	1/1	0.79	0.32	71,71,71,71	0
57	MG	14	3087	1/1	0.79	0.18	75,75,75,75	0
57	MG	1H	3196	1/1	0.80	0.28	103,103,103,103	0
57	MG	1H	3152	1/1	0.80	0.28	87,87,87,87	0
57	MG	1H	3178	1/1	0.80	0.27	80,80,80,80	0
57	MG	1H	3160	1/1	0.80	0.30	79,79,79,79	0
57	MG	1H	3364	1/1	0.80	0.14	85,85,85,85	0
57	MG	1H	3552	1/1	0.80	0.10	113,113,113,113	0
57	MG	1H	3057	1/1	0.80	0.29	71,71,71,71	0
57	MG	14	3046	1/1	0.80	0.12	77,77,77,77	0
57	MG	14	3455	1/1	0.80	0.17	115,115,115,115	0
57	MG	1H	3188	1/1	0.80	0.24	88,88,88,88	0
57	MG	14	3158	1/1	0.80	0.19	84,84,84,84	0
57	MG	14	3114	1/1	0.80	0.13	77,77,77,77	0
57	MG	14	3125	1/1	0.80	0.20	92,92,92,92	0
57	MG	21	301	1/1	0.80	0.26	77,77,77,77	0
57	MG	14	3170	1/1	0.80	0.14	76,76,76,76	0
57	MG	16	207	1/1	0.81	0.16	91,91,91,91	0
57	MG	14	3177	1/1	0.81	0.27	81,81,81,81	0
57	MG	13	1614	1/1	0.81	0.30	102,102,102,102	0
57	MG	1G	1645	1/1	0.81	0.12	124,124,124,124	0
57	MG	14	3183	1/1	0.81	0.24	88,88,88,88	0
57	MG	14	3058	1/1	0.81	0.25	83,83,83,83	0
57	MG	14	3151	1/1	0.81	0.24	108,108,108,108	0
57	MG	14	3193	1/1	0.81	0.33	96,96,96,96	0
57	MG	1G	1614	1/1	0.81	0.32	91,91,91,91	0
57	MG	2L	102	1/1	0.81	0.13	126,126,126,126	0
57	MG	14	3079	1/1	0.81	0.17	86,86,86,86	0
57	MG	1J	201	1/1	0.81	0.25	97,97,97,97	0
57	MG	1H	3391	1/1	0.81	0.26	90,90,90,90	0
57	MG	1G	1631	1/1	0.81	0.15	103,103,103,103	0
57	MG	1H	3078	1/1	0.81	0.29	85,85,85,85	0
57	MG	14	3166	1/1	0.81	0.23	95,95,95,95	0
57	MG	14	3138	1/1	0.81	0.27	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3095	1/1	0.81	0.39	72,72,72,72	0
57	MG	14	3108	1/1	0.82	0.26	103,103,103,103	0
57	MG	1H	3133	1/1	0.82	0.12	72,72,72,72	0
57	MG	1H	3540	1/1	0.82	0.29	110,110,110,110	0
57	MG	14	3152	1/1	0.82	0.23	99,99,99,99	0
57	MG	1H	3062	1/1	0.82	0.17	64,64,64,64	0
57	MG	1H	3411	1/1	0.82	0.12	95,95,95,95	0
57	MG	14	3130	1/1	0.82	0.24	92,92,92,92	0
57	MG	1G	1625	1/1	0.82	0.34	89,89,89,89	0
57	MG	14	3333	1/1	0.82	0.13	97,97,97,97	0
57	MG	1G	1626	1/1	0.82	0.13	119,119,119,119	0
57	MG	1H	3175	1/1	0.82	0.18	73,73,73,73	0
57	MG	14	3099	1/1	0.82	0.26	101,101,101,101	0
57	MG	14	3167	1/1	0.82	0.12	95,95,95,95	0
57	MG	14	3169	1/1	0.82	0.14	88,88,88,88	0
57	MG	1H	3138	1/1	0.82	0.25	98,98,98,98	0
57	MG	14	3173	1/1	0.82	0.16	90,90,90,90	0
57	MG	1H	3026	1/1	0.82	0.17	82,82,82,82	0
57	MG	1G	1636	1/1	0.82	0.23	87,87,87,87	0
57	MG	1H	3213	1/1	0.83	0.28	83,83,83,83	0
57	MG	1H	3015	1/1	0.83	0.24	77,77,77,77	0
57	MG	14	3141	1/1	0.83	0.20	85,85,85,85	0
57	MG	1H	3086	1/1	0.83	0.17	67,67,67,67	0
57	MG	1H	3229	1/1	0.83	0.16	84,84,84,84	0
57	MG	1H	3087	1/1	0.83	0.27	75,75,75,75	0
57	MG	1H	3151	1/1	0.83	0.24	79,79,79,79	0
57	MG	13	1655	1/1	0.83	0.36	83,83,83,83	0
57	MG	1H	3035	1/1	0.83	0.21	83,83,83,83	0
57	MG	1H	3094	1/1	0.83	0.30	64,64,64,64	0
57	MG	88	201	1/1	0.83	0.21	83,83,83,83	0
57	MG	1H	3013	1/1	0.83	0.25	94,94,94,94	0
57	MG	1H	3113	1/1	0.83	0.20	70,70,70,70	0
57	MG	14	3456	1/1	0.83	0.09	118,118,118,118	0
57	MG	14	3121	1/1	0.83	0.35	92,92,92,92	0
57	MG	1H	3051	1/1	0.83	0.22	74,74,74,74	0
57	MG	1H	3169	1/1	0.83	0.30	91,91,91,91	0
57	MG	14	3132	1/1	0.83	0.19	90,90,90,90	0
57	MG	1H	3509	1/1	0.83	0.20	114,114,114,114	0
57	MG	13	1670	1/1	0.83	0.39	85,85,85,85	0
57	MG	14	3080	1/1	0.83	0.13	71,71,71,71	0
57	MG	14	3155	1/1	0.84	0.15	83,83,83,83	0
57	MG	14	3093	1/1	0.84	0.23	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3055	1/1	0.84	0.17	62,62,62,62	0
57	MG	1H	3012	1/1	0.84	0.12	81,81,81,81	0
57	MG	13	1628	1/1	0.84	0.47	90,90,90,90	0
57	MG	13	1623	1/1	0.84	0.21	70,70,70,70	0
57	MG	1H	3109	1/1	0.84	0.36	79,79,79,79	0
57	MG	13	1675	1/1	0.84	0.11	91,91,91,91	0
57	MG	1H	3114	1/1	0.84	0.12	71,71,71,71	0
57	MG	1H	3187	1/1	0.84	0.38	83,83,83,83	0
57	MG	14	3171	1/1	0.84	0.27	86,86,86,86	0
57	MG	14	3172	1/1	0.84	0.29	82,82,82,82	0
57	MG	14	3004	1/1	0.84	0.27	81,81,81,81	0
57	MG	14	3014	1/1	0.84	0.21	72,72,72,72	0
57	MG	14	3120	1/1	0.84	0.14	84,84,84,84	0
57	MG	1H	3063	1/1	0.84	0.25	59,59,59,59	0
57	MG	1H	3069	1/1	0.84	0.24	76,76,76,76	0
57	MG	14	3126	1/1	0.84	0.27	89,89,89,89	0
57	MG	13	1631	1/1	0.84	0.27	106,106,106,106	0
57	MG	14	3027	1/1	0.84	0.18	85,85,85,85	0
57	MG	1H	3008	1/1	0.84	0.23	81,81,81,81	0
57	MG	1H	3036	1/1	0.84	0.23	73,73,73,73	0
57	MG	1H	3163	1/1	0.84	0.20	86,86,86,86	0
57	MG	1H	3047	1/1	0.84	0.34	64,64,64,64	0
57	MG	14	3341	1/1	0.84	0.29	78,78,78,78	0
57	MG	14	3425	1/1	0.84	0.13	106,106,106,106	0
57	MG	14	3063	1/1	0.84	0.17	93,93,93,93	0
57	MG	1H	3009	1/1	0.84	0.12	82,82,82,82	0
57	MG	14	3072	1/1	0.84	0.23	88,88,88,88	0
57	MG	1H	3225	1/1	0.84	0.36	74,74,74,74	0
57	MG	13	1632	1/1	0.84	0.14	95,95,95,95	0
57	MG	14	3148	1/1	0.84	0.18	113,113,113,113	0
57	MG	1H	3170	1/1	0.84	0.15	80,80,80,80	0
57	MG	16	210	1/1	0.84	0.25	86,86,86,86	0
57	MG	1H	3232	1/1	0.84	0.17	100,100,100,100	0
57	MG	45	201	1/1	0.84	0.27	84,84,84,84	0
57	MG	14	3090	1/1	0.84	0.25	77,77,77,77	0
57	MG	1G	1644	1/1	0.85	0.11	130,130,130,130	0
57	MG	14	3091	1/1	0.85	0.24	92,92,92,92	0
57	MG	1H	3179	1/1	0.85	0.21	74,74,74,74	0
57	MG	1H	3180	1/1	0.85	0.18	81,81,81,81	0
57	MG	1H	3097	1/1	0.85	0.16	43,43,43,43	0
57	MG	1H	3100	1/1	0.85	0.28	77,77,77,77	0
57	MG	1H	3239	1/1	0.85	0.13	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3241	1/1	0.85	0.15	82,82,82,82	0
57	MG	1H	3161	1/1	0.85	0.30	77,77,77,77	0
57	MG	1H	3371	1/1	0.85	0.11	88,88,88,88	0
57	MG	1G	1609	1/1	0.85	0.35	96,96,96,96	0
57	MG	1G	1610	1/1	0.85	0.17	84,84,84,84	0
57	MG	13	1736	1/1	0.85	0.09	129,129,129,129	0
57	MG	14	3118	1/1	0.85	0.12	96,96,96,96	0
57	MG	14	3119	1/1	0.85	0.16	69,69,69,69	0
57	MG	14	3178	1/1	0.85	0.11	83,83,83,83	0
57	MG	14	3007	1/1	0.85	0.15	61,61,61,61	0
57	MG	1G	1613	1/1	0.85	0.37	93,93,93,93	0
57	MG	1H	3194	1/1	0.85	0.25	80,80,80,80	0
57	MG	14	3185	1/1	0.85	0.24	93,93,93,93	0
57	MG	1H	3110	1/1	0.85	0.34	86,86,86,86	0
57	MG	1H	3059	1/1	0.85	0.34	72,72,72,72	0
57	MG	13	1646	1/1	0.85	0.34	91,91,91,91	0
57	MG	1H	3207	1/1	0.85	0.36	77,77,77,77	0
57	MG	14	3195	1/1	0.85	0.25	98,98,98,98	0
57	MG	14	3204	1/1	0.85	0.16	120,120,120,120	0
57	MG	1H	3525	1/1	0.85	0.16	99,99,99,99	0
57	MG	1H	3049	1/1	0.85	0.21	79,79,79,79	0
57	MG	1G	1627	1/1	0.85	0.16	122,122,122,122	0
57	MG	13	1653	1/1	0.85	0.15	95,95,95,95	0
57	MG	14	3452	1/1	0.85	0.13	122,122,122,122	0
57	MG	1H	3173	1/1	0.85	0.12	77,77,77,77	0
57	MG	14	3067	1/1	0.85	0.17	77,77,77,77	0
57	MG	14	3461	1/1	0.85	0.12	108,108,108,108	0
57	MG	1H	3018	1/1	0.85	0.25	63,63,63,63	0
57	MG	14	3074	1/1	0.85	0.22	95,95,95,95	0
57	MG	1H	3548	1/1	0.85	0.23	98,98,98,98	0
57	MG	1H	3093	1/1	0.85	0.29	73,73,73,73	0
57	MG	13	1605	1/1	0.85	0.17	88,88,88,88	0
57	MG	14	3082	1/1	0.85	0.20	80,80,80,80	0
57	MG	1G	1641	1/1	0.85	0.19	115,115,115,115	0
57	MG	13	1639	1/1	0.85	0.34	80,80,80,80	0
57	MG	16	209	1/1	0.86	0.12	86,86,86,86	0
57	MG	14	3113	1/1	0.86	0.27	74,74,74,74	0
57	MG	1H	3181	1/1	0.86	0.28	98,98,98,98	0
57	MG	14	3028	1/1	0.86	0.18	67,67,67,67	0
57	MG	1G	1634	1/1	0.86	0.11	98,98,98,98	0
57	MG	1G	1635	1/1	0.86	0.23	94,94,94,94	0
57	MG	1H	3155	1/1	0.86	0.26	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3219	1/1	0.86	0.20	83,83,83,83	0
57	MG	14	3062	1/1	0.86	0.23	97,97,97,97	0
57	MG	14	3128	1/1	0.86	0.22	88,88,88,88	0
57	MG	1H	3081	1/1	0.86	0.13	77,77,77,77	0
57	MG	1G	1640	1/1	0.86	0.30	80,80,80,80	0
57	MG	1H	3111	1/1	0.86	0.21	94,94,94,94	0
57	MG	1G	1604	1/1	0.86	0.14	132,132,132,132	0
57	MG	1H	3071	1/1	0.86	0.16	101,101,101,101	0
57	MG	1G	1607	1/1	0.86	0.16	107,107,107,107	0
57	MG	1H	3191	1/1	0.86	0.19	79,79,79,79	0
57	MG	1H	3192	1/1	0.86	0.27	83,83,83,83	0
57	MG	1H	3535	1/1	0.86	0.17	110,110,110,110	0
57	MG	14	3143	1/1	0.86	0.23	93,93,93,93	0
57	MG	14	3083	1/1	0.86	0.23	58,58,58,58	0
57	MG	1H	3193	1/1	0.86	0.44	89,89,89,89	0
57	MG	14	3355	1/1	0.86	0.13	99,99,99,99	0
57	MG	13	1611	1/1	0.86	0.17	78,78,78,78	0
57	MG	1G	1617	1/1	0.86	0.12	89,89,89,89	0
57	MG	14	3150	1/1	0.86	0.16	75,75,75,75	0
57	MG	1H	3162	1/1	0.86	0.33	92,92,92,92	0
57	MG	1H	3075	1/1	0.86	0.25	75,75,75,75	0
57	MG	1H	3164	1/1	0.86	0.23	85,85,85,85	0
57	MG	14	3002	1/1	0.86	0.18	63,63,63,63	0
57	MG	14	3156	1/1	0.86	0.22	81,81,81,81	0
57	MG	1H	3064	1/1	0.86	0.33	82,82,82,82	0
57	MG	16	203	1/1	0.86	0.19	84,84,84,84	0
57	MG	14	3012	1/1	0.86	0.20	69,69,69,69	0
57	MG	16	204	1/1	0.86	0.16	89,89,89,89	0
57	MG	1H	3209	1/1	0.86	0.38	92,92,92,92	0
57	MG	13	1610	1/1	0.86	0.42	81,81,81,81	0
57	MG	1H	3154	1/1	0.87	0.24	67,67,67,67	0
57	MG	13	1616	1/1	0.87	0.22	101,101,101,101	0
57	MG	14	3005	1/1	0.87	0.32	83,83,83,83	0
57	MG	1H	3076	1/1	0.87	0.22	75,75,75,75	0
57	MG	14	3010	1/1	0.87	0.32	84,84,84,84	0
57	MG	14	3105	1/1	0.87	0.18	92,92,92,92	0
57	MG	1H	3158	1/1	0.87	0.21	71,71,71,71	0
57	MG	1H	3226	1/1	0.87	0.24	92,92,92,92	0
57	MG	13	1652	1/1	0.87	0.20	82,82,82,82	0
57	MG	16	201	1/1	0.87	0.23	73,73,73,73	0
57	MG	14	3112	1/1	0.87	0.23	68,68,68,68	0
57	MG	13	1624	1/1	0.87	0.25	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3025	1/1	0.87	0.15	78,78,78,78	0
57	MG	1H	3185	1/1	0.87	0.25	76,76,76,76	0
57	MG	1H	3040	1/1	0.87	0.17	76,76,76,76	0
57	MG	1H	3042	1/1	0.87	0.15	67,67,67,67	0
57	MG	14	3038	1/1	0.87	0.22	68,68,68,68	0
57	MG	14	3123	1/1	0.87	0.12	75,75,75,75	0
57	MG	1H	3112	1/1	0.87	0.28	79,79,79,79	0
57	MG	14	3047	1/1	0.87	0.16	87,87,87,87	0
57	MG	13	1621	1/1	0.87	0.27	94,94,94,94	0
57	MG	14	3057	1/1	0.87	0.12	93,93,93,93	0
57	MG	14	3191	1/1	0.87	0.21	76,76,76,76	0
57	MG	14	3131	1/1	0.87	0.14	84,84,84,84	0
57	MG	13	1704	1/1	0.87	0.21	111,111,111,111	0
57	MG	1H	3141	1/1	0.87	0.12	75,75,75,75	0
57	MG	3I	301	1/1	0.87	0.08	70,70,70,70	0
57	MG	1H	3142	1/1	0.87	0.24	87,87,87,87	0
57	MG	14	3137	1/1	0.87	0.16	76,76,76,76	0
57	MG	13	1664	1/1	0.87	0.31	91,91,91,91	0
57	MG	14	3068	1/1	0.87	0.21	78,78,78,78	0
57	MG	14	3431	1/1	0.87	0.09	107,107,107,107	0
57	MG	1H	3146	1/1	0.87	0.35	85,85,85,85	0
57	MG	1H	3204	1/1	0.87	0.26	80,80,80,80	0
57	MG	1H	3421	1/1	0.87	0.26	93,93,93,93	0
57	MG	1H	3432	1/1	0.87	0.09	116,116,116,116	0
57	MG	1H	3205	1/1	0.87	0.29	71,71,71,71	0
57	MG	1H	3206	1/1	0.87	0.28	55,55,55,55	0
57	MG	1G	1611	1/1	0.87	0.35	84,84,84,84	0
57	MG	14	3086	1/1	0.87	0.23	73,73,73,73	0
57	MG	13	1741	1/1	0.87	0.14	95,95,95,95	0
57	MG	1G	1723	1/1	0.87	0.10	127,127,127,127	0
57	MG	1H	3150	1/1	0.87	0.23	81,81,81,81	0
57	MG	1H	3073	1/1	0.87	0.26	84,84,84,84	0
57	MG	1H	3004	1/1	0.87	0.19	64,64,64,64	0
57	MG	14	3056	1/1	0.88	0.19	74,74,74,74	0
57	MG	1H	3402	1/1	0.88	0.17	71,71,71,71	0
57	MG	13	1636	1/1	0.88	0.22	81,81,81,81	0
57	MG	1H	3101	1/1	0.88	0.10	72,72,72,72	0
57	MG	1H	3116	1/1	0.88	0.17	82,82,82,82	0
57	MG	1H	3215	1/1	0.88	0.38	94,94,94,94	0
57	MG	1H	3217	1/1	0.88	0.35	79,79,79,79	0
57	MG	14	3372	1/1	0.88	0.09	112,112,112,112	0
57	MG	1H	3190	1/1	0.88	0.15	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3070	1/1	0.88	0.30	66,66,66,66	0
57	MG	13	1657	1/1	0.88	0.30	75,75,75,75	0
57	MG	14	3444	1/1	0.88	0.26	102,102,102,102	0
57	MG	1H	3512	1/1	0.88	0.20	100,100,100,100	0
57	MG	14	3453	1/1	0.88	0.11	118,118,118,118	0
57	MG	13	1649	1/1	0.88	0.17	83,83,83,83	0
57	MG	1G	1653	1/1	0.88	0.10	125,125,125,125	0
57	MG	1G	1633	1/1	0.88	0.08	102,102,102,102	0
57	MG	13	1615	1/1	0.88	0.27	75,75,75,75	0
57	MG	14	3035	1/1	0.88	0.15	69,69,69,69	0
57	MG	1J	203	1/1	0.88	0.18	92,92,92,92	0
57	MG	1H	3383	1/1	0.88	0.17	74,74,74,74	0
57	MG	14	3040	1/1	0.88	0.26	80,80,80,80	0
57	MG	14	3043	1/1	0.88	0.27	96,96,96,96	0
57	MG	1H	3533	1/1	0.88	0.24	99,99,99,99	0
57	MG	1H	3044	1/1	0.88	0.28	80,80,80,80	0
57	MG	1G	1619	1/1	0.88	0.10	118,118,118,118	0
57	MG	1H	3168	1/1	0.89	0.18	89,89,89,89	0
57	MG	1H	3223	1/1	0.89	0.24	79,79,79,79	0
57	MG	14	3039	1/1	0.89	0.20	85,85,85,85	0
57	MG	1G	1659	1/1	0.89	0.07	120,120,120,120	0
57	MG	1G	1667	1/1	0.89	0.09	111,111,111,111	0
57	MG	2K	103	1/1	0.89	0.17	88,88,88,88	0
57	MG	14	3145	1/1	0.89	0.16	71,71,71,71	0
57	MG	1G	1720	1/1	0.89	0.09	135,135,135,135	0
57	MG	13	1699	1/1	0.89	0.10	114,114,114,114	0
57	MG	14	3054	1/1	0.89	0.21	67,67,67,67	0
57	MG	14	3202	1/1	0.89	0.12	106,106,106,106	0
57	MG	1G	1726	1/1	0.89	0.22	94,94,94,94	0
57	MG	14	3205	1/1	0.89	0.06	102,102,102,102	0
57	MG	14	3207	1/1	0.89	0.12	70,70,70,70	0
57	MG	14	3270	1/1	0.89	0.10	74,74,74,74	0
57	MG	13	1650	1/1	0.89	0.27	85,85,85,85	0
57	MG	1H	3228	1/1	0.89	0.08	81,81,81,81	0
57	MG	1G	1608	1/1	0.89	0.17	100,100,100,100	0
57	MG	1H	3145	1/1	0.89	0.18	74,74,74,74	0
57	MG	1H	3413	1/1	0.89	0.22	93,93,93,93	0
57	MG	14	3430	1/1	0.89	0.16	102,102,102,102	0
57	MG	14	3065	1/1	0.89	0.23	70,70,70,70	0
57	MG	1H	3174	1/1	0.89	0.17	73,73,73,73	0
57	MG	14	3160	1/1	0.89	0.11	85,85,85,85	0
57	MG	14	3006	1/1	0.89	0.10	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3031	1/1	0.89	0.20	90,90,90,90	0
57	MG	14	3122	1/1	0.89	0.20	90,90,90,90	0
57	MG	1H	3445	1/1	0.89	0.17	87,87,87,87	0
57	MG	1H	3126	1/1	0.89	0.14	71,71,71,71	0
57	MG	1H	3237	1/1	0.89	0.31	85,85,85,85	0
57	MG	14	3015	1/1	0.89	0.13	65,65,65,65	0
57	MG	1H	3201	1/1	0.89	0.23	80,80,80,80	0
57	MG	16	208	1/1	0.89	0.17	86,86,86,86	0
57	MG	1H	3218	1/1	0.89	0.33	70,70,70,70	0
57	MG	1H	3514	1/1	0.89	0.12	112,112,112,112	0
57	MG	3I	201	1/1	0.89	0.19	75,75,75,75	0
57	MG	1H	3264	1/1	0.89	0.10	55,55,55,55	0
57	MG	1G	1651	1/1	0.89	0.29	97,97,97,97	0
57	MG	1H	3023	1/1	0.90	0.15	71,71,71,71	0
57	MG	1H	3025	1/1	0.90	0.18	52,52,52,52	0
57	MG	1H	3401	1/1	0.90	0.14	99,99,99,99	0
57	MG	14	3101	1/1	0.90	0.14	87,87,87,87	0
57	MG	14	3051	1/1	0.90	0.20	70,70,70,70	0
57	MG	1H	3123	1/1	0.90	0.18	68,68,68,68	0
57	MG	13	1608	1/1	0.90	0.09	93,93,93,93	0
57	MG	14	3199	1/1	0.90	0.33	99,99,99,99	0
57	MG	1H	3536	1/1	0.90	0.15	104,104,104,104	0
57	MG	14	3203	1/1	0.90	0.15	95,95,95,95	0
57	MG	14	3009	1/1	0.90	0.09	77,77,77,77	0
57	MG	14	3061	1/1	0.90	0.17	60,60,60,60	0
57	MG	88	203	1/1	0.90	0.16	83,83,83,83	0
57	MG	14	3259	1/1	0.90	0.08	97,97,97,97	0
57	MG	14	3111	1/1	0.90	0.13	83,83,83,83	0
57	MG	14	3011	1/1	0.90	0.23	76,76,76,76	0
57	MG	1H	3030	1/1	0.90	0.18	89,89,89,89	0
57	MG	1H	3543	1/1	0.90	0.10	166,166,166,166	0
57	MG	14	3359	1/1	0.90	0.08	122,122,122,122	0
57	MG	14	3115	1/1	0.90	0.26	78,78,78,78	0
57	MG	14	3388	1/1	0.90	0.17	72,72,72,72	0
57	MG	14	3406	1/1	0.90	0.08	121,121,121,121	0
57	MG	14	3420	1/1	0.90	0.07	119,119,119,119	0
57	MG	14	3117	1/1	0.90	0.10	69,69,69,69	0
57	MG	1H	3199	1/1	0.90	0.14	81,81,81,81	0
57	MG	13	1635	1/1	0.90	0.22	83,83,83,83	0
57	MG	1H	3422	1/1	0.90	0.08	114,114,114,114	0
57	MG	14	3071	1/1	0.90	0.14	82,82,82,82	0
57	MG	14	3450	1/1	0.90	0.23	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3011	1/1	0.90	0.24	79,79,79,79	0
57	MG	14	3022	1/1	0.90	0.14	77,77,77,77	0
57	MG	14	3023	1/1	0.90	0.20	58,58,58,58	0
57	MG	14	3024	1/1	0.90	0.12	88,88,88,88	0
57	MG	1G	1686	1/1	0.90	0.07	113,113,113,113	0
57	MG	1G	1704	1/1	0.90	0.12	127,127,127,127	0
57	MG	1G	1711	1/1	0.90	0.08	156,156,156,156	0
57	MG	1H	3221	1/1	0.90	0.25	81,81,81,81	0
57	MG	1H	3065	1/1	0.90	0.18	72,72,72,72	0
57	MG	1H	3017	1/1	0.90	0.19	56,56,56,56	0
57	MG	1H	3134	1/1	0.90	0.30	77,77,77,77	0
57	MG	1H	3369	1/1	0.90	0.14	90,90,90,90	0
57	MG	13	1630	1/1	0.90	0.20	86,86,86,86	0
57	MG	14	3139	1/1	0.90	0.38	88,88,88,88	0
57	MG	1H	3107	1/1	0.91	0.22	62,62,62,62	0
57	MG	32	301	1/1	0.91	0.12	137,137,137,137	0
57	MG	13	1663	1/1	0.91	0.10	77,77,77,77	0
57	MG	14	3096	1/1	0.91	0.16	84,84,84,84	0
57	MG	13	1622	1/1	0.91	0.17	111,111,111,111	0
57	MG	14	3100	1/1	0.91	0.15	77,77,77,77	0
57	MG	14	3196	1/1	0.91	0.10	85,85,85,85	0
57	MG	14	3197	1/1	0.91	0.23	92,92,92,92	0
57	MG	13	1660	1/1	0.91	0.22	91,91,91,91	0
57	MG	1H	3165	1/1	0.91	0.13	85,85,85,85	0
57	MG	1H	3459	1/1	0.91	0.13	88,88,88,88	0
57	MG	14	3052	1/1	0.91	0.26	59,59,59,59	0
57	MG	14	3053	1/1	0.91	0.39	82,82,82,82	0
57	MG	1H	3484	1/1	0.91	0.20	97,97,97,97	0
57	MG	1H	3492	1/1	0.91	0.07	107,107,107,107	0
57	MG	14	3263	1/1	0.91	0.09	86,86,86,86	0
57	MG	16	205	1/1	0.91	0.10	84,84,84,84	0
57	MG	14	3284	1/1	0.91	0.14	107,107,107,107	0
57	MG	14	3314	1/1	0.91	0.10	78,78,78,78	0
57	MG	1G	1618	1/1	0.91	0.20	91,91,91,91	0
57	MG	13	1603	1/1	0.91	0.18	92,92,92,92	0
57	MG	14	3347	1/1	0.91	0.09	97,97,97,97	0
57	MG	14	3349	1/1	0.91	0.08	99,99,99,99	0
57	MG	1H	3347	1/1	0.91	0.07	113,113,113,113	0
57	MG	14	3356	1/1	0.91	0.20	78,78,78,78	0
57	MG	1H	3362	1/1	0.91	0.09	78,78,78,78	0
57	MG	1H	3092	1/1	0.91	0.13	67,67,67,67	0
57	MG	1H	3203	1/1	0.91	0.26	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3395	1/1	0.91	0.18	98,98,98,98	0
57	MG	13	1674	1/1	0.91	0.16	105,105,105,105	0
57	MG	14	3415	1/1	0.91	0.21	93,93,93,93	0
57	MG	14	3162	1/1	0.91	0.17	91,91,91,91	0
57	MG	14	3018	1/1	0.91	0.15	82,82,82,82	0
57	MG	14	3429	1/1	0.91	0.21	109,109,109,109	0
57	MG	1H	3380	1/1	0.91	0.15	76,76,76,76	0
57	MG	13	1613	1/1	0.91	0.19	94,94,94,94	0
57	MG	14	3434	1/1	0.91	0.20	110,110,110,110	0
57	MG	14	3438	1/1	0.91	0.12	111,111,111,111	0
57	MG	13	1678	1/1	0.91	0.08	114,114,114,114	0
57	MG	1G	1687	1/1	0.91	0.08	111,111,111,111	0
57	MG	14	3445	1/1	0.91	0.07	119,119,119,119	0
57	MG	14	3124	1/1	0.91	0.25	64,64,64,64	0
57	MG	1G	1702	1/1	0.91	0.07	117,117,117,117	0
57	MG	1H	3082	1/1	0.91	0.19	69,69,69,69	0
57	MG	1G	1630	1/1	0.91	0.14	132,132,132,132	0
57	MG	1H	3099	1/1	0.91	0.17	53,53,53,53	0
57	MG	14	3029	1/1	0.91	0.21	80,80,80,80	0
57	MG	1G	1713	1/1	0.91	0.09	120,120,120,120	0
57	MG	14	3033	1/1	0.91	0.20	57,57,57,57	0
57	MG	14	3034	1/1	0.91	0.20	75,75,75,75	0
57	MG	1H	3084	1/1	0.91	0.20	77,77,77,77	0
57	MG	14	3181	1/1	0.91	0.17	91,91,91,91	0
57	MG	1J	208	1/1	0.91	0.07	124,124,124,124	0
57	MG	14	3136	1/1	0.91	0.26	95,95,95,95	0
57	MG	14	3184	1/1	0.91	0.16	78,78,78,78	0
57	MG	35	202	1/1	0.91	0.09	80,80,80,80	0
57	MG	1H	3058	1/1	0.91	0.24	68,68,68,68	0
57	MG	14	3186	1/1	0.91	0.13	95,95,95,95	0
57	MG	E5	102	1/1	0.91	0.18	68,68,68,68	0
60	SPE	1G	1725	13/13	0.91	0.12	110,113,117,118	0
57	MG	13	1625	1/1	0.92	0.15	68,68,68,68	0
57	MG	1H	3079	1/1	0.92	0.20	85,85,85,85	0
57	MG	1H	3386	1/1	0.92	0.10	72,72,72,72	0
57	MG	1H	3080	1/1	0.92	0.15	75,75,75,75	0
57	MG	1H	3392	1/1	0.92	0.09	74,74,74,74	0
57	MG	1G	1663	1/1	0.92	0.09	112,112,112,112	0
57	MG	14	3206	1/1	0.92	0.06	97,97,97,97	0
57	MG	1H	3048	1/1	0.92	0.11	68,68,68,68	0
57	MG	1G	1678	1/1	0.92	0.07	98,98,98,98	0
57	MG	13	1633	1/1	0.92	0.09	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	1715	1/1	0.92	0.11	119,119,119,119	0
57	MG	14	3275	1/1	0.92	0.09	85,85,85,85	0
57	MG	14	3098	1/1	0.92	0.20	63,63,63,63	0
57	MG	14	3289	1/1	0.92	0.07	89,89,89,89	0
57	MG	14	3291	1/1	0.92	0.11	71,71,71,71	0
57	MG	1G	1688	1/1	0.92	0.09	123,123,123,123	0
57	MG	1H	3102	1/1	0.92	0.09	52,52,52,52	0
57	MG	1H	3234	1/1	0.92	0.26	84,84,84,84	0
57	MG	1H	3418	1/1	0.92	0.09	122,122,122,122	0
57	MG	14	3154	1/1	0.92	0.21	78,78,78,78	0
57	MG	1H	3420	1/1	0.92	0.17	94,94,94,94	0
57	MG	14	3104	1/1	0.92	0.15	89,89,89,89	0
57	MG	1H	3103	1/1	0.92	0.15	64,64,64,64	0
57	MG	14	3106	1/1	0.92	0.20	79,79,79,79	0
57	MG	14	3379	1/1	0.92	0.07	107,107,107,107	0
57	MG	14	3159	1/1	0.92	0.11	80,80,80,80	0
57	MG	1H	3149	1/1	0.92	0.27	81,81,81,81	0
57	MG	14	3400	1/1	0.92	0.07	135,135,135,135	0
57	MG	1H	3427	1/1	0.92	0.12	102,102,102,102	0
57	MG	1H	3189	1/1	0.92	0.18	83,83,83,83	0
57	MG	1H	3444	1/1	0.92	0.21	72,72,72,72	0
57	MG	14	3423	1/1	0.92	0.11	118,118,118,118	0
57	MG	1H	3006	1/1	0.92	0.23	77,77,77,77	0
57	MG	1H	3454	1/1	0.92	0.15	104,104,104,104	0
57	MG	14	3055	1/1	0.92	0.14	64,64,64,64	0
57	MG	2L	101	1/1	0.92	0.24	83,83,83,83	0
57	MG	1G	1632	1/1	0.92	0.10	108,108,108,108	0
57	MG	4L	101	1/1	0.92	0.12	102,102,102,102	0
57	MG	14	3439	1/1	0.92	0.20	100,100,100,100	0
57	MG	1H	3007	1/1	0.92	0.17	57,57,57,57	0
57	MG	13	1672	1/1	0.92	0.09	92,92,92,92	0
57	MG	14	3174	1/1	0.92	0.13	78,78,78,78	0
57	MG	14	3447	1/1	0.92	0.06	107,107,107,107	0
57	MG	1H	3486	1/1	0.92	0.20	99,99,99,99	0
57	MG	21	302	1/1	0.92	0.21	85,85,85,85	0
57	MG	1H	3489	1/1	0.92	0.12	107,107,107,107	0
57	MG	1H	3286	1/1	0.92	0.13	65,65,65,65	0
57	MG	13	1609	1/1	0.92	0.15	88,88,88,88	0
57	MG	14	3460	1/1	0.92	0.19	92,92,92,92	0
57	MG	1H	3360	1/1	0.92	0.10	102,102,102,102	0
57	MG	1H	3504	1/1	0.92	0.12	104,104,104,104	0
57	MG	14	3182	1/1	0.92	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3127	1/1	0.92	0.11	70,70,70,70	0
57	MG	1G	1643	1/1	0.92	0.10	100,100,100,100	0
57	MG	14	3129	1/1	0.92	0.25	90,90,90,90	0
57	MG	14	3073	1/1	0.92	0.20	61,61,61,61	0
57	MG	1H	3506	1/1	0.92	0.13	103,103,103,103	0
57	MG	14	3075	1/1	0.92	0.16	65,65,65,65	0
57	MG	1H	3020	1/1	0.92	0.15	60,60,60,60	0
57	MG	1H	3043	1/1	0.92	0.11	64,64,64,64	0
57	MG	1H	3136	1/1	0.92	0.12	63,63,63,63	0
57	MG	14	3081	1/1	0.92	0.15	79,79,79,79	0
59	ZN	C5	201	1/1	0.92	0.06	167,167,167,167	0
57	MG	2I	201	1/1	0.92	0.11	97,97,97,97	0
57	MG	88	202	1/1	0.93	0.12	71,71,71,71	0
57	MG	1H	3499	1/1	0.93	0.19	89,89,89,89	0
57	MG	14	3225	1/1	0.93	0.10	79,79,79,79	0
57	MG	14	3257	1/1	0.93	0.09	118,118,118,118	0
57	MG	14	3084	1/1	0.93	0.18	67,67,67,67	0
57	MG	14	3085	1/1	0.93	0.15	52,52,52,52	0
57	MG	1H	3061	1/1	0.93	0.17	62,62,62,62	0
57	MG	1H	3379	1/1	0.93	0.11	87,87,87,87	0
57	MG	1G	1603	1/1	0.93	0.12	91,91,91,91	0
57	MG	14	3089	1/1	0.93	0.06	73,73,73,73	0
57	MG	1H	3095	1/1	0.93	0.09	76,76,76,76	0
57	MG	14	3302	1/1	0.93	0.16	94,94,94,94	0
57	MG	1H	3041	1/1	0.93	0.12	57,57,57,57	0
57	MG	1H	3513	1/1	0.93	0.14	104,104,104,104	0
57	MG	14	3338	1/1	0.93	0.09	112,112,112,112	0
57	MG	1H	3121	1/1	0.93	0.10	89,89,89,89	0
57	MG	1H	3523	1/1	0.93	0.09	102,102,102,102	0
57	MG	1H	3171	1/1	0.93	0.18	88,88,88,88	0
57	MG	14	3351	1/1	0.93	0.08	101,101,101,101	0
57	MG	14	3097	1/1	0.93	0.11	84,84,84,84	0
57	MG	13	1644	1/1	0.93	0.14	99,99,99,99	0
57	MG	1H	3396	1/1	0.93	0.09	81,81,81,81	0
57	MG	14	3360	1/1	0.93	0.10	107,107,107,107	0
57	MG	14	3368	1/1	0.93	0.14	92,92,92,92	0
57	MG	1G	1670	1/1	0.93	0.20	109,109,109,109	0
57	MG	14	3378	1/1	0.93	0.08	101,101,101,101	0
57	MG	14	3032	1/1	0.93	0.26	72,72,72,72	0
57	MG	1H	3098	1/1	0.93	0.17	59,59,59,59	0
57	MG	14	3391	1/1	0.93	0.11	87,87,87,87	0
57	MG	14	3392	1/1	0.93	0.06	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3394	1/1	0.93	0.16	91,91,91,91	0
57	MG	1G	1684	1/1	0.93	0.07	109,109,109,109	0
57	MG	1H	3052	1/1	0.93	0.18	58,58,58,58	0
57	MG	14	3405	1/1	0.93	0.07	118,118,118,118	0
57	MG	1G	1616	1/1	0.93	0.17	84,84,84,84	0
57	MG	14	3414	1/1	0.93	0.13	99,99,99,99	0
57	MG	1H	3053	1/1	0.93	0.10	47,47,47,47	0
57	MG	14	3419	1/1	0.93	0.16	119,119,119,119	0
57	MG	1H	3537	1/1	0.93	0.10	112,112,112,112	0
57	MG	14	3042	1/1	0.93	0.16	54,54,54,54	0
57	MG	14	3424	1/1	0.93	0.07	117,117,117,117	0
57	MG	14	3168	1/1	0.93	0.11	70,70,70,70	0
57	MG	1G	1703	1/1	0.93	0.06	107,107,107,107	0
57	MG	1H	3066	1/1	0.93	0.19	65,65,65,65	0
57	MG	1G	1707	1/1	0.93	0.09	115,115,115,115	0
57	MG	1H	3541	1/1	0.93	0.09	109,109,109,109	0
57	MG	1H	3202	1/1	0.93	0.19	80,80,80,80	0
57	MG	1H	3083	1/1	0.93	0.19	80,80,80,80	0
57	MG	1G	1714	1/1	0.93	0.07	126,126,126,126	0
57	MG	14	3116	1/1	0.93	0.11	77,77,77,77	0
57	MG	13	1654	1/1	0.93	0.25	85,85,85,85	0
57	MG	1G	1721	1/1	0.93	0.05	128,128,128,128	0
57	MG	1G	1722	1/1	0.93	0.13	116,116,116,116	0
57	MG	1H	3070	1/1	0.93	0.11	51,51,51,51	0
57	MG	1H	3551	1/1	0.93	0.07	86,86,86,86	0
57	MG	13	1719	1/1	0.93	0.06	118,118,118,118	0
57	MG	1H	3072	1/1	0.93	0.10	60,60,60,60	0
57	MG	14	3457	1/1	0.93	0.05	134,134,134,134	0
57	MG	1H	3240	1/1	0.93	0.17	86,86,86,86	0
57	MG	1H	3088	1/1	0.93	0.10	87,87,87,87	0
57	MG	1H	3183	1/1	0.93	0.19	75,75,75,75	0
57	MG	1H	3045	1/1	0.93	0.27	63,63,63,63	0
57	MG	1H	3341	1/1	0.93	0.07	113,113,113,113	0
57	MG	14	3003	1/1	0.93	0.13	68,68,68,68	0
57	MG	1H	3460	1/1	0.93	0.23	85,85,85,85	0
57	MG	1J	207	1/1	0.93	0.11	119,119,119,119	0
57	MG	1H	3212	1/1	0.93	0.09	87,87,87,87	0
57	MG	1J	210	1/1	0.93	0.04	135,135,135,135	0
57	MG	19	301	1/1	0.93	0.20	61,61,61,61	0
57	MG	1H	3354	1/1	0.93	0.09	78,78,78,78	0
57	MG	1H	3021	1/1	0.93	0.17	60,60,60,60	0
57	MG	14	3008	1/1	0.93	0.12	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3076	1/1	0.93	0.10	80,80,80,80	0
57	MG	1H	3491	1/1	0.93	0.11	100,100,100,100	0
57	MG	13	1701	1/1	0.93	0.06	124,124,124,124	0
57	MG	1H	3115	1/1	0.93	0.13	64,64,64,64	0
57	MG	13	1740	1/1	0.93	0.05	162,162,162,162	0
57	MG	1H	3326	1/1	0.94	0.10	109,109,109,109	0
57	MG	1H	3338	1/1	0.94	0.07	99,99,99,99	0
57	MG	1H	3500	1/1	0.94	0.08	90,90,90,90	0
57	MG	13	1671	1/1	0.94	0.10	108,108,108,108	0
57	MG	1H	3001	1/1	0.94	0.21	49,49,49,49	0
57	MG	1G	1716	1/1	0.94	0.10	110,110,110,110	0
57	MG	1G	1719	1/1	0.94	0.08	115,115,115,115	0
57	MG	14	3069	1/1	0.94	0.07	56,56,56,56	0
57	MG	14	3295	1/1	0.94	0.12	88,88,88,88	0
57	MG	1H	3353	1/1	0.94	0.08	62,62,62,62	0
57	MG	14	3306	1/1	0.94	0.15	93,93,93,93	0
57	MG	1G	1615	1/1	0.94	0.12	89,89,89,89	0
57	MG	14	3324	1/1	0.94	0.06	90,90,90,90	0
57	MG	1H	3510	1/1	0.94	0.07	104,104,104,104	0
57	MG	1H	3153	1/1	0.94	0.24	71,71,71,71	0
57	MG	1H	3028	1/1	0.94	0.21	62,62,62,62	0
57	MG	13	1626	1/1	0.94	0.08	96,96,96,96	0
57	MG	1H	3129	1/1	0.94	0.15	85,85,85,85	0
57	MG	1H	3216	1/1	0.94	0.45	79,79,79,79	0
57	MG	1G	1622	1/1	0.94	0.11	104,104,104,104	0
57	MG	1H	3157	1/1	0.94	0.26	89,89,89,89	0
57	MG	1H	3377	1/1	0.94	0.09	94,94,94,94	0
57	MG	13	1618	1/1	0.94	0.09	72,72,72,72	0
57	MG	14	3362	1/1	0.94	0.07	99,99,99,99	0
57	MG	13	1640	1/1	0.94	0.05	97,97,97,97	0
57	MG	14	3371	1/1	0.94	0.07	108,108,108,108	0
57	MG	1H	3105	1/1	0.94	0.08	78,78,78,78	0
57	MG	14	3373	1/1	0.94	0.08	94,94,94,94	0
57	MG	13	1718	1/1	0.94	0.06	130,130,130,130	0
57	MG	1H	3539	1/1	0.94	0.16	95,95,95,95	0
57	MG	14	3381	1/1	0.94	0.08	136,136,136,136	0
57	MG	14	3384	1/1	0.94	0.06	88,88,88,88	0
57	MG	13	1607	1/1	0.94	0.16	83,83,83,83	0
57	MG	1H	3224	1/1	0.94	0.06	72,72,72,72	0
57	MG	13	1722	1/1	0.94	0.13	99,99,99,99	0
57	MG	1H	3399	1/1	0.94	0.06	109,109,109,109	0
57	MG	1H	3137	1/1	0.94	0.18	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3397	1/1	0.94	0.10	162,162,162,162	0
57	MG	14	3092	1/1	0.94	0.11	67,67,67,67	0
57	MG	1H	3549	1/1	0.94	0.10	94,94,94,94	0
57	MG	13	1723	1/1	0.94	0.09	118,118,118,118	0
57	MG	14	3412	1/1	0.94	0.10	106,106,106,106	0
57	MG	14	3413	1/1	0.94	0.08	125,125,125,125	0
57	MG	13	1727	1/1	0.94	0.06	124,124,124,124	0
57	MG	14	3016	1/1	0.94	0.13	69,69,69,69	0
57	MG	14	3417	1/1	0.94	0.05	117,117,117,117	0
57	MG	1H	3195	1/1	0.94	0.10	85,85,85,85	0
57	MG	1G	1639	1/1	0.94	0.32	90,90,90,90	0
57	MG	14	3422	1/1	0.94	0.10	104,104,104,104	0
57	MG	13	1728	1/1	0.94	0.06	117,117,117,117	0
57	MG	1H	3415	1/1	0.94	0.11	95,95,95,95	0
57	MG	14	3021	1/1	0.94	0.22	63,63,63,63	0
57	MG	14	3427	1/1	0.94	0.06	121,121,121,121	0
57	MG	13	1731	1/1	0.94	0.11	109,109,109,109	0
57	MG	13	1735	1/1	0.94	0.08	105,105,105,105	0
57	MG	13	1617	1/1	0.94	0.18	69,69,69,69	0
57	MG	1H	3236	1/1	0.94	0.11	93,93,93,93	0
57	MG	1G	1646	1/1	0.94	0.23	78,78,78,78	0
57	MG	1H	3144	1/1	0.94	0.09	71,71,71,71	0
57	MG	13	1683	1/1	0.94	0.10	119,119,119,119	0
57	MG	1H	3434	1/1	0.94	0.08	96,96,96,96	0
57	MG	13	1689	1/1	0.94	0.11	98,98,98,98	0
57	MG	13	1691	1/1	0.94	0.08	107,107,107,107	0
57	MG	1H	3452	1/1	0.94	0.06	115,115,115,115	0
57	MG	1H	3148	1/1	0.94	0.12	88,88,88,88	0
57	MG	14	3036	1/1	0.94	0.23	85,85,85,85	0
57	MG	1H	3246	1/1	0.94	0.08	54,54,54,54	0
57	MG	13	1658	1/1	0.94	0.44	83,83,83,83	0
57	MG	1G	1666	1/1	0.94	0.08	110,110,110,110	0
57	MG	1H	3466	1/1	0.94	0.10	103,103,103,103	0
57	MG	1H	3481	1/1	0.94	0.09	92,92,92,92	0
57	MG	14	3045	1/1	0.94	0.16	72,72,72,72	0
57	MG	1G	1674	1/1	0.94	0.08	106,106,106,106	0
57	MG	Q8	101	1/1	0.94	0.20	82,82,82,82	0
57	MG	1H	3268	1/1	0.94	0.11	70,70,70,70	0
57	MG	1H	3270	1/1	0.94	0.14	78,78,78,78	0
57	MG	14	3200	1/1	0.94	0.10	86,86,86,86	0
57	MG	14	3201	1/1	0.94	0.10	82,82,82,82	0
57	MG	1H	3281	1/1	0.94	0.07	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3024	1/1	0.94	0.17	64,64,64,64	0
57	MG	29	301	1/1	0.94	0.13	65,65,65,65	0
57	MG	1G	1693	1/1	0.94	0.07	121,121,121,121	0
57	MG	1G	1606	1/1	0.94	0.12	87,87,87,87	0
57	MG	1H	3301	1/1	0.94	0.07	86,86,86,86	0
57	MG	1H	3304	1/1	0.94	0.07	64,64,64,64	0
57	MG	14	3222	1/1	0.94	0.09	73,73,73,73	0
57	MG	1G	1706	1/1	0.94	0.06	138,138,138,138	0
57	MG	14	3245	1/1	0.94	0.09	74,74,74,74	0
57	MG	14	3255	1/1	0.94	0.08	110,110,110,110	0
60	SPE	14	3458	13/13	0.94	0.16	92,101,106,108	0
57	MG	1H	3528	1/1	0.95	0.06	117,117,117,117	0
57	MG	14	3328	1/1	0.95	0.09	95,95,95,95	0
57	MG	1H	3214	1/1	0.95	0.20	77,77,77,77	0
57	MG	14	3334	1/1	0.95	0.08	83,83,83,83	0
57	MG	14	3336	1/1	0.95	0.09	109,109,109,109	0
57	MG	1H	3424	1/1	0.95	0.12	84,84,84,84	0
57	MG	13	1606	1/1	0.95	0.13	88,88,88,88	0
57	MG	1G	1680	1/1	0.95	0.10	103,103,103,103	0
57	MG	14	3348	1/1	0.95	0.06	102,102,102,102	0
57	MG	1G	1681	1/1	0.95	0.04	131,131,131,131	0
57	MG	1H	3534	1/1	0.95	0.06	113,113,113,113	0
57	MG	1H	3358	1/1	0.95	0.06	100,100,100,100	0
57	MG	13	1703	1/1	0.95	0.08	71,71,71,71	0
57	MG	1H	3435	1/1	0.95	0.16	100,100,100,100	0
57	MG	1G	1692	1/1	0.95	0.09	103,103,103,103	0
57	MG	1H	3436	1/1	0.95	0.08	87,87,87,87	0
57	MG	1G	1696	1/1	0.95	0.09	109,109,109,109	0
57	MG	14	3370	1/1	0.95	0.08	90,90,90,90	0
57	MG	14	3037	1/1	0.95	0.23	54,54,54,54	0
57	MG	1G	1698	1/1	0.95	0.07	138,138,138,138	0
57	MG	1G	1699	1/1	0.95	0.06	113,113,113,113	0
57	MG	14	3375	1/1	0.95	0.15	116,116,116,116	0
57	MG	1G	1700	1/1	0.95	0.12	107,107,107,107	0
57	MG	1H	3002	1/1	0.95	0.09	51,51,51,51	0
57	MG	13	1696	1/1	0.95	0.13	114,114,114,114	0
57	MG	14	3044	1/1	0.95	0.10	71,71,71,71	0
57	MG	1H	3027	1/1	0.95	0.11	60,60,60,60	0
57	MG	1H	3370	1/1	0.95	0.14	80,80,80,80	0
57	MG	1H	3547	1/1	0.95	0.06	131,131,131,131	0
57	MG	14	3048	1/1	0.95	0.15	72,72,72,72	0
57	MG	1G	1709	1/1	0.95	0.08	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3455	1/1	0.95	0.09	120,120,120,120	0
57	MG	14	3399	1/1	0.95	0.05	122,122,122,122	0
57	MG	13	1739	1/1	0.95	0.08	119,119,119,119	0
57	MG	1H	3029	1/1	0.95	0.11	59,59,59,59	0
57	MG	1H	3463	1/1	0.95	0.15	70,70,70,70	0
57	MG	14	3410	1/1	0.95	0.09	107,107,107,107	0
57	MG	1H	3249	1/1	0.95	0.07	61,61,61,61	0
57	MG	1H	3261	1/1	0.95	0.14	61,61,61,61	0
57	MG	14	3188	1/1	0.95	0.14	69,69,69,69	0
57	MG	1H	3016	1/1	0.95	0.32	52,52,52,52	0
57	MG	1H	3485	1/1	0.95	0.12	102,102,102,102	0
57	MG	14	3059	1/1	0.95	0.11	58,58,58,58	0
57	MG	1H	3384	1/1	0.95	0.09	59,59,59,59	0
57	MG	14	3421	1/1	0.95	0.12	96,96,96,96	0
57	MG	1H	3488	1/1	0.95	0.09	84,84,84,84	0
57	MG	13	1706	1/1	0.95	0.10	88,88,88,88	0
57	MG	13	1724	1/1	0.95	0.07	116,116,116,116	0
57	MG	14	3198	1/1	0.95	0.32	88,88,88,88	0
57	MG	1H	3279	1/1	0.95	0.13	68,68,68,68	0
57	MG	1H	3054	1/1	0.95	0.12	63,63,63,63	0
57	MG	52	300	1/1	0.95	0.05	133,133,133,133	0
57	MG	1H	3494	1/1	0.95	0.16	87,87,87,87	0
57	MG	1H	3285	1/1	0.95	0.07	69,69,69,69	0
57	MG	1H	3208	1/1	0.95	0.06	69,69,69,69	0
57	MG	21	303	1/1	0.95	0.10	61,61,61,61	0
57	MG	1H	3019	1/1	0.95	0.17	53,53,53,53	0
57	MG	1H	3502	1/1	0.95	0.08	90,90,90,90	0
57	MG	14	3214	1/1	0.95	0.07	83,83,83,83	0
57	MG	14	3215	1/1	0.95	0.06	98,98,98,98	0
57	MG	14	3448	1/1	0.95	0.08	120,120,120,120	0
57	MG	13	1712	1/1	0.95	0.08	106,106,106,106	0
57	MG	14	3451	1/1	0.95	0.21	110,110,110,110	0
57	MG	1H	3505	1/1	0.95	0.07	112,112,112,112	0
57	MG	14	3228	1/1	0.95	0.09	64,64,64,64	0
57	MG	14	3454	1/1	0.95	0.08	108,108,108,108	0
57	MG	14	3243	1/1	0.95	0.15	93,93,93,93	0
57	MG	1H	3410	1/1	0.95	0.08	108,108,108,108	0
57	MG	1H	3313	1/1	0.95	0.06	62,62,62,62	0
57	MG	14	3459	1/1	0.95	0.09	68,68,68,68	0
57	MG	1G	1601	1/1	0.95	0.13	92,92,92,92	0
57	MG	1H	3230	1/1	0.95	0.12	90,90,90,90	0
57	MG	14	3262	1/1	0.95	0.07	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3334	1/1	0.95	0.10	103,103,103,103	0
57	MG	14	3265	1/1	0.95	0.07	100,100,100,100	0
57	MG	13	1684	1/1	0.95	0.09	105,105,105,105	0
57	MG	14	3272	1/1	0.95	0.08	71,71,71,71	0
57	MG	14	3273	1/1	0.95	0.07	61,61,61,61	0
57	MG	1H	3419	1/1	0.95	0.24	73,73,73,73	0
57	MG	1J	209	1/1	0.95	0.05	131,131,131,131	0
57	MG	14	3276	1/1	0.95	0.10	85,85,85,85	0
57	MG	1H	3519	1/1	0.95	0.10	104,104,104,104	0
57	MG	1G	1654	1/1	0.95	0.12	102,102,102,102	0
57	MG	1G	1655	1/1	0.95	0.08	90,90,90,90	0
57	MG	1G	1656	1/1	0.95	0.07	89,89,89,89	0
57	MG	14	3300	1/1	0.95	0.09	86,86,86,86	0
57	MG	14	3301	1/1	0.95	0.14	89,89,89,89	0
57	MG	B5	101	1/1	0.95	0.09	99,99,99,99	0
57	MG	1H	3022	1/1	0.95	0.13	56,56,56,56	0
57	MG	1H	3524	1/1	0.95	0.09	61,61,61,61	0
57	MG	14	3311	1/1	0.95	0.07	84,84,84,84	0
57	MG	14	3312	1/1	0.95	0.06	109,109,109,109	0
57	MG	1H	3091	1/1	0.95	0.42	77,77,77,77	0
57	MG	14	3365	1/1	0.96	0.10	93,93,93,93	0
57	MG	1H	3299	1/1	0.96	0.10	105,105,105,105	0
57	MG	1H	3034	1/1	0.96	0.13	74,74,74,74	0
57	MG	1H	3472	1/1	0.96	0.12	63,63,63,63	0
57	MG	1H	3474	1/1	0.96	0.09	83,83,83,83	0
57	MG	1H	3480	1/1	0.96	0.23	90,90,90,90	0
57	MG	14	3374	1/1	0.96	0.05	94,94,94,94	0
57	MG	13	1705	1/1	0.96	0.05	108,108,108,108	0
57	MG	14	3377	1/1	0.96	0.13	72,72,72,72	0
57	MG	1G	1694	1/1	0.96	0.06	105,105,105,105	0
57	MG	1H	3387	1/1	0.96	0.07	87,87,87,87	0
57	MG	1G	1697	1/1	0.96	0.06	125,125,125,125	0
57	MG	14	3382	1/1	0.96	0.05	116,116,116,116	0
57	MG	14	3383	1/1	0.96	0.06	91,91,91,91	0
57	MG	1H	3306	1/1	0.96	0.07	79,79,79,79	0
57	MG	14	3385	1/1	0.96	0.19	82,82,82,82	0
57	MG	1H	3307	1/1	0.96	0.07	56,56,56,56	0
57	MG	14	3389	1/1	0.96	0.21	72,72,72,72	0
57	MG	14	3390	1/1	0.96	0.14	73,73,73,73	0
57	MG	1H	3394	1/1	0.96	0.12	83,83,83,83	0
57	MG	1G	1701	1/1	0.96	0.06	115,115,115,115	0
57	MG	1H	3311	1/1	0.96	0.09	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3221	1/1	0.96	0.06	65,65,65,65	0
57	MG	1H	3397	1/1	0.96	0.07	87,87,87,87	0
57	MG	14	3398	1/1	0.96	0.07	86,86,86,86	0
57	MG	1H	3312	1/1	0.96	0.10	69,69,69,69	0
57	MG	1H	3400	1/1	0.96	0.06	79,79,79,79	0
57	MG	14	3404	1/1	0.96	0.07	121,121,121,121	0
57	MG	13	1732	1/1	0.96	0.07	108,108,108,108	0
57	MG	1G	1708	1/1	0.96	0.11	127,127,127,127	0
57	MG	14	3248	1/1	0.96	0.07	76,76,76,76	0
57	MG	14	3250	1/1	0.96	0.12	84,84,84,84	0
57	MG	14	3254	1/1	0.96	0.11	87,87,87,87	0
57	MG	1H	3220	1/1	0.96	0.11	71,71,71,71	0
57	MG	1H	3333	1/1	0.96	0.06	98,98,98,98	0
57	MG	13	1734	1/1	0.96	0.10	143,143,143,143	0
57	MG	1H	3335	1/1	0.96	0.06	83,83,83,83	0
57	MG	1H	3337	1/1	0.96	0.06	98,98,98,98	0
57	MG	13	1686	1/1	0.96	0.08	107,107,107,107	0
57	MG	14	3267	1/1	0.96	0.09	119,119,119,119	0
57	MG	41	201	1/1	0.96	0.10	81,81,81,81	0
57	MG	1H	3108	1/1	0.96	0.17	68,68,68,68	0
57	MG	14	3049	1/1	0.96	0.16	69,69,69,69	0
57	MG	1H	3346	1/1	0.96	0.05	75,75,75,75	0
57	MG	2K	101	1/1	0.96	0.06	80,80,80,80	0
57	MG	14	3280	1/1	0.96	0.08	76,76,76,76	0
57	MG	1H	3511	1/1	0.96	0.04	113,113,113,113	0
57	MG	14	3433	1/1	0.96	0.13	90,90,90,90	0
57	MG	14	3287	1/1	0.96	0.06	74,74,74,74	0
57	MG	14	3436	1/1	0.96	0.06	136,136,136,136	0
57	MG	1H	3068	1/1	0.96	0.27	66,66,66,66	0
57	MG	14	3290	1/1	0.96	0.12	71,71,71,71	0
57	MG	14	3442	1/1	0.96	0.08	83,83,83,83	0
57	MG	1H	3255	1/1	0.96	0.07	72,72,72,72	0
57	MG	14	3293	1/1	0.96	0.06	70,70,70,70	0
57	MG	14	3294	1/1	0.96	0.06	66,66,66,66	0
57	MG	1H	3423	1/1	0.96	0.04	115,115,115,115	0
57	MG	1H	3356	1/1	0.96	0.07	79,79,79,79	0
57	MG	13	1709	1/1	0.96	0.06	128,128,128,128	0
57	MG	1H	3127	1/1	0.96	0.21	69,69,69,69	0
57	MG	1H	3128	1/1	0.96	0.06	66,66,66,66	0
57	MG	14	3307	1/1	0.96	0.09	80,80,80,80	0
57	MG	1H	3526	1/1	0.96	0.16	96,96,96,96	0
57	MG	1H	3363	1/1	0.96	0.06	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	1737	1/1	0.96	0.14	107,107,107,107	0
57	MG	14	3315	1/1	0.96	0.07	83,83,83,83	0
57	MG	14	3318	1/1	0.96	0.07	65,65,65,65	0
57	MG	14	3323	1/1	0.96	0.06	84,84,84,84	0
57	MG	1H	3365	1/1	0.96	0.10	82,82,82,82	0
57	MG	1G	1657	1/1	0.96	0.05	114,114,114,114	0
57	MG	14	3066	1/1	0.96	0.12	63,63,63,63	0
57	MG	1H	3276	1/1	0.96	0.11	80,80,80,80	0
57	MG	14	3335	1/1	0.96	0.06	94,94,94,94	0
57	MG	1G	1660	1/1	0.96	0.09	128,128,128,128	0
57	MG	1H	3448	1/1	0.96	0.23	76,76,76,76	0
57	MG	14	3339	1/1	0.96	0.04	106,106,106,106	0
57	MG	13	1697	1/1	0.96	0.08	110,110,110,110	0
57	MG	14	3343	1/1	0.96	0.10	84,84,84,84	0
57	MG	14	3345	1/1	0.96	0.10	100,100,100,100	0
57	MG	1H	3453	1/1	0.96	0.09	82,82,82,82	0
57	MG	1G	1669	1/1	0.96	0.07	114,114,114,114	0
57	MG	25	301	1/1	0.96	0.11	120,120,120,120	0
57	MG	1H	3046	1/1	0.96	0.09	43,43,43,43	0
57	MG	14	3189	1/1	0.96	0.22	81,81,81,81	0
57	MG	14	3352	1/1	0.96	0.06	95,95,95,95	0
57	MG	1H	3003	1/1	0.96	0.14	67,67,67,67	0
57	MG	1H	3456	1/1	0.96	0.09	92,92,92,92	0
57	MG	14	3357	1/1	0.96	0.10	116,116,116,116	0
59	ZN	G8	201	1/1	0.96	0.12	150,150,150,150	0
57	MG	1H	3032	1/1	0.96	0.18	68,68,68,68	0
57	MG	1H	3287	1/1	0.96	0.06	76,76,76,76	0
57	MG	1G	1683	1/1	0.96	0.10	132,132,132,132	0
57	MG	1H	3471	1/1	0.97	0.13	83,83,83,83	0
57	MG	14	3344	1/1	0.97	0.05	104,104,104,104	0
57	MG	1H	3382	1/1	0.97	0.07	43,43,43,43	0
57	MG	14	3346	1/1	0.97	0.05	98,98,98,98	0
57	MG	1H	3473	1/1	0.97	0.11	98,98,98,98	0
57	MG	13	1725	1/1	0.97	0.06	99,99,99,99	0
57	MG	1G	1658	1/1	0.97	0.05	97,97,97,97	0
57	MG	14	3350	1/1	0.97	0.05	88,88,88,88	0
57	MG	16	211	1/1	0.97	0.05	93,93,93,93	0
57	MG	1H	3477	1/1	0.97	0.16	91,91,91,91	0
57	MG	14	3354	1/1	0.97	0.08	80,80,80,80	0
57	MG	1G	1662	1/1	0.97	0.08	118,118,118,118	0
57	MG	13	1707	1/1	0.97	0.05	88,88,88,88	0
57	MG	14	3026	1/1	0.97	0.10	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3385	1/1	0.97	0.13	94,94,94,94	0
57	MG	13	1698	1/1	0.97	0.12	93,93,93,93	0
57	MG	14	3361	1/1	0.97	0.05	87,87,87,87	0
57	MG	13	1682	1/1	0.97	0.06	109,109,109,109	0
57	MG	1H	3317	1/1	0.97	0.07	70,70,70,70	0
57	MG	1G	1672	1/1	0.97	0.09	117,117,117,117	0
57	MG	14	3369	1/1	0.97	0.05	90,90,90,90	0
57	MG	1G	1673	1/1	0.97	0.07	80,80,80,80	0
57	MG	1H	3321	1/1	0.97	0.08	55,55,55,55	0
57	MG	1G	1675	1/1	0.97	0.05	86,86,86,86	0
57	MG	1G	1676	1/1	0.97	0.04	104,104,104,104	0
57	MG	1H	3325	1/1	0.97	0.06	88,88,88,88	0
57	MG	1H	3395	1/1	0.97	0.05	92,92,92,92	0
57	MG	1H	3243	1/1	0.97	0.05	63,63,63,63	0
57	MG	1H	3328	1/1	0.97	0.07	81,81,81,81	0
57	MG	14	3041	1/1	0.97	0.10	66,66,66,66	0
57	MG	13	1714	1/1	0.97	0.06	94,94,94,94	0
57	MG	13	1733	1/1	0.97	0.04	118,118,118,118	0
57	MG	13	1700	1/1	0.97	0.04	110,110,110,110	0
57	MG	13	1604	1/1	0.97	0.07	79,79,79,79	0
57	MG	1G	1691	1/1	0.97	0.06	104,104,104,104	0
57	MG	14	3210	1/1	0.97	0.06	78,78,78,78	0
57	MG	14	3211	1/1	0.97	0.07	67,67,67,67	0
57	MG	14	3213	1/1	0.97	0.10	70,70,70,70	0
57	MG	1H	3501	1/1	0.97	0.05	108,108,108,108	0
57	MG	1H	3262	1/1	0.97	0.06	59,59,59,59	0
57	MG	1H	3503	1/1	0.97	0.07	104,104,104,104	0
57	MG	1H	3405	1/1	0.97	0.07	75,75,75,75	0
57	MG	14	3396	1/1	0.97	0.05	71,71,71,71	0
57	MG	1H	3408	1/1	0.97	0.05	87,87,87,87	0
57	MG	1H	3339	1/1	0.97	0.06	99,99,99,99	0
57	MG	14	3229	1/1	0.97	0.07	74,74,74,74	0
57	MG	14	3230	1/1	0.97	0.05	56,56,56,56	0
57	MG	14	3233	1/1	0.97	0.09	85,85,85,85	0
57	MG	14	3238	1/1	0.97	0.08	67,67,67,67	0
57	MG	14	3241	1/1	0.97	0.07	61,61,61,61	0
57	MG	14	3407	1/1	0.97	0.14	111,111,111,111	0
57	MG	1H	3507	1/1	0.97	0.14	90,90,90,90	0
57	MG	14	3411	1/1	0.97	0.04	115,115,115,115	0
57	MG	1H	3508	1/1	0.97	0.17	144,144,144,144	0
57	MG	14	3247	1/1	0.97	0.12	87,87,87,87	0
57	MG	13	1619	1/1	0.97	0.08	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3343	1/1	0.97	0.07	115,115,115,115	0
57	MG	1H	3067	1/1	0.97	0.06	55,55,55,55	0
57	MG	1H	3104	1/1	0.97	0.12	68,68,68,68	0
57	MG	14	3256	1/1	0.97	0.08	99,99,99,99	0
57	MG	1H	3348	1/1	0.97	0.05	66,66,66,66	0
57	MG	14	3060	1/1	0.97	0.11	65,65,65,65	0
57	MG	14	3260	1/1	0.97	0.16	77,77,77,77	0
57	MG	1H	3350	1/1	0.97	0.06	58,58,58,58	0
57	MG	1H	3516	1/1	0.97	0.04	122,122,122,122	0
57	MG	14	3426	1/1	0.97	0.05	99,99,99,99	0
57	MG	1H	3351	1/1	0.97	0.14	66,66,66,66	0
57	MG	14	3428	1/1	0.97	0.04	110,110,110,110	0
57	MG	1H	3522	1/1	0.97	0.05	112,112,112,112	0
57	MG	14	3268	1/1	0.97	0.18	89,89,89,89	0
57	MG	1H	3271	1/1	0.97	0.07	84,84,84,84	0
57	MG	1H	3272	1/1	0.97	0.11	79,79,79,79	0
57	MG	14	3146	1/1	0.97	0.05	62,62,62,62	0
57	MG	1H	3355	1/1	0.97	0.07	58,58,58,58	0
57	MG	14	3437	1/1	0.97	0.07	111,111,111,111	0
57	MG	1H	3033	1/1	0.97	0.11	63,63,63,63	0
57	MG	14	3278	1/1	0.97	0.05	83,83,83,83	0
57	MG	14	3279	1/1	0.97	0.06	93,93,93,93	0
57	MG	1H	3428	1/1	0.97	0.06	93,93,93,93	0
57	MG	14	3282	1/1	0.97	0.06	82,82,82,82	0
57	MG	1H	3431	1/1	0.97	0.05	102,102,102,102	0
57	MG	14	3446	1/1	0.97	0.04	118,118,118,118	0
57	MG	14	3286	1/1	0.97	0.06	58,58,58,58	0
57	MG	1H	3531	1/1	0.97	0.05	114,114,114,114	0
57	MG	14	3288	1/1	0.97	0.07	59,59,59,59	0
57	MG	1H	3277	1/1	0.97	0.09	79,79,79,79	0
57	MG	1H	3433	1/1	0.97	0.06	98,98,98,98	0
57	MG	13	1720	1/1	0.97	0.04	121,121,121,121	0
57	MG	13	1694	1/1	0.97	0.06	92,92,92,92	0
57	MG	1H	3231	1/1	0.97	0.06	103,103,103,103	0
57	MG	14	3077	1/1	0.97	0.15	85,85,85,85	0
57	MG	14	3296	1/1	0.97	0.06	76,76,76,76	0
57	MG	14	3297	1/1	0.97	0.06	90,90,90,90	0
57	MG	1H	3442	1/1	0.97	0.04	107,107,107,107	0
57	MG	1H	3443	1/1	0.97	0.05	112,112,112,112	0
57	MG	13	1685	1/1	0.97	0.06	79,79,79,79	0
57	MG	14	3305	1/1	0.97	0.07	64,64,64,64	0
57	MG	1H	3037	1/1	0.97	0.08	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3446	1/1	0.97	0.04	100,100,100,100	0
57	MG	1H	3544	1/1	0.97	0.06	105,105,105,105	0
57	MG	1J	206	1/1	0.97	0.04	99,99,99,99	0
57	MG	14	3164	1/1	0.97	0.04	83,83,83,83	0
57	MG	1H	3295	1/1	0.97	0.06	58,58,58,58	0
57	MG	1H	3296	1/1	0.97	0.06	56,56,56,56	0
57	MG	1H	3038	1/1	0.97	0.07	61,61,61,61	0
57	MG	14	3320	1/1	0.97	0.07	70,70,70,70	0
57	MG	14	3321	1/1	0.97	0.08	89,89,89,89	0
57	MG	1H	3372	1/1	0.97	0.17	66,66,66,66	0
57	MG	1H	3373	1/1	0.97	0.12	79,79,79,79	0
57	MG	14	3326	1/1	0.97	0.11	87,87,87,87	0
57	MG	1H	3375	1/1	0.97	0.05	80,80,80,80	0
57	MG	1H	3457	1/1	0.97	0.06	102,102,102,102	0
57	MG	1H	3132	1/1	0.97	0.14	55,55,55,55	0
57	MG	1H	3039	1/1	0.97	0.05	56,56,56,56	0
57	MG	1H	3462	1/1	0.97	0.05	99,99,99,99	0
57	MG	M5	101	1/1	0.97	0.26	81,81,81,81	0
57	MG	14	3337	1/1	0.97	0.04	116,116,116,116	0
57	MG	13	1680	1/1	0.97	0.06	89,89,89,89	0
57	MG	1H	3465	1/1	0.97	0.07	112,112,112,112	0
57	MG	1H	3381	1/1	0.97	0.06	58,58,58,58	0
57	MG	13	1738	1/1	0.98	0.06	138,138,138,138	0
57	MG	14	3342	1/1	0.98	0.05	105,105,105,105	0
57	MG	1H	3409	1/1	0.98	0.07	83,83,83,83	0
57	MG	1H	3275	1/1	0.98	0.06	72,72,72,72	0
57	MG	13	1730	1/1	0.98	0.05	110,110,110,110	0
57	MG	1H	3475	1/1	0.98	0.05	99,99,99,99	0
57	MG	1H	3476	1/1	0.98	0.13	94,94,94,94	0
57	MG	1H	3412	1/1	0.98	0.07	90,90,90,90	0
57	MG	1H	3478	1/1	0.98	0.07	79,79,79,79	0
57	MG	1H	3319	1/1	0.98	0.04	58,58,58,58	0
57	MG	1H	3366	1/1	0.98	0.04	56,56,56,56	0
57	MG	14	3013	1/1	0.98	0.11	56,56,56,56	0
57	MG	14	3353	1/1	0.98	0.11	89,89,89,89	0
57	MG	1H	3483	1/1	0.98	0.04	99,99,99,99	0
57	MG	1H	3416	1/1	0.98	0.04	80,80,80,80	0
57	MG	13	1716	1/1	0.98	0.07	116,116,116,116	0
57	MG	1H	3323	1/1	0.98	0.08	78,78,78,78	0
57	MG	1H	3487	1/1	0.98	0.04	108,108,108,108	0
57	MG	1H	3324	1/1	0.98	0.06	69,69,69,69	0
57	MG	1H	3278	1/1	0.98	0.04	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1661	1/1	0.98	0.15	118,118,118,118	0
57	MG	14	3364	1/1	0.98	0.03	98,98,98,98	0
57	MG	1H	3490	1/1	0.98	0.10	95,95,95,95	0
57	MG	14	3366	1/1	0.98	0.04	99,99,99,99	0
57	MG	14	3367	1/1	0.98	0.07	101,101,101,101	0
57	MG	1H	3242	1/1	0.98	0.04	50,50,50,50	0
57	MG	1G	1664	1/1	0.98	0.06	82,82,82,82	0
57	MG	1G	1665	1/1	0.98	0.06	82,82,82,82	0
57	MG	14	3216	1/1	0.98	0.12	62,62,62,62	0
57	MG	14	3217	1/1	0.98	0.04	76,76,76,76	0
57	MG	1H	3106	1/1	0.98	0.09	73,73,73,73	0
57	MG	1H	3376	1/1	0.98	0.04	71,71,71,71	0
57	MG	14	3223	1/1	0.98	0.10	61,61,61,61	0
57	MG	14	3376	1/1	0.98	0.05	82,82,82,82	0
57	MG	14	3224	1/1	0.98	0.05	76,76,76,76	0
57	MG	1G	1668	1/1	0.98	0.06	106,106,106,106	0
57	MG	1H	3426	1/1	0.98	0.14	82,82,82,82	0
57	MG	14	3380	1/1	0.98	0.09	106,106,106,106	0
57	MG	1H	3284	1/1	0.98	0.05	62,62,62,62	0
57	MG	14	3031	1/1	0.98	0.14	51,51,51,51	0
57	MG	14	3231	1/1	0.98	0.06	78,78,78,78	0
57	MG	1G	1671	1/1	0.98	0.05	101,101,101,101	0
57	MG	14	3236	1/1	0.98	0.05	69,69,69,69	0
57	MG	14	3386	1/1	0.98	0.12	65,65,65,65	0
57	MG	1H	3498	1/1	0.98	0.04	113,113,113,113	0
57	MG	14	3239	1/1	0.98	0.06	60,60,60,60	0
57	MG	1H	3118	1/1	0.98	0.07	63,63,63,63	0
57	MG	F8	101	1/1	0.98	0.10	85,85,85,85	0
57	MG	14	3244	1/1	0.98	0.06	68,68,68,68	0
57	MG	14	3393	1/1	0.98	0.06	89,89,89,89	0
57	MG	I8	101	1/1	0.98	0.07	95,95,95,95	0
57	MG	1H	3429	1/1	0.98	0.05	87,87,87,87	0
57	MG	1H	3430	1/1	0.98	0.08	94,94,94,94	0
57	MG	1G	1679	1/1	0.98	0.14	105,105,105,105	0
57	MG	14	3252	1/1	0.98	0.04	69,69,69,69	0
57	MG	1H	3248	1/1	0.98	0.05	57,57,57,57	0
57	MG	1H	3336	1/1	0.98	0.04	88,88,88,88	0
57	MG	14	3401	1/1	0.98	0.15	89,89,89,89	0
57	MG	14	3402	1/1	0.98	0.05	111,111,111,111	0
57	MG	14	3403	1/1	0.98	0.04	78,78,78,78	0
57	MG	1G	1682	1/1	0.98	0.09	123,123,123,123	0
57	MG	13	1717	1/1	0.98	0.07	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3258	1/1	0.98	0.07	97,97,97,97	0
57	MG	1H	3289	1/1	0.98	0.05	91,91,91,91	0
57	MG	14	3408	1/1	0.98	0.04	77,77,77,77	0
57	MG	14	3409	1/1	0.98	0.10	87,87,87,87	0
57	MG	1G	1685	1/1	0.98	0.05	129,129,129,129	0
57	MG	14	3261	1/1	0.98	0.07	64,64,64,64	0
57	MG	1H	3291	1/1	0.98	0.05	57,57,57,57	0
57	MG	1H	3340	1/1	0.98	0.04	109,109,109,109	0
57	MG	14	3264	1/1	0.98	0.07	88,88,88,88	0
57	MG	1H	3437	1/1	0.98	0.07	76,76,76,76	0
57	MG	14	3416	1/1	0.98	0.04	87,87,87,87	0
57	MG	14	3266	1/1	0.98	0.04	77,77,77,77	0
57	MG	14	3418	1/1	0.98	0.05	97,97,97,97	0
57	MG	1G	1689	1/1	0.98	0.07	92,92,92,92	0
57	MG	1G	1690	1/1	0.98	0.07	113,113,113,113	0
57	MG	14	3269	1/1	0.98	0.05	104,104,104,104	0
57	MG	1H	3441	1/1	0.98	0.06	100,100,100,100	0
57	MG	14	3271	1/1	0.98	0.05	67,67,67,67	0
57	MG	1H	3294	1/1	0.98	0.12	68,68,68,68	0
57	MG	13	1690	1/1	0.98	0.04	117,117,117,117	0
57	MG	14	3274	1/1	0.98	0.07	62,62,62,62	0
57	MG	1H	3390	1/1	0.98	0.08	48,48,48,48	0
57	MG	1G	1695	1/1	0.98	0.09	126,126,126,126	0
57	MG	1H	3345	1/1	0.98	0.09	85,85,85,85	0
57	MG	13	1687	1/1	0.98	0.07	89,89,89,89	0
57	MG	1H	3515	1/1	0.98	0.07	78,78,78,78	0
57	MG	14	3432	1/1	0.98	0.12	103,103,103,103	0
57	MG	14	3281	1/1	0.98	0.10	75,75,75,75	0
57	MG	1H	3447	1/1	0.98	0.03	98,98,98,98	0
57	MG	14	3435	1/1	0.98	0.04	122,122,122,122	0
57	MG	1H	3517	1/1	0.98	0.20	85,85,85,85	0
57	MG	14	3285	1/1	0.98	0.05	89,89,89,89	0
57	MG	1H	3297	1/1	0.98	0.06	56,56,56,56	0
57	MG	1H	3520	1/1	0.98	0.06	88,88,88,88	0
57	MG	14	3440	1/1	0.98	0.15	87,87,87,87	0
57	MG	14	3441	1/1	0.98	0.13	103,103,103,103	0
57	MG	1H	3521	1/1	0.98	0.04	65,65,65,65	0
57	MG	1H	3449	1/1	0.98	0.11	92,92,92,92	0
57	MG	1G	1705	1/1	0.98	0.03	117,117,117,117	0
57	MG	1H	3450	1/1	0.98	0.07	87,87,87,87	0
57	MG	13	1726	1/1	0.98	0.06	107,107,107,107	0
57	MG	2K	102	1/1	0.98	0.11	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3302	1/1	0.98	0.05	54,54,54,54	0
57	MG	14	3449	1/1	0.98	0.05	105,105,105,105	0
57	MG	1G	1710	1/1	0.98	0.04	113,113,113,113	0
57	MG	1H	3527	1/1	0.98	0.04	97,97,97,97	0
57	MG	1H	3398	1/1	0.98	0.04	86,86,86,86	0
57	MG	1H	3529	1/1	0.98	0.04	110,110,110,110	0
57	MG	1H	3266	1/1	0.98	0.10	92,92,92,92	0
57	MG	14	3303	1/1	0.98	0.04	52,52,52,52	0
57	MG	1G	1715	1/1	0.98	0.05	110,110,110,110	0
57	MG	1H	3305	1/1	0.98	0.07	72,72,72,72	0
57	MG	1G	1717	1/1	0.98	0.04	126,126,126,126	0
57	MG	14	3309	1/1	0.98	0.04	48,48,48,48	0
57	MG	14	3310	1/1	0.98	0.04	71,71,71,71	0
57	MG	1G	1718	1/1	0.98	0.04	124,124,124,124	0
57	MG	1H	3458	1/1	0.98	0.12	89,89,89,89	0
57	MG	14	3313	1/1	0.98	0.06	67,67,67,67	0
57	MG	13	1695	1/1	0.98	0.05	91,91,91,91	0
57	MG	1H	3198	1/1	0.98	0.24	75,75,75,75	0
57	MG	1H	3461	1/1	0.98	0.05	80,80,80,80	0
57	MG	14	3319	1/1	0.98	0.09	72,72,72,72	0
57	MG	1H	3403	1/1	0.98	0.07	68,68,68,68	0
57	MG	1G	1724	1/1	0.98	0.06	126,126,126,126	0
57	MG	1H	3308	1/1	0.98	0.06	62,62,62,62	0
57	MG	1H	3538	1/1	0.98	0.05	107,107,107,107	0
57	MG	14	3325	1/1	0.98	0.04	88,88,88,88	0
57	MG	1H	3464	1/1	0.98	0.12	57,57,57,57	0
57	MG	14	3327	1/1	0.98	0.05	108,108,108,108	0
57	MG	13	1721	1/1	0.98	0.11	77,77,77,77	0
57	MG	14	3329	1/1	0.98	0.13	93,93,93,93	0
57	MG	14	3332	1/1	0.98	0.08	63,63,63,63	0
57	MG	1H	3406	1/1	0.98	0.03	95,95,95,95	0
57	MG	7A	101	1/1	0.98	0.16	110,110,110,110	0
57	MG	1H	3542	1/1	0.98	0.04	103,103,103,103	0
57	MG	1H	3468	1/1	0.98	0.05	82,82,82,82	0
58	SF4	3E	301	8/8	0.98	0.04	95,98,106,108	0
57	MG	1H	3469	1/1	0.98	0.06	84,84,84,84	0
57	MG	14	3001	1/1	0.98	0.05	51,51,51,51	0
57	MG	1H	3470	1/1	0.98	0.11	105,105,105,105	0
57	MG	14	3340	1/1	0.98	0.06	63,63,63,63	0
57	MG	1H	3273	1/1	0.99	0.07	56,56,56,56	0
57	MG	1H	3318	1/1	0.99	0.08	74,74,74,74	0
57	MG	1H	3274	1/1	0.99	0.03	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3378	1/1	0.99	0.04	54,54,54,54	0
57	MG	14	3277	1/1	0.99	0.11	64,64,64,64	0
57	MG	1H	3320	1/1	0.99	0.03	71,71,71,71	0
57	MG	13	1729	1/1	0.99	0.04	110,110,110,110	0
57	MG	14	3387	1/1	0.99	0.08	83,83,83,83	0
57	MG	1H	3244	1/1	0.99	0.04	47,47,47,47	0
57	MG	1H	3245	1/1	0.99	0.08	58,58,58,58	0
57	MG	13	1688	1/1	0.99	0.04	96,96,96,96	0
57	MG	14	3283	1/1	0.99	0.05	105,105,105,105	0
57	MG	1H	3247	1/1	0.99	0.05	67,67,67,67	0
57	MG	1H	3327	1/1	0.99	0.10	81,81,81,81	0
57	MG	1H	3280	1/1	0.99	0.03	47,47,47,47	0
57	MG	1H	3329	1/1	0.99	0.04	53,53,53,53	0
57	MG	14	3192	1/1	0.99	0.03	80,80,80,80	0
57	MG	1H	3388	1/1	0.99	0.10	49,49,49,49	0
57	MG	1H	3330	1/1	0.99	0.03	74,74,74,74	0
57	MG	1H	3331	1/1	0.99	0.03	88,88,88,88	0
57	MG	14	3292	1/1	0.99	0.08	71,71,71,71	0
57	MG	13	1708	1/1	0.99	0.03	91,91,91,91	0
57	MG	1H	3393	1/1	0.99	0.04	63,63,63,63	0
57	MG	1H	3282	1/1	0.99	0.10	54,54,54,54	0
57	MG	13	1676	1/1	0.99	0.03	67,67,67,67	0
57	MG	1H	3250	1/1	0.99	0.04	54,54,54,54	0
57	MG	14	3298	1/1	0.99	0.03	95,95,95,95	0
57	MG	1H	3252	1/1	0.99	0.04	52,52,52,52	0
57	MG	1H	3253	1/1	0.99	0.04	58,58,58,58	0
57	MG	1H	3288	1/1	0.99	0.04	58,58,58,58	0
57	MG	1H	3467	1/1	0.99	0.12	74,74,74,74	0
57	MG	14	3304	1/1	0.99	0.04	61,61,61,61	0
57	MG	1H	3254	1/1	0.99	0.04	49,49,49,49	0
57	MG	1H	3290	1/1	0.99	0.08	87,87,87,87	0
57	MG	1H	3342	1/1	0.99	0.05	83,83,83,83	0
57	MG	14	3308	1/1	0.99	0.06	64,64,64,64	0
57	MG	14	3208	1/1	0.99	0.10	63,63,63,63	0
57	MG	14	3209	1/1	0.99	0.05	61,61,61,61	0
57	MG	13	1710	1/1	0.99	0.08	73,73,73,73	0
57	MG	1H	3344	1/1	0.99	0.04	60,60,60,60	0
57	MG	14	3212	1/1	0.99	0.05	60,60,60,60	0
57	MG	1H	3292	1/1	0.99	0.03	62,62,62,62	0
57	MG	1H	3546	1/1	0.99	0.06	105,105,105,105	0
57	MG	14	3316	1/1	0.99	0.03	100,100,100,100	0
57	MG	14	3317	1/1	0.99	0.03	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3258	1/1	0.99	0.04	56,56,56,56	0
57	MG	1H	3407	1/1	0.99	0.04	69,69,69,69	0
57	MG	1H	3259	1/1	0.99	0.04	59,59,59,59	0
57	MG	14	3218	1/1	0.99	0.04	55,55,55,55	0
57	MG	14	3322	1/1	0.99	0.03	58,58,58,58	0
57	MG	14	3219	1/1	0.99	0.02	59,59,59,59	0
57	MG	14	3220	1/1	0.99	0.06	65,65,65,65	0
57	MG	1H	3260	1/1	0.99	0.05	70,70,70,70	0
57	MG	1H	3349	1/1	0.99	0.04	61,61,61,61	0
57	MG	1H	3479	1/1	0.99	0.03	95,95,95,95	0
57	MG	13	1711	1/1	0.99	0.04	70,70,70,70	0
57	MG	13	1702	1/1	0.99	0.04	70,70,70,70	0
57	MG	14	3330	1/1	0.99	0.04	94,94,94,94	0
57	MG	14	3331	1/1	0.99	0.02	56,56,56,56	0
57	MG	14	3227	1/1	0.99	0.04	52,52,52,52	0
57	MG	1H	3482	1/1	0.99	0.06	107,107,107,107	0
57	MG	1H	3352	1/1	0.99	0.04	70,70,70,70	0
57	MG	1H	3414	1/1	0.99	0.06	52,52,52,52	0
57	MG	1H	3300	1/1	0.99	0.04	73,73,73,73	0
57	MG	14	3232	1/1	0.99	0.04	75,75,75,75	0
57	MG	1H	3263	1/1	0.99	0.06	53,53,53,53	0
57	MG	14	3234	1/1	0.99	0.03	62,62,62,62	0
57	MG	14	3235	1/1	0.99	0.03	55,55,55,55	0
57	MG	1H	3417	1/1	0.99	0.03	100,100,100,100	0
57	MG	14	3237	1/1	0.99	0.04	67,67,67,67	0
57	MG	13	1713	1/1	0.99	0.05	96,96,96,96	0
57	MG	1H	3265	1/1	0.99	0.06	74,74,74,74	0
57	MG	14	3240	1/1	0.99	0.11	63,63,63,63	0
57	MG	1H	3357	1/1	0.99	0.07	64,64,64,64	0
57	MG	14	3242	1/1	0.99	0.04	82,82,82,82	0
57	MG	16	212	1/1	0.99	0.02	78,78,78,78	0
57	MG	13	1681	1/1	0.99	0.11	91,91,91,91	0
57	MG	1H	3359	1/1	0.99	0.06	92,92,92,92	0
57	MG	14	3246	1/1	0.99	0.10	93,93,93,93	0
57	MG	1H	3267	1/1	0.99	0.05	103,103,103,103	0
57	MG	1H	3361	1/1	0.99	0.04	53,53,53,53	0
57	MG	14	3249	1/1	0.99	0.09	85,85,85,85	0
57	MG	1H	3495	1/1	0.99	0.05	87,87,87,87	0
57	MG	14	3251	1/1	0.99	0.15	113,113,113,113	0
57	MG	1H	3496	1/1	0.99	0.09	89,89,89,89	0
57	MG	14	3358	1/1	0.99	0.08	78,78,78,78	0
57	MG	14	3253	1/1	0.99	0.03	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3425	1/1	0.99	0.04	81,81,81,81	0
57	MG	13	1677	1/1	0.99	0.04	90,90,90,90	0
57	MG	1H	3269	1/1	0.99	0.05	83,83,83,83	0
57	MG	14	3363	1/1	0.99	0.02	83,83,83,83	0
57	MG	1H	3309	1/1	0.99	0.03	73,73,73,73	0
57	MG	I8	102	1/1	0.99	0.09	70,70,70,70	0
57	MG	1H	3310	1/1	0.99	0.02	76,76,76,76	0
57	MG	1H	3005	1/1	0.99	0.10	67,67,67,67	0
57	MG	1H	3367	1/1	0.99	0.08	69,69,69,69	0
57	MG	1H	3368	1/1	0.99	0.09	72,72,72,72	0
57	MG	1G	1677	1/1	0.99	0.03	83,83,83,83	0
57	MG	13	1620	1/1	0.99	0.05	68,68,68,68	0
57	MG	13	1693	1/1	0.99	0.08	95,95,95,95	0
57	MG	1H	3314	1/1	0.99	0.09	65,65,65,65	0
57	MG	1H	3315	1/1	0.99	0.04	61,61,61,61	0
57	MG	1H	3316	1/1	0.99	0.04	76,76,76,76	0
58	SF4	32	302	8/8	0.99	0.04	115,120,128,136	0
57	MG	1H	3438	1/1	0.99	0.03	95,95,95,95	0
59	ZN	5A	101	1/1	0.99	0.04	129,129,129,129	0
57	MG	1H	3439	1/1	0.99	0.04	76,76,76,76	0
57	MG	1H	3440	1/1	0.99	0.08	83,83,83,83	0
57	MG	1H	3374	1/1	0.99	0.08	57,57,57,57	0
57	MG	1H	3332	1/1	1.00	0.03	84,84,84,84	0
57	MG	1H	3322	1/1	1.00	0.03	59,59,59,59	0
57	MG	14	3299	1/1	1.00	0.05	63,63,63,63	0
57	MG	1H	3389	1/1	1.00	0.05	63,63,63,63	0
57	MG	1H	3257	1/1	1.00	0.03	49,49,49,49	0
57	MG	14	3226	1/1	1.00	0.03	54,54,54,54	0
57	MG	1H	3451	1/1	1.00	0.01	55,55,55,55	0
57	MG	1H	3283	1/1	1.00	0.03	59,59,59,59	0
57	MG	1H	3518	1/1	1.00	0.03	57,57,57,57	0
57	MG	1H	3186	1/1	1.00	0.02	56,56,56,56	0
57	MG	1H	3298	1/1	1.00	0.03	52,52,52,52	0
59	ZN	5I	101	1/1	1.00	0.02	94,94,94,94	0
57	MG	1H	3251	1/1	1.00	0.05	49,49,49,49	0
57	MG	13	1679	1/1	1.00	0.03	89,89,89,89	0
57	MG	1H	3293	1/1	1.00	0.02	60,60,60,60	0
57	MG	1H	3256	1/1	1.00	0.02	48,48,48,48	0
57	MG	1H	3303	1/1	1.00	0.03	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.