



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 16, 2026 – 05:03 am BST

PDB ID : 5EL7 / pdb_00005el7
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA^{Lys} in the A-site with a U-U mismatch in the second position and antibiotic paromomycin
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-11-04
Resolution : 3.15 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

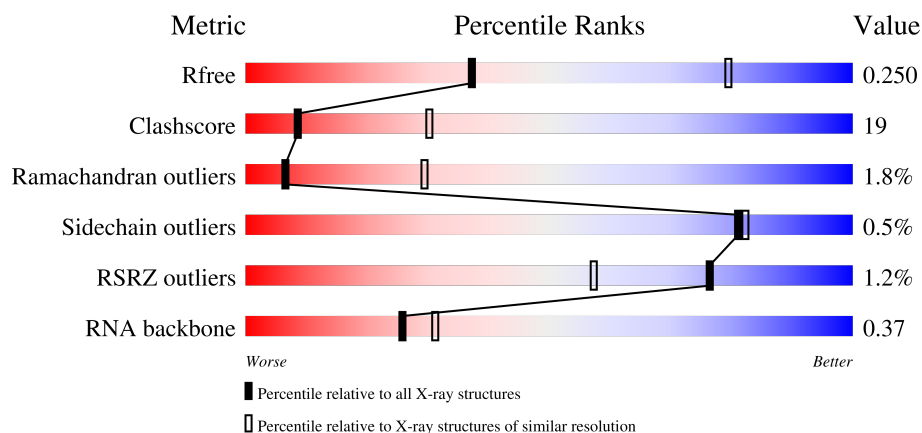
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

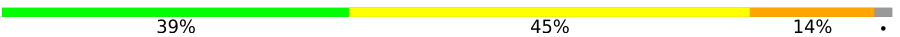
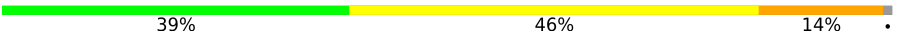
The reported resolution of this entry is 3.15 Å.

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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

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	
1	1G	1522	
2	12	256	

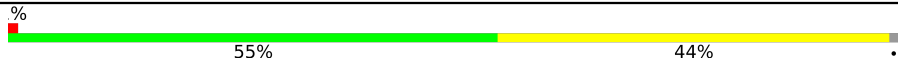
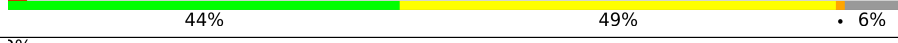
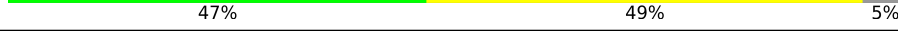
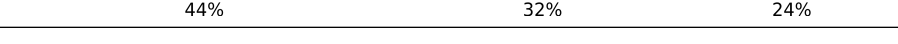
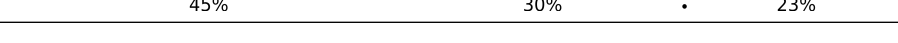
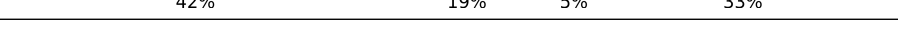
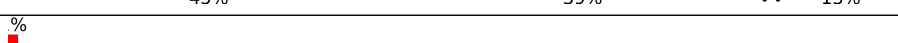
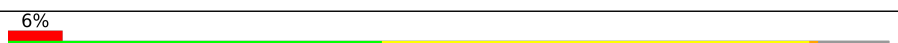
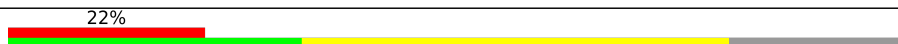
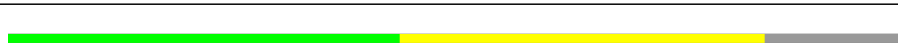
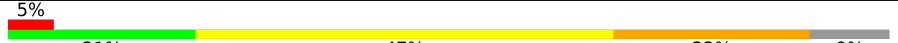
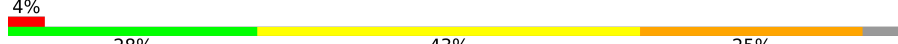
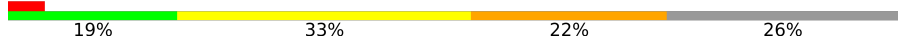
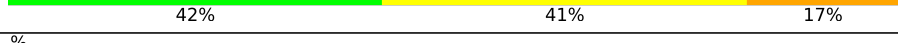
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Mol	Chain	Length	Quality of chain
2	1E	256	
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	

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

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

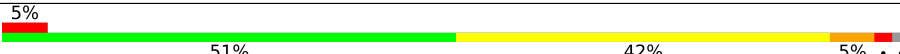
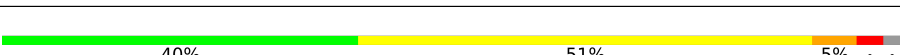
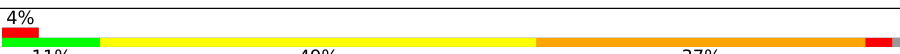
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Mol	Chain	Length	Quality of chain
40	A8	112	
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50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

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Mol	Chain	Length	Quality of chain
53	N8	60	
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	
56	3L	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	1625	-	-	-	X
57	MG	13	1659	-	-	-	X
57	MG	14	3035	-	-	-	X
57	MG	14	3170	-	-	-	X
57	MG	1H	3211	-	-	-	X
59	SF4	32	301	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296184 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1506	Total	C	N	O	P	0	0	0
			32368	14408	5999	10456	1505			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	-	expression tag	GB 55771382
13	1543	C	-	expression tag	GB 55771382
13	1544	U	-	expression tag	GB 55771382
1G	1542	G	-	expression tag	GB 55771382
1G	1543	C	-	expression tag	GB 55771382
1G	1544	U	-	expression tag	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	210	Total	C	N	O	S	0	0	0
			1721	1100	309	308	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	196	Total	C	N	O	S	0	0	0
			1541	975	298	267	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
			1690	1058	336	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	148	Total	C	N	O	S	0	0	0
			1134	718	215	197	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	139	Total	C	N	O	S	0	0	0
			1115	692	222	195	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				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	91	Total	C	N	O	S	0	0	0
			734	459	144	130	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	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	119	Total	C	N	O	S	0	0	0
			942	582	194	164	2			
13	4A	111	Total	C	N	O	S	0	0	0
			893	552	183	156	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	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	88	Total	C	N	O	S	0	0	0
			733	459	147	125	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	81	Total	C	N	O	S	0	0	0
			654	417	122	113	2			
19	AA	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

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

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

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

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

- Molecule 22 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	69	Total	C	N	O	P	S	0	0	0
			1477	662	257	488	69	1			
22	1L	73	Total	C	N	O	P	S	0	0	0
			1563	700	271	518	73	1			

- Molecule 23 is a RNA chain called E. coli 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	76	Total	C	N	O	P	0	0	0
			1611	721	281	534	75			

- 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
			439	197	91	131	20			
25	4L	19	Total	C	N	O	P	0	0	0
			417	187	86	125	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2833	Total	C	N	O	P	0	0	0
			61028	27159	11418	19618	2833			
26	14	2861	Total	C	N	O	P	0	0	0
			61630	27429	11535	19806	2860			

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 rRNA.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
29	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	179	Total	C	N	O	S	0	0	0
			1458	931	266	257	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	74	Total	C	N	O	S	0	0	0
			573	359	117	97				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
35	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1113	709	210	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
			875	550	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	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	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
			774	499	141	133	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
44	A5	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			743	482	134	126	1			
45	B5	94	Total	C	N	O	S	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	105	Total	C	N	O	S	0	0	0
			796	513	150	128	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	171	Total	C	N	O	S	0	0	0
			1373	876	247	247	3			
47	D5	132	Total	C	N	O	S	0	0	0
			1074	691	193	188	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	76	Total	C	N	O	S	0	0	0
			606	376	128	101	1			
48	E5	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			568	352	115	100	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	G5	66	Total	C	N	O	S	0	0	0
			558	346	113	98	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	47	Total	C	N	O	S	0	0	0
			366	234	61	66	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	3L	75	Total	C	N	O	P	0	0	0
			1601	717	280	530	74			

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

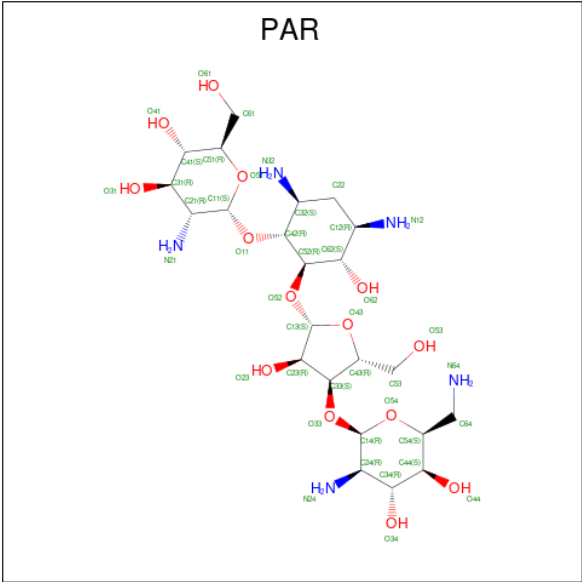
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	150	Total	Mg	0	0
			150	150		
57	5E	1	Total	Mg	0	0
			1	1		
57	1I	1	Total	Mg	0	0
			1	1		
57	3I	1	Total	Mg	0	0
			1	1		
57	5I	1	Total	Mg	0	0
			1	1		
57	BI	1	Total	Mg	0	0
			1	1		
57	2K	3	Total	Mg	0	0
			3	3		
57	1H	502	Total	Mg	0	0
			502	502		
57	16	12	Total	Mg	0	0
			12	12		
57	11	3	Total	Mg	0	0
			3	3		
57	21	3	Total	Mg	0	0
			3	3		
57	31	1	Total	Mg	0	0
			1	1		
57	41	2	Total	Mg	0	0
			2	2		
57	78	1	Total	Mg	0	0
			1	1		
57	88	1	Total	Mg	0	0
			1	1		
57	I8	1	Total	Mg	0	0
			1	1		
57	L8	1	Total	Mg	0	0
			1	1		
57	P8	1	Total	Mg	0	0
			1	1		
57	Q8	1	Total	Mg	0	0
			1	1		

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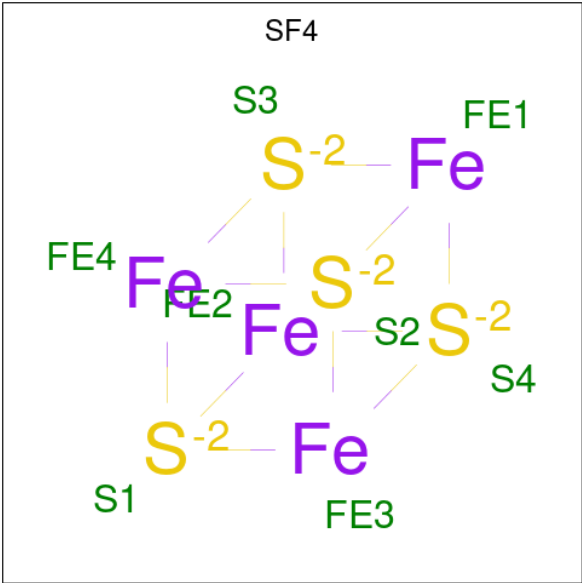
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	93	Total 93	Mg 93	0	0
57	7A	1	Total 1	Mg 1	0	0
57	2L	4	Total 4	Mg 4	0	0
57	14	454	Total 454	Mg 454	0	0
57	1J	6	Total 6	Mg 6	0	0
57	29	4	Total 4	Mg 4	0	0
57	39	2	Total 2	Mg 2	0	0
57	35	2	Total 2	Mg 2	0	0
57	45	3	Total 3	Mg 3	0	0
57	55	1	Total 1	Mg 1	0	0
57	85	1	Total 1	Mg 1	0	0
57	C5	1	Total 1	Mg 1	0	0
57	E5	1	Total 1	Mg 1	0	0
57	M5	1	Total 1	Mg 1	0	0

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	13	1	Total	C	N	O	0	0
			42	23	5	14		
58	1G	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	3E	1	Total	Fe	S	0	0
			8	4	4		
59	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	5I	1	Total 1	Zn 1	0	0
60	G8	1	Total 1	Zn 1	0	0
60	5A	1	Total 1	Zn 1	0	0
60	C5	1	Total 1	Zn 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	319	Total 319	O 319	0	0
61	3E	3	Total 3	O 3	0	0
61	4E	3	Total 3	O 3	0	0
61	8E	1	Total 1	O 1	0	0
61	1I	1	Total 1	O 1	0	0
61	3I	3	Total 3	O 3	0	0
61	5I	1	Total 1	O 1	0	0
61	6I	2	Total 2	O 2	0	0
61	8I	2	Total 2	O 2	0	0
61	BI	5	Total 5	O 5	0	0
61	1F	1	Total 1	O 1	0	0
61	1K	1	Total 1	O 1	0	0
61	2K	7	Total 7	O 7	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1H	1158	Total 1158	O 1158	0	0
61	16	26	Total 26	O 26	0	0
61	11	12	Total 12	O 12	0	0
61	21	6	Total 6	O 6	0	0
61	31	9	Total 9	O 9	0	0
61	58	1	Total 1	O 1	0	0
61	78	6	Total 6	O 6	0	0
61	88	2	Total 2	O 2	0	0
61	C8	2	Total 2	O 2	0	0
61	E8	3	Total 3	O 3	0	0
61	F8	2	Total 2	O 2	0	0
61	G8	2	Total 2	O 2	0	0
61	I8	5	Total 5	O 5	0	0
61	J8	3	Total 3	O 3	0	0
61	K8	2	Total 2	O 2	0	0
61	L8	2	Total 2	O 2	0	0
61	P8	1	Total 1	O 1	0	0
61	Q8	9	Total 9	O 9	0	0
61	1G	226	Total 226	O 226	0	0
61	32	3	Total 3	O 3	0	0
61	42	1	Total 1	O 1	0	0

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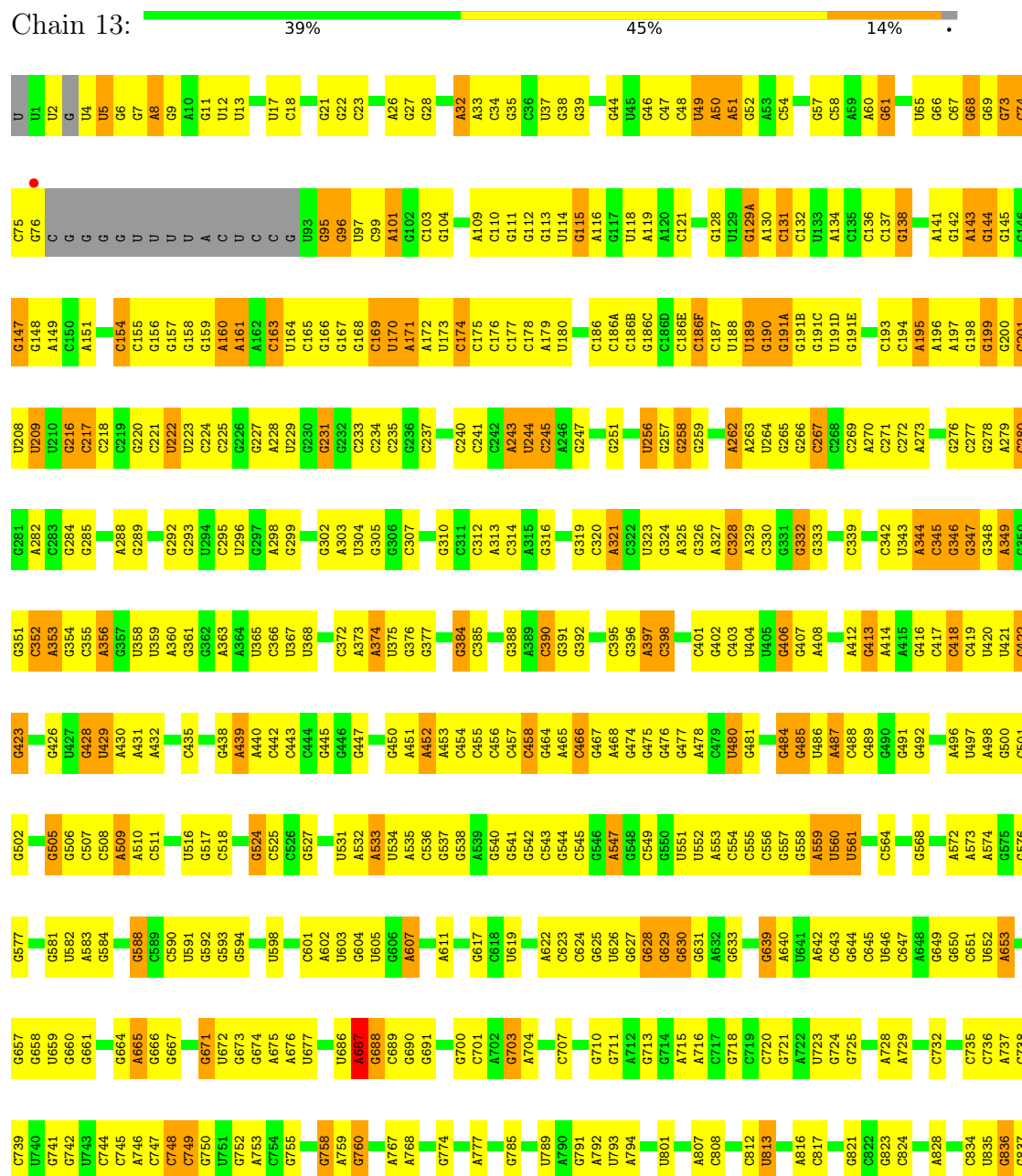
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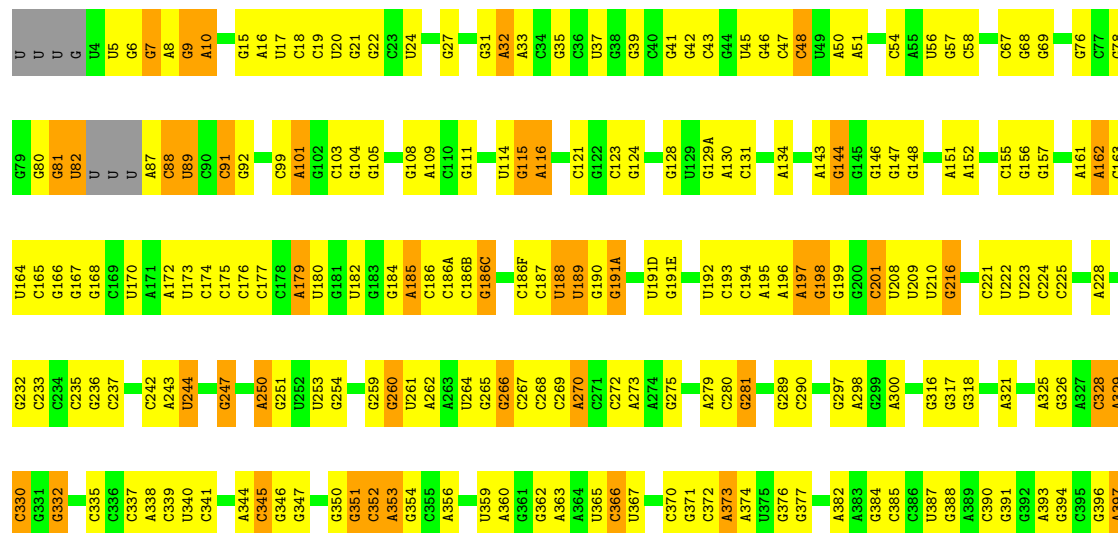
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	3A	1	Total 1	O 1	0	0
61	6A	3	Total 3	O 3	0	0
61	8A	1	Total 1	O 1	0	0
61	BA	3	Total 3	O 3	0	0
61	2L	1	Total 1	O 1	0	0
61	4L	3	Total 3	O 3	0	0
61	14	1015	Total 1015	O 1015	0	0
61	1J	18	Total 18	O 18	0	0
61	19	12	Total 12	O 12	0	0
61	29	6	Total 6	O 6	0	0
61	39	8	Total 8	O 8	0	0
61	35	5	Total 5	O 5	0	0
61	55	1	Total 1	O 1	0	0
61	75	1	Total 1	O 1	0	0
61	85	2	Total 2	O 2	0	0
61	A5	2	Total 2	O 2	0	0
61	B5	1	Total 1	O 1	0	0
61	C5	4	Total 4	O 4	0	0
61	H5	3	Total 3	O 3	0	0
61	L5	2	Total 2	O 2	0	0
61	M5	10	Total 10	O 10	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 rRNA

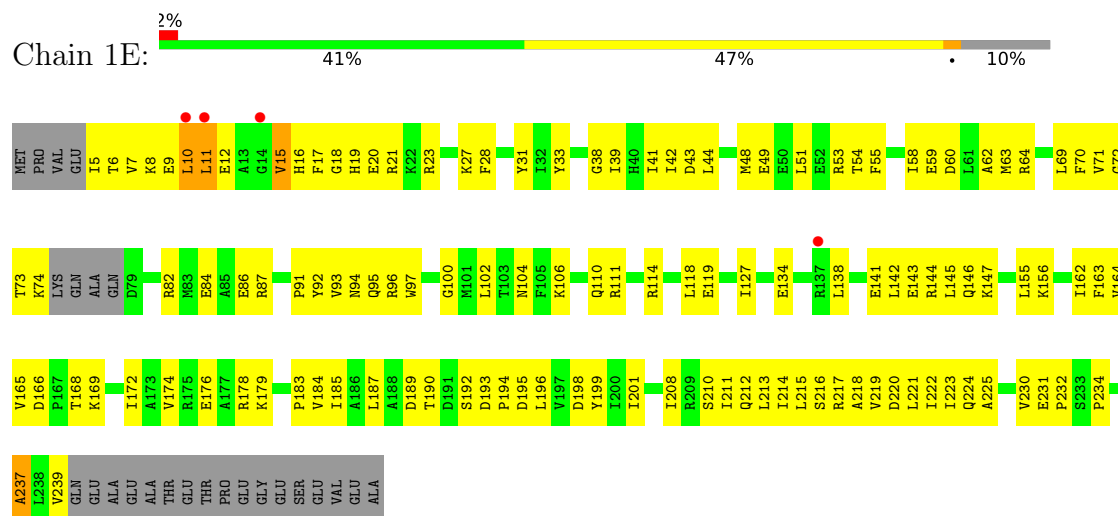




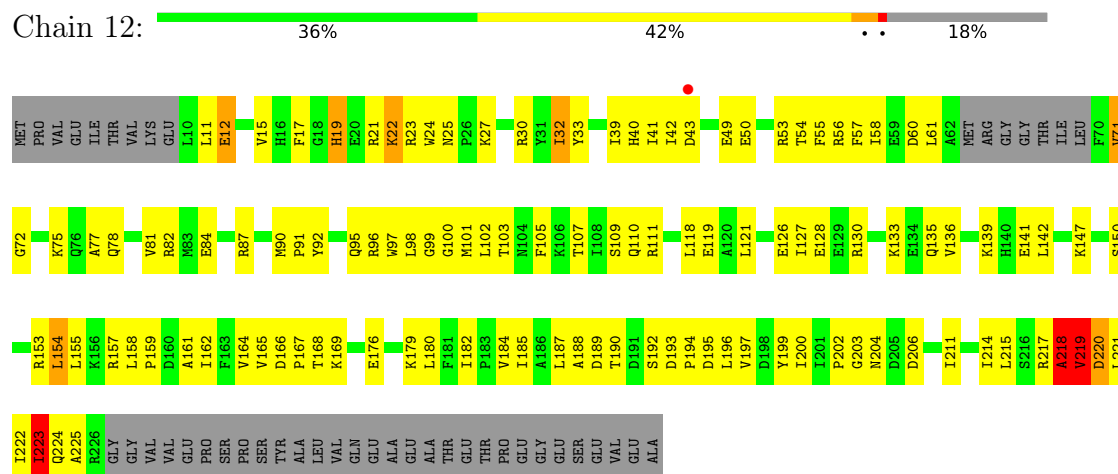


U U G C U

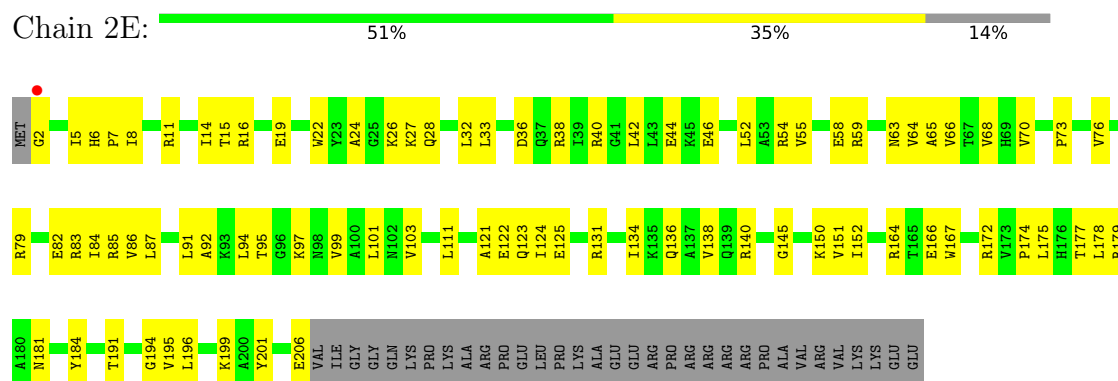
• Molecule 2: 30S ribosomal protein S2



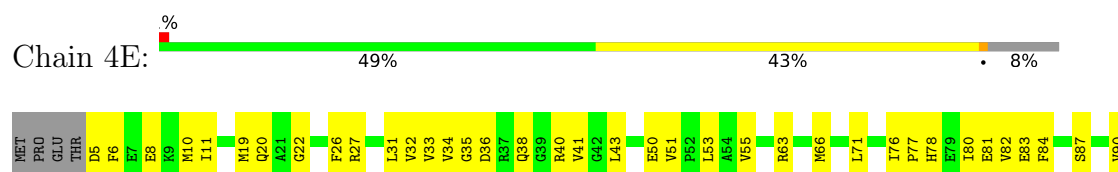
• Molecule 2: 30S ribosomal protein S2

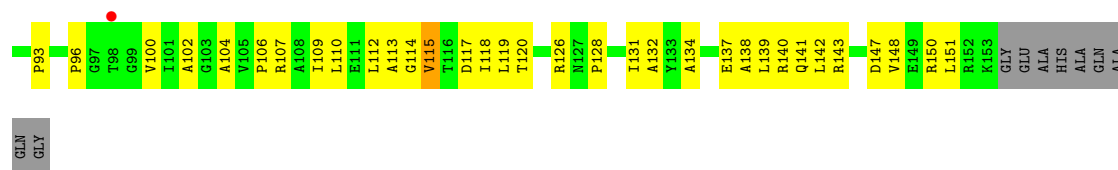


• Molecule 3: 30S ribosomal protein S3



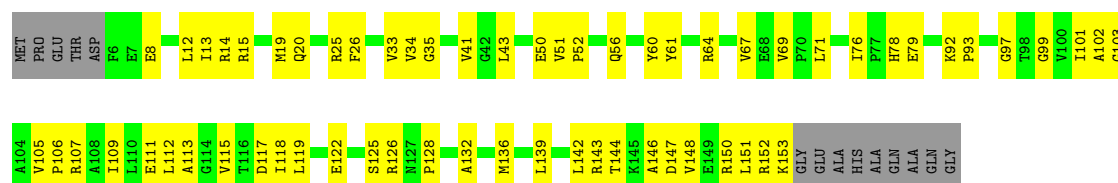
• Molecule 3: 30S ribosomal protein S3





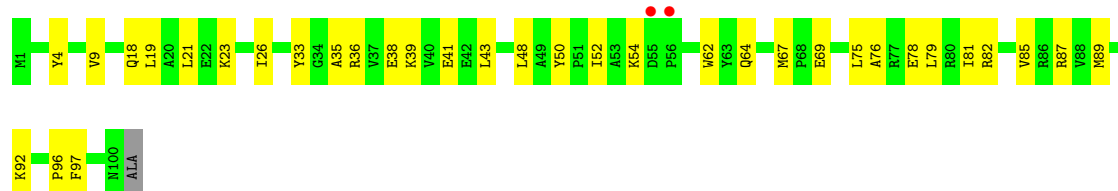
- Molecule 5: 30S ribosomal protein S5

Chain 42: 53% 38% 9%



- Molecule 6: 30S ribosomal protein S6

Chain 5E: 2% 65% 34%



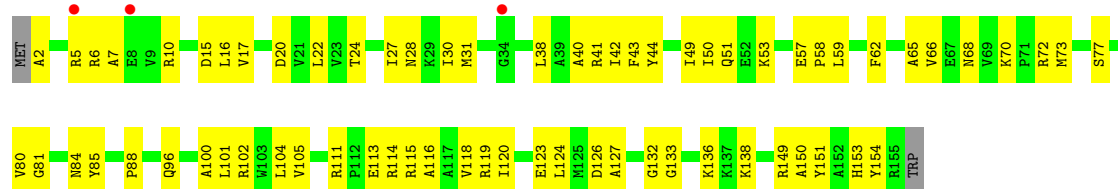
- Molecule 6: 30S ribosomal protein S6

Chain 52: 64% 34% 2%



- Molecule 7: 30S ribosomal protein S7

Chain 6E: 2% 55% 44%



- Molecule 7: 30S ribosomal protein S7

Chain 62: 48% 40% 11%



• Molecule 8: 30S ribosomal protein S8



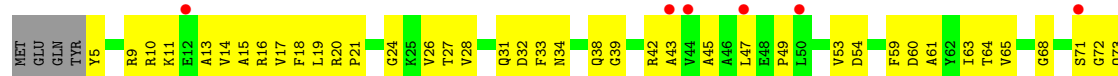
• Molecule 8: 30S ribosomal protein S8



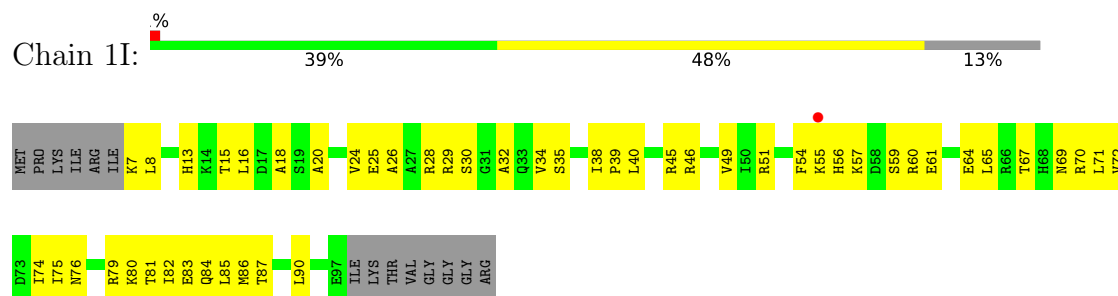
• Molecule 9: 30S ribosomal protein S9



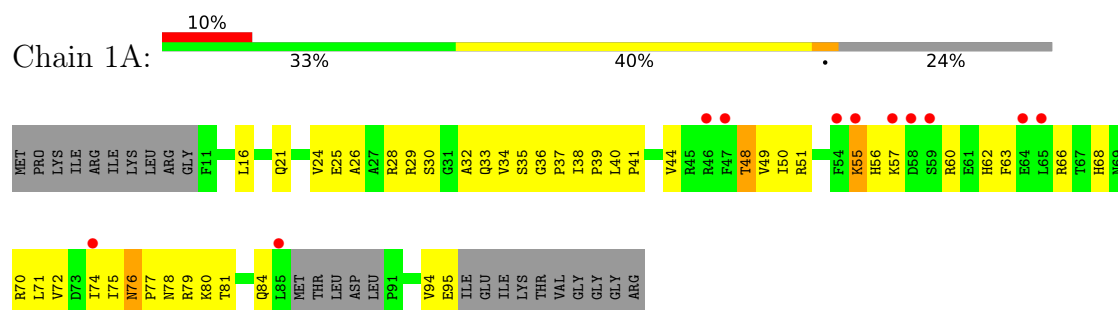
• Molecule 9: 30S ribosomal protein S9



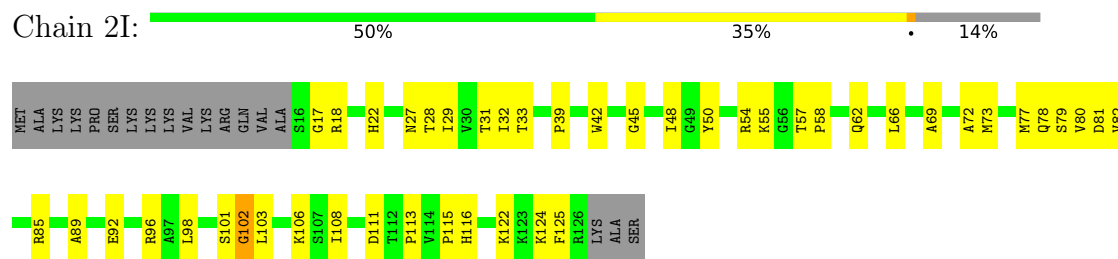
- Molecule 10: 30S ribosomal protein S10



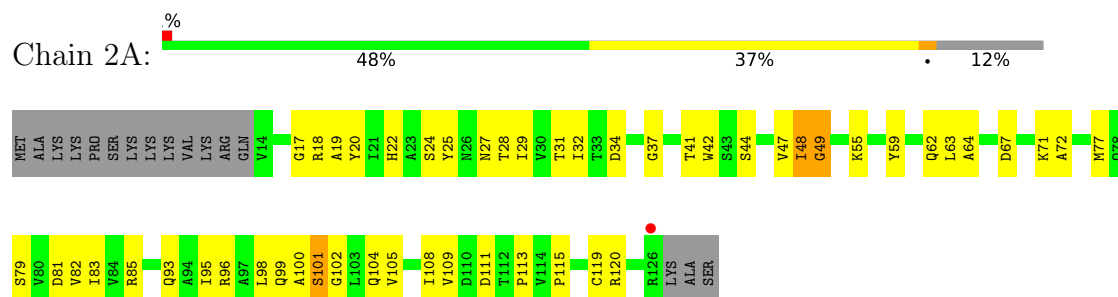
- Molecule 10: 30S ribosomal protein S10



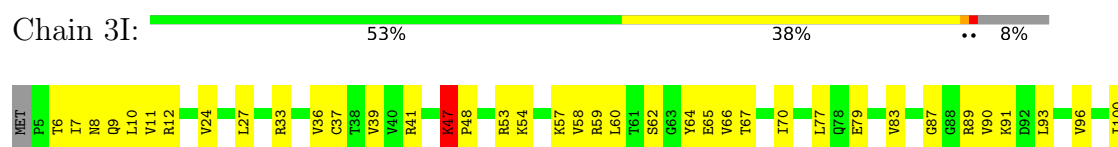
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

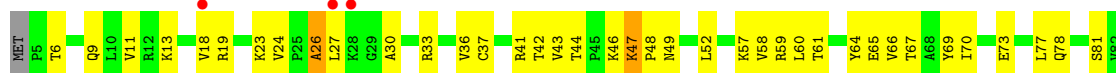


- Molecule 12: 30S ribosomal protein S12





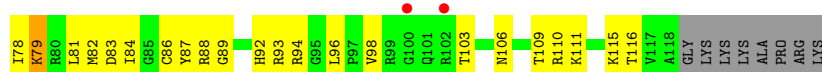
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



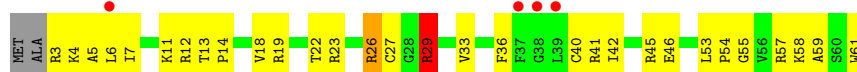
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z

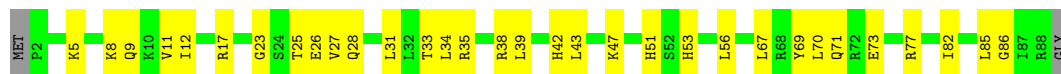


- Molecule 14: 30S ribosomal protein S14 type Z



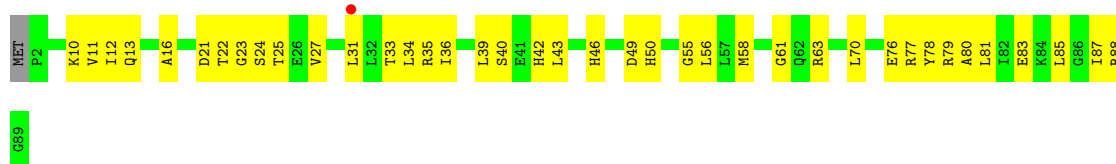
- Molecule 15: 30S ribosomal protein S15

Chain 6I: 



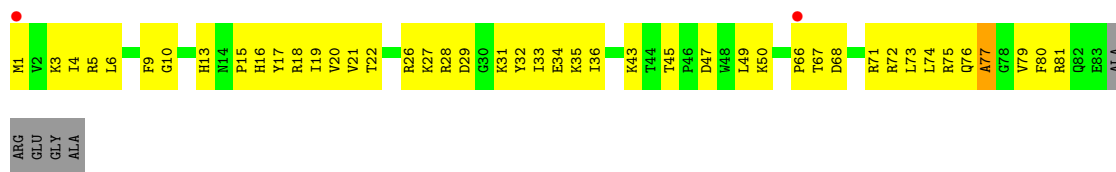
- Molecule 15: 30S ribosomal protein S15

Chain 6A: 

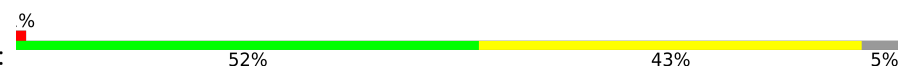


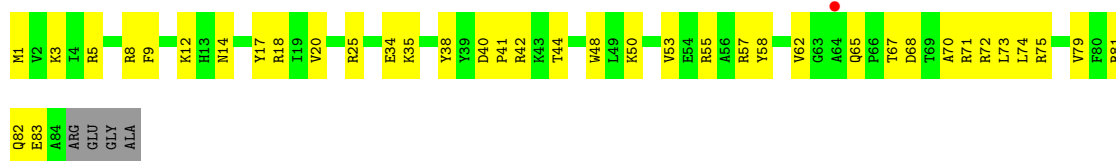
- Molecule 16: 30S ribosomal protein S16

Chain 7I: 



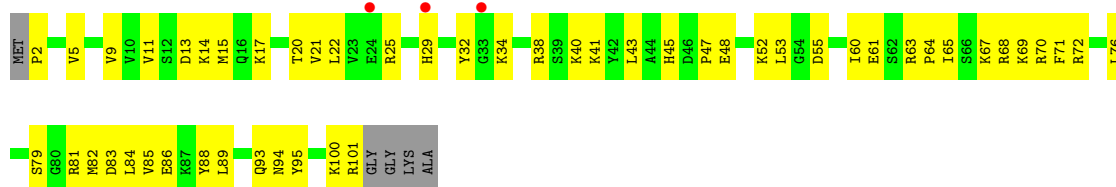
- Molecule 16: 30S ribosomal protein S16

Chain 7A: 



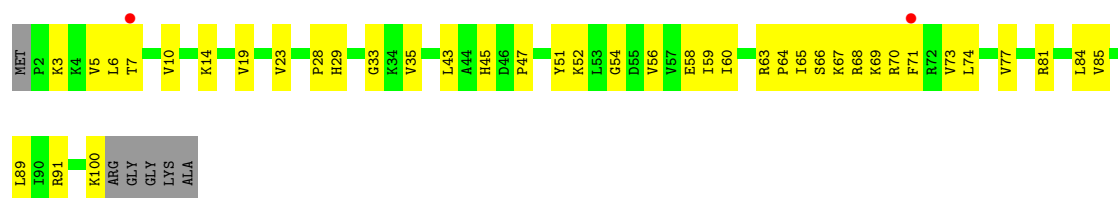
- Molecule 17: 30S ribosomal protein S17

Chain 8I: 

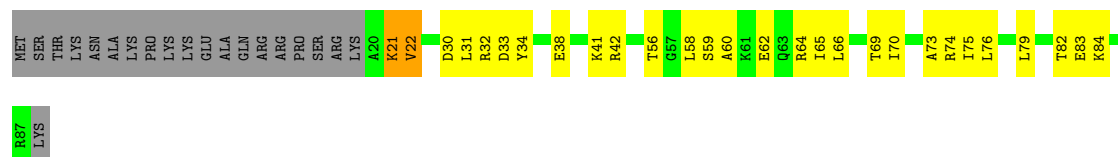


- Molecule 17: 30S ribosomal protein S17

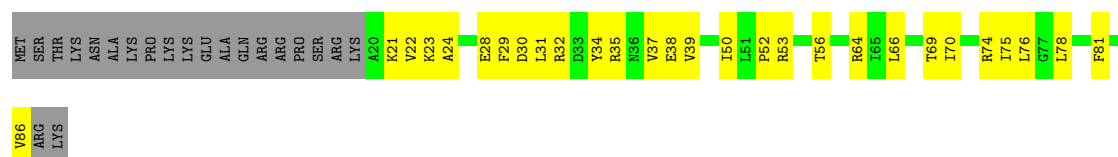
Chain 8A: 



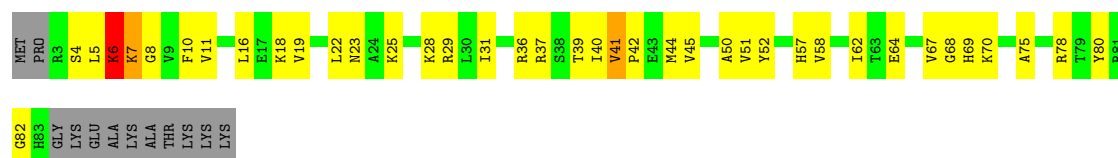
- Molecule 18: 30S ribosomal protein S18



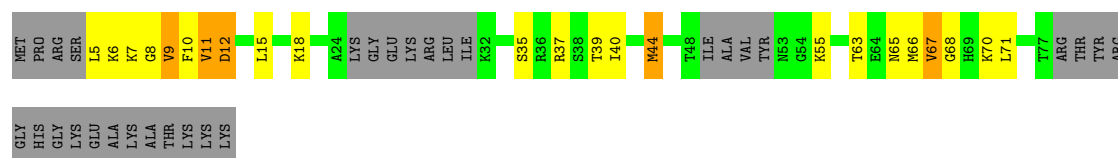
- Molecule 18: 30S ribosomal protein S18



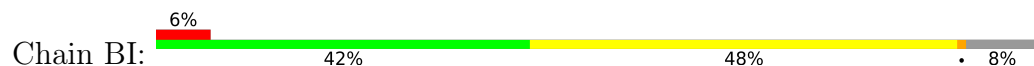
- Molecule 19: 30S ribosomal protein S19

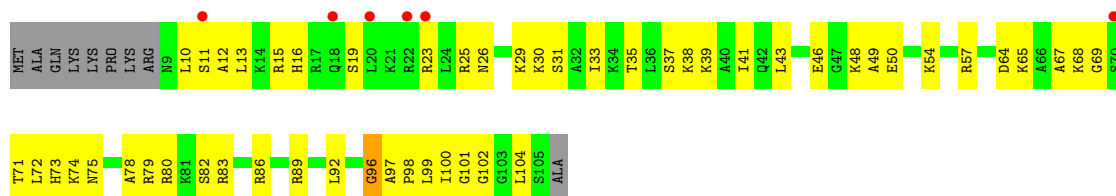


- Molecule 19: 30S ribosomal protein S19

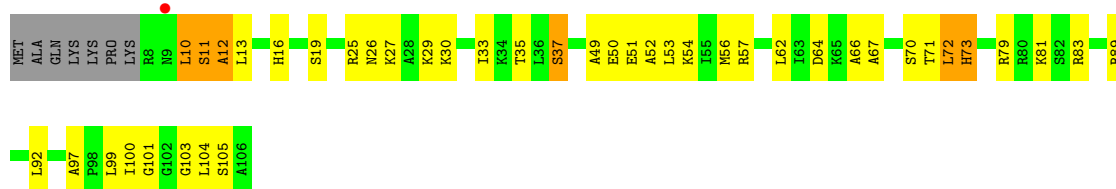


- Molecule 20: 30S ribosomal protein S20

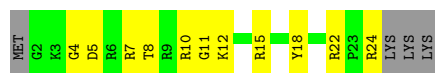




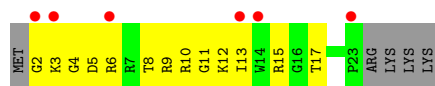
- Molecule 20: 30S ribosomal protein S20



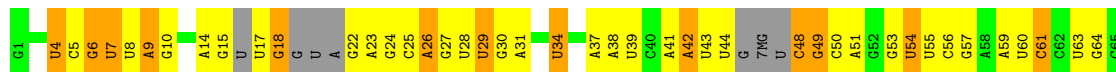
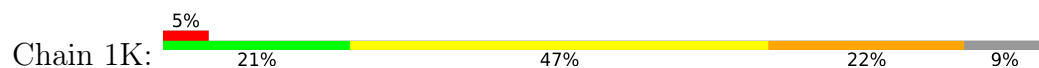
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx

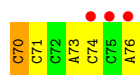


- Molecule 22: tRNA^{Lys}



- Molecule 22: tRNA^{Lys}





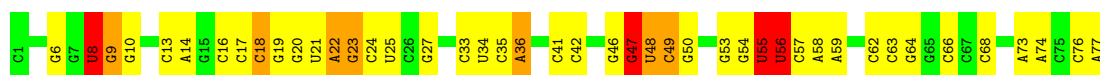
- Molecule 23: E. coli tRNA^{fMet}

Chain 2K: 51% 44% ..



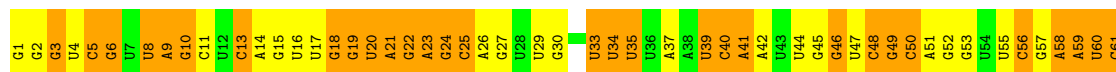
- Molecule 23: E. coli tRNA^{fMet}

Chain 2L: 43% 43% 9% 5%



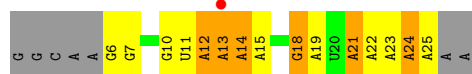
- Molecule 24: tRNA^{Lys}

Chain 3K: 3% 13% 37% 50%



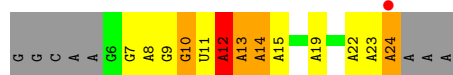
- Molecule 25: mRNA

Chain 4K: 4% 19% 33% 22% 26%



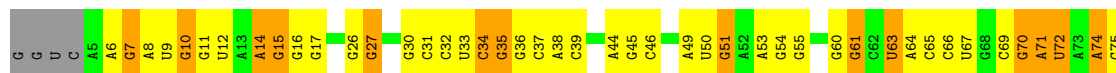
- Molecule 25: mRNA

Chain 4L: 4% 22% 30% 15% 30%



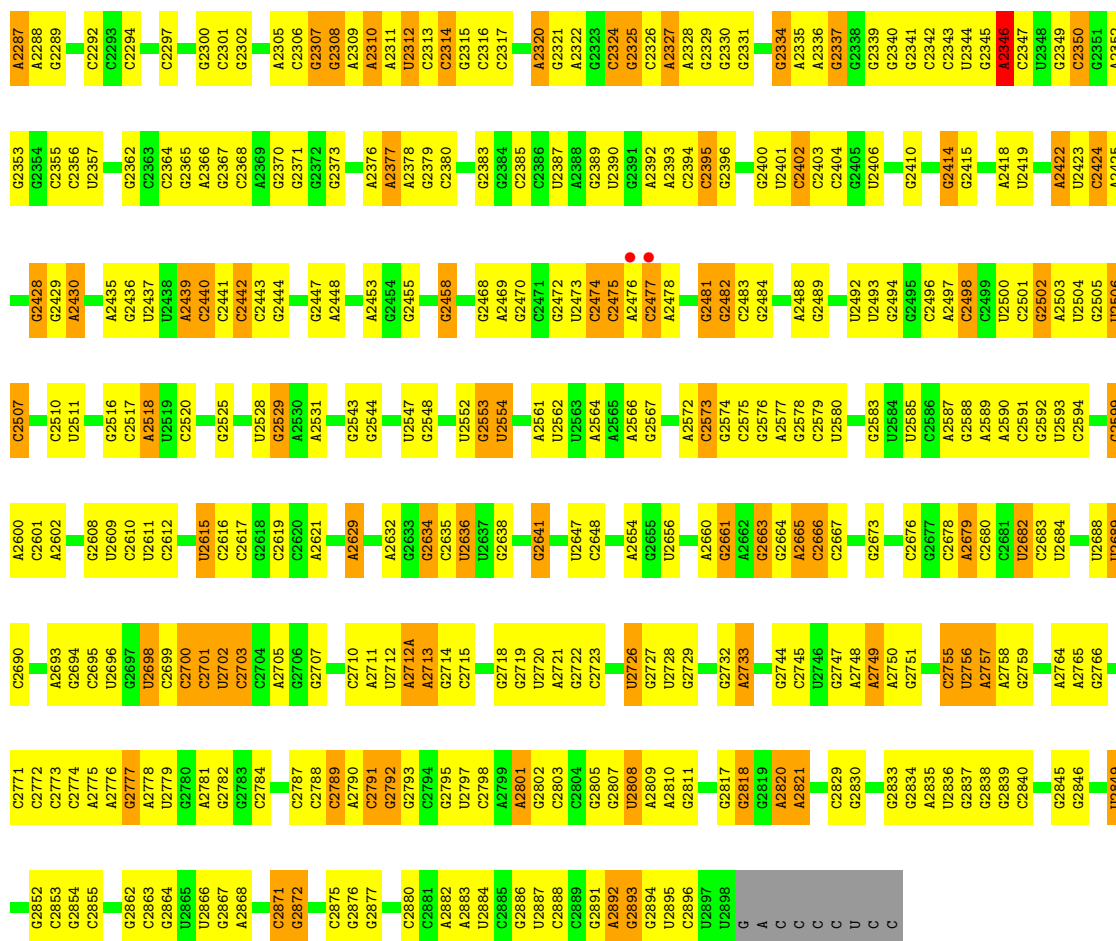
- Molecule 26: 23S rRNA

Chain 1H: 40% 43% 14%



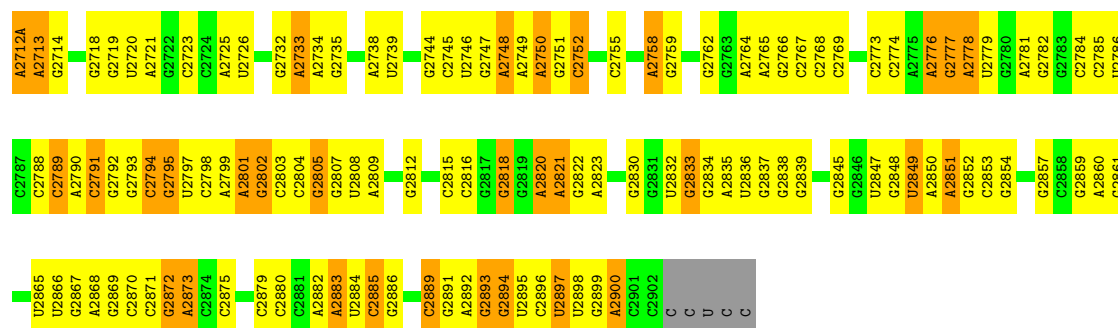
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G	A1027	G953	G796	C797	U724	A	G598	C517	C445	U363D	G298	G254	A181	G82
G	G954	G954	G725	G797	G725	C	G599	G518	G446	A363E	A299	G258	A182	G83
C	G1030	G955	G726	A800	A726	C	G600	U519	A447	A363F	A300	G259	A183	A84
C	G1031	G956	G727	G801	G727	C	G601	G520	U448	G364	G301	G260	C184	G85
G	U1032	A957	G728	A802	G728	C	G602		A449		C302	G261	U185	C86
U	U1033	U958	G729	A803	G729	G654H	G603	C527	U450	G370	G303	A262	G188	G89
A	A1034	A959	C730	A804	C730	G654I	A603	C451	C451	A371	G304	C263	G189	U90
U	U1035	A960	G731	G805	G731	G654J	G604	A528	C452	G372	G305	C264	A190	A91
U	U1036	C961	C732	C806	C732	G654K	C605	A529	C453	U373	U306	A265		
A	G1037	C962	G733	U807	G733	G654L	U606	G530	A454	A374	G307	G266		
C	U1038	U963	A734		A734	G654M	U607	C531	C455	C375	G308	C267	G194	G94
C	G1039		A735		A735	A654N		A532	C456	C376	G309	C268	A195	G95
U	C971	C812	C736	C812	C736	A654O	G609A	G583	A457		G310	U269	A196	U104
U	G972	C	C737	C	C737		G610	U534	G458	U380	A311	U270	A197	U105
A	A973	A	G738	C817	G738		G611	C535	U459	U381	G312	C270C	C198	C106
C	G974	G		G818			U612	A536	A460	U382		C270D	C199	C107
U	C974A	C893	G741	A821	G741		U613	C537	C461	C385	G313	C270E	A204	U108
G	G975	C894	G742		G742		G614	G539	C462	G386	G314	G270F	A207	G110
	G978	U895	U747	C825	U747		G615	C546	U464	G389	G315	C270G	C208	
A983		A	U748	U826	G748		G616	A547	G465	A390	C319	C270H		
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C988		A901	C754		C754		A621	U553	A471	U405	A324	G270M	G215	A118
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C992		U905	A835		A835		U625	U557	G475	A401	G328	C270Q	G219	G123
C993		G906	G836		G836		G626	G558	A476		A330	G270R	G220	G124
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C995		C908	C838		C838		G628	G563	A478	U406	G332	G270T	A222	A126
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A1002		C912	G770		G770		A633	A567	A482	G411	C336	G270X	G226	
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C1006		A918	G772		G772		G635	U569	C484	G418	G338	G271	A228	G138
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C1015		G938	A783		A783		G647	A578	U499	G430	G355	A278	G242	C155
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C1023		A947	G791		G791		C	U589	U511			A289	G250	G173
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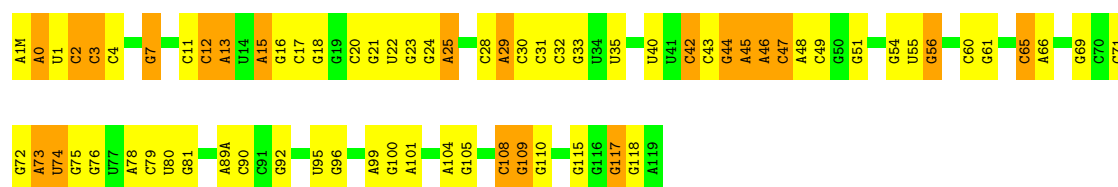


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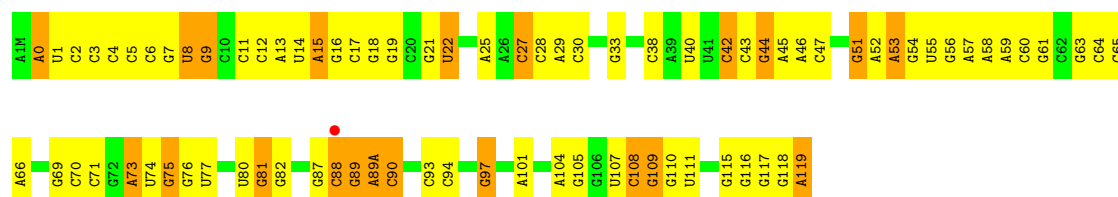
- Molecule 27: 5S rRNA

Chain 16: 42% 41% 17%



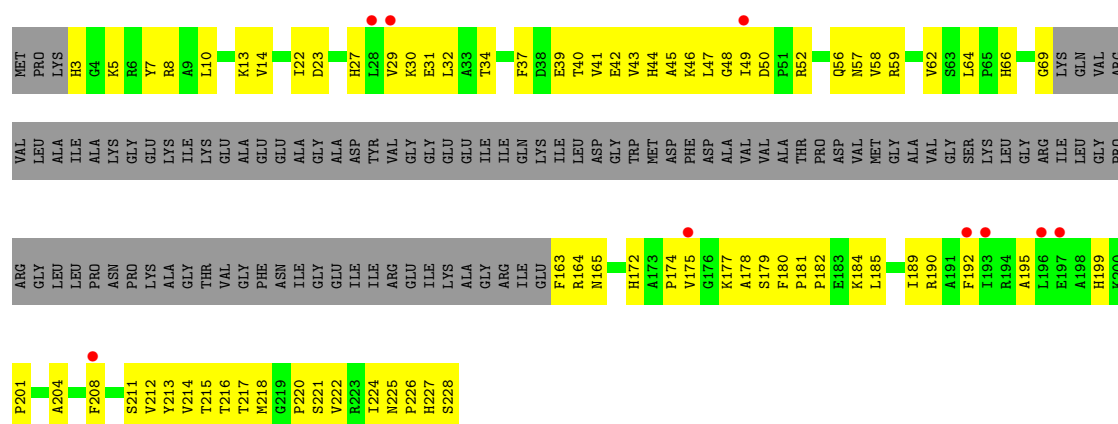
- Molecule 27: 5S rRNA

Chain 1J: 33% 50% 17%



- Molecule 28: 50S ribosomal protein L1

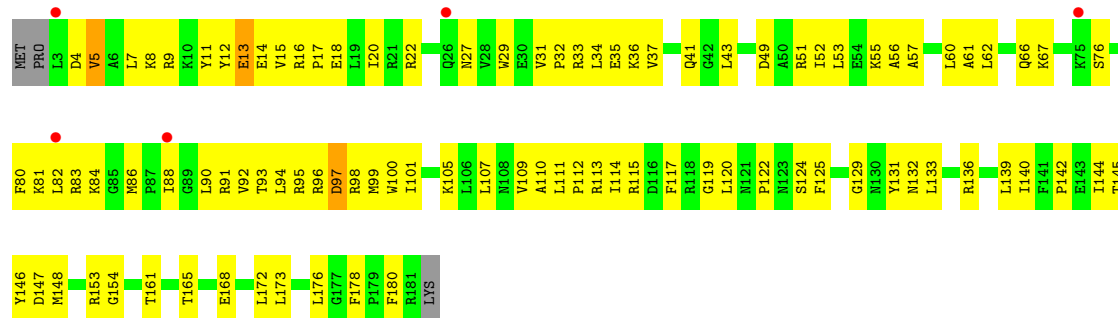
Chain 71: 4% 25% 33% 42%



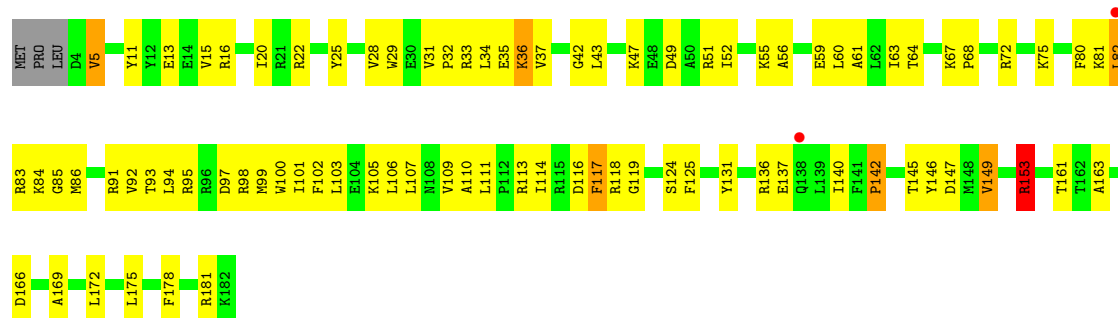
- Molecule 28: 50S ribosomal protein L1



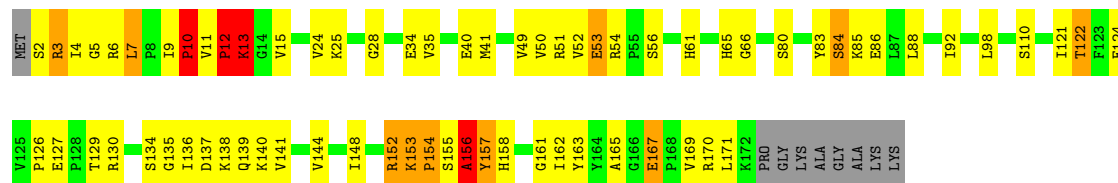
• Molecule 32: 50S ribosomal protein L5



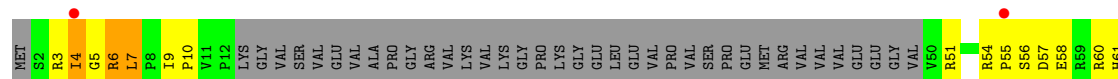
• Molecule 32: 50S ribosomal protein L5

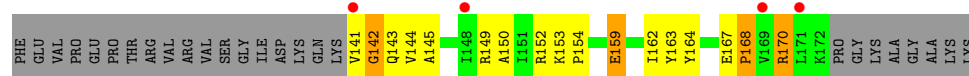
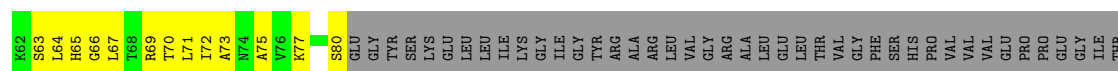


• Molecule 33: 50S ribosomal protein L6



• Molecule 33: 50S ribosomal protein L6





• Molecule 34: 50S ribosomal protein L9

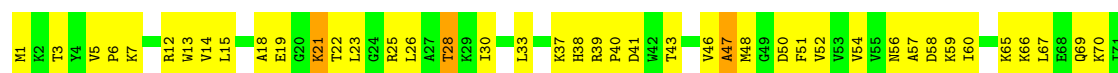


• Molecule 34: 50S ribosomal protein L9



GLU

• Molecule 35: 50S ribosomal protein L13



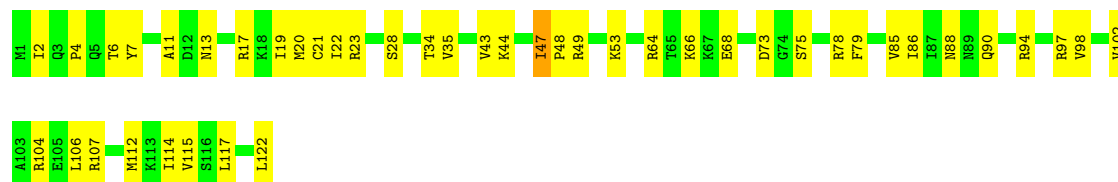
• Molecule 35: 50S ribosomal protein L13





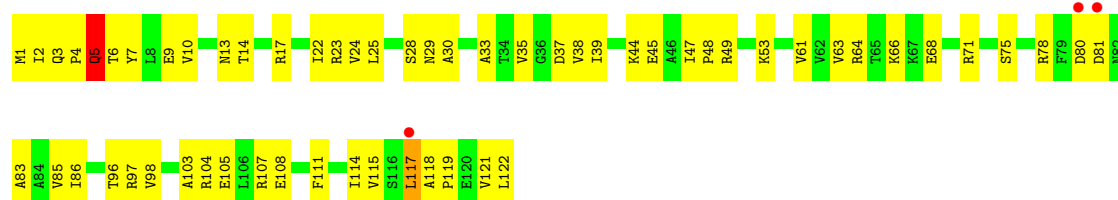
- Molecule 36: 50S ribosomal protein L14

Chain 68: 64% 35%



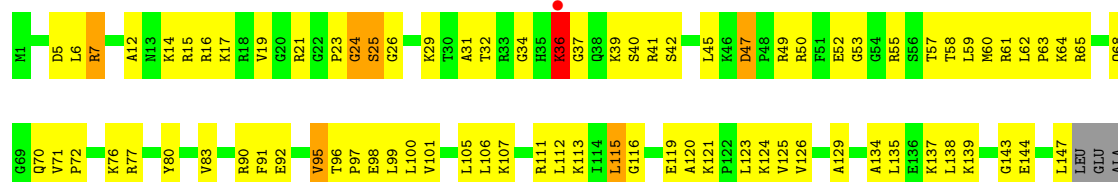
- Molecule 36: 50S ribosomal protein L14

Chain 25: 2% 52% 47%



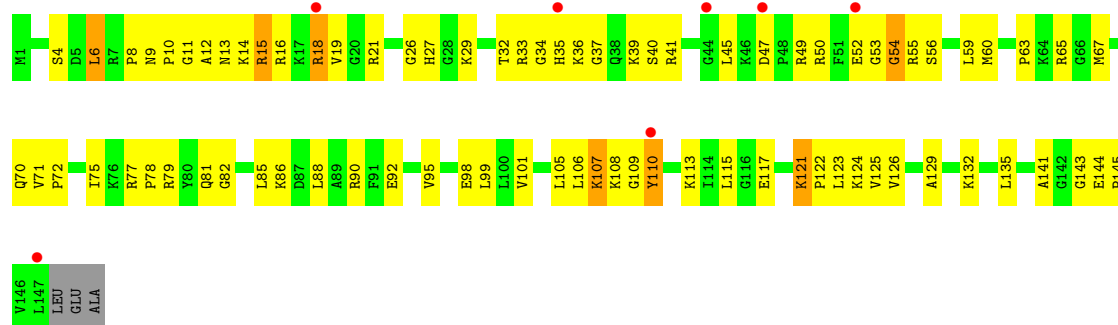
- Molecule 37: 50S ribosomal protein L15

Chain 78: 43% 50%

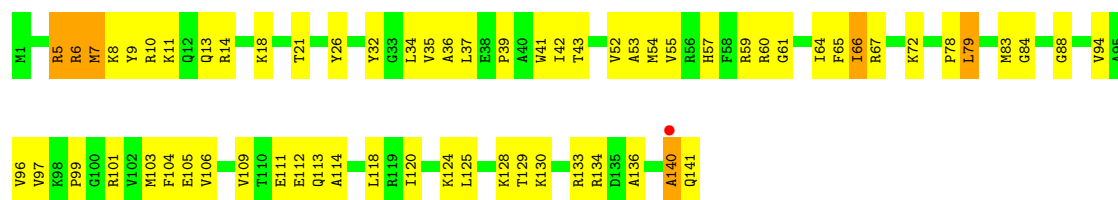


- Molecule 37: 50S ribosomal protein L15

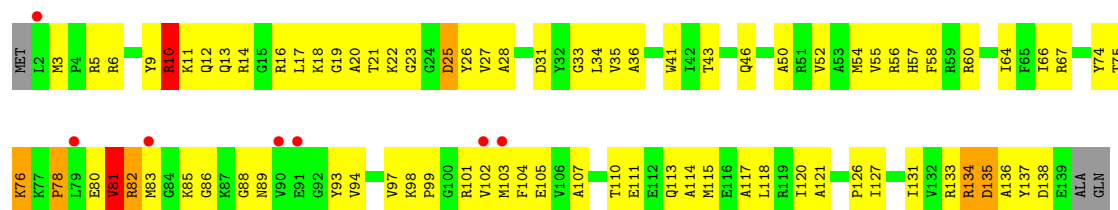
Chain 35: 5% 45% 49% 5%



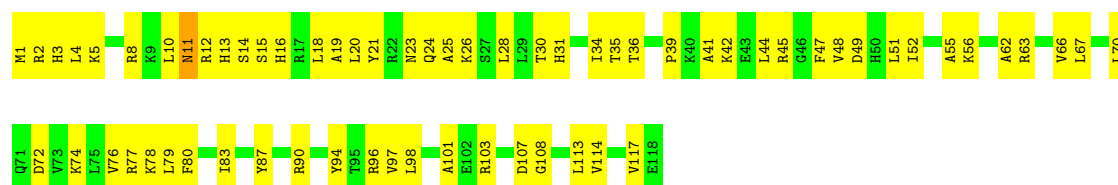
- Molecule 38: 50S ribosomal protein L16



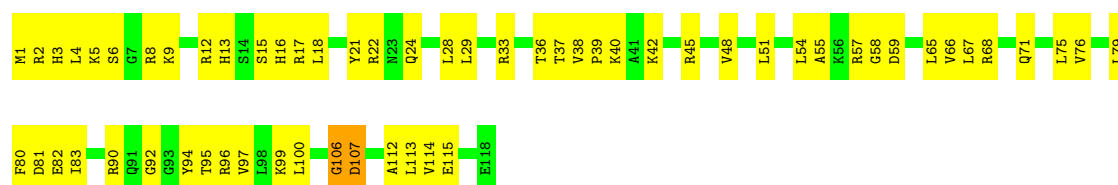
• Molecule 38: 50S ribosomal protein L16



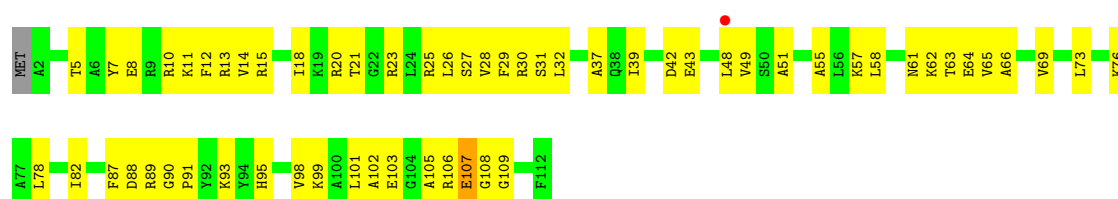
• Molecule 39: 50S ribosomal protein L17



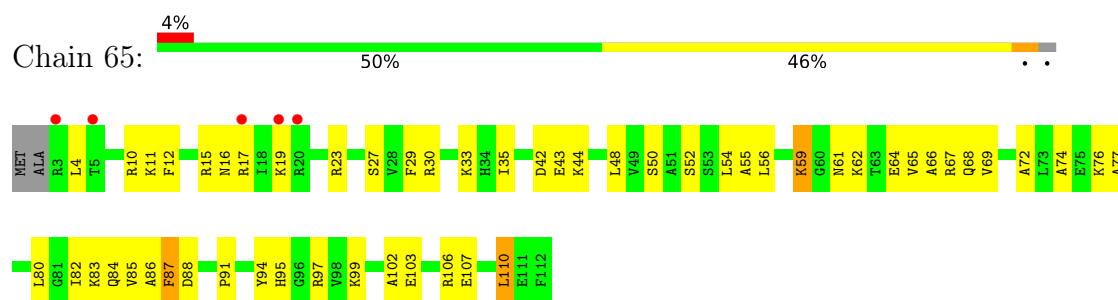
• Molecule 39: 50S ribosomal protein L17



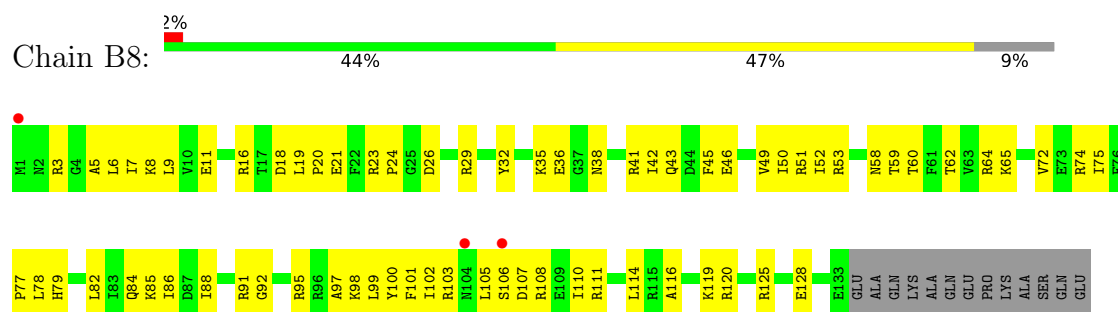
• Molecule 40: 50S ribosomal protein L18



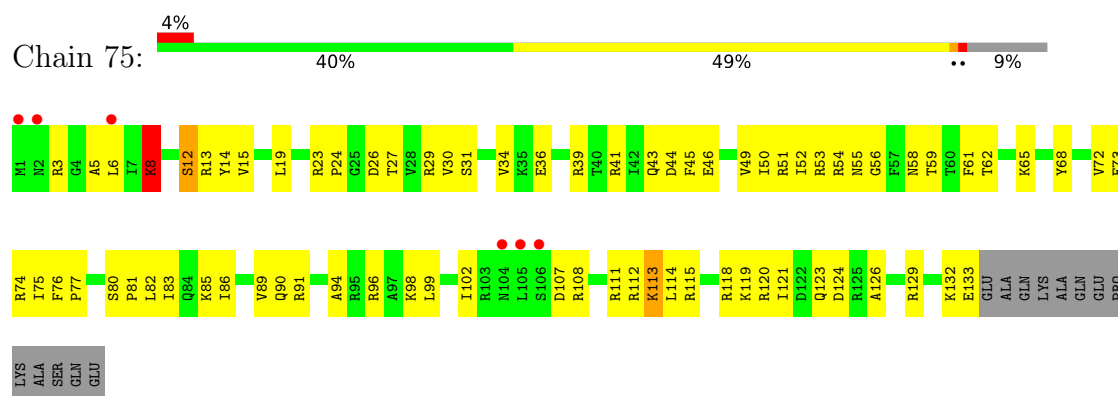
- Molecule 40: 50S ribosomal protein L18



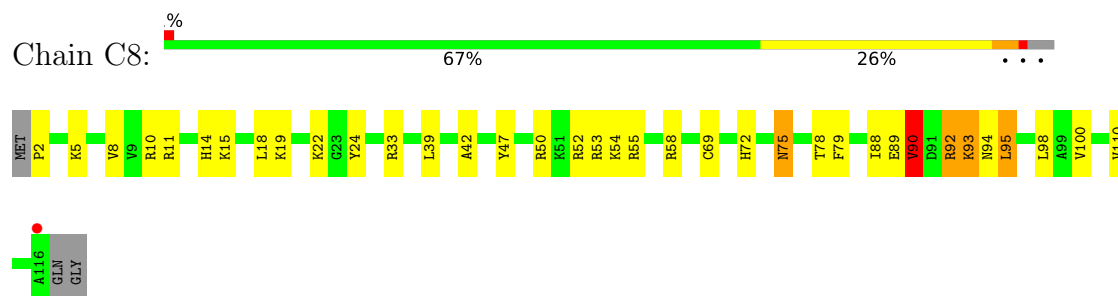
- Molecule 41: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L19

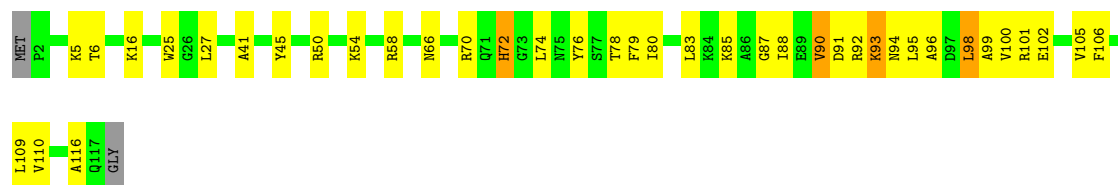


- Molecule 42: 50S ribosomal protein L20

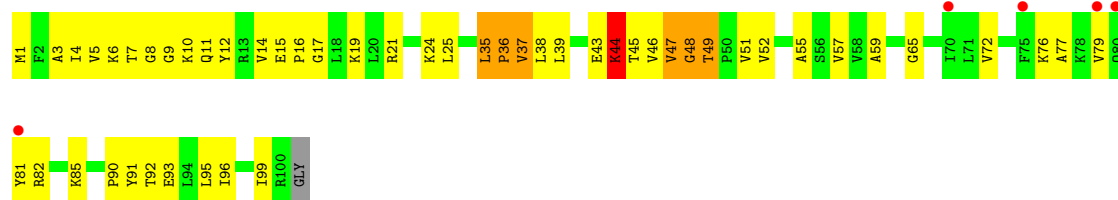


- Molecule 42: 50S ribosomal protein L20

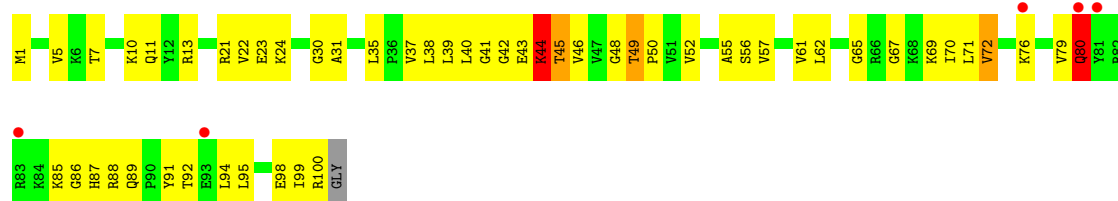




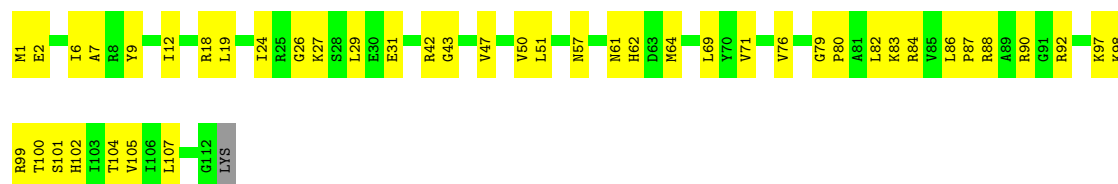
- Molecule 43: 50S ribosomal protein L21



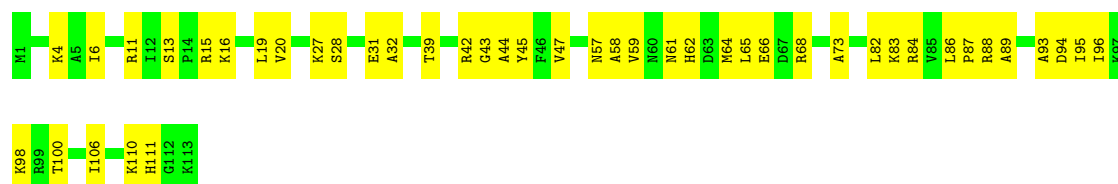
- Molecule 43: 50S ribosomal protein L21



- Molecule 44: 50S ribosomal protein L22

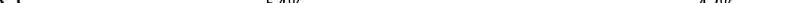


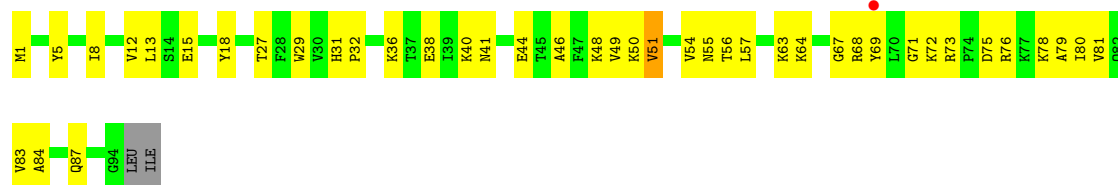
- Molecule 44: 50S ribosomal protein L22

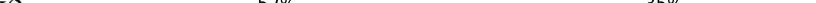


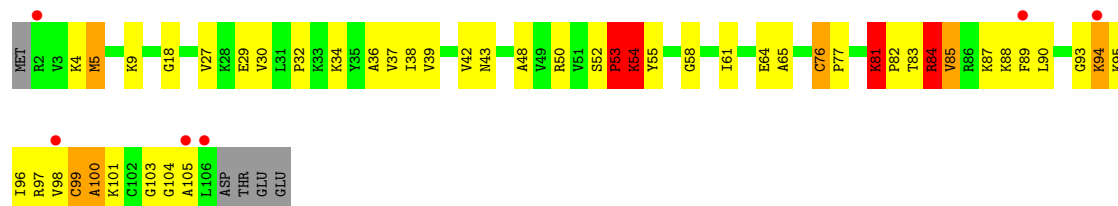
- Molecule 45: 50S ribosomal protein L23

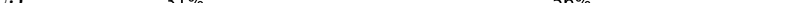
V81	Q82	V83	E93	Q94	L95	ILE	H1	K2	T3	A4	Y5	D6	V7	I8	L9	A10	P11	V12	L13	A17	G24	K25	Y26	T27	F28	W29	V30	H31	T35	K36	T37	F38	I39	K40	N41	A42	V43	E44	V49	K50	V51	V52	N55	G61	K62	K63	K64	K65	L66	G67	R68	Y69	L70	D75	K76	K77	K78	A79	T80
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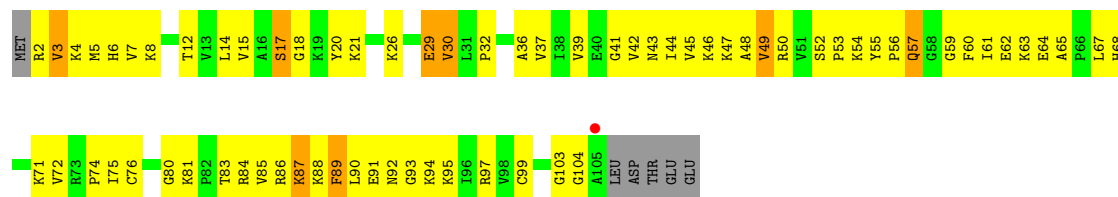
- Chain B5:  %

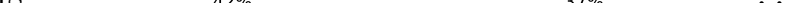


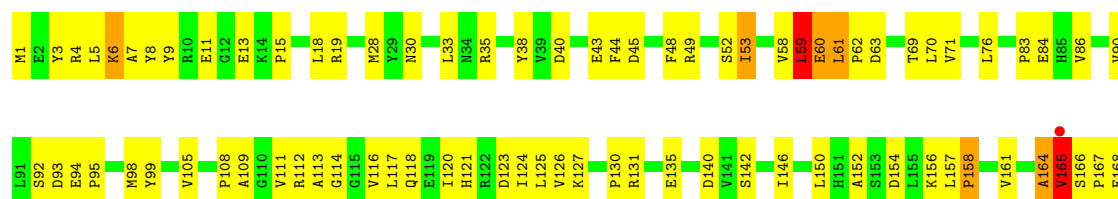
- Chain G8: 



- Chain C5: 



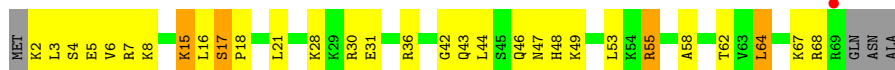
- Chain H8:  42% 37% •• 17%



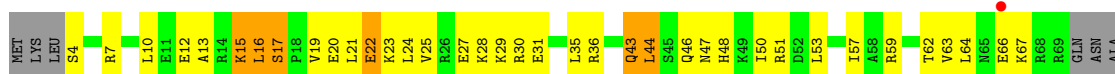




- Molecule 50: 50S ribosomal protein L29



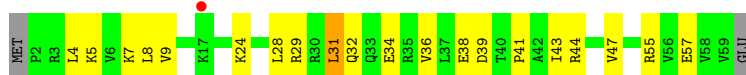
- Molecule 50: 50S ribosomal protein L29



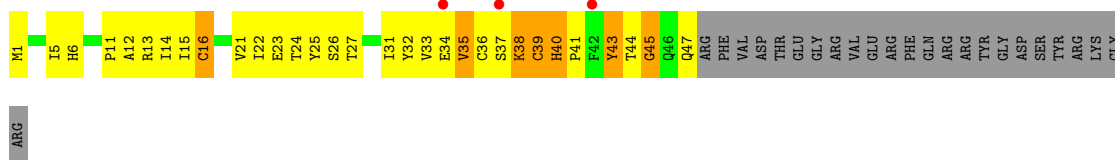
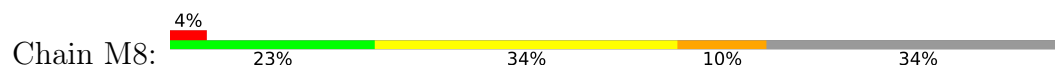
- Molecule 51: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L31



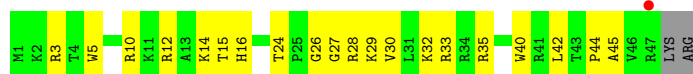
- Molecule 53: 50S ribosomal protein L32



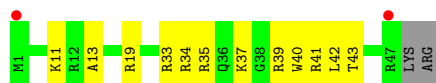
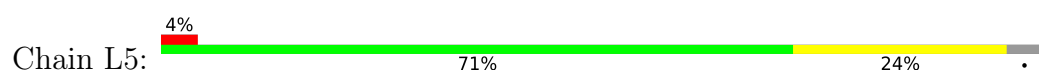
- Molecule 53: 50S ribosomal protein L32



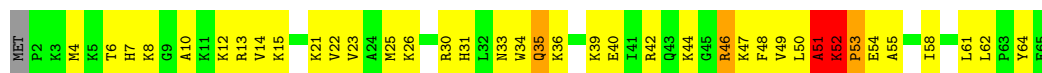
- Molecule 54: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L34



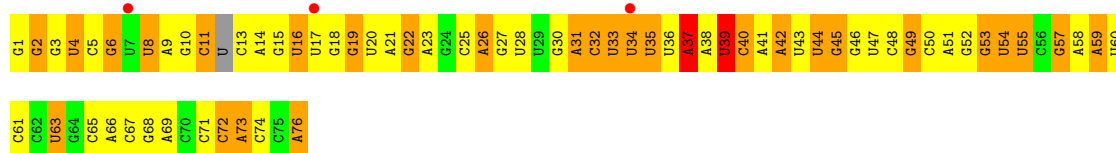
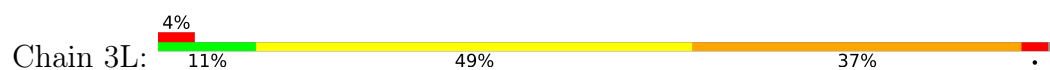
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNA^{Lys}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.70Å 449.50Å 620.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.17 – 3.15 152.17 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (152.17-3.15) 91.9 (152.17-3.15)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.247 0.194 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	80.1	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	296184	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: SF4, T6A, PSU, MG, 5MU, U8U, G7M, OMC, PAR, 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	0.37	0/35994	0.63	5/56171 (0.0%)
1	1G	0.32	0/36231	0.56	1/56544 (0.0%)
2	12	0.40	2/1752 (0.1%)	0.83	5/2360 (0.2%)
2	1E	0.39	1/1908 (0.1%)	0.72	2/2573 (0.1%)
3	22	0.34	0/1564	0.64	0/2109
3	2E	0.42	0/1629	0.64	0/2195
4	32	0.44	1/1732 (0.1%)	0.75	0/2318
4	3E	0.45	1/1720 (0.1%)	0.75	0/2305
5	42	0.38	0/1150	0.66	0/1548
5	4E	0.40	0/1158	0.67	0/1559
6	52	0.46	1/855 (0.1%)	0.62	0/1154
6	5E	0.41	0/850	0.69	0/1147
7	62	0.47	1/1127 (0.1%)	0.75	2/1507 (0.1%)
7	6E	0.33	0/1259	0.57	0/1686
8	72	0.30	0/1127	0.61	0/1517
8	7E	0.39	0/1135	0.73	1/1527 (0.1%)
9	82	0.33	0/971	0.78	3/1304 (0.2%)
9	8E	0.35	0/1019	0.69	0/1367
10	1A	0.60	1/658 (0.2%)	0.67	0/885
10	1I	0.47	0/747	0.74	0/1006
11	2A	0.32	0/850	0.64	0/1150
11	2I	0.37	0/838	0.65	0/1133
12	3A	0.41	0/972	0.75	0/1301
12	3I	0.53	0/972	0.88	1/1301 (0.1%)
13	4A	0.36	0/903	0.73	1/1211 (0.1%)
13	4I	0.42	0/952	0.76	1/1277 (0.1%)
14	5A	0.35	0/495	0.82	0/657
14	5I	0.41	0/500	0.82	2/664 (0.3%)
15	6A	0.34	0/744	0.58	0/992
15	6I	0.37	0/740	0.58	0/987
16	7A	0.41	0/721	0.71	0/970
16	7I	0.39	0/716	0.74	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.35	0/836	0.57	0/1117
17	8I	0.42	0/847	0.75	2/1131 (0.2%)
18	9A	0.39	0/549	0.67	0/732
18	9I	0.39	0/554	0.83	2/739 (0.3%)
19	AA	0.41	0/490	0.76	0/662
19	AI	0.46	0/668	0.85	0/899
20	BA	0.37	0/764	0.81	1/1007 (0.1%)
20	BI	0.37	0/748	0.74	1/986 (0.1%)
21	1B	0.40	0/192	0.67	0/252
21	1F	0.39	0/203	0.71	0/266
22	1K	0.34	0/1516	0.55	0/2350
22	1L	0.30	1/1613 (0.1%)	0.48	0/2504
23	2K	0.45	2/1721 (0.1%)	0.64	0/2682
23	2L	0.38	0/1721	0.59	0/2682
24	3K	0.31	0/1777	0.59	0/2767
25	4K	0.40	0/495	0.70	1/771 (0.1%)
25	4L	0.37	0/470	0.63	1/732 (0.1%)
26	14	0.42	4/69023 (0.0%)	0.67	11/107740 (0.0%)
26	1H	0.47	0/68351	0.73	14/106700 (0.0%)
27	16	0.40	0/2928	0.68	0/4568
27	1J	0.36	0/2928	0.64	0/4568
28	71	0.29	0/1055	0.66	0/1425
28	79	0.29	0/459	0.61	0/608
29	11	0.77	6/2170 (0.3%)	1.06	11/2926 (0.4%)
29	19	0.57	0/2175	1.00	7/2933 (0.2%)
30	21	0.51	0/1591	1.03	5/2146 (0.2%)
30	29	0.66	4/1596 (0.3%)	1.08	12/2153 (0.6%)
31	31	0.50	0/1620	0.84	0/2194
31	39	0.48	1/1637 (0.1%)	0.91	2/2218 (0.1%)
32	41	0.40	0/1481	0.77	2/1994 (0.1%)
32	49	0.52	3/1482 (0.2%)	0.75	0/1994
33	51	0.52	1/1337 (0.1%)	1.01	12/1809 (0.7%)
33	59	0.43	0/582	0.95	2/783 (0.3%)
34	61	0.44	0/1151	0.87	6/1558 (0.4%)
34	69	0.44	1/1146 (0.1%)	0.80	4/1551 (0.3%)
35	15	0.38	0/1131	0.70	0/1525
35	58	0.47	1/1131 (0.1%)	0.80	2/1525 (0.1%)
36	25	0.53	2/942 (0.2%)	0.80	0/1269
36	68	0.44	0/942	0.70	0/1269
37	35	0.56	1/1139 (0.1%)	1.02	2/1514 (0.1%)
37	78	0.54	0/1139	0.98	3/1514 (0.2%)
38	45	0.72	5/1120 (0.4%)	0.93	3/1498 (0.2%)
38	88	0.72	2/1134 (0.2%)	0.99	2/1519 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	55	0.47	0/981	0.80	0/1312
39	98	0.45	0/981	0.83	0/1312
40	65	0.46	0/886	0.89	1/1180 (0.1%)
40	A8	0.50	0/884	0.78	0/1178
41	75	0.54	2/1123 (0.2%)	0.77	0/1500
41	B8	0.52	0/1123	0.84	0/1500
42	85	0.42	0/977	0.76	0/1301
42	C8	0.47	0/968	0.78	0/1289
43	95	0.54	0/785	0.93	0/1052
43	D8	0.45	0/785	0.93	4/1052 (0.4%)
44	A5	0.53	0/910	0.77	0/1220
44	E8	0.48	0/901	0.75	0/1209
45	B5	0.50	0/749	0.82	0/1007
45	F8	0.53	0/757	0.95	3/1017 (0.3%)
46	C5	0.49	0/807	1.06	6/1076 (0.6%)
46	G8	0.68	1/809 (0.1%)	1.27	10/1080 (0.9%)
47	D5	0.46	0/1098	0.85	3/1487 (0.2%)
47	H8	0.44	1/1403 (0.1%)	0.81	2/1901 (0.1%)
48	E5	0.46	0/616	0.86	0/821
48	I8	0.65	0/614	0.98	0/819
49	F5	0.48	0/744	0.91	3/989 (0.3%)
49	J8	0.55	0/744	0.88	0/989
50	G5	0.52	0/560	0.93	1/741 (0.1%)
50	K8	0.86	4/570 (0.7%)	0.96	1/755 (0.1%)
51	H5	0.38	0/464	0.68	0/623
51	L8	0.49	0/464	0.76	0/623
52	M8	0.41	0/375	1.05	3/507 (0.6%)
53	J5	0.46	0/448	0.80	0/606
53	N8	0.54	0/381	0.83	0/516
54	L5	0.53	0/409	0.86	0/540
54	P8	0.61	0/409	0.93	0/540
55	M5	0.60	0/524	0.92	1/691 (0.1%)
55	Q8	0.56	0/524	1.20	5/691 (0.7%)
56	3L	0.36	0/1729	0.59	0/2690
All	All	0.43	50/317045 (0.0%)	0.71	175/474982 (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	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	3
4	3E	0	1
8	7E	0	1
9	82	0	1
9	8E	0	2
10	1A	0	1
11	2A	0	1
11	2I	0	1
12	3I	0	4
13	4A	0	3
13	4I	0	2
14	5A	0	3
14	5I	0	1
16	7I	0	2
18	9I	0	1
19	AA	0	1
19	AI	0	3
20	BA	0	3
20	BI	0	1
29	11	0	7
29	19	0	5
30	21	0	8
30	29	0	7
31	31	0	2
31	39	0	8
32	41	0	1
32	49	0	6
33	51	0	5
33	59	0	5
34	61	0	4
34	69	0	3
35	58	0	2
37	35	0	4
37	78	0	4
38	45	0	4
39	55	0	1
40	65	0	1
40	A8	0	1
41	75	0	1
42	85	0	4
42	C8	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	95	0	3
43	D8	0	3
44	A5	0	1
45	F8	0	1
46	C5	0	3
46	G8	0	4
47	D5	0	1
47	H8	0	4
49	F5	0	1
49	J8	0	1
50	G5	0	4
50	K8	0	3
52	M8	0	4
54	P8	0	1
55	M5	0	2
55	Q8	0	2
All	All	0	169

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	K8	55	ARG	NE-CZ	-11.03	1.21	1.33
32	49	153	ARG	CZ-NH2	-10.09	1.20	1.33
38	88	5	ARG	NE-CZ	-9.70	1.22	1.33
10	1A	76	ASN	C-N	-9.30	1.12	1.33
37	35	121	LYS	C-N	9.19	1.55	1.33

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	19	271	ILE	N-CA-C	14.58	127.33	111.88
46	G8	81	LYS	CA-C-N	11.56	154.73	127.00
46	G8	81	LYS	C-N-CA	11.56	154.73	127.00
45	F8	3	THR	N-CA-C	-11.47	93.51	110.48
46	G8	81	LYS	C-N-CD	-10.64	97.20	120.60

There are no chirality outliers.

5 of 169 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	11	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	169	LYS	Peptide
2	1E	234	PRO	Peptide
4	3E	82	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16234	756	0
1	1G	32368	0	16343	754	1
2	12	1721	0	1758	120	0
2	1E	1874	0	1926	115	0
3	22	1541	0	1606	79	0
3	2E	1605	0	1668	60	0
4	32	1702	0	1765	104	0
4	3E	1690	0	1738	96	0
5	42	1134	0	1200	72	0
5	4E	1142	0	1204	52	0
6	52	842	0	857	29	0
6	5E	837	0	852	31	0
7	62	1115	0	1165	57	0
7	6E	1242	0	1286	52	0
8	72	1107	0	1165	54	0
8	7E	1115	0	1177	70	0
9	82	953	0	983	72	0
9	8E	1000	0	1031	69	0
10	1A	646	0	662	48	0
10	1I	734	0	761	54	0
11	2A	835	0	847	46	0
11	2I	823	0	833	39	0
12	3A	956	0	1046	54	0
12	3I	956	0	1046	39	0
13	4A	893	0	946	56	0
13	4I	942	0	997	50	0
14	5A	486	0	524	29	0
14	5I	491	0	530	37	0
15	6A	733	0	771	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	28	0
16	7A	705	0	725	41	0
16	7I	700	0	720	52	0
17	8A	823	0	891	41	0
17	8I	834	0	904	61	0
18	9A	544	0	605	25	0
18	9I	549	0	607	23	0
19	AA	481	0	468	19	0
19	AI	654	0	675	52	0
20	BA	762	0	861	41	0
20	BI	746	0	843	51	0
21	1B	188	0	195	20	0
21	1F	199	0	208	13	0
22	1K	1477	0	758	30	0
22	1L	1563	0	799	31	0
23	2K	1646	0	844	19	0
23	2L	1646	0	844	33	0
24	3K	1611	0	817	74	0
25	4K	439	0	218	11	0
25	4L	417	0	207	11	0
26	14	61630	0	31072	1413	1
26	1H	61028	0	30762	1441	0
27	16	2617	0	1328	70	0
27	1J	2617	0	1328	77	0
28	7I	1033	0	1048	72	0
28	79	456	0	460	32	0
29	11	2120	0	2197	160	0
29	19	2125	0	2199	136	0
30	21	1558	0	1624	97	0
30	29	1563	0	1629	137	0
31	31	1585	0	1632	95	0
31	39	1602	0	1649	104	0
32	41	1457	0	1514	95	0
32	49	1458	0	1516	72	0
33	51	1312	0	1384	66	0
33	59	573	0	597	44	0
34	61	1136	0	1223	60	0
34	69	1131	0	1218	75	0
35	15	1104	0	1180	52	0
35	58	1104	0	1180	65	0
36	25	932	0	996	56	0
36	68	932	0	996	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	35	1122	0	1206	97	0
37	78	1122	0	1206	109	0
38	45	1099	0	1154	98	0
38	88	1113	0	1157	59	0
39	55	967	0	1033	54	0
39	98	967	0	1033	67	0
40	65	876	0	938	62	0
40	A8	875	0	936	54	0
41	75	1109	0	1170	74	0
41	B8	1109	0	1170	62	0
42	85	959	0	1019	56	0
42	C8	950	0	1011	55	0
43	95	774	0	849	83	0
43	D8	774	0	849	58	0
44	A5	899	0	964	34	0
44	E8	890	0	951	35	0
45	B5	735	0	785	44	0
45	F8	743	0	794	39	0
46	C5	794	0	886	76	0
46	G8	796	0	886	53	0
47	D5	1074	0	1086	63	0
47	H8	1373	0	1402	85	0
48	E5	608	0	622	37	0
48	I8	606	0	625	33	0
49	F5	737	0	813	43	0
49	J8	737	0	813	27	0
50	G5	558	0	610	34	0
50	K8	568	0	614	31	0
51	H5	459	0	512	15	0
51	L8	459	0	512	18	0
52	M8	366	0	370	33	0
53	J5	434	0	454	24	0
53	N8	369	0	388	23	0
54	L5	401	0	436	14	0
54	P8	401	0	436	17	0
55	M5	516	0	582	35	0
55	Q8	516	0	582	54	0
56	3L	1601	0	814	69	0
57	11	3	0	0	0	0
57	13	150	0	0	0	0
57	14	454	0	0	0	0
57	16	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1G	93	0	0	0	0
57	1H	502	0	0	0	0
57	1I	1	0	0	0	0
57	1J	6	0	0	0	0
57	2I	3	0	0	0	0
57	29	4	0	0	0	0
57	2K	3	0	0	0	0
57	2L	4	0	0	0	0
57	3I	1	0	0	0	0
57	35	2	0	0	0	0
57	39	2	0	0	0	0
57	3I	1	0	0	0	0
57	41	2	0	0	0	0
57	45	3	0	0	0	0
57	55	1	0	0	0	0
57	5E	1	0	0	0	0
57	5I	1	0	0	0	0
57	78	1	0	0	0	0
57	7A	1	0	0	0	0
57	85	1	0	0	0	0
57	88	1	0	0	0	0
57	BI	1	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	I8	1	0	0	0	0
57	L8	1	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	13	42	0	45	3	0
58	1G	42	0	45	2	0
59	32	8	0	0	2	0
59	3E	8	0	0	0	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	11	12	0	0	1	0
61	13	319	0	0	23	0
61	14	1015	0	0	117	0
61	16	26	0	0	6	0
61	19	12	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1F	1	0	0	0	0
61	1G	226	0	0	16	0
61	1H	1158	0	0	132	0
61	1I	1	0	0	0	0
61	1J	18	0	0	2	0
61	1K	1	0	0	0	0
61	2I	6	0	0	1	0
61	29	6	0	0	0	0
61	2K	7	0	0	0	0
61	2L	1	0	0	0	0
61	3I	9	0	0	0	0
61	32	3	0	0	0	0
61	35	5	0	0	1	0
61	39	8	0	0	1	0
61	3A	1	0	0	0	0
61	3E	3	0	0	0	0
61	3I	3	0	0	1	0
61	3K	1	0	0	0	0
61	42	1	0	0	0	0
61	4E	3	0	0	1	0
61	4K	4	0	0	0	0
61	4L	3	0	0	0	0
61	55	1	0	0	0	0
61	58	1	0	0	0	0
61	5I	1	0	0	1	0
61	6A	3	0	0	0	0
61	6I	2	0	0	0	0
61	75	1	0	0	0	0
61	78	6	0	0	1	0
61	85	2	0	0	0	0
61	88	2	0	0	0	0
61	8A	1	0	0	0	0
61	8E	1	0	0	0	0
61	8I	2	0	0	0	0
61	A5	2	0	0	0	0
61	B5	1	0	0	0	0
61	BA	3	0	0	1	0
61	BI	5	0	0	0	0
61	C5	4	0	0	0	0
61	C8	2	0	0	0	0
61	E8	3	0	0	0	0
61	F8	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	G8	2	0	0	0	0
61	H5	3	0	0	0	0
61	I8	5	0	0	1	0
61	J8	3	0	0	0	0
61	K8	2	0	0	0	0
61	L5	2	0	0	0	0
61	L8	2	0	0	0	0
61	M5	10	0	0	0	0
61	P8	1	0	0	0	0
61	Q8	9	0	0	2	0
All	All	296184	0	196368	8991	1

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

The worst 5 of 8991 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)
37:35:81:GLN:NE2	37:35:106:LEU:HA	1.45	1.29
37:35:81:GLN:CD	37:35:106:LEU:HA	1.58	1.29
15:6A:27:VAL:O	15:6A:31:LEU:HD13	1.26	1.27
26:14:2572:A:C5	30:29:144:ARG:NH1	2.04	1.25
29:19:69:ARG:NH2	29:19:130:ALA:H	1.33	1.21

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	206/256 (80%)	175 (85%)	24 (12%)	7 (3%)	3	16
2	1E	227/256 (89%)	188 (83%)	37 (16%)	2 (1%)	14	43
3	22	192/239 (80%)	169 (88%)	23 (12%)	0	100	100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	182 (88%)	22 (11%)	2 (1%)	12	41
4	3E	205/209 (98%)	188 (92%)	16 (8%)	1 (0%)	24	55
5	42	146/162 (90%)	136 (93%)	10 (7%)	0	100	100
5	4E	147/162 (91%)	141 (96%)	5 (3%)	1 (1%)	18	49
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	135/156 (86%)	122 (90%)	12 (9%)	1 (1%)	18	49
7	6E	152/156 (97%)	140 (92%)	12 (8%)	0	100	100
8	72	135/138 (98%)	126 (93%)	7 (5%)	2 (2%)	8	33
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	18	49
9	82	119/128 (93%)	108 (91%)	9 (8%)	2 (2%)	7	30
9	8E	124/128 (97%)	105 (85%)	18 (14%)	1 (1%)	16	46
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	89/105 (85%)	82 (92%)	7 (8%)	0	100	100
11	2A	111/129 (86%)	98 (88%)	11 (10%)	2 (2%)	6	29
11	2I	109/129 (84%)	95 (87%)	12 (11%)	2 (2%)	6	29
12	3A	120/132 (91%)	103 (86%)	13 (11%)	4 (3%)	3	17
12	3I	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	16	46
13	4A	109/126 (86%)	92 (84%)	15 (14%)	2 (2%)	6	29
13	4I	117/126 (93%)	98 (84%)	18 (15%)	1 (1%)	14	43
14	5A	57/61 (93%)	47 (82%)	9 (16%)	1 (2%)	6	29
14	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	16
15	6A	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	6I	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
16	7A	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
16	7I	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100
18	9I	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	33
19	AA	56/93 (60%)	49 (88%)	4 (7%)	3 (5%)	1	9
19	AI	79/93 (85%)	70 (89%)	7 (9%)	2 (2%)	4	22
20	BA	97/106 (92%)	83 (86%)	12 (12%)	2 (2%)	5	26
20	BI	95/106 (90%)	82 (86%)	13 (14%)	0	100	100
21	1B	20/27 (74%)	18 (90%)	2 (10%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	129/229 (56%)	120 (93%)	9 (7%)	0	100	100
28	79	45/229 (20%)	41 (91%)	4 (9%)	0	100	100
29	11	271/276 (98%)	244 (90%)	17 (6%)	10 (4%)	2	15
29	19	272/276 (99%)	245 (90%)	21 (8%)	6 (2%)	5	25
30	21	201/206 (98%)	156 (78%)	36 (18%)	9 (4%)	2	12
30	29	202/206 (98%)	154 (76%)	39 (19%)	9 (4%)	2	12
31	31	200/210 (95%)	179 (90%)	20 (10%)	1 (0%)	24	55
31	39	202/210 (96%)	161 (80%)	31 (15%)	10 (5%)	1	10
32	41	177/182 (97%)	153 (86%)	21 (12%)	3 (2%)	7	30
32	49	177/182 (97%)	153 (86%)	22 (12%)	2 (1%)	11	39
33	51	169/180 (94%)	135 (80%)	24 (14%)	10 (6%)	1	8
33	59	68/180 (38%)	49 (72%)	14 (21%)	5 (7%)	1	4
34	61	144/148 (97%)	116 (81%)	26 (18%)	2 (1%)	9	34
34	69	143/148 (97%)	113 (79%)	27 (19%)	3 (2%)	5	26
35	15	136/140 (97%)	125 (92%)	10 (7%)	1 (1%)	18	49
35	58	136/140 (97%)	116 (85%)	16 (12%)	4 (3%)	3	20
36	25	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	46
36	68	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
37	35	145/150 (97%)	116 (80%)	25 (17%)	4 (3%)	4	20
37	78	145/150 (97%)	115 (79%)	26 (18%)	4 (3%)	4	20
38	45	136/141 (96%)	109 (80%)	23 (17%)	4 (3%)	3	20
38	88	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	2	16
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	98	116/118 (98%)	102 (88%)	13 (11%)	1 (1%)	14	43
40	65	108/112 (96%)	88 (82%)	18 (17%)	2 (2%)	6	28
40	A8	109/112 (97%)	90 (83%)	19 (17%)	0	100	100
41	75	131/146 (90%)	116 (88%)	15 (12%)	0	100	100
41	B8	131/146 (90%)	118 (90%)	12 (9%)	1 (1%)	16	46
42	85	114/118 (97%)	101 (89%)	12 (10%)	1 (1%)	14	43
42	C8	113/118 (96%)	100 (88%)	10 (9%)	3 (3%)	4	21
43	95	98/101 (97%)	75 (76%)	19 (19%)	4 (4%)	2	14
43	D8	98/101 (97%)	86 (88%)	8 (8%)	4 (4%)	2	14
44	A5	111/113 (98%)	104 (94%)	6 (5%)	1 (1%)	14	43
44	E8	110/113 (97%)	100 (91%)	10 (9%)	0	100	100
45	B5	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	5	25
45	F8	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	11	39
46	C5	102/110 (93%)	74 (72%)	21 (21%)	7 (7%)	1	5
46	G8	103/110 (94%)	85 (82%)	13 (13%)	5 (5%)	1	11
47	D5	126/206 (61%)	99 (79%)	20 (16%)	7 (6%)	1	9
47	H8	169/206 (82%)	132 (78%)	31 (18%)	6 (4%)	2	16
48	E5	75/85 (88%)	64 (85%)	9 (12%)	2 (3%)	4	21
48	I8	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
49	F5	92/98 (94%)	84 (91%)	7 (8%)	1 (1%)	11	39
49	J8	92/98 (94%)	85 (92%)	4 (4%)	3 (3%)	3	17
50	G5	64/72 (89%)	57 (89%)	6 (9%)	1 (2%)	7	32
50	K8	66/72 (92%)	58 (88%)	6 (9%)	2 (3%)	3	19
51	H5	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
51	L8	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
52	M8	45/71 (63%)	30 (67%)	14 (31%)	1 (2%)	5	25
53	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
53	N8	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	4 (9%)	0	100	100
55	M5	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	Q8	62/65 (95%)	51 (82%)	8 (13%)	3 (5%)	2	11
All	All	10975/12333 (89%)	9578 (87%)	1200 (11%)	197 (2%)	6	29

5 of 197 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
29	11	28	GLU
29	11	40	THR
29	11	237	GLU
29	11	273	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	182/220 (83%)	182 (100%)	0	100	100
2	1E	200/220 (91%)	199 (100%)	1 (0%)	81	82
3	22	154/188 (82%)	154 (100%)	0	100	100
3	2E	159/188 (85%)	158 (99%)	1 (1%)	78	81
4	32	180/181 (99%)	178 (99%)	2 (1%)	65	75
4	3E	178/181 (98%)	175 (98%)	3 (2%)	53	70
5	42	114/123 (93%)	114 (100%)	0	100	100
5	4E	115/123 (94%)	113 (98%)	2 (2%)	53	70
6	52	90/90 (100%)	89 (99%)	1 (1%)	65	75
6	5E	90/90 (100%)	90 (100%)	0	100	100
7	62	114/127 (90%)	113 (99%)	1 (1%)	70	77
7	6E	125/127 (98%)	125 (100%)	0	100	100
8	72	118/119 (99%)	118 (100%)	0	100	100
8	7E	119/119 (100%)	119 (100%)	0	100	100
9	82	92/99 (93%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	8E	97/99 (98%)	97 (100%)	0	100	100
10	1A	71/92 (77%)	70 (99%)	1 (1%)	59	73
10	1I	81/92 (88%)	79 (98%)	2 (2%)	42	65
11	2A	85/99 (86%)	85 (100%)	0	100	100
11	2I	84/99 (85%)	84 (100%)	0	100	100
12	3A	103/109 (94%)	103 (100%)	0	100	100
12	3I	103/109 (94%)	103 (100%)	0	100	100
13	4A	91/101 (90%)	91 (100%)	0	100	100
13	4I	94/101 (93%)	94 (100%)	0	100	100
14	5A	49/50 (98%)	49 (100%)	0	100	100
14	5I	49/50 (98%)	49 (100%)	0	100	100
15	6A	79/80 (99%)	79 (100%)	0	100	100
15	6I	79/80 (99%)	78 (99%)	1 (1%)	61	73
16	7A	72/74 (97%)	72 (100%)	0	100	100
16	7I	72/74 (97%)	72 (100%)	0	100	100
17	8A	94/97 (97%)	94 (100%)	0	100	100
17	8I	95/97 (98%)	95 (100%)	0	100	100
18	9A	58/77 (75%)	58 (100%)	0	100	100
18	9I	58/77 (75%)	58 (100%)	0	100	100
19	AA	52/80 (65%)	51 (98%)	1 (2%)	50	69
19	AI	71/80 (89%)	71 (100%)	0	100	100
20	BA	76/82 (93%)	75 (99%)	1 (1%)	61	73
20	BI	75/82 (92%)	75 (100%)	0	100	100
21	1B	17/22 (77%)	17 (100%)	0	100	100
21	1F	18/22 (82%)	18 (100%)	0	100	100
28	7I	109/181 (60%)	109 (100%)	0	100	100
28	79	48/181 (26%)	47 (98%)	1 (2%)	47	67
29	11	214/218 (98%)	213 (100%)	1 (0%)	81	82
29	19	214/218 (98%)	212 (99%)	2 (1%)	70	77
30	21	165/166 (99%)	165 (100%)	0	100	100
30	29	165/166 (99%)	164 (99%)	1 (1%)	78	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	31	161/166 (97%)	161 (100%)	0	100	100
31	39	163/166 (98%)	163 (100%)	0	100	100
32	41	153/156 (98%)	153 (100%)	0	100	100
32	49	153/156 (98%)	152 (99%)	1 (1%)	76	80
33	51	142/148 (96%)	139 (98%)	3 (2%)	47	67
33	59	59/148 (40%)	59 (100%)	0	100	100
34	61	122/124 (98%)	122 (100%)	0	100	100
34	69	122/124 (98%)	121 (99%)	1 (1%)	73	78
35	15	117/119 (98%)	116 (99%)	1 (1%)	70	77
35	58	117/119 (98%)	115 (98%)	2 (2%)	53	70
36	25	100/100 (100%)	99 (99%)	1 (1%)	68	76
36	68	100/100 (100%)	99 (99%)	1 (1%)	68	76
37	35	114/116 (98%)	114 (100%)	0	100	100
37	78	114/116 (98%)	114 (100%)	0	100	100
38	45	109/111 (98%)	108 (99%)	1 (1%)	70	77
38	88	109/111 (98%)	109 (100%)	0	100	100
39	55	101/101 (100%)	101 (100%)	0	100	100
39	98	101/101 (100%)	101 (100%)	0	100	100
40	65	87/88 (99%)	87 (100%)	0	100	100
40	A8	86/88 (98%)	86 (100%)	0	100	100
41	75	117/127 (92%)	115 (98%)	2 (2%)	53	70
41	B8	117/127 (92%)	116 (99%)	1 (1%)	70	77
42	85	93/94 (99%)	93 (100%)	0	100	100
42	C8	92/94 (98%)	92 (100%)	0	100	100
43	95	82/82 (100%)	82 (100%)	0	100	100
43	D8	82/82 (100%)	82 (100%)	0	100	100
44	A5	92/92 (100%)	90 (98%)	2 (2%)	45	67
44	E8	91/92 (99%)	91 (100%)	0	100	100
45	B5	74/78 (95%)	74 (100%)	0	100	100
45	F8	75/78 (96%)	75 (100%)	0	100	100
46	C5	85/91 (93%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	G8	85/91 (93%)	85 (100%)	0	100	100
47	D5	118/179 (66%)	118 (100%)	0	100	100
47	H8	152/179 (85%)	152 (100%)	0	100	100
48	E5	61/67 (91%)	61 (100%)	0	100	100
48	I8	61/67 (91%)	61 (100%)	0	100	100
49	F5	79/83 (95%)	79 (100%)	0	100	100
49	J8	79/83 (95%)	78 (99%)	1 (1%)	61	73
50	G5	62/67 (92%)	60 (97%)	2 (3%)	34	61
50	K8	62/67 (92%)	61 (98%)	1 (2%)	55	71
51	H5	50/52 (96%)	48 (96%)	2 (4%)	28	56
51	L8	50/52 (96%)	50 (100%)	0	100	100
52	M8	42/63 (67%)	40 (95%)	2 (5%)	23	52
53	J5	48/52 (92%)	48 (100%)	0	100	100
53	N8	43/52 (83%)	43 (100%)	0	100	100
54	L5	38/42 (90%)	38 (100%)	0	100	100
54	P8	38/42 (90%)	38 (100%)	0	100	100
55	M5	54/55 (98%)	54 (100%)	0	100	100
55	Q8	54/55 (98%)	54 (100%)	0	100	100
All	All	9274/10193 (91%)	9228 (100%)	46 (0%)	81	82

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	BA	37	SER
35	15	90	MET
28	79	207	THR
30	29	73	GLU
38	45	10	ARG

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

Mol	Chain	Res	Type
13	4A	62	ASN
45	B5	41	ASN
19	AA	57	HIS

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Mol	Chain	Res	Type
33	59	147	ASN
49	F5	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	365 (24%)	32 (2%)
1	1G	1503/1522 (98%)	366 (24%)	35 (2%)
22	1K	66/76 (86%)	32 (48%)	3 (4%)
22	1L	70/76 (92%)	38 (54%)	3 (4%)
23	2K	76/77 (98%)	19 (25%)	2 (2%)
23	2L	76/77 (98%)	18 (23%)	1 (1%)
24	3K	75/76 (98%)	49 (65%)	3 (4%)
25	4K	19/27 (70%)	11 (57%)	1 (5%)
25	4L	18/27 (66%)	10 (55%)	1 (5%)
26	14	2852/2917 (97%)	752 (26%)	45 (1%)
26	1H	2828/2917 (96%)	685 (24%)	52 (1%)
27	16	121/122 (99%)	26 (21%)	3 (2%)
27	1J	121/122 (99%)	31 (25%)	3 (2%)
56	3L	73/76 (96%)	44 (60%)	5 (6%)
All	All	9391/9634 (97%)	2446 (26%)	189 (2%)

5 of 2446 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	8	A
1	13	28	G

5 of 189 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	913	A
26	14	71	A
1	1G	1126	U
1	1G	1533	C
26	14	479	A

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

23 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$
22	PSU	1K	55	22	18,21,22	1.15	1 (5%)	22,30,33	1.83	4 (18%)
23	OMC	2K	33	23	19,22,23	1.81	3 (15%)	26,31,34	0.80	0
22	PSU	1K	39	22	18,21,22	1.10	1 (5%)	22,30,33	1.73	4 (18%)
22	PSU	1L	55	22	18,21,22	1.09	1 (5%)	22,30,33	1.70	5 (22%)
23	G7M	2K	47	23	23,26,27	2.61	7 (30%)	35,39,42	1.64	8 (22%)
22	5MU	1L	54	22	19,22,23	3.90	5 (26%)	28,32,35	3.27	8 (28%)
23	4SU	2K	8	23	18,21,22	1.89	5 (27%)	26,30,33	2.54	5 (19%)
22	U8U	1K	34	22,25	19,24,25	2.52	7 (36%)	23,34,37	1.09	2 (8%)
23	PSU	2L	56	23	18,21,22	1.06	1 (5%)	22,30,33	1.80	5 (22%)
23	OMC	2L	33	23	19,22,23	1.97	4 (21%)	26,31,34	1.07	1 (3%)
23	5MU	2K	55	23	19,22,23	3.81	5 (26%)	28,32,35	3.40	6 (21%)
22	T6A	1K	37	22	31,34,35	2.39	6 (19%)	44,49,52	2.61	15 (34%)
23	4SU	2L	8	23	18,21,22	1.83	3 (16%)	26,30,33	2.71	6 (23%)
23	5MU	2L	55	23	19,22,23	3.93	5 (26%)	28,32,35	3.41	10 (35%)
22	PSU	1L	39	22	18,21,22	1.01	1 (5%)	22,30,33	1.73	3 (13%)
23	PSU	2K	56	23	18,21,22	1.15	1 (5%)	22,30,33	1.89	5 (22%)
22	5MU	1K	54	22	19,22,23	3.80	5 (26%)	28,32,35	3.18	9 (32%)
56	PSU	3L	39	56	18,21,22	1.14	2 (11%)	22,30,33	1.99	5 (22%)
22	U8U	1L	34	22,25	19,24,25	2.59	7 (36%)	23,34,37	1.27	3 (13%)
24	PSU	3K	39	24	18,21,22	1.28	1 (5%)	22,30,33	1.72	4 (18%)
22	T6A	1L	37	22	31,34,35	2.18	6 (19%)	44,49,52	2.40	14 (31%)
23	G7M	2L	47	23	23,26,27	2.55	9 (39%)	35,39,42	1.72	10 (28%)
56	T6A	3L	37	56	31,34,35	2.17	4 (12%)	44,49,52	2.32	16 (36%)

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
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	PSU	1K	39	22	-	2/7/25/26	0/2/2/2
22	PSU	1L	55	22	-	3/7/25/26	0/2/2/2
23	G7M	2K	47	23	-	1/7/25/26	0/3/3/3
22	5MU	1L	54	22	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
22	U8U	1K	34	22,25	-	2/9/28/29	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/9/27/28	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	4/23/41/42	0/3/3/3
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	3/7/25/26	0/2/2/2
22	PSU	1L	39	22	-	2/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
56	PSU	3L	39	56	-	2/7/25/26	0/2/2/2
22	U8U	1L	34	22,25	-	2/9/28/29	0/2/2/2
24	PSU	3K	39	24	-	3/7/25/26	0/2/2/2
22	T6A	1L	37	22	-	7/23/41/42	0/3/3/3
23	G7M	2L	47	23	-	2/7/25/26	0/3/3/3
56	T6A	3L	37	56	-	9/23/41/42	0/3/3/3

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	54	5MU	C2-N1	12.57	1.58	1.38
23	2L	55	5MU	C2-N1	12.55	1.58	1.38
23	2K	55	5MU	C2-N1	12.48	1.58	1.38
22	1K	54	5MU	C2-N1	12.00	1.57	1.38
22	1K	37	T6A	C10-N11	7.66	1.52	1.35

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2K	55	5MU	C5-C4-N3	11.43	125.06	115.31
23	2L	55	5MU	C5-C4-N3	11.29	124.95	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1L	54	5MU	C5-C4-N3	10.66	124.41	115.31
22	1K	54	5MU	C5-C4-N3	10.55	124.32	115.31
23	2L	8	4SU	C4-N3-C2	-9.01	118.59	127.34

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	3K	39	PSU	C3'-C4'-C5'-O5'
22	1L	34	U8U	N-C-C5-C4
22	1L	34	U8U	N-C-C5-C6
22	1L	37	T6A	C5-C6-N6-C10
22	1L	37	T6A	N1-C6-N6-C10

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	8	4SU	1	0
22	1K	34	U8U	1	0
23	2L	56	PSU	3	0
23	2K	55	5MU	2	0
23	2L	8	4SU	2	0
23	2L	55	5MU	2	0
22	1K	54	5MU	1	0
56	3L	39	PSU	1	0
22	1L	37	T6A	2	0
23	2L	47	G7M	4	0
56	3L	37	T6A	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1269 ligands modelled in this entry, 1265 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	$\# Z > 2$
58	PAR	13	1749	-	45,45,45	0.85	0	64,67,67	2.01	16 (25%)
58	PAR	1G	1691	-	45,45,45	0.71	0	64,67,67	1.73	17 (26%)
59	SF4	32	301	-	0,12,12	-	-	-		
59	SF4	3E	301	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	13	1749	-	-	4/18/94/94	0/4/4/4
58	PAR	1G	1691	-	-	6/18/94/94	0/4/4/4
59	SF4	32	301	-	-	-	0/6/5/5
59	SF4	3E	301	4	-	-	0/6/5/5

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1749	PAR	C22-C12-C62	-4.86	102.69	110.04
58	13	1749	PAR	C14-O33-C33	-4.70	106.32	117.96
58	1G	1691	PAR	O11-C11-C21	-4.60	100.30	108.22
58	13	1749	PAR	C11-O51-C51	4.53	122.58	113.69
58	13	1749	PAR	C14-O54-C54	4.32	122.17	113.69

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

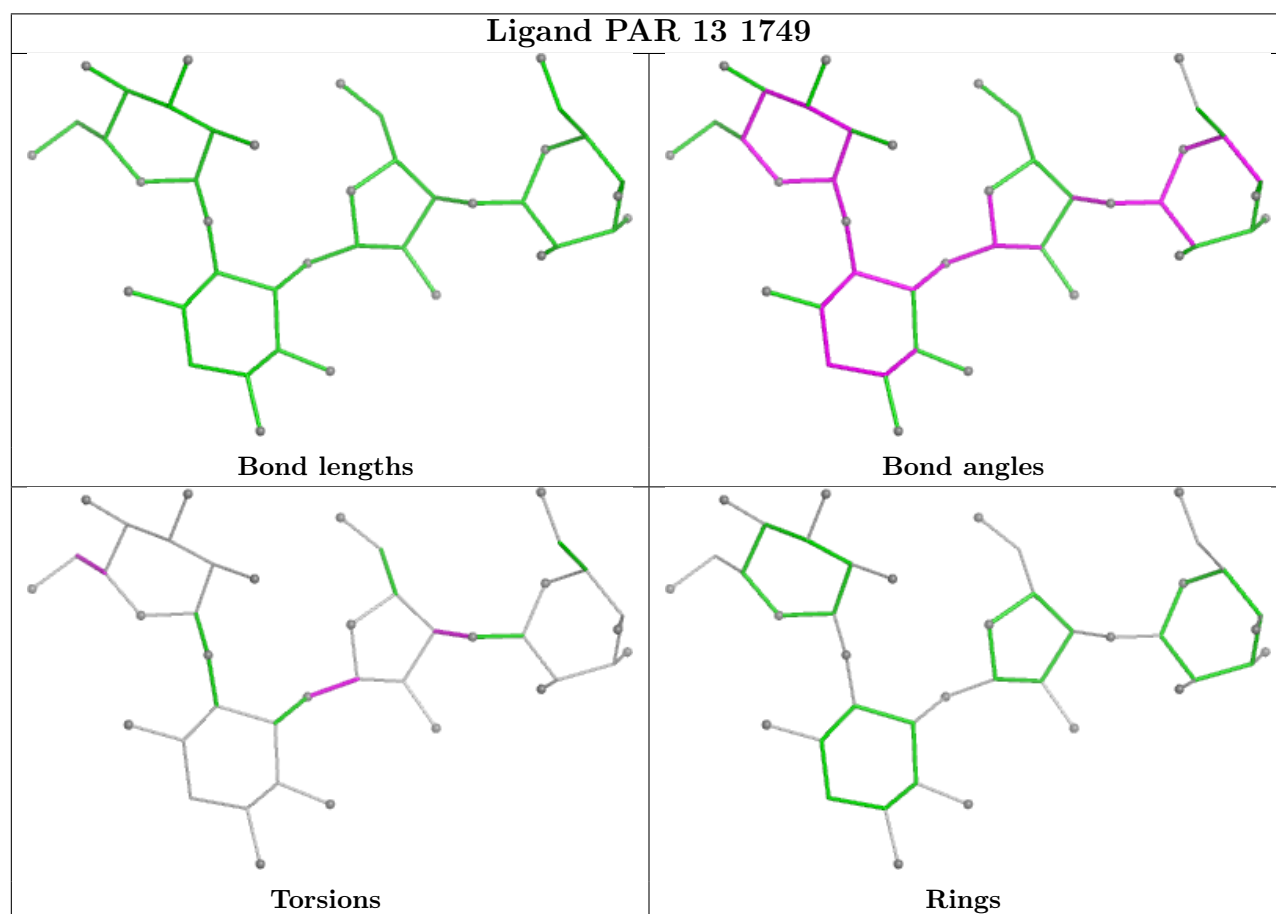
Mol	Chain	Res	Type	Atoms
58	13	1749	PAR	C41-C51-C61-O61
58	1G	1691	PAR	C33-C43-C53-O53
58	1G	1691	PAR	O43-C43-C53-O53
58	13	1749	PAR	O51-C51-C61-O61
58	1G	1691	PAR	O43-C13-O52-C52

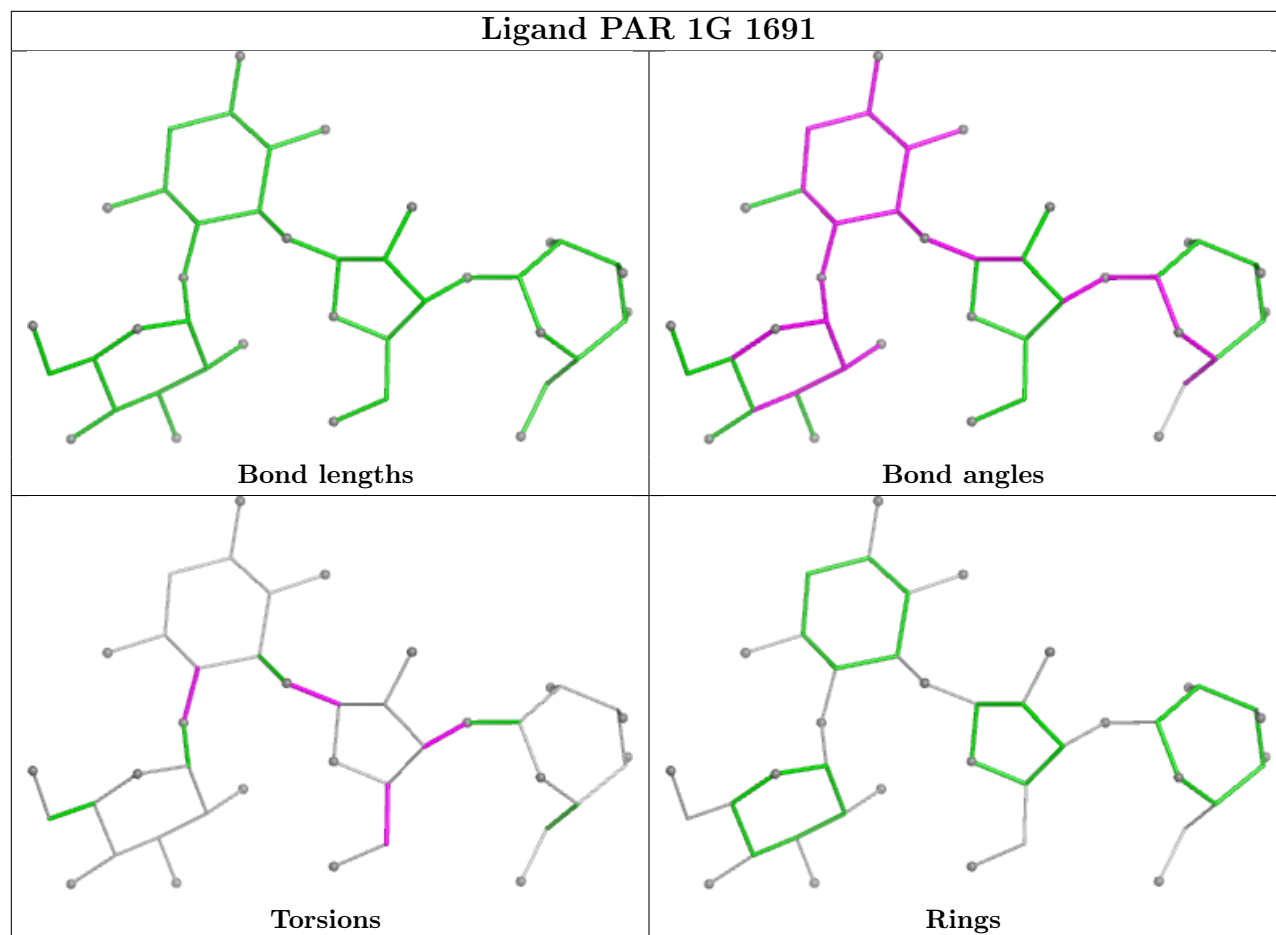
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	13	1749	PAR	3	0
58	1G	1691	PAR	2	0
59	32	301	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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
4	3E	1
34	69	1
10	1A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3E	36:ARG	C	37:PRO	N	1.17
1	69	79:ILE	C	80:PRO	N	1.16
1	1A	76:ASN	C	77:PRO	N	1.12

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1496/1522 (98%)	-0.59	3 (0%) 91 84	58, 99, 162, 246	0
1	1G	1506/1522 (98%)	-0.52	5 (0%) 90 81	73, 114, 168, 253	0
2	12	210/256 (82%)	0.15	1 (0%) 87 75	127, 152, 169, 182	0
2	1E	231/256 (90%)	-0.01	4 (1%) 69 48	105, 136, 157, 168	0
3	22	196/239 (82%)	0.00	0 100 100	122, 138, 165, 170	0
3	2E	205/239 (85%)	-0.34	1 (0%) 87 75	81, 103, 128, 138	0
4	32	208/209 (99%)	0.25	5 (2%) 59 39	98, 118, 136, 144	0
4	3E	207/209 (99%)	-0.03	3 (1%) 73 53	80, 101, 121, 129	0
5	42	148/162 (91%)	0.06	0 100 100	104, 121, 137, 147	0
5	4E	149/162 (91%)	-0.19	1 (0%) 84 69	79, 96, 112, 121	0
6	52	101/101 (100%)	-0.50	0 100 100	83, 101, 118, 131	0
6	5E	100/101 (99%)	-0.13	2 (2%) 65 44	83, 100, 115, 121	0
7	62	139/156 (89%)	-0.23	2 (1%) 73 53	111, 124, 135, 141	0
7	6E	154/156 (98%)	-0.15	3 (1%) 66 45	101, 115, 132, 141	0
8	72	137/138 (99%)	0.01	2 (1%) 72 52	104, 124, 136, 142	0
8	7E	138/138 (100%)	-0.15	4 (2%) 53 34	91, 106, 118, 127	0
9	82	121/128 (94%)	0.69	11 (9%) 15 8	110, 151, 165, 175	0
9	8E	126/128 (98%)	0.18	1 (0%) 82 66	89, 128, 147, 153	0
10	1A	80/105 (76%)	0.80	11 (13%) 6 4	116, 145, 154, 156	0
10	1I	91/105 (86%)	0.08	1 (1%) 78 60	80, 121, 156, 161	0
11	2A	113/129 (87%)	-0.20	1 (0%) 81 64	86, 110, 123, 130	0
11	2I	111/129 (86%)	-0.27	0 100 100	77, 102, 118, 125	0
12	3A	122/132 (92%)	0.08	4 (3%) 49 29	84, 102, 126, 145	0
12	3I	122/132 (92%)	-0.41	0 100 100	67, 77, 99, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	0.12	3 (2%) 56 35	109, 138, 154, 162	0
13	4I	119/126 (94%)	0.15	4 (3%) 48 28	84, 113, 128, 142	0
14	5A	59/61 (96%)	0.84	4 (6%) 23 13	122, 135, 145, 150	0
14	5I	60/61 (98%)	-0.03	1 (1%) 69 48	82, 92, 108, 112	0
15	6A	88/89 (98%)	-0.17	1 (1%) 78 60	89, 109, 128, 132	0
15	6I	87/89 (97%)	-0.20	0 100 100	83, 99, 116, 124	0
16	7A	84/88 (95%)	0.07	1 (1%) 76 57	92, 107, 125, 140	0
16	7I	83/88 (94%)	0.42	2 (2%) 59 39	97, 106, 136, 155	0
17	8A	99/105 (94%)	-0.01	2 (2%) 65 44	95, 114, 127, 134	0
17	8I	100/105 (95%)	0.07	3 (3%) 52 32	88, 104, 115, 121	0
18	9A	67/88 (76%)	-0.43	0 100 100	93, 111, 130, 132	0
18	9I	68/88 (77%)	-0.32	0 100 100	87, 102, 124, 127	0
19	AA	62/93 (66%)	0.15	0 100 100	123, 142, 153, 156	0
19	AI	81/93 (87%)	-0.14	0 100 100	91, 110, 132, 138	0
20	BA	99/106 (93%)	-0.08	1 (1%) 79 62	90, 110, 133, 142	0
20	BI	97/106 (91%)	0.28	6 (6%) 26 15	104, 121, 147, 152	0
21	1B	22/27 (81%)	1.62	6 (27%) 1 1	119, 130, 141, 145	0
21	1F	23/27 (85%)	0.20	0 100 100	89, 102, 110, 112	0
22	1K	64/76 (84%)	-0.05	4 (6%) 26 15	84, 173, 191, 198	0
22	1L	68/76 (89%)	0.11	3 (4%) 39 22	115, 198, 216, 220	0
23	2K	72/77 (93%)	-0.57	0 100 100	74, 96, 123, 139	0
23	2L	72/77 (93%)	-0.45	0 100 100	81, 109, 138, 153	0
24	3K	75/76 (98%)	-0.14	2 (2%) 56 35	76, 207, 224, 234	0
25	4K	20/27 (74%)	0.21	1 (5%) 34 20	73, 133, 219, 222	0
25	4L	19/27 (70%)	0.38	1 (5%) 32 18	92, 146, 215, 217	0
26	14	2861/2917 (98%)	-0.75	2 (0%) 92 88	54, 86, 192, 250	0
26	1H	2833/2917 (97%)	-0.82	6 (0%) 91 84	44, 76, 171, 250	0
27	16	122/122 (100%)	-0.82	0 100 100	69, 93, 114, 188	0
27	1J	122/122 (100%)	-0.43	1 (0%) 82 66	87, 113, 134, 182	0
28	71	133/229 (58%)	0.54	9 (6%) 23 13	135, 198, 223, 231	0
28	79	57/229 (24%)	0.38	3 (5%) 32 18	141, 174, 199, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	11	273/276 (98%)	-0.21	4 (1%) 72 52	43, 68, 86, 96	0
29	19	274/276 (99%)	-0.13	3 (1%) 78 60	52, 75, 91, 115	0
30	21	203/206 (98%)	0.20	11 (5%) 31 18	55, 93, 129, 137	0
30	29	204/206 (99%)	0.06	3 (1%) 72 52	63, 94, 125, 142	0
31	31	202/210 (96%)	-0.29	0 100 100	49, 80, 114, 128	0
31	39	204/210 (97%)	-0.19	0 100 100	60, 101, 144, 170	0
32	41	179/182 (98%)	-0.06	5 (2%) 55 34	80, 101, 132, 143	0
32	49	179/182 (98%)	-0.09	2 (1%) 78 60	107, 123, 144, 167	0
33	51	171/180 (95%)	-0.09	0 100 100	84, 103, 118, 126	0
33	59	74/180 (41%)	0.67	6 (8%) 18 10	127, 155, 176, 191	0
34	61	146/148 (98%)	-0.15	1 (0%) 84 69	80, 125, 142, 155	0
34	69	145/148 (97%)	-0.03	3 (2%) 63 42	86, 121, 142, 152	0
35	15	138/140 (98%)	0.07	3 (2%) 62 41	80, 104, 132, 141	0
35	58	138/140 (98%)	-0.02	2 (1%) 73 53	67, 94, 126, 137	0
36	25	122/122 (100%)	-0.18	3 (2%) 58 37	69, 87, 103, 112	0
36	68	122/122 (100%)	-0.13	0 100 100	61, 79, 95, 103	0
37	35	147/150 (98%)	0.20	7 (4%) 35 20	60, 102, 129, 139	0
37	78	147/150 (98%)	-0.04	1 (0%) 84 69	50, 84, 111, 117	0
38	45	138/141 (97%)	0.38	7 (5%) 33 19	74, 100, 118, 130	0
38	88	141/141 (100%)	-0.24	1 (0%) 84 69	61, 80, 100, 123	0
39	55	118/118 (100%)	-0.34	0 100 100	64, 80, 96, 107	0
39	98	118/118 (100%)	-0.15	0 100 100	66, 89, 106, 118	0
40	65	110/112 (98%)	0.14	5 (4%) 38 22	84, 106, 121, 127	0
40	A8	111/112 (99%)	-0.23	1 (0%) 81 64	76, 88, 107, 116	0
41	75	133/146 (91%)	0.15	6 (4%) 38 22	76, 95, 122, 143	0
41	B8	133/146 (91%)	0.07	3 (2%) 61 40	71, 94, 126, 141	0
42	85	116/118 (98%)	-0.08	0 100 100	67, 90, 121, 132	0
42	C8	115/118 (97%)	0.15	1 (0%) 81 64	60, 84, 111, 120	0
43	95	100/101 (99%)	0.14	5 (5%) 34 20	68, 117, 131, 142	0
43	D8	100/101 (99%)	0.16	5 (5%) 34 20	62, 103, 123, 129	0
44	A5	113/113 (100%)	-0.21	0 100 100	61, 75, 104, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	E8	112/113 (99%)	-0.32	0 100 100	60, 76, 104, 136	0
45	B5	94/96 (97%)	-0.23	1 (1%) 78 60	72, 83, 104, 119	0
45	F8	95/96 (98%)	-0.44	0 100 100	59, 74, 97, 107	0
46	C5	104/110 (94%)	0.33	1 (0%) 79 62	89, 114, 147, 154	0
46	G8	105/110 (95%)	0.25	6 (5%) 29 17	72, 94, 124, 135	0
47	D5	132/206 (64%)	-0.04	2 (1%) 72 52	104, 132, 155, 163	0
47	H8	171/206 (83%)	-0.16	1 (0%) 85 72	87, 118, 188, 193	0
48	E5	77/85 (90%)	0.23	1 (1%) 75 55	69, 87, 102, 123	0
48	I8	76/85 (89%)	-0.04	2 (2%) 57 36	59, 72, 85, 100	0
49	F5	94/98 (95%)	0.23	5 (5%) 32 18	66, 84, 115, 128	0
49	J8	94/98 (95%)	-0.10	1 (1%) 78 60	54, 77, 114, 120	0
50	G5	66/72 (91%)	-0.06	1 (1%) 72 52	81, 101, 121, 132	0
50	K8	68/72 (94%)	-0.01	1 (1%) 72 52	67, 84, 98, 115	0
51	H5	58/60 (96%)	-0.13	1 (1%) 69 48	77, 98, 128, 136	0
51	L8	58/60 (96%)	-0.43	0 100 100	65, 83, 107, 123	0
52	M8	47/71 (66%)	0.13	3 (6%) 25 14	102, 135, 150, 157	0
53	J5	56/60 (93%)	-0.09	1 (1%) 67 47	59, 87, 127, 134	0
53	N8	48/60 (80%)	-0.08	0 100 100	55, 86, 128, 132	0
54	L5	47/49 (95%)	-0.24	2 (4%) 40 23	54, 62, 83, 88	0
54	P8	47/49 (95%)	-0.28	1 (2%) 63 42	49, 55, 72, 81	0
55	M5	64/65 (98%)	0.20	3 (4%) 36 21	68, 78, 93, 111	0
55	Q8	64/65 (98%)	-0.13	0 100 100	62, 70, 84, 97	0
56	3L	73/76 (96%)	0.16	3 (4%) 41 24	84, 205, 228, 235	0
All	All	20602/21967 (93%)	-0.32	255 (1%) 76 57	43, 99, 165, 253	0

The worst 5 of 255 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	B8	1	MET	8.1
41	75	1	MET	7.1
41	B8	104	ASN	6.0
22	1L	76	A	5.5
21	1B	2	GLY	5.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	3L	39	20/21	0.77	0.11	118,132,140,141	0
22	PSU	1L	55	20/21	0.82	0.08	126,149,158,158	0
23	5MU	2L	55	21/22	0.85	0.09	105,114,119,125	0
24	PSU	3K	39	20/21	0.86	0.07	109,116,128,137	0
23	PSU	2L	56	20/21	0.87	0.06	106,110,116,120	0
22	5MU	1K	54	21/22	0.88	0.07	118,126,140,143	0
22	PSU	1K	55	20/21	0.88	0.07	107,132,143,147	0
56	T6A	3L	37	32/33	0.88	0.10	121,132,147,147	0
23	G7M	2L	47	24/25	0.89	0.08	114,121,128,132	0
22	5MU	1L	54	21/22	0.90	0.07	131,141,157,158	0
23	5MU	2K	55	21/22	0.91	0.07	90,103,110,112	0
23	4SU	2L	8	20/21	0.91	0.07	100,111,114,121	0
23	PSU	2K	56	20/21	0.91	0.07	95,100,104,111	0
22	T6A	1L	37	32/33	0.91	0.15	104,115,143,144	0
23	G7M	2K	47	24/25	0.92	0.06	90,101,110,116	0
22	T6A	1K	37	32/33	0.93	0.18	66,85,127,129	0
22	U8U	1L	34	23/24	0.93	0.13	115,123,131,134	0
23	4SU	2K	8	20/21	0.94	0.07	87,92,97,98	0
22	U8U	1K	34	23/24	0.94	0.09	81,89,100,107	0
22	PSU	1K	39	20/21	0.95	0.07	79,97,103,106	0
22	PSU	1L	39	20/21	0.95	0.07	104,123,128,130	0
23	OMC	2L	33	21/22	0.95	0.09	96,100,104,113	0
23	OMC	2K	33	21/22	0.96	0.08	73,80,83,87	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3232	1/1	0.30	0.25	130,130,130,130	0
57	MG	13	1646	1/1	0.32	0.26	109,109,109,109	0
57	MG	1G	1628	1/1	0.44	0.22	124,124,124,124	0
57	MG	1H	3282	1/1	0.47	0.30	96,96,96,96	0
57	MG	13	1650	1/1	0.49	0.35	100,100,100,100	0
57	MG	13	1642	1/1	0.49	0.36	107,107,107,107	0
57	MG	14	3031	1/1	0.53	0.30	105,105,105,105	0
57	MG	1H	3183	1/1	0.54	0.35	92,92,92,92	0
57	MG	1H	3018	1/1	0.56	0.28	80,80,80,80	0
57	MG	45	202	1/1	0.59	0.28	102,102,102,102	0
57	MG	1G	1621	1/1	0.60	0.31	103,103,103,103	0
57	MG	1H	3178	1/1	0.61	0.25	93,93,93,93	0
57	MG	1G	1692	1/1	0.62	0.31	105,105,105,105	0
57	MG	14	3162	1/1	0.62	0.23	67,67,67,67	0
57	MG	14	3248	1/1	0.63	0.24	75,75,75,75	0
57	MG	14	3241	1/1	0.63	0.35	84,84,84,84	0
57	MG	14	3265	1/1	0.64	0.23	79,79,79,79	0
57	MG	14	3266	1/1	0.64	0.29	84,84,84,84	0
57	MG	1G	1631	1/1	0.64	0.29	107,107,107,107	0
57	MG	14	3157	1/1	0.65	0.28	99,99,99,99	0
57	MG	13	1668	1/1	0.65	0.23	95,95,95,95	0
57	MG	1G	1645	1/1	0.65	0.31	88,88,88,88	0
57	MG	14	3120	1/1	0.65	0.24	67,67,67,67	0
57	MG	1G	1647	1/1	0.66	0.26	115,115,115,115	0
57	MG	1H	3272	1/1	0.66	0.37	95,95,95,95	0
57	MG	14	3170	1/1	0.66	0.45	86,86,86,86	0
57	MG	1H	3277	1/1	0.67	0.25	77,77,77,77	0
57	MG	14	3116	1/1	0.67	0.31	87,87,87,87	0
57	MG	16	207	1/1	0.67	0.26	77,77,77,77	0
57	MG	1H	3080	1/1	0.68	0.27	82,82,82,82	0
57	MG	1G	1694	1/1	0.68	0.27	98,98,98,98	0
57	MG	14	3260	1/1	0.68	0.15	117,117,117,117	0
57	MG	14	3016	1/1	0.68	0.27	73,73,73,73	0
57	MG	13	1625	1/1	0.68	0.57	96,96,96,96	0
57	MG	16	205	1/1	0.68	0.20	81,81,81,81	0
57	MG	2L	104	1/1	0.69	0.20	72,72,72,72	0
57	MG	14	3142	1/1	0.69	0.26	82,82,82,82	0
57	MG	1J	203	1/1	0.69	0.32	93,93,93,93	0
57	MG	1H	3210	1/1	0.69	0.21	74,74,74,74	0
57	MG	13	1662	1/1	0.70	0.18	119,119,119,119	0
57	MG	13	1661	1/1	0.70	0.30	102,102,102,102	0
57	MG	14	3257	1/1	0.70	0.36	87,87,87,87	0
57	MG	1H	3015	1/1	0.70	0.17	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3237	1/1	0.71	0.28	72,72,72,72	0
57	MG	13	1667	1/1	0.71	0.24	97,97,97,97	0
57	MG	14	3242	1/1	0.71	0.16	95,95,95,95	0
57	MG	14	3186	1/1	0.71	0.29	84,84,84,84	0
57	MG	2L	103	1/1	0.71	0.31	80,80,80,80	0
57	MG	1J	202	1/1	0.72	0.25	94,94,94,94	0
57	MG	14	3183	1/1	0.73	0.26	74,74,74,74	0
57	MG	1H	3177	1/1	0.73	0.27	81,81,81,81	0
57	MG	13	1636	1/1	0.73	0.28	75,75,75,75	0
57	MG	14	3144	1/1	0.73	0.31	80,80,80,80	0
57	MG	14	3035	1/1	0.73	0.41	83,83,83,83	0
57	MG	14	3102	1/1	0.73	0.21	86,86,86,86	0
57	MG	13	1648	1/1	0.73	0.39	90,90,90,90	0
57	MG	1H	3140	1/1	0.74	0.21	62,62,62,62	0
57	MG	14	3269	1/1	0.74	0.26	102,102,102,102	0
57	MG	1H	3014	1/1	0.74	0.26	75,75,75,75	0
57	MG	2K	101	1/1	0.74	0.23	95,95,95,95	0
57	MG	1H	3110	1/1	0.74	0.25	84,84,84,84	0
57	MG	14	3224	1/1	0.75	0.16	80,80,80,80	0
57	MG	14	3075	1/1	0.75	0.34	70,70,70,70	0
57	MG	1H	3115	1/1	0.75	0.23	82,82,82,82	0
57	MG	1H	3275	1/1	0.75	0.26	95,95,95,95	0
57	MG	13	1643	1/1	0.75	0.23	89,89,89,89	0
57	MG	13	1669	1/1	0.75	0.23	74,74,74,74	0
57	MG	14	3254	1/1	0.75	0.26	81,81,81,81	0
57	MG	14	3004	1/1	0.75	0.37	77,77,77,77	0
57	MG	1G	1640	1/1	0.75	0.22	100,100,100,100	0
57	MG	16	203	1/1	0.75	0.16	79,79,79,79	0
57	MG	1H	3247	1/1	0.75	0.36	77,77,77,77	0
57	MG	14	3036	1/1	0.75	0.32	76,76,76,76	0
57	MG	14	3063	1/1	0.75	0.24	76,76,76,76	0
57	MG	14	3206	1/1	0.75	0.26	95,95,95,95	0
57	MG	14	3211	1/1	0.75	0.25	78,78,78,78	0
57	MG	14	3104	1/1	0.76	0.29	81,81,81,81	0
57	MG	14	3259	1/1	0.76	0.19	97,97,97,97	0
57	MG	1I	201	1/1	0.76	0.21	100,100,100,100	0
57	MG	41	202	1/1	0.76	0.23	82,82,82,82	0
57	MG	14	3239	1/1	0.76	0.36	87,87,87,87	0
57	MG	1H	3493	1/1	0.76	0.20	94,94,94,94	0
57	MG	14	3198	1/1	0.76	0.18	81,81,81,81	0
57	MG	1H	3245	1/1	0.76	0.35	69,69,69,69	0
57	MG	13	1659	1/1	0.76	0.40	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3108	1/1	0.77	0.36	82,82,82,82	0
57	MG	1H	3218	1/1	0.77	0.33	70,70,70,70	0
57	MG	1H	3139	1/1	0.77	0.32	71,71,71,71	0
57	MG	2L	102	1/1	0.77	0.26	96,96,96,96	0
57	MG	14	3267	1/1	0.77	0.26	83,83,83,83	0
57	MG	1G	1637	1/1	0.77	0.19	77,77,77,77	0
57	MG	1H	3279	1/1	0.77	0.32	71,71,71,71	0
57	MG	14	3215	1/1	0.77	0.31	64,64,64,64	0
57	MG	35	202	1/1	0.77	0.20	75,75,75,75	0
57	MG	13	1666	1/1	0.77	0.29	77,77,77,77	0
57	MG	14	3175	1/1	0.78	0.20	90,90,90,90	0
57	MG	1G	1623	1/1	0.78	0.32	77,77,77,77	0
57	MG	14	3106	1/1	0.78	0.38	82,82,82,82	0
57	MG	14	3108	1/1	0.78	0.16	90,90,90,90	0
57	MG	14	3199	1/1	0.78	0.30	84,84,84,84	0
57	MG	14	3202	1/1	0.78	0.21	90,90,90,90	0
57	MG	14	3017	1/1	0.78	0.22	97,97,97,97	0
57	MG	1H	3185	1/1	0.78	0.32	90,90,90,90	0
57	MG	1H	3199	1/1	0.78	0.37	75,75,75,75	0
57	MG	1H	3288	1/1	0.78	0.23	80,80,80,80	0
57	MG	1G	1638	1/1	0.78	0.30	88,88,88,88	0
57	MG	1H	3126	1/1	0.78	0.22	70,70,70,70	0
57	MG	14	3168	1/1	0.78	0.23	89,89,89,89	0
57	MG	16	201	1/1	0.78	0.22	87,87,87,87	0
57	MG	1H	3122	1/1	0.79	0.20	73,73,73,73	0
57	MG	1H	3027	1/1	0.79	0.31	63,63,63,63	0
57	MG	1H	3197	1/1	0.79	0.18	67,67,67,67	0
57	MG	1H	3128	1/1	0.79	0.21	64,64,64,64	0
57	MG	1H	3208	1/1	0.79	0.21	76,76,76,76	0
57	MG	14	3110	1/1	0.79	0.23	86,86,86,86	0
57	MG	13	1629	1/1	0.79	0.19	98,98,98,98	0
57	MG	1H	3211	1/1	0.79	0.53	80,80,80,80	0
57	MG	1H	3213	1/1	0.79	0.20	92,92,92,92	0
57	MG	1H	3214	1/1	0.79	0.30	92,92,92,92	0
57	MG	13	1673	1/1	0.79	0.28	90,90,90,90	0
57	MG	1H	3230	1/1	0.79	0.26	78,78,78,78	0
57	MG	14	3163	1/1	0.79	0.31	72,72,72,72	0
57	MG	1H	3236	1/1	0.79	0.37	75,75,75,75	0
57	MG	14	3264	1/1	0.79	0.36	90,90,90,90	0
57	MG	13	1676	1/1	0.79	0.30	101,101,101,101	0
57	MG	1G	1626	1/1	0.79	0.32	73,73,73,73	0
57	MG	14	3033	1/1	0.79	0.23	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	14	3185	1/1	0.79	0.22	89,89,89,89	0
57	MG	13	1652	1/1	0.79	0.40	89,89,89,89	0
57	MG	1H	3180	1/1	0.79	0.27	76,76,76,76	0
57	MG	29	301	1/1	0.79	0.24	80,80,80,80	0
57	MG	14	3039	1/1	0.79	0.24	73,73,73,73	0
57	MG	1G	1633	1/1	0.79	0.27	100,100,100,100	0
57	MG	1H	3091	1/1	0.80	0.18	57,57,57,57	0
57	MG	14	3048	1/1	0.80	0.35	75,75,75,75	0
57	MG	1H	3276	1/1	0.80	0.22	98,98,98,98	0
57	MG	11	303	1/1	0.80	0.27	65,65,65,65	0
57	MG	1H	3196	1/1	0.80	0.34	88,88,88,88	0
57	MG	1G	1609	1/1	0.80	0.23	108,108,108,108	0
57	MG	1G	1611	1/1	0.80	0.25	74,74,74,74	0
57	MG	1H	3154	1/1	0.80	0.18	75,75,75,75	0
57	MG	13	1633	1/1	0.80	0.16	85,85,85,85	0
57	MG	1H	3287	1/1	0.80	0.26	80,80,80,80	0
57	MG	14	3210	1/1	0.80	0.27	80,80,80,80	0
57	MG	1G	1627	1/1	0.80	0.21	86,86,86,86	0
57	MG	13	1647	1/1	0.80	0.23	104,104,104,104	0
57	MG	1H	3291	1/1	0.80	0.40	88,88,88,88	0
57	MG	1H	3135	1/1	0.80	0.18	81,81,81,81	0
57	MG	29	304	1/1	0.80	0.11	71,71,71,71	0
57	MG	13	1603	1/1	0.80	0.21	76,76,76,76	0
57	MG	1H	3212	1/1	0.80	0.30	77,77,77,77	0
57	MG	14	3044	1/1	0.81	0.27	76,76,76,76	0
57	MG	13	1604	1/1	0.81	0.31	112,112,112,112	0
57	MG	1G	1622	1/1	0.81	0.30	76,76,76,76	0
57	MG	1H	3010	1/1	0.81	0.26	59,59,59,59	0
57	MG	14	3180	1/1	0.81	0.14	69,69,69,69	0
57	MG	13	1679	1/1	0.81	0.25	86,86,86,86	0
57	MG	1H	3168	1/1	0.81	0.34	80,80,80,80	0
57	MG	14	3105	1/1	0.81	0.27	55,55,55,55	0
57	MG	13	1682	1/1	0.81	0.32	90,90,90,90	0
57	MG	1H	3284	1/1	0.81	0.22	75,75,75,75	0
57	MG	1G	1632	1/1	0.81	0.20	132,132,132,132	0
57	MG	14	3203	1/1	0.81	0.16	89,89,89,89	0
57	MG	1H	3251	1/1	0.81	0.21	78,78,78,78	0
57	MG	1G	1636	1/1	0.81	0.29	89,89,89,89	0
57	MG	14	3129	1/1	0.81	0.20	69,69,69,69	0
57	MG	1G	1604	1/1	0.81	0.28	87,87,87,87	0
57	MG	1H	3258	1/1	0.81	0.13	79,79,79,79	0
57	MG	13	1635	1/1	0.81	0.09	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	1G	1618	1/1	0.81	0.20	86,86,86,86	0
57	MG	1H	3193	1/1	0.82	0.50	84,84,84,84	0
57	MG	14	3213	1/1	0.82	0.26	87,87,87,87	0
57	MG	13	1688	1/1	0.82	0.30	90,90,90,90	0
57	MG	14	3220	1/1	0.82	0.31	88,88,88,88	0
57	MG	13	1656	1/1	0.82	0.33	62,62,62,62	0
57	MG	14	3190	1/1	0.82	0.42	82,82,82,82	0
57	MG	14	3192	1/1	0.82	0.27	100,100,100,100	0
57	MG	14	3270	1/1	0.82	0.25	83,83,83,83	0
57	MG	14	3107	1/1	0.82	0.31	81,81,81,81	0
57	MG	13	1641	1/1	0.82	0.25	69,69,69,69	0
57	MG	88	201	1/1	0.82	0.44	82,82,82,82	0
57	MG	1H	3156	1/1	0.82	0.22	61,61,61,61	0
57	MG	35	201	1/1	0.82	0.26	71,71,71,71	0
57	MG	14	3094	1/1	0.82	0.30	85,85,85,85	0
57	MG	1H	3087	1/1	0.82	0.25	68,68,68,68	0
57	MG	1G	1619	1/1	0.83	0.24	92,92,92,92	0
57	MG	1H	3252	1/1	0.83	0.32	80,80,80,80	0
57	MG	1H	3191	1/1	0.83	0.12	95,95,95,95	0
57	MG	13	1644	1/1	0.83	0.17	80,80,80,80	0
57	MG	5I	101	1/1	0.83	0.19	88,88,88,88	0
57	MG	14	3226	1/1	0.83	0.24	78,78,78,78	0
57	MG	14	3143	1/1	0.83	0.20	73,73,73,73	0
57	MG	13	1618	1/1	0.83	0.28	64,64,64,64	0
57	MG	14	3155	1/1	0.83	0.17	66,66,66,66	0
57	MG	14	3021	1/1	0.83	0.27	53,53,53,53	0
57	MG	16	206	1/1	0.83	0.27	81,81,81,81	0
57	MG	1G	1629	1/1	0.83	0.29	83,83,83,83	0
57	MG	1G	1630	1/1	0.83	0.23	113,113,113,113	0
57	MG	1H	3066	1/1	0.83	0.20	57,57,57,57	0
57	MG	13	1665	1/1	0.83	0.32	82,82,82,82	0
57	MG	14	3179	1/1	0.83	0.28	74,74,74,74	0
57	MG	21	303	1/1	0.83	0.25	69,69,69,69	0
57	MG	1G	1635	1/1	0.83	0.28	97,97,97,97	0
57	MG	14	3058	1/1	0.83	0.19	66,66,66,66	0
57	MG	1H	3280	1/1	0.83	0.19	80,80,80,80	0
57	MG	14	3188	1/1	0.83	0.24	66,66,66,66	0
57	MG	1H	3242	1/1	0.83	0.31	80,80,80,80	0
57	MG	1H	3209	1/1	0.83	0.20	78,78,78,78	0
57	MG	1G	1639	1/1	0.83	0.22	97,97,97,97	0
57	MG	13	1689	1/1	0.83	0.27	99,99,99,99	0
57	MG	1H	3186	1/1	0.83	0.10	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	1G	1614	1/1	0.83	0.19	99,99,99,99	0
57	MG	1G	1616	1/1	0.83	0.26	86,86,86,86	0
57	MG	1H	3289	1/1	0.83	0.29	82,82,82,82	0
57	MG	1H	3233	1/1	0.84	0.26	70,70,70,70	0
57	MG	13	1674	1/1	0.84	0.23	78,78,78,78	0
57	MG	1H	3278	1/1	0.84	0.30	82,82,82,82	0
57	MG	13	1621	1/1	0.84	0.17	67,67,67,67	0
57	MG	1H	3036	1/1	0.84	0.15	78,78,78,78	0
57	MG	1G	1601	1/1	0.84	0.19	86,86,86,86	0
57	MG	14	3189	1/1	0.84	0.22	69,69,69,69	0
57	MG	1H	3246	1/1	0.84	0.28	85,85,85,85	0
57	MG	1H	3047	1/1	0.84	0.19	61,61,61,61	0
57	MG	1H	3120	1/1	0.84	0.14	63,63,63,63	0
57	MG	14	3261	1/1	0.84	0.21	102,102,102,102	0
57	MG	1G	1613	1/1	0.84	0.29	73,73,73,73	0
57	MG	1H	3159	1/1	0.84	0.17	56,56,56,56	0
57	MG	1H	3254	1/1	0.84	0.26	82,82,82,82	0
57	MG	1H	3255	1/1	0.84	0.12	88,88,88,88	0
57	MG	1H	3257	1/1	0.84	0.28	84,84,84,84	0
57	MG	1H	3011	1/1	0.84	0.35	72,72,72,72	0
57	MG	1J	201	1/1	0.84	0.20	85,85,85,85	0
57	MG	1H	3263	1/1	0.84	0.46	93,93,93,93	0
57	MG	14	3077	1/1	0.84	0.34	80,80,80,80	0
57	MG	14	3219	1/1	0.84	0.27	64,64,64,64	0
57	MG	13	1637	1/1	0.84	0.26	86,86,86,86	0
57	MG	14	3221	1/1	0.84	0.22	73,73,73,73	0
57	MG	13	1645	1/1	0.84	0.23	93,93,93,93	0
57	MG	14	3176	1/1	0.84	0.10	88,88,88,88	0
57	MG	55	201	1/1	0.84	0.35	83,83,83,83	0
57	MG	14	3233	1/1	0.85	0.31	79,79,79,79	0
57	MG	1H	3117	1/1	0.85	0.31	72,72,72,72	0
57	MG	1H	3283	1/1	0.85	0.34	82,82,82,82	0
57	MG	1H	3059	1/1	0.85	0.23	66,66,66,66	0
57	MG	13	1622	1/1	0.85	0.24	81,81,81,81	0
57	MG	1G	1608	1/1	0.85	0.21	91,91,91,91	0
57	MG	13	1602	1/1	0.85	0.28	88,88,88,88	0
57	MG	14	3109	1/1	0.85	0.20	60,60,60,60	0
57	MG	14	3026	1/1	0.85	0.27	72,72,72,72	0
57	MG	14	3113	1/1	0.85	0.27	73,73,73,73	0
57	MG	1H	3082	1/1	0.85	0.17	49,49,49,49	0
57	MG	14	3263	1/1	0.85	0.30	80,80,80,80	0
57	MG	13	1672	1/1	0.85	0.26	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	14	3034	1/1	0.85	0.25	57,57,57,57	0
57	MG	14	3131	1/1	0.85	0.19	78,78,78,78	0
57	MG	1H	3090	1/1	0.85	0.24	57,57,57,57	0
57	MG	1H	3007	1/1	0.85	0.19	68,68,68,68	0
57	MG	1H	3151	1/1	0.85	0.20	91,91,91,91	0
57	MG	14	3357	1/1	0.85	0.08	84,84,84,84	0
57	MG	14	3212	1/1	0.85	0.34	80,80,80,80	0
57	MG	16	204	1/1	0.85	0.23	90,90,90,90	0
57	MG	14	3046	1/1	0.85	0.19	58,58,58,58	0
57	MG	1G	1642	1/1	0.85	0.42	82,82,82,82	0
57	MG	1H	3240	1/1	0.85	0.17	72,72,72,72	0
57	MG	1H	3033	1/1	0.85	0.18	62,62,62,62	0
57	MG	13	1640	1/1	0.85	0.16	71,71,71,71	0
57	MG	1H	3111	1/1	0.85	0.20	80,80,80,80	0
57	MG	13	1628	1/1	0.85	0.44	96,96,96,96	0
57	MG	1H	3051	1/1	0.86	0.16	93,93,93,93	0
57	MG	1H	3025	1/1	0.86	0.20	56,56,56,56	0
57	MG	1H	3187	1/1	0.86	0.11	88,88,88,88	0
57	MG	14	3243	1/1	0.86	0.21	86,86,86,86	0
57	MG	1H	3114	1/1	0.86	0.21	78,78,78,78	0
57	MG	14	3191	1/1	0.86	0.30	73,73,73,73	0
57	MG	14	3255	1/1	0.86	0.18	87,87,87,87	0
57	MG	14	3062	1/1	0.86	0.18	85,85,85,85	0
57	MG	14	3134	1/1	0.86	0.17	98,98,98,98	0
57	MG	1H	3152	1/1	0.86	0.15	87,87,87,87	0
57	MG	14	3013	1/1	0.86	0.21	74,74,74,74	0
57	MG	1H	3008	1/1	0.86	0.20	57,57,57,57	0
57	MG	14	3205	1/1	0.86	0.39	77,77,77,77	0
57	MG	14	3146	1/1	0.86	0.30	76,76,76,76	0
57	MG	14	3147	1/1	0.86	0.16	72,72,72,72	0
57	MG	14	3088	1/1	0.86	0.23	65,65,65,65	0
57	MG	13	1660	1/1	0.86	0.28	83,83,83,83	0
57	MG	14	3097	1/1	0.86	0.27	65,65,65,65	0
57	MG	1H	3034	1/1	0.86	0.16	54,54,54,54	0
57	MG	14	3443	1/1	0.86	0.10	108,108,108,108	0
57	MG	1H	3035	1/1	0.86	0.24	57,57,57,57	0
57	MG	13	1678	1/1	0.86	0.25	83,83,83,83	0
57	MG	1H	3041	1/1	0.86	0.23	72,72,72,72	0
57	MG	1H	3129	1/1	0.86	0.26	76,76,76,76	0
57	MG	14	3225	1/1	0.86	0.35	80,80,80,80	0
57	MG	1H	3181	1/1	0.86	0.35	77,77,77,77	0
57	MG	1H	3285	1/1	0.86	0.28	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	1H	3021	1/1	0.86	0.17	90,90,90,90	0
57	MG	14	3111	1/1	0.86	0.20	79,79,79,79	0
57	MG	14	3240	1/1	0.87	0.21	85,85,85,85	0
57	MG	14	3043	1/1	0.87	0.17	75,75,75,75	0
57	MG	1H	3044	1/1	0.87	0.21	62,62,62,62	0
57	MG	1H	3205	1/1	0.87	0.20	77,77,77,77	0
57	MG	14	3244	1/1	0.87	0.25	77,77,77,77	0
57	MG	13	1605	1/1	0.87	0.20	68,68,68,68	0
57	MG	14	3053	1/1	0.87	0.30	77,77,77,77	0
57	MG	14	3195	1/1	0.87	0.13	105,105,105,105	0
57	MG	1G	1625	1/1	0.87	0.21	89,89,89,89	0
57	MG	14	3140	1/1	0.87	0.19	81,81,81,81	0
57	MG	1H	3105	1/1	0.87	0.27	79,79,79,79	0
57	MG	1H	3106	1/1	0.87	0.31	74,74,74,74	0
57	MG	1H	3248	1/1	0.87	0.19	79,79,79,79	0
57	MG	13	1653	1/1	0.87	0.18	66,66,66,66	0
57	MG	14	3078	1/1	0.87	0.16	86,86,86,86	0
57	MG	14	3150	1/1	0.87	0.19	68,68,68,68	0
57	MG	14	3082	1/1	0.87	0.24	55,55,55,55	0
57	MG	14	3268	1/1	0.87	0.19	60,60,60,60	0
57	MG	13	1655	1/1	0.87	0.31	71,71,71,71	0
57	MG	13	1681	1/1	0.87	0.33	86,86,86,86	0
57	MG	14	3271	1/1	0.87	0.24	80,80,80,80	0
57	MG	14	3272	1/1	0.87	0.31	77,77,77,77	0
57	MG	1G	1605	1/1	0.87	0.17	92,92,92,92	0
57	MG	1H	3076	1/1	0.87	0.18	76,76,76,76	0
57	MG	14	3022	1/1	0.87	0.29	60,60,60,60	0
57	MG	13	1611	1/1	0.87	0.29	79,79,79,79	0
57	MG	13	1675	1/1	0.87	0.23	79,79,79,79	0
57	MG	1H	3259	1/1	0.87	0.37	74,74,74,74	0
57	MG	14	3229	1/1	0.87	0.24	74,74,74,74	0
57	MG	1H	3083	1/1	0.87	0.17	74,74,74,74	0
57	MG	1H	3265	1/1	0.87	0.12	89,89,89,89	0
57	MG	1H	3023	1/1	0.87	0.29	81,81,81,81	0
57	MG	1H	3238	1/1	0.87	0.12	78,78,78,78	0
57	MG	14	3059	1/1	0.88	0.23	69,69,69,69	0
57	MG	14	3061	1/1	0.88	0.20	61,61,61,61	0
57	MG	1H	3157	1/1	0.88	0.23	64,64,64,64	0
57	MG	13	1626	1/1	0.88	0.15	87,87,87,87	0
57	MG	1H	3162	1/1	0.88	0.18	61,61,61,61	0
57	MG	14	3238	1/1	0.88	0.29	69,69,69,69	0
57	MG	14	3167	1/1	0.88	0.17	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3164	1/1	0.88	0.13	47,47,47,47	0
57	MG	1H	3286	1/1	0.88	0.18	82,82,82,82	0
57	MG	14	3171	1/1	0.88	0.25	73,73,73,73	0
57	MG	14	3081	1/1	0.88	0.41	74,74,74,74	0
57	MG	13	1684	1/1	0.88	0.18	85,85,85,85	0
57	MG	14	3245	1/1	0.88	0.19	79,79,79,79	0
57	MG	14	3085	1/1	0.88	0.23	65,65,65,65	0
57	MG	1H	3200	1/1	0.88	0.22	73,73,73,73	0
57	MG	1H	3202	1/1	0.88	0.22	58,58,58,58	0
57	MG	1H	3204	1/1	0.88	0.23	86,86,86,86	0
57	MG	1H	3169	1/1	0.88	0.13	85,85,85,85	0
57	MG	1H	3498	1/1	0.88	0.06	85,85,85,85	0
57	MG	1H	3171	1/1	0.88	0.23	68,68,68,68	0
57	MG	1H	3174	1/1	0.88	0.26	59,59,59,59	0
57	MG	1H	3112	1/1	0.88	0.26	66,66,66,66	0
57	MG	13	1631	1/1	0.88	0.14	73,73,73,73	0
57	MG	14	3027	1/1	0.88	0.21	83,83,83,83	0
57	MG	1H	3061	1/1	0.88	0.25	68,68,68,68	0
57	MG	1H	3142	1/1	0.88	0.26	85,85,85,85	0
57	MG	14	3200	1/1	0.88	0.15	69,69,69,69	0
57	MG	1H	3062	1/1	0.88	0.26	66,66,66,66	0
57	MG	13	1658	1/1	0.88	0.21	88,88,88,88	0
57	MG	13	1624	1/1	0.88	0.13	81,81,81,81	0
57	MG	1G	1634	1/1	0.88	0.19	93,93,93,93	0
57	MG	14	3040	1/1	0.88	0.18	64,64,64,64	0
57	MG	78	201	1/1	0.88	0.23	75,75,75,75	0
57	MG	1H	3232	1/1	0.88	0.24	65,65,65,65	0
57	MG	13	1654	1/1	0.88	0.31	75,75,75,75	0
57	MG	1G	1602	1/1	0.88	0.16	72,72,72,72	0
57	MG	14	3050	1/1	0.88	0.22	59,59,59,59	0
57	MG	14	3145	1/1	0.88	0.30	74,74,74,74	0
57	MG	1H	3188	1/1	0.88	0.34	74,74,74,74	0
57	MG	1H	3190	1/1	0.88	0.31	74,74,74,74	0
57	MG	14	3149	1/1	0.88	0.14	96,96,96,96	0
57	MG	1H	3144	1/1	0.89	0.30	75,75,75,75	0
57	MG	1H	3182	1/1	0.89	0.26	72,72,72,72	0
57	MG	1H	3147	1/1	0.89	0.14	51,51,51,51	0
57	MG	1H	3060	1/1	0.89	0.21	55,55,55,55	0
57	MG	14	3055	1/1	0.89	0.27	57,57,57,57	0
57	MG	13	1634	1/1	0.89	0.29	71,71,71,71	0
57	MG	1H	3267	1/1	0.89	0.09	67,67,67,67	0
57	MG	1H	3013	1/1	0.89	0.23	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3063	1/1	0.89	0.17	52,52,52,52	0
57	MG	14	3156	1/1	0.89	0.24	75,75,75,75	0
57	MG	1H	3220	1/1	0.89	0.26	73,73,73,73	0
57	MG	14	3069	1/1	0.89	0.32	67,67,67,67	0
57	MG	14	3072	1/1	0.89	0.23	69,69,69,69	0
57	MG	1G	1657	1/1	0.89	0.10	105,105,105,105	0
57	MG	14	3076	1/1	0.89	0.20	77,77,77,77	0
57	MG	1H	3221	1/1	0.89	0.12	60,60,60,60	0
57	MG	1H	3229	1/1	0.89	0.21	73,73,73,73	0
57	MG	1G	1610	1/1	0.89	0.15	114,114,114,114	0
57	MG	1H	3092	1/1	0.89	0.21	57,57,57,57	0
57	MG	14	3178	1/1	0.89	0.11	71,71,71,71	0
57	MG	1H	3231	1/1	0.89	0.26	65,65,65,65	0
57	MG	1H	3121	1/1	0.89	0.24	79,79,79,79	0
57	MG	14	3182	1/1	0.89	0.31	67,67,67,67	0
57	MG	1H	3099	1/1	0.89	0.13	60,60,60,60	0
57	MG	1H	3234	1/1	0.89	0.10	72,72,72,72	0
57	MG	1H	3235	1/1	0.89	0.10	65,65,65,65	0
57	MG	1H	3194	1/1	0.89	0.30	66,66,66,66	0
57	MG	1H	3101	1/1	0.89	0.15	58,58,58,58	0
57	MG	1H	3065	1/1	0.89	0.13	56,56,56,56	0
57	MG	1H	3241	1/1	0.89	0.34	71,71,71,71	0
57	MG	1H	3198	1/1	0.89	0.23	76,76,76,76	0
57	MG	1H	3006	1/1	0.89	0.15	86,86,86,86	0
57	MG	1H	3132	1/1	0.89	0.23	75,75,75,75	0
57	MG	1H	3201	1/1	0.89	0.20	65,65,65,65	0
57	MG	1H	3107	1/1	0.89	0.15	64,64,64,64	0
57	MG	14	3037	1/1	0.89	0.25	63,63,63,63	0
57	MG	14	3118	1/1	0.89	0.18	66,66,66,66	0
57	MG	13	1615	1/1	0.89	0.18	91,91,91,91	0
57	MG	14	3127	1/1	0.89	0.18	48,48,48,48	0
57	MG	13	1630	1/1	0.89	0.18	92,92,92,92	0
57	MG	14	3130	1/1	0.89	0.21	71,71,71,71	0
57	MG	14	3042	1/1	0.89	0.27	58,58,58,58	0
57	MG	1H	3206	1/1	0.89	0.24	56,56,56,56	0
57	MG	13	1687	1/1	0.89	0.18	70,70,70,70	0
57	MG	14	3216	1/1	0.89	0.30	74,74,74,74	0
57	MG	14	3217	1/1	0.89	0.23	76,76,76,76	0
57	MG	1G	1615	1/1	0.90	0.18	92,92,92,92	0
57	MG	13	1750	1/1	0.90	0.18	76,76,76,76	0
57	MG	1H	3476	1/1	0.90	0.07	93,93,93,93	0
57	MG	14	3064	1/1	0.90	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3222	1/1	0.90	0.23	64,64,64,64	0
57	MG	14	3223	1/1	0.90	0.32	75,75,75,75	0
57	MG	1H	3134	1/1	0.90	0.28	76,76,76,76	0
57	MG	14	3071	1/1	0.90	0.12	73,73,73,73	0
57	MG	1H	3005	1/1	0.90	0.34	74,74,74,74	0
57	MG	14	3006	1/1	0.90	0.21	66,66,66,66	0
57	MG	14	3230	1/1	0.90	0.21	70,70,70,70	0
57	MG	14	3009	1/1	0.90	0.22	68,68,68,68	0
57	MG	1H	3499	1/1	0.90	0.21	67,67,67,67	0
57	MG	14	3236	1/1	0.90	0.19	88,88,88,88	0
57	MG	1H	3138	1/1	0.90	0.22	55,55,55,55	0
57	MG	16	202	1/1	0.90	0.15	73,73,73,73	0
57	MG	1H	3176	1/1	0.90	0.34	67,67,67,67	0
57	MG	1H	3054	1/1	0.90	0.19	59,59,59,59	0
57	MG	14	3023	1/1	0.90	0.15	54,54,54,54	0
57	MG	14	3091	1/1	0.90	0.18	85,85,85,85	0
57	MG	14	3024	1/1	0.90	0.13	58,58,58,58	0
57	MG	1H	3113	1/1	0.90	0.39	82,82,82,82	0
57	MG	14	3099	1/1	0.90	0.16	57,57,57,57	0
57	MG	1H	3269	1/1	0.90	0.23	73,73,73,73	0
57	MG	1H	3067	1/1	0.90	0.18	52,52,52,52	0
57	MG	1H	3070	1/1	0.90	0.14	45,45,45,45	0
57	MG	1H	3100	1/1	0.90	0.15	44,44,44,44	0
57	MG	1H	3207	1/1	0.90	0.09	56,56,56,56	0
57	MG	1H	3119	1/1	0.90	0.14	71,71,71,71	0
57	MG	13	1670	1/1	0.90	0.30	78,78,78,78	0
57	MG	1H	3243	1/1	0.90	0.30	62,62,62,62	0
57	MG	1H	3281	1/1	0.90	0.38	69,69,69,69	0
57	MG	14	3112	1/1	0.90	0.31	88,88,88,88	0
57	MG	1H	3103	1/1	0.90	0.31	82,82,82,82	0
57	MG	14	3194	1/1	0.90	0.17	68,68,68,68	0
57	MG	1H	3077	1/1	0.90	0.25	74,74,74,74	0
57	MG	1H	3125	1/1	0.90	0.31	61,61,61,61	0
57	MG	1H	3158	1/1	0.90	0.38	68,68,68,68	0
57	MG	14	3123	1/1	0.90	0.37	70,70,70,70	0
57	MG	1H	3250	1/1	0.90	0.15	67,67,67,67	0
57	MG	14	3128	1/1	0.90	0.13	60,60,60,60	0
57	MG	14	3421	1/1	0.90	0.09	75,75,75,75	0
57	MG	1G	1646	1/1	0.90	0.30	84,84,84,84	0
57	MG	14	3052	1/1	0.90	0.18	62,62,62,62	0
57	MG	14	3207	1/1	0.90	0.09	71,71,71,71	0
57	MG	14	3208	1/1	0.90	0.22	75,75,75,75	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	0.90	0.16	53,53,53,53	0
57	MG	14	3133	1/1	0.90	0.19	71,71,71,71	0
57	MG	1G	1648	1/1	0.90	0.16	86,86,86,86	0
57	MG	14	3136	1/1	0.90	0.26	59,59,59,59	0
57	MG	45	201	1/1	0.90	0.21	72,72,72,72	0
57	MG	13	1614	1/1	0.90	0.27	64,64,64,64	0
57	MG	1H	3045	1/1	0.90	0.16	54,54,54,54	0
57	MG	14	3067	1/1	0.91	0.10	68,68,68,68	0
57	MG	1H	3086	1/1	0.91	0.19	71,71,71,71	0
57	MG	1H	3244	1/1	0.91	0.36	84,84,84,84	0
57	MG	41	201	1/1	0.91	0.18	75,75,75,75	0
57	MG	1H	3160	1/1	0.91	0.29	67,67,67,67	0
57	MG	1H	3189	1/1	0.91	0.23	87,87,87,87	0
57	MG	14	3148	1/1	0.91	0.20	69,69,69,69	0
57	MG	1H	3161	1/1	0.91	0.20	72,72,72,72	0
57	MG	13	1609	1/1	0.91	0.24	58,58,58,58	0
57	MG	14	3153	1/1	0.91	0.10	79,79,79,79	0
57	MG	14	3154	1/1	0.91	0.39	74,74,74,74	0
57	MG	14	3025	1/1	0.91	0.13	58,58,58,58	0
57	MG	14	3231	1/1	0.91	0.48	76,76,76,76	0
57	MG	1H	3215	1/1	0.91	0.22	65,65,65,65	0
57	MG	14	3083	1/1	0.91	0.17	61,61,61,61	0
57	MG	14	3084	1/1	0.91	0.20	56,56,56,56	0
57	MG	13	1651	1/1	0.91	0.19	68,68,68,68	0
57	MG	14	3165	1/1	0.91	0.11	78,78,78,78	0
57	MG	14	3166	1/1	0.91	0.15	61,61,61,61	0
57	MG	14	3030	1/1	0.91	0.15	68,68,68,68	0
57	MG	1H	3037	1/1	0.91	0.24	55,55,55,55	0
57	MG	14	3093	1/1	0.91	0.18	51,51,51,51	0
57	MG	1H	3004	1/1	0.91	0.19	54,54,54,54	0
57	MG	14	3173	1/1	0.91	0.20	69,69,69,69	0
57	MG	14	3095	1/1	0.91	0.12	85,85,85,85	0
57	MG	13	1607	1/1	0.91	0.18	74,74,74,74	0
57	MG	14	3098	1/1	0.91	0.12	67,67,67,67	0
57	MG	13	1686	1/1	0.91	0.17	96,96,96,96	0
57	MG	1H	3175	1/1	0.91	0.32	65,65,65,65	0
57	MG	14	3258	1/1	0.91	0.45	83,83,83,83	0
57	MG	1H	3471	1/1	0.91	0.06	82,82,82,82	0
57	MG	13	1639	1/1	0.91	0.12	84,84,84,84	0
57	MG	13	1612	1/1	0.91	0.29	85,85,85,85	0
57	MG	14	3041	1/1	0.91	0.20	64,64,64,64	0
57	MG	1H	3148	1/1	0.91	0.20	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3266	1/1	0.91	0.13	75,75,75,75	0
57	MG	13	1677	1/1	0.91	0.26	76,76,76,76	0
57	MG	1H	3055	1/1	0.91	0.20	72,72,72,72	0
57	MG	7A	101	1/1	0.91	0.42	89,89,89,89	0
57	MG	2L	101	1/1	0.91	0.20	70,70,70,70	0
57	MG	14	3051	1/1	0.91	0.17	62,62,62,62	0
57	MG	1H	3271	1/1	0.91	0.22	74,74,74,74	0
57	MG	13	1649	1/1	0.91	0.34	78,78,78,78	0
57	MG	14	3121	1/1	0.91	0.33	77,77,77,77	0
57	MG	14	3054	1/1	0.91	0.34	67,67,67,67	0
57	MG	1G	1624	1/1	0.91	0.16	87,87,87,87	0
57	MG	14	3003	1/1	0.91	0.20	65,65,65,65	0
57	MG	13	1671	1/1	0.91	0.18	71,71,71,71	0
57	MG	14	3060	1/1	0.91	0.20	74,74,74,74	0
57	MG	1H	3085	1/1	0.91	0.28	71,71,71,71	0
57	MG	14	3209	1/1	0.91	0.31	64,64,64,64	0
57	MG	14	3007	1/1	0.91	0.14	50,50,50,50	0
57	MG	1H	3131	1/1	0.91	0.24	67,67,67,67	0
57	MG	14	3010	1/1	0.91	0.23	69,69,69,69	0
57	MG	14	3139	1/1	0.91	0.22	58,58,58,58	0
57	MG	14	3066	1/1	0.91	0.10	53,53,53,53	0
57	MG	1H	3150	1/1	0.92	0.05	50,50,50,50	0
57	MG	14	3045	1/1	0.92	0.14	64,64,64,64	0
57	MG	14	3164	1/1	0.92	0.24	65,65,65,65	0
57	MG	1G	1612	1/1	0.92	0.21	67,67,67,67	0
57	MG	14	3227	1/1	0.92	0.35	83,83,83,83	0
57	MG	14	3228	1/1	0.92	0.22	81,81,81,81	0
57	MG	14	3103	1/1	0.92	0.32	68,68,68,68	0
57	MG	1H	3050	1/1	0.92	0.21	66,66,66,66	0
57	MG	13	1657	1/1	0.92	0.34	73,73,73,73	0
57	MG	14	3169	1/1	0.92	0.10	65,65,65,65	0
57	MG	1H	3411	1/1	0.92	0.07	81,81,81,81	0
57	MG	1H	3093	1/1	0.92	0.32	71,71,71,71	0
57	MG	1H	3069	1/1	0.92	0.36	65,65,65,65	0
57	MG	1H	3124	1/1	0.92	0.15	74,74,74,74	0
57	MG	1G	1620	1/1	0.92	0.21	79,79,79,79	0
57	MG	1H	3019	1/1	0.92	0.25	78,78,78,78	0
57	MG	1H	3261	1/1	0.92	0.16	67,67,67,67	0
57	MG	1H	3228	1/1	0.92	0.34	69,69,69,69	0
57	MG	1H	3071	1/1	0.92	0.24	54,54,54,54	0
57	MG	1H	3192	1/1	0.92	0.36	82,82,82,82	0
57	MG	1H	3074	1/1	0.92	0.16	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	14	3246	1/1	0.92	0.14	76,76,76,76	0
57	MG	14	3247	1/1	0.92	0.13	67,67,67,67	0
57	MG	1H	3075	1/1	0.92	0.12	60,60,60,60	0
57	MG	1H	3020	1/1	0.92	0.17	107,107,107,107	0
57	MG	14	3126	1/1	0.92	0.30	64,64,64,64	0
57	MG	14	3256	1/1	0.92	0.12	91,91,91,91	0
57	MG	1H	3056	1/1	0.92	0.14	52,52,52,52	0
57	MG	14	3068	1/1	0.92	0.15	67,67,67,67	0
57	MG	1H	3166	1/1	0.92	0.12	70,70,70,70	0
57	MG	1H	3078	1/1	0.92	0.18	60,60,60,60	0
57	MG	1H	3109	1/1	0.92	0.27	65,65,65,65	0
57	MG	1H	3058	1/1	0.92	0.13	53,53,53,53	0
57	MG	1H	3172	1/1	0.92	0.13	73,73,73,73	0
57	MG	13	1616	1/1	0.92	0.15	48,48,48,48	0
57	MG	L8	101	1/1	0.92	0.25	72,72,72,72	0
57	MG	1H	3022	1/1	0.92	0.16	81,81,81,81	0
57	MG	14	3204	1/1	0.92	0.18	90,90,90,90	0
57	MG	13	1601	1/1	0.92	0.12	68,68,68,68	0
57	MG	1H	3143	1/1	0.92	0.33	89,89,89,89	0
57	MG	13	1685	1/1	0.92	0.15	101,101,101,101	0
57	MG	1G	1641	1/1	0.92	0.45	78,78,78,78	0
57	MG	14	3087	1/1	0.92	0.15	97,97,97,97	0
57	MG	1G	1606	1/1	0.92	0.21	67,67,67,67	0
57	MG	14	3089	1/1	0.92	0.17	56,56,56,56	0
57	MG	14	3090	1/1	0.92	0.08	60,60,60,60	0
57	MG	1G	1643	1/1	0.92	0.39	67,67,67,67	0
57	MG	14	3214	1/1	0.92	0.36	73,73,73,73	0
57	MG	14	3151	1/1	0.92	0.08	72,72,72,72	0
57	MG	1G	1607	1/1	0.92	0.12	91,91,91,91	0
57	MG	39	301	1/1	0.92	0.05	95,95,95,95	0
57	MG	13	1751	1/1	0.92	0.17	87,87,87,87	0
57	MG	13	1680	1/1	0.92	0.21	75,75,75,75	0
57	MG	14	3096	1/1	0.92	0.17	65,65,65,65	0
57	MG	1H	3149	1/1	0.92	0.10	61,61,61,61	0
57	MG	14	3158	1/1	0.92	0.09	70,70,70,70	0
57	MG	1H	3167	1/1	0.93	0.14	63,63,63,63	0
57	MG	1H	3095	1/1	0.93	0.29	65,65,65,65	0
57	MG	1H	3096	1/1	0.93	0.18	67,67,67,67	0
57	MG	1H	3097	1/1	0.93	0.12	51,51,51,51	0
57	MG	14	3172	1/1	0.93	0.18	63,63,63,63	0
57	MG	1H	3274	1/1	0.93	0.09	70,70,70,70	0
57	MG	14	3174	1/1	0.93	0.20	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3234	1/1	0.93	0.08	64,64,64,64	0
57	MG	14	3119	1/1	0.93	0.34	63,63,63,63	0
57	MG	21	301	1/1	0.93	0.24	66,66,66,66	0
57	MG	1H	3118	1/1	0.93	0.07	60,60,60,60	0
57	MG	14	3122	1/1	0.93	0.08	104,104,104,104	0
57	MG	1H	3016	1/1	0.93	0.21	49,49,49,49	0
57	MG	14	3181	1/1	0.93	0.18	63,63,63,63	0
57	MG	14	3125	1/1	0.93	0.13	54,54,54,54	0
57	MG	1H	3146	1/1	0.93	0.33	51,51,51,51	0
57	MG	1H	3203	1/1	0.93	0.15	64,64,64,64	0
57	MG	1H	3038	1/1	0.93	0.18	53,53,53,53	0
57	MG	14	3187	1/1	0.93	0.13	80,80,80,80	0
57	MG	13	1663	1/1	0.93	0.42	71,71,71,71	0
57	MG	P8	101	1/1	0.93	0.27	66,66,66,66	0
57	MG	14	3251	1/1	0.93	0.20	82,82,82,82	0
57	MG	1H	3068	1/1	0.93	0.28	69,69,69,69	0
57	MG	1H	3123	1/1	0.93	0.18	71,71,71,71	0
57	MG	1H	3104	1/1	0.93	0.20	62,62,62,62	0
57	MG	14	3135	1/1	0.93	0.30	71,71,71,71	0
57	MG	1H	3084	1/1	0.93	0.13	82,82,82,82	0
57	MG	14	3138	1/1	0.93	0.13	68,68,68,68	0
57	MG	1H	3057	1/1	0.93	0.27	53,53,53,53	0
57	MG	1H	3249	1/1	0.93	0.23	61,61,61,61	0
57	MG	14	3141	1/1	0.93	0.17	50,50,50,50	0
57	MG	14	3038	1/1	0.93	0.12	76,76,76,76	0
57	MG	1H	3184	1/1	0.93	0.22	67,67,67,67	0
57	MG	1H	3043	1/1	0.93	0.17	70,70,70,70	0
57	MG	13	1613	1/1	0.93	0.14	65,65,65,65	0
57	MG	1H	3130	1/1	0.93	0.26	67,67,67,67	0
57	MG	1G	1649	1/1	0.93	0.09	115,115,115,115	0
57	MG	1H	3088	1/1	0.93	0.18	53,53,53,53	0
57	MG	1H	3452	1/1	0.93	0.07	89,89,89,89	0
57	MG	1H	3465	1/1	0.93	0.15	53,53,53,53	0
57	MG	14	3047	1/1	0.93	0.17	42,42,42,42	0
57	MG	1H	3012	1/1	0.93	0.24	42,42,42,42	0
57	MG	1H	3133	1/1	0.93	0.41	80,80,80,80	0
57	MG	14	3100	1/1	0.93	0.12	43,43,43,43	0
57	MG	13	1619	1/1	0.93	0.18	90,90,90,90	0
57	MG	1H	3496	1/1	0.93	0.07	94,94,94,94	0
57	MG	1H	3260	1/1	0.93	0.19	65,65,65,65	0
57	MG	29	303	1/1	0.93	0.20	67,67,67,67	0
57	MG	14	3159	1/1	0.93	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	1627	1/1	0.93	0.20	64,64,64,64	0
57	MG	39	302	1/1	0.93	0.07	63,63,63,63	0
57	MG	1H	3165	1/1	0.93	0.31	72,72,72,72	0
57	MG	14	3056	1/1	0.93	0.45	82,82,82,82	0
57	MG	14	3005	1/1	0.93	0.14	70,70,70,70	0
57	MG	13	1620	1/1	0.93	0.20	58,58,58,58	0
57	MG	1H	3195	1/1	0.93	0.21	73,73,73,73	0
60	ZN	G8	201	1/1	0.93	0.16	146,146,146,146	0
60	ZN	C5	202	1/1	0.93	0.08	169,169,169,169	0
57	MG	14	3193	1/1	0.94	0.10	70,70,70,70	0
57	MG	1H	3145	1/1	0.94	0.17	46,46,46,46	0
57	MG	1H	3049	1/1	0.94	0.15	68,68,68,68	0
57	MG	14	3101	1/1	0.94	0.27	64,64,64,64	0
57	MG	21	302	1/1	0.94	0.26	50,50,50,50	0
57	MG	1H	3028	1/1	0.94	0.13	51,51,51,51	0
57	MG	1H	3072	1/1	0.94	0.32	73,73,73,73	0
57	MG	14	3250	1/1	0.94	0.12	65,65,65,65	0
57	MG	14	3057	1/1	0.94	0.23	41,41,41,41	0
57	MG	1H	3029	1/1	0.94	0.17	49,49,49,49	0
57	MG	14	3015	1/1	0.94	0.18	77,77,77,77	0
57	MG	1H	3098	1/1	0.94	0.37	63,63,63,63	0
57	MG	13	1742	1/1	0.94	0.06	100,100,100,100	0
57	MG	14	3019	1/1	0.94	0.23	58,58,58,58	0
57	MG	13	1744	1/1	0.94	0.10	94,94,94,94	0
57	MG	14	3161	1/1	0.94	0.13	73,73,73,73	0
57	MG	13	1748	1/1	0.94	0.12	115,115,115,115	0
57	MG	13	1623	1/1	0.94	0.20	61,61,61,61	0
57	MG	14	3115	1/1	0.94	0.28	71,71,71,71	0
57	MG	1H	3127	1/1	0.94	0.15	56,56,56,56	0
57	MG	1H	3079	1/1	0.94	0.15	47,47,47,47	0
57	MG	13	1617	1/1	0.94	0.11	53,53,53,53	0
57	MG	13	1608	1/1	0.94	0.12	75,75,75,75	0
57	MG	1H	3403	1/1	0.94	0.09	89,89,89,89	0
57	MG	14	3073	1/1	0.94	0.11	57,57,57,57	0
57	MG	3I	201	1/1	0.94	0.11	57,57,57,57	0
57	MG	1H	3428	1/1	0.94	0.06	87,87,87,87	0
57	MG	1G	1644	1/1	0.94	0.22	67,67,67,67	0
57	MG	1H	3039	1/1	0.94	0.10	90,90,90,90	0
57	MG	1H	3226	1/1	0.94	0.07	64,64,64,64	0
57	MG	14	3448	1/1	0.94	0.06	92,92,92,92	0
57	MG	14	3452	1/1	0.94	0.11	113,113,113,113	0
57	MG	1H	3040	1/1	0.94	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	1664	1/1	0.94	0.46	81,81,81,81	0
57	MG	1H	3024	1/1	0.94	0.24	45,45,45,45	0
57	MG	13	1729	1/1	0.94	0.06	91,91,91,91	0
57	MG	29	302	1/1	0.94	0.17	40,40,40,40	0
57	MG	1G	1684	1/1	0.94	0.10	121,121,121,121	0
57	MG	1H	3089	1/1	0.94	0.19	51,51,51,51	0
57	MG	1H	3026	1/1	0.94	0.23	40,40,40,40	0
57	MG	1H	3170	1/1	0.94	0.38	72,72,72,72	0
57	MG	1H	3046	1/1	0.94	0.35	73,73,73,73	0
57	MG	1H	3116	1/1	0.94	0.19	63,63,63,63	0
57	MG	1H	3273	1/1	0.94	0.09	57,57,57,57	0
57	MG	1H	3237	1/1	0.94	0.12	61,61,61,61	0
57	MG	45	203	1/1	0.94	0.25	71,71,71,71	0
57	MG	14	3049	1/1	0.94	0.19	63,63,63,63	0
57	MG	1H	3173	1/1	0.94	0.15	63,63,63,63	0
57	MG	2K	102	1/1	0.94	0.07	92,92,92,92	0
57	MG	1H	3290	1/1	0.95	0.24	62,62,62,62	0
57	MG	1H	3225	1/1	0.95	0.22	67,67,67,67	0
57	MG	5E	201	1/1	0.95	0.12	81,81,81,81	0
57	MG	1H	3081	1/1	0.95	0.10	47,47,47,47	0
57	MG	13	1610	1/1	0.95	0.11	79,79,79,79	0
57	MG	1H	3433	1/1	0.95	0.06	86,86,86,86	0
57	MG	1H	3136	1/1	0.95	0.51	73,73,73,73	0
57	MG	14	3029	1/1	0.95	0.15	59,59,59,59	0
57	MG	1H	3137	1/1	0.95	0.14	72,72,72,72	0
57	MG	1H	3163	1/1	0.95	0.19	59,59,59,59	0
57	MG	14	3032	1/1	0.95	0.08	47,47,47,47	0
57	MG	14	3086	1/1	0.95	0.14	61,61,61,61	0
57	MG	14	3423	1/1	0.95	0.07	144,144,144,144	0
57	MG	14	3428	1/1	0.95	0.08	104,104,104,104	0
57	MG	14	3431	1/1	0.95	0.06	90,90,90,90	0
57	MG	1H	3009	1/1	0.95	0.14	54,54,54,54	0
57	MG	14	3446	1/1	0.95	0.05	109,109,109,109	0
57	MG	1H	3487	1/1	0.95	0.06	91,91,91,91	0
57	MG	1H	3264	1/1	0.95	0.19	74,74,74,74	0
57	MG	14	3117	1/1	0.95	0.19	66,66,66,66	0
57	MG	1H	3053	1/1	0.95	0.30	56,56,56,56	0
57	MG	1H	3102	1/1	0.95	0.28	70,70,70,70	0
57	MG	14	3092	1/1	0.95	0.14	56,56,56,56	0
57	MG	2K	103	1/1	0.95	0.20	61,61,61,61	0
57	MG	14	3152	1/1	0.95	0.19	67,67,67,67	0
57	MG	14	3012	1/1	0.95	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3252	1/1	0.95	0.12	67,67,67,67	0
57	MG	14	3253	1/1	0.95	0.10	63,63,63,63	0
57	MG	1H	3268	1/1	0.95	0.15	81,81,81,81	0
57	MG	14	3124	1/1	0.95	0.30	64,64,64,64	0
57	MG	1H	3042	1/1	0.95	0.13	79,79,79,79	0
57	MG	1H	3270	1/1	0.95	0.11	71,71,71,71	0
57	MG	1H	3048	1/1	0.95	0.07	80,80,80,80	0
57	MG	1H	3253	1/1	0.95	0.25	76,76,76,76	0
57	MG	E5	101	1/1	0.95	0.28	72,72,72,72	0
58	PAR	13	1749	42/42	0.95	0.09	64,70,78,81	0
57	MG	14	3160	1/1	0.95	0.17	51,51,51,51	0
57	MG	14	3020	1/1	0.95	0.19	51,51,51,51	0
57	MG	16	212	1/1	0.96	0.05	88,88,88,88	0
57	MG	14	3070	1/1	0.96	0.27	52,52,52,52	0
57	MG	14	3114	1/1	0.96	0.29	63,63,63,63	0
57	MG	1G	1674	1/1	0.96	0.04	107,107,107,107	0
57	MG	1G	1679	1/1	0.96	0.07	91,91,91,91	0
57	MG	1G	1683	1/1	0.96	0.05	96,96,96,96	0
57	MG	14	3074	1/1	0.96	0.15	62,62,62,62	0
57	MG	13	1727	1/1	0.96	0.09	110,110,110,110	0
57	MG	14	3262	1/1	0.96	0.05	72,72,72,72	0
57	MG	1H	3153	1/1	0.96	0.13	59,59,59,59	0
57	MG	1G	1693	1/1	0.96	0.09	92,92,92,92	0
57	MG	1H	3224	1/1	0.96	0.18	63,63,63,63	0
57	MG	14	3080	1/1	0.96	0.27	46,46,46,46	0
57	MG	1H	3435	1/1	0.96	0.05	94,94,94,94	0
57	MG	13	1606	1/1	0.96	0.19	52,52,52,52	0
57	MG	1H	3455	1/1	0.96	0.05	103,103,103,103	0
57	MG	13	1739	1/1	0.96	0.06	104,104,104,104	0
57	MG	1H	3470	1/1	0.96	0.05	100,100,100,100	0
57	MG	1H	3003	1/1	0.96	0.18	57,57,57,57	0
57	MG	14	3308	1/1	0.96	0.06	96,96,96,96	0
57	MG	14	3324	1/1	0.96	0.05	107,107,107,107	0
57	MG	14	3340	1/1	0.96	0.09	73,73,73,73	0
57	MG	1H	3256	1/1	0.96	0.26	71,71,71,71	0
57	MG	14	3365	1/1	0.96	0.04	88,88,88,88	0
57	MG	14	3406	1/1	0.96	0.10	76,76,76,76	0
57	MG	14	3417	1/1	0.96	0.04	87,87,87,87	0
57	MG	Q8	101	1/1	0.96	0.09	73,73,73,73	0
57	MG	1H	3478	1/1	0.96	0.04	85,85,85,85	0
57	MG	14	3427	1/1	0.96	0.09	102,102,102,102	0
57	MG	1H	3480	1/1	0.96	0.06	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	3008	1/1	0.96	0.05	72,72,72,72	0
57	MG	1H	3481	1/1	0.96	0.04	92,92,92,92	0
57	MG	14	3444	1/1	0.96	0.06	87,87,87,87	0
57	MG	14	3137	1/1	0.96	0.15	72,72,72,72	0
57	MG	1H	3064	1/1	0.96	0.10	54,54,54,54	0
57	MG	14	3011	1/1	0.96	0.34	72,72,72,72	0
57	MG	1H	3491	1/1	0.96	0.12	75,75,75,75	0
57	MG	14	3235	1/1	0.96	0.25	69,69,69,69	0
57	MG	1H	3179	1/1	0.96	0.10	49,49,49,49	0
57	MG	1J	206	1/1	0.96	0.06	94,94,94,94	0
57	MG	13	1638	1/1	0.96	0.26	58,58,58,58	0
57	MG	13	1710	1/1	0.96	0.09	108,108,108,108	0
57	MG	1H	3141	1/1	0.96	0.08	67,67,67,67	0
57	MG	1H	3501	1/1	0.96	0.11	72,72,72,72	0
57	MG	1H	3216	1/1	0.96	0.08	57,57,57,57	0
57	MG	1H	3369	1/1	0.96	0.09	74,74,74,74	0
57	MG	1H	3381	1/1	0.96	0.10	95,95,95,95	0
57	MG	1H	3387	1/1	0.96	0.05	64,64,64,64	0
57	MG	14	3197	1/1	0.96	0.06	56,56,56,56	0
57	MG	13	1724	1/1	0.96	0.06	114,114,114,114	0
57	MG	1G	1617	1/1	0.96	0.24	61,61,61,61	0
57	MG	1H	3406	1/1	0.96	0.07	87,87,87,87	0
57	MG	14	3065	1/1	0.96	0.12	54,54,54,54	0
57	MG	M5	101	1/1	0.96	0.12	77,77,77,77	0
57	MG	1H	3409	1/1	0.96	0.04	69,69,69,69	0
58	PAR	1G	1691	42/42	0.96	0.08	70,82,88,95	0
57	MG	14	3028	1/1	0.96	0.15	60,60,60,60	0
57	MG	1G	1655	1/1	0.96	0.04	120,120,120,120	0
57	MG	1H	3017	1/1	0.97	0.06	55,55,55,55	0
57	MG	1H	3458	1/1	0.97	0.06	87,87,87,87	0
57	MG	13	1734	1/1	0.97	0.04	86,86,86,86	0
57	MG	1H	3467	1/1	0.97	0.07	77,77,77,77	0
57	MG	14	3079	1/1	0.97	0.11	64,64,64,64	0
57	MG	1H	3468	1/1	0.97	0.04	71,71,71,71	0
57	MG	1H	3227	1/1	0.97	0.07	70,70,70,70	0
57	MG	1H	3094	1/1	0.97	0.04	52,52,52,52	0
57	MG	1H	3473	1/1	0.97	0.06	85,85,85,85	0
57	MG	1H	3475	1/1	0.97	0.04	88,88,88,88	0
57	MG	14	3201	1/1	0.97	0.17	58,58,58,58	0
57	MG	13	1737	1/1	0.97	0.09	147,147,147,147	0
57	MG	13	1738	1/1	0.97	0.04	97,97,97,97	0
57	MG	13	1708	1/1	0.97	0.04	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	1653	1/1	0.97	0.04	110,110,110,110	0
57	MG	13	1741	1/1	0.97	0.05	79,79,79,79	0
57	MG	1H	3482	1/1	0.97	0.05	72,72,72,72	0
57	MG	1G	1665	1/1	0.97	0.09	97,97,97,97	0
57	MG	1G	1666	1/1	0.97	0.04	106,106,106,106	0
57	MG	1G	1667	1/1	0.97	0.08	100,100,100,100	0
57	MG	1G	1669	1/1	0.97	0.05	114,114,114,114	0
57	MG	14	3280	1/1	0.97	0.05	54,54,54,54	0
57	MG	14	3303	1/1	0.97	0.05	63,63,63,63	0
57	MG	1G	1672	1/1	0.97	0.04	91,91,91,91	0
57	MG	14	3318	1/1	0.97	0.07	67,67,67,67	0
57	MG	1H	3485	1/1	0.97	0.04	76,76,76,76	0
57	MG	14	3329	1/1	0.97	0.06	90,90,90,90	0
57	MG	14	3330	1/1	0.97	0.06	113,113,113,113	0
57	MG	1G	1676	1/1	0.97	0.08	86,86,86,86	0
57	MG	14	3342	1/1	0.97	0.05	58,58,58,58	0
57	MG	14	3351	1/1	0.97	0.05	72,72,72,72	0
57	MG	1H	3334	1/1	0.97	0.06	82,82,82,82	0
57	MG	1G	1682	1/1	0.97	0.13	127,127,127,127	0
57	MG	14	3366	1/1	0.97	0.06	76,76,76,76	0
57	MG	14	3372	1/1	0.97	0.04	73,73,73,73	0
57	MG	14	3374	1/1	0.97	0.05	96,96,96,96	0
57	MG	14	3377	1/1	0.97	0.10	67,67,67,67	0
57	MG	14	3383	1/1	0.97	0.04	101,101,101,101	0
57	MG	14	3384	1/1	0.97	0.05	95,95,95,95	0
57	MG	14	3388	1/1	0.97	0.09	82,82,82,82	0
57	MG	1H	3488	1/1	0.97	0.09	113,113,113,113	0
57	MG	14	3410	1/1	0.97	0.04	85,85,85,85	0
57	MG	14	3414	1/1	0.97	0.05	85,85,85,85	0
57	MG	1H	3489	1/1	0.97	0.07	125,125,125,125	0
57	MG	1G	1685	1/1	0.97	0.05	109,109,109,109	0
57	MG	14	3422	1/1	0.97	0.05	84,84,84,84	0
57	MG	1G	1686	1/1	0.97	0.05	92,92,92,92	0
57	MG	14	3425	1/1	0.97	0.07	122,122,122,122	0
57	MG	1G	1687	1/1	0.97	0.04	95,95,95,95	0
57	MG	1G	1690	1/1	0.97	0.04	118,118,118,118	0
57	MG	14	3430	1/1	0.97	0.04	90,90,90,90	0
57	MG	1H	3364	1/1	0.97	0.04	106,106,106,106	0
57	MG	14	3435	1/1	0.97	0.04	103,103,103,103	0
57	MG	14	3438	1/1	0.97	0.05	93,93,93,93	0
57	MG	14	3442	1/1	0.97	0.04	95,95,95,95	0
57	MG	1H	3492	1/1	0.97	0.08	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	1H	3052	1/1	0.97	0.19	57,57,57,57	0
57	MG	1H	3495	1/1	0.97	0.03	98,98,98,98	0
57	MG	1H	3376	1/1	0.97	0.04	88,88,88,88	0
57	MG	14	3449	1/1	0.97	0.10	95,95,95,95	0
57	MG	1H	3378	1/1	0.97	0.08	84,84,84,84	0
57	MG	14	3453	1/1	0.97	0.07	88,88,88,88	0
57	MG	14	3454	1/1	0.97	0.06	79,79,79,79	0
57	MG	13	1726	1/1	0.97	0.09	85,85,85,85	0
57	MG	1H	3383	1/1	0.97	0.05	78,78,78,78	0
57	MG	1H	3386	1/1	0.97	0.04	84,84,84,84	0
57	MG	13	1632	1/1	0.97	0.10	77,77,77,77	0
57	MG	13	1745	1/1	0.97	0.04	117,117,117,117	0
57	MG	1H	3001	1/1	0.97	0.06	53,53,53,53	0
57	MG	1H	3002	1/1	0.97	0.13	39,39,39,39	0
57	MG	1H	3219	1/1	0.97	0.09	62,62,62,62	0
57	MG	14	3177	1/1	0.97	0.28	79,79,79,79	0
57	MG	1H	3420	1/1	0.97	0.04	64,64,64,64	0
57	MG	13	1715	1/1	0.97	0.07	110,110,110,110	0
57	MG	1H	3431	1/1	0.97	0.04	52,52,52,52	0
57	MG	13	1730	1/1	0.97	0.06	82,82,82,82	0
57	MG	1H	3222	1/1	0.97	0.05	68,68,68,68	0
57	MG	14	3014	1/1	0.97	0.10	72,72,72,72	0
57	MG	14	3184	1/1	0.97	0.10	60,60,60,60	0
57	MG	85	201	1/1	0.97	0.18	72,72,72,72	0
57	MG	1H	3442	1/1	0.97	0.06	86,86,86,86	0
57	MG	31	301	1/1	0.97	0.08	61,61,61,61	0
57	MG	1H	3451	1/1	0.97	0.04	95,95,95,95	0
57	MG	14	3249	1/1	0.97	0.16	60,60,60,60	0
57	MG	14	3018	1/1	0.97	0.12	49,49,49,49	0
57	MG	1H	3030	1/1	0.97	0.15	45,45,45,45	0
57	MG	13	1720	1/1	0.98	0.04	86,86,86,86	0
57	MG	1H	3262	1/1	0.98	0.07	68,68,68,68	0
57	MG	1H	3413	1/1	0.98	0.03	78,78,78,78	0
57	MG	1H	3032	1/1	0.98	0.08	61,61,61,61	0
57	MG	16	209	1/1	0.98	0.07	73,73,73,73	0
57	MG	16	210	1/1	0.98	0.11	88,88,88,88	0
57	MG	1G	1654	1/1	0.98	0.04	93,93,93,93	0
57	MG	16	211	1/1	0.98	0.04	84,84,84,84	0
57	MG	1G	1656	1/1	0.98	0.11	105,105,105,105	0
57	MG	1H	3422	1/1	0.98	0.05	79,79,79,79	0
57	MG	1H	3424	1/1	0.98	0.04	68,68,68,68	0
57	MG	14	3196	1/1	0.98	0.07	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3282	1/1	0.98	0.06	58,58,58,58	0
57	MG	1H	3425	1/1	0.98	0.05	83,83,83,83	0
57	MG	14	3306	1/1	0.98	0.07	55,55,55,55	0
57	MG	1H	3426	1/1	0.98	0.03	57,57,57,57	0
57	MG	14	3312	1/1	0.98	0.04	77,77,77,77	0
57	MG	14	3315	1/1	0.98	0.08	81,81,81,81	0
57	MG	14	3316	1/1	0.98	0.06	102,102,102,102	0
57	MG	14	3317	1/1	0.98	0.04	59,59,59,59	0
57	MG	1G	1668	1/1	0.98	0.06	111,111,111,111	0
57	MG	14	3319	1/1	0.98	0.07	91,91,91,91	0
57	MG	14	3320	1/1	0.98	0.08	83,83,83,83	0
57	MG	14	3323	1/1	0.98	0.05	72,72,72,72	0
57	MG	1H	3223	1/1	0.98	0.14	64,64,64,64	0
57	MG	14	3325	1/1	0.98	0.04	78,78,78,78	0
57	MG	14	3326	1/1	0.98	0.04	74,74,74,74	0
57	MG	14	3328	1/1	0.98	0.06	93,93,93,93	0
57	MG	1G	1670	1/1	0.98	0.05	108,108,108,108	0
57	MG	13	1705	1/1	0.98	0.07	76,76,76,76	0
57	MG	14	3336	1/1	0.98	0.04	83,83,83,83	0
57	MG	14	3338	1/1	0.98	0.03	72,72,72,72	0
57	MG	1H	3432	1/1	0.98	0.05	75,75,75,75	0
57	MG	1G	1675	1/1	0.98	0.04	88,88,88,88	0
57	MG	14	3345	1/1	0.98	0.05	68,68,68,68	0
57	MG	13	1707	1/1	0.98	0.09	90,90,90,90	0
57	MG	14	3354	1/1	0.98	0.06	78,78,78,78	0
57	MG	1G	1678	1/1	0.98	0.03	115,115,115,115	0
57	MG	14	3364	1/1	0.98	0.07	73,73,73,73	0
57	MG	1H	3434	1/1	0.98	0.08	73,73,73,73	0
57	MG	14	3132	1/1	0.98	0.08	58,58,58,58	0
57	MG	14	3369	1/1	0.98	0.08	56,56,56,56	0
57	MG	14	3370	1/1	0.98	0.04	81,81,81,81	0
57	MG	1G	1680	1/1	0.98	0.04	103,103,103,103	0
57	MG	14	3373	1/1	0.98	0.04	93,93,93,93	0
57	MG	13	1683	1/1	0.98	0.10	67,67,67,67	0
57	MG	1H	3439	1/1	0.98	0.06	81,81,81,81	0
57	MG	14	3378	1/1	0.98	0.04	93,93,93,93	0
57	MG	14	3380	1/1	0.98	0.03	93,93,93,93	0
57	MG	1H	3441	1/1	0.98	0.07	94,94,94,94	0
57	MG	13	1709	1/1	0.98	0.04	75,75,75,75	0
57	MG	1H	3444	1/1	0.98	0.03	77,77,77,77	0
57	MG	14	3389	1/1	0.98	0.05	81,81,81,81	0
57	MG	14	3399	1/1	0.98	0.07	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	3400	1/1	0.98	0.04	86,86,86,86	0
57	MG	14	3405	1/1	0.98	0.03	83,83,83,83	0
57	MG	1H	3449	1/1	0.98	0.05	69,69,69,69	0
57	MG	14	3407	1/1	0.98	0.05	74,74,74,74	0
57	MG	1G	1688	1/1	0.98	0.06	100,100,100,100	0
57	MG	14	3412	1/1	0.98	0.04	120,120,120,120	0
57	MG	1G	1689	1/1	0.98	0.04	126,126,126,126	0
57	MG	14	3415	1/1	0.98	0.03	77,77,77,77	0
57	MG	14	3416	1/1	0.98	0.07	66,66,66,66	0
57	MG	1G	1603	1/1	0.98	0.09	81,81,81,81	0
57	MG	1H	3450	1/1	0.98	0.03	87,87,87,87	0
57	MG	13	1702	1/1	0.98	0.06	76,76,76,76	0
57	MG	1H	3155	1/1	0.98	0.05	75,75,75,75	0
57	MG	1H	3292	1/1	0.98	0.04	50,50,50,50	0
57	MG	14	3426	1/1	0.98	0.04	80,80,80,80	0
57	MG	1H	3457	1/1	0.98	0.04	82,82,82,82	0
57	MG	1H	3299	1/1	0.98	0.09	50,50,50,50	0
57	MG	14	3429	1/1	0.98	0.06	98,98,98,98	0
57	MG	1H	3463	1/1	0.98	0.05	82,82,82,82	0
57	MG	1H	3303	1/1	0.98	0.04	63,63,63,63	0
57	MG	14	3432	1/1	0.98	0.07	83,83,83,83	0
57	MG	14	3434	1/1	0.98	0.04	82,82,82,82	0
57	MG	14	3001	1/1	0.98	0.05	103,103,103,103	0
57	MG	1H	3466	1/1	0.98	0.04	83,83,83,83	0
57	MG	14	3439	1/1	0.98	0.04	96,96,96,96	0
57	MG	14	3440	1/1	0.98	0.04	94,94,94,94	0
57	MG	1H	3311	1/1	0.98	0.05	53,53,53,53	0
57	MG	1H	3316	1/1	0.98	0.04	63,63,63,63	0
57	MG	1H	3469	1/1	0.98	0.04	100,100,100,100	0
57	MG	1H	3319	1/1	0.98	0.08	67,67,67,67	0
57	MG	14	3447	1/1	0.98	0.04	101,101,101,101	0
57	MG	1H	3325	1/1	0.98	0.06	69,69,69,69	0
57	MG	1H	3472	1/1	0.98	0.10	93,93,93,93	0
57	MG	14	3451	1/1	0.98	0.12	77,77,77,77	0
57	MG	1H	3326	1/1	0.98	0.10	49,49,49,49	0
57	MG	1H	3327	1/1	0.98	0.10	55,55,55,55	0
57	MG	13	1731	1/1	0.98	0.04	86,86,86,86	0
57	MG	1H	3337	1/1	0.98	0.06	73,73,73,73	0
57	MG	1H	3359	1/1	0.98	0.04	52,52,52,52	0
57	MG	1H	3363	1/1	0.98	0.04	61,61,61,61	0
57	MG	1J	205	1/1	0.98	0.06	95,95,95,95	0
57	MG	13	1732	1/1	0.98	0.10	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3483	1/1	0.98	0.04	106,106,106,106	0
57	MG	1H	3366	1/1	0.98	0.04	65,65,65,65	0
57	MG	1H	3486	1/1	0.98	0.06	61,61,61,61	0
57	MG	13	1711	1/1	0.98	0.05	99,99,99,99	0
57	MG	1H	3372	1/1	0.98	0.04	89,89,89,89	0
57	MG	1H	3073	1/1	0.98	0.10	36,36,36,36	0
57	MG	13	1735	1/1	0.98	0.06	118,118,118,118	0
57	MG	1H	3380	1/1	0.98	0.07	55,55,55,55	0
57	MG	13	1736	1/1	0.98	0.07	95,95,95,95	0
57	MG	1H	3494	1/1	0.98	0.05	126,126,126,126	0
57	MG	BI	201	1/1	0.98	0.04	103,103,103,103	0
57	MG	1H	3384	1/1	0.98	0.06	73,73,73,73	0
57	MG	13	1712	1/1	0.98	0.04	75,75,75,75	0
57	MG	13	1713	1/1	0.98	0.05	89,89,89,89	0
57	MG	1H	3399	1/1	0.98	0.04	61,61,61,61	0
57	MG	1H	3502	1/1	0.98	0.06	59,59,59,59	0
57	MG	1H	3402	1/1	0.98	0.04	73,73,73,73	0
59	SF4	3E	301	8/8	0.98	0.06	71,78,87,91	0
57	MG	1H	3239	1/1	0.98	0.07	67,67,67,67	0
57	MG	13	1704	1/1	0.98	0.04	105,105,105,105	0
57	MG	1H	3298	1/1	0.99	0.05	61,61,61,61	0
57	MG	1H	3423	1/1	0.99	0.03	55,55,55,55	0
57	MG	13	1703	1/1	0.99	0.06	95,95,95,95	0
57	MG	1H	3300	1/1	0.99	0.04	54,54,54,54	0
57	MG	1H	3301	1/1	0.99	0.07	49,49,49,49	0
57	MG	1H	3427	1/1	0.99	0.03	88,88,88,88	0
57	MG	1H	3302	1/1	0.99	0.09	47,47,47,47	0
57	MG	1H	3429	1/1	0.99	0.04	75,75,75,75	0
57	MG	1H	3430	1/1	0.99	0.03	85,85,85,85	0
57	MG	13	1725	1/1	0.99	0.10	71,71,71,71	0
57	MG	1H	3305	1/1	0.99	0.05	53,53,53,53	0
57	MG	1H	3306	1/1	0.99	0.03	60,60,60,60	0
57	MG	1H	3307	1/1	0.99	0.05	57,57,57,57	0
57	MG	1H	3308	1/1	0.99	0.05	61,61,61,61	0
57	MG	1H	3436	1/1	0.99	0.03	65,65,65,65	0
57	MG	1H	3437	1/1	0.99	0.03	57,57,57,57	0
57	MG	1H	3438	1/1	0.99	0.04	75,75,75,75	0
57	MG	1H	3310	1/1	0.99	0.03	58,58,58,58	0
57	MG	1H	3440	1/1	0.99	0.03	87,87,87,87	0
57	MG	13	1691	1/1	0.99	0.02	79,79,79,79	0
57	MG	1H	3313	1/1	0.99	0.05	72,72,72,72	0
57	MG	1G	1650	1/1	0.99	0.09	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	1G	1651	1/1	0.99	0.04	81,81,81,81	0
57	MG	1G	1652	1/1	0.99	0.03	82,82,82,82	0
57	MG	1H	3314	1/1	0.99	0.04	75,75,75,75	0
57	MG	1H	3445	1/1	0.99	0.03	97,97,97,97	0
57	MG	1H	3446	1/1	0.99	0.02	93,93,93,93	0
57	MG	1H	3447	1/1	0.99	0.07	97,97,97,97	0
57	MG	1H	3448	1/1	0.99	0.05	62,62,62,62	0
57	MG	1G	1658	1/1	0.99	0.04	94,94,94,94	0
57	MG	1G	1659	1/1	0.99	0.06	79,79,79,79	0
57	MG	1G	1660	1/1	0.99	0.03	96,96,96,96	0
57	MG	1G	1661	1/1	0.99	0.07	111,111,111,111	0
57	MG	1G	1662	1/1	0.99	0.04	76,76,76,76	0
57	MG	1G	1663	1/1	0.99	0.03	87,87,87,87	0
57	MG	1G	1664	1/1	0.99	0.07	91,91,91,91	0
57	MG	1H	3315	1/1	0.99	0.03	73,73,73,73	0
57	MG	13	1692	1/1	0.99	0.05	81,81,81,81	0
57	MG	1H	3318	1/1	0.99	0.05	54,54,54,54	0
57	MG	13	1728	1/1	0.99	0.04	91,91,91,91	0
57	MG	1H	3453	1/1	0.99	0.04	83,83,83,83	0
57	MG	1H	3454	1/1	0.99	0.03	62,62,62,62	0
57	MG	1G	1671	1/1	0.99	0.04	117,117,117,117	0
57	MG	1H	3320	1/1	0.99	0.03	67,67,67,67	0
57	MG	14	3273	1/1	0.99	0.04	58,58,58,58	0
57	MG	14	3275	1/1	0.99	0.03	61,61,61,61	0
57	MG	14	3276	1/1	0.99	0.03	62,62,62,62	0
57	MG	14	3278	1/1	0.99	0.04	65,65,65,65	0
57	MG	1G	1673	1/1	0.99	0.06	84,84,84,84	0
57	MG	14	3281	1/1	0.99	0.03	66,66,66,66	0
57	MG	1H	3456	1/1	0.99	0.02	72,72,72,72	0
57	MG	14	3283	1/1	0.99	0.04	74,74,74,74	0
57	MG	14	3285	1/1	0.99	0.07	59,59,59,59	0
57	MG	14	3290	1/1	0.99	0.03	64,64,64,64	0
57	MG	14	3291	1/1	0.99	0.03	66,66,66,66	0
57	MG	14	3295	1/1	0.99	0.02	58,58,58,58	0
57	MG	14	3296	1/1	0.99	0.05	59,59,59,59	0
57	MG	14	3298	1/1	0.99	0.03	79,79,79,79	0
57	MG	14	3299	1/1	0.99	0.05	60,60,60,60	0
57	MG	14	3300	1/1	0.99	0.03	57,57,57,57	0
57	MG	14	3302	1/1	0.99	0.03	68,68,68,68	0
57	MG	1H	3321	1/1	0.99	0.04	77,77,77,77	0
57	MG	14	3304	1/1	0.99	0.11	59,59,59,59	0
57	MG	1H	3322	1/1	0.99	0.03	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	14	3307	1/1	0.99	0.05	79,79,79,79	0
57	MG	1G	1677	1/1	0.99	0.03	105,105,105,105	0
57	MG	14	3309	1/1	0.99	0.09	73,73,73,73	0
57	MG	14	3310	1/1	0.99	0.04	68,68,68,68	0
57	MG	14	3311	1/1	0.99	0.04	66,66,66,66	0
57	MG	1H	3459	1/1	0.99	0.05	91,91,91,91	0
57	MG	14	3313	1/1	0.99	0.03	72,72,72,72	0
57	MG	14	3314	1/1	0.99	0.06	75,75,75,75	0
57	MG	1H	3460	1/1	0.99	0.06	62,62,62,62	0
57	MG	1H	3461	1/1	0.99	0.02	85,85,85,85	0
57	MG	1G	1681	1/1	0.99	0.03	85,85,85,85	0
57	MG	1H	3462	1/1	0.99	0.10	54,54,54,54	0
57	MG	1H	3323	1/1	0.99	0.03	61,61,61,61	0
57	MG	1H	3464	1/1	0.99	0.06	62,62,62,62	0
57	MG	14	3321	1/1	0.99	0.03	89,89,89,89	0
57	MG	14	3322	1/1	0.99	0.06	74,74,74,74	0
57	MG	1H	3324	1/1	0.99	0.03	47,47,47,47	0
57	MG	13	1693	1/1	0.99	0.06	72,72,72,72	0
57	MG	13	1694	1/1	0.99	0.05	79,79,79,79	0
57	MG	13	1695	1/1	0.99	0.05	76,76,76,76	0
57	MG	14	3327	1/1	0.99	0.06	67,67,67,67	0
57	MG	1H	3328	1/1	0.99	0.07	52,52,52,52	0
57	MG	1H	3329	1/1	0.99	0.04	55,55,55,55	0
57	MG	1H	3331	1/1	0.99	0.03	66,66,66,66	0
57	MG	14	3333	1/1	0.99	0.04	59,59,59,59	0
57	MG	1H	3333	1/1	0.99	0.07	75,75,75,75	0
57	MG	14	3337	1/1	0.99	0.11	76,76,76,76	0
57	MG	1H	3217	1/1	0.99	0.06	59,59,59,59	0
57	MG	14	3339	1/1	0.99	0.03	86,86,86,86	0
57	MG	1H	3474	1/1	0.99	0.08	89,89,89,89	0
57	MG	14	3341	1/1	0.99	0.06	62,62,62,62	0
57	MG	1H	3335	1/1	0.99	0.03	61,61,61,61	0
57	MG	14	3343	1/1	0.99	0.03	63,63,63,63	0
57	MG	14	3344	1/1	0.99	0.03	72,72,72,72	0
57	MG	13	1696	1/1	0.99	0.06	86,86,86,86	0
57	MG	14	3346	1/1	0.99	0.07	75,75,75,75	0
57	MG	14	3348	1/1	0.99	0.04	88,88,88,88	0
57	MG	14	3349	1/1	0.99	0.04	81,81,81,81	0
57	MG	14	3350	1/1	0.99	0.03	56,56,56,56	0
57	MG	1H	3477	1/1	0.99	0.03	65,65,65,65	0
57	MG	14	3352	1/1	0.99	0.06	65,65,65,65	0
57	MG	1H	3339	1/1	0.99	0.03	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3356	1/1	0.99	0.02	61,61,61,61	0
57	MG	1H	3479	1/1	0.99	0.02	89,89,89,89	0
57	MG	14	3358	1/1	0.99	0.03	54,54,54,54	0
57	MG	14	3360	1/1	0.99	0.04	83,83,83,83	0
57	MG	14	3361	1/1	0.99	0.04	69,69,69,69	0
57	MG	14	3363	1/1	0.99	0.03	68,68,68,68	0
57	MG	1H	3341	1/1	0.99	0.03	57,57,57,57	0
57	MG	1H	3342	1/1	0.99	0.03	71,71,71,71	0
57	MG	1H	3344	1/1	0.99	0.05	49,49,49,49	0
57	MG	14	3367	1/1	0.99	0.12	60,60,60,60	0
57	MG	14	3368	1/1	0.99	0.05	72,72,72,72	0
57	MG	1H	3346	1/1	0.99	0.03	58,58,58,58	0
57	MG	1H	3484	1/1	0.99	0.03	90,90,90,90	0
57	MG	14	3371	1/1	0.99	0.03	83,83,83,83	0
57	MG	1H	3347	1/1	0.99	0.03	69,69,69,69	0
57	MG	1H	3349	1/1	0.99	0.04	53,53,53,53	0
57	MG	1H	3350	1/1	0.99	0.05	69,69,69,69	0
57	MG	14	3375	1/1	0.99	0.03	91,91,91,91	0
57	MG	1H	3352	1/1	0.99	0.06	72,72,72,72	0
57	MG	1H	3353	1/1	0.99	0.03	57,57,57,57	0
57	MG	14	3379	1/1	0.99	0.05	94,94,94,94	0
57	MG	1H	3490	1/1	0.99	0.04	83,83,83,83	0
57	MG	14	3381	1/1	0.99	0.06	52,52,52,52	0
57	MG	14	3382	1/1	0.99	0.04	91,91,91,91	0
57	MG	1H	3354	1/1	0.99	0.06	62,62,62,62	0
57	MG	1H	3356	1/1	0.99	0.02	58,58,58,58	0
57	MG	14	3385	1/1	0.99	0.07	70,70,70,70	0
57	MG	14	3387	1/1	0.99	0.02	97,97,97,97	0
57	MG	1H	3357	1/1	0.99	0.03	68,68,68,68	0
57	MG	13	1733	1/1	0.99	0.05	73,73,73,73	0
57	MG	14	3390	1/1	0.99	0.04	82,82,82,82	0
57	MG	14	3391	1/1	0.99	0.03	86,86,86,86	0
57	MG	14	3392	1/1	0.99	0.03	87,87,87,87	0
57	MG	14	3393	1/1	0.99	0.06	79,79,79,79	0
57	MG	14	3395	1/1	0.99	0.06	78,78,78,78	0
57	MG	14	3396	1/1	0.99	0.03	62,62,62,62	0
57	MG	14	3397	1/1	0.99	0.05	64,64,64,64	0
57	MG	14	3398	1/1	0.99	0.06	83,83,83,83	0
57	MG	1H	3360	1/1	0.99	0.03	60,60,60,60	0
57	MG	1H	3361	1/1	0.99	0.04	53,53,53,53	0
57	MG	14	3402	1/1	0.99	0.04	88,88,88,88	0
57	MG	14	3403	1/1	0.99	0.03	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	14	3404	1/1	0.99	0.08	94,94,94,94	0
57	MG	1H	3497	1/1	0.99	0.03	97,97,97,97	0
57	MG	1H	3362	1/1	0.99	0.03	60,60,60,60	0
57	MG	13	1698	1/1	0.99	0.04	93,93,93,93	0
57	MG	14	3408	1/1	0.99	0.03	78,78,78,78	0
57	MG	14	3409	1/1	0.99	0.03	80,80,80,80	0
57	MG	1H	3500	1/1	0.99	0.03	71,71,71,71	0
57	MG	14	3411	1/1	0.99	0.03	74,74,74,74	0
57	MG	13	1699	1/1	0.99	0.05	73,73,73,73	0
57	MG	14	3413	1/1	0.99	0.02	97,97,97,97	0
57	MG	1H	3365	1/1	0.99	0.04	70,70,70,70	0
57	MG	13	1700	1/1	0.99	0.04	93,93,93,93	0
57	MG	1H	3367	1/1	0.99	0.03	54,54,54,54	0
57	MG	1H	3368	1/1	0.99	0.05	60,60,60,60	0
57	MG	14	3419	1/1	0.99	0.06	70,70,70,70	0
57	MG	14	3420	1/1	0.99	0.05	65,65,65,65	0
57	MG	13	1714	1/1	0.99	0.03	93,93,93,93	0
57	MG	1H	3370	1/1	0.99	0.06	70,70,70,70	0
57	MG	1H	3371	1/1	0.99	0.04	85,85,85,85	0
57	MG	14	3424	1/1	0.99	0.03	107,107,107,107	0
57	MG	13	1701	1/1	0.99	0.02	70,70,70,70	0
57	MG	16	208	1/1	0.99	0.04	67,67,67,67	0
57	MG	1H	3373	1/1	0.99	0.08	66,66,66,66	0
57	MG	1H	3374	1/1	0.99	0.04	55,55,55,55	0
57	MG	1H	3375	1/1	0.99	0.07	57,57,57,57	0
57	MG	13	1716	1/1	0.99	0.03	66,66,66,66	0
57	MG	11	302	1/1	0.99	0.03	57,57,57,57	0
57	MG	1H	3377	1/1	0.99	0.06	76,76,76,76	0
57	MG	14	3433	1/1	0.99	0.05	71,71,71,71	0
57	MG	13	1740	1/1	0.99	0.03	92,92,92,92	0
57	MG	1H	3379	1/1	0.99	0.07	86,86,86,86	0
57	MG	14	3436	1/1	0.99	0.02	108,108,108,108	0
57	MG	13	1717	1/1	0.99	0.05	66,66,66,66	0
57	MG	13	1718	1/1	0.99	0.04	78,78,78,78	0
57	MG	1H	3382	1/1	0.99	0.04	70,70,70,70	0
57	MG	14	3441	1/1	0.99	0.07	72,72,72,72	0
57	MG	13	1743	1/1	0.99	0.04	87,87,87,87	0
57	MG	13	1719	1/1	0.99	0.06	72,72,72,72	0
57	MG	1H	3385	1/1	0.99	0.03	57,57,57,57	0
57	MG	14	3445	1/1	0.99	0.03	87,87,87,87	0
57	MG	I8	101	1/1	0.99	0.05	65,65,65,65	0
57	MG	13	1690	1/1	0.99	0.05	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	1746	1/1	0.99	0.04	83,83,83,83	0
57	MG	1H	3389	1/1	0.99	0.05	59,59,59,59	0
57	MG	14	3450	1/1	0.99	0.04	63,63,63,63	0
57	MG	1H	3390	1/1	0.99	0.07	57,57,57,57	0
57	MG	1H	3391	1/1	0.99	0.03	49,49,49,49	0
57	MG	1H	3392	1/1	0.99	0.03	69,69,69,69	0
57	MG	1H	3393	1/1	0.99	0.04	56,56,56,56	0
57	MG	1H	3394	1/1	0.99	0.06	70,70,70,70	0
57	MG	1H	3395	1/1	0.99	0.05	59,59,59,59	0
57	MG	1H	3397	1/1	0.99	0.04	85,85,85,85	0
57	MG	1J	204	1/1	0.99	0.03	82,82,82,82	0
57	MG	1H	3398	1/1	0.99	0.03	50,50,50,50	0
57	MG	13	1747	1/1	0.99	0.03	72,72,72,72	0
57	MG	1H	3400	1/1	0.99	0.07	67,67,67,67	0
57	MG	13	1721	1/1	0.99	0.03	70,70,70,70	0
57	MG	13	1722	1/1	0.99	0.03	92,92,92,92	0
57	MG	1H	3404	1/1	0.99	0.04	76,76,76,76	0
57	MG	13	1723	1/1	0.99	0.06	84,84,84,84	0
57	MG	1H	3407	1/1	0.99	0.04	50,50,50,50	0
57	MG	1H	3408	1/1	0.99	0.07	50,50,50,50	0
57	MG	1H	3293	1/1	0.99	0.08	63,63,63,63	0
57	MG	1H	3410	1/1	0.99	0.02	56,56,56,56	0
57	MG	14	3218	1/1	0.99	0.13	54,54,54,54	0
57	MG	1H	3295	1/1	0.99	0.03	52,52,52,52	0
57	MG	1H	3412	1/1	0.99	0.05	66,66,66,66	0
57	MG	1H	3296	1/1	0.99	0.06	49,49,49,49	0
57	MG	C5	201	1/1	0.99	0.03	110,110,110,110	0
57	MG	1H	3414	1/1	0.99	0.03	53,53,53,53	0
57	MG	1H	3415	1/1	0.99	0.07	52,52,52,52	0
57	MG	1H	3416	1/1	0.99	0.06	48,48,48,48	0
57	MG	1H	3417	1/1	0.99	0.02	56,56,56,56	0
57	MG	1H	3418	1/1	0.99	0.03	69,69,69,69	0
59	SF4	32	301	8/8	0.99	0.03	100,111,117,118	0
57	MG	1H	3297	1/1	0.99	0.04	49,49,49,49	0
60	ZN	5A	101	1/1	0.99	0.03	128,128,128,128	0
57	MG	1H	3421	1/1	0.99	0.03	78,78,78,78	0
57	MG	14	3286	1/1	1.00	0.02	63,63,63,63	0
57	MG	14	3376	1/1	1.00	0.03	52,52,52,52	0
57	MG	14	3287	1/1	1.00	0.04	56,56,56,56	0
57	MG	14	3288	1/1	1.00	0.04	50,50,50,50	0
57	MG	14	3289	1/1	1.00	0.03	58,58,58,58	0
57	MG	1H	3332	1/1	1.00	0.04	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3331	1/1	1.00	0.02	66,66,66,66	0
57	MG	14	3332	1/1	1.00	0.06	63,63,63,63	0
57	MG	14	3437	1/1	1.00	0.02	93,93,93,93	0
57	MG	1H	3317	1/1	1.00	0.07	45,45,45,45	0
57	MG	14	3334	1/1	1.00	0.03	61,61,61,61	0
57	MG	14	3335	1/1	1.00	0.04	87,87,87,87	0
57	MG	14	3386	1/1	1.00	0.04	56,56,56,56	0
57	MG	14	3292	1/1	1.00	0.02	61,61,61,61	0
57	MG	14	3293	1/1	1.00	0.02	51,51,51,51	0
57	MG	14	3294	1/1	1.00	0.02	54,54,54,54	0
57	MG	1H	3405	1/1	1.00	0.02	69,69,69,69	0
57	MG	1H	3348	1/1	1.00	0.02	65,65,65,65	0
57	MG	14	3297	1/1	1.00	0.03	74,74,74,74	0
57	MG	13	1697	1/1	1.00	0.04	90,90,90,90	0
57	MG	14	3394	1/1	1.00	0.02	78,78,78,78	0
57	MG	1H	3312	1/1	1.00	0.03	76,76,76,76	0
57	MG	14	3002	1/1	1.00	0.02	49,49,49,49	0
57	MG	14	3301	1/1	1.00	0.02	56,56,56,56	0
57	MG	1H	3351	1/1	1.00	0.01	69,69,69,69	0
57	MG	14	3347	1/1	1.00	0.04	67,67,67,67	0
57	MG	1H	3388	1/1	1.00	0.03	57,57,57,57	0
57	MG	14	3401	1/1	1.00	0.02	66,66,66,66	0
57	MG	1H	3336	1/1	1.00	0.03	61,61,61,61	0
57	MG	14	3305	1/1	1.00	0.04	57,57,57,57	0
57	MG	1H	3294	1/1	1.00	0.02	56,56,56,56	0
57	MG	1H	3338	1/1	1.00	0.06	53,53,53,53	0
57	MG	14	3353	1/1	1.00	0.03	67,67,67,67	0
57	MG	1H	3355	1/1	1.00	0.01	68,68,68,68	0
57	MG	14	3355	1/1	1.00	0.02	59,59,59,59	0
57	MG	1H	3304	1/1	1.00	0.02	55,55,55,55	0
57	MG	1H	3340	1/1	1.00	0.02	54,54,54,54	0
57	MG	1H	3358	1/1	1.00	0.02	67,67,67,67	0
57	MG	14	3359	1/1	1.00	0.02	67,67,67,67	0
57	MG	1H	3396	1/1	1.00	0.02	60,60,60,60	0
57	MG	1H	3419	1/1	1.00	0.06	63,63,63,63	0
57	MG	14	3362	1/1	1.00	0.06	62,62,62,62	0
57	MG	14	3274	1/1	1.00	0.02	62,62,62,62	0
57	MG	11	301	1/1	1.00	0.02	46,46,46,46	0
57	MG	14	3418	1/1	1.00	0.05	75,75,75,75	0
57	MG	1H	3443	1/1	1.00	0.02	67,67,67,67	0
57	MG	14	3277	1/1	1.00	0.01	67,67,67,67	0
57	MG	1H	3309	1/1	1.00	0.03	48,48,48,48	0

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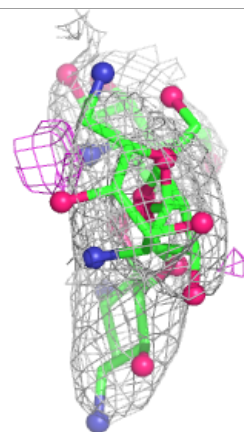
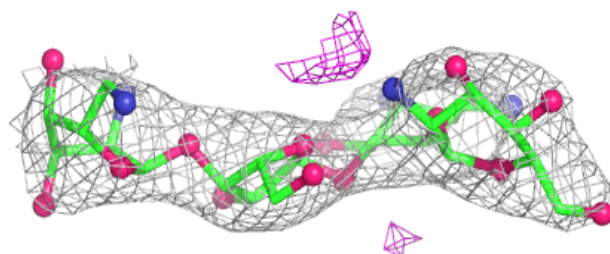
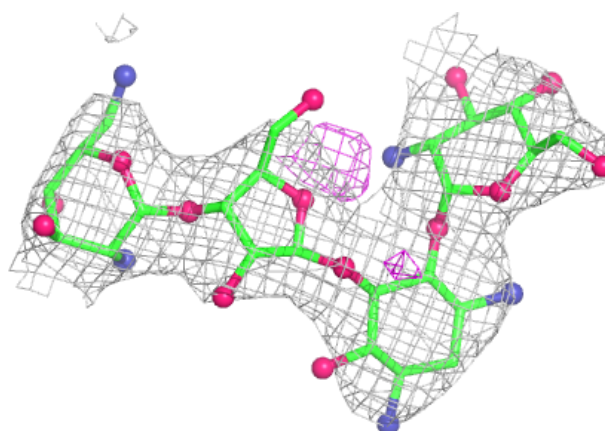
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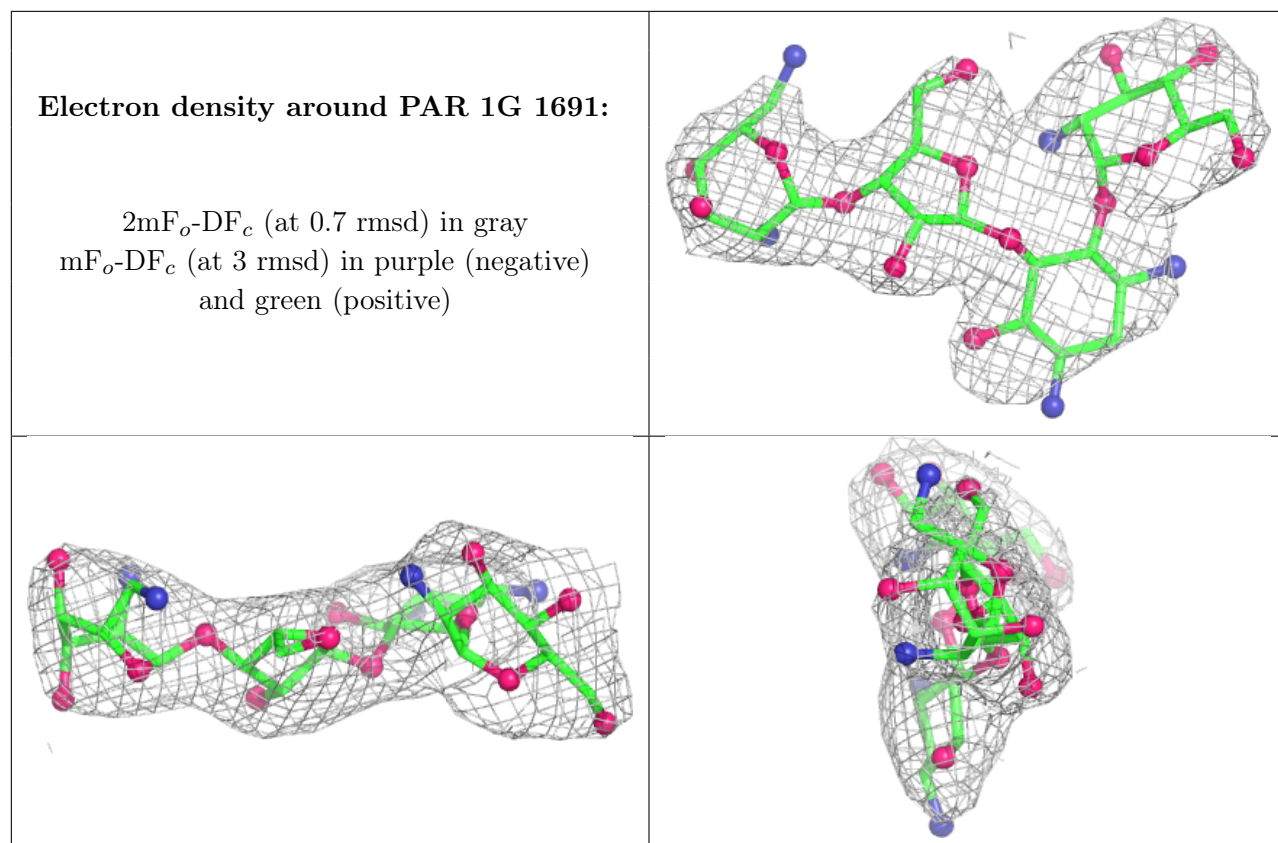
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3279	1/1	1.00	0.04	62,62,62,62	0
57	MG	1H	3330	1/1	1.00	0.03	57,57,57,57	0
57	MG	1H	3343	1/1	1.00	0.04	74,74,74,74	0
57	MG	13	1706	1/1	1.00	0.02	71,71,71,71	0
60	ZN	5I	102	1/1	1.00	0.01	88,88,88,88	0
57	MG	1H	3401	1/1	1.00	0.01	52,52,52,52	0
57	MG	14	3284	1/1	1.00	0.02	57,57,57,57	0
57	MG	1H	3345	1/1	1.00	0.02	56,56,56,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR 13 1749:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.