



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:22 AM UTC

PDB ID : 5EL6 / pdb_00005el6
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA^{Lys} in the A-site with a U-U mismatch in the first position and antibiotic paromomycin
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-11-04
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

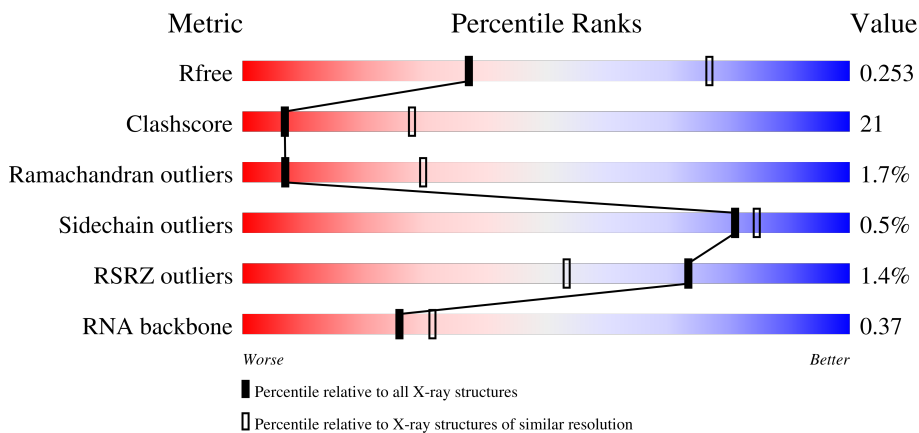
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



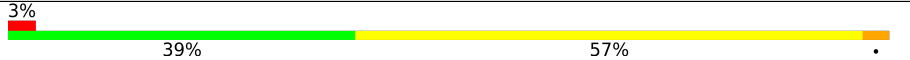
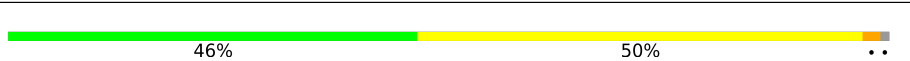
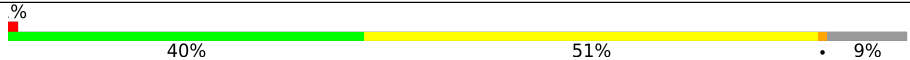
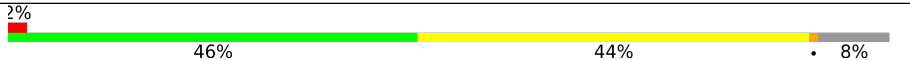
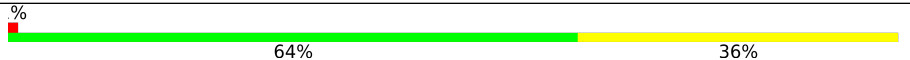
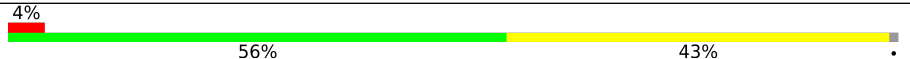
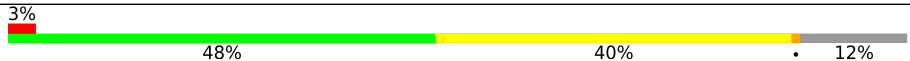
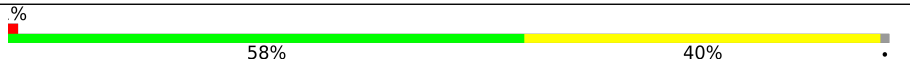
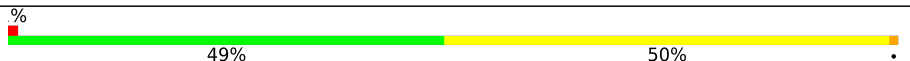
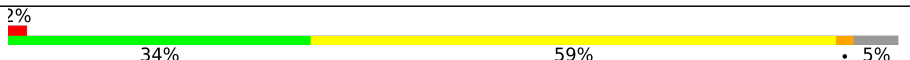
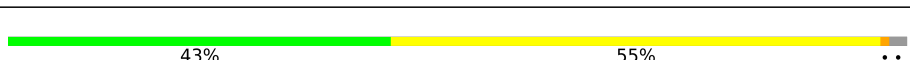
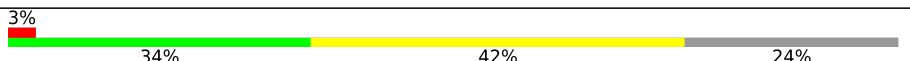
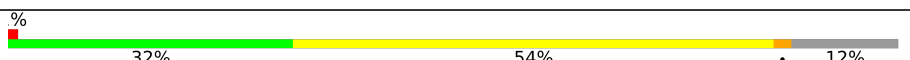
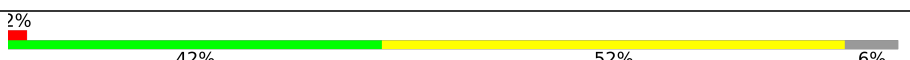
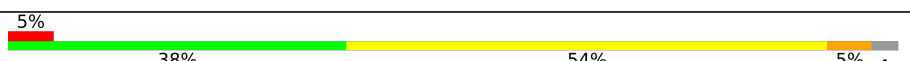
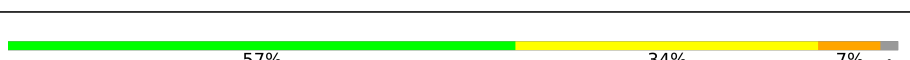
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	35% 47% 16% .
1	1G	1522	32% 50% 17% .
2	12	256	35% 43% . 18%

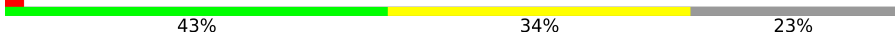
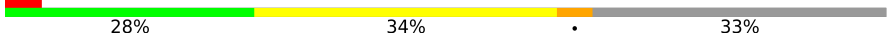
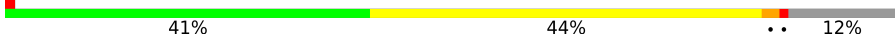
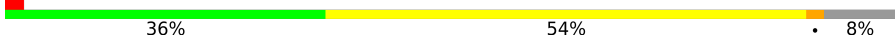
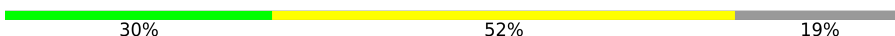
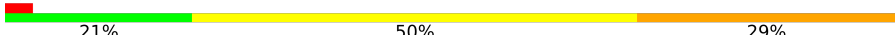
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Mol	Chain	Length	Quality of chain
2	1E	256	
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
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	
24	3L	76	
25	4K	27	
25	4L	27	
26	14	2912	
26	1H	2912	
27	16	122	

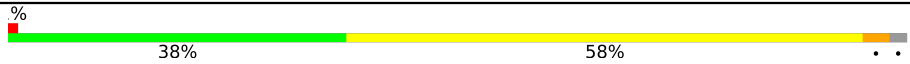
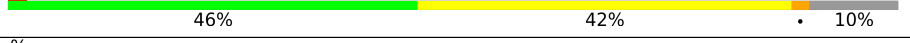
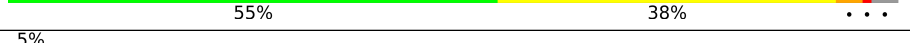
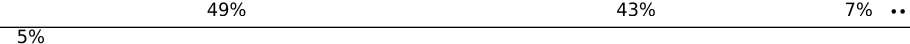
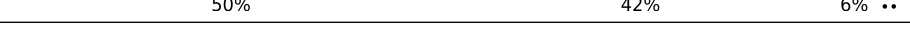
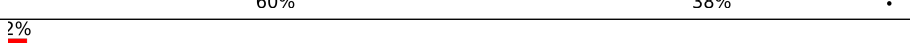
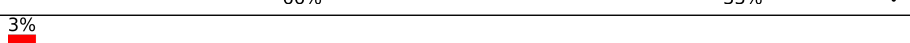
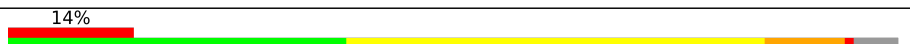
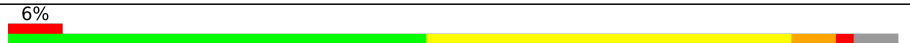
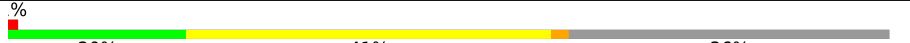
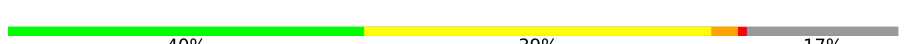
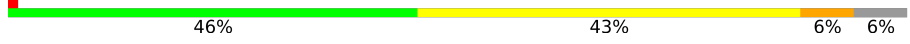
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Mol	Chain	Length	Quality of chain
27	1J	122	% 26% 53% 20%
28	71	229	24% 34% 42%
28	79	229	8% 17% 75%
29	11	276	% 52% 42% ..
29	19	276	3% 50% 45% ..
30	21	206	46% 45% 7% ..
30	29	206	% 39% 52% 6% ..
31	31	210	2% 50% 44% ..
31	39	210	% 44% 46% 6% ..
32	41	182	% 43% 54% ..
32	49	182	2% 42% 55% ..
33	51	180	3% 52% 38% 5% 5%
33	59	180	2% 13% 22% 62%
34	61	148	% 47% 51% ..
34	69	148	6% 49% 44% 5% ..
35	15	140	2% 62% 36% ..
35	58	140	3% 46% 48% ..
36	25	122	59% 40% .
36	68	122	3% 65% 34% .
37	35	150	4% 43% 49% 6% ..
37	78	150	% 46% 46% 5% ..
38	45	141	9% 39% 54% ..
38	88	141	2% 53% 42% 5%
39	55	118	40% 58% ..
39	98	118	47% 49% .

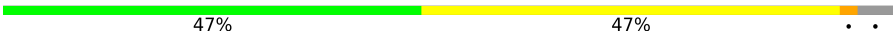
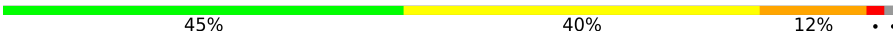
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Mol	Chain	Length	Quality of chain
40	65	112	
40	A8	112	
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	

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Mol	Chain	Length	Quality of chain
53	J5	60	
53	N8	60	
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1702	-	-	-	X
56	MG	14	3039	-	-	-	X
56	MG	14	3287	-	-	-	X
56	MG	1H	3052	-	-	-	X
56	MG	1H	3291	-	-	-	X
58	SF4	32	301	-	-	X	-
58	SF4	3E	302	-	-	X	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 294257 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	1507	Total	C	N	O	P	0	0	0
			32391	14418	6004	10463	1506			

- 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
			1698	1064	338	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	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	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	91	Total	C	N	O	S	0	0	0
			734	459	144	130	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			658	419	123	114	2			
19	AA	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	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			
24	3L	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	18	Total	C	N	O	P	0	0	0
			395	177	81	119	18			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	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	69	Total	C	N	O		0	0	0
			539	339	109	91				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	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
			881	556	176	149			
40	65	110	Total	C	N	O	0	0	0
			876	553	175	148			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	B8	132	Total	C	N	O	0	0	0
			1101	686	227	188			
41	75	133	Total	C	N	O	S	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
			950	603	199	147	1		
42	85	116	Total	C	N	O	S	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
			774	499	141	133	1		
43	95	100	Total	C	N	O	S	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
			890	560	175	153	2		
44	A5	111	Total	C	N	O	S	0	0
			886	558	174	152	2		

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	105	Total	C	N	O	S	0	0	0
			796	513	150	128	5			
46	C5	105	Total	C	N	O	S	0	0	0
			799	513	153	128	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			
50	G5	68	Total	C	N	O	S	0	0	0
			568	352	115	100	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	131	Total	Mg	0	0
			131	131		

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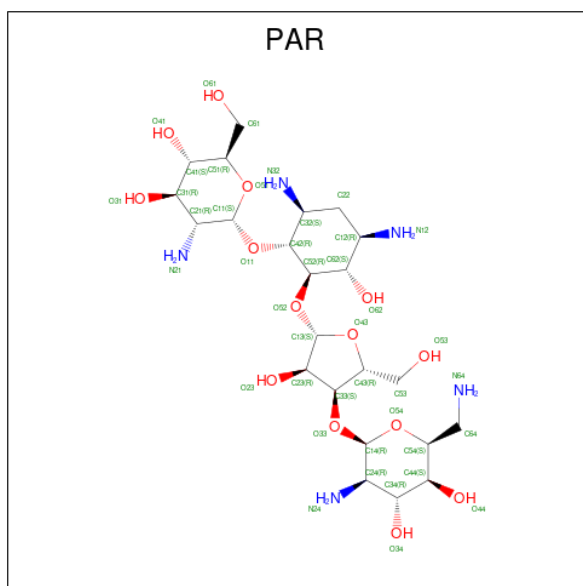
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	3E	1	Total 1	Mg 1	0	0
56	5E	1	Total 1	Mg 1	0	0
56	3I	1	Total 1	Mg 1	0	0
56	5I	1	Total 1	Mg 1	0	0
56	1K	1	Total 1	Mg 1	0	0
56	2K	3	Total 3	Mg 3	0	0
56	3K	1	Total 1	Mg 1	0	0
56	4K	1	Total 1	Mg 1	0	0
56	1H	429	Total 429	Mg 429	0	0
56	16	11	Total 11	Mg 11	0	0
56	21	2	Total 2	Mg 2	0	0
56	41	1	Total 1	Mg 1	0	0
56	78	1	Total 1	Mg 1	0	0
56	88	2	Total 2	Mg 2	0	0
56	I8	3	Total 3	Mg 3	0	0
56	L8	1	Total 1	Mg 1	0	0
56	P8	1	Total 1	Mg 1	0	0
56	Q8	1	Total 1	Mg 1	0	0
56	1G	81	Total 81	Mg 81	0	0
56	2L	3	Total 3	Mg 3	0	0
56	14	382	Total 382	Mg 382	0	0

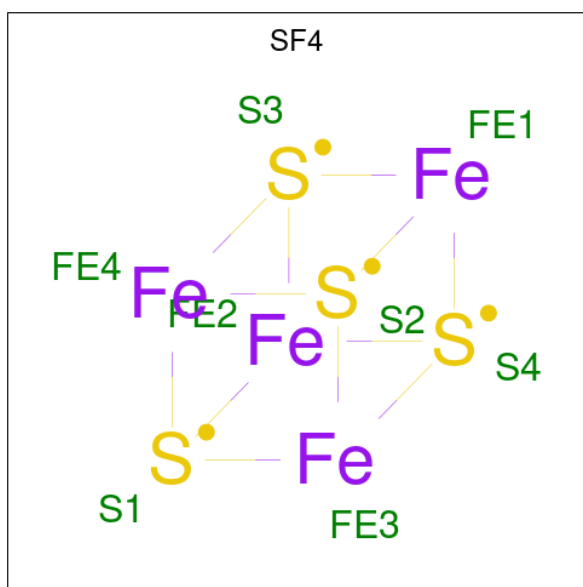
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1J	5	Total	Mg	0	0
			5	5		
56	29	1	Total	Mg	0	0
			1	1		
56	39	1	Total	Mg	0	0
			1	1		
56	35	1	Total	Mg	0	0
			1	1		
56	45	3	Total	Mg	0	0
			3	3		
56	85	1	Total	Mg	0	0
			1	1		
56	C5	1	Total	Mg	0	0
			1	1		
56	E5	1	Total	Mg	0	0
			1	1		

- Molecule 57 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).





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

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

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	13	144	Total	O	0	0
			144	144		
60	3E	2	Total	O	0	0
			2	2		
60	1I	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	5I	2	Total 2	O 2	0	0
60	6I	1	Total 1	O 1	0	0
60	7I	1	Total 1	O 1	0	0
60	BI	1	Total 1	O 1	0	0
60	3K	1	Total 1	O 1	0	0
60	4K	3	Total 3	O 3	0	0
60	1H	540	Total 540	O 540	0	0
60	16	22	Total 22	O 22	0	0
60	11	10	Total 10	O 10	0	0
60	31	7	Total 7	O 7	0	0
60	58	2	Total 2	O 2	0	0
60	78	4	Total 4	O 4	0	0
60	98	1	Total 1	O 1	0	0
60	G8	1	Total 1	O 1	0	0
60	I8	2	Total 2	O 2	0	0
60	L8	3	Total 3	O 3	0	0
60	P8	1	Total 1	O 1	0	0
60	1G	68	Total 68	O 68	0	0
60	32	2	Total 2	O 2	0	0
60	14	367	Total 367	O 367	0	0
60	1J	12	Total 12	O 12	0	0

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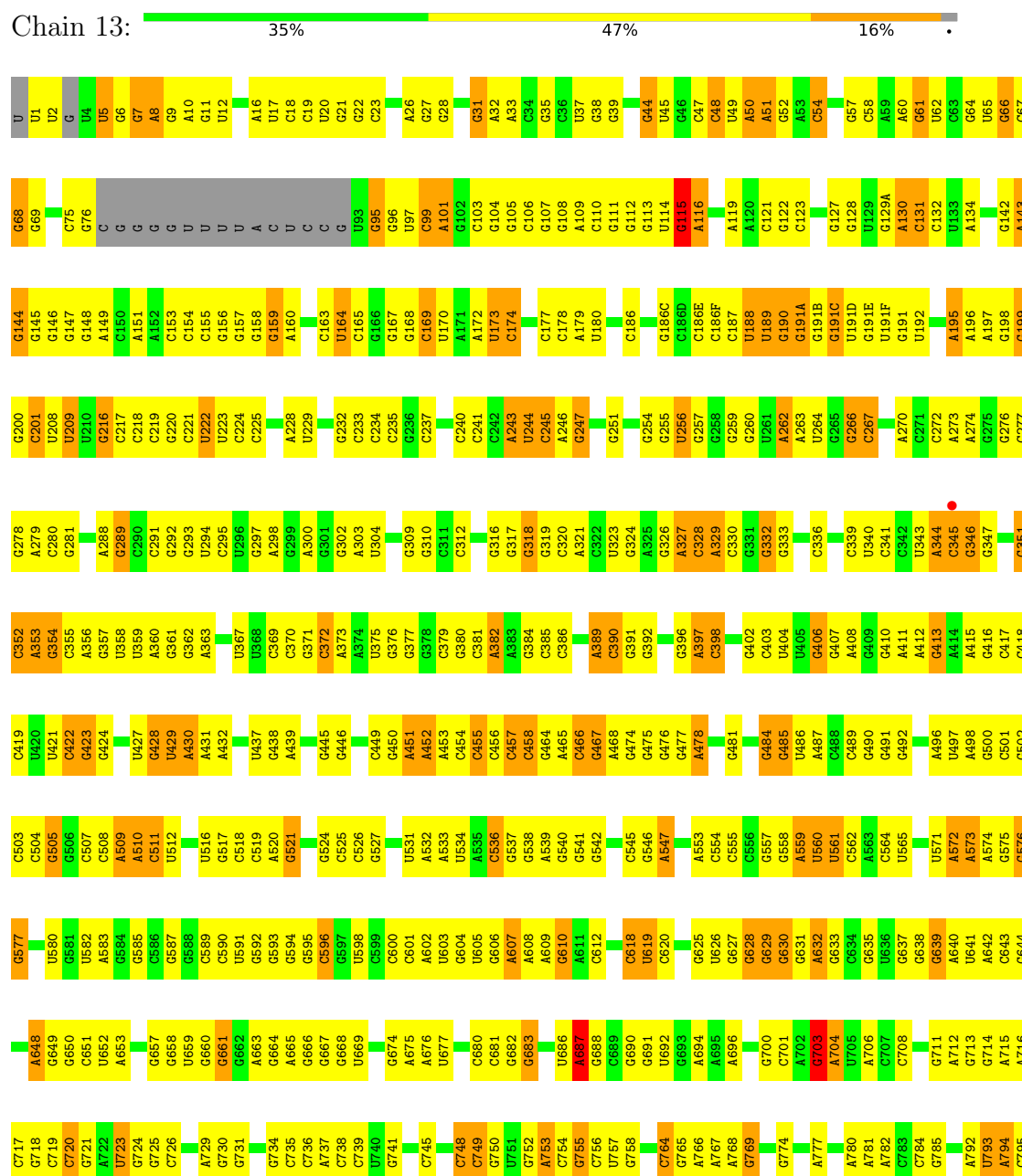
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	19	8	Total 8	O 8	0	0
60	29	2	Total 2	O 2	0	0
60	39	3	Total 3	O 3	0	0
60	35	2	Total 2	O 2	0	0
60	55	2	Total 2	O 2	0	0
60	H5	1	Total 1	O 1	0	0
60	L5	1	Total 1	O 1	0	0

3 Residue-property plots

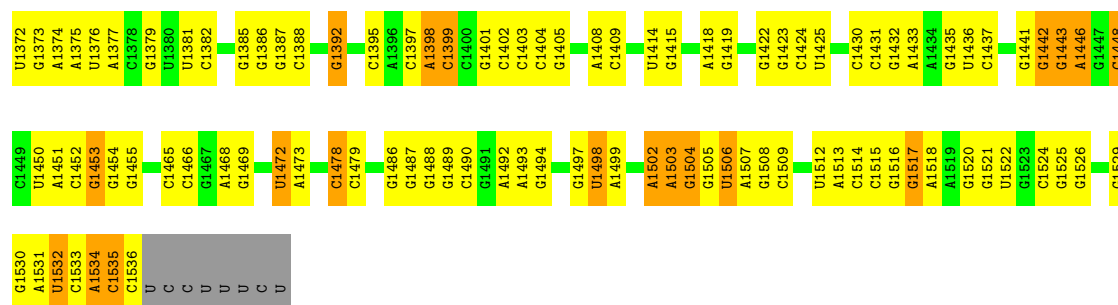
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

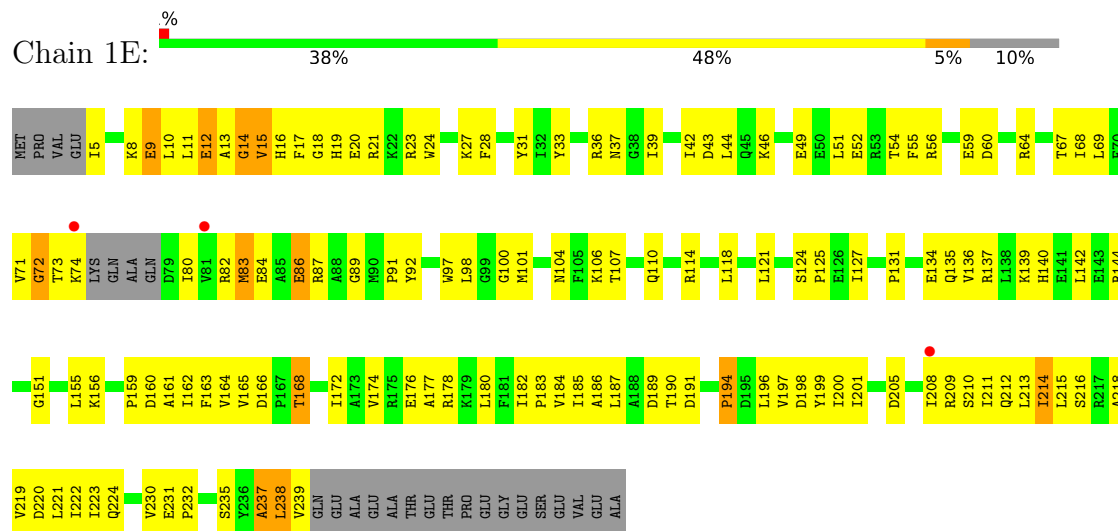




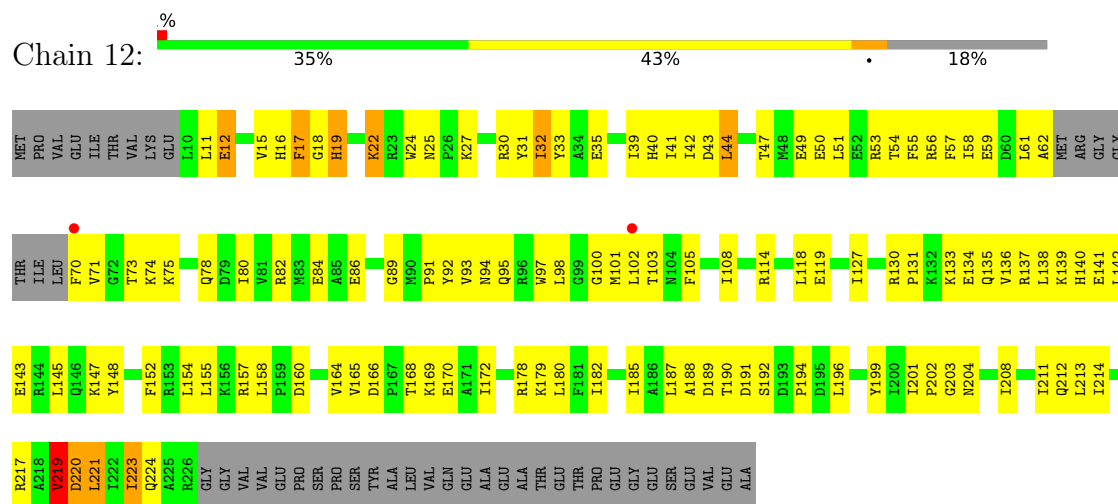
G1309	A1248	G1184	G1117	C1051	U992	G937	G741	G650	G588	G521	G438	U367	G289
G1312	G1249	G1187	C1118	U1052	G993	G838	G742	C651	C589	G527	A439	G371	U296
U1313	A1250	A1188	C1119	G1053	A994	U920	U743	U652	C590	G528	G446	G372	G297
G1314	A1251	C1189	G1120	C1054	G995	G922	G744	A653	U591	G529	G447	A374	A300
U1315	G1253	U1121	U1121	A1055	A996	A923	G745	G658	G592	G530	A448	G375	A303
G1316	C1254	G1190	U1122	C1056	G997	C924	C746	U659	G593	U531	C449	G376	U304
C1317	G1255	A1191	A1123	C1059	G998	G925	C747	G660	G594	A532	G450	G377	G305
A1318	U1256	G1192	G1124	G1060	C998A	G926	C748	G661	G595	A533	A451		
C1319	G1193	U1194	U1125	G1061	U999	G927	C749	G662	C596	U534	G452		
C1320	U1257	C1195	U1126	U1062	A1000	G928	G750	A663	U598	A535	A453		
C1321	G1258	C1063	G1127	C1063	G1001	G929	U751	G664	C599	C536			
C1322	U1259	U1196	C1128	G1064	G1002	G930	G752		C600	G537	C456		
G1323	G1197	G1197	C1129		G1003	C934		A665	C601	G538	C457		
A1324	A1261	G1198	A1130	A1067	A1004	A935	G755	G666	C602	A539	C458		
C1325	C1262	U1199	C1131	G1068	A1005		G756	G667	A603	G540	G464		
C1326		C1200	C1132	C1069	G1006	A938	U757	U668	U603	G541	G465		
G1265	G1265	A1201	G1133	U1070	C1007		G758	U669	G604	G542	C466		
G1266	G1266	G1202	G1134	C1071	C1008	G942	A759		U605	C543	G467		
G1267	C1267	C1203	U1135	G1072	G1009		G760	G673	G606	G544	A468		
A1268	U1268	A1204	U1136	U1073		A946	G761	G674	A607		G474		
U1205	U1205	U1205	C1137	U1077	A1014	G947		U677	A608	A547	G475		
G1270	C1270	G1206	G1138	U1078	A1015	C948	G763	U678	A609		G476		
G1271	G1271	G1207	G1139	G1079		A949	G764	C679		G396			
G1272	G1272	C1208	C1140	A1080	C1018	U952		C680	A614	A397			
G1273	C1273	C1209	C1141	G1079	C1019	G953	G765	C681	C615	C398			
C1210	C1210	U1211	G1143	U1082	U1020	G954	G769	G682	C616				
U1212	U1212	U1212	G1144	G1083	G1021	U955	G770		C617	C401			
A1213	C1213	A1213	C1145	U1084	G1022	A973	G771		C618	G402			
C1214	C1214	C1214	A1146	G1085	G1023	U956	U772		C619	G403			
G1215	C1215	G1215	C1147	U1086	G1024	U957			U619	C404			
G1216	G1216	G1216	U1148	U1087	U1025		A777		A621	U405			
C1217	C1217	C1217	U1149	G1087	G1026	U960	G778		A622	A487			
C1282	U1281	C1218	C1150	G1088	C1027	U961			A623	C406			
G1283	U1219	U1219	U1151	U1089	C1028	A964	A782		C624	G407			
C1284	C1284	U1220	A1152	U1090	C1028A	G965			G625	A408			
G1285	G1285	G1221	C1153	U1091	U1028	A966	U789		A626	G409			
A1286	A1286	G1222	G1154	A1092	G1029	C967	G791		U626	G410			
A1287	C1223	C1223	G1155	A1093	C1030	A968	G792		C627	A411			
A1288	G1224	G1224	G1156	U1094	G1031	A969	A792		U628	A412			
U1351	A1225	A1225	A1157	U1095	A1032	G970	U793		G629	A495			
G1290	C1226	C1226	C1158	C1096	G1032A	G971	A794		G630	G414			
G1291	A1227	A1227	U1159	C1097	G1032B	G972	C707		G631	G415			
U1292			U1159	C1098	G1033	C972	C708		A632	G416			
C1354	U1292		G1160	G1099	G1034	G973	G803		G633	U571			
G1355	G1293	U1232	C1161	C1100	A1035	A974	U804		C634	A572			
G1356	G1294	G1233	C1162	A1101	G1036	A975	C805		G635	A573			
A1357	G1295	C1234	C1163	A1102	C1037	G976			U636	A574			
U1358	C1296	U1235	G1164	C1103	G1038	G902	U723		G637	C504			
C1359	C1297	A1236	C1165	G1104	C1039	G903	G724		G638	G505			
A1360	C1298	C1237	G1166	A1105	U1040	A978	C817		G639	G576			
G1361	A1298	A1238		G1106	A1041	C979	G818		G640	G577			
G1362	G1300	A1239	G1171	C1107	A1042	C980	A819		U641	G579			
C1362A	U1301	U1240	G1177	U1108	C1043	U981	U820		A642	U580			
A1363	U1302	G1241		C1109	A1044	U982	G821		C643	G581			
U1364	G1303	C1242	G1178	A1110	G1045	A983	U827		G644	U582			
	C1304	C1243	A1179	C1110	A1046	C984	A828		C645	A583			
G1365	G1305	C1244	A1180	C1111	U1047	C985	G829		U646	G584			
A1306	A1306	A1245	G1181	C1112	G1047	C986	G830		C647	G585			
G1368	G1368	U1307	G1182	C1113	U1048	G987	U831		A648	C566			
G1370	G1370	C1246	G1183	C1114	G1049	G917			G649	C567			
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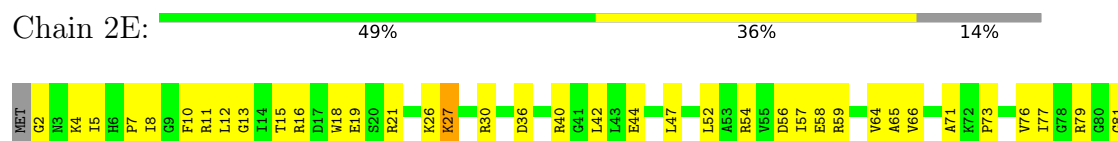
• Molecule 2: 30S ribosomal protein S2

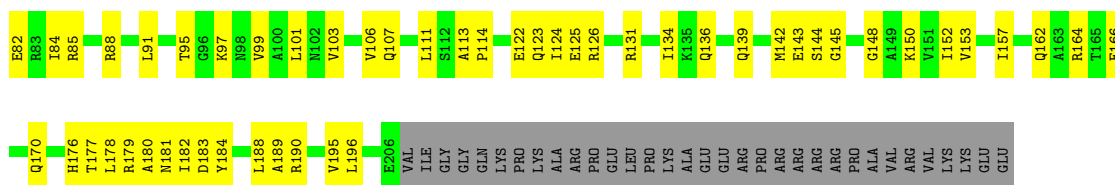


• Molecule 2: 30S ribosomal protein S2

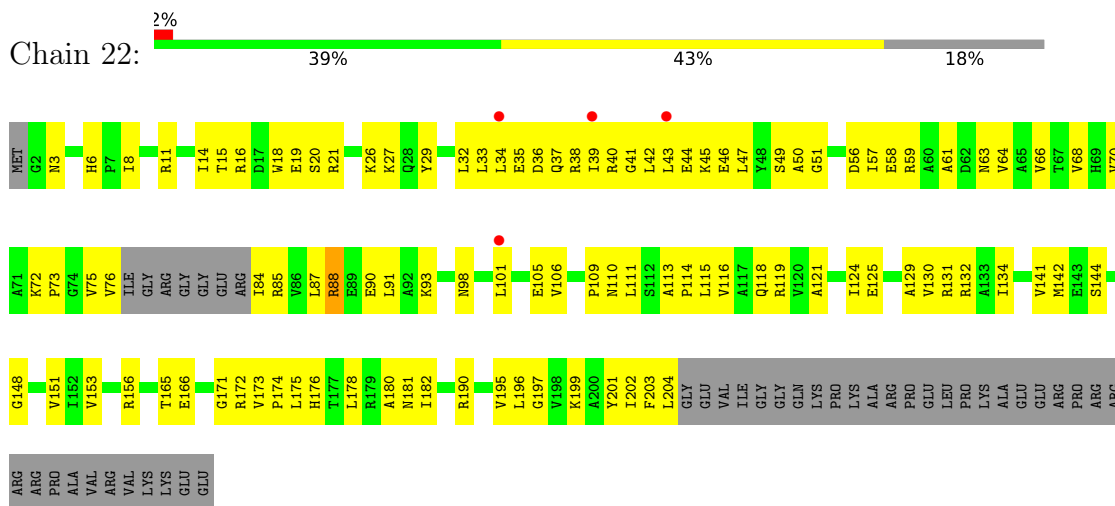


• Molecule 3: 30S ribosomal protein S3





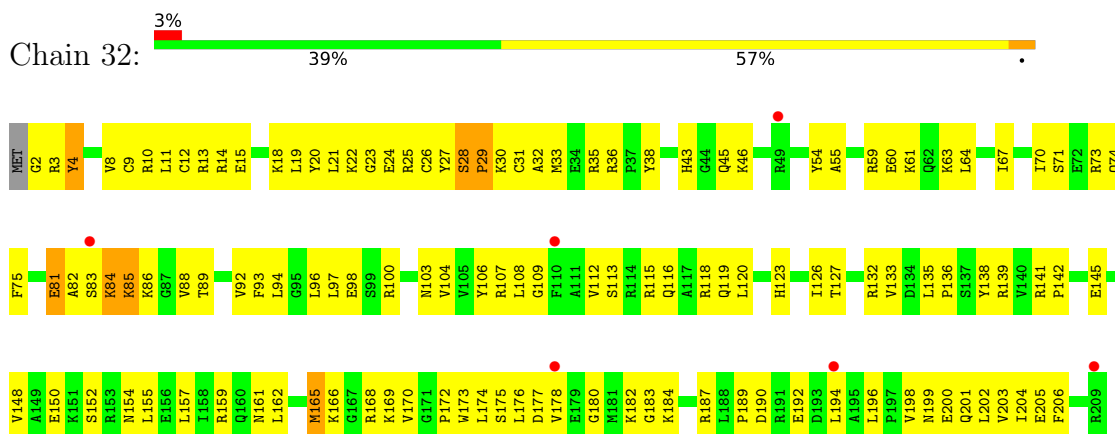
• Molecule 3: 30S ribosomal protein S3



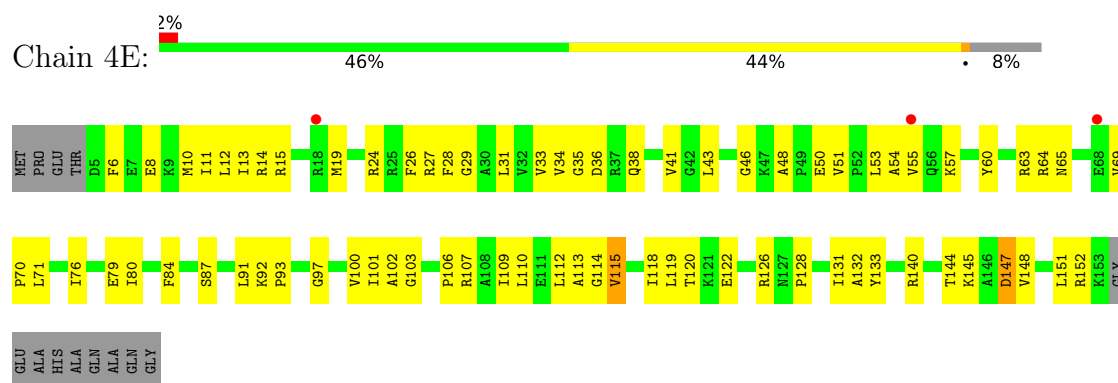
• Molecule 4: 30S ribosomal protein S4



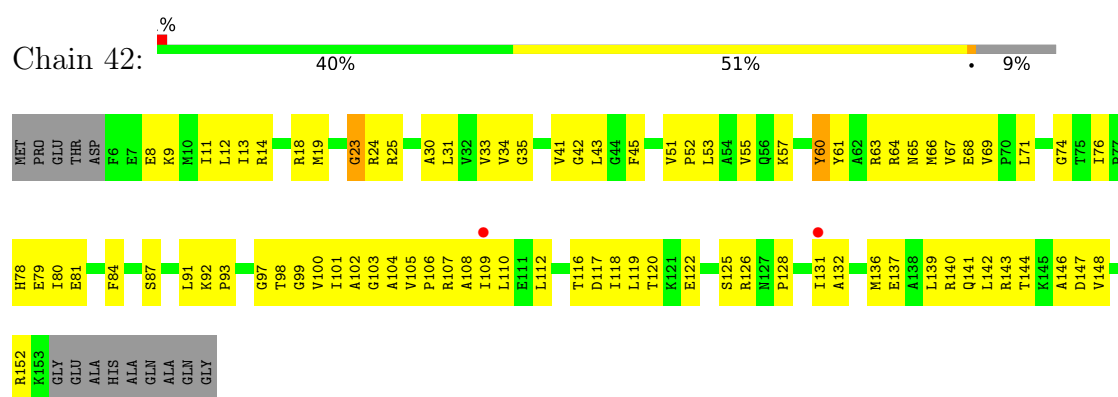
• Molecule 4: 30S ribosomal protein S4



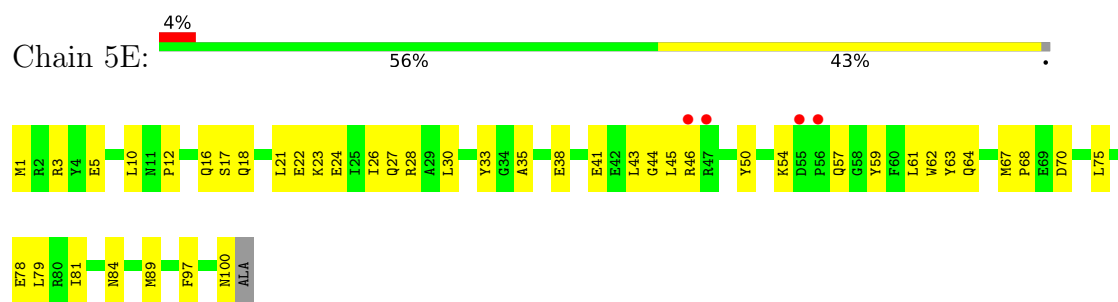
- Molecule 5: 30S ribosomal protein S5



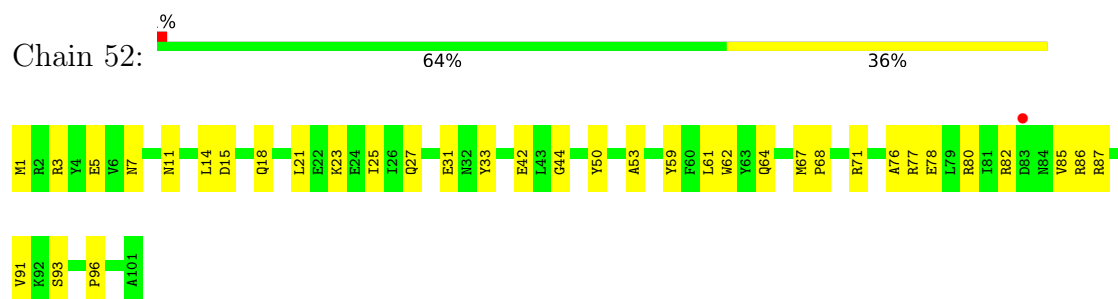
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

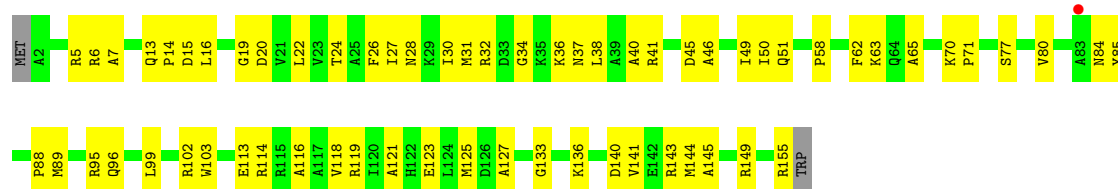


- Molecule 6: 30S ribosomal protein S6

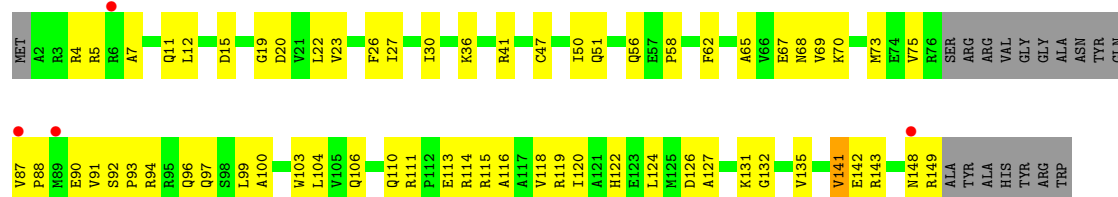


- Molecule 7: 30S ribosomal protein S7

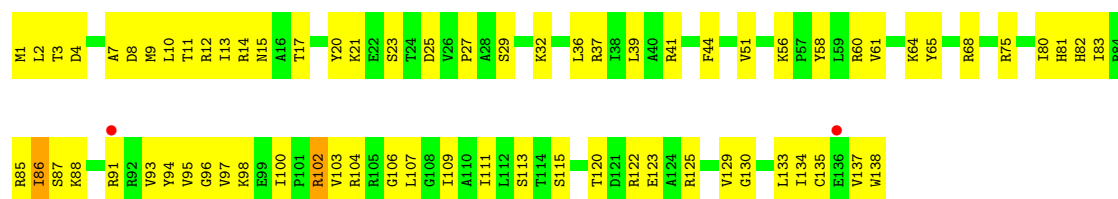




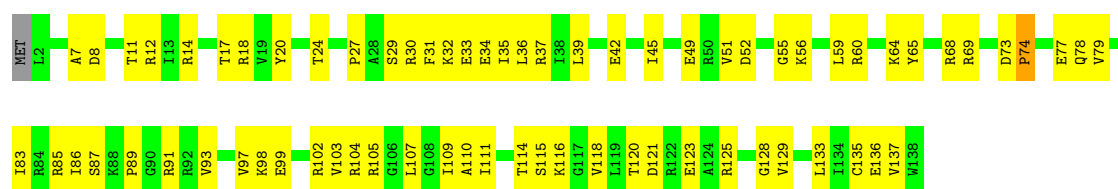
• Molecule 7: 30S ribosomal protein S7



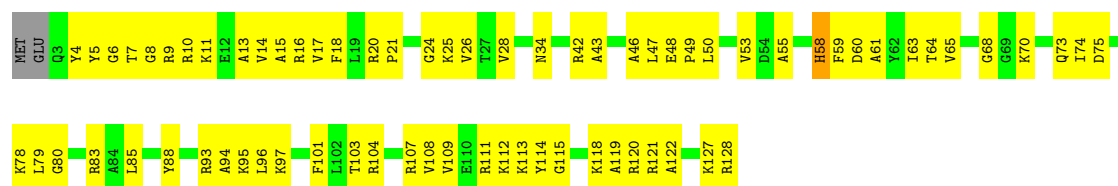
• Molecule 8: 30S ribosomal protein S8



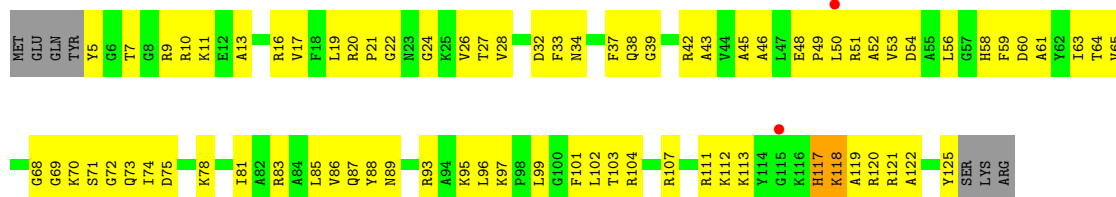
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9



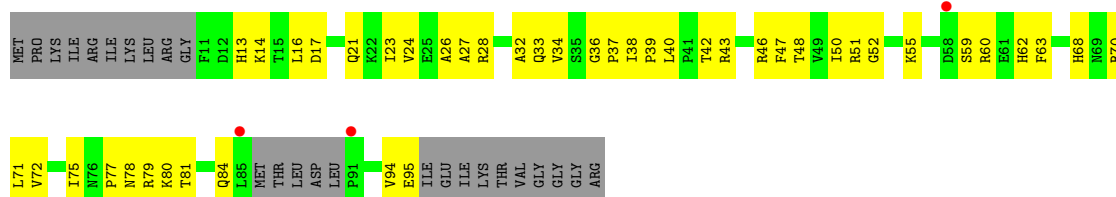
• Molecule 9: 30S ribosomal protein S9



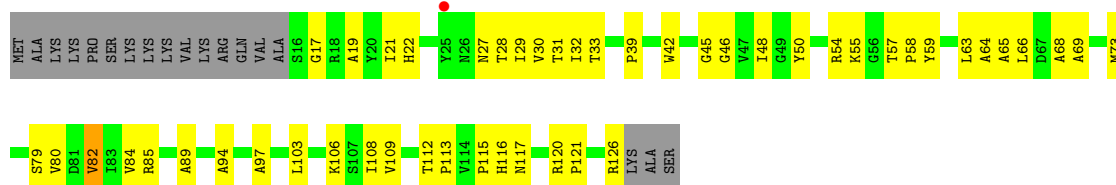
• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S11





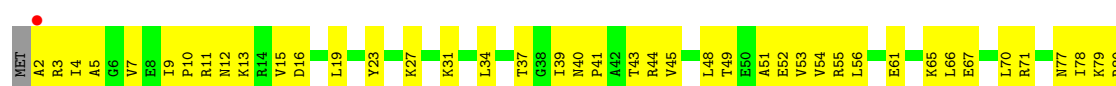
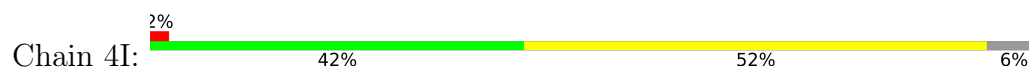
- Molecule 12: 30S ribosomal protein S12



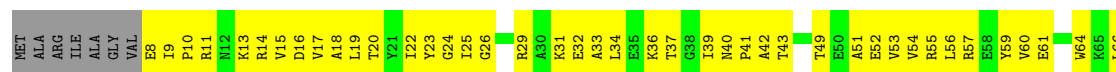
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

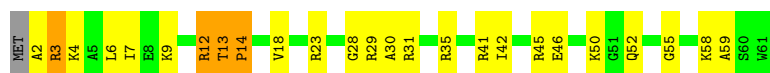


- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z

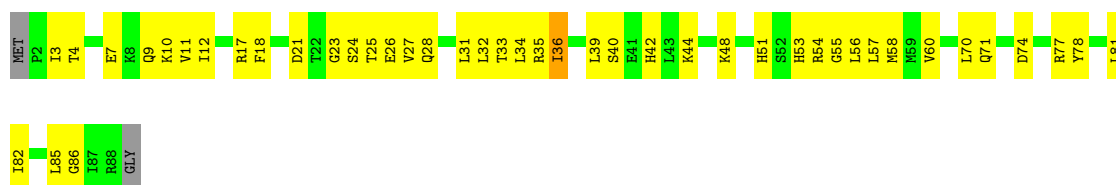




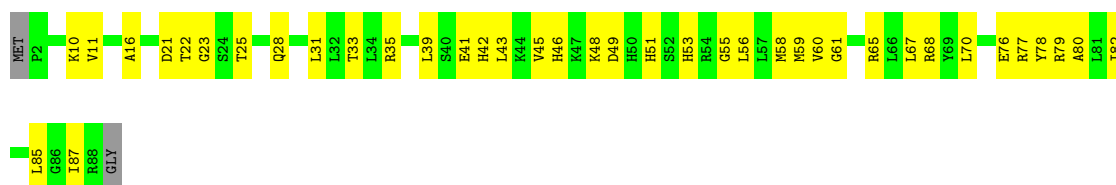
- Molecule 14: 30S ribosomal protein S14 type Z



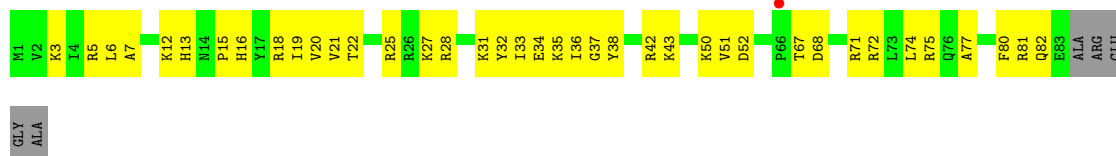
- Molecule 15: 30S ribosomal protein S15



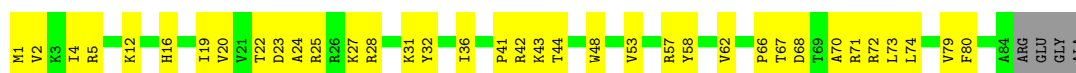
- Molecule 15: 30S ribosomal protein S15



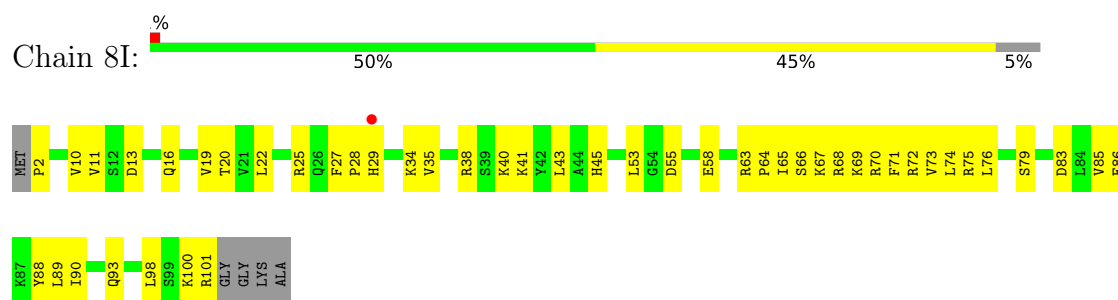
- Molecule 16: 30S ribosomal protein S16



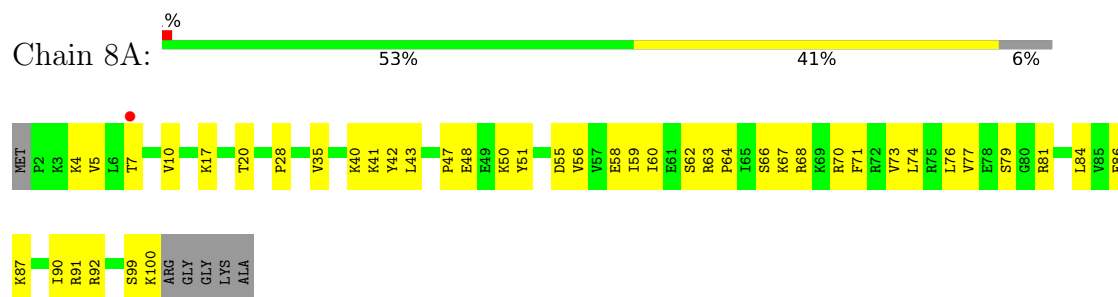
- Molecule 16: 30S ribosomal protein S16



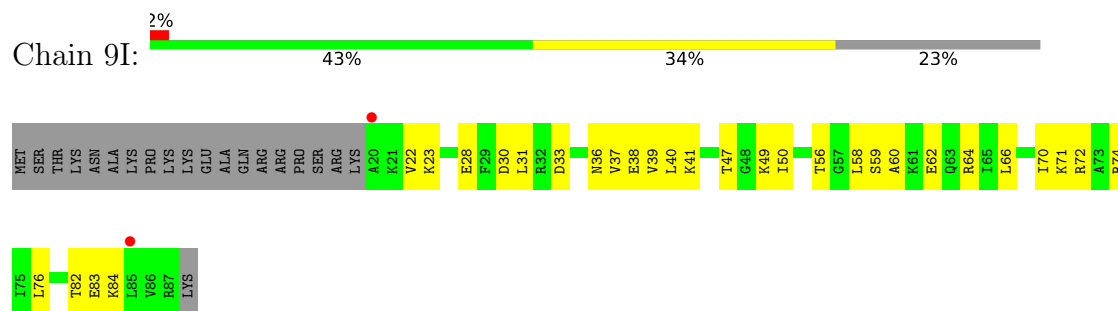
- Molecule 17: 30S ribosomal protein S17



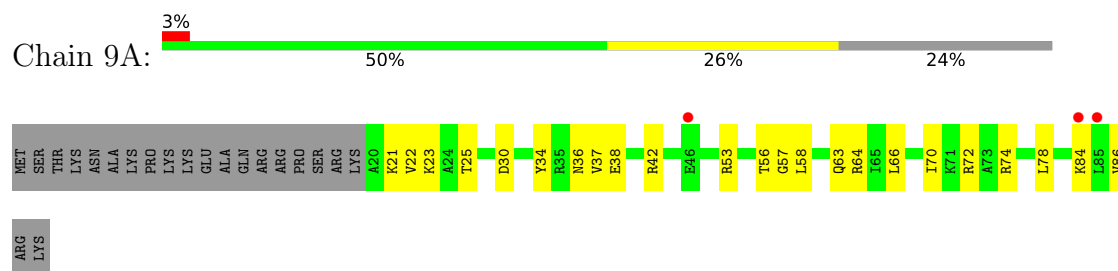
- Molecule 17: 30S ribosomal protein S17



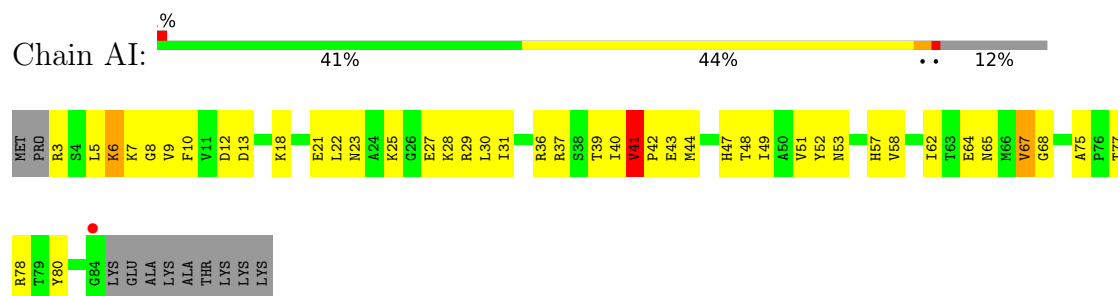
- Molecule 18: 30S ribosomal protein S18



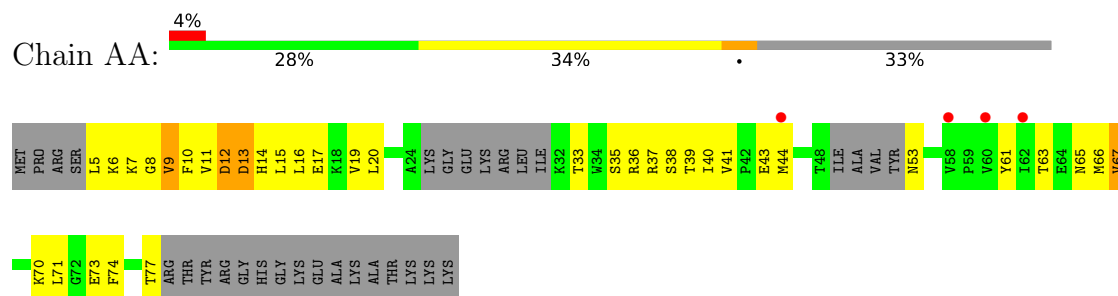
- Molecule 18: 30S ribosomal protein S18



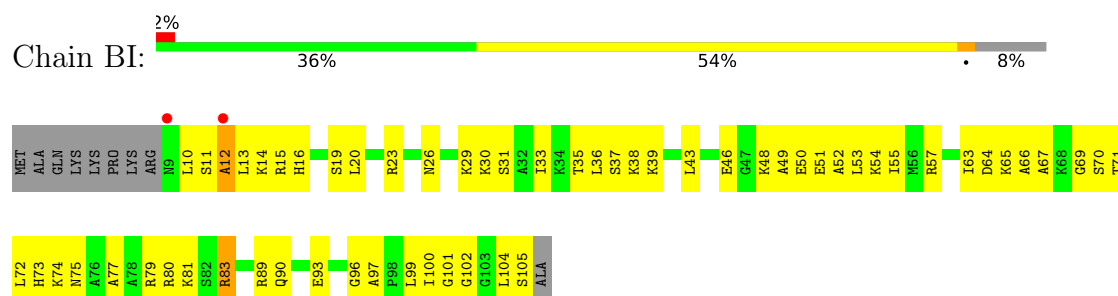
- Molecule 19: 30S ribosomal protein S19



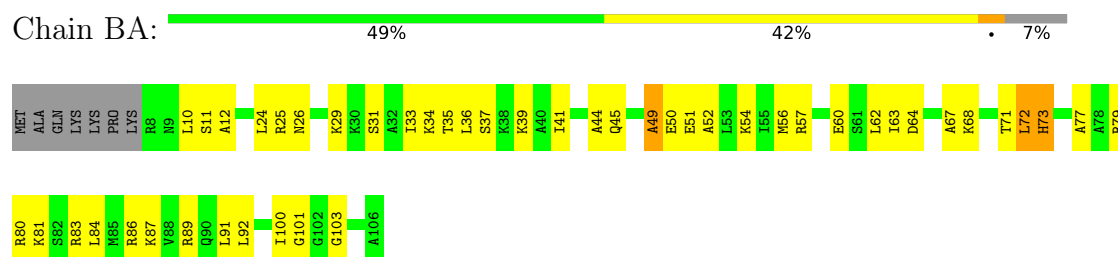
- Molecule 19: 30S ribosomal protein S19



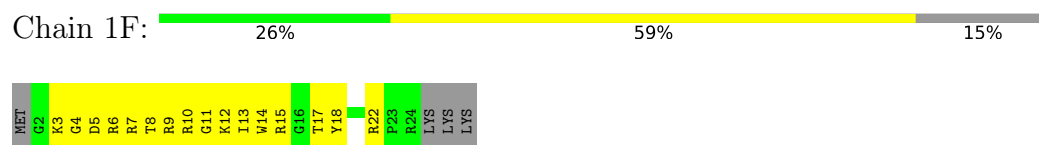
- Molecule 20: 30S ribosomal protein S20



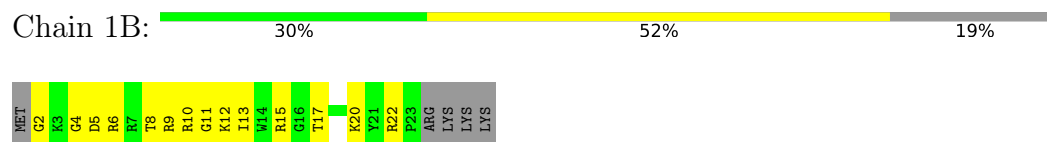
- Molecule 20: 30S ribosomal protein S20



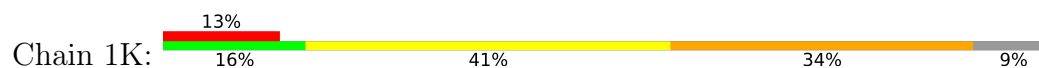
- Molecule 21: 30S ribosomal protein Thx

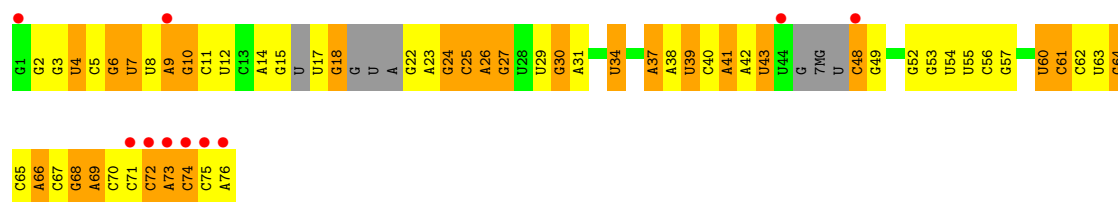


- Molecule 21: 30S ribosomal protein Thx

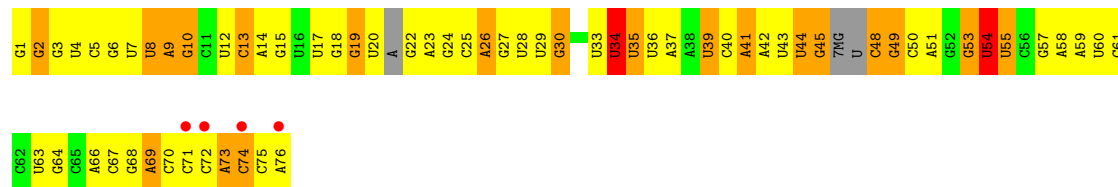
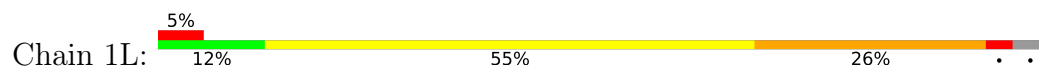


- Molecule 22: tRNA^{Lys}

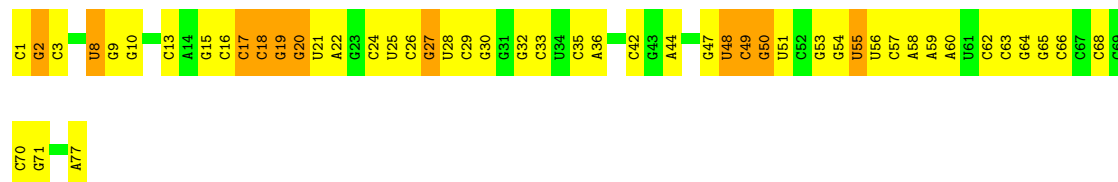




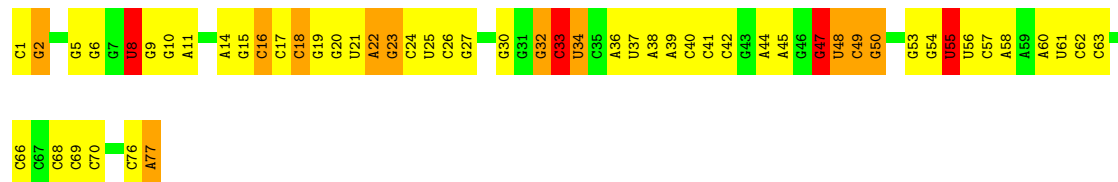
• Molecule 22: tRNA^{Lys}



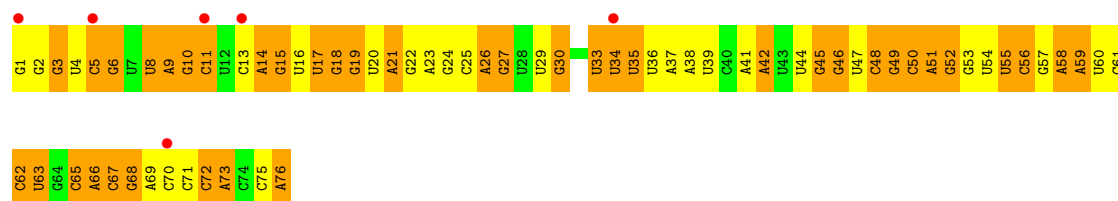
• Molecule 23: E. coli tRNA^{fMet}



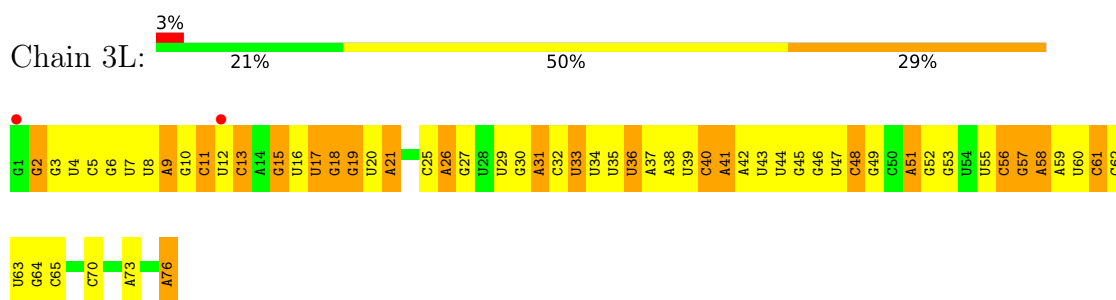
• Molecule 23: E. coli tRNA^{fMet}



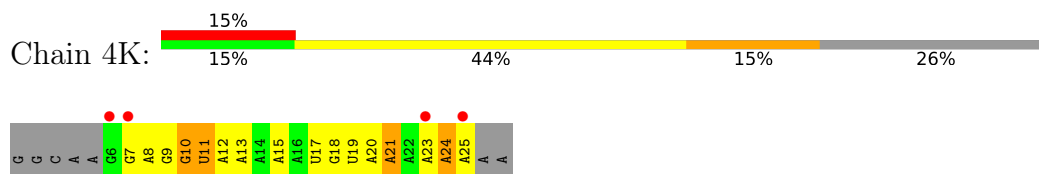
• Molecule 24: tRNA^{Lys}



• Molecule 24: tRNA^{Lys}



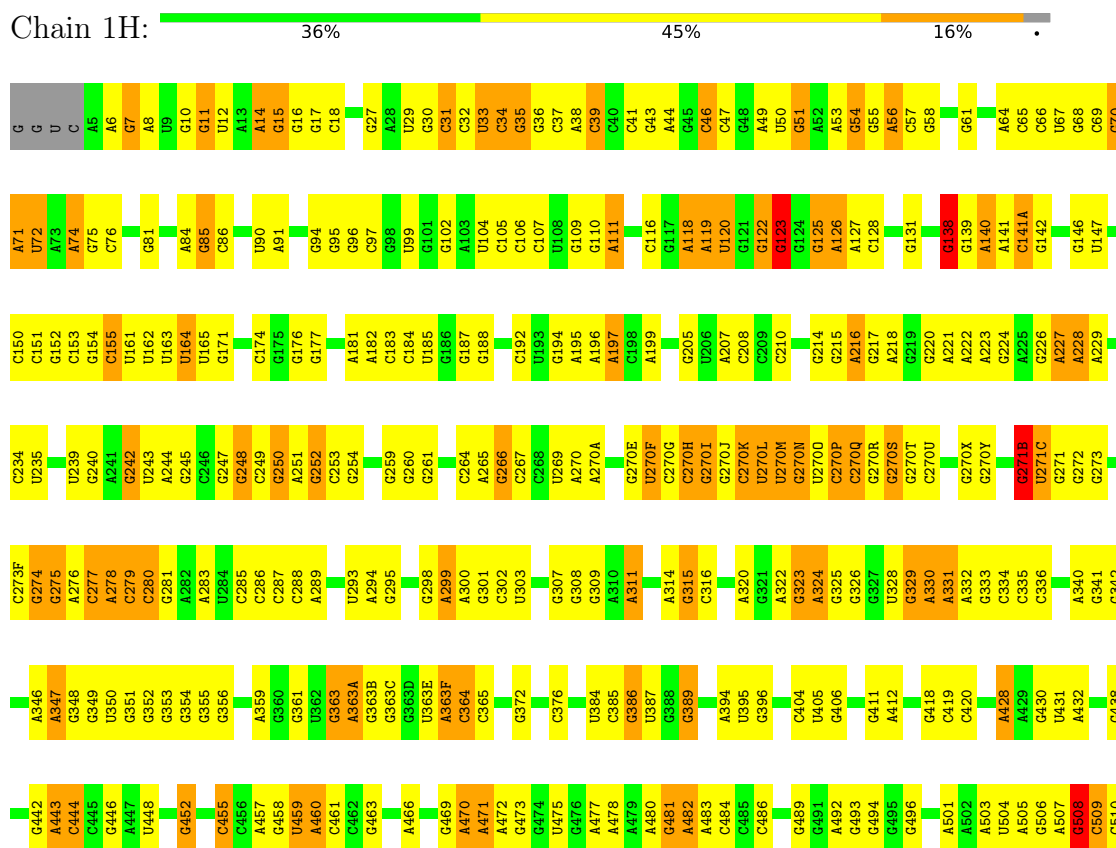
• Molecule 25: mRNA



• Molecule 25: mRNA

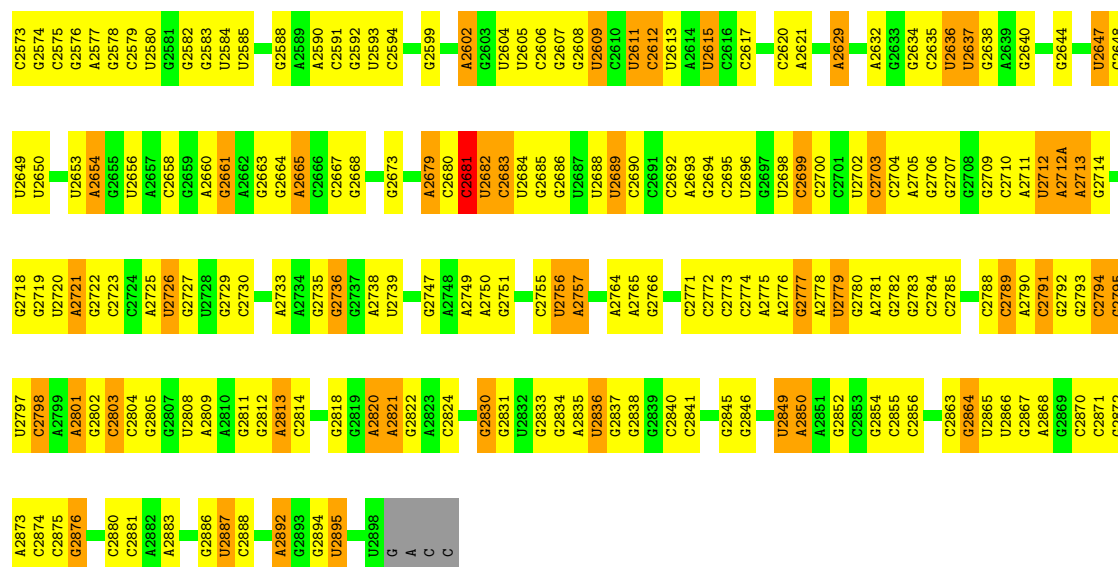


• Molecule 26: 23S rRNA



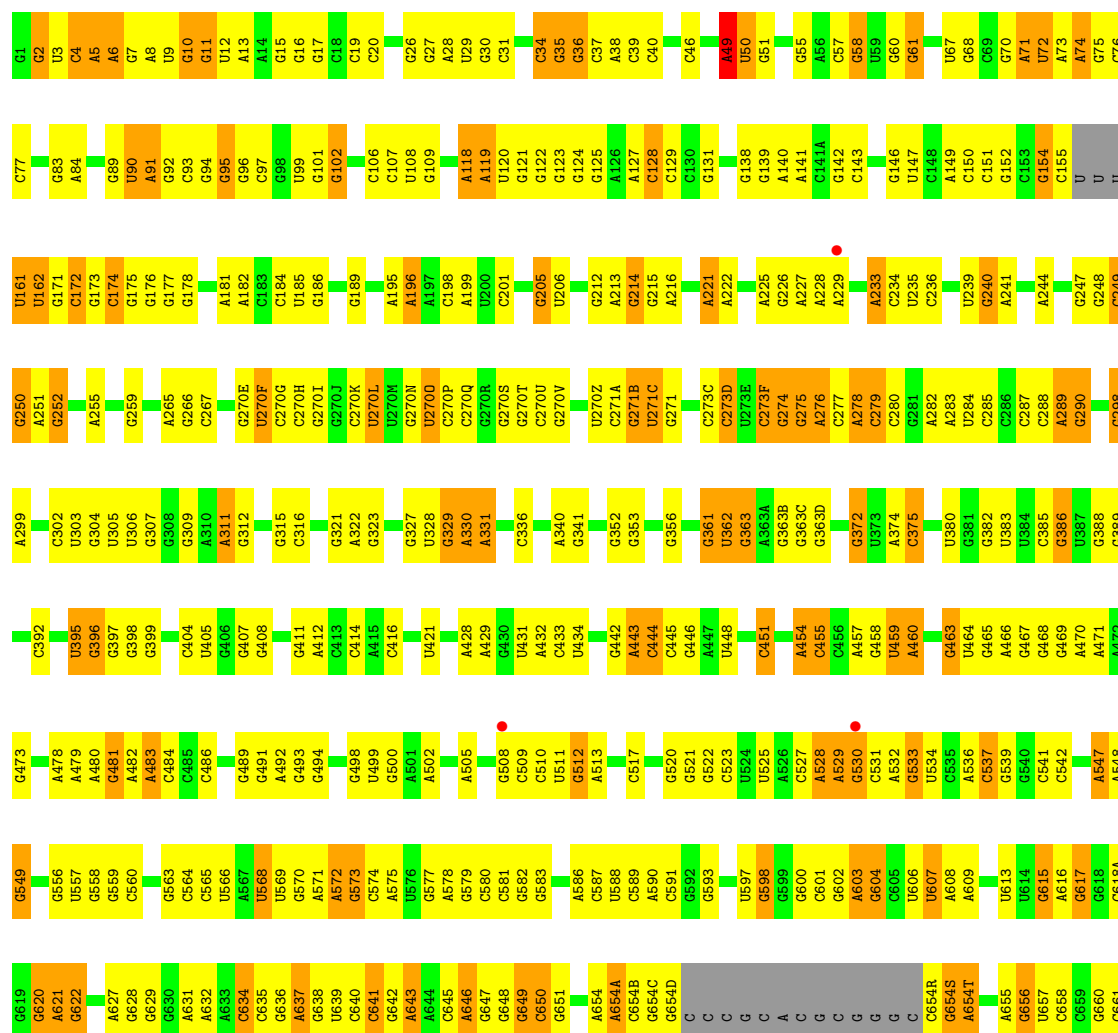
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C1437	G1371	G1296	G1219	C1146	C1013	C936	C857	U779	G704	A652	C587	A513
G1440	U1372	C1297	A1220	G1149	G1016	G938	U858	G780	U709	A654	U588	A514
G1441	A1373	C1298	C1221	G1150	U1019	A941	U860	A781	G710	A654A	C517	C517
G1442	G1374	G1299	C1222	G1151	A1020	G942	A861	A782	G711	A654B	G518	G518
G1443	C1375	U1300	C1223	G1154	A1021	U943	A863	A783	G712	G654C	U519	U519
G1444	G1376	A1301	G1224	A1155	G1022	G944	A864	A784	G713	C	G593	G593
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	G1378	G1303	G1226	A1157	G1024	G946	C866	U787	G715	C		
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G1448		U1312	G1229	G1164	A1027	C952	A870	C791	C719	C	G598	A528
A1449	A1384	U1313	G1229A	U1165	G1033	G953	A870	C792	C719	A	G599	A529
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G1455	G1389	G1319	A1237	G1170	G1038	U959	G	C797	U724	G654P	C505	C537
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• Molecule 26: 23S rRNA

Chain 14: 37% 45% 16%

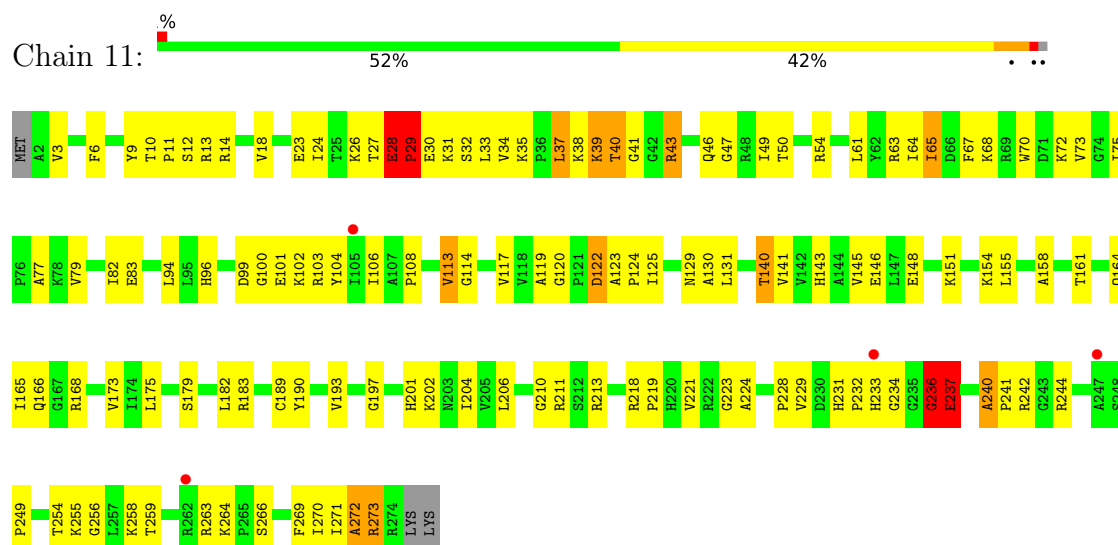


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G1601	U1534	G1461	U1394	G1323	A1241	U1167	U1105	A	G975	A	G975	G674
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G1755	C1593	G1513	G1513	G1371	G1310	G1224	A1155	G1093	G889	A	G889	G750
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C1757	G1595	G1515	G1515	A1373	G1310	G1224	A1155	G1093	G891	A	G891	G752
A1758	C1596	G1516	G1516	G1374	G1310	G1224	A1155	G1093	G892	A	G892	G753
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U1761	G1598	G1518	G1518	G1377	G1310	G1224	A1155	G1093	G895	A	G895	G756
G1762	C1599	U1519	U1519	A1378	G1310	G1224	A1155	G1093	G896	A	G896	G757
A1763	G1600	C1587	C1587	C1446	G1310	G1224	A1155	G1093	G897	A	G897	G758
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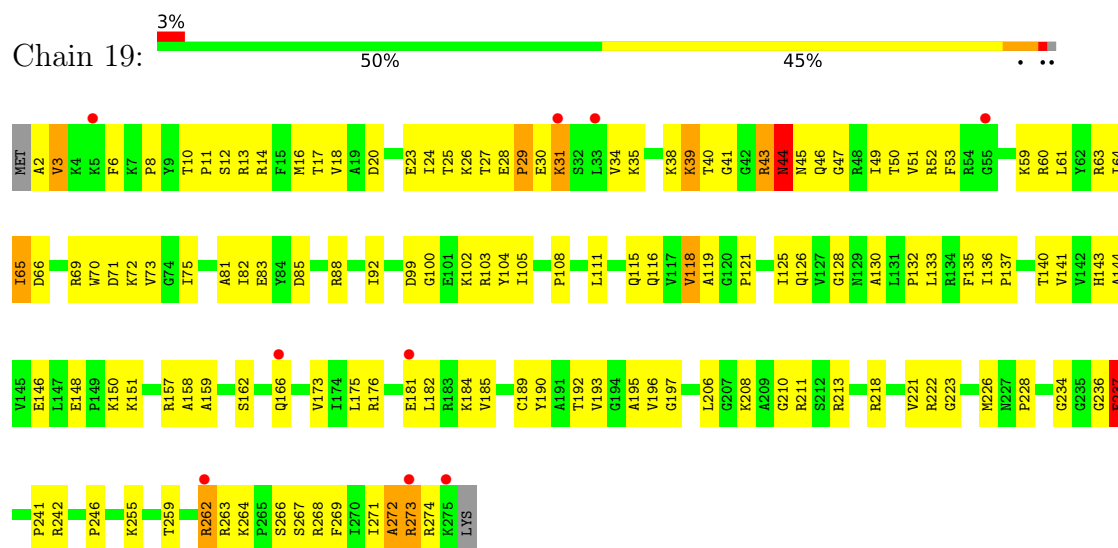
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G2818	U2746	C2679	C2606	C2620	A2448	G2379	U2312	G2243	G2160	C2097	G1929	G1839	G1769
G2819	G2747	C2680	G2607	G2625	U2449	G2380	C2313	U2244	C2161	U2098	G1930	A1847	G1770
A2820	A2748	U2681	U2608	G2626	G2453	C2381	C2314	U2245	C2162	G2099	U1931	A1853	G1771
A2821	A2749	U2682	C2610	U2528	A2454	G2382	C2316	A2247	C2163	G2024	A1936	A1853	G1772
G2822	A2750	U2683	U2611	G2629	G2455	G2383	C2317	C2248	C2164	C2025	A1937	A1854	A1773
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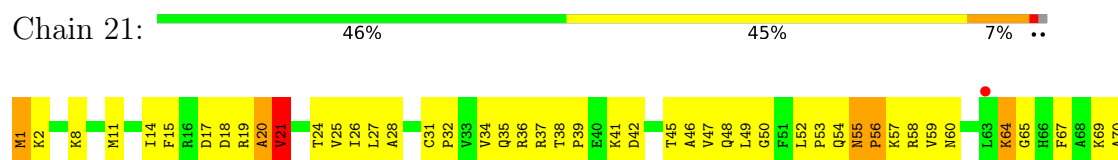
- Molecule 29: 50S ribosomal protein L2

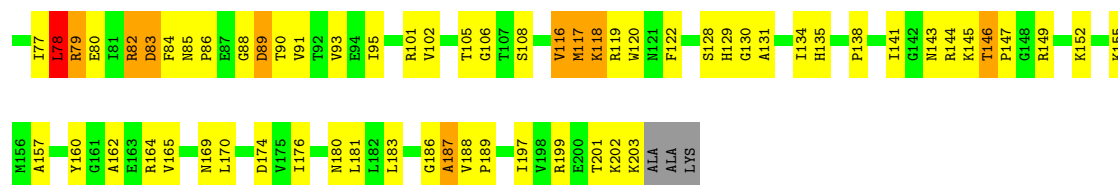


- Molecule 29: 50S ribosomal protein L2

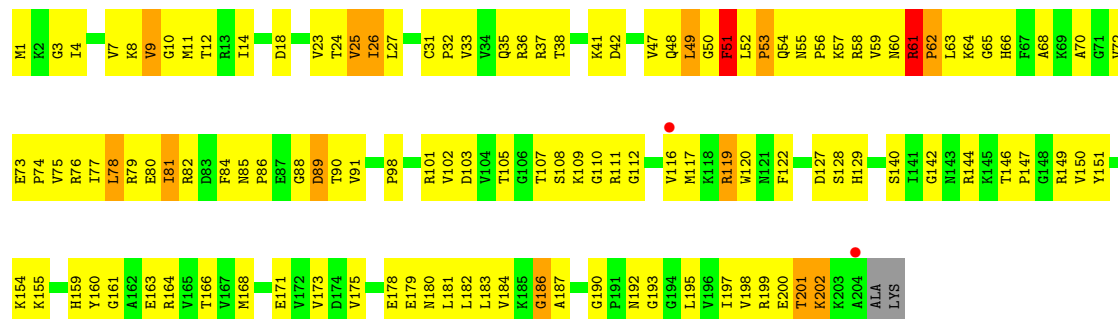
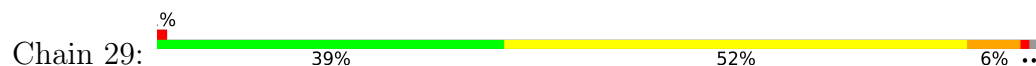


- Molecule 30: 50S ribosomal protein L3

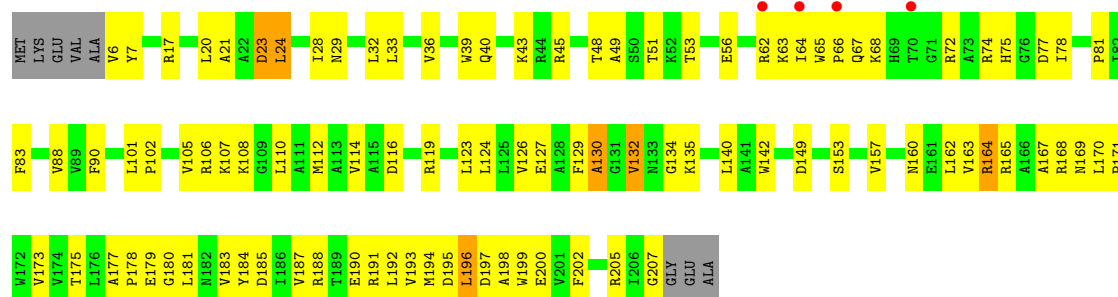




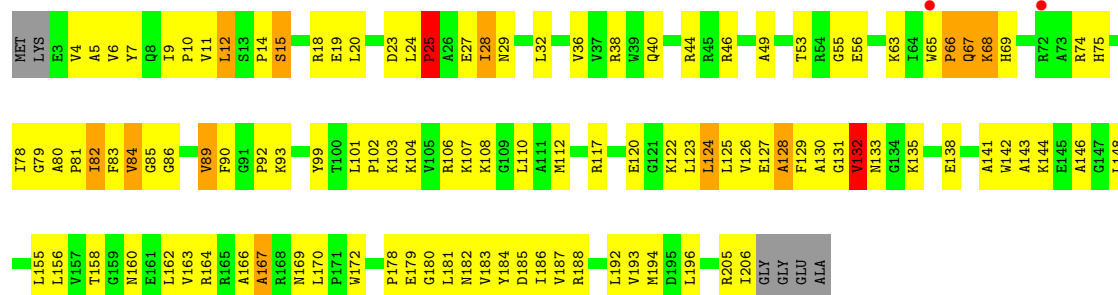
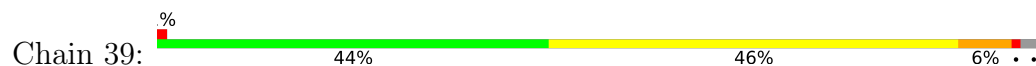
• Molecule 30: 50S ribosomal protein L3



• Molecule 31: 50S ribosomal protein L4



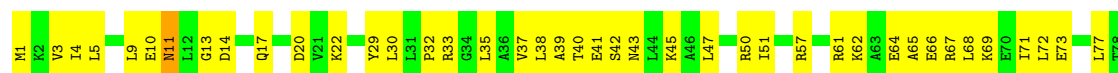
• Molecule 31: 50S ribosomal protein L4



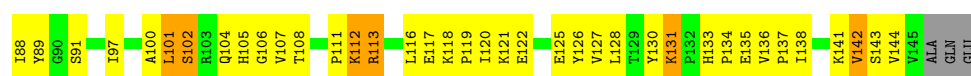
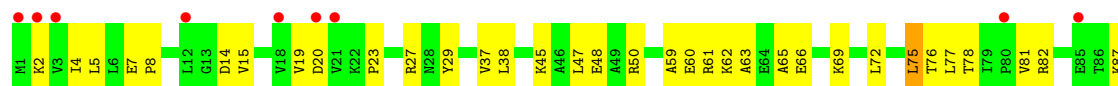
• Molecule 32: 50S ribosomal protein L5



• Molecule 34: 50S ribosomal protein L9



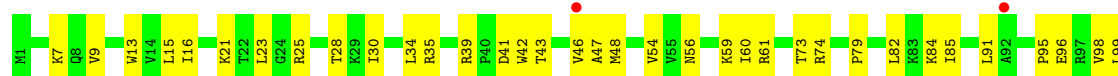
• Molecule 34: 50S ribosomal protein L9



• Molecule 35: 50S ribosomal protein L13

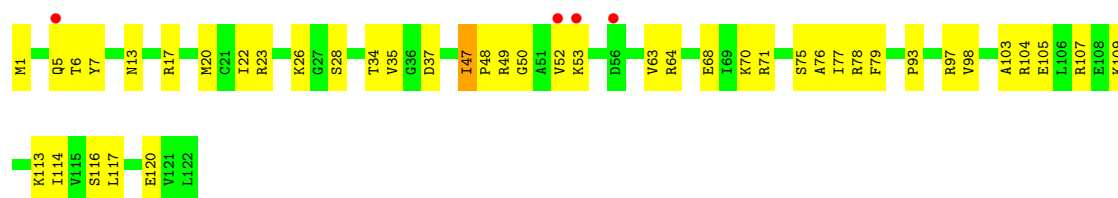


• Molecule 35: 50S ribosomal protein L13



• Molecule 36: 50S ribosomal protein L14





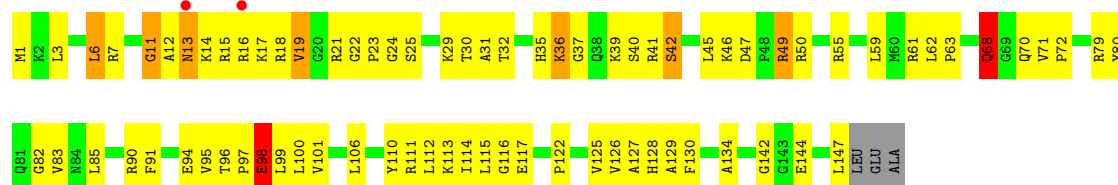
• Molecule 36: 50S ribosomal protein L14

Chain 25: 59% 40%



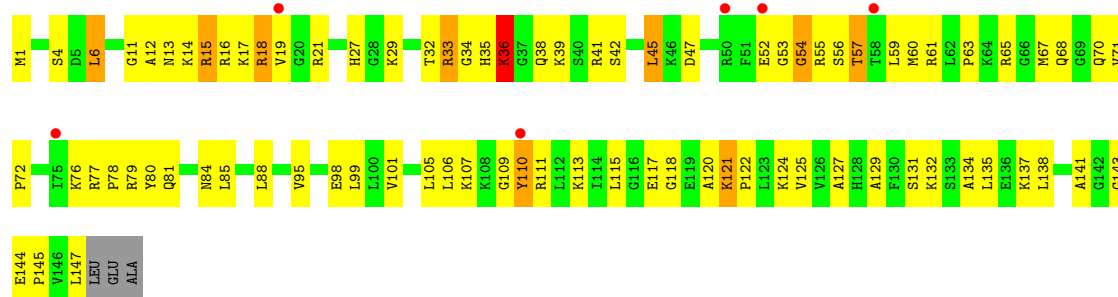
• Molecule 37: 50S ribosomal protein L15

Chain 78: 46% 46% 5% ..



• Molecule 37: 50S ribosomal protein L15

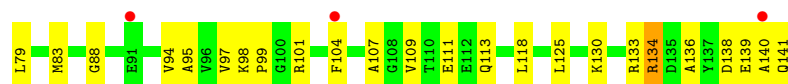
Chain 35: 4% 43% 49% 6% ..



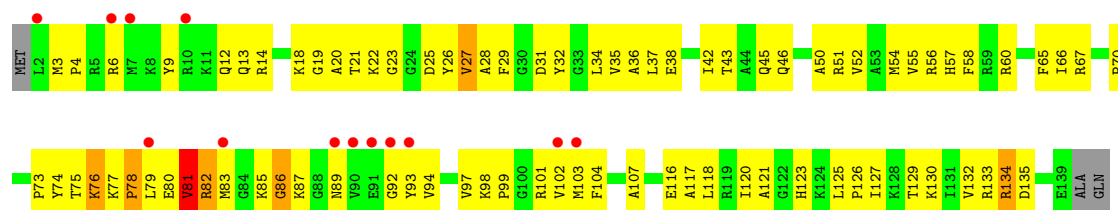
• Molecule 38: 50S ribosomal protein L16

Chain 88: 2% 53% 42% 5%

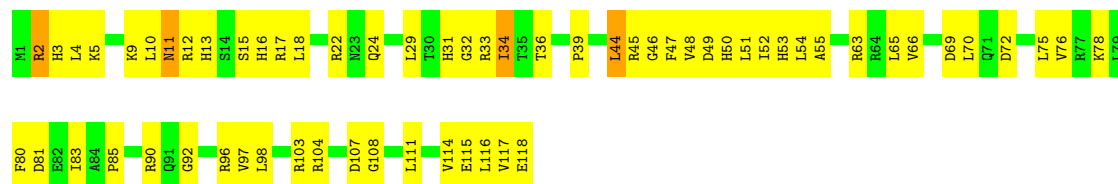




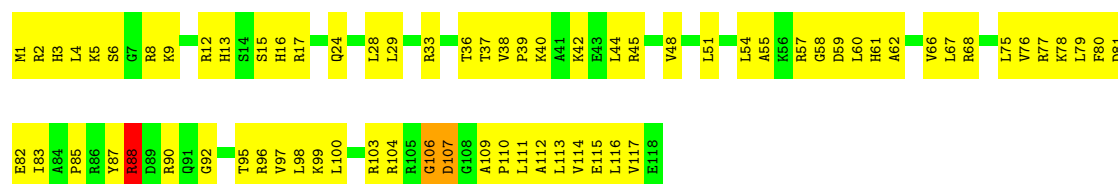
- Molecule 38: 50S ribosomal protein L16



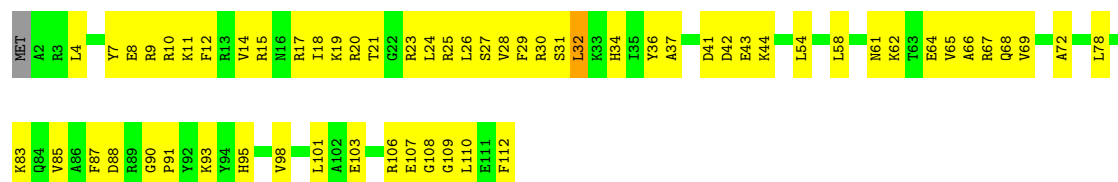
- Molecule 39: 50S ribosomal protein L17



- Molecule 39: 50S ribosomal protein L17

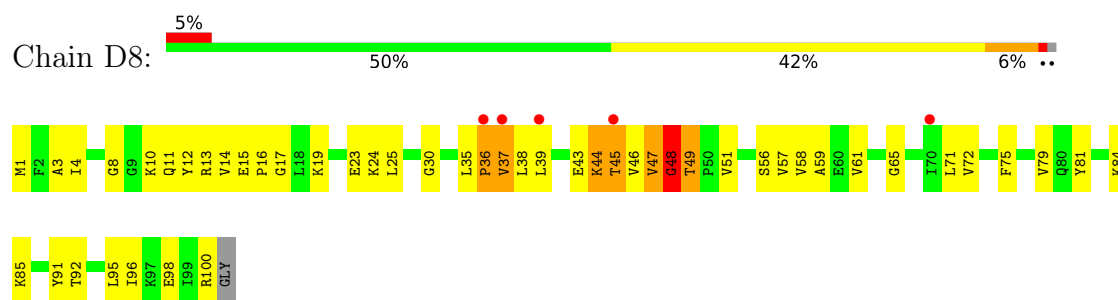


- Molecule 40: 50S ribosomal protein L18

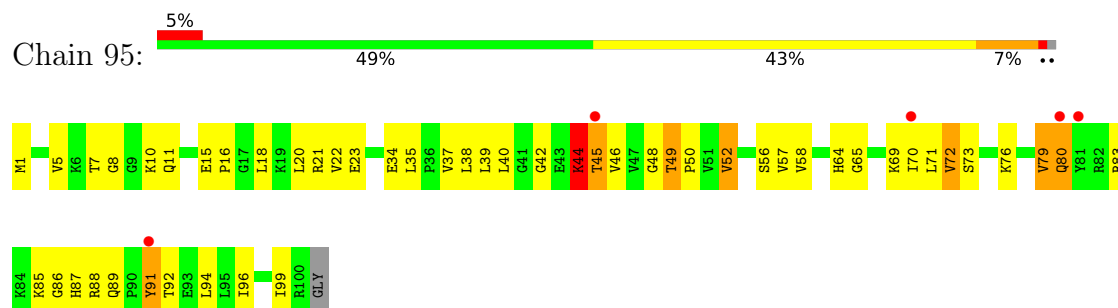


- Molecule 40: 50S ribosomal protein L18

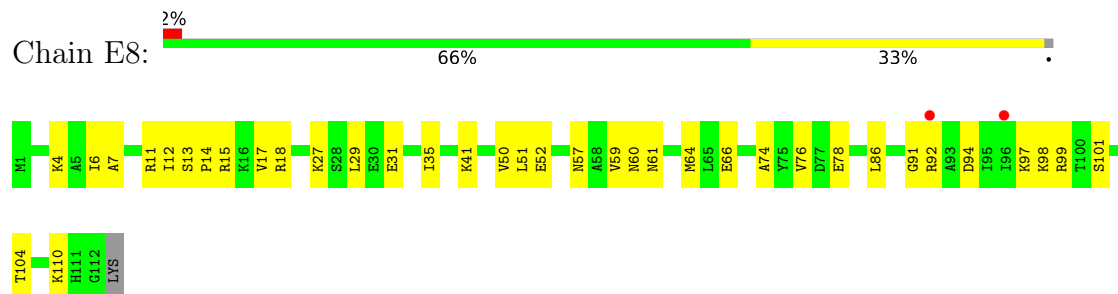




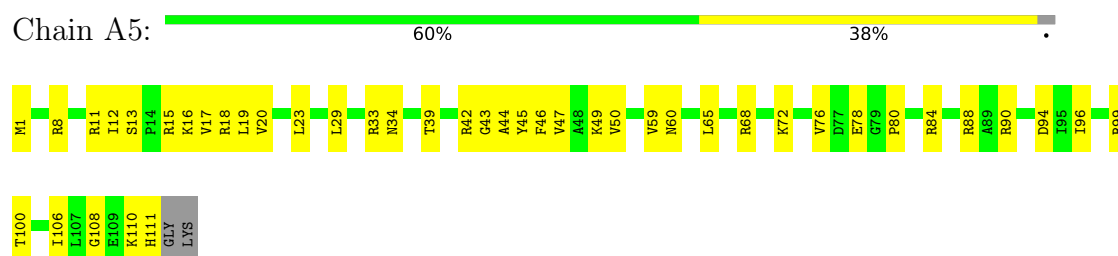
- Molecule 43: 50S ribosomal protein L21



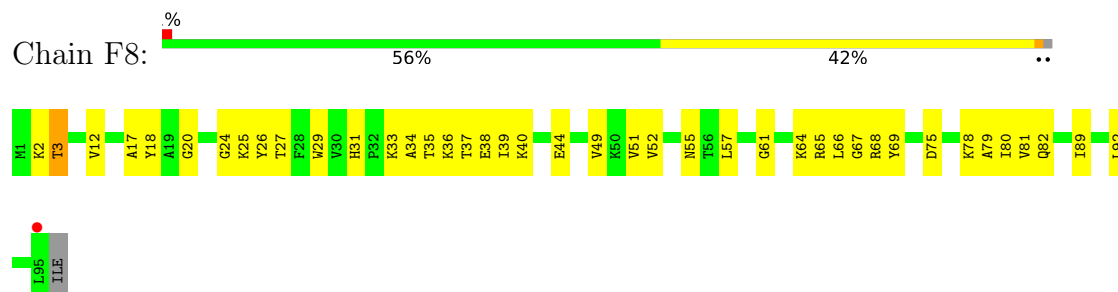
- Molecule 44: 50S ribosomal protein L22



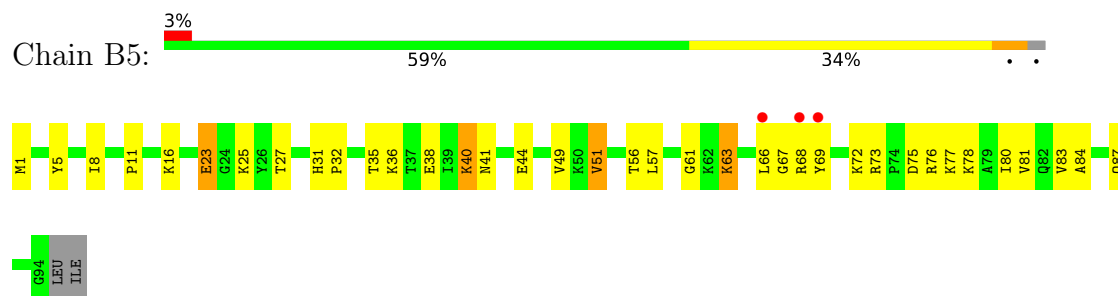
- Molecule 44: 50S ribosomal protein L22



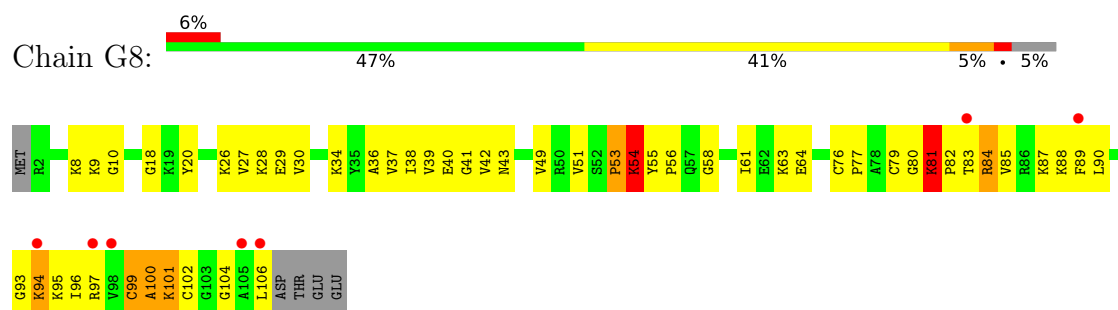
- Molecule 45: 50S ribosomal protein L23



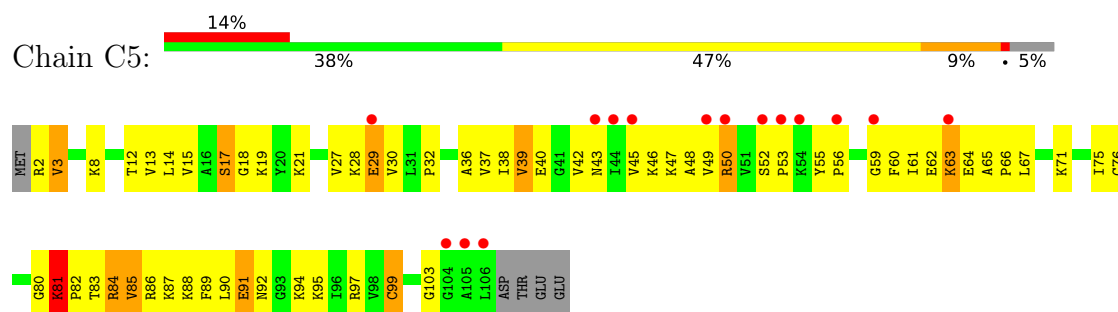
- Molecule 45: 50S ribosomal protein L23



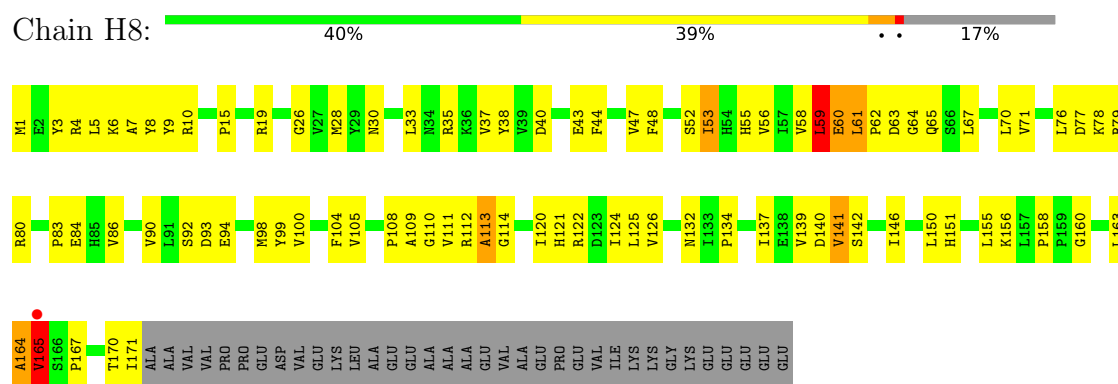
- Molecule 46: 50S ribosomal protein L24



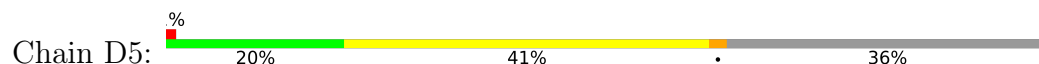
- Molecule 46: 50S ribosomal protein L24

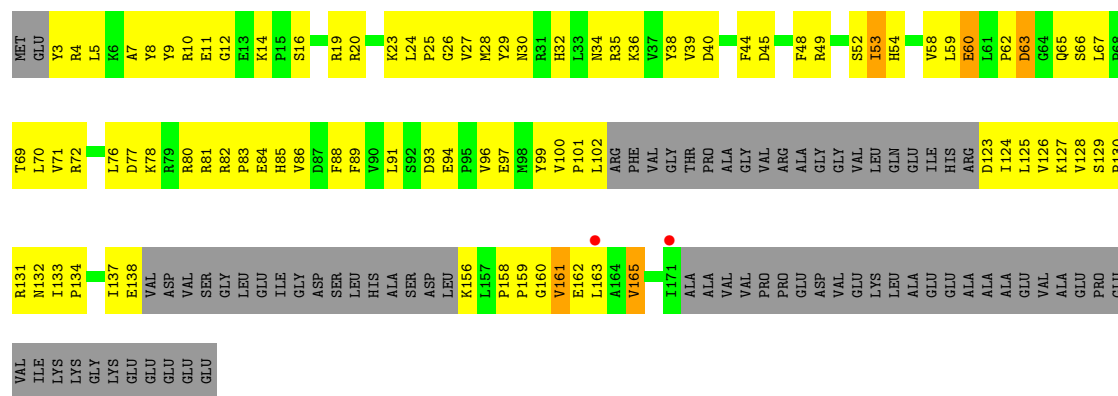


- Molecule 47: 50S ribosomal protein L25

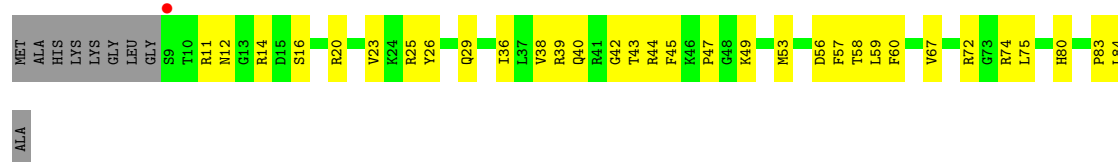


- Molecule 47: 50S ribosomal protein L25

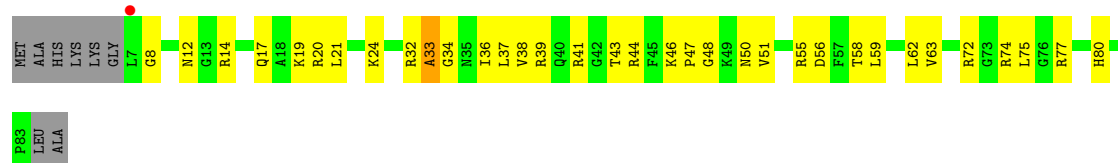




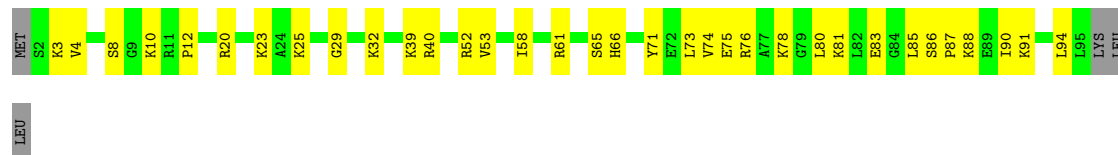
• Molecule 48: 50S ribosomal protein L27



• Molecule 48: 50S ribosomal protein L27

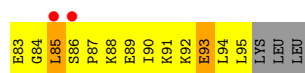


• Molecule 49: 50S ribosomal protein L28



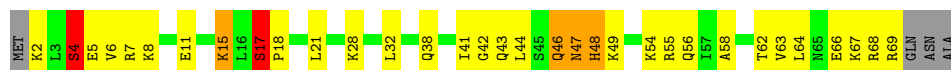
• Molecule 49: 50S ribosomal protein L28





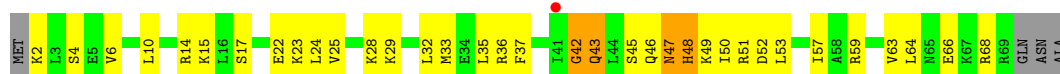
- Molecule 50: 50S ribosomal protein L29

Chain K8: 49% 38% 6% 6%



- Molecule 50: 50S ribosomal protein L29

Chain G5: 46% 43% 6% 6%



- Molecule 51: 50S ribosomal protein L30

Chain L8: 70% 27%



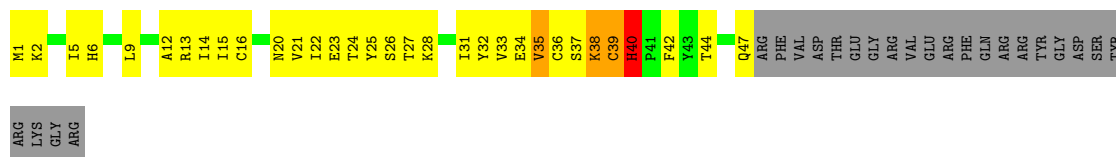
- Molecule 51: 50S ribosomal protein L30

Chain H5: 70% 27%



- Molecule 52: 50S ribosomal protein L31

Chain M8: 21% 39% 34%



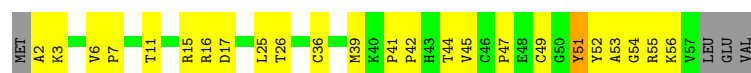
- Molecule 53: 50S ribosomal protein L32

Chain N8: 43% 35% 20%

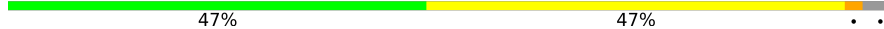


- Molecule 53: 50S ribosomal protein L32

Chain J5:  53% 38% 7%



- Molecule 54: 50S ribosomal protein L34

Chain P8:  47% 47% 6%

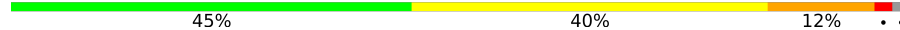


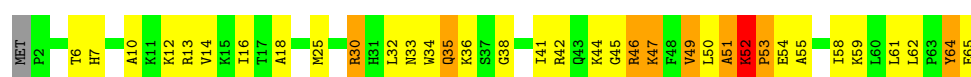
- Molecule 54: 50S ribosomal protein L34

Chain L5:  4% 55% 41%



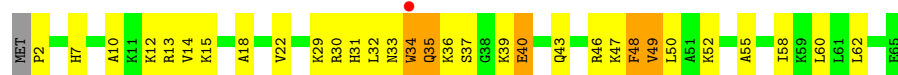
- Molecule 55: 50S ribosomal protein L35

Chain Q8:  45% 40% 12%



- Molecule 55: 50S ribosomal protein L35

Chain M5:  2% 51% 40% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.40Å 446.00Å 617.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.24 – 3.10 151.24 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (151.24-3.10) 93.3 (151.24-3.10)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.249 0.199 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (0.19%)	wwPDB-VP
Wilson B-factor (Å ²)	91.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	294257	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MU, OMC, U8U, SF4, ZN, 4SU, PAR, PSU, T6A, G7M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	13	0.51	0/35994	0.76	9/56171 (0.0%)
1	1G	0.43	0/36258	0.66	4/56589 (0.0%)
2	12	0.50	0/1752	0.83	4/2360 (0.2%)
2	1E	0.43	0/1908	0.75	2/2573 (0.1%)
3	22	0.56	4/1564 (0.3%)	0.67	0/2109
3	2E	0.54	0/1629	0.71	0/2195
4	32	0.48	0/1732	0.75	0/2318
4	3E	0.55	0/1728	0.82	1/2313 (0.0%)
5	42	0.45	0/1150	0.75	0/1548
5	4E	0.53	0/1158	0.78	0/1559
6	52	0.50	0/855	0.73	0/1154
6	5E	0.60	0/850	0.73	0/1147
7	62	0.42	0/1122	0.74	3/1500 (0.2%)
7	6E	0.44	0/1259	0.63	0/1686
8	72	0.36	0/1127	0.67	0/1517
8	7E	0.69	4/1135 (0.4%)	0.77	0/1527
9	82	0.41	0/971	0.73	0/1304
9	8E	0.42	0/1019	0.79	0/1367
10	1A	0.50	0/658	0.71	0/885
10	1I	0.47	0/747	0.82	1/1006 (0.1%)
11	2A	0.42	0/850	0.68	0/1150
11	2I	0.50	0/838	0.78	2/1133 (0.2%)
12	3A	0.52	0/972	0.83	2/1301 (0.2%)
12	3I	0.71	0/972	1.07	3/1301 (0.2%)
13	4A	0.50	0/903	0.83	1/1211 (0.1%)
13	4I	0.54	0/952	0.77	0/1277
14	5A	0.43	0/495	0.90	2/657 (0.3%)
14	5I	0.54	0/500	0.86	2/664 (0.3%)
15	6A	0.45	0/740	0.67	0/987
15	6I	0.52	0/740	0.73	0/987
16	7A	0.47	0/721	0.76	0/970
16	7I	0.51	0/716	0.81	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.42	0/836	0.67	0/1117
17	8I	0.47	0/847	0.77	0/1131
18	9A	0.48	0/549	0.71	0/732
18	9I	0.59	0/554	0.84	0/739
19	AA	0.46	0/490	0.79	0/662
19	AI	0.54	1/672 (0.1%)	0.83	0/904
20	BA	0.44	0/764	0.83	0/1007
20	BI	0.50	1/748 (0.1%)	0.76	1/986 (0.1%)
21	1B	0.37	0/192	0.68	0/252
21	1F	0.46	0/203	0.64	0/266
22	1K	0.49	0/1516	0.67	0/2350
22	1L	0.44	1/1613 (0.1%)	0.57	0/2504
23	2K	0.56	1/1721 (0.1%)	0.74	0/2682
23	2L	0.46	0/1721	0.66	0/2682
24	3K	0.47	0/1777	0.65	0/2767
24	3L	0.44	0/1777	0.60	0/2767
25	4K	0.57	0/494	0.68	0/767
25	4L	0.42	0/445	0.56	0/693
26	14	0.57	0/69023	0.81	22/107740 (0.0%)
26	1H	0.66	0/68351	0.90	33/106700 (0.0%)
27	16	0.54	0/2928	0.83	1/4568 (0.0%)
27	1J	0.47	0/2928	0.72	0/4568
28	71	0.41	0/1055	0.74	0/1425
28	79	0.45	0/459	0.75	0/608
29	11	0.89	3/2170 (0.1%)	1.32	16/2926 (0.5%)
29	19	0.84	5/2175 (0.2%)	1.17	11/2933 (0.4%)
30	21	0.66	0/1591	1.07	8/2146 (0.4%)
30	29	0.68	2/1596 (0.1%)	1.06	7/2153 (0.3%)
31	31	0.71	2/1620 (0.1%)	0.96	0/2194
31	39	0.82	1/1637 (0.1%)	1.06	5/2218 (0.2%)
32	41	0.51	0/1481	0.81	0/1994
32	49	0.41	0/1482	0.72	0/1994
33	51	0.60	0/1337	1.03	6/1809 (0.3%)
33	59	0.69	1/548 (0.2%)	1.21	7/738 (0.9%)
34	61	0.51	0/1151	0.84	1/1558 (0.1%)
34	69	0.50	0/1146	0.85	4/1551 (0.3%)
35	15	0.49	0/1131	0.82	0/1525
35	58	0.59	0/1131	0.89	2/1525 (0.1%)
36	25	0.61	1/942 (0.1%)	0.82	0/1269
36	68	0.62	0/942	0.85	0/1269
37	35	0.75	2/1139 (0.2%)	1.11	5/1514 (0.3%)
37	78	0.80	2/1139 (0.2%)	1.14	5/1514 (0.3%)
38	45	0.65	1/1120 (0.1%)	0.95	3/1498 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	88	0.80	1/1134 (0.1%)	1.14	6/1519 (0.4%)
39	55	0.70	2/981 (0.2%)	0.87	0/1312
39	98	0.56	0/981	0.88	0/1312
40	65	0.52	0/886	0.93	0/1180
40	A8	0.60	0/891	0.90	0/1187
41	75	0.61	0/1123	0.86	1/1500 (0.1%)
41	B8	0.69	0/1115	0.99	0/1490
42	85	0.53	0/977	0.79	0/1301
42	C8	0.64	0/968	0.90	0/1289
43	95	0.64	0/785	1.04	2/1052 (0.2%)
43	D8	0.58	0/785	0.93	2/1052 (0.2%)
44	A5	0.66	0/897	0.89	0/1204
44	E8	0.64	0/901	0.88	0/1209
45	B5	0.65	0/749	1.01	5/1007 (0.5%)
45	F8	0.72	0/757	1.17	4/1017 (0.4%)
46	C5	0.88	4/812 (0.5%)	1.14	5/1083 (0.5%)
46	G8	0.85	0/809	1.30	11/1080 (1.0%)
47	D5	0.52	0/1099	0.88	1/1490 (0.1%)
47	H8	0.49	0/1403	0.84	1/1901 (0.1%)
48	E5	0.59	0/616	0.97	0/821
48	I8	0.75	0/614	1.01	0/819
49	F5	0.61	0/744	0.99	4/989 (0.4%)
49	J8	0.68	0/744	0.95	0/989
50	G5	0.58	0/570	0.89	0/755
50	K8	0.72	0/570	1.08	3/755 (0.4%)
51	H5	0.45	0/464	0.74	0/623
51	L8	0.59	0/464	0.83	0/623
52	M8	0.55	0/375	1.09	1/507 (0.2%)
53	J5	0.59	0/448	0.84	0/606
53	N8	0.84	1/381 (0.3%)	0.97	0/516
54	L5	0.72	0/409	1.03	0/540
54	P8	0.90	0/409	1.08	1/540 (0.2%)
55	M5	0.74	0/524	1.18	3/691 (0.4%)
55	Q8	0.74	0/524	1.33	8/691 (1.2%)
All	All	0.57	40/317065 (0.0%)	0.83	231/475024 (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	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	5
4	32	0	6
4	3E	0	2
5	42	0	1
7	62	0	1
8	72	0	1
9	82	0	1
10	1A	0	2
11	2A	0	1
12	3I	0	2
13	4A	0	5
13	4I	0	2
14	5A	0	1
14	5I	0	1
19	AA	0	2
19	AI	0	2
20	BA	0	3
20	BI	0	2
28	71	0	3
29	11	0	8
29	19	0	4
30	21	0	10
30	29	0	6
31	31	0	2
31	39	0	9
32	49	0	3
33	51	0	6
33	59	0	5
34	61	0	4
34	69	0	4
35	58	0	1
37	35	0	4
37	78	0	7
38	45	0	6
38	88	0	3
39	55	0	1
39	98	0	2
40	65	0	2
40	A8	0	1
41	75	0	1
41	B8	0	2
42	85	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	C8	0	4
43	95	0	3
43	D8	0	3
44	A5	0	1
45	B5	0	1
45	F8	0	3
46	C5	0	4
46	G8	0	7
47	D5	0	1
47	H8	0	4
49	F5	0	1
49	J8	0	1
50	G5	0	3
50	K8	0	3
52	M8	0	4
54	P8	0	1
55	M5	0	1
55	Q8	0	2
All	All	0	191

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	39	66	PRO	N-CD	-23.05	1.15	1.47
29	19	262	ARG	CZ-NH2	-11.90	1.18	1.33
37	35	121	LYS	C-N	11.64	1.61	1.33
8	7E	102	ARG	NE-CZ	-10.12	1.22	1.33
29	11	29	PRO	N-CD	-9.47	1.34	1.47

The worst 5 of 231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	11	28	GLU	CA-C-N	18.89	143.45	119.84
29	11	28	GLU	C-N-CA	18.89	143.45	119.84
29	19	196	VAL	CA-C-N	-16.44	101.47	121.85
29	19	196	VAL	C-N-CA	-16.44	101.47	121.85
45	F8	3	THR	N-CA-C	-11.35	93.69	110.48

There are no chirality outliers.

5 of 191 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	12	GLU	Peptide
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	237	ALA	Peptide
2	1E	9	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16234	903	0
1	1G	32391	0	16353	953	1
2	12	1721	0	1758	127	0
2	1E	1874	0	1926	130	0
3	22	1541	0	1606	94	0
3	2E	1605	0	1668	67	0
4	32	1702	0	1765	147	0
4	3E	1698	0	1760	127	0
5	42	1134	0	1200	81	0
5	4E	1142	0	1204	68	0
6	52	842	0	857	30	0
6	5E	837	0	852	47	0
7	62	1110	0	1163	64	0
7	6E	1242	0	1286	54	0
8	72	1107	0	1165	65	0
8	7E	1115	0	1177	76	0
9	82	953	0	983	92	0
9	8E	1000	0	1031	64	0
10	1A	646	0	662	42	0
10	1I	734	0	761	49	0
11	2A	835	0	847	36	0
11	2I	823	0	833	42	0
12	3A	956	0	1046	70	0
12	3I	956	0	1046	49	0
13	4A	893	0	946	73	0
13	4I	942	0	997	70	0
14	5A	486	0	525	51	0
14	5I	491	0	529	30	0
15	6A	729	0	768	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	6I	729	0	768	40	0
16	7A	705	0	725	46	0
16	7I	700	0	720	53	0
17	8A	823	0	891	39	0
17	8I	834	0	904	55	0
18	9A	544	0	605	23	0
18	9I	549	0	607	31	0
19	AA	481	0	468	46	0
19	AI	658	0	678	52	0
20	BA	762	0	861	45	0
20	BI	746	0	843	63	0
21	1B	188	0	195	14	0
21	1F	199	0	208	16	0
22	1K	1477	0	758	51	0
22	1L	1563	0	799	55	0
23	2K	1646	0	844	30	0
23	2L	1646	0	844	57	0
24	3K	1611	0	817	79	0
24	3L	1611	0	817	55	0
25	4K	439	0	219	11	0
25	4L	395	0	196	12	0
26	14	61630	0	31073	1539	1
26	1H	61028	0	30758	1549	0
27	16	2617	0	1328	67	0
27	1J	2617	0	1328	89	0
28	71	1033	0	1048	77	0
28	79	456	0	460	53	0
29	11	2120	0	2197	146	0
29	19	2125	0	2199	137	0
30	21	1558	0	1623	112	0
30	29	1563	0	1629	138	0
31	31	1585	0	1632	107	0
31	39	1602	0	1649	138	0
32	41	1457	0	1514	109	0
32	49	1458	0	1515	87	0
33	51	1312	0	1384	73	0
33	59	539	0	563	38	0
34	61	1136	0	1223	59	0
34	69	1131	0	1218	62	0
35	15	1104	0	1180	42	0
35	58	1104	0	1180	78	0
36	25	932	0	996	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	68	932	0	996	46	0
37	35	1122	0	1206	101	0
37	78	1122	0	1206	108	0
38	45	1099	0	1154	89	0
38	88	1113	0	1157	63	0
39	55	967	0	1033	67	0
39	98	967	0	1033	54	0
40	65	876	0	938	78	0
40	A8	881	0	943	59	0
41	75	1109	0	1170	64	0
41	B8	1101	0	1158	64	0
42	85	959	0	1019	69	0
42	C8	950	0	1011	67	0
43	95	774	0	849	66	0
43	D8	774	0	849	59	0
44	A5	886	0	948	32	0
44	E8	890	0	951	33	0
45	B5	735	0	785	39	0
45	F8	743	0	794	32	0
46	C5	799	0	888	72	0
46	G8	796	0	886	61	0
47	D5	1074	0	1087	77	0
47	H8	1373	0	1402	80	0
48	E5	608	0	622	33	0
48	I8	606	0	625	30	0
49	F5	737	0	813	51	0
49	J8	737	0	813	29	0
50	G5	568	0	614	43	0
50	K8	568	0	614	41	0
51	H5	459	0	512	11	0
51	L8	459	0	512	14	0
52	M8	366	0	370	49	0
53	J5	434	0	454	24	0
53	N8	369	0	388	24	0
54	L5	401	0	436	22	0
54	P8	401	0	436	21	0
55	M5	516	0	582	35	0
55	Q8	516	0	582	42	0
56	13	131	0	0	0	0
56	14	382	0	0	0	0
56	16	11	0	0	0	0
56	1G	81	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1H	429	0	0	0	0
56	1J	5	0	0	0	0
56	1K	1	0	0	0	0
56	2I	2	0	0	0	0
56	2J	1	0	0	0	0
56	2K	3	0	0	0	0
56	2L	3	0	0	0	0
56	35	1	0	0	0	0
56	39	1	0	0	0	0
56	3E	1	0	0	0	0
56	3I	1	0	0	0	0
56	3K	1	0	0	0	0
56	4I	1	0	0	0	0
56	45	3	0	0	0	0
56	4K	1	0	0	0	0
56	5E	1	0	0	0	0
56	5I	1	0	0	0	0
56	78	1	0	0	0	0
56	85	1	0	0	0	0
56	88	2	0	0	0	0
56	C5	1	0	0	0	0
56	E5	1	0	0	0	0
56	I8	3	0	0	0	0
56	L8	1	0	0	0	0
56	P8	1	0	0	0	0
56	Q8	1	0	0	0	0
57	13	42	0	45	3	0
57	1G	42	0	45	2	0
58	32	8	0	0	3	0
58	3E	8	0	0	3	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	C5	1	0	0	0	0
59	G8	1	0	0	0	0
60	11	10	0	0	3	0
60	13	144	0	0	15	0
60	14	367	0	0	32	0
60	16	22	0	0	1	0
60	19	8	0	0	0	0
60	1G	68	0	0	4	0
60	1H	540	0	0	71	0
60	1I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1J	12	0	0	3	0
60	29	2	0	0	1	0
60	31	7	0	0	0	0
60	32	2	0	0	0	0
60	35	2	0	0	0	0
60	39	3	0	0	1	0
60	3E	2	0	0	1	0
60	3K	1	0	0	0	0
60	4K	3	0	0	1	0
60	55	2	0	0	2	0
60	58	2	0	0	0	0
60	5I	2	0	0	0	0
60	6I	1	0	0	0	0
60	78	4	0	0	1	0
60	7I	1	0	0	0	0
60	98	1	0	0	1	0
60	BI	1	0	0	0	0
60	G8	1	0	0	0	0
60	H5	1	0	0	0	0
60	I8	2	0	0	0	0
60	L5	1	0	0	0	0
60	L8	3	0	0	1	0
60	P8	1	0	0	0	0
All	All	294257	0	196338	9976	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 21.

The worst 5 of 9976 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:943:U:OP2	37:78:36:LYS:NZ	1.64	1.30
31:39:38:ARG:NH2	31:39:99:TYR:CE1	1.96	1.30
44:E8:92:ARG:NH1	44:E8:94:ASP:OD1	1.71	1.22
35:58:49:GLY:O	35:58:119:ARG:NH1	1.77	1.16
29:11:183:ARG:NH1	29:11:269:PHE:HB2	1.61	1.15

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]	2.16	0.04

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%)	171 (83%)	30 (15%)	5 (2%)	4	22
2	1E	227/256 (89%)	188 (83%)	36 (16%)	3 (1%)	9	35
3	22	192/239 (80%)	172 (90%)	20 (10%)	0	100	100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	175 (85%)	29 (14%)	2 (1%)	12	41
4	3E	205/209 (98%)	188 (92%)	15 (7%)	2 (1%)	12	41
5	42	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	18	49
5	4E	147/162 (91%)	139 (95%)	7 (5%)	1 (1%)	18	49
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	134/156 (86%)	122 (91%)	12 (9%)	0	100	100
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	18	49
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	18	49
9	82	119/128 (93%)	111 (93%)	7 (6%)	1 (1%)	16	47
9	8E	124/128 (97%)	106 (86%)	16 (13%)	2 (2%)	7	30
10	1A	76/105 (72%)	70 (92%)	6 (8%)	0	100	100
10	1I	89/105 (85%)	80 (90%)	9 (10%)	0	100	100
11	2A	111/129 (86%)	100 (90%)	9 (8%)	2 (2%)	6	28
11	2I	109/129 (84%)	98 (90%)	9 (8%)	2 (2%)	6	28
12	3A	120/132 (91%)	98 (82%)	19 (16%)	3 (2%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	3I	120/132 (91%)	105 (88%)	14 (12%)	1 (1%)	16	47
13	4A	109/126 (86%)	93 (85%)	15 (14%)	1 (1%)	14	44
13	4I	117/126 (93%)	95 (81%)	22 (19%)	0	100	100
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	6	28
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	16
15	6A	85/89 (96%)	78 (92%)	7 (8%)	0	100	100
15	6I	85/89 (96%)	77 (91%)	7 (8%)	1 (1%)	10	37
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	7I	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	8A	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	8I	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	9A	65/88 (74%)	61 (94%)	4 (6%)	0	100	100
18	9I	66/88 (75%)	62 (94%)	2 (3%)	2 (3%)	3	19
19	AA	56/93 (60%)	47 (84%)	7 (12%)	2 (4%)	2	16
19	AI	80/93 (86%)	67 (84%)	10 (12%)	3 (4%)	2	15
20	BA	97/106 (92%)	86 (89%)	9 (9%)	2 (2%)	5	25
20	BI	95/106 (90%)	84 (88%)	11 (12%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	7I	129/229 (56%)	119 (92%)	10 (8%)	0	100	100
28	79	45/229 (20%)	41 (91%)	4 (9%)	0	100	100
29	11	271/276 (98%)	243 (90%)	19 (7%)	9 (3%)	3	17
29	19	272/276 (99%)	242 (89%)	23 (8%)	7 (3%)	4	21
30	21	201/206 (98%)	158 (79%)	35 (17%)	8 (4%)	2	13
30	29	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	2	13
31	31	200/210 (95%)	183 (92%)	14 (7%)	3 (2%)	8	32
31	39	202/210 (96%)	155 (77%)	40 (20%)	7 (4%)	3	16
32	41	177/182 (97%)	154 (87%)	21 (12%)	2 (1%)	11	39
32	49	177/182 (97%)	152 (86%)	23 (13%)	2 (1%)	11	39
33	51	169/180 (94%)	135 (80%)	25 (15%)	9 (5%)	1	10
33	59	63/180 (35%)	48 (76%)	13 (21%)	2 (3%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	61	144/148 (97%)	120 (83%)	22 (15%)	2 (1%)	9	34
34	69	143/148 (97%)	114 (80%)	28 (20%)	1 (1%)	18	49
35	15	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	18	49
35	58	136/140 (97%)	114 (84%)	18 (13%)	4 (3%)	3	19
36	25	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
36	68	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
37	35	145/150 (97%)	115 (79%)	25 (17%)	5 (3%)	3	16
37	78	145/150 (97%)	117 (81%)	24 (17%)	4 (3%)	4	20
38	45	136/141 (96%)	115 (85%)	18 (13%)	3 (2%)	5	24
38	88	139/141 (99%)	118 (85%)	17 (12%)	4 (3%)	3	19
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14	44
39	98	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	14	44
40	65	108/112 (96%)	84 (78%)	23 (21%)	1 (1%)	14	44
40	A8	109/112 (97%)	87 (80%)	22 (20%)	0	100	100
41	75	131/146 (90%)	121 (92%)	10 (8%)	0	100	100
41	B8	130/146 (89%)	115 (88%)	14 (11%)	1 (1%)	16	47
42	85	114/118 (97%)	105 (92%)	7 (6%)	2 (2%)	6	28
42	C8	113/118 (96%)	103 (91%)	7 (6%)	3 (3%)	4	20
43	95	98/101 (97%)	73 (74%)	20 (20%)	5 (5%)	1	10
43	D8	98/101 (97%)	86 (88%)	8 (8%)	4 (4%)	2	13
44	A5	109/113 (96%)	103 (94%)	4 (4%)	2 (2%)	6	28
44	E8	110/113 (97%)	103 (94%)	7 (6%)	0	100	100
45	B5	92/96 (96%)	81 (88%)	9 (10%)	2 (2%)	5	24
45	F8	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
46	C5	103/110 (94%)	72 (70%)	24 (23%)	7 (7%)	1	5
46	G8	103/110 (94%)	87 (84%)	13 (13%)	3 (3%)	3	19
47	D5	128/206 (62%)	104 (81%)	20 (16%)	4 (3%)	3	18
47	H8	169/206 (82%)	136 (80%)	26 (15%)	7 (4%)	2	13
48	E5	75/85 (88%)	67 (89%)	5 (7%)	3 (4%)	2	13
48	I8	74/85 (87%)	69 (93%)	5 (7%)	0	100	100
49	F5	92/98 (94%)	85 (92%)	5 (5%)	2 (2%)	5	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	J8	92/98 (94%)	84 (91%)	7 (8%)	1 (1%)	11	39
50	G5	66/72 (92%)	62 (94%)	2 (3%)	2 (3%)	3	19
50	K8	66/72 (92%)	59 (89%)	4 (6%)	3 (4%)	2	12
51	H5	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	M8	45/71 (63%)	31 (69%)	13 (29%)	1 (2%)	5	24
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	4 (9%)	0	100	100
55	M5	62/65 (95%)	50 (81%)	9 (14%)	3 (5%)	2	11
55	Q8	62/65 (95%)	51 (82%)	8 (13%)	3 (5%)	2	11
All	All	10971/12333 (89%)	9586 (87%)	1202 (11%)	183 (2%)	7	30

5 of 183 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	8E	127	LYS
18	9I	22	VAL
29	11	28	GLU
29	11	40	THR
30	21	83	ASP

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%)	196 (98%)	4 (2%)	48	72
3	22	154/188 (82%)	154 (100%)	0	100	100
3	2E	159/188 (85%)	158 (99%)	1 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	32	180/181 (99%)	179 (99%)	1 (1%)	78	83
4	3E	180/181 (99%)	178 (99%)	2 (1%)	65	78
5	42	114/123 (93%)	114 (100%)	0	100	100
5	4E	115/123 (94%)	113 (98%)	2 (2%)	53	74
6	52	90/90 (100%)	89 (99%)	1 (1%)	65	78
6	5E	90/90 (100%)	90 (100%)	0	100	100
7	62	114/127 (90%)	114 (100%)	0	100	100
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
9	8E	97/99 (98%)	96 (99%)	1 (1%)	68	79
10	1A	71/92 (77%)	71 (100%)	0	100	100
10	1I	81/92 (88%)	81 (100%)	0	100	100
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%)	102 (99%)	1 (1%)	68	79
12	3I	103/109 (94%)	102 (99%)	1 (1%)	68	79
13	4A	91/101 (90%)	90 (99%)	1 (1%)	65	78
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%)	79 (100%)	0	100	100
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%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AI	71/80 (89%)	71 (100%)	0	100	100
20	BA	76/82 (93%)	76 (100%)	0	100	100
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	71	109/181 (60%)	109 (100%)	0	100	100
28	79	48/181 (26%)	48 (100%)	0	100	100
29	11	214/218 (98%)	214 (100%)	0	100	100
29	19	214/218 (98%)	212 (99%)	2 (1%)	70	80
30	21	165/166 (99%)	165 (100%)	0	100	100
30	29	165/166 (99%)	164 (99%)	1 (1%)	78	83
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%)	152 (99%)	1 (1%)	76	82
32	49	153/156 (98%)	153 (100%)	0	100	100
33	51	142/148 (96%)	141 (99%)	1 (1%)	76	82
33	59	56/148 (38%)	56 (100%)	0	100	100
34	61	122/124 (98%)	122 (100%)	0	100	100
34	69	122/124 (98%)	121 (99%)	1 (1%)	73	81
35	15	117/119 (98%)	117 (100%)	0	100	100
35	58	117/119 (98%)	116 (99%)	1 (1%)	70	80
36	25	100/100 (100%)	99 (99%)	1 (1%)	68	79
36	68	100/100 (100%)	99 (99%)	1 (1%)	68	79
37	35	114/116 (98%)	114 (100%)	0	100	100
37	78	114/116 (98%)	112 (98%)	2 (2%)	51	73
38	45	109/111 (98%)	109 (100%)	0	100	100
38	88	109/111 (98%)	109 (100%)	0	100	100
39	55	101/101 (100%)	99 (98%)	2 (2%)	48	72
39	98	101/101 (100%)	100 (99%)	1 (1%)	68	79
40	65	87/88 (99%)	87 (100%)	0	100	100
40	A8	87/88 (99%)	86 (99%)	1 (1%)	65	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	75	117/127 (92%)	117 (100%)	0	100	100
41	B8	116/127 (91%)	114 (98%)	2 (2%)	53	74
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%)	81 (99%)	1 (1%)	63	78
43	D8	82/82 (100%)	82 (100%)	0	100	100
44	A5	91/92 (99%)	89 (98%)	2 (2%)	45	71
44	E8	91/92 (99%)	90 (99%)	1 (1%)	65	78
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
46	G8	85/91 (93%)	85 (100%)	0	100	100
47	D5	118/179 (66%)	117 (99%)	1 (1%)	73	81
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%)	79 (100%)	0	100	100
50	G5	62/67 (92%)	62 (100%)	0	100	100
50	K8	62/67 (92%)	61 (98%)	1 (2%)	55	75
51	H5	50/52 (96%)	50 (100%)	0	100	100
51	L8	50/52 (96%)	50 (100%)	0	100	100
52	M8	42/63 (67%)	42 (100%)	0	100	100
53	J5	48/52 (92%)	46 (96%)	2 (4%)	26	58
53	N8	43/52 (83%)	42 (98%)	1 (2%)	44	70
54	L5	38/42 (90%)	37 (97%)	1 (3%)	40	68
54	P8	38/42 (90%)	37 (97%)	1 (3%)	40	68
55	M5	54/55 (98%)	54 (100%)	0	100	100
55	Q8	54/55 (98%)	54 (100%)	0	100	100
All	All	9272/10193 (91%)	9229 (100%)	43 (0%)	81	85

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	4A	115	LYS
39	55	88	ARG
29	19	31	LYS
34	69	108	THR
44	A5	39	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
15	6A	53	HIS
36	25	5	GLN
18	9A	36	ASN
31	39	8	GLN
45	B5	87	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	349 (23%)	32 (2%)
1	1G	1505/1522 (98%)	385 (25%)	30 (1%)
22	1K	66/76 (86%)	31 (46%)	3 (4%)
22	1L	71/76 (93%)	32 (45%)	5 (7%)
23	2K	76/77 (98%)	23 (30%)	1 (1%)
23	2L	76/77 (98%)	19 (25%)	2 (2%)
24	3K	75/76 (98%)	45 (60%)	3 (4%)
24	3L	75/76 (98%)	33 (44%)	0
25	4K	18/27 (66%)	11 (61%)	1 (5%)
25	4L	17/27 (62%)	10 (58%)	0
26	14	2852/2912 (97%)	738 (25%)	51 (1%)
26	1H	2828/2912 (97%)	735 (25%)	51 (1%)
27	16	121/122 (99%)	17 (14%)	2 (1%)
27	1J	121/122 (99%)	33 (27%)	2 (1%)
All	All	9394/9624 (97%)	2461 (26%)	183 (1%)

5 of 2461 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	7	G

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Mol	Chain	Res	Type
1	13	8	A

5 of 183 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	1139	G
26	14	791	C
1	1G	1300	G
26	14	34	C
26	14	1396	U

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

22 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	T6A	1K	37	22	31,34,35	2.16	9 (29%)	43,49,52	2.05	11 (25%)
22	5MU	1K	54	22	19,22,23	3.76	5 (26%)	27,32,35	2.99	6 (22%)
22	T6A	1L	37	22	31,34,35	2.03	5 (16%)	43,49,52	2.29	15 (34%)
24	PSU	3K	39	24	18,21,22	1.32	3 (16%)	21,30,33	1.96	7 (33%)
23	PSU	2L	56	23	18,21,22	1.26	1 (5%)	21,30,33	1.98	4 (19%)
23	5MU	2L	55	23	19,22,23	3.92	5 (26%)	27,32,35	3.47	10 (37%)
24	PSU	3L	39	24	18,21,22	1.20	1 (5%)	21,30,33	1.54	2 (9%)
23	G7M	2K	47	23	23,26,27	2.56	9 (39%)	34,39,42	1.63	10 (29%)
22	PSU	1L	55	22	18,21,22	1.17	1 (5%)	21,30,33	1.69	4 (19%)
22	PSU	1L	39	22	18,21,22	1.15	1 (5%)	21,30,33	1.72	3 (14%)
23	G7M	2L	47	23	23,26,27	2.69	8 (34%)	34,39,42	1.79	7 (20%)
23	4SU	2L	8	23	18,21,22	1.87	3 (16%)	25,30,33	2.68	4 (16%)
23	OMC	2L	33	23	19,22,23	1.82	4 (21%)	25,31,34	1.29	2 (8%)
22	U8U	1K	34	22	20,24,25	2.41	6 (30%)	22,34,37	0.94	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	2K	56	23	18,21,22	1.27	2 (11%)	21,30,33	1.86	4 (19%)
23	5MU	2K	55	23	19,22,23	3.75	5 (26%)	27,32,35	3.43	7 (25%)
22	U8U	1L	34	22,25	20,24,25	2.41	6 (30%)	22,34,37	0.80	2 (9%)
22	5MU	1L	54	22	19,22,23	4.03	5 (26%)	27,32,35	3.38	9 (33%)
23	OMC	2K	33	23	19,22,23	1.72	3 (15%)	25,31,34	1.16	2 (8%)
23	4SU	2K	8	23	18,21,22	1.98	5 (27%)	25,30,33	2.83	8 (32%)
22	PSU	1K	55	22	18,21,22	1.21	1 (5%)	21,30,33	1.60	4 (19%)
22	PSU	1K	39	22	18,21,22	0.96	1 (5%)	21,30,33	1.64	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	T6A	1K	37	22	-	5/23/41/42	0/3/3/3
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
22	T6A	1L	37	22	-	5/23/41/42	0/3/3/3
24	PSU	3K	39	24	-	2/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	1/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	3/7/25/26	0/2/2/2
24	PSU	3L	39	24	-	0/7/25/26	0/2/2/2
23	G7M	2K	47	23	-	1/7/25/26	0/3/3/3
22	PSU	1L	55	22	-	2/7/25/26	0/2/2/2
22	PSU	1L	39	22	-	1/7/25/26	0/2/2/2
23	G7M	2L	47	23	-	3/7/25/26	0/3/3/3
23	4SU	2L	8	23	-	1/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	3/9/27/28	0/2/2/2
22	U8U	1K	34	22	-	0/10/28/29	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
22	U8U	1L	34	22,25	-	5/10/28/29	0/2/2/2
22	5MU	1L	54	22	-	3/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
23	4SU	2K	8	23	-	2/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	1/7/25/26	0/2/2/2

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	54	5MU	C2-N1	13.27	1.59	1.38
23	2L	55	5MU	C2-N1	12.75	1.58	1.38
22	1K	54	5MU	C2-N1	11.98	1.57	1.38
23	2K	55	5MU	C2-N1	11.80	1.56	1.38
23	2K	47	G7M	C4-N3	6.57	1.49	1.34

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2K	55	5MU	C5-C4-N3	11.11	124.98	115.32
23	2L	55	5MU	C5-C4-N3	10.45	124.40	115.32
22	1K	54	5MU	C5-C4-N3	10.24	124.22	115.32
22	1L	54	5MU	C5-C4-N3	10.12	124.12	115.32
23	2L	8	4SU	C4-N3-C2	-8.63	119.04	127.31

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1L	34	U8U	N-C-C5-C4
22	1L	34	U8U	C5-C-N-CA
22	1L	37	T6A	C5-C6-N6-C10
22	1L	37	T6A	N1-C6-N6-C10
22	1L	54	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	37	T6A	2	0
23	2L	55	5MU	3	0
22	1L	55	PSU	2	0
22	1L	39	PSU	2	0
23	2L	47	G7M	1	0
23	2L	8	4SU	4	0
23	2L	33	OMC	3	0
22	1K	34	U8U	1	0
23	2K	55	5MU	3	0
22	1L	34	U8U	1	0
22	1L	54	5MU	2	0
22	1K	39	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1081 ligands modelled in this entry, 1077 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
57	PAR	13	1730	-	44,45,45	0.87	1 (2%)	63,67,67	2.16	21 (33%)
58	SF4	3E	302	4	0,12,12	-	-	-		
58	SF4	32	301	4	0,12,12	-	-	-		
57	PAR	1G	1681	-	44,45,45	0.78	1 (2%)	63,67,67	1.74	11 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PAR	13	1730	-	-	5/18/94/94	0/4/4/4
58	SF4	3E	302	4	-	-	0/6/5/5
58	SF4	32	301	4	-	-	0/6/5/5
57	PAR	1G	1681	-	-	4/18/94/94	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1G	1681	PAR	C31-C21	-2.75	1.50	1.53
57	13	1730	PAR	O54-C14	2.12	1.47	1.41

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1G	1681	PAR	O52-C13-O43	-6.44	104.79	111.37
57	13	1730	PAR	O52-C13-O43	-5.89	105.35	111.37
57	13	1730	PAR	C32-C22-C12	-5.75	101.16	111.02
57	1G	1681	PAR	C13-O52-C52	-4.70	106.84	117.98
57	1G	1681	PAR	C14-O54-C54	4.68	122.86	113.72

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

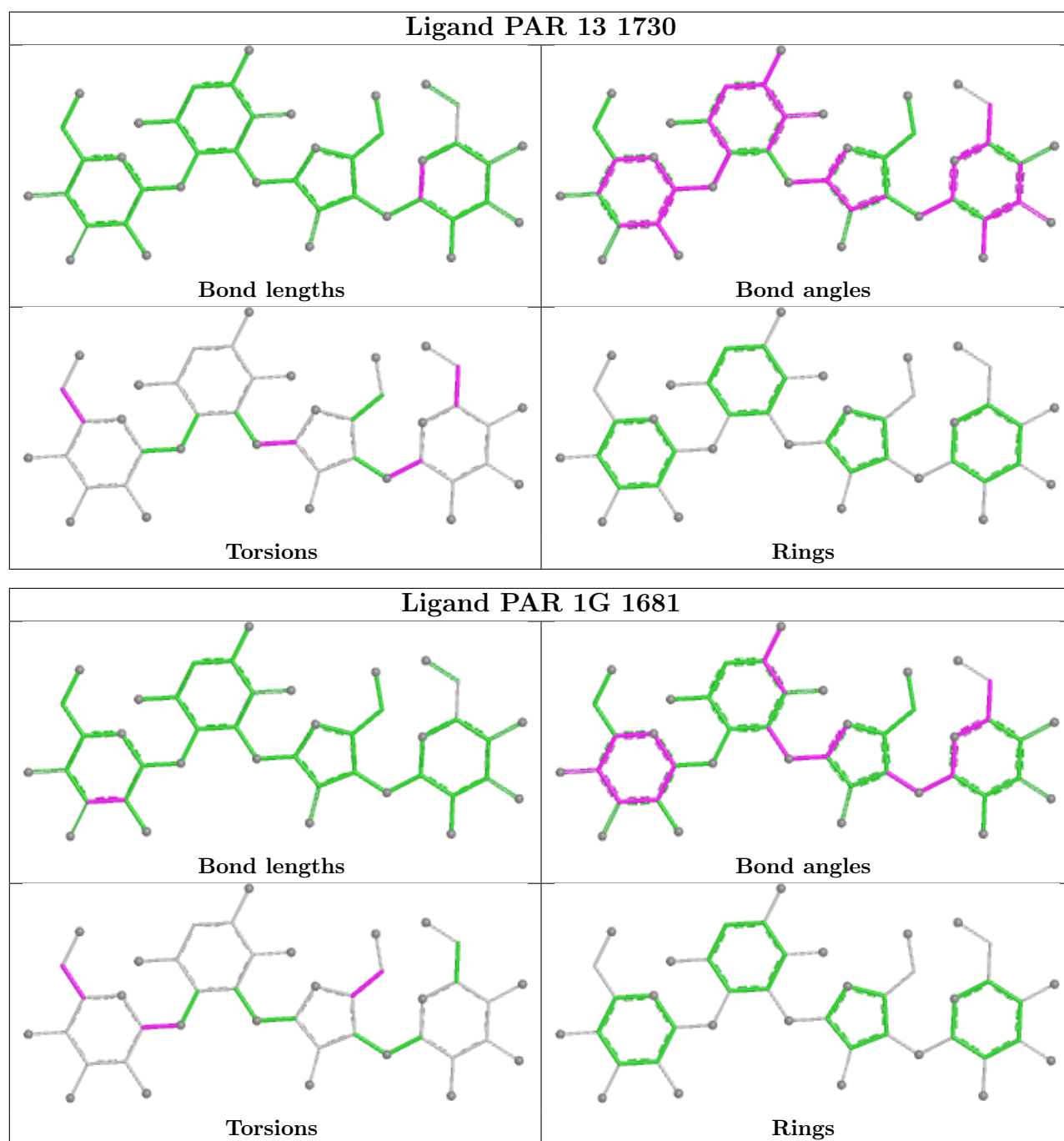
Mol	Chain	Res	Type	Atoms
57	13	1730	PAR	O54-C54-C64-N64
57	1G	1681	PAR	O51-C51-C61-O61
57	1G	1681	PAR	C41-C51-C61-O61
57	13	1730	PAR	C41-C51-C61-O61
57	1G	1681	PAR	O51-C11-O11-C42

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	13	1730	PAR	3	0
58	3E	302	SF4	3	0
58	32	301	SF4	3	0
57	1G	1681	PAR	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
25	4K	1
37	35	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4K	24:A	O3'	25:A	P	4.27
1	35	121:LYS	C	122:PRO	N	1.61

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%)	-0.74	2 (0%) 92 86	64, 104, 160, 189	0
1	1G	1507/1522 (99%)	-0.71	4 (0%) 90 80	78, 123, 164, 193	0
2	12	210/256 (82%)	0.10	2 (0%) 79 61	121, 148, 157, 163	0
2	1E	231/256 (90%)	0.01	3 (1%) 75 56	112, 136, 153, 161	0
3	22	196/239 (82%)	0.12	4 (2%) 65 44	128, 141, 155, 161	0
3	2E	205/239 (85%)	-0.38	0 100 100	90, 109, 133, 144	0
4	32	208/209 (99%)	0.28	6 (2%) 53 32	101, 123, 139, 150	0
4	3E	207/209 (99%)	-0.09	1 (0%) 87 73	88, 106, 126, 133	0
5	42	148/162 (91%)	0.22	2 (1%) 73 53	110, 128, 140, 145	0
5	4E	149/162 (91%)	0.07	3 (2%) 65 44	80, 101, 118, 130	0
6	52	101/101 (100%)	-0.07	1 (0%) 79 61	96, 111, 126, 136	0
6	5E	100/101 (99%)	0.01	4 (4%) 42 23	84, 102, 119, 129	0
7	62	138/156 (88%)	-0.03	4 (2%) 53 32	120, 131, 141, 145	0
7	6E	154/156 (98%)	-0.16	1 (0%) 85 70	105, 124, 144, 159	0
8	72	137/138 (99%)	-0.31	0 100 100	111, 131, 141, 147	0
8	7E	138/138 (100%)	0.21	2 (1%) 73 53	92, 110, 121, 130	0
9	82	121/128 (94%)	-0.04	2 (1%) 69 48	115, 146, 155, 160	0
9	8E	126/128 (98%)	-0.22	0 100 100	93, 132, 149, 152	0
10	1A	80/105 (76%)	0.16	3 (3%) 44 25	125, 141, 153, 156	0
10	1I	91/105 (86%)	-0.23	1 (1%) 78 59	84, 125, 153, 158	0
11	2A	113/129 (87%)	0.18	2 (1%) 67 47	90, 119, 128, 133	0
11	2I	111/129 (86%)	0.24	1 (0%) 81 63	82, 112, 129, 144	0
12	3A	122/132 (92%)	0.55	13 (10%) 11 6	88, 112, 132, 146	0
12	3I	122/132 (92%)	-0.15	4 (3%) 49 29	73, 82, 106, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	0.03	1 (0%) 81 63	124, 141, 150, 165	0
13	4I	119/126 (94%)	-0.25	2 (1%) 69 48	94, 120, 135, 146	0
14	5A	59/61 (96%)	0.21	3 (5%) 33 18	130, 140, 148, 150	0
14	5I	60/61 (98%)	-0.53	0 100 100	88, 100, 112, 125	0
15	6A	87/89 (97%)	-0.59	0 100 100	93, 117, 132, 135	0
15	6I	87/89 (97%)	-0.24	0 100 100	84, 103, 120, 126	0
16	7A	84/88 (95%)	-0.08	0 100 100	93, 111, 130, 141	0
16	7I	83/88 (94%)	0.07	1 (1%) 76 58	102, 112, 135, 147	0
17	8A	99/105 (94%)	-0.38	1 (1%) 79 61	108, 120, 133, 138	0
17	8I	100/105 (95%)	-0.07	1 (1%) 79 61	89, 111, 126, 131	0
18	9A	67/88 (76%)	-0.12	3 (4%) 38 20	106, 117, 135, 139	0
18	9I	68/88 (77%)	0.18	2 (2%) 53 32	89, 105, 124, 127	0
19	AA	62/93 (66%)	0.38	4 (6%) 25 13	123, 149, 157, 163	0
19	AI	82/93 (88%)	-0.17	1 (1%) 76 58	99, 118, 134, 142	0
20	BA	99/106 (93%)	-0.45	0 100 100	94, 116, 141, 150	0
20	BI	97/106 (91%)	-0.09	2 (2%) 63 42	114, 126, 144, 148	0
21	1B	22/27 (81%)	-0.07	0 100 100	124, 136, 143, 147	0
21	1F	23/27 (85%)	-0.74	0 100 100	99, 109, 116, 120	0
22	1K	64/76 (84%)	0.77	10 (15%) 5 2	93, 158, 171, 173	0
22	1L	68/76 (89%)	0.17	4 (5%) 28 15	125, 171, 178, 184	0
23	2K	72/77 (93%)	-0.29	0 100 100	77, 104, 130, 146	0
23	2L	72/77 (93%)	-0.35	0 100 100	84, 122, 150, 165	0
24	3K	75/76 (98%)	0.46	6 (8%) 18 10	81, 170, 184, 189	0
24	3L	75/76 (98%)	0.06	2 (2%) 56 35	89, 167, 182, 188	0
25	4K	20/27 (74%)	0.78	4 (20%) 3 1	76, 144, 177, 178	0
25	4L	18/27 (66%)	0.12	0 100 100	103, 157, 182, 183	0
26	14	2861/2912 (98%)	-0.80	9 (0%) 90 80	58, 92, 173, 197	0
26	1H	2833/2912 (97%)	-0.84	10 (0%) 88 76	50, 80, 164, 199	0
27	16	122/122 (100%)	-0.98	0 100 100	75, 98, 119, 170	0
27	1J	122/122 (100%)	-0.76	1 (0%) 82 65	93, 123, 141, 174	0
28	7I	133/229 (58%)	0.12	1 (0%) 82 65	137, 169, 179, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	79	57/229 (24%)	0.17	1 (1%) 67 47	139, 160, 169, 174	0
29	11	273/276 (98%)	0.09	4 (1%) 72 52	48, 74, 92, 101	0
29	19	274/276 (99%)	0.14	9 (3%) 49 29	60, 82, 99, 116	0
30	21	203/206 (98%)	-0.07	1 (0%) 87 73	58, 95, 135, 146	0
30	29	204/206 (99%)	-0.27	2 (0%) 79 61	67, 99, 134, 144	0
31	31	202/210 (96%)	-0.26	4 (1%) 65 44	54, 85, 119, 138	0
31	39	204/210 (97%)	-0.14	2 (0%) 79 61	64, 112, 147, 163	0
32	41	179/182 (98%)	-0.39	2 (1%) 78 59	87, 107, 136, 148	0
32	49	179/182 (98%)	0.09	3 (1%) 69 48	121, 137, 156, 168	0
33	51	171/180 (95%)	-0.01	6 (3%) 47 27	89, 110, 125, 137	0
33	59	69/180 (38%)	0.55	4 (5%) 29 16	131, 151, 162, 166	0
34	61	146/148 (98%)	-0.12	1 (0%) 84 68	85, 129, 142, 149	0
34	69	145/148 (97%)	0.08	9 (6%) 26 14	91, 126, 142, 151	0
35	15	138/140 (98%)	0.20	3 (2%) 62 41	87, 114, 138, 154	0
35	58	138/140 (98%)	0.10	4 (2%) 53 32	69, 97, 124, 140	0
36	25	122/122 (100%)	0.20	0 100 100	76, 96, 112, 118	0
36	68	122/122 (100%)	0.09	4 (3%) 49 29	63, 84, 101, 110	0
37	35	147/150 (98%)	0.19	6 (4%) 41 23	65, 110, 135, 148	0
37	78	147/150 (98%)	-0.11	2 (1%) 73 53	50, 89, 113, 128	0
38	45	138/141 (97%)	0.37	13 (9%) 14 8	84, 111, 129, 137	0
38	88	141/141 (100%)	-0.17	3 (2%) 63 42	58, 84, 107, 125	0
39	55	118/118 (100%)	-0.46	0 100 100	70, 86, 108, 121	0
39	98	118/118 (100%)	-0.17	0 100 100	71, 92, 112, 126	0
40	65	110/112 (98%)	-0.32	1 (0%) 81 63	91, 116, 132, 137	0
40	A8	111/112 (99%)	-0.38	0 100 100	76, 94, 117, 123	0
41	75	133/146 (91%)	0.06	7 (5%) 32 17	86, 102, 130, 142	0
41	B8	132/146 (90%)	0.01	3 (2%) 61 39	78, 99, 128, 138	0
42	85	116/118 (98%)	0.07	1 (0%) 81 63	76, 101, 130, 139	0
42	C8	115/118 (97%)	0.12	2 (1%) 69 48	65, 83, 114, 118	0
43	95	100/101 (99%)	0.36	5 (5%) 34 18	76, 123, 139, 141	0
43	D8	100/101 (99%)	0.42	5 (5%) 34 18	64, 105, 128, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	A5	111/113 (98%)	-0.06	0 100 100	68, 84, 114, 141	0
44	E8	112/113 (99%)	0.08	2 (1%) 67 47	64, 82, 112, 142	0
45	B5	94/96 (97%)	-0.14	3 (3%) 50 30	75, 91, 115, 123	0
45	F8	95/96 (98%)	-0.24	1 (1%) 78 59	62, 79, 111, 125	0
46	C5	105/110 (95%)	0.71	15 (14%) 6 3	91, 124, 146, 152	0
46	G8	105/110 (95%)	0.26	7 (6%) 24 13	79, 101, 127, 132	0
47	D5	132/206 (64%)	-0.09	2 (1%) 72 52	115, 136, 152, 155	0
47	H8	171/206 (83%)	-0.07	1 (0%) 85 70	90, 124, 164, 168	0
48	E5	77/85 (90%)	-0.08	1 (1%) 75 56	75, 96, 113, 135	0
48	I8	76/85 (89%)	-0.27	1 (1%) 75 56	65, 78, 91, 107	0
49	F5	94/98 (95%)	0.48	6 (6%) 25 14	70, 90, 123, 133	0
49	J8	94/98 (95%)	-0.05	0 100 100	61, 81, 120, 128	0
50	G5	68/72 (94%)	-0.13	1 (1%) 72 52	88, 109, 129, 150	0
50	K8	68/72 (94%)	-0.08	0 100 100	66, 84, 104, 128	0
51	H5	58/60 (96%)	-0.18	0 100 100	85, 106, 134, 140	0
51	L8	58/60 (96%)	-0.22	0 100 100	65, 87, 115, 132	0
52	M8	47/71 (66%)	-0.14	0 100 100	111, 137, 156, 163	0
53	J5	56/60 (93%)	-0.16	0 100 100	67, 92, 137, 147	0
53	N8	48/60 (80%)	-0.30	0 100 100	61, 87, 134, 141	0
54	L5	47/49 (95%)	-0.33	2 (4%) 40 22	57, 68, 85, 103	0
54	P8	47/49 (95%)	-0.64	0 100 100	53, 60, 79, 88	0
55	M5	64/65 (98%)	0.06	1 (1%) 70 49	75, 86, 103, 126	0
55	Q8	64/65 (98%)	-0.12	0 100 100	64, 74, 92, 108	0
All	All	20598/21957 (93%)	-0.35	283 (1%) 73 53	48, 105, 159, 199	0

The worst 5 of 283 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	75	104	ASN	6.6
43	D8	37	VAL	6.0
41	75	106	SER	6.0
22	1K	76	A	5.9
38	45	90	VAL	5.6

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
22	PSU	1K	55	20/21	0.84	0.09	102,113,120,131	0
23	OMC	2L	33	21/22	0.84	0.10	105,114,118,121	0
23	G7M	2L	47	24/25	0.86	0.10	126,133,141,145	0
23	5MU	2L	55	21/22	0.86	0.08	119,131,141,145	0
23	PSU	2K	56	20/21	0.86	0.08	99,110,121,122	0
23	PSU	2L	56	20/21	0.86	0.07	115,126,131,135	0
23	4SU	2L	8	20/21	0.88	0.08	114,124,129,130	0
24	PSU	3K	39	20/21	0.88	0.09	141,151,156,159	0
24	PSU	3L	39	20/21	0.88	0.08	145,155,159,162	0
22	PSU	1L	55	20/21	0.89	0.06	129,139,149,150	0
22	U8U	1L	34	23/24	0.89	0.09	123,133,138,150	0
22	PSU	1L	39	20/21	0.90	0.08	135,144,149,150	0
22	5MU	1K	54	21/22	0.90	0.08	110,117,132,137	0
23	5MU	2K	55	21/22	0.90	0.09	106,117,125,127	0
22	5MU	1L	54	21/22	0.91	0.07	133,141,146,152	0
22	T6A	1L	37	32/33	0.92	0.10	132,140,153,154	0
23	G7M	2K	47	24/25	0.93	0.08	102,114,127,133	0
22	PSU	1K	39	20/21	0.93	0.10	98,115,125,127	0
22	U8U	1K	34	23/24	0.94	0.08	84,92,100,108	0
22	T6A	1K	37	32/33	0.95	0.11	79,94,121,123	0
23	OMC	2K	33	21/22	0.96	0.11	77,83,91,93	0
23	4SU	2K	8	20/21	0.96	0.07	91,98,107,109	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1K	101	1/1	0.19	0.40	138,138,138,138	0
56	MG	2K	102	1/1	0.20	0.35	126,126,126,126	0
56	MG	1G	1656	1/1	0.51	0.23	138,138,138,138	0
56	MG	1J	203	1/1	0.52	0.26	113,113,113,113	0
56	MG	14	3250	1/1	0.55	0.30	99,99,99,99	0
56	MG	14	3055	1/1	0.55	0.33	112,112,112,112	0
56	MG	1G	1616	1/1	0.56	0.36	96,96,96,96	0
56	MG	14	3302	1/1	0.57	0.36	110,110,110,110	0
56	MG	1G	1640	1/1	0.57	0.28	108,108,108,108	0
56	MG	14	3130	1/1	0.58	0.34	78,78,78,78	0
56	MG	16	204	1/1	0.58	0.25	98,98,98,98	0
56	MG	14	3288	1/1	0.58	0.27	109,109,109,109	0
56	MG	1G	1602	1/1	0.58	0.36	105,105,105,105	0
56	MG	1H	3284	1/1	0.58	0.28	88,88,88,88	0
56	MG	14	3220	1/1	0.59	0.28	107,107,107,107	0
56	MG	13	1681	1/1	0.59	0.28	106,106,106,106	0
56	MG	14	3287	1/1	0.59	0.41	105,105,105,105	0
56	MG	14	3229	1/1	0.60	0.28	86,86,86,86	0
56	MG	14	3181	1/1	0.60	0.36	98,98,98,98	0
56	MG	1H	3045	1/1	0.60	0.29	116,116,116,116	0
56	MG	1H	3277	1/1	0.61	0.27	100,100,100,100	0
56	MG	1J	202	1/1	0.61	0.25	104,104,104,104	0
56	MG	14	3266	1/1	0.61	0.30	90,90,90,90	0
56	MG	13	1700	1/1	0.62	0.26	111,111,111,111	0
56	MG	14	3142	1/1	0.62	0.18	111,111,111,111	0
56	MG	1H	3280	1/1	0.62	0.23	88,88,88,88	0
56	MG	1G	1664	1/1	0.62	0.27	119,119,119,119	0
56	MG	2L	102	1/1	0.62	0.28	98,98,98,98	0
56	MG	13	1608	1/1	0.62	0.28	91,91,91,91	0
56	MG	1H	3295	1/1	0.63	0.23	85,85,85,85	0
56	MG	14	3039	1/1	0.63	0.43	103,103,103,103	0
56	MG	13	1628	1/1	0.63	0.33	95,95,95,95	0
56	MG	1G	1630	1/1	0.63	0.35	108,108,108,108	0
56	MG	1G	1665	1/1	0.63	0.24	93,93,93,93	0
56	MG	13	1691	1/1	0.64	0.20	109,109,109,109	0
56	MG	14	3301	1/1	0.64	0.27	99,99,99,99	0
56	MG	14	3260	1/1	0.64	0.31	90,90,90,90	0
56	MG	1G	1629	1/1	0.64	0.29	104,104,104,104	0
56	MG	14	3172	1/1	0.64	0.24	98,98,98,98	0
56	MG	14	3280	1/1	0.65	0.37	99,99,99,99	0
56	MG	14	3110	1/1	0.65	0.30	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	13	1702	1/1	0.65	0.45	103,103,103,103	0
56	MG	13	1692	1/1	0.65	0.28	100,100,100,100	0
56	MG	14	3255	1/1	0.65	0.33	87,87,87,87	0
56	MG	14	3303	1/1	0.65	0.35	98,98,98,98	0
56	MG	1H	3318	1/1	0.65	0.24	96,96,96,96	0
56	MG	1H	3326	1/1	0.65	0.20	91,91,91,91	0
56	MG	14	3274	1/1	0.66	0.25	99,99,99,99	0
56	MG	13	1646	1/1	0.66	0.37	95,95,95,95	0
56	MG	1H	3015	1/1	0.66	0.38	77,77,77,77	0
56	MG	1H	3319	1/1	0.66	0.26	102,102,102,102	0
56	MG	14	3299	1/1	0.66	0.23	96,96,96,96	0
56	MG	13	1679	1/1	0.67	0.22	107,107,107,107	0
56	MG	13	1671	1/1	0.67	0.22	102,102,102,102	0
56	MG	4K	101	1/1	0.67	0.25	156,156,156,156	0
56	MG	1H	3308	1/1	0.68	0.40	99,99,99,99	0
56	MG	14	3381	1/1	0.68	0.20	102,102,102,102	0
56	MG	1G	1660	1/1	0.68	0.32	97,97,97,97	0
56	MG	14	3298	1/1	0.68	0.33	94,94,94,94	0
56	MG	1H	3184	1/1	0.69	0.29	96,96,96,96	0
56	MG	14	3017	1/1	0.69	0.27	92,92,92,92	0
56	MG	13	1606	1/1	0.69	0.24	115,115,115,115	0
56	MG	1G	1662	1/1	0.69	0.21	133,133,133,133	0
56	MG	1G	1633	1/1	0.69	0.25	83,83,83,83	0
56	MG	1H	3123	1/1	0.69	0.33	77,77,77,77	0
56	MG	14	3139	1/1	0.69	0.23	93,93,93,93	0
56	MG	45	202	1/1	0.69	0.26	103,103,103,103	0
56	MG	1H	3169	1/1	0.70	0.18	95,95,95,95	0
56	MG	13	1648	1/1	0.70	0.33	82,82,82,82	0
56	MG	1H	3321	1/1	0.70	0.26	85,85,85,85	0
56	MG	1H	3189	1/1	0.70	0.25	84,84,84,84	0
56	MG	1G	1638	1/1	0.70	0.36	81,81,81,81	0
56	MG	1H	3260	1/1	0.70	0.34	88,88,88,88	0
56	MG	16	208	1/1	0.70	0.22	82,82,82,82	0
56	MG	1H	3274	1/1	0.70	0.28	85,85,85,85	0
56	MG	C5	201	1/1	0.70	0.22	109,109,109,109	0
56	MG	14	3264	1/1	0.71	0.20	92,92,92,92	0
56	MG	1G	1641	1/1	0.71	0.22	92,92,92,92	0
56	MG	14	3210	1/1	0.71	0.24	96,96,96,96	0
56	MG	1H	3297	1/1	0.71	0.19	101,101,101,101	0
56	MG	1H	3306	1/1	0.71	0.23	84,84,84,84	0
56	MG	13	1622	1/1	0.71	0.20	94,94,94,94	0
56	MG	14	3169	1/1	0.71	0.20	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	13	1664	1/1	0.71	0.27	99,99,99,99	0
56	MG	14	3227	1/1	0.72	0.22	81,81,81,81	0
56	MG	1H	3263	1/1	0.72	0.34	94,94,94,94	0
56	MG	1H	3281	1/1	0.72	0.22	81,81,81,81	0
56	MG	1H	3223	1/1	0.72	0.27	88,88,88,88	0
56	MG	1H	3311	1/1	0.72	0.24	96,96,96,96	0
56	MG	14	3133	1/1	0.72	0.28	97,97,97,97	0
56	MG	13	1623	1/1	0.72	0.26	105,105,105,105	0
56	MG	1G	1603	1/1	0.73	0.20	101,101,101,101	0
56	MG	13	1678	1/1	0.73	0.23	83,83,83,83	0
56	MG	14	3164	1/1	0.73	0.25	83,83,83,83	0
56	MG	13	1689	1/1	0.73	0.29	92,92,92,92	0
56	MG	1H	3293	1/1	0.73	0.23	98,98,98,98	0
56	MG	14	3012	1/1	0.73	0.30	82,82,82,82	0
56	MG	14	3193	1/1	0.73	0.27	78,78,78,78	0
56	MG	1H	3270	1/1	0.73	0.31	70,70,70,70	0
56	MG	1H	3323	1/1	0.73	0.28	91,91,91,91	0
56	MG	1H	3209	1/1	0.73	0.20	82,82,82,82	0
56	MG	1H	3302	1/1	0.73	0.28	89,89,89,89	0
56	MG	14	3248	1/1	0.73	0.35	94,94,94,94	0
56	MG	14	3122	1/1	0.73	0.33	91,91,91,91	0
56	MG	14	3251	1/1	0.73	0.21	106,106,106,106	0
56	MG	1H	3032	1/1	0.73	0.20	80,80,80,80	0
56	MG	1H	3234	1/1	0.73	0.18	99,99,99,99	0
56	MG	13	1629	1/1	0.74	0.33	90,90,90,90	0
56	MG	14	3183	1/1	0.74	0.32	89,89,89,89	0
56	MG	14	3056	1/1	0.74	0.09	62,62,62,62	0
56	MG	13	1676	1/1	0.74	0.14	127,127,127,127	0
56	MG	13	1696	1/1	0.74	0.26	111,111,111,111	0
56	MG	14	3127	1/1	0.74	0.23	71,71,71,71	0
56	MG	1H	3047	1/1	0.74	0.25	92,92,92,92	0
56	MG	14	3232	1/1	0.74	0.23	127,127,127,127	0
56	MG	14	3239	1/1	0.74	0.24	79,79,79,79	0
56	MG	1H	3298	1/1	0.74	0.29	93,93,93,93	0
56	MG	1H	3300	1/1	0.74	0.22	77,77,77,77	0
56	MG	1H	3301	1/1	0.74	0.21	128,128,128,128	0
56	MG	3K	101	1/1	0.74	0.17	162,162,162,162	0
56	MG	14	3037	1/1	0.74	0.24	70,70,70,70	0
56	MG	13	1604	1/1	0.74	0.30	93,93,93,93	0
56	MG	14	3069	1/1	0.75	0.34	91,91,91,91	0
56	MG	1G	1667	1/1	0.75	0.25	100,100,100,100	0
56	MG	1H	3134	1/1	0.75	0.25	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3141	1/1	0.75	0.24	69,69,69,69	0
56	MG	1G	1658	1/1	0.75	0.23	124,124,124,124	0
56	MG	13	1685	1/1	0.75	0.40	95,95,95,95	0
56	MG	13	1647	1/1	0.75	0.24	95,95,95,95	0
56	MG	1H	3128	1/1	0.75	0.25	83,83,83,83	0
56	MG	14	3154	1/1	0.75	0.23	90,90,90,90	0
56	MG	45	201	1/1	0.75	0.21	96,96,96,96	0
56	MG	1G	1612	1/1	0.75	0.24	93,93,93,93	0
56	MG	14	3235	1/1	0.75	0.25	104,104,104,104	0
56	MG	1H	3183	1/1	0.76	0.27	90,90,90,90	0
56	MG	14	3061	1/1	0.76	0.22	97,97,97,97	0
56	MG	88	202	1/1	0.76	0.23	87,87,87,87	0
56	MG	14	3167	1/1	0.76	0.24	99,99,99,99	0
56	MG	1H	3212	1/1	0.76	0.28	89,89,89,89	0
56	MG	14	3119	1/1	0.76	0.27	86,86,86,86	0
56	MG	14	3022	1/1	0.76	0.33	83,83,83,83	0
56	MG	14	3031	1/1	0.76	0.27	76,76,76,76	0
56	MG	14	3191	1/1	0.76	0.18	76,76,76,76	0
56	MG	1G	1643	1/1	0.76	0.30	91,91,91,91	0
56	MG	1G	1651	1/1	0.76	0.37	93,93,93,93	0
56	MG	1G	1634	1/1	0.76	0.29	109,109,109,109	0
56	MG	14	3140	1/1	0.76	0.26	87,87,87,87	0
56	MG	14	3168	1/1	0.77	0.28	66,66,66,66	0
56	MG	14	3135	1/1	0.77	0.20	78,78,78,78	0
56	MG	1H	3317	1/1	0.77	0.31	105,105,105,105	0
56	MG	13	1655	1/1	0.77	0.24	103,103,103,103	0
56	MG	1H	3200	1/1	0.77	0.27	87,87,87,87	0
56	MG	14	3308	1/1	0.77	0.24	82,82,82,82	0
56	MG	1H	3081	1/1	0.77	0.24	85,85,85,85	0
56	MG	14	3277	1/1	0.77	0.32	92,92,92,92	0
56	MG	14	3243	1/1	0.77	0.17	89,89,89,89	0
56	MG	14	3286	1/1	0.77	0.23	83,83,83,83	0
56	MG	13	1660	1/1	0.77	0.30	81,81,81,81	0
56	MG	14	3101	1/1	0.77	0.27	91,91,91,91	0
56	MG	1H	3315	1/1	0.78	0.15	91,91,91,91	0
56	MG	14	3240	1/1	0.78	0.31	87,87,87,87	0
56	MG	14	3272	1/1	0.78	0.29	93,93,93,93	0
56	MG	14	3273	1/1	0.78	0.26	94,94,94,94	0
56	MG	1G	1668	1/1	0.78	0.24	106,106,106,106	0
56	MG	14	3310	1/1	0.78	0.18	120,120,120,120	0
56	MG	1G	1646	1/1	0.78	0.33	86,86,86,86	0
56	MG	1H	3194	1/1	0.78	0.17	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3307	1/1	0.78	0.21	82,82,82,82	0
56	MG	14	3252	1/1	0.78	0.19	73,73,73,73	0
56	MG	1G	1657	1/1	0.78	0.23	90,90,90,90	0
56	MG	14	3064	1/1	0.78	0.23	84,84,84,84	0
56	MG	14	3159	1/1	0.79	0.30	81,81,81,81	0
56	MG	14	3300	1/1	0.79	0.31	89,89,89,89	0
56	MG	13	1633	1/1	0.79	0.15	65,65,65,65	0
56	MG	1H	3013	1/1	0.79	0.34	89,89,89,89	0
56	MG	1H	3291	1/1	0.79	0.41	99,99,99,99	0
56	MG	14	3060	1/1	0.79	0.29	92,92,92,92	0
56	MG	14	3020	1/1	0.79	0.27	76,76,76,76	0
56	MG	14	3062	1/1	0.79	0.23	81,81,81,81	0
56	MG	78	201	1/1	0.79	0.34	75,75,75,75	0
56	MG	1G	1620	1/1	0.79	0.10	94,94,94,94	0
56	MG	14	3032	1/1	0.79	0.36	88,88,88,88	0
56	MG	14	3146	1/1	0.79	0.23	61,61,61,61	0
56	MG	1H	3052	1/1	0.79	0.54	99,99,99,99	0
56	MG	1H	3224	1/1	0.80	0.34	88,88,88,88	0
56	MG	1H	3227	1/1	0.80	0.15	50,50,50,50	0
56	MG	13	1699	1/1	0.80	0.23	81,81,81,81	0
56	MG	1H	3244	1/1	0.80	0.26	84,84,84,84	0
56	MG	1H	3044	1/1	0.80	0.40	89,89,89,89	0
56	MG	14	3259	1/1	0.80	0.24	84,84,84,84	0
56	MG	14	3221	1/1	0.80	0.15	91,91,91,91	0
56	MG	1H	3094	1/1	0.80	0.17	91,91,91,91	0
56	MG	14	3305	1/1	0.80	0.20	86,86,86,86	0
56	MG	13	1654	1/1	0.80	0.28	88,88,88,88	0
56	MG	13	1688	1/1	0.80	0.27	94,94,94,94	0
56	MG	1H	3219	1/1	0.80	0.32	89,89,89,89	0
56	MG	1H	3186	1/1	0.80	0.14	71,71,71,71	0
56	MG	14	3276	1/1	0.80	0.19	102,102,102,102	0
56	MG	39	301	1/1	0.80	0.16	80,80,80,80	0
56	MG	14	3180	1/1	0.80	0.22	79,79,79,79	0
56	MG	1G	1622	1/1	0.80	0.36	99,99,99,99	0
56	MG	14	3244	1/1	0.80	0.16	74,74,74,74	0
56	MG	1H	3097	1/1	0.81	0.17	103,103,103,103	0
56	MG	14	3131	1/1	0.81	0.28	76,76,76,76	0
56	MG	1H	3110	1/1	0.81	0.19	65,65,65,65	0
56	MG	14	3023	1/1	0.81	0.22	55,55,55,55	0
56	MG	13	1684	1/1	0.81	0.14	114,114,114,114	0
56	MG	1G	1644	1/1	0.81	0.26	86,86,86,86	0
56	MG	14	3290	1/1	0.81	0.25	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3295	1/1	0.81	0.23	114,114,114,114	0
56	MG	1H	3187	1/1	0.81	0.20	95,95,95,95	0
56	MG	1H	3254	1/1	0.81	0.35	95,95,95,95	0
56	MG	1H	3257	1/1	0.81	0.31	94,94,94,94	0
56	MG	13	1672	1/1	0.81	0.15	81,81,81,81	0
56	MG	1G	1611	1/1	0.81	0.29	108,108,108,108	0
56	MG	1H	3192	1/1	0.81	0.18	81,81,81,81	0
56	MG	13	1674	1/1	0.81	0.32	92,92,92,92	0
56	MG	1H	3039	1/1	0.81	0.30	80,80,80,80	0
56	MG	14	3068	1/1	0.81	0.12	89,89,89,89	0
56	MG	1H	3152	1/1	0.81	0.28	99,99,99,99	0
56	MG	1H	3163	1/1	0.81	0.30	48,48,48,48	0
56	MG	1H	3216	1/1	0.81	0.29	80,80,80,80	0
56	MG	1H	3167	1/1	0.81	0.22	81,81,81,81	0
56	MG	1H	3220	1/1	0.81	0.25	87,87,87,87	0
56	MG	14	3203	1/1	0.81	0.17	68,68,68,68	0
56	MG	13	1695	1/1	0.81	0.32	103,103,103,103	0
56	MG	14	3058	1/1	0.82	0.19	80,80,80,80	0
56	MG	1H	3204	1/1	0.82	0.14	100,100,100,100	0
56	MG	1H	3322	1/1	0.82	0.20	68,68,68,68	0
56	MG	14	3281	1/1	0.82	0.40	89,89,89,89	0
56	MG	1G	1642	1/1	0.82	0.24	123,123,123,123	0
56	MG	14	3150	1/1	0.82	0.26	91,91,91,91	0
56	MG	14	3003	1/1	0.82	0.26	69,69,69,69	0
56	MG	14	3238	1/1	0.82	0.25	78,78,78,78	0
56	MG	14	3291	1/1	0.82	0.31	94,94,94,94	0
56	MG	1H	3264	1/1	0.82	0.13	84,84,84,84	0
56	MG	14	3296	1/1	0.82	0.37	91,91,91,91	0
56	MG	14	3297	1/1	0.82	0.18	124,124,124,124	0
56	MG	14	3162	1/1	0.82	0.28	83,83,83,83	0
56	MG	13	1602	1/1	0.82	0.21	89,89,89,89	0
56	MG	14	3075	1/1	0.82	0.51	90,90,90,90	0
56	MG	1H	3180	1/1	0.82	0.23	76,76,76,76	0
56	MG	1H	3314	1/1	0.82	0.18	92,92,92,92	0
56	MG	1H	3055	1/1	0.82	0.28	88,88,88,88	0
56	MG	14	3120	1/1	0.82	0.21	71,71,71,71	0
56	MG	14	3307	1/1	0.82	0.24	108,108,108,108	0
56	MG	1G	1632	1/1	0.82	0.28	102,102,102,102	0
56	MG	14	3258	1/1	0.82	0.29	99,99,99,99	0
56	MG	1H	3051	1/1	0.82	0.16	84,84,84,84	0
56	MG	14	3188	1/1	0.82	0.32	92,92,92,92	0
56	MG	1H	3199	1/1	0.82	0.26	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1636	1/1	0.82	0.20	101,101,101,101	0
56	MG	14	3197	1/1	0.82	0.33	84,84,84,84	0
56	MG	1G	1637	1/1	0.82	0.27	97,97,97,97	0
56	MG	1H	3140	1/1	0.82	0.13	69,69,69,69	0
56	MG	1H	3276	1/1	0.83	0.23	85,85,85,85	0
56	MG	1H	3065	1/1	0.83	0.27	55,55,55,55	0
56	MG	1H	3217	1/1	0.83	0.23	67,67,67,67	0
56	MG	1H	3040	1/1	0.83	0.36	72,72,72,72	0
56	MG	14	3234	1/1	0.83	0.26	89,89,89,89	0
56	MG	13	1632	1/1	0.83	0.28	73,73,73,73	0
56	MG	13	1677	1/1	0.83	0.23	91,91,91,91	0
56	MG	1H	3104	1/1	0.83	0.22	71,71,71,71	0
56	MG	1H	3025	1/1	0.83	0.17	77,77,77,77	0
56	MG	1H	3048	1/1	0.83	0.20	92,92,92,92	0
56	MG	14	3070	1/1	0.83	0.18	71,71,71,71	0
56	MG	1H	3327	1/1	0.83	0.24	95,95,95,95	0
56	MG	16	202	1/1	0.83	0.23	86,86,86,86	0
56	MG	1H	3125	1/1	0.83	0.14	87,87,87,87	0
56	MG	14	3176	1/1	0.83	0.26	88,88,88,88	0
56	MG	14	3114	1/1	0.83	0.28	81,81,81,81	0
56	MG	1H	3050	1/1	0.83	0.26	78,78,78,78	0
56	MG	13	1620	1/1	0.83	0.15	82,82,82,82	0
56	MG	1H	3138	1/1	0.83	0.29	61,61,61,61	0
56	MG	14	3030	1/1	0.83	0.32	87,87,87,87	0
56	MG	1H	3035	1/1	0.83	0.13	76,76,76,76	0
56	MG	1H	3053	1/1	0.83	0.29	82,82,82,82	0
56	MG	14	3132	1/1	0.83	0.31	91,91,91,91	0
56	MG	13	1626	1/1	0.83	0.29	87,87,87,87	0
56	MG	35	201	1/1	0.83	0.23	76,76,76,76	0
56	MG	14	3214	1/1	0.83	0.35	87,87,87,87	0
56	MG	1H	3061	1/1	0.83	0.27	62,62,62,62	0
56	MG	14	3278	1/1	0.83	0.24	96,96,96,96	0
56	MG	1G	1652	1/1	0.84	0.26	88,88,88,88	0
56	MG	1G	1654	1/1	0.84	0.35	86,86,86,86	0
56	MG	1H	3010	1/1	0.84	0.33	57,57,57,57	0
56	MG	Q8	101	1/1	0.84	0.25	83,83,83,83	0
56	MG	13	1661	1/1	0.84	0.10	93,93,93,93	0
56	MG	1H	3305	1/1	0.84	0.25	68,68,68,68	0
56	MG	14	3071	1/1	0.84	0.19	84,84,84,84	0
56	MG	1G	1604	1/1	0.84	0.23	97,97,97,97	0
56	MG	14	3083	1/1	0.84	0.26	87,87,87,87	0
56	MG	1H	3158	1/1	0.84	0.24	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3261	1/1	0.84	0.13	90,90,90,90	0
56	MG	14	3113	1/1	0.84	0.18	78,78,78,78	0
56	MG	1H	3159	1/1	0.84	0.27	83,83,83,83	0
56	MG	14	3115	1/1	0.84	0.26	66,66,66,66	0
56	MG	1H	3162	1/1	0.84	0.28	87,87,87,87	0
56	MG	1H	3265	1/1	0.84	0.15	74,74,74,74	0
56	MG	13	1642	1/1	0.84	0.19	73,73,73,73	0
56	MG	14	3126	1/1	0.84	0.36	83,83,83,83	0
56	MG	14	3004	1/1	0.84	0.24	83,83,83,83	0
56	MG	1H	3101	1/1	0.84	0.17	64,64,64,64	0
56	MG	1H	3019	1/1	0.84	0.35	89,89,89,89	0
56	MG	13	1643	1/1	0.84	0.20	79,79,79,79	0
56	MG	13	1645	1/1	0.84	0.19	66,66,66,66	0
56	MG	1H	3221	1/1	0.84	0.28	78,78,78,78	0
56	MG	13	1686	1/1	0.84	0.35	73,73,73,73	0
56	MG	1H	3036	1/1	0.84	0.23	77,77,77,77	0
56	MG	13	1687	1/1	0.84	0.23	76,76,76,76	0
56	MG	14	3245	1/1	0.84	0.17	88,88,88,88	0
56	MG	14	3246	1/1	0.84	0.17	72,72,72,72	0
56	MG	14	3143	1/1	0.84	0.34	70,70,70,70	0
56	MG	13	1697	1/1	0.84	0.24	96,96,96,96	0
56	MG	16	203	1/1	0.84	0.17	91,91,91,91	0
56	MG	1H	3239	1/1	0.84	0.11	81,81,81,81	0
56	MG	16	207	1/1	0.84	0.23	76,76,76,76	0
56	MG	14	3256	1/1	0.84	0.22	76,76,76,76	0
56	MG	1H	3041	1/1	0.84	0.28	77,77,77,77	0
56	MG	1H	3246	1/1	0.84	0.28	88,88,88,88	0
56	MG	13	1656	1/1	0.85	0.23	88,88,88,88	0
56	MG	1G	1663	1/1	0.85	0.18	97,97,97,97	0
56	MG	13	1693	1/1	0.85	0.43	88,88,88,88	0
56	MG	14	3261	1/1	0.85	0.34	83,83,83,83	0
56	MG	1H	3132	1/1	0.85	0.30	78,78,78,78	0
56	MG	14	3086	1/1	0.85	0.35	82,82,82,82	0
56	MG	14	3271	1/1	0.85	0.17	74,74,74,74	0
56	MG	14	3096	1/1	0.85	0.23	60,60,60,60	0
56	MG	3E	301	1/1	0.85	0.33	94,94,94,94	0
56	MG	1H	3137	1/1	0.85	0.16	73,73,73,73	0
56	MG	2L	101	1/1	0.85	0.26	72,72,72,72	0
56	MG	1G	1631	1/1	0.85	0.23	91,91,91,91	0
56	MG	1H	3072	1/1	0.85	0.20	72,72,72,72	0
56	MG	14	3199	1/1	0.85	0.23	59,59,59,59	0
56	MG	14	3201	1/1	0.85	0.19	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	5E	201	1/1	0.85	0.22	84,84,84,84	0
56	MG	1H	3236	1/1	0.85	0.35	91,91,91,91	0
56	MG	1G	1635	1/1	0.85	0.18	93,93,93,93	0
56	MG	1H	3093	1/1	0.85	0.18	72,72,72,72	0
56	MG	1H	3198	1/1	0.85	0.20	67,67,67,67	0
56	MG	14	3128	1/1	0.85	0.23	73,73,73,73	0
56	MG	13	1605	1/1	0.85	0.23	75,75,75,75	0
56	MG	14	3230	1/1	0.85	0.19	72,72,72,72	0
56	MG	14	3024	1/1	0.85	0.25	74,74,74,74	0
56	MG	14	3233	1/1	0.85	0.39	80,80,80,80	0
56	MG	1H	3248	1/1	0.85	0.21	83,83,83,83	0
56	MG	1H	3299	1/1	0.85	0.34	86,86,86,86	0
56	MG	1H	3250	1/1	0.85	0.24	87,87,87,87	0
56	MG	13	1673	1/1	0.85	0.20	102,102,102,102	0
56	MG	14	3304	1/1	0.85	0.23	90,90,90,90	0
56	MG	13	1690	1/1	0.85	0.38	81,81,81,81	0
56	MG	14	3242	1/1	0.85	0.10	70,70,70,70	0
56	MG	1H	3258	1/1	0.85	0.11	72,72,72,72	0
56	MG	1G	1649	1/1	0.85	0.27	96,96,96,96	0
56	MG	1H	3206	1/1	0.85	0.29	94,94,94,94	0
56	MG	13	1669	1/1	0.85	0.23	72,72,72,72	0
56	MG	1H	3038	1/1	0.85	0.22	81,81,81,81	0
56	MG	14	3157	1/1	0.85	0.32	66,66,66,66	0
56	MG	1G	1610	1/1	0.85	0.16	102,102,102,102	0
56	MG	1H	3114	1/1	0.85	0.16	67,67,67,67	0
56	MG	1H	3007	1/1	0.85	0.27	80,80,80,80	0
56	MG	1G	1614	1/1	0.85	0.25	93,93,93,93	0
56	MG	14	3033	1/1	0.86	0.29	84,84,84,84	0
56	MG	1H	3088	1/1	0.86	0.13	54,54,54,54	0
56	MG	14	3206	1/1	0.86	0.22	82,82,82,82	0
56	MG	13	1636	1/1	0.86	0.36	85,85,85,85	0
56	MG	14	3212	1/1	0.86	0.29	69,69,69,69	0
56	MG	14	3053	1/1	0.86	0.30	61,61,61,61	0
56	MG	14	3217	1/1	0.86	0.15	87,87,87,87	0
56	MG	13	1644	1/1	0.86	0.22	84,84,84,84	0
56	MG	1G	1626	1/1	0.86	0.15	95,95,95,95	0
56	MG	14	3222	1/1	0.86	0.24	80,80,80,80	0
56	MG	13	1667	1/1	0.86	0.18	85,85,85,85	0
56	MG	1H	3099	1/1	0.86	0.24	75,75,75,75	0
56	MG	1H	3262	1/1	0.86	0.30	77,77,77,77	0
56	MG	14	3231	1/1	0.86	0.22	84,84,84,84	0
56	MG	13	1694	1/1	0.86	0.18	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3294	1/1	0.86	0.22	74,74,74,74	0
56	MG	1H	3028	1/1	0.86	0.32	72,72,72,72	0
56	MG	14	3149	1/1	0.86	0.32	92,92,92,92	0
56	MG	1H	3108	1/1	0.86	0.18	62,62,62,62	0
56	MG	1H	3042	1/1	0.86	0.28	93,93,93,93	0
56	MG	13	1652	1/1	0.86	0.22	74,74,74,74	0
56	MG	1H	3275	1/1	0.86	0.29	74,74,74,74	0
56	MG	14	3002	1/1	0.86	0.21	62,62,62,62	0
56	MG	14	3079	1/1	0.86	0.23	72,72,72,72	0
56	MG	14	3165	1/1	0.86	0.20	60,60,60,60	0
56	MG	I8	103	1/1	0.86	0.23	86,86,86,86	0
56	MG	1H	3309	1/1	0.86	0.21	79,79,79,79	0
56	MG	14	3306	1/1	0.86	0.19	110,110,110,110	0
56	MG	14	3007	1/1	0.86	0.29	63,63,63,63	0
56	MG	1H	3034	1/1	0.86	0.34	78,78,78,78	0
56	MG	1H	3312	1/1	0.86	0.18	67,67,67,67	0
56	MG	14	3019	1/1	0.86	0.33	84,84,84,84	0
56	MG	1J	201	1/1	0.86	0.27	90,90,90,90	0
56	MG	1H	3164	1/1	0.86	0.17	73,73,73,73	0
56	MG	1H	3046	1/1	0.86	0.33	87,87,87,87	0
56	MG	13	1653	1/1	0.86	0.17	89,89,89,89	0
56	MG	1H	3249	1/1	0.86	0.31	86,86,86,86	0
56	MG	1H	3170	1/1	0.86	0.14	81,81,81,81	0
56	MG	1G	1615	1/1	0.86	0.18	119,119,119,119	0
56	MG	1G	1653	1/1	0.86	0.17	85,85,85,85	0
56	MG	1H	3290	1/1	0.87	0.16	80,80,80,80	0
56	MG	1H	3018	1/1	0.87	0.30	78,78,78,78	0
56	MG	14	3285	1/1	0.87	0.27	72,72,72,72	0
56	MG	14	3015	1/1	0.87	0.26	63,63,63,63	0
56	MG	13	1649	1/1	0.87	0.17	75,75,75,75	0
56	MG	1H	3269	1/1	0.87	0.28	97,97,97,97	0
56	MG	I8	102	1/1	0.87	0.38	83,83,83,83	0
56	MG	14	3192	1/1	0.87	0.18	80,80,80,80	0
56	MG	14	3293	1/1	0.87	0.10	99,99,99,99	0
56	MG	14	3134	1/1	0.87	0.15	74,74,74,74	0
56	MG	1H	3296	1/1	0.87	0.26	92,92,92,92	0
56	MG	1H	3033	1/1	0.87	0.15	68,68,68,68	0
56	MG	14	3249	1/1	0.87	0.23	78,78,78,78	0
56	MG	14	3076	1/1	0.87	0.27	89,89,89,89	0
56	MG	14	3202	1/1	0.87	0.17	79,79,79,79	0
56	MG	1H	3273	1/1	0.87	0.26	84,84,84,84	0
56	MG	14	3253	1/1	0.87	0.28	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3084	1/1	0.87	0.17	82,82,82,82	0
56	MG	1H	3232	1/1	0.87	0.10	71,71,71,71	0
56	MG	1G	1609	1/1	0.87	0.23	94,94,94,94	0
56	MG	14	3097	1/1	0.87	0.19	74,74,74,74	0
56	MG	1H	3054	1/1	0.87	0.19	87,87,87,87	0
56	MG	14	3102	1/1	0.87	0.21	76,76,76,76	0
56	MG	14	3263	1/1	0.87	0.20	82,82,82,82	0
56	MG	14	3309	1/1	0.87	0.34	90,90,90,90	0
56	MG	1H	3089	1/1	0.87	0.21	74,74,74,74	0
56	MG	14	3265	1/1	0.87	0.27	89,89,89,89	0
56	MG	1H	3304	1/1	0.87	0.43	73,73,73,73	0
56	MG	14	3046	1/1	0.87	0.19	66,66,66,66	0
56	MG	1H	3043	1/1	0.87	0.28	87,87,87,87	0
56	MG	13	1675	1/1	0.87	0.14	124,124,124,124	0
56	MG	1H	3283	1/1	0.87	0.27	85,85,85,85	0
56	MG	1G	1618	1/1	0.87	0.20	101,101,101,101	0
56	MG	14	3170	1/1	0.87	0.36	81,81,81,81	0
56	MG	1H	3124	1/1	0.87	0.15	59,59,59,59	0
56	MG	13	1651	1/1	0.88	0.12	86,86,86,86	0
56	MG	14	3204	1/1	0.88	0.19	82,82,82,82	0
56	MG	5I	101	1/1	0.88	0.14	88,88,88,88	0
56	MG	1G	1647	1/1	0.88	0.19	102,102,102,102	0
56	MG	13	1698	1/1	0.88	0.28	81,81,81,81	0
56	MG	14	3213	1/1	0.88	0.16	89,89,89,89	0
56	MG	1G	1601	1/1	0.88	0.18	96,96,96,96	0
56	MG	1H	3118	1/1	0.88	0.16	61,61,61,61	0
56	MG	14	3050	1/1	0.88	0.21	73,73,73,73	0
56	MG	1H	3153	1/1	0.88	0.11	60,60,60,60	0
56	MG	1H	3225	1/1	0.88	0.32	74,74,74,74	0
56	MG	1H	3156	1/1	0.88	0.25	77,77,77,77	0
56	MG	1H	3230	1/1	0.88	0.20	73,73,73,73	0
56	MG	1H	3310	1/1	0.88	0.24	72,72,72,72	0
56	MG	1H	3191	1/1	0.88	0.15	90,90,90,90	0
56	MG	14	3289	1/1	0.88	0.17	91,91,91,91	0
56	MG	1G	1661	1/1	0.88	0.16	150,150,150,150	0
56	MG	1H	3157	1/1	0.88	0.35	83,83,83,83	0
56	MG	14	3292	1/1	0.88	0.19	86,86,86,86	0
56	MG	13	1611	1/1	0.88	0.15	61,61,61,61	0
56	MG	14	3156	1/1	0.88	0.14	62,62,62,62	0
56	MG	13	1663	1/1	0.88	0.16	75,75,75,75	0
56	MG	1H	3240	1/1	0.88	0.14	56,56,56,56	0
56	MG	1H	3241	1/1	0.88	0.29	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3058	1/1	0.88	0.12	62,62,62,62	0
56	MG	13	1621	1/1	0.88	0.19	95,95,95,95	0
56	MG	1H	3287	1/1	0.88	0.36	86,86,86,86	0
56	MG	1H	3288	1/1	0.88	0.10	94,94,94,94	0
56	MG	1H	3005	1/1	0.88	0.16	62,62,62,62	0
56	MG	14	3247	1/1	0.88	0.29	73,73,73,73	0
56	MG	14	3087	1/1	0.88	0.30	79,79,79,79	0
56	MG	1H	3067	1/1	0.88	0.20	63,63,63,63	0
56	MG	16	201	1/1	0.88	0.16	92,92,92,92	0
56	MG	14	3009	1/1	0.88	0.23	52,52,52,52	0
56	MG	1H	3207	1/1	0.88	0.28	81,81,81,81	0
56	MG	1H	3251	1/1	0.88	0.15	63,63,63,63	0
56	MG	1H	3253	1/1	0.88	0.13	60,60,60,60	0
56	MG	16	205	1/1	0.88	0.26	84,84,84,84	0
56	MG	14	3257	1/1	0.88	0.11	68,68,68,68	0
56	MG	16	206	1/1	0.88	0.13	84,84,84,84	0
56	MG	14	3117	1/1	0.88	0.34	77,77,77,77	0
56	MG	1H	3135	1/1	0.88	0.22	81,81,81,81	0
56	MG	13	1665	1/1	0.88	0.23	64,64,64,64	0
56	MG	14	3262	1/1	0.88	0.39	91,91,91,91	0
56	MG	1H	3172	1/1	0.88	0.18	82,82,82,82	0
56	MG	1H	3179	1/1	0.88	0.23	93,93,93,93	0
56	MG	E5	101	1/1	0.88	0.27	83,83,83,83	0
56	MG	14	3190	1/1	0.89	0.18	95,95,95,95	0
56	MG	14	3021	1/1	0.89	0.31	78,78,78,78	0
56	MG	1G	1606	1/1	0.89	0.21	82,82,82,82	0
56	MG	1H	3085	1/1	0.89	0.19	82,82,82,82	0
56	MG	13	1668	1/1	0.89	0.15	80,80,80,80	0
56	MG	14	3198	1/1	0.89	0.27	80,80,80,80	0
56	MG	14	3025	1/1	0.89	0.18	69,69,69,69	0
56	MG	14	3268	1/1	0.89	0.13	86,86,86,86	0
56	MG	1H	3012	1/1	0.89	0.21	79,79,79,79	0
56	MG	13	1612	1/1	0.89	0.19	79,79,79,79	0
56	MG	14	3123	1/1	0.89	0.15	82,82,82,82	0
56	MG	14	3125	1/1	0.89	0.22	54,54,54,54	0
56	MG	1H	3259	1/1	0.89	0.14	80,80,80,80	0
56	MG	1H	3014	1/1	0.89	0.39	69,69,69,69	0
56	MG	14	3211	1/1	0.89	0.27	74,74,74,74	0
56	MG	13	1683	1/1	0.89	0.26	91,91,91,91	0
56	MG	1H	3197	1/1	0.89	0.18	80,80,80,80	0
56	MG	14	3284	1/1	0.89	0.11	84,84,84,84	0
56	MG	1G	1619	1/1	0.89	0.12	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3215	1/1	0.89	0.20	83,83,83,83	0
56	MG	14	3047	1/1	0.89	0.15	57,57,57,57	0
56	MG	1H	3428	1/1	0.89	0.21	54,54,54,54	0
56	MG	14	3051	1/1	0.89	0.22	90,90,90,90	0
56	MG	1G	1621	1/1	0.89	0.26	61,61,61,61	0
56	MG	14	3224	1/1	0.89	0.26	75,75,75,75	0
56	MG	1H	3064	1/1	0.89	0.18	54,54,54,54	0
56	MG	1H	3017	1/1	0.89	0.31	77,77,77,77	0
56	MG	14	3141	1/1	0.89	0.14	90,90,90,90	0
56	MG	1G	1627	1/1	0.89	0.23	85,85,85,85	0
56	MG	13	1637	1/1	0.89	0.32	68,68,68,68	0
56	MG	1H	3202	1/1	0.89	0.24	75,75,75,75	0
56	MG	1H	3203	1/1	0.89	0.25	75,75,75,75	0
56	MG	1H	3271	1/1	0.89	0.28	94,94,94,94	0
56	MG	14	3237	1/1	0.89	0.15	62,62,62,62	0
56	MG	14	3152	1/1	0.89	0.24	91,91,91,91	0
56	MG	14	3067	1/1	0.89	0.19	74,74,74,74	0
56	MG	13	1627	1/1	0.89	0.33	81,81,81,81	0
56	MG	2L	103	1/1	0.89	0.25	79,79,79,79	0
56	MG	1H	3205	1/1	0.89	0.23	83,83,83,83	0
56	MG	14	3160	1/1	0.89	0.18	57,57,57,57	0
56	MG	1H	3173	1/1	0.89	0.34	79,79,79,79	0
56	MG	1H	3177	1/1	0.89	0.17	82,82,82,82	0
56	MG	1H	3020	1/1	0.89	0.21	60,60,60,60	0
56	MG	1H	3083	1/1	0.89	0.11	75,75,75,75	0
56	MG	14	3011	1/1	0.89	0.31	58,58,58,58	0
56	MG	1H	3115	1/1	0.89	0.24	76,76,76,76	0
56	MG	14	3013	1/1	0.89	0.25	83,83,83,83	0
56	MG	14	3091	1/1	0.89	0.42	87,87,87,87	0
56	MG	14	3014	1/1	0.89	0.21	49,49,49,49	0
56	MG	13	1662	1/1	0.89	0.23	82,82,82,82	0
56	MG	1H	3252	1/1	0.89	0.16	72,72,72,72	0
56	MG	1H	3285	1/1	0.89	0.19	72,72,72,72	0
56	MG	14	3184	1/1	0.89	0.24	86,86,86,86	0
56	MG	1H	3316	1/1	0.89	0.29	87,87,87,87	0
56	MG	1H	3278	1/1	0.90	0.27	92,92,92,92	0
56	MG	1H	3160	1/1	0.90	0.14	69,69,69,69	0
56	MG	13	1617	1/1	0.90	0.18	77,77,77,77	0
56	MG	13	1639	1/1	0.90	0.29	85,85,85,85	0
56	MG	13	1640	1/1	0.90	0.15	91,91,91,91	0
56	MG	1H	3166	1/1	0.90	0.11	68,68,68,68	0
56	MG	1H	3255	1/1	0.90	0.14	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1645	1/1	0.90	0.28	88,88,88,88	0
56	MG	1H	3256	1/1	0.90	0.15	76,76,76,76	0
56	MG	1H	3289	1/1	0.90	0.20	82,82,82,82	0
56	MG	14	3219	1/1	0.90	0.24	78,78,78,78	0
56	MG	14	3148	1/1	0.90	0.24	72,72,72,72	0
56	MG	1H	3121	1/1	0.90	0.29	53,53,53,53	0
56	MG	14	3081	1/1	0.90	0.26	62,62,62,62	0
56	MG	14	3223	1/1	0.90	0.24	83,83,83,83	0
56	MG	14	3082	1/1	0.90	0.21	63,63,63,63	0
56	MG	14	3226	1/1	0.90	0.18	72,72,72,72	0
56	MG	1H	3098	1/1	0.90	0.13	69,69,69,69	0
56	MG	14	3228	1/1	0.90	0.23	93,93,93,93	0
56	MG	1H	3292	1/1	0.90	0.07	61,61,61,61	0
56	MG	1H	3151	1/1	0.90	0.09	52,52,52,52	0
56	MG	1H	3226	1/1	0.90	0.18	55,55,55,55	0
56	MG	14	3093	1/1	0.90	0.21	85,85,85,85	0
56	MG	14	3161	1/1	0.90	0.27	73,73,73,73	0
56	MG	14	3095	1/1	0.90	0.20	56,56,56,56	0
56	MG	1H	3171	1/1	0.90	0.20	74,74,74,74	0
56	MG	1H	3429	1/1	0.90	0.16	66,66,66,66	0
56	MG	14	3166	1/1	0.90	0.31	85,85,85,85	0
56	MG	14	3098	1/1	0.90	0.23	68,68,68,68	0
56	MG	14	3028	1/1	0.90	0.34	79,79,79,79	0
56	MG	1H	3009	1/1	0.90	0.23	66,66,66,66	0
56	MG	1G	1659	1/1	0.90	0.27	85,85,85,85	0
56	MG	1H	3231	1/1	0.90	0.25	56,56,56,56	0
56	MG	1G	1625	1/1	0.90	0.32	76,76,76,76	0
56	MG	14	3179	1/1	0.90	0.41	84,84,84,84	0
56	MG	13	1625	1/1	0.90	0.38	82,82,82,82	0
56	MG	14	3116	1/1	0.90	0.24	63,63,63,63	0
56	MG	14	3182	1/1	0.90	0.21	73,73,73,73	0
56	MG	1H	3155	1/1	0.90	0.21	86,86,86,86	0
56	MG	1H	3178	1/1	0.90	0.18	74,74,74,74	0
56	MG	1H	3126	1/1	0.90	0.15	72,72,72,72	0
56	MG	1G	1666	1/1	0.90	0.24	85,85,85,85	0
56	MG	14	3254	1/1	0.90	0.27	78,78,78,78	0
56	MG	13	1607	1/1	0.90	0.30	85,85,85,85	0
56	MG	14	3124	1/1	0.90	0.15	70,70,70,70	0
56	MG	1H	3182	1/1	0.90	0.18	77,77,77,77	0
56	MG	13	1731	1/1	0.90	0.19	94,94,94,94	0
56	MG	1H	3090	1/1	0.90	0.31	72,72,72,72	0
56	MG	14	3057	1/1	0.90	0.24	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3213	1/1	0.90	0.47	84,84,84,84	0
56	MG	1H	3215	1/1	0.90	0.36	81,81,81,81	0
56	MG	14	3099	1/1	0.91	0.21	62,62,62,62	0
56	MG	1H	3142	1/1	0.91	0.19	68,68,68,68	0
56	MG	14	3044	1/1	0.91	0.26	68,68,68,68	0
56	MG	14	3103	1/1	0.91	0.16	66,66,66,66	0
56	MG	14	3107	1/1	0.91	0.15	87,87,87,87	0
56	MG	14	3163	1/1	0.91	0.30	76,76,76,76	0
56	MG	1H	3147	1/1	0.91	0.10	72,72,72,72	0
56	MG	1G	1628	1/1	0.91	0.13	98,98,98,98	0
56	MG	13	1722	1/1	0.91	0.10	93,93,93,93	0
56	MG	14	3283	1/1	0.91	0.17	80,80,80,80	0
56	MG	1H	3049	1/1	0.91	0.08	65,65,65,65	0
56	MG	1H	3303	1/1	0.91	0.23	73,73,73,73	0
56	MG	13	1670	1/1	0.91	0.20	95,95,95,95	0
56	MG	1H	3030	1/1	0.91	0.24	69,69,69,69	0
56	MG	21	302	1/1	0.91	0.12	78,78,78,78	0
56	MG	14	3173	1/1	0.91	0.13	82,82,82,82	0
56	MG	14	3236	1/1	0.91	0.13	79,79,79,79	0
56	MG	41	201	1/1	0.91	0.18	71,71,71,71	0
56	MG	1H	3243	1/1	0.91	0.06	56,56,56,56	0
56	MG	1H	3075	1/1	0.91	0.10	79,79,79,79	0
56	MG	1H	3076	1/1	0.91	0.14	65,65,65,65	0
56	MG	1H	3210	1/1	0.91	0.20	73,73,73,73	0
56	MG	1H	3127	1/1	0.91	0.16	53,53,53,53	0
56	MG	1H	3100	1/1	0.91	0.14	56,56,56,56	0
56	MG	1H	3282	1/1	0.91	0.14	78,78,78,78	0
56	MG	1H	3185	1/1	0.91	0.19	78,78,78,78	0
56	MG	1H	3130	1/1	0.91	0.12	60,60,60,60	0
56	MG	1H	3161	1/1	0.91	0.21	84,84,84,84	0
56	MG	1H	3188	1/1	0.91	0.34	76,76,76,76	0
56	MG	14	3194	1/1	0.91	0.21	86,86,86,86	0
56	MG	2K	101	1/1	0.91	0.31	86,86,86,86	0
56	MG	14	3080	1/1	0.91	0.18	67,67,67,67	0
56	MG	1H	3008	1/1	0.91	0.12	74,74,74,74	0
56	MG	13	1601	1/1	0.91	0.18	59,59,59,59	0
56	MG	2K	103	1/1	0.91	0.17	71,71,71,71	0
56	MG	1H	3195	1/1	0.91	0.34	78,78,78,78	0
56	MG	1H	3324	1/1	0.91	0.17	69,69,69,69	0
56	MG	14	3205	1/1	0.91	0.08	80,80,80,80	0
56	MG	14	3382	1/1	0.91	0.14	100,100,100,100	0
56	MG	14	3147	1/1	0.91	0.22	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3325	1/1	0.91	0.19	76,76,76,76	0
56	MG	1H	3196	1/1	0.91	0.35	80,80,80,80	0
56	MG	1H	3112	1/1	0.91	0.19	66,66,66,66	0
56	MG	1H	3228	1/1	0.91	0.21	57,57,57,57	0
56	MG	14	3153	1/1	0.91	0.26	78,78,78,78	0
56	MG	13	1603	1/1	0.91	0.25	92,92,92,92	0
56	MG	85	201	1/1	0.91	0.54	88,88,88,88	0
56	MG	14	3155	1/1	0.91	0.13	71,71,71,71	0
56	MG	1H	3024	1/1	0.91	0.34	70,70,70,70	0
56	MG	1H	3080	1/1	0.92	0.10	86,86,86,86	0
56	MG	14	3174	1/1	0.92	0.34	81,81,81,81	0
56	MG	14	3175	1/1	0.92	0.20	96,96,96,96	0
56	MG	1H	3096	1/1	0.92	0.27	78,78,78,78	0
56	MG	14	3177	1/1	0.92	0.26	87,87,87,87	0
56	MG	14	3178	1/1	0.92	0.44	90,90,90,90	0
56	MG	1G	1617	1/1	0.92	0.11	125,125,125,125	0
56	MG	1H	3272	1/1	0.92	0.14	89,89,89,89	0
56	MG	1H	3201	1/1	0.92	0.29	70,70,70,70	0
56	MG	13	1650	1/1	0.92	0.30	79,79,79,79	0
56	MG	14	3090	1/1	0.92	0.17	70,70,70,70	0
56	MG	13	1641	1/1	0.92	0.25	75,75,75,75	0
56	MG	88	201	1/1	0.92	0.22	81,81,81,81	0
56	MG	14	3048	1/1	0.92	0.27	55,55,55,55	0
56	MG	14	3008	1/1	0.92	0.28	65,65,65,65	0
56	MG	1H	3011	1/1	0.92	0.29	71,71,71,71	0
56	MG	14	3010	1/1	0.92	0.24	54,54,54,54	0
56	MG	1H	3027	1/1	0.92	0.24	48,48,48,48	0
56	MG	14	3195	1/1	0.92	0.08	107,107,107,107	0
56	MG	14	3196	1/1	0.92	0.23	69,69,69,69	0
56	MG	14	3100	1/1	0.92	0.14	91,91,91,91	0
56	MG	1H	3150	1/1	0.92	0.10	70,70,70,70	0
56	MG	1H	3087	1/1	0.92	0.11	65,65,65,65	0
56	MG	14	3200	1/1	0.92	0.22	67,67,67,67	0
56	MG	1H	3102	1/1	0.92	0.23	55,55,55,55	0
56	MG	14	3059	1/1	0.92	0.22	55,55,55,55	0
56	MG	14	3109	1/1	0.92	0.24	72,72,72,72	0
56	MG	1H	3070	1/1	0.92	0.24	50,50,50,50	0
56	MG	14	3111	1/1	0.92	0.22	69,69,69,69	0
56	MG	1H	3107	1/1	0.92	0.24	73,73,73,73	0
56	MG	13	1610	1/1	0.92	0.15	72,72,72,72	0
56	MG	1G	1605	1/1	0.92	0.23	85,85,85,85	0
56	MG	14	3066	1/1	0.92	0.17	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3214	1/1	0.92	0.15	68,68,68,68	0
56	MG	1H	3175	1/1	0.92	0.28	70,70,70,70	0
56	MG	13	1615	1/1	0.92	0.14	85,85,85,85	0
56	MG	14	3216	1/1	0.92	0.18	70,70,70,70	0
56	MG	14	3121	1/1	0.92	0.18	84,84,84,84	0
56	MG	1H	3059	1/1	0.92	0.16	48,48,48,48	0
56	MG	29	301	1/1	0.92	0.16	63,63,63,63	0
56	MG	1H	3218	1/1	0.92	0.10	76,76,76,76	0
56	MG	14	3267	1/1	0.92	0.22	66,66,66,66	0
56	MG	14	3073	1/1	0.92	0.29	81,81,81,81	0
56	MG	14	3269	1/1	0.92	0.25	75,75,75,75	0
56	MG	45	203	1/1	0.92	0.20	73,73,73,73	0
56	MG	1G	1639	1/1	0.92	0.34	80,80,80,80	0
56	MG	14	3029	1/1	0.92	0.21	83,83,83,83	0
56	MG	1H	3113	1/1	0.92	0.12	67,67,67,67	0
56	MG	1H	3222	1/1	0.93	0.28	79,79,79,79	0
56	MG	14	3207	1/1	0.93	0.12	89,89,89,89	0
56	MG	14	3208	1/1	0.93	0.10	67,67,67,67	0
56	MG	13	1638	1/1	0.93	0.30	87,87,87,87	0
56	MG	14	3088	1/1	0.93	0.21	73,73,73,73	0
56	MG	13	1630	1/1	0.93	0.37	71,71,71,71	0
56	MG	1G	1613	1/1	0.93	0.10	100,100,100,100	0
56	MG	1H	3174	1/1	0.93	0.16	85,85,85,85	0
56	MG	14	3094	1/1	0.93	0.12	82,82,82,82	0
56	MG	14	3275	1/1	0.93	0.16	68,68,68,68	0
56	MG	1H	3062	1/1	0.93	0.21	54,54,54,54	0
56	MG	1H	3294	1/1	0.93	0.32	71,71,71,71	0
56	MG	14	3218	1/1	0.93	0.20	60,60,60,60	0
56	MG	14	3158	1/1	0.93	0.09	71,71,71,71	0
56	MG	1H	3176	1/1	0.93	0.19	68,68,68,68	0
56	MG	1H	3359	1/1	0.93	0.16	66,66,66,66	0
56	MG	14	3036	1/1	0.93	0.20	73,73,73,73	0
56	MG	1H	3380	1/1	0.93	0.08	70,70,70,70	0
56	MG	14	3038	1/1	0.93	0.18	86,86,86,86	0
56	MG	3I	201	1/1	0.93	0.12	62,62,62,62	0
56	MG	1H	3086	1/1	0.93	0.21	41,41,41,41	0
56	MG	14	3105	1/1	0.93	0.11	52,52,52,52	0
56	MG	1H	3016	1/1	0.93	0.19	48,48,48,48	0
56	MG	1G	1624	1/1	0.93	0.18	76,76,76,76	0
56	MG	1H	3106	1/1	0.93	0.16	77,77,77,77	0
56	MG	14	3049	1/1	0.93	0.11	58,58,58,58	0
56	MG	14	3171	1/1	0.93	0.16	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3268	1/1	0.93	0.26	79,79,79,79	0
56	MG	1H	3181	1/1	0.93	0.04	74,74,74,74	0
56	MG	13	1631	1/1	0.93	0.38	93,93,93,93	0
56	MG	1G	1682	1/1	0.93	0.12	91,91,91,91	0
56	MG	1H	3238	1/1	0.93	0.12	82,82,82,82	0
56	MG	1H	3208	1/1	0.93	0.22	63,63,63,63	0
56	MG	1H	3131	1/1	0.93	0.12	62,62,62,62	0
56	MG	2I	301	1/1	0.93	0.17	57,57,57,57	0
56	MG	1H	3031	1/1	0.93	0.15	65,65,65,65	0
56	MG	1H	3242	1/1	0.93	0.27	64,64,64,64	0
56	MG	14	3005	1/1	0.93	0.18	44,44,44,44	0
56	MG	1H	3211	1/1	0.93	0.17	71,71,71,71	0
56	MG	1H	3133	1/1	0.93	0.23	69,69,69,69	0
56	MG	13	1624	1/1	0.93	0.11	71,71,71,71	0
56	MG	1H	3092	1/1	0.93	0.17	67,67,67,67	0
56	MG	14	3129	1/1	0.93	0.21	58,58,58,58	0
56	MG	1H	3136	1/1	0.93	0.13	68,68,68,68	0
56	MG	1H	3313	1/1	0.93	0.06	66,66,66,66	0
56	MG	1H	3002	1/1	0.93	0.17	49,49,49,49	0
56	MG	14	3072	1/1	0.93	0.17	55,55,55,55	0
56	MG	1H	3003	1/1	0.93	0.12	54,54,54,54	0
56	MG	1H	3079	1/1	0.93	0.12	61,61,61,61	0
56	MG	1H	3021	1/1	0.93	0.19	57,57,57,57	0
56	MG	14	3078	1/1	0.93	0.14	64,64,64,64	0
56	MG	14	3018	1/1	0.93	0.22	73,73,73,73	0
56	MG	1H	3119	1/1	0.93	0.27	78,78,78,78	0
56	MG	1H	3143	1/1	0.93	0.28	77,77,77,77	0
56	MG	14	3145	1/1	0.93	0.14	67,67,67,67	0
56	MG	1H	3320	1/1	0.93	0.07	68,68,68,68	0
56	MG	1G	1648	1/1	0.93	0.27	78,78,78,78	0
59	ZN	G8	201	1/1	0.93	0.19	144,144,144,144	0
56	MG	14	3189	1/1	0.94	0.25	73,73,73,73	0
56	MG	1H	3165	1/1	0.94	0.23	79,79,79,79	0
56	MG	14	3144	1/1	0.94	0.30	58,58,58,58	0
56	MG	14	3054	1/1	0.94	0.09	83,83,83,83	0
56	MG	14	3016	1/1	0.94	0.18	60,60,60,60	0
56	MG	13	1701	1/1	0.94	0.17	121,121,121,121	0
56	MG	1H	3068	1/1	0.94	0.12	56,56,56,56	0
56	MG	1H	3229	1/1	0.94	0.13	45,45,45,45	0
56	MG	1H	3146	1/1	0.94	0.19	59,59,59,59	0
56	MG	14	3104	1/1	0.94	0.10	64,64,64,64	0
56	MG	1G	1607	1/1	0.94	0.12	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1608	1/1	0.94	0.06	101,101,101,101	0
56	MG	1H	3069	1/1	0.94	0.13	60,60,60,60	0
56	MG	1H	3006	1/1	0.94	0.14	61,61,61,61	0
56	MG	1H	3071	1/1	0.94	0.16	56,56,56,56	0
56	MG	14	3112	1/1	0.94	0.18	61,61,61,61	0
56	MG	14	3026	1/1	0.94	0.26	68,68,68,68	0
56	MG	1H	3286	1/1	0.94	0.09	64,64,64,64	0
56	MG	1H	3235	1/1	0.94	0.14	85,85,85,85	0
56	MG	1H	3193	1/1	0.94	0.25	72,72,72,72	0
56	MG	13	1613	1/1	0.94	0.14	77,77,77,77	0
56	MG	1H	3074	1/1	0.94	0.20	69,69,69,69	0
56	MG	1H	3060	1/1	0.94	0.18	52,52,52,52	0
56	MG	1H	3029	1/1	0.94	0.29	69,69,69,69	0
56	MG	1H	3077	1/1	0.94	0.09	63,63,63,63	0
56	MG	14	3077	1/1	0.94	0.13	60,60,60,60	0
56	MG	1H	3095	1/1	0.94	0.15	73,73,73,73	0
56	MG	1H	3001	1/1	0.94	0.23	53,53,53,53	0
56	MG	14	3040	1/1	0.94	0.31	84,84,84,84	0
56	MG	14	3041	1/1	0.94	0.09	49,49,49,49	0
56	MG	14	3042	1/1	0.94	0.16	58,58,58,58	0
56	MG	14	3043	1/1	0.94	0.14	52,52,52,52	0
56	MG	14	3085	1/1	0.94	0.26	51,51,51,51	0
56	MG	1H	3245	1/1	0.94	0.24	74,74,74,74	0
56	MG	14	3045	1/1	0.94	0.20	64,64,64,64	0
56	MG	14	3270	1/1	0.94	0.25	84,84,84,84	0
56	MG	1G	1623	1/1	0.94	0.19	83,83,83,83	0
56	MG	1H	3117	1/1	0.94	0.18	82,82,82,82	0
56	MG	13	1619	1/1	0.94	0.16	69,69,69,69	0
56	MG	14	3136	1/1	0.94	0.13	62,62,62,62	0
56	MG	13	1616	1/1	0.94	0.29	77,77,77,77	0
56	MG	1H	3066	1/1	0.94	0.10	48,48,48,48	0
56	MG	1H	3122	1/1	0.94	0.16	50,50,50,50	0
56	MG	14	3052	1/1	0.94	0.13	71,71,71,71	0
56	MG	14	3279	1/1	0.94	0.09	73,73,73,73	0
56	MG	14	3065	1/1	0.95	0.10	68,68,68,68	0
56	MG	14	3092	1/1	0.95	0.06	75,75,75,75	0
56	MG	13	1680	1/1	0.95	0.33	87,87,87,87	0
56	MG	1H	3082	1/1	0.95	0.17	65,65,65,65	0
56	MG	14	3151	1/1	0.95	0.33	81,81,81,81	0
56	MG	1H	3129	1/1	0.95	0.07	56,56,56,56	0
56	MG	1H	3145	1/1	0.95	0.24	77,77,77,77	0
56	MG	13	1659	1/1	0.95	0.10	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3027	1/1	0.95	0.26	71,71,71,71	0
56	MG	1H	3247	1/1	0.95	0.20	73,73,73,73	0
56	MG	14	3187	1/1	0.95	0.21	75,75,75,75	0
56	MG	1H	3103	1/1	0.95	0.10	51,51,51,51	0
56	MG	1H	3148	1/1	0.95	0.11	49,49,49,49	0
56	MG	1H	3026	1/1	0.95	0.28	50,50,50,50	0
56	MG	1H	3105	1/1	0.95	0.13	64,64,64,64	0
56	MG	1H	3168	1/1	0.95	0.09	65,65,65,65	0
56	MG	14	3034	1/1	0.95	0.25	74,74,74,74	0
56	MG	14	3035	1/1	0.95	0.26	84,84,84,84	0
56	MG	14	3108	1/1	0.95	0.10	75,75,75,75	0
56	MG	1H	3057	1/1	0.95	0.18	52,52,52,52	0
56	MG	14	3138	1/1	0.95	0.18	55,55,55,55	0
56	MG	13	1682	1/1	0.95	0.07	73,73,73,73	0
56	MG	13	1666	1/1	0.95	0.05	89,89,89,89	0
56	MG	13	1618	1/1	0.95	0.07	97,97,97,97	0
56	MG	1H	3111	1/1	0.95	0.12	60,60,60,60	0
56	MG	1H	3022	1/1	0.95	0.13	52,52,52,52	0
56	MG	14	3063	1/1	0.95	0.10	77,77,77,77	0
56	MG	14	3089	1/1	0.95	0.22	54,54,54,54	0
57	PAR	13	1730	42/42	0.95	0.08	67,77,86,91	0
56	MG	1H	3421	1/1	0.95	0.09	83,83,83,83	0
56	MG	1G	1678	1/1	0.96	0.07	92,92,92,92	0
56	MG	13	1723	1/1	0.96	0.10	73,73,73,73	0
56	MG	L8	101	1/1	0.96	0.35	88,88,88,88	0
56	MG	1H	3387	1/1	0.96	0.08	72,72,72,72	0
56	MG	1H	3399	1/1	0.96	0.06	91,91,91,91	0
56	MG	14	3241	1/1	0.96	0.26	68,68,68,68	0
56	MG	1H	3414	1/1	0.96	0.07	83,83,83,83	0
56	MG	1H	3237	1/1	0.96	0.08	77,77,77,77	0
56	MG	14	3185	1/1	0.96	0.08	74,74,74,74	0
56	MG	14	3186	1/1	0.96	0.43	83,83,83,83	0
56	MG	1H	3109	1/1	0.96	0.06	59,59,59,59	0
56	MG	1H	3154	1/1	0.96	0.28	69,69,69,69	0
56	MG	14	3006	1/1	0.96	0.30	58,58,58,58	0
56	MG	13	1728	1/1	0.96	0.07	127,127,127,127	0
56	MG	14	3311	1/1	0.96	0.12	83,83,83,83	0
56	MG	14	3340	1/1	0.96	0.07	83,83,83,83	0
56	MG	14	3137	1/1	0.96	0.07	62,62,62,62	0
56	MG	1H	3139	1/1	0.96	0.13	64,64,64,64	0
56	MG	1H	3073	1/1	0.96	0.10	47,47,47,47	0
56	MG	1H	3190	1/1	0.96	0.24	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3063	1/1	0.96	0.12	55,55,55,55	0
56	MG	14	3225	1/1	0.96	0.07	71,71,71,71	0
56	MG	1H	3004	1/1	0.96	0.11	41,41,41,41	0
56	MG	13	1614	1/1	0.96	0.03	81,81,81,81	0
56	MG	1H	3056	1/1	0.96	0.15	40,40,40,40	0
56	MG	1H	3078	1/1	0.96	0.07	57,57,57,57	0
56	MG	13	1634	1/1	0.96	0.16	53,53,53,53	0
56	MG	13	1635	1/1	0.96	0.07	54,54,54,54	0
56	MG	1H	3149	1/1	0.96	0.33	65,65,65,65	0
56	MG	13	1657	1/1	0.96	0.09	80,80,80,80	0
56	MG	13	1658	1/1	0.96	0.04	82,82,82,82	0
57	PAR	1G	1681	42/42	0.96	0.07	79,90,98,101	0
56	MG	1H	3374	1/1	0.96	0.08	88,88,88,88	0
56	MG	14	3282	1/1	0.97	0.43	84,84,84,84	0
56	MG	14	3074	1/1	0.97	0.13	45,45,45,45	0
56	MG	1G	1674	1/1	0.97	0.04	123,123,123,123	0
56	MG	1G	1676	1/1	0.97	0.07	111,111,111,111	0
56	MG	13	1725	1/1	0.97	0.10	102,102,102,102	0
56	MG	1G	1679	1/1	0.97	0.10	138,138,138,138	0
56	MG	14	3317	1/1	0.97	0.07	64,64,64,64	0
56	MG	14	3334	1/1	0.97	0.06	85,85,85,85	0
56	MG	14	3338	1/1	0.97	0.10	111,111,111,111	0
56	MG	1H	3344	1/1	0.97	0.09	75,75,75,75	0
56	MG	14	3341	1/1	0.97	0.05	94,94,94,94	0
56	MG	14	3358	1/1	0.97	0.04	64,64,64,64	0
56	MG	14	3365	1/1	0.97	0.04	88,88,88,88	0
56	MG	14	3367	1/1	0.97	0.06	94,94,94,94	0
56	MG	14	3370	1/1	0.97	0.05	99,99,99,99	0
56	MG	14	3371	1/1	0.97	0.04	72,72,72,72	0
56	MG	14	3379	1/1	0.97	0.10	107,107,107,107	0
56	MG	1G	1655	1/1	0.97	0.12	94,94,94,94	0
56	MG	1H	3023	1/1	0.97	0.36	57,57,57,57	0
56	MG	1H	3091	1/1	0.97	0.05	61,61,61,61	0
56	MG	1H	3266	1/1	0.97	0.09	60,60,60,60	0
56	MG	14	3084	1/1	0.97	0.15	73,73,73,73	0
56	MG	1J	205	1/1	0.97	0.10	109,109,109,109	0
56	MG	1H	3267	1/1	0.97	0.13	69,69,69,69	0
56	MG	1H	3389	1/1	0.97	0.08	64,64,64,64	0
56	MG	1H	3116	1/1	0.97	0.07	56,56,56,56	0
56	MG	1H	3408	1/1	0.97	0.04	80,80,80,80	0
56	MG	1H	3413	1/1	0.97	0.06	107,107,107,107	0
56	MG	13	1732	1/1	0.97	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3037	1/1	0.97	0.34	63,63,63,63	0
56	MG	1G	1650	1/1	0.97	0.08	91,91,91,91	0
56	MG	1H	3423	1/1	0.97	0.09	147,147,147,147	0
56	MG	13	1707	1/1	0.97	0.04	85,85,85,85	0
56	MG	14	3118	1/1	0.97	0.06	66,66,66,66	0
56	MG	1G	1671	1/1	0.97	0.07	90,90,90,90	0
59	ZN	C5	202	1/1	0.97	0.06	165,165,165,165	0
56	MG	1H	3418	1/1	0.98	0.05	88,88,88,88	0
56	MG	1H	3330	1/1	0.98	0.04	60,60,60,60	0
56	MG	14	3352	1/1	0.98	0.04	78,78,78,78	0
56	MG	P8	101	1/1	0.98	0.04	78,78,78,78	0
56	MG	14	3360	1/1	0.98	0.04	75,75,75,75	0
56	MG	1H	3343	1/1	0.98	0.05	65,65,65,65	0
56	MG	14	3366	1/1	0.98	0.08	92,92,92,92	0
56	MG	1G	1672	1/1	0.98	0.10	121,121,121,121	0
56	MG	1H	3424	1/1	0.98	0.06	89,89,89,89	0
56	MG	1H	3427	1/1	0.98	0.04	84,84,84,84	0
56	MG	13	1705	1/1	0.98	0.04	94,94,94,94	0
56	MG	1H	3348	1/1	0.98	0.07	100,100,100,100	0
56	MG	1H	3358	1/1	0.98	0.06	68,68,68,68	0
56	MG	13	1609	1/1	0.98	0.08	73,73,73,73	0
56	MG	1H	3373	1/1	0.98	0.04	82,82,82,82	0
56	MG	1H	3144	1/1	0.98	0.03	54,54,54,54	0
56	MG	1J	204	1/1	0.98	0.09	99,99,99,99	0
56	MG	1H	3120	1/1	0.98	0.10	41,41,41,41	0
56	MG	1H	3386	1/1	0.98	0.04	52,52,52,52	0
56	MG	13	1724	1/1	0.98	0.04	108,108,108,108	0
56	MG	1H	3388	1/1	0.98	0.06	63,63,63,63	0
56	MG	1H	3279	1/1	0.98	0.09	51,51,51,51	0
56	MG	1H	3391	1/1	0.98	0.03	107,107,107,107	0
56	MG	13	1714	1/1	0.98	0.04	104,104,104,104	0
56	MG	13	1727	1/1	0.98	0.05	115,115,115,115	0
56	MG	14	3106	1/1	0.98	0.37	69,69,69,69	0
56	MG	1H	3409	1/1	0.98	0.04	86,86,86,86	0
56	MG	1H	3233	1/1	0.98	0.05	50,50,50,50	0
56	MG	14	3209	1/1	0.98	0.11	67,67,67,67	0
56	MG	14	3336	1/1	0.98	0.04	77,77,77,77	0
56	MG	1H	3328	1/1	0.98	0.04	52,52,52,52	0
56	MG	1H	3367	1/1	0.99	0.04	71,71,71,71	0
56	MG	1H	3369	1/1	0.99	0.03	69,69,69,69	0
56	MG	1H	3372	1/1	0.99	0.04	53,53,53,53	0
56	MG	13	1708	1/1	0.99	0.04	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	13	1709	1/1	0.99	0.03	94,94,94,94	0
56	MG	1H	3376	1/1	0.99	0.03	60,60,60,60	0
56	MG	1H	3377	1/1	0.99	0.05	77,77,77,77	0
56	MG	1H	3378	1/1	0.99	0.03	68,68,68,68	0
56	MG	1G	1669	1/1	0.99	0.05	82,82,82,82	0
56	MG	1G	1670	1/1	0.99	0.03	88,88,88,88	0
56	MG	1H	3379	1/1	0.99	0.02	61,61,61,61	0
56	MG	13	1726	1/1	0.99	0.03	82,82,82,82	0
56	MG	1G	1673	1/1	0.99	0.04	85,85,85,85	0
56	MG	1H	3381	1/1	0.99	0.04	59,59,59,59	0
56	MG	1G	1675	1/1	0.99	0.04	116,116,116,116	0
56	MG	1H	3382	1/1	0.99	0.02	60,60,60,60	0
56	MG	1G	1677	1/1	0.99	0.04	119,119,119,119	0
56	MG	1H	3383	1/1	0.99	0.03	65,65,65,65	0
56	MG	1H	3384	1/1	0.99	0.04	109,109,109,109	0
56	MG	1G	1680	1/1	0.99	0.03	120,120,120,120	0
56	MG	1H	3385	1/1	0.99	0.04	78,78,78,78	0
56	MG	13	1711	1/1	0.99	0.05	92,92,92,92	0
56	MG	13	1712	1/1	0.99	0.03	78,78,78,78	0
56	MG	13	1729	1/1	0.99	0.05	103,103,103,103	0
56	MG	14	3001	1/1	0.99	0.02	51,51,51,51	0
56	MG	13	1713	1/1	0.99	0.02	88,88,88,88	0
56	MG	1H	3390	1/1	0.99	0.04	88,88,88,88	0
56	MG	13	1703	1/1	0.99	0.09	70,70,70,70	0
56	MG	1H	3392	1/1	0.99	0.03	71,71,71,71	0
56	MG	1H	3393	1/1	0.99	0.06	70,70,70,70	0
56	MG	1H	3395	1/1	0.99	0.03	74,74,74,74	0
56	MG	1H	3396	1/1	0.99	0.02	58,58,58,58	0
56	MG	1H	3397	1/1	0.99	0.03	71,71,71,71	0
56	MG	1H	3398	1/1	0.99	0.03	83,83,83,83	0
56	MG	13	1715	1/1	0.99	0.03	100,100,100,100	0
56	MG	1H	3404	1/1	0.99	0.08	64,64,64,64	0
56	MG	1H	3405	1/1	0.99	0.06	52,52,52,52	0
56	MG	1H	3406	1/1	0.99	0.04	65,65,65,65	0
56	MG	1H	3407	1/1	0.99	0.03	86,86,86,86	0
56	MG	14	3313	1/1	0.99	0.04	64,64,64,64	0
56	MG	14	3314	1/1	0.99	0.04	73,73,73,73	0
56	MG	14	3316	1/1	0.99	0.02	67,67,67,67	0
56	MG	13	1717	1/1	0.99	0.05	74,74,74,74	0
56	MG	14	3318	1/1	0.99	0.06	71,71,71,71	0
56	MG	14	3319	1/1	0.99	0.07	62,62,62,62	0
56	MG	14	3320	1/1	0.99	0.03	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3321	1/1	0.99	0.05	73,73,73,73	0
56	MG	14	3322	1/1	0.99	0.04	72,72,72,72	0
56	MG	14	3324	1/1	0.99	0.05	77,77,77,77	0
56	MG	14	3329	1/1	0.99	0.03	55,55,55,55	0
56	MG	14	3330	1/1	0.99	0.03	65,65,65,65	0
56	MG	14	3332	1/1	0.99	0.05	64,64,64,64	0
56	MG	14	3333	1/1	0.99	0.04	79,79,79,79	0
56	MG	1H	3329	1/1	0.99	0.04	59,59,59,59	0
56	MG	1H	3410	1/1	0.99	0.04	53,53,53,53	0
56	MG	14	3337	1/1	0.99	0.05	79,79,79,79	0
56	MG	1H	3411	1/1	0.99	0.03	100,100,100,100	0
56	MG	1H	3412	1/1	0.99	0.04	68,68,68,68	0
56	MG	13	1718	1/1	0.99	0.04	67,67,67,67	0
56	MG	14	3342	1/1	0.99	0.05	94,94,94,94	0
56	MG	14	3344	1/1	0.99	0.04	95,95,95,95	0
56	MG	14	3345	1/1	0.99	0.07	118,118,118,118	0
56	MG	14	3347	1/1	0.99	0.06	77,77,77,77	0
56	MG	14	3348	1/1	0.99	0.03	83,83,83,83	0
56	MG	14	3349	1/1	0.99	0.03	90,90,90,90	0
56	MG	14	3350	1/1	0.99	0.06	76,76,76,76	0
56	MG	1H	3333	1/1	0.99	0.07	63,63,63,63	0
56	MG	14	3353	1/1	0.99	0.06	69,69,69,69	0
56	MG	14	3354	1/1	0.99	0.08	87,87,87,87	0
56	MG	14	3355	1/1	0.99	0.04	92,92,92,92	0
56	MG	14	3357	1/1	0.99	0.08	77,77,77,77	0
56	MG	1H	3415	1/1	0.99	0.04	94,94,94,94	0
56	MG	1H	3416	1/1	0.99	0.09	104,104,104,104	0
56	MG	14	3361	1/1	0.99	0.04	60,60,60,60	0
56	MG	14	3362	1/1	0.99	0.04	77,77,77,77	0
56	MG	14	3364	1/1	0.99	0.05	73,73,73,73	0
56	MG	1H	3334	1/1	0.99	0.04	51,51,51,51	0
56	MG	1H	3419	1/1	0.99	0.02	73,73,73,73	0
56	MG	1H	3420	1/1	0.99	0.10	76,76,76,76	0
56	MG	14	3369	1/1	0.99	0.11	84,84,84,84	0
56	MG	1H	3335	1/1	0.99	0.03	50,50,50,50	0
56	MG	1H	3422	1/1	0.99	0.05	100,100,100,100	0
56	MG	14	3373	1/1	0.99	0.03	87,87,87,87	0
56	MG	14	3374	1/1	0.99	0.04	129,129,129,129	0
56	MG	14	3375	1/1	0.99	0.05	111,111,111,111	0
56	MG	14	3376	1/1	0.99	0.03	90,90,90,90	0
56	MG	14	3377	1/1	0.99	0.05	60,60,60,60	0
56	MG	14	3378	1/1	0.99	0.02	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3338	1/1	0.99	0.03	59,59,59,59	0
56	MG	14	3380	1/1	0.99	0.02	83,83,83,83	0
56	MG	1H	3341	1/1	0.99	0.03	57,57,57,57	0
56	MG	1H	3425	1/1	0.99	0.04	92,92,92,92	0
56	MG	13	1719	1/1	0.99	0.05	86,86,86,86	0
56	MG	13	1720	1/1	0.99	0.13	115,115,115,115	0
56	MG	1H	3345	1/1	0.99	0.05	58,58,58,58	0
56	MG	1H	3346	1/1	0.99	0.08	63,63,63,63	0
56	MG	13	1721	1/1	0.99	0.03	79,79,79,79	0
56	MG	1H	3350	1/1	0.99	0.05	72,72,72,72	0
56	MG	1H	3352	1/1	0.99	0.05	71,71,71,71	0
56	MG	1H	3354	1/1	0.99	0.11	65,65,65,65	0
56	MG	1H	3356	1/1	0.99	0.03	61,61,61,61	0
56	MG	1H	3357	1/1	0.99	0.03	58,58,58,58	0
56	MG	13	1706	1/1	0.99	0.05	87,87,87,87	0
56	MG	16	209	1/1	0.99	0.04	64,64,64,64	0
56	MG	16	210	1/1	0.99	0.09	81,81,81,81	0
56	MG	16	211	1/1	0.99	0.06	85,85,85,85	0
56	MG	13	1704	1/1	0.99	0.04	85,85,85,85	0
56	MG	1H	3360	1/1	0.99	0.02	57,57,57,57	0
58	SF4	3E	302	8/8	0.99	0.05	76,86,96,96	0
58	SF4	32	301	8/8	0.99	0.03	92,113,120,129	0
56	MG	1H	3364	1/1	0.99	0.04	56,56,56,56	0
59	ZN	5A	101	1/1	0.99	0.04	139,139,139,139	0
56	MG	1H	3365	1/1	0.99	0.03	54,54,54,54	0
56	MG	14	3356	1/1	1.00	0.05	98,98,98,98	0
56	MG	13	1716	1/1	1.00	0.02	88,88,88,88	0
56	MG	1H	3400	1/1	1.00	0.05	52,52,52,52	0
56	MG	14	3359	1/1	1.00	0.03	55,55,55,55	0
56	MG	14	3315	1/1	1.00	0.06	71,71,71,71	0
56	MG	1H	3401	1/1	1.00	0.03	55,55,55,55	0
56	MG	1H	3402	1/1	1.00	0.04	60,60,60,60	0
56	MG	14	3363	1/1	1.00	0.01	51,51,51,51	0
56	MG	1H	3403	1/1	1.00	0.03	61,61,61,61	0
56	MG	1H	3355	1/1	1.00	0.02	58,58,58,58	0
56	MG	1H	3342	1/1	1.00	0.04	59,59,59,59	0
56	MG	13	1710	1/1	1.00	0.03	72,72,72,72	0
56	MG	14	3368	1/1	1.00	0.04	49,49,49,49	0
56	MG	1H	3331	1/1	1.00	0.02	51,51,51,51	0
56	MG	14	3323	1/1	1.00	0.03	66,66,66,66	0
56	MG	1H	3336	1/1	1.00	0.04	49,49,49,49	0
56	MG	14	3372	1/1	1.00	0.02	87,87,87,87	0

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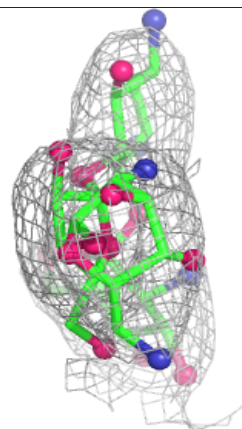
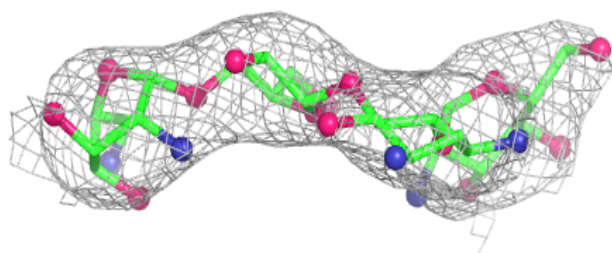
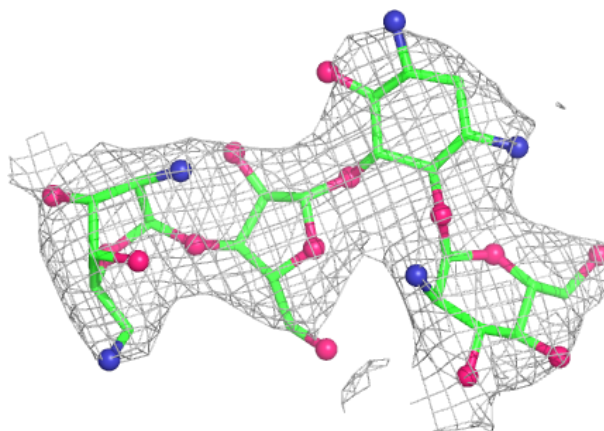
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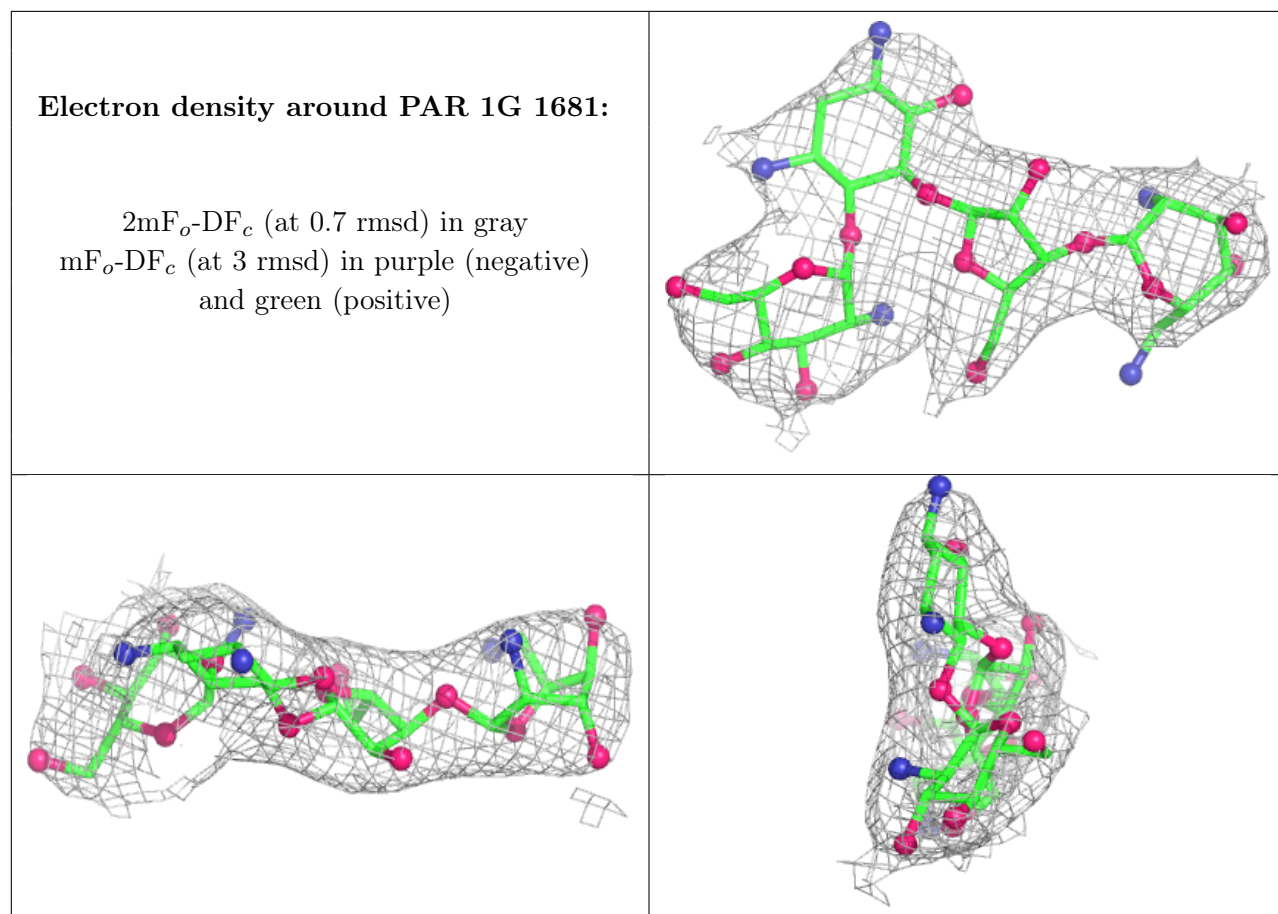
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3325	1/1	1.00	0.03	76,76,76,76	0
56	MG	14	3326	1/1	1.00	0.02	61,61,61,61	0
56	MG	14	3327	1/1	1.00	0.02	84,84,84,84	0
56	MG	14	3328	1/1	1.00	0.05	64,64,64,64	0
56	MG	1H	3337	1/1	1.00	0.05	55,55,55,55	0
56	MG	1H	3361	1/1	1.00	0.03	82,82,82,82	0
56	MG	14	3331	1/1	1.00	0.06	63,63,63,63	0
56	MG	1H	3362	1/1	1.00	0.02	64,64,64,64	0
56	MG	1H	3363	1/1	1.00	0.03	69,69,69,69	0
56	MG	1H	3347	1/1	1.00	0.02	78,78,78,78	0
56	MG	14	3335	1/1	1.00	0.02	63,63,63,63	0
56	MG	1H	3332	1/1	1.00	0.02	66,66,66,66	0
56	MG	1H	3366	1/1	1.00	0.11	59,59,59,59	0
56	MG	1H	3349	1/1	1.00	0.03	74,74,74,74	0
56	MG	14	3339	1/1	1.00	0.02	64,64,64,64	0
56	MG	1H	3417	1/1	1.00	0.01	62,62,62,62	0
56	MG	I8	101	1/1	1.00	0.04	59,59,59,59	0
56	MG	1H	3368	1/1	1.00	0.04	57,57,57,57	0
56	MG	14	3343	1/1	1.00	0.02	71,71,71,71	0
56	MG	1H	3339	1/1	1.00	0.02	70,70,70,70	0
56	MG	1H	3370	1/1	1.00	0.01	76,76,76,76	0
56	MG	14	3346	1/1	1.00	0.01	64,64,64,64	0
56	MG	1H	3371	1/1	1.00	0.02	63,63,63,63	0
56	MG	1H	3394	1/1	1.00	0.05	60,60,60,60	0
56	MG	1H	3351	1/1	1.00	0.02	73,73,73,73	0
56	MG	1H	3340	1/1	1.00	0.03	58,58,58,58	0
56	MG	14	3351	1/1	1.00	0.02	65,65,65,65	0
56	MG	1H	3353	1/1	1.00	0.03	53,53,53,53	0
59	ZN	5I	102	1/1	1.00	0.02	99,99,99,99	0
56	MG	1H	3426	1/1	1.00	0.03	54,54,54,54	0
56	MG	1H	3375	1/1	1.00	0.02	67,67,67,67	0
56	MG	14	3312	1/1	1.00	0.05	70,70,70,70	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 1730:

$2mF_o-DF_c$ (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.