



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 10:56 am BST

PDB ID : 4WSD
Title : Complex of 70S ribosome with tRNA-Phe and mRNA with C-A mismatch in the second position in the A-site and with antibiotic paromomycin.
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-10-27
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

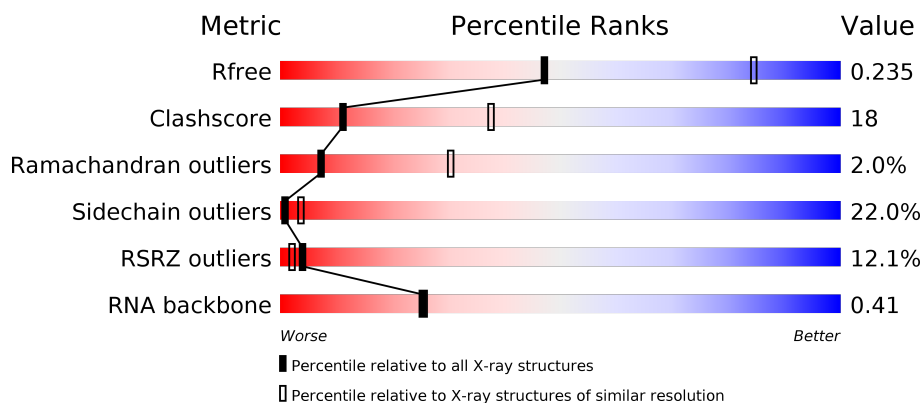
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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 on 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	 30% 44% 20% 5%
1	1G	1522	 4% 31% 45% 19%
2	12	256	 8% 38% 40% 13% 7%
2	1E	256	 7% 39% 44% 9% 7%

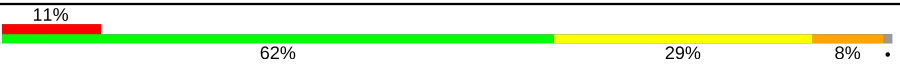

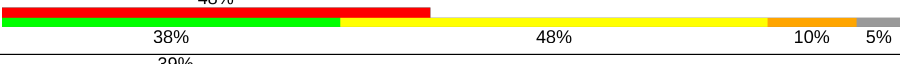
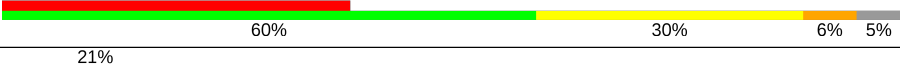
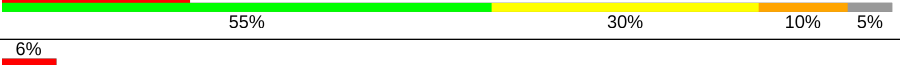

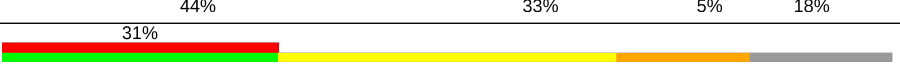
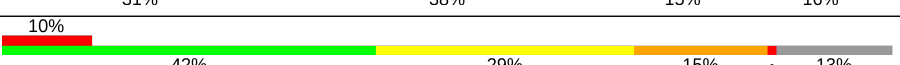
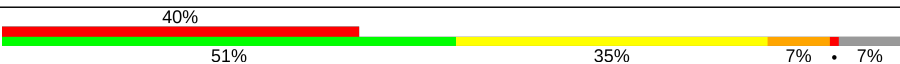



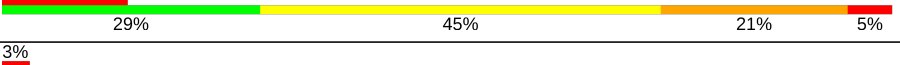
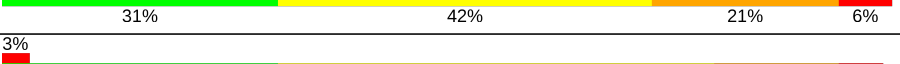
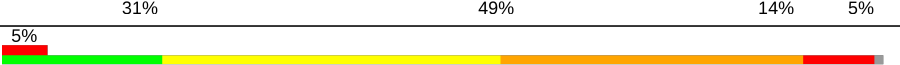


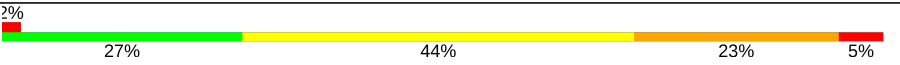
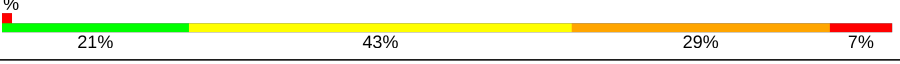
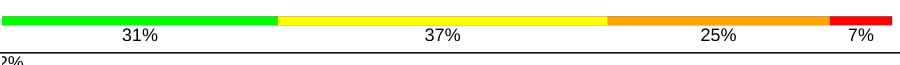
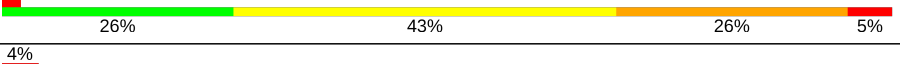

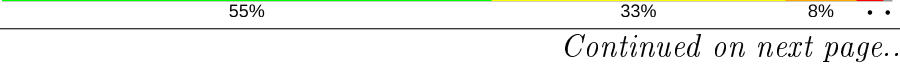


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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	77	
23	2L	77	
24	3K	76	
25	4K	30	
25	4L	30	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	11	276	
28	19	276	

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Mol	Chain	Length	Quality of chain
29	21	206	
29	29	206	
30	31	210	
30	39	210	
31	41	182	
31	49	182	
32	51	180	
32	59	180	
33	61	148	
33	69	148	
34	15	140	
34	58	140	
35	25	122	
35	68	122	
36	35	150	
36	78	150	
37	45	141	
37	88	141	
38	55	118	
38	98	118	
39	65	112	
39	A8	112	
40	75	146	
40	B8	146	
41	85	118	

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Mol	Chain	Length	Quality of chain
41	C8	118	
42	95	101	
42	D8	101	
43	A5	113	
43	E8	113	
44	B5	96	
44	F8	96	
45	C5	110	
45	G8	110	
46	D5	206	
46	H8	206	
47	E5	85	
47	I8	85	
48	F5	98	
48	J8	98	
49	G5	72	
49	K8	72	
50	H5	60	
50	L8	60	
51	I5	71	
51	M8	71	
52	J5	60	
52	N8	60	
53	K5	54	
53	O8	54	

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Mol	Chain	Length	Quality of chain
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	
56	1L	76	
57	3L	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	13	1710	-	-	-	X
58	MG	14	3143	-	-	-	X
58	MG	14	3158	-	-	-	X
58	MG	14	3193	-	-	-	X
58	MG	1H	3020	-	-	-	X
58	MG	1H	3056	-	-	-	X
58	MG	1H	3162	-	-	-	X
58	MG	1H	3247	-	-	-	X
58	MG	1H	3254	-	-	-	X
58	MG	1H	3262	-	-	-	X
58	MG	1H	3310	-	-	-	X
58	MG	1H	3334	-	-	-	X
58	MG	1H	3337	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300252 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1498	Total	C	N	O	P	0	0	0
			32207	14334	5973	10402	1498			
1	1G	1498	Total	C	N	O	P	0	0	0
			32204	14334	5973	10400	1497			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	12	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- 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	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	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	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	42	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	101	Total	C	N	O	S	0	0	0
			842	531	155	153	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	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			
7	62	152	Total	C	N	O	S	0	0	0
			1243	774	249	214	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	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O	0	0	0
			1009	639	197	173			
9	82	124	Total	C	N	O	0	0	0
			983	624	190	169			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1A	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
11	2A	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	3A	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	118	Total	C	N	O	S	0	0	0
			938	580	193	163	2			
13	4A	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4I	119	ALA	GLY	conflict	UNP P80377
4A	119	ALA	GLY	conflict	UNP P80377

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	5A	58	Total	C	N	O	S	0	0	0
			475	303	99	69	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			
15	6A	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	84	Total	C	N	O	S	0	0	0
			705	446	140	118	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	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	72	Total	C	N	O	0	0	0
			590	376	117	97			
18	9A	72	Total	C	N	O	0	0	0
			590	376	117	97			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	81	Total	C	N	O	S	0	0	0
			647	413	119	113	2			
19	AA	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	1B	25	Total	C	N	O	0	0	0
			217	134	52	31			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	3K	75	Total	C	N	O	P	S	0	0	0
			1603	719	285	524	74	1			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	13	Total	C	N	O	P	0	0	0
			279	126	55	85	13			
25	4L	11	Total	C	N	O	P	0	0	0
			235	106	45	73	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
26	14	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			

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

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
28	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	21	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
29	29	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
30	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
32	59	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
33	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
34	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
35	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	78	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			
36	35	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	88	138	Total	C	N	O	S	0	0	0
			1086	693	208	179	6			
37	45	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
38	55	117	Total	C	N	O		0	0	0
			959	599	202	158				

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
39	65	111	Total	C	N	O	0	0	0
			881	556	176	149			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
40	75	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
41	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
42	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	E8	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			
43	A5	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	F8	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			
44	B5	94	Total	C	N	O		0	0	0
			735	477	133	125				

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	G8	104	Total	C	N	O	S	0	0	0
			791	510	149	127	5			
45	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
46	D5	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	80	Total	C	N	O	S	0	0	0
			626	388	132	105	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	E5	77	Total	C	N	O	S	0	0	0
			612	379	129	103	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I8	6	ALA	GLY	conflict	UNP P60493
I8	8	ALA	GLY	conflict	UNP P60493
E5	6	ALA	GLY	conflict	UNP P60493
E5	8	ALA	GLY	conflict	UNP P60493

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	J8	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			
48	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	K8	67	Total	C	N	O	S	0	0	0
			563	349	114	99	1			
49	G5	67	Total	C	N	O	S	0	0	0
			563	349	114	99	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	L8	57	Total	C	N	O	0	0	0
			452	288	88	76			
50	H5	59	Total	C	N	O	0	0	0
			468	298	90	80			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M8	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
51	I5	60	Total	C	N	O	S	0	0	0
			481	305	84	87	5			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	N8	58	Total	C	N	O	S	0	0	0
			453	285	89	74	5			
52	J5	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
53	K5	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	P8	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			
54	L5	46	Total	C	N	O	S	0	0	0
			398	245	98	53	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Q8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
55	M5	60	Total	C	N	O	S	0	0	0
			477	303	98	74	2			

- Molecule 56 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	76	Total	C	N	O	P S	0	0	0
			1627	730	290	531	75 1			

- Molecule 57 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	3L	76	Total	C	N	O	P S	0	0	0
			1624	725	290	532	76 1			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

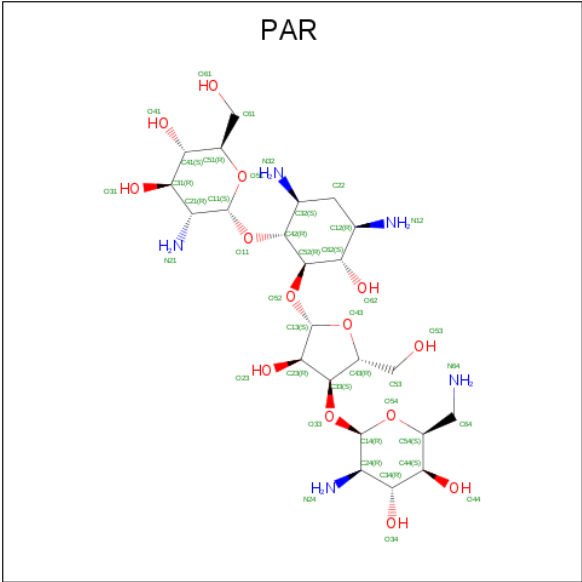
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	98	2	Total 2	Mg 2	0	0
58	P8	1	Total 1	Mg 1	0	0
58	J5	1	Total 1	Mg 1	0	0
58	C5	1	Total 1	Mg 1	0	0
58	2I	1	Total 1	Mg 1	0	0
58	13	148	Total 148	Mg 148	0	0
58	1J	5	Total 5	Mg 5	0	0
58	5I	2	Total 2	Mg 2	0	0
58	16	13	Total 13	Mg 13	0	0
58	25	1	Total 1	Mg 1	0	0
58	3K	1	Total 1	Mg 1	0	0
58	21	2	Total 2	Mg 2	0	0
58	2K	5	Total 5	Mg 5	0	0
58	L8	1	Total 1	Mg 1	0	0
58	I8	1	Total 1	Mg 1	0	0
58	2A	2	Total 2	Mg 2	0	0
58	5E	1	Total 1	Mg 1	0	0
58	29	4	Total 4	Mg 4	0	0
58	7A	1	Total 1	Mg 1	0	0
58	41	2	Total 2	Mg 2	0	0
58	78	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1G	96	Total 96	Mg 96	0	0
58	11	4	Total 4	Mg 4	0	0
58	1H	520	Total 520	Mg 520	0	0
58	88	2	Total 2	Mg 2	0	0
58	49	1	Total 1	Mg 1	0	0
58	14	407	Total 407	Mg 407	0	0
58	3E	2	Total 2	Mg 2	0	0
58	55	1	Total 1	Mg 1	0	0
58	3L	2	Total 2	Mg 2	0	0
58	4K	1	Total 1	Mg 1	0	0
58	1K	2	Total 2	Mg 2	0	0
58	G8	1	Total 1	Mg 1	0	0
58	2L	3	Total 3	Mg 3	0	0

- Molecule 59 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	13	1	Total	C	N	O	0	0
			42	23	5	14		
59	1G	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	32	1	Total	Zn	0	0
			1	1		
60	3E	1	Total	Zn	0	0
			1	1		
60	5I	1	Total	Zn	0	0
			1	1		
60	5A	1	Total	Zn	0	0
			1	1		
60	G8	1	Total	Zn	0	0
			1	1		
60	C5	1	Total	Zn	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	197	Total	O	0	0
			197	197		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	3E	3	Total 3	O 3	0	0
61	8E	2	Total 2	O 2	0	0
61	1I	2	Total 2	O 2	0	0
61	3I	1	Total 1	O 1	0	0
61	5I	2	Total 2	O 2	0	0
61	6I	1	Total 1	O 1	0	0
61	7I	1	Total 1	O 1	0	0
61	1K	5	Total 5	O 5	0	0
61	2K	6	Total 6	O 6	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	2	Total 2	O 2	0	0
61	1H	999	Total 999	O 999	0	0
61	16	21	Total 21	O 21	0	0
61	11	13	Total 13	O 13	0	0
61	21	4	Total 4	O 4	0	0
61	31	4	Total 4	O 4	0	0
61	58	2	Total 2	O 2	0	0
61	78	5	Total 5	O 5	0	0
61	B8	1	Total 1	O 1	0	0
61	C8	3	Total 3	O 3	0	0
61	D8	1	Total 1	O 1	0	0

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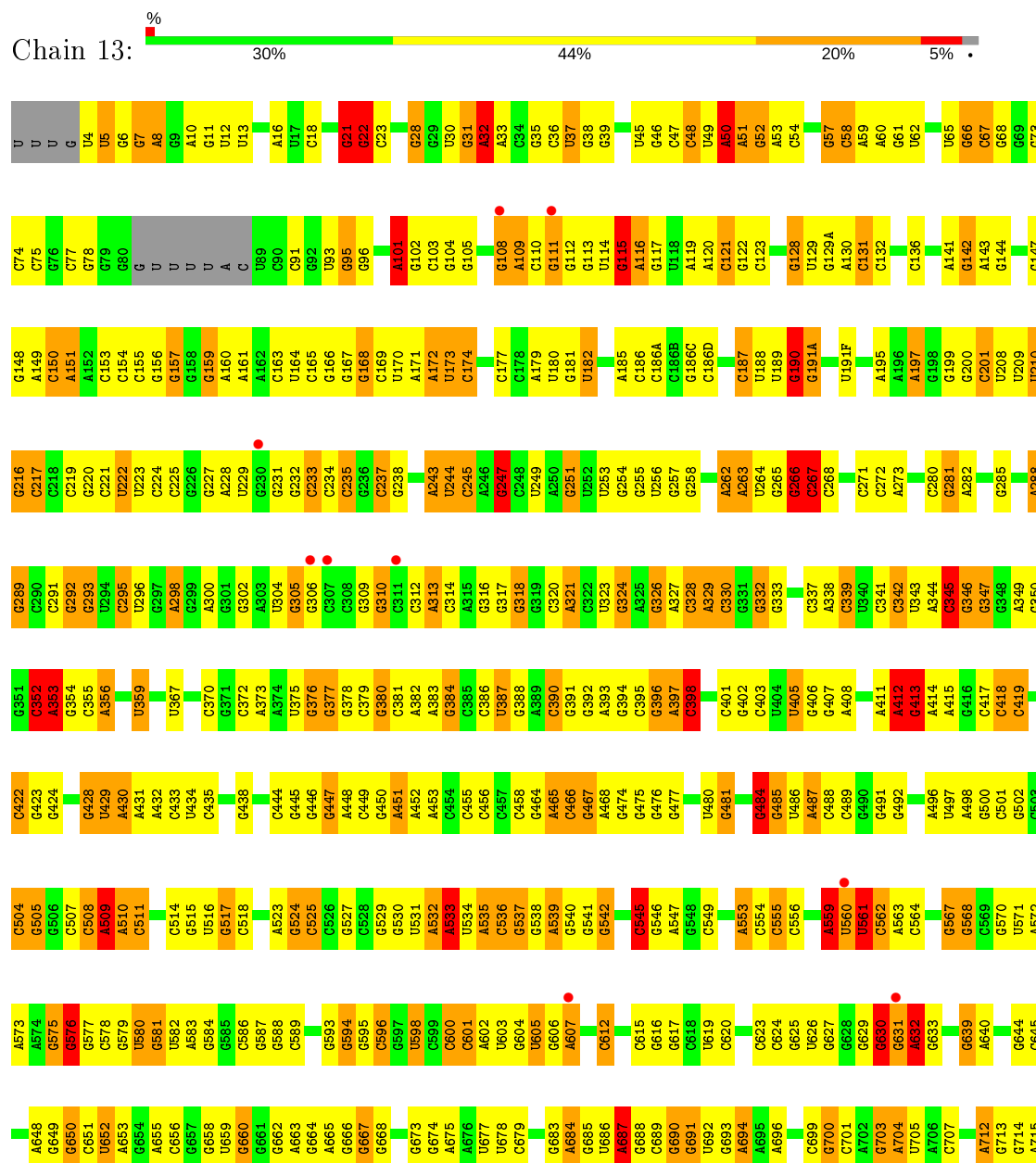
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	G8	4	Total 4	O 4	0	0
61	I8	7	Total 7	O 7	0	0
61	L8	1	Total 1	O 1	0	0
61	P8	1	Total 1	O 1	0	0
61	Q8	2	Total 2	O 2	0	0
61	1G	82	Total 82	O 82	0	0
61	7A	1	Total 1	O 1	0	0
61	BA	1	Total 1	O 1	0	0
61	3L	6	Total 6	O 6	0	0
61	14	598	Total 598	O 598	0	0
61	19	13	Total 13	O 13	0	0
61	39	7	Total 7	O 7	0	0
61	35	1	Total 1	O 1	0	0
61	85	1	Total 1	O 1	0	0
61	A5	1	Total 1	O 1	0	0
61	G5	1	Total 1	O 1	0	0
61	L5	1	Total 1	O 1	0	0

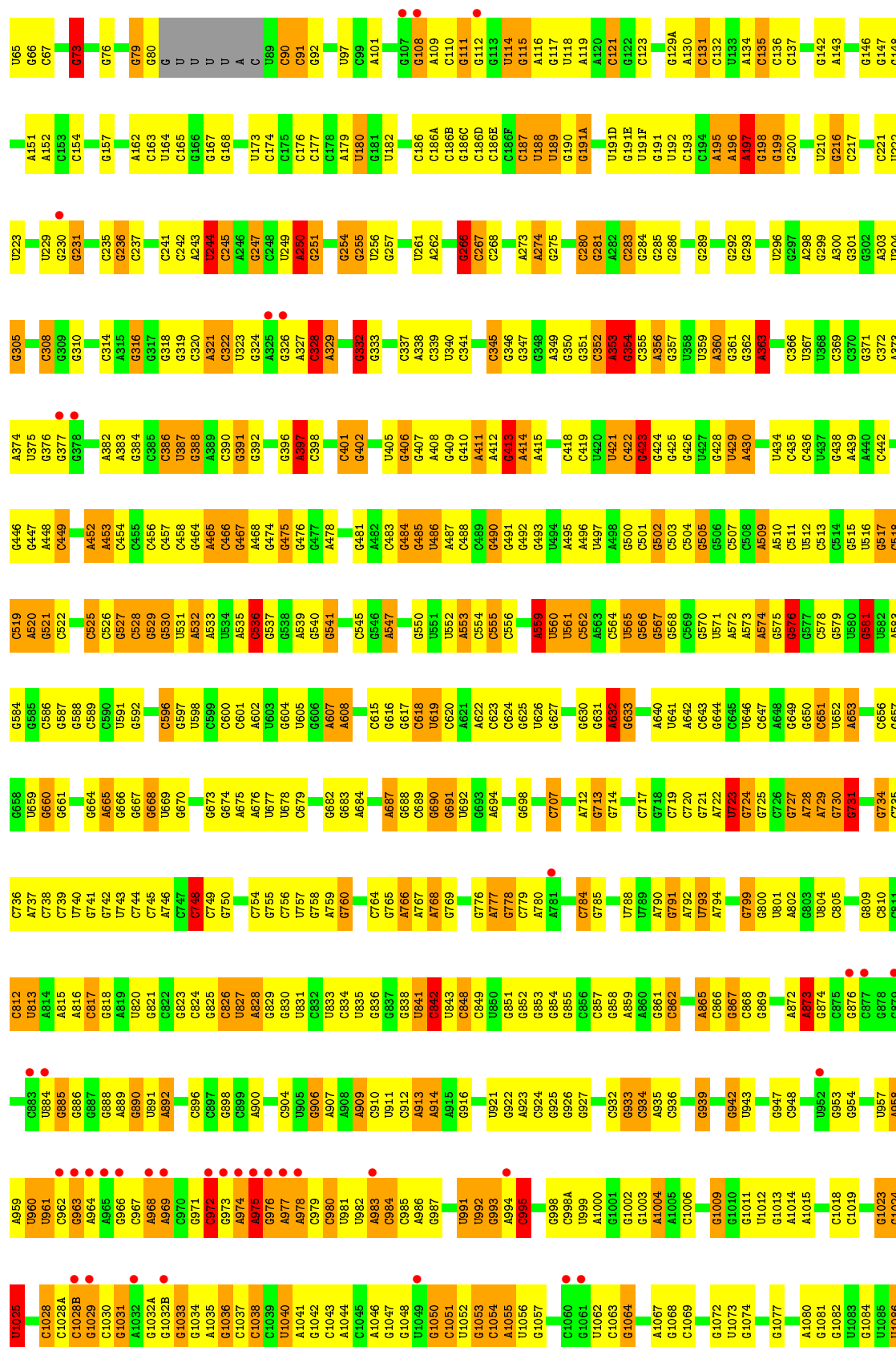
3 Residue-property plots [i](#)

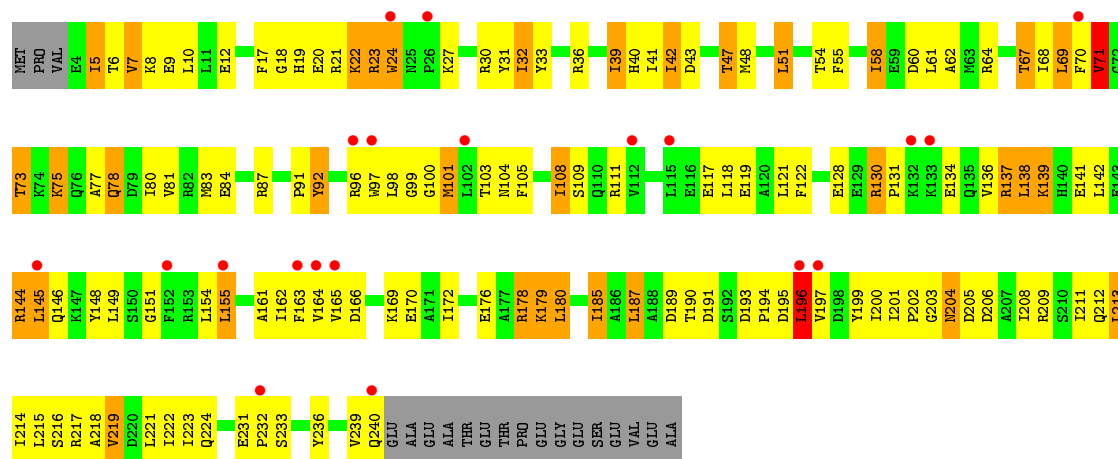
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

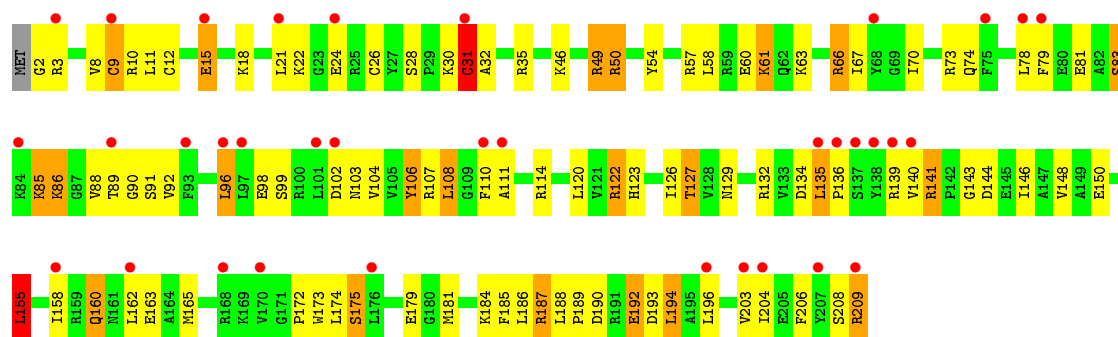
- Molecule 1: 16S ribosomal RNA



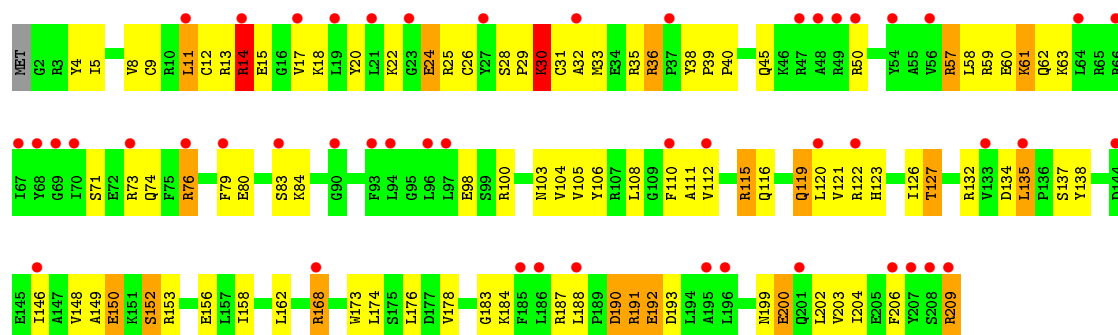








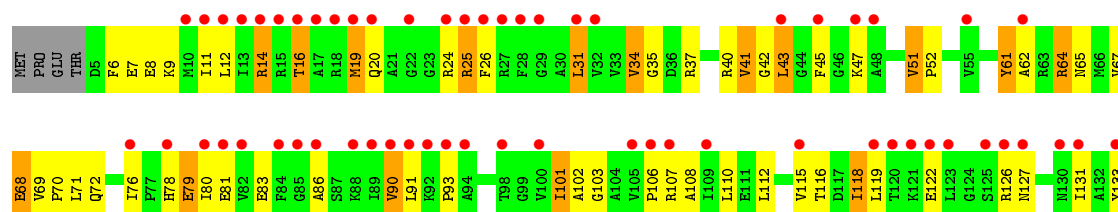
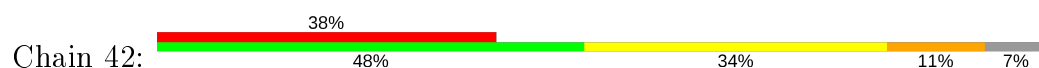
• Molecule 4: 30S ribosomal protein S4

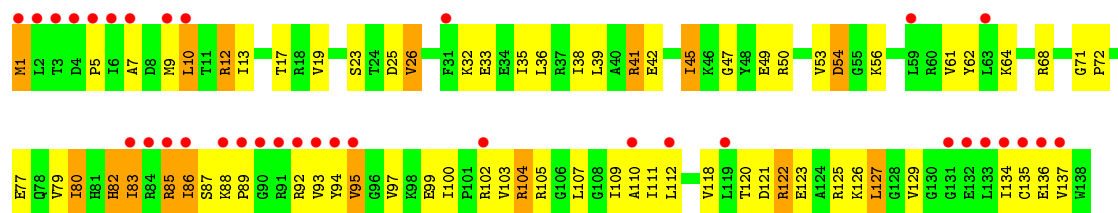


• Molecule 5: 30S ribosomal protein S5

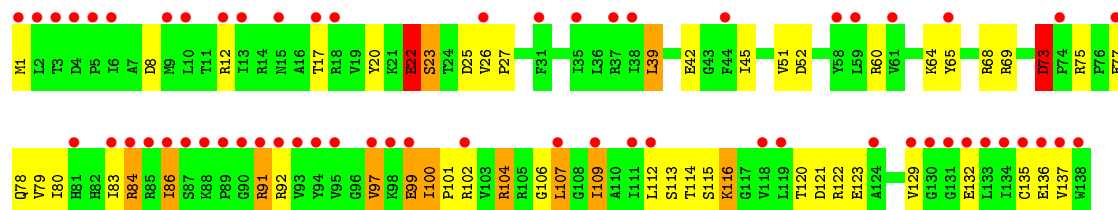
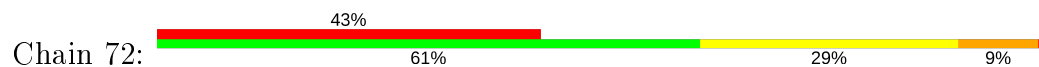


• Molecule 5: 30S ribosomal protein S5

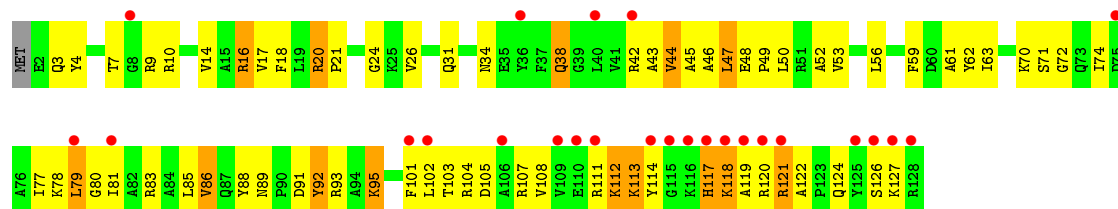




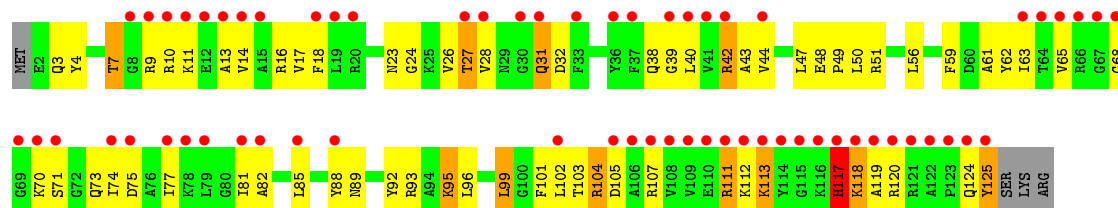
• Molecule 8: 30S ribosomal protein S8



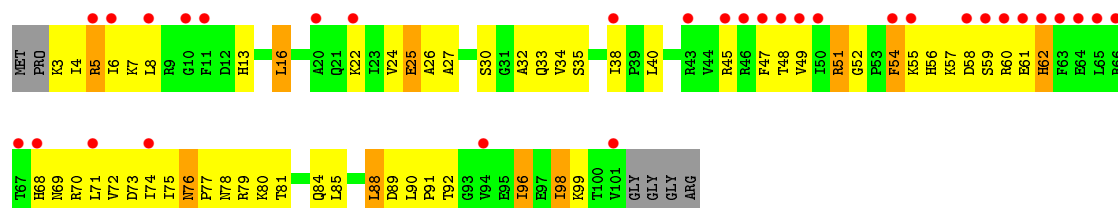
• Molecule 9: 30S ribosomal protein S9



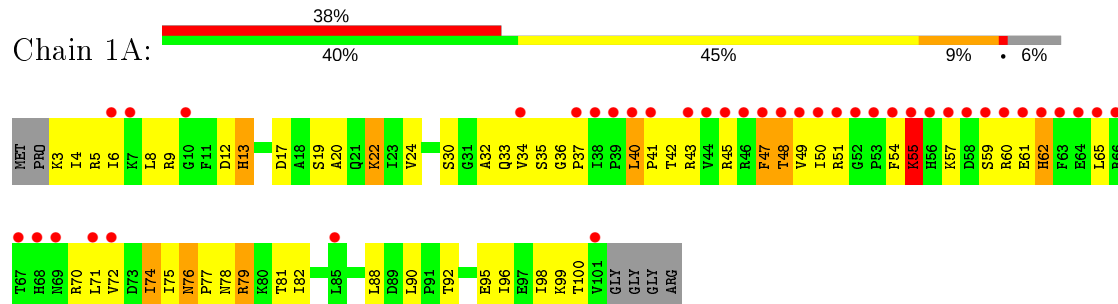
• Molecule 9: 30S ribosomal protein S9



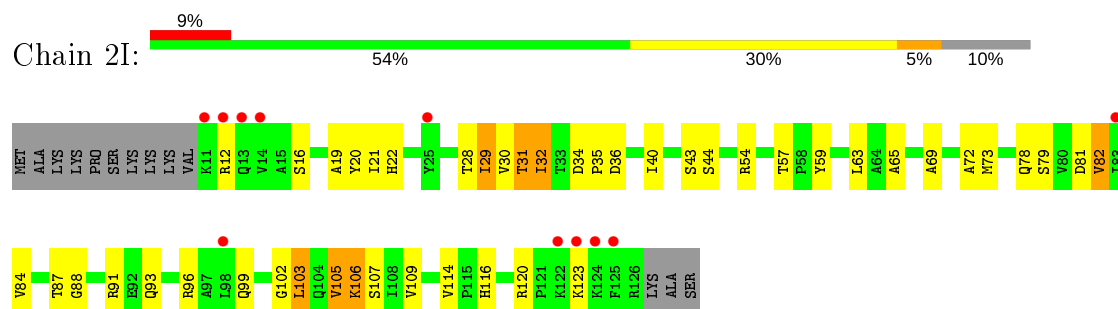
• Molecule 10: 30S ribosomal protein S10



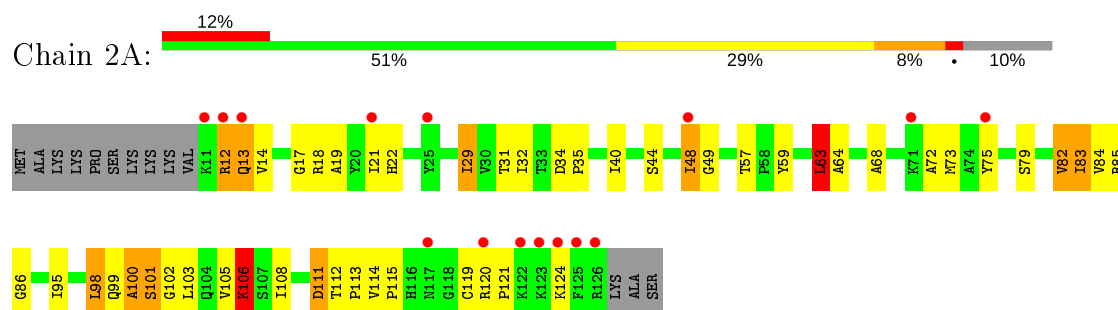
- Molecule 10: 30S ribosomal protein S10



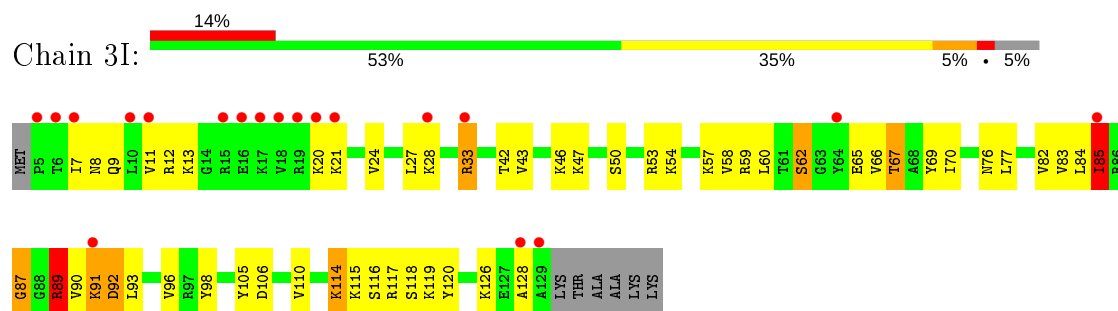
- Molecule 11: 30S ribosomal protein S11



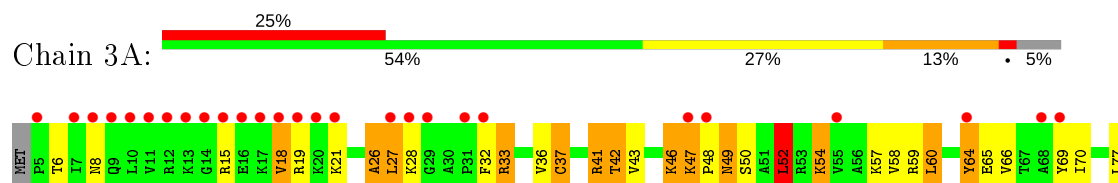
- Molecule 11: 30S ribosomal protein S11

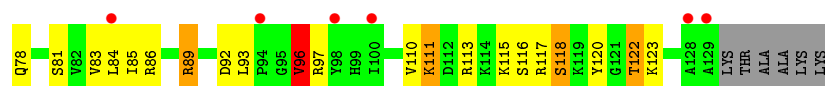


- Molecule 12: 30S ribosomal protein S12

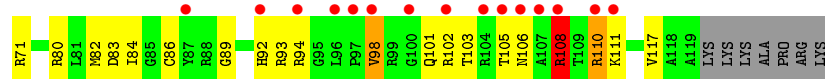
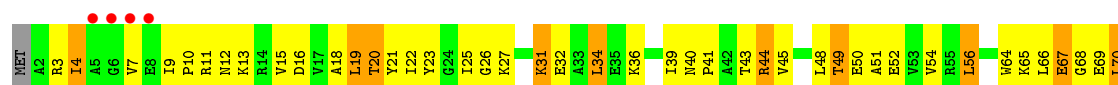
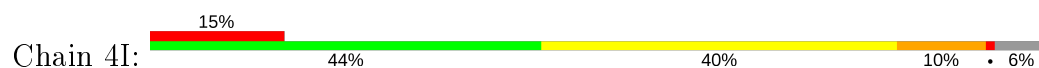


- Molecule 12: 30S ribosomal protein S12

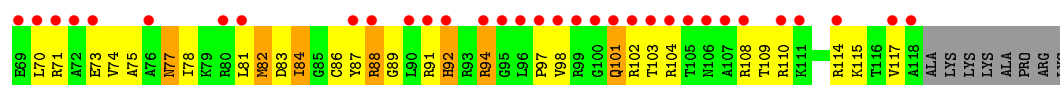
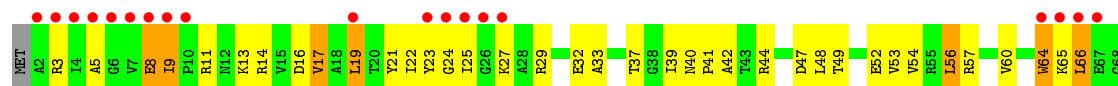
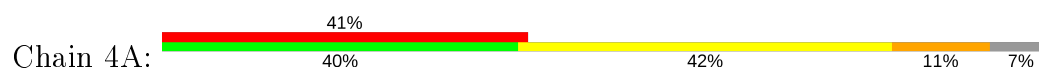




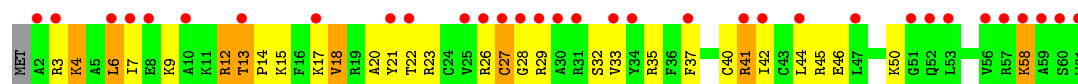
- Molecule 13: 30S ribosomal protein S13



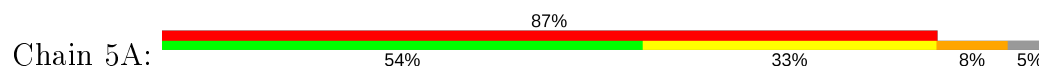
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



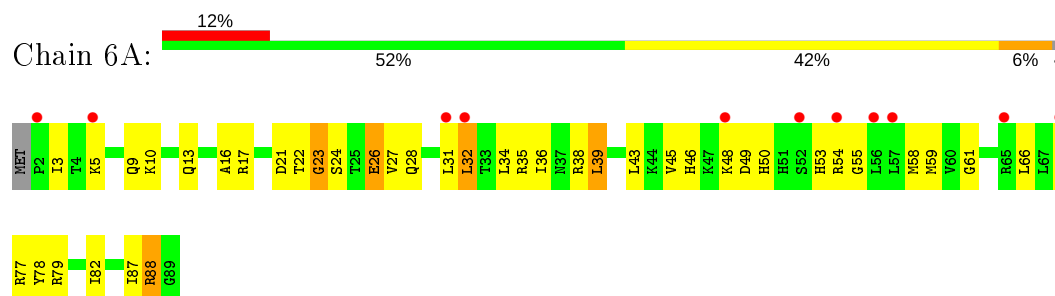
- Molecule 14: 30S ribosomal protein S14 type Z



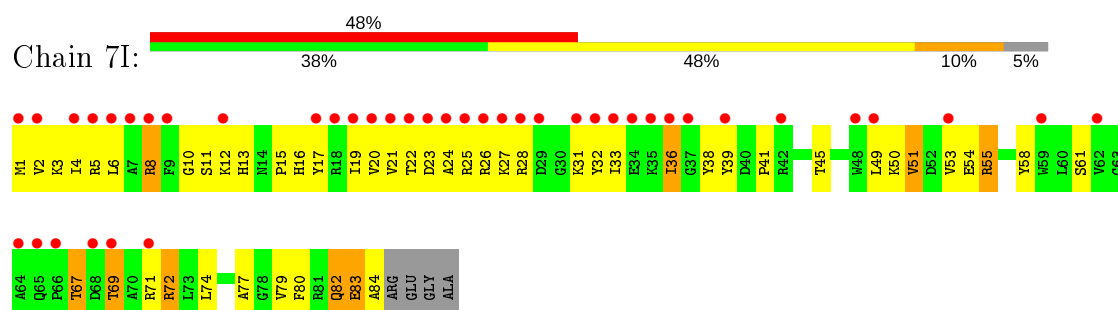
- Molecule 15: 30S ribosomal protein S15



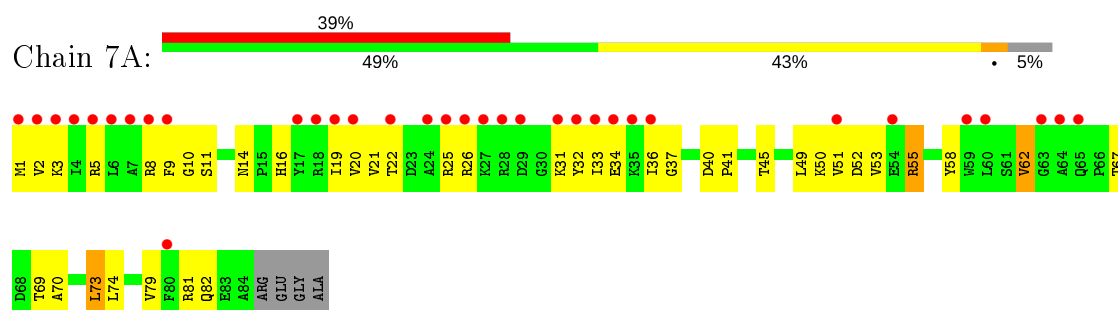
- Molecule 15: 30S ribosomal protein S15



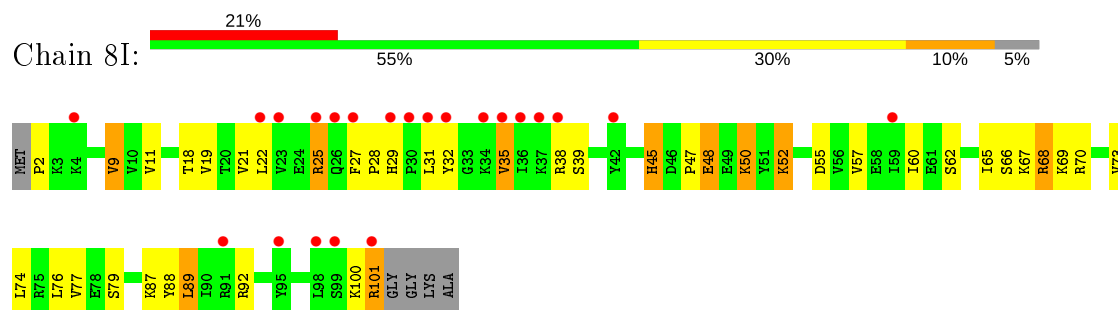
- Molecule 16: 30S ribosomal protein S16



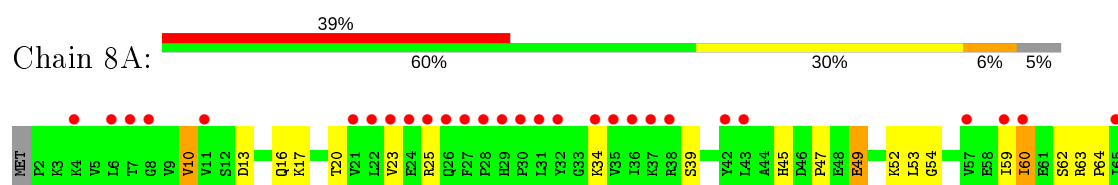
- Molecule 16: 30S ribosomal protein S16

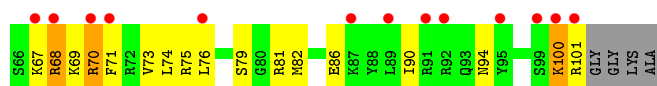


- Molecule 17: 30S ribosomal protein S17

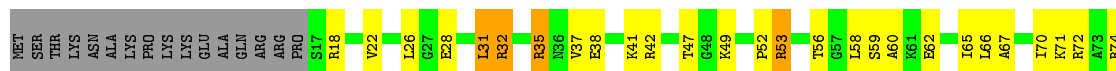


- Molecule 17: 30S ribosomal protein S17





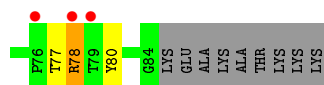
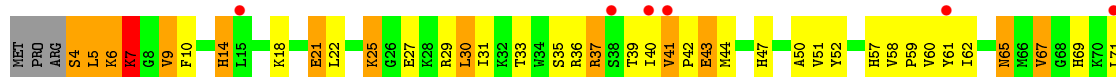
- Molecule 18: 30S ribosomal protein S18



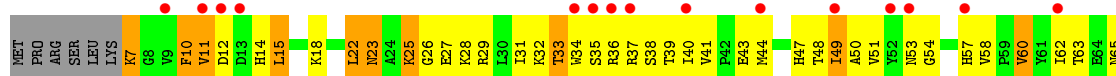
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

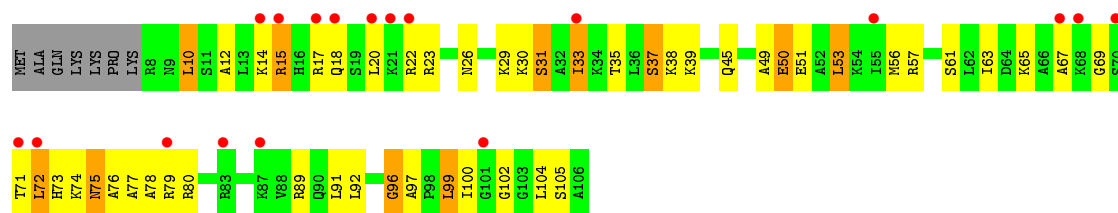


- Molecule 19: 30S ribosomal protein S19

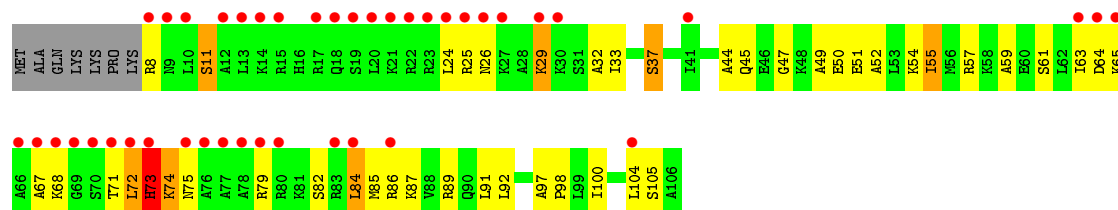
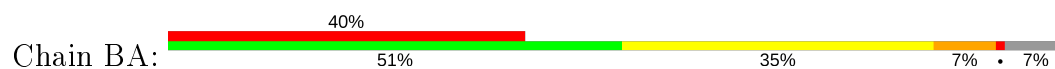


- Molecule 20: 30S ribosomal protein S20

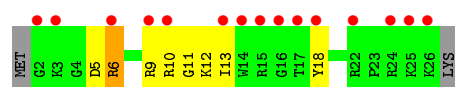




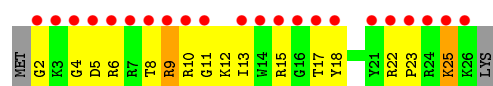
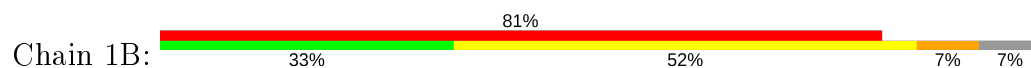
• Molecule 20: 30S ribosomal protein S20



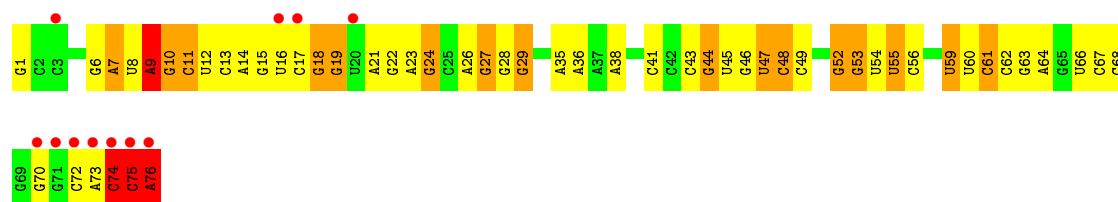
• Molecule 21: 30S ribosomal protein Thx



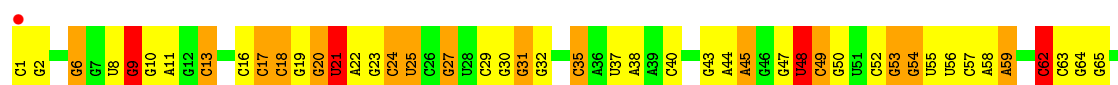
• Molecule 21: 30S ribosomal protein Thx



• Molecule 22: tRNA-Phe

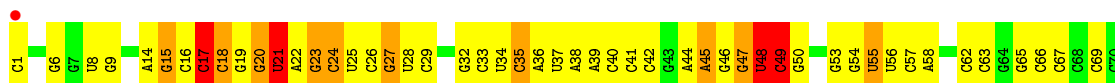


• Molecule 23: tRNA-fMet

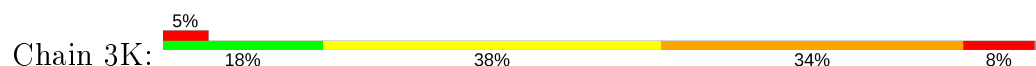




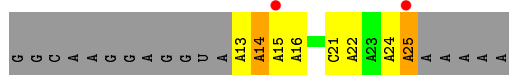
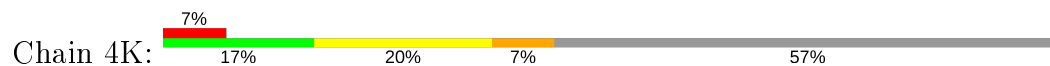
● Molecule 23: tRNA-fMet



● Molecule 24: tRNA-Phe



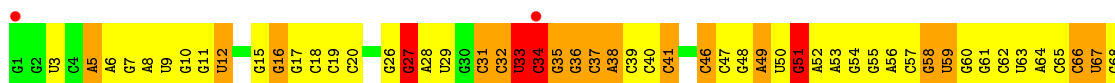
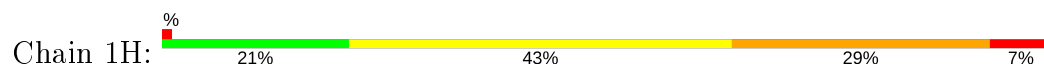
● Molecule 25: mRNA



● Molecule 25: mRNA



● Molecule 26: 23S ribosomal RNA



G977	G978	G979	G916	U851	C791	C729	G668	A627	U568	A502	G439	A374	U306	C263	A199	G130
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G979	G980	G981	A918	G853	A793	C731	A670	G629	G570	A504	U441	C376	G308	A285	C201	G132
G980	G981	G982	G919	G854	G732	C732	G671	G630	A571	A505	C377	C378	G309	G286	U202	G133
G981	G982	G983	G920	G855	G733	C733	G672	A631	A572	G506	A443	C379	A310	C203	C203	G134
G982	G983	G984	G921	G856	G734	C734	G673	A632	G573	A507	C444	C380	A311	A204	G205	G135
G983	G984	G985	G922	G857	A735	C735	G674	A633	G574	G508	C445	U380	G312	U270F	U206	G136
G984	G985	G986	G923	U858	A736	C736	A675	A634	C574	C509	G446	G381	G313	C270G	U207	G137
G985	G986	G987	C924	G859	C737	C737	A676	C635	A575	C510	G447	C382	G314	C270H	A207	G137A
G986	G987	G988	A926	U860	G738	C738	A677	G636	G576	U511	U448	U383	C316	G270I	C208	G138
G987	G988	G989	G928	G862	G739	C739	G678	A637	A578	G512	U449	U384	C317	G270J	C209	G139
G988	G989	G990	G929	G863	U802	C740	G679	G638	G579	A513	G450	C385	C318	G270K	C210	A140
G989	G990	G991	G930	A864	U803	G741	G680	U639	C580	A514	C451	G386	C319	U270L	A211	A141
G990	G991	G992	U830	G865	A804	G742	G681	C640	C581	A515	G452	U387	A320	U270M	G212	C141A
G991	G992	G993	G931	C865	G805	G743	G682	G641	G582	C516	C453	G388	G321	G270N	A213	G142
G992	G993	G994	G932	A866	G806	G744	G683	G642	U583	C517	A454	G389	A322	U270O	G214	C143
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G994	G995	G996	G933	U868	G808	U747	A685	A644	G585	U519	C456	G391	A324	G270Q	A216	G145
G995	G996	G997	G936	U869	G809	G748	G686	C645	A586	G520	A457	C392	G325	G270R	G217	G146
G996	G997	G998	A937	A870	U810	C749	G687	A646	C587	G521	G458	C393	G326	G270S	A218	U147
G997	G998	G999	U837	G871	U811	A750	U688	G647	U588	G522	U459	A394	G327	G270T	C222	U148
G998	G999	G1000	G938	G872	G812	A751	A689	G648	C589	C523	U460	U395	U328	G270Y	A223	A149
G999	G1000	G1001	A941	U873	U813	A752	G690	G649	G590	U524	C461	U396	G329	U270Z	G224	C150
G1000	G1001	G1002	G942	C814	C814	C753	G691	G650	G592	A525	C462	U397	A331	G271A	A225	C151
G1001	G1002	G1003	U943	C815	C816	C754	G692	G651	G593	U526	G463	U398	A332	G271B	G226	G152
G1002	G1003	G1004	G944	C817	C818	C755	G693	C652	U594	C527	U464	G400	A333	G271C	G227	C153
G1003	G1004	G1005	A945	G880	G819	G756	G694	A653	C595	A528	G465	A401	A334	G271D	G228	G154
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G1006	G1007	G1008	G948	G883	A820	G759	G697	A654B	G598	G531	G468	U405	A337	G271G	U162	C231
G1007	G1008	G1009	G949	C884	A821	G760	G698	G654C	G599	A532	G469	G406	C336	G271H	U163	U163
G1008	G1009	G1010	C949	G885	U822	A761	G699	G654D	G600	G533	A470	G407	C337	G271I	U164	U164
G1009	G1010	G1011	A950	C886	U823	U762	G700	C654E	G601	U534	A471	G408	U339	G271J	U165	C172
G1010	G1011	G1012	C951	G887	A824	G763	G701	G654F	G602	C535	A472	G409	A340	G271K	G172	G173
G1011	G1012	G1013	G952	C888	C825	A764	G702	G654G	A603	A536	G473	G410	A341	G271L	G236	G173
G1012	G1013	G1014	A953	G889	U826	G765	G703	A654H	G604	C537	G474	G411	G344	G271M	C237	G174
G1013	G1014	G1015	G954	U827	C827	C766	G704	A654I	G605	G539	U475	A412	G345	G271N	C238	G175
G1014	G1015	G1016	C955	U828	U828	U767	A705	G654J	C606	G540	C413	C414	G352	G271O	U239	G176
G1015	G1016	G1017	G956	C893	A829	G768	A706	G654K	U606	G541	C414	A415	G353	G271P	G240	G177
G1016	G1017	G1018	A957	G894	G830	G769	G707	G654L	U607	C542	A476	A416	G354	G271Q	A241	G178
G1017	G1019	G1020	U958	U895	G831	G770	U709	G654M	A608	C543	A477	G417	G355	G271R	G242	G179
G1019	G1020	G1021	A959	U896	G832	C771	G710	G654N	A609	C544	G481	C417	G356	G271S	G243	G180
G1020	G1021	G1022	C960	C834	U833	A774	G712	G654O	G609A	G545	A482	G418	G357	G271T	A244	A181
G1021	G1022	G1023	G961	C835	A835	G775	G713	C654P	C610	C611	A483	C287	A357	G271U	G245	G182
G1022	G1023	G1024	G962	U836	G836	C776	G714	G654Q	G612	G613	A484	C288	U358	G271V	G246	C183
G1023	G1024	G1025	C963	A900	C837	A777	U715	C654R	U614	U615	C485	A289	G361	G271W	U185	C184
G1024	G1026	G1027	C964	A901	C838	G778	G716	G654S	G615	G616	C486	G290	G362	G271X	G186	G187
G1026	G1027	G1028	G965	C902	U839	U779	G717	A655	G617	U617	G488	A294	U362	G271Y	G249	G188
G1027	G1028	G1029	G966	C903	C840	G780	A718	U657	G618	U619	G489	A295	A363A	G271Z	G250	G189
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G1029	G1030	G1031	U968	U907	G842	A782	C720	C659	G620	G621	A492	A428	G363C	G271B	G252	G189
G1030	G1031	G1032	C970	U908	G843	A783	C721	G660	G622	G623	A493	A429	G363D	G271C	G253	A190
G1031	G1032	G1033	C971	C904	A784	A784	C722	G661	G624	G625	G494	A430	C364	G271D	G254	A191
G1032	G1033	G1034	U1035	A910	G845	G785	G723	G662	A621	G622	A495	A432	C365	G271E	U193	C192
G1033	G1034	G1035	A911	C912	C846	C786	G724	G663	G623	G624	G496	A433	C366	G271F	G255	U194
G1034	G1035	G1036	U1036	G912	C847	U787	G725	G664	G625	G626	G497	A434	C367	G271G	G256	G195
G1035	G1036	G1037	C974	U913	G848	A788	G726	G665	G627	G628	G498	A435	C368	G271H	G261	A196
G1036	G1037	G1038	G975	C914	A849	A789	G727	G666	G629	G630	G499	A436	C369	G271I	G262	A197
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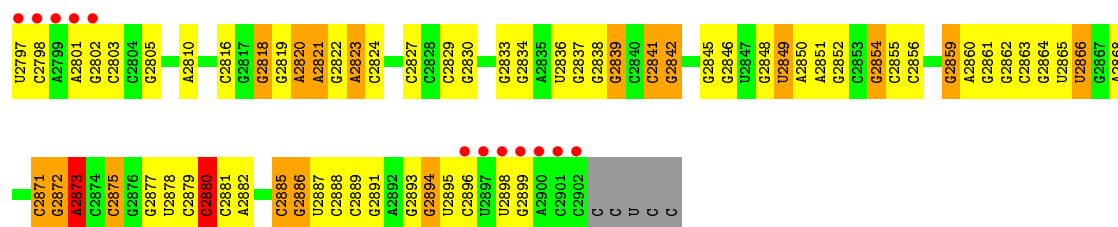
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A1901	G1823	A1762	C1671	A1611	C1548	G1485	G1423	U1300	G1238	A1174	U1105	G1044
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A1952	A1811	C1660	G1600	C1660	A1473	G1538	C1473	U1351	A1286	C1161	G1161	G1093
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C1957	G1816	A1755	A1664	C1664	A1477	G1543	A1477	G1356	C1291	G1165	C1166	A1098
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- Molecule 26: 23S ribosomal RNA



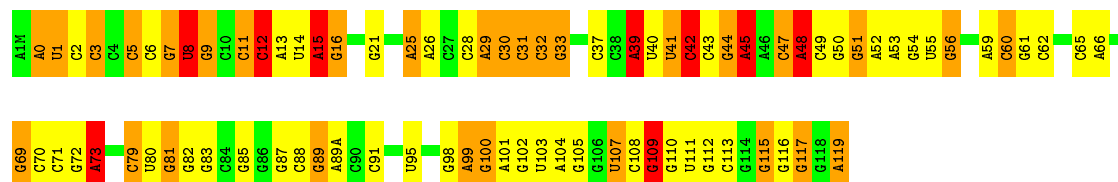
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A1803	G1728	G1649	C1585	G1517	A1449	G1382	G1319	A1254	C1041	G979	A917
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G1807	G1732	A1654	C1588	G1521	C1451	G1386	U1323	C1258	A1045	A983	G921
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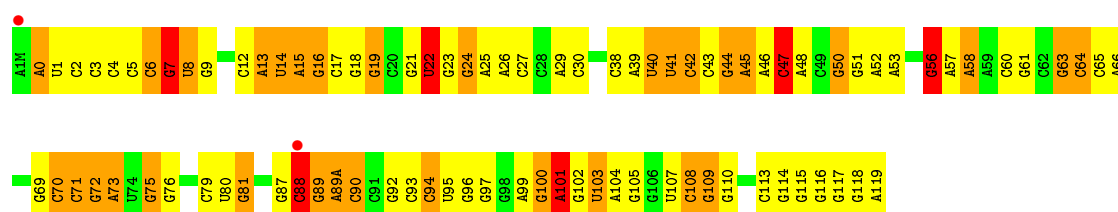
• Molecule 27: 5S ribosomal RNA

Chain 16: 31% 37% 25% 7%



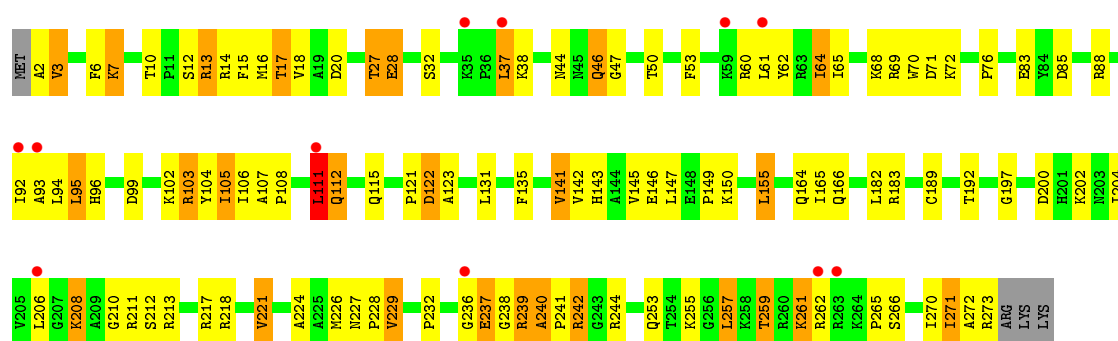
• Molecule 27: 5S ribosomal RNA

Chain 1J: 26% 43% 26% 5%



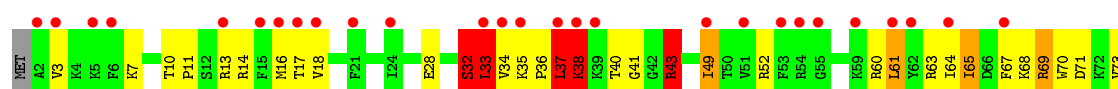
• Molecule 28: 50S ribosomal protein L2

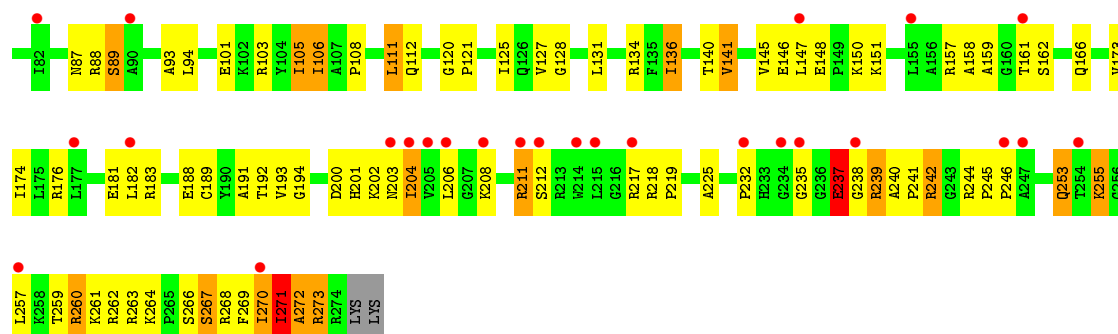
Chain 11: 4% 58% 31% 10%



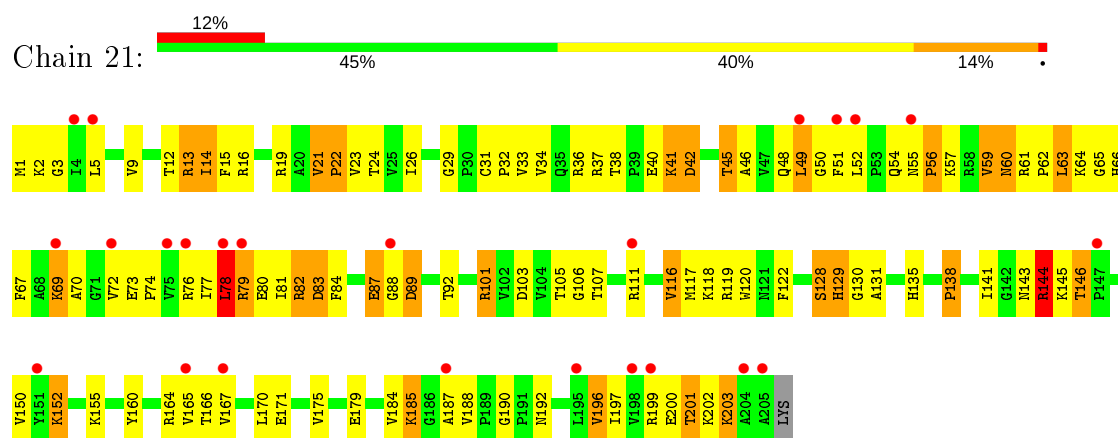
• Molecule 28: 50S ribosomal protein L2

Chain 19: 19% 55% 33% 8%

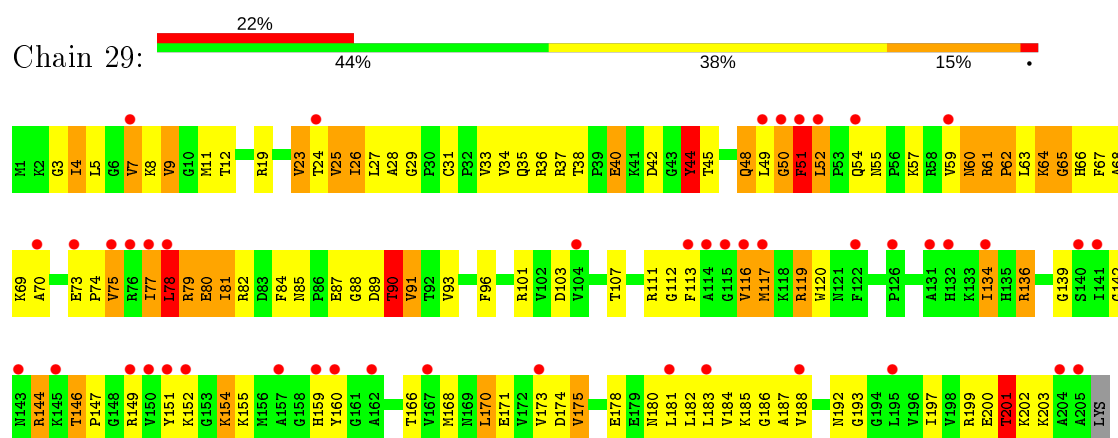




• Molecule 29: 50S ribosomal protein L3

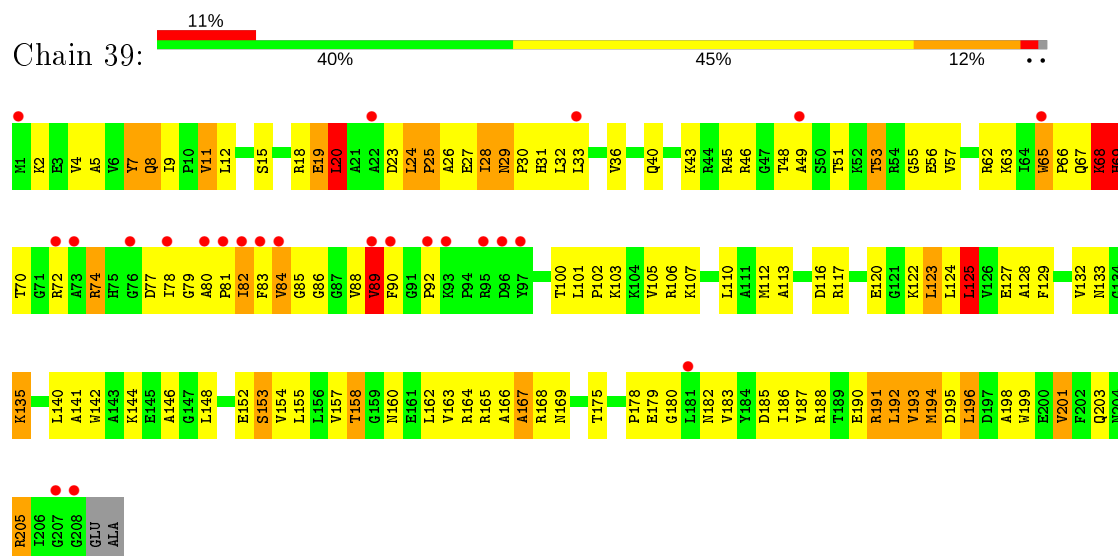


• Molecule 30: 50S ribosomal protein L4

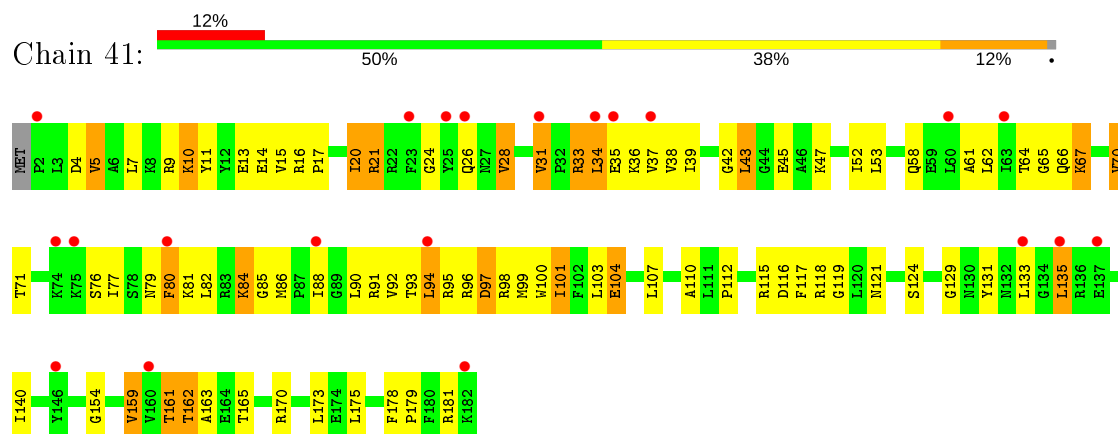




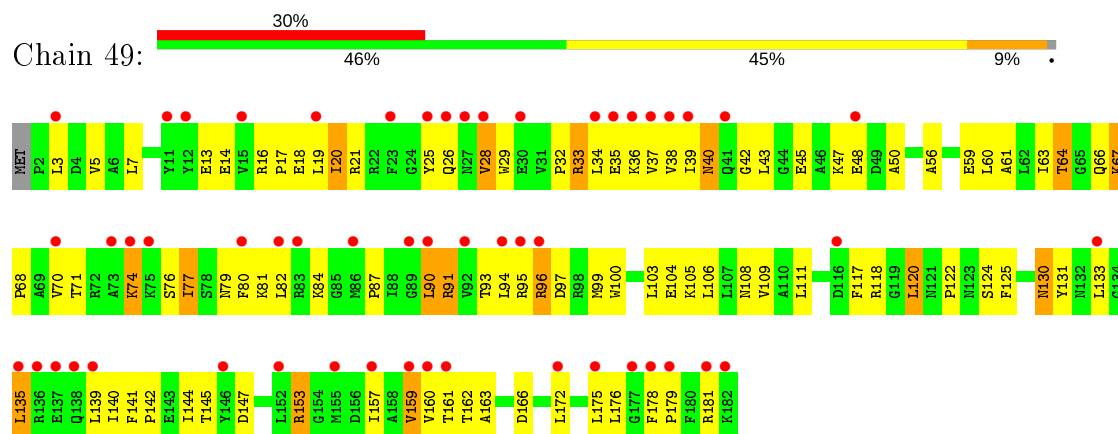
• Molecule 30: 50S ribosomal protein L4



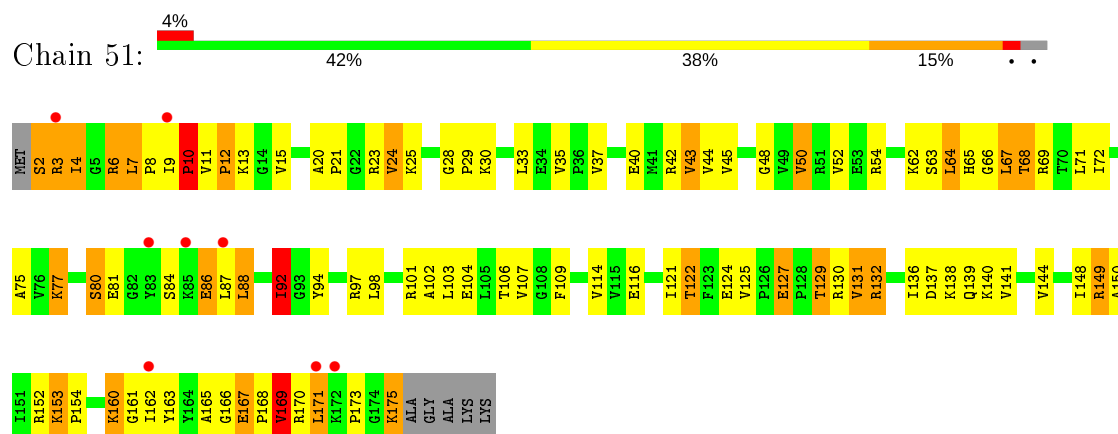
• Molecule 31: 50S ribosomal protein L5



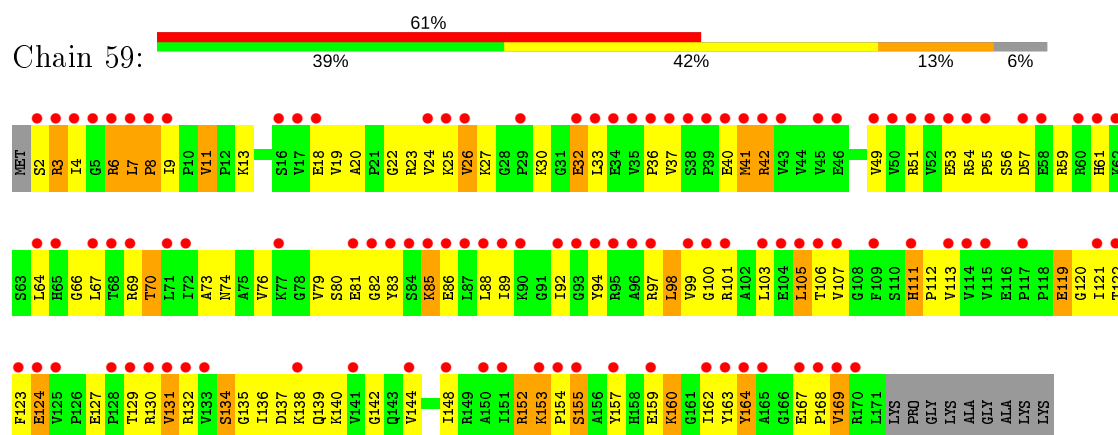
• Molecule 31: 50S ribosomal protein L5



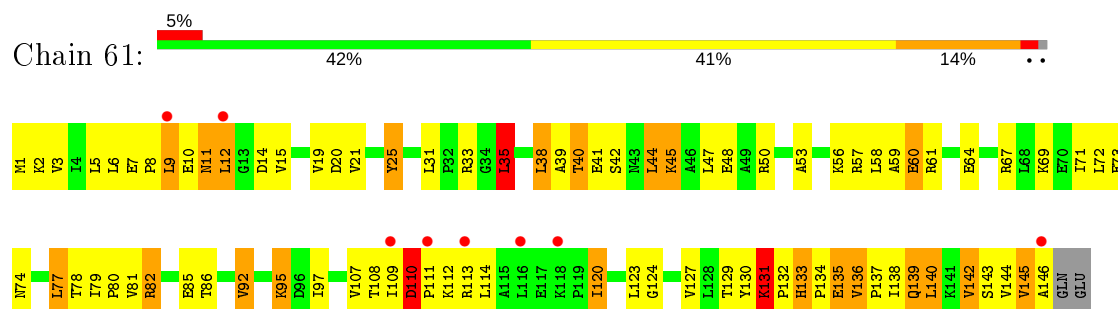
- Molecule 32: 50S ribosomal protein L6



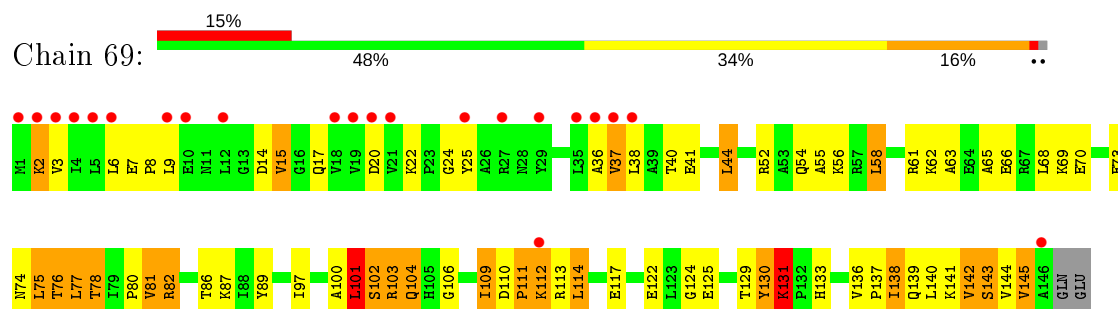
- Molecule 32: 50S ribosomal protein L6



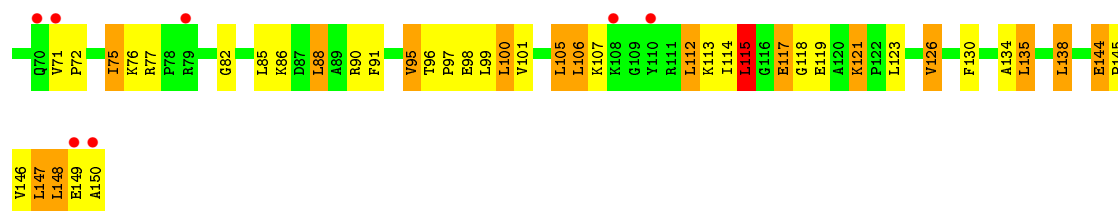
- Molecule 33: 50S ribosomal protein L9



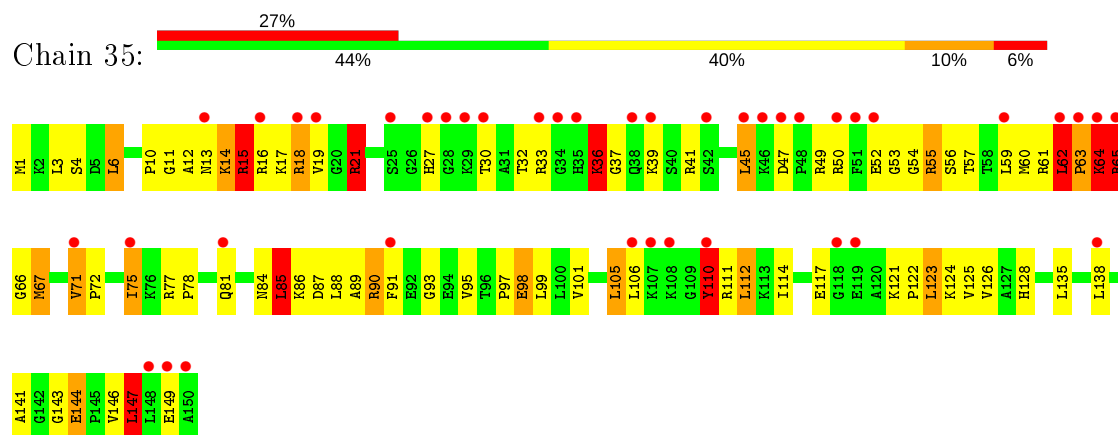
- Molecule 33: 50S ribosomal protein L9



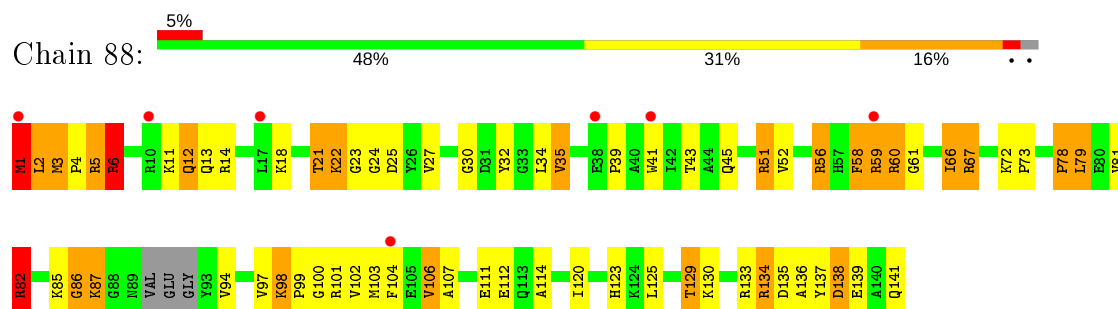
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-
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| L3 | |
| S4 | |
| D5 | |
| L6 | |
| R7 | |
| P8 | |
| R9 | |
| P10 | |
| G11 | |
| A12 | |
| I13 | |
| K14 | |
| R15 | |
| L16 | |
| K17 | |
| R18 | |
| V19 | |
| G20 | |
| R21 | |
| H27 | |
| G28 | |
| K29 | |
| T30 | |
| A31 | |
| T32 | |
| R33 | |
| G34 | |
| H35 | |
| K36 | |
| G37 | |
| Q38 | |
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| R41 | |
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| G43 | |
| G44 | |
| L45 | |
| K46 | |
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| P48 | |
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| G63 | |
| G64 | |
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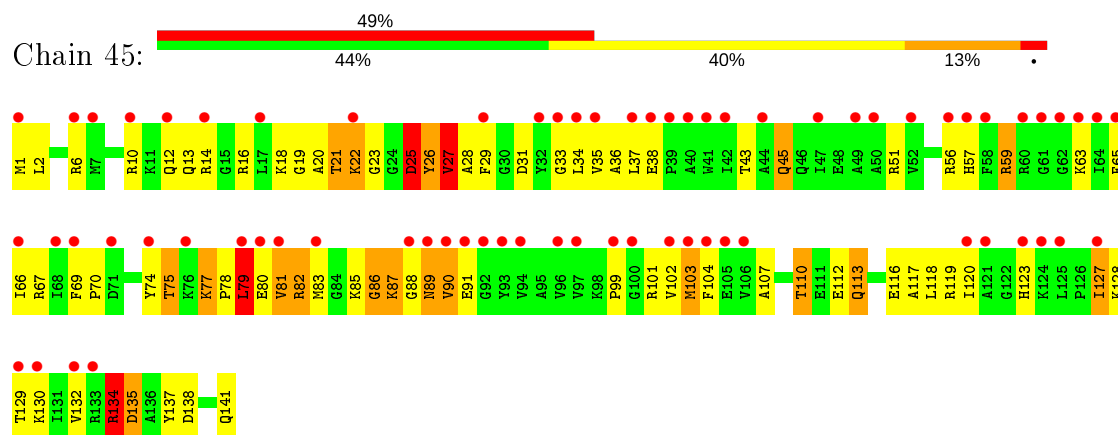
• Molecule 36: 50S ribosomal protein L15



• Molecule 37: 50S ribosomal protein L16

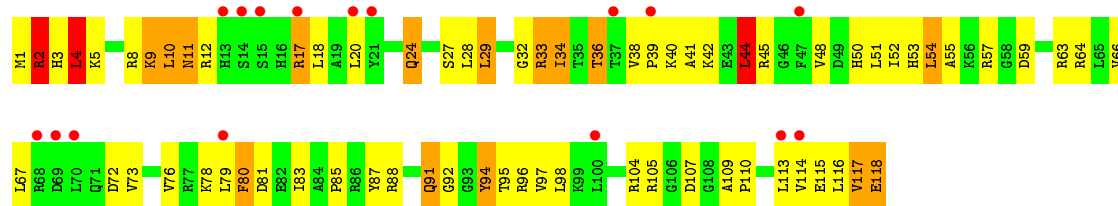


• Molecule 37: 50S ribosomal protein L16

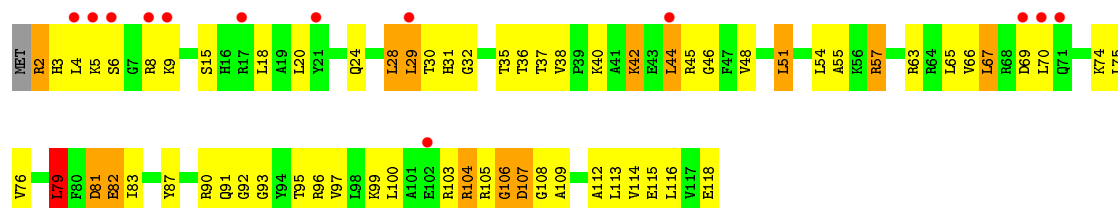


• Molecule 38: 50S ribosomal protein L17

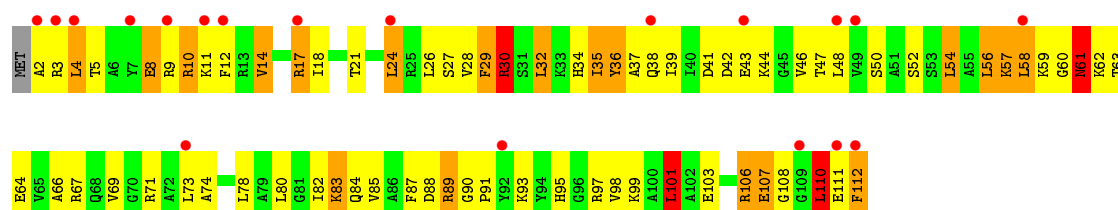




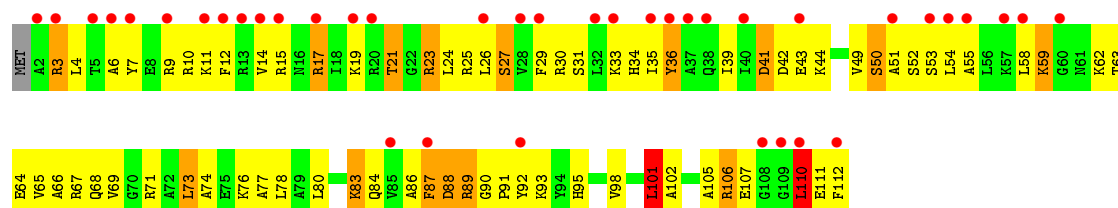
• Molecule 38: 50S ribosomal protein L17



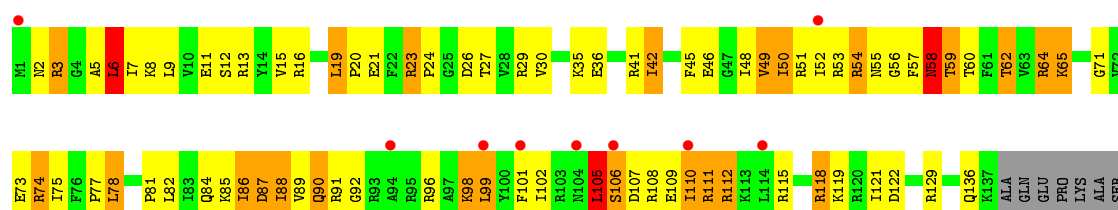
• Molecule 39: 50S ribosomal protein L18

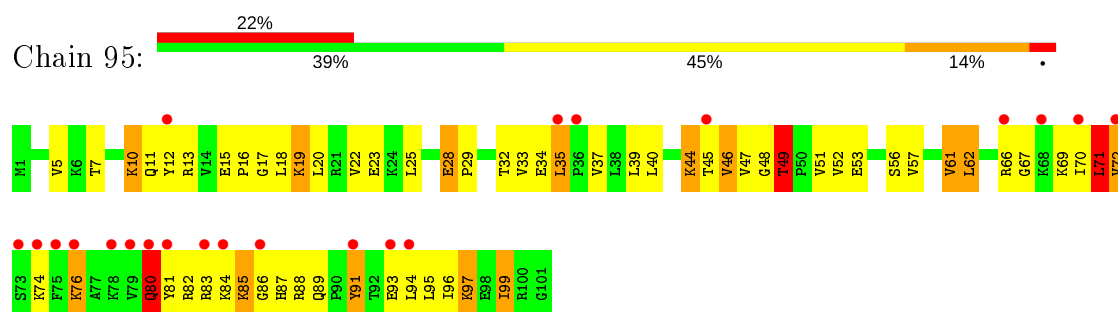


• Molecule 39: 50S ribosomal protein L18

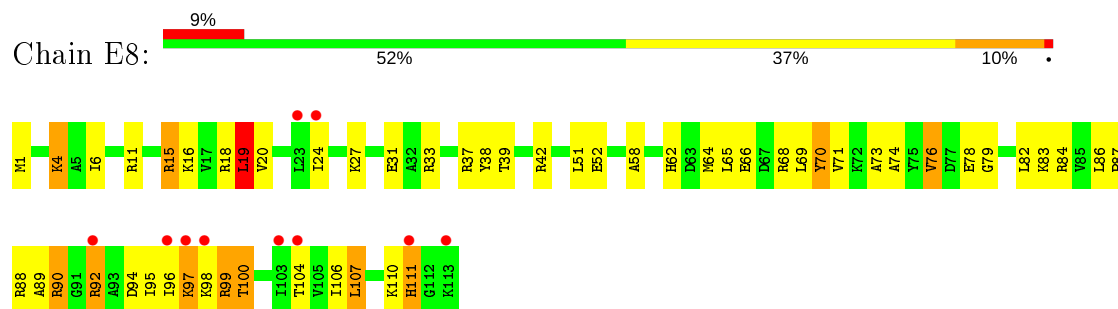


• Molecule 40: 50S ribosomal protein L19

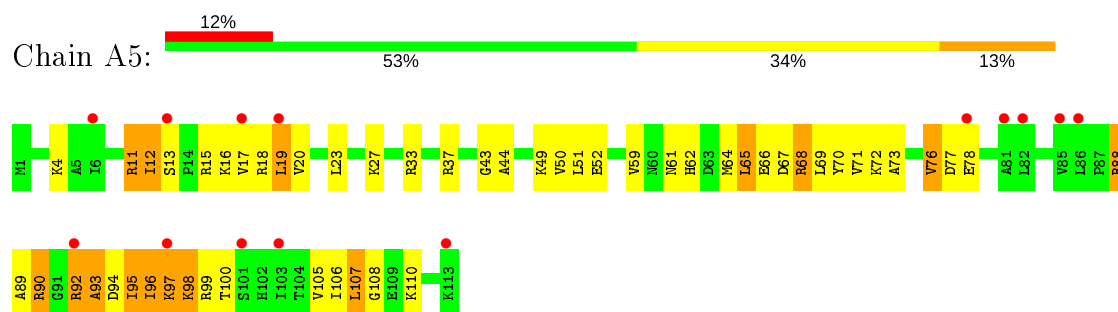




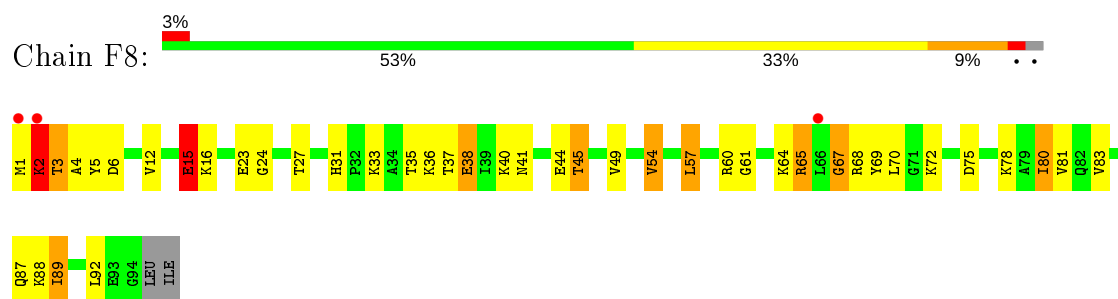
- Molecule 43: 50S ribosomal protein L22



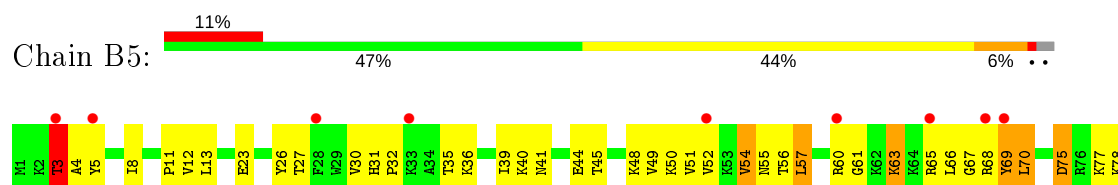
- Molecule 43: 50S ribosomal protein L22



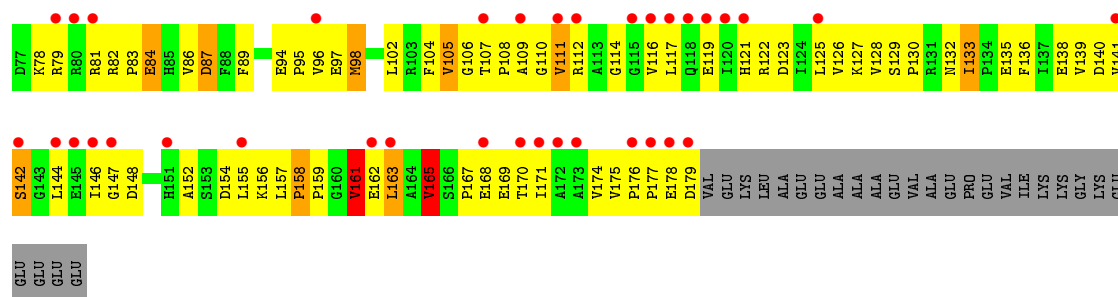
- Molecule 44: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L23



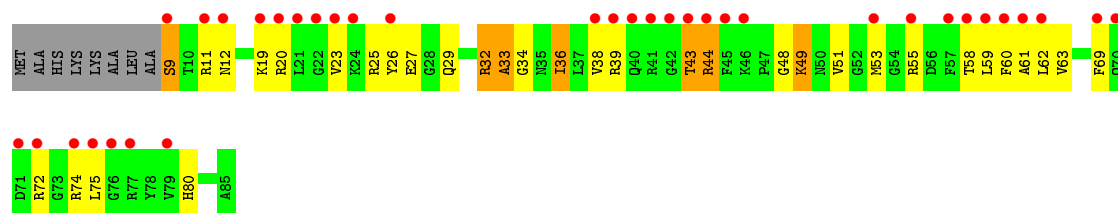
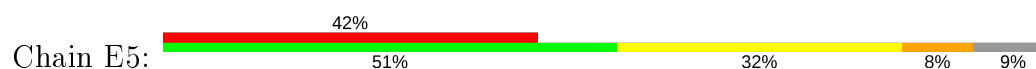




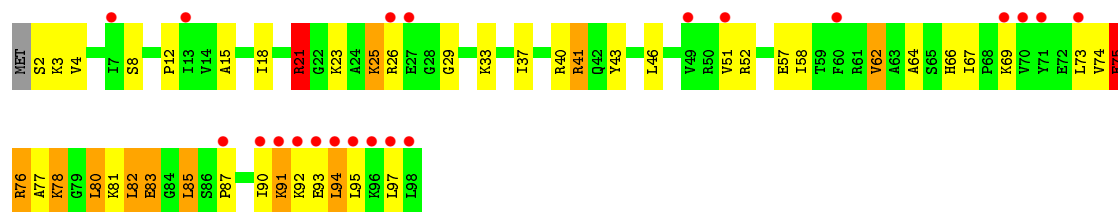
- Molecule 47: 50S ribosomal protein L27



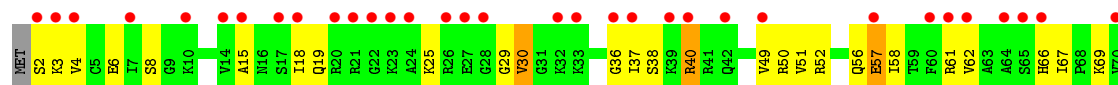
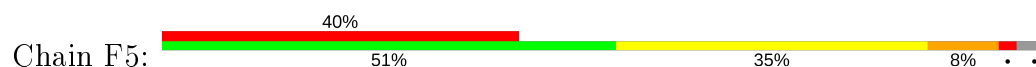
- Molecule 47: 50S ribosomal protein L27

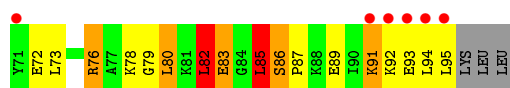


- Molecule 48: 50S ribosomal protein L28

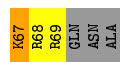
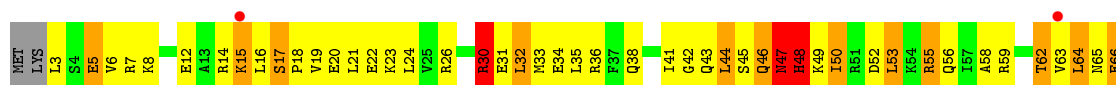


- Molecule 48: 50S ribosomal protein L28

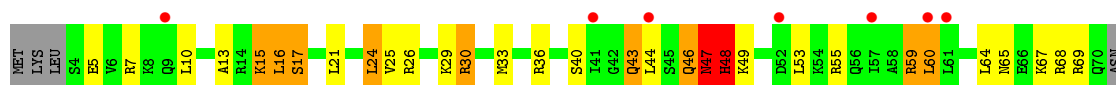




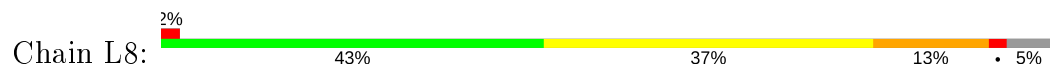
- Molecule 49: 50S ribosomal protein L29



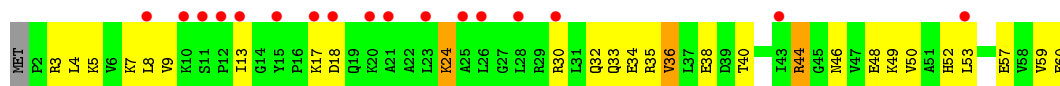
- Molecule 49: 50S ribosomal protein L29



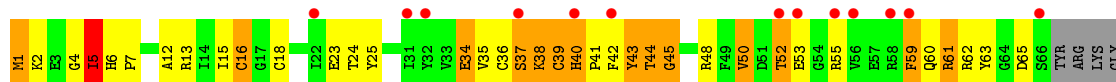
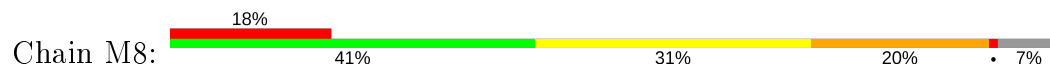
- Molecule 50: 50S ribosomal protein L30



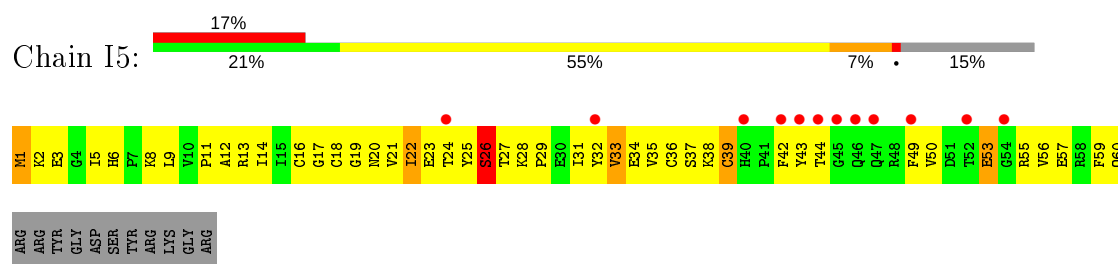
- Molecule 50: 50S ribosomal protein L30



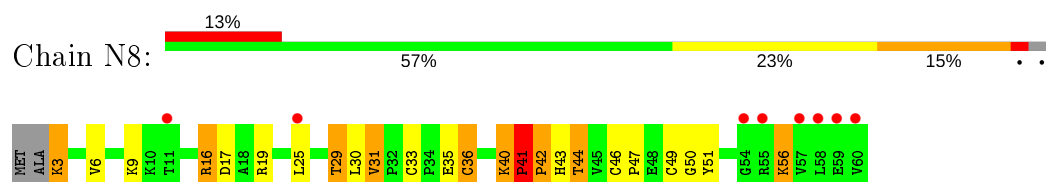
- Molecule 51: 50S ribosomal protein L31



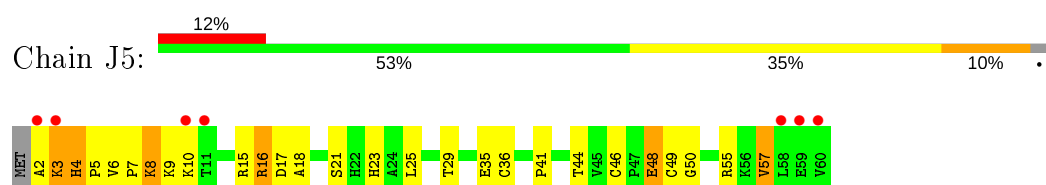
- Molecule 51: 50S ribosomal protein L31



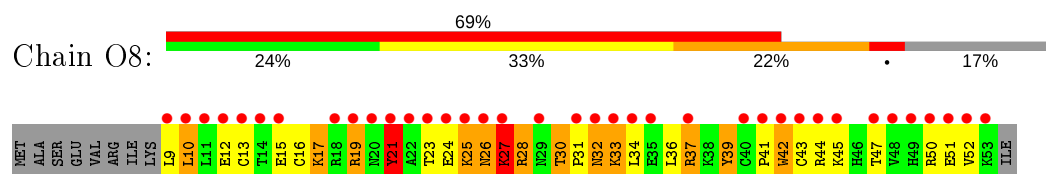
- Molecule 52: 50S ribosomal protein L32



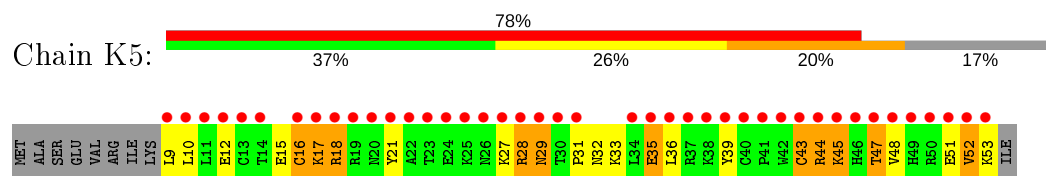
- Molecule 52: 50S ribosomal protein L32



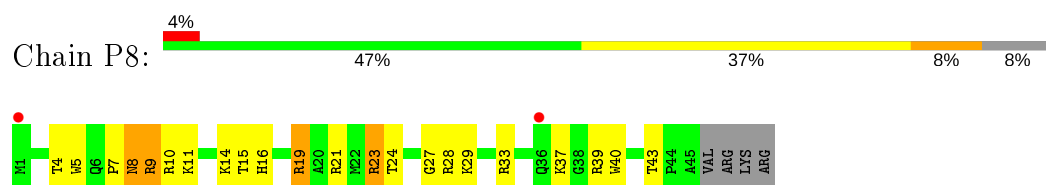
- Molecule 53: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L34

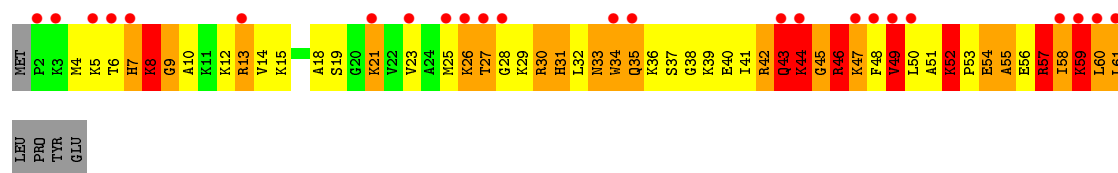


- Molecule 54: 50S ribosomal protein L34

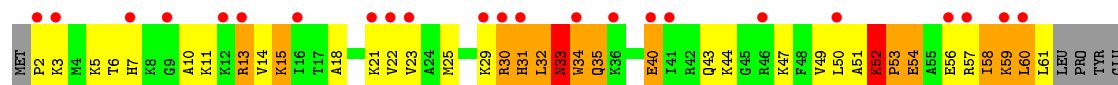




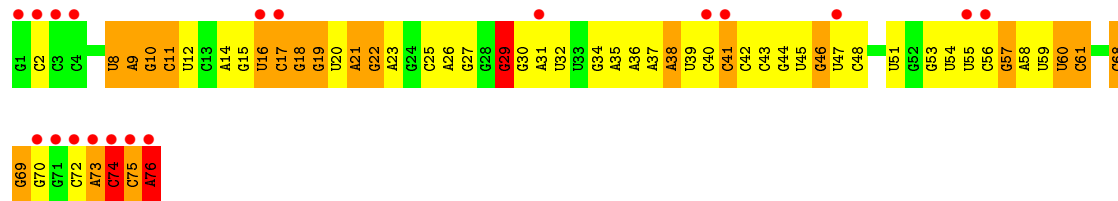
- Molecule 55: 50S ribosomal protein L35



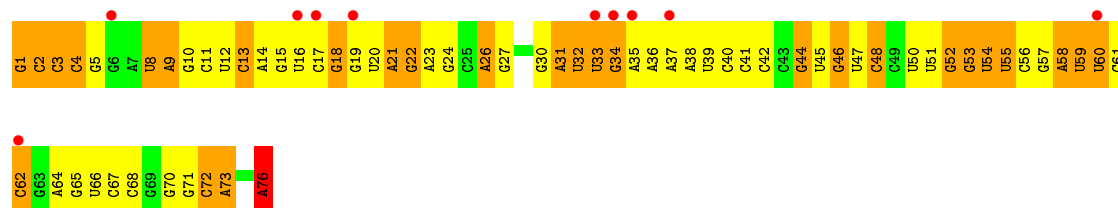
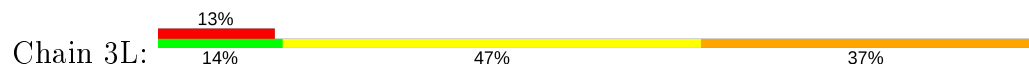
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNA-Phe



- Molecule 57: tRNA-Phe



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.40 Å 449.20 Å 621.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	255.47 – 2.95 255.48 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (255.47-2.95) 94.1 (255.48-2.95)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.89 (at 2.96 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.193 , 0.235 0.194 , 0.235	Depositor DCC
R_{free} test set	1999 reflections (0.16%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 77.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	300252	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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: 5MU, OMC, PAR, MIA, MG, ZN, 4SU, 7MG, PSU

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	0.93	27/36052 (0.1%)	1.65	832/56266 (1.5%)
1	1G	0.76	3/36049 (0.0%)	1.45	463/56262 (0.8%)
2	12	0.40	0/1959	0.65	2/2642 (0.1%)
2	1E	0.46	0/1959	0.72	1/2642 (0.0%)
3	22	0.42	0/1636	0.65	1/2205 (0.0%)
3	2E	0.60	0/1629	0.76	0/2195
4	32	0.56	0/1732	0.76	0/2318
4	3E	0.75	2/1732 (0.1%)	0.83	1/2318 (0.0%)
5	42	0.50	0/1171	0.74	1/1576 (0.1%)
5	4E	0.65	0/1171	0.80	0/1576
6	52	0.61	0/855	0.77	1/1154 (0.1%)
6	5E	0.63	0/855	0.78	0/1154
7	62	0.49	0/1261	0.62	0/1689
7	6E	0.55	0/1275	0.68	0/1709
8	72	0.45	0/1135	0.64	0/1527
8	7E	0.62	0/1135	0.83	0/1527
9	82	0.47	0/1002	0.70	0/1346
9	8E	0.54	0/1028	0.75	1/1379 (0.1%)
10	1A	0.41	0/814	0.65	0/1095
10	1I	0.58	0/814	0.73	0/1095
11	2A	0.53	0/879	0.74	1/1187 (0.1%)
11	2I	0.61	0/879	0.80	1/1187 (0.1%)
12	3A	0.62	0/991	0.84	2/1327 (0.2%)
12	3I	0.82	0/991	1.02	3/1327 (0.2%)
13	4A	0.39	0/943	0.63	0/1265
13	4I	0.59	0/948	0.79	1/1272 (0.1%)
14	5A	0.42	0/484	0.69	0/643
14	5I	0.81	1/500 (0.2%)	0.83	0/664
15	6A	0.55	0/744	0.67	1/992 (0.1%)
15	6I	0.62	0/744	0.82	0/992
16	7A	0.59	0/721	0.73	0/970
16	7I	0.58	0/721	0.79	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.60	1/847 (0.1%)	0.70	0/1131
17	8I	0.62	0/847	0.80	0/1131
18	9A	0.57	0/595	0.73	0/790
18	9I	0.61	0/595	0.87	1/790 (0.1%)
19	AA	0.40	0/638	0.64	0/860
19	AI	0.61	0/661	0.87	1/890 (0.1%)
20	BA	0.53	0/764	0.81	0/1007
20	BI	0.48	0/764	0.74	0/1007
21	1B	0.52	0/221	0.64	0/288
21	1F	0.57	0/221	0.81	0/288
22	1K	0.62	3/1673 (0.2%)	1.31	20/2606 (0.8%)
23	2K	1.06	5/1721 (0.3%)	1.71	46/2682 (1.7%)
23	2L	0.81	1/1721 (0.1%)	1.49	33/2682 (1.2%)
24	3K	0.64	1/1712 (0.1%)	1.32	18/2663 (0.7%)
25	4K	1.10	0/313	1.39	1/485 (0.2%)
25	4L	1.01	1/262 (0.4%)	1.64	6/403 (1.5%)
26	14	1.05	136/70167 (0.2%)	1.79	2340/109541 (2.1%)
26	1H	1.28	361/70233 (0.5%)	2.08	3902/109643 (3.6%)
27	16	1.03	6/2928 (0.2%)	1.88	107/4568 (2.3%)
27	1J	0.83	1/2928 (0.0%)	1.52	38/4568 (0.8%)
28	11	0.99	4/2165 (0.2%)	1.09	6/2919 (0.2%)
28	19	0.85	0/2170	1.02	5/2926 (0.2%)
29	21	0.79	0/1601	1.01	4/2160 (0.2%)
29	29	0.75	0/1601	1.02	6/2160 (0.3%)
30	31	0.90	1/1620 (0.1%)	1.05	6/2194 (0.3%)
30	39	0.71	1/1662 (0.1%)	0.96	3/2249 (0.1%)
31	41	0.65	0/1498	0.85	1/2016 (0.0%)
31	49	0.43	0/1498	0.68	0/2016
32	51	0.70	0/1362	0.92	2/1841 (0.1%)
32	59	0.43	0/1332	0.72	1/1802 (0.1%)
33	61	0.57	0/1151	0.83	3/1558 (0.2%)
33	69	0.54	0/1151	0.81	2/1558 (0.1%)
34	15	0.57	0/1131	0.77	0/1525
34	58	0.67	0/1131	0.89	2/1525 (0.1%)
35	25	0.71	0/942	0.88	2/1269 (0.2%)
35	68	0.79	0/942	0.88	1/1269 (0.1%)
36	35	0.76	0/1161	1.19	5/1544 (0.3%)
36	78	0.87	0/1161	1.12	3/1544 (0.2%)
37	45	0.74	1/1142 (0.1%)	0.99	2/1527 (0.1%)
37	88	0.97	3/1106 (0.3%)	1.20	5/1478 (0.3%)
38	55	0.78	0/973	1.02	2/1302 (0.2%)
38	98	0.70	0/981	0.99	1/1312 (0.1%)
39	65	0.61	0/891	0.94	2/1187 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	A8	0.76	0/891	1.01	3/1187 (0.3%)
40	75	0.67	0/1155	0.85	0/1542
40	B8	0.80	0/1155	0.96	2/1542 (0.1%)
41	85	0.66	0/981	0.82	0/1306
41	C8	0.84	1/981 (0.1%)	1.04	3/1306 (0.2%)
42	95	0.71	0/789	0.93	3/1057 (0.3%)
42	D8	0.75	0/789	0.94	1/1057 (0.1%)
43	A5	0.84	1/910 (0.1%)	0.91	0/1220
43	E8	0.78	0/910	0.97	2/1220 (0.2%)
44	B5	0.86	1/749 (0.1%)	0.88	0/1007
44	F8	1.00	1/756 (0.1%)	1.03	3/1014 (0.3%)
45	C5	0.74	0/807	0.97	2/1076 (0.2%)
45	G8	0.84	0/804	1.09	5/1073 (0.5%)
46	D5	0.47	0/1460	0.71	0/1982
46	H8	0.55	0/1427	0.86	3/1935 (0.2%)
47	E5	0.72	0/620	0.88	0/827
47	I8	0.88	0/634	0.97	1/847 (0.1%)
48	F5	0.77	0/744	1.03	2/989 (0.2%)
48	J8	0.87	0/769	0.98	3/1022 (0.3%)
49	G5	0.66	0/565	0.88	0/748
49	K8	1.00	2/565 (0.4%)	1.11	1/748 (0.1%)
50	H5	0.60	0/473	0.77	0/635
50	L8	0.72	0/457	0.99	2/613 (0.3%)
51	I5	0.47	0/492	0.80	0/663
51	M8	0.64	0/545	0.87	1/733 (0.1%)
52	J5	0.73	0/472	0.94	0/639
52	N8	0.74	0/467	0.98	1/632 (0.2%)
53	K5	0.74	0/396	0.98	1/529 (0.2%)
53	O8	0.82	1/396 (0.3%)	1.05	1/529 (0.2%)
54	L5	0.81	0/406	0.94	0/536
54	P8	1.07	0/399	1.26	5/526 (1.0%)
55	M5	1.07	2/483 (0.4%)	1.16	1/634 (0.2%)
55	Q8	1.43	2/486 (0.4%)	1.85	9/638 (1.4%)
56	1L	0.49	0/1717	1.05	5/2674 (0.2%)
57	3L	0.68	2/1698 (0.1%)	1.27	11/2646 (0.4%)
All	All	0.96	572/322340 (0.2%)	1.61	7960/482707 (1.6%)

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	1E	0	2
4	32	0	2
9	82	0	1
10	1A	0	1
11	2A	0	1
12	3I	0	1
13	4I	0	2
14	5A	0	1
19	AI	0	2
20	BA	0	2
20	BI	0	1
28	11	0	2
28	19	0	5
29	21	0	4
29	29	0	5
30	31	0	3
30	39	0	7
31	41	0	2
31	49	0	1
32	59	0	1
33	61	0	4
33	69	0	3
36	35	0	3
36	78	0	3
37	45	0	6
37	88	0	4
38	55	0	2
38	98	0	2
39	65	0	1
40	75	0	2
40	B8	0	2
41	85	0	2
41	C8	0	1
42	95	0	2
42	D8	0	1
43	A5	0	2
44	B5	0	1
45	C5	0	1
45	G8	0	3
46	D5	0	1
46	H8	0	3
47	I8	0	2
48	F5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
48	J8	0	2
49	G5	0	4
49	K8	0	2
51	I5	0	1
51	M8	0	2
52	N8	0	1
53	K5	0	4
53	O8	0	2
55	M5	0	3
55	Q8	0	8
All	All	0	127

The worst 5 of 572 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	2430	A	N9-C4	-14.70	1.29	1.37
26	14	783	A	N9-C4	-13.46	1.29	1.37
26	1H	774	A	N9-C4	-13.24	1.29	1.37
26	1H	676	A	N9-C4	-13.22	1.29	1.37
26	1H	783	A	N3-C4	-13.21	1.26	1.34

The worst 5 of 7960 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	783	A	C2-N3-C4	-29.75	95.72	110.60
26	1H	1899	G	N3-C4-N9	-29.71	108.17	126.00
26	1H	945	A	C6-C5-N7	-23.71	115.70	132.30
26	1H	676	A	C2-N3-C4	-23.41	98.89	110.60
26	1H	1899	G	N3-C4-C5	22.92	140.06	128.60

There are no chirality outliers.

5 of 127 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	237	ALA	Peptide
12	3I	87	GLY	Peptide
13	4I	105	THR	Peptide
13	4I	4	ILE	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	32207	0	16256	718	0
1	1G	32204	0	16255	829	0
2	12	1924	0	1975	99	0
2	1E	1924	0	1975	100	0
3	22	1612	0	1677	90	0
3	2E	1605	0	1668	52	0
4	32	1702	0	1763	86	0
4	3E	1702	0	1762	62	0
5	42	1155	0	1213	55	0
5	4E	1155	0	1213	53	0
6	52	842	0	857	31	0
6	5E	842	0	857	26	0
7	62	1243	0	1284	58	0
7	6E	1256	0	1296	42	0
8	72	1115	0	1177	41	0
8	7E	1115	0	1177	57	0
9	82	983	0	1006	61	0
9	8E	1009	0	1037	61	0
10	1A	801	0	849	45	0
10	1I	801	0	849	51	0
11	2A	864	0	881	32	0
11	2I	864	0	881	27	0
12	3A	975	0	1062	47	0
12	3I	975	0	1062	48	0
13	4A	933	0	992	64	0
13	4I	938	0	997	56	0
14	5A	475	0	511	29	0
14	5I	491	0	529	24	0
15	6A	733	0	771	33	0
15	6I	733	0	771	28	0
16	7A	705	0	725	29	0
16	7I	705	0	725	53	0
17	8A	834	0	904	22	0
17	8I	834	0	904	33	0
18	9A	590	0	662	18	0
18	9I	590	0	662	26	0
19	AA	624	0	636	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	647	0	665	53	0
20	BA	762	0	861	30	0
20	BI	762	0	861	48	0
21	1B	217	0	234	20	0
21	1F	217	0	234	8	0
22	1K	1627	0	836	35	0
23	2K	1646	0	845	27	0
23	2L	1646	0	845	32	0
24	3K	1603	0	824	57	0
25	4K	279	0	142	4	0
25	4L	235	0	121	14	0
26	14	62647	0	31578	1347	0
26	1H	62707	0	31600	1532	1
27	16	2617	0	1328	54	0
27	1J	2617	0	1328	106	0
28	11	2115	0	2195	85	0
28	19	2120	0	2197	88	0
29	21	1568	0	1634	89	0
29	29	1568	0	1634	92	0
30	31	1585	0	1632	93	0
30	39	1627	0	1680	104	0
31	41	1473	0	1535	80	0
31	49	1473	0	1535	62	0
32	51	1336	0	1418	71	0
32	59	1307	0	1382	63	0
33	61	1136	0	1223	54	0
33	69	1136	0	1223	54	0
34	15	1104	0	1180	53	0
34	58	1104	0	1180	54	0
35	25	932	0	996	48	0
35	68	932	0	996	35	0
36	35	1144	0	1228	101	0
36	78	1144	0	1228	98	0
37	45	1121	0	1179	74	0
37	88	1086	0	1129	64	0
38	55	959	0	1021	45	0
38	98	967	0	1033	53	0
39	65	881	0	943	70	0
39	A8	881	0	943	59	0
40	75	1141	0	1202	63	0
40	B8	1141	0	1202	70	0
41	85	963	0	1022	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	C8	963	0	1022	85	0
42	95	778	0	852	70	0
42	D8	778	0	852	34	0
43	A5	899	0	964	31	0
43	E8	899	0	964	33	0
44	B5	735	0	785	31	0
44	F8	742	0	803	42	0
45	C5	794	0	883	57	0
45	G8	791	0	882	59	0
46	D5	1428	0	1454	70	0
46	H8	1397	0	1430	84	0
47	E5	612	0	633	30	0
47	I8	626	0	642	26	0
48	F5	737	0	813	32	0
48	J8	762	0	848	37	0
49	G5	563	0	612	21	1
49	K8	563	0	612	36	0
50	H5	468	0	518	13	0
50	L8	452	0	503	21	0
51	I5	481	0	479	46	0
51	M8	533	0	526	43	0
52	J5	458	0	480	32	0
52	N8	453	0	475	28	0
53	K5	389	0	404	21	0
53	O8	389	0	404	28	0
54	L5	398	0	441	17	0
54	P8	391	0	432	17	0
55	M5	477	0	540	45	0
55	Q8	480	0	549	95	0
56	1L	1627	0	836	40	0
57	3L	1624	0	827	68	0
58	11	4	0	0	0	0
58	13	148	0	0	0	0
58	14	407	0	0	0	0
58	16	13	0	0	0	0
58	1G	96	0	0	0	0
58	1H	520	0	0	0	0
58	1J	5	0	0	0	0
58	1K	2	0	0	0	0
58	21	2	0	0	0	0
58	25	1	0	0	0	0
58	29	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2A	2	0	0	0	0
58	2I	1	0	0	0	0
58	2K	5	0	0	0	0
58	2L	3	0	0	0	0
58	3E	2	0	0	0	0
58	3K	1	0	0	0	0
58	3L	2	0	0	0	0
58	4I	2	0	0	0	0
58	49	1	0	0	0	0
58	4K	1	0	0	0	0
58	55	1	0	0	0	0
58	5E	1	0	0	0	0
58	5I	2	0	0	0	0
58	78	1	0	0	0	0
58	7A	1	0	0	0	0
58	88	2	0	0	0	0
58	98	2	0	0	0	0
58	C5	1	0	0	0	0
58	G8	1	0	0	0	0
58	I8	1	0	0	0	0
58	J5	1	0	0	0	0
58	L8	1	0	0	0	0
58	P8	1	0	0	0	0
59	13	42	0	45	1	0
59	1G	42	0	45	2	0
60	32	1	0	0	0	0
60	3E	1	0	0	0	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	11	13	0	0	3	0
61	13	197	0	0	29	0
61	14	598	0	0	153	0
61	16	21	0	0	4	0
61	19	13	0	0	3	0
61	1G	82	0	0	18	0
61	1H	999	0	0	280	0
61	1I	2	0	0	1	0
61	1K	5	0	0	0	0
61	21	4	0	0	0	0
61	2K	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	31	4	0	0	0	0
61	35	1	0	0	0	0
61	39	7	0	0	1	0
61	3E	3	0	0	0	0
61	3I	1	0	0	0	0
61	3K	1	0	0	0	0
61	3L	6	0	0	1	0
61	4K	2	0	0	0	0
61	58	2	0	0	0	0
61	5I	2	0	0	1	0
61	6I	1	0	0	0	0
61	78	5	0	0	1	0
61	7A	1	0	0	0	0
61	7I	1	0	0	0	0
61	85	1	0	0	0	0
61	8E	2	0	0	0	0
61	A5	1	0	0	0	0
61	B8	1	0	0	0	0
61	BA	1	0	0	0	0
61	C8	3	0	0	0	0
61	D8	1	0	0	0	0
61	G5	1	0	0	0	0
61	G8	4	0	0	1	0
61	I8	7	0	0	0	0
61	L5	1	0	0	0	0
61	L8	1	0	0	1	0
61	P8	1	0	0	0	0
61	Q8	2	0	0	0	0
All	All	300252	0	200448	8632	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 18.

The worst 5 of 8632 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)
26:14:2701:C:H3'	26:14:2702:U:H5''	1.27	1.15
26:1H:2592:G:OP1	61:1H:4524:HOH:O	1.68	1.10
40:B8:50:ILE:HD11	40:B8:102:ILE:HD11	1.32	1.10
26:1H:1614:A:OP1	61:1H:3947:HOH:O	1.70	1.09
26:1H:945:A:OP1	61:1H:4167:HOH:O	1.70	1.09

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)
26:1H:277:C:O2'	49:G5:49:LYS:NZ[2_564]	2.14	0.06

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	235/256 (92%)	192 (82%)	37 (16%)	6 (3%)	5	24
2	1E	235/256 (92%)	197 (84%)	37 (16%)	1 (0%)	34	69
3	22	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	29	64
3	2E	203/239 (85%)	184 (91%)	19 (9%)	0	100	100
4	32	206/209 (99%)	179 (87%)	25 (12%)	2 (1%)	15	48
4	3E	206/209 (99%)	192 (93%)	12 (6%)	2 (1%)	15	48
5	42	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	4E	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	56
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
7	62	148/156 (95%)	137 (93%)	11 (7%)	0	100	100
7	6E	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
8	72	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	10	38
8	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22	56
9	82	122/128 (95%)	113 (93%)	8 (7%)	1 (1%)	19	53
9	8E	125/128 (98%)	105 (84%)	19 (15%)	1 (1%)	19	53
10	1A	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
10	1I	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
11	2A	114/129 (88%)	102 (90%)	8 (7%)	4 (4%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2I	114/129 (88%)	99 (87%)	14 (12%)	1 (1%)	17	51
12	3A	123/132 (93%)	101 (82%)	18 (15%)	4 (3%)	4	18
12	3I	123/132 (93%)	103 (84%)	20 (16%)	0	100	100
13	4A	115/126 (91%)	96 (84%)	18 (16%)	1 (1%)	17	51
13	4I	116/126 (92%)	96 (83%)	19 (16%)	1 (1%)	17	51
14	5A	56/61 (92%)	46 (82%)	9 (16%)	1 (2%)	8	33
14	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	17
15	6A	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	6I	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	7A	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
16	7I	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
17	8A	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	8I	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
18	9A	70/88 (80%)	65 (93%)	5 (7%)	0	100	100
18	9I	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	11	39
19	AA	76/93 (82%)	59 (78%)	15 (20%)	2 (3%)	5	24
19	AI	79/93 (85%)	65 (82%)	11 (14%)	3 (4%)	3	15
20	BA	97/106 (92%)	84 (87%)	12 (12%)	1 (1%)	15	48
20	BI	97/106 (92%)	86 (89%)	10 (10%)	1 (1%)	15	48
21	1B	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	1F	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
28	11	270/276 (98%)	253 (94%)	12 (4%)	5 (2%)	8	32
28	19	271/276 (98%)	248 (92%)	16 (6%)	7 (3%)	5	24
29	21	203/206 (98%)	164 (81%)	30 (15%)	9 (4%)	2	12
29	29	203/206 (98%)	156 (77%)	35 (17%)	12 (6%)	1	7
30	31	200/210 (95%)	182 (91%)	15 (8%)	3 (2%)	10	38
30	39	206/210 (98%)	165 (80%)	34 (16%)	7 (3%)	3	17
31	41	179/182 (98%)	156 (87%)	21 (12%)	2 (1%)	14	46
31	49	179/182 (98%)	155 (87%)	22 (12%)	2 (1%)	14	46
32	51	172/180 (96%)	146 (85%)	18 (10%)	8 (5%)	2	11
32	59	168/180 (93%)	131 (78%)	30 (18%)	7 (4%)	3	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	61	144/148 (97%)	117 (81%)	23 (16%)	4 (3%)	5	22
33	69	144/148 (97%)	112 (78%)	29 (20%)	3 (2%)	7	29
34	15	136/140 (97%)	120 (88%)	15 (11%)	1 (1%)	22	56
34	58	136/140 (97%)	116 (85%)	16 (12%)	4 (3%)	4	21
35	25	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	9	34
35	68	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
36	35	148/150 (99%)	117 (79%)	27 (18%)	4 (3%)	5	23
36	78	148/150 (99%)	113 (76%)	29 (20%)	6 (4%)	3	13
37	45	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	22	56
37	88	134/141 (95%)	112 (84%)	15 (11%)	7 (5%)	2	9
38	55	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	9	34
38	98	116/118 (98%)	104 (90%)	10 (9%)	2 (2%)	9	34
39	65	109/112 (97%)	88 (81%)	18 (16%)	3 (3%)	5	22
39	A8	109/112 (97%)	91 (84%)	16 (15%)	2 (2%)	8	33
40	75	135/146 (92%)	115 (85%)	17 (13%)	3 (2%)	6	28
40	B8	135/146 (92%)	119 (88%)	15 (11%)	1 (1%)	22	56
41	85	115/118 (98%)	102 (89%)	12 (10%)	1 (1%)	17	51
41	C8	115/118 (98%)	104 (90%)	9 (8%)	2 (2%)	9	34
42	95	99/101 (98%)	77 (78%)	17 (17%)	5 (5%)	2	9
42	D8	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	48
43	A5	111/113 (98%)	102 (92%)	7 (6%)	2 (2%)	8	33
43	E8	111/113 (98%)	100 (90%)	11 (10%)	0	100	100
44	B5	92/96 (96%)	83 (90%)	5 (5%)	4 (4%)	2	12
44	F8	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	6	28
45	C5	102/110 (93%)	75 (74%)	21 (21%)	6 (6%)	1	7
45	G8	102/110 (93%)	80 (78%)	15 (15%)	7 (7%)	1	4
46	D5	177/206 (86%)	134 (76%)	33 (19%)	10 (6%)	2	8
46	H8	173/206 (84%)	142 (82%)	25 (14%)	6 (4%)	3	17
47	E5	75/85 (88%)	67 (89%)	6 (8%)	2 (3%)	5	23
47	I8	78/85 (92%)	68 (87%)	9 (12%)	1 (1%)	12	41
48	F5	92/98 (94%)	87 (95%)	4 (4%)	1 (1%)	14	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	J8	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	7	29
49	G5	65/72 (90%)	61 (94%)	2 (3%)	2 (3%)	4	19
49	K8	65/72 (90%)	58 (89%)	4 (6%)	3 (5%)	2	11
50	H5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	L8	55/60 (92%)	51 (93%)	3 (6%)	1 (2%)	8	33
51	I5	58/71 (82%)	29 (50%)	25 (43%)	4 (7%)	1	4
51	M8	64/71 (90%)	43 (67%)	18 (28%)	3 (5%)	2	11
52	J5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	8	33
52	N8	56/60 (93%)	48 (86%)	6 (11%)	2 (4%)	3	16
53	K5	43/54 (80%)	27 (63%)	14 (33%)	2 (5%)	2	11
53	O8	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	2	11
54	L5	44/49 (90%)	42 (96%)	2 (4%)	0	100	100
54	P8	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
55	M5	58/65 (89%)	49 (84%)	6 (10%)	3 (5%)	2	9
55	Q8	58/65 (89%)	30 (52%)	21 (36%)	7 (12%)	0	1
All	All	11318/12054 (94%)	9776 (86%)	1313 (12%)	229 (2%)	7	30

5 of 229 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	21	83	ASP
36	78	57	THR
41	C8	89	GLU
41	C8	90	VAL
45	G8	54	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	205/220 (93%)	161 (78%)	44 (22%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
2	1E	205/220 (93%)	161 (78%)	44 (22%)	1	4	
3	22	160/188 (85%)	128 (80%)	32 (20%)	1	5	
3	2E	159/188 (85%)	128 (80%)	31 (20%)	1	6	
4	32	180/181 (99%)	150 (83%)	30 (17%)	2	9	
4	3E	180/181 (99%)	139 (77%)	41 (23%)	1	3	
5	42	116/123 (94%)	90 (78%)	26 (22%)	1	3	
5	4E	116/123 (94%)	94 (81%)	22 (19%)	1	6	
6	52	90/90 (100%)	71 (79%)	19 (21%)	1	4	
6	5E	90/90 (100%)	77 (86%)	13 (14%)	3	13	
7	62	126/127 (99%)	106 (84%)	20 (16%)	2	10	
7	6E	126/127 (99%)	101 (80%)	25 (20%)	1	6	
8	72	119/119 (100%)	99 (83%)	20 (17%)	2	9	
8	7E	119/119 (100%)	95 (80%)	24 (20%)	1	5	
9	82	95/99 (96%)	79 (83%)	16 (17%)	2	9	
9	8E	98/99 (99%)	73 (74%)	25 (26%)	0	2	
10	1A	89/92 (97%)	70 (79%)	19 (21%)	1	4	
10	1I	89/92 (97%)	72 (81%)	17 (19%)	1	6	
11	2A	88/99 (89%)	72 (82%)	16 (18%)	1	7	
11	2I	88/99 (89%)	72 (82%)	16 (18%)	1	7	
12	3A	104/109 (95%)	81 (78%)	23 (22%)	1	3	
12	3I	104/109 (95%)	89 (86%)	15 (14%)	3	13	
13	4A	94/101 (93%)	70 (74%)	24 (26%)	0	2	
13	4I	94/101 (93%)	73 (78%)	21 (22%)	1	3	
14	5A	48/50 (96%)	40 (83%)	8 (17%)	2	9	
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	2	
15	6A	79/80 (99%)	66 (84%)	13 (16%)	2	9	
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2	8	
16	7A	72/74 (97%)	64 (89%)	8 (11%)	6	22	
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	6	
17	8A	95/97 (98%)	81 (85%)	14 (15%)	3	12	
17	8I	95/97 (98%)	76 (80%)	19 (20%)	1	5	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	9A	63/77 (82%)	52 (82%)	11 (18%)	2	8
18	9I	63/77 (82%)	55 (87%)	8 (13%)	4	17
19	AA	67/80 (84%)	50 (75%)	17 (25%)	0	2
19	AI	70/80 (88%)	53 (76%)	17 (24%)	0	2
20	BA	76/82 (93%)	64 (84%)	12 (16%)	2	10
20	BI	76/82 (93%)	62 (82%)	14 (18%)	1	7
21	1B	20/22 (91%)	18 (90%)	2 (10%)	7	26
21	1F	20/22 (91%)	19 (95%)	1 (5%)	24	57
28	11	214/218 (98%)	173 (81%)	41 (19%)	1	6
28	19	214/218 (98%)	169 (79%)	45 (21%)	1	4
29	21	165/166 (99%)	124 (75%)	41 (25%)	0	2
29	29	165/166 (99%)	123 (74%)	42 (26%)	0	2
30	31	161/166 (97%)	128 (80%)	33 (20%)	1	5
30	39	165/166 (99%)	127 (77%)	38 (23%)	1	3
31	41	155/156 (99%)	120 (77%)	35 (23%)	1	3
31	49	155/156 (99%)	124 (80%)	31 (20%)	1	5
32	51	145/148 (98%)	108 (74%)	37 (26%)	0	2
32	59	142/148 (96%)	109 (77%)	33 (23%)	1	3
33	61	122/124 (98%)	88 (72%)	34 (28%)	0	1
33	69	122/124 (98%)	88 (72%)	34 (28%)	0	1
34	15	117/119 (98%)	91 (78%)	26 (22%)	1	3
34	58	117/119 (98%)	94 (80%)	23 (20%)	1	6
35	25	100/100 (100%)	79 (79%)	21 (21%)	1	4
35	68	100/100 (100%)	85 (85%)	15 (15%)	3	12
36	35	116/116 (100%)	84 (72%)	32 (28%)	0	1
36	78	116/116 (100%)	78 (67%)	38 (33%)	0	1
37	45	111/111 (100%)	86 (78%)	25 (22%)	1	3
37	88	104/111 (94%)	78 (75%)	26 (25%)	0	2
38	55	100/101 (99%)	79 (79%)	21 (21%)	1	4
38	98	101/101 (100%)	73 (72%)	28 (28%)	0	1
39	65	87/88 (99%)	64 (74%)	23 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
39	A8	87/88 (99%)	57 (66%)	30 (34%)	0	1	
40	75	120/127 (94%)	87 (72%)	33 (28%)	0	1	
40	B8	120/127 (94%)	82 (68%)	38 (32%)	0	1	
41	85	93/94 (99%)	73 (78%)	20 (22%)	1	4	
41	C8	93/94 (99%)	80 (86%)	13 (14%)	3	14	
42	95	82/82 (100%)	58 (71%)	24 (29%)	0	1	
42	D8	82/82 (100%)	68 (83%)	14 (17%)	2	8	
43	A5	92/92 (100%)	71 (77%)	21 (23%)	1	3	
43	E8	92/92 (100%)	68 (74%)	24 (26%)	0	2	
44	B5	74/78 (95%)	58 (78%)	16 (22%)	1	4	
44	F8	76/78 (97%)	60 (79%)	16 (21%)	1	4	
45	C5	85/91 (93%)	63 (74%)	22 (26%)	0	2	
45	G8	85/91 (93%)	62 (73%)	23 (27%)	0	1	
46	D5	158/179 (88%)	123 (78%)	35 (22%)	1	3	
46	H8	154/179 (86%)	121 (79%)	33 (21%)	1	4	
47	E5	62/67 (92%)	53 (86%)	9 (14%)	3	13	
47	I8	61/67 (91%)	48 (79%)	13 (21%)	1	4	
48	F5	79/83 (95%)	62 (78%)	17 (22%)	1	4	
48	J8	82/83 (99%)	65 (79%)	17 (21%)	1	4	
49	G5	62/67 (92%)	44 (71%)	18 (29%)	0	1	
49	K8	62/67 (92%)	37 (60%)	25 (40%)	0	0	
50	H5	51/52 (98%)	37 (72%)	14 (28%)	0	1	
50	L8	49/52 (94%)	35 (71%)	14 (29%)	0	1	
51	I5	54/63 (86%)	44 (82%)	10 (18%)	1	7	
51	M8	59/63 (94%)	42 (71%)	17 (29%)	0	1	
52	J5	51/52 (98%)	39 (76%)	12 (24%)	1	3	
52	N8	51/52 (98%)	39 (76%)	12 (24%)	1	3	
53	K5	44/52 (85%)	36 (82%)	8 (18%)	1	7	
53	O8	44/52 (85%)	29 (66%)	15 (34%)	0	1	
54	L5	39/42 (93%)	33 (85%)	6 (15%)	2	11	
54	P8	38/42 (90%)	32 (84%)	6 (16%)	2	10	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	M5	49/55 (89%)	34 (69%)	15 (31%)	0	1
55	Q8	50/55 (91%)	32 (64%)	18 (36%)	0	1
All	All	9552/9998 (96%)	7454 (78%)	2098 (22%)	1	4

5 of 2098 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	J8	4	VAL
4	32	190	ASP
45	C5	44	ILE
49	K8	30	ARG
55	Q8	46	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	22	176	HIS
4	32	123	HIS
49	G5	48	HIS
4	32	119	GLN
7	62	84	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1495/1522 (98%)	329 (22%)	34 (2%)
1	1G	1495/1522 (98%)	353 (23%)	37 (2%)
22	1K	74/76 (97%)	33 (44%)	3 (4%)
23	2K	76/77 (98%)	21 (27%)	2 (2%)
23	2L	76/77 (98%)	16 (21%)	1 (1%)
24	3K	72/76 (94%)	40 (55%)	6 (8%)
25	4K	12/30 (40%)	4 (33%)	0
25	4L	10/30 (33%)	3 (30%)	1 (10%)
26	14	2908/2917 (99%)	721 (24%)	52 (1%)
26	1H	2911/2917 (99%)	701 (24%)	51 (1%)
27	16	121/122 (99%)	27 (22%)	1 (0%)
27	1J	121/122 (99%)	35 (28%)	2 (1%)
56	1L	74/76 (97%)	34 (45%)	3 (4%)
57	3L	75/76 (98%)	37 (49%)	4 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9520/9640 (98%)	2354 (24%)	197 (2%)

5 of 2354 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	7	G
1	13	8	A
1	13	21	G

5 of 197 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2439	A
1	1G	561	U
26	14	2402	C
26	1H	2475	C
1	1G	250	A

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

28 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
56	5MU	1L	54	56	15,22,23	2.18	3 (20%)	16,32,35	1.86	2 (12%)
24	PSU	3K	39	24	17,21,22	1.04	1 (5%)	20,30,33	3.43	6 (30%)
23	OMC	2K	33	23	15,22,23	2.35	4 (26%)	17,31,34	1.58	3 (17%)
56	PSU	1L	39	56	17,21,22	1.14	1 (5%)	20,30,33	3.51	4 (20%)
57	PSU	3L	32	57	17,21,22	1.19	2 (11%)	20,30,33	3.37	9 (45%)
22	PSU	1K	39	22	17,21,22	1.00	1 (5%)	20,30,33	3.15	6 (30%)
23	PSU	2L	56	23	17,21,22	1.18	1 (5%)	20,30,33	3.23	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	1L	32	56	17,21,22	1.05	1 (5%)	20,30,33	3.07	7 (35%)
22	4SU	1K	8	22	14,21,22	3.27	2 (14%)	15,30,33	1.43	2 (13%)
24	PSU	3K	32	24	17,21,22	1.09	1 (5%)	20,30,33	3.04	5 (25%)
57	4SU	3L	8	57	14,21,22	3.60	2 (14%)	15,30,33	1.62	2 (13%)
23	7MG	2L	47	23	22,26,27	3.63	7 (31%)	28,39,42	2.55	12 (42%)
23	7MG	2K	47	23	22,26,27	3.35	7 (31%)	28,39,42	2.47	12 (42%)
22	MIA	1K	37	22	24,31,32	2.49	4 (16%)	26,44,47	3.34	7 (26%)
22	5MU	1K	54	22	15,22,23	2.27	3 (20%)	16,32,35	1.78	2 (12%)
57	PSU	3L	55	57	17,21,22	1.12	1 (5%)	20,30,33	3.56	7 (35%)
23	4SU	2L	8	23	14,21,22	3.54	2 (14%)	15,30,33	1.16	2 (13%)
23	5MU	2L	55	23	15,22,23	2.33	3 (20%)	16,32,35	1.99	3 (18%)
56	MIA	1L	37	56	24,31,32	2.41	4 (16%)	26,44,47	3.20	7 (26%)
57	5MU	3L	54	57	15,22,23	2.30	3 (20%)	16,32,35	1.85	3 (18%)
24	MIA	3K	37	24,58	24,31,32	2.57	5 (20%)	26,44,47	2.48	8 (30%)
57	7MG	3L	46	57	22,26,27	3.59	7 (31%)	28,39,42	2.74	12 (42%)
22	PSU	1K	32	58,22	17,21,22	1.09	1 (5%)	20,30,33	3.09	5 (25%)
23	PSU	2K	56	23	17,21,22	1.11	2 (11%)	20,30,33	2.98	6 (30%)
23	5MU	2K	55	58,23	15,22,23	2.20	3 (20%)	16,32,35	1.64	2 (12%)
23	OMC	2L	33	23	15,22,23	2.23	4 (26%)	17,31,34	1.60	3 (17%)
23	4SU	2K	8	23	14,21,22	3.18	2 (14%)	15,30,33	0.65	0
22	PSU	1K	55	22	17,21,22	1.16	1 (5%)	20,30,33	3.88	6 (30%)

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
56	5MU	1L	54	56	-	0/5/25/26	0/2/2/2
24	PSU	3K	39	24	-	2/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/7/27/28	0/2/2/2
56	PSU	1L	39	56	-	0/7/25/26	0/2/2/2
57	PSU	3L	32	57	-	1/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
56	PSU	1L	32	56	-	1/7/25/26	0/2/2/2
22	4SU	1K	8	22	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	3K	32	24	-	0/7/25/26	0/2/2/2
57	4SU	3L	8	57	-	0/5/25/26	0/2/2/2
23	7MG	2L	47	23	-	0/7/37/38	0/3/3/3
23	7MG	2K	47	23	-	2/7/37/38	0/3/3/3
22	MIA	1K	37	22	-	2/11/33/34	0/3/3/3
22	5MU	1K	54	22	-	0/5/25/26	0/2/2/2
57	PSU	3L	55	57	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	2/5/25/26	0/2/2/2
23	5MU	2L	55	23	-	3/5/25/26	0/2/2/2
56	MIA	1L	37	56	-	9/11/33/34	0/3/3/3
57	5MU	3L	54	57	-	2/5/25/26	0/2/2/2
24	MIA	3K	37	24,58	-	6/11/33/34	0/3/3/3
57	7MG	3L	46	57	-	0/7/37/38	0/3/3/3
22	PSU	1K	32	58,22	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	58,23	-	0/5/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/7/27/28	0/2/2/2
23	4SU	2K	8	23	-	0/5/25/26	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2

The worst 5 of 78 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	7MG	C4-N3	11.23	1.48	1.34
57	3L	8	4SU	C5-C4	10.65	1.50	1.38
23	2L	8	4SU	C5-C4	10.22	1.50	1.38
23	2K	47	7MG	C4-N3	10.20	1.47	1.34
57	3L	46	7MG	C4-N3	10.13	1.47	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1L	39	PSU	N1-C2-N3	-12.99	118.11	128.43
22	1K	55	PSU	N1-C2-N3	-12.63	118.39	128.43
57	3L	55	PSU	N1-C2-N3	-12.37	118.59	128.43
22	1K	37	MIA	C11-S10-C2	11.81	111.09	102.27
24	3K	39	PSU	N1-C2-N3	-11.45	119.33	128.43

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	3L	32	PSU	C4'-C5'-O5'-P
22	1K	37	MIA	C12-C13-C14-C15
22	1K	37	MIA	C12-C13-C14-C16
56	1L	37	MIA	O4'-C4'-C5'-O5'
56	1L	37	MIA	C5-C6-N6-C12

There are no ring outliers.

22 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1L	54	5MU	2	0
24	3K	39	PSU	2	0
56	1L	39	PSU	1	0
57	3L	32	PSU	3	0
23	2L	56	PSU	2	0
22	1K	8	4SU	1	0
57	3L	8	4SU	5	0
23	2L	47	7MG	3	0
23	2K	47	7MG	3	0
22	1K	54	5MU	1	0
57	3L	55	PSU	2	0
23	2L	8	4SU	2	0
23	2L	55	5MU	2	0
56	1L	37	MIA	1	0
57	3L	54	5MU	2	0
24	3K	37	MIA	2	0
57	3L	46	7MG	3	0
23	2K	56	PSU	2	0
23	2K	55	5MU	3	0
23	2L	33	OMC	2	0
23	2K	8	4SU	1	0
22	1K	55	PSU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1246 ligands modelled in this entry, 1244 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	PAR	13	1749	-	45,45,45	0.71	1 (2%)	64,67,67	1.59	15 (23%)
59	PAR	1G	1697	-	45,45,45	0.87	3 (6%)	64,67,67	1.64	15 (23%)

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
59	PAR	13	1749	-	-	5/18/94/94	0/4/4/4
59	PAR	1G	1697	-	-	5/18/94/94	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1G	1697	PAR	C24-N24	-2.79	1.43	1.47
59	1G	1697	PAR	C34-C24	-2.37	1.50	1.53
59	1G	1697	PAR	C31-C21	-2.02	1.51	1.53
59	13	1749	PAR	C21-N21	-2.02	1.44	1.47

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1G	1697	PAR	C13-O52-C52	-4.53	106.75	117.96
59	1G	1697	PAR	C14-O33-C33	-4.08	107.88	117.96
59	13	1749	PAR	C14-O54-C54	3.94	121.42	113.69
59	1G	1697	PAR	C34-C24-N24	-3.36	104.17	111.05
59	1G	1697	PAR	O11-C11-C21	-3.31	102.51	108.22

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	13	1749	PAR	C33-C43-C53-O53

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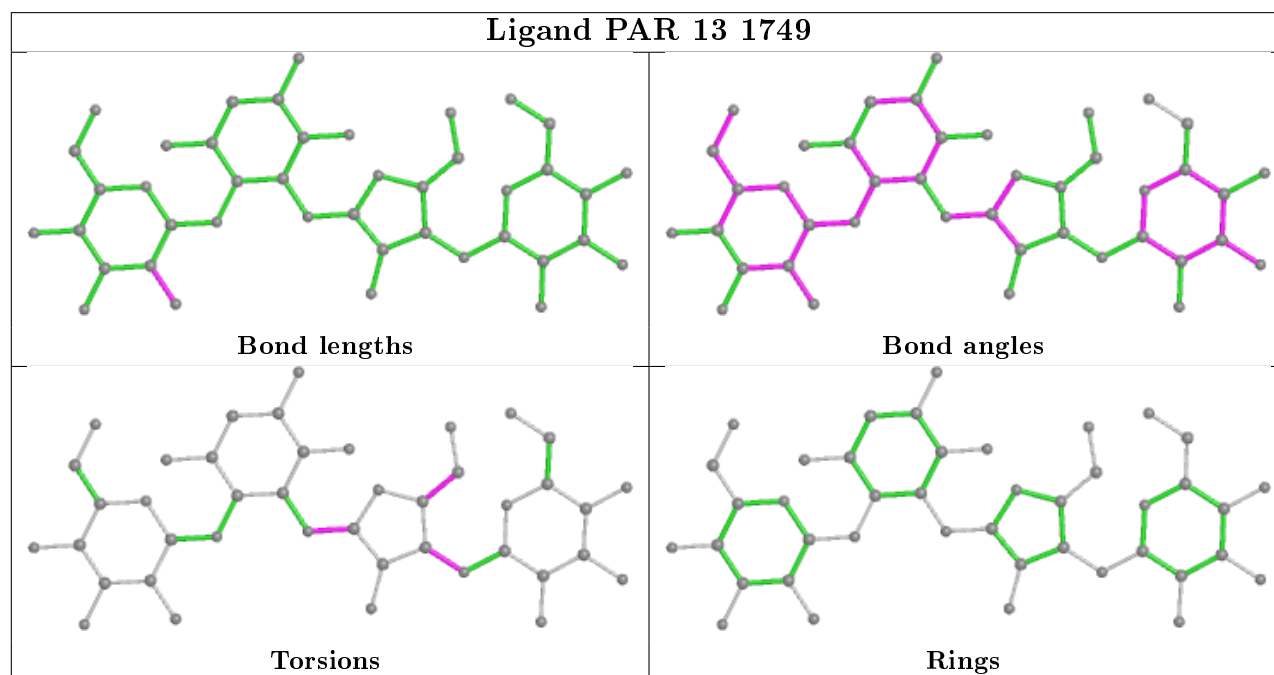
Mol	Chain	Res	Type	Atoms
59	13	1749	PAR	O43-C43-C53-O53
59	1G	1697	PAR	C44-C54-C64-N64
59	13	1749	PAR	O43-C13-O52-C52
59	1G	1697	PAR	O43-C43-C53-O53

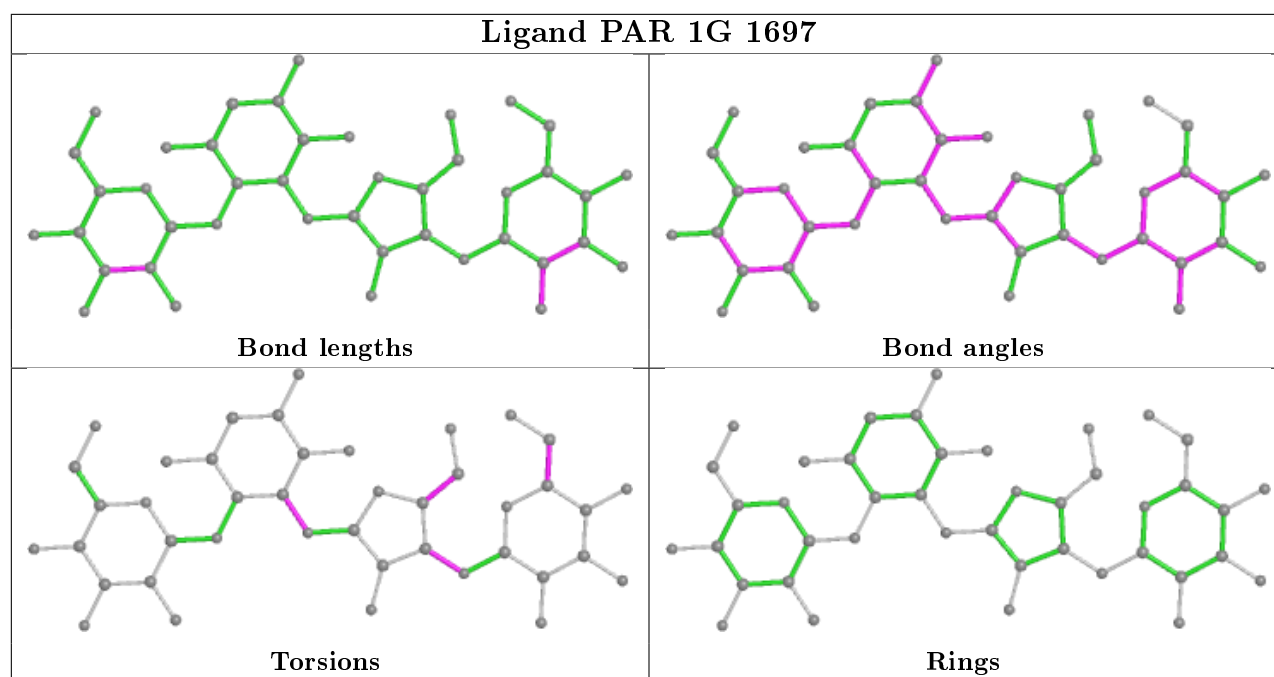
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	13	1749	PAR	1	0
59	1G	1697	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
1	1G	1
1	13	1
25	4L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	13	1530:G	O3'	1531:A	P	3.82
1	1G	1530:G	O3'	1531:A	P	3.28
1	4L	21:C	O3'	22:A	P	3.02

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	1498/1522 (98%)	0.27	14 (0%) 84 71	53, 93, 174, 276	0
1	1G	1498/1522 (98%)	0.40	67 (4%) 33 21	69, 116, 188, 285	0
2	12	237/256 (92%)	0.39	20 (8%) 11 6	141, 173, 195, 205	0
2	1E	237/256 (92%)	0.49	19 (8%) 12 7	105, 141, 169, 176	0
3	22	206/239 (86%)	1.37	63 (30%) 0 0	136, 162, 182, 190	0
3	2E	205/239 (85%)	0.72	19 (9%) 8 5	82, 102, 138, 147	0
4	32	208/209 (99%)	1.28	49 (23%) 0 0	93, 114, 138, 145	0
4	3E	208/209 (99%)	0.84	35 (16%) 1 1	75, 100, 123, 134	0
5	42	151/162 (93%)	1.85	61 (40%) 0 0	111, 135, 154, 184	0
5	4E	151/162 (93%)	1.15	35 (23%) 0 0	72, 93, 117, 160	0
6	52	101/101 (100%)	0.01	0 100 100	82, 100, 119, 142	0
6	5E	101/101 (100%)	0.33	2 (1%) 65 48	77, 96, 118, 141	0
7	62	152/156 (97%)	0.65	19 (12%) 3 2	112, 127, 147, 160	0
7	6E	155/156 (99%)	0.63	18 (11%) 4 2	92, 111, 146, 163	0
8	72	138/138 (100%)	2.12	60 (43%) 0 0	102, 132, 151, 155	0
8	7E	138/138 (100%)	1.25	35 (25%) 0 0	84, 101, 113, 121	0
9	82	124/128 (96%)	2.50	63 (50%) 0 0	115, 150, 165, 171	0
9	8E	127/128 (99%)	0.85	25 (19%) 1 0	80, 127, 148, 158	0
10	1A	99/105 (94%)	2.50	40 (40%) 0 0	131, 155, 176, 184	0
10	1I	99/105 (94%)	1.36	32 (32%) 0 0	73, 125, 159, 162	0
11	2A	116/129 (89%)	0.89	15 (12%) 3 2	85, 108, 130, 159	0
11	2I	116/129 (89%)	0.53	11 (9%) 8 5	69, 100, 127, 165	0
12	3A	125/132 (94%)	1.21	33 (26%) 0 0	83, 106, 134, 167	0
12	3I	125/132 (94%)	0.88	19 (15%) 2 1	60, 71, 107, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	4A	117/126 (92%)	2.11	52 (44%)	0	0	118, 155, 179, 185	0
13	4I	118/126 (93%)	0.75	19 (16%)	1	1	74, 112, 132, 145	0
14	5A	58/61 (95%)	6.47	53 (91%)	0	0	134, 159, 174, 179	0
14	5I	60/61 (98%)	2.20	33 (55%)	0	0	80, 91, 106, 119	0
15	6A	88/89 (98%)	0.60	11 (12%)	3	2	87, 112, 127, 133	0
15	6I	88/89 (98%)	0.65	10 (11%)	5	3	69, 98, 116, 127	0
16	7A	84/88 (95%)	1.85	34 (40%)	0	0	87, 103, 126, 159	0
16	7I	84/88 (95%)	2.10	42 (50%)	0	0	93, 107, 141, 158	0
17	8A	100/105 (95%)	1.74	41 (41%)	0	0	93, 110, 128, 148	0
17	8I	100/105 (95%)	1.09	22 (22%)	0	0	83, 101, 113, 116	0
18	9A	72/88 (81%)	0.44	5 (6%)	16	10	92, 115, 144, 170	0
18	9I	72/88 (81%)	0.28	0	100	100	83, 100, 136, 168	0
19	AA	78/93 (83%)	1.81	29 (37%)	0	0	150, 182, 192, 196	0
19	AI	81/93 (87%)	0.56	9 (11%)	5	3	88, 113, 138, 146	0
20	BA	99/106 (93%)	1.65	42 (42%)	0	0	85, 111, 137, 149	0
20	BI	99/106 (93%)	0.96	18 (18%)	1	1	102, 117, 153, 161	0
21	1B	25/27 (92%)	5.51	22 (88%)	0	0	119, 140, 152, 167	0
21	1F	25/27 (92%)	2.57	15 (60%)	0	0	88, 97, 113, 142	0
22	1K	70/76 (92%)	0.76	11 (15%)	2	1	76, 203, 247, 250	0
23	2K	72/77 (93%)	0.16	2 (2%)	53	36	68, 91, 119, 138	0
23	2L	72/77 (93%)	-0.08	2 (2%)	53	36	80, 113, 149, 166	0
24	3K	72/76 (94%)	0.31	4 (5%)	24	15	71, 230, 258, 260	0
25	4K	13/30 (43%)	0.91	2 (15%)	2	1	64, 80, 130, 131	0
25	4L	11/30 (36%)	1.08	1 (9%)	9	5	93, 124, 136, 143	0
26	14	2909/2917 (99%)	0.35	53 (1%)	68	51	50, 84, 241, 338	0
26	1H	2912/2917 (99%)	0.38	28 (0%)	82	68	37, 70, 222, 303	0
27	16	122/122 (100%)	-0.03	0	100	100	63, 87, 110, 193	0
27	1J	122/122 (100%)	-0.16	2 (1%)	72	55	86, 120, 149, 192	0
28	11	272/276 (98%)	0.62	11 (4%)	38	25	38, 62, 78, 83	0
28	19	273/276 (98%)	1.21	53 (19%)	1	0	46, 71, 87, 97	0
29	21	205/206 (99%)	1.00	24 (11%)	4	2	50, 88, 129, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
29	29	205/206 (99%)	1.26	45 (21%)	0 0	61, 93, 141, 174	0
30	31	202/210 (96%)	0.47	6 (2%)	50 34	43, 73, 113, 131	0
30	39	208/210 (99%)	0.64	24 (11%)	4 3	56, 103, 167, 189	0
31	41	181/182 (99%)	0.71	21 (11%)	4 2	78, 98, 131, 148	0
31	49	181/182 (99%)	1.35	54 (29%)	0 0	120, 142, 168, 178	0
32	51	174/180 (96%)	0.54	8 (4%)	32 20	77, 102, 120, 135	0
32	59	170/180 (94%)	3.51	109 (64%)	0 0	142, 193, 215, 227	0
33	61	146/148 (98%)	0.41	8 (5%)	25 15	71, 129, 146, 151	0
33	69	146/148 (98%)	0.77	22 (15%)	2 1	81, 122, 150, 157	0
34	15	138/140 (98%)	1.44	40 (28%)	0 0	77, 106, 136, 163	0
34	58	138/140 (98%)	0.73	11 (7%)	12 7	62, 89, 128, 145	0
35	25	122/122 (100%)	0.72	9 (7%)	14 8	66, 87, 103, 109	0
35	68	122/122 (100%)	0.53	3 (2%)	57 40	57, 73, 89, 100	0
36	35	150/150 (100%)	1.45	41 (27%)	0 0	58, 106, 138, 169	0
36	78	150/150 (100%)	0.71	13 (8%)	10 6	43, 77, 104, 157	0
37	45	141/141 (100%)	2.47	69 (48%)	0 0	75, 107, 136, 152	0
37	88	138/141 (97%)	0.73	7 (5%)	28 17	50, 76, 98, 128	0
38	55	117/118 (99%)	0.82	13 (11%)	5 3	59, 76, 91, 110	0
38	98	118/118 (100%)	0.99	16 (13%)	3 1	61, 81, 102, 110	0
39	65	111/112 (99%)	1.46	39 (35%)	0 0	91, 114, 131, 139	0
39	A8	111/112 (99%)	1.00	19 (17%)	1 1	73, 84, 108, 123	0
40	75	137/146 (93%)	0.84	20 (14%)	2 1	78, 95, 150, 184	0
40	B8	137/146 (93%)	0.59	9 (6%)	18 10	69, 89, 145, 175	0
41	85	117/118 (99%)	0.92	23 (19%)	1 0	66, 94, 138, 155	0
41	C8	117/118 (99%)	0.93	18 (15%)	2 1	52, 79, 111, 129	0
42	95	101/101 (100%)	0.95	22 (21%)	0 0	66, 124, 140, 157	0
42	D8	101/101 (100%)	0.72	12 (11%)	4 2	54, 103, 129, 140	0
43	A5	113/113 (100%)	1.12	14 (12%)	4 2	60, 72, 105, 150	0
43	E8	113/113 (100%)	0.88	10 (8%)	10 5	56, 72, 105, 146	0
44	B5	94/96 (97%)	1.07	11 (11%)	4 2	68, 83, 109, 120	0
44	F8	94/96 (97%)	0.49	3 (3%)	47 31	55, 69, 90, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	C5	104/110 (94%)	1.55	28 (26%) 0 0	92, 115, 146, 153	0
45	G8	104/110 (94%)	0.46	3 (2%) 51 35	70, 90, 131, 142	0
46	D5	179/206 (86%)	1.27	44 (24%) 0 0	113, 151, 230, 237	0
46	H8	175/206 (84%)	0.30	4 (2%) 60 43	80, 119, 203, 216	0
47	E5	77/85 (90%)	2.07	36 (46%) 0 0	67, 88, 106, 145	0
47	I8	80/85 (94%)	1.11	13 (16%) 1 1	54, 67, 101, 108	0
48	F5	94/98 (95%)	1.74	39 (41%) 0 0	60, 79, 122, 132	0
48	J8	97/98 (98%)	1.39	21 (21%) 0 0	50, 69, 122, 149	0
49	G5	67/72 (93%)	0.69	7 (10%) 6 4	80, 100, 121, 144	0
49	K8	67/72 (93%)	0.68	2 (2%) 50 34	61, 77, 95, 125	0
50	H5	59/60 (98%)	1.48	17 (28%) 0 0	77, 100, 140, 153	0
50	L8	57/60 (95%)	0.53	1 (1%) 68 51	57, 79, 102, 109	0
51	I5	60/71 (84%)	1.03	12 (20%) 1 0	151, 187, 203, 206	0
51	M8	66/71 (92%)	0.88	13 (19%) 1 0	104, 144, 179, 189	0
52	J5	59/60 (98%)	1.06	7 (11%) 4 2	57, 81, 150, 183	0
52	N8	58/60 (96%)	1.28	8 (13%) 2 1	48, 97, 160, 163	0
53	K5	45/54 (83%)	7.57	42 (93%) 0 0	123, 152, 165, 172	0
53	O8	45/54 (83%)	4.33	37 (82%) 0 0	107, 137, 157, 161	0
54	L5	46/49 (93%)	1.25	6 (13%) 3 2	45, 58, 72, 85	0
54	P8	45/49 (91%)	0.69	2 (4%) 34 21	40, 48, 61, 75	0
55	M5	60/65 (92%)	1.93	23 (38%) 0 0	71, 79, 100, 124	0
55	Q8	60/65 (92%)	1.99	24 (40%) 0 0	56, 72, 98, 109	0
56	1L	72/76 (94%)	1.69	19 (26%) 0 0	122, 239, 257, 262	0
57	3L	71/76 (93%)	0.72	10 (14%) 2 1	82, 208, 243, 253	0
All	All	21028/21694 (96%)	0.79	2541 (12%) 4 2	37, 97, 186, 338	0

The worst 5 of 2541 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	59	100	GLY	23.3
32	59	4	ILE	21.1
53	K5	13	CYS	18.8
53	K5	50	ARG	17.1
53	K5	42	TRP	16.4

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	0.76	0.16	112,129,148,149	0
56	5MU	1L	54	21/22	0.77	0.27	134,151,174,175	0
57	5MU	3L	54	21/22	0.78	0.18	115,149,174,177	0
57	PSU	3L	55	20/21	0.78	0.15	121,143,168,174	0
57	4SU	3L	8	20/21	0.80	0.09	153,160,176,185	0
56	PSU	1L	32	20/21	0.80	0.32	124,129,142,152	0
57	7MG	3L	46	24/25	0.83	0.10	147,158,169,181	0
24	MIA	3K	37	29/30	0.84	0.28	103,119,131,151	0
57	PSU	3L	32	20/21	0.86	0.18	119,134,142,142	0
56	PSU	1L	39	20/21	0.89	0.27	110,121,135,138	0
22	4SU	1K	8	20/21	0.89	0.10	129,144,162,164	0
23	PSU	2L	56	20/21	0.91	0.10	96,107,114,116	0
56	MIA	1L	37	29/30	0.91	0.35	102,116,122,128	0
23	5MU	2L	55	21/22	0.92	0.13	101,107,114,117	0
24	PSU	3K	32	20/21	0.93	0.18	108,124,131,143	0
23	PSU	2K	56	20/21	0.93	0.13	84,91,100,103	0
24	PSU	3K	39	20/21	0.93	0.14	113,120,126,127	0
23	4SU	2L	8	20/21	0.93	0.11	94,105,113,115	0
22	PSU	1K	32	20/21	0.94	0.23	89,96,103,114	0
22	5MU	1K	54	21/22	0.94	0.13	106,112,129,132	0
22	PSU	1K	39	20/21	0.95	0.17	72,86,90,90	0
23	7MG	2K	47	24/25	0.95	0.14	82,93,103,108	0
22	MIA	1K	37	29/30	0.95	0.25	70,75,87,93	0
23	5MU	2K	55	21/22	0.96	0.12	81,93,97,102	0
23	4SU	2K	8	20/21	0.96	0.17	75,84,93,98	0
23	7MG	2L	47	24/25	0.96	0.10	107,115,120,123	0
23	OMC	2L	33	21/22	0.97	0.21	87,93,96,103	0
23	OMC	2K	33	21/22	0.98	0.25	65,68,74,78	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1H	3491	1/1	0.32	0.13	105,105,105,105	0
60	ZN	G8	202	1/1	0.39	0.17	164,164,164,164	0
58	MG	1G	1607	1/1	0.46	0.26	85,85,85,85	0
58	MG	1H	3292	1/1	0.47	0.38	84,84,84,84	0
58	MG	1G	1661	1/1	0.47	0.17	99,99,99,99	0
58	MG	14	3266	1/1	0.51	0.26	84,84,84,84	0
58	MG	3K	101	1/1	0.52	0.23	80,80,80,80	0
58	MG	1H	3302	1/1	0.53	0.18	77,77,77,77	0
58	MG	14	3178	1/1	0.55	0.25	88,88,88,88	0
58	MG	1H	3334	1/1	0.55	0.46	95,95,95,95	0
58	MG	14	3193	1/1	0.55	0.41	89,89,89,89	0
58	MG	14	3143	1/1	0.55	0.45	85,85,85,85	0
58	MG	1H	3500	1/1	0.55	0.12	54,54,54,54	0
58	MG	29	304	1/1	0.56	0.28	95,95,95,95	0
58	MG	1H	3310	1/1	0.56	0.46	105,105,105,105	0
58	MG	14	3039	1/1	0.56	0.18	74,74,74,74	0
58	MG	14	3269	1/1	0.58	0.27	77,77,77,77	0
58	MG	1H	3214	1/1	0.58	0.26	67,67,67,67	0
58	MG	1H	3012	1/1	0.58	0.38	78,78,78,78	0
58	MG	1H	3392	1/1	0.59	0.09	94,94,94,94	0
60	ZN	C5	202	1/1	0.59	0.19	181,181,181,181	0
58	MG	14	3035	1/1	0.59	0.21	72,72,72,72	0
58	MG	1H	3045	1/1	0.60	0.29	72,72,72,72	0
58	MG	1H	3475	1/1	0.61	0.16	109,109,109,109	0
58	MG	1H	3027	1/1	0.62	0.24	76,76,76,76	0
58	MG	1H	3047	1/1	0.63	0.34	76,76,76,76	0
58	MG	1H	3273	1/1	0.64	0.19	84,84,84,84	0
58	MG	1H	3262	1/1	0.64	0.43	96,96,96,96	0
58	MG	1H	3025	1/1	0.65	0.30	90,90,90,90	0
58	MG	13	1666	1/1	0.66	0.32	82,82,82,82	0
58	MG	14	3272	1/1	0.66	0.21	85,85,85,85	0
58	MG	13	1684	1/1	0.67	0.33	94,94,94,94	0
58	MG	14	3298	1/1	0.67	0.13	93,93,93,93	0
58	MG	1H	3403	1/1	0.67	0.11	72,72,72,72	0
58	MG	13	1622	1/1	0.67	0.30	66,66,66,66	0
58	MG	1H	3314	1/1	0.67	0.34	84,84,84,84	0
58	MG	14	3337	1/1	0.67	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3185	1/1	0.67	0.18	81,81,81,81	0
58	MG	1H	3051	1/1	0.67	0.24	97,97,97,97	0
58	MG	1H	3205	1/1	0.68	0.18	68,68,68,68	0
58	MG	13	1710	1/1	0.68	0.43	148,148,148,148	0
58	MG	13	1664	1/1	0.68	0.16	74,74,74,74	0
58	MG	1H	3248	1/1	0.69	0.36	75,75,75,75	0
58	MG	14	3285	1/1	0.69	0.39	104,104,104,104	0
58	MG	1H	3337	1/1	0.69	0.43	86,86,86,86	0
58	MG	1H	3019	1/1	0.69	0.25	85,85,85,85	0
58	MG	14	3048	1/1	0.69	0.23	76,76,76,76	0
58	MG	14	3265	1/1	0.69	0.21	90,90,90,90	0
58	MG	14	3049	1/1	0.69	0.22	86,86,86,86	0
58	MG	1H	3249	1/1	0.69	0.33	76,76,76,76	0
58	MG	14	3077	1/1	0.70	0.14	77,77,77,77	0
58	MG	14	3029	1/1	0.70	0.15	87,87,87,87	0
58	MG	14	3186	1/1	0.70	0.22	85,85,85,85	0
58	MG	1H	3345	1/1	0.70	0.26	81,81,81,81	0
58	MG	5I	101	1/1	0.70	0.21	81,81,81,81	0
58	MG	1H	3081	1/1	0.70	0.33	90,90,90,90	0
58	MG	1H	3499	1/1	0.71	0.08	105,105,105,105	0
58	MG	13	1665	1/1	0.71	0.25	88,88,88,88	0
58	MG	1H	3056	1/1	0.72	0.54	97,97,97,97	0
58	MG	14	3406	1/1	0.72	0.30	112,112,112,112	0
58	MG	13	1608	1/1	0.72	0.26	85,85,85,85	0
58	MG	1H	3092	1/1	0.72	0.31	57,57,57,57	0
58	MG	14	3255	1/1	0.72	0.32	92,92,92,92	0
58	MG	14	3010	1/1	0.72	0.23	78,78,78,78	0
58	MG	1G	1660	1/1	0.72	0.30	98,98,98,98	0
58	MG	1H	3454	1/1	0.72	0.23	67,67,67,67	0
58	MG	1H	3513	1/1	0.72	0.21	82,82,82,82	0
58	MG	1H	3161	1/1	0.72	0.13	89,89,89,89	0
58	MG	1H	3275	1/1	0.73	0.35	82,82,82,82	0
58	MG	1H	3218	1/1	0.73	0.28	55,55,55,55	0
58	MG	14	3276	1/1	0.73	0.31	80,80,80,80	0
58	MG	14	3289	1/1	0.73	0.16	78,78,78,78	0
58	MG	1H	3293	1/1	0.73	0.23	67,67,67,67	0
58	MG	14	3158	1/1	0.73	0.45	95,95,95,95	0
58	MG	1H	3282	1/1	0.73	0.27	98,98,98,98	0
58	MG	14	3361	1/1	0.73	0.05	76,76,76,76	0
58	MG	14	3160	1/1	0.73	0.14	82,82,82,82	0
58	MG	1H	3208	1/1	0.74	0.22	70,70,70,70	0
58	MG	7A	101	1/1	0.74	0.32	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3038	1/1	0.74	0.35	86,86,86,86	0
58	MG	13	1694	1/1	0.74	0.23	78,78,78,78	0
58	MG	1H	3326	1/1	0.74	0.19	90,90,90,90	0
58	MG	13	1704	1/1	0.74	0.32	102,102,102,102	0
58	MG	1H	3247	1/1	0.74	0.54	92,92,92,92	0
58	MG	1G	1635	1/1	0.74	0.33	92,92,92,92	0
58	MG	1H	3269	1/1	0.74	0.29	72,72,72,72	0
58	MG	1H	3254	1/1	0.74	0.43	78,78,78,78	0
58	MG	16	203	1/1	0.75	0.22	81,81,81,81	0
58	MG	1J	204	1/1	0.75	0.30	94,94,94,94	0
58	MG	14	3019	1/1	0.75	0.33	84,84,84,84	0
58	MG	14	3271	1/1	0.75	0.19	86,86,86,86	0
58	MG	1H	3519	1/1	0.75	0.11	101,101,101,101	0
58	MG	1H	3469	1/1	0.75	0.10	99,99,99,99	0
58	MG	14	3381	1/1	0.75	0.09	91,91,91,91	0
58	MG	1H	3024	1/1	0.75	0.30	77,77,77,77	0
58	MG	14	3045	1/1	0.75	0.27	70,70,70,70	0
58	MG	1H	3267	1/1	0.75	0.17	71,71,71,71	0
58	MG	14	3211	1/1	0.76	0.15	81,81,81,81	0
58	MG	1H	3180	1/1	0.76	0.32	77,77,77,77	0
58	MG	14	3020	1/1	0.76	0.15	75,75,75,75	0
58	MG	1H	3271	1/1	0.76	0.37	80,80,80,80	0
58	MG	98	202	1/1	0.76	0.31	95,95,95,95	0
58	MG	14	3293	1/1	0.76	0.34	94,94,94,94	0
58	MG	14	3144	1/1	0.76	0.34	81,81,81,81	0
58	MG	1H	3258	1/1	0.76	0.23	64,64,64,64	0
58	MG	1H	3303	1/1	0.76	0.21	76,76,76,76	0
58	MG	14	3015	1/1	0.76	0.21	80,80,80,80	0
58	MG	14	3051	1/1	0.76	0.33	102,102,102,102	0
58	MG	1H	3157	1/1	0.77	0.26	84,84,84,84	0
58	MG	1H	3281	1/1	0.77	0.39	98,98,98,98	0
58	MG	1H	3049	1/1	0.77	0.32	69,69,69,69	0
58	MG	1H	3198	1/1	0.77	0.22	70,70,70,70	0
58	MG	1H	3010	1/1	0.77	0.40	87,87,87,87	0
58	MG	1H	3137	1/1	0.77	0.31	71,71,71,71	0
58	MG	14	3392	1/1	0.77	0.23	77,77,77,77	0
58	MG	13	1609	1/1	0.77	0.16	81,81,81,81	0
58	MG	1H	3290	1/1	0.77	0.24	84,84,84,84	0
58	MG	1H	3257	1/1	0.77	0.19	69,69,69,69	0
58	MG	14	3254	1/1	0.77	0.18	92,92,92,92	0
58	MG	14	3397	1/1	0.77	0.10	52,52,52,52	0
58	MG	1H	3316	1/1	0.78	0.28	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3021	1/1	0.78	0.34	68,68,68,68	0
58	MG	3L	101	1/1	0.78	0.25	99,99,99,99	0
58	MG	11	304	1/1	0.78	0.26	73,73,73,73	0
58	MG	1H	3020	1/1	0.78	0.49	90,90,90,90	0
58	MG	1H	3484	1/1	0.78	0.12	73,73,73,73	0
58	MG	13	1708	1/1	0.78	0.29	90,90,90,90	0
58	MG	1H	3052	1/1	0.78	0.33	83,83,83,83	0
58	MG	1H	3177	1/1	0.78	0.39	86,86,86,86	0
58	MG	13	1745	1/1	0.78	0.14	107,107,107,107	0
58	MG	1H	3220	1/1	0.78	0.17	74,74,74,74	0
58	MG	1H	3054	1/1	0.78	0.32	92,92,92,92	0
58	MG	1H	3196	1/1	0.78	0.38	102,102,102,102	0
58	MG	1H	3035	1/1	0.79	0.37	89,89,89,89	0
58	MG	13	1675	1/1	0.79	0.14	78,78,78,78	0
58	MG	14	3263	1/1	0.79	0.29	76,76,76,76	0
58	MG	1H	3162	1/1	0.79	0.43	89,89,89,89	0
58	MG	14	3082	1/1	0.79	0.23	63,63,63,63	0
58	MG	1H	3287	1/1	0.79	0.34	77,77,77,77	0
58	MG	1G	1675	1/1	0.79	0.18	90,90,90,90	0
58	MG	14	3372	1/1	0.79	0.11	76,76,76,76	0
58	MG	14	3166	1/1	0.79	0.35	81,81,81,81	0
58	MG	14	3379	1/1	0.79	0.07	106,106,106,106	0
58	MG	1H	3389	1/1	0.79	0.07	74,74,74,74	0
58	MG	3L	102	1/1	0.79	0.11	151,151,151,151	0
58	MG	1G	1688	1/1	0.79	0.10	102,102,102,102	0
58	MG	14	3268	1/1	0.79	0.14	87,87,87,87	0
58	MG	1H	3321	1/1	0.79	0.25	72,72,72,72	0
58	MG	1H	3426	1/1	0.79	0.12	88,88,88,88	0
58	MG	41	202	1/1	0.80	0.34	81,81,81,81	0
58	MG	1G	1601	1/1	0.80	0.29	90,90,90,90	0
58	MG	1H	3234	1/1	0.80	0.32	67,67,67,67	0
58	MG	1H	3133	1/1	0.80	0.23	53,53,53,53	0
58	MG	1H	3331	1/1	0.80	0.15	67,67,67,67	0
58	MG	14	3389	1/1	0.80	0.13	75,75,75,75	0
58	MG	1H	3240	1/1	0.80	0.18	77,77,77,77	0
58	MG	1H	3195	1/1	0.80	0.38	81,81,81,81	0
58	MG	1H	3259	1/1	0.80	0.33	82,82,82,82	0
58	MG	14	3116	1/1	0.80	0.26	80,80,80,80	0
58	MG	13	1699	1/1	0.80	0.14	61,61,61,61	0
58	MG	1H	3295	1/1	0.80	0.40	87,87,87,87	0
58	MG	1H	3301	1/1	0.80	0.31	59,59,59,59	0
58	MG	1H	3283	1/1	0.80	0.24	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	13	1615	1/1	0.80	0.34	84,84,84,84	0
58	MG	14	3159	1/1	0.80	0.11	73,73,73,73	0
58	MG	1H	3184	1/1	0.80	0.33	78,78,78,78	0
58	MG	14	3050	1/1	0.81	0.39	94,94,94,94	0
58	MG	14	3229	1/1	0.81	0.34	91,91,91,91	0
58	MG	1H	3040	1/1	0.81	0.47	76,76,76,76	0
58	MG	1H	3492	1/1	0.81	0.28	82,82,82,82	0
58	MG	13	1701	1/1	0.81	0.21	99,99,99,99	0
58	MG	14	3274	1/1	0.81	0.23	88,88,88,88	0
58	MG	14	3338	1/1	0.81	0.12	74,74,74,74	0
58	MG	13	1652	1/1	0.81	0.16	85,85,85,85	0
58	MG	13	1736	1/1	0.81	0.08	116,116,116,116	0
58	MG	14	3151	1/1	0.81	0.53	91,91,91,91	0
58	MG	14	3370	1/1	0.81	0.10	106,106,106,106	0
58	MG	1G	1636	1/1	0.81	0.38	106,106,106,106	0
58	MG	13	1700	1/1	0.81	0.30	92,92,92,92	0
58	MG	14	3385	1/1	0.81	0.12	91,91,91,91	0
58	MG	1G	1647	1/1	0.81	0.16	94,94,94,94	0
58	MG	1H	3339	1/1	0.81	0.33	75,75,75,75	0
58	MG	1H	3431	1/1	0.81	0.10	94,94,94,94	0
58	MG	1H	3268	1/1	0.81	0.25	71,71,71,71	0
58	MG	14	3023	1/1	0.81	0.26	90,90,90,90	0
58	MG	14	3376	1/1	0.81	0.06	119,119,119,119	0
58	MG	1G	1606	1/1	0.81	0.17	83,83,83,83	0
58	MG	1H	3043	1/1	0.81	0.22	77,77,77,77	0
58	MG	14	3292	1/1	0.81	0.26	84,84,84,84	0
58	MG	16	206	1/1	0.81	0.21	74,74,74,74	0
58	MG	1H	3155	1/1	0.81	0.10	58,58,58,58	0
58	MG	14	3172	1/1	0.81	0.13	72,72,72,72	0
58	MG	1H	3315	1/1	0.82	0.32	80,80,80,80	0
58	MG	1H	3272	1/1	0.82	0.24	68,68,68,68	0
58	MG	1G	1680	1/1	0.82	0.38	101,101,101,101	0
58	MG	13	1712	1/1	0.82	0.14	80,80,80,80	0
58	MG	14	3147	1/1	0.82	0.16	81,81,81,81	0
58	MG	1H	3023	1/1	0.82	0.53	88,88,88,88	0
58	MG	13	1651	1/1	0.82	0.23	79,79,79,79	0
58	MG	1H	3308	1/1	0.82	0.26	75,75,75,75	0
58	MG	1H	3192	1/1	0.82	0.17	71,71,71,71	0
58	MG	1H	3174	1/1	0.82	0.25	70,70,70,70	0
58	MG	13	1606	1/1	0.82	0.43	88,88,88,88	0
58	MG	14	3407	1/1	0.82	0.09	117,117,117,117	0
58	MG	1H	3156	1/1	0.82	0.17	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2L	102	1/1	0.82	0.20	85,85,85,85	0
58	MG	14	3220	1/1	0.82	0.30	66,66,66,66	0
58	MG	1J	202	1/1	0.82	0.34	88,88,88,88	0
58	MG	1H	3340	1/1	0.82	0.35	82,82,82,82	0
58	MG	14	3047	1/1	0.83	0.15	92,92,92,92	0
58	MG	1H	3457	1/1	0.83	0.15	82,82,82,82	0
58	MG	14	3244	1/1	0.83	0.13	68,68,68,68	0
58	MG	14	3148	1/1	0.83	0.19	65,65,65,65	0
58	MG	1H	3159	1/1	0.83	0.28	73,73,73,73	0
58	MG	13	1705	1/1	0.83	0.44	91,91,91,91	0
58	MG	1H	3474	1/1	0.83	0.10	100,100,100,100	0
58	MG	14	3367	1/1	0.83	0.07	103,103,103,103	0
58	MG	14	3169	1/1	0.83	0.22	92,92,92,92	0
58	MG	14	3121	1/1	0.83	0.30	75,75,75,75	0
58	MG	1H	3077	1/1	0.83	0.18	54,54,54,54	0
58	MG	1H	3246	1/1	0.83	0.27	75,75,75,75	0
58	MG	13	1723	1/1	0.83	0.13	70,70,70,70	0
58	MG	1H	3187	1/1	0.83	0.17	78,78,78,78	0
58	MG	1H	3188	1/1	0.83	0.31	73,73,73,73	0
58	MG	1H	3346	1/1	0.83	0.16	80,80,80,80	0
58	MG	14	3034	1/1	0.83	0.27	82,82,82,82	0
58	MG	1H	3422	1/1	0.83	0.15	66,66,66,66	0
58	MG	1H	3327	1/1	0.83	0.35	77,77,77,77	0
58	MG	14	3126	1/1	0.83	0.21	79,79,79,79	0
58	MG	11	301	1/1	0.83	0.26	50,50,50,50	0
58	MG	1H	3075	1/1	0.83	0.19	76,76,76,76	0
58	MG	1H	3030	1/1	0.83	0.21	67,67,67,67	0
58	MG	14	3300	1/1	0.83	0.20	63,63,63,63	0
58	MG	16	204	1/1	0.83	0.19	67,67,67,67	0
58	MG	1H	3348	1/1	0.83	0.33	73,73,73,73	0
58	MG	14	3234	1/1	0.83	0.16	80,80,80,80	0
58	MG	1H	3421	1/1	0.83	0.15	46,46,46,46	0
58	MG	1G	1646	1/1	0.84	0.37	95,95,95,95	0
58	MG	1G	1649	1/1	0.84	0.23	101,101,101,101	0
58	MG	14	3286	1/1	0.84	0.14	71,71,71,71	0
58	MG	1H	3266	1/1	0.84	0.24	91,91,91,91	0
58	MG	13	1636	1/1	0.84	0.27	77,77,77,77	0
58	MG	1H	3136	1/1	0.84	0.18	73,73,73,73	0
58	MG	13	1680	1/1	0.84	0.18	97,97,97,97	0
58	MG	14	3242	1/1	0.84	0.20	78,78,78,78	0
58	MG	13	1683	1/1	0.84	0.12	76,76,76,76	0
58	MG	1H	3033	1/1	0.84	0.37	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3123	1/1	0.84	0.24	78,78,78,78	0
58	MG	13	1692	1/1	0.84	0.18	79,79,79,79	0
58	MG	14	3227	1/1	0.84	0.11	84,84,84,84	0
58	MG	1H	3224	1/1	0.84	0.49	92,92,92,92	0
58	MG	14	3299	1/1	0.84	0.17	76,76,76,76	0
58	MG	14	3140	1/1	0.84	0.23	69,69,69,69	0
58	MG	1H	3333	1/1	0.84	0.28	71,71,71,71	0
58	MG	1H	3007	1/1	0.84	0.36	64,64,64,64	0
58	MG	16	205	1/1	0.84	0.20	81,81,81,81	0
58	MG	1H	3277	1/1	0.84	0.27	70,70,70,70	0
58	MG	1H	3153	1/1	0.84	0.29	72,72,72,72	0
58	MG	14	3025	1/1	0.84	0.21	81,81,81,81	0
58	MG	1H	3242	1/1	0.84	0.33	77,77,77,77	0
58	MG	1H	3297	1/1	0.85	0.31	78,78,78,78	0
58	MG	1H	3514	1/1	0.85	0.09	77,77,77,77	0
58	MG	13	1706	1/1	0.85	0.38	81,81,81,81	0
58	MG	14	3164	1/1	0.85	0.34	78,78,78,78	0
58	MG	1H	3119	1/1	0.85	0.33	91,91,91,91	0
58	MG	1H	3098	1/1	0.85	0.41	71,71,71,71	0
58	MG	1H	3228	1/1	0.85	0.22	83,83,83,83	0
58	MG	1G	1625	1/1	0.85	0.12	129,129,129,129	0
58	MG	1J	205	1/1	0.85	0.20	78,78,78,78	0
58	MG	14	3248	1/1	0.85	0.20	79,79,79,79	0
58	MG	1H	3185	1/1	0.85	0.27	72,72,72,72	0
58	MG	1H	3241	1/1	0.85	0.29	71,71,71,71	0
58	MG	1H	3322	1/1	0.85	0.22	88,88,88,88	0
58	MG	1H	3138	1/1	0.85	0.14	65,65,65,65	0
58	MG	14	3386	1/1	0.85	0.12	94,94,94,94	0
58	MG	1H	3183	1/1	0.85	0.18	60,60,60,60	0
58	MG	1H	3154	1/1	0.85	0.19	59,59,59,59	0
58	MG	1H	3026	1/1	0.85	0.32	80,80,80,80	0
58	MG	14	3118	1/1	0.85	0.15	72,72,72,72	0
58	MG	14	3404	1/1	0.85	0.12	66,66,66,66	0
58	MG	1H	3175	1/1	0.85	0.19	65,65,65,65	0
58	MG	1G	1630	1/1	0.85	0.14	78,78,78,78	0
58	MG	14	3167	1/1	0.85	0.19	86,86,86,86	0
58	MG	14	3168	1/1	0.85	0.32	92,92,92,92	0
58	MG	14	3296	1/1	0.85	0.16	74,74,74,74	0
58	MG	14	3236	1/1	0.85	0.21	86,86,86,86	0
58	MG	1H	3330	1/1	0.85	0.23	75,75,75,75	0
58	MG	14	3076	1/1	0.85	0.13	73,73,73,73	0
58	MG	1H	3440	1/1	0.85	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	88	202	1/1	0.85	0.22	64,64,64,64	0
58	MG	14	3145	1/1	0.86	0.33	87,87,87,87	0
58	MG	14	3231	1/1	0.86	0.21	70,70,70,70	0
58	MG	1G	1633	1/1	0.86	0.31	82,82,82,82	0
58	MG	14	3180	1/1	0.86	0.15	74,74,74,74	0
58	MG	14	3273	1/1	0.86	0.12	62,62,62,62	0
58	MG	1H	3165	1/1	0.86	0.24	60,60,60,60	0
58	MG	14	3369	1/1	0.86	0.07	102,102,102,102	0
58	MG	14	3075	1/1	0.86	0.13	89,89,89,89	0
58	MG	1H	3031	1/1	0.86	0.41	90,90,90,90	0
58	MG	1H	3113	1/1	0.86	0.21	68,68,68,68	0
58	MG	14	3387	1/1	0.86	0.17	93,93,93,93	0
58	MG	14	3190	1/1	0.86	0.14	53,53,53,53	0
58	MG	1H	3335	1/1	0.86	0.22	59,59,59,59	0
58	MG	13	1647	1/1	0.86	0.13	87,87,87,87	0
58	MG	14	3090	1/1	0.86	0.15	68,68,68,68	0
58	MG	1G	1685	1/1	0.86	0.11	88,88,88,88	0
58	MG	14	3258	1/1	0.86	0.12	82,82,82,82	0
58	MG	1H	3509	1/1	0.86	0.12	68,68,68,68	0
58	MG	1H	3250	1/1	0.86	0.46	86,86,86,86	0
58	MG	1H	3343	1/1	0.86	0.54	99,99,99,99	0
58	MG	14	3282	1/1	0.86	0.45	88,88,88,88	0
58	MG	14	3060	1/1	0.86	0.17	58,58,58,58	0
58	MG	3E	301	1/1	0.86	0.14	109,109,109,109	0
58	MG	1H	3243	1/1	0.86	0.27	81,81,81,81	0
58	MG	1H	3252	1/1	0.86	0.15	60,60,60,60	0
58	MG	14	3012	1/1	0.86	0.13	69,69,69,69	0
58	MG	1H	3341	1/1	0.86	0.16	96,96,96,96	0
58	MG	1H	3042	1/1	0.86	0.17	64,64,64,64	0
58	MG	1H	3217	1/1	0.86	0.25	54,54,54,54	0
58	MG	16	209	1/1	0.87	0.26	65,65,65,65	0
58	MG	1H	3284	1/1	0.87	0.25	74,74,74,74	0
58	MG	1H	3200	1/1	0.87	0.17	35,35,35,35	0
58	MG	2K	103	1/1	0.87	0.31	88,88,88,88	0
58	MG	1H	3202	1/1	0.87	0.23	58,58,58,58	0
58	MG	14	3001	1/1	0.87	0.28	89,89,89,89	0
58	MG	13	1677	1/1	0.87	0.29	74,74,74,74	0
58	MG	78	201	1/1	0.87	0.25	80,80,80,80	0
58	MG	14	3201	1/1	0.87	0.19	69,69,69,69	0
58	MG	1H	3478	1/1	0.87	0.13	91,91,91,91	0
58	MG	1H	3199	1/1	0.87	0.19	44,44,44,44	0
58	MG	1H	3221	1/1	0.87	0.26	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3080	1/1	0.87	0.14	56,56,56,56	0
58	MG	14	3250	1/1	0.87	0.22	72,72,72,72	0
58	MG	13	1648	1/1	0.87	0.36	78,78,78,78	0
58	MG	1H	3078	1/1	0.87	0.21	67,67,67,67	0
58	MG	13	1707	1/1	0.87	0.45	80,80,80,80	0
58	MG	13	1644	1/1	0.87	0.36	78,78,78,78	0
58	MG	14	3239	1/1	0.87	0.37	98,98,98,98	0
58	MG	13	1630	1/1	0.87	0.16	67,67,67,67	0
58	MG	5I	102	1/1	0.87	0.26	90,90,90,90	0
58	MG	13	1687	1/1	0.87	0.21	98,98,98,98	0
58	MG	1H	3329	1/1	0.87	0.33	85,85,85,85	0
58	MG	1H	3338	1/1	0.87	0.34	80,80,80,80	0
58	MG	14	3277	1/1	0.87	0.13	104,104,104,104	0
58	MG	14	3281	1/1	0.87	0.30	84,84,84,84	0
58	MG	1H	3376	1/1	0.87	0.18	67,67,67,67	0
58	MG	1G	1671	1/1	0.87	0.18	82,82,82,82	0
58	MG	1H	3044	1/1	0.87	0.21	61,61,61,61	0
58	MG	14	3294	1/1	0.87	0.15	94,94,94,94	0
58	MG	1G	1631	1/1	0.87	0.25	82,82,82,82	0
58	MG	1H	3430	1/1	0.87	0.09	73,73,73,73	0
58	MG	14	3223	1/1	0.87	0.10	80,80,80,80	0
58	MG	1H	3285	1/1	0.87	0.12	80,80,80,80	0
58	MG	1H	3354	1/1	0.87	0.13	49,49,49,49	0
58	MG	14	3400	1/1	0.87	0.09	65,65,65,65	0
58	MG	14	3253	1/1	0.87	0.18	151,151,151,151	0
58	MG	1H	3520	1/1	0.87	0.51	97,97,97,97	0
58	MG	14	3016	1/1	0.88	0.32	91,91,91,91	0
58	MG	1H	3311	1/1	0.88	0.31	81,81,81,81	0
58	MG	1H	3383	1/1	0.88	0.12	61,61,61,61	0
58	MG	1H	3309	1/1	0.88	0.17	70,70,70,70	0
58	MG	13	1738	1/1	0.88	0.07	84,84,84,84	0
58	MG	13	1627	1/1	0.88	0.31	90,90,90,90	0
58	MG	14	3390	1/1	0.88	0.12	109,109,109,109	0
58	MG	1G	1678	1/1	0.88	0.29	108,108,108,108	0
58	MG	13	1725	1/1	0.88	0.08	77,77,77,77	0
58	MG	14	3044	1/1	0.88	0.16	57,57,57,57	0
58	MG	1H	3204	1/1	0.88	0.14	41,41,41,41	0
58	MG	1G	1670	1/1	0.88	0.12	88,88,88,88	0
58	MG	14	3275	1/1	0.88	0.18	86,86,86,86	0
58	MG	1H	3342	1/1	0.88	0.30	89,89,89,89	0
58	MG	14	3245	1/1	0.88	0.29	77,77,77,77	0
58	MG	13	1739	1/1	0.88	0.07	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3503	1/1	0.88	0.28	73,73,73,73	0
58	MG	1H	3485	1/1	0.88	0.09	87,87,87,87	0
58	MG	1H	3169	1/1	0.88	0.37	85,85,85,85	0
58	MG	14	3122	1/1	0.88	0.36	79,79,79,79	0
58	MG	13	1669	1/1	0.88	0.11	68,68,68,68	0
58	MG	1H	3186	1/1	0.88	0.17	74,74,74,74	0
58	MG	13	1643	1/1	0.88	0.35	78,78,78,78	0
58	MG	13	1721	1/1	0.88	0.09	83,83,83,83	0
58	MG	1H	3497	1/1	0.88	0.14	42,42,42,42	0
58	MG	1G	1676	1/1	0.88	0.35	95,95,95,95	0
58	MG	14	3176	1/1	0.88	0.19	58,58,58,58	0
58	MG	14	3042	1/1	0.88	0.24	87,87,87,87	0
58	MG	29	303	1/1	0.88	0.19	73,73,73,73	0
58	MG	2L	103	1/1	0.88	0.21	93,93,93,93	0
58	MG	1H	3460	1/1	0.88	0.16	81,81,81,81	0
58	MG	14	3165	1/1	0.88	0.21	83,83,83,83	0
58	MG	1H	3515	1/1	0.88	0.05	83,83,83,83	0
58	MG	14	3243	1/1	0.88	0.35	70,70,70,70	0
58	MG	14	3046	1/1	0.88	0.24	68,68,68,68	0
58	MG	14	3215	1/1	0.88	0.09	73,73,73,73	0
58	MG	1G	1677	1/1	0.88	0.14	97,97,97,97	0
58	MG	1G	1679	1/1	0.88	0.39	120,120,120,120	0
58	MG	1H	3434	1/1	0.88	0.09	63,63,63,63	0
58	MG	13	1671	1/1	0.88	0.22	95,95,95,95	0
58	MG	1G	1668	1/1	0.88	0.12	84,84,84,84	0
58	MG	2A	202	1/1	0.88	0.27	98,98,98,98	0
58	MG	1H	3398	1/1	0.88	0.10	57,57,57,57	0
58	MG	1H	3253	1/1	0.88	0.23	76,76,76,76	0
58	MG	1G	1665	1/1	0.88	0.52	127,127,127,127	0
58	MG	14	3216	1/1	0.88	0.08	63,63,63,63	0
58	MG	14	3087	1/1	0.88	0.16	48,48,48,48	0
58	MG	1G	1626	1/1	0.88	0.35	99,99,99,99	0
58	MG	14	3181	1/1	0.88	0.28	79,79,79,79	0
58	MG	1H	3373	1/1	0.88	0.08	75,75,75,75	0
58	MG	1H	3034	1/1	0.88	0.38	73,73,73,73	0
58	MG	2A	201	1/1	0.88	0.13	91,91,91,91	0
58	MG	14	3251	1/1	0.88	0.30	84,84,84,84	0
58	MG	14	3163	1/1	0.88	0.17	71,71,71,71	0
58	MG	13	1646	1/1	0.88	0.26	61,61,61,61	0
58	MG	1H	3015	1/1	0.89	0.16	73,73,73,73	0
58	MG	1H	3135	1/1	0.89	0.28	61,61,61,61	0
58	MG	14	3162	1/1	0.89	0.24	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3032	1/1	0.89	0.23	82,82,82,82	0
58	MG	1H	3279	1/1	0.89	0.25	67,67,67,67	0
58	MG	1G	1658	1/1	0.89	0.11	92,92,92,92	0
58	MG	14	3283	1/1	0.89	0.23	82,82,82,82	0
58	MG	13	1673	1/1	0.89	0.22	73,73,73,73	0
58	MG	13	1634	1/1	0.89	0.17	47,47,47,47	0
58	MG	98	201	1/1	0.89	0.21	56,56,56,56	0
58	MG	1G	1662	1/1	0.89	0.34	83,83,83,83	0
58	MG	13	1688	1/1	0.89	0.35	97,97,97,97	0
58	MG	1H	3038	1/1	0.89	0.45	73,73,73,73	0
58	MG	14	3290	1/1	0.89	0.20	79,79,79,79	0
58	MG	14	3278	1/1	0.89	0.14	89,89,89,89	0
58	MG	1H	3480	1/1	0.89	0.11	88,88,88,88	0
58	MG	14	3183	1/1	0.89	0.14	66,66,66,66	0
58	MG	14	3279	1/1	0.89	0.15	74,74,74,74	0
58	MG	13	1670	1/1	0.89	0.33	91,91,91,91	0
58	MG	1H	3294	1/1	0.89	0.68	61,61,61,61	0
58	MG	1G	1655	1/1	0.89	0.24	86,86,86,86	0
58	MG	14	3173	1/1	0.89	0.17	79,79,79,79	0
58	MG	1H	3318	1/1	0.89	0.27	85,85,85,85	0
58	MG	14	3334	1/1	0.89	0.09	49,49,49,49	0
58	MG	14	3196	1/1	0.89	0.12	65,65,65,65	0
58	MG	13	1709	1/1	0.89	0.32	84,84,84,84	0
58	MG	14	3146	1/1	0.89	0.10	64,64,64,64	0
58	MG	14	3195	1/1	0.89	0.24	70,70,70,70	0
58	MG	1H	3289	1/1	0.89	0.47	89,89,89,89	0
58	MG	1G	1610	1/1	0.89	0.10	88,88,88,88	0
58	MG	1H	3320	1/1	0.89	0.27	71,71,71,71	0
58	MG	13	1633	1/1	0.89	0.15	49,49,49,49	0
58	MG	1H	3147	1/1	0.89	0.27	63,63,63,63	0
58	MG	1H	3209	1/1	0.89	0.10	57,57,57,57	0
58	MG	1H	3235	1/1	0.89	0.34	83,83,83,83	0
58	MG	13	1654	1/1	0.89	0.15	76,76,76,76	0
58	MG	1H	3453	1/1	0.89	0.08	105,105,105,105	0
58	MG	1H	3211	1/1	0.89	0.39	78,78,78,78	0
58	MG	13	1672	1/1	0.89	0.10	72,72,72,72	0
58	MG	13	1713	1/1	0.89	0.40	88,88,88,88	0
58	MG	1H	3130	1/1	0.89	0.12	59,59,59,59	0
58	MG	14	3352	1/1	0.89	0.18	99,99,99,99	0
58	MG	14	3026	1/1	0.89	0.15	71,71,71,71	0
58	MG	1G	1637	1/1	0.90	0.23	79,79,79,79	0
58	MG	1H	3306	1/1	0.90	0.45	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3232	1/1	0.90	0.58	52,52,52,52	0
58	MG	14	3115	1/1	0.90	0.27	66,66,66,66	0
58	MG	14	3237	1/1	0.90	0.15	79,79,79,79	0
58	MG	1H	3466	1/1	0.90	0.06	67,67,67,67	0
58	MG	1G	1602	1/1	0.90	0.20	93,93,93,93	0
58	MG	1G	1605	1/1	0.90	0.36	83,83,83,83	0
58	MG	1H	3423	1/1	0.90	0.11	59,59,59,59	0
58	MG	1H	3332	1/1	0.90	0.26	74,74,74,74	0
58	MG	14	3398	1/1	0.90	0.09	70,70,70,70	0
58	MG	1H	3270	1/1	0.90	0.38	77,77,77,77	0
58	MG	25	201	1/1	0.90	0.48	102,102,102,102	0
58	MG	1H	3448	1/1	0.90	0.09	51,51,51,51	0
58	MG	1H	3110	1/1	0.90	0.13	45,45,45,45	0
58	MG	1H	3018	1/1	0.90	0.37	73,73,73,73	0
58	MG	1H	3245	1/1	0.90	0.32	81,81,81,81	0
58	MG	14	3297	1/1	0.90	0.09	75,75,75,75	0
58	MG	1H	3280	1/1	0.90	0.45	82,82,82,82	0
58	MG	1H	3109	1/1	0.90	0.10	46,46,46,46	0
58	MG	13	1662	1/1	0.90	0.29	115,115,115,115	0
58	MG	1H	3493	1/1	0.90	0.22	79,79,79,79	0
58	MG	1G	1648	1/1	0.90	0.20	79,79,79,79	0
58	MG	13	1655	1/1	0.90	0.08	77,77,77,77	0
58	MG	1H	3471	1/1	0.90	0.08	63,63,63,63	0
58	MG	14	3358	1/1	0.90	0.08	82,82,82,82	0
58	MG	14	3240	1/1	0.90	0.11	83,83,83,83	0
58	MG	1G	1681	1/1	0.90	0.22	75,75,75,75	0
58	MG	1G	1674	1/1	0.90	0.23	98,98,98,98	0
58	MG	14	3033	1/1	0.90	0.21	76,76,76,76	0
58	MG	14	3261	1/1	0.90	0.13	84,84,84,84	0
58	MG	1G	1682	1/1	0.90	0.19	103,103,103,103	0
58	MG	1H	3091	1/1	0.90	0.23	77,77,77,77	0
58	MG	1H	3100	1/1	0.90	0.25	64,64,64,64	0
58	MG	14	3391	1/1	0.90	0.09	97,97,97,97	0
58	MG	1H	3207	1/1	0.90	0.17	56,56,56,56	0
58	MG	14	3184	1/1	0.90	0.26	91,91,91,91	0
58	MG	1H	3127	1/1	0.90	0.12	50,50,50,50	0
58	MG	14	3024	1/1	0.90	0.27	82,82,82,82	0
58	MG	16	210	1/1	0.90	0.15	73,73,73,73	0
58	MG	13	1682	1/1	0.90	0.22	73,73,73,73	0
58	MG	1G	1692	1/1	0.90	0.09	83,83,83,83	0
58	MG	1H	3428	1/1	0.90	0.15	74,74,74,74	0
58	MG	1H	3344	1/1	0.90	0.28	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3175	1/1	0.90	0.20	87,87,87,87	0
58	MG	1H	3230	1/1	0.90	0.52	91,91,91,91	0
58	MG	1H	3046	1/1	0.90	0.25	84,84,84,84	0
58	MG	1G	1687	1/1	0.90	0.09	104,104,104,104	0
58	MG	1H	3459	1/1	0.90	0.21	73,73,73,73	0
58	MG	13	1653	1/1	0.90	0.28	87,87,87,87	0
58	MG	1H	3009	1/1	0.90	0.49	73,73,73,73	0
58	MG	P8	101	1/1	0.90	0.29	73,73,73,73	0
58	MG	1H	3488	1/1	0.90	0.10	69,69,69,69	0
58	MG	1H	3118	1/1	0.91	0.17	53,53,53,53	0
58	MG	1H	3048	1/1	0.91	0.42	81,81,81,81	0
58	MG	14	3402	1/1	0.91	0.11	76,76,76,76	0
58	MG	1H	3236	1/1	0.91	0.26	79,79,79,79	0
58	MG	14	3074	1/1	0.91	0.16	73,73,73,73	0
58	MG	L8	101	1/1	0.91	0.42	79,79,79,79	0
58	MG	1G	1618	1/1	0.91	0.17	78,78,78,78	0
58	MG	1G	1657	1/1	0.91	0.22	107,107,107,107	0
58	MG	1H	3508	1/1	0.91	0.12	55,55,55,55	0
58	MG	14	3031	1/1	0.91	0.20	78,78,78,78	0
58	MG	1H	3105	1/1	0.91	0.22	71,71,71,71	0
58	MG	13	1696	1/1	0.91	0.10	70,70,70,70	0
58	MG	13	1702	1/1	0.91	0.38	81,81,81,81	0
58	MG	1H	3120	1/1	0.91	0.36	70,70,70,70	0
58	MG	3E	302	1/1	0.91	0.25	108,108,108,108	0
58	MG	1G	1667	1/1	0.91	0.21	92,92,92,92	0
58	MG	2K	102	1/1	0.91	0.15	80,80,80,80	0
58	MG	14	3259	1/1	0.91	0.17	102,102,102,102	0
58	MG	14	3191	1/1	0.91	0.12	70,70,70,70	0
58	MG	14	3366	1/1	0.91	0.10	94,94,94,94	0
58	MG	1H	3017	1/1	0.91	0.41	66,66,66,66	0
58	MG	1H	3016	1/1	0.91	0.41	97,97,97,97	0
58	MG	1G	1628	1/1	0.91	0.37	88,88,88,88	0
58	MG	14	3403	1/1	0.91	0.08	66,66,66,66	0
58	MG	14	3011	1/1	0.91	0.24	70,70,70,70	0
58	MG	1G	1604	1/1	0.91	0.17	98,98,98,98	0
58	MG	14	3206	1/1	0.91	0.14	50,50,50,50	0
58	MG	14	3280	1/1	0.91	0.40	87,87,87,87	0
58	MG	1H	3325	1/1	0.91	0.37	92,92,92,92	0
58	MG	1H	3059	1/1	0.91	0.26	56,56,56,56	0
58	MG	14	3182	1/1	0.91	0.24	86,86,86,86	0
60	ZN	5A	101	1/1	0.91	0.12	143,143,143,143	0
58	MG	16	202	1/1	0.91	0.29	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3464	1/1	0.91	0.11	84,84,84,84	0
58	MG	1H	3371	1/1	0.91	0.09	45,45,45,45	0
58	MG	1G	1624	1/1	0.91	0.14	85,85,85,85	0
58	MG	1G	1613	1/1	0.91	0.08	87,87,87,87	0
58	MG	1H	3206	1/1	0.91	0.13	54,54,54,54	0
58	MG	1H	3178	1/1	0.91	0.10	63,63,63,63	0
58	MG	14	3246	1/1	0.91	0.16	85,85,85,85	0
58	MG	14	3070	1/1	0.91	0.11	79,79,79,79	0
58	MG	1G	1650	1/1	0.91	0.33	81,81,81,81	0
58	MG	1H	3011	1/1	0.91	0.13	72,72,72,72	0
58	MG	1H	3305	1/1	0.91	0.21	75,75,75,75	0
58	MG	14	3154	1/1	0.91	0.12	68,68,68,68	0
58	MG	1H	3510	1/1	0.91	0.25	51,51,51,51	0
58	MG	13	1703	1/1	0.91	0.15	89,89,89,89	0
58	MG	1H	3223	1/1	0.91	0.26	60,60,60,60	0
58	MG	1H	3039	1/1	0.91	0.39	75,75,75,75	0
58	MG	11	303	1/1	0.91	0.12	41,41,41,41	0
58	MG	1G	1614	1/1	0.91	0.24	91,91,91,91	0
58	MG	13	1733	1/1	0.91	0.10	104,104,104,104	0
58	MG	14	3365	1/1	0.91	0.19	83,83,83,83	0
58	MG	1H	3378	1/1	0.91	0.09	79,79,79,79	0
58	MG	13	1661	1/1	0.91	0.22	97,97,97,97	0
58	MG	14	3326	1/1	0.91	0.16	61,61,61,61	0
58	MG	1H	3494	1/1	0.91	0.11	82,82,82,82	0
58	MG	1H	3265	1/1	0.91	0.22	79,79,79,79	0
58	MG	1G	1672	1/1	0.91	0.26	88,88,88,88	0
58	MG	1H	3472	1/1	0.91	0.07	72,72,72,72	0
58	MG	1G	1643	1/1	0.92	0.28	74,74,74,74	0
58	MG	14	3395	1/1	0.92	0.24	75,75,75,75	0
58	MG	1G	1620	1/1	0.92	0.18	77,77,77,77	0
58	MG	14	3129	1/1	0.92	0.25	69,69,69,69	0
58	MG	1H	3288	1/1	0.92	0.18	58,58,58,58	0
58	MG	1H	3487	1/1	0.92	0.12	100,100,100,100	0
58	MG	1H	3101	1/1	0.92	0.28	72,72,72,72	0
58	MG	1H	3079	1/1	0.92	0.15	53,53,53,53	0
58	MG	14	3235	1/1	0.92	0.19	80,80,80,80	0
58	MG	1H	3261	1/1	0.92	0.21	64,64,64,64	0
58	MG	1H	3313	1/1	0.92	0.30	78,78,78,78	0
58	MG	13	1686	1/1	0.92	0.19	80,80,80,80	0
58	MG	14	3353	1/1	0.92	0.12	82,82,82,82	0
58	MG	1G	1616	1/1	0.92	0.29	86,86,86,86	0
58	MG	14	3204	1/1	0.92	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3417	1/1	0.92	0.11	66,66,66,66	0
58	MG	1H	3298	1/1	0.92	0.22	68,68,68,68	0
58	MG	14	3371	1/1	0.92	0.08	79,79,79,79	0
58	MG	13	1642	1/1	0.92	0.24	64,64,64,64	0
58	MG	1G	1659	1/1	0.92	0.20	95,95,95,95	0
58	MG	14	3394	1/1	0.92	0.12	53,53,53,53	0
58	MG	16	208	1/1	0.92	0.29	77,77,77,77	0
58	MG	1H	3449	1/1	0.92	0.08	74,74,74,74	0
58	MG	13	1691	1/1	0.92	0.26	75,75,75,75	0
58	MG	18	101	1/1	0.92	0.08	56,56,56,56	0
58	MG	1H	3164	1/1	0.92	0.30	58,58,58,58	0
58	MG	1G	1651	1/1	0.92	0.17	77,77,77,77	0
58	MG	14	3106	1/1	0.92	0.19	62,62,62,62	0
58	MG	14	3004	1/1	0.92	0.23	78,78,78,78	0
58	MG	1H	3447	1/1	0.92	0.14	55,55,55,55	0
58	MG	14	3221	1/1	0.92	0.27	72,72,72,72	0
58	MG	1H	3233	1/1	0.92	0.25	70,70,70,70	0
58	MG	13	1693	1/1	0.92	0.42	94,94,94,94	0
58	MG	1H	3463	1/1	0.92	0.15	66,66,66,66	0
58	MG	1H	3146	1/1	0.92	0.32	67,67,67,67	0
58	MG	13	1742	1/1	0.92	0.21	95,95,95,95	0
58	MG	41	201	1/1	0.92	0.15	67,67,67,67	0
58	MG	1H	3006	1/1	0.92	0.23	57,57,57,57	0
58	MG	88	201	1/1	0.92	0.16	84,84,84,84	0
58	MG	14	3156	1/1	0.92	0.21	63,63,63,63	0
58	MG	4K	101	1/1	0.92	0.21	73,73,73,73	0
58	MG	1G	1656	1/1	0.92	0.14	140,140,140,140	0
58	MG	1H	3400	1/1	0.92	0.20	54,54,54,54	0
58	MG	1H	3299	1/1	0.92	0.56	98,98,98,98	0
58	MG	13	1657	1/1	0.92	0.28	89,89,89,89	0
58	MG	13	1698	1/1	0.92	0.15	80,80,80,80	0
58	MG	2K	105	1/1	0.92	0.06	81,81,81,81	0
58	MG	14	3321	1/1	0.92	0.11	55,55,55,55	0
58	MG	1H	3470	1/1	0.92	0.06	73,73,73,73	0
58	MG	1H	3496	1/1	0.92	0.12	59,59,59,59	0
58	MG	1H	3131	1/1	0.92	0.28	57,57,57,57	0
58	MG	1H	3473	1/1	0.92	0.07	85,85,85,85	0
58	MG	1H	3264	1/1	0.92	0.18	67,67,67,67	0
58	MG	1H	3150	1/1	0.92	0.35	69,69,69,69	0
58	MG	1H	3352	1/1	0.92	0.13	45,45,45,45	0
58	MG	14	3084	1/1	0.92	0.10	81,81,81,81	0
58	MG	1H	3082	1/1	0.92	0.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3383	1/1	0.92	0.09	66,66,66,66	0
58	MG	1H	3436	1/1	0.92	0.09	67,67,67,67	0
58	MG	14	3171	1/1	0.92	0.26	80,80,80,80	0
58	MG	14	3018	1/1	0.92	0.16	50,50,50,50	0
58	MG	13	1737	1/1	0.92	0.06	93,93,93,93	0
58	MG	1H	3274	1/1	0.92	0.28	83,83,83,83	0
58	MG	1H	3122	1/1	0.92	0.20	68,68,68,68	0
58	MG	1H	3481	1/1	0.92	0.09	132,132,132,132	0
58	MG	1H	3041	1/1	0.92	0.19	88,88,88,88	0
58	MG	1H	3121	1/1	0.92	0.23	35,35,35,35	0
58	MG	C5	201	1/1	0.92	0.32	105,105,105,105	0
58	MG	1H	3112	1/1	0.92	0.22	71,71,71,71	0
58	MG	13	1660	1/1	0.93	0.30	86,86,86,86	0
58	MG	14	3007	1/1	0.93	0.33	68,68,68,68	0
58	MG	13	1674	1/1	0.93	0.16	77,77,77,77	0
58	MG	14	3179	1/1	0.93	0.27	72,72,72,72	0
58	MG	1G	1663	1/1	0.93	0.14	112,112,112,112	0
58	MG	14	3083	1/1	0.93	0.18	88,88,88,88	0
58	MG	1H	3359	1/1	0.93	0.13	60,60,60,60	0
58	MG	14	3307	1/1	0.93	0.12	49,49,49,49	0
58	MG	1H	3128	1/1	0.93	0.20	66,66,66,66	0
58	MG	14	3217	1/1	0.93	0.17	101,101,101,101	0
58	MG	1H	3191	1/1	0.93	0.45	70,70,70,70	0
58	MG	14	3097	1/1	0.93	0.21	77,77,77,77	0
58	MG	1H	3089	1/1	0.93	0.31	72,72,72,72	0
58	MG	14	3363	1/1	0.93	0.12	54,54,54,54	0
58	MG	1H	3149	1/1	0.93	0.22	61,61,61,61	0
58	MG	13	1711	1/1	0.93	0.26	76,76,76,76	0
58	MG	14	3104	1/1	0.93	0.15	74,74,74,74	0
58	MG	16	212	1/1	0.93	0.04	81,81,81,81	0
58	MG	1H	3036	1/1	0.93	0.30	65,65,65,65	0
58	MG	14	3362	1/1	0.93	0.06	56,56,56,56	0
58	MG	14	3022	1/1	0.93	0.20	78,78,78,78	0
58	MG	1H	3095	1/1	0.93	0.18	49,49,49,49	0
58	MG	14	3138	1/1	0.93	0.11	94,94,94,94	0
58	MG	1H	3148	1/1	0.93	0.24	78,78,78,78	0
58	MG	14	3124	1/1	0.93	0.23	76,76,76,76	0
58	MG	1H	3443	1/1	0.93	0.11	66,66,66,66	0
58	MG	14	3027	1/1	0.93	0.31	81,81,81,81	0
58	MG	16	207	1/1	0.93	0.25	88,88,88,88	0
58	MG	14	3098	1/1	0.93	0.16	71,71,71,71	0
58	MG	14	3230	1/1	0.93	0.60	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	13	1728	1/1	0.93	0.13	95,95,95,95	0
58	MG	1H	3094	1/1	0.93	0.21	54,54,54,54	0
58	MG	14	3354	1/1	0.93	0.15	56,56,56,56	0
58	MG	14	3028	1/1	0.93	0.17	99,99,99,99	0
58	MG	1G	1695	1/1	0.93	0.08	96,96,96,96	0
58	MG	1H	3212	1/1	0.93	0.29	70,70,70,70	0
58	MG	14	3110	1/1	0.93	0.10	55,55,55,55	0
58	MG	1H	3414	1/1	0.93	0.28	64,64,64,64	0
58	MG	1H	3222	1/1	0.93	0.11	58,58,58,58	0
58	MG	14	3014	1/1	0.93	0.17	77,77,77,77	0
58	MG	13	1641	1/1	0.93	0.11	69,69,69,69	0
58	MG	14	3368	1/1	0.93	0.06	89,89,89,89	0
58	MG	1G	1696	1/1	0.93	0.04	109,109,109,109	0
58	MG	14	3009	1/1	0.93	0.15	66,66,66,66	0
58	MG	14	3333	1/1	0.93	0.13	67,67,67,67	0
58	MG	13	1607	1/1	0.93	0.28	71,71,71,71	0
58	MG	1G	1627	1/1	0.93	0.18	88,88,88,88	0
58	MG	13	1678	1/1	0.93	0.11	89,89,89,89	0
58	MG	14	3373	1/1	0.93	0.06	64,64,64,64	0
58	MG	1G	1609	1/1	0.93	0.11	81,81,81,81	0
58	MG	1H	3179	1/1	0.93	0.39	67,67,67,67	0
58	MG	13	1656	1/1	0.93	0.25	79,79,79,79	0
58	MG	1H	3319	1/1	0.93	0.22	83,83,83,83	0
58	MG	13	1612	1/1	0.93	0.29	89,89,89,89	0
58	MG	1H	3465	1/1	0.93	0.14	76,76,76,76	0
58	MG	13	1610	1/1	0.93	0.20	66,66,66,66	0
58	MG	13	1676	1/1	0.93	0.09	88,88,88,88	0
58	MG	1H	3237	1/1	0.93	0.28	72,72,72,72	0
58	MG	1H	3251	1/1	0.93	0.28	79,79,79,79	0
58	MG	1H	3193	1/1	0.93	0.14	60,60,60,60	0
58	MG	1H	3163	1/1	0.93	0.28	65,65,65,65	0
58	MG	14	3030	1/1	0.93	0.16	70,70,70,70	0
58	MG	14	3161	1/1	0.93	0.21	74,74,74,74	0
60	ZN	32	301	1/1	0.93	0.38	112,112,112,112	0
58	MG	13	1695	1/1	0.93	0.19	83,83,83,83	0
58	MG	1H	3413	1/1	0.93	0.09	50,50,50,50	0
58	MG	1H	3255	1/1	0.93	0.34	83,83,83,83	0
58	MG	14	3375	1/1	0.93	0.11	89,89,89,89	0
58	MG	14	3219	1/1	0.93	0.18	51,51,51,51	0
58	MG	14	3393	1/1	0.93	0.17	76,76,76,76	0
58	MG	1H	3215	1/1	0.93	0.12	60,60,60,60	0
58	MG	1H	3022	1/1	0.93	0.12	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3284	1/1	0.93	0.43	94,94,94,94	0
58	MG	14	3213	1/1	0.93	0.19	75,75,75,75	0
58	MG	1H	3439	1/1	0.93	0.13	51,51,51,51	0
58	MG	14	3197	1/1	0.93	0.19	73,73,73,73	0
58	MG	1H	3468	1/1	0.94	0.11	63,63,63,63	0
58	MG	14	3344	1/1	0.94	0.13	64,64,64,64	0
58	MG	1G	1611	1/1	0.94	0.10	91,91,91,91	0
58	MG	1G	1619	1/1	0.94	0.24	92,92,92,92	0
58	MG	14	3137	1/1	0.94	0.20	78,78,78,78	0
58	MG	1H	3367	1/1	0.94	0.10	54,54,54,54	0
58	MG	1H	3210	1/1	0.94	0.34	67,67,67,67	0
58	MG	14	3134	1/1	0.94	0.17	62,62,62,62	0
58	MG	1H	3203	1/1	0.94	0.38	79,79,79,79	0
58	MG	14	3335	1/1	0.94	0.16	80,80,80,80	0
58	MG	14	3332	1/1	0.94	0.16	64,64,64,64	0
58	MG	14	3301	1/1	0.94	0.15	87,87,87,87	0
58	MG	1H	3114	1/1	0.94	0.16	66,66,66,66	0
58	MG	1H	3216	1/1	0.94	0.27	71,71,71,71	0
58	MG	14	3202	1/1	0.94	0.25	64,64,64,64	0
58	MG	1H	3197	1/1	0.94	0.21	63,63,63,63	0
58	MG	1H	3076	1/1	0.94	0.24	51,51,51,51	0
58	MG	2K	101	1/1	0.94	0.22	66,66,66,66	0
58	MG	14	3233	1/1	0.94	0.10	63,63,63,63	0
58	MG	16	201	1/1	0.94	0.41	79,79,79,79	0
58	MG	14	3214	1/1	0.94	0.25	75,75,75,75	0
58	MG	13	1618	1/1	0.94	0.20	63,63,63,63	0
58	MG	1H	3229	1/1	0.94	0.20	50,50,50,50	0
58	MG	14	3177	1/1	0.94	0.20	84,84,84,84	0
58	MG	14	3209	1/1	0.94	0.17	81,81,81,81	0
58	MG	14	3218	1/1	0.94	0.15	71,71,71,71	0
58	MG	1H	3394	1/1	0.94	0.15	70,70,70,70	0
58	MG	14	3053	1/1	0.94	0.19	45,45,45,45	0
58	MG	1H	3381	1/1	0.94	0.16	62,62,62,62	0
58	MG	14	3205	1/1	0.94	0.16	58,58,58,58	0
58	MG	14	3208	1/1	0.94	0.14	83,83,83,83	0
58	MG	14	3377	1/1	0.94	0.14	107,107,107,107	0
58	MG	13	1690	1/1	0.94	0.28	90,90,90,90	0
58	MG	1H	3420	1/1	0.94	0.14	50,50,50,50	0
58	MG	14	3153	1/1	0.94	0.34	60,60,60,60	0
58	MG	13	1717	1/1	0.94	0.07	76,76,76,76	0
58	MG	1H	3144	1/1	0.94	0.30	49,49,49,49	0
58	MG	13	1625	1/1	0.94	0.15	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3252	1/1	0.94	0.34	91,91,91,91	0
58	MG	13	1722	1/1	0.94	0.10	76,76,76,76	0
58	MG	1G	1691	1/1	0.94	0.19	89,89,89,89	0
58	MG	14	3141	1/1	0.94	0.11	46,46,46,46	0
58	MG	14	3312	1/1	0.94	0.12	88,88,88,88	0
58	MG	13	1605	1/1	0.94	0.31	76,76,76,76	0
58	MG	1H	3141	1/1	0.94	0.14	40,40,40,40	0
58	MG	21	302	1/1	0.94	0.17	68,68,68,68	0
58	MG	14	3287	1/1	0.94	0.15	96,96,96,96	0
58	MG	14	3256	1/1	0.94	0.42	57,57,57,57	0
58	MG	14	3062	1/1	0.94	0.35	75,75,75,75	0
58	MG	1H	3219	1/1	0.94	0.12	70,70,70,70	0
58	MG	14	3317	1/1	0.94	0.12	48,48,48,48	0
58	MG	14	3396	1/1	0.94	0.11	53,53,53,53	0
58	MG	14	3043	1/1	0.94	0.25	76,76,76,76	0
58	MG	1H	3458	1/1	0.94	0.12	45,45,45,45	0
58	MG	13	1679	1/1	0.94	0.15	75,75,75,75	0
58	MG	14	3355	1/1	0.94	0.09	64,64,64,64	0
58	MG	1H	3382	1/1	0.94	0.09	71,71,71,71	0
58	MG	1H	3312	1/1	0.94	0.13	73,73,73,73	0
58	MG	49	201	1/1	0.94	0.22	128,128,128,128	0
58	MG	14	3089	1/1	0.94	0.24	81,81,81,81	0
58	MG	1H	3387	1/1	0.94	0.14	65,65,65,65	0
58	MG	1H	3393	1/1	0.94	0.10	58,58,58,58	0
58	MG	14	3346	1/1	0.94	0.10	74,74,74,74	0
58	MG	1H	3005	1/1	0.94	0.31	53,53,53,53	0
58	MG	14	3157	1/1	0.94	0.15	71,71,71,71	0
58	MG	14	3378	1/1	0.94	0.07	71,71,71,71	0
58	MG	1H	3495	1/1	0.94	0.09	47,47,47,47	0
58	MG	14	3348	1/1	0.94	0.08	76,76,76,76	0
58	MG	14	3111	1/1	0.94	0.18	92,92,92,92	0
58	MG	1H	3347	1/1	0.94	0.45	78,78,78,78	0
58	MG	13	1743	1/1	0.94	0.07	60,60,60,60	0
58	MG	14	3003	1/1	0.94	0.24	77,77,77,77	0
58	MG	1H	3511	1/1	0.94	0.11	82,82,82,82	0
58	MG	13	1747	1/1	0.94	0.07	96,96,96,96	0
58	MG	14	3096	1/1	0.94	0.24	73,73,73,73	0
58	MG	14	3127	1/1	0.94	0.14	54,54,54,54	0
58	MG	13	1624	1/1	0.94	0.29	68,68,68,68	0
58	MG	1H	3518	1/1	0.94	0.13	94,94,94,94	0
58	MG	1H	3406	1/1	0.94	0.19	49,49,49,49	0
58	MG	14	3091	1/1	0.94	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3305	1/1	0.94	0.09	69,69,69,69	0
58	MG	14	3295	1/1	0.94	0.18	79,79,79,79	0
58	MG	13	1616	1/1	0.94	0.22	65,65,65,65	0
58	MG	14	3086	1/1	0.94	0.17	67,67,67,67	0
58	MG	1G	1642	1/1	0.94	0.18	92,92,92,92	0
58	MG	14	3198	1/1	0.94	0.26	94,94,94,94	0
58	MG	14	3380	1/1	0.94	0.07	76,76,76,76	0
58	MG	1G	1632	1/1	0.94	0.30	83,83,83,83	0
58	MG	1H	3317	1/1	0.94	0.22	84,84,84,84	0
58	MG	14	3073	1/1	0.94	0.25	91,91,91,91	0
58	MG	1H	3231	1/1	0.94	0.26	74,74,74,74	0
58	MG	1H	3256	1/1	0.95	0.15	58,58,58,58	0
58	MG	1H	3151	1/1	0.95	0.28	73,73,73,73	0
58	MG	14	3224	1/1	0.95	0.19	77,77,77,77	0
58	MG	14	3130	1/1	0.95	0.29	85,85,85,85	0
58	MG	14	3103	1/1	0.95	0.32	78,78,78,78	0
58	MG	1H	3375	1/1	0.95	0.05	81,81,81,81	0
58	MG	1H	3506	1/1	0.95	0.09	44,44,44,44	0
58	MG	13	1727	1/1	0.95	0.09	55,55,55,55	0
58	MG	1H	3226	1/1	0.95	0.17	89,89,89,89	0
58	MG	1H	3071	1/1	0.95	0.18	39,39,39,39	0
58	MG	1H	3173	1/1	0.95	0.24	65,65,65,65	0
58	MG	14	3203	1/1	0.95	0.28	83,83,83,83	0
58	MG	1H	3415	1/1	0.95	0.12	63,63,63,63	0
58	MG	1H	3507	1/1	0.95	0.10	43,43,43,43	0
58	MG	14	3081	1/1	0.95	0.21	80,80,80,80	0
58	MG	14	3405	1/1	0.95	0.17	75,75,75,75	0
58	MG	1H	3158	1/1	0.95	0.11	44,44,44,44	0
58	MG	14	3059	1/1	0.95	0.13	55,55,55,55	0
58	MG	1H	3467	1/1	0.95	0.18	69,69,69,69	0
58	MG	1H	3028	1/1	0.95	0.32	64,64,64,64	0
58	MG	1H	3504	1/1	0.95	0.12	66,66,66,66	0
58	MG	1H	3074	1/1	0.95	0.40	88,88,88,88	0
58	MG	1H	3142	1/1	0.95	0.21	39,39,39,39	0
58	MG	1H	3452	1/1	0.95	0.08	74,74,74,74	0
58	MG	14	3152	1/1	0.95	0.21	75,75,75,75	0
58	MG	14	3194	1/1	0.95	0.13	61,61,61,61	0
58	MG	1H	3213	1/1	0.95	0.15	43,43,43,43	0
58	MG	1H	3505	1/1	0.95	0.09	41,41,41,41	0
58	MG	13	1740	1/1	0.95	0.10	70,70,70,70	0
58	MG	1H	3351	1/1	0.95	0.15	53,53,53,53	0
58	MG	14	3360	1/1	0.95	0.07	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3170	1/1	0.95	0.41	77,77,77,77	0
58	MG	13	1611	1/1	0.95	0.28	71,71,71,71	0
58	MG	1H	3244	1/1	0.95	0.38	98,98,98,98	0
58	MG	13	1730	1/1	0.95	0.07	67,67,67,67	0
58	MG	1H	3124	1/1	0.95	0.18	39,39,39,39	0
58	MG	14	3142	1/1	0.95	0.36	88,88,88,88	0
58	MG	13	1649	1/1	0.95	0.17	79,79,79,79	0
58	MG	13	1744	1/1	0.95	0.08	89,89,89,89	0
58	MG	1H	3139	1/1	0.95	0.25	52,52,52,52	0
58	MG	14	3017	1/1	0.95	0.20	63,63,63,63	0
58	MG	1H	3479	1/1	0.95	0.09	79,79,79,79	0
58	MG	13	1716	1/1	0.95	0.08	73,73,73,73	0
58	MG	14	3002	1/1	0.95	0.23	64,64,64,64	0
58	MG	13	1613	1/1	0.95	0.27	83,83,83,83	0
58	MG	1H	3323	1/1	0.95	0.34	78,78,78,78	0
58	MG	1H	3232	1/1	0.95	0.11	72,72,72,72	0
58	MG	14	3150	1/1	0.95	0.18	50,50,50,50	0
58	MG	14	3267	1/1	0.95	0.13	79,79,79,79	0
58	MG	1H	3390	1/1	0.95	0.12	56,56,56,56	0
58	MG	1G	1644	1/1	0.95	0.21	110,110,110,110	0
58	MG	14	3249	1/1	0.95	0.23	65,65,65,65	0
58	MG	13	1681	1/1	0.95	0.11	66,66,66,66	0
58	MG	1H	3276	1/1	0.95	0.12	55,55,55,55	0
58	MG	1H	3068	1/1	0.95	0.17	50,50,50,50	0
58	MG	1H	3106	1/1	0.95	0.17	49,49,49,49	0
58	MG	14	3102	1/1	0.95	0.19	73,73,73,73	0
58	MG	1H	3462	1/1	0.95	0.09	79,79,79,79	0
58	MG	14	3225	1/1	0.95	0.20	57,57,57,57	0
58	MG	1H	3053	1/1	0.95	0.37	66,66,66,66	0
58	MG	14	3303	1/1	0.95	0.14	53,53,53,53	0
58	MG	2K	104	1/1	0.95	0.12	80,80,80,80	0
58	MG	1H	3361	1/1	0.95	0.09	64,64,64,64	0
58	MG	14	3057	1/1	0.95	0.21	62,62,62,62	0
58	MG	1H	3476	1/1	0.95	0.11	70,70,70,70	0
58	MG	1H	3455	1/1	0.95	0.15	66,66,66,66	0
58	MG	14	3094	1/1	0.95	0.12	76,76,76,76	0
58	MG	13	1628	1/1	0.95	0.18	58,58,58,58	0
58	MG	13	1746	1/1	0.95	0.07	84,84,84,84	0
58	MG	14	3099	1/1	0.95	0.17	55,55,55,55	0
58	MG	13	1734	1/1	0.95	0.07	100,100,100,100	0
58	MG	1H	3456	1/1	0.95	0.08	80,80,80,80	0
58	MG	1H	3444	1/1	0.95	0.09	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3066	1/1	0.95	0.25	48,48,48,48	0
58	MG	1H	3418	1/1	0.95	0.10	70,70,70,70	0
58	MG	1G	1634	1/1	0.95	0.15	84,84,84,84	0
58	MG	13	1667	1/1	0.95	0.22	82,82,82,82	0
58	MG	14	3382	1/1	0.95	0.09	81,81,81,81	0
58	MG	14	3063	1/1	0.95	0.22	70,70,70,70	0
58	MG	1G	1638	1/1	0.95	0.30	84,84,84,84	0
58	MG	11	302	1/1	0.95	0.12	35,35,35,35	0
58	MG	1G	1653	1/1	0.95	0.29	78,78,78,78	0
58	MG	14	3071	1/1	0.95	0.15	42,42,42,42	0
58	MG	1G	1669	1/1	0.95	0.12	80,80,80,80	0
58	MG	1H	3300	1/1	0.95	0.31	72,72,72,72	0
58	MG	13	1635	1/1	0.95	0.19	48,48,48,48	0
58	MG	14	3339	1/1	0.95	0.09	62,62,62,62	0
58	MG	14	3036	1/1	0.95	0.19	67,67,67,67	0
58	MG	14	3329	1/1	0.95	0.09	54,54,54,54	0
58	MG	14	3340	1/1	0.95	0.09	67,67,67,67	0
58	MG	14	3247	1/1	0.95	0.26	85,85,85,85	0
58	MG	14	3330	1/1	0.95	0.11	53,53,53,53	0
58	MG	1H	3037	1/1	0.95	0.30	62,62,62,62	0
58	MG	1H	3380	1/1	0.95	0.12	77,77,77,77	0
58	MG	1H	3083	1/1	0.95	0.30	68,68,68,68	0
58	MG	13	1650	1/1	0.95	0.27	72,72,72,72	0
58	MG	14	3364	1/1	0.95	0.08	75,75,75,75	0
58	MG	1H	3143	1/1	0.95	0.22	50,50,50,50	0
58	MG	13	1689	1/1	0.95	0.20	118,118,118,118	0
58	MG	1H	3073	1/1	0.95	0.24	73,73,73,73	0
58	MG	1H	3134	1/1	0.95	0.22	50,50,50,50	0
58	MG	1H	3085	1/1	0.95	0.13	69,69,69,69	0
58	MG	1H	3307	1/1	0.95	0.24	60,60,60,60	0
58	MG	1H	3029	1/1	0.95	0.31	72,72,72,72	0
58	MG	1H	3369	1/1	0.95	0.18	55,55,55,55	0
58	MG	1H	3324	1/1	0.95	0.18	76,76,76,76	0
58	MG	1H	3296	1/1	0.95	0.22	72,72,72,72	0
58	MG	2I	201	1/1	0.95	0.17	77,77,77,77	0
58	MG	1H	3072	1/1	0.96	0.26	61,61,61,61	0
58	MG	14	3107	1/1	0.96	0.20	58,58,58,58	0
58	MG	1G	1666	1/1	0.96	0.15	84,84,84,84	0
58	MG	14	3331	1/1	0.96	0.09	56,56,56,56	0
58	MG	1H	3450	1/1	0.96	0.10	62,62,62,62	0
58	MG	1K	102	1/1	0.96	0.21	72,72,72,72	0
58	MG	1H	3129	1/1	0.96	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	13	1614	1/1	0.96	0.23	86,86,86,86	0
58	MG	1H	3374	1/1	0.96	0.07	90,90,90,90	0
58	MG	14	3069	1/1	0.96	0.18	60,60,60,60	0
58	MG	1H	3070	1/1	0.96	0.31	68,68,68,68	0
58	MG	1G	1654	1/1	0.96	0.23	85,85,85,85	0
58	MG	14	3132	1/1	0.96	0.15	44,44,44,44	0
58	MG	14	3192	1/1	0.96	0.11	59,59,59,59	0
58	MG	1H	3364	1/1	0.96	0.14	47,47,47,47	0
58	MG	14	3310	1/1	0.96	0.07	56,56,56,56	0
58	MG	1H	3055	1/1	0.96	0.31	85,85,85,85	0
58	MG	1H	3402	1/1	0.96	0.09	53,53,53,53	0
58	MG	1H	3416	1/1	0.96	0.11	67,67,67,67	0
58	MG	14	3212	1/1	0.96	0.17	75,75,75,75	0
58	MG	1H	3111	1/1	0.96	0.27	44,44,44,44	0
58	MG	14	3313	1/1	0.96	0.08	48,48,48,48	0
58	MG	1G	1622	1/1	0.96	0.21	81,81,81,81	0
58	MG	13	1748	1/1	0.96	0.10	82,82,82,82	0
58	MG	14	3187	1/1	0.96	0.14	47,47,47,47	0
58	MG	1H	3238	1/1	0.96	0.65	52,52,52,52	0
58	MG	13	1659	1/1	0.96	0.36	68,68,68,68	0
58	MG	14	3041	1/1	0.96	0.18	66,66,66,66	0
58	MG	1G	1608	1/1	0.96	0.16	72,72,72,72	0
58	MG	13	1632	1/1	0.96	0.24	71,71,71,71	0
58	MG	14	3125	1/1	0.96	0.20	70,70,70,70	0
58	MG	14	3040	1/1	0.96	0.15	82,82,82,82	0
58	MG	1H	3108	1/1	0.96	0.12	50,50,50,50	0
58	MG	1H	3088	1/1	0.96	0.18	77,77,77,77	0
58	MG	14	3114	1/1	0.96	0.36	79,79,79,79	0
58	MG	13	1626	1/1	0.96	0.33	90,90,90,90	0
58	MG	1G	1683	1/1	0.96	0.07	61,61,61,61	0
58	MG	1G	1664	1/1	0.96	0.14	92,92,92,92	0
58	MG	1H	3435	1/1	0.96	0.08	82,82,82,82	0
58	MG	1H	3410	1/1	0.96	0.10	33,33,33,33	0
58	MG	1G	1615	1/1	0.96	0.17	85,85,85,85	0
58	MG	14	3136	1/1	0.96	0.25	49,49,49,49	0
58	MG	1H	3182	1/1	0.96	0.34	61,61,61,61	0
58	MG	1H	3396	1/1	0.96	0.07	69,69,69,69	0
58	MG	14	3120	1/1	0.96	0.07	54,54,54,54	0
58	MG	1H	3498	1/1	0.96	0.11	47,47,47,47	0
58	MG	13	1645	1/1	0.96	0.26	69,69,69,69	0
58	MG	13	1735	1/1	0.96	0.12	84,84,84,84	0
58	MG	1H	3102	1/1	0.96	0.24	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3004	1/1	0.96	0.35	68,68,68,68	0
58	MG	1H	3425	1/1	0.96	0.16	49,49,49,49	0
58	MG	14	3207	1/1	0.96	0.12	68,68,68,68	0
58	MG	13	1639	1/1	0.96	0.16	55,55,55,55	0
60	ZN	5I	103	1/1	0.96	0.18	91,91,91,91	0
58	MG	1H	3516	1/1	0.96	0.07	86,86,86,86	0
58	MG	1H	3227	1/1	0.96	0.35	87,87,87,87	0
58	MG	14	3008	1/1	0.96	0.19	65,65,65,65	0
58	MG	1H	3172	1/1	0.96	0.35	79,79,79,79	0
58	MG	1H	3357	1/1	0.96	0.10	35,35,35,35	0
59	PAR	1G	1697	42/42	0.96	0.19	75,80,88,91	0
58	MG	1H	3349	1/1	0.96	0.14	40,40,40,40	0
58	MG	14	3085	1/1	0.96	0.21	52,52,52,52	0
58	MG	14	3199	1/1	0.96	0.35	96,96,96,96	0
58	MG	1H	3107	1/1	0.96	0.18	52,52,52,52	0
58	MG	14	3357	1/1	0.96	0.10	69,69,69,69	0
58	MG	1H	3461	1/1	0.96	0.13	51,51,51,51	0
58	MG	1H	3181	1/1	0.96	0.23	63,63,63,63	0
58	MG	13	1629	1/1	0.96	0.24	69,69,69,69	0
58	MG	1K	101	1/1	0.96	0.08	85,85,85,85	0
58	MG	1H	3225	1/1	0.96	0.19	79,79,79,79	0
58	MG	5E	201	1/1	0.96	0.21	67,67,67,67	0
58	MG	1H	3115	1/1	0.96	0.21	37,37,37,37	0
58	MG	13	1637	1/1	0.96	0.12	66,66,66,66	0
58	MG	1H	3013	1/1	0.96	0.23	52,52,52,52	0
58	MG	1H	3168	1/1	0.96	0.20	64,64,64,64	0
58	MG	14	3095	1/1	0.96	0.13	83,83,83,83	0
58	MG	14	3037	1/1	0.96	0.16	82,82,82,82	0
58	MG	14	3374	1/1	0.96	0.10	86,86,86,86	0
58	MG	1H	3201	1/1	0.96	0.16	41,41,41,41	0
58	MG	1G	1629	1/1	0.96	0.28	96,96,96,96	0
58	MG	1H	3486	1/1	0.96	0.14	50,50,50,50	0
58	MG	1H	3064	1/1	0.96	0.18	43,43,43,43	0
58	MG	1H	3517	1/1	0.96	0.13	57,57,57,57	0
58	MG	1H	3152	1/1	0.96	0.27	71,71,71,71	0
58	MG	1H	3050	1/1	0.96	0.27	63,63,63,63	0
58	MG	J5	101	1/1	0.96	0.11	52,52,52,52	0
58	MG	1H	3408	1/1	0.96	0.14	49,49,49,49	0
58	MG	1G	1686	1/1	0.96	0.10	84,84,84,84	0
58	MG	14	3318	1/1	0.96	0.10	47,47,47,47	0
58	MG	1G	1640	1/1	0.96	0.14	83,83,83,83	0
58	MG	1H	3096	1/1	0.96	0.21	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1G	1652	1/1	0.96	0.19	81,81,81,81	0
58	MG	1H	3412	1/1	0.96	0.09	50,50,50,50	0
58	MG	1G	1645	1/1	0.96	0.19	142,142,142,142	0
58	MG	1H	3104	1/1	0.96	0.17	68,68,68,68	0
58	MG	13	1658	1/1	0.96	0.26	92,92,92,92	0
58	MG	1H	3189	1/1	0.96	0.14	61,61,61,61	0
58	MG	1H	3171	1/1	0.96	0.15	58,58,58,58	0
58	MG	14	3078	1/1	0.96	0.18	63,63,63,63	0
58	MG	14	3068	1/1	0.96	0.16	60,60,60,60	0
58	MG	14	3174	1/1	0.96	0.17	84,84,84,84	0
58	MG	14	3327	1/1	0.96	0.06	58,58,58,58	0
58	MG	13	1729	1/1	0.96	0.12	86,86,86,86	0
58	MG	14	3388	1/1	0.96	0.10	79,79,79,79	0
58	MG	1H	3032	1/1	0.96	0.23	82,82,82,82	0
58	MG	14	3319	1/1	0.96	0.16	65,65,65,65	0
58	MG	14	3270	1/1	0.96	0.20	95,95,95,95	0
58	MG	1G	1603	1/1	0.96	0.18	87,87,87,87	0
58	MG	1J	201	1/1	0.96	0.40	76,76,76,76	0
58	MG	1H	3377	1/1	0.96	0.09	61,61,61,61	0
58	MG	1H	3239	1/1	0.96	0.10	67,67,67,67	0
58	MG	1G	1690	1/1	0.96	0.12	104,104,104,104	0
58	MG	1H	3386	1/1	0.96	0.14	50,50,50,50	0
58	MG	14	3101	1/1	0.97	0.15	65,65,65,65	0
58	MG	1H	3451	1/1	0.97	0.10	55,55,55,55	0
58	MG	13	1714	1/1	0.97	0.12	45,45,45,45	0
58	MG	1H	3278	1/1	0.97	0.21	106,106,106,106	0
58	MG	13	1603	1/1	0.97	0.34	50,50,50,50	0
58	MG	14	3189	1/1	0.97	0.15	46,46,46,46	0
58	MG	55	201	1/1	0.97	0.18	58,58,58,58	0
58	MG	14	3080	1/1	0.97	0.21	62,62,62,62	0
58	MG	1H	3140	1/1	0.97	0.30	69,69,69,69	0
58	MG	21	301	1/1	0.97	0.27	54,54,54,54	0
58	MG	14	3135	1/1	0.97	0.12	54,54,54,54	0
58	MG	1H	3116	1/1	0.97	0.37	51,51,51,51	0
58	MG	13	1720	1/1	0.97	0.12	82,82,82,82	0
58	MG	14	3323	1/1	0.97	0.10	65,65,65,65	0
58	MG	14	3241	1/1	0.97	0.28	80,80,80,80	0
58	MG	1H	3103	1/1	0.97	0.20	58,58,58,58	0
58	MG	1H	3260	1/1	0.97	0.22	35,35,35,35	0
58	MG	14	3351	1/1	0.97	0.18	87,87,87,87	0
58	MG	14	3072	1/1	0.97	0.22	74,74,74,74	0
58	MG	14	3066	1/1	0.97	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	29	302	1/1	0.97	0.19	57,57,57,57	0
58	MG	1H	3166	1/1	0.97	0.24	64,64,64,64	0
58	MG	1H	3397	1/1	0.97	0.08	49,49,49,49	0
58	MG	13	1602	1/1	0.97	0.27	49,49,49,49	0
58	MG	14	3260	1/1	0.97	0.20	100,100,100,100	0
58	MG	1H	3483	1/1	0.97	0.07	90,90,90,90	0
58	MG	1G	1689	1/1	0.97	0.10	84,84,84,84	0
58	MG	1H	3160	1/1	0.97	0.35	79,79,79,79	0
58	MG	13	1685	1/1	0.97	0.18	74,74,74,74	0
58	MG	1H	3512	1/1	0.97	0.09	44,44,44,44	0
58	MG	1H	3145	1/1	0.97	0.38	76,76,76,76	0
58	MG	1H	3304	1/1	0.97	0.12	71,71,71,71	0
58	MG	13	1724	1/1	0.97	0.11	96,96,96,96	0
58	MG	14	3264	1/1	0.97	0.19	77,77,77,77	0
58	MG	14	3315	1/1	0.97	0.16	57,57,57,57	0
58	MG	1H	3432	1/1	0.97	0.10	70,70,70,70	0
58	MG	1H	3058	1/1	0.97	0.24	36,36,36,36	0
58	MG	14	3210	1/1	0.97	0.14	51,51,51,51	0
58	MG	14	3093	1/1	0.97	0.18	63,63,63,63	0
58	MG	1H	3061	1/1	0.97	0.28	56,56,56,56	0
58	MG	14	3108	1/1	0.97	0.23	50,50,50,50	0
58	MG	14	3226	1/1	0.97	0.20	67,67,67,67	0
58	MG	1H	3437	1/1	0.97	0.18	54,54,54,54	0
58	MG	1H	3328	1/1	0.97	0.25	56,56,56,56	0
58	MG	1H	3069	1/1	0.97	0.15	52,52,52,52	0
58	MG	1H	3366	1/1	0.97	0.14	56,56,56,56	0
58	MG	1G	1612	1/1	0.97	0.22	83,83,83,83	0
58	MG	29	301	1/1	0.97	0.21	64,64,64,64	0
58	MG	1H	3501	1/1	0.97	0.09	42,42,42,42	0
58	MG	1H	3370	1/1	0.97	0.07	55,55,55,55	0
58	MG	1G	1673	1/1	0.97	0.09	92,92,92,92	0
58	MG	1H	3336	1/1	0.97	0.13	62,62,62,62	0
58	MG	1H	3350	1/1	0.97	0.09	51,51,51,51	0
58	MG	13	1663	1/1	0.97	0.34	62,62,62,62	0
58	MG	13	1620	1/1	0.97	0.30	72,72,72,72	0
58	MG	1H	3263	1/1	0.97	0.49	56,56,56,56	0
58	MG	14	3328	1/1	0.97	0.11	49,49,49,49	0
58	MG	1H	3190	1/1	0.97	0.25	69,69,69,69	0
58	MG	1H	3490	1/1	0.97	0.10	64,64,64,64	0
58	MG	1H	3362	1/1	0.97	0.15	41,41,41,41	0
58	MG	14	3131	1/1	0.97	0.28	87,87,87,87	0
58	MG	1H	3060	1/1	0.97	0.30	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3482	1/1	0.97	0.10	54,54,54,54	0
58	MG	14	3238	1/1	0.97	0.11	86,86,86,86	0
58	MG	1H	3363	1/1	0.97	0.14	40,40,40,40	0
58	MG	1J	203	1/1	0.97	0.18	100,100,100,100	0
59	PAR	13	1749	42/42	0.97	0.23	52,62,69,75	0
58	MG	14	3005	1/1	0.97	0.28	60,60,60,60	0
58	MG	16	211	1/1	0.97	0.09	70,70,70,70	0
58	MG	1H	3286	1/1	0.97	0.15	71,71,71,71	0
58	MG	14	3342	1/1	0.97	0.09	49,49,49,49	0
58	MG	1G	1617	1/1	0.97	0.12	74,74,74,74	0
58	MG	14	3021	1/1	0.97	0.23	73,73,73,73	0
58	MG	14	3064	1/1	0.97	0.20	86,86,86,86	0
58	MG	13	1623	1/1	0.97	0.23	62,62,62,62	0
58	MG	13	1621	1/1	0.97	0.14	74,74,74,74	0
58	MG	14	3113	1/1	0.97	0.23	62,62,62,62	0
58	MG	14	3067	1/1	0.97	0.15	81,81,81,81	0
58	MG	1H	3395	1/1	0.97	0.14	36,36,36,36	0
58	MG	1H	3194	1/1	0.97	0.15	40,40,40,40	0
58	MG	13	1631	1/1	0.97	0.22	82,82,82,82	0
58	MG	14	3065	1/1	0.97	0.17	62,62,62,62	0
58	MG	13	1719	1/1	0.97	0.10	67,67,67,67	0
58	MG	13	1638	1/1	0.97	0.25	62,62,62,62	0
58	MG	1H	3003	1/1	0.97	0.24	49,49,49,49	0
58	MG	13	1668	1/1	0.97	0.18	66,66,66,66	0
58	MG	1H	3014	1/1	0.97	0.15	58,58,58,58	0
58	MG	1H	3391	1/1	0.97	0.05	60,60,60,60	0
58	MG	14	3384	1/1	0.98	0.07	68,68,68,68	0
58	MG	14	3311	1/1	0.98	0.09	65,65,65,65	0
58	MG	14	3092	1/1	0.98	0.16	48,48,48,48	0
58	MG	1H	3008	1/1	0.98	0.33	68,68,68,68	0
58	MG	1H	3132	1/1	0.98	0.27	62,62,62,62	0
58	MG	1H	3429	1/1	0.98	0.05	72,72,72,72	0
58	MG	1G	1621	1/1	0.98	0.10	90,90,90,90	0
58	MG	14	3117	1/1	0.98	0.22	57,57,57,57	0
58	MG	14	3325	1/1	0.98	0.09	76,76,76,76	0
58	MG	13	1718	1/1	0.98	0.09	69,69,69,69	0
58	MG	1H	3117	1/1	0.98	0.14	43,43,43,43	0
58	MG	1H	3446	1/1	0.98	0.09	59,59,59,59	0
60	ZN	3E	303	1/1	0.98	0.44	97,97,97,97	0
58	MG	1H	3401	1/1	0.98	0.18	47,47,47,47	0
58	MG	14	3079	1/1	0.98	0.20	73,73,73,73	0
58	MG	13	1715	1/1	0.98	0.12	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3086	1/1	0.98	0.19	54,54,54,54	0
58	MG	14	3347	1/1	0.98	0.11	48,48,48,48	0
58	MG	14	3356	1/1	0.98	0.08	65,65,65,65	0
58	MG	13	1726	1/1	0.98	0.08	93,93,93,93	0
58	MG	14	3052	1/1	0.98	0.23	59,59,59,59	0
58	MG	13	1619	1/1	0.98	0.15	75,75,75,75	0
58	MG	14	3105	1/1	0.98	0.27	45,45,45,45	0
58	MG	1H	3372	1/1	0.98	0.15	64,64,64,64	0
58	MG	1H	3065	1/1	0.98	0.21	43,43,43,43	0
58	MG	14	3149	1/1	0.98	0.10	62,62,62,62	0
58	MG	14	3359	1/1	0.98	0.08	73,73,73,73	0
58	MG	1H	3099	1/1	0.98	0.33	63,63,63,63	0
58	MG	14	3112	1/1	0.98	0.19	65,65,65,65	0
58	MG	1H	3502	1/1	0.98	0.11	66,66,66,66	0
58	MG	1H	3433	1/1	0.98	0.04	73,73,73,73	0
58	MG	13	1604	1/1	0.98	0.41	81,81,81,81	0
58	MG	1H	3291	1/1	0.98	0.14	86,86,86,86	0
58	MG	13	1697	1/1	0.98	0.13	73,73,73,73	0
58	MG	14	3139	1/1	0.98	0.22	63,63,63,63	0
58	MG	1H	3176	1/1	0.98	0.30	82,82,82,82	0
58	MG	14	3350	1/1	0.98	0.08	92,92,92,92	0
58	MG	1H	3489	1/1	0.98	0.17	53,53,53,53	0
58	MG	1H	3093	1/1	0.98	0.20	53,53,53,53	0
58	MG	14	3309	1/1	0.98	0.14	59,59,59,59	0
58	MG	14	3054	1/1	0.98	0.15	51,51,51,51	0
58	MG	14	3401	1/1	0.98	0.08	45,45,45,45	0
58	MG	1G	1693	1/1	0.98	0.12	82,82,82,82	0
58	MG	1H	3407	1/1	0.98	0.12	43,43,43,43	0
58	MG	1H	3355	1/1	0.98	0.14	57,57,57,57	0
58	MG	14	3349	1/1	0.98	0.14	62,62,62,62	0
58	MG	14	3188	1/1	0.98	0.11	53,53,53,53	0
58	MG	14	3170	1/1	0.98	0.10	84,84,84,84	0
58	MG	1H	3001	1/1	0.98	0.38	53,53,53,53	0
58	MG	1H	3353	1/1	0.98	0.15	40,40,40,40	0
58	MG	1H	3097	1/1	0.98	0.33	69,69,69,69	0
58	MG	1H	3404	1/1	0.98	0.15	48,48,48,48	0
58	MG	14	3262	1/1	0.98	0.07	78,78,78,78	0
58	MG	14	3308	1/1	0.98	0.07	46,46,46,46	0
58	MG	14	3100	1/1	0.98	0.23	66,66,66,66	0
58	MG	14	3128	1/1	0.98	0.16	58,58,58,58	0
58	MG	1H	3062	1/1	0.98	0.17	44,44,44,44	0
58	MG	14	3399	1/1	0.98	0.11	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	14	3155	1/1	0.98	0.22	65,65,65,65	0
58	MG	14	3061	1/1	0.98	0.20	58,58,58,58	0
58	MG	14	3341	1/1	0.98	0.14	41,41,41,41	0
58	MG	16	213	1/1	0.98	0.12	66,66,66,66	0
58	MG	1H	3067	1/1	0.98	0.25	46,46,46,46	0
58	MG	14	3320	1/1	0.98	0.10	42,42,42,42	0
58	MG	14	3336	1/1	0.98	0.10	60,60,60,60	0
58	MG	14	3006	1/1	0.98	0.21	62,62,62,62	0
58	MG	1H	3167	1/1	0.98	0.20	56,56,56,56	0
58	MG	14	3222	1/1	0.98	0.21	75,75,75,75	0
58	MG	14	3119	1/1	0.98	0.14	49,49,49,49	0
58	MG	1H	3379	1/1	0.98	0.04	72,72,72,72	0
58	MG	1H	3084	1/1	0.98	0.33	69,69,69,69	0
58	MG	1H	3438	1/1	0.98	0.14	55,55,55,55	0
58	MG	G8	201	1/1	0.98	0.21	73,73,73,73	0
58	MG	14	3200	1/1	0.98	0.22	94,94,94,94	0
58	MG	1H	3384	1/1	0.98	0.12	34,34,34,34	0
58	MG	14	3291	1/1	0.98	0.18	70,70,70,70	0
58	MG	1H	3385	1/1	0.98	0.12	45,45,45,45	0
58	MG	13	1617	1/1	0.98	0.17	60,60,60,60	0
58	MG	1H	3125	1/1	0.98	0.19	47,47,47,47	0
58	MG	14	3228	1/1	0.98	0.26	85,85,85,85	0
58	MG	13	1640	1/1	0.98	0.10	64,64,64,64	0
58	MG	14	3322	1/1	0.98	0.06	72,72,72,72	0
58	MG	13	1732	1/1	0.98	0.07	78,78,78,78	0
58	MG	1H	3411	1/1	0.98	0.12	46,46,46,46	0
58	MG	14	3055	1/1	0.98	0.21	54,54,54,54	0
58	MG	1G	1684	1/1	0.98	0.09	70,70,70,70	0
58	MG	14	3302	1/1	0.98	0.24	83,83,83,83	0
58	MG	14	3316	1/1	0.98	0.10	62,62,62,62	0
58	MG	1H	3409	1/1	0.98	0.11	41,41,41,41	0
58	MG	1G	1639	1/1	0.98	0.16	80,80,80,80	0
58	MG	14	3314	1/1	0.98	0.12	58,58,58,58	0
58	MG	14	3304	1/1	0.98	0.11	50,50,50,50	0
58	MG	1H	3057	1/1	0.98	0.18	44,44,44,44	0
58	MG	1H	3087	1/1	0.98	0.22	75,75,75,75	0
58	MG	14	3324	1/1	0.99	0.14	62,62,62,62	0
58	MG	1H	3442	1/1	0.99	0.14	54,54,54,54	0
58	MG	14	3345	1/1	0.99	0.14	51,51,51,51	0
58	MG	14	3133	1/1	0.99	0.21	77,77,77,77	0
58	MG	1H	3368	1/1	0.99	0.14	56,56,56,56	0
58	MG	1H	3477	1/1	0.99	0.17	62,62,62,62	0

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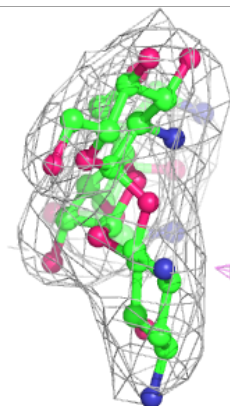
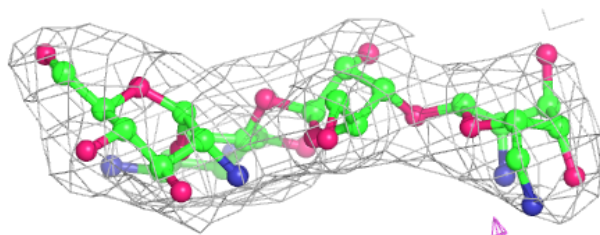
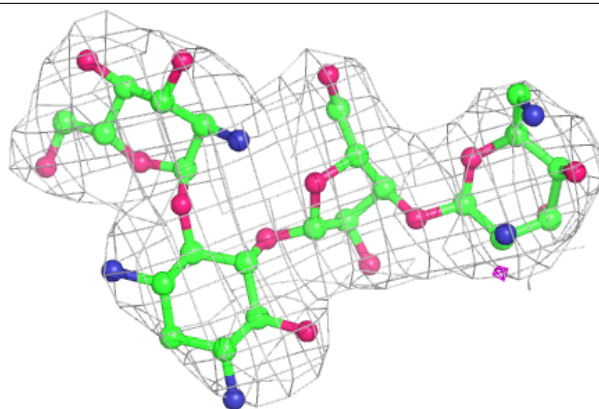
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1H	3388	1/1	0.99	0.08	59,59,59,59	0
58	MG	14	3056	1/1	0.99	0.26	58,58,58,58	0
58	MG	1H	3445	1/1	0.99	0.11	44,44,44,44	0
58	MG	1G	1641	1/1	0.99	0.13	98,98,98,98	0
58	MG	1H	3123	1/1	0.99	0.29	49,49,49,49	0
58	MG	1H	3126	1/1	0.99	0.28	60,60,60,60	0
58	MG	2L	101	1/1	0.99	0.15	88,88,88,88	0
58	MG	13	1731	1/1	0.99	0.10	68,68,68,68	0
58	MG	1H	3399	1/1	0.99	0.10	52,52,52,52	0
58	MG	1H	3419	1/1	0.99	0.10	47,47,47,47	0
58	MG	14	3306	1/1	0.99	0.12	52,52,52,52	0
58	MG	14	3109	1/1	0.99	0.19	62,62,62,62	0
58	MG	14	3257	1/1	0.99	0.17	58,58,58,58	0
58	MG	13	1741	1/1	0.99	0.14	82,82,82,82	0
58	MG	14	3343	1/1	0.99	0.08	47,47,47,47	0
58	MG	1H	3063	1/1	0.99	0.17	64,64,64,64	0
58	MG	14	3088	1/1	0.99	0.20	45,45,45,45	0
58	MG	1H	3090	1/1	0.99	0.11	37,37,37,37	0
58	MG	1H	3427	1/1	0.99	0.12	41,41,41,41	0
58	MG	1H	3405	1/1	0.99	0.11	43,43,43,43	0
58	MG	14	3013	1/1	0.99	0.25	56,56,56,56	0
58	MG	14	3288	1/1	0.99	0.13	78,78,78,78	0
58	MG	1H	3356	1/1	0.99	0.12	52,52,52,52	0
58	MG	1H	3360	1/1	0.99	0.12	46,46,46,46	0
58	MG	1G	1623	1/1	0.99	0.22	91,91,91,91	0
58	MG	13	1601	1/1	0.99	0.20	52,52,52,52	0
58	MG	1G	1694	1/1	0.99	0.12	67,67,67,67	0
58	MG	14	3058	1/1	0.99	0.22	58,58,58,58	0
58	MG	1H	3365	1/1	0.99	0.10	44,44,44,44	0
58	MG	1H	3002	1/1	0.99	0.22	60,60,60,60	0
58	MG	1H	3424	1/1	0.99	0.15	73,73,73,73	0
58	MG	1H	3441	1/1	0.99	0.08	51,51,51,51	0
58	MG	1H	3358	1/1	1.00	0.09	43,43,43,43	0

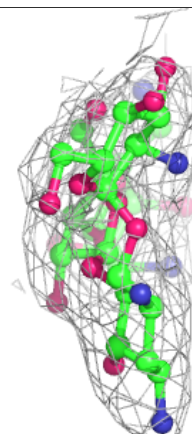
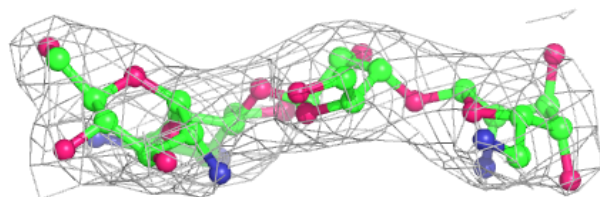
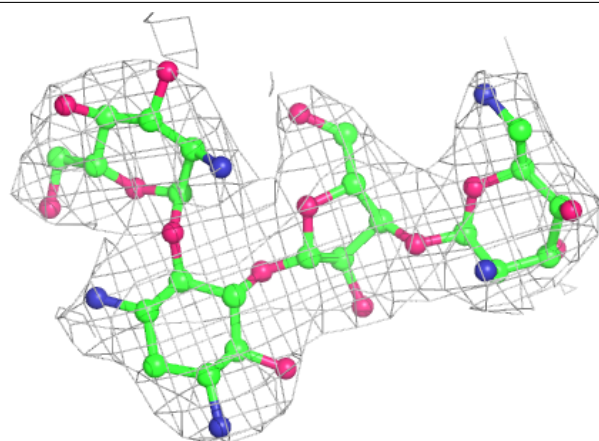
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR 1G 1697:

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

**Electron density around PAR 13 1749:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.