



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 10:02 PM UTC

PDB ID : 5IB7 / pdb\_00005ib7  
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA<sup>fMet</sup>, near-cognate tRNA<sup>Lys</sup> with U-G mismatch in the A-site and antibiotic paromomycin  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2016-02-22  
Resolution : 2.99 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

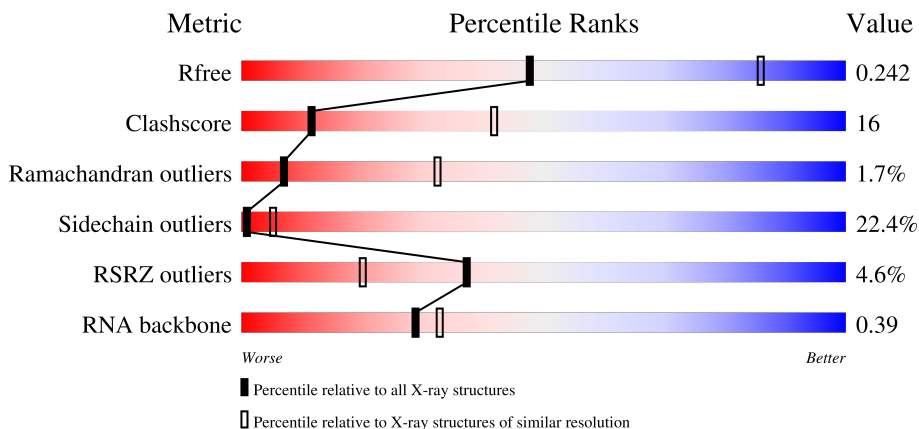
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 Å.

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



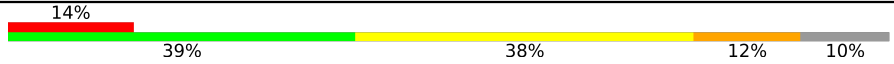
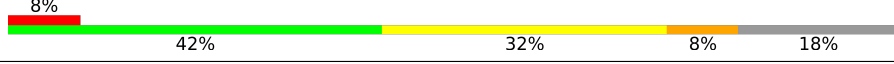
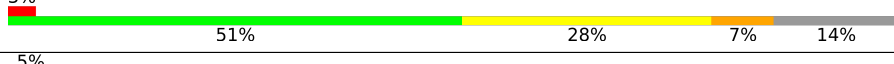
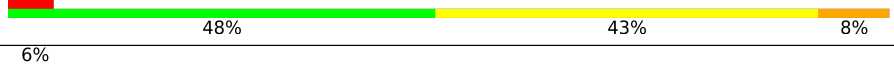
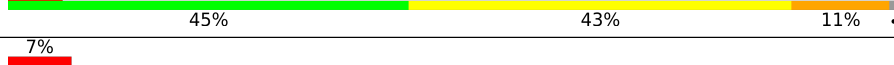

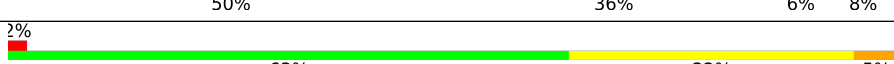

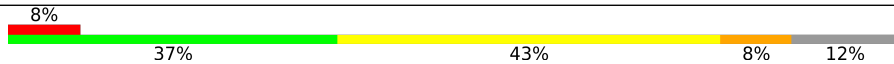


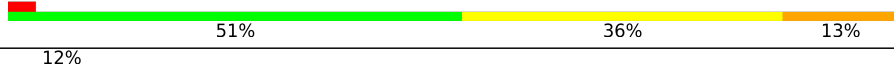
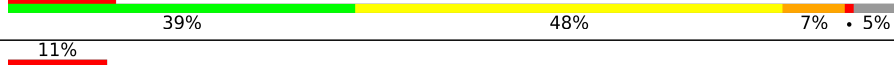

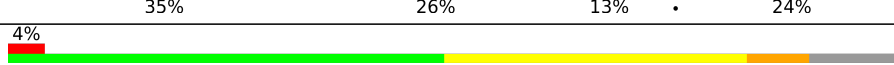










Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	13	1522	
1	1G	1522	
2	12	256	

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

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

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Mol	Chain	Length	Quality of chain
27	1J	122	
28	71	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	

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Mol	Chain	Length	Quality of chain
40	A8	112	3% 37% 47% 15%
41	75	146	3% 38% 40% 12% 9%
41	B8	146	8% 34% 42% 15% 8%
42	85	118	7% 56% 30% 13%
42	C8	118	3% 52% 38% 6%
43	95	101	4% 54% 38% 6%
43	D8	101	3% 47% 41% 10%
44	A5	113	2% 60% 29% 9%
44	E8	113	4% 53% 35% 10%
45	B5	96	4% 53% 33% 11%
45	F8	96	2% 61% 30% 7%
46	C5	110	29% 40% 36% 15% 5%
46	G8	110	12% 46% 29% 16% 6%
47	D5	206	2% 32% 40% 13% 14%
47	H8	206	38% 33% 10% 17%
48	E5	85	5% 45% 36% 7% 11%
48	I8	85	5% 48% 33% 9% 9%
49	F5	98	4% 52% 32% 11%
49	J8	98	6% 49% 33% 15%
50	G5	72	7% 43% 40% 10%
50	K8	72	3% 35% 42% 12% 6% 6%
51	H5	60	58% 35%
51	L8	60	52% 37% 8%
52	M8	71	7% 35% 32% 10% 7% 15%
53	J5	60	10% 55% 35% 7%

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Mol	Chain	Length	Quality of chain
53	N8	60	
54	O8	54	
55	L5	49	
55	P8	49	
56	M5	65	
56	Q8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	13	1643	-	-	-	X
57	MG	13	1669	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	13	1676	-	-	-	X
57	MG	14	3088	-	-	-	X
57	MG	14	3197	-	-	-	X
57	MG	14	3208	-	-	-	X
57	MG	1H	3151	-	-	-	X
57	MG	1H	3157	-	-	-	X
57	MG	1H	3206	-	-	-	X
59	SF4	32	302	-	-	X	-

## 2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 297444 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
			Total	C	N	O	P			
1	13	1499	Total 32223	C 14342	N 5973	O 10409	P 1499	0	0	0
1	1G	1508	Total 32414	C 14427	N 6005	O 10474	P 1508	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	-	expression tag	GB 55771382
13	1543	C	-	expression tag	GB 55771382
13	1544	U	-	expression tag	GB 55771382
1G	1542	G	-	expression tag	GB 55771382
1G	1543	C	-	expression tag	GB 55771382
1G	1544	U	-	expression tag	GB 55771382

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	150	Total	C	N	O	S	0	0	0
			1141	719	217	201	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O	0	0	0
			1000	634	196	170			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	82	121	Total	C	N	O	0	0	0
			953	605	186	162			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	94	Total	C	N	O	S	0	0	0
			749	468	147	133	1			
10	1A	80	Total	C	N	O	0	0	0	
			646	403	129	114				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	111	Total	C	N	O	S	0	0	0
			823	512	154	154	3			
11	2A	113	Total	C	N	O	S	0	0	0
			835	520	156	156	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			661	422	123	114	2			
19	AA	65	Total	C	N	O	S	0	0	0
			510	324	92	92	2			

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

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

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

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

- Molecule 22 is a RNA chain called tRNA<sup>Lys</sup>.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
22	1K	72	Total	C	N	O	P	S	0	0	0
			1542	691	269	509	72	1			

- Molecule 23 is a RNA chain called tRNA<sup>fMet</sup>.

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<sup>Lys</sup>.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1483	664	260	490	69			
24	1L	66	Total	C	N	O	P	0	0	0
			1401	626	244	465	66			
24	3L	72	Total	C	N	O	P	0	0	0
			1528	684	270	503	71			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	19	Total	C	N	O	P	0	0	0
			420	188	89	124	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	4L	19	419	188	89	123	19	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	1H	2860	61609	27418	11525	19806	2860	0	0	0
26	14	2826	60877	27092	11393	19566	2826	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1059B	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	71	132	1027	648	193	185	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	21	203	Total	C	N	O	S	0	0	0
			1546	978	295	267	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	180	Total	C	N	O	S	0	0	0
			1459	931	266	258	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
33	59	169	Total	C	N	O	S	0	0	0
			1295	823	241	230	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	137	Total	C	N	O	S	0	0	0
			1096	706	205	181	4			
35	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1117	712	211	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	B8	135	1119	697	230	191	1	0	0	0
41	75	133	1109	691	228	189	1	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
45	B5	94	Total	C	N	O	S	0	0	0
			735	477	133	125				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	170	Total	C	N	O	S	0	0	0
			1365	870	246	246	3			
47	D5	177	Total	C	N	O	S	0	0	0
			1411	901	253	255	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	96	Total	C	N	O	S	0	0	0
			747	469	148	129	1			
49	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	M8	60	Total 475	C 300	N 84	O 86	S 5	0	0	0

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

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

- Molecule 54 is a protein called 50S ribosomal protein L33.

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

- Molecule 55 is a protein called 50S ribosomal protein L34.

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

- Molecule 56 is a protein called 50S ribosomal protein L35.

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

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

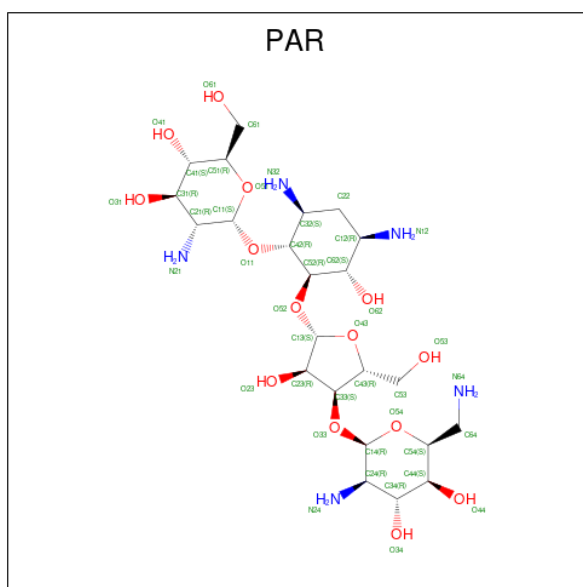
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	140	Total	Mg	0	0
			140	140		
57	3I	1	Total	Mg	0	0
			1	1		
57	4I	1	Total	Mg	0	0
			1	1		
57	5I	1	Total	Mg	0	0
			1	1		
57	2K	2	Total	Mg	0	0
			2	2		
57	1H	525	Total	Mg	0	0
			525	525		
57	16	11	Total	Mg	0	0
			11	11		
57	21	3	Total	Mg	0	0
			3	3		
57	31	2	Total	Mg	0	0
			2	2		
57	41	1	Total	Mg	0	0
			1	1		
57	78	1	Total	Mg	0	0
			1	1		
57	88	3	Total	Mg	0	0
			3	3		
57	I8	2	Total	Mg	0	0
			2	2		
57	P8	1	Total	Mg	0	0
			1	1		
57	Q8	1	Total	Mg	0	0
			1	1		
57	1G	102	Total	Mg	0	0
			102	102		
57	32	1	Total	Mg	0	0
			1	1		
57	42	1	Total	Mg	0	0
			1	1		

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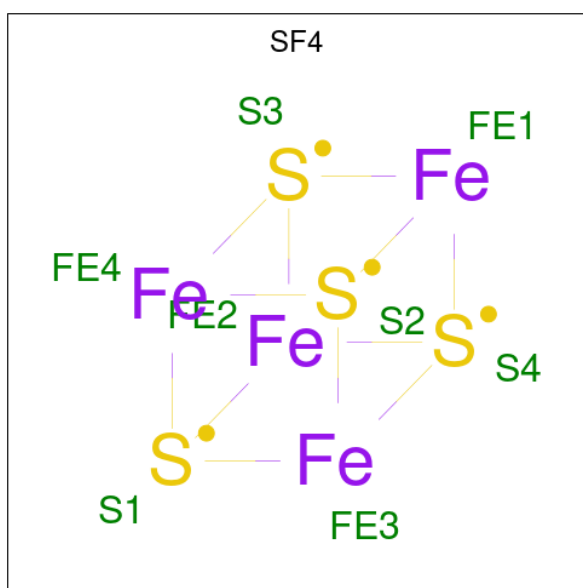
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	52	1	Total Mg 1 1	0	0
57	7A	1	Total Mg 1 1	0	0
57	2L	2	Total Mg 2 2	0	0
57	4L	1	Total Mg 1 1	0	0
57	14	435	Total Mg 435 435	0	0
57	1J	8	Total Mg 8 8	0	0
57	19	1	Total Mg 1 1	0	0
57	29	1	Total Mg 1 1	0	0
57	39	2	Total Mg 2 2	0	0
57	25	1	Total Mg 1 1	0	0
57	35	1	Total Mg 1 1	0	0
57	45	2	Total Mg 2 2	0	0
57	C5	1	Total Mg 1 1	0	0
57	E5	1	Total Mg 1 1	0	0
57	M5	1	Total Mg 1 1	0	0

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



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

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

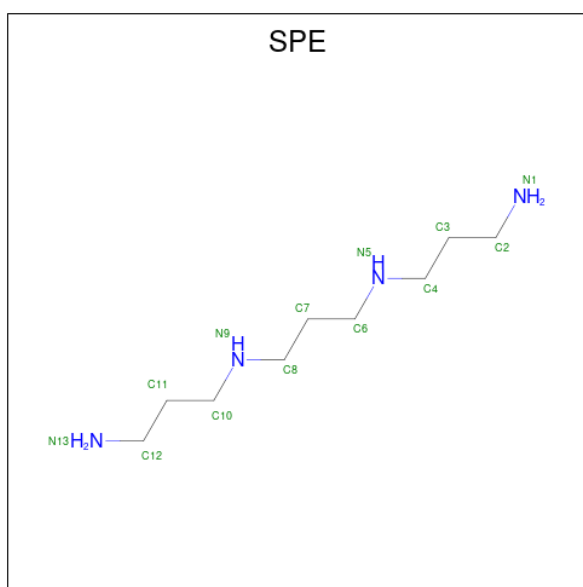


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe S		
59	3E	1	8	4 4	0	0
59	32	1	8	4 4	0	0

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

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

- Molecule 61 is THERMINE (CCD ID: SPE) (formula: C<sub>9</sub>H<sub>24</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	1	Total C N 13 9 4	0	0
61	14	1	Total C N 13 9 4	0	0
61	14	1	Total C N 13 9 4	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	13	320	Total O 320 320	0	0
62	4E	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	8E	2	Total O 2 2	0	0
62	1I	2	Total O 2 2	0	0
62	3I	2	Total O 2 2	0	0
62	5I	2	Total O 2 2	0	0
62	6I	3	Total O 3 3	0	0
62	7I	1	Total O 1 1	0	0
62	BI	2	Total O 2 2	0	0
62	1F	1	Total O 1 1	0	0
62	1K	2	Total O 2 2	0	0
62	2K	8	Total O 8 8	0	0
62	4K	5	Total O 5 5	0	0
62	1H	1470	Total O 1470 1470	0	0
62	16	12	Total O 12 12	0	0
62	11	17	Total O 17 17	0	0
62	21	7	Total O 7 7	0	0
62	31	5	Total O 5 5	0	0
62	41	1	Total O 1 1	0	0
62	58	2	Total O 2 2	0	0
62	78	10	Total O 10 10	0	0
62	B8	1	Total O 1 1	0	0
62	C8	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	F8	2	Total O 2 2	0	0
62	G8	2	Total O 2 2	0	0
62	I8	6	Total O 6 6	0	0
62	J8	4	Total O 4 4	0	0
62	L8	3	Total O 3 3	0	0
62	P8	1	Total O 1 1	0	0
62	Q8	5	Total O 5 5	0	0
62	1G	317	Total O 317 317	0	0
62	32	1	Total O 1 1	0	0
62	52	4	Total O 4 4	0	0
62	1A	1	Total O 1 1	0	0
62	6A	2	Total O 2 2	0	0
62	7A	5	Total O 5 5	0	0
62	9A	2	Total O 2 2	0	0
62	BA	2	Total O 2 2	0	0
62	2L	6	Total O 6 6	0	0
62	4L	6	Total O 6 6	0	0
62	14	1144	Total O 1144 1144	0	0
62	1J	12	Total O 12 12	0	0
62	19	15	Total O 15 15	0	0
62	29	4	Total O 4 4	0	0

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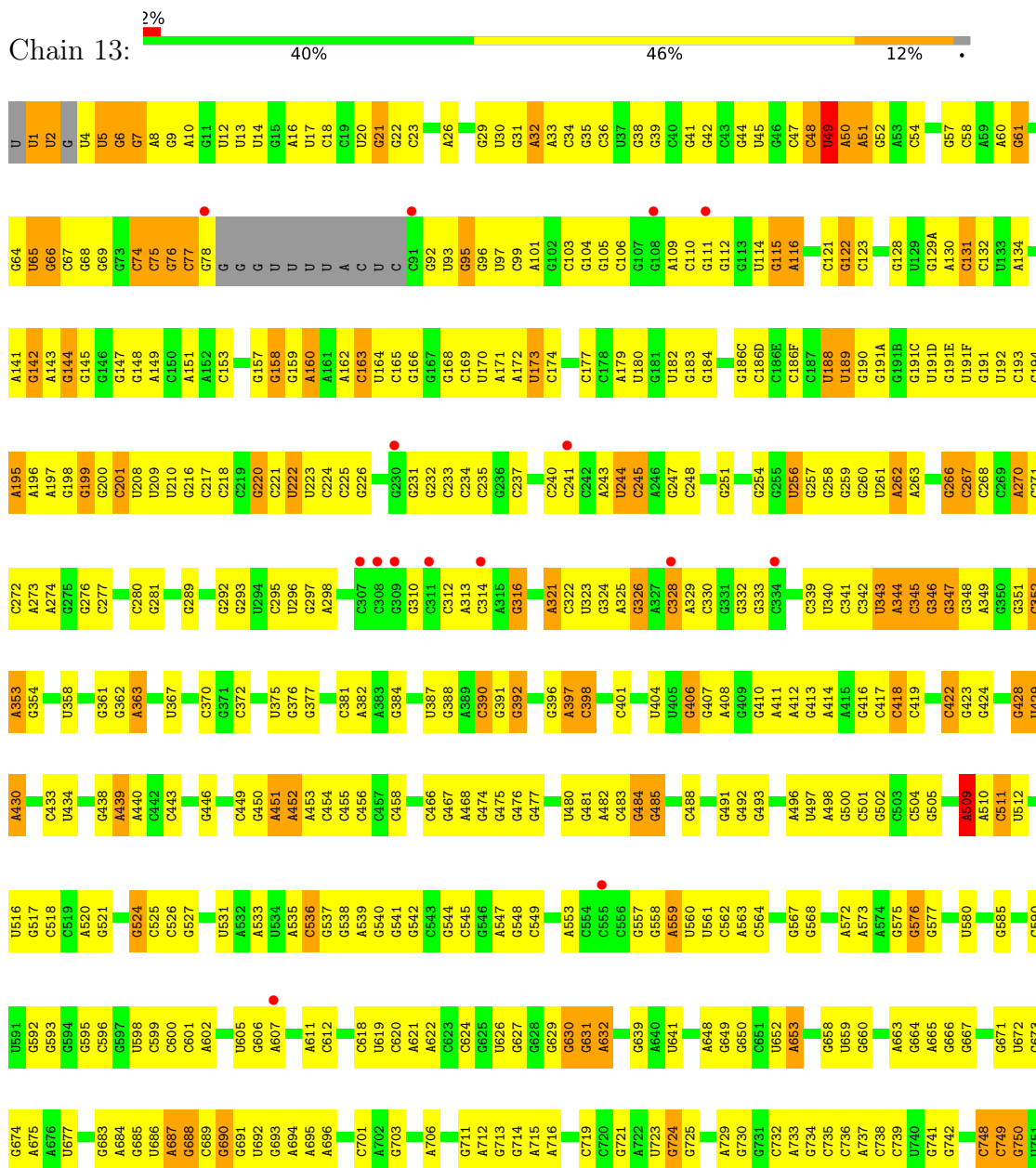
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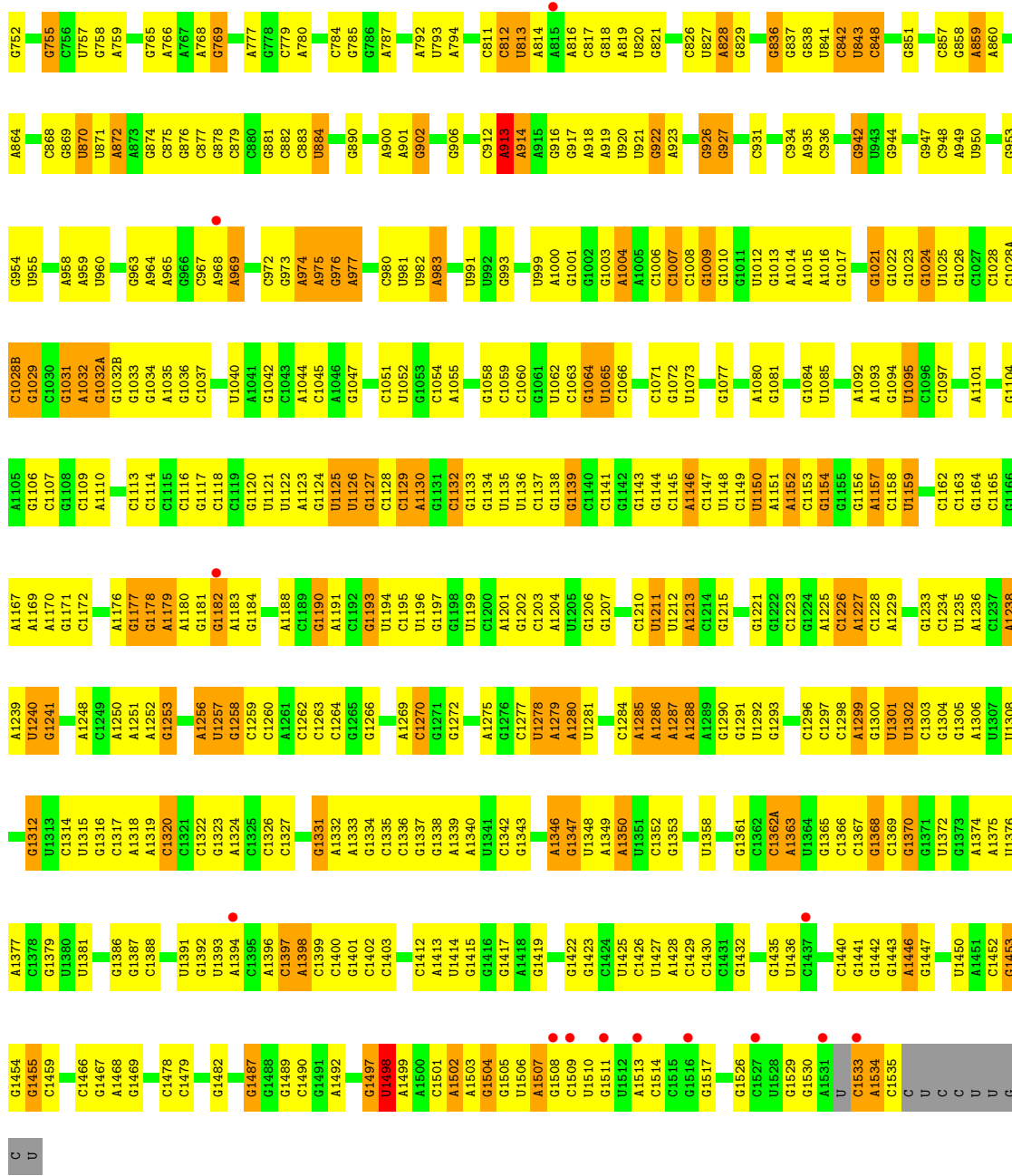
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	39	5	Total 5	O 5	0	0
62	15	1	Total 1	O 1	0	0
62	25	6	Total 6	O 6	0	0
62	35	8	Total 8	O 8	0	0
62	55	3	Total 3	O 3	0	0
62	85	2	Total 2	O 2	0	0
62	A5	1	Total 1	O 1	0	0
62	B5	1	Total 1	O 1	0	0
62	C5	3	Total 3	O 3	0	0
62	F5	1	Total 1	O 1	0	0
62	H5	2	Total 2	O 2	0	0
62	M5	9	Total 9	O 9	0	0

### 3 Residue-property plots [i](#)

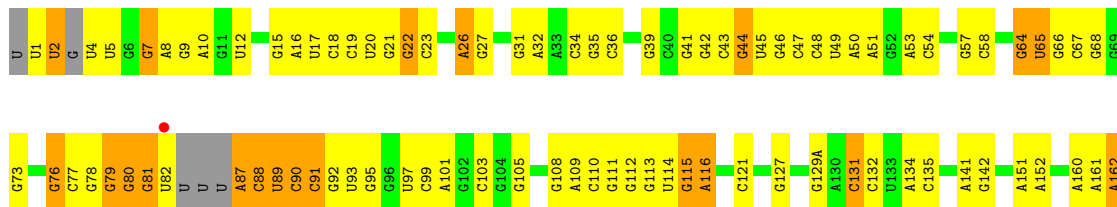
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

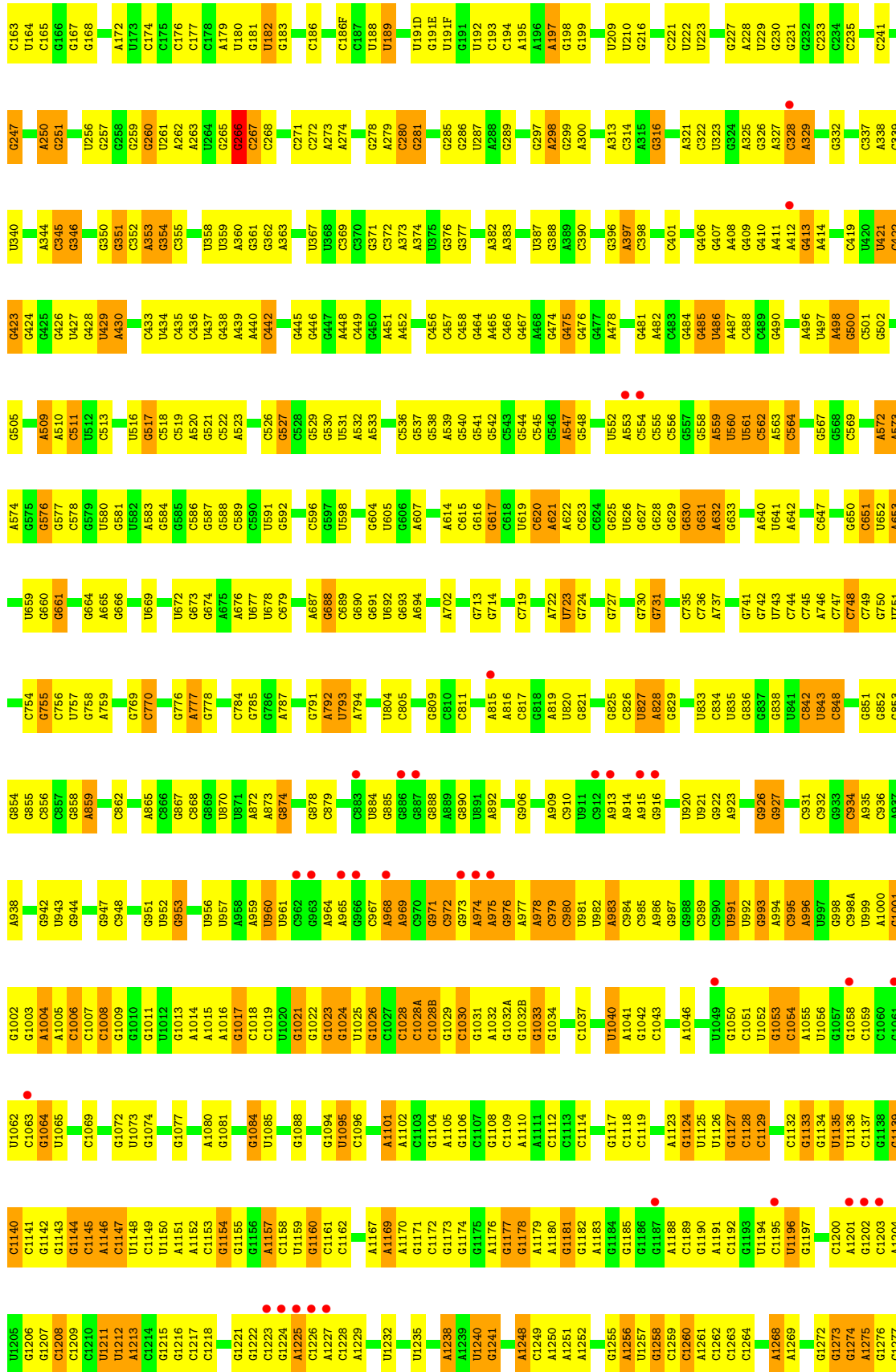
- Molecule 1: 16S ribosomal RNA

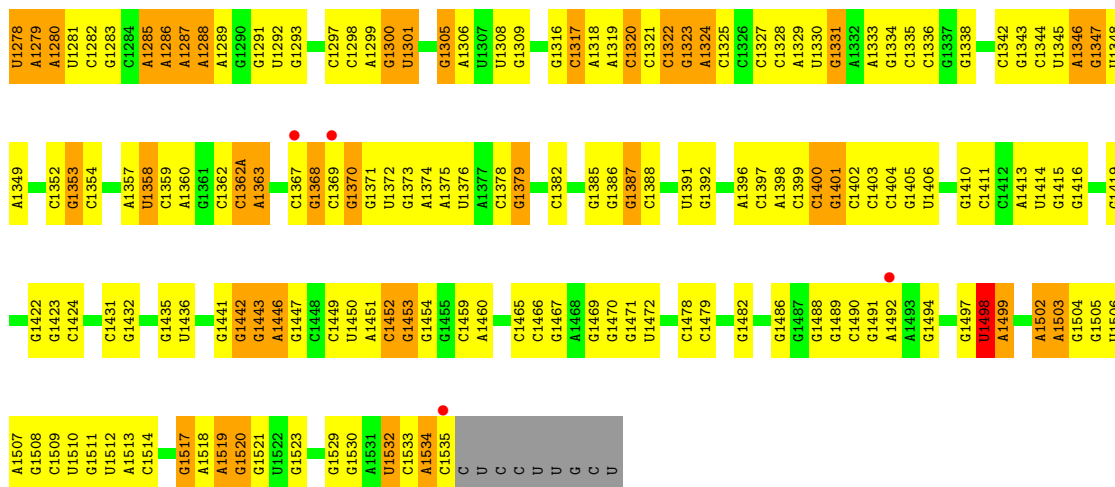




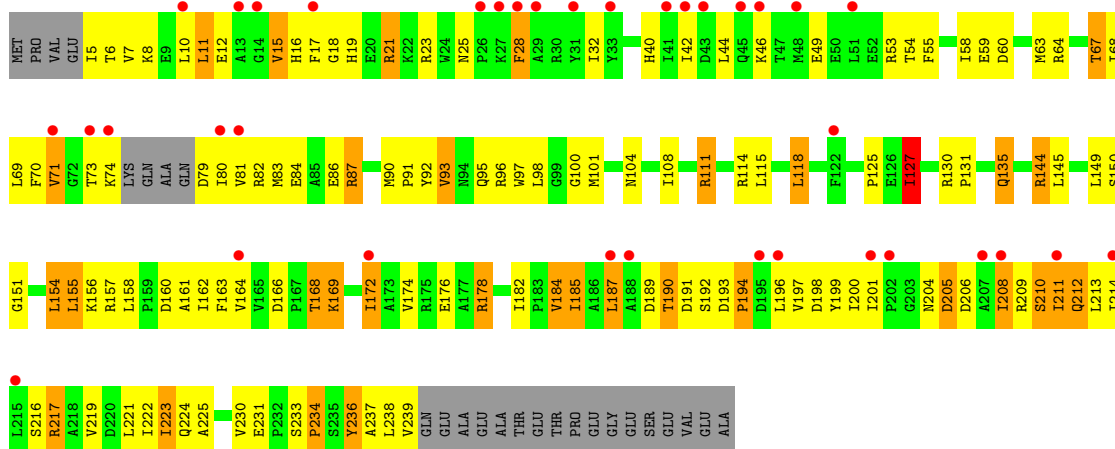
• Molecule 1: 16S ribosomal RNA



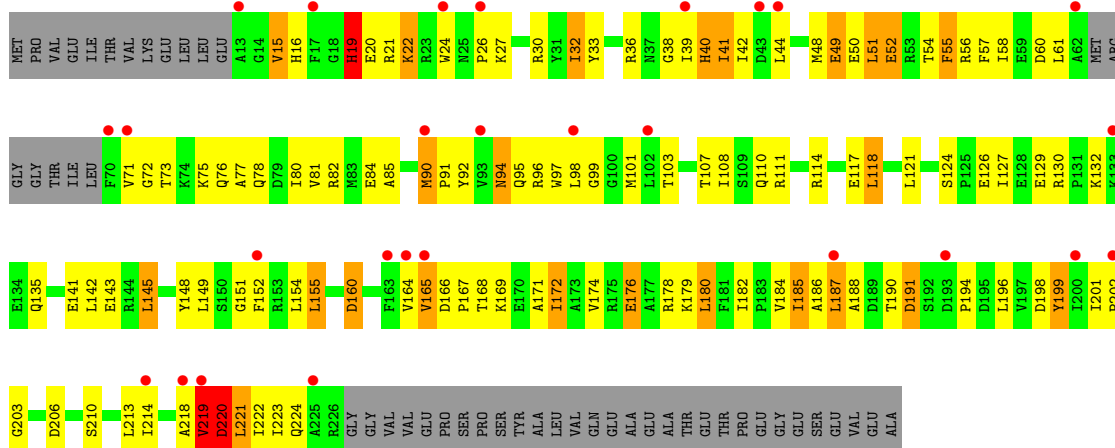
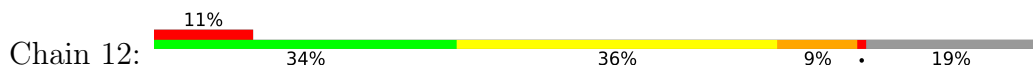




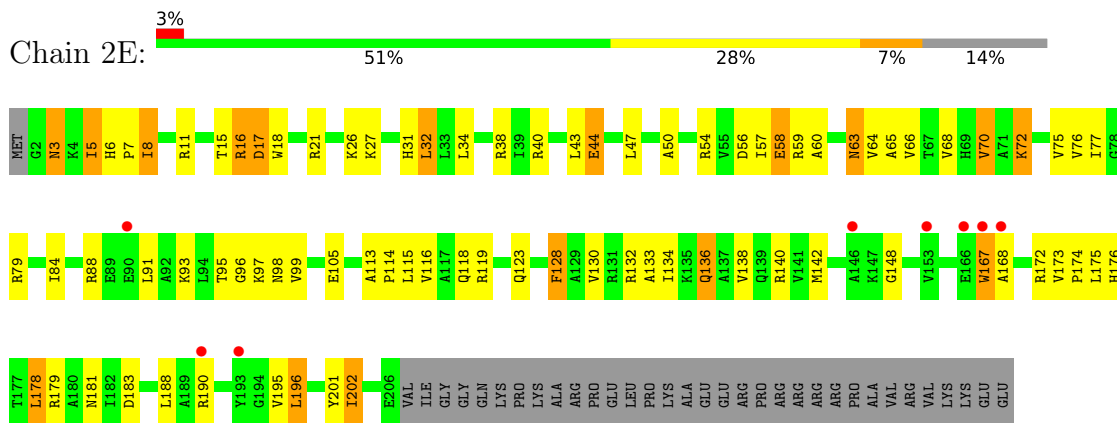
• Molecule 2: 30S ribosomal protein S2



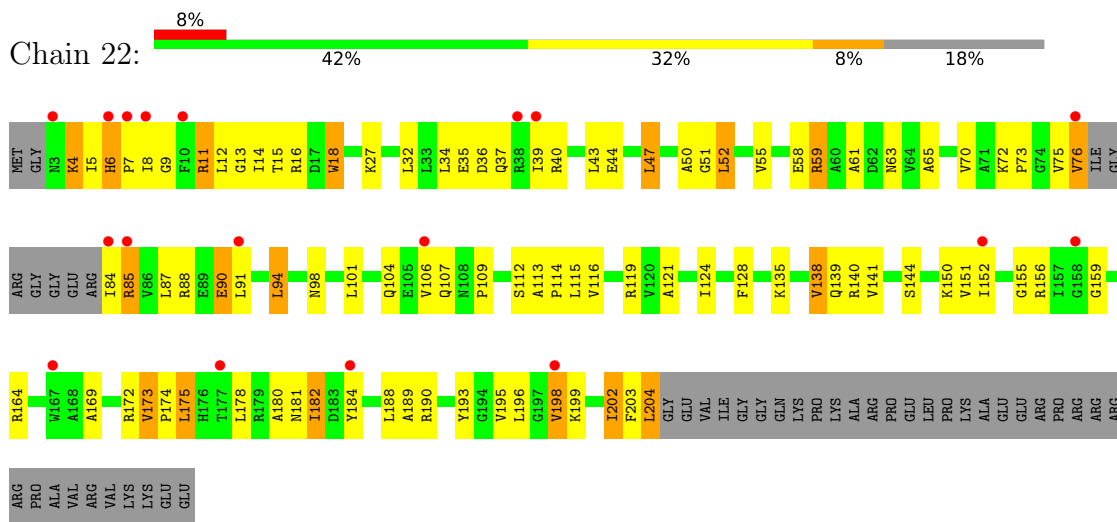
• Molecule 2: 30S ribosomal protein S2



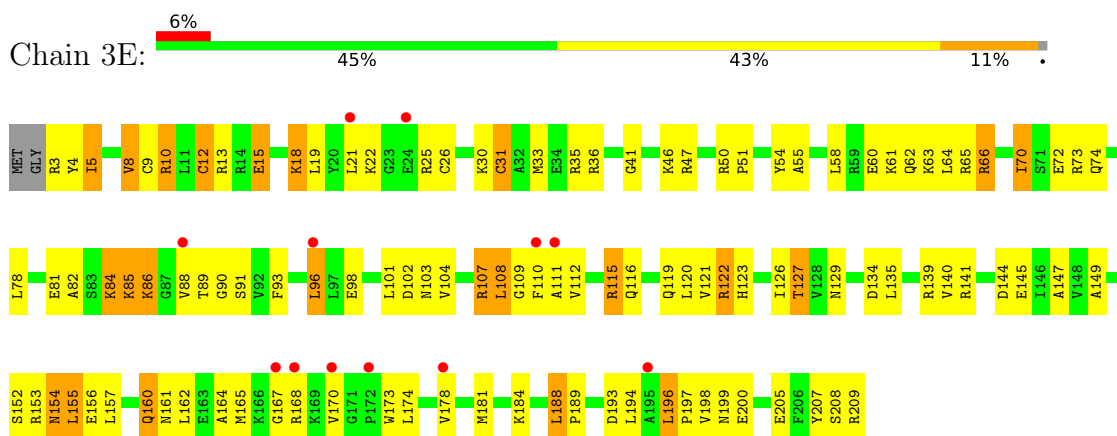
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

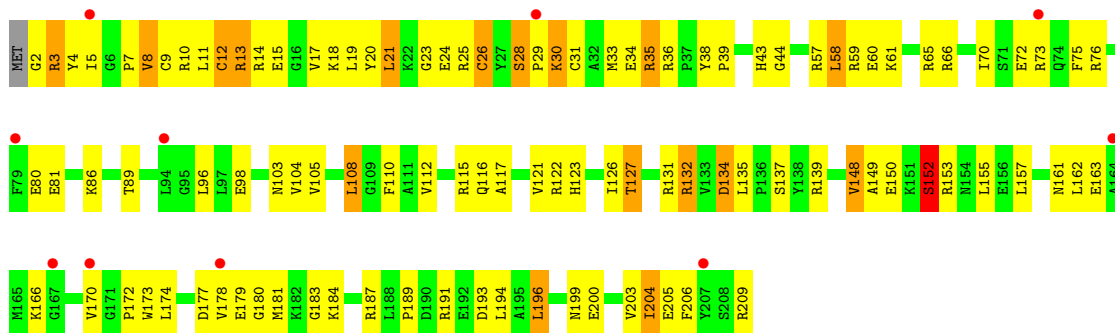


• Molecule 4: 30S ribosomal protein S4

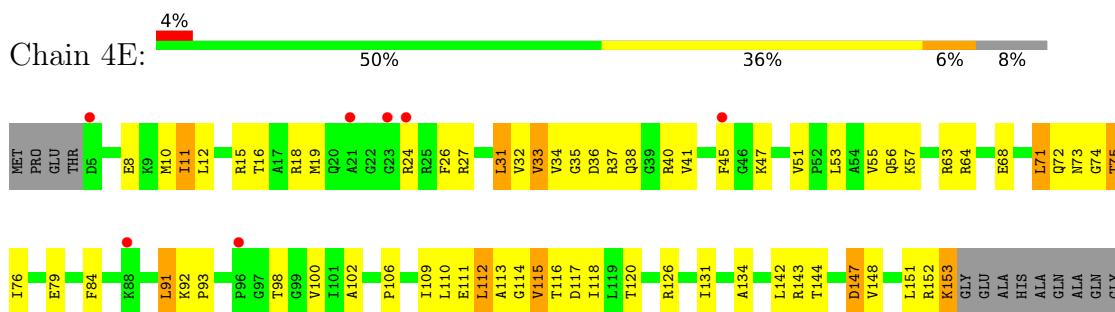


• Molecule 4: 30S ribosomal protein S4

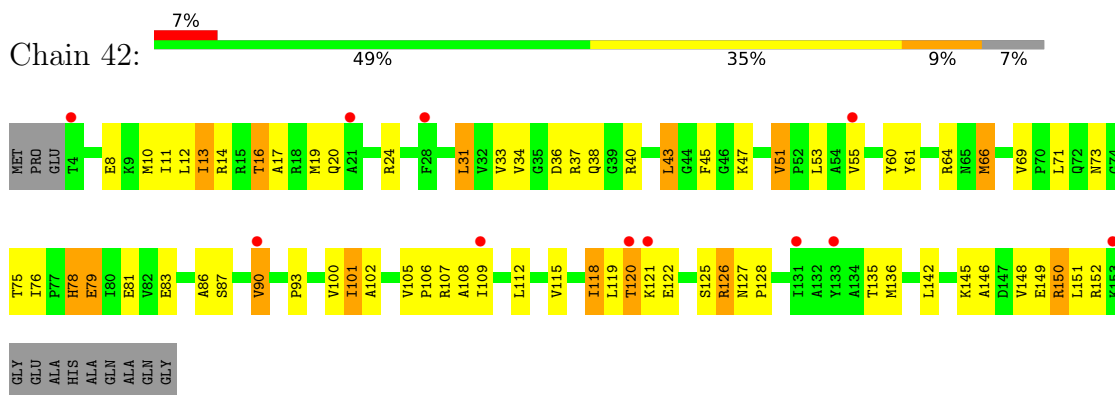




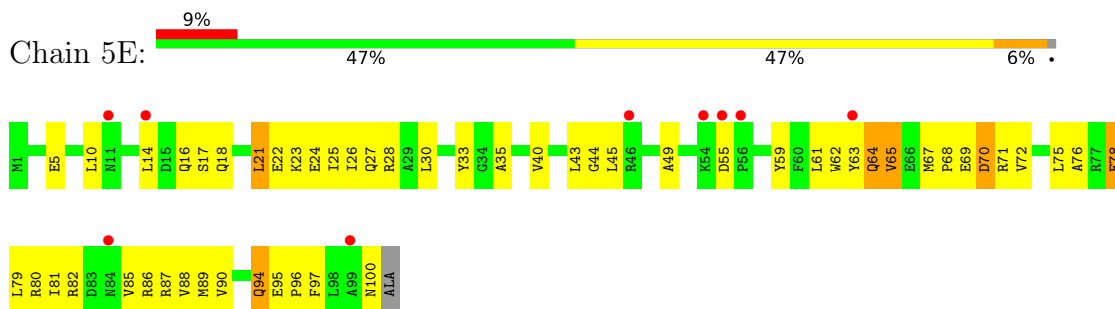
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

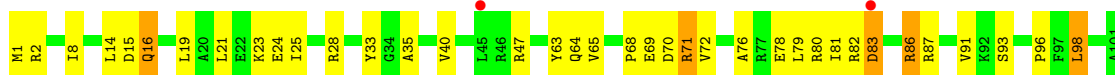


• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

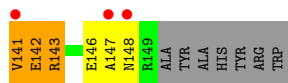




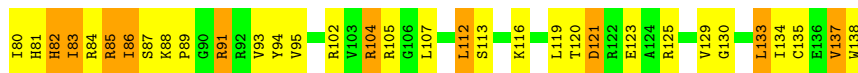
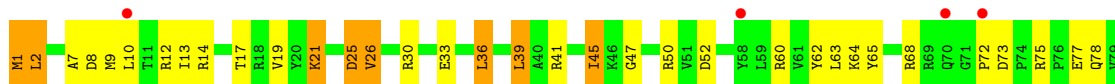
- Molecule 7: 30S ribosomal protein S7



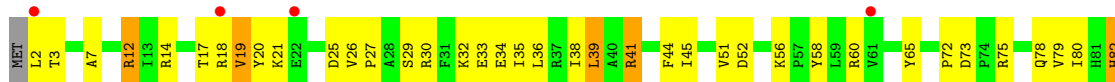
- Molecule 7: 30S ribosomal protein S7



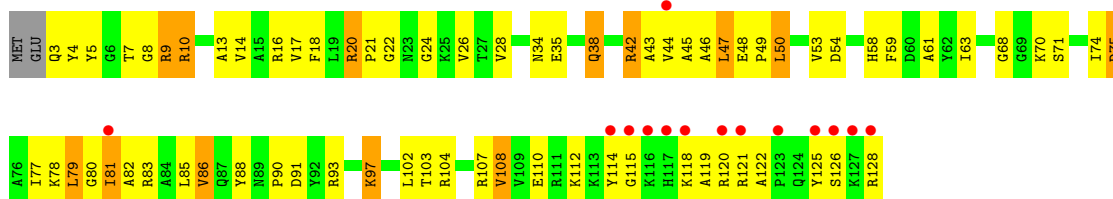
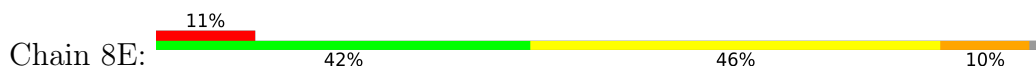
- Molecule 8: 30S ribosomal protein S8



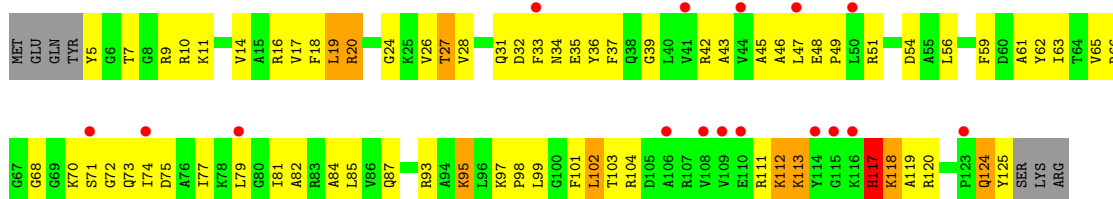
- Molecule 8: 30S ribosomal protein S8



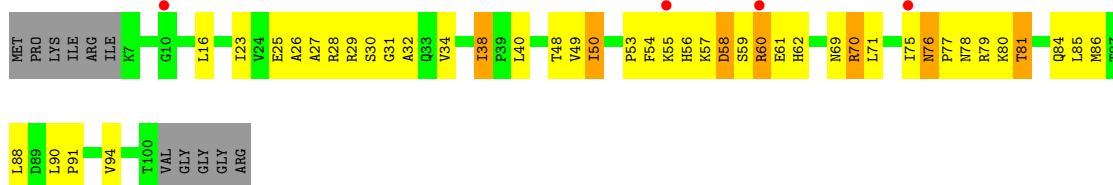
- Molecule 9: 30S ribosomal protein S9



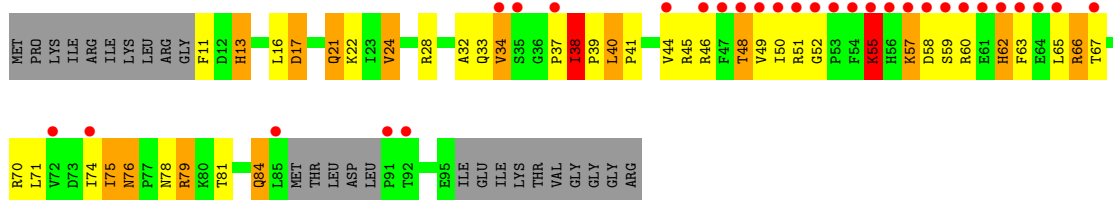
- Molecule 9: 30S ribosomal protein S9



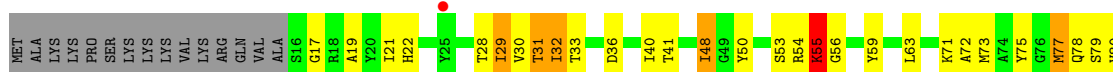
- Molecule 10: 30S ribosomal protein S10

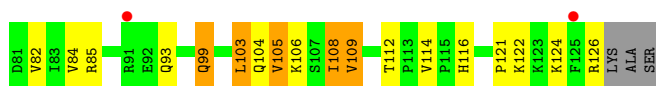


- Molecule 10: 30S ribosomal protein S10

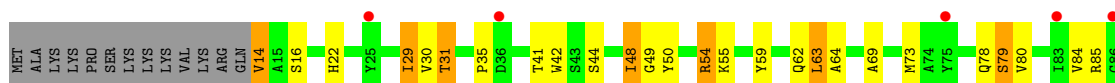


- Molecule 11: 30S ribosomal protein S11

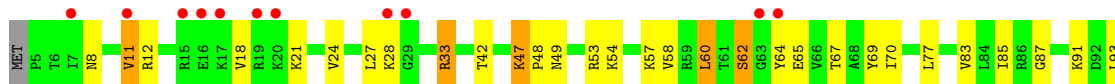




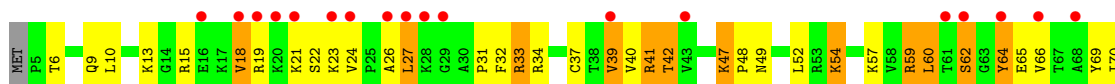
- Molecule 11: 30S ribosomal protein S11



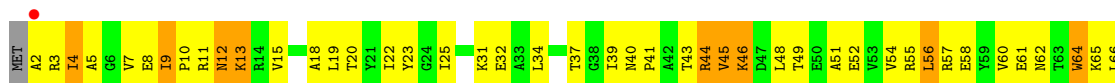
- Molecule 12: 30S ribosomal protein S12



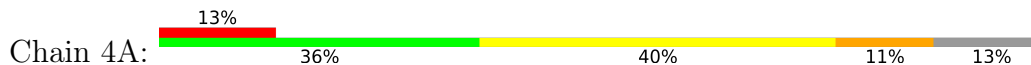
- Molecule 12: 30S ribosomal protein S12

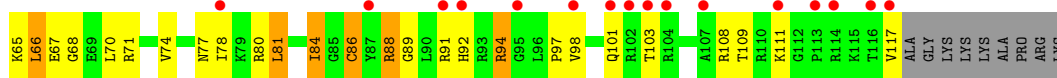
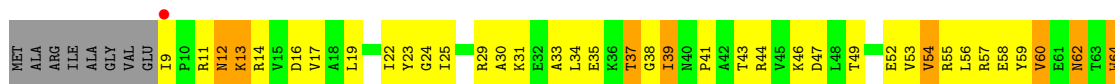


- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13

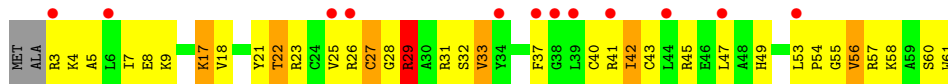




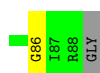
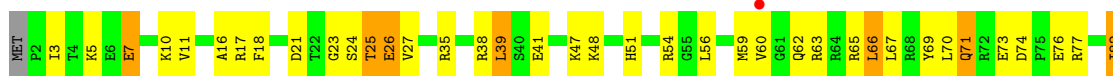
• Molecule 14: 30S ribosomal protein S14 type Z



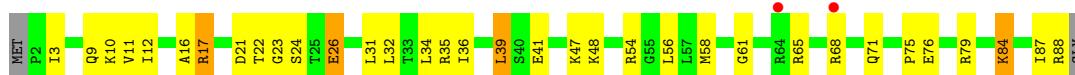
• Molecule 14: 30S ribosomal protein S14 type Z



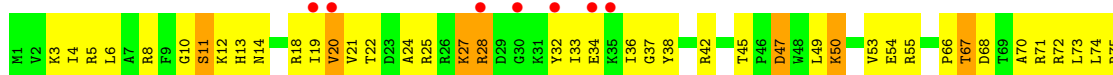
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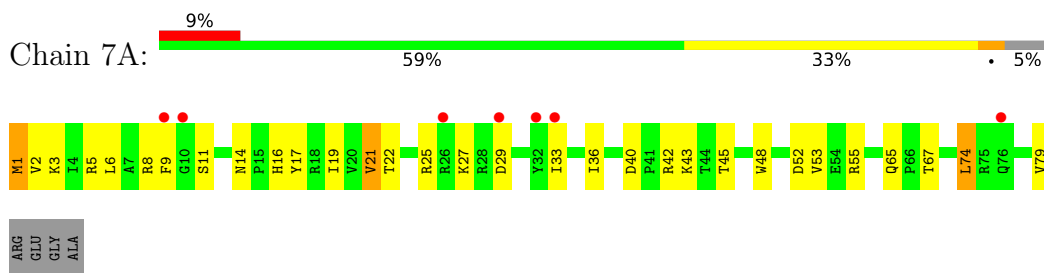
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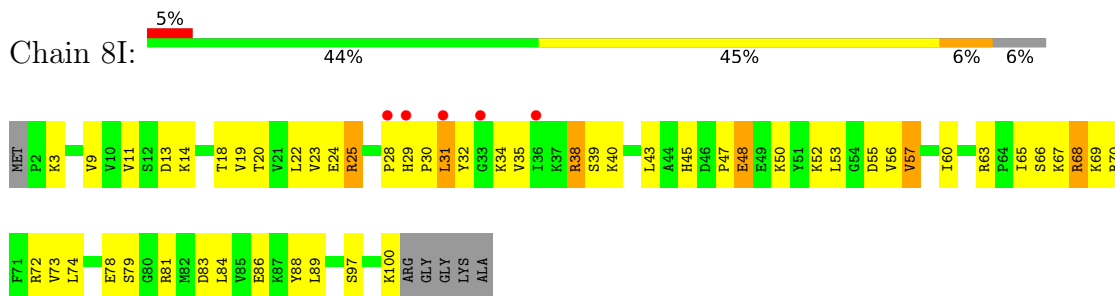
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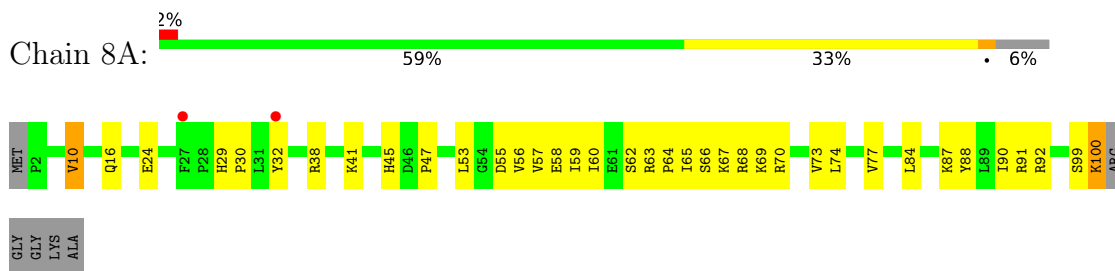
- Molecule 16: 30S ribosomal protein S16



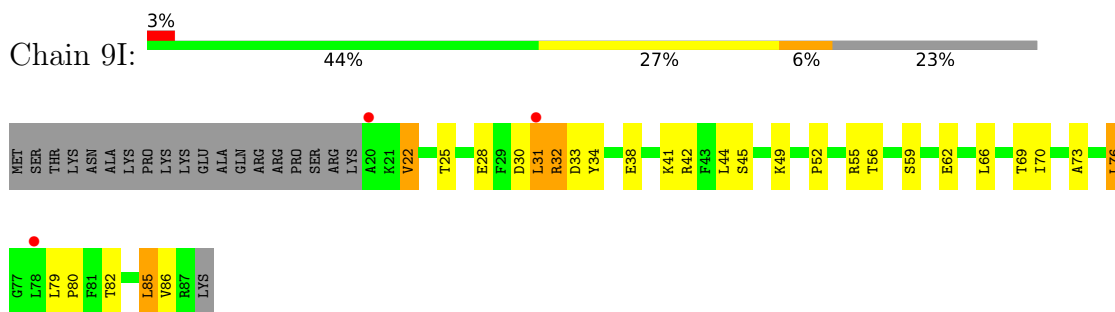
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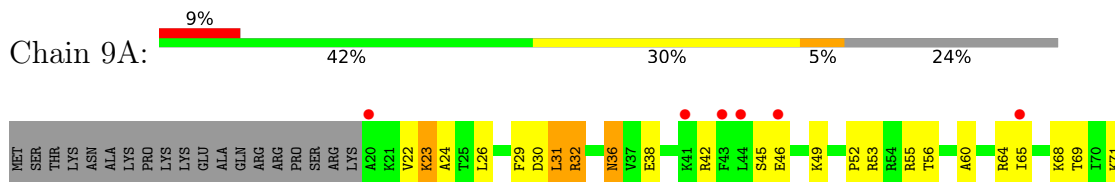
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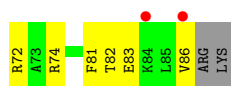


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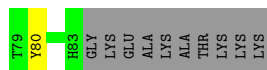
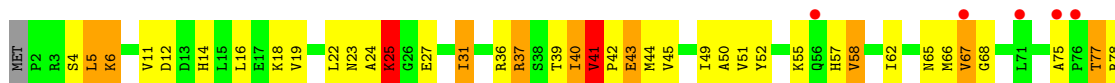


- Molecule 18: 30S ribosomal protein S18

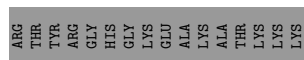
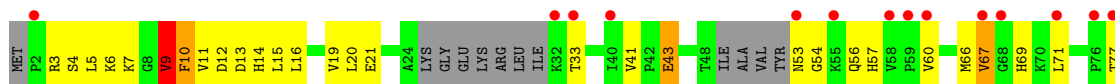
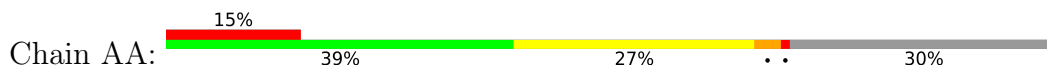




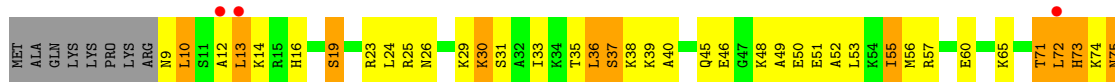
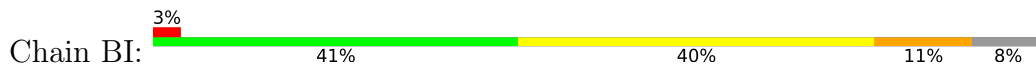
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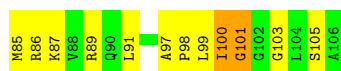
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20

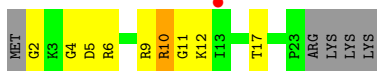


- Molecule 21: 30S ribosomal protein Thx





- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA<sup>Lys</sup>



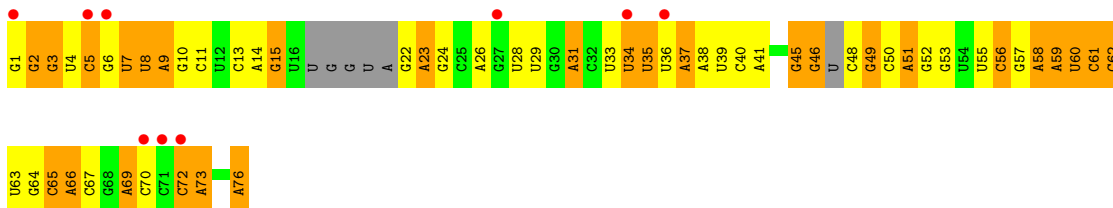
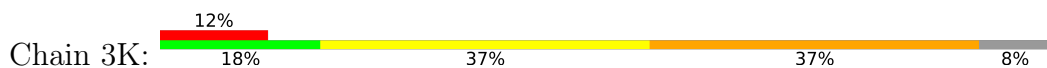
- Molecule 23: tRNA<sup>fMet</sup>



- Molecule 23: tRNA<sup>fMet</sup>

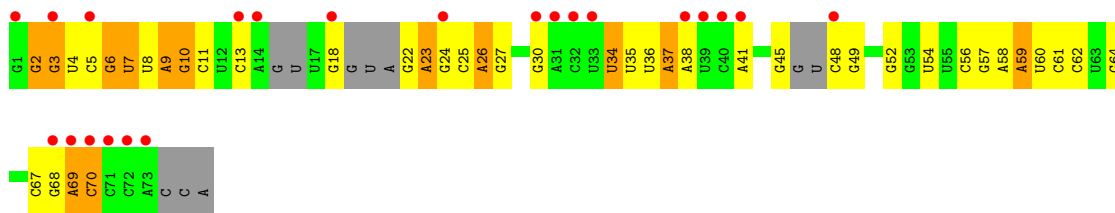


- Molecule 24: tRNA<sup>Lys</sup>

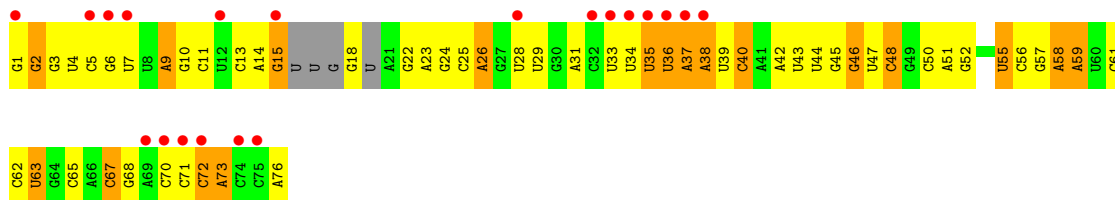
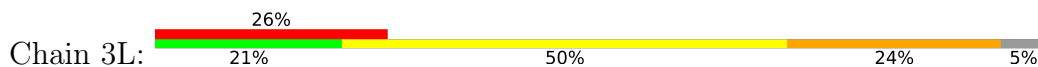


- Molecule 24: tRNA<sup>Lys</sup>

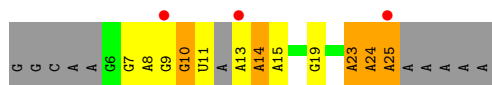




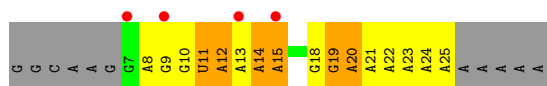
• Molecule 24: tRNA<sup>Lys</sup>



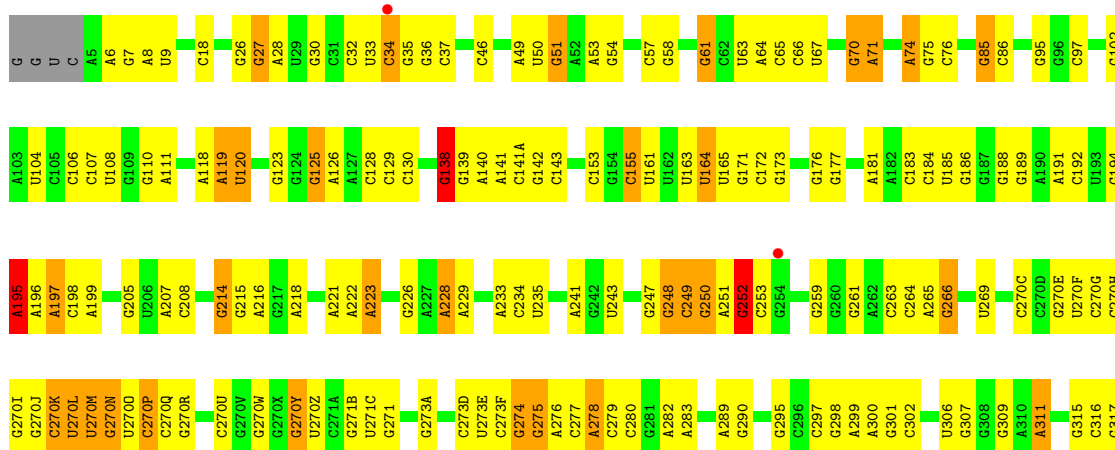
• Molecule 25: mRNA



• Molecule 25: mRNA

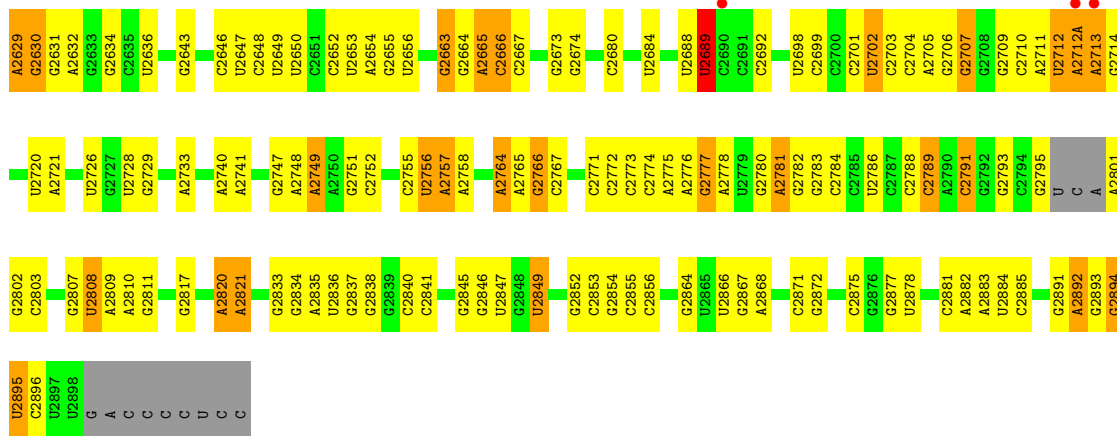


• Molecule 26: 23S ribosomal RNA

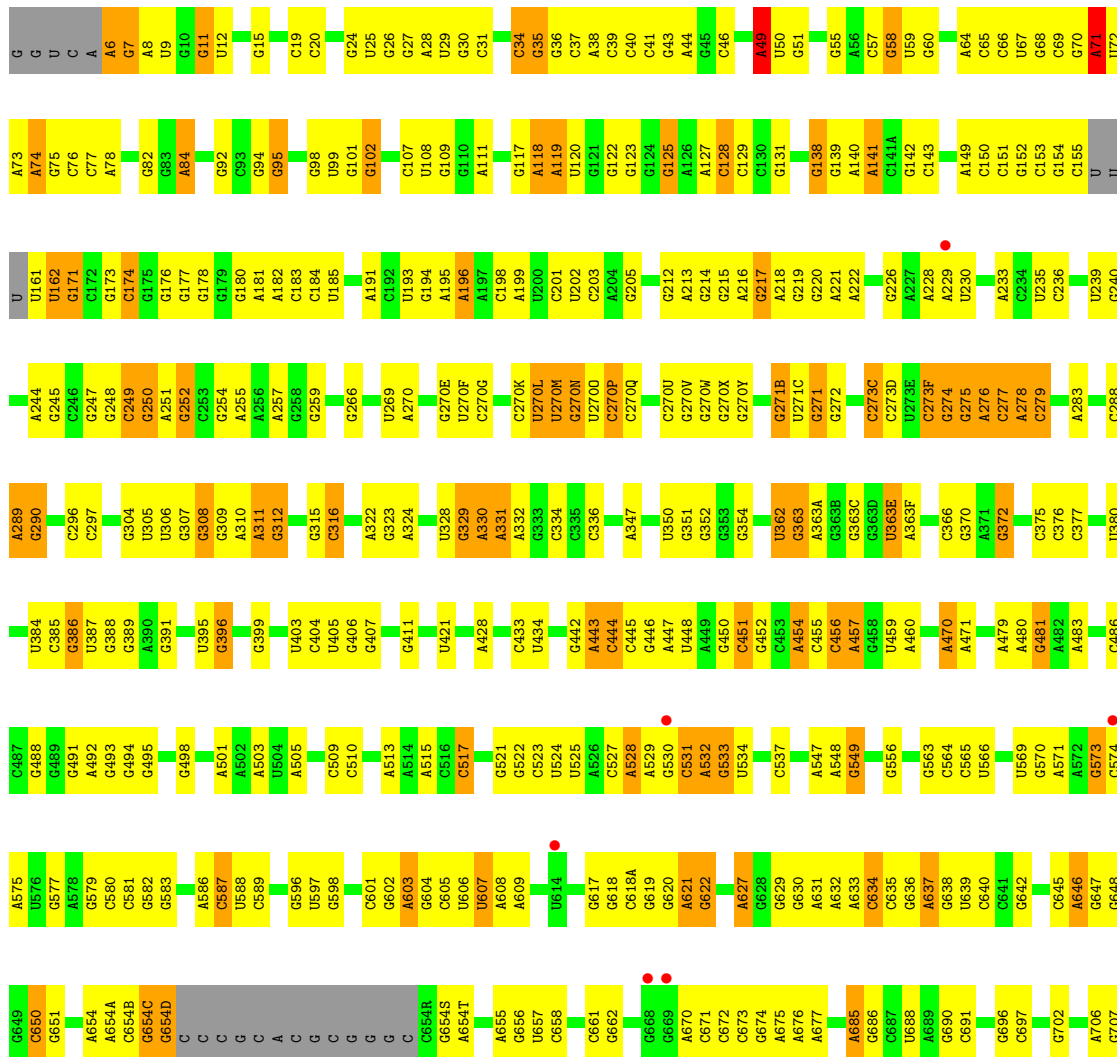


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● Molecule 26: 23S ribosomal RNA

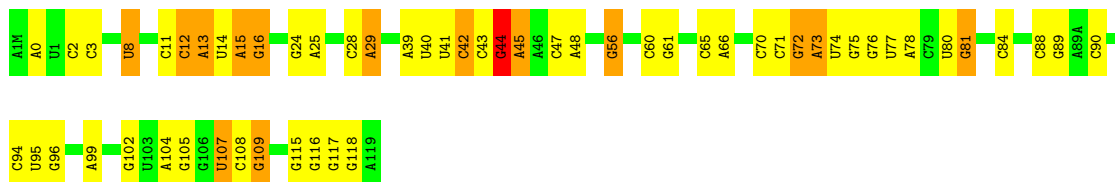




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G2908	U2686	C2525	C2525	A2437	A2366	A2298	G2229	C2145	G2068	G2002	C1908
U2909	U2687	U2526	U2526	A2438	A2367	G2299	C2229	C2146	G2069	C1909	C1909
C2910	C2688	U2527	U2527	C2440	G2370	G2299	U2232	C2147	A2071	C2006	A1912
G2911	C2689	C2528	C2528	C2441	G2371	G2299	U2232	C2148	U2074	C2007	A1912
U2912	C2690	G2529	G2529	C2442	G2372	G2299	U2233	C2148	U2074	C2008	A1913

- Molecule 27: 5S ribosomal RNA

Chain 16: 




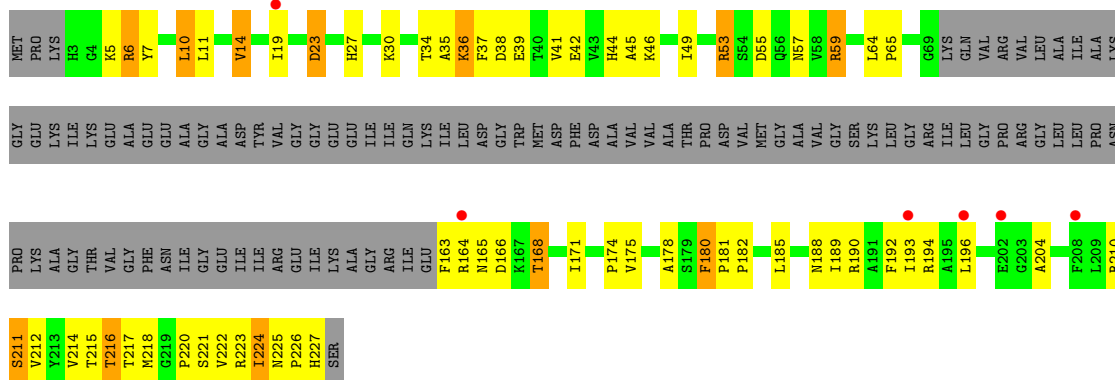
- Molecule 27: 5S ribosomal RNA

Chain 1J: 



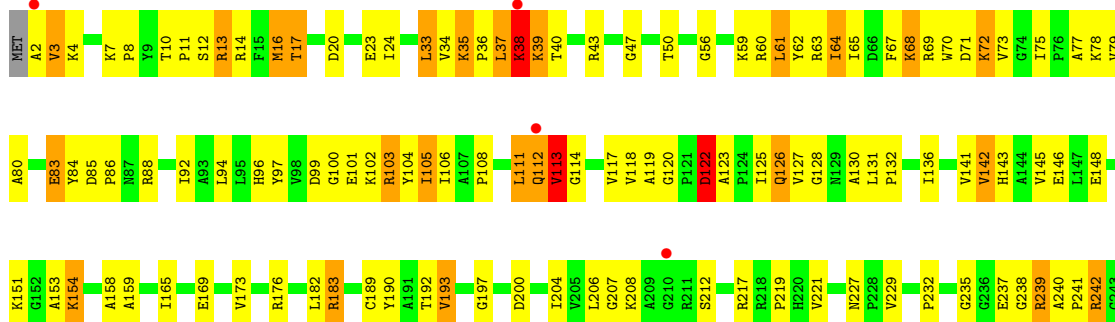
- Molecule 28: 50S ribosomal protein L1

Chain 71: 



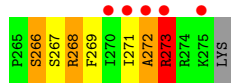
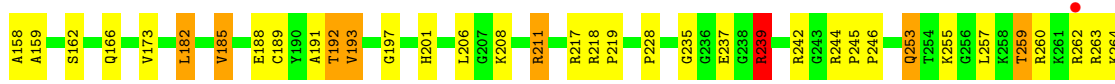
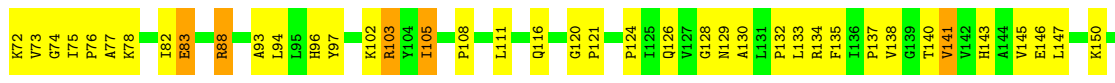
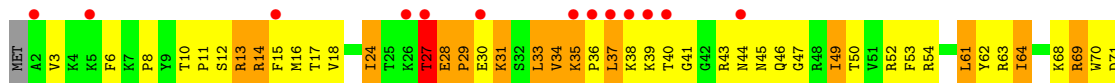
- Molecule 29: 50S ribosomal protein L2

Chain 11: 

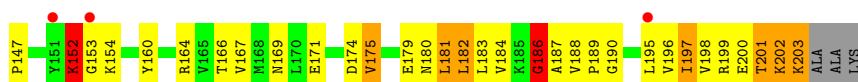
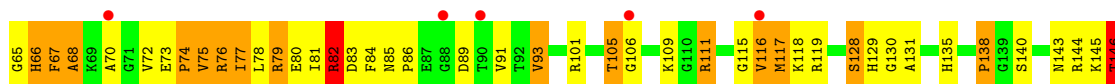
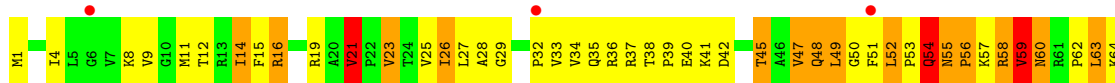




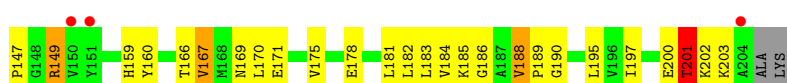
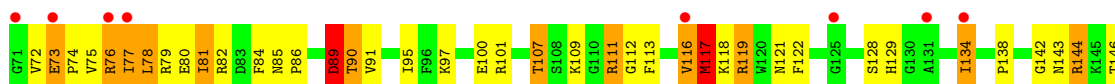
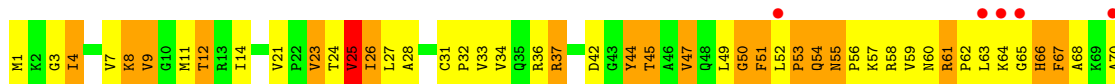
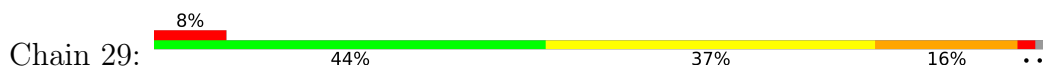
• Molecule 29: 50S ribosomal protein L2



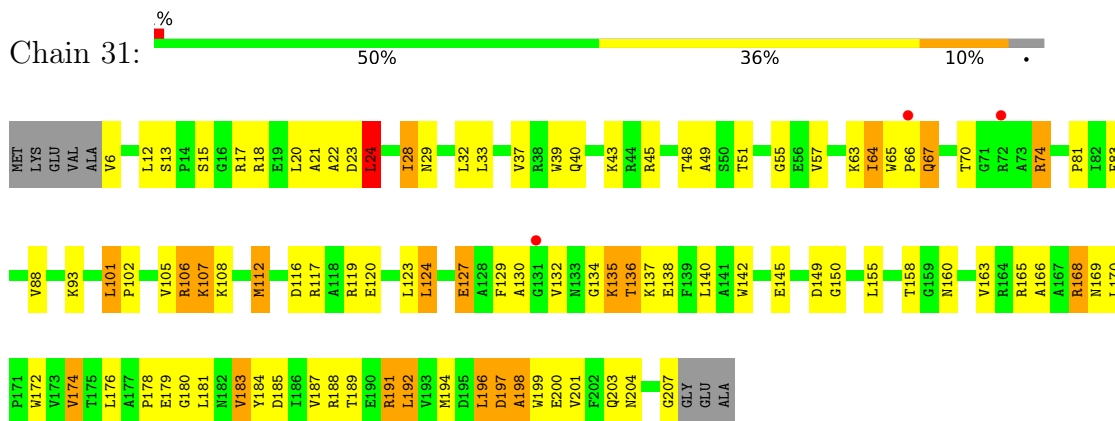
• Molecule 30: 50S ribosomal protein L3



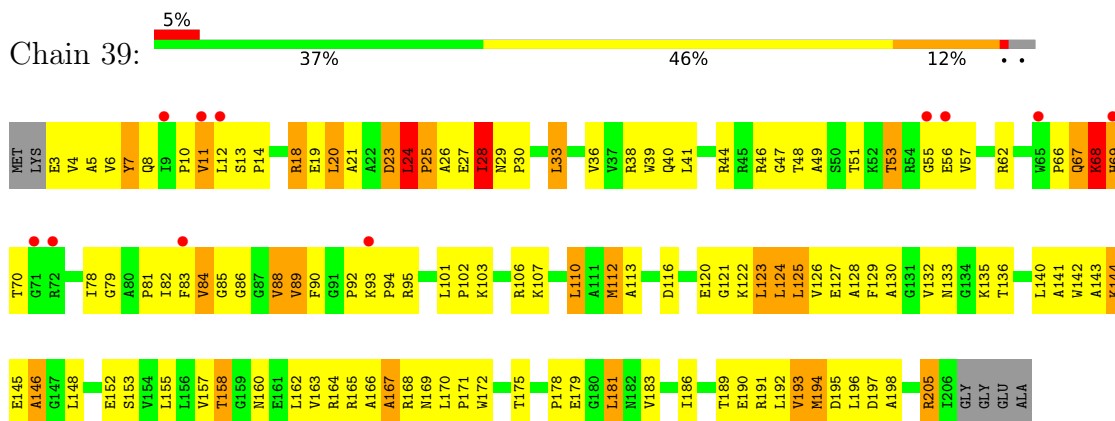
• Molecule 30: 50S ribosomal protein L3



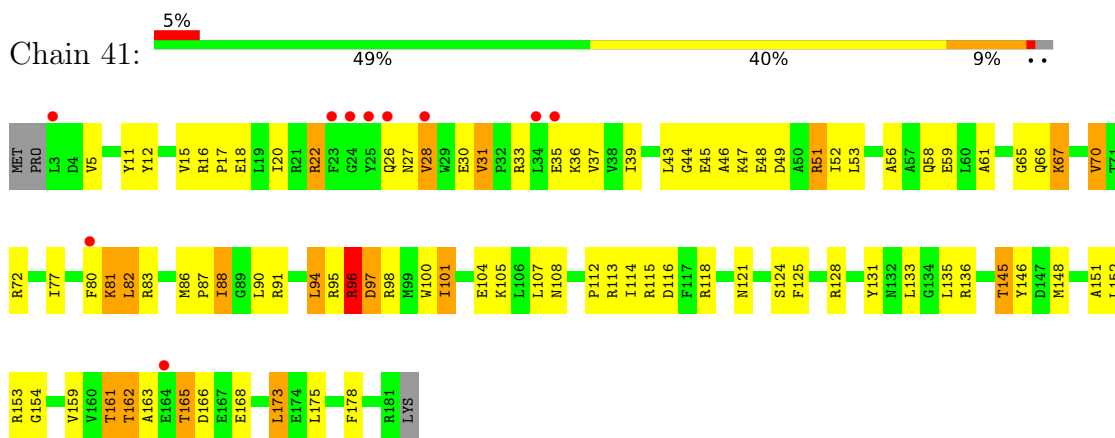
• Molecule 31: 50S ribosomal protein L4



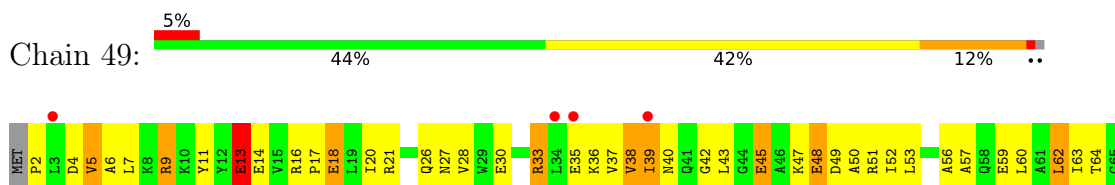
• Molecule 31: 50S ribosomal protein L4

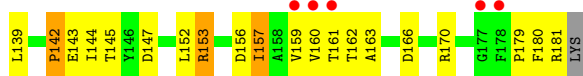
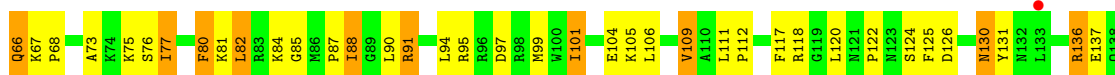


• Molecule 32: 50S ribosomal protein L5

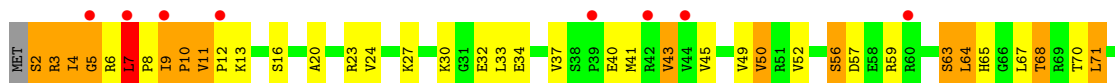


• Molecule 32: 50S ribosomal protein L5

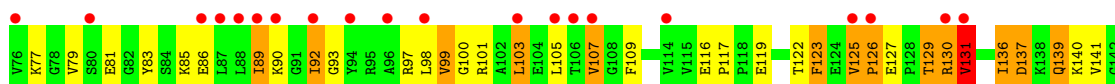
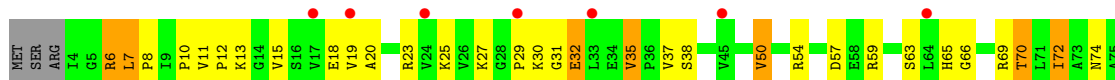




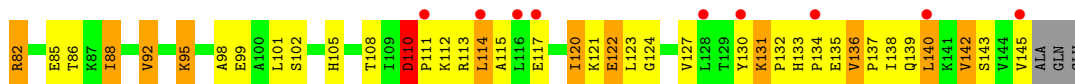
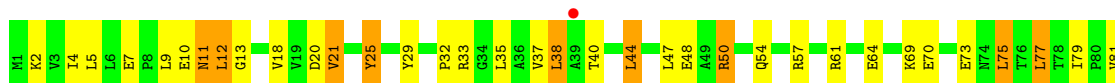
• Molecule 33: 50S ribosomal protein L6



• Molecule 33: 50S ribosomal protein L6

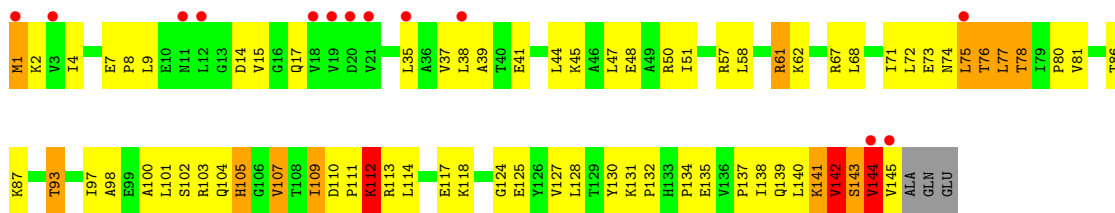


• Molecule 34: 50S ribosomal protein L9

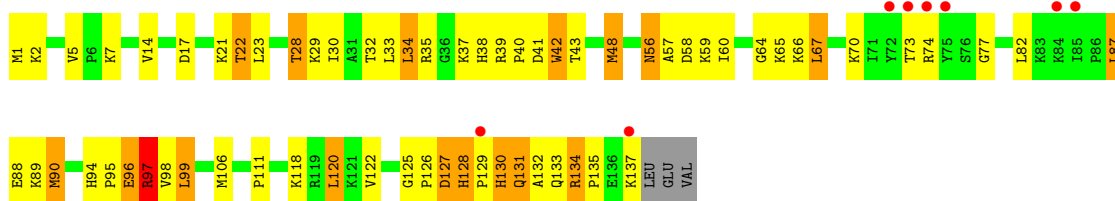


• Molecule 34: 50S ribosomal protein L9

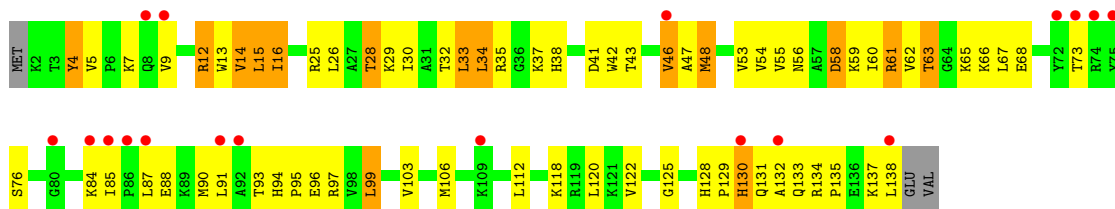




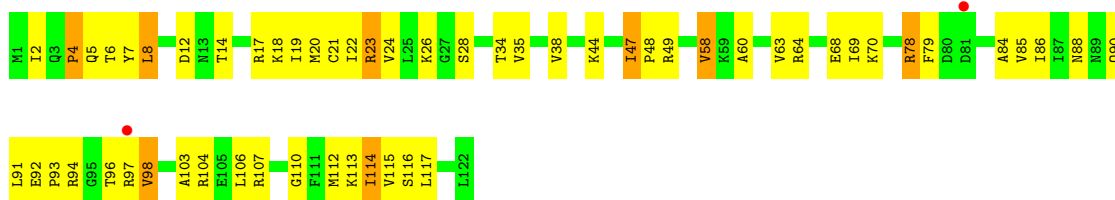
• Molecule 35: 50S ribosomal protein L13



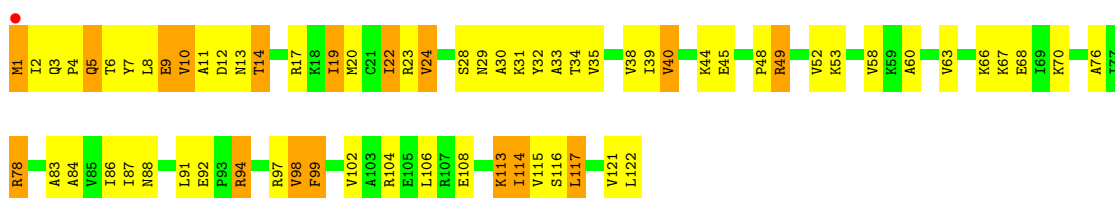
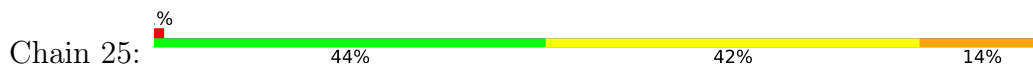
• Molecule 35: 50S ribosomal protein L13



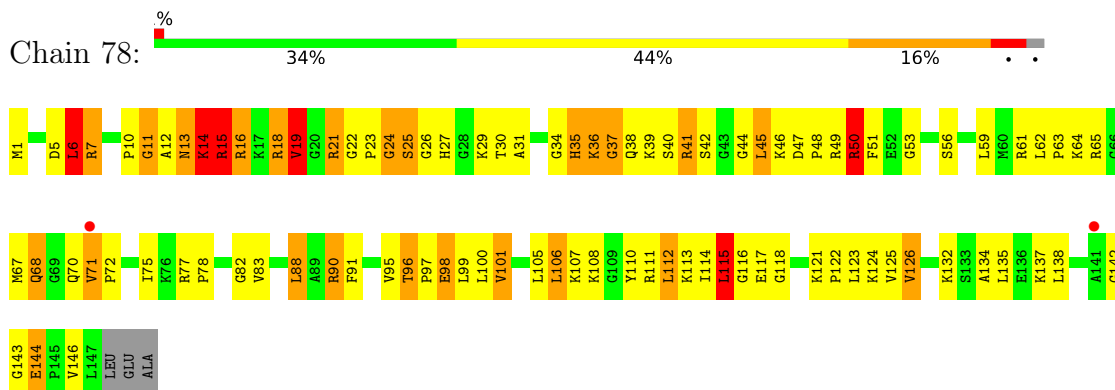
• Molecule 36: 50S ribosomal protein L14



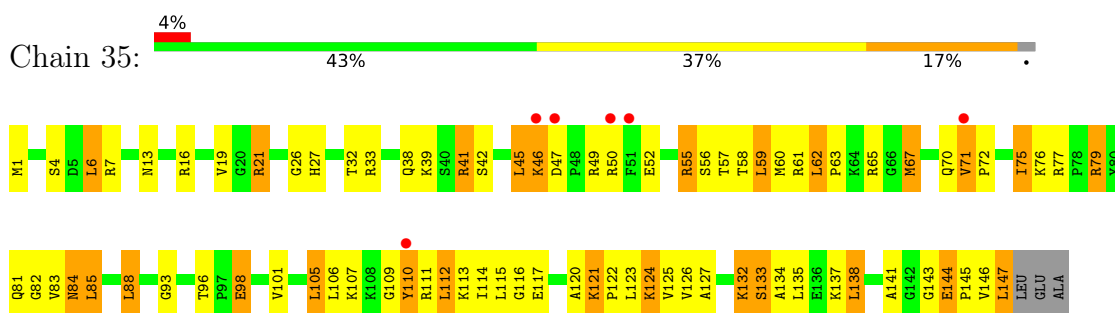
• Molecule 36: 50S ribosomal protein L14



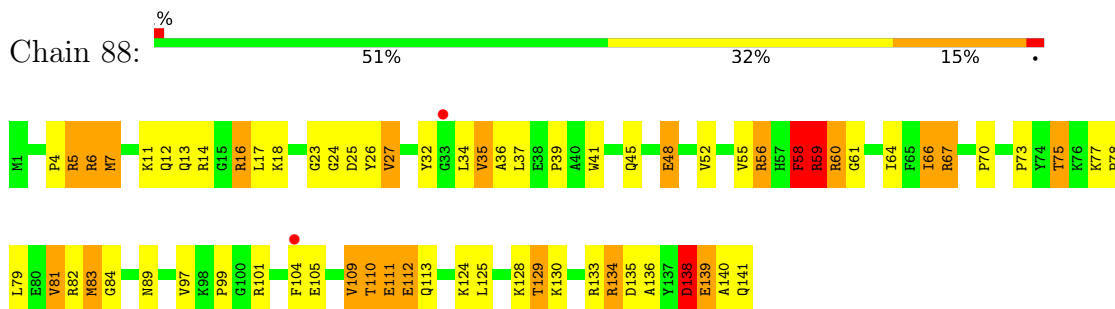
- Molecule 37: 50S ribosomal protein L15



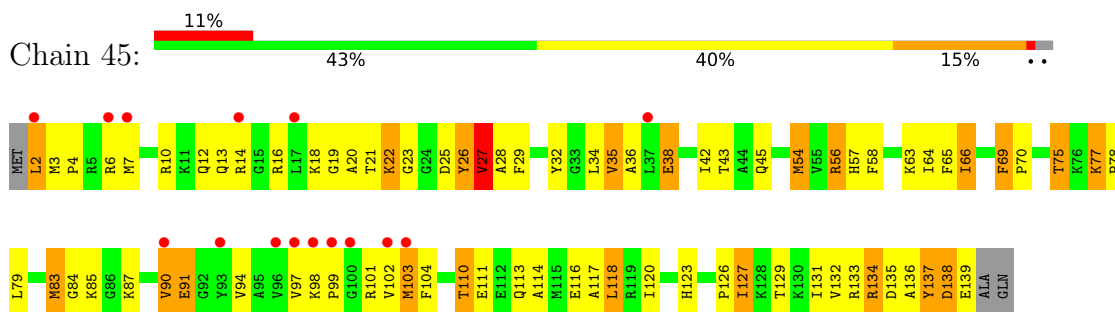
- Molecule 37: 50S ribosomal protein L15



- Molecule 38: 50S ribosomal protein L16

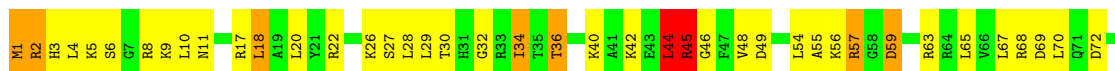


- Molecule 38: 50S ribosomal protein L16

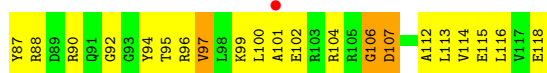


- Molecule 39: 50S ribosomal protein L17





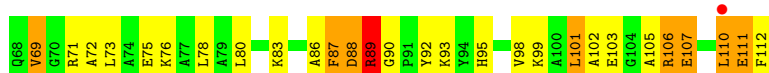
- Molecule 39: 50S ribosomal protein L17



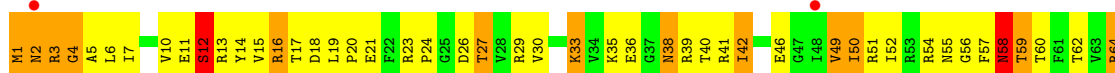
- Molecule 40: 50S ribosomal protein L18



- Molecule 40: 50S ribosomal protein L18

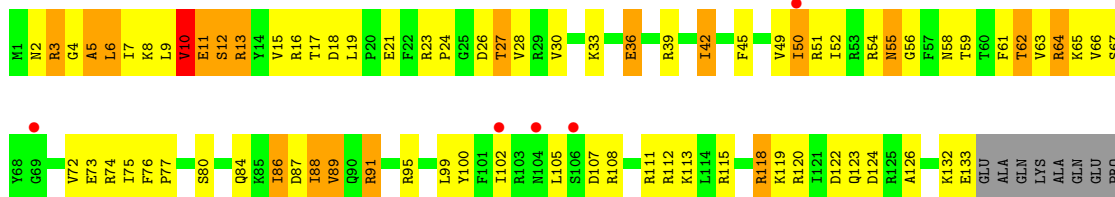


- Molecule 41: 50S ribosomal protein L19



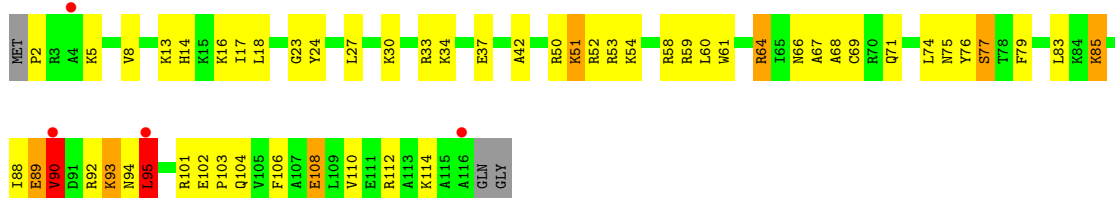
PRO  
LYS  
ALA  
SER  
GLN  
GLU

• Molecule 41: 50S ribosomal protein L19

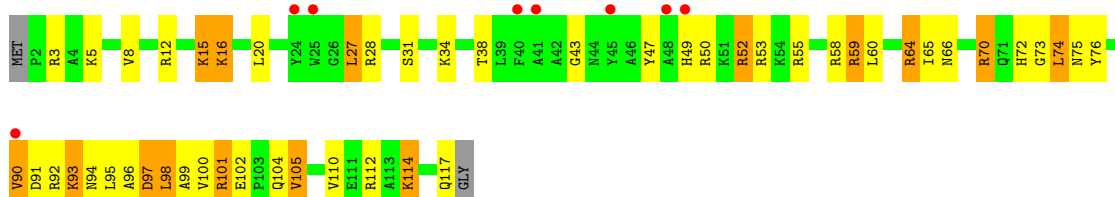


LYS  
ALA  
SER  
GLN  
GLU

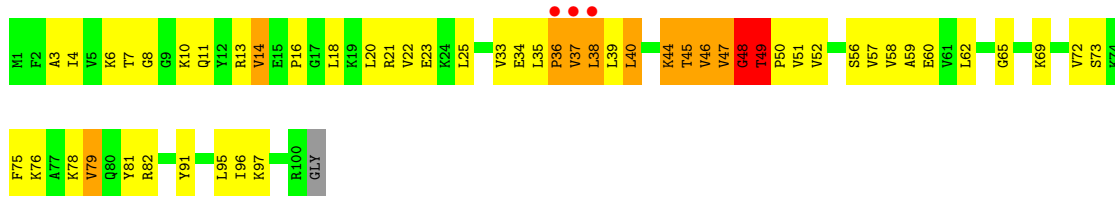
• Molecule 42: 50S ribosomal protein L20



• Molecule 42: 50S ribosomal protein L20

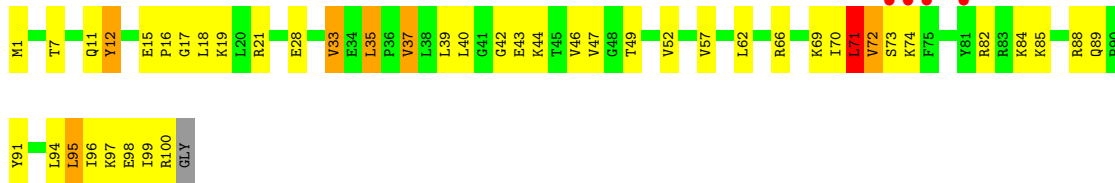


• Molecule 43: 50S ribosomal protein L21



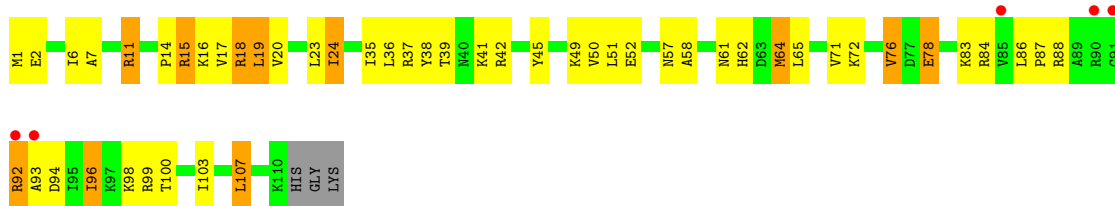
• Molecule 43: 50S ribosomal protein L21

Chain 95: 



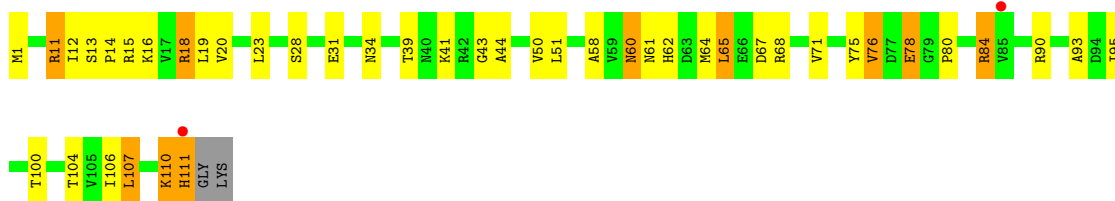
- Molecule 44: 50S ribosomal protein L22

Chain E8: 



- Molecule 44: 50S ribosomal protein L22

Chain A5: 



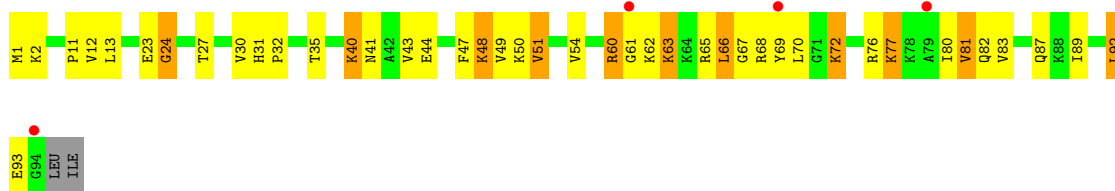
- Molecule 45: 50S ribosomal protein L23

Chain F8: 



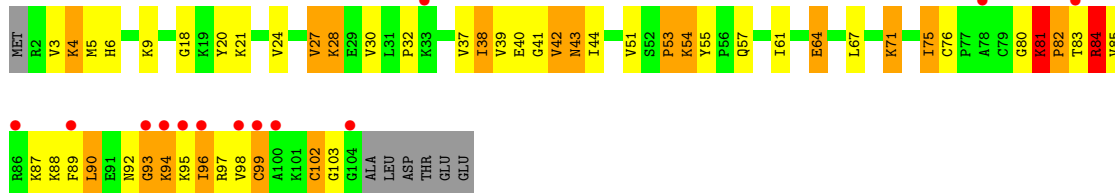
- Molecule 45: 50S ribosomal protein L23

Chain B5: 



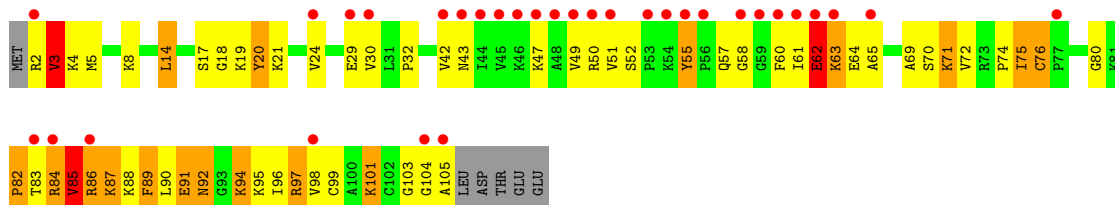
- Molecule 46: 50S ribosomal protein L24

Chain G8: 12% 46% 29% 16% 6%



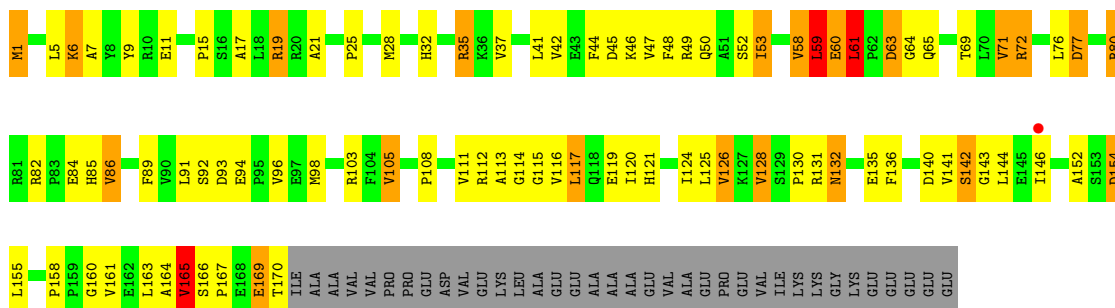
- Molecule 46: 50S ribosomal protein L24

Chain C5: 29% 40% 36% 15% 5%



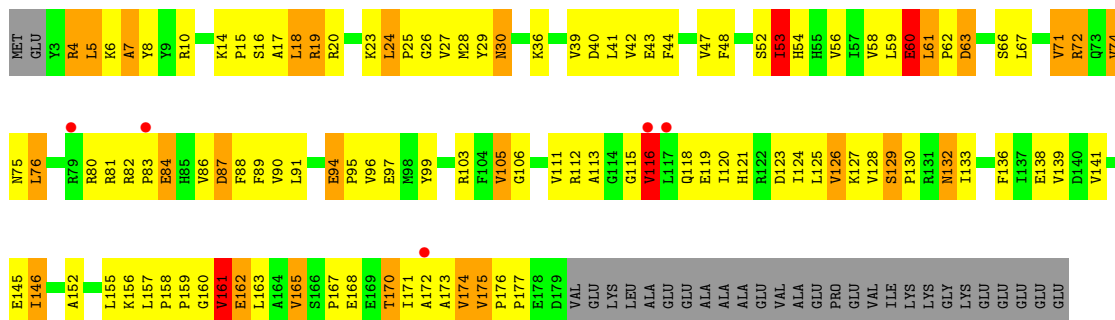
- Molecule 47: 50S ribosomal protein L25

Chain H8: 38% 33% 10% 17%

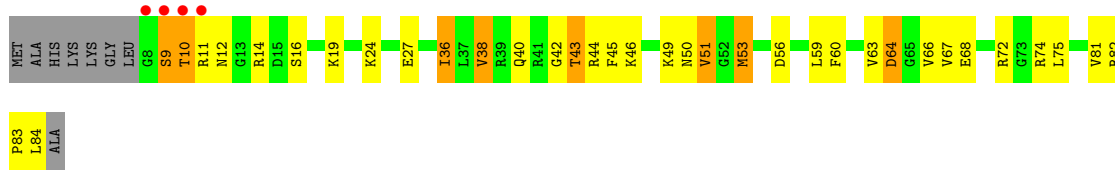


- Molecule 47: 50S ribosomal protein L25

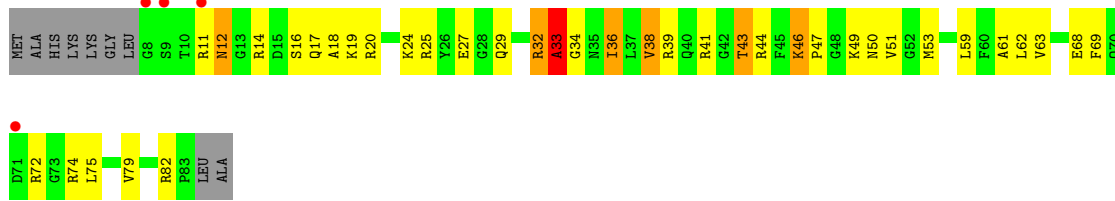
Chain D5: 2% 32% 40% 13% 14%



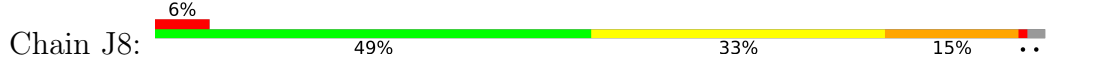
- Molecule 48: 50S ribosomal protein L27



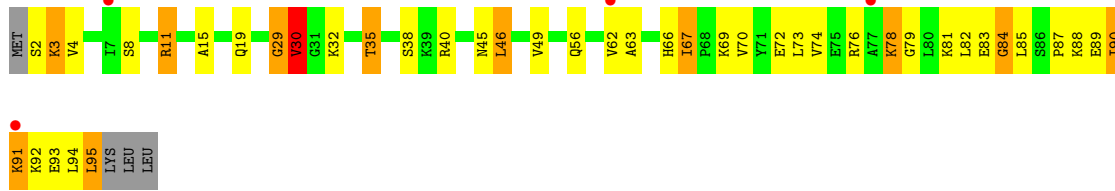
• Molecule 48: 50S ribosomal protein L27



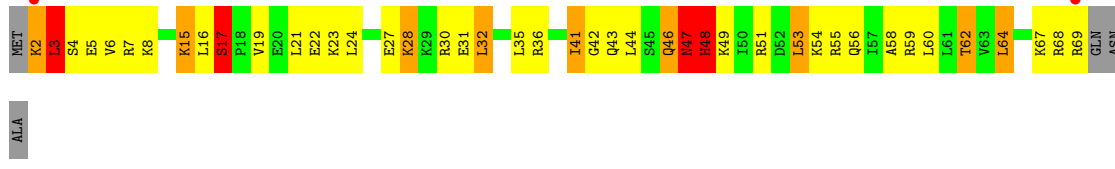
• Molecule 49: 50S ribosomal protein L28



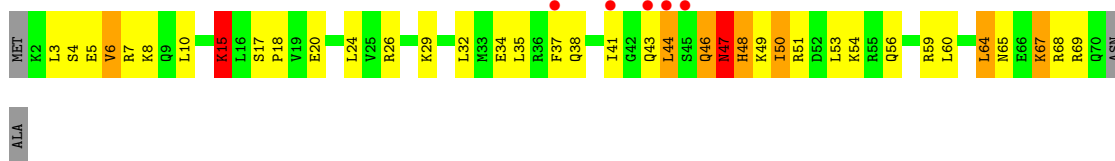
• Molecule 49: 50S ribosomal protein L28



• Molecule 50: 50S ribosomal protein L29



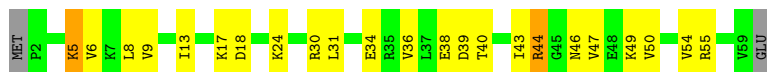
- Molecule 50: 50S ribosomal protein L29



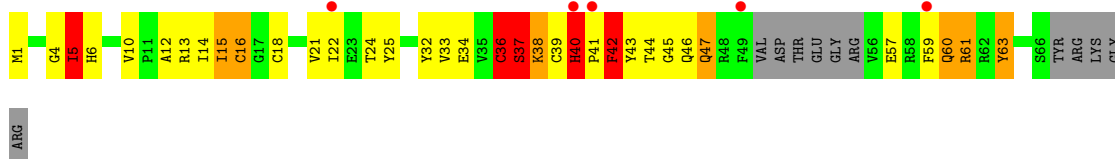
- Molecule 51: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L31



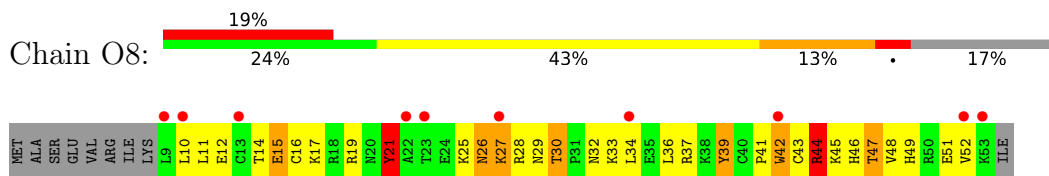
- Molecule 53: 50S ribosomal protein L32



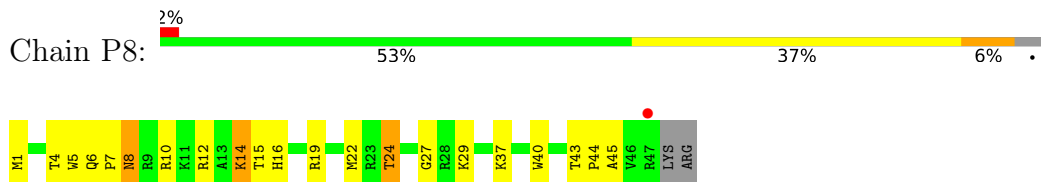
- Molecule 53: 50S ribosomal protein L32



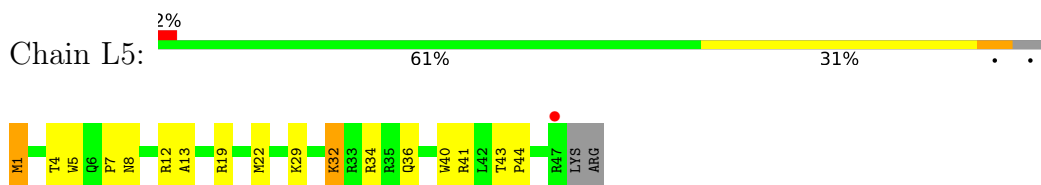
- Molecule 54: 50S ribosomal protein L33



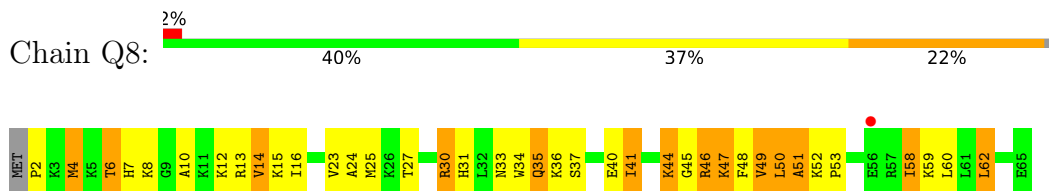
• Molecule 55: 50S ribosomal protein L34



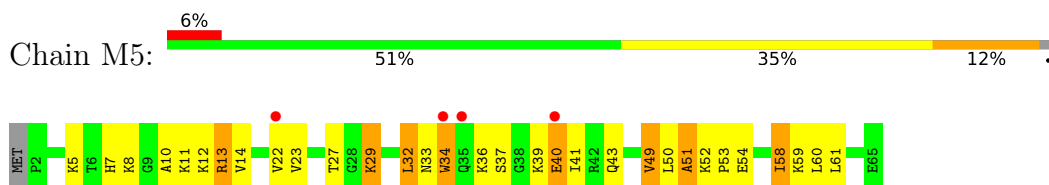
• Molecule 55: 50S ribosomal protein L34



• Molecule 56: 50S ribosomal protein L35



• Molecule 56: 50S ribosomal protein L35



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.30Å 448.80Å 620.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.08 – 2.99 147.08 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (147.08-2.99) 90.8 (147.08-2.99)	Depositor EDS
$R_{merge}$	0.34	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.92 (at 3.01Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.202 , 0.241 0.204 , 0.242	Depositor DCC
$R_{free}$ test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.3	Xtrriage
Anisotropy	0.342	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 70.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	297444	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SPE, OMC, 4SU, 5MU, PAR, ZN, T6A, PSU, SF4, 7MG, U8U, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	13	0.39	0/36068	0.65	8/56287 (0.0%)
1	1G	0.34	0/36282	0.58	2/56623 (0.0%)
2	12	0.34	0/1727	0.67	2/2326 (0.1%)
2	1E	0.36	0/1908	0.64	0/2573
3	22	0.35	1/1560 (0.1%)	0.54	0/2104
3	2E	0.42	1/1629 (0.1%)	0.62	1/2195 (0.0%)
4	32	0.38	1/1732 (0.1%)	0.66	0/2318
4	3E	0.40	1/1728 (0.1%)	0.64	0/2313
5	42	0.33	0/1156	0.57	0/1557
5	4E	0.39	0/1158	0.64	0/1559
6	52	0.43	0/855	0.59	0/1154
6	5E	0.40	0/850	0.58	0/1147
7	62	0.34	0/1122	0.68	3/1500 (0.2%)
7	6E	0.34	0/1259	0.52	0/1686
8	72	0.30	0/1127	0.58	2/1517 (0.1%)
8	7E	0.34	0/1135	0.60	0/1527
9	82	0.30	0/971	0.63	1/1304 (0.1%)
9	8E	0.33	0/1019	0.63	0/1367
10	1A	0.84	2/658 (0.3%)	0.60	0/885
10	1I	0.36	0/762	0.63	0/1027
11	2A	0.33	0/850	0.62	0/1150
11	2I	0.43	0/838	0.72	0/1133
12	3A	0.40	0/963	0.68	0/1290
12	3I	0.56	0/972	0.88	0/1301
13	4A	0.31	0/889	0.62	0/1192
13	4I	0.44	0/943	0.71	0/1265
14	5A	0.30	0/495	0.74	2/657 (0.3%)
14	5I	0.41	0/495	0.78	2/657 (0.3%)
15	6A	0.34	0/740	0.56	0/987
15	6I	0.41	0/740	0.61	0/987
16	7A	0.37	0/721	0.70	0/970
16	7I	0.39	0/716	0.71	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.35	0/836	0.59	0/1117
17	8I	0.43	0/836	0.69	0/1117
18	9A	0.41	0/549	0.65	0/732
18	9I	0.38	0/554	0.66	0/739
19	AA	0.38	0/520	0.72	2/700 (0.3%)
19	AI	0.37	0/676	0.86	3/910 (0.3%)
20	BA	0.32	0/764	0.83	7/1007 (0.7%)
20	BI	0.44	1/748 (0.1%)	0.62	0/986
21	1B	0.35	0/192	0.68	0/252
21	1F	0.36	0/203	0.63	0/266
22	1K	0.32	0/1589	0.50	0/2464
23	2K	0.44	1/1721 (0.1%)	0.66	0/2682
23	2L	0.39	1/1721 (0.1%)	0.58	0/2682
24	1L	0.24	0/1560	0.41	0/2418
24	3K	0.32	0/1654	0.53	0/2570
24	3L	0.31	0/1705	0.49	0/2650
25	4K	0.41	0/473	0.56	0/735
25	4L	0.38	0/473	0.66	0/737
26	14	0.46	0/68181	0.72	19/106432 (0.0%)
26	1H	0.55	1/68997 (0.0%)	0.79	29/107696 (0.0%)
27	16	0.45	0/2928	0.76	1/4568 (0.0%)
27	1J	0.39	0/2928	0.64	0/4568
28	7I	0.24	0/1049	0.52	0/1417
29	11	0.64	0/2170	1.01	11/2926 (0.4%)
29	19	0.61	0/2175	0.95	3/2933 (0.1%)
30	21	0.58	0/1579	1.14	14/2131 (0.7%)
30	29	0.49	0/1596	0.88	5/2153 (0.2%)
31	31	0.57	0/1620	0.87	0/2194
31	39	0.50	0/1637	0.96	4/2218 (0.2%)
32	41	0.42	0/1481	0.70	0/1994
32	49	0.33	0/1483	0.67	1/1997 (0.1%)
33	51	0.52	0/1354	1.04	13/1833 (0.7%)
33	59	0.34	0/1320	0.75	1/1787 (0.1%)
34	61	0.40	0/1146	0.75	4/1551 (0.3%)
34	69	0.38	0/1146	0.78	3/1551 (0.2%)
35	15	0.36	0/1123	0.65	0/1515
35	58	0.48	0/1123	0.82	5/1514 (0.3%)
36	25	0.41	0/942	0.74	0/1269
36	68	0.50	0/942	0.82	2/1269 (0.2%)
37	35	0.51	0/1139	0.88	0/1514
37	78	0.62	0/1139	1.17	9/1514 (0.6%)
38	45	0.60	3/1120 (0.3%)	0.93	0/1498
38	88	0.68	1/1138 (0.1%)	0.98	1/1523 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	55	0.49	0/981	0.80	0/1312
39	98	0.49	0/981	0.87	0/1312
40	65	0.43	0/886	0.88	2/1180 (0.2%)
40	A8	0.52	0/891	0.85	0/1187
41	75	0.47	0/1123	0.81	3/1500 (0.2%)
41	B8	0.57	0/1133	0.94	4/1514 (0.3%)
42	85	0.46	0/977	0.75	1/1301 (0.1%)
42	C8	0.55	0/968	0.83	2/1289 (0.2%)
43	95	0.43	0/781	0.79	0/1048
43	D8	0.44	0/785	0.78	0/1052
44	A5	0.54	0/897	0.78	0/1204
44	E8	0.55	0/886	0.79	0/1189
45	B5	0.52	0/749	0.80	2/1007 (0.2%)
45	F8	0.57	0/764	0.85	0/1025
46	C5	0.49	0/807	0.91	1/1076 (0.1%)
46	G8	0.65	0/796	1.15	7/1062 (0.7%)
47	D5	0.46	1/1443 (0.1%)	0.66	1/1960 (0.1%)
47	H8	0.45	1/1395 (0.1%)	0.80	1/1890 (0.1%)
48	E5	0.49	0/611	0.86	0/814
48	I8	0.66	0/619	1.02	2/825 (0.2%)
49	F5	0.49	0/744	1.00	5/989 (0.5%)
49	J8	0.62	0/754	0.97	2/1003 (0.2%)
50	G5	0.49	0/578	0.87	1/766 (0.1%)
50	K8	0.66	0/577	1.11	3/763 (0.4%)
51	H5	0.41	0/464	0.66	0/623
51	L8	0.49	0/464	0.73	0/623
52	M8	0.47	0/485	1.15	5/652 (0.8%)
53	J5	0.52	0/448	0.79	0/606
53	N8	0.56	0/381	0.86	0/516
54	O8	0.58	0/396	1.07	2/529 (0.4%)
55	L5	0.57	0/409	0.86	0/540
55	P8	0.74	0/409	0.95	0/540
56	M5	0.63	0/524	1.01	2/691 (0.3%)
56	Q8	0.71	0/524	1.19	3/691 (0.4%)
All	All	0.46	16/317928 (0.0%)	0.73	209/476129 (0.0%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	2
9	82	0	1
9	8E	0	2
10	1A	0	1
11	2A	0	1
12	3A	0	1
12	3I	0	2
13	4A	0	1
13	4I	0	1
14	5A	0	1
19	AA	0	2
19	AI	0	1
20	BA	0	2
29	11	0	5
29	19	0	3
30	21	0	8
30	29	0	5
31	39	0	7
32	41	0	1
32	49	0	2
33	51	0	5
33	59	0	1
34	61	0	3
34	69	0	4
35	58	0	1
37	35	0	2
37	78	0	6
38	45	0	2
38	88	0	4
39	55	0	1
39	98	0	2
40	65	0	1
40	A8	0	2
41	75	0	3
41	B8	0	3
42	85	0	4
42	C8	0	2
43	D8	0	3
44	A5	0	1
45	B5	0	2
46	C5	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	G8	0	5
47	D5	0	3
47	H8	0	6
48	E5	0	2
48	I8	0	1
49	F5	0	1
49	J8	0	1
50	G5	0	2
50	K8	0	2
52	M8	0	3
54	O8	0	1
55	P8	0	1
56	M5	0	2
56	Q8	0	3
All	All	0	145

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1A	38	ILE	C-N	15.98	1.71	1.33
47	D5	94	GLU	C-N	11.91	1.61	1.33
10	1A	76	ASN	C-N	11.67	1.61	1.33
3	22	173	VAL	C-N	9.13	1.55	1.33
20	BI	97	ALA	C-N	7.53	1.51	1.33

The worst 5 of 209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	21	152	LYS	CA-C-N	-11.16	102.73	122.83
30	21	152	LYS	C-N-CA	-11.16	102.73	122.83
37	78	15	ARG	CA-C-N	10.09	138.50	121.86
37	78	15	ARG	C-N-CA	10.09	138.50	121.86
52	M8	40	HIS	CA-C-N	9.96	132.29	119.84

There are no chirality outliers.

5 of 145 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	234	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	1E	236	TYR	Peptide
9	8E	4	TYR	Peptide

## 5.2 Too-close contacts [i](#)

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	32223	0	16267	696	0
1	1G	32414	0	16360	759	0
2	12	1696	0	1730	90	0
2	1E	1874	0	1926	97	0
3	22	1537	0	1603	85	0
3	2E	1605	0	1668	55	0
4	32	1702	0	1765	95	0
4	3E	1698	0	1759	85	0
5	42	1141	0	1199	43	0
5	4E	1142	0	1204	41	0
6	52	842	0	857	19	0
6	5E	837	0	852	36	0
7	62	1110	0	1163	54	0
7	6E	1242	0	1286	50	0
8	72	1107	0	1165	50	0
8	7E	1115	0	1177	46	0
9	82	953	0	983	65	0
9	8E	1000	0	1031	63	0
10	1A	646	0	662	46	0
10	1I	749	0	767	42	0
11	2A	835	0	847	26	0
11	2I	823	0	833	31	0
12	3A	947	0	1033	45	0
12	3I	956	0	1046	35	0
13	4A	879	0	935	46	0
13	4I	933	0	992	56	0
14	5A	486	0	525	38	0
14	5I	486	0	524	30	0
15	6A	729	0	768	27	0
15	6I	729	0	768	23	0
16	7A	705	0	725	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	7I	700	0	720	47	0
17	8A	823	0	891	23	0
17	8I	823	0	891	34	0
18	9A	544	0	605	19	0
18	9I	549	0	607	23	0
19	AA	510	0	507	22	0
19	AI	661	0	683	44	0
20	BA	762	0	861	44	0
20	BI	746	0	843	46	0
21	1B	188	0	195	9	0
21	1F	199	0	208	10	0
22	1K	1542	0	790	25	0
23	2K	1646	0	845	18	0
23	2L	1646	0	845	25	0
24	1L	1401	0	713	22	0
24	3K	1483	0	756	50	0
24	3L	1528	0	778	42	0
25	4K	420	0	209	7	0
25	4L	419	0	208	17	0
26	14	60877	0	30690	1175	0
26	1H	61609	0	31058	1201	0
27	16	2617	0	1328	50	0
27	1J	2617	0	1328	77	0
28	71	1027	0	1043	57	0
29	11	2120	0	2197	102	0
29	19	2125	0	2199	111	0
30	21	1546	0	1602	92	0
30	29	1563	0	1629	98	0
31	31	1585	0	1632	70	0
31	39	1602	0	1649	96	0
32	41	1457	0	1514	68	0
32	49	1459	0	1507	67	0
33	51	1328	0	1396	63	0
33	59	1295	0	1366	58	0
34	61	1131	0	1218	39	0
34	69	1131	0	1218	51	0
35	15	1096	0	1168	48	0
35	58	1096	0	1169	49	0
36	25	932	0	996	49	0
36	68	932	0	996	43	0
37	35	1122	0	1206	79	0
37	78	1122	0	1206	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	45	1099	0	1154	76	0
38	88	1117	0	1168	60	0
39	55	967	0	1033	43	0
39	98	967	0	1033	48	0
40	65	876	0	938	64	0
40	A8	881	0	943	55	0
41	75	1109	0	1170	63	0
41	B8	1119	0	1177	73	0
42	85	959	0	1019	42	0
42	C8	950	0	1011	62	0
43	95	770	0	838	32	0
43	D8	774	0	849	42	0
44	A5	886	0	948	25	0
44	E8	876	0	941	33	0
45	B5	735	0	785	31	0
45	F8	750	0	814	20	0
46	C5	794	0	885	55	0
46	G8	783	0	869	48	0
47	D5	1411	0	1436	82	0
47	H8	1365	0	1391	61	0
48	E5	603	0	620	35	0
48	I8	611	0	631	34	0
49	F5	737	0	813	32	0
49	J8	747	0	817	42	0
50	G5	576	0	625	28	0
50	K8	575	0	634	41	0
51	H5	459	0	512	11	0
51	L8	459	0	512	13	0
52	M8	475	0	465	35	0
53	J5	434	0	454	21	0
53	N8	369	0	388	21	0
54	O8	389	0	404	25	0
55	L5	401	0	436	11	0
55	P8	401	0	436	13	0
56	M5	516	0	582	26	0
56	Q8	516	0	582	39	0
57	13	140	0	0	0	0
57	14	435	0	0	0	0
57	16	11	0	0	0	0
57	19	1	0	0	0	0
57	1G	102	0	0	0	0
57	1H	525	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1J	8	0	0	0	0
57	2I	3	0	0	0	0
57	25	1	0	0	0	0
57	29	1	0	0	0	0
57	2K	2	0	0	0	0
57	2L	2	0	0	0	0
57	3I	2	0	0	0	0
57	32	1	0	0	0	0
57	35	1	0	0	0	0
57	39	2	0	0	0	0
57	3I	1	0	0	0	0
57	4I	1	0	0	0	0
57	42	1	0	0	0	0
57	45	2	0	0	0	0
57	4I	1	0	0	0	0
57	4L	1	0	0	0	0
57	52	1	0	0	0	0
57	5I	1	0	0	0	0
57	78	1	0	0	0	0
57	7A	1	0	0	0	0
57	88	3	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	I8	2	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	13	42	0	43	0	0
58	1G	42	0	45	1	0
59	32	8	0	0	3	0
59	3E	8	0	0	1	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	14	26	0	45	8	0
61	1G	13	0	24	0	0
62	11	17	0	0	4	0
62	13	320	0	0	12	0
62	14	1144	0	0	65	0
62	15	1	0	0	0	0
62	16	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	19	15	0	0	3	0
62	1A	1	0	0	0	0
62	1F	1	0	0	0	0
62	1G	317	0	0	21	0
62	1H	1470	0	0	90	0
62	1I	2	0	0	0	0
62	1J	12	0	0	1	0
62	1K	2	0	0	0	0
62	21	7	0	0	1	0
62	25	6	0	0	0	0
62	29	4	0	0	0	0
62	2K	8	0	0	1	0
62	2L	6	0	0	0	0
62	31	5	0	0	0	0
62	32	1	0	0	0	0
62	35	8	0	0	1	0
62	39	5	0	0	1	0
62	3I	2	0	0	0	0
62	41	1	0	0	0	0
62	4E	3	0	0	0	0
62	4K	5	0	0	0	0
62	4L	6	0	0	0	0
62	52	4	0	0	0	0
62	55	3	0	0	0	0
62	58	2	0	0	0	0
62	5I	2	0	0	0	0
62	6A	2	0	0	0	0
62	6I	3	0	0	0	0
62	78	10	0	0	0	0
62	7A	5	0	0	0	0
62	7I	1	0	0	0	0
62	85	2	0	0	0	0
62	8E	2	0	0	0	0
62	9A	2	0	0	0	0
62	A5	1	0	0	0	0
62	B5	1	0	0	0	0
62	B8	1	0	0	0	0
62	BA	2	0	0	0	0
62	BI	2	0	0	1	0
62	C5	3	0	0	0	0
62	C8	3	0	0	0	0
62	F5	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	F8	2	0	0	0	0
62	G8	2	0	0	0	0
62	H5	2	0	0	1	0
62	I8	6	0	0	1	0
62	J8	4	0	0	0	0
62	L8	3	0	0	1	0
62	M5	9	0	0	1	0
62	P8	1	0	0	0	0
62	Q8	5	0	0	2	0
All	All	297444	0	197360	7614	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 7614 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1A:38:ILE:C	10:1A:39:PRO:N	1.71	1.49
38:45:27:VAL:HB	38:45:28:ALA:HA	1.19	1.13
29:11:182:LEU:H	29:11:272:ALA:HB3	1.23	1.02
37:78:63:PRO:HB2	56:Q8:30:ARG:HH21	1.23	1.01
26:14:330:A:H2	26:14:1210:A:HO2'	1.05	0.98

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	12	203/256 (79%)	173 (85%)	25 (12%)	5 (2%)	<b>4</b> <b>23</b>
2	1E	227/256 (89%)	185 (82%)	39 (17%)	3 (1%)	<b>9</b> <b>38</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	22	191/239 (80%)	171 (90%)	20 (10%)	0	100	100
3	2E	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	32	206/209 (99%)	184 (89%)	21 (10%)	1 (0%)	24	60
4	3E	205/209 (98%)	192 (94%)	12 (6%)	1 (0%)	24	60
5	42	148/162 (91%)	141 (95%)	7 (5%)	0	100	100
5	4E	147/162 (91%)	141 (96%)	5 (3%)	1 (1%)	18	53
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	62	134/156 (86%)	123 (92%)	10 (8%)	1 (1%)	18	53
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	8	35
8	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	18	53
9	82	119/128 (93%)	109 (92%)	9 (8%)	1 (1%)	16	50
9	8E	124/128 (97%)	108 (87%)	16 (13%)	0	100	100
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	92/105 (88%)	85 (92%)	7 (8%)	0	100	100
11	2A	111/129 (86%)	101 (91%)	8 (7%)	2 (2%)	6	31
11	2I	109/129 (84%)	94 (86%)	12 (11%)	3 (3%)	4	21
12	3A	119/132 (90%)	100 (84%)	15 (13%)	4 (3%)	3	17
12	3I	120/132 (91%)	107 (89%)	12 (10%)	1 (1%)	16	50
13	4A	107/126 (85%)	88 (82%)	18 (17%)	1 (1%)	14	48
13	4I	115/126 (91%)	96 (84%)	18 (16%)	1 (1%)	14	48
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	6	31
14	5I	57/61 (93%)	48 (84%)	7 (12%)	2 (4%)	3	16
15	6A	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
15	6I	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	12	45
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9I	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	8	35
19	AA	59/93 (63%)	49 (83%)	8 (14%)	2 (3%)	3	17
19	AI	80/93 (86%)	68 (85%)	9 (11%)	3 (4%)	2	15
20	BA	97/106 (92%)	83 (86%)	13 (13%)	1 (1%)	12	45
20	BI	95/106 (90%)	84 (88%)	10 (10%)	1 (1%)	11	43
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	128/229 (56%)	120 (94%)	8 (6%)	0	100	100
29	11	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	6	31
29	19	272/276 (99%)	246 (90%)	23 (8%)	3 (1%)	11	43
30	21	201/206 (98%)	158 (79%)	33 (16%)	10 (5%)	1	10
30	29	202/206 (98%)	149 (74%)	42 (21%)	11 (5%)	1	9
31	31	200/210 (95%)	181 (90%)	17 (8%)	2 (1%)	12	45
31	39	202/210 (96%)	162 (80%)	34 (17%)	6 (3%)	3	19
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	7	32
32	49	178/182 (98%)	155 (87%)	22 (12%)	1 (1%)	21	56
33	51	172/180 (96%)	141 (82%)	20 (12%)	11 (6%)	1	6
33	59	167/180 (93%)	129 (77%)	32 (19%)	6 (4%)	2	16
34	61	143/148 (97%)	122 (85%)	19 (13%)	2 (1%)	9	36
34	69	143/148 (97%)	111 (78%)	29 (20%)	3 (2%)	5	27
35	15	135/140 (96%)	122 (90%)	13 (10%)	0	100	100
35	58	135/140 (96%)	114 (84%)	17 (13%)	4 (3%)	3	19
36	25	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	68	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
37	35	145/150 (97%)	119 (82%)	26 (18%)	0	100	100
37	78	145/150 (97%)	114 (79%)	22 (15%)	9 (6%)	1	6
38	45	136/141 (96%)	115 (85%)	19 (14%)	2 (2%)	8	35
38	88	139/141 (99%)	116 (84%)	18 (13%)	5 (4%)	2	16
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	48
39	98	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	14	48
40	65	108/112 (96%)	89 (82%)	16 (15%)	3 (3%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	A8	109/112 (97%)	90 (83%)	19 (17%)	0	100	100
41	75	131/146 (90%)	117 (89%)	12 (9%)	2 (2%)	8	35
41	B8	133/146 (91%)	118 (89%)	15 (11%)	0	100	100
42	85	114/118 (97%)	104 (91%)	9 (8%)	1 (1%)	14	48
42	C8	113/118 (96%)	104 (92%)	6 (5%)	3 (3%)	4	22
43	95	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	3	19
43	D8	98/101 (97%)	88 (90%)	6 (6%)	4 (4%)	2	13
44	A5	109/113 (96%)	101 (93%)	7 (6%)	1 (1%)	14	48
44	E8	108/113 (96%)	100 (93%)	8 (7%)	0	100	100
45	B5	92/96 (96%)	84 (91%)	6 (6%)	2 (2%)	5	26
45	F8	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
46	C5	102/110 (93%)	74 (72%)	21 (21%)	7 (7%)	1	5
46	G8	101/110 (92%)	81 (80%)	16 (16%)	4 (4%)	2	14
47	D5	175/206 (85%)	136 (78%)	31 (18%)	8 (5%)	2	11
47	H8	168/206 (82%)	136 (81%)	25 (15%)	7 (4%)	2	13
48	E5	74/85 (87%)	66 (89%)	6 (8%)	2 (3%)	4	22
48	I8	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	9	38
49	F5	92/98 (94%)	79 (86%)	12 (13%)	1 (1%)	11	43
49	J8	94/98 (96%)	83 (88%)	9 (10%)	2 (2%)	5	27
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	3	19
50	K8	66/72 (92%)	60 (91%)	3 (4%)	3 (4%)	2	12
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	M8	56/71 (79%)	40 (71%)	15 (27%)	1 (2%)	6	31
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
54	O8	43/54 (80%)	30 (70%)	12 (28%)	1 (2%)	5	25
55	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
55	P8	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
56	M5	62/65 (95%)	52 (84%)	9 (14%)	1 (2%)	7	34
56	Q8	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11128/12158 (92%)	9762 (88%)	1180 (11%)	186 (2%)	7	32

5 of 186 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	2I	55	LYS
12	3I	48	PRO
18	9I	22	VAL
19	AI	41	VAL
30	21	83	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	179/220 (81%)	141 (79%)	38 (21%)	1	6
2	1E	200/220 (91%)	157 (78%)	43 (22%)	1	6
3	22	154/188 (82%)	129 (84%)	25 (16%)	2	12
3	2E	159/188 (85%)	126 (79%)	33 (21%)	1	7
4	32	180/181 (99%)	151 (84%)	29 (16%)	2	12
4	3E	180/181 (99%)	145 (81%)	35 (19%)	1	8
5	42	114/123 (93%)	87 (76%)	27 (24%)	1	4
5	4E	115/123 (94%)	92 (80%)	23 (20%)	1	7
6	52	90/90 (100%)	72 (80%)	18 (20%)	1	7
6	5E	90/90 (100%)	76 (84%)	14 (16%)	2	13
7	62	114/127 (90%)	88 (77%)	26 (23%)	1	5
7	6E	125/127 (98%)	103 (82%)	22 (18%)	2	10
8	72	118/119 (99%)	97 (82%)	21 (18%)	2	10
8	7E	119/119 (100%)	94 (79%)	25 (21%)	1	6
9	82	92/99 (93%)	77 (84%)	15 (16%)	2	12
9	8E	97/99 (98%)	77 (79%)	20 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1A	71/92 (77%)	48 (68%)	23 (32%)	0	1
10	1I	81/92 (88%)	68 (84%)	13 (16%)	2	12
11	2A	85/99 (86%)	67 (79%)	18 (21%)	1	6
11	2I	84/99 (85%)	67 (80%)	17 (20%)	1	7
12	3A	102/109 (94%)	78 (76%)	24 (24%)	1	4
12	3I	103/109 (94%)	92 (89%)	11 (11%)	6	26
13	4A	90/101 (89%)	65 (72%)	25 (28%)	0	2
13	4I	94/101 (93%)	72 (77%)	22 (23%)	1	4
14	5A	49/50 (98%)	39 (80%)	10 (20%)	1	7
14	5I	49/50 (98%)	35 (71%)	14 (29%)	0	2
15	6A	79/80 (99%)	68 (86%)	11 (14%)	3	17
15	6I	79/80 (99%)	63 (80%)	16 (20%)	1	7
16	7A	72/74 (97%)	62 (86%)	10 (14%)	3	17
16	7I	72/74 (97%)	60 (83%)	12 (17%)	2	12
17	8A	94/97 (97%)	79 (84%)	15 (16%)	2	12
17	8I	94/97 (97%)	77 (82%)	17 (18%)	2	9
18	9A	58/77 (75%)	46 (79%)	12 (21%)	1	7
18	9I	58/77 (75%)	50 (86%)	8 (14%)	3	17
19	AA	56/80 (70%)	47 (84%)	9 (16%)	2	12
19	AI	72/80 (90%)	61 (85%)	11 (15%)	3	14
20	BA	76/82 (93%)	67 (88%)	9 (12%)	5	22
20	BI	75/82 (92%)	59 (79%)	16 (21%)	1	6
21	1B	17/22 (77%)	16 (94%)	1 (6%)	18	50
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	5
28	7I	108/181 (60%)	91 (84%)	17 (16%)	2	13
29	11	214/218 (98%)	164 (77%)	50 (23%)	1	4
29	19	214/218 (98%)	167 (78%)	47 (22%)	1	5
30	21	162/166 (98%)	114 (70%)	48 (30%)	0	2
30	29	165/166 (99%)	125 (76%)	40 (24%)	1	4
31	31	161/166 (97%)	123 (76%)	38 (24%)	1	4
31	39	163/166 (98%)	122 (75%)	41 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	41	153/156 (98%)	120 (78%)	33 (22%)	1	6
32	49	152/156 (97%)	121 (80%)	31 (20%)	1	7
33	51	143/148 (97%)	103 (72%)	40 (28%)	0	2
33	59	140/148 (95%)	106 (76%)	34 (24%)	1	4
34	61	122/124 (98%)	82 (67%)	40 (33%)	0	1
34	69	122/124 (98%)	92 (75%)	30 (25%)	1	4
35	15	116/119 (98%)	86 (74%)	30 (26%)	0	3
35	58	116/119 (98%)	87 (75%)	29 (25%)	0	3
36	25	100/100 (100%)	69 (69%)	31 (31%)	0	1
36	68	100/100 (100%)	82 (82%)	18 (18%)	2	10
37	35	114/116 (98%)	77 (68%)	37 (32%)	0	1
37	78	114/116 (98%)	73 (64%)	41 (36%)	0	1
38	45	109/111 (98%)	86 (79%)	23 (21%)	1	6
38	88	110/111 (99%)	86 (78%)	24 (22%)	1	6
39	55	101/101 (100%)	77 (76%)	24 (24%)	1	4
39	98	101/101 (100%)	72 (71%)	29 (29%)	0	2
40	65	87/88 (99%)	60 (69%)	27 (31%)	0	1
40	A8	87/88 (99%)	63 (72%)	24 (28%)	0	2
41	75	117/127 (92%)	90 (77%)	27 (23%)	1	5
41	B8	117/127 (92%)	81 (69%)	36 (31%)	0	1
42	85	93/94 (99%)	72 (77%)	21 (23%)	1	5
42	C8	92/94 (98%)	76 (83%)	16 (17%)	2	10
43	95	81/82 (99%)	66 (82%)	15 (18%)	1	9
43	D8	82/82 (100%)	60 (73%)	22 (27%)	0	2
44	A5	91/92 (99%)	69 (76%)	22 (24%)	1	4
44	E8	90/92 (98%)	70 (78%)	20 (22%)	1	5
45	B5	74/78 (95%)	55 (74%)	19 (26%)	0	3
45	F8	77/78 (99%)	59 (77%)	18 (23%)	1	4
46	C5	85/91 (93%)	61 (72%)	24 (28%)	0	2
46	G8	84/91 (92%)	60 (71%)	24 (29%)	0	2
47	D5	156/179 (87%)	113 (72%)	43 (28%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	H8	151/179 (84%)	116 (77%)	35 (23%)	1	4
48	E5	61/67 (91%)	55 (90%)	6 (10%)	7	30
48	I8	62/67 (92%)	52 (84%)	10 (16%)	2	12
49	F5	79/83 (95%)	61 (77%)	18 (23%)	1	5
49	J8	79/83 (95%)	63 (80%)	16 (20%)	1	7
50	G5	63/67 (94%)	45 (71%)	18 (29%)	0	2
50	K8	64/67 (96%)	43 (67%)	21 (33%)	0	1
51	H5	50/52 (96%)	39 (78%)	11 (22%)	1	5
51	L8	50/52 (96%)	38 (76%)	12 (24%)	1	4
52	M8	52/63 (82%)	38 (73%)	14 (27%)	0	2
53	J5	48/52 (92%)	42 (88%)	6 (12%)	4	20
53	N8	43/52 (83%)	36 (84%)	7 (16%)	2	12
54	O8	44/52 (85%)	28 (64%)	16 (36%)	0	1
55	L5	38/42 (90%)	31 (82%)	7 (18%)	1	9
55	P8	38/42 (90%)	30 (79%)	8 (21%)	1	6
56	M5	54/55 (98%)	44 (82%)	10 (18%)	1	9
56	Q8	54/55 (98%)	43 (80%)	11 (20%)	1	7
All	All	9397/10064 (93%)	7296 (78%)	2101 (22%)	1	5

5 of 2101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	65	110	LEU
43	95	35	LEU
40	65	106	ARG
53	J5	29	THR
39	98	105	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	12	76	GLN
44	A5	60	ASN
4	32	201	GLN
43	95	80	GLN

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Mol	Chain	Res	Type
29	19	253	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1497/1522 (98%)	332 (22%)	33 (2%)
1	1G	1506/1522 (98%)	352 (23%)	33 (2%)
22	1K	69/76 (90%)	27 (39%)	4 (5%)
23	2K	76/77 (98%)	21 (27%)	2 (2%)
23	2L	76/77 (98%)	15 (19%)	2 (2%)
24	1L	62/76 (81%)	24 (38%)	2 (3%)
24	3K	67/76 (88%)	37 (55%)	2 (2%)
24	3L	69/76 (90%)	30 (43%)	2 (2%)
25	4K	17/30 (56%)	9 (52%)	1 (5%)
25	4L	18/30 (60%)	12 (66%)	1 (5%)
26	14	2822/2917 (96%)	680 (24%)	42 (1%)
26	1H	2850/2917 (97%)	634 (22%)	52 (1%)
27	16	121/122 (99%)	24 (19%)	1 (0%)
27	1J	121/122 (99%)	32 (26%)	3 (2%)
All	All	9371/9640 (97%)	2229 (23%)	180 (1%)

5 of 2229 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	7	G
1	13	9	G

5 of 180 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	992	U
26	14	503	A
1	1G	1145	C
23	2L	33	OMC
26	14	960	A

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	OMC	2K	33	23	19,22,23	1.80	3 (15%)	25,31,34	1.04	2 (8%)
23	5MU	2K	55	23	19,22,23	3.96	5 (26%)	27,32,35	3.17	9 (33%)
22	U8U	1K	34	25,22	20,24,25	2.46	6 (30%)	22,34,37	1.08	1 (4%)
22	PSU	1K	55	22	18,21,22	1.34	1 (5%)	21,30,33	1.68	4 (19%)
22	5MU	1K	54	22	19,22,23	4.01	5 (26%)	27,32,35	2.94	7 (25%)
22	T6A	1K	37	22	31,34,35	1.99	8 (25%)	43,49,52	2.36	13 (30%)
23	7MG	2K	47	23	23,26,27	2.92	8 (34%)	27,39,42	2.94	9 (33%)
23	PSU	2K	56	23	18,21,22	1.36	3 (16%)	21,30,33	1.94	3 (14%)
23	PSU	2L	56	23	18,21,22	1.31	2 (11%)	21,30,33	1.54	2 (9%)
23	4SU	2K	8	23	18,21,22	1.74	3 (16%)	25,30,33	2.44	4 (16%)
23	4SU	2L	8	23	18,21,22	2.05	4 (22%)	25,30,33	2.42	5 (20%)
23	5MU	2L	55	23	19,22,23	4.06	5 (26%)	27,32,35	3.14	8 (29%)
22	PSU	1K	39	22	18,21,22	1.06	1 (5%)	21,30,33	1.65	4 (19%)
23	OMC	2L	33	23	19,22,23	1.77	4 (21%)	25,31,34	1.29	2 (8%)
23	7MG	2L	47	23	23,26,27	3.01	8 (34%)	27,39,42	2.90	9 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
22	U8U	1K	34	25,22	-	1/10/28/29	0/2/2/2
22	PSU	1K	55	22	-	3/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	6/23/41/42	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	7MG	2K	47	23	-	4/7/37/38	0/3/3/3
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	2/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	3/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/9/27/28	0/2/2/2
23	7MG	2L	47	23	-	2/7/37/38	0/3/3/3

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C2-N1	13.20	1.59	1.38
22	1K	54	5MU	C2-N1	12.93	1.58	1.38
23	2K	55	5MU	C2-N1	12.82	1.58	1.38
23	2L	47	7MG	C5-N7	8.08	1.45	1.35
23	2K	47	7MG	C5-N7	7.29	1.44	1.35

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	55	5MU	C5-C4-N3	9.70	123.75	115.32
23	2K	55	5MU	C5-C4-N3	9.50	123.58	115.32
22	1K	54	5MU	C5-C4-N3	9.23	123.34	115.32
23	2L	8	4SU	C4-N3-C2	-8.21	119.44	127.31
23	2L	47	7MG	C4-C5-N7	8.19	115.05	105.38

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

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

There are no ring outliers.

7 monomers are involved in 13 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1269 ligands modelled in this entry, 1262 are monoatomic - leaving 7 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
61	SPE	1G	1703	-	12,12,12	0.35	0	11,11,11	0.75	0
59	SF4	3E	301	4	0,12,12	-	-	-	-	-
58	PAR	1G	1702	-	44,45,45	0.67	1 (2%)	63,67,67	1.40	9 (14%)
61	SPE	14	3436	-	12,12,12	0.43	0	11,11,11	0.64	0
58	PAR	13	1741	1	44,45,45	0.67	0	63,67,67	1.52	10 (15%)
59	SF4	32	302	4	0,12,12	-	-	-	-	-
61	SPE	14	3437	26	12,12,12	0.83	0	11,11,11	0.96	1 (9%)

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
61	SPE	1G	1703	-	-	3/10/10/10	-
59	SF4	3E	301	4	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	1G	1702	-	-	2/18/94/94	0/4/4/4
61	SPE	14	3436	-	-	5/10/10/10	-
58	PAR	13	1741	1	-	5/18/94/94	0/4/4/4
61	SPE	14	3437	26	-	4/10/10/10	-
59	SF4	32	302	4	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1G	1702	PAR	C24-N24	-2.22	1.43	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1741	PAR	C32-C22-C12	4.52	118.76	111.02
58	1G	1702	PAR	C14-O33-C33	-3.73	109.14	117.98
58	13	1741	PAR	C11-O51-C51	3.65	120.85	113.72
58	1G	1702	PAR	C13-O52-C52	-3.43	109.84	117.98
58	13	1741	PAR	C22-C12-C62	3.28	115.00	110.08

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

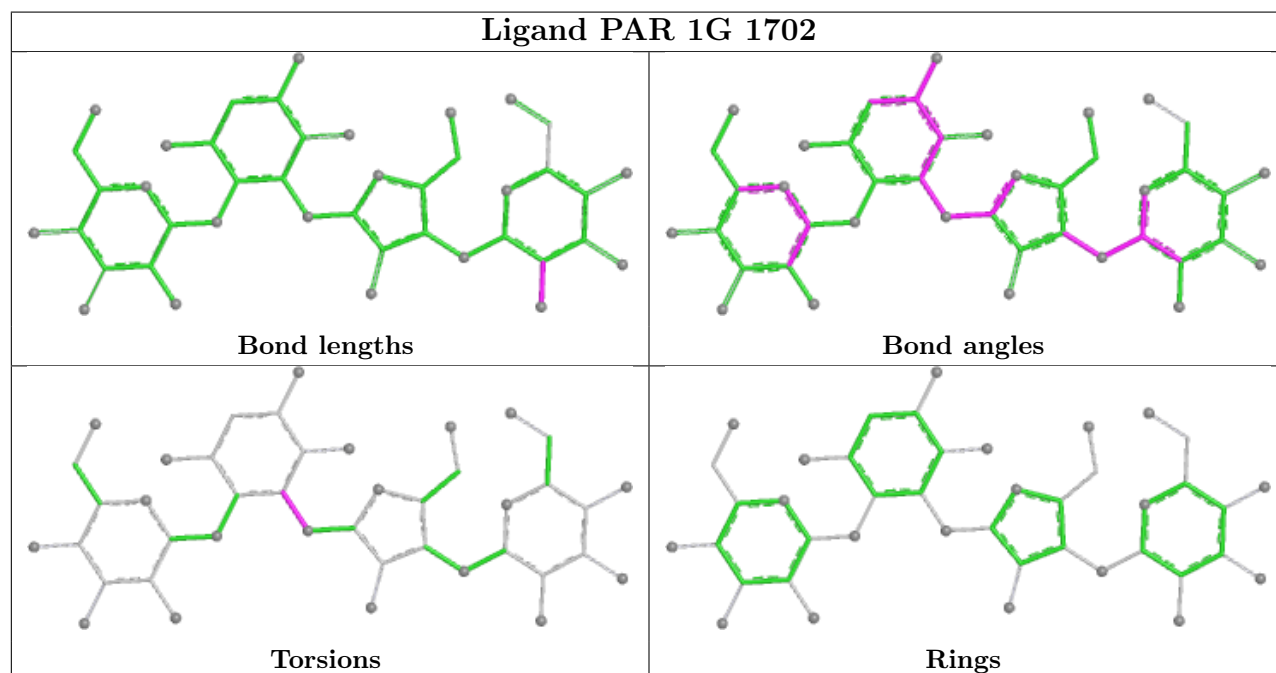
Mol	Chain	Res	Type	Atoms
58	13	1741	PAR	C44-C54-C64-N64
58	13	1741	PAR	O54-C54-C64-N64
61	1G	1703	SPE	C2-C3-C4-N5
61	14	3437	SPE	C6-C7-C8-N9
61	14	3437	SPE	N9-C10-C11-C12

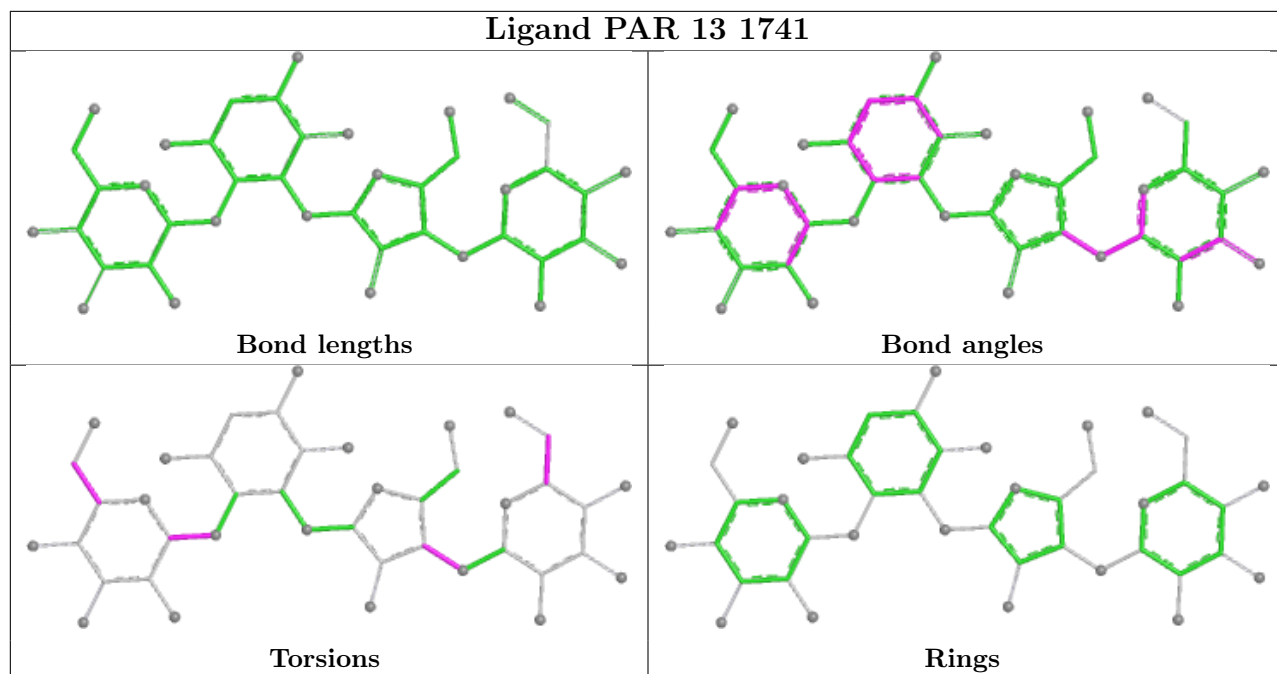
There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	3E	301	SF4	1	0
58	1G	1702	PAR	1	0
61	14	3436	SPE	2	0
59	32	302	SF4	3	0
61	14	3437	SPE	6	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
10	1A	2
26	1H	1
24	1L	1
47	D5	1
4	3E	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1H	1055:G	O3'	1059:G	P	14.13
1	1L	72:C	O3'	73:A	P	3.25
1	1A	38:ILE	C	39:PRO	N	1.71
1	1A	76:ASN	C	77:PRO	N	1.61
1	D5	94:GLU	C	95:PRO	N	1.61

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	13	1499/1522 (98%)	-0.15	28 (1%) 66 43	57, 100, 176, 247	0
1	1G	1508/1522 (99%)	-0.01	39 (2%) 57 34	71, 119, 192, 267	0
2	12	207/256 (80%)	0.90	27 (13%) 7 4	131, 164, 184, 192	0
2	1E	231/256 (90%)	0.99	36 (15%) 5 3	112, 143, 169, 174	0
3	22	195/239 (81%)	0.80	18 (9%) 14 8	135, 160, 173, 178	0
3	2E	205/239 (85%)	0.45	8 (3%) 43 24	88, 111, 143, 151	0
4	32	208/209 (99%)	0.52	10 (4%) 35 19	92, 113, 136, 142	0
4	3E	207/209 (99%)	0.72	12 (5%) 29 15	84, 108, 132, 144	0
5	42	150/162 (92%)	0.83	11 (7%) 21 11	108, 128, 148, 160	0
5	4E	149/162 (91%)	0.61	7 (4%) 36 19	82, 103, 121, 131	0
6	52	101/101 (100%)	0.46	2 (1%) 65 41	85, 104, 121, 132	0
6	5E	100/101 (99%)	0.58	9 (9%) 15 8	85, 105, 120, 132	0
7	62	138/156 (88%)	0.52	12 (8%) 16 8	116, 130, 141, 147	0
7	6E	154/156 (98%)	0.30	4 (2%) 57 34	102, 120, 150, 171	0
8	72	137/138 (99%)	0.74	7 (5%) 33 17	100, 131, 142, 149	0
8	7E	138/138 (100%)	0.46	4 (2%) 53 31	93, 110, 122, 134	0
9	82	121/128 (94%)	0.96	16 (13%) 7 4	116, 163, 174, 182	0
9	8E	126/128 (98%)	0.64	14 (11%) 10 6	87, 138, 157, 163	0
10	1A	80/105 (76%)	2.02	30 (37%) 1 1	133, 156, 169, 174	0
10	1I	94/105 (89%)	0.59	4 (4%) 40 21	81, 131, 168, 173	0
11	2A	113/129 (87%)	0.72	10 (8%) 15 8	84, 109, 124, 135	0
11	2I	111/129 (86%)	0.51	3 (2%) 56 33	72, 107, 123, 133	0
12	3A	121/132 (91%)	1.24	19 (15%) 5 3	90, 112, 135, 151	0
12	3I	122/132 (92%)	0.43	11 (9%) 15 8	66, 76, 102, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	109/126 (86%)	0.76	17 (15%) 5 3	123, 150, 180, 194	0
13	4I	117/126 (92%)	0.57	10 (8%) 16 8	88, 116, 131, 138	0
14	5A	59/61 (96%)	1.29	12 (20%) 3 2	137, 158, 180, 183	0
14	5I	59/61 (96%)	0.23	2 (3%) 48 27	81, 96, 114, 122	0
15	6A	87/89 (97%)	0.03	2 (2%) 61 38	84, 113, 128, 131	0
15	6I	87/89 (97%)	0.09	1 (1%) 78 57	80, 98, 113, 123	0
16	7A	84/88 (95%)	0.63	8 (9%) 14 7	92, 105, 129, 155	0
16	7I	83/88 (94%)	0.97	10 (12%) 9 5	96, 111, 137, 155	0
17	8A	99/105 (94%)	0.37	2 (2%) 65 41	97, 113, 130, 135	0
17	8I	99/105 (94%)	0.35	5 (5%) 33 17	89, 106, 115, 124	0
18	9A	67/88 (76%)	0.91	8 (11%) 9 5	92, 112, 132, 138	0
18	9I	68/88 (77%)	0.47	3 (4%) 39 21	88, 107, 131, 135	0
19	AA	65/93 (69%)	1.31	14 (21%) 2 1	162, 178, 187, 192	0
19	AI	82/93 (88%)	0.45	5 (6%) 27 14	96, 117, 138, 151	0
20	BA	99/106 (93%)	0.24	2 (2%) 65 41	90, 114, 140, 152	0
20	BI	97/106 (91%)	0.26	3 (3%) 51 30	106, 119, 145, 151	0
21	1B	22/27 (81%)	0.57	1 (4%) 38 20	127, 141, 145, 148	0
21	1F	23/27 (85%)	-0.16	0 100 100	92, 99, 107, 115	0
22	1K	67/76 (88%)	1.52	17 (25%) 1 1	90, 193, 226, 233	0
23	2K	72/77 (93%)	0.11	1 (1%) 73 51	67, 92, 124, 140	0
23	2L	72/77 (93%)	0.72	5 (6%) 23 12	80, 116, 152, 163	0
24	1L	66/76 (86%)	1.67	22 (33%) 1 1	145, 224, 245, 249	0
24	3K	70/76 (92%)	0.98	9 (12%) 7 5	76, 229, 251, 253	0
24	3L	72/76 (94%)	1.63	20 (27%) 1 1	85, 220, 238, 240	0
25	4K	19/30 (63%)	0.93	3 (15%) 5 3	71, 140, 219, 219	0
25	4L	19/30 (63%)	1.09	4 (21%) 2 1	98, 158, 230, 230	0
26	14	2826/2917 (96%)	-0.29	23 (0%) 82 64	50, 85, 199, 264	0
26	1H	2860/2917 (98%)	-0.47	28 (0%) 79 59	40, 69, 186, 257	0
27	16	122/122 (100%)	-0.62	0 100 100	61, 88, 107, 197	0
27	1J	122/122 (100%)	-0.08	2 (1%) 70 47	85, 119, 145, 205	0
28	71	132/229 (57%)	0.51	6 (4%) 38 20	146, 210, 235, 243	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	11	273/276 (98%)	-0.00	6 (2%) 62 39	41, 63, 79, 93	0
29	19	274/276 (99%)	0.38	19 (6%) 23 12	47, 73, 88, 107	0
30	21	203/206 (98%)	0.40	11 (5%) 31 16	48, 84, 120, 130	0
30	29	204/206 (99%)	0.46	16 (7%) 19 10	60, 95, 134, 149	0
31	31	202/210 (96%)	-0.10	3 (1%) 72 49	46, 76, 112, 127	0
31	39	204/210 (97%)	0.35	11 (5%) 31 16	57, 101, 148, 177	0
32	41	179/182 (98%)	0.28	10 (5%) 30 15	79, 100, 134, 146	0
32	49	180/182 (98%)	0.56	10 (5%) 30 15	117, 138, 156, 174	0
33	51	174/180 (96%)	0.51	12 (6%) 23 12	77, 102, 119, 130	0
33	59	169/180 (93%)	1.35	39 (23%) 2 1	152, 196, 220, 233	0
34	61	145/148 (97%)	0.40	10 (6%) 23 12	76, 131, 149, 157	0
34	69	145/148 (97%)	0.43	13 (8%) 15 8	86, 122, 149, 156	0
35	15	137/140 (97%)	1.06	18 (13%) 7 4	81, 108, 135, 151	0
35	58	137/140 (97%)	0.54	8 (5%) 29 15	63, 85, 121, 138	0
36	25	122/122 (100%)	0.18	1 (0%) 82 64	69, 88, 105, 117	0
36	68	122/122 (100%)	0.05	2 (1%) 70 47	56, 72, 90, 99	0
37	35	147/150 (98%)	0.45	6 (4%) 41 23	58, 102, 135, 152	0
37	78	147/150 (98%)	-0.04	2 (1%) 73 51	47, 80, 104, 115	0
38	45	138/141 (97%)	0.86	15 (10%) 10 6	76, 105, 124, 155	0
38	88	141/141 (100%)	0.01	2 (1%) 73 51	54, 75, 95, 123	0
39	55	118/118 (100%)	-0.07	1 (0%) 82 64	65, 80, 97, 112	0
39	98	118/118 (100%)	0.02	0 100 100	60, 78, 94, 106	0
40	65	110/112 (98%)	0.60	5 (4%) 38 20	89, 112, 132, 137	0
40	A8	111/112 (99%)	0.05	3 (2%) 56 33	72, 85, 105, 116	0
41	75	133/146 (91%)	0.23	5 (3%) 44 24	80, 96, 128, 151	0
41	B8	135/146 (92%)	0.63	12 (8%) 15 8	67, 84, 128, 139	0
42	85	116/118 (98%)	0.66	8 (6%) 23 12	63, 96, 127, 134	0
42	C8	115/118 (97%)	0.40	4 (3%) 47 27	53, 77, 102, 108	0
43	95	100/101 (99%)	0.73	4 (4%) 42 23	65, 116, 135, 142	0
43	D8	100/101 (99%)	0.48	3 (3%) 52 30	53, 101, 119, 126	0
44	A5	111/113 (98%)	0.23	2 (1%) 67 44	57, 75, 101, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	E8	110/113 (97%)	0.27	5 (4%) 38 20	53, 70, 94, 106	0
45	B5	94/96 (97%)	0.23	4 (4%) 40 21	68, 83, 104, 118	0
45	F8	95/96 (98%)	0.09	2 (2%) 63 40	49, 66, 97, 110	0
46	C5	104/110 (94%)	1.57	32 (30%) 1 1	92, 118, 156, 164	0
46	G8	103/110 (93%)	0.81	13 (12%) 8 5	73, 95, 122, 130	0
47	D5	177/206 (85%)	0.49	5 (2%) 55 32	108, 148, 226, 236	0
47	H8	170/206 (82%)	0.14	1 (0%) 85 69	80, 116, 202, 210	0
48	E5	76/85 (89%)	0.33	4 (5%) 32 16	66, 88, 102, 115	0
48	I8	77/85 (90%)	-0.10	4 (5%) 33 17	54, 69, 91, 102	0
49	F5	94/98 (95%)	0.54	4 (4%) 40 21	60, 83, 122, 136	0
49	J8	96/98 (97%)	0.43	6 (6%) 26 13	51, 71, 126, 138	0
50	G5	69/72 (95%)	0.46	5 (7%) 21 11	81, 104, 124, 138	0
50	K8	68/72 (94%)	0.19	2 (2%) 53 31	59, 79, 96, 120	0
51	H5	58/60 (96%)	0.32	0 100 100	77, 99, 122, 135	0
51	L8	58/60 (96%)	-0.17	0 100 100	60, 77, 103, 110	0
52	M8	60/71 (84%)	0.78	5 (8%) 17 9	102, 143, 168, 171	0
53	J5	56/60 (93%)	0.42	6 (10%) 11 6	58, 85, 131, 141	0
53	N8	48/60 (80%)	0.02	1 (2%) 63 40	46, 78, 119, 127	0
54	O8	45/54 (83%)	1.28	10 (22%) 2 1	117, 153, 171, 177	0
55	L5	47/49 (95%)	-0.27	1 (2%) 63 40	47, 60, 87, 97	0
55	P8	47/49 (95%)	-0.43	1 (2%) 63 40	42, 50, 72, 87	0
56	M5	64/65 (98%)	0.44	4 (6%) 26 13	68, 80, 97, 117	0
56	Q8	64/65 (98%)	0.01	1 (1%) 70 47	51, 65, 80, 98	0
All	All	20730/21798 (95%)	0.17	963 (4%) 37 20	40, 99, 184, 267	0

The worst 5 of 963 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	B8	104	ASN	9.4
9	82	115	GLY	8.7
24	3L	35	U	8.3
22	1K	76	A	7.7
24	3L	34	U	7.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
22	PSU	1K	55	20/21	0.83	0.10	107,127,140,145	0
23	7MG	2L	47	24/25	0.85	0.11	118,128,137,141	0
23	PSU	2L	56	20/21	0.85	0.08	109,121,126,126	0
22	5MU	1K	54	21/22	0.86	0.09	104,125,133,143	0
23	4SU	2L	8	20/21	0.86	0.12	107,118,124,125	0
23	5MU	2L	55	21/22	0.87	0.10	115,122,127,130	0
23	OMC	2L	33	21/22	0.87	0.13	94,103,107,109	0
23	7MG	2K	47	24/25	0.89	0.10	96,101,113,116	0
23	PSU	2K	56	20/21	0.89	0.07	91,101,110,117	0
23	5MU	2K	55	21/22	0.89	0.09	98,105,112,114	0
23	4SU	2K	8	20/21	0.90	0.12	89,95,101,103	0
22	U8U	1K	34	23/24	0.93	0.12	83,98,108,110	0
22	T6A	1K	37	32/33	0.94	0.16	81,92,114,116	0
22	PSU	1K	39	20/21	0.94	0.20	94,112,118,120	0
23	OMC	2K	33	21/22	0.95	0.15	73,79,82,94	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
57	MG	14	3017	1/1	0.31	0.30	119,119,119,119	0
57	MG	14	3187	1/1	0.40	0.28	117,117,117,117	0
57	MG	13	1678	1/1	0.46	0.24	112,112,112,112	0
57	MG	14	3072	1/1	0.49	0.29	94,94,94,94	0
57	MG	14	3129	1/1	0.57	0.31	118,118,118,118	0
57	MG	14	3060	1/1	0.59	0.33	98,98,98,98	0
57	MG	1H	3136	1/1	0.59	0.32	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	14	3154	1/1	0.61	0.26	95,95,95,95	0
57	MG	14	3177	1/1	0.61	0.33	101,101,101,101	0
57	MG	1H	3081	1/1	0.61	0.33	83,83,83,83	0
57	MG	13	1659	1/1	0.62	0.21	126,126,126,126	0
57	MG	1J	202	1/1	0.62	0.32	92,92,92,92	0
57	MG	1G	1640	1/1	0.63	0.29	108,108,108,108	0
57	MG	1H	3119	1/1	0.63	0.35	83,83,83,83	0
57	MG	1G	1623	1/1	0.63	0.26	115,115,115,115	0
57	MG	1H	3216	1/1	0.64	0.36	82,82,82,82	0
57	MG	1H	3204	1/1	0.65	0.25	91,91,91,91	0
57	MG	1G	1642	1/1	0.65	0.28	99,99,99,99	0
57	MG	1G	1628	1/1	0.65	0.26	113,113,113,113	0
57	MG	14	3153	1/1	0.65	0.35	90,90,90,90	0
57	MG	13	1671	1/1	0.66	0.41	79,79,79,79	0
57	MG	1H	3148	1/1	0.66	0.39	83,83,83,83	0
57	MG	14	3163	1/1	0.66	0.26	93,93,93,93	0
57	MG	1H	3237	1/1	0.67	0.25	81,81,81,81	0
57	MG	14	3144	1/1	0.67	0.29	102,102,102,102	0
57	MG	1G	1602	1/1	0.67	0.28	106,106,106,106	0
57	MG	13	1675	1/1	0.67	0.35	101,101,101,101	0
57	MG	1H	3221	1/1	0.68	0.18	73,73,73,73	0
57	MG	1H	3157	1/1	0.68	0.41	89,89,89,89	0
57	MG	4L	101	1/1	0.68	0.16	131,131,131,131	0
57	MG	1H	3242	1/1	0.68	0.34	90,90,90,90	0
57	MG	1H	3144	1/1	0.68	0.38	102,102,102,102	0
57	MG	1H	3206	1/1	0.68	0.42	93,93,93,93	0
57	MG	14	3208	1/1	0.68	0.41	88,88,88,88	0
57	MG	13	1651	1/1	0.68	0.31	98,98,98,98	0
57	MG	14	3136	1/1	0.69	0.37	92,92,92,92	0
57	MG	13	1676	1/1	0.69	0.41	93,93,93,93	0
57	MG	14	3183	1/1	0.69	0.23	103,103,103,103	0
57	MG	1G	1631	1/1	0.70	0.32	92,92,92,92	0
57	MG	1H	3043	1/1	0.70	0.26	75,75,75,75	0
57	MG	1H	3151	1/1	0.70	0.41	80,80,80,80	0
57	MG	1G	1609	1/1	0.71	0.38	92,92,92,92	0
57	MG	14	3101	1/1	0.72	0.27	87,87,87,87	0
57	MG	16	203	1/1	0.72	0.17	82,82,82,82	0
57	MG	14	3201	1/1	0.72	0.28	88,88,88,88	0
57	MG	13	1645	1/1	0.72	0.31	92,92,92,92	0
57	MG	1H	3172	1/1	0.72	0.18	83,83,83,83	0
57	MG	1H	3088	1/1	0.73	0.34	80,80,80,80	0
57	MG	14	3157	1/1	0.73	0.31	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3061	1/1	0.73	0.14	53,53,53,53	0
57	MG	14	3175	1/1	0.73	0.25	88,88,88,88	0
57	MG	14	3430	1/1	0.73	0.12	107,107,107,107	0
57	MG	1G	1608	1/1	0.73	0.21	93,93,93,93	0
57	MG	35	201	1/1	0.74	0.17	75,75,75,75	0
57	MG	1H	3044	1/1	0.75	0.29	67,67,67,67	0
57	MG	1H	3174	1/1	0.75	0.13	55,55,55,55	0
57	MG	1H	3201	1/1	0.75	0.29	104,104,104,104	0
57	MG	1G	1641	1/1	0.75	0.34	103,103,103,103	0
57	MG	13	1626	1/1	0.75	0.28	84,84,84,84	0
57	MG	1H	3150	1/1	0.75	0.34	98,98,98,98	0
57	MG	1H	3120	1/1	0.75	0.31	88,88,88,88	0
57	MG	14	3046	1/1	0.75	0.25	79,79,79,79	0
57	MG	13	1643	1/1	0.75	0.41	101,101,101,101	0
57	MG	13	1668	1/1	0.76	0.22	66,66,66,66	0
57	MG	1H	3106	1/1	0.76	0.32	87,87,87,87	0
57	MG	1H	3008	1/1	0.76	0.27	82,82,82,82	0
57	MG	13	1661	1/1	0.76	0.23	90,90,90,90	0
57	MG	1G	1605	1/1	0.76	0.31	104,104,104,104	0
57	MG	1H	3180	1/1	0.76	0.35	90,90,90,90	0
57	MG	1H	3235	1/1	0.76	0.27	71,71,71,71	0
57	MG	88	201	1/1	0.77	0.26	76,76,76,76	0
57	MG	1G	1635	1/1	0.77	0.20	105,105,105,105	0
57	MG	1H	3129	1/1	0.77	0.14	76,76,76,76	0
57	MG	1H	3230	1/1	0.77	0.25	82,82,82,82	0
57	MG	13	1641	1/1	0.77	0.18	81,81,81,81	0
57	MG	14	3197	1/1	0.77	0.48	77,77,77,77	0
57	MG	1H	3141	1/1	0.77	0.26	83,83,83,83	0
57	MG	14	3152	1/1	0.77	0.19	78,78,78,78	0
57	MG	14	3008	1/1	0.77	0.23	77,77,77,77	0
57	MG	13	1679	1/1	0.77	0.33	99,99,99,99	0
57	MG	4I	200	1/1	0.77	0.30	95,95,95,95	0
57	MG	45	201	1/1	0.77	0.20	101,101,101,101	0
57	MG	1H	3321	1/1	0.78	0.14	86,86,86,86	0
57	MG	1H	3085	1/1	0.78	0.31	70,70,70,70	0
57	MG	14	3169	1/1	0.78	0.28	85,85,85,85	0
57	MG	14	3097	1/1	0.78	0.22	97,97,97,97	0
57	MG	1H	3130	1/1	0.78	0.10	63,63,63,63	0
57	MG	14	3112	1/1	0.78	0.18	83,83,83,83	0
57	MG	14	3122	1/1	0.78	0.18	75,75,75,75	0
57	MG	1H	3006	1/1	0.78	0.16	74,74,74,74	0
57	MG	14	3134	1/1	0.78	0.27	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3222	1/1	0.78	0.22	69,69,69,69	0
57	MG	13	1628	1/1	0.78	0.23	91,91,91,91	0
57	MG	1H	3024	1/1	0.78	0.24	83,83,83,83	0
57	MG	1J	206	1/1	0.78	0.26	94,94,94,94	0
57	MG	1H	3029	1/1	0.78	0.26	77,77,77,77	0
57	MG	1H	3127	1/1	0.78	0.23	91,91,91,91	0
57	MG	14	3195	1/1	0.79	0.17	78,78,78,78	0
57	MG	1H	3156	1/1	0.79	0.28	83,83,83,83	0
57	MG	14	3198	1/1	0.79	0.31	81,81,81,81	0
57	MG	1H	3113	1/1	0.79	0.21	81,81,81,81	0
57	MG	13	1602	1/1	0.79	0.24	120,120,120,120	0
57	MG	1H	3205	1/1	0.79	0.35	79,79,79,79	0
57	MG	14	3102	1/1	0.79	0.28	85,85,85,85	0
57	MG	14	3025	1/1	0.79	0.25	80,80,80,80	0
57	MG	14	3186	1/1	0.79	0.14	108,108,108,108	0
57	MG	1H	3154	1/1	0.79	0.13	58,58,58,58	0
57	MG	E5	101	1/1	0.79	0.37	89,89,89,89	0
57	MG	14	3161	1/1	0.80	0.25	78,78,78,78	0
57	MG	14	3064	1/1	0.80	0.22	63,63,63,63	0
57	MG	14	3168	1/1	0.80	0.17	89,89,89,89	0
57	MG	1H	3197	1/1	0.80	0.30	77,77,77,77	0
57	MG	14	3088	1/1	0.80	0.41	87,87,87,87	0
57	MG	13	1709	1/1	0.80	0.19	99,99,99,99	0
57	MG	14	3181	1/1	0.80	0.25	75,75,75,75	0
57	MG	1H	3203	1/1	0.80	0.26	74,74,74,74	0
57	MG	1H	3075	1/1	0.80	0.24	76,76,76,76	0
57	MG	1H	3114	1/1	0.80	0.25	71,71,71,71	0
57	MG	13	1669	1/1	0.80	0.45	95,95,95,95	0
57	MG	14	3127	1/1	0.80	0.39	87,87,87,87	0
57	MG	1H	3207	1/1	0.80	0.29	92,92,92,92	0
57	MG	1H	3209	1/1	0.80	0.34	76,76,76,76	0
57	MG	13	1630	1/1	0.80	0.25	96,96,96,96	0
57	MG	14	3391	1/1	0.80	0.17	99,99,99,99	0
57	MG	1H	3126	1/1	0.80	0.31	86,86,86,86	0
57	MG	14	3146	1/1	0.80	0.18	75,75,75,75	0
57	MG	14	3023	1/1	0.80	0.20	76,76,76,76	0
57	MG	13	1660	1/1	0.80	0.31	88,88,88,88	0
57	MG	1G	1620	1/1	0.80	0.22	91,91,91,91	0
57	MG	1G	1622	1/1	0.80	0.13	125,125,125,125	0
57	MG	13	1633	1/1	0.81	0.19	73,73,73,73	0
57	MG	16	208	1/1	0.81	0.28	85,85,85,85	0
57	MG	1H	3077	1/1	0.81	0.29	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3231	1/1	0.81	0.30	66,66,66,66	0
57	MG	14	3132	1/1	0.81	0.26	82,82,82,82	0
57	MG	14	3133	1/1	0.81	0.36	88,88,88,88	0
57	MG	14	3058	1/1	0.81	0.20	84,84,84,84	0
57	MG	14	3135	1/1	0.81	0.30	79,79,79,79	0
57	MG	1H	3234	1/1	0.81	0.19	79,79,79,79	0
57	MG	13	1665	1/1	0.81	0.30	82,82,82,82	0
57	MG	14	3145	1/1	0.81	0.20	90,90,90,90	0
57	MG	14	3207	1/1	0.81	0.25	70,70,70,70	0
57	MG	13	1674	1/1	0.81	0.34	92,92,92,92	0
57	MG	14	3082	1/1	0.81	0.33	79,79,79,79	0
57	MG	1G	1654	1/1	0.81	0.13	108,108,108,108	0
57	MG	2L	102	1/1	0.81	0.11	132,132,132,132	0
57	MG	14	3099	1/1	0.81	0.21	78,78,78,78	0
57	MG	39	302	1/1	0.81	0.14	74,74,74,74	0
57	MG	1H	3050	1/1	0.81	0.33	72,72,72,72	0
57	MG	13	1656	1/1	0.81	0.26	74,74,74,74	0
57	MG	14	3103	1/1	0.81	0.41	96,96,96,96	0
57	MG	14	3093	1/1	0.82	0.23	84,84,84,84	0
57	MG	14	3015	1/1	0.82	0.32	63,63,63,63	0
57	MG	14	3138	1/1	0.82	0.28	78,78,78,78	0
57	MG	1H	3488	1/1	0.82	0.12	105,105,105,105	0
57	MG	1H	3145	1/1	0.82	0.30	80,80,80,80	0
57	MG	1G	1616	1/1	0.82	0.23	94,94,94,94	0
57	MG	1H	3193	1/1	0.82	0.27	61,61,61,61	0
57	MG	14	3109	1/1	0.82	0.20	67,67,67,67	0
57	MG	14	3048	1/1	0.82	0.25	51,51,51,51	0
57	MG	14	3119	1/1	0.82	0.28	81,81,81,81	0
57	MG	13	1647	1/1	0.82	0.25	88,88,88,88	0
57	MG	13	1654	1/1	0.82	0.42	101,101,101,101	0
57	MG	14	3128	1/1	0.82	0.37	89,89,89,89	0
57	MG	2L	101	1/1	0.82	0.33	91,91,91,91	0
57	MG	1G	1625	1/1	0.82	0.17	99,99,99,99	0
57	MG	1H	3176	1/1	0.82	0.23	83,83,83,83	0
57	MG	1G	1630	1/1	0.82	0.28	72,72,72,72	0
57	MG	13	1640	1/1	0.83	0.22	92,92,92,92	0
57	MG	16	205	1/1	0.83	0.16	69,69,69,69	0
57	MG	14	3054	1/1	0.83	0.31	79,79,79,79	0
57	MG	1H	3220	1/1	0.83	0.39	89,89,89,89	0
57	MG	1G	1637	1/1	0.83	0.31	103,103,103,103	0
57	MG	1H	3189	1/1	0.83	0.23	68,68,68,68	0
57	MG	14	3069	1/1	0.83	0.25	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	14	3192	1/1	0.83	0.22	74,74,74,74	0
57	MG	1H	3052	1/1	0.83	0.28	59,59,59,59	0
57	MG	1H	3055	1/1	0.83	0.12	48,48,48,48	0
57	MG	14	3084	1/1	0.83	0.24	79,79,79,79	0
57	MG	1H	3084	1/1	0.83	0.23	62,62,62,62	0
57	MG	14	3203	1/1	0.83	0.30	79,79,79,79	0
57	MG	13	1610	1/1	0.83	0.33	82,82,82,82	0
57	MG	1G	1612	1/1	0.83	0.16	106,106,106,106	0
57	MG	1H	3158	1/1	0.83	0.18	71,71,71,71	0
57	MG	1H	3169	1/1	0.83	0.22	91,91,91,91	0
57	MG	1H	3070	1/1	0.83	0.26	75,75,75,75	0
57	MG	1H	3147	1/1	0.83	0.44	84,84,84,84	0
57	MG	1H	3089	1/1	0.83	0.20	38,38,38,38	0
57	MG	16	202	1/1	0.83	0.23	82,82,82,82	0
57	MG	14	3113	1/1	0.83	0.12	52,52,52,52	0
57	MG	14	3114	1/1	0.83	0.12	70,70,70,70	0
61	SPE	14	3437	13/13	0.83	0.19	59,68,73,74	0
57	MG	1H	3095	1/1	0.84	0.25	70,70,70,70	0
57	MG	14	3032	1/1	0.84	0.20	64,64,64,64	0
57	MG	13	1667	1/1	0.84	0.43	89,89,89,89	0
57	MG	1H	3224	1/1	0.84	0.23	85,85,85,85	0
57	MG	14	3053	1/1	0.84	0.23	95,95,95,95	0
57	MG	1G	1613	1/1	0.84	0.38	89,89,89,89	0
57	MG	1H	3226	1/1	0.84	0.30	71,71,71,71	0
57	MG	1G	1617	1/1	0.84	0.13	116,116,116,116	0
57	MG	1H	3007	1/1	0.84	0.23	81,81,81,81	0
57	MG	14	3155	1/1	0.84	0.20	78,78,78,78	0
57	MG	13	1637	1/1	0.84	0.34	74,74,74,74	0
57	MG	1H	3233	1/1	0.84	0.20	93,93,93,93	0
57	MG	14	3076	1/1	0.84	0.36	81,81,81,81	0
57	MG	14	3165	1/1	0.84	0.33	77,77,77,77	0
57	MG	1H	3079	1/1	0.84	0.17	63,63,63,63	0
57	MG	1H	3009	1/1	0.84	0.31	71,71,71,71	0
57	MG	1H	3198	1/1	0.84	0.28	79,79,79,79	0
57	MG	13	1639	1/1	0.84	0.35	70,70,70,70	0
57	MG	1G	1633	1/1	0.84	0.13	118,118,118,118	0
57	MG	1G	1634	1/1	0.84	0.31	85,85,85,85	0
57	MG	1H	3057	1/1	0.84	0.28	75,75,75,75	0
57	MG	1H	3445	1/1	0.84	0.11	92,92,92,92	0
57	MG	1H	3087	1/1	0.84	0.14	71,71,71,71	0
57	MG	14	3107	1/1	0.84	0.23	54,54,54,54	0
57	MG	1H	3521	1/1	0.84	0.08	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3111	1/1	0.84	0.12	58,58,58,58	0
57	MG	13	1670	1/1	0.84	0.34	82,82,82,82	0
57	MG	1H	3134	1/1	0.84	0.15	57,57,57,57	0
57	MG	32	301	1/1	0.84	0.28	113,113,113,113	0
57	MG	14	3115	1/1	0.84	0.32	87,87,87,87	0
57	MG	1H	3160	1/1	0.84	0.26	71,71,71,71	0
57	MG	14	3393	1/1	0.84	0.13	165,165,165,165	0
57	MG	1H	3165	1/1	0.84	0.21	64,64,64,64	0
57	MG	14	3125	1/1	0.84	0.22	81,81,81,81	0
57	MG	1J	204	1/1	0.84	0.11	89,89,89,89	0
57	MG	31	302	1/1	0.84	0.17	77,77,77,77	0
57	MG	1H	3135	1/1	0.84	0.34	79,79,79,79	0
57	MG	1H	3217	1/1	0.84	0.33	82,82,82,82	0
57	MG	1G	1604	1/1	0.84	0.16	127,127,127,127	0
57	MG	14	3018	1/1	0.84	0.12	44,44,44,44	0
57	MG	1H	3066	1/1	0.84	0.24	60,60,60,60	0
57	MG	1H	3117	1/1	0.85	0.14	60,60,60,60	0
57	MG	14	3156	1/1	0.85	0.29	87,87,87,87	0
57	MG	14	3199	1/1	0.85	0.24	76,76,76,76	0
57	MG	14	3059	1/1	0.85	0.19	89,89,89,89	0
57	MG	1H	3187	1/1	0.85	0.28	44,44,44,44	0
57	MG	14	3020	1/1	0.85	0.15	75,75,75,75	0
57	MG	13	1635	1/1	0.85	0.24	81,81,81,81	0
57	MG	1H	3170	1/1	0.85	0.29	80,80,80,80	0
57	MG	1H	3137	1/1	0.85	0.25	70,70,70,70	0
57	MG	14	3035	1/1	0.85	0.24	58,58,58,58	0
57	MG	14	3142	1/1	0.85	0.30	80,80,80,80	0
57	MG	1H	3086	1/1	0.85	0.23	53,53,53,53	0
57	MG	1H	3102	1/1	0.85	0.20	60,60,60,60	0
57	MG	14	3051	1/1	0.85	0.21	61,61,61,61	0
57	MG	14	3094	1/1	0.85	0.26	73,73,73,73	0
57	MG	1G	1639	1/1	0.85	0.21	78,78,78,78	0
57	MG	1G	1610	1/1	0.85	0.28	91,91,91,91	0
57	MG	14	3196	1/1	0.85	0.29	71,71,71,71	0
57	MG	1H	3109	1/1	0.86	0.23	59,59,59,59	0
57	MG	1H	3163	1/1	0.86	0.36	91,91,91,91	0
57	MG	1G	1644	1/1	0.86	0.12	106,106,106,106	0
57	MG	13	1615	1/1	0.86	0.25	88,88,88,88	0
57	MG	14	3123	1/1	0.86	0.34	83,83,83,83	0
57	MG	14	3178	1/1	0.86	0.31	78,78,78,78	0
57	MG	14	3124	1/1	0.86	0.16	97,97,97,97	0
57	MG	1G	1663	1/1	0.86	0.10	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1G	1673	1/1	0.86	0.09	115,115,115,115	0
57	MG	1H	3033	1/1	0.86	0.19	70,70,70,70	0
57	MG	1G	1614	1/1	0.86	0.30	88,88,88,88	0
57	MG	14	3077	1/1	0.86	0.16	52,52,52,52	0
57	MG	1H	3243	1/1	0.86	0.24	82,82,82,82	0
57	MG	14	3083	1/1	0.86	0.13	72,72,72,72	0
57	MG	13	1616	1/1	0.86	0.27	74,74,74,74	0
57	MG	1H	3067	1/1	0.86	0.21	58,58,58,58	0
57	MG	1H	3069	1/1	0.86	0.26	69,69,69,69	0
57	MG	13	1620	1/1	0.86	0.36	86,86,86,86	0
57	MG	1H	3177	1/1	0.86	0.36	82,82,82,82	0
57	MG	1H	3071	1/1	0.86	0.30	79,79,79,79	0
57	MG	14	3213	1/1	0.86	0.31	87,87,87,87	0
57	MG	14	3366	1/1	0.86	0.21	82,82,82,82	0
57	MG	13	1677	1/1	0.86	0.32	77,77,77,77	0
57	MG	14	3149	1/1	0.86	0.14	72,72,72,72	0
57	MG	1H	3012	1/1	0.86	0.27	58,58,58,58	0
57	MG	1H	3223	1/1	0.86	0.30	85,85,85,85	0
57	MG	14	3104	1/1	0.86	0.20	78,78,78,78	0
57	MG	1H	3191	1/1	0.86	0.24	58,58,58,58	0
57	MG	1H	3192	1/1	0.86	0.37	75,75,75,75	0
57	MG	1H	3132	1/1	0.86	0.22	65,65,65,65	0
57	MG	14	3159	1/1	0.86	0.20	79,79,79,79	0
57	MG	1H	3004	1/1	0.86	0.45	89,89,89,89	0
61	SPE	14	3436	13/13	0.86	0.20	83,88,93,94	0
57	MG	1H	3108	1/1	0.86	0.22	64,64,64,64	0
57	MG	14	3080	1/1	0.87	0.19	68,68,68,68	0
57	MG	1H	3101	1/1	0.87	0.32	78,78,78,78	0
57	MG	1H	3166	1/1	0.87	0.30	78,78,78,78	0
57	MG	1G	1627	1/1	0.87	0.21	87,87,87,87	0
57	MG	16	206	1/1	0.87	0.13	77,77,77,77	0
57	MG	16	207	1/1	0.87	0.25	74,74,74,74	0
57	MG	1H	3195	1/1	0.87	0.15	55,55,55,55	0
57	MG	16	209	1/1	0.87	0.22	76,76,76,76	0
57	MG	14	3031	1/1	0.87	0.20	73,73,73,73	0
57	MG	13	1650	1/1	0.87	0.30	75,75,75,75	0
57	MG	1H	3068	1/1	0.87	0.28	72,72,72,72	0
57	MG	14	3148	1/1	0.87	0.27	85,85,85,85	0
57	MG	14	3036	1/1	0.87	0.20	85,85,85,85	0
57	MG	14	3043	1/1	0.87	0.18	71,71,71,71	0
57	MG	14	3209	1/1	0.87	0.30	83,83,83,83	0
57	MG	14	3211	1/1	0.87	0.24	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3171	1/1	0.87	0.29	73,73,73,73	0
57	MG	1H	3202	1/1	0.87	0.27	73,73,73,73	0
57	MG	14	3381	1/1	0.87	0.23	79,79,79,79	0
57	MG	1H	3051	1/1	0.87	0.21	60,60,60,60	0
57	MG	1H	3173	1/1	0.87	0.10	59,59,59,59	0
57	MG	14	3428	1/1	0.87	0.14	119,119,119,119	0
57	MG	13	1601	1/1	0.87	0.28	80,80,80,80	0
57	MG	1H	3111	1/1	0.87	0.29	79,79,79,79	0
57	MG	1H	3011	1/1	0.87	0.23	56,56,56,56	0
57	MG	1H	3038	1/1	0.87	0.23	50,50,50,50	0
57	MG	1H	3212	1/1	0.87	0.10	65,65,65,65	0
57	MG	14	3066	1/1	0.87	0.25	61,61,61,61	0
57	MG	1H	3213	1/1	0.87	0.23	71,71,71,71	0
57	MG	13	1644	1/1	0.87	0.32	85,85,85,85	0
57	MG	1H	3093	1/1	0.87	0.10	56,56,56,56	0
57	MG	1H	3020	1/1	0.87	0.16	73,73,73,73	0
57	MG	1G	1621	1/1	0.88	0.28	82,82,82,82	0
57	MG	14	3063	1/1	0.88	0.18	67,67,67,67	0
57	MG	13	1662	1/1	0.88	0.35	89,89,89,89	0
57	MG	14	3180	1/1	0.88	0.30	91,91,91,91	0
57	MG	1H	3098	1/1	0.88	0.23	46,46,46,46	0
57	MG	14	3003	1/1	0.88	0.21	78,78,78,78	0
57	MG	14	3006	1/1	0.88	0.28	75,75,75,75	0
57	MG	14	3074	1/1	0.88	0.13	69,69,69,69	0
57	MG	5I	101	1/1	0.88	0.12	79,79,79,79	0
57	MG	14	3194	1/1	0.88	0.36	80,80,80,80	0
57	MG	14	3130	1/1	0.88	0.23	66,66,66,66	0
57	MG	1H	3225	1/1	0.88	0.28	71,71,71,71	0
57	MG	1H	3001	1/1	0.88	0.38	84,84,84,84	0
57	MG	1H	3013	1/1	0.88	0.19	40,40,40,40	0
57	MG	1H	3002	1/1	0.88	0.17	48,48,48,48	0
57	MG	14	3200	1/1	0.88	0.12	89,89,89,89	0
57	MG	13	1624	1/1	0.88	0.16	59,59,59,59	0
57	MG	14	3087	1/1	0.88	0.22	76,76,76,76	0
57	MG	1H	3025	1/1	0.88	0.24	75,75,75,75	0
57	MG	14	3090	1/1	0.88	0.23	86,86,86,86	0
57	MG	1H	3005	1/1	0.88	0.13	68,68,68,68	0
57	MG	14	3210	1/1	0.88	0.32	91,91,91,91	0
57	MG	1H	3211	1/1	0.88	0.30	78,78,78,78	0
57	MG	14	3033	1/1	0.88	0.26	80,80,80,80	0
57	MG	14	3350	1/1	0.88	0.12	101,101,101,101	0
57	MG	14	3098	1/1	0.88	0.25	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3240	1/1	0.88	0.24	73,73,73,73	0
57	MG	13	1666	1/1	0.88	0.22	85,85,85,85	0
57	MG	1H	3034	1/1	0.88	0.13	46,46,46,46	0
57	MG	14	3395	1/1	0.88	0.08	118,118,118,118	0
57	MG	1H	3214	1/1	0.88	0.32	77,77,77,77	0
57	MG	1H	3168	1/1	0.88	0.29	80,80,80,80	0
57	MG	14	3433	1/1	0.88	0.15	114,114,114,114	0
57	MG	14	3049	1/1	0.88	0.53	83,83,83,83	0
57	MG	13	1631	1/1	0.88	0.12	78,78,78,78	0
57	MG	1H	3196	1/1	0.88	0.17	77,77,77,77	0
57	MG	14	3162	1/1	0.88	0.41	74,74,74,74	0
57	MG	1H	3522	1/1	0.88	0.07	110,110,110,110	0
57	MG	14	3057	1/1	0.88	0.19	49,49,49,49	0
57	MG	14	3167	1/1	0.88	0.13	78,78,78,78	0
57	MG	13	1636	1/1	0.88	0.21	74,74,74,74	0
57	MG	42	201	1/1	0.88	0.23	120,120,120,120	0
57	MG	1H	3078	1/1	0.89	0.10	58,58,58,58	0
57	MG	13	1617	1/1	0.89	0.09	51,51,51,51	0
57	MG	88	203	1/1	0.89	0.22	79,79,79,79	0
57	MG	1H	3178	1/1	0.89	0.23	63,63,63,63	0
57	MG	1H	3161	1/1	0.89	0.20	67,67,67,67	0
57	MG	1H	3182	1/1	0.89	0.25	60,60,60,60	0
57	MG	1H	3238	1/1	0.89	0.31	80,80,80,80	0
57	MG	1H	3040	1/1	0.89	0.31	44,44,44,44	0
57	MG	14	3100	1/1	0.89	0.19	71,71,71,71	0
57	MG	1H	3188	1/1	0.89	0.23	49,49,49,49	0
57	MG	1H	3164	1/1	0.89	0.26	69,69,69,69	0
57	MG	14	3151	1/1	0.89	0.09	70,70,70,70	0
57	MG	14	3052	1/1	0.89	0.13	54,54,54,54	0
57	MG	1H	3041	1/1	0.89	0.14	51,51,51,51	0
57	MG	1G	1695	1/1	0.89	0.10	107,107,107,107	0
57	MG	1H	3376	1/1	0.89	0.15	66,66,66,66	0
57	MG	1H	3105	1/1	0.89	0.16	72,72,72,72	0
57	MG	1H	3167	1/1	0.89	0.41	98,98,98,98	0
57	MG	1G	1618	1/1	0.89	0.27	78,78,78,78	0
57	MG	13	1622	1/1	0.89	0.23	63,63,63,63	0
57	MG	14	3390	1/1	0.89	0.12	94,94,94,94	0
57	MG	1H	3056	1/1	0.89	0.23	49,49,49,49	0
57	MG	16	201	1/1	0.89	0.20	62,62,62,62	0
57	MG	14	3121	1/1	0.89	0.17	61,61,61,61	0
57	MG	13	1653	1/1	0.89	0.33	73,73,73,73	0
57	MG	14	3429	1/1	0.89	0.24	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	14	3013	1/1	0.89	0.16	47,47,47,47	0
57	MG	1H	3153	1/1	0.89	0.24	77,77,77,77	0
57	MG	14	3170	1/1	0.89	0.24	81,81,81,81	0
57	MG	1J	203	1/1	0.89	0.22	73,73,73,73	0
57	MG	14	3172	1/1	0.89	0.19	77,77,77,77	0
57	MG	1H	3200	1/1	0.89	0.37	71,71,71,71	0
57	MG	14	3126	1/1	0.89	0.17	72,72,72,72	0
57	MG	1H	3072	1/1	0.89	0.19	58,58,58,58	0
57	MG	1H	3049	1/1	0.89	0.14	62,62,62,62	0
57	MG	14	3022	1/1	0.89	0.15	81,81,81,81	0
61	SPE	1G	1703	13/13	0.89	0.12	90,107,113,114	0
57	MG	1H	3229	1/1	0.89	0.44	90,90,90,90	0
57	MG	1H	3063	1/1	0.89	0.21	100,100,100,100	0
57	MG	13	1704	1/1	0.90	0.10	106,106,106,106	0
57	MG	1H	3100	1/1	0.90	0.37	68,68,68,68	0
57	MG	14	3002	1/1	0.90	0.22	57,57,57,57	0
57	MG	13	1642	1/1	0.90	0.15	103,103,103,103	0
57	MG	13	1724	1/1	0.90	0.08	117,117,117,117	0
57	MG	14	3007	1/1	0.90	0.12	60,60,60,60	0
57	MG	14	3166	1/1	0.90	0.28	79,79,79,79	0
57	MG	14	3096	1/1	0.90	0.15	65,65,65,65	0
57	MG	1H	3139	1/1	0.90	0.21	71,71,71,71	0
57	MG	1G	1611	1/1	0.90	0.26	76,76,76,76	0
57	MG	13	1655	1/1	0.90	0.27	82,82,82,82	0
57	MG	1H	3017	1/1	0.90	0.19	62,62,62,62	0
57	MG	13	1672	1/1	0.90	0.20	88,88,88,88	0
57	MG	1H	3023	1/1	0.90	0.15	50,50,50,50	0
57	MG	1H	3244	1/1	0.90	0.27	74,74,74,74	0
57	MG	1H	3309	1/1	0.90	0.10	54,54,54,54	0
57	MG	14	3024	1/1	0.90	0.13	81,81,81,81	0
57	MG	14	3108	1/1	0.90	0.11	72,72,72,72	0
57	MG	14	3184	1/1	0.90	0.29	78,78,78,78	0
57	MG	1H	3175	1/1	0.90	0.20	64,64,64,64	0
57	MG	14	3026	1/1	0.90	0.18	56,56,56,56	0
57	MG	14	3027	1/1	0.90	0.23	66,66,66,66	0
57	MG	1H	3339	1/1	0.90	0.09	106,106,106,106	0
57	MG	1H	3367	1/1	0.90	0.08	66,66,66,66	0
57	MG	1H	3374	1/1	0.90	0.12	83,83,83,83	0
57	MG	14	3116	1/1	0.90	0.17	88,88,88,88	0
57	MG	14	3117	1/1	0.90	0.17	64,64,64,64	0
57	MG	1G	1624	1/1	0.90	0.19	95,95,95,95	0
57	MG	1H	3080	1/1	0.90	0.14	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	14	3039	1/1	0.90	0.18	89,89,89,89	0
57	MG	1H	3434	1/1	0.90	0.12	95,95,95,95	0
57	MG	13	1673	1/1	0.90	0.24	84,84,84,84	0
57	MG	1H	3082	1/1	0.90	0.20	71,71,71,71	0
57	MG	1H	3496	1/1	0.90	0.10	89,89,89,89	0
57	MG	1H	3116	1/1	0.90	0.20	53,53,53,53	0
57	MG	1H	3215	1/1	0.90	0.18	63,63,63,63	0
57	MG	13	1664	1/1	0.90	0.32	78,78,78,78	0
57	MG	14	3243	1/1	0.90	0.09	58,58,58,58	0
57	MG	14	3252	1/1	0.90	0.17	90,90,90,90	0
57	MG	14	3297	1/1	0.90	0.10	71,71,71,71	0
57	MG	14	3347	1/1	0.90	0.10	88,88,88,88	0
57	MG	1G	1636	1/1	0.90	0.19	90,90,90,90	0
57	MG	1H	3003	1/1	0.90	0.24	65,65,65,65	0
57	MG	14	3376	1/1	0.90	0.11	102,102,102,102	0
57	MG	14	3379	1/1	0.90	0.10	84,84,84,84	0
57	MG	13	1625	1/1	0.90	0.21	82,82,82,82	0
57	MG	1H	3124	1/1	0.90	0.16	61,61,61,61	0
57	MG	1H	3065	1/1	0.90	0.24	65,65,65,65	0
57	MG	13	1657	1/1	0.90	0.14	68,68,68,68	0
57	MG	14	3137	1/1	0.90	0.33	99,99,99,99	0
57	MG	14	3421	1/1	0.90	0.09	97,97,97,97	0
57	MG	1H	3162	1/1	0.90	0.10	60,60,60,60	0
57	MG	1H	3194	1/1	0.90	0.09	63,63,63,63	0
57	MG	14	3143	1/1	0.90	0.08	57,57,57,57	0
57	MG	14	3431	1/1	0.90	0.12	116,116,116,116	0
57	MG	14	3067	1/1	0.90	0.21	78,78,78,78	0
57	MG	13	1658	1/1	0.90	0.35	82,82,82,82	0
57	MG	14	3070	1/1	0.90	0.15	52,52,52,52	0
57	MG	14	3147	1/1	0.90	0.17	69,69,69,69	0
57	MG	1G	1671	1/1	0.90	0.14	112,112,112,112	0
57	MG	78	201	1/1	0.90	0.12	66,66,66,66	0
57	MG	1G	1678	1/1	0.90	0.12	111,111,111,111	0
57	MG	1H	3227	1/1	0.90	0.22	72,72,72,72	0
57	MG	14	3079	1/1	0.90	0.18	48,48,48,48	0
57	MG	88	202	1/1	0.90	0.18	66,66,66,66	0
57	MG	13	1603	1/1	0.90	0.16	74,74,74,74	0
57	MG	13	1614	1/1	0.90	0.24	84,84,84,84	0
57	MG	1H	3219	1/1	0.91	0.22	71,71,71,71	0
57	MG	13	1663	1/1	0.91	0.14	107,107,107,107	0
57	MG	14	3202	1/1	0.91	0.29	84,84,84,84	0
57	MG	14	3061	1/1	0.91	0.25	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3204	1/1	0.91	0.14	72,72,72,72	0
57	MG	13	1613	1/1	0.91	0.16	87,87,87,87	0
57	MG	14	3110	1/1	0.91	0.14	69,69,69,69	0
57	MG	1H	3074	1/1	0.91	0.21	64,64,64,64	0
57	MG	1H	3143	1/1	0.91	0.20	50,50,50,50	0
57	MG	13	1627	1/1	0.91	0.37	71,71,71,71	0
57	MG	1H	3125	1/1	0.91	0.15	56,56,56,56	0
57	MG	14	3214	1/1	0.91	0.42	80,80,80,80	0
57	MG	1G	1674	1/1	0.91	0.10	107,107,107,107	0
57	MG	1H	3186	1/1	0.91	0.27	62,62,62,62	0
57	MG	14	3277	1/1	0.91	0.17	84,84,84,84	0
57	MG	14	3291	1/1	0.91	0.08	85,85,85,85	0
57	MG	14	3029	1/1	0.91	0.18	57,57,57,57	0
57	MG	14	3030	1/1	0.91	0.26	57,57,57,57	0
57	MG	14	3120	1/1	0.91	0.23	78,78,78,78	0
57	MG	1H	3146	1/1	0.91	0.15	52,52,52,52	0
57	MG	1H	3392	1/1	0.91	0.09	48,48,48,48	0
57	MG	1H	3423	1/1	0.91	0.18	84,84,84,84	0
57	MG	14	3081	1/1	0.91	0.16	56,56,56,56	0
57	MG	14	3384	1/1	0.91	0.15	78,78,78,78	0
57	MG	1H	3076	1/1	0.91	0.23	72,72,72,72	0
57	MG	1H	3053	1/1	0.91	0.27	75,75,75,75	0
57	MG	1H	3149	1/1	0.91	0.19	55,55,55,55	0
57	MG	14	3085	1/1	0.91	0.19	88,88,88,88	0
57	MG	14	3417	1/1	0.91	0.10	108,108,108,108	0
57	MG	13	1608	1/1	0.91	0.13	76,76,76,76	0
57	MG	1H	3110	1/1	0.91	0.12	79,79,79,79	0
57	MG	14	3131	1/1	0.91	0.12	64,64,64,64	0
57	MG	14	3047	1/1	0.91	0.17	65,65,65,65	0
57	MG	1H	3092	1/1	0.91	0.19	61,61,61,61	0
57	MG	13	1629	1/1	0.91	0.15	72,72,72,72	0
57	MG	14	3434	1/1	0.91	0.11	110,110,110,110	0
57	MG	14	3050	1/1	0.91	0.18	57,57,57,57	0
57	MG	1G	1638	1/1	0.91	0.13	127,127,127,127	0
57	MG	14	3010	1/1	0.91	0.18	57,57,57,57	0
57	MG	1J	205	1/1	0.91	0.13	73,73,73,73	0
57	MG	14	3191	1/1	0.91	0.18	67,67,67,67	0
57	MG	19	301	1/1	0.91	0.19	48,48,48,48	0
57	MG	29	301	1/1	0.91	0.23	58,58,58,58	0
57	MG	14	3012	1/1	0.91	0.18	57,57,57,57	0
57	MG	14	3139	1/1	0.91	0.13	68,68,68,68	0
57	MG	14	3141	1/1	0.91	0.22	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	13	1607	1/1	0.91	0.18	72,72,72,72	0
60	ZN	G8	201	1/1	0.91	0.17	139,139,139,139	0
57	MG	14	3055	1/1	0.91	0.18	60,60,60,60	0
57	MG	1H	3058	1/1	0.91	0.15	60,60,60,60	0
57	MG	14	3016	1/1	0.91	0.21	74,74,74,74	0
57	MG	1G	1704	1/1	0.92	0.18	84,84,84,84	0
57	MG	1H	3348	1/1	0.92	0.10	111,111,111,111	0
57	MG	13	1723	1/1	0.92	0.07	128,128,128,128	0
57	MG	7A	101	1/1	0.92	0.19	114,114,114,114	0
57	MG	1G	1606	1/1	0.92	0.09	73,73,73,73	0
57	MG	1H	3181	1/1	0.92	0.17	65,65,65,65	0
57	MG	1H	3014	1/1	0.92	0.13	53,53,53,53	0
57	MG	1H	3037	1/1	0.92	0.34	75,75,75,75	0
57	MG	1H	3396	1/1	0.92	0.09	59,59,59,59	0
57	MG	1H	3414	1/1	0.92	0.10	105,105,105,105	0
57	MG	1H	3415	1/1	0.92	0.10	72,72,72,72	0
57	MG	14	3206	1/1	0.92	0.16	85,85,85,85	0
57	MG	14	3075	1/1	0.92	0.19	73,73,73,73	0
57	MG	1H	3419	1/1	0.92	0.14	86,86,86,86	0
57	MG	1G	1615	1/1	0.92	0.16	86,86,86,86	0
57	MG	1H	3422	1/1	0.92	0.26	65,65,65,65	0
57	MG	1H	3083	1/1	0.92	0.63	83,83,83,83	0
57	MG	1H	3096	1/1	0.92	0.12	64,64,64,64	0
57	MG	1H	3444	1/1	0.92	0.09	74,74,74,74	0
57	MG	1H	3210	1/1	0.92	0.12	56,56,56,56	0
57	MG	1H	3458	1/1	0.92	0.17	82,82,82,82	0
57	MG	14	3019	1/1	0.92	0.21	57,57,57,57	0
57	MG	14	3281	1/1	0.92	0.07	69,69,69,69	0
57	MG	1H	3468	1/1	0.92	0.16	82,82,82,82	0
57	MG	1H	3232	1/1	0.92	0.11	48,48,48,48	0
57	MG	14	3312	1/1	0.92	0.08	92,92,92,92	0
57	MG	1H	3112	1/1	0.92	0.21	55,55,55,55	0
57	MG	1H	3503	1/1	0.92	0.11	91,91,91,91	0
57	MG	14	3355	1/1	0.92	0.07	104,104,104,104	0
57	MG	1H	3516	1/1	0.92	0.10	102,102,102,102	0
57	MG	1H	3054	1/1	0.92	0.22	52,52,52,52	0
57	MG	1H	3152	1/1	0.92	0.22	70,70,70,70	0
57	MG	1H	3236	1/1	0.92	0.27	67,67,67,67	0
57	MG	1H	3045	1/1	0.92	0.19	46,46,46,46	0
57	MG	14	3387	1/1	0.92	0.11	83,83,83,83	0
57	MG	1H	3048	1/1	0.92	0.08	45,45,45,45	0
57	MG	16	204	1/1	0.92	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3155	1/1	0.92	0.18	55,55,55,55	0
57	MG	13	1649	1/1	0.92	0.28	75,75,75,75	0
57	MG	14	3398	1/1	0.92	0.07	76,76,76,76	0
57	MG	14	3409	1/1	0.92	0.19	88,88,88,88	0
57	MG	14	3416	1/1	0.92	0.10	102,102,102,102	0
57	MG	1H	3118	1/1	0.92	0.09	69,69,69,69	0
57	MG	14	3164	1/1	0.92	0.24	78,78,78,78	0
57	MG	14	3424	1/1	0.92	0.08	109,109,109,109	0
57	MG	14	3037	1/1	0.92	0.13	65,65,65,65	0
57	MG	1H	3103	1/1	0.92	0.23	61,61,61,61	0
57	MG	14	3040	1/1	0.92	0.13	68,68,68,68	0
57	MG	14	3042	1/1	0.92	0.12	65,65,65,65	0
57	MG	1H	3249	1/1	0.92	0.11	63,63,63,63	0
57	MG	21	302	1/1	0.92	0.13	72,72,72,72	0
57	MG	14	3171	1/1	0.92	0.18	56,56,56,56	0
57	MG	31	301	1/1	0.92	0.05	63,63,63,63	0
57	MG	14	3173	1/1	0.92	0.25	79,79,79,79	0
57	MG	1H	3270	1/1	0.92	0.09	50,50,50,50	0
57	MG	1H	3271	1/1	0.92	0.10	51,51,51,51	0
57	MG	1G	1667	1/1	0.92	0.07	103,103,103,103	0
57	MG	1H	3159	1/1	0.92	0.22	80,80,80,80	0
57	MG	14	3118	1/1	0.92	0.28	61,61,61,61	0
57	MG	1H	3310	1/1	0.92	0.09	70,70,70,70	0
57	MG	1H	3104	1/1	0.92	0.09	43,43,43,43	0
57	MG	13	1605	1/1	0.92	0.14	71,71,71,71	0
57	MG	1G	1693	1/1	0.92	0.06	129,129,129,129	0
57	MG	14	3190	1/1	0.92	0.22	59,59,59,59	0
57	MG	1G	1603	1/1	0.92	0.09	88,88,88,88	0
57	MG	1G	1698	1/1	0.92	0.09	123,123,123,123	0
57	MG	1H	3274	1/1	0.93	0.09	97,97,97,97	0
57	MG	1H	3489	1/1	0.93	0.21	73,73,73,73	0
57	MG	14	3150	1/1	0.93	0.07	63,63,63,63	0
57	MG	14	3044	1/1	0.93	0.12	57,57,57,57	0
57	MG	14	3212	1/1	0.93	0.32	75,75,75,75	0
57	MG	1G	1699	1/1	0.93	0.05	133,133,133,133	0
57	MG	1H	3208	1/1	0.93	0.22	72,72,72,72	0
57	MG	14	3215	1/1	0.93	0.59	86,86,86,86	0
57	MG	1H	3497	1/1	0.93	0.07	107,107,107,107	0
57	MG	14	3105	1/1	0.93	0.12	73,73,73,73	0
57	MG	14	3106	1/1	0.93	0.25	57,57,57,57	0
57	MG	1H	3228	1/1	0.93	0.11	60,60,60,60	0
57	MG	1H	3505	1/1	0.93	0.14	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3160	1/1	0.93	0.12	65,65,65,65	0
57	MG	13	1611	1/1	0.93	0.21	70,70,70,70	0
57	MG	14	3316	1/1	0.93	0.08	69,69,69,69	0
57	MG	1H	3059	1/1	0.93	0.18	56,56,56,56	0
57	MG	1H	3341	1/1	0.93	0.07	78,78,78,78	0
57	MG	13	1612	1/1	0.93	0.10	86,86,86,86	0
57	MG	1H	3352	1/1	0.93	0.08	57,57,57,57	0
57	MG	14	3005	1/1	0.93	0.17	54,54,54,54	0
57	MG	14	3377	1/1	0.93	0.09	131,131,131,131	0
57	MG	1H	3366	1/1	0.93	0.07	68,68,68,68	0
57	MG	1H	3140	1/1	0.93	0.18	54,54,54,54	0
57	MG	1H	3368	1/1	0.93	0.11	69,69,69,69	0
57	MG	14	3009	1/1	0.93	0.20	57,57,57,57	0
57	MG	13	1717	1/1	0.93	0.09	99,99,99,99	0
57	MG	14	3011	1/1	0.93	0.09	44,44,44,44	0
57	MG	1H	3142	1/1	0.93	0.24	68,68,68,68	0
57	MG	14	3174	1/1	0.93	0.09	89,89,89,89	0
57	MG	1H	3388	1/1	0.93	0.08	55,55,55,55	0
57	MG	14	3176	1/1	0.93	0.16	82,82,82,82	0
57	MG	14	3413	1/1	0.93	0.09	107,107,107,107	0
57	MG	1H	3391	1/1	0.93	0.09	89,89,89,89	0
57	MG	1H	3064	1/1	0.93	0.05	51,51,51,51	0
57	MG	1H	3395	1/1	0.93	0.17	68,68,68,68	0
57	MG	14	3073	1/1	0.93	0.15	78,78,78,78	0
57	MG	13	1652	1/1	0.93	0.37	71,71,71,71	0
57	MG	13	1606	1/1	0.93	0.15	72,72,72,72	0
57	MG	13	1728	1/1	0.93	0.06	117,117,117,117	0
57	MG	1H	3179	1/1	0.93	0.15	80,80,80,80	0
57	MG	14	3189	1/1	0.93	0.18	51,51,51,51	0
57	MG	1H	3241	1/1	0.93	0.14	58,58,58,58	0
57	MG	1J	201	1/1	0.93	0.24	73,73,73,73	0
57	MG	1H	3022	1/1	0.93	0.15	49,49,49,49	0
57	MG	1G	1643	1/1	0.93	0.35	83,83,83,83	0
57	MG	13	1732	1/1	0.93	0.07	114,114,114,114	0
57	MG	1H	3131	1/1	0.93	0.29	83,83,83,83	0
57	MG	1H	3099	1/1	0.93	0.20	56,56,56,56	0
57	MG	1H	3447	1/1	0.93	0.22	70,70,70,70	0
57	MG	1G	1669	1/1	0.93	0.10	105,105,105,105	0
57	MG	1H	3453	1/1	0.93	0.13	93,93,93,93	0
57	MG	13	1634	1/1	0.93	0.21	75,75,75,75	0
57	MG	13	1701	1/1	0.93	0.10	108,108,108,108	0
57	MG	1H	3484	1/1	0.93	0.08	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3095	1/1	0.93	0.09	62,62,62,62	0
57	MG	1G	1685	1/1	0.93	0.09	110,110,110,110	0
57	MG	1G	1686	1/1	0.93	0.07	106,106,106,106	0
57	MG	1H	3487	1/1	0.93	0.11	85,85,85,85	0
57	MG	1H	3300	1/1	0.94	0.09	62,62,62,62	0
57	MG	1H	3090	1/1	0.94	0.12	42,42,42,42	0
57	MG	1G	1668	1/1	0.94	0.06	124,124,124,124	0
57	MG	1H	3047	1/1	0.94	0.12	55,55,55,55	0
57	MG	1H	3026	1/1	0.94	0.18	55,55,55,55	0
57	MG	13	1727	1/1	0.94	0.13	90,90,90,90	0
57	MG	14	3221	1/1	0.94	0.07	62,62,62,62	0
57	MG	1H	3133	1/1	0.94	0.06	55,55,55,55	0
57	MG	1G	1676	1/1	0.94	0.07	93,93,93,93	0
57	MG	14	3254	1/1	0.94	0.07	77,77,77,77	0
57	MG	14	3264	1/1	0.94	0.07	93,93,93,93	0
57	MG	14	3276	1/1	0.94	0.10	120,120,120,120	0
57	MG	14	3038	1/1	0.94	0.15	52,52,52,52	0
57	MG	14	3279	1/1	0.94	0.07	58,58,58,58	0
57	MG	1H	3476	1/1	0.94	0.17	82,82,82,82	0
57	MG	1H	3477	1/1	0.94	0.10	83,83,83,83	0
57	MG	14	3041	1/1	0.94	0.17	55,55,55,55	0
57	MG	14	3298	1/1	0.94	0.07	86,86,86,86	0
57	MG	14	3307	1/1	0.94	0.07	66,66,66,66	0
57	MG	1H	3483	1/1	0.94	0.15	91,91,91,91	0
57	MG	1G	1688	1/1	0.94	0.16	113,113,113,113	0
57	MG	14	3318	1/1	0.94	0.08	89,89,89,89	0
57	MG	14	3346	1/1	0.94	0.07	99,99,99,99	0
57	MG	1G	1692	1/1	0.94	0.11	101,101,101,101	0
57	MG	13	1682	1/1	0.94	0.06	93,93,93,93	0
57	MG	14	3354	1/1	0.94	0.17	60,60,60,60	0
57	MG	13	1731	1/1	0.94	0.06	112,112,112,112	0
57	MG	1G	1697	1/1	0.94	0.05	128,128,128,128	0
57	MG	1H	3354	1/1	0.94	0.08	60,60,60,60	0
57	MG	1H	3362	1/1	0.94	0.10	100,100,100,100	0
57	MG	1H	3363	1/1	0.94	0.09	96,96,96,96	0
57	MG	1H	3015	1/1	0.94	0.17	51,51,51,51	0
57	MG	1H	3498	1/1	0.94	0.10	98,98,98,98	0
57	MG	14	3385	1/1	0.94	0.14	67,67,67,67	0
57	MG	52	201	1/1	0.94	0.06	129,129,129,129	0
57	MG	13	1714	1/1	0.94	0.06	122,122,122,122	0
57	MG	13	1736	1/1	0.94	0.07	101,101,101,101	0
57	MG	1H	3511	1/1	0.94	0.11	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3515	1/1	0.94	0.11	58,58,58,58	0
57	MG	1H	3372	1/1	0.94	0.06	89,89,89,89	0
57	MG	14	3407	1/1	0.94	0.07	123,123,123,123	0
57	MG	14	3408	1/1	0.94	0.10	92,92,92,92	0
57	MG	1H	3520	1/1	0.94	0.08	105,105,105,105	0
57	MG	14	3004	1/1	0.94	0.15	63,63,63,63	0
57	MG	14	3414	1/1	0.94	0.07	97,97,97,97	0
57	MG	1H	3218	1/1	0.94	0.17	37,37,37,37	0
57	MG	1H	3239	1/1	0.94	0.20	67,67,67,67	0
57	MG	14	3185	1/1	0.94	0.31	86,86,86,86	0
57	MG	14	3422	1/1	0.94	0.17	108,108,108,108	0
57	MG	1H	3524	1/1	0.94	0.14	81,81,81,81	0
57	MG	14	3425	1/1	0.94	0.19	91,91,91,91	0
57	MG	1H	3525	1/1	0.94	0.10	68,68,68,68	0
57	MG	14	3188	1/1	0.94	0.25	72,72,72,72	0
57	MG	1G	1629	1/1	0.94	0.21	85,85,85,85	0
57	MG	1H	3386	1/1	0.94	0.07	42,42,42,42	0
57	MG	14	3432	1/1	0.94	0.12	116,116,116,116	0
57	MG	3I	201	1/1	0.94	0.16	60,60,60,60	0
57	MG	1H	3389	1/1	0.94	0.12	88,88,88,88	0
57	MG	14	3193	1/1	0.94	0.06	45,45,45,45	0
57	MG	13	1700	1/1	0.94	0.11	102,102,102,102	0
57	MG	1H	3122	1/1	0.94	0.05	52,52,52,52	0
57	MG	13	1648	1/1	0.94	0.12	67,67,67,67	0
57	MG	1H	3073	1/1	0.94	0.16	66,66,66,66	0
57	MG	13	1646	1/1	0.94	0.14	71,71,71,71	0
57	MG	1H	3261	1/1	0.94	0.08	63,63,63,63	0
57	MG	1H	3268	1/1	0.94	0.07	59,59,59,59	0
57	MG	1H	3046	1/1	0.94	0.08	33,33,33,33	0
57	MG	1H	3184	1/1	0.94	0.14	70,70,70,70	0
57	MG	4I	201	1/1	0.94	0.09	69,69,69,69	0
57	MG	1H	3128	1/1	0.94	0.34	85,85,85,85	0
58	PAR	1G	1702	42/42	0.94	0.10	83,92,100,103	0
57	MG	1H	3443	1/1	0.94	0.14	75,75,75,75	0
57	MG	1G	1655	1/1	0.94	0.09	110,110,110,110	0
57	MG	14	3091	1/1	0.94	0.12	78,78,78,78	0
57	MG	14	3028	1/1	0.94	0.19	45,45,45,45	0
57	MG	1H	3344	1/1	0.95	0.06	103,103,103,103	0
57	MG	14	3295	1/1	0.95	0.07	60,60,60,60	0
57	MG	2K	102	1/1	0.95	0.10	78,78,78,78	0
57	MG	14	3001	1/1	0.95	0.06	57,57,57,57	0
57	MG	1H	3350	1/1	0.95	0.10	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3042	1/1	0.95	0.16	65,65,65,65	0
57	MG	1H	3457	1/1	0.95	0.16	84,84,84,84	0
57	MG	2I	301	1/1	0.95	0.14	59,59,59,59	0
57	MG	14	3328	1/1	0.95	0.06	81,81,81,81	0
57	MG	14	3334	1/1	0.95	0.06	60,60,60,60	0
57	MG	14	3342	1/1	0.95	0.05	113,113,113,113	0
57	MG	1H	3021	1/1	0.95	0.09	49,49,49,49	0
57	MG	1H	3462	1/1	0.95	0.10	94,94,94,94	0
57	MG	13	1623	1/1	0.95	0.14	76,76,76,76	0
57	MG	1H	3010	1/1	0.95	0.28	39,39,39,39	0
57	MG	14	3179	1/1	0.95	0.06	77,77,77,77	0
57	MG	14	3362	1/1	0.95	0.05	114,114,114,114	0
57	MG	13	1712	1/1	0.95	0.09	89,89,89,89	0
57	MG	14	3372	1/1	0.95	0.07	86,86,86,86	0
57	MG	14	3373	1/1	0.95	0.10	65,65,65,65	0
57	MG	1H	3479	1/1	0.95	0.15	83,83,83,83	0
57	MG	14	3182	1/1	0.95	0.13	74,74,74,74	0
57	MG	14	3068	1/1	0.95	0.27	53,53,53,53	0
57	MG	13	1726	1/1	0.95	0.10	74,74,74,74	0
57	MG	13	1739	1/1	0.95	0.05	121,121,121,121	0
57	MG	14	3014	1/1	0.95	0.13	59,59,59,59	0
57	MG	P8	101	1/1	0.95	0.32	71,71,71,71	0
57	MG	14	3388	1/1	0.95	0.05	85,85,85,85	0
57	MG	1G	1645	1/1	0.95	0.08	81,81,81,81	0
57	MG	1G	1650	1/1	0.95	0.09	101,101,101,101	0
57	MG	1H	3267	1/1	0.95	0.14	56,56,56,56	0
57	MG	1H	3373	1/1	0.95	0.07	80,80,80,80	0
57	MG	14	3078	1/1	0.95	0.21	56,56,56,56	0
57	MG	14	3402	1/1	0.95	0.06	78,78,78,78	0
57	MG	1G	1662	1/1	0.95	0.07	91,91,91,91	0
57	MG	13	1632	1/1	0.95	0.08	78,78,78,78	0
57	MG	1G	1666	1/1	0.95	0.08	100,100,100,100	0
57	MG	1H	3492	1/1	0.95	0.15	78,78,78,78	0
57	MG	1H	3375	1/1	0.95	0.07	79,79,79,79	0
57	MG	1H	3032	1/1	0.95	0.11	47,47,47,47	0
57	MG	1H	3123	1/1	0.95	0.25	65,65,65,65	0
57	MG	1H	3500	1/1	0.95	0.10	94,94,94,94	0
57	MG	13	1708	1/1	0.95	0.08	65,65,65,65	0
57	MG	14	3423	1/1	0.95	0.06	120,120,120,120	0
57	MG	1H	3277	1/1	0.95	0.07	71,71,71,71	0
57	MG	1G	1677	1/1	0.95	0.14	92,92,92,92	0
57	MG	14	3426	1/1	0.95	0.13	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3427	1/1	0.95	0.08	65,65,65,65	0
57	MG	14	3092	1/1	0.95	0.16	66,66,66,66	0
57	MG	14	3205	1/1	0.95	0.23	59,59,59,59	0
57	MG	1H	3508	1/1	0.95	0.06	117,117,117,117	0
57	MG	1H	3390	1/1	0.95	0.12	64,64,64,64	0
57	MG	14	3034	1/1	0.95	0.22	40,40,40,40	0
57	MG	1H	3283	1/1	0.95	0.10	71,71,71,71	0
57	MG	1H	3293	1/1	0.95	0.08	73,73,73,73	0
57	MG	14	3435	1/1	0.95	0.12	92,92,92,92	0
57	MG	1G	1690	1/1	0.95	0.05	117,117,117,117	0
57	MG	1H	3519	1/1	0.95	0.06	116,116,116,116	0
57	MG	1H	3298	1/1	0.95	0.07	51,51,51,51	0
57	MG	1G	1619	1/1	0.95	0.08	102,102,102,102	0
57	MG	1G	1696	1/1	0.95	0.07	128,128,128,128	0
57	MG	1H	3016	1/1	0.95	0.13	44,44,44,44	0
57	MG	1J	207	1/1	0.95	0.08	97,97,97,97	0
57	MG	1J	208	1/1	0.95	0.07	103,103,103,103	0
57	MG	14	3233	1/1	0.95	0.12	65,65,65,65	0
57	MG	14	3236	1/1	0.95	0.11	44,44,44,44	0
57	MG	39	301	1/1	0.95	0.15	89,89,89,89	0
57	MG	1H	3036	1/1	0.95	0.06	37,37,37,37	0
57	MG	1H	3199	1/1	0.95	0.07	61,61,61,61	0
57	MG	13	1729	1/1	0.95	0.07	110,110,110,110	0
57	MG	1H	3331	1/1	0.95	0.10	70,70,70,70	0
58	PAR	13	1741	42/42	0.95	0.08	64,71,75,82	0
57	MG	1H	3334	1/1	0.95	0.07	77,77,77,77	0
57	MG	1G	1626	1/1	0.95	0.12	83,83,83,83	0
57	MG	1H	3018	1/1	0.95	0.15	41,41,41,41	0
57	MG	1H	3019	1/1	0.95	0.13	32,32,32,32	0
57	MG	14	3285	1/1	0.95	0.09	108,108,108,108	0
57	MG	13	1604	1/1	0.96	0.09	62,62,62,62	0
57	MG	14	3317	1/1	0.96	0.11	82,82,82,82	0
57	MG	1G	1632	1/1	0.96	0.06	91,91,91,91	0
57	MG	14	3326	1/1	0.96	0.05	77,77,77,77	0
57	MG	1H	3380	1/1	0.96	0.13	55,55,55,55	0
57	MG	14	3329	1/1	0.96	0.05	105,105,105,105	0
57	MG	14	3330	1/1	0.96	0.07	94,94,94,94	0
57	MG	14	3332	1/1	0.96	0.05	102,102,102,102	0
57	MG	1H	3383	1/1	0.96	0.13	68,68,68,68	0
57	MG	14	3335	1/1	0.96	0.06	81,81,81,81	0
57	MG	14	3339	1/1	0.96	0.07	107,107,107,107	0
57	MG	16	210	1/1	0.96	0.06	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3343	1/1	0.96	0.07	80,80,80,80	0
57	MG	1H	3121	1/1	0.96	0.18	39,39,39,39	0
57	MG	1H	3469	1/1	0.96	0.08	58,58,58,58	0
57	MG	1H	3470	1/1	0.96	0.08	83,83,83,83	0
57	MG	1H	3475	1/1	0.96	0.09	97,97,97,97	0
57	MG	13	1609	1/1	0.96	0.13	70,70,70,70	0
57	MG	14	3357	1/1	0.96	0.06	105,105,105,105	0
57	MG	14	3065	1/1	0.96	0.07	47,47,47,47	0
57	MG	14	3363	1/1	0.96	0.06	107,107,107,107	0
57	MG	13	1638	1/1	0.96	0.07	85,85,85,85	0
57	MG	14	3367	1/1	0.96	0.07	106,106,106,106	0
57	MG	14	3368	1/1	0.96	0.08	88,88,88,88	0
57	MG	14	3369	1/1	0.96	0.07	91,91,91,91	0
57	MG	1H	3138	1/1	0.96	0.12	54,54,54,54	0
57	MG	1H	3481	1/1	0.96	0.07	103,103,103,103	0
57	MG	1H	3185	1/1	0.96	0.28	64,64,64,64	0
57	MG	1H	3351	1/1	0.96	0.06	68,68,68,68	0
57	MG	1G	1646	1/1	0.96	0.06	86,86,86,86	0
57	MG	Q8	300	1/1	0.96	0.15	80,80,80,80	0
57	MG	14	3382	1/1	0.96	0.10	66,66,66,66	0
57	MG	1G	1653	1/1	0.96	0.06	97,97,97,97	0
57	MG	1G	1601	1/1	0.96	0.09	77,77,77,77	0
57	MG	14	3386	1/1	0.96	0.10	74,74,74,74	0
57	MG	13	1619	1/1	0.96	0.10	52,52,52,52	0
57	MG	1G	1660	1/1	0.96	0.07	74,74,74,74	0
57	MG	1G	1661	1/1	0.96	0.06	95,95,95,95	0
57	MG	13	1730	1/1	0.96	0.08	94,94,94,94	0
57	MG	1H	3400	1/1	0.96	0.06	53,53,53,53	0
57	MG	14	3021	1/1	0.96	0.20	38,38,38,38	0
57	MG	14	3140	1/1	0.96	0.04	51,51,51,51	0
57	MG	14	3399	1/1	0.96	0.08	123,123,123,123	0
57	MG	14	3400	1/1	0.96	0.06	108,108,108,108	0
57	MG	14	3401	1/1	0.96	0.11	110,110,110,110	0
57	MG	1H	3405	1/1	0.96	0.05	66,66,66,66	0
57	MG	14	3403	1/1	0.96	0.14	84,84,84,84	0
57	MG	14	3404	1/1	0.96	0.13	97,97,97,97	0
57	MG	14	3406	1/1	0.96	0.11	101,101,101,101	0
57	MG	1H	3407	1/1	0.96	0.09	72,72,72,72	0
57	MG	1H	3357	1/1	0.96	0.06	52,52,52,52	0
57	MG	1H	3358	1/1	0.96	0.10	45,45,45,45	0
57	MG	14	3412	1/1	0.96	0.06	97,97,97,97	0
57	MG	14	3086	1/1	0.96	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3416	1/1	0.96	0.06	89,89,89,89	0
57	MG	1G	1672	1/1	0.96	0.08	110,110,110,110	0
57	MG	14	3089	1/1	0.96	0.21	54,54,54,54	0
57	MG	14	3418	1/1	0.96	0.05	90,90,90,90	0
57	MG	14	3420	1/1	0.96	0.05	107,107,107,107	0
57	MG	1H	3417	1/1	0.96	0.16	83,83,83,83	0
57	MG	1H	3418	1/1	0.96	0.05	46,46,46,46	0
57	MG	13	1720	1/1	0.96	0.10	109,109,109,109	0
57	MG	1H	3421	1/1	0.96	0.06	82,82,82,82	0
57	MG	1H	3512	1/1	0.96	0.09	87,87,87,87	0
57	MG	1G	1682	1/1	0.96	0.05	123,123,123,123	0
57	MG	1G	1684	1/1	0.96	0.10	96,96,96,96	0
57	MG	1H	3285	1/1	0.96	0.14	55,55,55,55	0
57	MG	14	3222	1/1	0.96	0.11	59,59,59,59	0
57	MG	14	3230	1/1	0.96	0.07	63,63,63,63	0
57	MG	13	1721	1/1	0.96	0.09	106,106,106,106	0
57	MG	14	3158	1/1	0.96	0.06	66,66,66,66	0
57	MG	14	3237	1/1	0.96	0.10	51,51,51,51	0
57	MG	1H	3425	1/1	0.96	0.08	64,64,64,64	0
57	MG	1H	3428	1/1	0.96	0.08	89,89,89,89	0
57	MG	1G	1691	1/1	0.96	0.05	133,133,133,133	0
57	MG	14	3257	1/1	0.96	0.07	69,69,69,69	0
57	MG	14	3259	1/1	0.96	0.10	71,71,71,71	0
57	MG	14	3263	1/1	0.96	0.09	71,71,71,71	0
57	MG	1H	3431	1/1	0.96	0.06	98,98,98,98	0
57	MG	14	3271	1/1	0.96	0.05	94,94,94,94	0
57	MG	13	1722	1/1	0.96	0.06	87,87,87,87	0
57	MG	1H	3523	1/1	0.96	0.11	82,82,82,82	0
57	MG	1H	3440	1/1	0.96	0.06	92,92,92,92	0
57	MG	13	1737	1/1	0.96	0.12	99,99,99,99	0
57	MG	14	3284	1/1	0.96	0.07	72,72,72,72	0
57	MG	13	1706	1/1	0.96	0.05	117,117,117,117	0
57	MG	14	3286	1/1	0.96	0.08	73,73,73,73	0
57	MG	13	1680	1/1	0.96	0.08	64,64,64,64	0
57	MG	45	202	1/1	0.96	0.23	64,64,64,64	0
57	MG	C5	201	1/1	0.96	0.07	113,113,113,113	0
57	MG	14	3292	1/1	0.96	0.09	74,74,74,74	0
57	MG	M5	101	1/1	0.96	0.17	88,88,88,88	0
57	MG	1G	1700	1/1	0.96	0.06	109,109,109,109	0
57	MG	14	3296	1/1	0.96	0.06	72,72,72,72	0
57	MG	1H	3035	1/1	0.96	0.05	40,40,40,40	0
57	MG	1H	3062	1/1	0.96	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1H	3454	1/1	0.96	0.05	111,111,111,111	0
57	MG	1H	3455	1/1	0.96	0.07	76,76,76,76	0
57	MG	13	1710	1/1	0.97	0.05	96,96,96,96	0
57	MG	1H	3343	1/1	0.97	0.05	78,78,78,78	0
57	MG	14	3313	1/1	0.97	0.04	105,105,105,105	0
57	MG	14	3314	1/1	0.97	0.09	69,69,69,69	0
57	MG	1H	3499	1/1	0.97	0.04	112,112,112,112	0
57	MG	1H	3408	1/1	0.97	0.07	67,67,67,67	0
57	MG	1H	3501	1/1	0.97	0.09	90,90,90,90	0
57	MG	14	3319	1/1	0.97	0.06	95,95,95,95	0
57	MG	14	3322	1/1	0.97	0.08	58,58,58,58	0
57	MG	14	3323	1/1	0.97	0.07	81,81,81,81	0
57	MG	1H	3502	1/1	0.97	0.18	141,141,141,141	0
57	MG	1H	3410	1/1	0.97	0.11	83,83,83,83	0
57	MG	1H	3504	1/1	0.97	0.04	109,109,109,109	0
57	MG	1H	3412	1/1	0.97	0.10	75,75,75,75	0
57	MG	1H	3506	1/1	0.97	0.07	106,106,106,106	0
57	MG	13	1711	1/1	0.97	0.07	74,74,74,74	0
57	MG	1H	3346	1/1	0.97	0.05	92,92,92,92	0
57	MG	14	3336	1/1	0.97	0.06	94,94,94,94	0
57	MG	14	3337	1/1	0.97	0.09	104,104,104,104	0
57	MG	13	1698	1/1	0.97	0.06	83,83,83,83	0
57	MG	1H	3513	1/1	0.97	0.06	53,53,53,53	0
57	MG	1H	3245	1/1	0.97	0.06	47,47,47,47	0
57	MG	14	3344	1/1	0.97	0.06	93,93,93,93	0
57	MG	14	3345	1/1	0.97	0.09	99,99,99,99	0
57	MG	1H	3115	1/1	0.97	0.06	61,61,61,61	0
57	MG	1H	3251	1/1	0.97	0.07	48,48,48,48	0
57	MG	14	3348	1/1	0.97	0.06	96,96,96,96	0
57	MG	1H	3420	1/1	0.97	0.04	69,69,69,69	0
57	MG	1H	3256	1/1	0.97	0.06	47,47,47,47	0
57	MG	1H	3355	1/1	0.97	0.06	59,59,59,59	0
57	MG	1H	3356	1/1	0.97	0.06	54,54,54,54	0
57	MG	14	3359	1/1	0.97	0.05	93,93,93,93	0
57	MG	14	3360	1/1	0.97	0.05	96,96,96,96	0
57	MG	1H	3094	1/1	0.97	0.03	33,33,33,33	0
57	MG	13	1618	1/1	0.97	0.09	48,48,48,48	0
57	MG	13	1621	1/1	0.97	0.13	85,85,85,85	0
57	MG	1H	3432	1/1	0.97	0.06	93,93,93,93	0
57	MG	1H	3433	1/1	0.97	0.14	72,72,72,72	0
57	MG	1H	3097	1/1	0.97	0.05	65,65,65,65	0
57	MG	14	3370	1/1	0.97	0.07	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1G	1647	1/1	0.97	0.06	97,97,97,97	0
57	MG	1G	1648	1/1	0.97	0.09	115,115,115,115	0
57	MG	14	3375	1/1	0.97	0.04	93,93,93,93	0
57	MG	1G	1649	1/1	0.97	0.08	113,113,113,113	0
57	MG	1H	3435	1/1	0.97	0.10	62,62,62,62	0
57	MG	1G	1652	1/1	0.97	0.08	81,81,81,81	0
57	MG	14	3380	1/1	0.97	0.04	78,78,78,78	0
57	MG	1H	3437	1/1	0.97	0.07	92,92,92,92	0
57	MG	13	1703	1/1	0.97	0.06	70,70,70,70	0
57	MG	14	3383	1/1	0.97	0.06	90,90,90,90	0
57	MG	1H	3441	1/1	0.97	0.07	105,105,105,105	0
57	MG	1G	1656	1/1	0.97	0.06	100,100,100,100	0
57	MG	1G	1657	1/1	0.97	0.04	121,121,121,121	0
57	MG	1G	1659	1/1	0.97	0.05	115,115,115,115	0
57	MG	1H	3442	1/1	0.97	0.07	103,103,103,103	0
57	MG	13	1733	1/1	0.97	0.09	101,101,101,101	0
57	MG	13	1683	1/1	0.97	0.05	93,93,93,93	0
57	MG	13	1685	1/1	0.97	0.06	90,90,90,90	0
57	MG	13	1738	1/1	0.97	0.04	133,133,133,133	0
57	MG	14	3396	1/1	0.97	0.04	126,126,126,126	0
57	MG	14	3397	1/1	0.97	0.11	96,96,96,96	0
57	MG	13	1707	1/1	0.97	0.05	56,56,56,56	0
57	MG	1H	3190	1/1	0.97	0.35	91,91,91,91	0
57	MG	1H	3299	1/1	0.97	0.06	48,48,48,48	0
57	MG	1G	1670	1/1	0.97	0.05	134,134,134,134	0
57	MG	1H	3378	1/1	0.97	0.07	50,50,50,50	0
57	MG	1H	3379	1/1	0.97	0.05	73,73,73,73	0
57	MG	13	1740	1/1	0.97	0.05	98,98,98,98	0
57	MG	14	3405	1/1	0.97	0.04	108,108,108,108	0
57	MG	18	101	1/1	0.97	0.05	85,85,85,85	0
57	MG	1G	1675	1/1	0.97	0.05	103,103,103,103	0
57	MG	1H	3301	1/1	0.97	0.05	45,45,45,45	0
57	MG	1H	3384	1/1	0.97	0.10	67,67,67,67	0
57	MG	14	3410	1/1	0.97	0.05	85,85,85,85	0
57	MG	1H	3027	1/1	0.97	0.10	52,52,52,52	0
57	MG	14	3218	1/1	0.97	0.05	65,65,65,65	0
57	MG	1G	1679	1/1	0.97	0.09	94,94,94,94	0
57	MG	14	3415	1/1	0.97	0.12	103,103,103,103	0
57	MG	1G	1680	1/1	0.97	0.05	123,123,123,123	0
57	MG	14	3223	1/1	0.97	0.10	87,87,87,87	0
57	MG	14	3225	1/1	0.97	0.05	73,73,73,73	0
57	MG	14	3419	1/1	0.97	0.04	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3228	1/1	0.97	0.07	56,56,56,56	0
57	MG	1H	3474	1/1	0.97	0.07	93,93,93,93	0
57	MG	13	1691	1/1	0.97	0.07	92,92,92,92	0
57	MG	14	3056	1/1	0.97	0.09	54,54,54,54	0
57	MG	1H	3316	1/1	0.97	0.08	78,78,78,78	0
57	MG	14	3238	1/1	0.97	0.06	50,50,50,50	0
57	MG	1H	3317	1/1	0.97	0.06	66,66,66,66	0
57	MG	14	3244	1/1	0.97	0.06	54,54,54,54	0
57	MG	14	3245	1/1	0.97	0.05	63,63,63,63	0
57	MG	1G	1687	1/1	0.97	0.04	111,111,111,111	0
57	MG	1H	3478	1/1	0.97	0.04	101,101,101,101	0
57	MG	14	3255	1/1	0.97	0.13	79,79,79,79	0
57	MG	14	3256	1/1	0.97	0.08	83,83,83,83	0
57	MG	1G	1689	1/1	0.97	0.05	116,116,116,116	0
57	MG	14	3258	1/1	0.97	0.05	79,79,79,79	0
57	MG	14	3062	1/1	0.97	0.13	59,59,59,59	0
57	MG	1G	1607	1/1	0.97	0.10	86,86,86,86	0
57	MG	1H	3030	1/1	0.97	0.05	39,39,39,39	0
57	MG	14	3265	1/1	0.97	0.08	91,91,91,91	0
57	MG	14	3266	1/1	0.97	0.04	107,107,107,107	0
57	MG	14	3268	1/1	0.97	0.07	82,82,82,82	0
57	MG	1H	3329	1/1	0.97	0.05	85,85,85,85	0
57	MG	14	3275	1/1	0.97	0.06	65,65,65,65	0
57	MG	1H	3482	1/1	0.97	0.05	94,94,94,94	0
57	MG	1G	1694	1/1	0.97	0.06	113,113,113,113	0
57	MG	14	3278	1/1	0.97	0.04	102,102,102,102	0
57	MG	1H	3394	1/1	0.97	0.06	49,49,49,49	0
57	MG	1H	3031	1/1	0.97	0.06	51,51,51,51	0
57	MG	1H	3486	1/1	0.97	0.08	95,95,95,95	0
57	MG	14	3071	1/1	0.97	0.11	74,74,74,74	0
57	MG	13	1725	1/1	0.97	0.04	115,115,115,115	0
57	MG	1H	3397	1/1	0.97	0.08	51,51,51,51	0
57	MG	13	1694	1/1	0.97	0.12	82,82,82,82	0
57	MG	14	3293	1/1	0.97	0.06	63,63,63,63	0
57	MG	1G	1701	1/1	0.97	0.04	111,111,111,111	0
57	MG	1H	3490	1/1	0.97	0.07	89,89,89,89	0
57	MG	1H	3403	1/1	0.97	0.05	99,99,99,99	0
60	ZN	C5	202	1/1	0.97	0.04	165,165,165,165	0
57	MG	1H	3404	1/1	0.97	0.06	71,71,71,71	0
57	MG	14	3299	1/1	0.97	0.05	79,79,79,79	0
57	MG	14	3304	1/1	0.97	0.07	74,74,74,74	0
57	MG	14	3325	1/1	0.98	0.06	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	13	1735	1/1	0.98	0.06	100,100,100,100	0
57	MG	13	1688	1/1	0.98	0.05	109,109,109,109	0
57	MG	1H	3303	1/1	0.98	0.05	48,48,48,48	0
57	MG	1H	3307	1/1	0.98	0.06	44,44,44,44	0
57	MG	14	3331	1/1	0.98	0.11	90,90,90,90	0
57	MG	1H	3308	1/1	0.98	0.05	50,50,50,50	0
57	MG	13	1684	1/1	0.98	0.04	85,85,85,85	0
57	MG	1H	3393	1/1	0.98	0.04	50,50,50,50	0
57	MG	1H	3491	1/1	0.98	0.12	70,70,70,70	0
57	MG	13	1681	1/1	0.98	0.05	59,59,59,59	0
57	MG	14	3338	1/1	0.98	0.04	107,107,107,107	0
57	MG	1H	3494	1/1	0.98	0.09	72,72,72,72	0
57	MG	1H	3314	1/1	0.98	0.05	68,68,68,68	0
57	MG	1H	3246	1/1	0.98	0.04	55,55,55,55	0
57	MG	1H	3248	1/1	0.98	0.05	44,44,44,44	0
57	MG	1H	3318	1/1	0.98	0.07	59,59,59,59	0
57	MG	1H	3401	1/1	0.98	0.05	64,64,64,64	0
57	MG	13	1713	1/1	0.98	0.04	86,86,86,86	0
57	MG	1H	3323	1/1	0.98	0.10	57,57,57,57	0
57	MG	14	3349	1/1	0.98	0.05	83,83,83,83	0
57	MG	1H	3324	1/1	0.98	0.07	70,70,70,70	0
57	MG	14	3351	1/1	0.98	0.05	78,78,78,78	0
57	MG	14	3353	1/1	0.98	0.05	83,83,83,83	0
57	MG	1H	3250	1/1	0.98	0.06	41,41,41,41	0
57	MG	1H	3330	1/1	0.98	0.06	71,71,71,71	0
57	MG	1H	3409	1/1	0.98	0.04	85,85,85,85	0
57	MG	1H	3507	1/1	0.98	0.04	57,57,57,57	0
57	MG	13	1695	1/1	0.98	0.04	106,106,106,106	0
57	MG	1H	3509	1/1	0.98	0.04	47,47,47,47	0
57	MG	1H	3332	1/1	0.98	0.11	102,102,102,102	0
57	MG	14	3364	1/1	0.98	0.07	92,92,92,92	0
57	MG	14	3365	1/1	0.98	0.04	78,78,78,78	0
57	MG	1H	3253	1/1	0.98	0.05	42,42,42,42	0
57	MG	1H	3335	1/1	0.98	0.04	48,48,48,48	0
57	MG	1G	1651	1/1	0.98	0.06	76,76,76,76	0
57	MG	1H	3514	1/1	0.98	0.04	98,98,98,98	0
57	MG	1H	3336	1/1	0.98	0.04	62,62,62,62	0
57	MG	14	3371	1/1	0.98	0.05	107,107,107,107	0
57	MG	13	1716	1/1	0.98	0.05	71,71,71,71	0
57	MG	1H	3518	1/1	0.98	0.05	96,96,96,96	0
57	MG	14	3374	1/1	0.98	0.06	92,92,92,92	0
57	MG	1H	3340	1/1	0.98	0.05	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3260	1/1	0.98	0.06	42,42,42,42	0
57	MG	1G	1658	1/1	0.98	0.03	104,104,104,104	0
57	MG	14	3378	1/1	0.98	0.07	92,92,92,92	0
57	MG	14	3219	1/1	0.98	0.04	57,57,57,57	0
57	MG	14	3220	1/1	0.98	0.05	54,54,54,54	0
57	MG	13	1696	1/1	0.98	0.07	93,93,93,93	0
57	MG	1H	3264	1/1	0.98	0.15	50,50,50,50	0
57	MG	1H	3266	1/1	0.98	0.04	54,54,54,54	0
57	MG	14	3224	1/1	0.98	0.06	45,45,45,45	0
57	MG	1H	3347	1/1	0.98	0.10	67,67,67,67	0
57	MG	14	3227	1/1	0.98	0.04	58,58,58,58	0
57	MG	1H	3424	1/1	0.98	0.04	101,101,101,101	0
57	MG	1G	1664	1/1	0.98	0.08	80,80,80,80	0
57	MG	14	3389	1/1	0.98	0.04	93,93,93,93	0
57	MG	14	3231	1/1	0.98	0.07	55,55,55,55	0
57	MG	14	3045	1/1	0.98	0.15	53,53,53,53	0
57	MG	14	3392	1/1	0.98	0.04	63,63,63,63	0
57	MG	14	3234	1/1	0.98	0.06	57,57,57,57	0
57	MG	13	1718	1/1	0.98	0.07	90,90,90,90	0
57	MG	1H	3427	1/1	0.98	0.11	67,67,67,67	0
57	MG	1H	3039	1/1	0.98	0.13	33,33,33,33	0
57	MG	14	3241	1/1	0.98	0.05	78,78,78,78	0
57	MG	1H	3430	1/1	0.98	0.07	73,73,73,73	0
57	MG	2K	101	1/1	0.98	0.09	100,100,100,100	0
57	MG	13	1697	1/1	0.98	0.07	84,84,84,84	0
57	MG	14	3249	1/1	0.98	0.06	52,52,52,52	0
57	MG	14	3251	1/1	0.98	0.05	80,80,80,80	0
57	MG	1H	3273	1/1	0.98	0.10	78,78,78,78	0
57	MG	13	1687	1/1	0.98	0.04	103,103,103,103	0
57	MG	1H	3276	1/1	0.98	0.03	78,78,78,78	0
57	MG	1H	3107	1/1	0.98	0.06	60,60,60,60	0
57	MG	1H	3281	1/1	0.98	0.09	61,61,61,61	0
57	MG	1H	3359	1/1	0.98	0.06	44,44,44,44	0
57	MG	1H	3360	1/1	0.98	0.04	78,78,78,78	0
57	MG	14	3260	1/1	0.98	0.08	106,106,106,106	0
57	MG	1H	3361	1/1	0.98	0.04	52,52,52,52	0
57	MG	1H	3028	1/1	0.98	0.10	67,67,67,67	0
57	MG	1G	1681	1/1	0.98	0.05	96,96,96,96	0
57	MG	1H	3284	1/1	0.98	0.04	83,83,83,83	0
57	MG	14	3267	1/1	0.98	0.06	82,82,82,82	0
57	MG	1G	1683	1/1	0.98	0.10	121,121,121,121	0
57	MG	14	3269	1/1	0.98	0.10	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3270	1/1	0.98	0.05	67,67,67,67	0
57	MG	1H	3446	1/1	0.98	0.05	98,98,98,98	0
57	MG	1H	3091	1/1	0.98	0.17	41,41,41,41	0
57	MG	1H	3449	1/1	0.98	0.05	80,80,80,80	0
57	MG	1H	3451	1/1	0.98	0.03	102,102,102,102	0
57	MG	1H	3452	1/1	0.98	0.09	72,72,72,72	0
57	MG	1H	3287	1/1	0.98	0.05	71,71,71,71	0
57	MG	1H	3289	1/1	0.98	0.05	59,59,59,59	0
57	MG	14	3282	1/1	0.98	0.06	90,90,90,90	0
57	MG	14	3283	1/1	0.98	0.08	68,68,68,68	0
57	MG	1H	3369	1/1	0.98	0.04	44,44,44,44	0
57	MG	1H	3370	1/1	0.98	0.09	68,68,68,68	0
57	MG	1H	3371	1/1	0.98	0.07	56,56,56,56	0
57	MG	14	3287	1/1	0.98	0.04	88,88,88,88	0
57	MG	14	3288	1/1	0.98	0.07	49,49,49,49	0
57	MG	14	3289	1/1	0.98	0.04	74,74,74,74	0
57	MG	14	3290	1/1	0.98	0.07	59,59,59,59	0
57	MG	1H	3459	1/1	0.98	0.05	75,75,75,75	0
57	MG	1H	3460	1/1	0.98	0.04	96,96,96,96	0
57	MG	1H	3461	1/1	0.98	0.04	45,45,45,45	0
57	MG	1H	3290	1/1	0.98	0.05	55,55,55,55	0
57	MG	1H	3465	1/1	0.98	0.11	67,67,67,67	0
57	MG	1H	3467	1/1	0.98	0.06	84,84,84,84	0
57	MG	1H	3291	1/1	0.98	0.04	59,59,59,59	0
57	MG	1H	3292	1/1	0.98	0.11	43,43,43,43	0
57	MG	14	3303	1/1	0.98	0.07	74,74,74,74	0
57	MG	13	1699	1/1	0.98	0.04	83,83,83,83	0
57	MG	1H	3471	1/1	0.98	0.09	90,90,90,90	0
57	MG	25	201	1/1	0.98	0.04	115,115,115,115	0
57	MG	14	3308	1/1	0.98	0.05	94,94,94,94	0
57	MG	14	3311	1/1	0.98	0.04	67,67,67,67	0
57	MG	1H	3473	1/1	0.98	0.10	95,95,95,95	0
57	MG	1H	3294	1/1	0.98	0.07	54,54,54,54	0
57	MG	1H	3377	1/1	0.98	0.12	76,76,76,76	0
57	MG	14	3315	1/1	0.98	0.06	68,68,68,68	0
57	MG	1H	3295	1/1	0.98	0.04	89,89,89,89	0
57	MG	1H	3296	1/1	0.98	0.08	91,91,91,91	0
59	SF4	3E	301	8/8	0.98	0.04	82,91,95,98	0
57	MG	1H	3297	1/1	0.98	0.06	49,49,49,49	0
60	ZN	5A	101	1/1	0.98	0.04	146,146,146,146	0
57	MG	1H	3381	1/1	0.98	0.09	74,74,74,74	0
57	MG	14	3320	1/1	0.98	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1H	3183	1/1	0.98	0.15	70,70,70,70	0
57	MG	1H	3060	1/1	0.98	0.09	35,35,35,35	0
57	MG	14	3356	1/1	0.99	0.07	75,75,75,75	0
57	MG	1H	3411	1/1	0.99	0.03	63,63,63,63	0
57	MG	14	3358	1/1	0.99	0.04	86,86,86,86	0
57	MG	1G	1665	1/1	0.99	0.03	91,91,91,91	0
57	MG	13	1734	1/1	0.99	0.03	94,94,94,94	0
57	MG	14	3361	1/1	0.99	0.09	79,79,79,79	0
57	MG	1H	3413	1/1	0.99	0.08	78,78,78,78	0
57	MG	13	1693	1/1	0.99	0.03	85,85,85,85	0
57	MG	I8	102	1/1	0.99	0.07	62,62,62,62	0
57	MG	1H	3320	1/1	0.99	0.02	58,58,58,58	0
57	MG	1H	3364	1/1	0.99	0.03	44,44,44,44	0
57	MG	14	3261	1/1	0.99	0.05	59,59,59,59	0
57	MG	14	3262	1/1	0.99	0.04	83,83,83,83	0
57	MG	1H	3480	1/1	0.99	0.06	87,87,87,87	0
57	MG	1H	3365	1/1	0.99	0.09	67,67,67,67	0
57	MG	1H	3286	1/1	0.99	0.03	40,40,40,40	0
57	MG	1H	3262	1/1	0.99	0.07	43,43,43,43	0
57	MG	1H	3288	1/1	0.99	0.05	54,54,54,54	0
57	MG	1H	3485	1/1	0.99	0.04	77,77,77,77	0
57	MG	1H	3326	1/1	0.99	0.02	62,62,62,62	0
57	MG	1H	3327	1/1	0.99	0.05	50,50,50,50	0
57	MG	1H	3328	1/1	0.99	0.03	47,47,47,47	0
57	MG	14	3272	1/1	0.99	0.08	71,71,71,71	0
57	MG	14	3273	1/1	0.99	0.05	86,86,86,86	0
57	MG	14	3274	1/1	0.99	0.08	85,85,85,85	0
57	MG	1H	3263	1/1	0.99	0.05	46,46,46,46	0
57	MG	1H	3247	1/1	0.99	0.06	36,36,36,36	0
57	MG	1H	3426	1/1	0.99	0.06	74,74,74,74	0
57	MG	13	1690	1/1	0.99	0.09	70,70,70,70	0
57	MG	1H	3493	1/1	0.99	0.03	101,101,101,101	0
57	MG	14	3280	1/1	0.99	0.04	61,61,61,61	0
57	MG	13	1715	1/1	0.99	0.06	76,76,76,76	0
57	MG	1H	3495	1/1	0.99	0.03	97,97,97,97	0
57	MG	1H	3429	1/1	0.99	0.08	88,88,88,88	0
57	MG	1H	3333	1/1	0.99	0.09	77,77,77,77	0
57	MG	13	1705	1/1	0.99	0.08	97,97,97,97	0
57	MG	1H	3269	1/1	0.99	0.04	41,41,41,41	0
57	MG	13	1689	1/1	0.99	0.06	88,88,88,88	0
57	MG	14	3394	1/1	0.99	0.04	91,91,91,91	0
57	MG	1H	3337	1/1	0.99	0.04	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3338	1/1	0.99	0.03	66,66,66,66	0
57	MG	1H	3436	1/1	0.99	0.03	70,70,70,70	0
57	MG	1H	3382	1/1	0.99	0.03	49,49,49,49	0
57	MG	1H	3438	1/1	0.99	0.07	62,62,62,62	0
57	MG	1H	3439	1/1	0.99	0.06	67,67,67,67	0
57	MG	14	3294	1/1	0.99	0.09	75,75,75,75	0
57	MG	1H	3252	1/1	0.99	0.04	65,65,65,65	0
57	MG	1H	3272	1/1	0.99	0.05	63,63,63,63	0
57	MG	13	1702	1/1	0.99	0.14	85,85,85,85	0
57	MG	1H	3510	1/1	0.99	0.07	39,39,39,39	0
57	MG	1H	3387	1/1	0.99	0.03	33,33,33,33	0
57	MG	14	3300	1/1	0.99	0.07	89,89,89,89	0
57	MG	14	3301	1/1	0.99	0.03	85,85,85,85	0
57	MG	14	3302	1/1	0.99	0.03	58,58,58,58	0
57	MG	1H	3342	1/1	0.99	0.03	86,86,86,86	0
57	MG	14	3411	1/1	0.99	0.04	105,105,105,105	0
57	MG	1H	3254	1/1	0.99	0.02	46,46,46,46	0
57	MG	14	3305	1/1	0.99	0.03	49,49,49,49	0
57	MG	14	3306	1/1	0.99	0.04	58,58,58,58	0
57	MG	1H	3275	1/1	0.99	0.11	57,57,57,57	0
57	MG	1H	3345	1/1	0.99	0.03	102,102,102,102	0
57	MG	14	3309	1/1	0.99	0.05	55,55,55,55	0
57	MG	14	3310	1/1	0.99	0.05	54,54,54,54	0
57	MG	1H	3448	1/1	0.99	0.06	80,80,80,80	0
57	MG	1H	3517	1/1	0.99	0.06	91,91,91,91	0
57	MG	1H	3255	1/1	0.99	0.02	49,49,49,49	0
57	MG	13	1719	1/1	0.99	0.06	81,81,81,81	0
57	MG	14	3217	1/1	0.99	0.06	56,56,56,56	0
57	MG	1H	3304	1/1	0.99	0.03	58,58,58,58	0
57	MG	1H	3349	1/1	0.99	0.03	50,50,50,50	0
57	MG	1H	3305	1/1	0.99	0.05	63,63,63,63	0
57	MG	1H	3278	1/1	0.99	0.03	75,75,75,75	0
57	MG	1H	3456	1/1	0.99	0.03	94,94,94,94	0
57	MG	14	3321	1/1	0.99	0.09	69,69,69,69	0
57	MG	1H	3398	1/1	0.99	0.07	78,78,78,78	0
57	MG	1H	3399	1/1	0.99	0.07	73,73,73,73	0
57	MG	14	3324	1/1	0.99	0.03	48,48,48,48	0
57	MG	1H	3279	1/1	0.99	0.06	48,48,48,48	0
57	MG	14	3226	1/1	0.99	0.05	51,51,51,51	0
57	MG	14	3327	1/1	0.99	0.03	82,82,82,82	0
57	MG	1H	3353	1/1	0.99	0.06	48,48,48,48	0
57	MG	1H	3402	1/1	0.99	0.04	85,85,85,85	0

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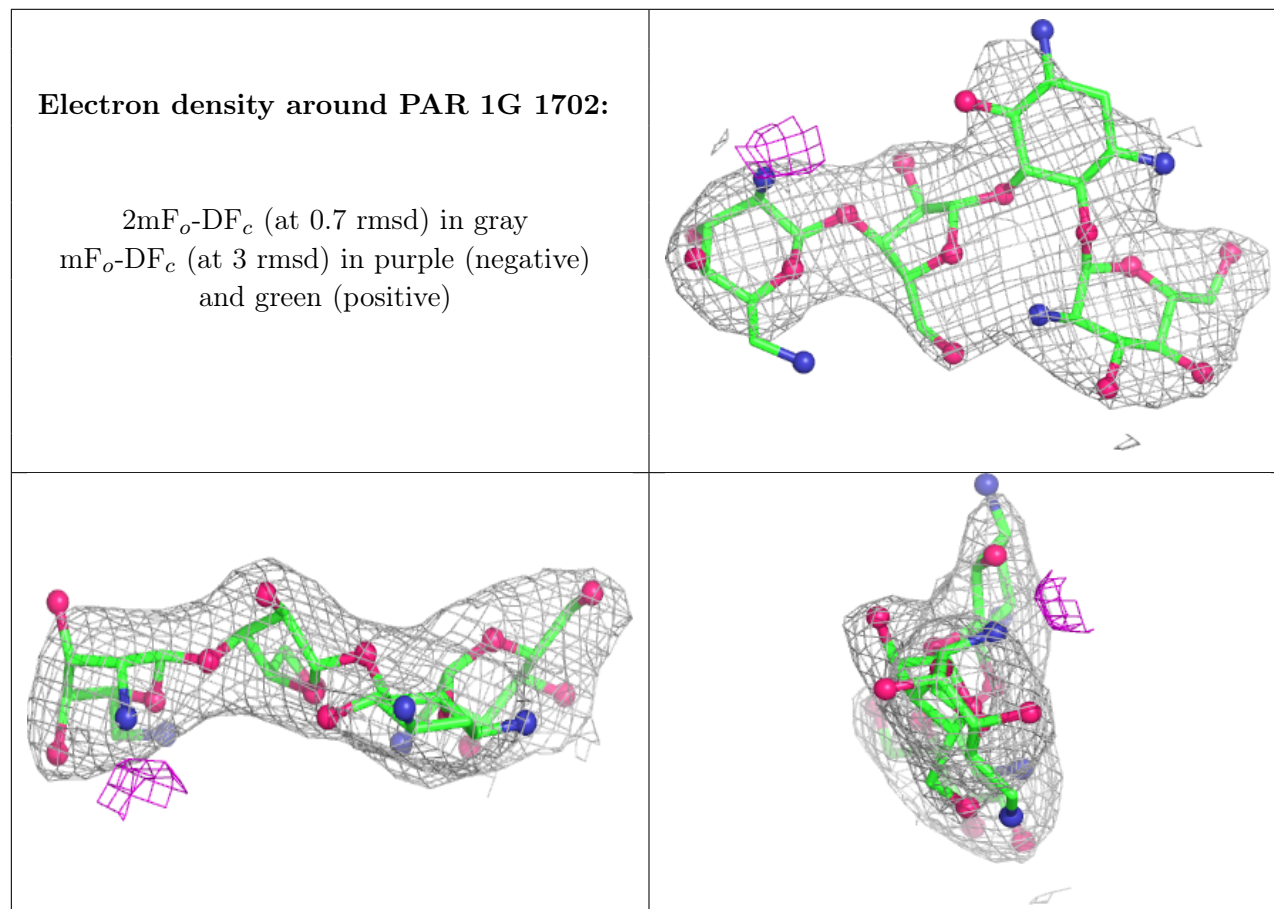
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3229	1/1	0.99	0.02	59,59,59,59	0
57	MG	1H	3280	1/1	0.99	0.04	36,36,36,36	0
57	MG	1H	3463	1/1	0.99	0.06	81,81,81,81	0
57	MG	14	3333	1/1	0.99	0.04	50,50,50,50	0
57	MG	14	3232	1/1	0.99	0.03	66,66,66,66	0
57	MG	1H	3464	1/1	0.99	0.06	63,63,63,63	0
57	MG	1H	3258	1/1	0.99	0.03	47,47,47,47	0
57	MG	14	3235	1/1	0.99	0.09	48,48,48,48	0
57	MG	1H	3466	1/1	0.99	0.03	72,72,72,72	0
57	MG	1H	3312	1/1	0.99	0.05	44,44,44,44	0
57	MG	14	3340	1/1	0.99	0.07	107,107,107,107	0
57	MG	14	3341	1/1	0.99	0.03	66,66,66,66	0
57	MG	16	211	1/1	0.99	0.08	73,73,73,73	0
57	MG	14	3239	1/1	0.99	0.04	77,77,77,77	0
57	MG	14	3240	1/1	0.99	0.04	73,73,73,73	0
57	MG	1H	3406	1/1	0.99	0.08	85,85,85,85	0
57	MG	1H	3313	1/1	0.99	0.07	47,47,47,47	0
57	MG	1H	3282	1/1	0.99	0.08	71,71,71,71	0
57	MG	1H	3315	1/1	0.99	0.02	63,63,63,63	0
57	MG	14	3246	1/1	0.99	0.03	61,61,61,61	0
59	SF4	32	302	8/8	0.99	0.04	100,109,118,124	0
60	ZN	5I	102	1/1	0.99	0.02	86,86,86,86	0
57	MG	14	3247	1/1	0.99	0.05	52,52,52,52	0
57	MG	14	3248	1/1	0.99	0.11	47,47,47,47	0
57	MG	14	3352	1/1	0.99	0.09	82,82,82,82	0
57	MG	1H	3472	1/1	0.99	0.03	83,83,83,83	0
57	MG	14	3250	1/1	0.99	0.03	79,79,79,79	0
57	MG	1H	3259	1/1	0.99	0.07	54,54,54,54	0
57	MG	14	3242	1/1	1.00	0.02	62,62,62,62	0
57	MG	1H	3302	1/1	1.00	0.02	51,51,51,51	0
57	MG	1H	3385	1/1	1.00	0.04	25,25,25,25	0
57	MG	14	3216	1/1	1.00	0.05	52,52,52,52	0
57	MG	1H	3325	1/1	1.00	0.04	46,46,46,46	0
57	MG	13	1686	1/1	1.00	0.05	76,76,76,76	0
57	MG	21	303	1/1	1.00	0.03	46,46,46,46	0
57	MG	1H	3257	1/1	1.00	0.02	43,43,43,43	0
57	MG	1H	3311	1/1	1.00	0.02	53,53,53,53	0
57	MG	1H	3319	1/1	1.00	0.08	57,57,57,57	0
57	MG	13	1692	1/1	1.00	0.06	72,72,72,72	0
57	MG	14	3253	1/1	1.00	0.03	58,58,58,58	0
57	MG	1H	3306	1/1	1.00	0.03	75,75,75,75	0
57	MG	1H	3322	1/1	1.00	0.04	58,58,58,58	0

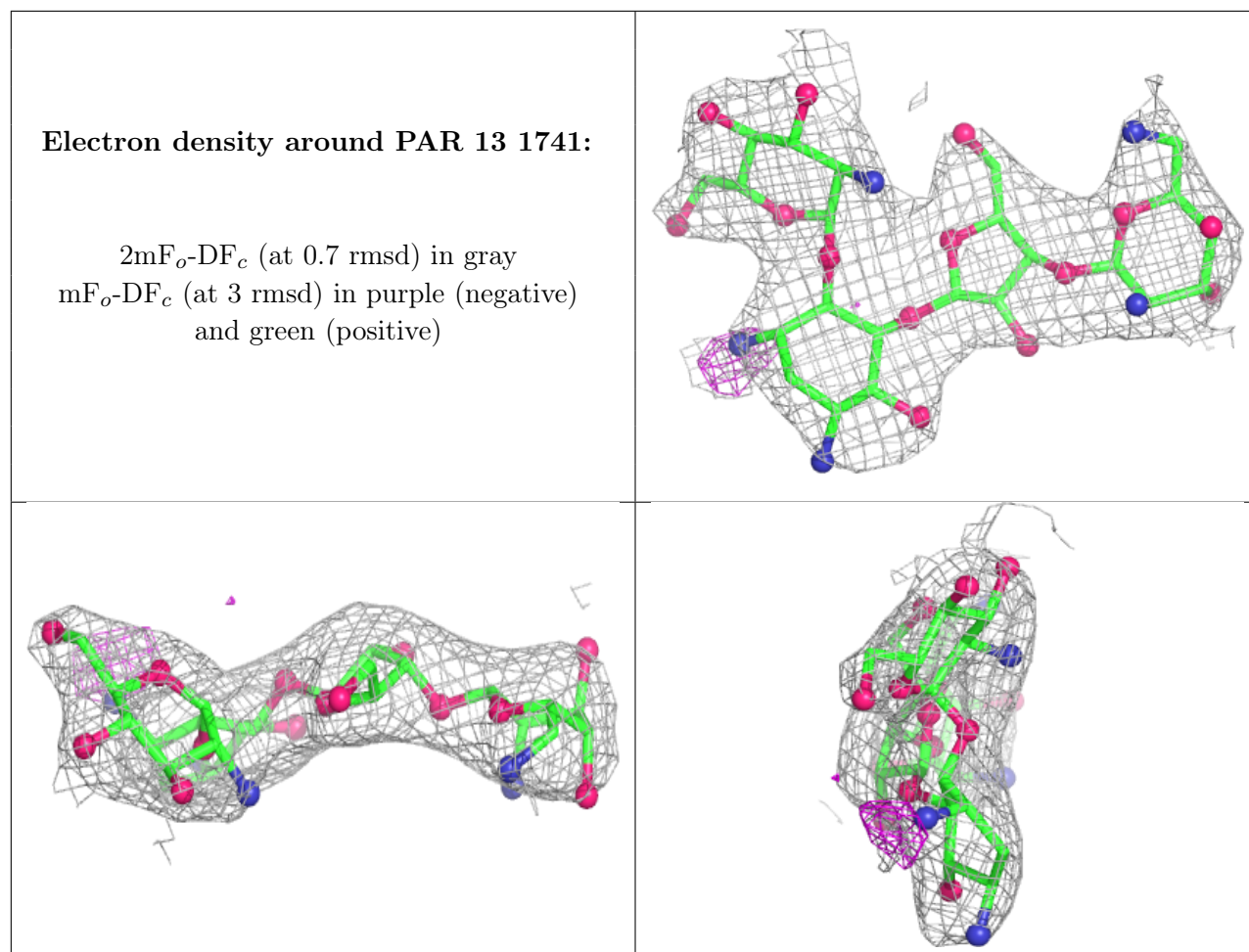
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3265	1/1	1.00	0.01	46,46,46,46	0
57	MG	1H	3450	1/1	1.00	0.01	44,44,44,44	0

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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.