



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 12:23 PM UTC

PDB ID : 4WQR / pdb_00004wqr
Title : Complex of 70S ribosome with tRNA-Phe and mRNA with C-A mismatch in the first position in the A-site.
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-10-22
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

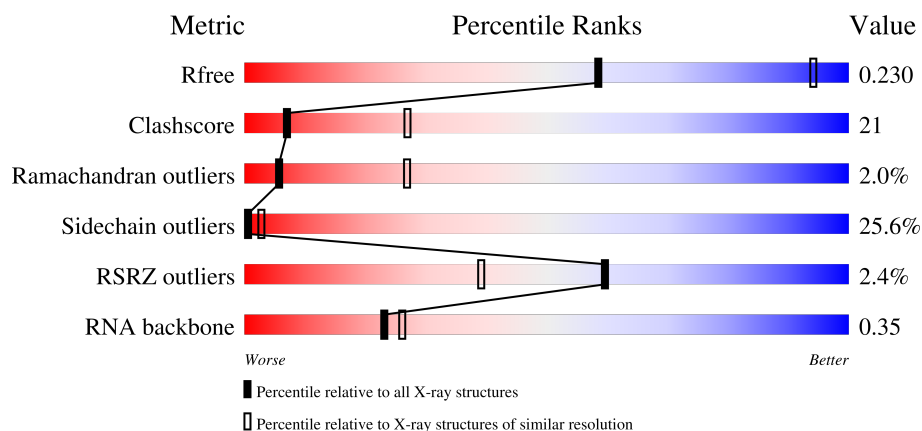
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

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

Mol	Chain	Length	Quality of chain
1	13	1522	2% 34% 49% 15%
1	1G	1522	2% 35% 47% 15%
2	12	256	3% 45% 37% 10% 7%
2	1E	256	5% 34% 45% 12% 7%

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

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

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Mol	Chain	Length	Quality of chain
28	11	276	
28	19	276	
29	21	206	
29	29	206	
30	31	210	
30	39	210	
31	41	182	
31	49	182	
32	51	180	
32	59	180	
33	61	148	
33	69	148	
34	15	140	
34	58	140	
35	25	122	
35	68	122	
36	35	150	
36	78	150	
37	45	141	
37	88	141	
38	55	118	
38	98	118	
39	65	112	
39	A8	112	
40	75	146	

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Mol	Chain	Length	Quality of chain
40	B8	146	
41	85	118	
41	C8	118	
42	95	101	
42	D8	101	
43	A5	113	
43	E8	113	
44	B5	96	
44	F8	96	
45	C5	110	
45	G8	110	
46	D5	206	
46	H8	206	
47	E5	85	
47	I8	85	
48	F5	98	
48	J8	98	
49	G5	72	
49	K8	72	
50	H5	60	
50	L8	60	
51	I5	71	
51	M8	71	
52	J5	60	
52	N8	60	

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Mol	Chain	Length	Quality of chain
53	K5	54	
53	O8	54	
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1648	-	-	-	X
56	MG	13	1680	-	-	-	X
56	MG	13	1689	-	-	-	X
56	MG	13	1693	-	-	-	X
56	MG	13	1704	-	-	-	X
56	MG	13	1712	-	-	-	X
56	MG	14	3112	-	-	-	X
56	MG	14	3128	-	-	-	X
56	MG	14	3218	-	-	-	X
56	MG	14	3240	-	-	-	X
56	MG	14	3241	-	-	-	X
56	MG	14	3252	-	-	-	X
56	MG	14	3254	-	-	-	X
56	MG	1G	1642	-	-	-	X
56	MG	1G	1655	-	-	-	X
56	MG	1G	1662	-	-	-	X
56	MG	1G	1664	-	-	-	X
56	MG	1G	1669	-	-	-	X
56	MG	1G	1677	-	-	-	X
56	MG	1G	1682	-	-	-	X
56	MG	2L	102	-	-	-	X
56	MG	4A	201	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 300537 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1498	Total	C	N	O	P	0	0	0
			32207	14334	5973	10402	1498			
1	1G	1497	Total	C	N	O	P	0	0	0
			32182	14324	5968	10394	1496			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	32	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	42	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	52	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	62	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	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
			1116	705	215	193	3			
8	72	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	82	127	Total	C	N	O		0	0	0
			1010	639	197	174				

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	2A	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	5A	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	6A	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	72	Total	C	N	O	0	0	0
			591	376	117	98			
18	9A	72	Total	C	N	O	0	0	0
			591	376	117	98			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BA	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	76	Total	C	N	O	P	S	0	0	0
			1626	729	290	531	75	1			
22	1L	76	Total	C	N	O	P	S	0	0	0
			1626	729	290	531	75	1			

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2K	18	C	U	conflict	GB 675817920
2L	18	C	U	conflict	GB 675817920

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
24	3L	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	14	Total	C	N	O	P	0	0	0
			301	136	60	91	14			
25	4L	6	Total	C	N	O	P	0	0	0
			131	59	27	39	6			

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

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	-	insertion	GB 48268
1H	493	G	-	insertion	GB 48268
1H	1228	G	-	insertion	GB 48268
14	161	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	1228	G	-	insertion	GB 48268

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			
31	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	68	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
35	25	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	78	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
36	35	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	88	138	Total	C	N	O	S	0	0	0
			1087	693	208	180	6			
37	45	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	98	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
38	55	117	Total	C	N	O		0	0	0
			960	599	202	159				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	A8	111	Total	C	N	O	0	0	0
			882	556	176	150			
39	65	111	Total	C	N	O	0	0	0
			882	556	176	150			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	C8	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
41	85	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	D8	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
42	95	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	E8	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
43	A5	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	F8	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			
44	B5	93	Total	C	N	O		0	0	0
			730	474	132	124				

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	80	Total	C	N	O	S	0	0	0
			627	388	132	106	1			
47	E5	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	J8	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
48	F5	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	G5	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	L8	57	Total	C	N	O		0	0	0
			452	288	88	76				
50	H5	59	Total	C	N	O		0	0	0
			469	298	90	81				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M8	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
51	I5	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	N8	58	Total	C	N	O	S	0	0	0
			454	285	89	75	5			
52	J5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	P8	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
54	L5	46	Total	C	N	O	S	0	0	0
			398	245	98	53	2			

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

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

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	151	Total	Mg	0	0
			151	151		
56	3E	2	Total	Mg	0	0
			2	2		
56	5E	1	Total	Mg	0	0
			1	1		
56	3I	1	Total	Mg	0	0
			1	1		
56	AI	1	Total	Mg	0	0
			1	1		
56	1K	2	Total	Mg	0	0
			2	2		
56	2K	3	Total	Mg	0	0
			3	3		
56	1H	529	Total	Mg	0	0
			529	529		
56	16	13	Total	Mg	0	0
			13	13		
56	11	4	Total	Mg	0	0
			4	4		
56	21	2	Total	Mg	0	0
			2	2		
56	31	1	Total	Mg	0	0
			1	1		
56	41	2	Total	Mg	0	0
			2	2		
56	78	2	Total	Mg	0	0
			2	2		
56	88	2	Total	Mg	0	0
			2	2		
56	98	1	Total	Mg	0	0
			1	1		
56	C8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	E8	1	Total 1	Mg 1	0	0
56	I8	2	Total 2	Mg 2	0	0
56	J8	2	Total 2	Mg 2	0	0
56	L8	1	Total 1	Mg 1	0	0
56	P8	1	Total 1	Mg 1	0	0
56	Q8	1	Total 1	Mg 1	0	0
56	1G	103	Total 103	Mg 103	0	0
56	4A	1	Total 1	Mg 1	0	0
56	6A	1	Total 1	Mg 1	0	0
56	2L	2	Total 2	Mg 2	0	0
56	14	389	Total 389	Mg 389	0	0
56	1J	9	Total 9	Mg 9	0	0
56	29	2	Total 2	Mg 2	0	0
56	49	1	Total 1	Mg 1	0	0
56	35	1	Total 1	Mg 1	0	0
56	75	1	Total 1	Mg 1	0	0
56	85	1	Total 1	Mg 1	0	0
56	C5	1	Total 1	Mg 1	0	0
56	F5	1	Total 1	Mg 1	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	3E	1	Total 1	Zn 1	0	0
57	5I	1	Total 1	Zn 1	0	0
57	G8	1	Total 1	Zn 1	0	0
57	32	1	Total 1	Zn 1	0	0
57	5A	1	Total 1	Zn 1	0	0
57	C5	1	Total 1	Zn 1	0	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	212	Total 212	O 212	0	0
58	3E	1	Total 1	O 1	0	0
58	4E	2	Total 2	O 2	0	0
58	8E	2	Total 2	O 2	0	0
58	1I	2	Total 2	O 2	0	0
58	3I	1	Total 1	O 1	0	0
58	5I	2	Total 2	O 2	0	0
58	1K	1	Total 1	O 1	0	0
58	3K	1	Total 1	O 1	0	0
58	4K	4	Total 4	O 4	0	0
58	1H	1097	Total 1097	O 1097	0	0
58	16	16	Total 16	O 16	0	0
58	11	9	Total 9	O 9	0	0
58	21	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	31	10	Total 10	O 10	0	0
58	58	1	Total 1	O 1	0	0
58	78	4	Total 4	O 4	0	0
58	98	1	Total 1	O 1	0	0
58	C8	2	Total 2	O 2	0	0
58	D8	1	Total 1	O 1	0	0
58	E8	2	Total 2	O 2	0	0
58	G8	3	Total 3	O 3	0	0
58	I8	6	Total 6	O 6	0	0
58	L8	2	Total 2	O 2	0	0
58	P8	2	Total 2	O 2	0	0
58	Q8	2	Total 2	O 2	0	0
58	1G	99	Total 99	O 99	0	0
58	7A	2	Total 2	O 2	0	0
58	BA	1	Total 1	O 1	0	0
58	14	730	Total 730	O 730	0	0
58	1J	12	Total 12	O 12	0	0
58	19	11	Total 11	O 11	0	0
58	29	6	Total 6	O 6	0	0
58	39	7	Total 7	O 7	0	0
58	55	1	Total 1	O 1	0	0

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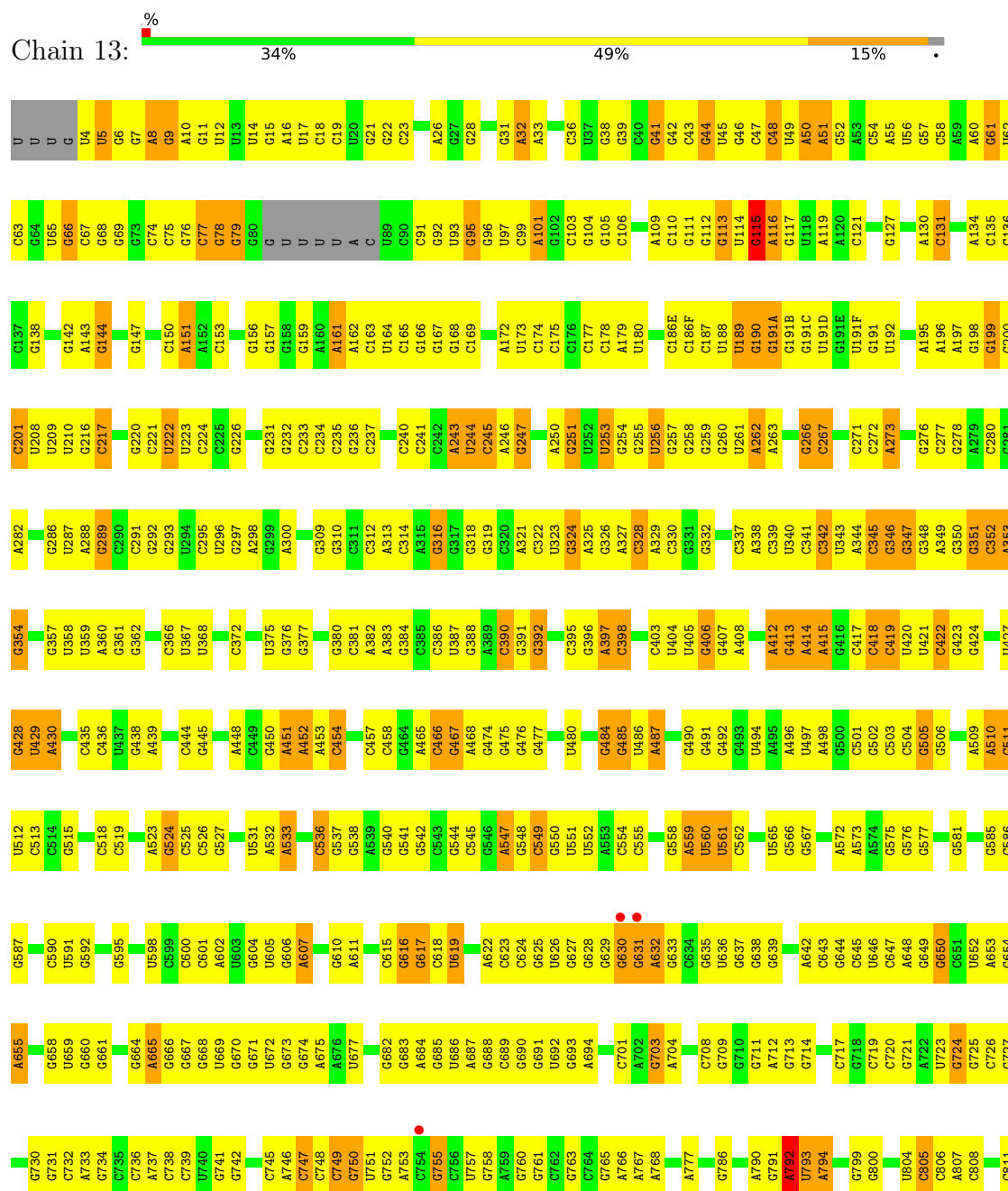
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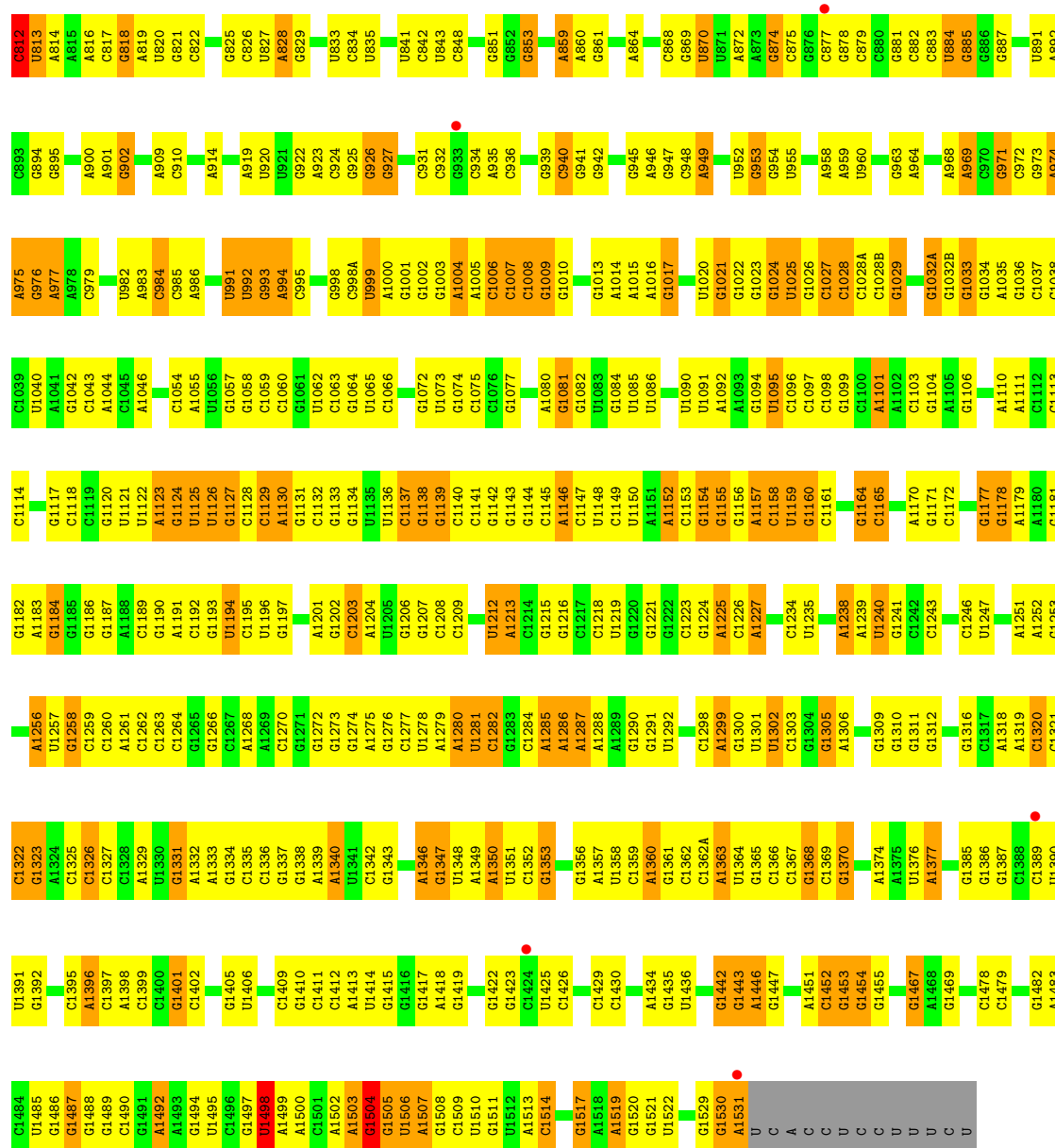
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	85	1	Total	O	0	0
			1	1		
58	A5	1	Total	O	0	0
			1	1		
58	H5	1	Total	O	0	0
			1	1		
58	L5	1	Total	O	0	0
			1	1		

3 Residue-property plots

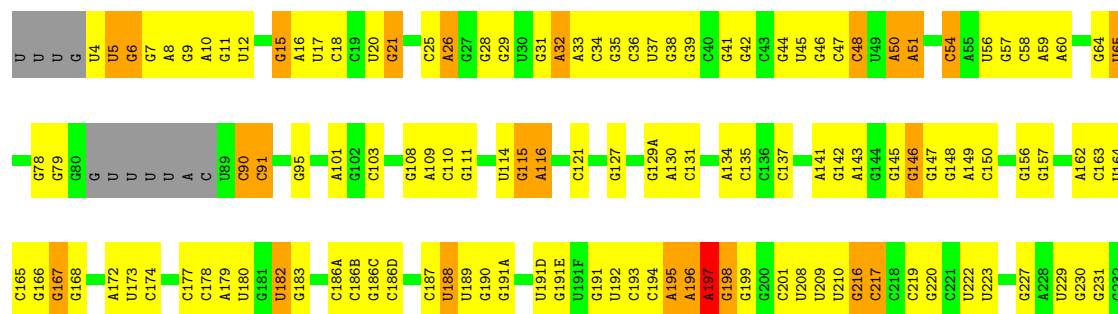
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S ribosomal RNA

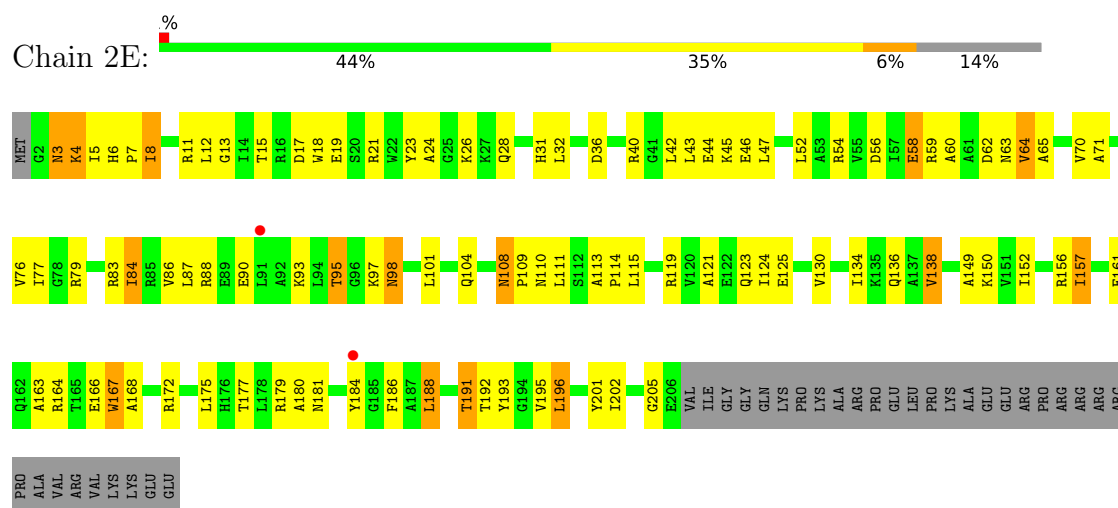




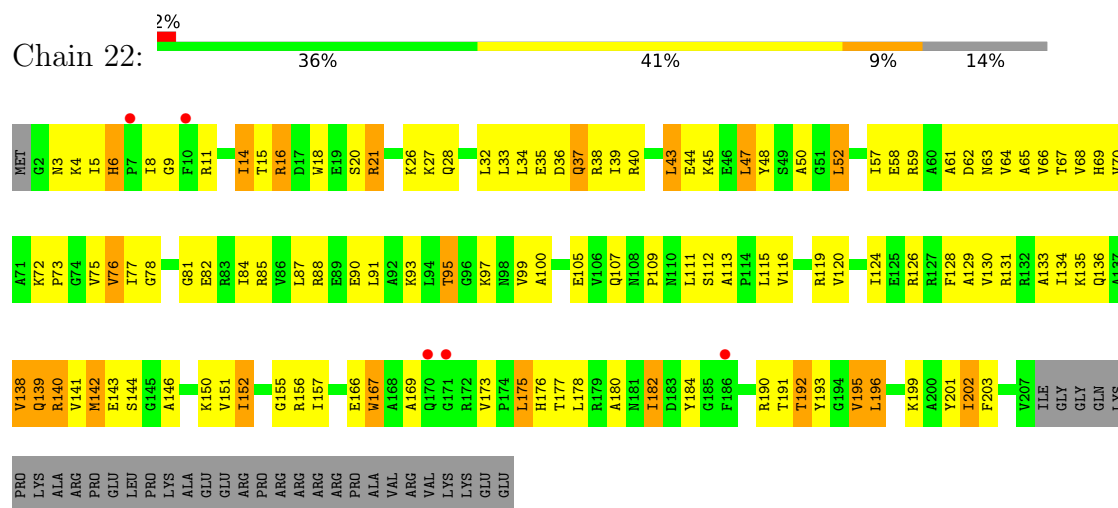
Molecule 1: 16S ribosomal RNA



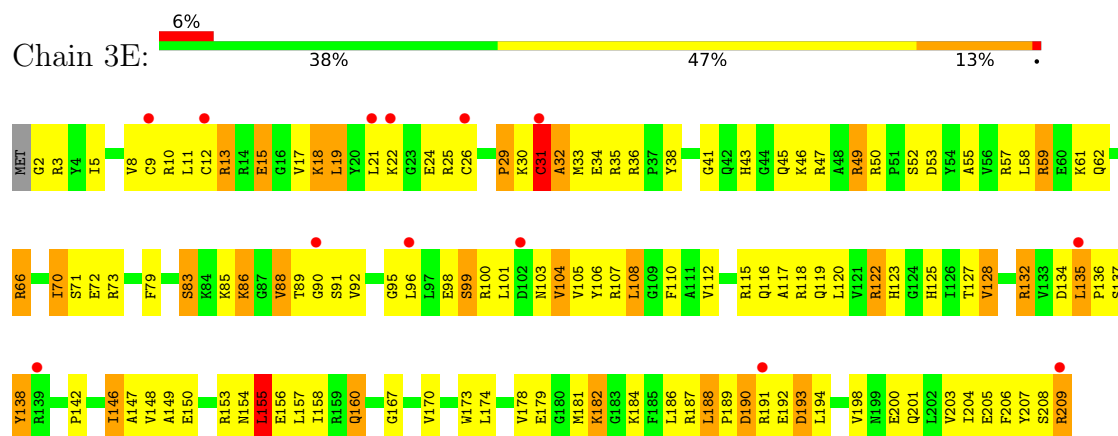
U1194	C1233	C233	C234	C235	C236	C237	C240	A243	U244	G247	C248	U249	A250	G251	U252	G259	G260	U261	A262	A263	U264	G265	C266	C267	C268	C280	G281	A282	C283	G284	G285	G286	U287	A288	G289	U296	G297	A298	G299	A300	G301	G302	A303	U304	G305	G309	G310	A313	A314	A315	G316	A317	G318								
C1195	C321	C322	C323	C324	A325	G326	A327	C328	A329	C330	G331	G332	C337	A338	C339	U340	C345	G346	G347	A348	A349	G350	G351	C352	A353	G354	C355	A356	G357	U358	A359	G360	G361	U362	A363	C366	U367	G371	C372	A373	U374	U375	G376	G377	A382	A383	G388	A389	C390	G396	A397	C398									
C403	U404	U405	G406	G407	A408	G409	A410	G411	U411	A412	G413	A414	A415	G416	C417	A418	U420	U421	C422	A423	G424	G425	G426	U427	G428	U429	A430	A431	A432	U433	U434	C435	A436	U437	G438	A439	A440	C442	C443	C444	G445	G446	G447	A448	G449	G450	A451	A452	A453	C457	C458	G459	A464	A465	C466	G467	A468	G474			
G475	G476	G477	U480	G481	A482	C483	G484	G485	U486	C487	C488	G489	G490	A496	U497	A498	G500	C501	G502	A503	C504	G505	G506	C507	A508	A509	A510	C511	U512	A513	C518	C519	G520	C521	C522	A523	G524	C525	C526	G527	C528	G529	G530	U531	A532	A533	U534	A535	C536	G537	A538	A539	G540	G541	G544						
C545	G546	A547	C554	C555	C556	A559	U560	U561	C562	A563	C564	G565	G566	G567	A568	C569	G570	U571	A572	C573	C574	G575	G576	G577	U578	A579	U580	G581	U582	A583	G584	G587	C588	C589	C590	U591	G592	C596	G597	U598	C599	C600	C601	G604	U605	A606	A607	A608	A609	A614	G615	G616	G617								
C618	U619	C620	A621	G622	C623	C624	G625	U626	G627	G628	G629	C630	G631	A632	G633	U636	G637	G638	G639	A640	U641	A642	U646	C647	A648	C649	G650	C651	U652	A653	U659	G660	G661	G662	A663	G664	A665	G668	U669	G670	G673	G674	A675	A676	U677	C680	G683	A684	G685	U686	A687	G688									
C689	G690	G691	U692	G693	A694	G702	G703	A704	U705	C706	G707	C708	G709	G710	G713	U714	A715	A716	C720	A721	U722	A723	U724	A728	A729	G730	G731	C735	G736	A737	C738	G741	G742	U743	G744	C745	A746	C747	C748	G749	G750	C754	G755	C756	C757	G758	G759	G760	G763	C764	U765	A766									
A767	A768	G775	G776	A777	G778	C779	G785	A790	G791	U792	A793	A794	U801	G802	G803	U804	C805	C806	A807	C808	C811	C812	U813	A815	A816	C817	G818	A819	U820	G821	C822	G823	C824	U825	C826	U827	A828	G829	G830	U831	G836	G837	G838	U841	C842	U843	C848	C849	U850												
G851	G852	G853	A854	G855	C856	C857	G858	A859	A860	G861	C862	C868	G869	U870	A871	A872	A873	G878	C879	G880	G881	C882	G885	G886	G887	G888	A889	G890	U891	A892	G895	A900	A901	G902	G903	C904	U905	G906	A907	A908	C909	G910	A913	A914	A915	G916	G917	A918	A919	G922	A923	G926									
G927	C934	A935	U936	G937	A938	C939	C940	G941	G942	U943	G944	G947	C948	A949	U950	G951	U952	G953	G954	U955	U956	U957	A958	A959	U960	U961	C962	G963	A964	U965	G966	A968	C970	G971	C972	G973	A974	U975	G976	A977	A978	C979	C980	U981	U982	A983	C984	C985	A986	G987	U991	U992	A994								
G988	G988A	U999	A1000	G1001	G1002	G1003	A1004	C1005	A1006	G1007	G1008	G1009	G1010	G1013	A1014	A1015	A1016	G1017	U1020	G1023	G1024	U1025	G1026	C1027	G1028	C1029	U1028B	G1029	C1030	G1031	C1032	A1032A	G1032B	G1033	G1034	A1035	G1036	C1037	U1038	G1039	U1040	A1041	C1042	G1043	A1046	G1047	U1048	U1049	G1050	C1051	U1052	G1053	A1054	A1055							
U1056	G1057	G1058	U1062	G1063	U1064	U1065	C1066	C1067	G1068	G1072	U1073	C1074	C1075	U1078	G1079	A1080	C1081	G1082	U1083	G1084	U1085	U1086	A1089	A1092	A1093	A1094	U1095	C1096	C1097	G1098	C1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	A1111	C1112	C1113	C1114	C1115	C1116	G1117	C1118	C1119	U1122	A1123	G1124	U1125	U1126							
G1127	C1128	A1130	G1131	C1132	G1133	U1136	C1137	G1138	A1139	C1140	G1141	G1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	G1155	A1156	A1157	C1158	U1159	G1160	C1161	C1162	C1163	G1171	C1172	G1173	G1174	G1175	U1176	G1177	G1178	A1180	G1181	G1182	A1183	G1184	G1185	G1186	U1187	A1188	C1189	U1190	A1191	C1192	G1193						
C1246	U1247	A1248	C1249	A1250	A1251	A1252	G1253	C1254	G1255	A1256	U1257	G1258	C1259	C1260	A1261	U1235	A1236	C1237	A1238	A1239	U1240	G1241	C1246	U1247	A1248	C1249	A1250	A1251	A1252	G1253	C1254	G1255	A1256	U1257	G1258	C1259	C1260	A1261	U1235	A1236	C1237	A1238	A1239	U1240	G1241	C1246	U1247	A1248	C1249	A1250	A1251	A1252	G1253	C1254	G1255	A1256	U1257	G1258	C1259	C1260	A1261



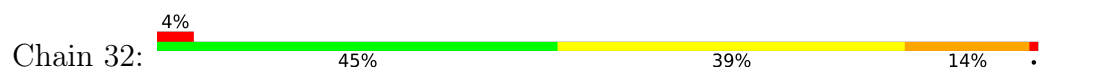
• Molecule 3: 30S ribosomal protein S3

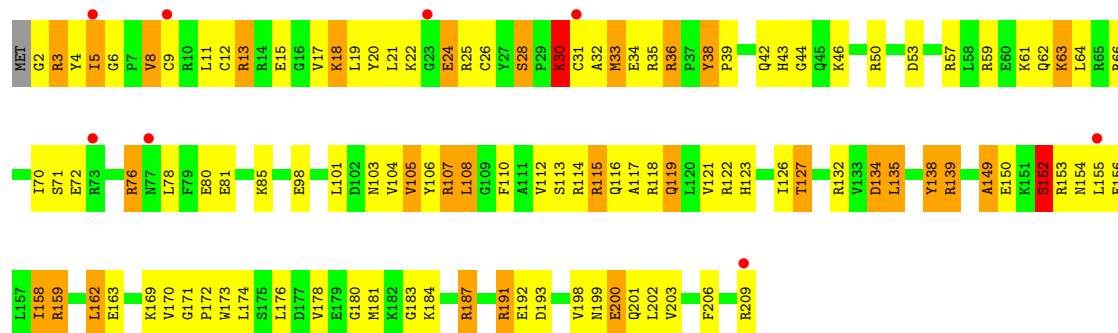


• Molecule 4: 30S ribosomal protein S4

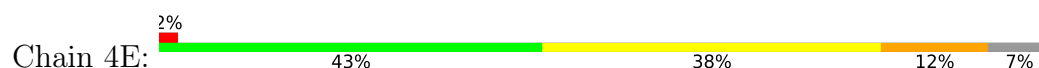


• Molecule 4: 30S ribosomal protein S4





• Molecule 5: 30S ribosomal protein S5



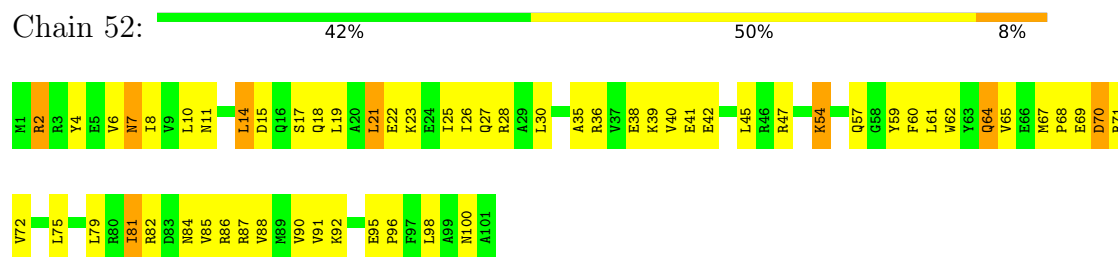
• Molecule 5: 30S ribosomal protein S5



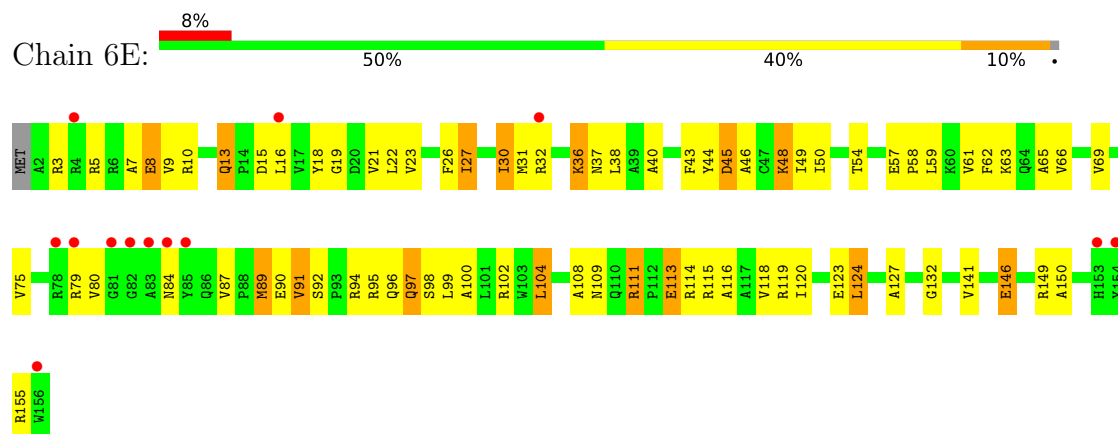
• Molecule 6: 30S ribosomal protein S6



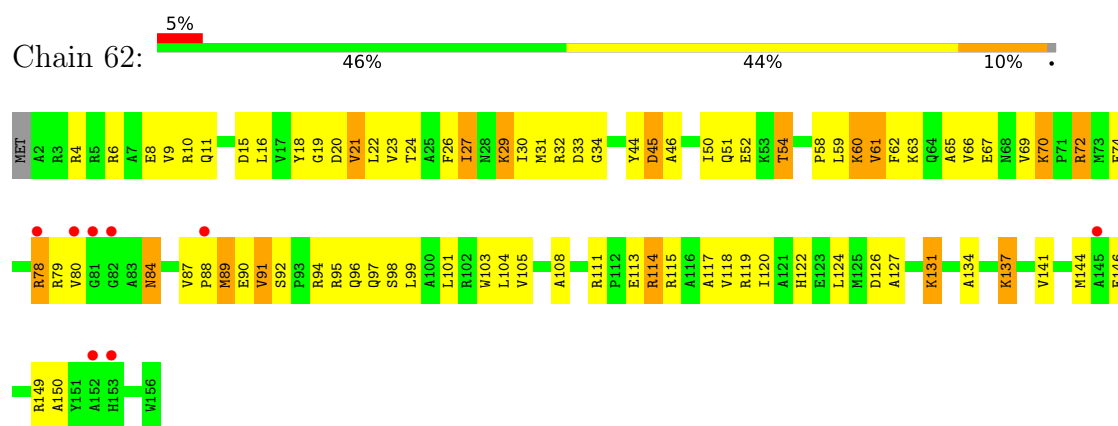
• Molecule 6: 30S ribosomal protein S6



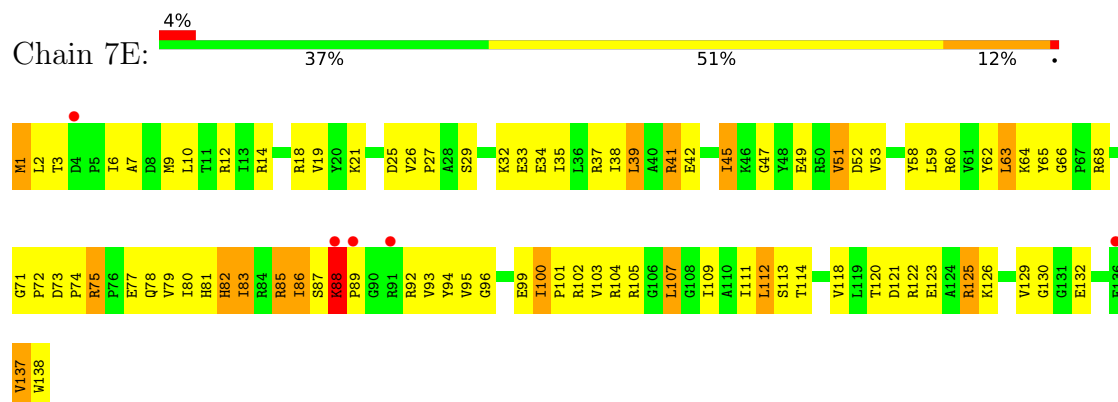
• Molecule 7: 30S ribosomal protein S7



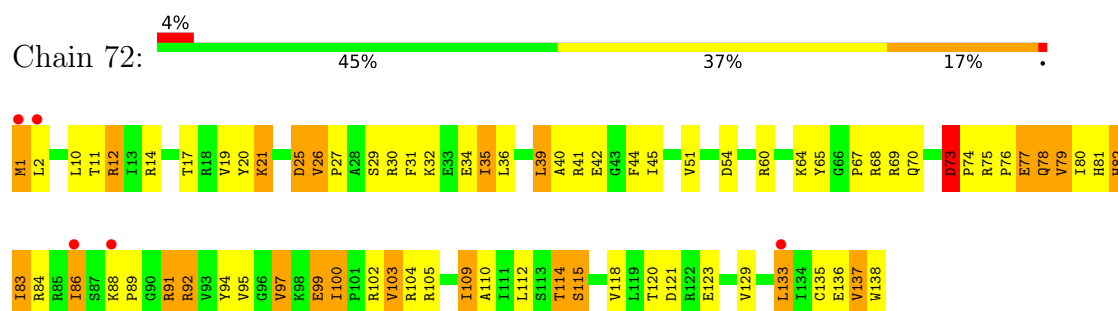
• Molecule 7: 30S ribosomal protein S7



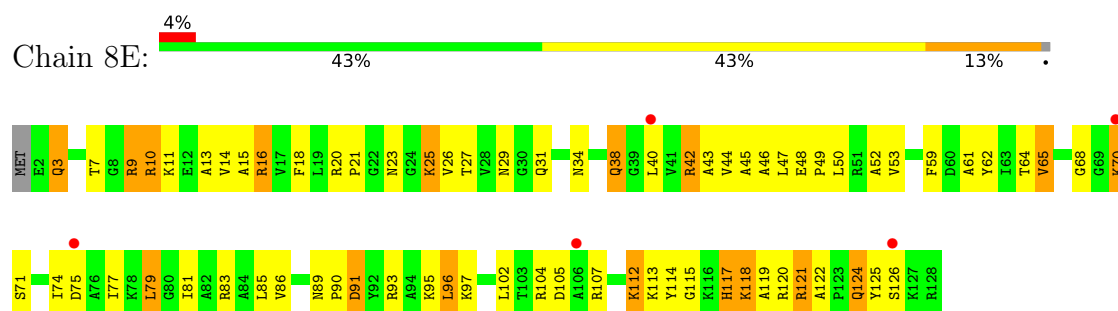
• Molecule 8: 30S ribosomal protein S8



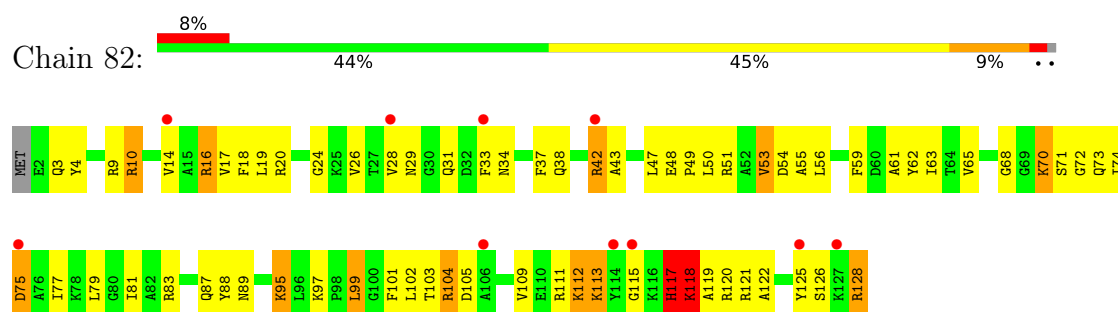
- Molecule 8: 30S ribosomal protein S8



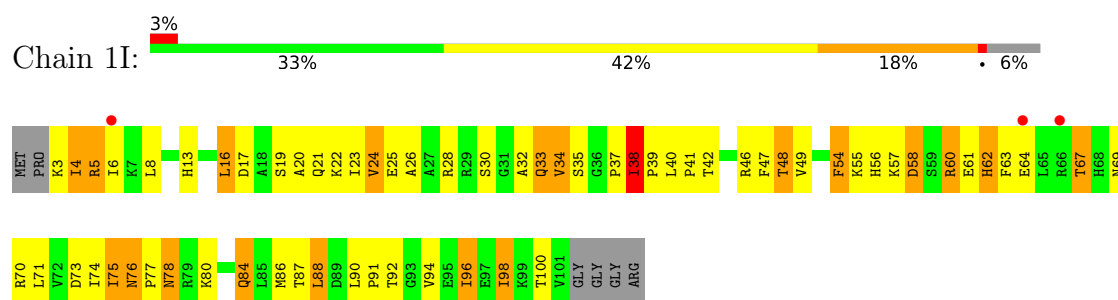
- Molecule 9: 30S ribosomal protein S9



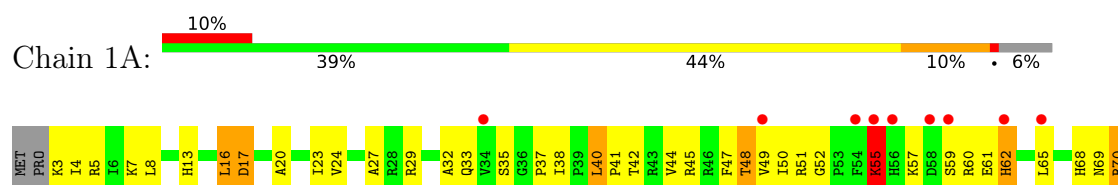
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

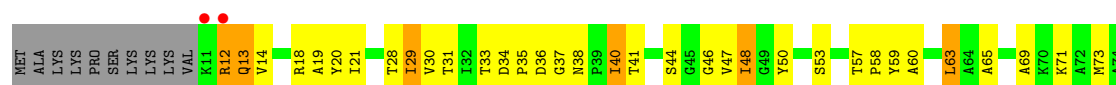
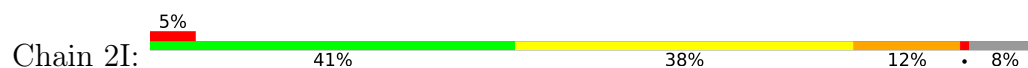


- Molecule 10: 30S ribosomal protein S10

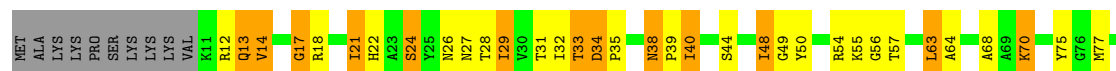




• Molecule 11: 30S ribosomal protein S11



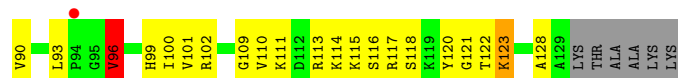
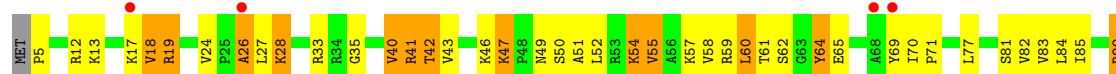
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12

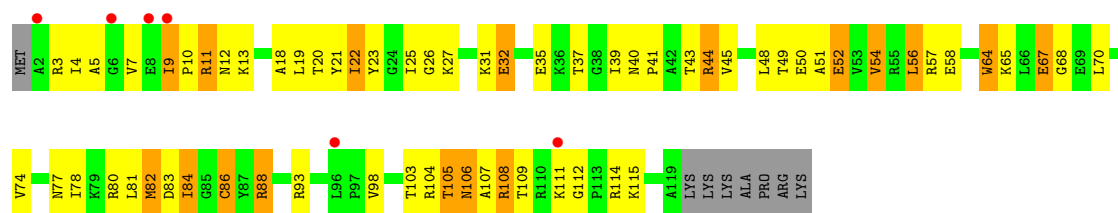


• Molecule 12: 30S ribosomal protein S12

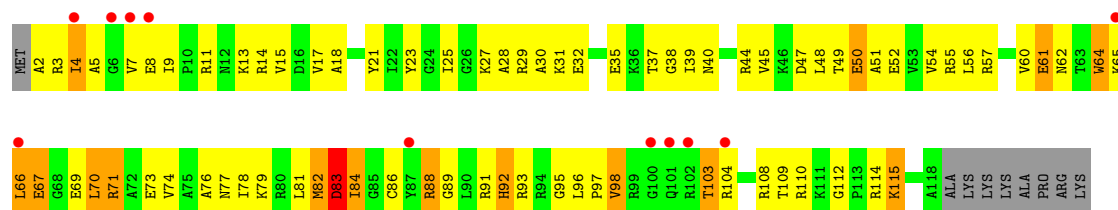


• Molecule 13: 30S ribosomal protein S13

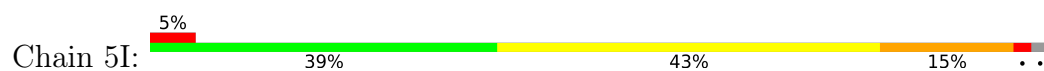




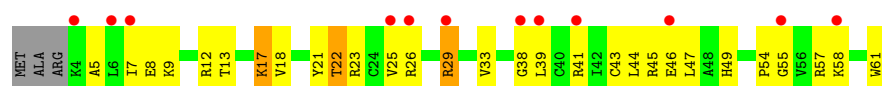
• Molecule 13: 30S ribosomal protein S13



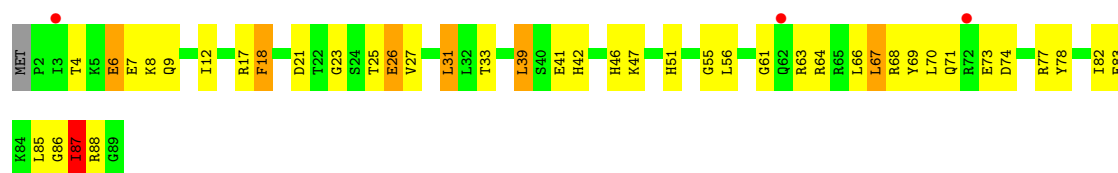
• Molecule 14: 30S ribosomal protein S14 type Z



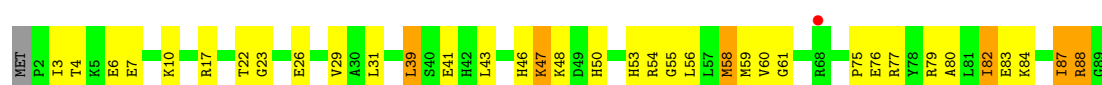
• Molecule 14: 30S ribosomal protein S14 type Z



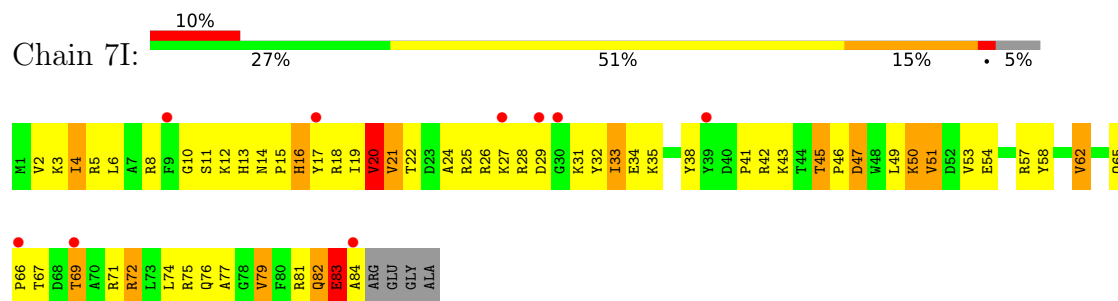
• Molecule 15: 30S ribosomal protein S15



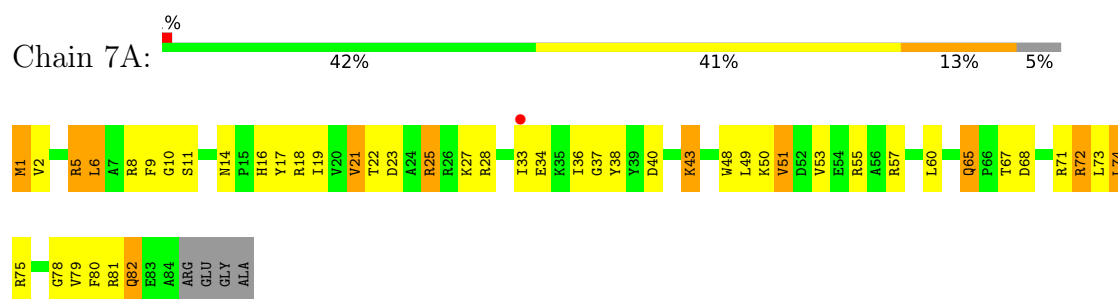
• Molecule 15: 30S ribosomal protein S15



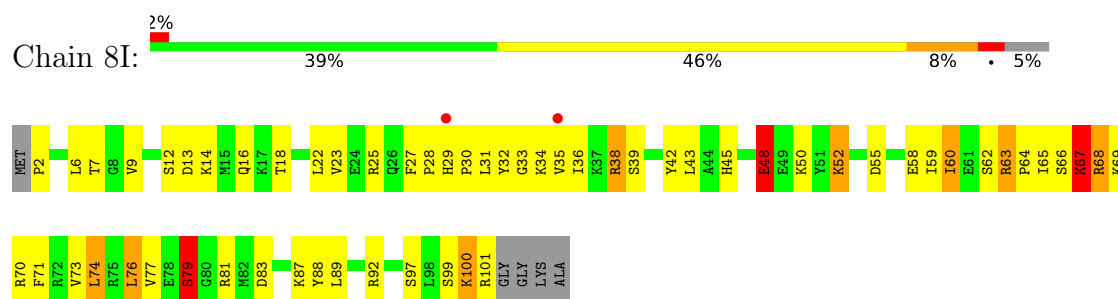
• Molecule 16: 30S ribosomal protein S16



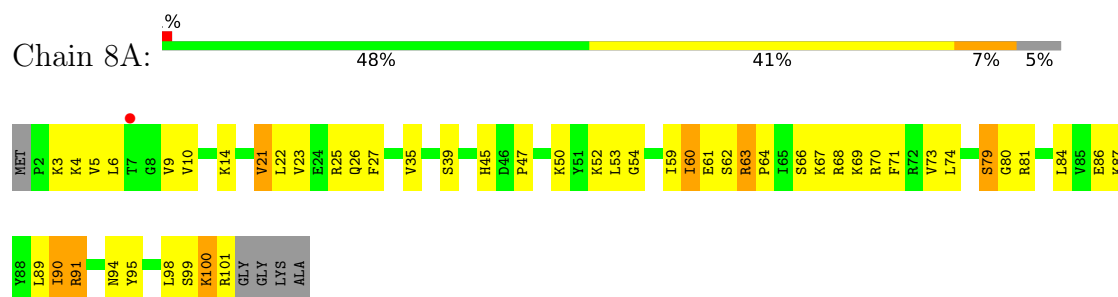
• Molecule 16: 30S ribosomal protein S16



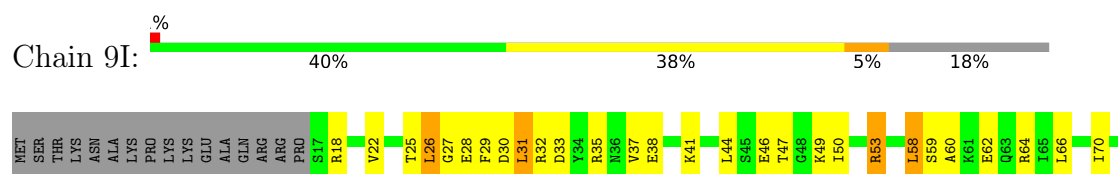
• Molecule 17: 30S ribosomal protein S17

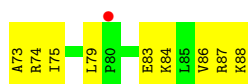


• Molecule 17: 30S ribosomal protein S17

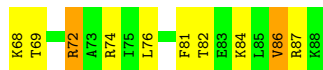


• Molecule 18: 30S ribosomal protein S18

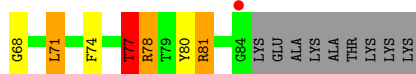
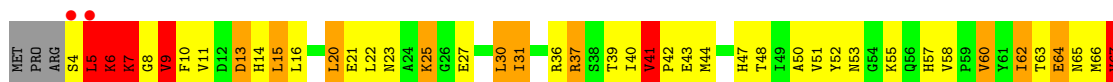




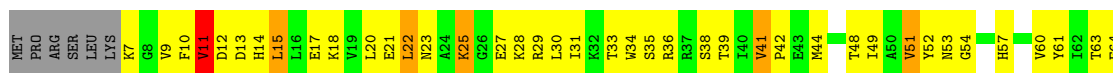
- Molecule 18: 30S ribosomal protein S18



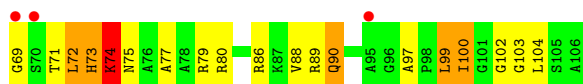
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19

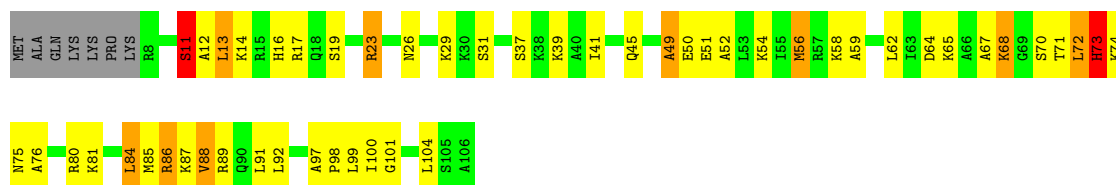


- Molecule 20: 30S ribosomal protein S20



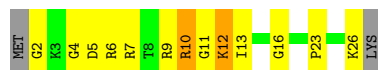
- Molecule 20: 30S ribosomal protein S20





- Molecule 21: 30S ribosomal protein Thx

Chain 1F: 44% 41% 7% 7%



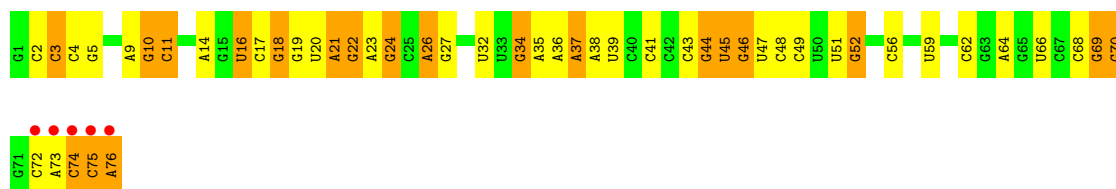
- Molecule 21: 30S ribosomal protein Thx

Chain 1B: 33% 44% 41% 7% 7%



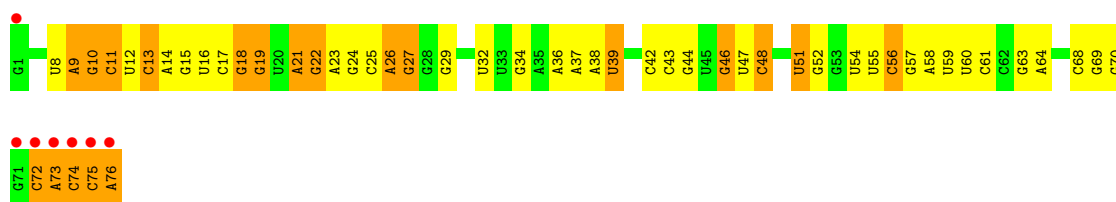
- Molecule 22: tRNA-Phe

Chain 1K: 7% 36% 38% 26%



- Molecule 22: tRNA-Phe

Chain 1L: 9% 32% 42% 26%



- Molecule 23: tRNA-fMet

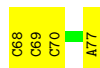
Chain 2K: % 35% 43% 19%





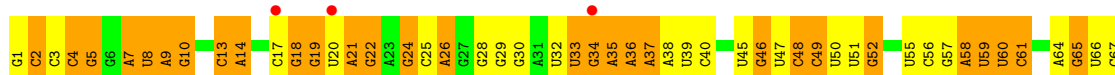
- Molecule 23: tRNA-fMet

Chain 2L: 34% 44% 18%



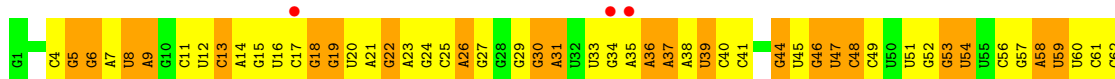
- Molecule 24: tRNA-Phe

Chain 3K: 4% 25% 29% 46%



- Molecule 24: tRNA-Phe

Chain 3L: 4% 17% 45% 38%



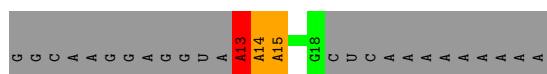
- Molecule 25: mRNA

Chain 4K: 10% 27% 10% 53%



- Molecule 25: mRNA

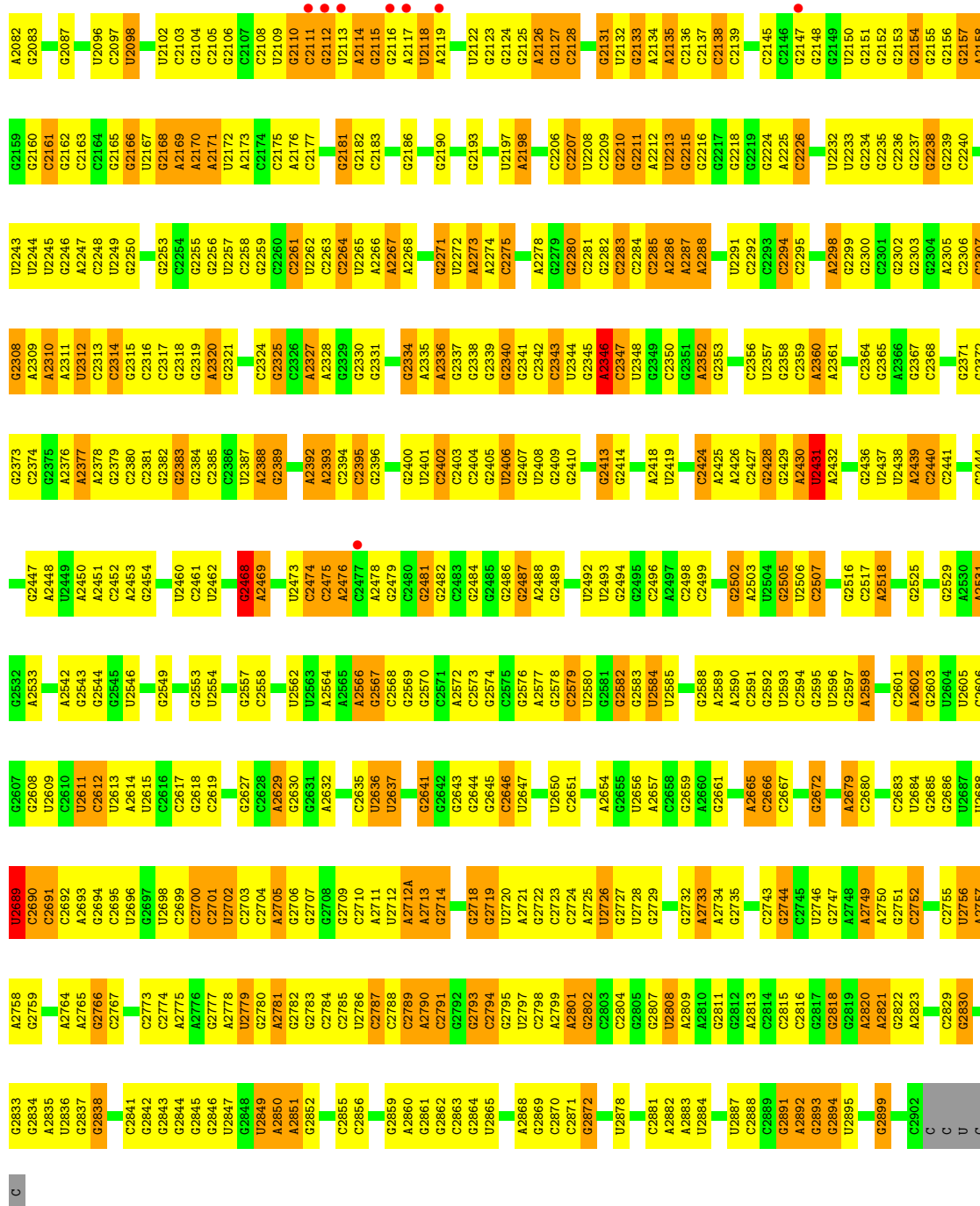
Chain 4L: 10% 7% 80%



- Molecule 26: 23S ribosomal RNA

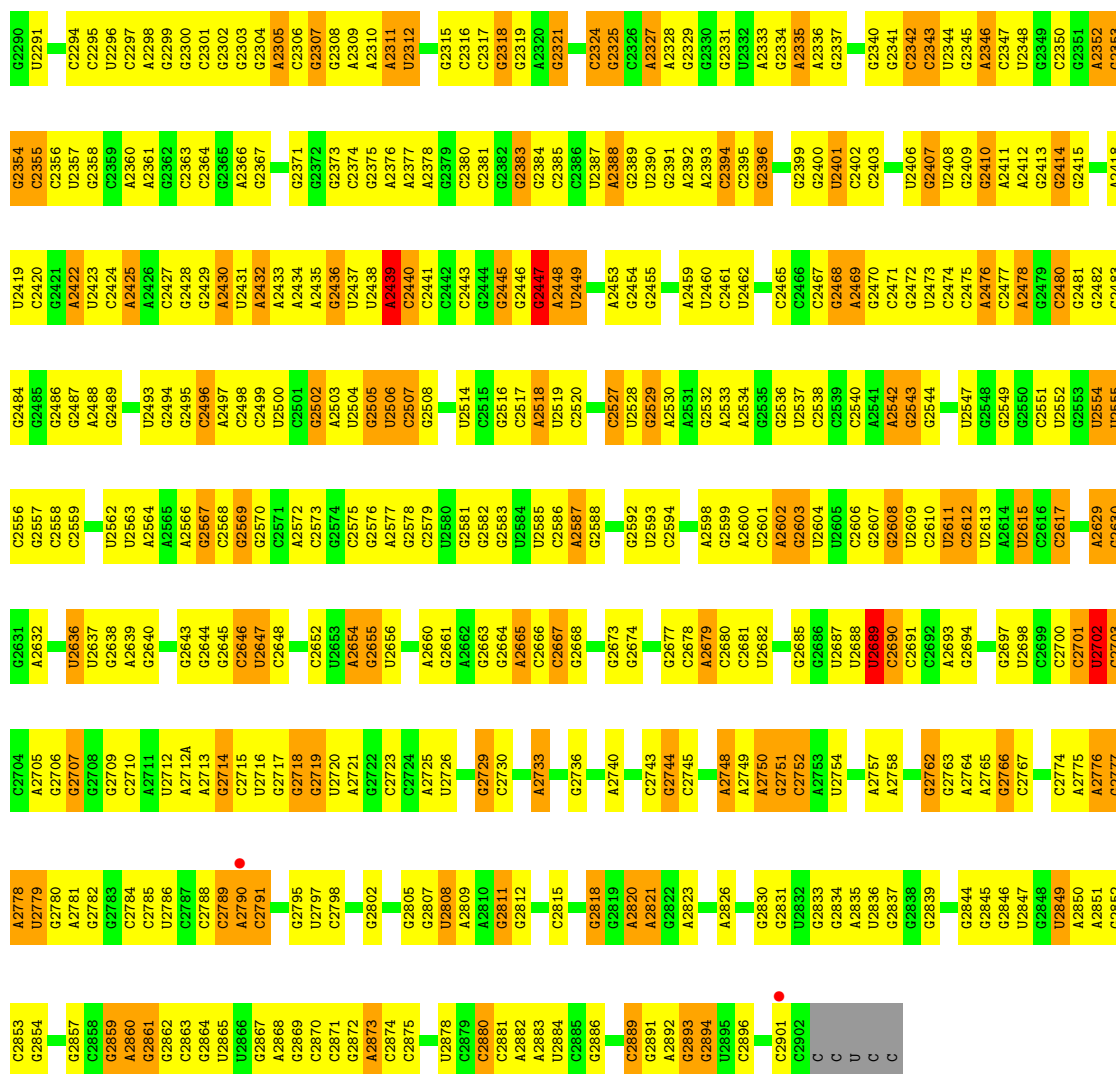
Chain 1H: 35% 49% 16%

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A2019	U1061	A1129	U1199	A1268	G1339	U1405	G1471	G1539	A1603	U1679	C1766	C1837	G1933	G2028
A2020	G1062	U1130	U1199	A1269	U1199	U1406	A1472	G1540	U1603	U1680	C1767	C1838	G1933	G2029
C2021	G1063	G1131	C1200	G1270	A1342	C1407	G1473	U1541	C1607	G1681	G1771	G1839	A1938	A2030
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G2023	U1065	U1133	C1202	A1272	C1346	U1409	G1475	A1543	A1609	C1683	A1773	C1844	U1946	G2032
G2027	U1066	C1135	G1203	U1273	G1347	G1410	G1478	C1544	A1610	C1684	G1776	A1847	G1950	U2033
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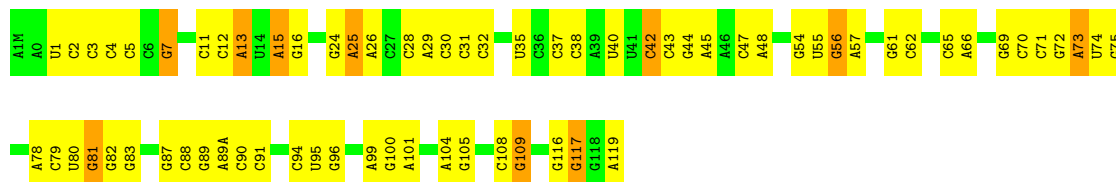


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			C1041	A973	G974	U839	G771	G696	A654	C581	A503		A337		
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			C1043	C974A	C908	A841	U773	C698	C654B	C583	A505		U839		
			U1044	G975	A909	C842	A774	A699	C654C	C584	G506		A340		
			A1045		A910	G843	G775	G700	G654D				A341		
			C1046	A980	C911	C844		A706	C654E	G585	C509		A342		
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			U1061	C996	A926	C864	G794	U724	G654T	U606	A449		A229		
			G1062	A996	C925	A863	G795	G725	A654U	U607	A526		A230		
			C1063	C997	G931	C865	C796	G726	A654V	A529	A449		A231		
			U1064	C998	C932	A866	C797	G727	A654W	G530	A449		A232		
			C1065	U999	A933	C867	G798	A729	A654X	C451	A447		A233		
			A1066	C1000	C934	U868	G798	C731	A655	C610	A447		A234		
			U1067	A1001	G934	U868	G798	C731	A656	C610	A447		A235		
			G1137	A1001	C935	G869	G801	A724	U657	U613	A447		A236		
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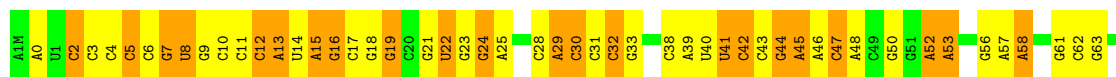
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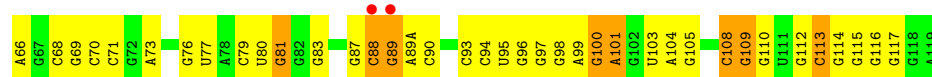


● Molecule 27: 5S ribosomal RNA



● Molecule 27: 5S ribosomal RNA





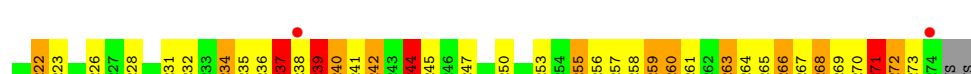
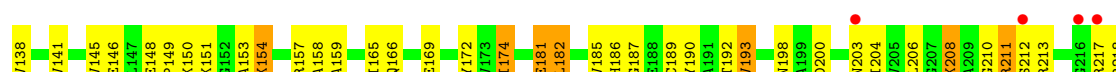
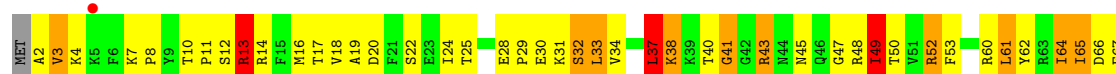
• Molecule 28: 50S ribosomal protein L2

Chain 11: 37% 46% 14% ..



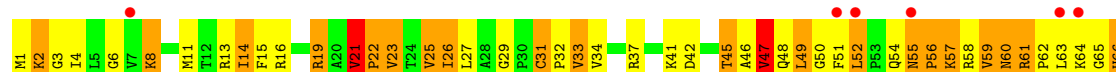
• Molecule 28: 50S ribosomal protein L2

Chain 19: 3% 39% 44% 13% ..



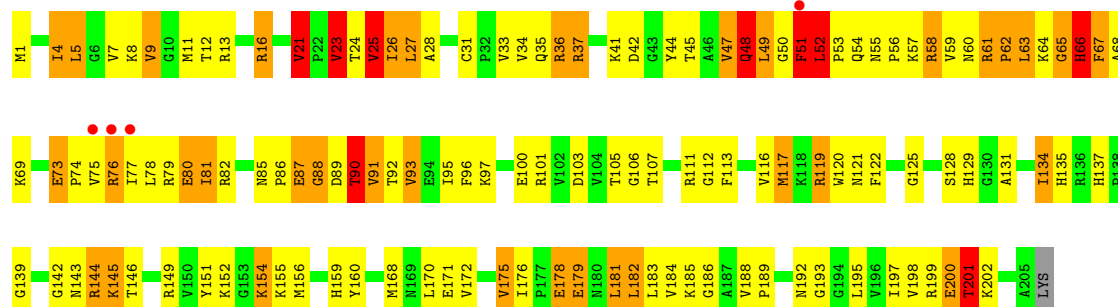
• Molecule 29: 50S ribosomal protein L3

Chain 21: 7% 38% 38% 20% .

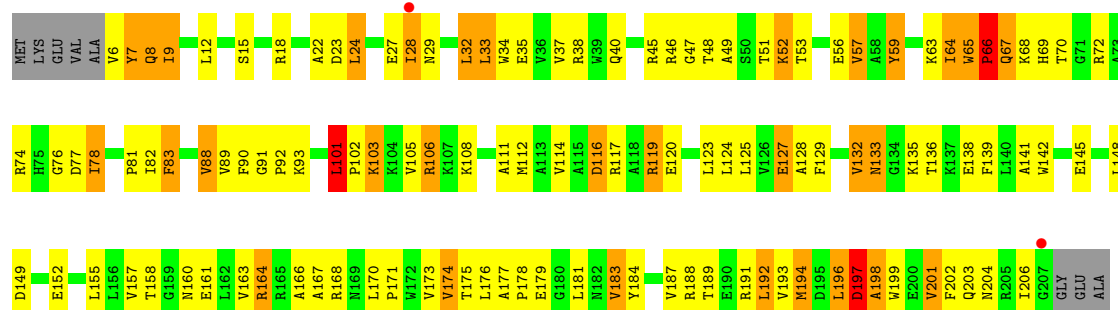




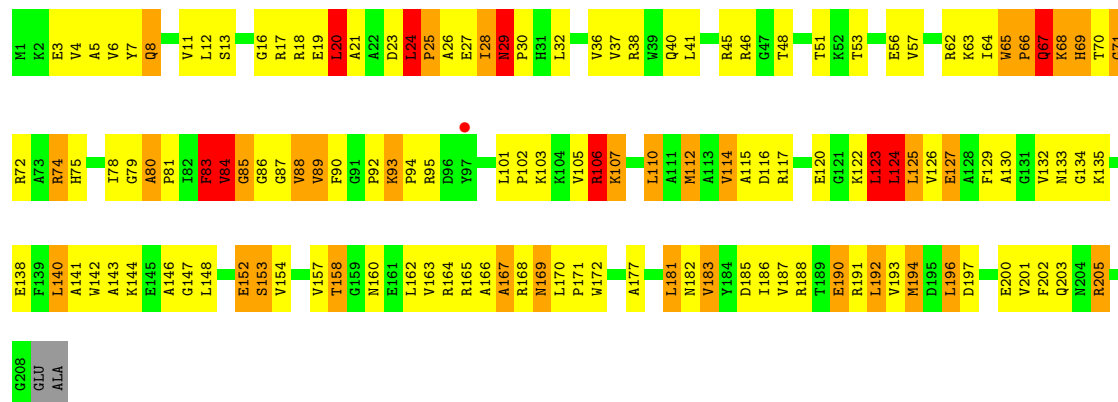
• Molecule 29: 50S ribosomal protein L3



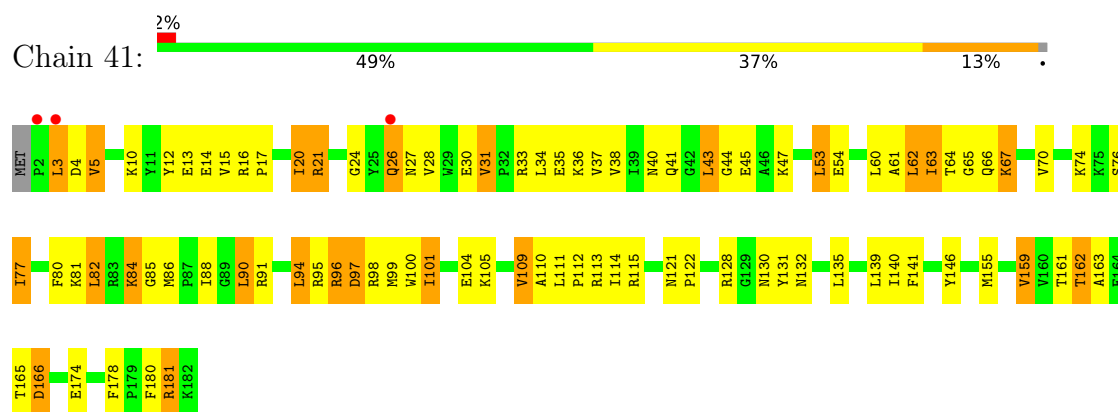
• Molecule 30: 50S ribosomal protein L4



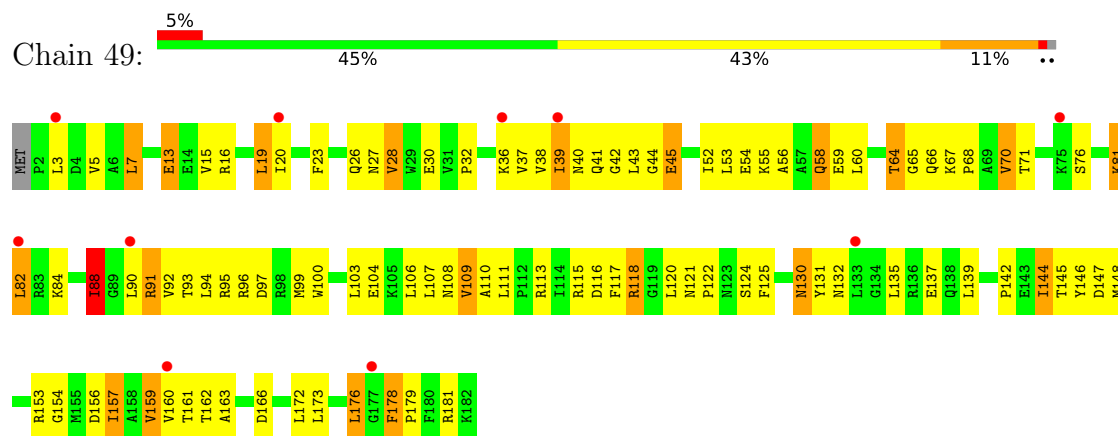
• Molecule 30: 50S ribosomal protein L4



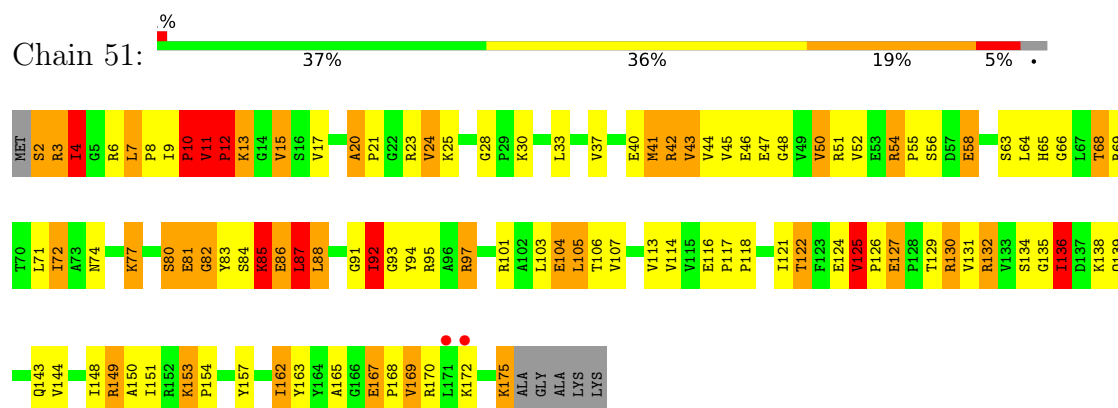
• Molecule 31: 50S ribosomal protein L5



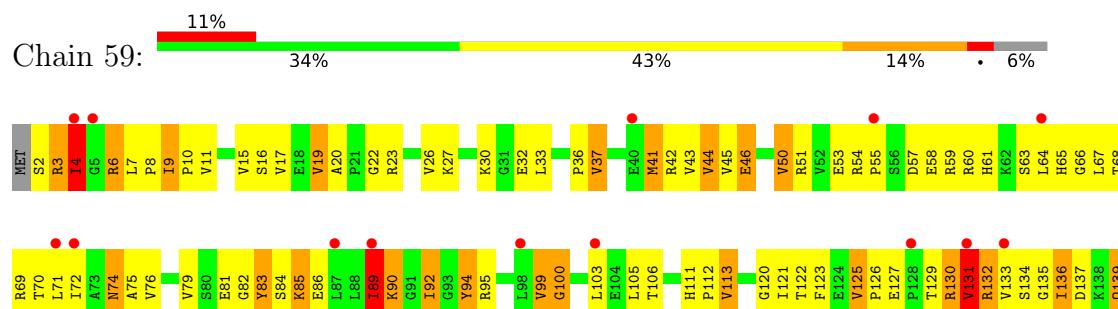
• Molecule 31: 50S ribosomal protein L5



• Molecule 32: 50S ribosomal protein L6

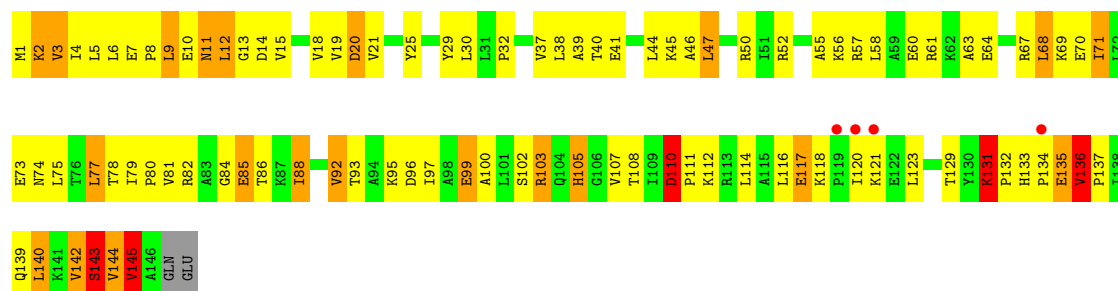


• Molecule 32: 50S ribosomal protein L6

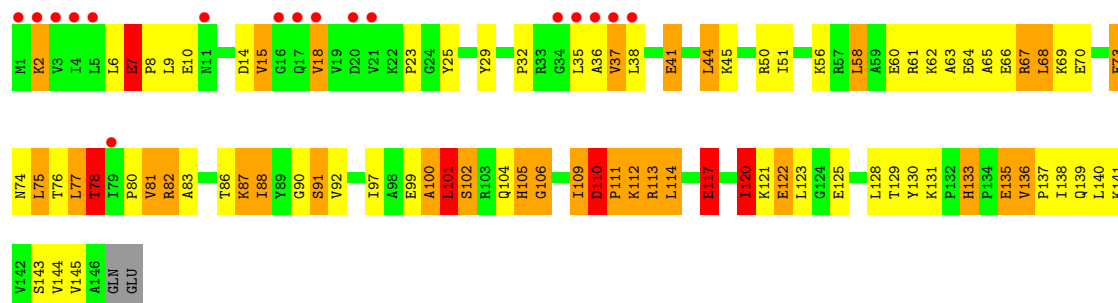




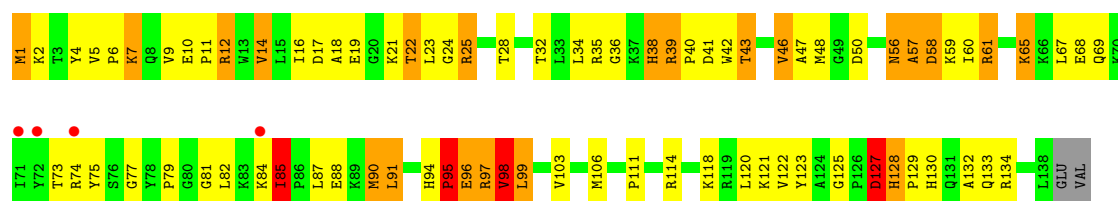
• Molecule 33: 50S ribosomal protein L9



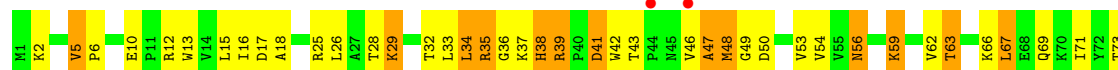
• Molecule 33: 50S ribosomal protein L9



• Molecule 34: 50S ribosomal protein L13

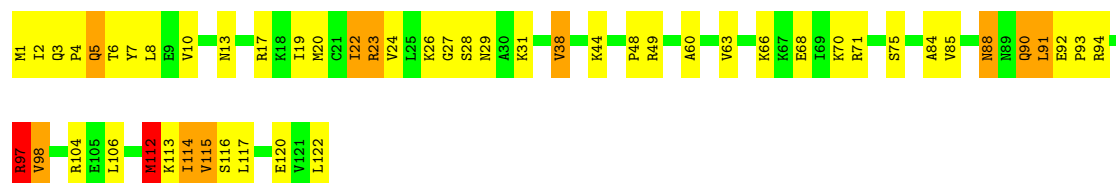


• Molecule 34: 50S ribosomal protein L13

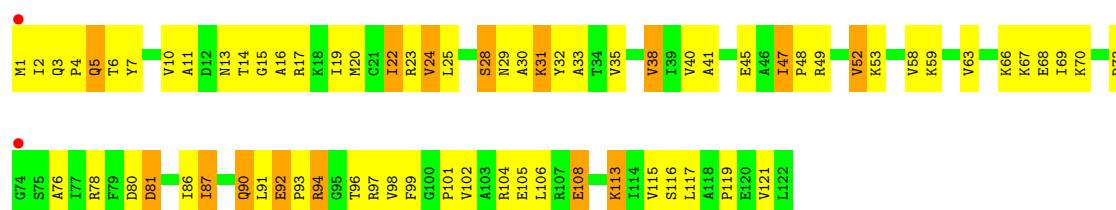




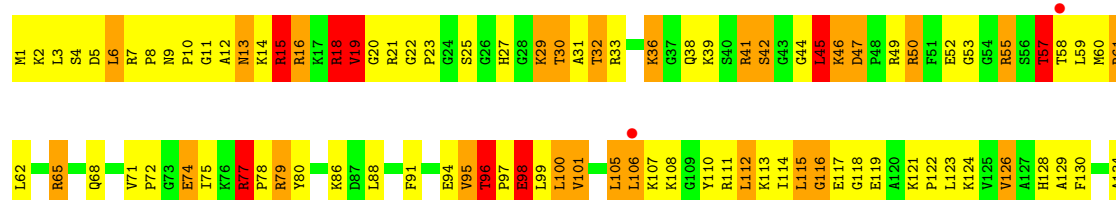
- Molecule 35: 50S ribosomal protein L14



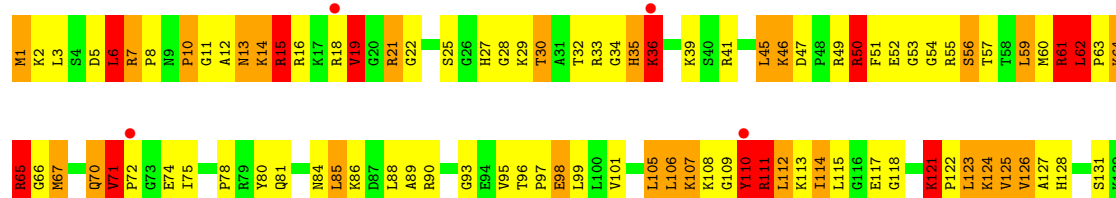
- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15

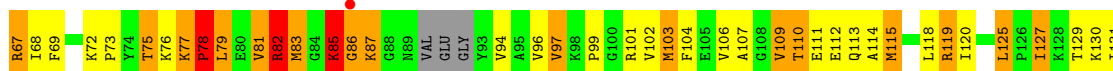
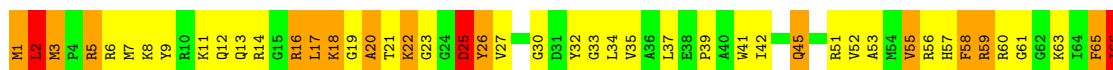


- Molecule 36: 50S ribosomal protein L15

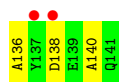




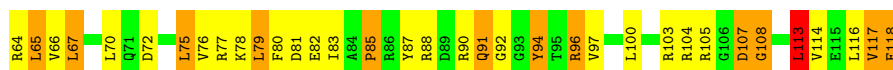
- Molecule 37: 50S ribosomal protein L16



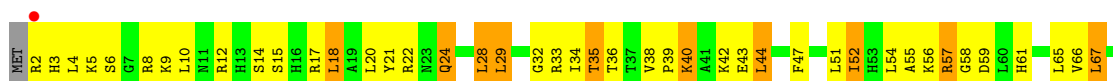
- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17

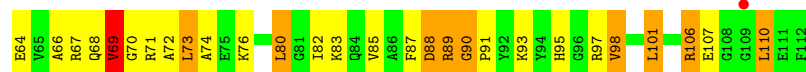
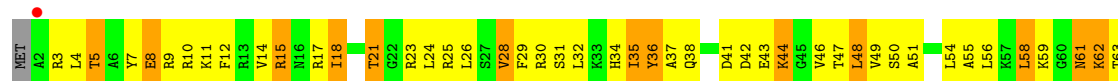


- Molecule 38: 50S ribosomal protein L17

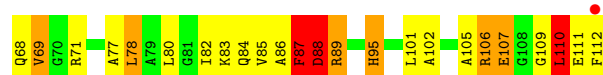
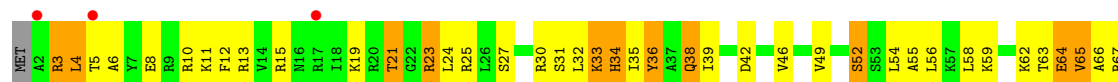
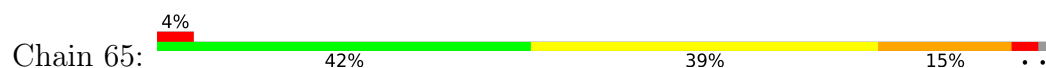




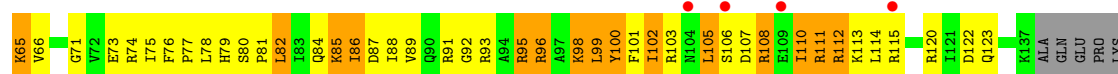
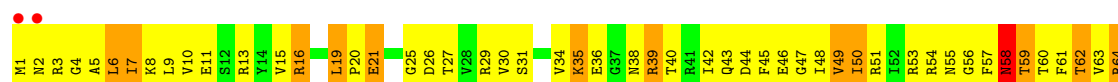
• Molecule 39: 50S ribosomal protein L18



• Molecule 39: 50S ribosomal protein L18



• Molecule 40: 50S ribosomal protein L19

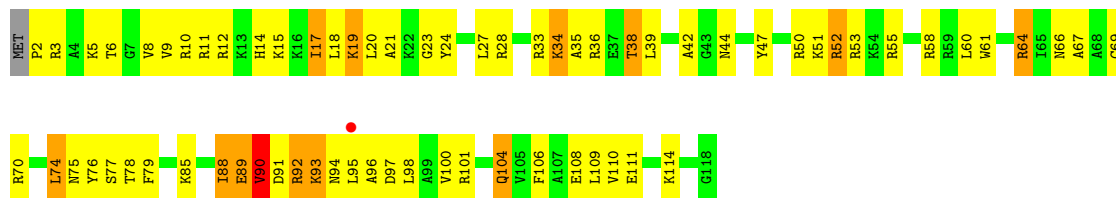


• Molecule 40: 50S ribosomal protein L19

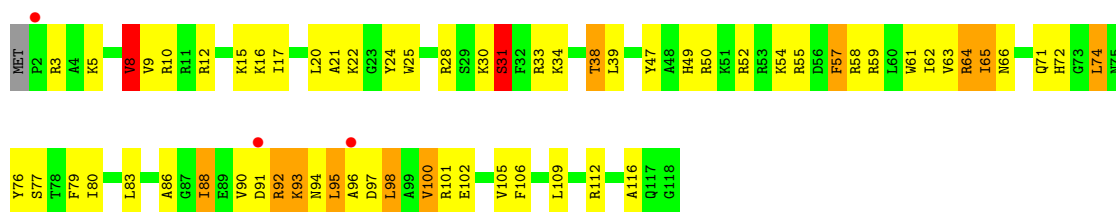


SER
GLN
GLU

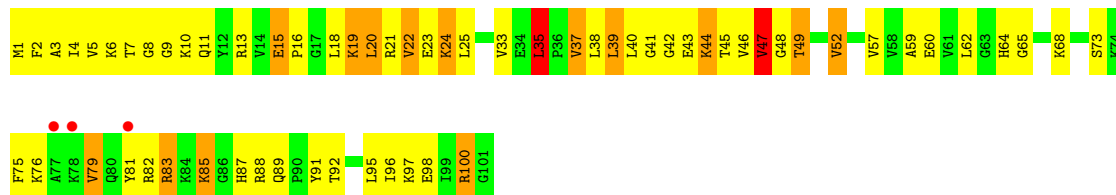
• Molecule 41: 50S ribosomal protein L20

Chain C8:  41% 47% 10% ..

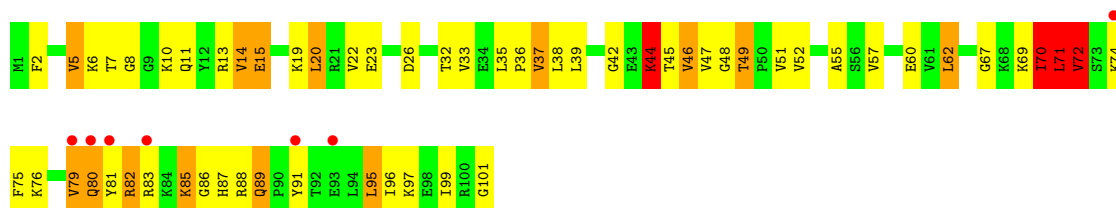
• Molecule 41: 50S ribosomal protein L20

Chain 85:  3% 46% 42% 9% ..

• Molecule 42: 50S ribosomal protein L21

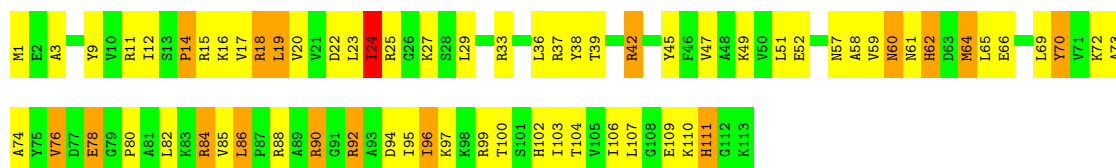
Chain D8:  3% 38% 47% 14% .

• Molecule 42: 50S ribosomal protein L21

Chain 95:  7% 42% 41% 14% .

• Molecule 43: 50S ribosomal protein L22

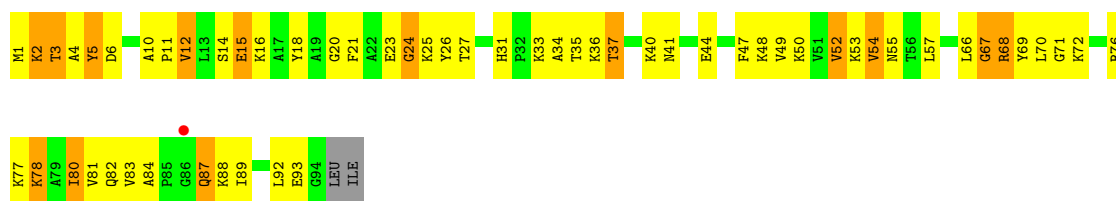
Chain E8:  41% 44% 14% .



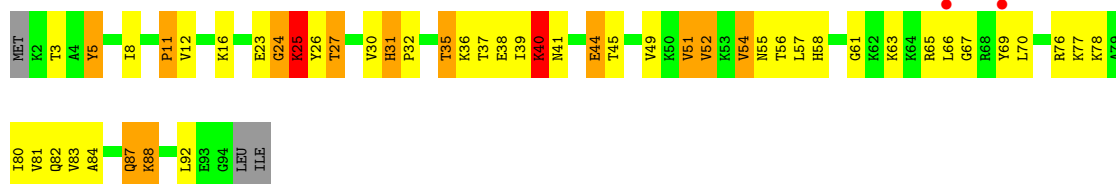
• Molecule 43: 50S ribosomal protein L22



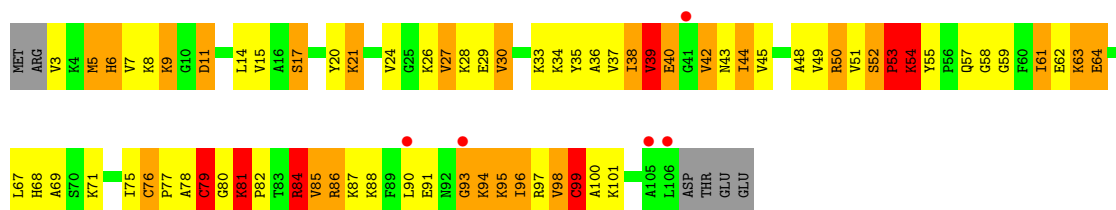
• Molecule 44: 50S ribosomal protein L23



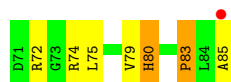
• Molecule 44: 50S ribosomal protein L23



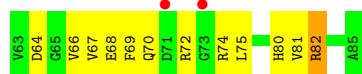
• Molecule 45: 50S ribosomal protein L24



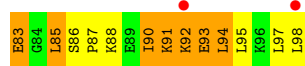
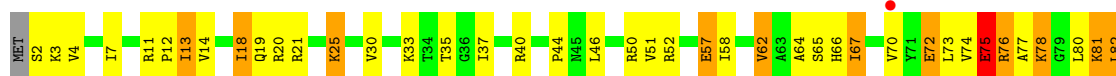
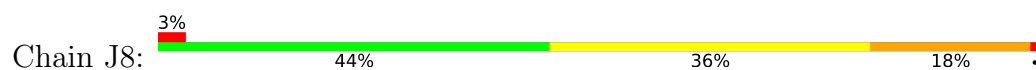
• Molecule 45: 50S ribosomal protein L24



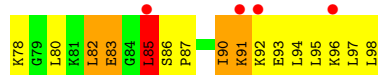
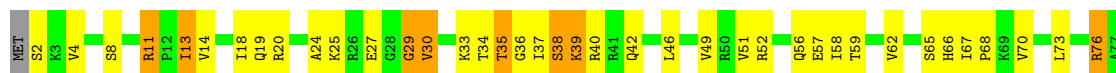
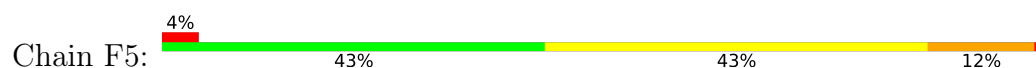
- Molecule 47: 50S ribosomal protein L27



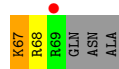
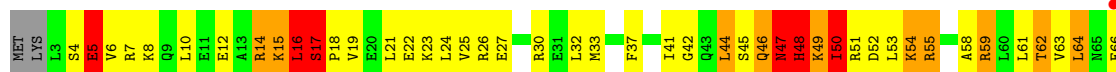
- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28

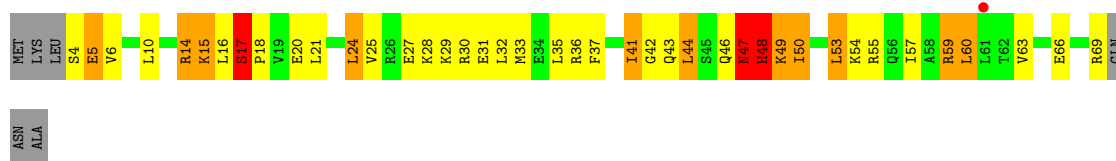


- Molecule 49: 50S ribosomal protein L29



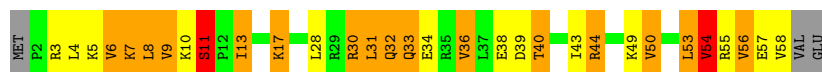
- Molecule 49: 50S ribosomal protein L29





- Molecule 50: 50S ribosomal protein L30

Chain L8: 43% 22% 27% 5%



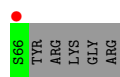
- Molecule 50: 50S ribosomal protein L30

Chain H5: 45% 35% 17%



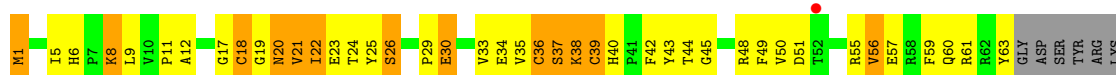
- Molecule 51: 50S ribosomal protein L31

Chain M8: 6% 25% 44% 20% 7%



- Molecule 51: 50S ribosomal protein L31

Chain I5: 30% 41% 18% 11%

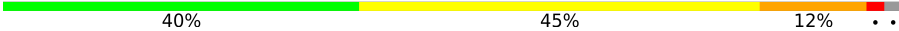


- Molecule 52: 50S ribosomal protein L32

Chain N8: 43% 32% 17% 5%



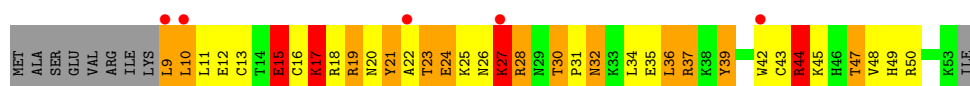
- Molecule 52: 50S ribosomal protein L32

Chain J5:  40% 45% 12% ..

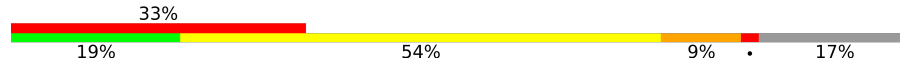


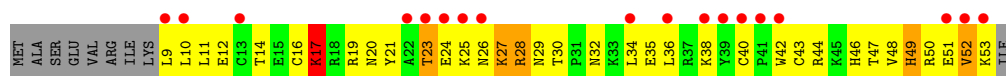
- Molecule 53: 50S ribosomal protein L33

Chain O8:  9% 19% 33% 24% 7% 17%



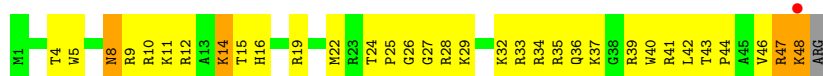
- Molecule 53: 50S ribosomal protein L33

Chain K5:  33% 19% 54% 9% 17%

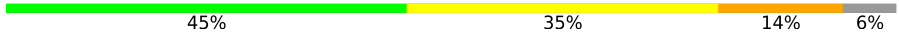


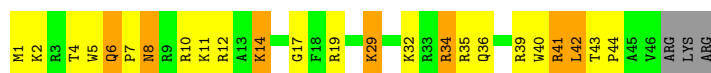
- Molecule 54: 50S ribosomal protein L34

Chain P8:  2% 31% 59% 8%

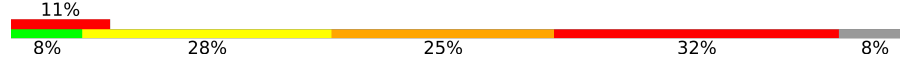


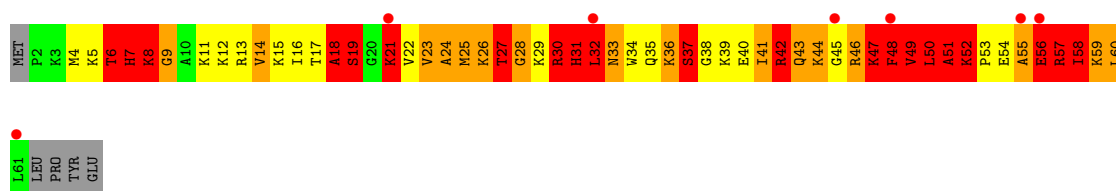
- Molecule 54: 50S ribosomal protein L34

Chain L5:  45% 35% 14% 6%

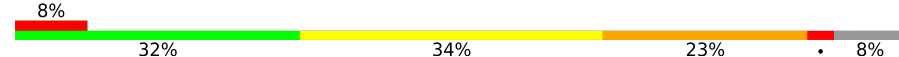


- Molecule 55: 50S ribosomal protein L35

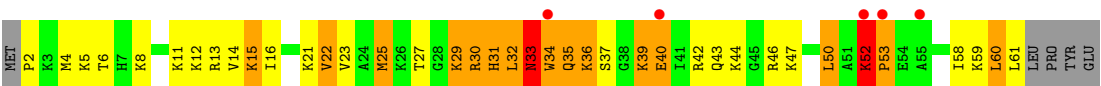
Chain Q8:  11% 8% 28% 25% 32% 8%



- Molecule 55: 50S ribosomal protein L35

Chain M5:  8% 32% 34% 23% 8%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.10Å 448.80Å 621.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.19 – 3.15 152.19 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (152.19-3.15) 93.3 (152.19-3.15)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.89 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.189 , 0.231 0.190 , 0.230	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	87.9	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	300537	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, MIA, 7MG, ZN, PSU, OMC, MG, 5MU

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	0.45	0/36052	0.73	9/56266 (0.0%)
1	1G	0.39	0/36025	0.65	10/56227 (0.0%)
2	12	0.52	0/1959	1.05	17/2642 (0.6%)
2	1E	0.60	0/1959	1.07	12/2642 (0.5%)
3	22	0.52	0/1636	1.03	6/2205 (0.3%)
3	2E	0.65	0/1629	1.02	2/2195 (0.1%)
4	32	0.63	0/1733	1.18	13/2318 (0.6%)
4	3E	0.72	0/1733	1.12	5/2318 (0.2%)
5	42	0.62	0/1171	1.10	5/1576 (0.3%)
5	4E	0.70	0/1171	1.14	3/1576 (0.2%)
6	52	0.69	0/856	1.02	0/1154
6	5E	0.72	0/856	1.07	1/1154 (0.1%)
7	62	0.55	0/1276	0.96	0/1709
7	6E	0.60	0/1276	1.04	7/1709 (0.4%)
8	72	0.52	0/1136	1.08	3/1527 (0.2%)
8	7E	0.69	0/1136	1.22	11/1527 (0.7%)
9	82	0.51	0/1029	1.01	5/1379 (0.4%)
9	8E	0.60	0/1029	1.08	2/1379 (0.1%)
10	1A	0.53	0/814	0.98	4/1095 (0.4%)
10	1I	0.68	1/814 (0.1%)	1.00	4/1095 (0.4%)
11	2A	0.67	0/900	1.25	10/1213 (0.8%)
11	2I	0.78	1/900 (0.1%)	1.26	5/1213 (0.4%)
12	3A	0.78	0/991	1.10	4/1327 (0.3%)
12	3I	0.90	0/991	1.34	10/1327 (0.8%)
13	4A	0.50	0/943	0.99	6/1265 (0.5%)
13	4I	0.64	0/948	1.08	3/1272 (0.2%)
14	5A	0.59	0/485	0.98	2/643 (0.3%)
14	5I	0.77	1/501 (0.2%)	1.18	5/664 (0.8%)
15	6A	0.61	0/745	0.96	1/992 (0.1%)
15	6I	0.79	0/745	1.24	2/992 (0.2%)
16	7A	0.65	0/721	1.04	2/970 (0.2%)
16	7I	0.66	0/721	1.04	5/970 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.64	0/847	0.98	1/1131 (0.1%)
17	8I	0.73	0/847	1.13	4/1131 (0.4%)
18	9A	0.65	0/596	1.00	0/790
18	9I	0.70	0/596	1.11	0/790
19	AA	0.60	0/638	1.12	5/860 (0.6%)
19	AI	0.78	2/661 (0.3%)	1.29	6/890 (0.7%)
20	BA	0.63	0/765	1.16	1/1007 (0.1%)
20	BI	0.58	0/765	1.11	3/1007 (0.3%)
21	1B	0.65	0/221	1.02	0/288
21	1F	0.59	0/221	1.00	0/288
22	1K	0.30	0/1739	0.49	0/2708
22	1L	0.24	0/1739	0.40	0/2708
23	2K	0.60	2/1721 (0.1%)	0.77	0/2682
23	2L	0.52	1/1721 (0.1%)	0.69	0/2682
24	3K	0.31	0/1809	0.60	0/2819
24	3L	0.28	0/1809	0.50	0/2819
25	4K	0.51	0/338	0.67	0/524
25	4L	0.51	0/147	0.83	2/227 (0.9%)
26	14	0.53	0/70167	0.80	28/109541 (0.0%)
26	1H	0.63	0/70233	0.90	51/109643 (0.0%)
27	16	0.55	0/2928	0.85	0/4568
27	1J	0.45	0/2928	0.73	0/4568
28	11	1.17	6/2170 (0.3%)	1.57	44/2926 (1.5%)
28	19	0.98	2/2170 (0.1%)	1.46	29/2926 (1.0%)
29	21	0.92	0/1601	1.50	28/2160 (1.3%)
29	29	0.93	1/1601 (0.1%)	1.42	20/2160 (0.9%)
30	31	1.01	1/1620 (0.1%)	1.43	18/2194 (0.8%)
30	39	0.85	1/1662 (0.1%)	1.42	22/2249 (1.0%)
31	41	0.74	0/1498	1.23	7/2016 (0.3%)
31	49	0.55	0/1498	1.04	8/2016 (0.4%)
32	51	0.86	0/1362	1.50	24/1841 (1.3%)
32	59	0.54	0/1332	1.18	12/1802 (0.7%)
33	61	0.72	0/1151	1.25	16/1558 (1.0%)
33	69	0.68	0/1151	1.21	15/1558 (1.0%)
34	15	0.66	0/1131	1.18	12/1525 (0.8%)
34	58	0.84	0/1131	1.27	11/1525 (0.7%)
35	25	0.81	0/943	1.27	6/1269 (0.5%)
35	68	0.94	2/943 (0.2%)	1.28	9/1269 (0.7%)
36	35	0.98	3/1162 (0.3%)	1.66	27/1544 (1.7%)
36	78	1.04	3/1162 (0.3%)	1.59	23/1544 (1.5%)
37	45	0.96	2/1143 (0.2%)	1.35	9/1527 (0.6%)
37	88	1.24	5/1107 (0.5%)	1.66	29/1478 (2.0%)
38	55	0.87	0/974	1.22	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	98	0.88	0/982	1.31	7/1312 (0.5%)
39	65	0.72	0/892	1.30	4/1187 (0.3%)
39	A8	0.88	0/892	1.39	8/1187 (0.7%)
40	75	0.80	0/1155	1.15	5/1542 (0.3%)
40	B8	0.86	0/1155	1.28	8/1542 (0.5%)
41	85	0.79	0/982	1.17	4/1306 (0.3%)
41	C8	0.95	1/982 (0.1%)	1.22	2/1306 (0.2%)
42	95	0.90	2/790 (0.3%)	1.39	7/1057 (0.7%)
42	D8	0.86	0/790	1.27	6/1057 (0.6%)
43	A5	0.92	0/911	1.21	4/1220 (0.3%)
43	E8	0.90	0/911	1.37	7/1220 (0.6%)
44	B5	0.97	1/744 (0.1%)	1.31	8/1000 (0.8%)
44	F8	1.06	0/756	1.38	10/1014 (1.0%)
45	C5	1.01	3/807 (0.4%)	1.36	8/1076 (0.7%)
45	G8	0.96	0/804	1.46	11/1073 (1.0%)
46	D5	0.59	0/1460	1.17	10/1982 (0.5%)
46	H8	0.74	2/1427 (0.1%)	1.32	16/1935 (0.8%)
47	E5	0.79	0/621	1.34	11/827 (1.3%)
47	I8	1.04	1/635 (0.2%)	1.39	3/847 (0.4%)
48	F5	0.86	0/770	1.34	6/1022 (0.6%)
48	J8	1.00	1/770 (0.1%)	1.30	3/1022 (0.3%)
49	G5	0.72	0/560	1.24	2/741 (0.3%)
49	K8	0.99	0/565	1.42	7/748 (0.9%)
50	H5	0.63	0/474	1.17	3/635 (0.5%)
50	L8	1.05	0/457	1.63	9/613 (1.5%)
51	I5	0.71	0/527	1.23	4/709 (0.6%)
51	M8	0.79	0/545	1.29	4/733 (0.5%)
52	J5	0.91	0/473	1.42	4/639 (0.6%)
52	N8	0.97	0/468	1.84	10/632 (1.6%)
53	K5	0.86	0/396	1.41	5/529 (0.9%)
53	O8	1.10	1/396 (0.3%)	1.39	8/529 (1.5%)
54	L5	1.06	0/406	1.47	5/536 (0.9%)
54	P8	1.26	0/426	1.48	3/561 (0.5%)
55	M5	1.29	2/483 (0.4%)	1.68	14/634 (2.2%)
55	Q8	1.93	16/486 (3.3%)	2.34	28/638 (4.4%)
All	All	0.62	64/322727 (0.0%)	0.94	898/483212 (0.2%)

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	1
2	1E	0	1
4	32	0	4
4	3E	0	1
9	82	0	2
10	1A	0	2
11	2A	0	2
12	3A	0	1
12	3I	0	1
15	6I	0	1
19	AI	0	2
20	BA	0	3
28	11	0	1
28	19	0	4
29	21	0	3
29	29	0	4
30	31	0	1
30	39	0	6
31	41	0	2
31	49	0	1
32	59	0	3
33	61	0	5
33	69	0	2
34	15	0	2
34	58	0	2
35	68	0	1
36	35	0	4
36	78	0	2
37	45	0	6
37	88	0	2
38	55	0	1
38	98	0	3
39	65	0	2
39	A8	0	2
40	75	0	1
40	B8	0	1
41	85	0	2
41	C8	0	2
42	95	0	1
43	A5	0	3
44	B5	0	2
44	F8	0	1
45	C5	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	G8	0	3
46	D5	0	2
46	H8	0	2
47	I8	0	2
48	F5	0	1
48	J8	0	2
49	G5	0	3
49	K8	0	3
51	I5	0	2
51	M8	0	2
52	N8	0	2
53	K5	0	3
53	O8	0	3
55	M5	0	3
55	Q8	0	13
All	All	0	142

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Q8	6	THR	CA-CB	11.77	1.70	1.53
55	Q8	49	VAL	CA-CB	10.68	1.69	1.54
37	88	82	ARG	CA-C	10.56	1.67	1.52
55	M5	52	LYS	CA-C	9.73	1.65	1.52
37	88	82	ARG	N-CA	9.63	1.58	1.46

The worst 5 of 898 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	88	86	GLY	N-CA-C	-16.90	94.81	112.04
52	N8	40	LYS	CA-C-N	-16.31	103.58	120.38
52	N8	40	LYS	C-N-CA	-16.31	103.58	120.38
28	19	272	ALA	N-CA-C	14.61	131.25	107.73
28	11	271	ILE	N-CA-C	14.50	127.25	111.88

There are no chirality outliers.

5 of 142 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
4	3E	31	CYS	Peptide

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Mol	Chain	Res	Type	Group
12	3I	87	GLY	Peptide
15	6I	87	ILE	Peptide
19	AI	6	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32207	0	16256	878	0
1	1G	32182	0	16244	871	0
2	12	1924	0	1975	87	0
2	1E	1924	0	1975	106	0
3	22	1612	0	1677	81	0
3	2E	1605	0	1668	65	0
4	32	1703	0	1763	98	0
4	3E	1703	0	1762	104	0
5	42	1155	0	1213	61	0
5	4E	1155	0	1213	56	0
6	52	843	0	857	46	0
6	5E	843	0	857	39	0
7	62	1257	0	1296	62	0
7	6E	1257	0	1296	50	0
8	72	1116	0	1177	57	0
8	7E	1116	0	1177	65	0
9	82	1010	0	1037	74	0
9	8E	1010	0	1037	60	0
10	1A	801	0	849	43	0
10	1I	801	0	849	63	0
11	2A	885	0	904	39	0
11	2I	885	0	904	45	0
12	3A	975	0	1062	46	0
12	3I	975	0	1062	45	0
13	4A	933	0	992	70	0
13	4I	938	0	997	51	0
14	5A	476	0	511	31	0
14	5I	492	0	529	30	0
15	6A	734	0	771	24	0
15	6I	734	0	771	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	7A	705	0	725	43	0
16	7I	705	0	725	55	0
17	8A	834	0	904	25	0
17	8I	834	0	904	51	0
18	9A	591	0	662	27	0
18	9I	591	0	662	29	0
19	AA	624	0	636	50	0
19	AI	647	0	665	59	0
20	BA	763	0	861	45	0
20	BI	763	0	861	44	0
21	1B	217	0	234	12	0
21	1F	217	0	234	13	0
22	1K	1626	0	834	29	0
22	1L	1626	0	834	41	0
23	2K	1646	0	845	37	0
23	2L	1646	0	845	39	0
24	3K	1619	0	822	52	0
24	3L	1619	0	822	60	0
25	4K	301	0	153	10	0
25	4L	131	0	66	5	0
26	14	62647	0	31580	1629	1
26	1H	62707	0	31607	1780	1
27	16	2617	0	1328	71	0
27	1J	2617	0	1328	100	0
28	11	2120	0	2197	129	0
28	19	2120	0	2197	122	0
29	21	1568	0	1634	112	0
29	29	1568	0	1634	127	0
30	31	1585	0	1632	106	0
30	39	1627	0	1680	107	0
31	41	1473	0	1535	77	0
31	49	1473	0	1535	72	0
32	51	1336	0	1418	99	0
32	59	1307	0	1382	73	0
33	61	1136	0	1223	63	0
33	69	1136	0	1223	56	0
34	15	1104	0	1180	55	0
34	58	1104	0	1180	73	0
35	25	933	0	996	49	0
35	68	933	0	996	44	0
36	35	1145	0	1228	118	0
36	78	1145	0	1228	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	45	1122	0	1179	86	0
37	88	1087	0	1129	91	0
38	55	960	0	1021	65	0
38	98	968	0	1033	72	0
39	65	882	0	943	62	0
39	A8	882	0	943	68	0
40	75	1141	0	1202	71	0
40	B8	1141	0	1202	79	0
41	85	964	0	1022	57	0
41	C8	964	0	1022	71	0
42	95	779	0	852	69	0
42	D8	779	0	852	43	0
43	A5	900	0	964	36	0
43	E8	900	0	964	50	0
44	B5	730	0	780	32	0
44	F8	742	0	803	59	0
45	C5	794	0	884	59	0
45	G8	791	0	882	58	0
46	D5	1428	0	1454	93	0
46	H8	1397	0	1430	86	0
47	E5	613	0	633	49	0
47	I8	627	0	642	34	0
48	F5	763	0	848	33	0
48	J8	763	0	848	38	0
49	G5	558	0	610	32	1
49	K8	563	0	612	45	1
50	H5	469	0	518	16	0
50	L8	452	0	503	32	0
51	I5	515	0	514	42	0
51	M8	533	0	526	49	0
52	J5	459	0	480	34	0
52	N8	454	0	475	33	0
53	K5	389	0	404	22	0
53	O8	389	0	404	33	0
54	L5	398	0	441	19	0
54	P8	418	0	467	24	0
55	M5	477	0	540	50	0
55	Q8	480	0	549	133	0
56	11	4	0	0	0	0
56	13	151	0	0	0	0
56	14	389	0	0	0	0
56	16	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1G	103	0	0	0	0
56	1H	529	0	0	0	0
56	1J	9	0	0	0	0
56	1K	2	0	0	0	0
56	2I	2	0	0	0	0
56	29	2	0	0	0	0
56	2K	3	0	0	0	0
56	2L	2	0	0	0	0
56	3I	1	0	0	0	0
56	35	1	0	0	0	0
56	3E	2	0	0	0	0
56	3I	1	0	0	0	0
56	4I	2	0	0	0	0
56	49	1	0	0	0	0
56	4A	1	0	0	0	0
56	5E	1	0	0	0	0
56	6A	1	0	0	0	0
56	75	1	0	0	0	0
56	78	2	0	0	0	0
56	85	1	0	0	0	0
56	88	2	0	0	0	0
56	98	1	0	0	0	0
56	AI	1	0	0	0	0
56	C5	1	0	0	0	0
56	C8	1	0	0	0	0
56	E8	1	0	0	0	0
56	F5	1	0	0	0	0
56	I8	2	0	0	0	0
56	J8	2	0	0	0	0
56	L8	1	0	0	0	0
56	P8	1	0	0	0	0
56	Q8	1	0	0	0	0
57	32	1	0	0	0	0
57	3E	1	0	0	0	0
57	5A	1	0	0	0	0
57	5I	1	0	0	0	0
57	C5	1	0	0	0	0
57	G8	1	0	0	0	0
58	11	9	0	0	0	0
58	13	212	0	0	36	0
58	14	730	0	0	169	0
58	16	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	19	11	0	0	0	0
58	1G	99	0	0	22	0
58	1H	1097	0	0	264	0
58	1I	2	0	0	0	0
58	1J	12	0	0	3	0
58	1K	1	0	0	0	0
58	21	5	0	0	3	0
58	29	6	0	0	0	0
58	31	10	0	0	0	0
58	39	7	0	0	0	0
58	3E	1	0	0	0	0
58	3I	1	0	0	0	0
58	3K	1	0	0	0	0
58	4E	2	0	0	0	0
58	4K	4	0	0	0	0
58	55	1	0	0	0	0
58	58	1	0	0	0	0
58	5I	2	0	0	0	0
58	78	4	0	0	0	0
58	7A	2	0	0	0	0
58	85	1	0	0	0	0
58	8E	2	0	0	0	0
58	98	1	0	0	0	0
58	A5	1	0	0	0	0
58	BA	1	0	0	0	0
58	C8	2	0	0	1	0
58	D8	1	0	0	0	0
58	E8	2	0	0	0	0
58	G8	3	0	0	0	0
58	H5	1	0	0	0	0
58	I8	6	0	0	0	0
58	L5	1	0	0	0	0
58	L8	2	0	0	0	0
58	P8	2	0	0	0	0
58	Q8	2	0	0	0	0
All	All	300537	0	200491	10068	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 10068 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)
4:32:9:CYS:SG	4:32:31:CYS:HB2	1.81	1.19
26:1H:2714:G:OP2	58:1H:3670:HOH:O	1.68	1.11
36:78:19:VAL:HG12	36:78:21:ARG:H	1.15	1.07
26:14:2593:U:O4	58:14:4084:HOH:O	1.72	1.07
26:1H:1614:A:OP1	58:1H:3921:HOH:O	1.73	1.06

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:K8:17:SER:OG	26:14:307:G:OP1[2_564]	1.99	0.21
26:1H:277:C:O2'	49:G5:49:LYS:NZ[2_564]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	235/256 (92%)	194 (83%)	38 (16%)	3 (1%)	9	36
2	1E	235/256 (92%)	198 (84%)	35 (15%)	2 (1%)	14	43
3	22	204/239 (85%)	180 (88%)	24 (12%)	0	100	100
3	2E	203/239 (85%)	179 (88%)	23 (11%)	1 (0%)	24	55
4	32	206/209 (99%)	181 (88%)	24 (12%)	1 (0%)	24	55
4	3E	206/209 (99%)	190 (92%)	14 (7%)	2 (1%)	12	41
5	42	149/162 (92%)	141 (95%)	8 (5%)	0	100	100
5	4E	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	18	49
6	52	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	5E	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
7	62	153/156 (98%)	146 (95%)	6 (4%)	1 (1%)	18	49
7	6E	153/156 (98%)	142 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	72	136/138 (99%)	126 (93%)	8 (6%)	2 (2%)	8	33
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	18	49
9	82	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16	46
9	8E	125/128 (98%)	107 (86%)	18 (14%)	0	100	100
10	1A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
10	1I	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
11	2A	117/129 (91%)	102 (87%)	12 (10%)	3 (3%)	4	21
11	2I	117/129 (91%)	103 (88%)	13 (11%)	1 (1%)	14	43
12	3A	123/132 (93%)	100 (81%)	18 (15%)	5 (4%)	2	14
12	3I	123/132 (93%)	105 (85%)	18 (15%)	0	100	100
13	4A	115/126 (91%)	94 (82%)	19 (16%)	2 (2%)	7	30
13	4I	116/126 (92%)	94 (81%)	22 (19%)	0	100	100
14	5A	56/61 (92%)	47 (84%)	8 (14%)	1 (2%)	6	29
14	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	16
15	6A	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	6I	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	7I	82/88 (93%)	75 (92%)	6 (7%)	1 (1%)	10	37
17	8A	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	8I	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	9A	70/88 (80%)	65 (93%)	5 (7%)	0	100	100
18	9I	70/88 (80%)	62 (89%)	7 (10%)	1 (1%)	9	34
19	AA	76/93 (82%)	61 (80%)	13 (17%)	2 (3%)	4	21
19	AI	79/93 (85%)	65 (82%)	10 (13%)	4 (5%)	1	10
20	BA	97/106 (92%)	84 (87%)	11 (11%)	2 (2%)	5	26
20	BI	97/106 (92%)	82 (84%)	14 (14%)	1 (1%)	12	41
21	1B	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
28	11	271/276 (98%)	252 (93%)	14 (5%)	5 (2%)	6	29
28	19	271/276 (98%)	252 (93%)	14 (5%)	5 (2%)	6	29
29	21	203/206 (98%)	161 (79%)	30 (15%)	12 (6%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	29	203/206 (98%)	156 (77%)	35 (17%)	12 (6%)	1	8
30	31	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	12	41
30	39	206/210 (98%)	159 (77%)	41 (20%)	6 (3%)	3	20
31	41	179/182 (98%)	159 (89%)	17 (10%)	3 (2%)	7	30
31	49	179/182 (98%)	158 (88%)	20 (11%)	1 (1%)	21	52
32	51	172/180 (96%)	148 (86%)	17 (10%)	7 (4%)	2	14
32	59	168/180 (93%)	129 (77%)	34 (20%)	5 (3%)	3	19
33	61	144/148 (97%)	117 (81%)	23 (16%)	4 (3%)	4	20
33	69	144/148 (97%)	119 (83%)	21 (15%)	4 (3%)	4	20
34	15	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	18	49
34	58	136/140 (97%)	116 (85%)	16 (12%)	4 (3%)	3	20
35	25	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
35	68	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	46
36	35	148/150 (99%)	114 (77%)	28 (19%)	6 (4%)	2	14
36	78	148/150 (99%)	121 (82%)	21 (14%)	6 (4%)	2	14
37	45	139/141 (99%)	114 (82%)	23 (16%)	2 (1%)	9	34
37	88	134/141 (95%)	110 (82%)	18 (13%)	6 (4%)	2	12
38	55	115/118 (98%)	104 (90%)	9 (8%)	2 (2%)	7	30
38	98	116/118 (98%)	97 (84%)	18 (16%)	1 (1%)	14	43
39	65	109/112 (97%)	87 (80%)	18 (16%)	4 (4%)	2	15
39	A8	109/112 (97%)	90 (83%)	18 (16%)	1 (1%)	14	43
40	75	135/146 (92%)	119 (88%)	15 (11%)	1 (1%)	18	49
40	B8	135/146 (92%)	122 (90%)	13 (10%)	0	100	100
41	85	115/118 (98%)	99 (86%)	15 (13%)	1 (1%)	14	43
41	C8	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	16
42	95	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	1	10
42	D8	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	27
43	A5	111/113 (98%)	100 (90%)	11 (10%)	0	100	100
43	E8	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
44	B5	91/96 (95%)	82 (90%)	8 (9%)	1 (1%)	11	39
44	F8	92/96 (96%)	84 (91%)	7 (8%)	1 (1%)	11	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	C5	102/110 (93%)	75 (74%)	22 (22%)	5 (5%)	1	11
45	G8	102/110 (93%)	82 (80%)	14 (14%)	6 (6%)	1	8
46	D5	177/206 (86%)	130 (73%)	37 (21%)	10 (6%)	1	9
46	H8	173/206 (84%)	136 (79%)	28 (16%)	9 (5%)	1	10
47	E5	75/85 (88%)	66 (88%)	8 (11%)	1 (1%)	9	36
47	I8	78/85 (92%)	65 (83%)	12 (15%)	1 (1%)	9	36
48	F5	95/98 (97%)	88 (93%)	6 (6%)	1 (1%)	11	39
48	J8	95/98 (97%)	86 (90%)	7 (7%)	2 (2%)	5	26
49	G5	64/72 (89%)	59 (92%)	3 (5%)	2 (3%)	3	18
49	K8	65/72 (90%)	60 (92%)	3 (5%)	2 (3%)	3	18
50	H5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	L8	55/60 (92%)	50 (91%)	4 (7%)	1 (2%)	6	29
51	I5	61/71 (86%)	34 (56%)	24 (39%)	3 (5%)	1	11
51	M8	64/71 (90%)	40 (62%)	21 (33%)	3 (5%)	2	11
52	J5	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	6	29
52	N8	56/60 (93%)	48 (86%)	6 (11%)	2 (4%)	2	16
53	K5	43/54 (80%)	26 (60%)	14 (33%)	3 (7%)	1	5
53	O8	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	2	11
54	L5	44/49 (90%)	42 (96%)	2 (4%)	0	100	100
54	P8	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
55	M5	58/65 (89%)	47 (81%)	9 (16%)	2 (3%)	3	16
55	Q8	58/65 (89%)	31 (53%)	16 (28%)	11 (19%)	0	0
All	All	11340/12054 (94%)	9786 (86%)	1332 (12%)	222 (2%)	6	27

5 of 222 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1E	237	ALA
18	9I	22	VAL
29	21	83	ASP
32	51	169	VAL
36	78	57	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	205/220 (93%)	168 (82%)	37 (18%)	2	8
2	1E	205/220 (93%)	148 (72%)	57 (28%)	0	2
3	22	160/188 (85%)	126 (79%)	34 (21%)	1	5
3	2E	159/188 (85%)	126 (79%)	33 (21%)	1	6
4	32	180/181 (99%)	141 (78%)	39 (22%)	1	5
4	3E	180/181 (99%)	130 (72%)	50 (28%)	0	2
5	42	116/123 (94%)	83 (72%)	33 (28%)	0	1
5	4E	116/123 (94%)	85 (73%)	31 (27%)	0	2
6	52	90/90 (100%)	72 (80%)	18 (20%)	1	6
6	5E	90/90 (100%)	76 (84%)	14 (16%)	2	12
7	62	126/127 (99%)	97 (77%)	29 (23%)	1	4
7	6E	126/127 (99%)	98 (78%)	28 (22%)	1	5
8	72	119/119 (100%)	87 (73%)	32 (27%)	0	2
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1	5
9	82	98/99 (99%)	79 (81%)	19 (19%)	1	7
9	8E	98/99 (99%)	75 (76%)	23 (24%)	1	4
10	1A	89/92 (97%)	70 (79%)	19 (21%)	1	5
10	1I	89/92 (97%)	67 (75%)	22 (25%)	1	3
11	2A	90/99 (91%)	64 (71%)	26 (29%)	0	1
11	2I	90/99 (91%)	69 (77%)	21 (23%)	1	4
12	3A	104/109 (95%)	82 (79%)	22 (21%)	1	5
12	3I	104/109 (95%)	84 (81%)	20 (19%)	1	7
13	4A	94/101 (93%)	69 (73%)	25 (27%)	0	2
13	4I	94/101 (93%)	71 (76%)	23 (24%)	1	3
14	5A	48/50 (96%)	41 (85%)	7 (15%)	3	14
14	5I	49/50 (98%)	37 (76%)	12 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	6A	79/80 (99%)	64 (81%)	15 (19%)	1	7
15	6I	79/80 (99%)	67 (85%)	12 (15%)	3	12
16	7A	72/74 (97%)	59 (82%)	13 (18%)	2	8
16	7I	72/74 (97%)	51 (71%)	21 (29%)	0	1
17	8A	95/97 (98%)	73 (77%)	22 (23%)	1	4
17	8I	95/97 (98%)	73 (77%)	22 (23%)	1	4
18	9A	63/77 (82%)	46 (73%)	17 (27%)	0	2
18	9I	63/77 (82%)	50 (79%)	13 (21%)	1	6
19	AA	67/80 (84%)	50 (75%)	17 (25%)	0	3
19	AI	70/80 (88%)	48 (69%)	22 (31%)	0	1
20	BA	76/82 (93%)	65 (86%)	11 (14%)	3	14
20	BI	76/82 (93%)	59 (78%)	17 (22%)	1	4
21	1B	20/22 (91%)	18 (90%)	2 (10%)	7	27
21	1F	20/22 (91%)	18 (90%)	2 (10%)	7	27
28	11	214/218 (98%)	160 (75%)	54 (25%)	0	3
28	19	214/218 (98%)	160 (75%)	54 (25%)	0	3
29	21	165/166 (99%)	119 (72%)	46 (28%)	0	2
29	29	165/166 (99%)	120 (73%)	45 (27%)	0	2
30	31	161/166 (97%)	116 (72%)	45 (28%)	0	2
30	39	165/166 (99%)	120 (73%)	45 (27%)	0	2
31	41	155/156 (99%)	119 (77%)	36 (23%)	1	4
31	49	155/156 (99%)	126 (81%)	29 (19%)	1	8
32	51	145/148 (98%)	99 (68%)	46 (32%)	0	1
32	59	142/148 (96%)	100 (70%)	42 (30%)	0	1
33	61	122/124 (98%)	88 (72%)	34 (28%)	0	2
33	69	122/124 (98%)	82 (67%)	40 (33%)	0	1
34	15	117/119 (98%)	93 (80%)	24 (20%)	1	6
34	58	117/119 (98%)	88 (75%)	29 (25%)	1	3
35	25	100/100 (100%)	73 (73%)	27 (27%)	0	2
35	68	100/100 (100%)	84 (84%)	16 (16%)	2	11
36	35	116/116 (100%)	70 (60%)	46 (40%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
36	78	116/116 (100%)	79 (68%)	37 (32%)	0	1	
37	45	111/111 (100%)	86 (78%)	25 (22%)	1	4	
37	88	104/111 (94%)	72 (69%)	32 (31%)	0	1	
38	55	100/101 (99%)	75 (75%)	25 (25%)	0	3	
38	98	101/101 (100%)	71 (70%)	30 (30%)	0	1	
39	65	87/88 (99%)	61 (70%)	26 (30%)	0	1	
39	A8	87/88 (99%)	60 (69%)	27 (31%)	0	1	
40	75	120/127 (94%)	77 (64%)	43 (36%)	0	0	
40	B8	120/127 (94%)	84 (70%)	36 (30%)	0	1	
41	85	93/94 (99%)	72 (77%)	21 (23%)	1	4	
41	C8	93/94 (99%)	76 (82%)	17 (18%)	2	8	
42	95	82/82 (100%)	61 (74%)	21 (26%)	0	3	
42	D8	82/82 (100%)	54 (66%)	28 (34%)	0	0	
43	A5	92/92 (100%)	63 (68%)	29 (32%)	0	1	
43	E8	92/92 (100%)	62 (67%)	30 (33%)	0	1	
44	B5	74/78 (95%)	52 (70%)	22 (30%)	0	1	
44	F8	76/78 (97%)	58 (76%)	18 (24%)	1	4	
45	C5	85/91 (93%)	54 (64%)	31 (36%)	0	0	
45	G8	85/91 (93%)	50 (59%)	35 (41%)	0	0	
46	D5	158/179 (88%)	115 (73%)	43 (27%)	0	2	
46	H8	154/179 (86%)	126 (82%)	28 (18%)	2	8	
47	E5	62/67 (92%)	51 (82%)	11 (18%)	2	8	
47	I8	61/67 (91%)	45 (74%)	16 (26%)	0	2	
48	F5	82/83 (99%)	64 (78%)	18 (22%)	1	5	
48	J8	82/83 (99%)	53 (65%)	29 (35%)	0	0	
49	G5	62/67 (92%)	41 (66%)	21 (34%)	0	0	
49	K8	62/67 (92%)	39 (63%)	23 (37%)	0	0	
50	H5	51/52 (98%)	33 (65%)	18 (35%)	0	0	
50	L8	49/52 (94%)	30 (61%)	19 (39%)	0	0	
51	I5	57/63 (90%)	45 (79%)	12 (21%)	1	6	
51	M8	59/63 (94%)	43 (73%)	16 (27%)	0	2	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	J5	51/52 (98%)	41 (80%)	10 (20%)	1	7
52	N8	51/52 (98%)	39 (76%)	12 (24%)	1	4
53	K5	44/52 (85%)	36 (82%)	8 (18%)	2	8
53	O8	44/52 (85%)	30 (68%)	14 (32%)	0	1
54	L5	39/42 (93%)	30 (77%)	9 (23%)	1	4
54	P8	41/42 (98%)	30 (73%)	11 (27%)	0	2
55	M5	49/55 (89%)	37 (76%)	12 (24%)	1	3
55	Q8	50/55 (91%)	29 (58%)	21 (42%)	0	0
All	All	9568/9998 (96%)	7120 (74%)	2448 (26%)	0	3

5 of 2448 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	49	91	ARG
46	D5	28	MET
33	69	7	GLU
31	49	82	LEU
38	55	67	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
11	2A	13	GLN
31	49	40	ASN
13	4A	77	ASN
19	AA	47	HIS
34	15	56	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1496/1522 (98%)	363 (24%)	29 (1%)
1	1G	1495/1522 (98%)	367 (24%)	36 (2%)
22	1K	75/76 (98%)	36 (48%)	1 (1%)
22	1L	75/76 (98%)	32 (42%)	3 (4%)
23	2K	76/77 (98%)	21 (27%)	3 (3%)
23	2L	76/77 (98%)	19 (25%)	4 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	3K	75/76 (98%)	39 (52%)	8 (10%)
24	3L	75/76 (98%)	41 (54%)	3 (4%)
25	4K	13/30 (43%)	6 (46%)	1 (7%)
25	4L	6/30 (20%)	2 (33%)	1 (16%)
26	14	2908/2917 (99%)	781 (26%)	51 (1%)
26	1H	2911/2917 (99%)	746 (25%)	61 (2%)
27	16	121/122 (99%)	21 (17%)	1 (0%)
27	1J	121/122 (99%)	35 (28%)	2 (1%)
All	All	9523/9640 (98%)	2509 (26%)	204 (2%)

5 of 2509 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	8	A
1	13	9	G
1	13	28	G

5 of 204 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	465	A
23	2L	20	G
26	14	2778	A
1	1G	560	U
1	1G	1157	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	MIA	1K	37	22	28,31,32	2.24	5 (17%)	38,44,47	2.46	10 (26%)
23	5MU	2L	55	23	19,22,23	3.96	5 (26%)	27,32,35	3.34	10 (37%)
22	MIA	1L	37	22	28,31,32	2.32	4 (14%)	38,44,47	3.32	14 (36%)
22	PSU	1K	32	22	18,21,22	2.37	5 (27%)	21,30,33	1.65	4 (19%)
22	PSU	1L	32	22	18,21,22	2.57	6 (33%)	21,30,33	1.58	4 (19%)
23	PSU	2K	56	23	18,21,22	2.40	4 (22%)	21,30,33	2.05	5 (23%)
23	7MG	2K	47	23	23,26,27	3.21	7 (30%)	27,39,42	2.79	11 (40%)
23	5MU	2K	55	23,56	19,22,23	4.01	5 (26%)	27,32,35	3.56	8 (29%)
23	4SU	2K	8	23	18,21,22	1.96	3 (16%)	25,30,33	3.00	6 (24%)
22	PSU	1K	39	22	18,21,22	2.27	5 (27%)	21,30,33	1.81	4 (19%)
23	4SU	2L	8	23	18,21,22	1.82	3 (16%)	25,30,33	2.57	5 (20%)
23	OMC	2L	33	23	19,22,23	1.78	3 (15%)	25,31,34	1.18	3 (12%)
23	7MG	2L	47	23	23,26,27	3.14	7 (30%)	27,39,42	2.93	10 (37%)
23	PSU	2L	56	23	18,21,22	2.66	5 (27%)	21,30,33	1.81	5 (23%)
23	OMC	2K	33	23	19,22,23	1.72	3 (15%)	25,31,34	1.09	3 (12%)
22	PSU	1L	39	22	18,21,22	2.61	5 (27%)	21,30,33	1.42	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	MIA	1K	37	22	-	5/15/33/34	0/3/3/3
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	MIA	1L	37	22	-	7/15/33/34	0/3/3/3
22	PSU	1K	32	22	-	0/7/25/26	0/2/2/2
22	PSU	1L	32	22	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	1/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	1/7/37/38	0/3/3/3
23	5MU	2K	55	23,56	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	2/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/9/27/28	0/2/2/2

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

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	55	5MU	C2-N1	13.27	1.59	1.38
23	2L	55	5MU	C2-N1	12.92	1.58	1.38
23	2K	47	7MG	C4-N9	-8.82	1.27	1.37
22	1K	37	MIA	C13-C14	8.33	1.57	1.32
23	2L	47	7MG	C5-N7	8.30	1.46	1.35

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1L	37	MIA	C11-S10-C2	11.21	110.67	102.25
23	2K	55	5MU	C5-C4-N3	10.61	124.55	115.32
23	2L	55	5MU	C5-C4-N3	10.46	124.42	115.32
22	1L	37	MIA	C12-C13-C14	-10.00	109.05	127.01
23	2K	8	4SU	C4-N3-C2	-9.63	118.09	127.31

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	MIA	C5-C6-N6-C12
22	1K	37	MIA	N1-C2-S10-C11
22	1K	37	MIA	N3-C2-S10-C11
22	1K	37	MIA	C12-C13-C14-C16
22	1L	37	MIA	C5-C6-N6-C12

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	37	MIA	2	0
23	2L	55	5MU	1	0
23	2K	56	PSU	1	0
23	2K	47	7MG	4	0

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1245 ligands modelled in this entry, 1245 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	13	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	13	1530:G	O3'	1531:A	P	3.03

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1498/1522 (98%)	-0.40	8 (0%) 87 75	61, 110, 194, 290	0
1	1G	1497/1522 (98%)	-0.20	27 (1%) 67 47	73, 129, 204, 306	0
2	12	237/256 (92%)	0.37	7 (2%) 52 32	151, 185, 205, 218	0
2	1E	237/256 (92%)	0.21	13 (5%) 30 17	119, 155, 183, 193	0
3	22	206/239 (86%)	0.38	5 (2%) 59 39	149, 166, 190, 202	0
3	2E	205/239 (85%)	-0.04	2 (0%) 79 62	98, 122, 159, 171	0
4	32	208/209 (99%)	0.45	8 (3%) 44 26	107, 128, 153, 160	0
4	3E	208/209 (99%)	0.38	13 (6%) 26 15	92, 122, 146, 155	0
5	42	151/162 (93%)	0.24	3 (1%) 65 44	118, 139, 159, 195	0
5	4E	151/162 (93%)	0.02	4 (2%) 57 36	88, 109, 135, 174	0
6	52	101/101 (100%)	-0.38	0 100 100	92, 115, 133, 160	0
6	5E	101/101 (100%)	-0.16	0 100 100	87, 110, 132, 154	0
7	62	155/156 (99%)	0.05	8 (5%) 33 19	124, 143, 178, 199	0
7	6E	155/156 (99%)	0.13	13 (8%) 17 10	110, 129, 160, 179	0
8	72	138/138 (100%)	0.20	5 (3%) 46 27	115, 145, 160, 163	0
8	7E	138/138 (100%)	0.06	5 (3%) 46 27	93, 118, 128, 142	0
9	82	127/128 (99%)	0.57	10 (7%) 18 10	123, 171, 189, 197	0
9	8E	127/128 (99%)	0.32	5 (3%) 43 25	94, 149, 170, 180	0
10	1A	99/105 (94%)	0.68	10 (10%) 12 7	139, 174, 192, 197	0
10	1I	99/105 (94%)	0.21	3 (3%) 52 32	90, 148, 181, 187	0
11	2A	119/129 (92%)	-0.04	2 (1%) 69 48	94, 125, 152, 183	0
11	2I	119/129 (92%)	0.05	6 (5%) 34 20	77, 113, 153, 182	0
12	3A	125/132 (94%)	0.18	5 (4%) 42 24	91, 114, 144, 175	0
12	3I	125/132 (94%)	-0.24	2 (1%) 70 50	74, 84, 117, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	117/126 (92%)	0.40	11 (9%) 14 8	127, 171, 192, 200	0
13	4I	118/126 (93%)	0.20	6 (5%) 33 19	86, 127, 148, 156	0
14	5A	58/61 (95%)	1.39	12 (20%) 2 2	152, 166, 179, 184	0
14	5I	60/61 (98%)	0.43	3 (5%) 34 20	92, 113, 128, 135	0
15	6A	88/89 (98%)	-0.15	1 (1%) 78 60	96, 125, 143, 148	0
15	6I	88/89 (98%)	0.01	3 (3%) 48 28	82, 104, 122, 129	0
16	7A	84/88 (95%)	0.10	1 (1%) 76 57	100, 117, 142, 174	0
16	7I	84/88 (95%)	0.82	9 (10%) 11 6	110, 126, 158, 174	0
17	8A	100/105 (95%)	0.14	1 (1%) 79 62	105, 122, 138, 160	0
17	8I	100/105 (95%)	0.01	2 (2%) 65 44	97, 114, 125, 129	0
18	9A	72/88 (81%)	-0.32	0 100 100	106, 128, 167, 178	0
18	9I	72/88 (81%)	-0.17	1 (1%) 73 53	90, 113, 143, 175	0
19	AA	78/93 (83%)	0.36	5 (6%) 25 14	160, 189, 203, 207	0
19	AI	81/93 (87%)	0.10	3 (3%) 45 26	103, 127, 156, 165	0
20	BA	99/106 (93%)	0.11	0 100 100	97, 118, 150, 162	0
20	BI	99/106 (93%)	0.61	11 (11%) 10 6	115, 131, 165, 172	0
21	1B	25/27 (92%)	1.60	9 (36%) 1 1	125, 153, 169, 189	0
21	1F	25/27 (92%)	0.38	0 100 100	100, 112, 127, 154	0
22	1K	73/76 (96%)	-0.04	5 (6%) 23 13	97, 221, 259, 264	0
22	1L	73/76 (96%)	0.17	7 (9%) 13 8	134, 254, 277, 285	0
23	2K	72/77 (93%)	-0.45	1 (1%) 73 53	73, 95, 128, 139	0
23	2L	72/77 (93%)	-0.28	0 100 100	87, 121, 153, 165	0
24	3K	76/76 (100%)	0.39	3 (3%) 43 25	77, 253, 279, 282	0
24	3L	76/76 (100%)	0.31	3 (3%) 43 25	89, 259, 278, 280	0
25	4K	14/30 (46%)	-0.07	0 100 100	76, 107, 151, 155	0
25	4L	6/30 (20%)	0.46	0 100 100	100, 108, 158, 160	0
26	14	2909/2917 (99%)	-0.62	9 (0%) 90 81	53, 91, 249, 335	0
26	1H	2912/2917 (99%)	-0.75	10 (0%) 90 81	40, 77, 231, 309	0
27	16	122/122 (100%)	-0.81	0 100 100	69, 98, 122, 202	0
27	1J	122/122 (100%)	-0.14	2 (1%) 70 50	89, 133, 162, 212	0
28	11	273/276 (98%)	-0.34	0 100 100	43, 66, 84, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	19	273/276 (98%)	0.06	7 (2%) 57 36	54, 80, 97, 112	0
29	21	205/206 (99%)	0.19	15 (7%) 21 12	49, 94, 143, 161	0
29	29	205/206 (99%)	0.09	4 (1%) 65 44	64, 99, 146, 173	0
30	31	202/210 (96%)	-0.32	2 (0%) 79 62	47, 80, 119, 141	0
30	39	208/210 (99%)	-0.11	1 (0%) 87 75	60, 109, 170, 198	0
31	41	181/182 (99%)	-0.11	3 (1%) 69 48	83, 109, 145, 156	0
31	49	181/182 (99%)	0.28	10 (5%) 30 17	127, 154, 181, 199	0
32	51	174/180 (96%)	-0.16	2 (1%) 78 60	85, 109, 129, 142	0
32	59	170/180 (94%)	0.71	19 (11%) 10 6	155, 205, 228, 248	0
33	61	146/148 (98%)	0.01	4 (2%) 56 35	80, 139, 157, 163	0
33	69	146/148 (98%)	0.64	17 (11%) 9 6	88, 135, 157, 168	0
34	15	138/140 (98%)	0.22	8 (5%) 29 16	85, 116, 149, 165	0
34	58	138/140 (98%)	0.06	4 (2%) 53 34	69, 95, 137, 156	0
35	25	122/122 (100%)	-0.19	2 (1%) 70 50	73, 93, 108, 124	0
35	68	122/122 (100%)	-0.42	0 100 100	61, 80, 99, 112	0
36	35	150/150 (100%)	0.26	4 (2%) 56 35	62, 113, 145, 183	0
36	78	150/150 (100%)	0.08	3 (2%) 65 44	49, 85, 116, 166	0
37	45	141/141 (100%)	0.61	13 (9%) 14 8	81, 111, 145, 155	0
37	88	138/141 (97%)	-0.10	2 (1%) 73 53	56, 83, 107, 138	0
38	55	117/118 (99%)	-0.19	1 (0%) 81 64	64, 84, 99, 117	0
38	98	118/118 (100%)	-0.16	1 (0%) 82 66	63, 87, 109, 120	0
39	65	111/112 (99%)	0.37	4 (3%) 46 27	98, 128, 148, 162	0
39	A8	111/112 (99%)	-0.05	2 (1%) 67 47	75, 94, 123, 133	0
40	75	137/146 (93%)	0.18	9 (6%) 24 14	83, 101, 161, 195	0
40	B8	137/146 (93%)	0.19	6 (4%) 39 22	76, 97, 154, 179	0
41	85	117/118 (99%)	0.05	3 (2%) 57 36	73, 104, 150, 174	0
41	C8	117/118 (99%)	0.11	1 (0%) 81 64	56, 82, 115, 134	0
42	95	101/101 (100%)	0.39	7 (6%) 23 13	71, 134, 155, 175	0
42	D8	101/101 (100%)	0.25	3 (2%) 52 32	61, 111, 141, 155	0
43	A5	113/113 (100%)	-0.20	0 100 100	66, 80, 117, 174	0
43	E8	113/113 (100%)	-0.29	0 100 100	58, 76, 112, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	B5	93/96 (96%)	-0.12	2 (2%) 62 41	71, 89, 113, 121	0
44	F8	94/96 (97%)	-0.24	1 (1%) 78 60	56, 73, 97, 117	0
45	C5	104/110 (94%)	0.31	5 (4%) 35 20	89, 122, 160, 166	0
45	G8	104/110 (94%)	0.21	5 (4%) 35 20	75, 98, 142, 149	0
46	D5	179/206 (86%)	0.18	1 (0%) 85 72	124, 161, 240, 246	0
46	H8	175/206 (84%)	0.06	2 (1%) 78 60	86, 128, 212, 218	0
47	E5	77/85 (90%)	0.30	3 (3%) 43 25	77, 96, 116, 162	0
47	I8	80/85 (94%)	-0.02	3 (3%) 44 26	58, 77, 114, 117	0
48	F5	97/98 (98%)	0.22	4 (4%) 41 24	63, 89, 143, 161	0
48	J8	97/98 (98%)	-0.13	3 (3%) 51 31	54, 77, 128, 161	0
49	G5	66/72 (91%)	0.03	1 (1%) 72 52	89, 112, 130, 148	0
49	K8	67/72 (93%)	-0.03	2 (2%) 52 32	65, 81, 99, 132	0
50	H5	59/60 (98%)	-0.14	0 100 100	80, 109, 155, 173	0
50	L8	57/60 (95%)	-0.48	0 100 100	64, 83, 112, 120	0
51	I5	63/71 (88%)	0.04	1 (1%) 70 50	167, 206, 219, 221	0
51	M8	66/71 (92%)	0.37	4 (6%) 27 15	114, 161, 192, 200	0
52	J5	59/60 (98%)	0.05	0 100 100	66, 91, 159, 212	0
52	N8	58/60 (96%)	0.06	0 100 100	53, 100, 178, 183	0
53	K5	45/54 (83%)	1.68	18 (40%) 1 1	141, 181, 194, 201	0
53	O8	45/54 (83%)	0.58	5 (11%) 10 6	117, 148, 168, 171	0
54	L5	46/49 (93%)	-0.39	0 100 100	53, 63, 75, 86	0
54	P8	48/49 (97%)	-0.43	1 (2%) 63 42	46, 51, 88, 112	0
55	M5	60/65 (92%)	0.40	5 (8%) 17 10	73, 86, 108, 133	0
55	Q8	60/65 (92%)	0.90	7 (11%) 9 5	61, 73, 104, 119	0
All	All	21056/21694 (97%)	-0.17	512 (2%) 59 39	40, 109, 201, 335	0

The worst 5 of 512 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1J	88	C	8.1
22	1K	73	A	7.5
40	B8	1	MET	7.2
7	62	81	GLY	7.0
14	5A	6	LEU	6.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	4SU	2L	8	20/21	0.81	0.12	124,129,135,138	0
23	5MU	2L	55	21/22	0.86	0.09	126,131,137,141	0
23	7MG	2K	47	24/25	0.87	0.08	97,107,122,130	0
23	7MG	2L	47	24/25	0.88	0.09	130,140,145,148	0
23	PSU	2L	56	20/21	0.89	0.08	121,128,134,135	0
23	5MU	2K	55	21/22	0.90	0.10	99,108,119,128	0
23	PSU	2K	56	20/21	0.90	0.07	97,104,114,116	0
23	4SU	2K	8	20/21	0.91	0.10	86,95,103,110	0
22	MIA	1L	37	29/30	0.93	0.10	121,132,138,150	0
22	PSU	1L	39	20/21	0.93	0.08	113,140,153,154	0
22	PSU	1K	32	20/21	0.93	0.09	112,119,129,131	0
22	PSU	1L	32	20/21	0.94	0.09	139,147,158,158	0
22	PSU	1K	39	20/21	0.95	0.08	90,106,111,114	0
23	OMC	2L	33	21/22	0.96	0.07	105,111,114,116	0
23	OMC	2K	33	21/22	0.96	0.10	79,84,93,100	0
22	MIA	1K	37	29/30	0.97	0.08	88,98,114,119	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	13	1705	1/1	0.23	0.36	138,138,138,138	0
56	MG	1G	1673	1/1	0.26	0.30	138,138,138,138	0
56	MG	14	3182	1/1	0.32	0.27	152,152,152,152	0
56	MG	1H	3332	1/1	0.34	0.32	138,138,138,138	0
56	MG	6A	101	1/1	0.35	0.30	126,126,126,126	0
56	MG	1G	1685	1/1	0.40	0.27	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1655	1/1	0.40	0.43	124,124,124,124	0
56	MG	1G	1641	1/1	0.40	0.33	121,121,121,121	0
56	MG	13	1696	1/1	0.43	0.31	137,137,137,137	0
56	MG	1G	1683	1/1	0.45	0.29	123,123,123,123	0
56	MG	14	3233	1/1	0.45	0.27	112,112,112,112	0
56	MG	1J	204	1/1	0.46	0.39	100,100,100,100	0
56	MG	13	1639	1/1	0.49	0.33	98,98,98,98	0
56	MG	13	1658	1/1	0.49	0.26	92,92,92,92	0
56	MG	13	1682	1/1	0.52	0.29	92,92,92,92	0
56	MG	75	201	1/1	0.52	0.23	108,108,108,108	0
56	MG	14	3204	1/1	0.54	0.21	126,126,126,126	0
56	MG	13	1708	1/1	0.54	0.32	116,116,116,116	0
56	MG	1G	1678	1/1	0.55	0.28	114,114,114,114	0
56	MG	14	3240	1/1	0.55	0.52	103,103,103,103	0
56	MG	14	3252	1/1	0.56	0.45	117,117,117,117	0
56	MG	13	1668	1/1	0.57	0.36	111,111,111,111	0
56	MG	13	1671	1/1	0.58	0.23	110,110,110,110	0
56	MG	14	3197	1/1	0.58	0.38	94,94,94,94	0
56	MG	13	1615	1/1	0.59	0.32	103,103,103,103	0
56	MG	13	1677	1/1	0.59	0.40	109,109,109,109	0
56	MG	1H	3142	1/1	0.59	0.23	101,101,101,101	0
56	MG	1H	3269	1/1	0.59	0.27	99,99,99,99	0
56	MG	1G	1620	1/1	0.60	0.34	111,111,111,111	0
56	MG	1H	3335	1/1	0.60	0.34	97,97,97,97	0
56	MG	13	1712	1/1	0.61	0.42	114,114,114,114	0
56	MG	3E	301	1/1	0.61	0.22	128,128,128,128	0
56	MG	13	1685	1/1	0.62	0.28	123,123,123,123	0
56	MG	13	1616	1/1	0.62	0.39	98,98,98,98	0
56	MG	1H	3318	1/1	0.62	0.12	86,86,86,86	0
56	MG	13	1672	1/1	0.63	0.18	118,118,118,118	0
56	MG	1J	207	1/1	0.63	0.25	109,109,109,109	0
56	MG	1H	3226	1/1	0.63	0.33	97,97,97,97	0
56	MG	1H	3229	1/1	0.64	0.29	112,112,112,112	0
56	MG	14	3178	1/1	0.64	0.28	95,95,95,95	0
56	MG	13	1711	1/1	0.64	0.23	109,109,109,109	0
56	MG	1H	3214	1/1	0.64	0.14	79,79,79,79	0
56	MG	1H	3022	1/1	0.64	0.35	78,78,78,78	0
56	MG	14	3215	1/1	0.64	0.32	111,111,111,111	0
56	MG	1H	3183	1/1	0.65	0.24	76,76,76,76	0
56	MG	14	3254	1/1	0.65	0.54	81,81,81,81	0
56	MG	14	3082	1/1	0.65	0.38	97,97,97,97	0
56	MG	14	3239	1/1	0.65	0.27	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1659	1/1	0.65	0.33	110,110,110,110	0
56	MG	1G	1675	1/1	0.66	0.28	96,96,96,96	0
56	MG	14	3037	1/1	0.66	0.29	103,103,103,103	0
56	MG	14	3250	1/1	0.66	0.24	108,108,108,108	0
56	MG	1H	3259	1/1	0.66	0.25	115,115,115,115	0
56	MG	2L	102	1/1	0.67	0.44	103,103,103,103	0
56	MG	1H	3270	1/1	0.67	0.22	106,106,106,106	0
56	MG	1H	3294	1/1	0.67	0.30	122,122,122,122	0
56	MG	14	3146	1/1	0.67	0.25	105,105,105,105	0
56	MG	1H	3300	1/1	0.67	0.32	90,90,90,90	0
56	MG	13	1699	1/1	0.67	0.34	98,98,98,98	0
56	MG	16	209	1/1	0.68	0.24	90,90,90,90	0
56	MG	1G	1668	1/1	0.68	0.25	116,116,116,116	0
56	MG	13	1693	1/1	0.68	0.45	109,109,109,109	0
56	MG	1G	1684	1/1	0.68	0.26	113,113,113,113	0
56	MG	1H	3328	1/1	0.69	0.18	86,86,86,86	0
56	MG	13	1692	1/1	0.69	0.24	114,114,114,114	0
56	MG	14	3008	1/1	0.69	0.29	58,58,58,58	0
56	MG	13	1702	1/1	0.69	0.22	112,112,112,112	0
56	MG	1H	3279	1/1	0.69	0.31	100,100,100,100	0
56	MG	1G	1676	1/1	0.69	0.17	157,157,157,157	0
56	MG	13	1654	1/1	0.69	0.18	105,105,105,105	0
56	MG	13	1609	1/1	0.69	0.28	94,94,94,94	0
56	MG	1G	1647	1/1	0.69	0.35	102,102,102,102	0
56	MG	13	1709	1/1	0.69	0.32	127,127,127,127	0
56	MG	1H	3329	1/1	0.70	0.18	99,99,99,99	0
56	MG	1H	3184	1/1	0.70	0.31	94,94,94,94	0
56	MG	14	3230	1/1	0.70	0.22	103,103,103,103	0
56	MG	13	1701	1/1	0.70	0.33	103,103,103,103	0
56	MG	16	201	1/1	0.70	0.23	96,96,96,96	0
56	MG	2K	101	1/1	0.70	0.20	86,86,86,86	0
56	MG	13	1690	1/1	0.70	0.22	96,96,96,96	0
56	MG	14	3118	1/1	0.70	0.20	92,92,92,92	0
56	MG	1G	1677	1/1	0.70	0.46	106,106,106,106	0
56	MG	1G	1623	1/1	0.70	0.27	114,114,114,114	0
56	MG	13	1704	1/1	0.70	0.43	95,95,95,95	0
56	MG	13	1700	1/1	0.70	0.24	100,100,100,100	0
56	MG	13	1686	1/1	0.71	0.33	106,106,106,106	0
56	MG	1H	3274	1/1	0.71	0.32	87,87,87,87	0
56	MG	1H	3324	1/1	0.71	0.17	93,93,93,93	0
56	MG	14	3119	1/1	0.71	0.39	88,88,88,88	0
56	MG	13	1703	1/1	0.72	0.32	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3127	1/1	0.72	0.28	84,84,84,84	0
56	MG	16	207	1/1	0.72	0.26	87,87,87,87	0
56	MG	14	3110	1/1	0.72	0.31	88,88,88,88	0
56	MG	1G	1651	1/1	0.72	0.20	102,102,102,102	0
56	MG	13	1640	1/1	0.72	0.18	95,95,95,95	0
56	MG	16	210	1/1	0.72	0.29	97,97,97,97	0
56	MG	13	1676	1/1	0.72	0.24	104,104,104,104	0
56	MG	1G	1669	1/1	0.72	0.44	103,103,103,103	0
56	MG	1G	1670	1/1	0.72	0.29	98,98,98,98	0
56	MG	1G	1671	1/1	0.72	0.35	96,96,96,96	0
57	ZN	G8	201	1/1	0.72	0.19	188,188,188,188	0
56	MG	13	1689	1/1	0.73	0.48	97,97,97,97	0
56	MG	14	3128	1/1	0.73	0.43	98,98,98,98	0
56	MG	1G	1662	1/1	0.73	0.44	100,100,100,100	0
56	MG	14	3246	1/1	0.73	0.25	98,98,98,98	0
56	MG	1G	1639	1/1	0.73	0.40	99,99,99,99	0
56	MG	1H	3281	1/1	0.73	0.16	60,60,60,60	0
56	MG	14	3183	1/1	0.73	0.38	83,83,83,83	0
56	MG	13	1632	1/1	0.73	0.39	77,77,77,77	0
56	MG	1H	3273	1/1	0.73	0.40	97,97,97,97	0
56	MG	14	3114	1/1	0.73	0.33	72,72,72,72	0
56	MG	13	1653	1/1	0.73	0.22	111,111,111,111	0
56	MG	14	3097	1/1	0.74	0.34	80,80,80,80	0
56	MG	13	1662	1/1	0.74	0.32	113,113,113,113	0
56	MG	14	3213	1/1	0.74	0.34	93,93,93,93	0
56	MG	1J	201	1/1	0.74	0.18	114,114,114,114	0
56	MG	14	3218	1/1	0.75	0.40	82,82,82,82	0
56	MG	1H	3250	1/1	0.75	0.27	90,90,90,90	0
56	MG	1H	3171	1/1	0.75	0.27	101,101,101,101	0
56	MG	1G	1624	1/1	0.75	0.31	85,85,85,85	0
56	MG	13	1614	1/1	0.75	0.34	97,97,97,97	0
56	MG	13	1680	1/1	0.75	0.65	97,97,97,97	0
56	MG	1G	1642	1/1	0.75	0.49	110,110,110,110	0
56	MG	1G	1664	1/1	0.76	0.41	88,88,88,88	0
56	MG	14	3194	1/1	0.76	0.16	140,140,140,140	0
56	MG	14	3117	1/1	0.76	0.36	84,84,84,84	0
56	MG	13	1638	1/1	0.76	0.28	107,107,107,107	0
56	MG	1G	1635	1/1	0.76	0.28	96,96,96,96	0
56	MG	1G	1618	1/1	0.76	0.23	85,85,85,85	0
56	MG	13	1710	1/1	0.76	0.36	125,125,125,125	0
56	MG	1J	206	1/1	0.76	0.25	91,91,91,91	0
56	MG	14	3157	1/1	0.76	0.30	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1672	1/1	0.76	0.33	100,100,100,100	0
56	MG	13	1750	1/1	0.76	0.21	97,97,97,97	0
56	MG	1H	3271	1/1	0.77	0.35	90,90,90,90	0
56	MG	14	3148	1/1	0.77	0.35	75,75,75,75	0
56	MG	1G	1658	1/1	0.77	0.38	96,96,96,96	0
56	MG	16	206	1/1	0.77	0.21	76,76,76,76	0
56	MG	1H	3327	1/1	0.77	0.30	110,110,110,110	0
56	MG	1G	1638	1/1	0.77	0.28	154,154,154,154	0
56	MG	14	3112	1/1	0.77	0.43	90,90,90,90	0
56	MG	14	3258	1/1	0.77	0.20	90,90,90,90	0
56	MG	14	3113	1/1	0.77	0.39	96,96,96,96	0
56	MG	AI	101	1/1	0.77	0.22	119,119,119,119	0
56	MG	1H	3295	1/1	0.77	0.29	94,94,94,94	0
56	MG	1G	1601	1/1	0.77	0.25	94,94,94,94	0
56	MG	1H	3098	1/1	0.77	0.21	74,74,74,74	0
56	MG	1H	3120	1/1	0.77	0.18	68,68,68,68	0
56	MG	1H	3211	1/1	0.78	0.16	88,88,88,88	0
56	MG	1G	1629	1/1	0.78	0.37	89,89,89,89	0
56	MG	1H	3212	1/1	0.78	0.35	92,92,92,92	0
56	MG	13	1635	1/1	0.78	0.28	73,73,73,73	0
56	MG	1H	3059	1/1	0.78	0.27	63,63,63,63	0
56	MG	1G	1640	1/1	0.78	0.19	99,99,99,99	0
56	MG	11	304	1/1	0.78	0.29	68,68,68,68	0
56	MG	14	3145	1/1	0.78	0.23	90,90,90,90	0
56	MG	13	1648	1/1	0.78	0.50	89,89,89,89	0
56	MG	14	3028	1/1	0.78	0.32	81,81,81,81	0
56	MG	1H	3304	1/1	0.78	0.21	79,79,79,79	0
56	MG	14	3170	1/1	0.78	0.26	88,88,88,88	0
56	MG	14	3387	1/1	0.78	0.27	74,74,74,74	0
56	MG	14	3079	1/1	0.78	0.30	69,69,69,69	0
56	MG	1G	1648	1/1	0.78	0.16	115,115,115,115	0
56	MG	1H	3200	1/1	0.78	0.19	98,98,98,98	0
56	MG	14	3102	1/1	0.78	0.29	76,76,76,76	0
56	MG	14	3109	1/1	0.78	0.31	85,85,85,85	0
56	MG	16	205	1/1	0.78	0.21	88,88,88,88	0
56	MG	1H	3035	1/1	0.79	0.27	86,86,86,86	0
56	MG	14	3002	1/1	0.79	0.24	67,67,67,67	0
56	MG	13	1688	1/1	0.79	0.21	102,102,102,102	0
56	MG	13	1694	1/1	0.79	0.29	95,95,95,95	0
56	MG	13	1610	1/1	0.79	0.18	72,72,72,72	0
56	MG	14	3196	1/1	0.79	0.26	91,91,91,91	0
56	MG	14	3255	1/1	0.79	0.27	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3071	1/1	0.79	0.24	88,88,88,88	0
56	MG	14	3203	1/1	0.79	0.39	111,111,111,111	0
56	MG	13	1679	1/1	0.79	0.28	95,95,95,95	0
56	MG	1J	202	1/1	0.79	0.33	81,81,81,81	0
56	MG	1H	3296	1/1	0.79	0.26	81,81,81,81	0
56	MG	14	3089	1/1	0.79	0.28	87,87,87,87	0
56	MG	13	1619	1/1	0.79	0.18	82,82,82,82	0
56	MG	29	302	1/1	0.79	0.39	85,85,85,85	0
56	MG	4A	201	1/1	0.79	0.41	115,115,115,115	0
56	MG	1H	3030	1/1	0.79	0.28	70,70,70,70	0
56	MG	1G	1682	1/1	0.80	0.44	102,102,102,102	0
56	MG	1H	3047	1/1	0.80	0.21	71,71,71,71	0
56	MG	14	3241	1/1	0.80	0.51	90,90,90,90	0
56	MG	1G	1619	1/1	0.80	0.18	130,130,130,130	0
56	MG	1H	3164	1/1	0.80	0.31	70,70,70,70	0
56	MG	14	3083	1/1	0.80	0.30	93,93,93,93	0
56	MG	1G	1679	1/1	0.80	0.19	105,105,105,105	0
56	MG	14	3031	1/1	0.80	0.27	73,73,73,73	0
56	MG	14	3234	1/1	0.80	0.37	80,80,80,80	0
56	MG	1H	3165	1/1	0.81	0.21	68,68,68,68	0
56	MG	1G	1611	1/1	0.81	0.26	91,91,91,91	0
56	MG	1H	3252	1/1	0.81	0.25	83,83,83,83	0
56	MG	1H	3034	1/1	0.81	0.20	91,91,91,91	0
56	MG	1H	3106	1/1	0.81	0.21	78,78,78,78	0
56	MG	14	3232	1/1	0.81	0.25	109,109,109,109	0
56	MG	1H	3108	1/1	0.81	0.23	58,58,58,58	0
56	MG	1H	3116	1/1	0.81	0.12	61,61,61,61	0
56	MG	1H	3203	1/1	0.81	0.25	76,76,76,76	0
56	MG	14	3125	1/1	0.81	0.18	105,105,105,105	0
56	MG	14	3126	1/1	0.81	0.19	71,71,71,71	0
56	MG	1H	3207	1/1	0.81	0.28	79,79,79,79	0
56	MG	14	3141	1/1	0.81	0.28	84,84,84,84	0
56	MG	14	3029	1/1	0.81	0.33	84,84,84,84	0
56	MG	2K	102	1/1	0.81	0.34	76,76,76,76	0
56	MG	1H	3046	1/1	0.81	0.24	80,80,80,80	0
56	MG	14	3068	1/1	0.81	0.29	73,73,73,73	0
56	MG	1G	1674	1/1	0.81	0.12	94,94,94,94	0
56	MG	14	3171	1/1	0.81	0.25	91,91,91,91	0
56	MG	1H	3131	1/1	0.81	0.24	79,79,79,79	0
56	MG	13	1606	1/1	0.81	0.30	80,80,80,80	0
56	MG	13	1678	1/1	0.81	0.26	110,110,110,110	0
56	MG	1H	3297	1/1	0.81	0.23	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3230	1/1	0.81	0.32	66,66,66,66	0
56	MG	14	3100	1/1	0.81	0.17	70,70,70,70	0
56	MG	98	201	1/1	0.81	0.50	99,99,99,99	0
56	MG	1G	1665	1/1	0.82	0.43	104,104,104,104	0
56	MG	13	1691	1/1	0.82	0.19	101,101,101,101	0
56	MG	13	1605	1/1	0.82	0.30	81,81,81,81	0
56	MG	14	3019	1/1	0.82	0.34	56,56,56,56	0
56	MG	14	3227	1/1	0.82	0.54	103,103,103,103	0
56	MG	1G	1634	1/1	0.82	0.23	110,110,110,110	0
56	MG	14	3122	1/1	0.82	0.23	81,81,81,81	0
56	MG	13	1650	1/1	0.82	0.33	98,98,98,98	0
56	MG	1G	1636	1/1	0.82	0.37	94,94,94,94	0
56	MG	13	1622	1/1	0.82	0.34	85,85,85,85	0
56	MG	14	3044	1/1	0.82	0.33	82,82,82,82	0
56	MG	1H	3181	1/1	0.82	0.21	99,99,99,99	0
56	MG	1H	3305	1/1	0.82	0.24	87,87,87,87	0
56	MG	1H	3308	1/1	0.82	0.28	81,81,81,81	0
56	MG	14	3149	1/1	0.82	0.32	89,89,89,89	0
56	MG	1H	3312	1/1	0.82	0.31	82,82,82,82	0
56	MG	14	3168	1/1	0.82	0.22	74,74,74,74	0
56	MG	41	302	1/1	0.82	0.25	94,94,94,94	0
56	MG	1H	3123	1/1	0.82	0.26	73,73,73,73	0
56	MG	14	3093	1/1	0.82	0.36	63,63,63,63	0
56	MG	1H	3275	1/1	0.82	0.24	94,94,94,94	0
56	MG	1H	3325	1/1	0.82	0.12	64,64,64,64	0
56	MG	14	3186	1/1	0.82	0.20	86,86,86,86	0
56	MG	13	1636	1/1	0.82	0.19	93,93,93,93	0
56	MG	13	1641	1/1	0.82	0.32	90,90,90,90	0
56	MG	1H	3290	1/1	0.82	0.27	94,94,94,94	0
56	MG	C5	201	1/1	0.82	0.20	102,102,102,102	0
56	MG	1H	3133	1/1	0.82	0.20	61,61,61,61	0
56	MG	13	1643	1/1	0.83	0.22	96,96,96,96	0
56	MG	1G	1617	1/1	0.83	0.26	99,99,99,99	0
56	MG	1H	3326	1/1	0.83	0.22	94,94,94,94	0
56	MG	1H	3045	1/1	0.83	0.22	75,75,75,75	0
56	MG	14	3235	1/1	0.83	0.10	76,76,76,76	0
56	MG	14	3237	1/1	0.83	0.26	78,78,78,78	0
56	MG	1H	3285	1/1	0.83	0.28	89,89,89,89	0
56	MG	14	3096	1/1	0.83	0.30	78,78,78,78	0
56	MG	1H	3236	1/1	0.83	0.28	78,78,78,78	0
56	MG	1H	3245	1/1	0.83	0.20	91,91,91,91	0
56	MG	1H	3026	1/1	0.83	0.33	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	13	1670	1/1	0.83	0.35	92,92,92,92	0
56	MG	1H	3257	1/1	0.83	0.24	82,82,82,82	0
56	MG	14	3016	1/1	0.83	0.21	68,68,68,68	0
56	MG	1H	3299	1/1	0.83	0.24	93,93,93,93	0
56	MG	13	1683	1/1	0.83	0.25	78,78,78,78	0
56	MG	1H	3156	1/1	0.83	0.34	78,78,78,78	0
56	MG	1H	3223	1/1	0.83	0.16	69,69,69,69	0
56	MG	1H	3224	1/1	0.83	0.34	89,89,89,89	0
56	MG	14	3039	1/1	0.83	0.34	79,79,79,79	0
56	MG	14	3123	1/1	0.83	0.22	82,82,82,82	0
56	MG	1H	3225	1/1	0.83	0.25	79,79,79,79	0
56	MG	14	3217	1/1	0.83	0.24	88,88,88,88	0
56	MG	1H	3188	1/1	0.83	0.17	62,62,62,62	0
56	MG	1H	3227	1/1	0.83	0.37	93,93,93,93	0
56	MG	14	3018	1/1	0.84	0.23	68,68,68,68	0
56	MG	1G	1637	1/1	0.84	0.21	124,124,124,124	0
56	MG	14	3026	1/1	0.84	0.33	90,90,90,90	0
56	MG	14	3210	1/1	0.84	0.30	88,88,88,88	0
56	MG	1H	3036	1/1	0.84	0.27	85,85,85,85	0
56	MG	1H	3105	1/1	0.84	0.33	68,68,68,68	0
56	MG	1G	1602	1/1	0.84	0.31	72,72,72,72	0
56	MG	14	3036	1/1	0.84	0.22	68,68,68,68	0
56	MG	14	3224	1/1	0.84	0.30	90,90,90,90	0
56	MG	1G	1609	1/1	0.84	0.26	101,101,101,101	0
56	MG	1H	3006	1/1	0.84	0.30	55,55,55,55	0
56	MG	14	3040	1/1	0.84	0.19	49,49,49,49	0
56	MG	1G	1612	1/1	0.84	0.13	94,94,94,94	0
56	MG	14	3135	1/1	0.84	0.21	54,54,54,54	0
56	MG	14	3050	1/1	0.84	0.22	81,81,81,81	0
56	MG	1H	3243	1/1	0.84	0.26	88,88,88,88	0
56	MG	1H	3033	1/1	0.84	0.25	75,75,75,75	0
56	MG	1H	3246	1/1	0.84	0.25	88,88,88,88	0
56	MG	1G	1657	1/1	0.84	0.32	87,87,87,87	0
56	MG	14	3154	1/1	0.84	0.15	79,79,79,79	0
56	MG	14	3249	1/1	0.84	0.10	69,69,69,69	0
56	MG	1H	3187	1/1	0.84	0.23	89,89,89,89	0
56	MG	14	3164	1/1	0.84	0.12	74,74,74,74	0
56	MG	14	3253	1/1	0.84	0.39	86,86,86,86	0
56	MG	14	3166	1/1	0.84	0.22	112,112,112,112	0
56	MG	1G	1622	1/1	0.84	0.30	90,90,90,90	0
56	MG	13	1645	1/1	0.84	0.25	83,83,83,83	0
56	MG	1H	3198	1/1	0.84	0.25	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3173	1/1	0.84	0.32	82,82,82,82	0
56	MG	13	1663	1/1	0.84	0.17	82,82,82,82	0
56	MG	1H	3264	1/1	0.84	0.21	76,76,76,76	0
56	MG	1J	205	1/1	0.84	0.26	98,98,98,98	0
56	MG	1H	3070	1/1	0.84	0.30	74,74,74,74	0
56	MG	14	3185	1/1	0.84	0.22	64,64,64,64	0
56	MG	14	3107	1/1	0.84	0.26	76,76,76,76	0
56	MG	14	3191	1/1	0.84	0.20	94,94,94,94	0
56	MG	14	3015	1/1	0.84	0.21	69,69,69,69	0
56	MG	78	202	1/1	0.84	0.17	78,78,78,78	0
57	ZN	C5	202	1/1	0.84	0.14	181,181,181,181	0
56	MG	1H	3172	1/1	0.85	0.27	70,70,70,70	0
56	MG	14	3130	1/1	0.85	0.29	75,75,75,75	0
56	MG	1H	3309	1/1	0.85	0.19	87,87,87,87	0
56	MG	1H	3238	1/1	0.85	0.19	71,71,71,71	0
56	MG	1H	3174	1/1	0.85	0.20	78,78,78,78	0
56	MG	88	201	1/1	0.85	0.28	79,79,79,79	0
56	MG	1H	3128	1/1	0.85	0.17	71,71,71,71	0
56	MG	1H	3213	1/1	0.85	0.36	86,86,86,86	0
56	MG	1H	3249	1/1	0.85	0.38	89,89,89,89	0
56	MG	1G	1607	1/1	0.85	0.20	92,92,92,92	0
56	MG	1H	3028	1/1	0.85	0.24	77,77,77,77	0
56	MG	13	1646	1/1	0.85	0.22	100,100,100,100	0
56	MG	1H	3256	1/1	0.85	0.39	74,74,74,74	0
56	MG	13	1751	1/1	0.85	0.23	70,70,70,70	0
56	MG	13	1695	1/1	0.85	0.18	88,88,88,88	0
56	MG	1G	1656	1/1	0.85	0.38	102,102,102,102	0
56	MG	13	1687	1/1	0.85	0.38	79,79,79,79	0
56	MG	1H	3085	1/1	0.85	0.26	74,74,74,74	0
56	MG	1H	3301	1/1	0.85	0.34	84,84,84,84	0
56	MG	1K	101	1/1	0.85	0.21	88,88,88,88	0
56	MG	1H	3205	1/1	0.85	0.29	80,80,80,80	0
56	MG	1G	1616	1/1	0.86	0.34	79,79,79,79	0
56	MG	1H	3286	1/1	0.86	0.31	91,91,91,91	0
56	MG	1H	3316	1/1	0.86	0.31	64,64,64,64	0
56	MG	13	1743	1/1	0.86	0.08	156,156,156,156	0
56	MG	14	3223	1/1	0.86	0.31	86,86,86,86	0
56	MG	1G	1652	1/1	0.86	0.53	86,86,86,86	0
56	MG	1G	1653	1/1	0.86	0.30	91,91,91,91	0
56	MG	1G	1680	1/1	0.86	0.45	107,107,107,107	0
56	MG	14	3053	1/1	0.86	0.23	55,55,55,55	0
56	MG	14	3064	1/1	0.86	0.21	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1681	1/1	0.86	0.36	106,106,106,106	0
56	MG	1G	1654	1/1	0.86	0.25	86,86,86,86	0
56	MG	1H	3175	1/1	0.86	0.37	92,92,92,92	0
56	MG	14	3081	1/1	0.86	0.25	71,71,71,71	0
56	MG	13	1667	1/1	0.86	0.25	87,87,87,87	0
56	MG	13	1625	1/1	0.86	0.19	61,61,61,61	0
56	MG	14	3245	1/1	0.86	0.27	84,84,84,84	0
56	MG	1G	1686	1/1	0.86	0.32	84,84,84,84	0
56	MG	14	3092	1/1	0.86	0.19	68,68,68,68	0
56	MG	1H	3109	1/1	0.86	0.33	93,93,93,93	0
56	MG	1H	3083	1/1	0.86	0.25	55,55,55,55	0
56	MG	1G	1632	1/1	0.86	0.21	86,86,86,86	0
56	MG	1H	3160	1/1	0.86	0.18	92,92,92,92	0
56	MG	1H	3118	1/1	0.86	0.38	93,93,93,93	0
56	MG	1G	1666	1/1	0.86	0.25	94,94,94,94	0
56	MG	14	3336	1/1	0.86	0.12	123,123,123,123	0
56	MG	1G	1603	1/1	0.86	0.23	83,83,83,83	0
56	MG	1H	3276	1/1	0.86	0.22	81,81,81,81	0
56	MG	13	1642	1/1	0.86	0.31	89,89,89,89	0
56	MG	14	3020	1/1	0.86	0.18	72,72,72,72	0
56	MG	1H	3087	1/1	0.86	0.23	72,72,72,72	0
56	MG	14	3027	1/1	0.86	0.23	91,91,91,91	0
56	MG	14	3201	1/1	0.86	0.20	86,86,86,86	0
56	MG	14	3202	1/1	0.86	0.13	115,115,115,115	0
56	MG	49	301	1/1	0.86	0.12	116,116,116,116	0
56	MG	3I	201	1/1	0.86	0.24	70,70,70,70	0
56	MG	1G	1615	1/1	0.86	0.13	103,103,103,103	0
56	MG	14	3208	1/1	0.86	0.22	94,94,94,94	0
56	MG	14	3121	1/1	0.86	0.31	79,79,79,79	0
56	MG	1H	3097	1/1	0.87	0.31	41,41,41,41	0
56	MG	14	3136	1/1	0.87	0.19	60,60,60,60	0
56	MG	14	3226	1/1	0.87	0.29	83,83,83,83	0
56	MG	14	3001	1/1	0.87	0.23	58,58,58,58	0
56	MG	14	3076	1/1	0.87	0.21	79,79,79,79	0
56	MG	1H	3228	1/1	0.87	0.19	71,71,71,71	0
56	MG	13	1698	1/1	0.87	0.27	90,90,90,90	0
56	MG	14	3011	1/1	0.87	0.36	57,57,57,57	0
56	MG	1H	3055	1/1	0.87	0.26	52,52,52,52	0
56	MG	16	202	1/1	0.87	0.32	66,66,66,66	0
56	MG	1H	3206	1/1	0.87	0.17	77,77,77,77	0
56	MG	1G	1650	1/1	0.87	0.28	111,111,111,111	0
56	MG	13	1657	1/1	0.87	0.05	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3169	1/1	0.87	0.27	81,81,81,81	0
56	MG	14	3022	1/1	0.87	0.23	61,61,61,61	0
56	MG	14	3024	1/1	0.87	0.22	79,79,79,79	0
56	MG	13	1669	1/1	0.87	0.17	142,142,142,142	0
56	MG	1H	3244	1/1	0.87	0.23	89,89,89,89	0
56	MG	1H	3073	1/1	0.87	0.18	53,53,53,53	0
56	MG	1H	3111	1/1	0.87	0.20	100,100,100,100	0
56	MG	1H	3313	1/1	0.87	0.29	80,80,80,80	0
56	MG	14	3032	1/1	0.87	0.17	60,60,60,60	0
56	MG	14	3034	1/1	0.87	0.28	64,64,64,64	0
56	MG	1H	3280	1/1	0.87	0.12	80,80,80,80	0
56	MG	1H	3186	1/1	0.87	0.34	89,89,89,89	0
56	MG	13	1732	1/1	0.87	0.11	132,132,132,132	0
56	MG	1J	203	1/1	0.87	0.25	79,79,79,79	0
56	MG	1G	1661	1/1	0.87	0.27	87,87,87,87	0
56	MG	1H	3251	1/1	0.87	0.21	96,96,96,96	0
56	MG	13	1634	1/1	0.87	0.29	80,80,80,80	0
56	MG	14	3124	1/1	0.87	0.22	81,81,81,81	0
56	MG	14	3052	1/1	0.87	0.50	74,74,74,74	0
56	MG	1H	3196	1/1	0.87	0.24	90,90,90,90	0
56	MG	14	3060	1/1	0.87	0.27	65,65,65,65	0
56	MG	13	1660	1/1	0.87	0.16	108,108,108,108	0
56	MG	14	3131	1/1	0.87	0.41	93,93,93,93	0
56	MG	14	3132	1/1	0.87	0.13	75,75,75,75	0
56	MG	1H	3082	1/1	0.88	0.26	64,64,64,64	0
56	MG	14	3009	1/1	0.88	0.32	63,63,63,63	0
56	MG	1H	3291	1/1	0.88	0.15	71,71,71,71	0
56	MG	14	3219	1/1	0.88	0.45	89,89,89,89	0
56	MG	14	3220	1/1	0.88	0.13	77,77,77,77	0
56	MG	14	3139	1/1	0.88	0.26	69,69,69,69	0
56	MG	1H	3293	1/1	0.88	0.25	82,82,82,82	0
56	MG	1H	3044	1/1	0.88	0.34	75,75,75,75	0
56	MG	14	3085	1/1	0.88	0.27	77,77,77,77	0
56	MG	14	3229	1/1	0.88	0.23	82,82,82,82	0
56	MG	14	3147	1/1	0.88	0.17	95,95,95,95	0
56	MG	13	1707	1/1	0.88	0.09	104,104,104,104	0
56	MG	13	1603	1/1	0.88	0.22	74,74,74,74	0
56	MG	1H	3124	1/1	0.88	0.21	89,89,89,89	0
56	MG	14	3156	1/1	0.88	0.24	80,80,80,80	0
56	MG	14	3021	1/1	0.88	0.21	80,80,80,80	0
56	MG	1H	3216	1/1	0.88	0.37	68,68,68,68	0
56	MG	13	1665	1/1	0.88	0.40	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3048	1/1	0.88	0.29	84,84,84,84	0
56	MG	1H	3099	1/1	0.88	0.20	64,64,64,64	0
56	MG	1H	3102	1/1	0.88	0.37	75,75,75,75	0
56	MG	14	3248	1/1	0.88	0.25	85,85,85,85	0
56	MG	1H	3190	1/1	0.88	0.23	88,88,88,88	0
56	MG	13	1621	1/1	0.88	0.18	97,97,97,97	0
56	MG	14	3251	1/1	0.88	0.22	102,102,102,102	0
56	MG	14	3177	1/1	0.88	0.41	80,80,80,80	0
56	MG	1G	1644	1/1	0.88	0.39	74,74,74,74	0
56	MG	13	1629	1/1	0.88	0.24	87,87,87,87	0
56	MG	1H	3014	1/1	0.88	0.21	57,57,57,57	0
56	MG	1G	1605	1/1	0.88	0.23	101,101,101,101	0
56	MG	1H	3315	1/1	0.88	0.24	77,77,77,77	0
56	MG	14	3187	1/1	0.88	0.11	62,62,62,62	0
56	MG	14	3120	1/1	0.88	0.23	78,78,78,78	0
56	MG	14	3193	1/1	0.88	0.26	74,74,74,74	0
56	MG	1H	3232	1/1	0.88	0.17	90,90,90,90	0
56	MG	1H	3234	1/1	0.88	0.22	74,74,74,74	0
56	MG	1H	3235	1/1	0.88	0.31	82,82,82,82	0
56	MG	1H	3202	1/1	0.88	0.19	80,80,80,80	0
56	MG	13	1631	1/1	0.88	0.20	82,82,82,82	0
56	MG	1H	3241	1/1	0.88	0.35	70,70,70,70	0
56	MG	14	3127	1/1	0.88	0.21	83,83,83,83	0
56	MG	1H	3283	1/1	0.88	0.14	67,67,67,67	0
56	MG	85	201	1/1	0.88	0.57	87,87,87,87	0
56	MG	1H	3081	1/1	0.88	0.27	63,63,63,63	0
56	MG	14	3212	1/1	0.88	0.28	90,90,90,90	0
56	MG	1H	3115	1/1	0.88	0.12	59,59,59,59	0
56	MG	14	3165	1/1	0.89	0.23	81,81,81,81	0
56	MG	1H	3237	1/1	0.89	0.13	62,62,62,62	0
56	MG	13	1656	1/1	0.89	0.19	83,83,83,83	0
56	MG	J8	102	1/1	0.89	0.09	66,66,66,66	0
56	MG	1H	3094	1/1	0.89	0.32	76,76,76,76	0
56	MG	1H	3278	1/1	0.89	0.12	82,82,82,82	0
56	MG	1H	3052	1/1	0.89	0.29	52,52,52,52	0
56	MG	14	3174	1/1	0.89	0.18	96,96,96,96	0
56	MG	1H	3010	1/1	0.89	0.19	47,47,47,47	0
56	MG	1H	3058	1/1	0.89	0.33	69,69,69,69	0
56	MG	13	1624	1/1	0.89	0.35	71,71,71,71	0
56	MG	1H	3066	1/1	0.89	0.16	62,62,62,62	0
56	MG	1H	3067	1/1	0.89	0.26	74,74,74,74	0
56	MG	1H	3148	1/1	0.89	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3019	1/1	0.89	0.15	71,71,71,71	0
56	MG	1H	3255	1/1	0.89	0.14	68,68,68,68	0
56	MG	1H	3159	1/1	0.89	0.16	65,65,65,65	0
56	MG	1H	3524	1/1	0.89	0.27	49,49,49,49	0
56	MG	14	3073	1/1	0.89	0.23	58,58,58,58	0
56	MG	14	3007	1/1	0.89	0.23	54,54,54,54	0
56	MG	14	3198	1/1	0.89	0.13	82,82,82,82	0
56	MG	1H	3021	1/1	0.89	0.16	58,58,58,58	0
56	MG	14	3134	1/1	0.89	0.25	88,88,88,88	0
56	MG	1H	3163	1/1	0.89	0.29	74,74,74,74	0
56	MG	1H	3231	1/1	0.89	0.19	63,63,63,63	0
56	MG	1H	3265	1/1	0.89	0.40	92,92,92,92	0
56	MG	1G	1628	1/1	0.89	0.29	76,76,76,76	0
56	MG	1H	3267	1/1	0.89	0.16	84,84,84,84	0
56	MG	1G	1630	1/1	0.89	0.26	76,76,76,76	0
56	MG	14	3214	1/1	0.89	0.25	81,81,81,81	0
56	MG	1G	1631	1/1	0.89	0.22	89,89,89,89	0
56	MG	1K	102	1/1	0.89	0.41	93,93,93,93	0
56	MG	1H	3303	1/1	0.89	0.17	88,88,88,88	0
56	MG	1H	3023	1/1	0.89	0.25	57,57,57,57	0
56	MG	31	301	1/1	0.89	0.12	62,62,62,62	0
56	MG	13	1618	1/1	0.89	0.29	71,71,71,71	0
56	MG	14	3163	1/1	0.89	0.29	71,71,71,71	0
56	MG	13	1644	1/1	0.89	0.24	77,77,77,77	0
56	MG	1H	3078	1/1	0.90	0.21	60,60,60,60	0
56	MG	1H	3242	1/1	0.90	0.22	86,86,86,86	0
56	MG	14	3133	1/1	0.90	0.28	82,82,82,82	0
56	MG	1H	3079	1/1	0.90	0.15	52,52,52,52	0
56	MG	1H	3080	1/1	0.90	0.23	53,53,53,53	0
56	MG	1H	3282	1/1	0.90	0.28	68,68,68,68	0
56	MG	13	1674	1/1	0.90	0.34	95,95,95,95	0
56	MG	13	1607	1/1	0.90	0.25	78,78,78,78	0
56	MG	1H	3248	1/1	0.90	0.09	81,81,81,81	0
56	MG	1H	3333	1/1	0.90	0.42	99,99,99,99	0
56	MG	13	1613	1/1	0.90	0.28	83,83,83,83	0
56	MG	14	3225	1/1	0.90	0.09	96,96,96,96	0
56	MG	14	3084	1/1	0.90	0.11	56,56,56,56	0
56	MG	1H	3025	1/1	0.90	0.17	86,86,86,86	0
56	MG	14	3086	1/1	0.90	0.14	53,53,53,53	0
56	MG	14	3155	1/1	0.90	0.11	82,82,82,82	0
56	MG	14	3017	1/1	0.90	0.22	85,85,85,85	0
56	MG	1H	3121	1/1	0.90	0.25	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2K	103	1/1	0.90	0.15	59,59,59,59	0
56	MG	1H	3003	1/1	0.90	0.26	63,63,63,63	0
56	MG	14	3236	1/1	0.90	0.17	89,89,89,89	0
56	MG	13	1628	1/1	0.90	0.36	77,77,77,77	0
56	MG	13	1602	1/1	0.90	0.23	68,68,68,68	0
56	MG	16	208	1/1	0.90	0.15	70,70,70,70	0
56	MG	14	3105	1/1	0.90	0.25	75,75,75,75	0
56	MG	1H	3258	1/1	0.90	0.27	68,68,68,68	0
56	MG	1H	3013	1/1	0.90	0.19	53,53,53,53	0
56	MG	11	302	1/1	0.90	0.28	82,82,82,82	0
56	MG	14	3111	1/1	0.90	0.18	86,86,86,86	0
56	MG	14	3176	1/1	0.90	0.20	71,71,71,71	0
56	MG	1H	3100	1/1	0.90	0.18	71,71,71,71	0
56	MG	21	302	1/1	0.90	0.21	73,73,73,73	0
56	MG	1H	3140	1/1	0.90	0.23	59,59,59,59	0
56	MG	14	3116	1/1	0.90	0.16	77,77,77,77	0
56	MG	13	1630	1/1	0.90	0.19	57,57,57,57	0
56	MG	1H	3144	1/1	0.90	0.34	78,78,78,78	0
56	MG	1H	3307	1/1	0.90	0.40	80,80,80,80	0
56	MG	14	3372	1/1	0.90	0.12	88,88,88,88	0
56	MG	14	3188	1/1	0.90	0.10	83,83,83,83	0
56	MG	14	3190	1/1	0.90	0.30	77,77,77,77	0
56	MG	14	3038	1/1	0.90	0.17	74,74,74,74	0
56	MG	1H	3233	1/1	0.90	0.24	75,75,75,75	0
56	MG	1H	3199	1/1	0.90	0.32	86,86,86,86	0
56	MG	1H	3103	1/1	0.90	0.23	76,76,76,76	0
56	MG	1H	3154	1/1	0.90	0.15	66,66,66,66	0
56	MG	14	3051	1/1	0.90	0.43	71,71,71,71	0
56	MG	13	1623	1/1	0.90	0.26	85,85,85,85	0
56	MG	1H	3020	1/1	0.90	0.18	56,56,56,56	0
56	MG	14	3056	1/1	0.90	0.20	64,64,64,64	0
56	MG	14	3129	1/1	0.90	0.29	76,76,76,76	0
56	MG	14	3206	1/1	0.90	0.25	90,90,90,90	0
56	MG	14	3207	1/1	0.90	0.40	93,93,93,93	0
56	MG	14	3057	1/1	0.90	0.24	80,80,80,80	0
56	MG	1H	3247	1/1	0.91	0.20	65,65,65,65	0
56	MG	14	3144	1/1	0.91	0.19	72,72,72,72	0
56	MG	1H	3219	1/1	0.91	0.36	82,82,82,82	0
56	MG	14	3216	1/1	0.91	0.15	70,70,70,70	0
56	MG	14	3090	1/1	0.91	0.16	90,90,90,90	0
56	MG	1H	3074	1/1	0.91	0.25	65,65,65,65	0
56	MG	1H	3076	1/1	0.91	0.21	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3134	1/1	0.91	0.44	90,90,90,90	0
56	MG	14	3222	1/1	0.91	0.25	87,87,87,87	0
56	MG	1H	3287	1/1	0.91	0.17	85,85,85,85	0
56	MG	1H	3011	1/1	0.91	0.22	54,54,54,54	0
56	MG	13	1684	1/1	0.91	0.31	95,95,95,95	0
56	MG	14	3104	1/1	0.91	0.36	86,86,86,86	0
56	MG	14	3160	1/1	0.91	0.35	88,88,88,88	0
56	MG	14	3161	1/1	0.91	0.23	70,70,70,70	0
56	MG	14	3033	1/1	0.91	0.25	69,69,69,69	0
56	MG	14	3231	1/1	0.91	0.14	77,77,77,77	0
56	MG	14	3106	1/1	0.91	0.25	70,70,70,70	0
56	MG	1G	1645	1/1	0.91	0.32	92,92,92,92	0
56	MG	14	3108	1/1	0.91	0.30	64,64,64,64	0
56	MG	14	3035	1/1	0.91	0.27	71,71,71,71	0
56	MG	1H	3330	1/1	0.91	0.29	94,94,94,94	0
56	MG	1H	3029	1/1	0.91	0.20	65,65,65,65	0
56	MG	14	3238	1/1	0.91	0.38	77,77,77,77	0
56	MG	1H	3049	1/1	0.91	0.17	74,74,74,74	0
56	MG	13	1747	1/1	0.91	0.06	140,140,140,140	0
56	MG	1H	3406	1/1	0.91	0.13	86,86,86,86	0
56	MG	1H	3499	1/1	0.91	0.09	77,77,77,77	0
56	MG	1H	3114	1/1	0.91	0.09	59,59,59,59	0
56	MG	13	1651	1/1	0.91	0.24	73,73,73,73	0
56	MG	14	3179	1/1	0.91	0.16	86,86,86,86	0
56	MG	2L	101	1/1	0.91	0.24	88,88,88,88	0
56	MG	1H	3004	1/1	0.91	0.23	57,57,57,57	0
56	MG	1H	3005	1/1	0.91	0.24	46,46,46,46	0
56	MG	1H	3063	1/1	0.91	0.25	47,47,47,47	0
56	MG	13	1675	1/1	0.91	0.13	92,92,92,92	0
56	MG	1H	3042	1/1	0.91	0.25	53,53,53,53	0
56	MG	14	3066	1/1	0.91	0.27	65,65,65,65	0
56	MG	1G	1627	1/1	0.91	0.35	77,77,77,77	0
56	MG	14	3010	1/1	0.91	0.18	58,58,58,58	0
56	MG	1H	3008	1/1	0.91	0.20	56,56,56,56	0
56	MG	14	3074	1/1	0.91	0.19	63,63,63,63	0
56	MG	1H	3125	1/1	0.91	0.26	77,77,77,77	0
56	MG	14	3077	1/1	0.91	0.22	78,78,78,78	0
56	MG	13	1612	1/1	0.91	0.27	70,70,70,70	0
56	MG	1G	1667	1/1	0.91	0.29	97,97,97,97	0
56	MG	1H	3176	1/1	0.91	0.46	90,90,90,90	0
56	MG	1H	3215	1/1	0.91	0.34	71,71,71,71	0
56	MG	14	3205	1/1	0.91	0.28	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3101	1/1	0.91	0.31	80,80,80,80	0
56	MG	14	3137	1/1	0.91	0.21	53,53,53,53	0
56	MG	14	3138	1/1	0.91	0.09	57,57,57,57	0
56	MG	14	3209	1/1	0.91	0.18	71,71,71,71	0
56	MG	1H	3217	1/1	0.91	0.11	61,61,61,61	0
56	MG	14	3140	1/1	0.91	0.22	65,65,65,65	0
56	MG	14	3069	1/1	0.92	0.29	63,63,63,63	0
56	MG	1H	3135	1/1	0.92	0.19	68,68,68,68	0
56	MG	1H	3001	1/1	0.92	0.25	45,45,45,45	0
56	MG	13	1745	1/1	0.92	0.08	119,119,119,119	0
56	MG	14	3005	1/1	0.92	0.22	48,48,48,48	0
56	MG	1H	3110	1/1	0.92	0.25	64,64,64,64	0
56	MG	14	3211	1/1	0.92	0.45	82,82,82,82	0
56	MG	1H	3193	1/1	0.92	0.24	67,67,67,67	0
56	MG	1H	3146	1/1	0.92	0.14	42,42,42,42	0
56	MG	14	3142	1/1	0.92	0.20	73,73,73,73	0
56	MG	14	3143	1/1	0.92	0.33	70,70,70,70	0
56	MG	P8	101	1/1	0.92	0.18	70,70,70,70	0
56	MG	1H	3272	1/1	0.92	0.26	71,71,71,71	0
56	MG	14	3013	1/1	0.92	0.14	66,66,66,66	0
56	MG	1H	3197	1/1	0.92	0.08	68,68,68,68	0
56	MG	1H	3068	1/1	0.92	0.24	67,67,67,67	0
56	MG	1H	3323	1/1	0.92	0.22	87,87,87,87	0
56	MG	14	3150	1/1	0.92	0.21	64,64,64,64	0
56	MG	14	3151	1/1	0.92	0.20	52,52,52,52	0
56	MG	14	3152	1/1	0.92	0.14	61,61,61,61	0
56	MG	1H	3149	1/1	0.92	0.27	77,77,77,77	0
56	MG	1H	3090	1/1	0.92	0.31	66,66,66,66	0
56	MG	1H	3037	1/1	0.92	0.18	64,64,64,64	0
56	MG	1H	3239	1/1	0.92	0.24	84,84,84,84	0
56	MG	14	3158	1/1	0.92	0.15	75,75,75,75	0
56	MG	1G	1614	1/1	0.92	0.27	78,78,78,78	0
56	MG	1H	3240	1/1	0.92	0.31	77,77,77,77	0
56	MG	1H	3158	1/1	0.92	0.13	55,55,55,55	0
56	MG	1H	3095	1/1	0.92	0.39	78,78,78,78	0
56	MG	1H	3096	1/1	0.92	0.23	70,70,70,70	0
56	MG	1H	3050	1/1	0.92	0.24	62,62,62,62	0
56	MG	1H	3051	1/1	0.92	0.24	72,72,72,72	0
56	MG	1G	1621	1/1	0.92	0.13	92,92,92,92	0
56	MG	1H	3075	1/1	0.92	0.19	53,53,53,53	0
56	MG	1H	3490	1/1	0.92	0.12	92,92,92,92	0
56	MG	1H	3170	1/1	0.92	0.23	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1626	1/1	0.92	0.27	78,78,78,78	0
56	MG	1H	3041	1/1	0.92	0.18	57,57,57,57	0
56	MG	13	1673	1/1	0.92	0.16	83,83,83,83	0
56	MG	14	3115	1/1	0.92	0.29	86,86,86,86	0
56	MG	1H	3126	1/1	0.92	0.25	88,88,88,88	0
56	MG	16	203	1/1	0.92	0.11	91,91,91,91	0
56	MG	14	3041	1/1	0.92	0.41	76,76,76,76	0
56	MG	14	3184	1/1	0.92	0.23	53,53,53,53	0
56	MG	14	3043	1/1	0.92	0.22	57,57,57,57	0
56	MG	14	3257	1/1	0.92	0.48	99,99,99,99	0
56	MG	13	1620	1/1	0.92	0.34	69,69,69,69	0
56	MG	14	3259	1/1	0.92	0.15	67,67,67,67	0
56	MG	14	3045	1/1	0.92	0.16	60,60,60,60	0
56	MG	14	3360	1/1	0.92	0.19	112,112,112,112	0
56	MG	14	3047	1/1	0.92	0.23	59,59,59,59	0
56	MG	14	3378	1/1	0.92	0.08	92,92,92,92	0
56	MG	14	3385	1/1	0.92	0.20	113,113,113,113	0
56	MG	14	3189	1/1	0.92	0.54	86,86,86,86	0
56	MG	13	1659	1/1	0.92	0.10	107,107,107,107	0
56	MG	1H	3180	1/1	0.92	0.28	67,67,67,67	0
56	MG	14	3192	1/1	0.92	0.26	85,85,85,85	0
56	MG	1H	3104	1/1	0.92	0.11	67,67,67,67	0
56	MG	1H	3182	1/1	0.92	0.34	82,82,82,82	0
56	MG	1H	3018	1/1	0.92	0.31	83,83,83,83	0
56	MG	1H	3302	1/1	0.92	0.08	81,81,81,81	0
56	MG	14	3059	1/1	0.92	0.13	59,59,59,59	0
56	MG	14	3199	1/1	0.92	0.21	84,84,84,84	0
56	MG	35	201	1/1	0.92	0.22	76,76,76,76	0
56	MG	14	3200	1/1	0.92	0.15	82,82,82,82	0
56	MG	11	303	1/1	0.92	0.09	75,75,75,75	0
56	MG	1H	3064	1/1	0.92	0.15	45,45,45,45	0
56	MG	21	301	1/1	0.92	0.26	55,55,55,55	0
56	MG	1H	3263	1/1	0.92	0.25	82,82,82,82	0
56	MG	1H	3510	1/1	0.93	0.10	99,99,99,99	0
56	MG	14	3023	1/1	0.93	0.16	66,66,66,66	0
56	MG	1H	3107	1/1	0.93	0.20	84,84,84,84	0
56	MG	5E	201	1/1	0.93	0.14	93,93,93,93	0
56	MG	14	3095	1/1	0.93	0.23	72,72,72,72	0
56	MG	14	3221	1/1	0.93	0.16	88,88,88,88	0
56	MG	1H	3007	1/1	0.93	0.19	40,40,40,40	0
56	MG	1H	3038	1/1	0.93	0.20	76,76,76,76	0
56	MG	16	204	1/1	0.93	0.24	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3218	1/1	0.93	0.15	76,76,76,76	0
56	MG	1H	3306	1/1	0.93	0.17	81,81,81,81	0
56	MG	1H	3189	1/1	0.93	0.28	77,77,77,77	0
56	MG	1H	3129	1/1	0.93	0.16	77,77,77,77	0
56	MG	1H	3277	1/1	0.93	0.35	84,84,84,84	0
56	MG	14	3167	1/1	0.93	0.24	71,71,71,71	0
56	MG	1H	3311	1/1	0.93	0.10	70,70,70,70	0
56	MG	1H	3191	1/1	0.93	0.09	59,59,59,59	0
56	MG	1H	3039	1/1	0.93	0.28	70,70,70,70	0
56	MG	1G	1633	1/1	0.93	0.24	92,92,92,92	0
56	MG	1H	3132	1/1	0.93	0.35	74,74,74,74	0
56	MG	13	1655	1/1	0.93	0.19	80,80,80,80	0
56	MG	1H	3317	1/1	0.93	0.15	66,66,66,66	0
56	MG	1H	3168	1/1	0.93	0.22	84,84,84,84	0
56	MG	1H	3319	1/1	0.93	0.21	76,76,76,76	0
56	MG	14	3046	1/1	0.93	0.19	65,65,65,65	0
56	MG	14	3242	1/1	0.93	0.36	78,78,78,78	0
56	MG	14	3243	1/1	0.93	0.42	81,81,81,81	0
56	MG	14	3244	1/1	0.93	0.19	80,80,80,80	0
56	MG	78	201	1/1	0.93	0.24	70,70,70,70	0
56	MG	14	3049	1/1	0.93	0.28	71,71,71,71	0
56	MG	13	1681	1/1	0.93	0.34	83,83,83,83	0
56	MG	13	1697	1/1	0.93	0.35	75,75,75,75	0
56	MG	1H	3138	1/1	0.93	0.20	69,69,69,69	0
56	MG	1H	3056	1/1	0.93	0.20	54,54,54,54	0
56	MG	14	3054	1/1	0.93	0.26	59,59,59,59	0
56	MG	14	3055	1/1	0.93	0.15	60,60,60,60	0
56	MG	1H	3088	1/1	0.93	0.17	61,61,61,61	0
56	MG	1H	3143	1/1	0.93	0.20	68,68,68,68	0
56	MG	1H	3261	1/1	0.93	0.20	58,58,58,58	0
56	MG	13	1617	1/1	0.93	0.22	70,70,70,70	0
56	MG	14	3061	1/1	0.93	0.29	71,71,71,71	0
56	MG	14	3287	1/1	0.93	0.08	99,99,99,99	0
56	MG	14	3334	1/1	0.93	0.06	116,116,116,116	0
56	MG	14	3195	1/1	0.93	0.51	96,96,96,96	0
56	MG	14	3063	1/1	0.93	0.10	62,62,62,62	0
56	MG	14	3365	1/1	0.93	0.08	87,87,87,87	0
56	MG	14	3006	1/1	0.93	0.24	60,60,60,60	0
56	MG	14	3373	1/1	0.93	0.06	125,125,125,125	0
56	MG	14	3065	1/1	0.93	0.46	49,49,49,49	0
56	MG	1H	3208	1/1	0.93	0.15	71,71,71,71	0
56	MG	14	3067	1/1	0.93	0.40	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1606	1/1	0.93	0.18	94,94,94,94	0
56	MG	1H	3122	1/1	0.93	0.41	78,78,78,78	0
56	MG	14	3070	1/1	0.93	0.32	59,59,59,59	0
56	MG	1G	1608	1/1	0.93	0.14	90,90,90,90	0
56	MG	1H	3266	1/1	0.93	0.38	75,75,75,75	0
56	MG	14	3012	1/1	0.93	0.21	49,49,49,49	0
56	MG	1H	3404	1/1	0.93	0.12	86,86,86,86	0
56	MG	14	3014	1/1	0.93	0.20	81,81,81,81	0
56	MG	1H	3298	1/1	0.93	0.24	73,73,73,73	0
56	MG	1G	1613	1/1	0.93	0.44	87,87,87,87	0
56	MG	1H	3431	1/1	0.93	0.07	117,117,117,117	0
56	MG	1H	3489	1/1	0.93	0.10	86,86,86,86	0
56	MG	1H	3092	1/1	0.93	0.17	52,52,52,52	0
56	MG	1G	1663	1/1	0.93	0.14	89,89,89,89	0
56	MG	3E	302	1/1	0.93	0.07	125,125,125,125	0
56	MG	88	202	1/1	0.94	0.12	69,69,69,69	0
56	MG	1H	3192	1/1	0.94	0.17	81,81,81,81	0
56	MG	14	3175	1/1	0.94	0.22	88,88,88,88	0
56	MG	J8	101	1/1	0.94	0.24	72,72,72,72	0
56	MG	1H	3388	1/1	0.94	0.08	63,63,63,63	0
56	MG	L8	101	1/1	0.94	0.18	72,72,72,72	0
56	MG	13	1661	1/1	0.94	0.12	95,95,95,95	0
56	MG	14	3180	1/1	0.94	0.31	93,93,93,93	0
56	MG	Q8	101	1/1	0.94	0.12	53,53,53,53	0
56	MG	1H	3195	1/1	0.94	0.14	68,68,68,68	0
56	MG	1H	3415	1/1	0.94	0.06	100,100,100,100	0
56	MG	1H	3427	1/1	0.94	0.15	78,78,78,78	0
56	MG	1H	3430	1/1	0.94	0.11	71,71,71,71	0
56	MG	1H	3169	1/1	0.94	0.16	74,74,74,74	0
56	MG	1H	3445	1/1	0.94	0.12	91,91,91,91	0
56	MG	1H	3450	1/1	0.94	0.06	119,119,119,119	0
56	MG	1H	3473	1/1	0.94	0.11	92,92,92,92	0
56	MG	14	3075	1/1	0.94	0.29	61,61,61,61	0
56	MG	13	1633	1/1	0.94	0.32	73,73,73,73	0
56	MG	13	1649	1/1	0.94	0.14	79,79,79,79	0
56	MG	1H	3493	1/1	0.94	0.06	113,113,113,113	0
56	MG	14	3080	1/1	0.94	0.18	54,54,54,54	0
56	MG	1H	3498	1/1	0.94	0.13	64,64,64,64	0
56	MG	13	1739	1/1	0.94	0.08	118,118,118,118	0
56	MG	1H	3253	1/1	0.94	0.33	64,64,64,64	0
56	MG	1H	3518	1/1	0.94	0.14	74,74,74,74	0
56	MG	1H	3112	1/1	0.94	0.32	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3030	1/1	0.94	0.10	74,74,74,74	0
56	MG	1H	3529	1/1	0.94	0.11	55,55,55,55	0
56	MG	1H	3113	1/1	0.94	0.17	73,73,73,73	0
56	MG	1H	3150	1/1	0.94	0.12	52,52,52,52	0
56	MG	1H	3177	1/1	0.94	0.09	62,62,62,62	0
56	MG	1H	3179	1/1	0.94	0.12	59,59,59,59	0
56	MG	1H	3289	1/1	0.94	0.18	77,77,77,77	0
56	MG	14	3366	1/1	0.94	0.10	83,83,83,83	0
56	MG	14	3371	1/1	0.94	0.08	108,108,108,108	0
56	MG	1H	3152	1/1	0.94	0.21	53,53,53,53	0
56	MG	13	1664	1/1	0.94	0.29	71,71,71,71	0
56	MG	1H	3321	1/1	0.94	0.07	72,72,72,72	0
56	MG	1H	3322	1/1	0.94	0.14	77,77,77,77	0
56	MG	1H	3292	1/1	0.94	0.33	79,79,79,79	0
56	MG	16	213	1/1	0.94	0.07	102,102,102,102	0
56	MG	11	301	1/1	0.94	0.19	48,48,48,48	0
56	MG	14	3159	1/1	0.94	0.07	60,60,60,60	0
56	MG	1H	3031	1/1	0.94	0.14	63,63,63,63	0
56	MG	1H	3157	1/1	0.94	0.18	65,65,65,65	0
56	MG	14	3162	1/1	0.94	0.20	60,60,60,60	0
56	MG	13	1604	1/1	0.94	0.17	89,89,89,89	0
56	MG	29	301	1/1	0.94	0.15	49,49,49,49	0
56	MG	13	1637	1/1	0.94	0.28	59,59,59,59	0
56	MG	1H	3119	1/1	0.94	0.35	86,86,86,86	0
56	MG	1H	3061	1/1	0.94	0.18	61,61,61,61	0
56	MG	1H	3012	1/1	0.94	0.25	52,52,52,52	0
56	MG	1H	3024	1/1	0.94	0.26	53,53,53,53	0
56	MG	1H	3166	1/1	0.94	0.20	60,60,60,60	0
56	MG	F5	101	1/1	0.94	0.30	74,74,74,74	0
56	MG	1H	3334	1/1	0.94	0.15	77,77,77,77	0
56	MG	1G	1643	1/1	0.94	0.25	79,79,79,79	0
56	MG	1H	3523	1/1	0.95	0.26	37,37,37,37	0
56	MG	1H	3254	1/1	0.95	0.26	84,84,84,84	0
56	MG	1H	3527	1/1	0.95	0.10	69,69,69,69	0
56	MG	1H	3320	1/1	0.95	0.21	86,86,86,86	0
56	MG	1H	3053	1/1	0.95	0.16	48,48,48,48	0
56	MG	1H	3086	1/1	0.95	0.30	67,67,67,67	0
56	MG	14	3072	1/1	0.95	0.15	75,75,75,75	0
56	MG	1H	3054	1/1	0.95	0.09	53,53,53,53	0
56	MG	1H	3147	1/1	0.95	0.17	49,49,49,49	0
56	MG	1H	3201	1/1	0.95	0.14	79,79,79,79	0
56	MG	1H	3260	1/1	0.95	0.36	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3025	1/1	0.95	0.20	53,53,53,53	0
56	MG	1H	3072	1/1	0.95	0.13	46,46,46,46	0
56	MG	13	1601	1/1	0.95	0.12	83,83,83,83	0
56	MG	13	1741	1/1	0.95	0.05	138,138,138,138	0
56	MG	1H	3057	1/1	0.95	0.14	40,40,40,40	0
56	MG	1H	3153	1/1	0.95	0.13	57,57,57,57	0
56	MG	1H	3016	1/1	0.95	0.19	61,61,61,61	0
56	MG	1H	3268	1/1	0.95	0.30	80,80,80,80	0
56	MG	1H	3209	1/1	0.95	0.15	60,60,60,60	0
56	MG	14	3088	1/1	0.95	0.16	44,44,44,44	0
56	MG	1H	3377	1/1	0.95	0.07	100,100,100,100	0
56	MG	1H	3210	1/1	0.95	0.11	95,95,95,95	0
56	MG	1H	3077	1/1	0.95	0.17	69,69,69,69	0
56	MG	13	1742	1/1	0.95	0.08	102,102,102,102	0
56	MG	14	3278	1/1	0.95	0.07	84,84,84,84	0
56	MG	14	3094	1/1	0.95	0.20	82,82,82,82	0
56	MG	14	3295	1/1	0.95	0.10	87,87,87,87	0
56	MG	14	3329	1/1	0.95	0.10	89,89,89,89	0
56	MG	41	301	1/1	0.95	0.13	77,77,77,77	0
56	MG	13	1713	1/1	0.95	0.08	77,77,77,77	0
56	MG	14	3354	1/1	0.95	0.22	77,77,77,77	0
56	MG	14	3356	1/1	0.95	0.09	85,85,85,85	0
56	MG	13	1727	1/1	0.95	0.10	117,117,117,117	0
56	MG	14	3363	1/1	0.95	0.09	96,96,96,96	0
56	MG	14	3099	1/1	0.95	0.16	68,68,68,68	0
56	MG	13	1729	1/1	0.95	0.07	111,111,111,111	0
56	MG	1H	3117	1/1	0.95	0.35	63,63,63,63	0
56	MG	1H	3136	1/1	0.95	0.16	66,66,66,66	0
56	MG	1G	1693	1/1	0.95	0.06	125,125,125,125	0
56	MG	1H	3310	1/1	0.95	0.27	82,82,82,82	0
56	MG	E8	201	1/1	0.95	0.10	79,79,79,79	0
56	MG	14	3048	1/1	0.95	0.16	65,65,65,65	0
56	MG	1H	3455	1/1	0.95	0.07	111,111,111,111	0
56	MG	1H	3464	1/1	0.95	0.06	111,111,111,111	0
56	MG	1H	3469	1/1	0.95	0.13	96,96,96,96	0
56	MG	1H	3137	1/1	0.95	0.18	67,67,67,67	0
56	MG	14	3003	1/1	0.95	0.14	45,45,45,45	0
56	MG	1H	3484	1/1	0.95	0.10	89,89,89,89	0
56	MG	1H	3487	1/1	0.95	0.06	101,101,101,101	0
56	MG	13	1608	1/1	0.95	0.13	75,75,75,75	0
56	MG	1H	3222	1/1	0.95	0.27	77,77,77,77	0
56	MG	1G	1604	1/1	0.95	0.11	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3172	1/1	0.95	0.13	93,93,93,93	0
56	MG	1H	3314	1/1	0.95	0.17	110,110,110,110	0
56	MG	14	3228	1/1	0.95	0.08	192,192,192,192	0
56	MG	1H	3032	1/1	0.95	0.23	46,46,46,46	0
56	MG	1H	3194	1/1	0.95	0.19	48,48,48,48	0
56	MG	1H	3141	1/1	0.95	0.10	53,53,53,53	0
56	MG	1H	3084	1/1	0.95	0.13	66,66,66,66	0
56	MG	1H	3331	1/1	0.96	0.30	74,74,74,74	0
56	MG	14	3087	1/1	0.96	0.07	59,59,59,59	0
56	MG	1H	3511	1/1	0.96	0.10	76,76,76,76	0
56	MG	1H	3517	1/1	0.96	0.06	71,71,71,71	0
56	MG	1G	1687	1/1	0.96	0.06	121,121,121,121	0
56	MG	14	3247	1/1	0.96	0.08	61,61,61,61	0
56	MG	1H	3091	1/1	0.96	0.12	43,43,43,43	0
56	MG	1G	1696	1/1	0.96	0.05	98,98,98,98	0
56	MG	14	3042	1/1	0.96	0.13	48,48,48,48	0
56	MG	1G	1697	1/1	0.96	0.07	108,108,108,108	0
56	MG	13	1724	1/1	0.96	0.07	102,102,102,102	0
56	MG	1H	3060	1/1	0.96	0.29	48,48,48,48	0
56	MG	14	3098	1/1	0.96	0.20	53,53,53,53	0
56	MG	1H	3284	1/1	0.96	0.09	190,190,190,190	0
56	MG	1H	3528	1/1	0.96	0.08	77,77,77,77	0
56	MG	13	1706	1/1	0.96	0.09	108,108,108,108	0
56	MG	1H	3262	1/1	0.96	0.10	57,57,57,57	0
56	MG	14	3269	1/1	0.96	0.08	90,90,90,90	0
56	MG	13	1652	1/1	0.96	0.06	79,79,79,79	0
56	MG	14	3282	1/1	0.96	0.07	92,92,92,92	0
56	MG	14	3004	1/1	0.96	0.15	53,53,53,53	0
56	MG	14	3289	1/1	0.96	0.07	77,77,77,77	0
56	MG	1G	1610	1/1	0.96	0.05	98,98,98,98	0
56	MG	14	3297	1/1	0.96	0.06	107,107,107,107	0
56	MG	14	3315	1/1	0.96	0.08	71,71,71,71	0
56	MG	14	3324	1/1	0.96	0.06	107,107,107,107	0
56	MG	1H	3405	1/1	0.96	0.09	75,75,75,75	0
56	MG	1H	3288	1/1	0.96	0.08	60,60,60,60	0
56	MG	14	3335	1/1	0.96	0.07	91,91,91,91	0
56	MG	1H	3151	1/1	0.96	0.18	71,71,71,71	0
56	MG	14	3338	1/1	0.96	0.06	107,107,107,107	0
56	MG	14	3340	1/1	0.96	0.10	83,83,83,83	0
56	MG	1H	3417	1/1	0.96	0.07	65,65,65,65	0
56	MG	1H	3422	1/1	0.96	0.08	83,83,83,83	0
56	MG	14	3058	1/1	0.96	0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	13	1744	1/1	0.96	0.04	144,144,144,144	0
56	MG	1G	1660	1/1	0.96	0.11	92,92,92,92	0
56	MG	1H	3428	1/1	0.96	0.13	100,100,100,100	0
56	MG	1H	3221	1/1	0.96	0.33	92,92,92,92	0
56	MG	1H	3065	1/1	0.96	0.28	51,51,51,51	0
56	MG	1H	3442	1/1	0.96	0.05	100,100,100,100	0
56	MG	1H	3178	1/1	0.96	0.27	68,68,68,68	0
56	MG	14	3383	1/1	0.96	0.09	93,93,93,93	0
56	MG	1H	3040	1/1	0.96	0.08	47,47,47,47	0
56	MG	13	1627	1/1	0.96	0.10	57,57,57,57	0
56	MG	1H	3461	1/1	0.96	0.09	105,105,105,105	0
56	MG	1G	1625	1/1	0.96	0.39	82,82,82,82	0
56	MG	13	1738	1/1	0.96	0.11	113,113,113,113	0
56	MG	1H	3069	1/1	0.96	0.21	45,45,45,45	0
56	MG	13	1748	1/1	0.96	0.09	156,156,156,156	0
56	MG	1H	3139	1/1	0.96	0.14	65,65,65,65	0
56	MG	1H	3185	1/1	0.96	0.40	68,68,68,68	0
56	MG	14	3181	1/1	0.96	0.33	86,86,86,86	0
56	MG	1H	3071	1/1	0.96	0.14	51,51,51,51	0
56	MG	13	1749	1/1	0.96	0.08	101,101,101,101	0
56	MG	13	1666	1/1	0.96	0.07	99,99,99,99	0
56	MG	1H	3496	1/1	0.96	0.09	59,59,59,59	0
56	MG	C8	201	1/1	0.96	0.17	74,74,74,74	0
56	MG	1H	3089	1/1	0.96	0.08	44,44,44,44	0
56	MG	13	1740	1/1	0.96	0.11	91,91,91,91	0
57	ZN	3E	303	1/1	0.96	0.27	110,110,110,110	0
56	MG	1H	3502	1/1	0.96	0.10	49,49,49,49	0
56	MG	1H	3508	1/1	0.96	0.06	96,96,96,96	0
56	MG	1G	1701	1/1	0.97	0.05	128,128,128,128	0
56	MG	14	3272	1/1	0.97	0.06	59,59,59,59	0
56	MG	14	3274	1/1	0.97	0.09	99,99,99,99	0
56	MG	14	3276	1/1	0.97	0.07	64,64,64,64	0
56	MG	1G	1703	1/1	0.97	0.05	124,124,124,124	0
56	MG	14	3281	1/1	0.97	0.11	79,79,79,79	0
56	MG	1H	3363	1/1	0.97	0.05	89,89,89,89	0
56	MG	1H	3043	1/1	0.97	0.09	50,50,50,50	0
56	MG	1H	3488	1/1	0.97	0.08	102,102,102,102	0
56	MG	1H	3378	1/1	0.97	0.13	83,83,83,83	0
56	MG	1H	3093	1/1	0.97	0.36	61,61,61,61	0
56	MG	14	3305	1/1	0.97	0.10	112,112,112,112	0
56	MG	14	3313	1/1	0.97	0.10	81,81,81,81	0
56	MG	1H	3491	1/1	0.97	0.05	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3321	1/1	0.97	0.08	97,97,97,97	0
56	MG	14	3322	1/1	0.97	0.06	101,101,101,101	0
56	MG	1H	3492	1/1	0.97	0.08	108,108,108,108	0
56	MG	14	3326	1/1	0.97	0.04	110,110,110,110	0
56	MG	14	3328	1/1	0.97	0.05	98,98,98,98	0
56	MG	1H	3397	1/1	0.97	0.06	96,96,96,96	0
56	MG	14	3330	1/1	0.97	0.05	104,104,104,104	0
56	MG	14	3091	1/1	0.97	0.14	54,54,54,54	0
56	MG	13	1721	1/1	0.97	0.11	94,94,94,94	0
56	MG	13	1746	1/1	0.97	0.04	127,127,127,127	0
56	MG	1H	3002	1/1	0.97	0.11	30,30,30,30	0
56	MG	1H	3410	1/1	0.97	0.07	62,62,62,62	0
56	MG	14	3348	1/1	0.97	0.06	97,97,97,97	0
56	MG	14	3349	1/1	0.97	0.05	110,110,110,110	0
56	MG	14	3352	1/1	0.97	0.08	106,106,106,106	0
56	MG	1H	3412	1/1	0.97	0.08	101,101,101,101	0
56	MG	14	3355	1/1	0.97	0.13	97,97,97,97	0
56	MG	1H	3204	1/1	0.97	0.21	76,76,76,76	0
56	MG	14	3359	1/1	0.97	0.06	97,97,97,97	0
56	MG	13	1611	1/1	0.97	0.21	70,70,70,70	0
56	MG	14	3361	1/1	0.97	0.06	115,115,115,115	0
56	MG	13	1726	1/1	0.97	0.05	91,91,91,91	0
56	MG	13	1626	1/1	0.97	0.04	65,65,65,65	0
56	MG	1H	3520	1/1	0.97	0.06	109,109,109,109	0
56	MG	14	3370	1/1	0.97	0.06	88,88,88,88	0
56	MG	14	3103	1/1	0.97	0.10	52,52,52,52	0
56	MG	1H	3521	1/1	0.97	0.05	49,49,49,49	0
56	MG	1H	3522	1/1	0.97	0.10	99,99,99,99	0
56	MG	1H	3027	1/1	0.97	0.22	64,64,64,64	0
56	MG	14	3380	1/1	0.97	0.07	58,58,58,58	0
56	MG	14	3382	1/1	0.97	0.08	85,85,85,85	0
56	MG	1H	3017	1/1	0.97	0.17	43,43,43,43	0
56	MG	13	1715	1/1	0.97	0.05	116,116,116,116	0
56	MG	13	1719	1/1	0.97	0.05	64,64,64,64	0
56	MG	14	3389	1/1	0.97	0.13	62,62,62,62	0
56	MG	1H	3130	1/1	0.97	0.31	82,82,82,82	0
56	MG	1H	3161	1/1	0.97	0.23	66,66,66,66	0
56	MG	1H	3145	1/1	0.97	0.15	49,49,49,49	0
56	MG	1H	3456	1/1	0.97	0.07	111,111,111,111	0
56	MG	13	1737	1/1	0.97	0.04	122,122,122,122	0
56	MG	1H	3349	1/1	0.97	0.11	70,70,70,70	0
56	MG	1H	3465	1/1	0.97	0.10	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1J	208	1/1	0.97	0.04	109,109,109,109	0
56	MG	1H	3466	1/1	0.97	0.05	106,106,106,106	0
56	MG	1G	1649	1/1	0.97	0.08	145,145,145,145	0
56	MG	1H	3355	1/1	0.97	0.14	53,53,53,53	0
56	MG	1G	1690	1/1	0.97	0.05	90,90,90,90	0
56	MG	1G	1691	1/1	0.97	0.05	119,119,119,119	0
56	MG	1H	3359	1/1	0.97	0.04	102,102,102,102	0
56	MG	14	3256	1/1	0.97	0.09	75,75,75,75	0
56	MG	1G	1695	1/1	0.97	0.07	103,103,103,103	0
56	MG	1H	3475	1/1	0.97	0.07	77,77,77,77	0
56	MG	1H	3480	1/1	0.97	0.04	122,122,122,122	0
56	MG	14	3266	1/1	0.97	0.05	69,69,69,69	0
56	MG	13	1647	1/1	0.98	0.30	75,75,75,75	0
56	MG	1H	3356	1/1	0.98	0.04	67,67,67,67	0
56	MG	1H	3433	1/1	0.98	0.06	77,77,77,77	0
56	MG	1H	3435	1/1	0.98	0.06	95,95,95,95	0
56	MG	1H	3439	1/1	0.98	0.06	76,76,76,76	0
56	MG	1H	3441	1/1	0.98	0.08	82,82,82,82	0
56	MG	1H	3357	1/1	0.98	0.06	52,52,52,52	0
56	MG	1H	3173	1/1	0.98	0.07	79,79,79,79	0
56	MG	14	3301	1/1	0.98	0.05	81,81,81,81	0
56	MG	14	3304	1/1	0.98	0.05	91,91,91,91	0
56	MG	1H	3361	1/1	0.98	0.04	105,105,105,105	0
56	MG	14	3312	1/1	0.98	0.07	97,97,97,97	0
56	MG	1H	3451	1/1	0.98	0.08	94,94,94,94	0
56	MG	1H	3062	1/1	0.98	0.10	35,35,35,35	0
56	MG	14	3317	1/1	0.98	0.11	89,89,89,89	0
56	MG	14	3319	1/1	0.98	0.06	88,88,88,88	0
56	MG	14	3153	1/1	0.98	0.05	60,60,60,60	0
56	MG	1H	3364	1/1	0.98	0.05	70,70,70,70	0
56	MG	14	3323	1/1	0.98	0.05	96,96,96,96	0
56	MG	1H	3457	1/1	0.98	0.10	91,91,91,91	0
56	MG	14	3325	1/1	0.98	0.04	103,103,103,103	0
56	MG	1H	3365	1/1	0.98	0.04	91,91,91,91	0
56	MG	14	3327	1/1	0.98	0.04	120,120,120,120	0
56	MG	1H	3366	1/1	0.98	0.04	68,68,68,68	0
56	MG	1H	3369	1/1	0.98	0.06	70,70,70,70	0
56	MG	1H	3372	1/1	0.98	0.08	65,65,65,65	0
56	MG	14	3333	1/1	0.98	0.04	91,91,91,91	0
56	MG	1H	3468	1/1	0.98	0.04	109,109,109,109	0
56	MG	1H	3220	1/1	0.98	0.05	61,61,61,61	0
56	MG	14	3101	1/1	0.98	0.04	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3337	1/1	0.98	0.06	83,83,83,83	0
56	MG	1H	3471	1/1	0.98	0.13	94,94,94,94	0
56	MG	1G	1688	1/1	0.98	0.04	73,73,73,73	0
56	MG	14	3341	1/1	0.98	0.04	103,103,103,103	0
56	MG	13	1723	1/1	0.98	0.04	105,105,105,105	0
56	MG	1H	3380	1/1	0.98	0.07	82,82,82,82	0
56	MG	14	3350	1/1	0.98	0.14	84,84,84,84	0
56	MG	14	3351	1/1	0.98	0.03	99,99,99,99	0
56	MG	1G	1692	1/1	0.98	0.05	111,111,111,111	0
56	MG	1H	3478	1/1	0.98	0.03	111,111,111,111	0
56	MG	1G	1694	1/1	0.98	0.04	104,104,104,104	0
56	MG	1H	3384	1/1	0.98	0.04	62,62,62,62	0
56	MG	14	3358	1/1	0.98	0.06	117,117,117,117	0
56	MG	1H	3483	1/1	0.98	0.04	117,117,117,117	0
56	MG	1H	3386	1/1	0.98	0.06	58,58,58,58	0
56	MG	1G	1699	1/1	0.98	0.08	122,122,122,122	0
56	MG	1H	3167	1/1	0.98	0.15	62,62,62,62	0
56	MG	14	3364	1/1	0.98	0.06	77,77,77,77	0
56	MG	1G	1702	1/1	0.98	0.09	146,146,146,146	0
56	MG	1H	3390	1/1	0.98	0.04	55,55,55,55	0
56	MG	14	3367	1/1	0.98	0.09	92,92,92,92	0
56	MG	1H	3015	1/1	0.98	0.09	57,57,57,57	0
56	MG	1H	3155	1/1	0.98	0.31	72,72,72,72	0
56	MG	1H	3162	1/1	0.98	0.05	55,55,55,55	0
56	MG	1G	1646	1/1	0.98	0.12	84,84,84,84	0
56	MG	14	3377	1/1	0.98	0.09	52,52,52,52	0
56	MG	1H	3336	1/1	0.98	0.07	52,52,52,52	0
56	MG	14	3379	1/1	0.98	0.08	60,60,60,60	0
56	MG	I8	101	1/1	0.98	0.07	88,88,88,88	0
56	MG	14	3381	1/1	0.98	0.12	79,79,79,79	0
56	MG	1H	3407	1/1	0.98	0.05	84,84,84,84	0
56	MG	1H	3494	1/1	0.98	0.07	95,95,95,95	0
56	MG	14	3384	1/1	0.98	0.05	110,110,110,110	0
56	MG	1H	3337	1/1	0.98	0.07	56,56,56,56	0
56	MG	14	3386	1/1	0.98	0.09	51,51,51,51	0
56	MG	1H	3411	1/1	0.98	0.03	101,101,101,101	0
56	MG	14	3388	1/1	0.98	0.07	80,80,80,80	0
56	MG	1H	3338	1/1	0.98	0.05	49,49,49,49	0
56	MG	1H	3501	1/1	0.98	0.04	70,70,70,70	0
56	MG	1H	3414	1/1	0.98	0.07	80,80,80,80	0
56	MG	1H	3503	1/1	0.98	0.04	115,115,115,115	0
56	MG	1H	3505	1/1	0.98	0.13	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3339	1/1	0.98	0.07	50,50,50,50	0
56	MG	1H	3509	1/1	0.98	0.03	82,82,82,82	0
56	MG	1H	3344	1/1	0.98	0.05	48,48,48,48	0
56	MG	1H	3419	1/1	0.98	0.05	53,53,53,53	0
56	MG	1J	209	1/1	0.98	0.06	94,94,94,94	0
56	MG	1H	3516	1/1	0.98	0.05	100,100,100,100	0
56	MG	1H	3420	1/1	0.98	0.05	65,65,65,65	0
56	MG	1H	3348	1/1	0.98	0.10	60,60,60,60	0
56	MG	14	3260	1/1	0.98	0.04	62,62,62,62	0
56	MG	14	3265	1/1	0.98	0.06	61,61,61,61	0
56	MG	14	3078	1/1	0.98	0.11	68,68,68,68	0
56	MG	1H	3423	1/1	0.98	0.04	93,93,93,93	0
56	MG	14	3270	1/1	0.98	0.04	75,75,75,75	0
56	MG	14	3271	1/1	0.98	0.05	63,63,63,63	0
56	MG	1H	3009	1/1	0.98	0.12	47,47,47,47	0
57	ZN	32	301	1/1	0.98	0.24	123,123,123,123	0
57	ZN	5A	101	1/1	0.98	0.04	160,160,160,160	0
56	MG	1H	3353	1/1	0.98	0.04	61,61,61,61	0
56	MG	1G	1700	1/1	0.99	0.03	126,126,126,126	0
56	MG	13	1716	1/1	0.99	0.05	89,89,89,89	0
56	MG	13	1731	1/1	0.99	0.05	69,69,69,69	0
56	MG	1H	3358	1/1	0.99	0.07	65,65,65,65	0
56	MG	14	3273	1/1	0.99	0.07	53,53,53,53	0
56	MG	1H	3408	1/1	0.99	0.03	58,58,58,58	0
56	MG	14	3275	1/1	0.99	0.02	71,71,71,71	0
56	MG	13	1722	1/1	0.99	0.11	94,94,94,94	0
56	MG	14	3277	1/1	0.99	0.03	67,67,67,67	0
56	MG	1H	3360	1/1	0.99	0.04	105,105,105,105	0
56	MG	14	3279	1/1	0.99	0.03	95,95,95,95	0
56	MG	14	3280	1/1	0.99	0.05	88,88,88,88	0
56	MG	13	1733	1/1	0.99	0.06	101,101,101,101	0
56	MG	1H	3413	1/1	0.99	0.03	71,71,71,71	0
56	MG	14	3283	1/1	0.99	0.03	57,57,57,57	0
56	MG	14	3285	1/1	0.99	0.03	57,57,57,57	0
56	MG	1H	3495	1/1	0.99	0.10	53,53,53,53	0
56	MG	14	3288	1/1	0.99	0.05	62,62,62,62	0
56	MG	1H	3362	1/1	0.99	0.04	72,72,72,72	0
56	MG	14	3290	1/1	0.99	0.03	61,61,61,61	0
56	MG	14	3291	1/1	0.99	0.04	54,54,54,54	0
56	MG	14	3292	1/1	0.99	0.03	90,90,90,90	0
56	MG	14	3293	1/1	0.99	0.04	68,68,68,68	0
56	MG	14	3294	1/1	0.99	0.05	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3497	1/1	0.99	0.05	51,51,51,51	0
56	MG	13	1734	1/1	0.99	0.07	87,87,87,87	0
56	MG	14	3298	1/1	0.99	0.04	59,59,59,59	0
56	MG	14	3299	1/1	0.99	0.04	82,82,82,82	0
56	MG	1H	3416	1/1	0.99	0.03	69,69,69,69	0
56	MG	14	3303	1/1	0.99	0.05	107,107,107,107	0
56	MG	1H	3500	1/1	0.99	0.03	80,80,80,80	0
56	MG	13	1717	1/1	0.99	0.05	105,105,105,105	0
56	MG	14	3306	1/1	0.99	0.03	49,49,49,49	0
56	MG	14	3307	1/1	0.99	0.06	70,70,70,70	0
56	MG	14	3308	1/1	0.99	0.04	68,68,68,68	0
56	MG	14	3309	1/1	0.99	0.04	86,86,86,86	0
56	MG	14	3310	1/1	0.99	0.04	78,78,78,78	0
56	MG	14	3311	1/1	0.99	0.04	82,82,82,82	0
56	MG	1H	3418	1/1	0.99	0.06	56,56,56,56	0
56	MG	1H	3340	1/1	0.99	0.03	41,41,41,41	0
56	MG	14	3314	1/1	0.99	0.05	64,64,64,64	0
56	MG	1H	3504	1/1	0.99	0.06	75,75,75,75	0
56	MG	14	3316	1/1	0.99	0.03	82,82,82,82	0
56	MG	1H	3341	1/1	0.99	0.04	49,49,49,49	0
56	MG	14	3318	1/1	0.99	0.03	63,63,63,63	0
56	MG	1H	3506	1/1	0.99	0.07	88,88,88,88	0
56	MG	14	3320	1/1	0.99	0.02	72,72,72,72	0
56	MG	1H	3507	1/1	0.99	0.06	94,94,94,94	0
56	MG	1H	3367	1/1	0.99	0.07	83,83,83,83	0
56	MG	1H	3368	1/1	0.99	0.04	76,76,76,76	0
56	MG	1H	3425	1/1	0.99	0.03	67,67,67,67	0
56	MG	1H	3426	1/1	0.99	0.08	53,53,53,53	0
56	MG	1H	3512	1/1	0.99	0.04	44,44,44,44	0
56	MG	1H	3513	1/1	0.99	0.03	58,58,58,58	0
56	MG	1H	3514	1/1	0.99	0.04	51,51,51,51	0
56	MG	1H	3515	1/1	0.99	0.03	46,46,46,46	0
56	MG	1H	3342	1/1	0.99	0.03	57,57,57,57	0
56	MG	14	3331	1/1	0.99	0.03	65,65,65,65	0
56	MG	14	3332	1/1	0.99	0.03	88,88,88,88	0
56	MG	1H	3370	1/1	0.99	0.05	51,51,51,51	0
56	MG	1H	3429	1/1	0.99	0.06	74,74,74,74	0
56	MG	1H	3519	1/1	0.99	0.09	94,94,94,94	0
56	MG	1H	3371	1/1	0.99	0.05	53,53,53,53	0
56	MG	13	1718	1/1	0.99	0.04	88,88,88,88	0
56	MG	1H	3373	1/1	0.99	0.07	63,63,63,63	0
56	MG	14	3339	1/1	0.99	0.04	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3434	1/1	0.99	0.03	72,72,72,72	0
56	MG	1H	3374	1/1	0.99	0.04	63,63,63,63	0
56	MG	14	3342	1/1	0.99	0.03	72,72,72,72	0
56	MG	14	3343	1/1	0.99	0.04	100,100,100,100	0
56	MG	14	3344	1/1	0.99	0.09	85,85,85,85	0
56	MG	14	3345	1/1	0.99	0.05	72,72,72,72	0
56	MG	14	3346	1/1	0.99	0.08	80,80,80,80	0
56	MG	14	3347	1/1	0.99	0.06	75,75,75,75	0
56	MG	1H	3526	1/1	0.99	0.02	46,46,46,46	0
56	MG	1H	3436	1/1	0.99	0.03	79,79,79,79	0
56	MG	1H	3437	1/1	0.99	0.16	82,82,82,82	0
56	MG	1H	3438	1/1	0.99	0.03	52,52,52,52	0
56	MG	1H	3375	1/1	0.99	0.05	75,75,75,75	0
56	MG	14	3353	1/1	0.99	0.07	99,99,99,99	0
56	MG	1H	3376	1/1	0.99	0.04	70,70,70,70	0
56	MG	1H	3346	1/1	0.99	0.07	64,64,64,64	0
56	MG	1H	3443	1/1	0.99	0.03	76,76,76,76	0
56	MG	14	3357	1/1	0.99	0.14	82,82,82,82	0
56	MG	1H	3444	1/1	0.99	0.04	97,97,97,97	0
56	MG	1H	3347	1/1	0.99	0.03	59,59,59,59	0
56	MG	1H	3446	1/1	0.99	0.05	84,84,84,84	0
56	MG	1H	3447	1/1	0.99	0.03	81,81,81,81	0
56	MG	14	3362	1/1	0.99	0.03	78,78,78,78	0
56	MG	1H	3448	1/1	0.99	0.09	68,68,68,68	0
56	MG	1H	3449	1/1	0.99	0.04	66,66,66,66	0
56	MG	16	211	1/1	0.99	0.03	84,84,84,84	0
56	MG	16	212	1/1	0.99	0.05	79,79,79,79	0
56	MG	1H	3379	1/1	0.99	0.06	79,79,79,79	0
56	MG	14	3368	1/1	0.99	0.05	53,53,53,53	0
56	MG	14	3369	1/1	0.99	0.03	96,96,96,96	0
56	MG	13	1725	1/1	0.99	0.06	90,90,90,90	0
56	MG	1H	3453	1/1	0.99	0.04	91,91,91,91	0
56	MG	1H	3454	1/1	0.99	0.05	106,106,106,106	0
56	MG	1H	3382	1/1	0.99	0.03	60,60,60,60	0
56	MG	14	3374	1/1	0.99	0.04	57,57,57,57	0
56	MG	14	3375	1/1	0.99	0.04	61,61,61,61	0
56	MG	14	3376	1/1	0.99	0.03	65,65,65,65	0
56	MG	13	1714	1/1	0.99	0.03	62,62,62,62	0
56	MG	1H	3385	1/1	0.99	0.03	66,66,66,66	0
56	MG	1H	3458	1/1	0.99	0.08	109,109,109,109	0
56	MG	1H	3459	1/1	0.99	0.06	64,64,64,64	0
56	MG	1H	3460	1/1	0.99	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3350	1/1	0.99	0.04	43,43,43,43	0
56	MG	1H	3462	1/1	0.99	0.06	81,81,81,81	0
56	MG	1H	3463	1/1	0.99	0.03	82,82,82,82	0
56	MG	1H	3351	1/1	0.99	0.03	50,50,50,50	0
56	MG	14	3062	1/1	0.99	0.05	69,69,69,69	0
56	MG	1H	3389	1/1	0.99	0.03	51,51,51,51	0
56	MG	13	1720	1/1	0.99	0.04	66,66,66,66	0
56	MG	1H	3467	1/1	0.99	0.06	86,86,86,86	0
56	MG	1H	3391	1/1	0.99	0.03	53,53,53,53	0
56	MG	1H	3392	1/1	0.99	0.05	42,42,42,42	0
56	MG	1H	3470	1/1	0.99	0.04	98,98,98,98	0
56	MG	1H	3396	1/1	0.99	0.12	79,79,79,79	0
56	MG	1H	3354	1/1	0.99	0.05	61,61,61,61	0
56	MG	1H	3474	1/1	0.99	0.03	91,91,91,91	0
56	MG	1H	3399	1/1	0.99	0.02	67,67,67,67	0
56	MG	1H	3476	1/1	0.99	0.09	65,65,65,65	0
56	MG	1H	3477	1/1	0.99	0.04	82,82,82,82	0
56	MG	1H	3400	1/1	0.99	0.03	68,68,68,68	0
56	MG	1H	3479	1/1	0.99	0.18	67,67,67,67	0
56	MG	1H	3401	1/1	0.99	0.08	50,50,50,50	0
56	MG	1H	3481	1/1	0.99	0.11	79,79,79,79	0
56	MG	1H	3402	1/1	0.99	0.04	49,49,49,49	0
56	MG	13	1728	1/1	0.99	0.04	95,95,95,95	0
56	MG	14	3261	1/1	0.99	0.03	54,54,54,54	0
56	MG	14	3263	1/1	0.99	0.05	60,60,60,60	0
56	MG	14	3264	1/1	0.99	0.04	53,53,53,53	0
57	ZN	5I	101	1/1	0.99	0.03	111,111,111,111	0
56	MG	1G	1698	1/1	0.99	0.04	91,91,91,91	0
56	MG	1H	3486	1/1	0.99	0.06	61,61,61,61	0
56	MG	14	3267	1/1	0.99	0.03	67,67,67,67	0
56	MG	14	3268	1/1	0.99	0.05	64,64,64,64	0
56	MG	1H	3452	1/1	1.00	0.04	69,69,69,69	0
56	MG	14	3286	1/1	1.00	0.03	58,58,58,58	0
56	MG	1H	3387	1/1	1.00	0.03	57,57,57,57	0
56	MG	13	1735	1/1	1.00	0.05	77,77,77,77	0
56	MG	1H	3345	1/1	1.00	0.03	47,47,47,47	0
56	MG	1H	3403	1/1	1.00	0.02	48,48,48,48	0
56	MG	14	3262	1/1	1.00	0.02	88,88,88,88	0
56	MG	1H	3381	1/1	1.00	0.07	46,46,46,46	0
56	MG	1H	3525	1/1	1.00	0.03	43,43,43,43	0
56	MG	13	1736	1/1	1.00	0.07	86,86,86,86	0
56	MG	1H	3421	1/1	1.00	0.08	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3296	1/1	1.00	0.04	53,53,53,53	0
56	MG	1H	3440	1/1	1.00	0.02	63,63,63,63	0
56	MG	1H	3482	1/1	1.00	0.05	66,66,66,66	0
56	MG	1G	1689	1/1	1.00	0.04	80,80,80,80	0
56	MG	14	3300	1/1	1.00	0.02	47,47,47,47	0
56	MG	1H	3383	1/1	1.00	0.09	48,48,48,48	0
56	MG	14	3302	1/1	1.00	0.03	73,73,73,73	0
56	MG	1H	3393	1/1	1.00	0.03	44,44,44,44	0
56	MG	1H	3485	1/1	1.00	0.03	81,81,81,81	0
56	MG	1H	3424	1/1	1.00	0.03	49,49,49,49	0
56	MG	1H	3394	1/1	1.00	0.02	54,54,54,54	0
56	MG	1H	3409	1/1	1.00	0.02	83,83,83,83	0
56	MG	I8	102	1/1	1.00	0.06	67,67,67,67	0
56	MG	1H	3395	1/1	1.00	0.02	48,48,48,48	0
56	MG	1H	3352	1/1	1.00	0.03	43,43,43,43	0
56	MG	13	1730	1/1	1.00	0.10	75,75,75,75	0
56	MG	1H	3398	1/1	1.00	0.03	63,63,63,63	0
56	MG	1H	3343	1/1	1.00	0.02	48,48,48,48	0
56	MG	1H	3432	1/1	1.00	0.03	83,83,83,83	0
56	MG	1H	3472	1/1	1.00	0.04	61,61,61,61	0
56	MG	14	3284	1/1	1.00	0.02	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.