



wwPDB X-ray Structure Validation Summary Report

Jan 6, 2024 – 10:50 pm GMT

PDB ID : 6GSJ
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet} and cognate tRNA^{Thr} in the A-site
Authors : Rozov, A.; Yusupov, M.; Yusupova, G.
Deposited on : 2018-06-14
Resolution : 2.96 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

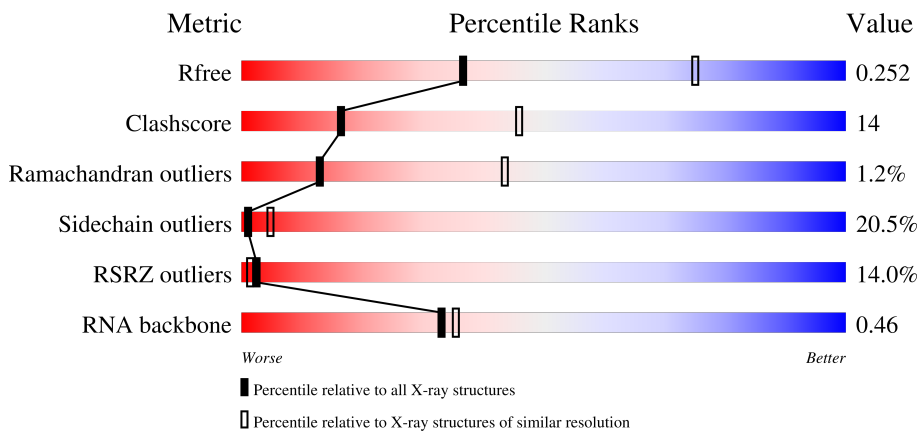
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 Å.

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



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

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

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

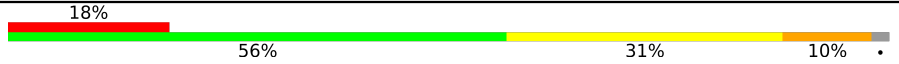
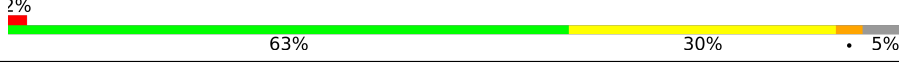
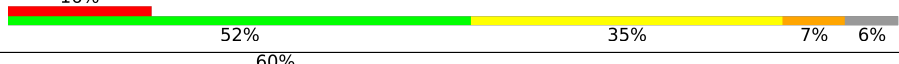


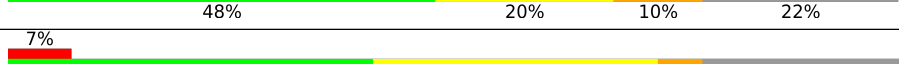
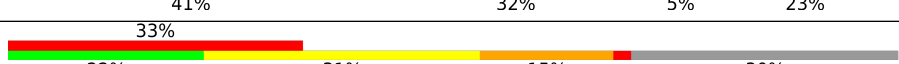
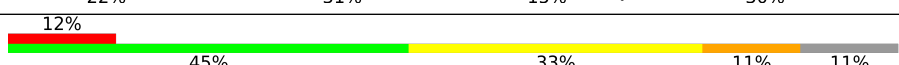
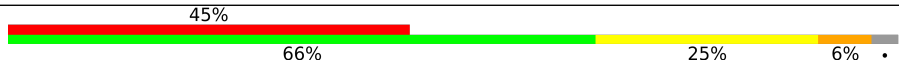

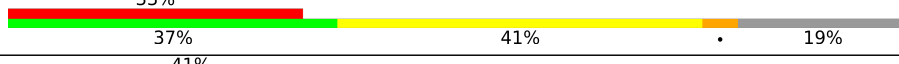

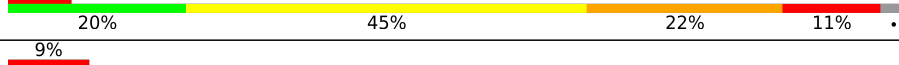

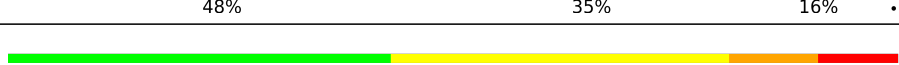
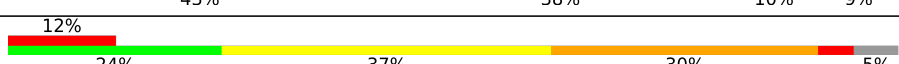
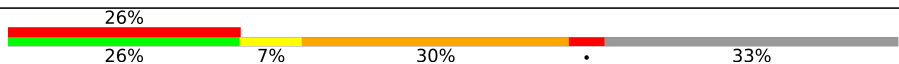
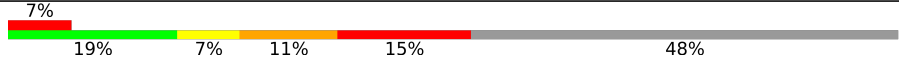
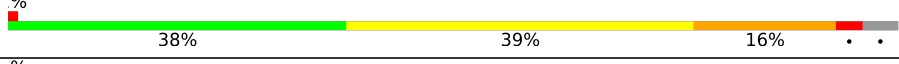






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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
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	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	11	276	


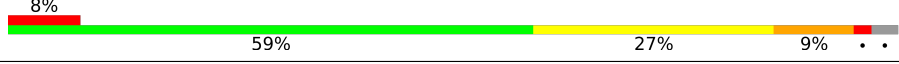
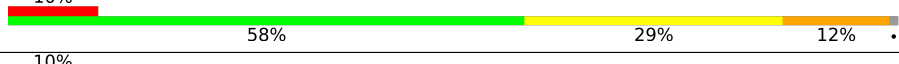


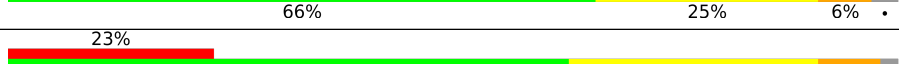
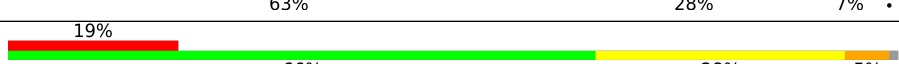
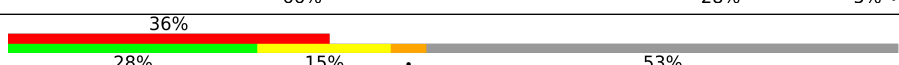
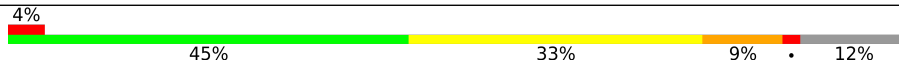
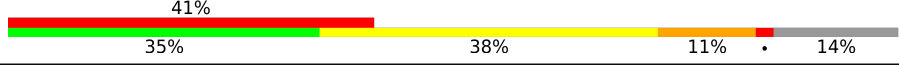
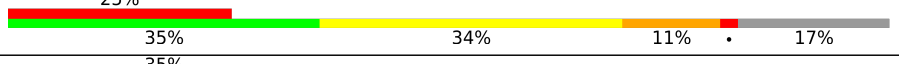
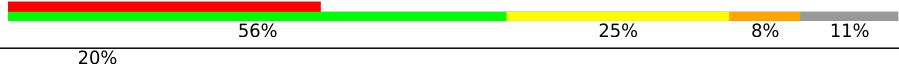


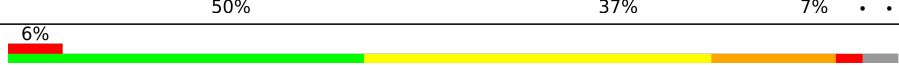
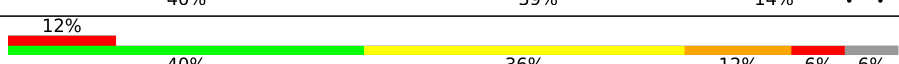


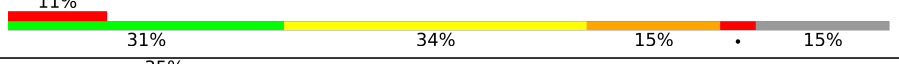
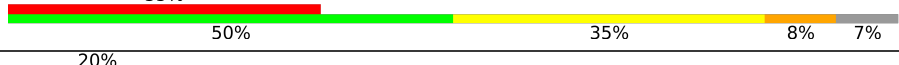





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Mol	Chain	Length	Quality of chain
28	19	276	34% 63% 28% 7%
29	21	206	20% 51% 37% 12%
29	29	206	21% 51% 35% 10%
30	31	210	19% 56% 35% 5%
30	39	210	25% 42% 42% 12%
31	41	182	12% 49% 38% 11%
31	49	182	34% 49% 37% 12%
32	51	180	3% 57% 28% 9%
32	59	180	41% 38% 42% 14% 6%
33	61	148	% 46% 39% 11%
33	69	148	2% 49% 40% 8%
34	15	140	51% 53% 34% 11%
34	58	140	29% 48% 36% 5% 11%
35	25	122	62% 62% 30% 8%
35	68	122	16% 73% 22% 5%
36	35	150	36% 45% 35% 17%
36	78	150	11% 42% 45% 8%
37	45	141	49% 50% 33% 14%
37	88	141	30% 53% 38% 9%
38	55	118	22% 49% 36% 14%
38	98	118	43% 43% 47% 9%
39	65	112	14% 34% 48% 16%
39	A8	112	19% 42% 46% 10%
40	75	146	25% 45% 40% 10%
40	B8	146	17% 41% 40% 12% 7%

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Mol	Chain	Length	Quality of chain
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	M8	71	
52	J5	60	
52	N8	60	
53	L5	49	
53	P8	49	

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Mol	Chain	Length	Quality of chain
54	M5	65	
54	Q8	65	
55	3L	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1665	-	-	-	X
56	MG	13	1685	-	-	-	X
56	MG	13	1686	-	-	-	X
56	MG	13	1689	-	-	-	X
56	MG	13	1696	-	-	-	X
56	MG	13	1706	-	-	-	X
56	MG	13	1710	-	-	-	X
56	MG	13	1712	-	-	-	X
56	MG	13	1725	-	-	-	X
56	MG	13	1763	-	-	-	X
56	MG	13	1764	-	-	-	X
56	MG	14	3178	-	-	-	X
56	MG	14	3179	-	-	-	X
56	MG	14	3191	-	-	-	X
56	MG	14	3245	-	-	-	X
56	MG	14	3262	-	-	-	X
56	MG	1G	1647	-	-	-	X
56	MG	1G	1667	-	-	-	X
56	MG	1G	1722	-	-	-	X
56	MG	1H	3046	-	-	-	X
56	MG	1H	3165	-	-	-	X
56	MG	1H	3196	-	-	-	X
56	MG	1H	3205	-	-	-	X
56	MG	1H	3219	-	-	-	X
56	MG	1H	3259	-	-	-	X
56	MG	1H	3264	-	-	-	X
56	MG	1H	3300	-	-	-	X
56	MG	1H	3332	-	-	-	X
56	MG	1H	3333	-	-	-	X
56	MG	1H	3370	-	-	-	X
56	MG	21	302	-	-	-	X
56	MG	78	202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	202	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 294252 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	13	1500	Total 32246	C 14352	N 5978	O 10416	P 1500	0	0	0
1	1G	1490	Total 32028	C 14255	N 5932	O 10351	P 1490	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	2E	205	Total 1605	C 1011	N 313	O 280	S 1	0	0	0
3	22	197	Total 1546	C 978	N 299	O 268	S 1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	94	Total	C	N	O	S	0	0	0
			749	468	147	133	1			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	4I	119	942	582	194	164	2	0	0	0
13	4A	109	879	544	181	152	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	5I	60	491	312	104	71	4	0	0	0
14	5A	59	486	309	103	70	4	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	69	Total	C	N	O	0	0	0
			554	355	106	93			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	AA	65	Total	C	N	O	S	0	0	0
			510	324	92	92	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			
20	BA	103	Total	C	N	O	S	0	0	0
			778	481	163	132	2			

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

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

- Molecule 22 is a RNA chain called tRNAThr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	74	Total	C	N	O	P	0	0	0
			1593	712	285	522	74			
22	1L	74	Total	C	N	O	P	0	0	0
			1593	712	285	522	74			

- Molecule 23 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	297	536	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1646	735	297	536	77	1			

- Molecule 24 is a RNA chain called tRNAThr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	72	Total	C	N	O	P	0	0	0
			1537	686	276	503	72			

- Molecule 25 is a RNA chain called RNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	18	Total	C	N	O	P	0	0	0
			391	176	80	117	18			
25	4L	14	Total	C	N	O	P	0	0	0
			303	137	63	89	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2850	Total	C	N	O	P	0	0	0
			61381	27319	11475	19737	2850			
26	14	2811	Total	C	N	O	P	0	0	0
			60561	26951	11337	19462	2811			

There are 14 discrepancies between the modelled and reference sequences:

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

- Molecule 27 is a RNA chain called 5S 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	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	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
			1556	984	297	269	6			
29	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	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	204	Total	C	N	O	S	0	0	0
			1602	1022	299	279	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
31	49	180	Total	C	N	O	S	0	0	0
			1459	931	266	258	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
			1328	842	249	236	1			
32	59	169	Total	C	N	O	S	0	0	0
			1295	823	241	230	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	61	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
33	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	125	Total	C	N	O	S	0	0	0
			995	645	183	163	4			
34	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	78	148	1127	701	230	193	3	0	0	0
36	35	147	1122	698	229	192	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	88	141	1117	712	211	187	7	0	0	0
37	45	138	1099	702	208	183	6	0	0	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				
39	A8	111	881	556	176	149		0	0	0
39	65	110	876	553	175	148		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	B8	136	1128	702	231	194	1	0	0	0
40	75	140	1164	723	238	202	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	C8	115	Total	C	N	O	S	0	0	0
			950	603	199	147	1			
41	85	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	D8	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			
42	95	100	Total	C	N	O	S	0	0	0
			770	496	140	133	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	G8	97	Total	C	N	O	S	0	0	0
			734	472	140	117	5			
45	C5	52	Total	C	N	O	S	0	0	0
			396	258	72	65	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	P8	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			
53	L5	48	Total	C	N	O	S	0	0	0
			406	249	100	55	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a RNA chain called tRNAThr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	3L	72	Total	C	N	O	P	0	0	0
			1538	687	276	503	72			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	205	Total	Mg	0	0
			205	205		
56	3E	1	Total	Mg	0	0
			1	1		
56	5E	1	Total	Mg	0	0
			1	1		
56	2I	1	Total	Mg	0	0
			1	1		
56	5I	2	Total	Mg	0	0
			2	2		

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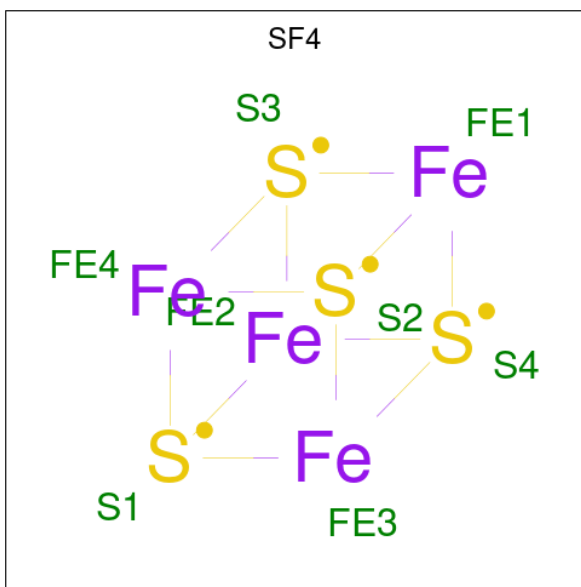
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	8I	1	Total Mg 1 1	0	0
56	BI	2	Total Mg 2 2	0	0
56	1K	1	Total Mg 1 1	0	0
56	2K	2	Total Mg 2 2	0	0
56	1H	622	Total Mg 622 622	0	0
56	16	15	Total Mg 15 15	0	0
56	11	1	Total Mg 1 1	0	0
56	21	4	Total Mg 4 4	0	0
56	31	2	Total Mg 2 2	0	0
56	41	1	Total Mg 1 1	0	0
56	68	2	Total Mg 2 2	0	0
56	78	2	Total Mg 2 2	0	0
56	88	3	Total Mg 3 3	0	0
56	98	1	Total Mg 1 1	0	0
56	D8	1	Total Mg 1 1	0	0
56	I8	2	Total Mg 2 2	0	0
56	P8	1	Total Mg 1 1	0	0
56	Q8	1	Total Mg 1 1	0	0
56	1G	155	Total Mg 155 155	0	0
56	42	1	Total Mg 1 1	0	0
56	2A	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	4A	1	Total Mg 1 1	0	0
56	9A	1	Total Mg 1 1	0	0
56	BA	2	Total Mg 2 2	0	0
56	1B	1	Total Mg 1 1	0	0
56	2L	2	Total Mg 2 2	0	0
56	4L	1	Total Mg 1 1	0	0
56	14	435	Total Mg 435 435	0	0
56	1J	6	Total Mg 6 6	0	0
56	19	1	Total Mg 1 1	0	0
56	29	3	Total Mg 3 3	0	0
56	39	1	Total Mg 1 1	0	0
56	25	1	Total Mg 1 1	0	0
56	35	3	Total Mg 3 3	0	0
56	45	2	Total Mg 2 2	0	0
56	55	1	Total Mg 1 1	0	0
56	85	1	Total Mg 1 1	0	0
56	E5	1	Total Mg 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	3E	1	Total	Fe S	0	0
			8	4 4		
57	32	1	Total	Fe S	0	0
			8	4 4		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	5I	1	Total	Zn	0	0
			1	1		
58	5A	1	Total	Zn	0	0
			1	1		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	13	339	Total	O	0	0
			339	339		
59	1E	1	Total	O	0	0
			1	1		
59	3E	2	Total	O	0	0
			2	2		
59	4E	2	Total	O	0	0
			2	2		
59	6E	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	8E	2	Total O 2 2	0	0
59	1I	3	Total O 3 3	0	0
59	3I	1	Total O 1 1	0	0
59	4I	2	Total O 2 2	0	0
59	5I	1	Total O 1 1	0	0
59	6I	1	Total O 1 1	0	0
59	7I	3	Total O 3 3	0	0
59	1F	2	Total O 2 2	0	0
59	1K	1	Total O 1 1	0	0
59	4K	2	Total O 2 2	0	0
59	1H	1047	Total O 1047 1047	0	0
59	16	19	Total O 19 19	0	0
59	11	11	Total O 11 11	0	0
59	21	8	Total O 8 8	0	0
59	31	7	Total O 7 7	0	0
59	58	3	Total O 3 3	0	0
59	78	6	Total O 6 6	0	0
59	D8	1	Total O 1 1	0	0
59	E8	1	Total O 1 1	0	0
59	G8	1	Total O 1 1	0	0
59	I8	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	J8	1	Total O 1 1	0	0
59	L8	4	Total O 4 4	0	0
59	P8	1	Total O 1 1	0	0
59	Q8	2	Total O 2 2	0	0
59	1G	289	Total O 289 289	0	0
59	32	2	Total O 2 2	0	0
59	42	1	Total O 1 1	0	0
59	52	4	Total O 4 4	0	0
59	1A	1	Total O 1 1	0	0
59	7A	4	Total O 4 4	0	0
59	9A	2	Total O 2 2	0	0
59	BA	2	Total O 2 2	0	0
59	2L	6	Total O 6 6	0	0
59	4L	3	Total O 3 3	0	0
59	14	730	Total O 730 730	0	0
59	19	10	Total O 10 10	0	0
59	29	2	Total O 2 2	0	0
59	39	5	Total O 5 5	0	0
59	15	1	Total O 1 1	0	0
59	25	6	Total O 6 6	0	0
59	35	6	Total O 6 6	0	0

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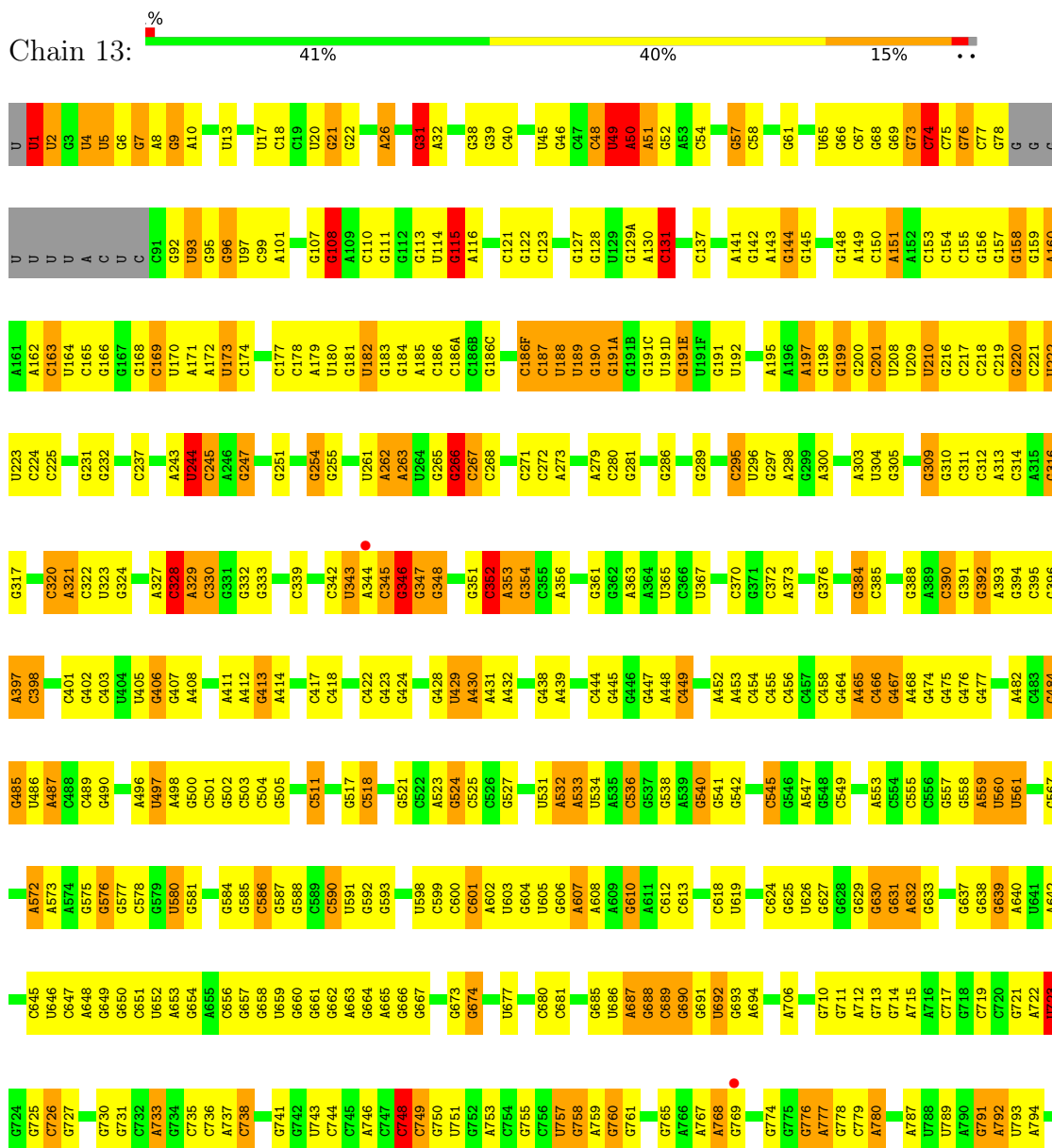
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	45	4	Total O 4 4	0	0
59	75	1	Total O 1 1	0	0
59	95	1	Total O 1 1	0	0
59	B5	3	Total O 3 3	0	0
59	H5	3	Total O 3 3	0	0
59	M5	2	Total O 2 2	0	0

3 Residue-property plots [i](#)

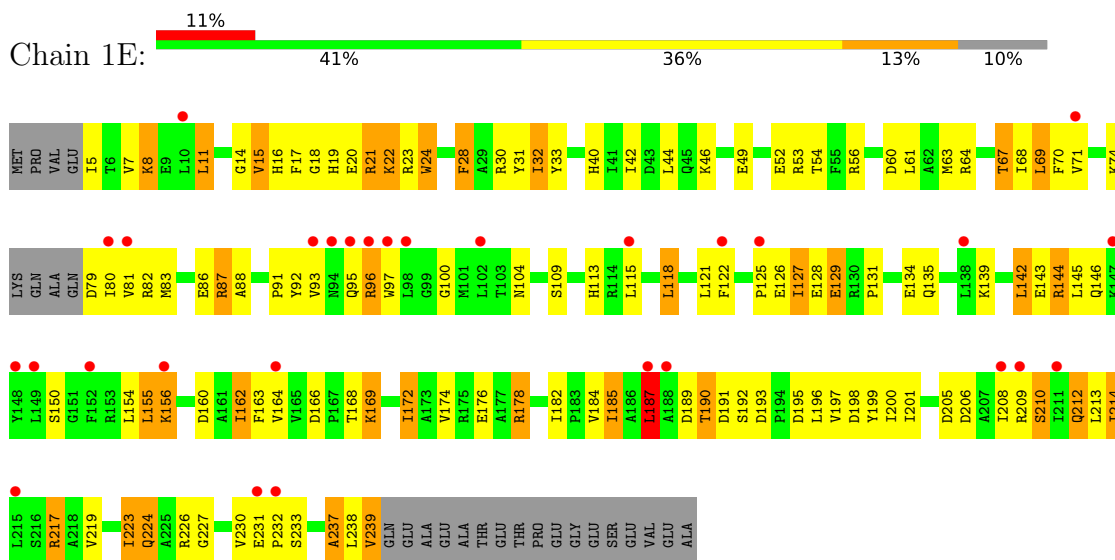
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S ribosomal RNA

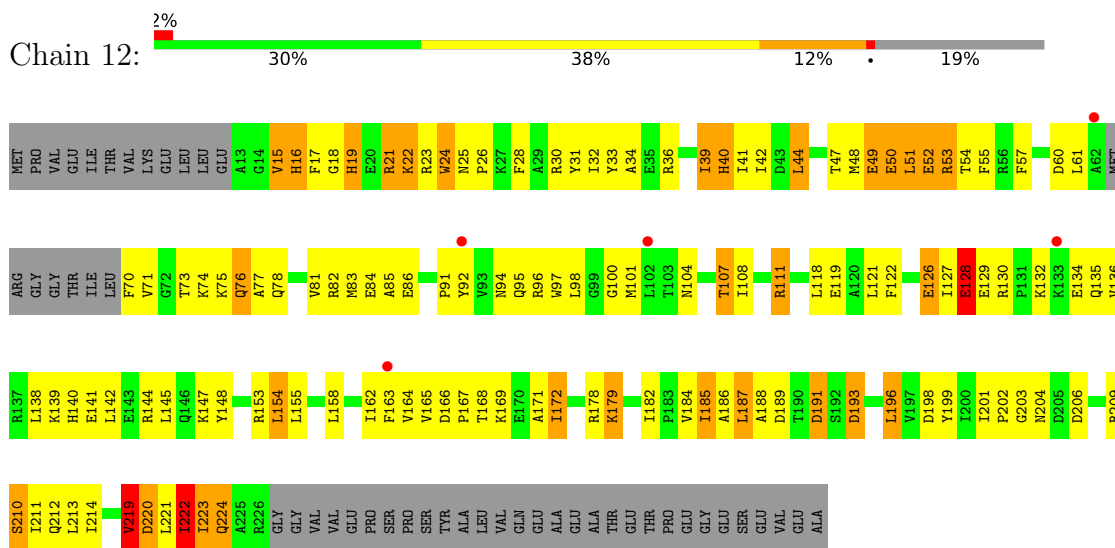




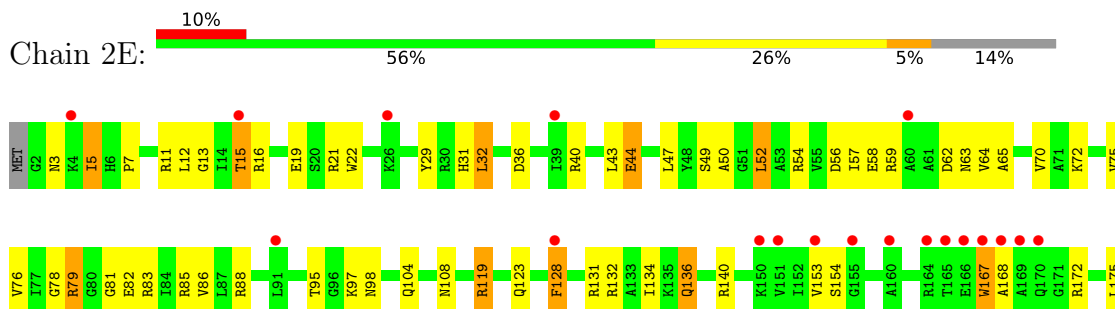
- Molecule 2: 30S ribosomal protein S2

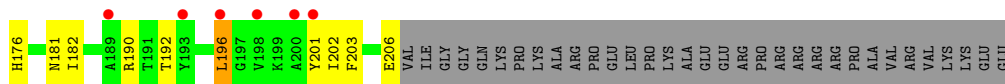


- Molecule 2: 30S ribosomal protein S2

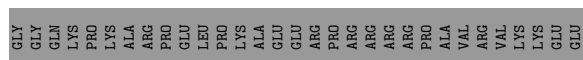
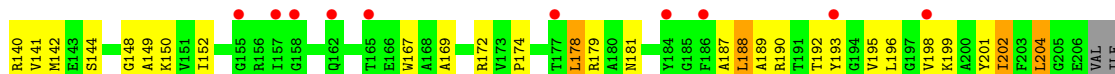
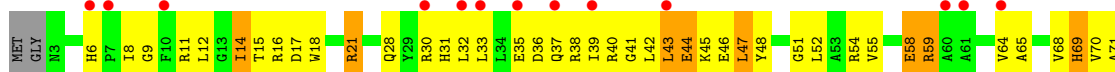


- Molecule 3: 30S ribosomal protein S3

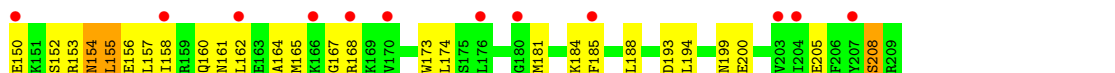
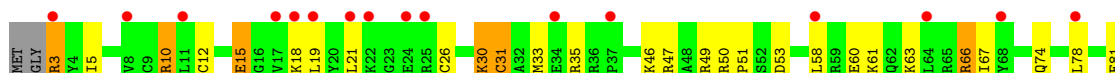




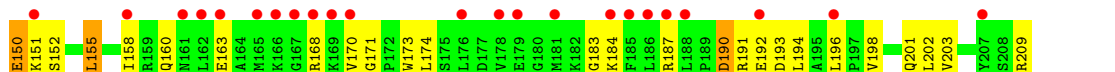
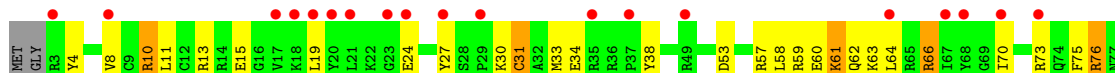
• Molecule 3: 30S ribosomal protein S3



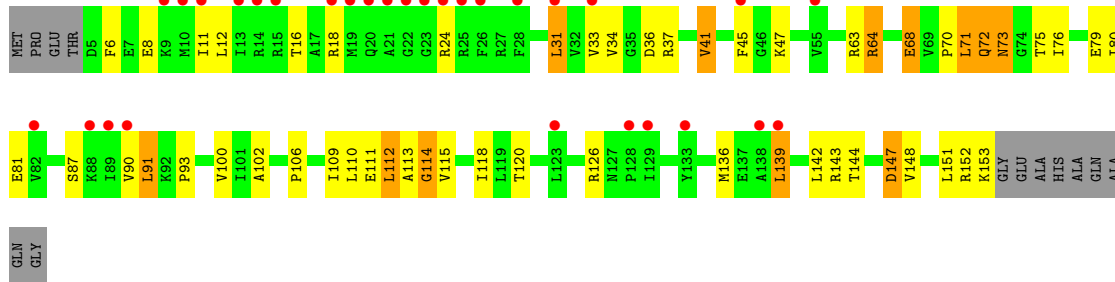
• Molecule 4: 30S ribosomal protein S4



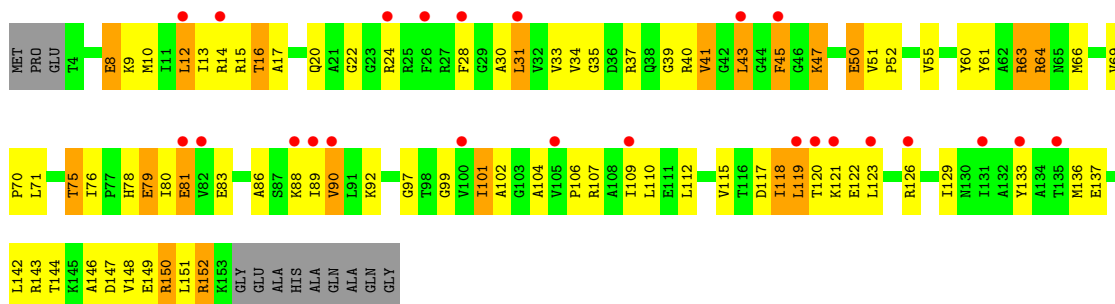
• Molecule 4: 30S ribosomal protein S4



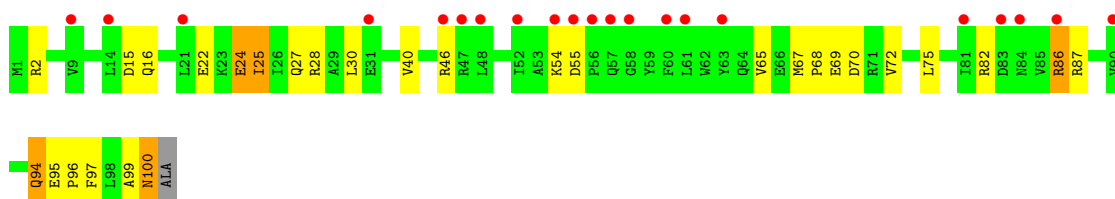
• Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

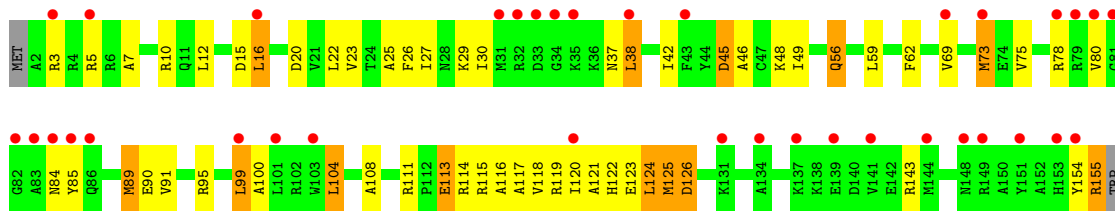


- Molecule 6: 30S ribosomal protein S6

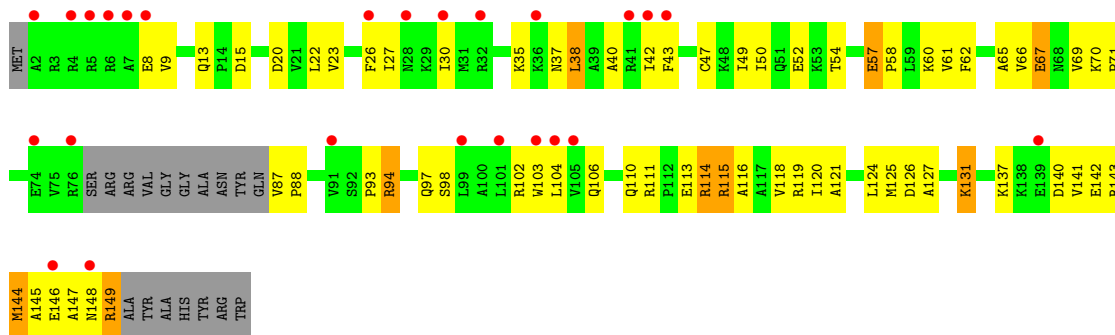


- Molecule 7: 30S ribosomal protein S7

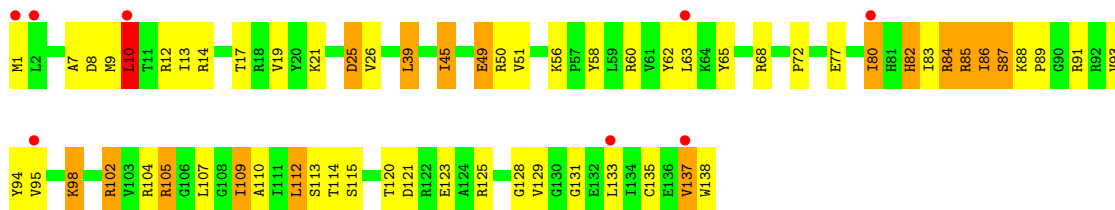




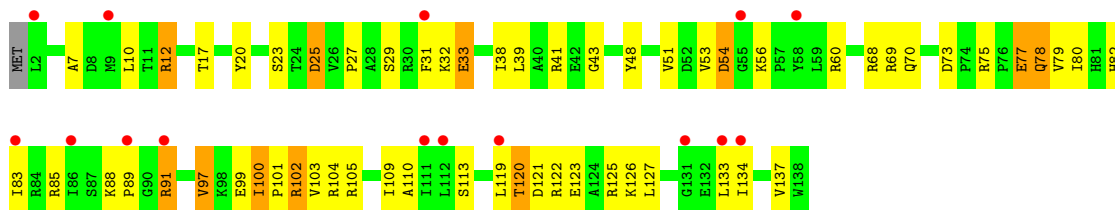
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

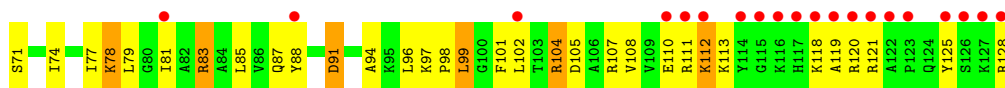


• Molecule 8: 30S ribosomal protein S8

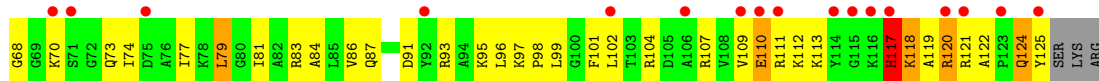
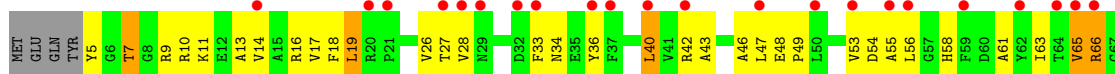


• Molecule 9: 30S ribosomal protein S9

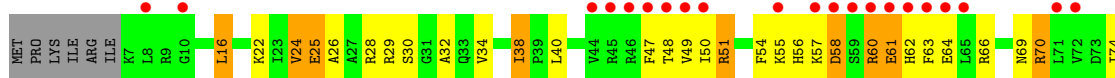




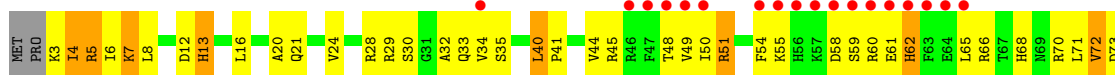
• Molecule 9: 30S ribosomal protein S9



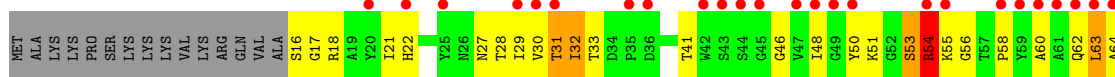
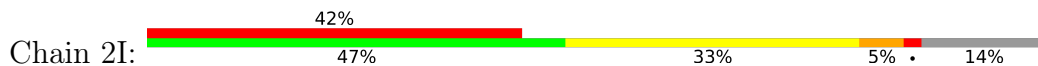
• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10

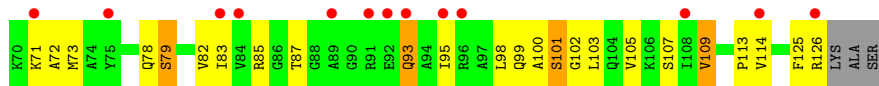


• Molecule 11: 30S ribosomal protein S11

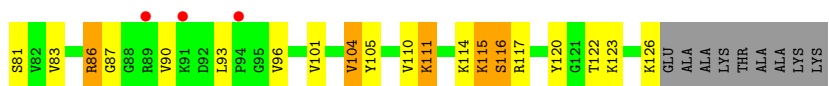
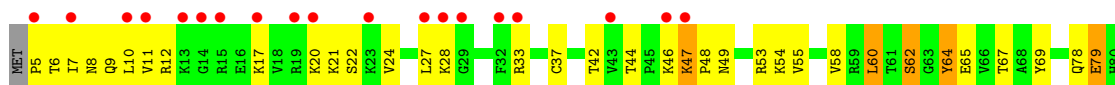


• Molecule 11: 30S ribosomal protein S11

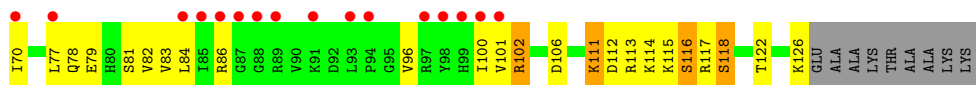
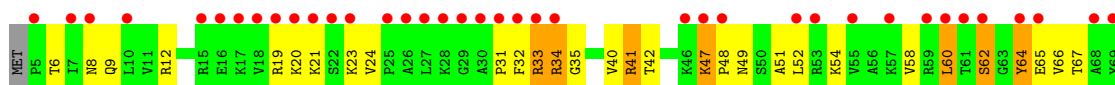
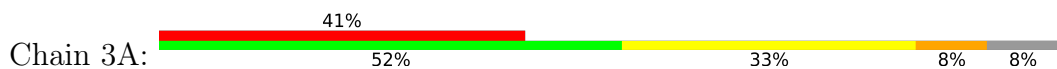




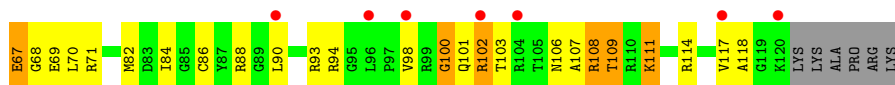
• Molecule 12: 30S ribosomal protein S12



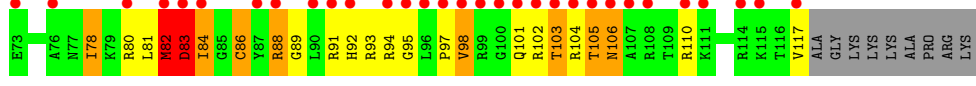
• Molecule 12: 30S ribosomal protein S12



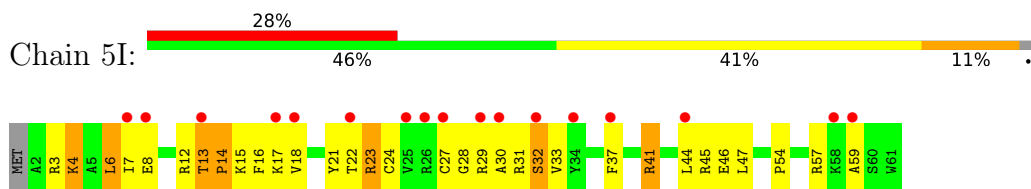
• Molecule 13: 30S ribosomal protein S13



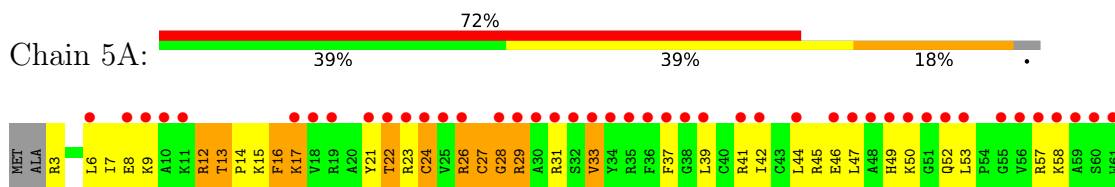
• Molecule 13: 30S ribosomal protein S13



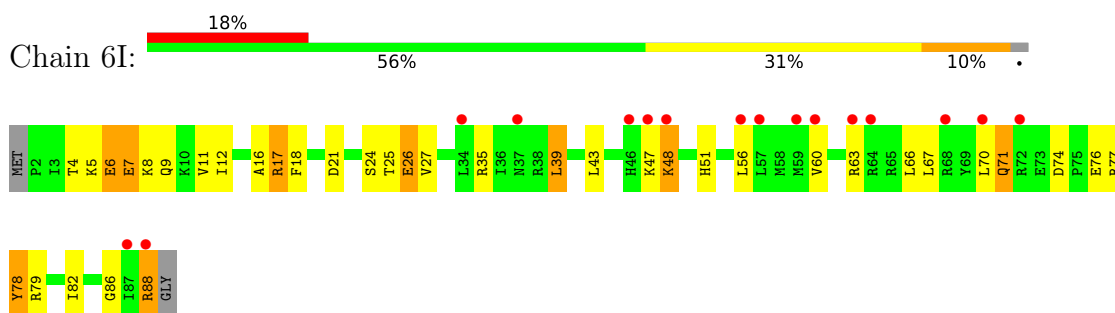
- Molecule 14: 30S ribosomal protein S14 type Z



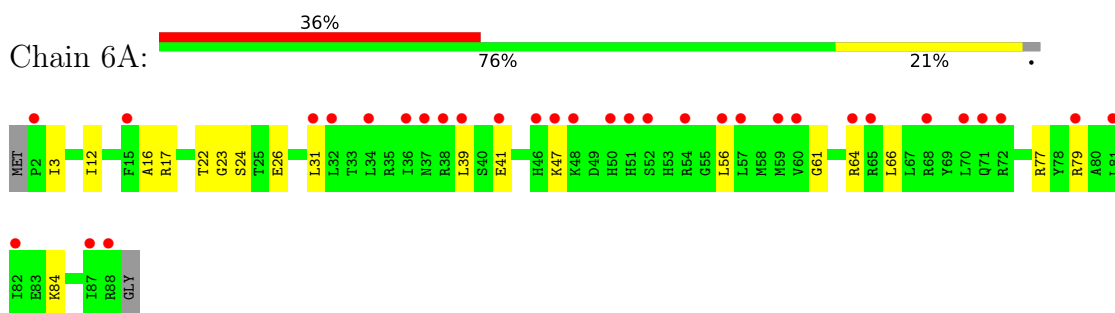
- Molecule 14: 30S ribosomal protein S14 type Z



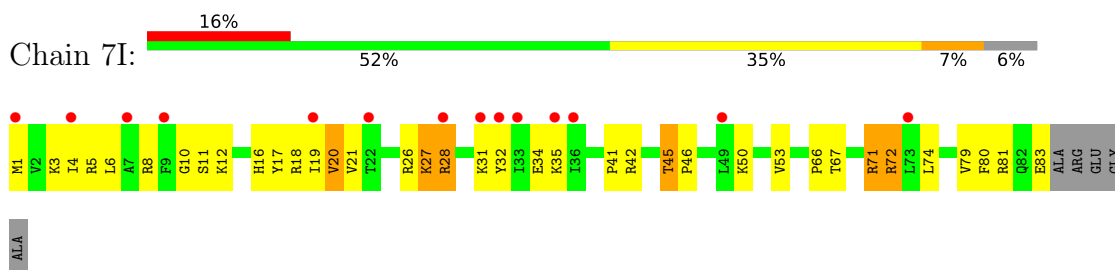
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

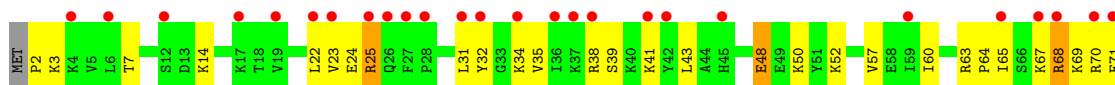


- Molecule 16: 30S ribosomal protein S16

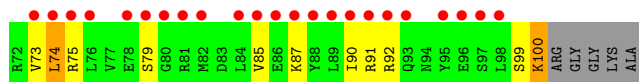
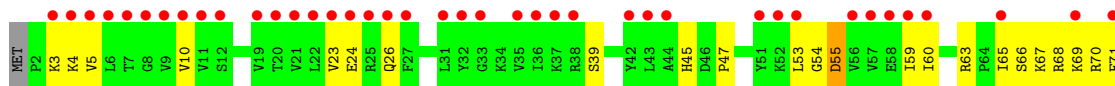




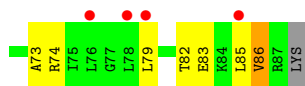
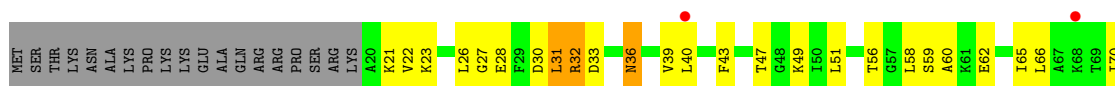
• Molecule 17: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

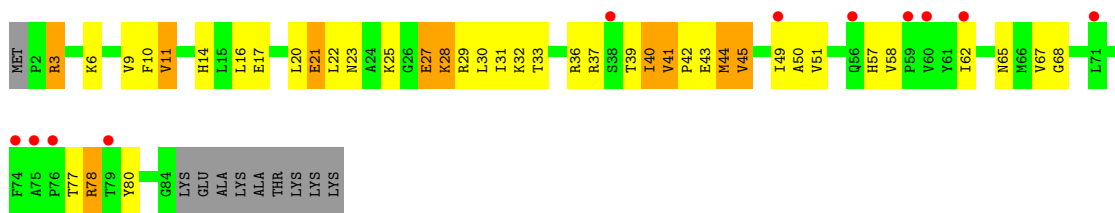


• Molecule 18: 30S ribosomal protein S18

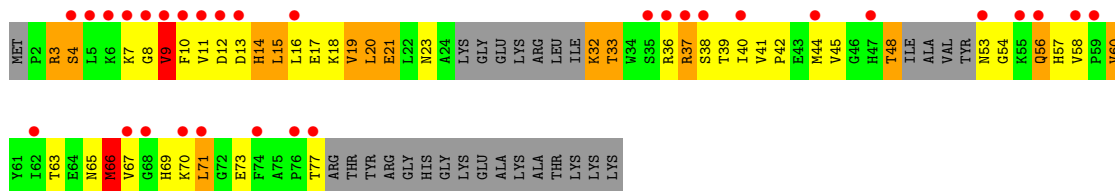
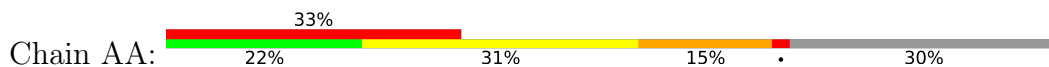


• Molecule 19: 30S ribosomal protein S19

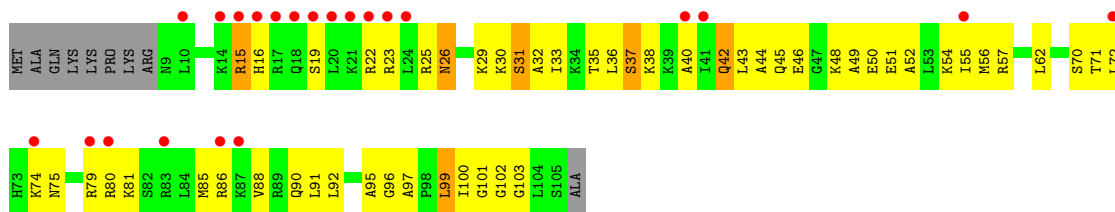
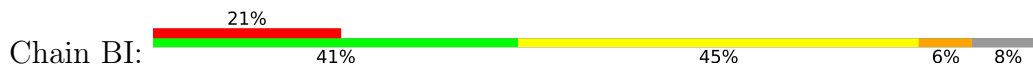




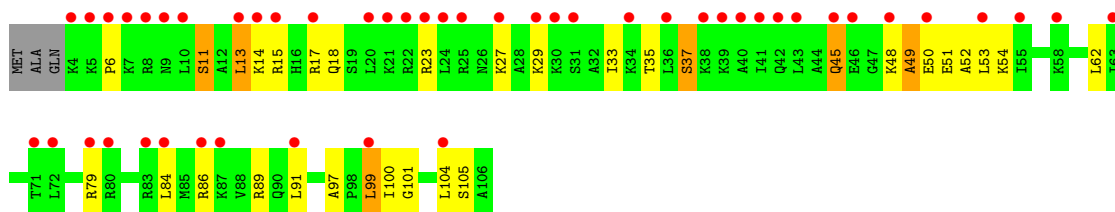
● Molecule 19: 30S ribosomal protein S19



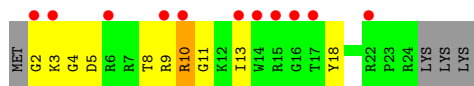
● Molecule 20: 30S ribosomal protein S20



● Molecule 20: 30S ribosomal protein S20

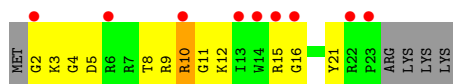


● Molecule 21: 30S ribosomal protein Thx

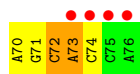
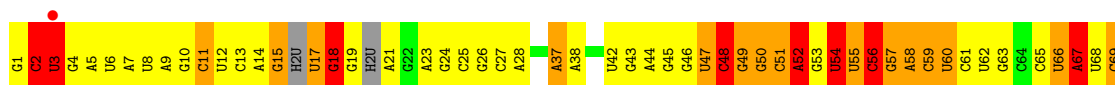
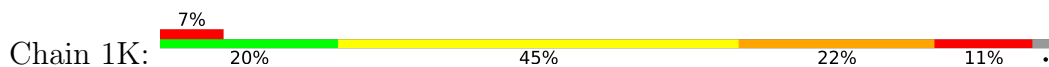


● Molecule 21: 30S ribosomal protein Thx

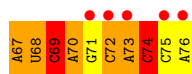
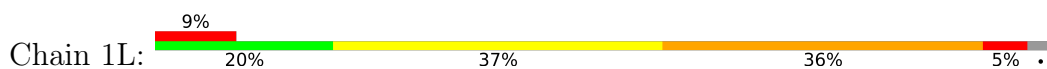




- Molecule 22: tRNATHr



- Molecule 22: tRNATHr



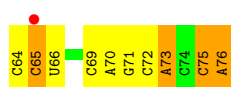
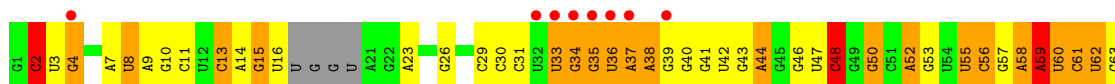
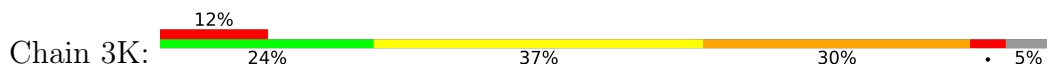
- Molecule 23: tRNAfMet



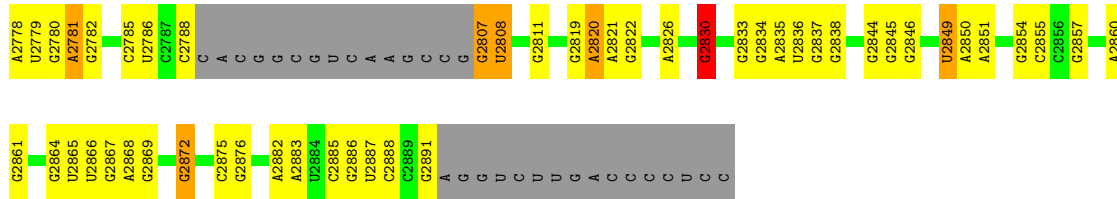
- Molecule 23: tRNAfMet



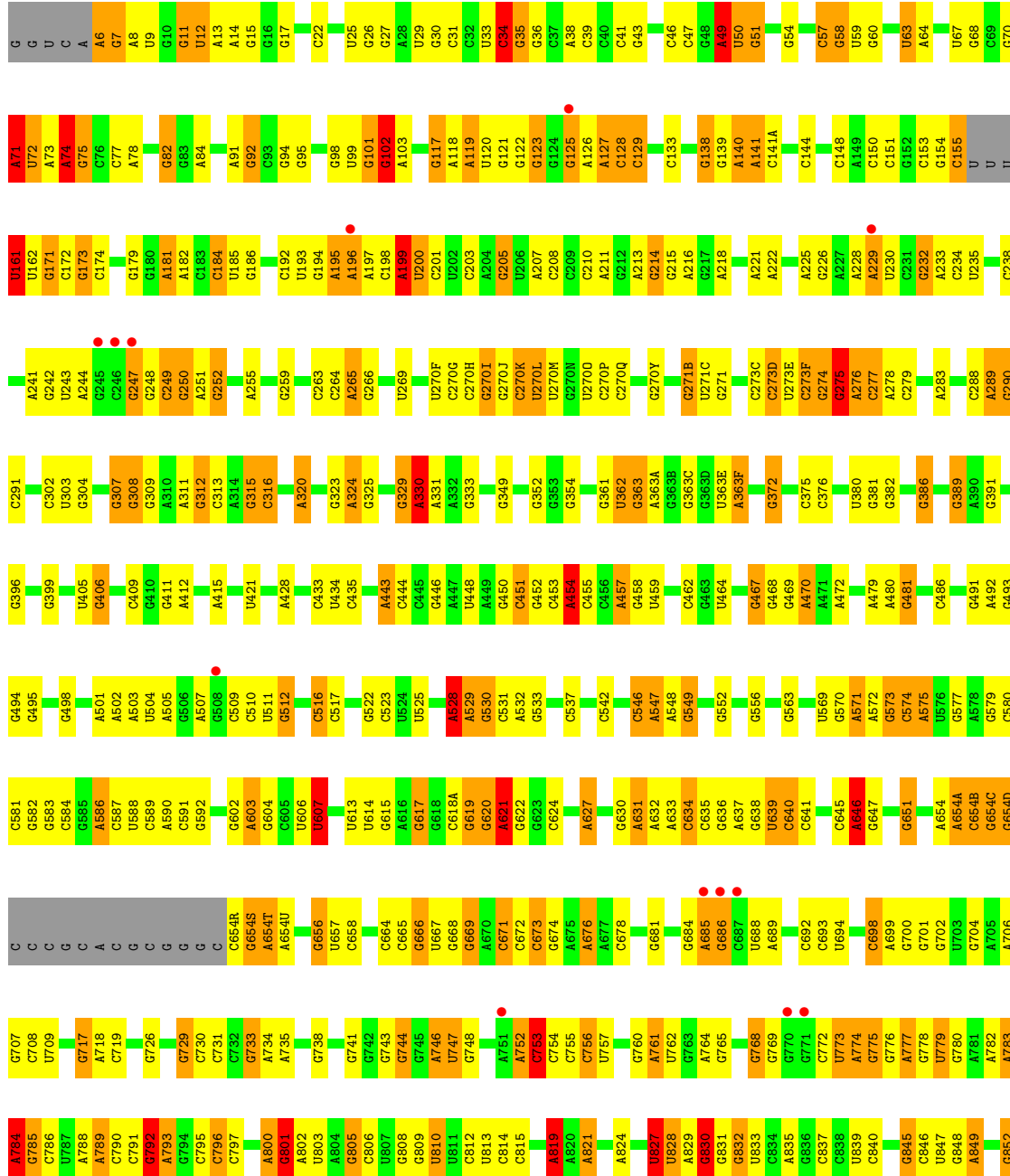
- Molecule 24: tRNATHr



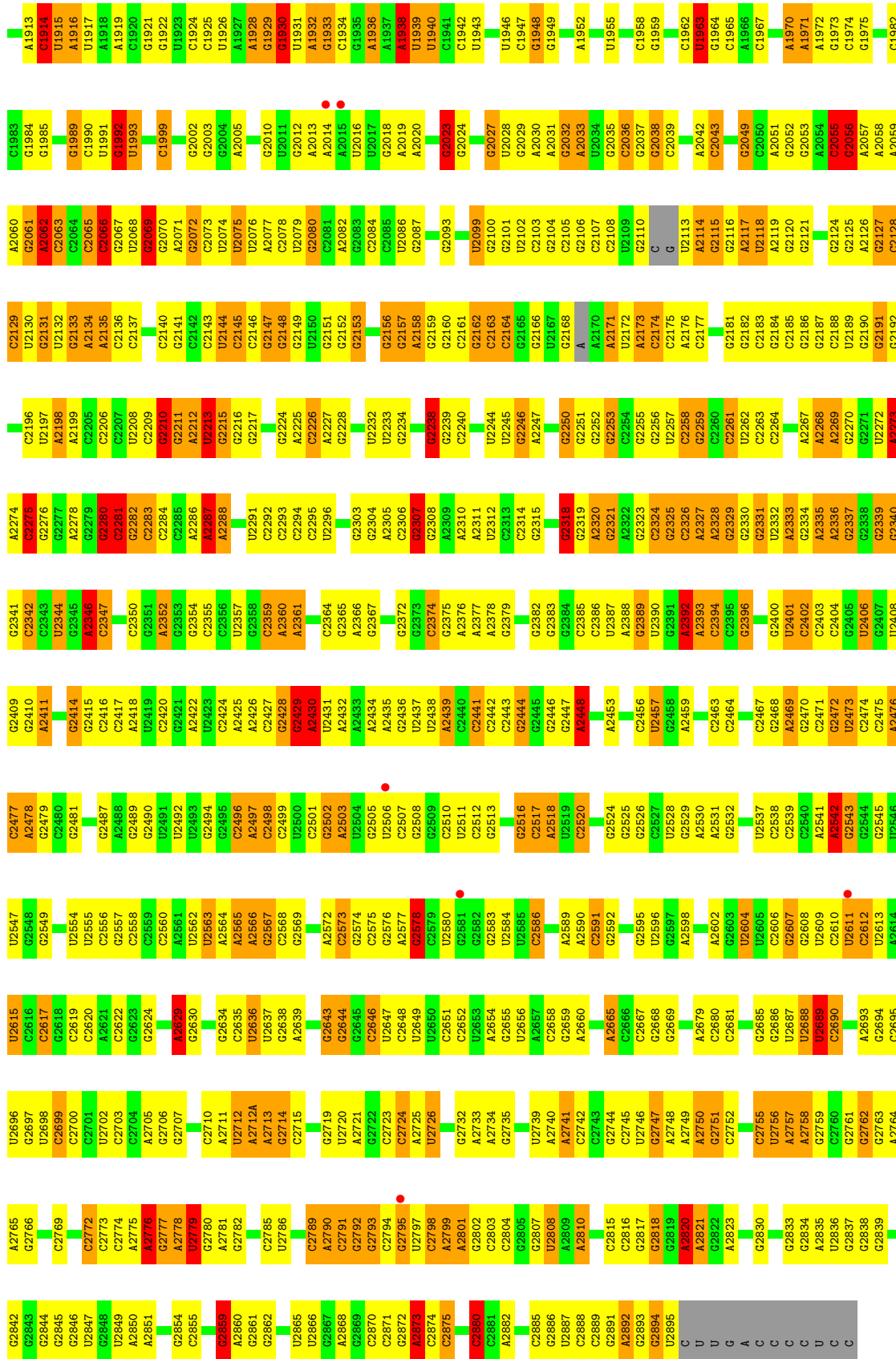
- Molecule 25: RNA (27-MER)



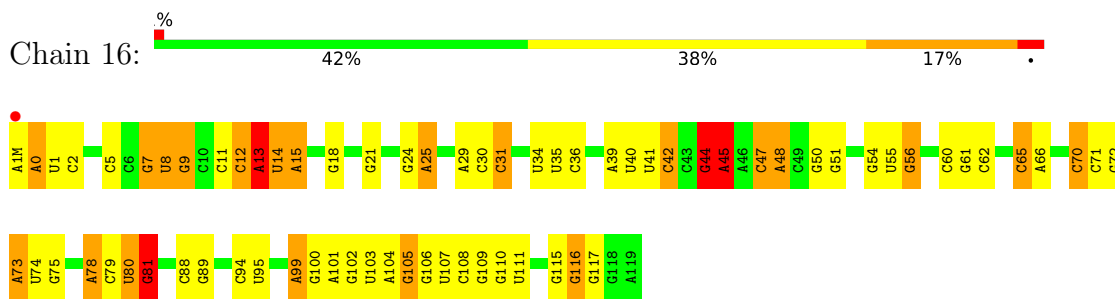
• Molecule 26: 23S ribosomal RNA



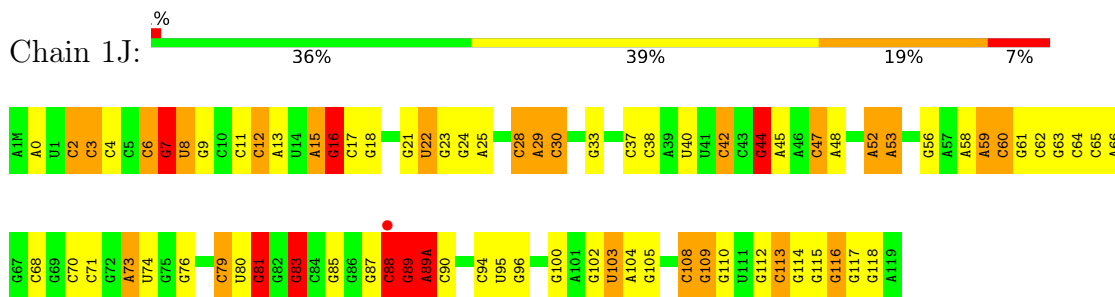
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U2005	G1707	G1707	G1475	U1396						
U2006	G1707	G1707	G1475	U1396						
U2007	G1707	G1707	G1475	U1396						
U2008	G1707	G1707	G1475	U1396						
U2009	G1707	G1707	G1475	U13						



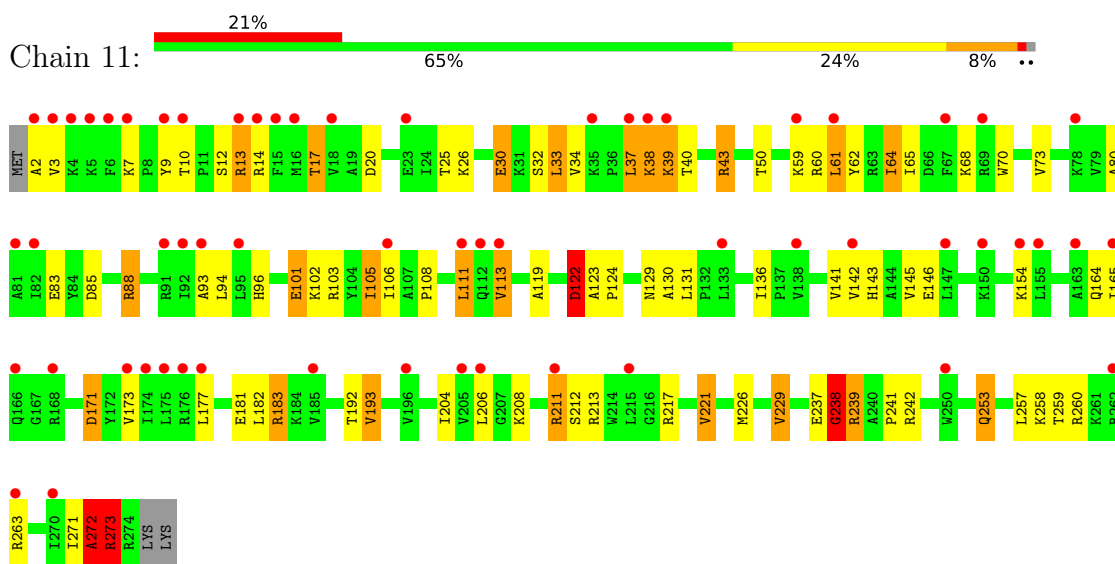
● Molecule 27: 5S ribosomal RNA



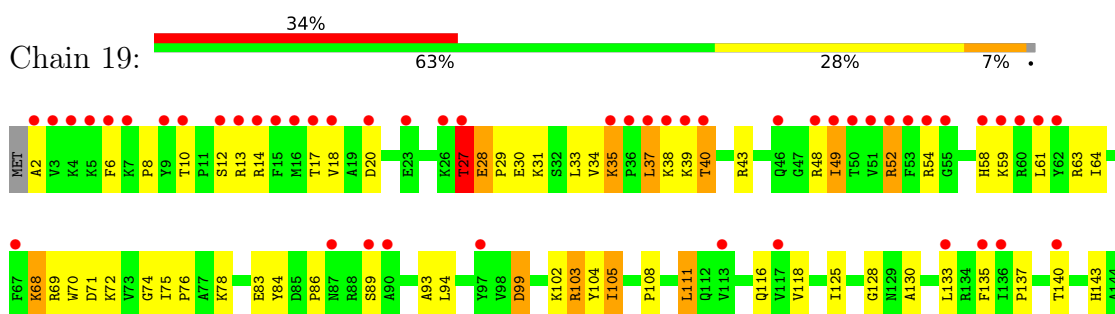
• Molecule 27: 5S ribosomal RNA

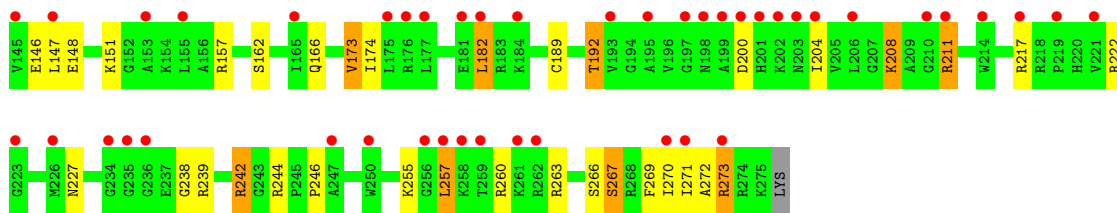


• Molecule 28: 50S ribosomal protein L2

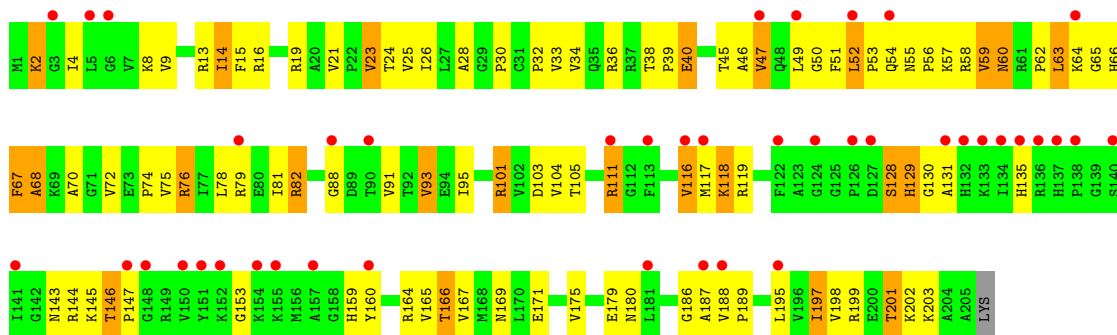


• Molecule 28: 50S ribosomal protein L2

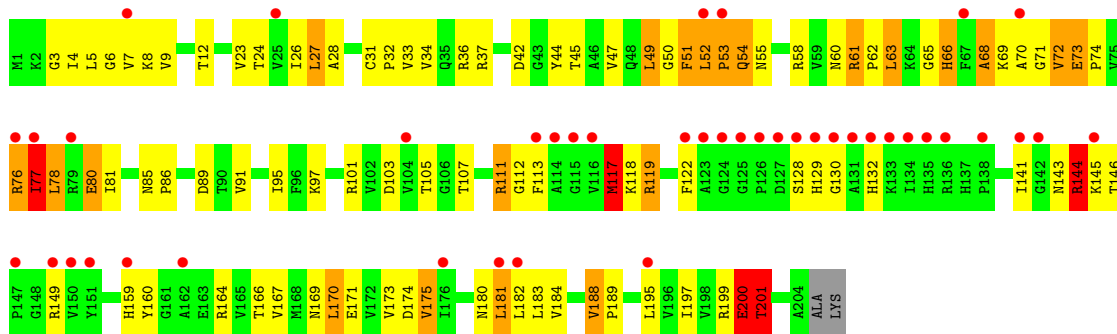




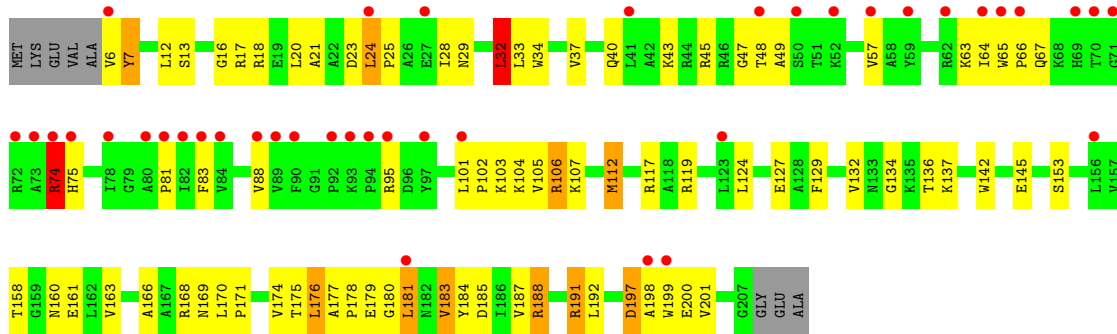
• Molecule 29: 50S ribosomal protein L3

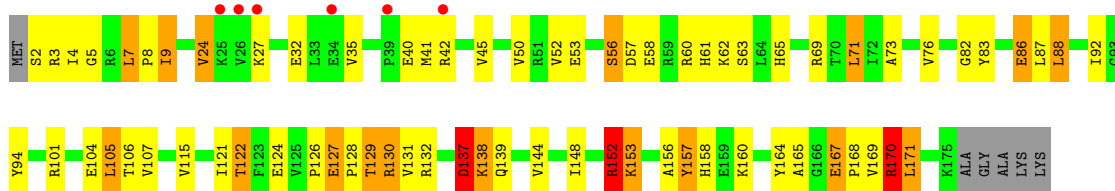


• Molecule 29: 50S ribosomal protein L3

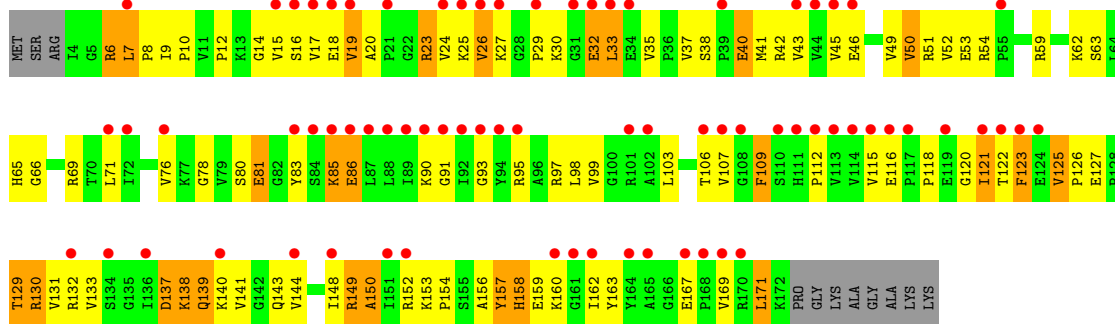
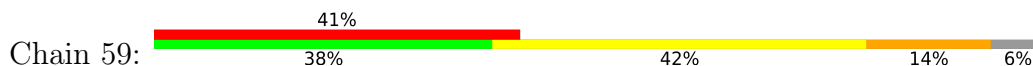


• Molecule 30: 50S ribosomal protein L4

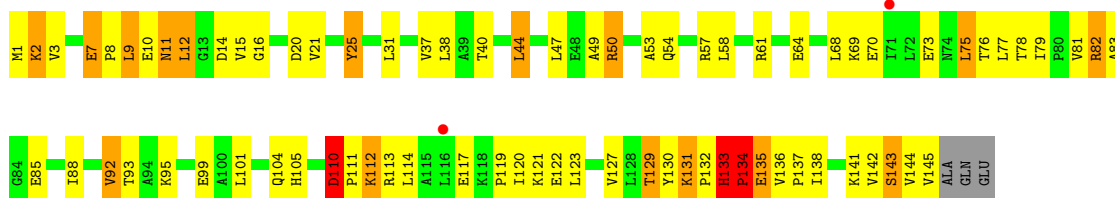




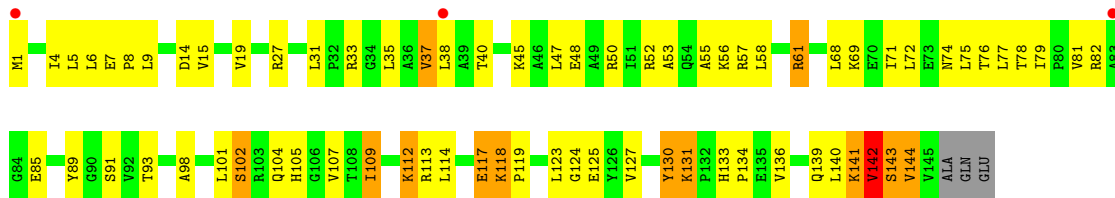
• Molecule 32: 50S ribosomal protein L6



• Molecule 33: 50S ribosomal protein L9

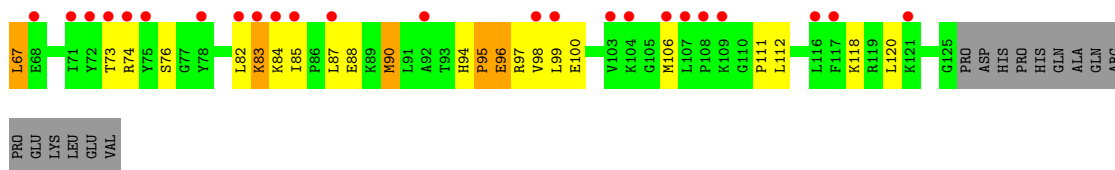


• Molecule 33: 50S ribosomal protein L9

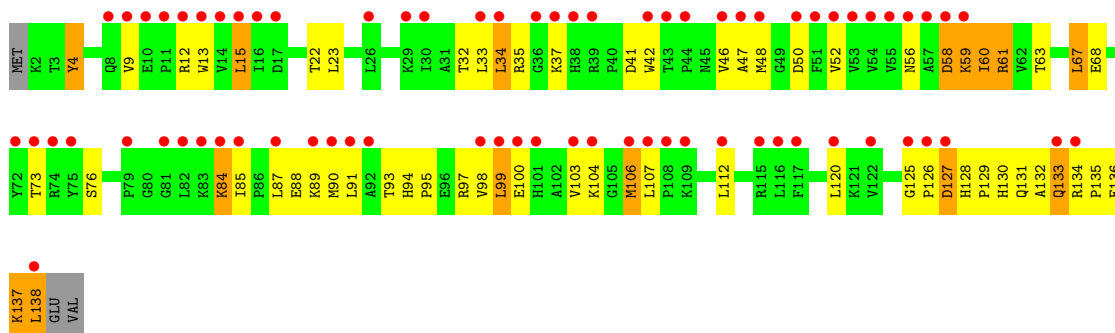


• Molecule 34: 50S ribosomal protein L13

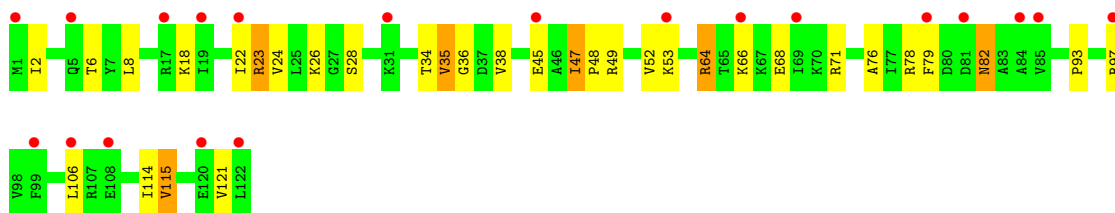
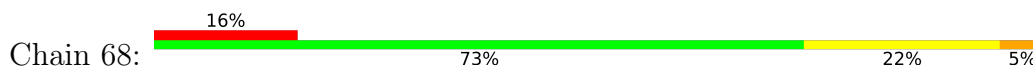




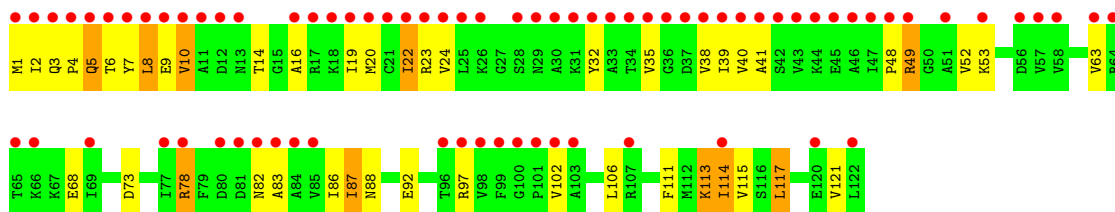
• Molecule 34: 50S ribosomal protein L13



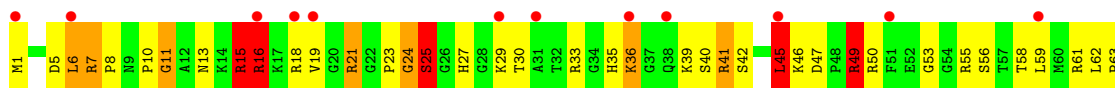
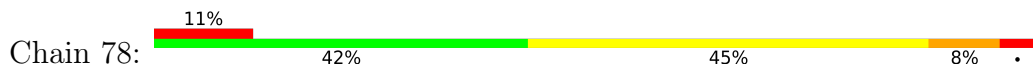
• Molecule 35: 50S ribosomal protein L14

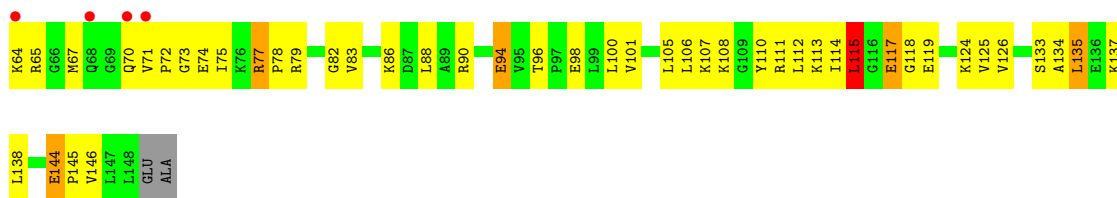


• Molecule 35: 50S ribosomal protein L14

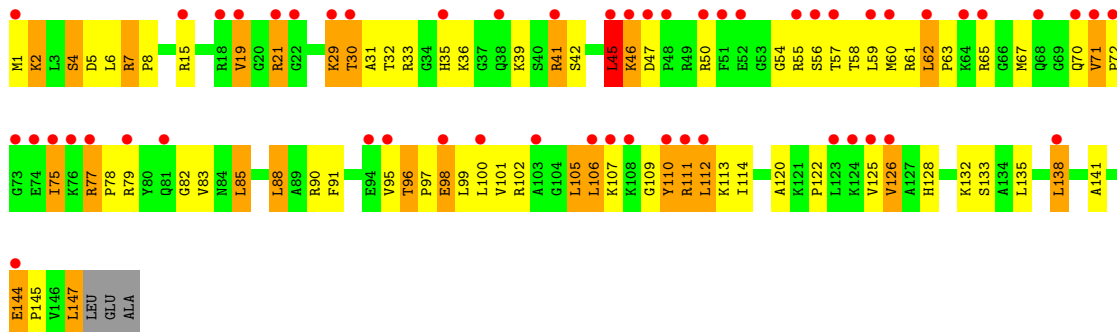


• Molecule 36: 50S ribosomal protein L15

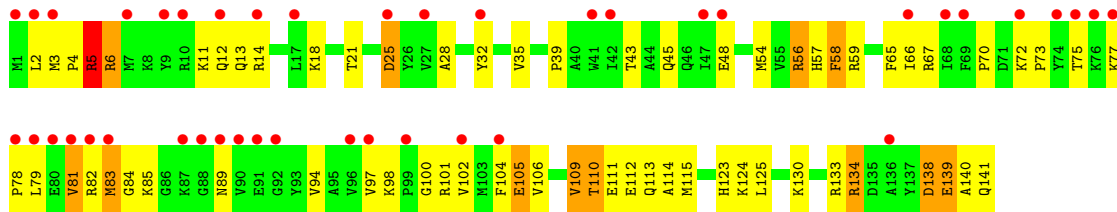




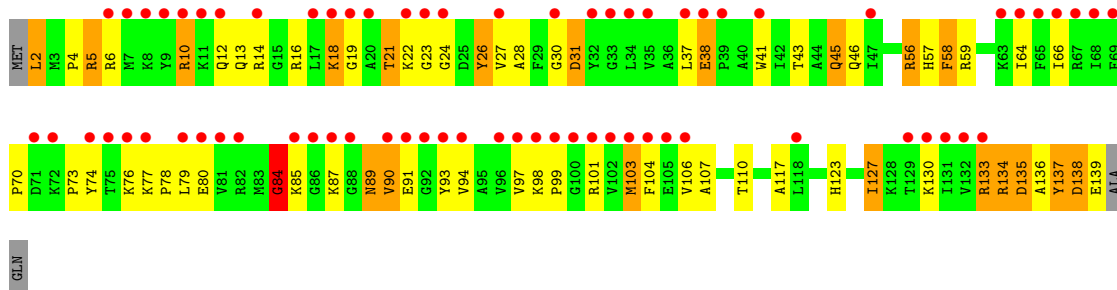
• Molecule 36: 50S ribosomal protein L15



• Molecule 37: 50S ribosomal protein L16

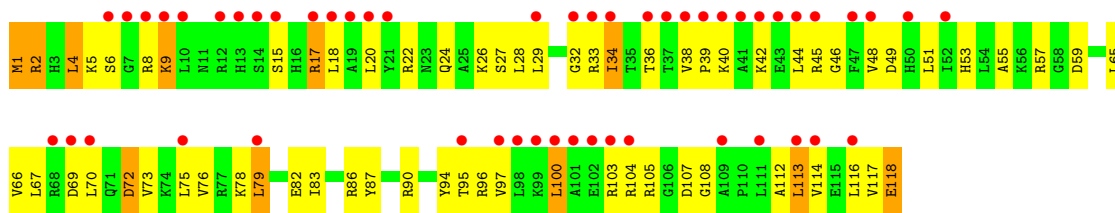


• Molecule 37: 50S ribosomal protein L16

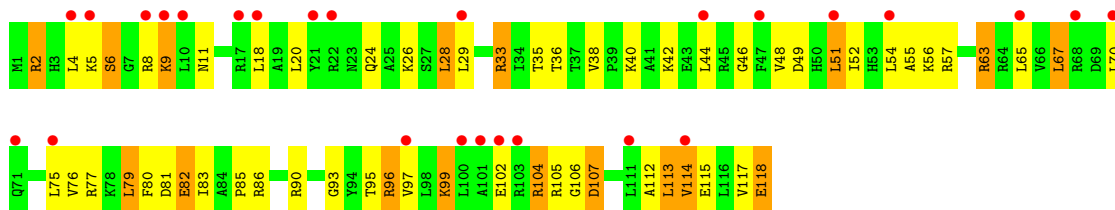


• Molecule 38: 50S ribosomal protein L17

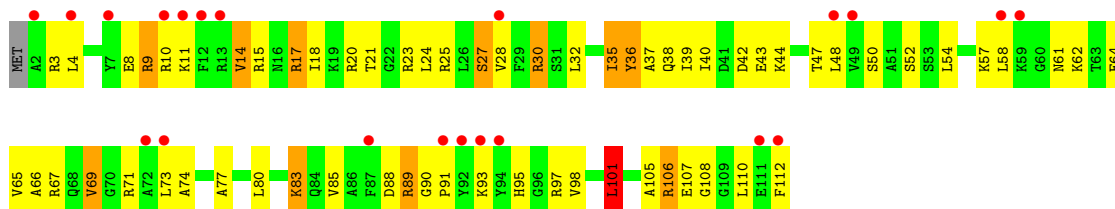
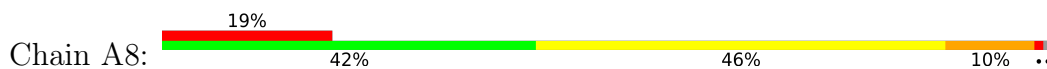




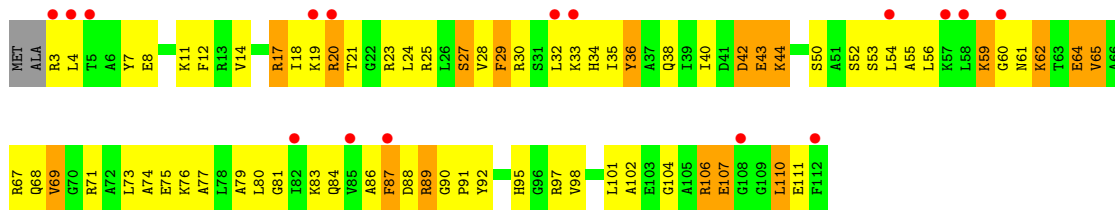
● Molecule 38: 50S ribosomal protein L17



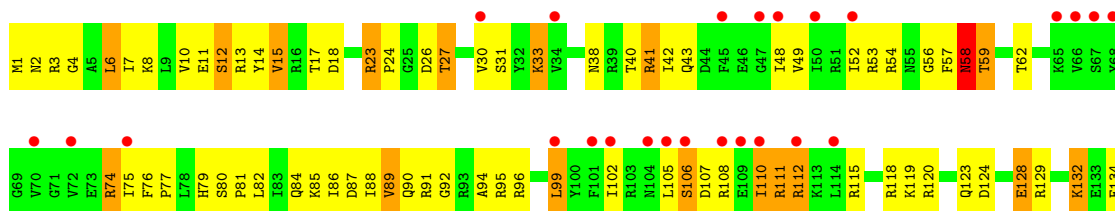
● Molecule 39: 50S ribosomal protein L18



● Molecule 39: 50S ribosomal protein L18

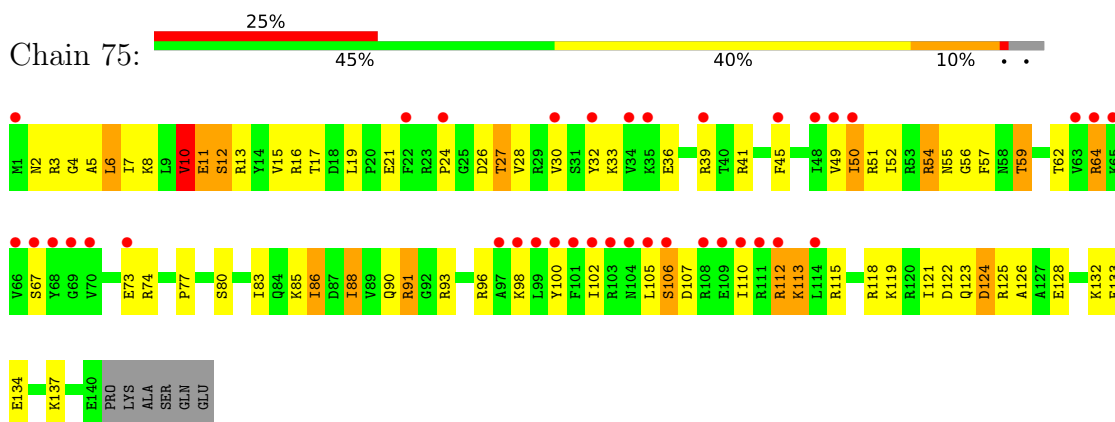


● Molecule 40: 50S ribosomal protein L19

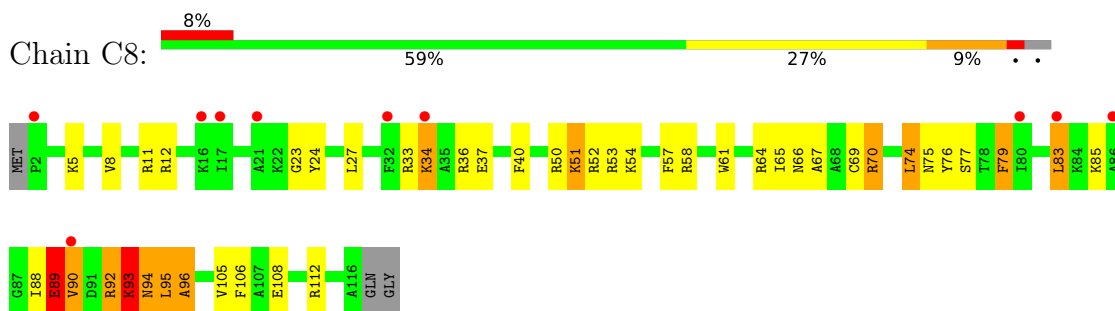


A135
Q136
LYS
ALA
GLN
GLU
PRO
LYS
ALA
SER
GLN
GLU

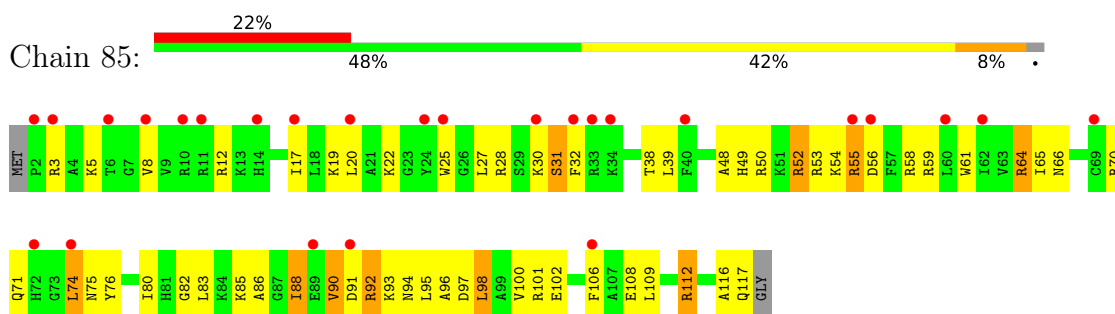
- Molecule 40: 50S ribosomal protein L19



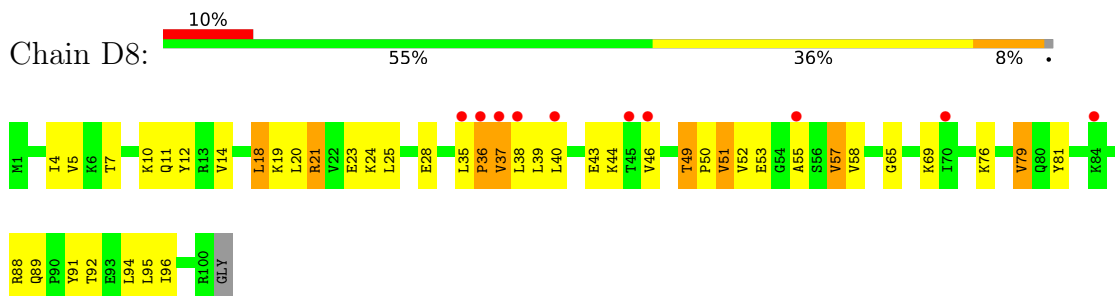
- Molecule 41: 50S ribosomal protein L20



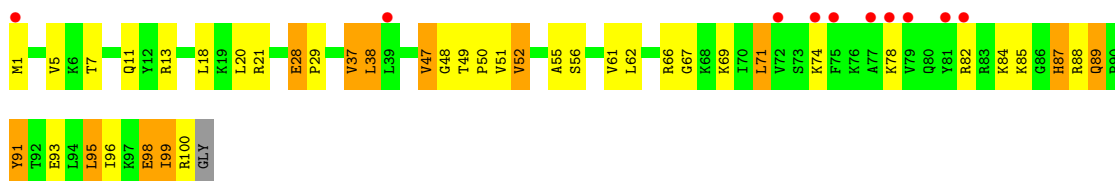
- Molecule 41: 50S ribosomal protein L20



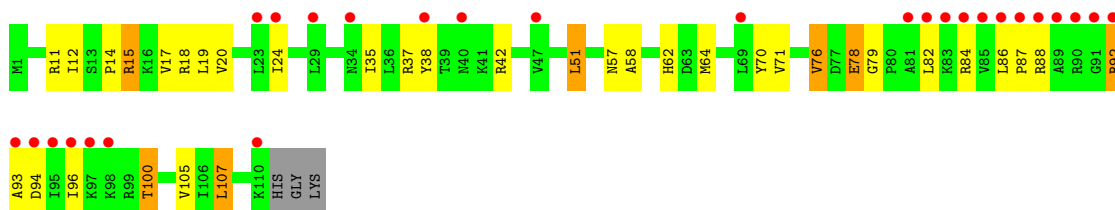
- Molecule 42: 50S ribosomal protein L21



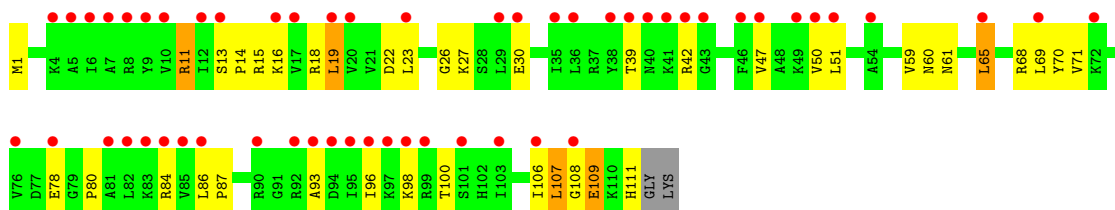
- Molecule 42: 50S ribosomal protein L21



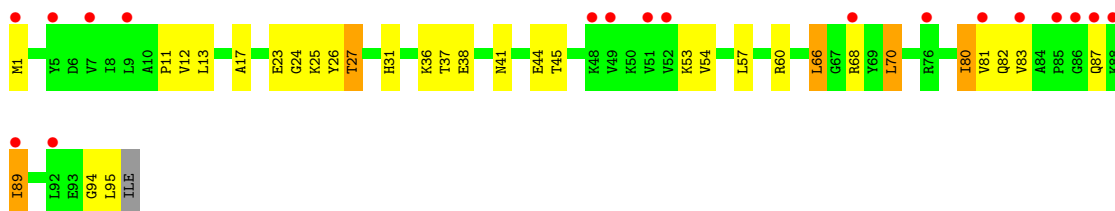
- Molecule 43: 50S ribosomal protein L22



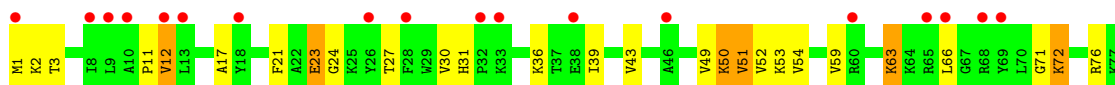
- Molecule 43: 50S ribosomal protein L22

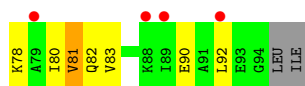


- Molecule 44: 50S ribosomal protein L23

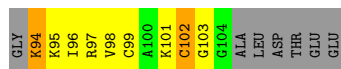


- Molecule 44: 50S ribosomal protein L23

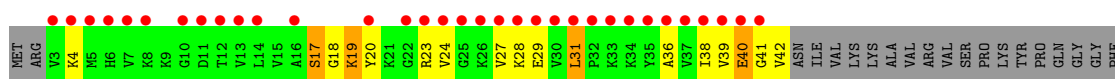
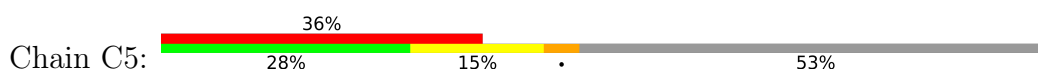




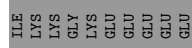
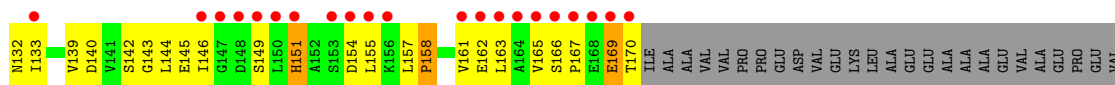
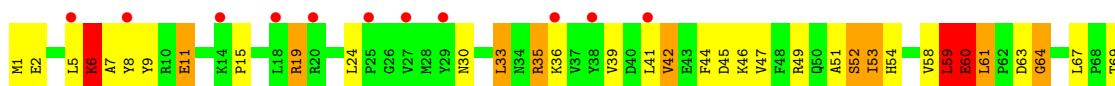
- Molecule 45: 50S ribosomal protein L24



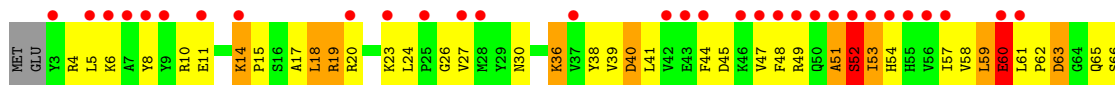
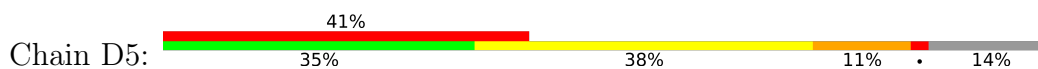
- Molecule 45: 50S ribosomal protein L24

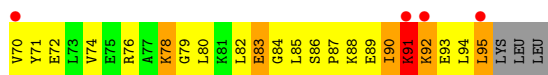


- Molecule 46: 50S ribosomal protein L25

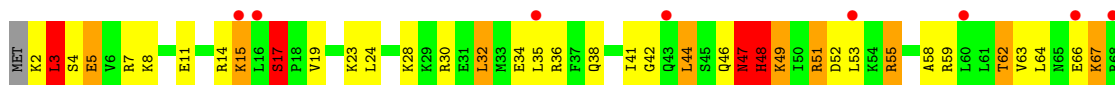


- Molecule 46: 50S ribosomal protein L25

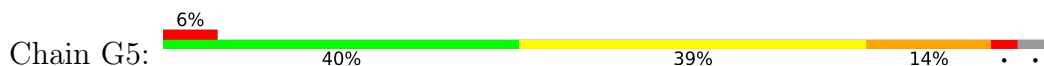




• Molecule 49: 50S ribosomal protein L29



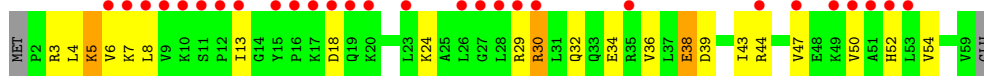
• Molecule 49: 50S ribosomal protein L29



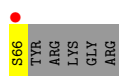
• Molecule 50: 50S ribosomal protein L30



• Molecule 50: 50S ribosomal protein L30



• Molecule 51: 50S ribosomal protein L31

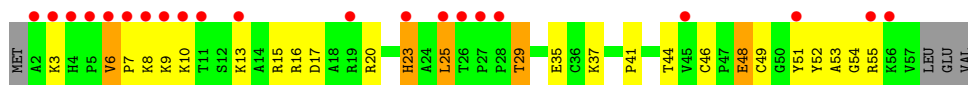


• Molecule 52: 50S ribosomal protein L32

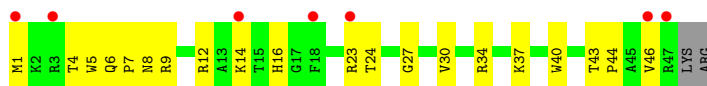




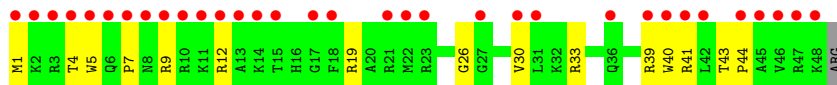
• Molecule 52: 50S ribosomal protein L32



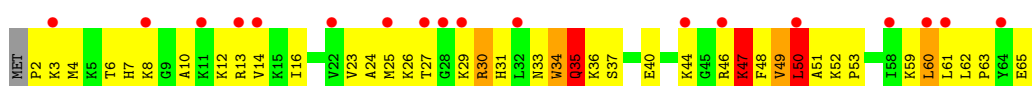
• Molecule 53: 50S ribosomal protein L34



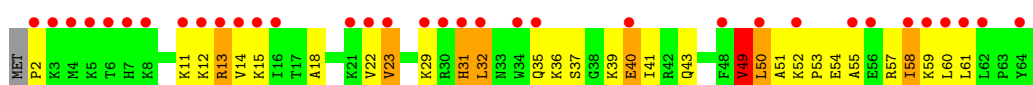
• Molecule 53: 50S ribosomal protein L34



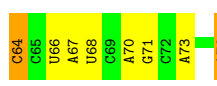
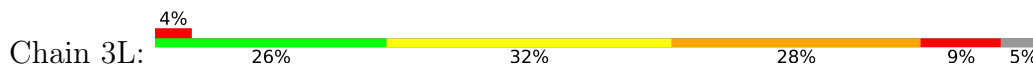
• Molecule 54: 50S ribosomal protein L35



• Molecule 54: 50S ribosomal protein L35



• Molecule 55: tRNAThr



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.41Å 449.24Å 618.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.62 – 2.96 309.20 – 2.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (224.62-2.96) 94.4 (309.20-2.96)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 2.96Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.196 , 0.252 0.196 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	82.0	Xtrriage
Anisotropy	0.292	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	294252	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, SF4, PSU, MG, 7MG, ZN, 5MU, AET, 4SU, OMC

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	0.73	2/36095 (0.0%)	1.34	310/56332 (0.6%)
1	1G	0.66	4/35850 (0.0%)	1.24	189/55949 (0.3%)
2	12	0.46	0/1727	0.62	1/2326 (0.0%)
2	1E	0.42	0/1908	0.63	1/2573 (0.0%)
3	22	0.43	0/1569	0.62	1/2116 (0.0%)
3	2E	0.44	0/1629	0.62	1/2195 (0.0%)
4	32	0.45	0/1728	0.62	0/2313
4	3E	0.47	0/1728	0.65	0/2313
5	42	0.44	0/1156	0.61	0/1557
5	4E	0.45	0/1158	0.63	0/1559
6	52	0.44	0/855	0.58	0/1154
6	5E	0.46	0/850	0.61	0/1147
7	62	0.41	0/1122	0.57	0/1500
7	6E	0.44	0/1259	0.56	0/1686
8	72	0.38	0/1127	0.59	0/1517
8	7E	0.41	0/1135	0.65	1/1527 (0.1%)
9	82	0.42	0/971	0.63	0/1304
9	8E	0.44	0/1019	0.65	1/1367 (0.1%)
10	1A	0.41	0/814	0.56	0/1095
10	1I	0.45	0/762	0.66	1/1027 (0.1%)
11	2A	0.39	0/850	0.59	0/1150
11	2I	0.45	0/838	0.65	0/1133
12	3A	0.46	0/972	0.71	0/1301
12	3I	0.60	0/972	0.79	1/1301 (0.1%)
13	4A	0.43	0/889	0.66	0/1192
13	4I	0.52	0/952	0.64	0/1277
14	5A	0.45	0/495	0.66	0/657
14	5I	0.47	0/500	0.73	1/664 (0.2%)
15	6A	0.40	0/740	0.54	0/987
15	6I	0.44	0/740	0.59	0/987
16	7A	0.45	0/721	0.64	0/970
16	7I	0.44	0/716	0.67	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.47	0/836	0.59	0/1117
17	8I	0.46	0/847	0.65	0/1131
18	9A	0.46	0/559	0.68	1/746 (0.1%)
18	9I	0.44	0/554	0.61	0/739
19	AA	0.53	0/520	0.78	0/700
19	AI	0.45	0/680	0.70	0/915
20	BA	0.39	0/781	0.58	0/1033
20	BI	0.39	0/748	0.59	0/986
21	1B	0.35	0/192	0.57	0/252
21	1F	0.41	0/203	0.63	0/266
22	1K	0.77	1/1675 (0.1%)	1.36	20/2608 (0.8%)
22	1L	0.71	0/1675	1.23	9/2608 (0.3%)
23	2K	0.77	1/1721 (0.1%)	1.37	16/2682 (0.6%)
23	2L	0.69	0/1721	1.30	10/2682 (0.4%)
24	3K	0.72	1/1716 (0.1%)	1.32	20/2668 (0.7%)
25	4K	0.88	0/440	1.28	2/684 (0.3%)
25	4L	0.84	0/341	1.57	9/529 (1.7%)
26	14	0.87	52/67828 (0.1%)	1.53	1188/105880 (1.1%)
26	1H	1.01	119/68741 (0.2%)	1.69	1859/107295 (1.7%)
27	16	0.77	0/2928	1.53	51/4568 (1.1%)
27	1J	0.73	1/2928 (0.0%)	1.44	41/4568 (0.9%)
28	11	0.63	0/2170	0.83	2/2926 (0.1%)
28	19	0.61	0/2175	0.82	2/2933 (0.1%)
29	21	0.55	0/1589	0.84	1/2145 (0.0%)
29	29	0.54	1/1596 (0.1%)	0.78	1/2153 (0.0%)
30	31	0.62	1/1620 (0.1%)	0.80	4/2194 (0.2%)
30	39	0.52	1/1637 (0.1%)	0.74	0/2218
31	41	0.50	1/1481 (0.1%)	0.73	1/1994 (0.1%)
31	49	0.45	0/1483	0.67	0/1997
32	51	0.50	0/1354	0.82	4/1833 (0.2%)
32	59	0.48	0/1320	0.70	1/1787 (0.1%)
33	61	0.44	0/1146	0.71	2/1551 (0.1%)
33	69	0.42	0/1146	0.65	0/1551
34	15	0.44	0/1123	0.66	0/1515
34	58	0.49	0/1017	0.78	2/1369 (0.1%)
35	25	0.49	0/942	0.70	1/1269 (0.1%)
35	68	0.54	0/942	0.71	0/1269
36	35	0.53	0/1139	0.86	3/1514 (0.2%)
36	78	0.58	0/1144	0.98	5/1521 (0.3%)
37	45	0.50	0/1120	0.78	0/1498
37	88	0.62	0/1138	0.85	0/1523
38	55	0.49	0/981	0.79	0/1312
38	98	0.48	0/981	0.78	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	65	0.47	0/886	0.74	1/1180 (0.1%)
39	A8	0.54	0/891	0.83	2/1187 (0.2%)
40	75	0.51	0/1178	0.73	1/1573 (0.1%)
40	B8	0.54	0/1142	0.75	1/1526 (0.1%)
41	85	0.51	0/977	0.68	0/1301
41	C8	0.57	0/968	0.76	1/1289 (0.1%)
42	95	0.47	0/781	0.77	0/1048
42	D8	0.52	0/785	0.77	1/1052 (0.1%)
43	A5	0.53	0/897	0.73	0/1204
43	E8	0.58	0/886	0.71	0/1189
44	B5	0.57	0/749	0.71	0/1007
44	F8	0.61	0/764	0.83	1/1025 (0.1%)
45	C5	0.56	0/401	0.74	0/535
45	G8	0.60	0/745	0.84	2/993 (0.2%)
46	D5	0.45	0/1443	0.70	2/1960 (0.1%)
46	H8	0.46	0/1395	0.80	2/1890 (0.1%)
47	E5	0.54	0/611	0.76	0/814
47	I8	0.68	1/619 (0.2%)	0.82	2/825 (0.2%)
48	F5	0.58	0/744	0.82	0/989
48	J8	0.66	0/754	0.92	3/1003 (0.3%)
49	G5	0.54	0/578	0.70	0/766
49	K8	0.63	0/577	0.93	2/763 (0.3%)
50	H5	0.46	0/464	0.63	0/623
50	L8	0.55	0/464	0.69	0/623
51	M8	0.56	0/485	0.77	0/652
52	J5	0.61	0/448	0.86	1/606 (0.2%)
52	N8	0.61	0/381	0.81	0/516
53	L5	0.55	0/414	0.73	0/547
53	P8	0.72	0/409	0.87	0/540
54	M5	0.62	0/524	0.88	1/691 (0.1%)
54	Q8	0.61	0/524	0.95	1/691 (0.1%)
55	3L	0.73	0/1672	1.37	22/2600 (0.8%)
All	All	0.77	186/315281 (0.1%)	1.34	3810/472388 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	6
2	1E	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	22	0	2
4	32	0	2
5	4E	0	1
9	82	0	1
9	8E	0	2
10	1A	0	1
11	2I	0	3
12	3A	0	1
12	3I	0	3
13	4A	0	4
13	4I	0	2
14	5A	0	3
16	7A	0	1
19	AA	0	7
20	BA	0	3
20	BI	0	1
28	11	0	4
28	19	0	2
29	21	0	6
29	29	0	6
30	31	0	3
30	39	0	5
31	49	0	2
32	51	0	4
32	59	0	2
33	61	0	5
33	69	0	3
34	58	0	2
36	35	0	3
36	78	0	5
37	45	0	5
37	88	0	2
38	98	0	1
39	65	0	1
39	A8	0	1
40	75	0	2
40	B8	0	3
41	85	0	2
41	C8	0	4
42	95	0	2
42	D8	0	2
44	B5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	G8	0	3
46	D5	0	6
46	H8	0	5
48	F5	0	4
48	J8	0	3
49	G5	0	4
49	K8	0	4
51	M8	0	4
54	M5	0	3
54	Q8	0	3
All	All	0	163

The worst 5 of 186 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	774	A	N9-C4	-13.04	1.30	1.37
26	1H	676	A	N9-C4	-11.33	1.31	1.37
26	1H	2430	A	N9-C4	-10.69	1.31	1.37
26	1H	945	A	N9-C4	-10.48	1.31	1.37
26	1H	783	A	N9-C4	-10.03	1.31	1.37

The worst 5 of 3810 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-22.84	112.30	126.00
26	1H	2430	A	N1-C6-N6	20.05	130.63	118.60
26	1H	2430	A	C2-N3-C4	-19.74	100.73	110.60
26	1H	783	A	C2-N3-C4	-18.96	101.12	110.60
26	1H	676	A	C2-N3-C4	-18.87	101.17	110.60

There are no chirality outliers.

5 of 163 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	11	LEU	Peptide
2	1E	15	VAL	Peptide
2	1E	237	ALA	Peptide
5	4E	114	GLY	Peptide
9	8E	4	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32246	0	16276	648	0
1	1G	32028	0	16165	605	0
2	12	1696	0	1730	102	0
2	1E	1874	0	1926	85	0
3	22	1546	0	1608	79	0
3	2E	1605	0	1668	37	0
4	32	1698	0	1761	87	1
4	3E	1698	0	1760	71	0
5	42	1141	0	1199	58	0
5	4E	1142	0	1204	34	0
6	52	842	0	857	18	0
6	5E	837	0	852	19	1
7	62	1110	0	1163	51	0
7	6E	1242	0	1286	41	0
8	72	1107	0	1165	37	0
8	7E	1115	0	1177	46	0
9	82	953	0	983	56	0
9	8E	1000	0	1031	58	0
10	1A	801	0	849	51	0
10	1I	749	0	767	45	0
11	2A	835	0	847	29	0
11	2I	823	0	832	30	0
12	3A	956	0	1046	32	0
12	3I	956	0	1046	33	0
13	4A	879	0	935	48	0
13	4I	942	0	997	56	0
14	5A	486	0	526	22	0
14	5I	491	0	529	27	0
15	6A	729	0	768	12	0
15	6I	729	0	768	28	0
16	7A	705	0	725	19	0
16	7I	700	0	720	28	0
17	8A	823	0	891	32	0
17	8I	834	0	904	33	0
18	9A	554	0	609	15	0
18	9I	549	0	607	25	0
19	AA	510	0	507	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	665	0	686	36	0
20	BA	778	0	863	26	0
20	BI	746	0	843	46	0
21	1B	188	0	195	14	0
21	1F	199	0	208	8	0
22	1K	1593	0	813	50	0
22	1L	1593	0	813	48	0
23	2K	1646	0	844	19	0
23	2L	1646	0	842	31	0
24	3K	1537	0	779	46	0
25	4K	391	0	197	7	0
25	4L	303	0	154	15	0
26	14	60561	0	30527	996	0
26	1H	61381	0	30944	1089	0
27	16	2617	0	1328	45	0
27	1J	2617	0	1328	68	0
28	11	2120	0	2197	58	0
28	19	2125	0	2199	67	0
29	21	1556	0	1612	74	0
29	29	1563	0	1629	82	0
30	31	1585	0	1632	70	0
30	39	1602	0	1649	84	0
31	41	1457	0	1514	64	0
31	49	1459	0	1507	54	0
32	51	1328	0	1396	46	0
32	59	1295	0	1366	78	0
33	61	1131	0	1218	49	0
33	69	1131	0	1218	46	0
34	15	1096	0	1168	51	0
34	58	995	0	1077	36	0
35	25	932	0	996	32	0
35	68	932	0	996	21	0
36	35	1122	0	1206	71	0
36	78	1127	0	1208	64	0
37	45	1099	0	1154	67	0
37	88	1117	0	1168	51	0
38	55	967	0	1033	45	0
38	98	967	0	1033	41	0
39	65	876	0	938	71	0
39	A8	881	0	943	43	0
40	75	1164	0	1221	59	0
40	B8	1128	0	1183	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	85	959	0	1019	61	0
41	C8	950	0	1011	43	0
42	95	770	0	838	32	0
42	D8	774	0	849	29	0
43	A5	886	0	948	23	0
43	E8	876	0	941	24	0
44	B5	735	0	785	19	0
44	F8	750	0	814	20	0
45	C5	396	0	444	18	0
45	G8	734	0	821	38	0
46	D5	1411	0	1436	71	0
46	H8	1365	0	1391	61	0
47	E5	603	0	620	22	0
47	I8	611	0	631	26	0
48	F5	737	0	813	32	0
48	J8	747	0	817	35	0
49	G5	576	0	625	31	0
49	K8	575	0	634	33	0
50	H5	459	0	512	18	0
50	L8	459	0	512	9	0
51	M8	475	0	465	33	0
52	J5	434	0	454	22	0
52	N8	369	0	388	23	0
53	L5	406	0	438	10	0
53	P8	401	0	436	10	0
54	M5	516	0	582	22	0
54	Q8	516	0	582	37	0
55	3L	1538	0	781	38	0
56	11	1	0	0	0	0
56	13	205	0	0	0	0
56	14	435	0	0	0	0
56	16	15	0	0	0	0
56	19	1	0	0	0	0
56	1B	1	0	0	0	0
56	1G	155	0	0	0	0
56	1H	622	0	0	0	0
56	1J	6	0	0	0	0
56	1K	1	0	0	0	0
56	21	4	0	0	0	0
56	25	1	0	0	0	0
56	29	3	0	0	0	0
56	2A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2I	1	0	0	0	0
56	2K	2	0	0	0	0
56	2L	2	0	0	0	0
56	31	2	0	0	0	0
56	35	3	0	0	0	0
56	39	1	0	0	0	0
56	3E	1	0	0	0	0
56	41	1	0	0	0	0
56	42	1	0	0	0	0
56	45	2	0	0	0	0
56	4A	1	0	0	0	0
56	4L	1	0	0	0	0
56	55	1	0	0	0	0
56	5E	1	0	0	0	0
56	5I	2	0	0	0	0
56	68	2	0	0	0	0
56	78	2	0	0	0	0
56	85	1	0	0	0	0
56	88	3	0	0	0	0
56	8I	1	0	0	0	0
56	98	1	0	0	0	0
56	9A	1	0	0	0	0
56	BA	2	0	0	0	0
56	BI	2	0	0	0	0
56	D8	1	0	0	0	0
56	E5	1	0	0	0	0
56	I8	2	0	0	0	0
56	P8	1	0	0	0	0
56	Q8	1	0	0	0	0
57	32	8	0	0	1	0
57	3E	8	0	0	1	0
58	5A	1	0	0	0	0
58	5I	1	0	0	0	0
59	11	11	0	0	0	0
59	13	339	0	0	42	0
59	14	730	0	0	89	0
59	15	1	0	0	0	0
59	16	19	0	0	0	0
59	19	10	0	0	1	0
59	1A	1	0	0	0	0
59	1E	1	0	0	1	0
59	1F	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1G	289	0	0	25	0
59	1H	1047	0	0	184	0
59	1I	3	0	0	1	0
59	1K	1	0	0	0	0
59	21	8	0	0	0	0
59	25	6	0	0	0	0
59	29	2	0	0	0	0
59	2L	6	0	0	0	0
59	31	7	0	0	0	0
59	32	2	0	0	0	0
59	35	6	0	0	0	0
59	39	5	0	0	0	0
59	3E	2	0	0	0	0
59	3I	1	0	0	0	0
59	42	1	0	0	0	0
59	45	4	0	0	0	0
59	4E	2	0	0	0	0
59	4I	2	0	0	1	0
59	4K	2	0	0	0	0
59	4L	3	0	0	1	0
59	52	4	0	0	0	0
59	58	3	0	0	0	0
59	5I	1	0	0	0	0
59	6E	1	0	0	0	0
59	6I	1	0	0	0	0
59	75	1	0	0	0	0
59	78	6	0	0	0	0
59	7A	4	0	0	1	0
59	7I	3	0	0	0	0
59	8E	2	0	0	0	0
59	95	1	0	0	0	0
59	9A	2	0	0	1	0
59	B5	3	0	0	0	0
59	BA	2	0	0	0	0
59	D8	1	0	0	0	0
59	E8	1	0	0	0	0
59	G8	1	0	0	0	0
59	H5	3	0	0	1	0
59	I8	2	0	0	1	0
59	J8	1	0	0	0	0
59	L8	4	0	0	0	0
59	M5	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	P8	1	0	0	0	0
59	Q8	2	0	0	1	0
All	All	294252	0	195096	6738	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 6738 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:810:U:OP1	59:1H:3720:HOH:O	1.68	1.09
29:29:54:GLN:HA	29:29:74:PRO:HA	1.35	1.08
26:14:1604:C:OP2	59:14:3509:HOH:O	1.71	1.07
37:45:27:VAL:HB	37:45:28:ALA:HA	1.32	1.07
26:14:2113:U:H3'	26:14:2114:A:H4'	1.34	1.06

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5E:15:ASP:OD2	4:32:27:TYR:OH[4_555]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	12	203/256 (79%)	161 (79%)	41 (20%)	1 (0%)	29 64
2	1E	227/256 (89%)	175 (77%)	49 (22%)	3 (1%)	12 41
3	22	193/239 (81%)	161 (83%)	31 (16%)	1 (0%)	29 64
3	2E	203/239 (85%)	181 (89%)	21 (10%)	1 (0%)	29 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	32	205/209 (98%)	186 (91%)	19 (9%)	0	100	100
4	3E	205/209 (98%)	175 (85%)	29 (14%)	1 (0%)	29	64
5	42	148/162 (91%)	136 (92%)	12 (8%)	0	100	100
5	4E	147/162 (91%)	140 (95%)	7 (5%)	0	100	100
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
6	5E	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
7	62	134/156 (86%)	127 (95%)	7 (5%)	0	100	100
7	6E	152/156 (97%)	142 (93%)	10 (7%)	0	100	100
8	72	135/138 (98%)	118 (87%)	16 (12%)	1 (1%)	22	56
8	7E	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	10	38
9	82	119/128 (93%)	103 (87%)	14 (12%)	2 (2%)	9	34
9	8E	124/128 (97%)	102 (82%)	22 (18%)	0	100	100
10	1A	97/105 (92%)	83 (86%)	14 (14%)	0	100	100
10	1I	92/105 (88%)	80 (87%)	12 (13%)	0	100	100
11	2A	111/129 (86%)	96 (86%)	14 (13%)	1 (1%)	17	51
11	2I	109/129 (84%)	94 (86%)	14 (13%)	1 (1%)	17	51
12	3A	120/132 (91%)	100 (83%)	19 (16%)	1 (1%)	19	53
12	3I	120/132 (91%)	104 (87%)	15 (12%)	1 (1%)	19	53
13	4A	107/126 (85%)	84 (78%)	17 (16%)	6 (6%)	2	8
13	4I	117/126 (93%)	86 (74%)	26 (22%)	5 (4%)	2	12
14	5A	57/61 (93%)	46 (81%)	10 (18%)	1 (2%)	8	33
14	5I	58/61 (95%)	50 (86%)	5 (9%)	3 (5%)	2	9
15	6A	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
15	6I	85/89 (96%)	71 (84%)	14 (16%)	0	100	100
16	7A	82/88 (93%)	74 (90%)	7 (8%)	1 (1%)	13	43
16	7I	81/88 (92%)	72 (89%)	9 (11%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	87 (89%)	11 (11%)	0	100	100
18	9A	67/88 (76%)	65 (97%)	2 (3%)	0	100	100
18	9I	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
19	AA	59/93 (63%)	43 (73%)	15 (25%)	1 (2%)	9	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AI	81/93 (87%)	67 (83%)	13 (16%)	1 (1%)	13	43
20	BA	101/106 (95%)	83 (82%)	17 (17%)	1 (1%)	15	48
20	BI	95/106 (90%)	84 (88%)	11 (12%)	0	100	100
21	1B	20/27 (74%)	17 (85%)	2 (10%)	1 (5%)	2	10
21	1F	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	11	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	8	33
28	19	272/276 (99%)	235 (86%)	36 (13%)	1 (0%)	34	69
29	21	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	5	25
29	29	202/206 (98%)	146 (72%)	48 (24%)	8 (4%)	3	14
30	31	200/210 (95%)	178 (89%)	22 (11%)	0	100	100
30	39	202/210 (96%)	163 (81%)	35 (17%)	4 (2%)	7	30
31	41	177/182 (97%)	153 (86%)	23 (13%)	1 (1%)	25	60
31	49	178/182 (98%)	149 (84%)	27 (15%)	2 (1%)	14	46
32	51	172/180 (96%)	132 (77%)	31 (18%)	9 (5%)	2	9
32	59	167/180 (93%)	125 (75%)	42 (25%)	0	100	100
33	61	143/148 (97%)	111 (78%)	28 (20%)	4 (3%)	5	22
33	69	143/148 (97%)	107 (75%)	34 (24%)	2 (1%)	11	39
34	15	135/140 (96%)	118 (87%)	16 (12%)	1 (1%)	22	56
34	58	123/140 (88%)	109 (89%)	13 (11%)	1 (1%)	19	53
35	25	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
35	68	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	35	145/150 (97%)	117 (81%)	26 (18%)	2 (1%)	11	39
36	78	146/150 (97%)	111 (76%)	30 (20%)	5 (3%)	3	17
37	45	136/141 (96%)	106 (78%)	29 (21%)	1 (1%)	22	56
37	88	139/141 (99%)	120 (86%)	15 (11%)	4 (3%)	4	21
38	55	116/118 (98%)	104 (90%)	10 (9%)	2 (2%)	9	34
38	98	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
39	65	108/112 (96%)	84 (78%)	23 (21%)	1 (1%)	17	51
39	A8	109/112 (97%)	85 (78%)	24 (22%)	0	100	100
40	75	138/146 (94%)	120 (87%)	16 (12%)	2 (1%)	11	39
40	B8	134/146 (92%)	112 (84%)	21 (16%)	1 (1%)	22	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	85	114/118 (97%)	99 (87%)	15 (13%)	0	100	100
41	C8	113/118 (96%)	97 (86%)	14 (12%)	2 (2%)	8	33
42	95	98/101 (97%)	79 (81%)	16 (16%)	3 (3%)	4	19
42	D8	98/101 (97%)	85 (87%)	13 (13%)	0	100	100
43	A5	109/113 (96%)	102 (94%)	7 (6%)	0	100	100
43	E8	108/113 (96%)	100 (93%)	8 (7%)	0	100	100
44	B5	92/96 (96%)	77 (84%)	14 (15%)	1 (1%)	14	46
44	F8	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
45	C5	48/110 (44%)	39 (81%)	8 (17%)	1 (2%)	7	29
45	G8	93/110 (84%)	64 (69%)	25 (27%)	4 (4%)	2	12
46	D5	175/206 (85%)	123 (70%)	45 (26%)	7 (4%)	3	14
46	H8	168/206 (82%)	127 (76%)	35 (21%)	6 (4%)	3	16
47	E5	74/85 (87%)	64 (86%)	8 (11%)	2 (3%)	5	23
47	I8	75/85 (88%)	66 (88%)	9 (12%)	0	100	100
48	F5	92/98 (94%)	78 (85%)	12 (13%)	2 (2%)	6	28
48	J8	94/98 (96%)	79 (84%)	13 (14%)	2 (2%)	7	29
49	G5	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	10	38
49	K8	66/72 (92%)	58 (88%)	7 (11%)	1 (2%)	10	38
50	H5	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
50	L8	56/60 (93%)	50 (89%)	6 (11%)	0	100	100
51	M8	56/71 (79%)	35 (62%)	19 (34%)	2 (4%)	3	16
52	J5	54/60 (90%)	45 (83%)	9 (17%)	0	100	100
52	N8	46/60 (77%)	37 (80%)	9 (20%)	0	100	100
53	L5	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
53	P8	45/49 (92%)	42 (93%)	2 (4%)	1 (2%)	6	28
54	M5	62/65 (95%)	54 (87%)	8 (13%)	0	100	100
54	Q8	62/65 (95%)	47 (76%)	12 (19%)	3 (5%)	2	11
All	All	10929/11875 (92%)	9262 (85%)	1532 (14%)	135 (1%)	13	43

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	4I	12	ASN

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Mol	Chain	Res	Type
28	11	239	ARG
33	61	134	PRO
34	58	96	GLU
36	78	36	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	179/220 (81%)	135 (75%)	44 (25%)	0	2
2	1E	200/220 (91%)	152 (76%)	48 (24%)	0	2
3	22	154/188 (82%)	120 (78%)	34 (22%)	1	3
3	2E	159/188 (85%)	128 (80%)	31 (20%)	1	6
4	32	180/181 (99%)	152 (84%)	28 (16%)	2	11
4	3E	180/181 (99%)	148 (82%)	32 (18%)	2	8
5	42	114/123 (93%)	86 (75%)	28 (25%)	0	2
5	4E	115/123 (94%)	95 (83%)	20 (17%)	2	8
6	52	90/90 (100%)	76 (84%)	14 (16%)	2	11
6	5E	90/90 (100%)	78 (87%)	12 (13%)	4	15
7	62	114/127 (90%)	90 (79%)	24 (21%)	1	4
7	6E	125/127 (98%)	103 (82%)	22 (18%)	2	8
8	72	118/119 (99%)	95 (80%)	23 (20%)	1	6
8	7E	119/119 (100%)	95 (80%)	24 (20%)	1	5
9	82	92/99 (93%)	69 (75%)	23 (25%)	0	2
9	8E	97/99 (98%)	77 (79%)	20 (21%)	1	4
10	1A	89/92 (97%)	69 (78%)	20 (22%)	1	3
10	1I	81/92 (88%)	68 (84%)	13 (16%)	2	10
11	2A	85/99 (86%)	72 (85%)	13 (15%)	2	11
11	2I	84/99 (85%)	68 (81%)	16 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	3A	103/109 (94%)	75 (73%)	28 (27%)	0	1
12	3I	103/109 (94%)	83 (81%)	20 (19%)	1	6
13	4A	90/101 (89%)	70 (78%)	20 (22%)	1	3
13	4I	94/101 (93%)	72 (77%)	22 (23%)	1	3
14	5A	49/50 (98%)	31 (63%)	18 (37%)	0	0
14	5I	49/50 (98%)	38 (78%)	11 (22%)	1	3
15	6A	79/80 (99%)	73 (92%)	6 (8%)	13	39
15	6I	79/80 (99%)	64 (81%)	15 (19%)	1	6
16	7A	72/74 (97%)	63 (88%)	9 (12%)	4	17
16	7I	72/74 (97%)	56 (78%)	16 (22%)	1	3
17	8A	94/97 (97%)	85 (90%)	9 (10%)	8	28
17	8I	95/97 (98%)	77 (81%)	18 (19%)	1	7
18	9A	58/77 (75%)	42 (72%)	16 (28%)	0	1
18	9I	58/77 (75%)	52 (90%)	6 (10%)	7	25
19	AA	56/80 (70%)	43 (77%)	13 (23%)	1	3
19	AI	72/80 (90%)	56 (78%)	16 (22%)	1	3
20	BA	76/82 (93%)	69 (91%)	7 (9%)	9	30
20	BI	75/82 (92%)	65 (87%)	10 (13%)	4	15
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	50
21	1F	18/22 (82%)	17 (94%)	1 (6%)	21	53
28	11	214/218 (98%)	172 (80%)	42 (20%)	1	6
28	19	214/218 (98%)	173 (81%)	41 (19%)	1	6
29	21	162/166 (98%)	132 (82%)	30 (18%)	1	7
29	29	165/166 (99%)	138 (84%)	27 (16%)	2	9
30	31	161/166 (97%)	131 (81%)	30 (19%)	1	7
30	39	163/166 (98%)	124 (76%)	39 (24%)	0	2
31	41	153/156 (98%)	121 (79%)	32 (21%)	1	4
31	49	152/156 (97%)	117 (77%)	35 (23%)	1	3
32	51	143/148 (97%)	120 (84%)	23 (16%)	2	10
32	59	140/148 (95%)	101 (72%)	39 (28%)	0	1
33	61	122/124 (98%)	91 (75%)	31 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	69	122/124 (98%)	95 (78%)	27 (22%)	1	3
34	15	116/119 (98%)	88 (76%)	28 (24%)	0	2
34	58	105/119 (88%)	83 (79%)	22 (21%)	1	4
35	25	100/100 (100%)	85 (85%)	15 (15%)	3	12
35	68	100/100 (100%)	88 (88%)	12 (12%)	5	19
36	35	114/116 (98%)	80 (70%)	34 (30%)	0	1
36	78	114/116 (98%)	77 (68%)	37 (32%)	0	1
37	45	109/111 (98%)	85 (78%)	24 (22%)	1	4
37	88	110/111 (99%)	96 (87%)	14 (13%)	4	17
38	55	101/101 (100%)	75 (74%)	26 (26%)	0	2
38	98	101/101 (100%)	74 (73%)	27 (27%)	0	2
39	65	87/88 (99%)	60 (69%)	27 (31%)	0	1
39	A8	87/88 (99%)	63 (72%)	24 (28%)	0	1
40	75	122/127 (96%)	95 (78%)	27 (22%)	1	3
40	B8	118/127 (93%)	82 (70%)	36 (30%)	0	1
41	85	93/94 (99%)	77 (83%)	16 (17%)	2	8
41	C8	92/94 (98%)	77 (84%)	15 (16%)	2	9
42	95	81/82 (99%)	64 (79%)	17 (21%)	1	4
42	D8	82/82 (100%)	62 (76%)	20 (24%)	0	2
43	A5	91/92 (99%)	74 (81%)	17 (19%)	1	7
43	E8	90/92 (98%)	79 (88%)	11 (12%)	5	19
44	B5	74/78 (95%)	60 (81%)	14 (19%)	1	7
44	F8	77/78 (99%)	66 (86%)	11 (14%)	3	13
45	C5	43/91 (47%)	35 (81%)	8 (19%)	1	7
45	G8	79/91 (87%)	64 (81%)	15 (19%)	1	6
46	D5	156/179 (87%)	124 (80%)	32 (20%)	1	5
46	H8	151/179 (84%)	108 (72%)	43 (28%)	0	1
47	E5	61/67 (91%)	51 (84%)	10 (16%)	2	9
47	I8	62/67 (92%)	55 (89%)	7 (11%)	6	21
48	F5	79/83 (95%)	62 (78%)	17 (22%)	1	4
48	J8	79/83 (95%)	64 (81%)	15 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	G5	63/67 (94%)	45 (71%)	18 (29%)	0	1
49	K8	64/67 (96%)	41 (64%)	23 (36%)	0	1
50	H5	50/52 (96%)	45 (90%)	5 (10%)	7	26
50	L8	50/52 (96%)	42 (84%)	8 (16%)	2	10
51	M8	52/63 (82%)	34 (65%)	18 (35%)	0	1
52	J5	48/52 (92%)	37 (77%)	11 (23%)	1	3
52	N8	43/52 (83%)	32 (74%)	11 (26%)	0	2
53	L5	38/42 (90%)	34 (90%)	4 (10%)	7	24
53	P8	38/42 (90%)	32 (84%)	6 (16%)	2	10
54	M5	54/55 (98%)	42 (78%)	12 (22%)	1	3
54	Q8	54/55 (98%)	48 (89%)	6 (11%)	6	22
All	All	9213/9831 (94%)	7323 (80%)	1890 (20%)	1	5

5 of 1890 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	N8	35	GLU
45	C5	4	LYS
9	82	47	LEU
43	A5	100	THR
36	35	132	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
29	29	54	GLN
41	85	94	ASN
49	G5	46	GLN
43	A5	60	ASN
49	K8	48	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1499/1522 (98%)	326 (21%)	36 (2%)
1	1G	1488/1522 (97%)	314 (21%)	31 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	1K	72/76 (94%)	39 (54%)	5 (6%)
22	1L	71/76 (93%)	40 (56%)	1 (1%)
23	2K	76/77 (98%)	18 (23%)	1 (1%)
23	2L	76/77 (98%)	18 (23%)	3 (3%)
24	3K	69/76 (90%)	36 (52%)	2 (2%)
25	4K	17/27 (62%)	10 (58%)	3 (17%)
25	4L	14/27 (51%)	6 (42%)	3 (21%)
26	14	2805/2917 (96%)	630 (22%)	35 (1%)
26	1H	2841/2917 (97%)	579 (20%)	45 (1%)
27	16	121/122 (99%)	17 (14%)	1 (0%)
27	1J	121/122 (99%)	33 (27%)	1 (0%)
55	3L	69/76 (90%)	31 (44%)	3 (4%)
All	All	9339/9634 (96%)	2097 (22%)	170 (1%)

5 of 2097 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	4	U
1	13	5	U
1	13	6	G
1	13	7	G

5 of 170 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	1145	C
26	14	960	A
1	1G	1359	C
55	3L	58	A
26	14	1534	G

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

20 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
55	PSU	3L	55	55	18,21,22	1.21	2 (11%)	22,30,33	1.78	4 (18%)
23	4SU	2K	8	23	18,21,22	1.81	3 (16%)	26,30,33	2.93	8 (30%)
23	OMC	2L	33	23	19,22,23	1.71	3 (15%)	26,31,34	0.81	0
22	5MU	1L	54	22	19,22,23	4.11	5 (26%)	28,32,35	3.23	10 (35%)
22	PSU	1K	55	22	18,21,22	1.31	2 (11%)	22,30,33	1.79	3 (13%)
55	5MU	3L	54	55	19,22,23	3.91	5 (26%)	28,32,35	3.27	9 (32%)
23	7MG	2K	47	23	22,26,27	3.02	8 (36%)	29,39,42	2.76	10 (34%)
23	7MG	2L	47	23	22,26,27	2.99	7 (31%)	29,39,42	2.83	10 (34%)
23	5MU	2K	55	23	19,22,23	3.86	5 (26%)	28,32,35	3.24	9 (32%)
22	PSU	1L	55	22	18,21,22	1.33	1 (5%)	22,30,33	1.75	5 (22%)
22	H2U	1K	17	22	18,21,22	2.27	4 (22%)	21,30,33	1.87	4 (19%)
22	AET	1K	37	22	28,35,36	2.57	4 (14%)	31,51,54	2.10	4 (12%)
23	OMC	2K	33	23	19,22,23	1.82	3 (15%)	26,31,34	1.24	5 (19%)
23	4SU	2L	8	23	18,21,22	1.78	3 (16%)	26,30,33	2.39	7 (26%)
23	PSU	2K	56	23	18,21,22	1.25	1 (5%)	22,30,33	1.95	4 (18%)
22	AET	1L	37	22	28,35,36	2.55	4 (14%)	31,51,54	1.99	9 (29%)
22	H2U	1L	17	22	18,21,22	2.46	4 (22%)	21,30,33	1.83	5 (23%)
22	5MU	1K	54	22	19,22,23	4.23	5 (26%)	28,32,35	3.46	13 (46%)
23	PSU	2L	56	23	18,21,22	1.19	2 (11%)	22,30,33	1.47	2 (9%)
23	5MU	2L	55	23	19,22,23	3.94	5 (26%)	28,32,35	3.39	9 (32%)

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
55	PSU	3L	55	55	-	2/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	2/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
22	5MU	1L	54	22	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
55	5MU	3L	54	55	-	2/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	2/7/37/38	0/3/3/3
23	7MG	2L	47	23	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
22	PSU	1L	55	22	-	2/7/25/26	0/2/2/2
22	H2U	1K	17	22	-	4/7/38/39	0/2/2/2
22	AET	1K	37	22	-	10/23/45/46	0/3/3/3
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2
23	4SU	2L	8	23	-	2/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	AET	1L	37	22	-	4/23/45/46	0/3/3/3
22	H2U	1L	17	22	-	5/7/38/39	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	2/7/25/26	0/2/2/2

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	54	5MU	C2-N1	14.25	1.61	1.38
22	1L	54	5MU	C2-N1	13.45	1.60	1.38
23	2L	55	5MU	C2-N1	12.71	1.58	1.38
23	2K	55	5MU	C2-N1	12.42	1.58	1.38
55	3L	54	5MU	C2-N1	12.18	1.58	1.38

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	55	5MU	C5-C4-N3	11.13	124.81	115.31
55	3L	54	5MU	C5-C4-N3	10.82	124.55	115.31
22	1K	54	5MU	C5-C4-N3	10.72	124.46	115.31
22	1L	54	5MU	C5-C4-N3	10.66	124.41	115.31
23	2K	55	5MU	C5-C4-N3	9.76	123.64	115.31

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	3L	54	5MU	C4'-C5'-O5'-P
22	1K	17	H2U	O4'-C1'-N1-C2
22	1K	17	H2U	O4'-C1'-N1-C6
22	1K	17	H2U	C2'-C1'-N1-C6
22	1L	17	H2U	O4'-C1'-N1-C2

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	3L	55	PSU	2	0
23	2K	8	4SU	1	0
23	2L	33	OMC	2	0
22	1L	54	5MU	1	0
55	3L	54	5MU	3	0
23	2K	47	7MG	3	0
23	2L	47	7MG	1	0
22	1K	37	AET	4	0
23	2L	8	4SU	1	0
22	1L	37	AET	3	0
22	1K	54	5MU	3	0
23	2L	55	5MU	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1498 ligands modelled in this entry, 1496 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	SF4	32	301	4	0,12,12	-	-	-		
57	SF4	3E	302	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	32	301	4	-	-	0/6/5/5
57	SF4	3E	302	4	-	-	0/6/5/5

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	32	301	SF4	1	0
57	3E	302	SF4	1	0

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
55	3L	1
24	3K	1
26	1H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3L	48:C	O3'	49:G	P	5.87
1	3K	48:C	O3'	49:G	P	5.53
1	1H	1053:C	O3'	1054:A	P	3.55

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1500/1522 (98%)	0.02	10 (0%) 87 76	60, 99, 150, 173	0
1	1G	1490/1522 (97%)	-0.07	8 (0%) 91 81	69, 111, 148, 171	0
2	12	207/256 (80%)	0.13	5 (2%) 59 42	116, 138, 149, 156	0
2	1E	231/256 (90%)	0.64	29 (12%) 3 2	107, 131, 148, 156	0
3	22	197/239 (82%)	0.56	26 (13%) 3 2	114, 131, 144, 153	0
3	2E	205/239 (85%)	0.70	25 (12%) 4 2	82, 106, 127, 136	0
4	32	207/209 (99%)	1.31	60 (28%) 0 0	91, 110, 129, 137	0
4	3E	207/209 (99%)	1.14	44 (21%) 0 0	82, 105, 125, 132	0
5	42	150/162 (92%)	0.69	24 (16%) 1 1	99, 117, 132, 142	0
5	4E	149/162 (91%)	1.12	30 (20%) 1 0	83, 100, 118, 125	0
6	52	101/101 (100%)	0.38	4 (3%) 38 25	87, 104, 119, 131	0
6	5E	100/101 (99%)	0.94	21 (21%) 1 0	88, 105, 119, 128	0
7	62	138/156 (88%)	0.84	25 (18%) 1 1	110, 120, 130, 136	0
7	6E	154/156 (98%)	1.34	36 (23%) 0 0	101, 116, 137, 150	0
8	72	137/138 (99%)	0.63	15 (10%) 5 3	97, 119, 130, 138	0
8	7E	138/138 (100%)	0.33	8 (5%) 23 14	91, 108, 122, 128	0
9	82	121/128 (94%)	1.51	39 (32%) 0 0	105, 135, 143, 150	0
9	8E	126/128 (98%)	0.95	30 (23%) 0 0	86, 127, 142, 150	0
10	1A	99/105 (94%)	0.90	21 (21%) 0 0	112, 135, 147, 153	0
10	1I	94/105 (89%)	1.02	25 (26%) 0 0	77, 120, 141, 143	0
11	2A	113/129 (87%)	1.55	36 (31%) 0 0	83, 108, 122, 131	0
11	2I	111/129 (86%)	2.10	54 (48%) 0 0	76, 105, 125, 137	0
12	3A	122/132 (92%)	1.97	54 (44%) 0 0	81, 99, 118, 132	0
12	3I	122/132 (92%)	0.81	22 (18%) 1 1	64, 77, 108, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	109/126 (86%)	1.11	31 (28%) 0 0	111, 131, 145, 152	0
13	4I	119/126 (94%)	0.46	10 (8%) 11 6	87, 116, 130, 141	0
14	5A	59/61 (96%)	3.96	44 (74%) 0 0	120, 129, 138, 142	0
14	5I	60/61 (98%)	1.31	17 (28%) 0 0	82, 95, 116, 123	0
15	6A	87/89 (97%)	1.41	32 (36%) 0 0	86, 108, 123, 126	0
15	6I	87/89 (97%)	0.94	16 (18%) 1 1	81, 100, 119, 128	0
16	7A	84/88 (95%)	0.40	2 (2%) 59 42	91, 101, 125, 143	0
16	7I	83/88 (94%)	0.90	14 (16%) 1 1	96, 110, 130, 143	0
17	8A	99/105 (94%)	2.78	63 (63%) 0 0	93, 107, 122, 127	0
17	8I	100/105 (95%)	1.71	38 (38%) 0 0	89, 105, 116, 119	0
18	9A	69/88 (78%)	-0.00	0 100 100	94, 110, 130, 139	0
18	9I	68/88 (77%)	0.52	6 (8%) 10 5	88, 106, 123, 131	0
19	AA	65/93 (69%)	2.25	31 (47%) 0 0	122, 140, 150, 156	0
19	AI	83/93 (89%)	0.66	11 (13%) 3 2	93, 112, 138, 145	0
20	BA	103/106 (97%)	1.98	48 (46%) 0 0	89, 110, 132, 136	0
20	BI	97/106 (91%)	1.01	22 (22%) 0 0	105, 116, 134, 137	0
21	1B	22/27 (81%)	2.07	9 (40%) 0 0	109, 122, 128, 128	0
21	1F	23/27 (85%)	2.23	11 (47%) 0 0	94, 102, 111, 117	0
22	1K	70/76 (92%)	0.16	5 (7%) 16 9	79, 151, 170, 173	0
22	1L	70/76 (92%)	0.29	7 (10%) 7 4	111, 158, 174, 179	0
23	2K	72/77 (93%)	0.21	2 (2%) 53 36	67, 93, 126, 137	0
23	2L	72/77 (93%)	-0.20	0 100 100	75, 104, 139, 145	0
24	3K	72/76 (94%)	0.41	9 (12%) 3 2	70, 157, 167, 169	0
25	4K	18/27 (66%)	2.13	7 (38%) 0 0	69, 124, 164, 170	0
25	4L	14/27 (51%)	0.68	2 (14%) 2 1	87, 122, 152, 154	0
26	14	2811/2917 (96%)	0.16	27 (0%) 82 68	52, 85, 154, 176	0
26	1H	2850/2917 (97%)	0.19	22 (0%) 86 73	41, 73, 157, 180	0
27	16	122/122 (100%)	-0.24	1 (0%) 86 73	67, 90, 108, 164	0
27	1J	122/122 (100%)	-0.21	1 (0%) 86 73	85, 110, 127, 162	0
28	11	273/276 (98%)	1.24	59 (21%) 0 0	45, 67, 87, 99	0
28	19	274/276 (99%)	1.65	94 (34%) 0 0	50, 73, 91, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	21	205/206 (99%)	1.17	42 (20%) 1 0	51, 88, 122, 131	0
29	29	204/206 (99%)	1.07	43 (21%) 1 0	58, 97, 127, 140	0
30	31	202/210 (96%)	1.11	40 (19%) 1 0	47, 80, 115, 131	0
30	39	204/210 (97%)	1.18	52 (25%) 0 0	57, 102, 138, 149	0
31	41	179/182 (98%)	0.58	22 (12%) 4 2	84, 104, 132, 151	0
31	49	180/182 (98%)	1.78	62 (34%) 0 0	103, 122, 144, 154	0
32	51	174/180 (96%)	0.30	6 (3%) 45 29	83, 101, 117, 136	0
32	59	169/180 (93%)	2.33	73 (43%) 0 0	129, 156, 164, 168	0
33	61	145/148 (97%)	0.02	2 (1%) 75 59	79, 121, 132, 139	0
33	69	145/148 (97%)	0.05	3 (2%) 63 46	84, 117, 137, 143	0
34	15	137/140 (97%)	2.19	72 (52%) 0 0	80, 106, 131, 138	0
34	58	125/140 (89%)	1.51	40 (32%) 0 0	69, 89, 105, 131	0
35	25	122/122 (100%)	2.55	76 (62%) 0 0	68, 89, 105, 119	0
35	68	122/122 (100%)	1.21	20 (16%) 1 1	60, 78, 97, 105	0
36	35	147/150 (98%)	1.67	54 (36%) 0 0	59, 99, 130, 139	0
36	78	148/150 (98%)	0.67	16 (10%) 5 3	52, 83, 109, 121	0
37	45	138/141 (97%)	2.41	69 (50%) 0 0	72, 100, 121, 133	0
37	88	141/141 (100%)	1.55	42 (29%) 0 0	56, 80, 102, 129	0
38	55	118/118 (100%)	1.17	26 (22%) 0 0	64, 84, 99, 110	0
38	98	118/118 (100%)	1.74	51 (43%) 0 0	63, 83, 102, 115	0
39	65	110/112 (98%)	0.78	16 (14%) 2 1	86, 106, 125, 130	0
39	A8	111/112 (99%)	1.03	21 (18%) 1 0	77, 88, 106, 113	0
40	75	140/146 (95%)	1.29	37 (26%) 0 0	82, 98, 145, 155	0
40	B8	136/146 (93%)	0.91	25 (18%) 1 1	73, 92, 131, 146	0
41	85	116/118 (98%)	1.22	26 (22%) 0 0	68, 93, 128, 140	0
41	C8	115/118 (97%)	0.71	10 (8%) 10 6	56, 79, 108, 116	0
42	95	100/101 (99%)	0.58	10 (10%) 7 4	66, 114, 131, 136	0
42	D8	100/101 (99%)	0.80	10 (10%) 7 4	55, 101, 120, 127	0
43	A5	111/113 (98%)	2.19	54 (48%) 0 0	66, 78, 103, 131	0
43	E8	110/113 (97%)	1.35	27 (24%) 0 0	59, 74, 98, 108	0
44	B5	94/96 (97%)	1.36	22 (23%) 0 0	72, 84, 105, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	F8	95/96 (98%)	0.97	18 (18%) 1 0	57, 70, 101, 112	0
45	C5	52/110 (47%)	3.37	40 (76%) 0 0	93, 103, 119, 123	0
45	G8	97/110 (88%)	0.57	4 (4%) 37 24	76, 96, 127, 133	0
46	D5	177/206 (85%)	2.26	84 (47%) 0 0	106, 131, 162, 166	0
46	H8	170/206 (82%)	1.48	52 (30%) 0 0	81, 116, 154, 162	0
47	E5	76/85 (89%)	1.84	30 (39%) 0 0	66, 87, 102, 110	0
47	I8	77/85 (90%)	1.21	17 (22%) 0 0	57, 72, 96, 104	0
48	F5	94/98 (95%)	1.90	40 (42%) 0 0	63, 83, 121, 129	0
48	J8	96/98 (97%)	1.87	39 (40%) 0 0	53, 75, 123, 138	0
49	G5	69/72 (95%)	0.71	4 (5%) 23 14	85, 106, 126, 142	0
49	K8	68/72 (94%)	1.03	9 (13%) 3 2	63, 84, 103, 121	0
50	H5	58/60 (96%)	2.18	28 (48%) 0 0	77, 98, 120, 127	0
50	L8	58/60 (96%)	0.68	7 (12%) 4 2	60, 81, 108, 113	0
51	M8	60/71 (84%)	0.63	8 (13%) 3 2	105, 135, 148, 152	0
52	J5	56/60 (93%)	1.47	21 (37%) 0 0	60, 85, 127, 136	0
52	N8	48/60 (80%)	1.26	12 (25%) 0 0	51, 87, 121, 128	0
53	L5	48/49 (97%)	3.07	33 (68%) 0 0	52, 61, 95, 104	0
53	P8	47/49 (95%)	1.00	7 (14%) 2 1	47, 52, 71, 89	0
54	M5	64/65 (98%)	2.36	35 (54%) 0 0	68, 81, 95, 115	0
54	Q8	64/65 (98%)	1.36	18 (28%) 0 0	56, 69, 83, 95	0
55	3L	70/76 (92%)	-0.03	3 (4%) 35 22	80, 150, 162, 164	0
All	All	20486/21509 (95%)	0.71	2870 (14%) 2 1	41, 98, 147, 180	0

The worst 5 of 2870 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	59	151	ILE	16.1
32	59	112	PRO	14.6
32	59	111	HIS	14.3
12	3A	64	TYR	13.4
32	59	114	VAL	13.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	H2U	1L	17	20/21	0.46	0.39	153,166,172,174	0
22	H2U	1K	17	20/21	0.54	0.26	153,168,175,178	0
55	PSU	3L	55	20/21	0.87	0.11	140,146,152,152	0
22	PSU	1L	55	20/21	0.90	0.10	122,134,145,147	0
23	4SU	2L	8	20/21	0.90	0.12	99,111,114,120	0
55	5MU	3L	54	21/22	0.91	0.09	136,142,145,152	0
22	5MU	1L	54	21/22	0.92	0.11	122,128,134,140	0
23	7MG	2L	47	24/25	0.92	0.13	113,120,131,141	0
22	5MU	1K	54	21/22	0.93	0.15	100,111,121,127	0
23	PSU	2L	56	20/21	0.93	0.10	108,116,121,124	0
23	4SU	2K	8	20/21	0.94	0.14	85,93,98,99	0
23	7MG	2K	47	24/25	0.94	0.15	94,102,111,114	0
23	5MU	2K	55	21/22	0.95	0.15	99,109,114,119	0
23	PSU	2K	56	20/21	0.95	0.10	96,104,114,115	0
22	PSU	1K	55	20/21	0.95	0.11	104,115,130,130	0
23	OMC	2L	33	21/22	0.96	0.16	93,95,98,101	0
22	AET	1L	37	33/34	0.96	0.23	94,112,119,124	0
23	OMC	2K	33	21/22	0.96	0.30	71,78,80,88	0
22	AET	1K	37	33/34	0.97	0.24	69,82,106,115	0
23	5MU	2L	55	21/22	0.98	0.10	116,121,123,124	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	1G	1666	1/1	0.12	0.09	122,122,122,122	0
56	MG	1G	1663	1/1	0.13	0.34	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	14	3245	1/1	0.40	0.42	104,104,104,104	0
56	MG	13	1726	1/1	0.41	0.27	99,99,99,99	0
56	MG	1H	3448	1/1	0.43	0.20	96,96,96,96	0
56	MG	1H	3430	1/1	0.44	0.34	80,80,80,80	0
56	MG	13	1763	1/1	0.44	0.56	131,131,131,131	0
56	MG	68	201	1/1	0.44	0.19	84,84,84,84	0
56	MG	1H	3345	1/1	0.47	0.26	87,87,87,87	0
56	MG	1H	3340	1/1	0.48	0.33	83,83,83,83	0
56	MG	14	3216	1/1	0.48	0.18	91,91,91,91	0
56	MG	13	1674	1/1	0.48	0.17	101,101,101,101	0
56	MG	14	3053	1/1	0.49	0.20	72,72,72,72	0
56	MG	BA	202	1/1	0.51	3.85	113,113,113,113	0
56	MG	13	1606	1/1	0.51	0.19	81,81,81,81	0
56	MG	13	1682	1/1	0.51	0.29	116,116,116,116	0
56	MG	13	1711	1/1	0.51	0.26	114,114,114,114	0
56	MG	13	1662	1/1	0.53	0.29	105,105,105,105	0
56	MG	68	202	1/1	0.53	0.19	90,90,90,90	0
56	MG	14	3179	1/1	0.54	0.43	83,83,83,83	0
56	MG	1H	3294	1/1	0.55	0.16	112,112,112,112	0
56	MG	35	201	1/1	0.55	0.20	84,84,84,84	0
56	MG	14	3211	1/1	0.56	0.26	111,111,111,111	0
56	MG	1G	1674	1/1	0.56	0.16	106,106,106,106	0
56	MG	14	3178	1/1	0.56	0.40	85,85,85,85	0
56	MG	1H	3301	1/1	0.56	0.19	95,95,95,95	0
56	MG	14	3193	1/1	0.57	0.20	88,88,88,88	0
56	MG	14	3201	1/1	0.57	0.38	91,91,91,91	0
56	MG	16	209	1/1	0.57	0.22	81,81,81,81	0
56	MG	1H	3481	1/1	0.58	0.13	122,122,122,122	0
56	MG	14	3427	1/1	0.58	0.08	104,104,104,104	0
56	MG	1H	3608	1/1	0.58	0.08	110,110,110,110	0
56	MG	1H	3176	1/1	0.59	0.27	93,93,93,93	0
56	MG	1H	3445	1/1	0.59	0.34	90,90,90,90	0
56	MG	1G	1661	1/1	0.60	0.18	94,94,94,94	0
56	MG	1H	3241	1/1	0.60	0.21	93,93,93,93	0
56	MG	1J	205	1/1	0.60	0.17	118,118,118,118	0
56	MG	1H	3523	1/1	0.60	0.18	82,82,82,82	0
56	MG	13	1706	1/1	0.61	1.38	111,111,111,111	0
56	MG	1H	3186	1/1	0.61	0.28	97,97,97,97	0
56	MG	1H	3463	1/1	0.61	0.07	101,101,101,101	0
56	MG	1H	3093	1/1	0.61	0.20	56,56,56,56	0
56	MG	1H	3172	1/1	0.61	0.40	96,96,96,96	0
56	MG	1H	3177	1/1	0.62	0.36	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	13	1631	1/1	0.62	0.08	88,88,88,88	0
56	MG	14	3424	1/1	0.62	0.09	94,94,94,94	0
56	MG	1H	3193	1/1	0.62	0.31	89,89,89,89	0
56	MG	14	3029	1/1	0.62	0.20	96,96,96,96	0
56	MG	1H	3138	1/1	0.62	0.23	75,75,75,75	0
56	MG	1H	3139	1/1	0.63	0.24	79,79,79,79	0
56	MG	16	213	1/1	0.63	0.09	98,98,98,98	0
56	MG	1G	1643	1/1	0.63	0.26	92,92,92,92	0
56	MG	1G	1630	1/1	0.64	0.18	95,95,95,95	0
56	MG	1H	3337	1/1	0.64	0.14	99,99,99,99	0
56	MG	55	201	1/1	0.64	0.31	85,85,85,85	0
56	MG	14	3292	1/1	0.65	0.19	88,88,88,88	0
56	MG	13	1804	1/1	0.65	0.14	137,137,137,137	0
56	MG	1H	3479	1/1	0.65	0.12	107,107,107,107	0
56	MG	1H	3328	1/1	0.65	0.27	86,86,86,86	0
56	MG	1H	3021	1/1	0.65	0.29	67,67,67,67	0
56	MG	13	1667	1/1	0.65	0.22	86,86,86,86	0
56	MG	13	1764	1/1	0.66	0.52	128,128,128,128	0
56	MG	14	3278	1/1	0.66	0.23	74,74,74,74	0
56	MG	1G	1672	1/1	0.66	0.36	96,96,96,96	0
56	MG	13	1608	1/1	0.66	0.12	111,111,111,111	0
56	MG	1H	3227	1/1	0.67	0.21	99,99,99,99	0
56	MG	5I	101	1/1	0.67	0.29	85,85,85,85	0
56	MG	14	3047	1/1	0.67	0.26	80,80,80,80	0
56	MG	1H	3292	1/1	0.67	0.19	108,108,108,108	0
56	MG	13	1619	1/1	0.67	0.11	95,95,95,95	0
56	MG	1G	1675	1/1	0.67	0.20	92,92,92,92	0
56	MG	1G	1715	1/1	0.68	0.07	119,119,119,119	0
56	MG	1G	1651	1/1	0.68	0.22	107,107,107,107	0
56	MG	14	3235	1/1	0.68	0.19	88,88,88,88	0
56	MG	16	211	1/1	0.68	0.31	79,79,79,79	0
56	MG	1H	3307	1/1	0.68	0.31	89,89,89,89	0
56	MG	1G	1665	1/1	0.68	0.17	107,107,107,107	0
56	MG	1H	3205	1/1	0.68	0.49	94,94,94,94	0
56	MG	1H	3333	1/1	0.68	0.51	96,96,96,96	0
56	MG	14	3183	1/1	0.68	0.21	96,96,96,96	0
56	MG	13	1741	1/1	0.68	0.27	99,99,99,99	0
56	MG	1H	3053	1/1	0.68	0.17	53,53,53,53	0
56	MG	13	1670	1/1	0.69	0.11	84,84,84,84	0
56	MG	1H	3465	1/1	0.69	0.11	111,111,111,111	0
56	MG	1G	1654	1/1	0.69	0.14	98,98,98,98	0
56	MG	13	1737	1/1	0.69	0.20	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3248	1/1	0.69	0.19	86,86,86,86	0
56	MG	14	3286	1/1	0.69	0.29	93,93,93,93	0
56	MG	16	207	1/1	0.70	0.25	110,110,110,110	0
56	MG	13	1788	1/1	0.70	0.08	123,123,123,123	0
56	MG	1H	3264	1/1	0.70	0.87	74,74,74,74	0
56	MG	1H	3482	1/1	0.70	0.07	142,142,142,142	0
56	MG	1H	3332	1/1	0.70	0.79	83,83,83,83	0
56	MG	1H	3266	1/1	0.70	0.28	83,83,83,83	0
56	MG	25	201	1/1	0.70	0.04	123,123,123,123	0
56	MG	1G	1604	1/1	0.70	0.21	87,87,87,87	0
56	MG	16	206	1/1	0.70	0.21	80,80,80,80	0
56	MG	14	3023	1/1	0.71	0.22	82,82,82,82	0
56	MG	1H	3265	1/1	0.71	0.19	72,72,72,72	0
56	MG	1H	3459	1/1	0.71	0.35	102,102,102,102	0
56	MG	1H	3070	1/1	0.71	0.15	78,78,78,78	0
56	MG	14	3229	1/1	0.71	0.36	92,92,92,92	0
56	MG	1H	3268	1/1	0.71	0.18	86,86,86,86	0
56	MG	1H	3252	1/1	0.71	0.10	102,102,102,102	0
56	MG	13	1686	1/1	0.71	0.60	129,129,129,129	0
56	MG	1G	1667	1/1	0.72	0.65	104,104,104,104	0
56	MG	14	3277	1/1	0.72	0.22	90,90,90,90	0
56	MG	1H	3185	1/1	0.72	0.21	87,87,87,87	0
56	MG	1H	3419	1/1	0.72	0.21	77,77,77,77	0
56	MG	1H	3426	1/1	0.72	0.29	80,80,80,80	0
56	MG	1H	3293	1/1	0.72	0.31	95,95,95,95	0
56	MG	1G	1722	1/1	0.72	0.51	111,111,111,111	0
56	MG	13	1696	1/1	0.72	2.85	104,104,104,104	0
56	MG	13	1689	1/1	0.72	0.64	105,105,105,105	0
56	MG	1H	3575	1/1	0.72	0.10	63,63,63,63	0
56	MG	1H	3283	1/1	0.72	0.24	79,79,79,79	0
56	MG	14	3206	1/1	0.73	0.27	87,87,87,87	0
56	MG	13	1712	1/1	0.73	1.39	106,106,106,106	0
56	MG	14	3318	1/1	0.73	0.14	84,84,84,84	0
56	MG	1G	1696	1/1	0.73	0.29	103,103,103,103	0
56	MG	13	1690	1/1	0.73	0.12	118,118,118,118	0
56	MG	1H	3269	1/1	0.73	0.28	80,80,80,80	0
56	MG	1H	3055	1/1	0.73	0.12	69,69,69,69	0
56	MG	13	1748	1/1	0.73	0.08	122,122,122,122	0
56	MG	13	1727	1/1	0.73	0.19	103,103,103,103	0
56	MG	1G	1605	1/1	0.74	0.16	105,105,105,105	0
56	MG	14	3215	1/1	0.74	0.26	94,94,94,94	0
56	MG	13	1673	1/1	0.74	0.27	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1G	1642	1/1	0.74	0.21	110,110,110,110	0
56	MG	1H	3564	1/1	0.74	0.18	95,95,95,95	0
56	MG	1H	3219	1/1	0.74	0.46	98,98,98,98	0
56	MG	14	3262	1/1	0.74	0.43	87,87,87,87	0
56	MG	1H	3441	1/1	0.74	0.10	115,115,115,115	0
56	MG	13	1607	1/1	0.74	0.20	78,78,78,78	0
56	MG	1H	3235	1/1	0.74	0.24	66,66,66,66	0
56	MG	14	3073	1/1	0.74	0.15	72,72,72,72	0
56	MG	14	3300	1/1	0.74	0.21	84,84,84,84	0
56	MG	14	3312	1/1	0.74	0.08	99,99,99,99	0
56	MG	14	3154	1/1	0.74	0.27	87,87,87,87	0
56	MG	1H	3270	1/1	0.74	0.28	87,87,87,87	0
56	MG	1H	3180	1/1	0.74	0.38	88,88,88,88	0
56	MG	13	1622	1/1	0.74	0.30	72,72,72,72	0
56	MG	1H	3054	1/1	0.74	0.29	78,78,78,78	0
56	MG	1H	3386	1/1	0.74	0.37	96,96,96,96	0
56	MG	13	1685	1/1	0.74	0.48	114,114,114,114	0
56	MG	1G	1656	1/1	0.75	0.15	99,99,99,99	0
56	MG	14	3041	1/1	0.75	0.26	85,85,85,85	0
56	MG	1G	1626	1/1	0.75	0.28	102,102,102,102	0
56	MG	14	3051	1/1	0.75	0.14	75,75,75,75	0
56	MG	1H	3568	1/1	0.75	0.10	89,89,89,89	0
56	MG	1H	3520	1/1	0.75	0.14	54,54,54,54	0
56	MG	14	3224	1/1	0.75	0.29	101,101,101,101	0
56	MG	78	202	1/1	0.75	1.41	87,87,87,87	0
56	MG	14	3435	1/1	0.75	0.08	121,121,121,121	0
56	MG	14	3168	1/1	0.75	0.30	65,65,65,65	0
56	MG	1G	1752	1/1	0.75	0.06	139,139,139,139	0
56	MG	21	301	1/1	0.75	0.14	64,64,64,64	0
56	MG	31	301	1/1	0.75	0.09	67,67,67,67	0
56	MG	13	1710	1/1	0.76	2.00	103,103,103,103	0
56	MG	1H	3599	1/1	0.76	0.11	85,85,85,85	0
56	MG	1H	3228	1/1	0.76	0.32	85,85,85,85	0
56	MG	1G	1718	1/1	0.76	0.17	140,140,140,140	0
56	MG	1G	1639	1/1	0.76	0.21	113,113,113,113	0
56	MG	14	3315	1/1	0.76	0.10	93,93,93,93	0
56	MG	1H	3046	1/1	0.76	0.67	73,73,73,73	0
56	MG	14	3217	1/1	0.76	0.12	96,96,96,96	0
56	MG	1H	3238	1/1	0.76	0.39	87,87,87,87	0
56	MG	2L	102	1/1	0.76	0.06	113,113,113,113	0
56	MG	1H	3213	1/1	0.76	0.15	69,69,69,69	0
56	MG	13	1734	1/1	0.76	0.23	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3184	1/1	0.76	0.12	85,85,85,85	0
56	MG	35	202	1/1	0.76	0.26	79,79,79,79	0
56	MG	14	3191	1/1	0.76	0.66	84,84,84,84	0
56	MG	1H	3096	1/1	0.77	0.24	63,63,63,63	0
56	MG	14	3065	1/1	0.77	0.22	90,90,90,90	0
56	MG	1G	1627	1/1	0.77	0.09	88,88,88,88	0
56	MG	1H	3162	1/1	0.77	0.26	70,70,70,70	0
56	MG	14	3275	1/1	0.77	0.31	77,77,77,77	0
56	MG	1G	1695	1/1	0.77	0.23	96,96,96,96	0
56	MG	1H	3202	1/1	0.77	0.30	84,84,84,84	0
56	MG	1H	3434	1/1	0.77	0.17	86,86,86,86	0
56	MG	1H	3300	1/1	0.77	0.52	86,86,86,86	0
56	MG	1G	1646	1/1	0.77	0.23	116,116,116,116	0
56	MG	1G	1734	1/1	0.77	0.12	94,94,94,94	0
56	MG	1H	3165	1/1	0.77	0.42	98,98,98,98	0
56	MG	1H	3562	1/1	0.77	0.10	97,97,97,97	0
56	MG	14	3319	1/1	0.77	0.07	104,104,104,104	0
56	MG	14	3330	1/1	0.77	0.16	82,82,82,82	0
56	MG	14	3205	1/1	0.77	0.27	75,75,75,75	0
56	MG	13	1666	1/1	0.77	0.13	92,92,92,92	0
56	MG	14	3210	1/1	0.77	0.33	100,100,100,100	0
56	MG	1H	3456	1/1	0.77	0.08	100,100,100,100	0
56	MG	1H	3370	1/1	0.77	1.53	84,84,84,84	0
56	MG	1H	3595	1/1	0.77	0.07	99,99,99,99	0
56	MG	1H	3597	1/1	0.77	0.10	92,92,92,92	0
56	MG	1H	3316	1/1	0.77	0.18	106,106,106,106	0
56	MG	14	3157	1/1	0.78	0.19	86,86,86,86	0
56	MG	4L	401	1/1	0.78	0.23	99,99,99,99	0
56	MG	14	3012	1/1	0.78	0.24	66,66,66,66	0
56	MG	21	302	1/1	0.78	1.24	76,76,76,76	0
56	MG	13	1665	1/1	0.78	0.42	117,117,117,117	0
56	MG	1H	3142	1/1	0.78	0.23	79,79,79,79	0
56	MG	14	3385	1/1	0.78	0.16	84,84,84,84	0
56	MG	1H	3462	1/1	0.78	0.08	95,95,95,95	0
56	MG	1G	1738	1/1	0.78	0.33	105,105,105,105	0
56	MG	1G	1739	1/1	0.78	0.09	107,107,107,107	0
56	MG	14	3276	1/1	0.78	0.24	92,92,92,92	0
56	MG	1G	1685	1/1	0.78	0.22	76,76,76,76	0
56	MG	14	3071	1/1	0.78	0.18	83,83,83,83	0
56	MG	1G	1647	1/1	0.78	0.44	92,92,92,92	0
56	MG	1H	3062	1/1	0.78	0.18	72,72,72,72	0
56	MG	1H	3579	1/1	0.79	0.09	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3068	1/1	0.79	0.21	78,78,78,78	0
56	MG	13	1757	1/1	0.79	0.11	119,119,119,119	0
56	MG	13	1725	1/1	0.79	0.80	101,101,101,101	0
56	MG	14	3317	1/1	0.79	0.12	153,153,153,153	0
56	MG	1H	3487	1/1	0.79	0.09	50,50,50,50	0
56	MG	1G	1673	1/1	0.79	0.23	104,104,104,104	0
56	MG	14	3162	1/1	0.79	0.14	89,89,89,89	0
56	MG	1H	3189	1/1	0.79	0.18	77,77,77,77	0
56	MG	14	3391	1/1	0.79	0.08	106,106,106,106	0
56	MG	1H	3016	1/1	0.79	0.27	66,66,66,66	0
56	MG	1H	3223	1/1	0.79	0.37	65,65,65,65	0
56	MG	1H	3196	1/1	0.79	0.43	68,68,68,68	0
56	MG	1G	1609	1/1	0.79	0.12	96,96,96,96	0
56	MG	1G	1659	1/1	0.79	0.36	104,104,104,104	0
56	MG	1G	1716	1/1	0.79	0.10	109,109,109,109	0
56	MG	1H	3473	1/1	0.79	0.12	112,112,112,112	0
56	MG	1H	3259	1/1	0.79	0.50	69,69,69,69	0
56	MG	1G	1669	1/1	0.80	0.22	85,85,85,85	0
56	MG	1H	3236	1/1	0.80	0.25	80,80,80,80	0
56	MG	1H	3284	1/1	0.80	0.30	79,79,79,79	0
56	MG	1H	3291	1/1	0.80	0.09	97,97,97,97	0
56	MG	14	3129	1/1	0.80	0.22	84,84,84,84	0
56	MG	13	1721	1/1	0.80	0.21	74,74,74,74	0
56	MG	1J	202	1/1	0.80	0.07	92,92,92,92	0
56	MG	1H	3229	1/1	0.80	0.13	83,83,83,83	0
56	MG	13	1789	1/1	0.80	0.08	63,63,63,63	0
56	MG	1H	3281	1/1	0.80	0.24	86,86,86,86	0
56	MG	1G	1701	1/1	0.80	0.36	94,94,94,94	0
56	MG	35	203	1/1	0.80	0.30	81,81,81,81	0
56	MG	14	3320	1/1	0.80	0.17	120,120,120,120	0
56	MG	1H	3422	1/1	0.81	0.27	90,90,90,90	0
56	MG	13	1801	1/1	0.81	0.12	113,113,113,113	0
56	MG	14	3160	1/1	0.81	0.47	86,86,86,86	0
56	MG	1G	1743	1/1	0.81	0.07	122,122,122,122	0
56	MG	1G	1748	1/1	0.81	0.07	107,107,107,107	0
56	MG	1H	3614	1/1	0.81	0.26	97,97,97,97	0
56	MG	1H	3121	1/1	0.81	0.24	67,67,67,67	0
56	MG	13	1729	1/1	0.81	0.11	95,95,95,95	0
56	MG	1H	3036	1/1	0.81	0.09	73,73,73,73	0
56	MG	14	3001	1/1	0.81	0.17	76,76,76,76	0
56	MG	14	3006	1/1	0.81	0.18	56,56,56,56	0
56	MG	13	1805	1/1	0.81	0.06	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3526	1/1	0.81	0.12	57,57,57,57	0
56	MG	1H	3209	1/1	0.81	0.23	80,80,80,80	0
56	MG	1H	3298	1/1	0.81	0.28	82,82,82,82	0
56	MG	14	3405	1/1	0.81	0.12	108,108,108,108	0
56	MG	14	3420	1/1	0.81	0.07	86,86,86,86	0
56	MG	14	3421	1/1	0.81	0.30	72,72,72,72	0
56	MG	14	3043	1/1	0.81	0.59	73,73,73,73	0
56	MG	1G	1699	1/1	0.81	0.14	90,90,90,90	0
56	MG	14	3432	1/1	0.81	0.12	91,91,91,91	0
56	MG	1H	3356	1/1	0.81	0.41	76,76,76,76	0
56	MG	1G	1708	1/1	0.81	0.16	105,105,105,105	0
56	MG	1H	3362	1/1	0.81	0.22	69,69,69,69	0
56	MG	1H	3210	1/1	0.81	0.22	68,68,68,68	0
56	MG	1H	3591	1/1	0.81	0.08	70,70,70,70	0
56	MG	1H	3146	1/1	0.81	0.14	71,71,71,71	0
56	MG	14	3124	1/1	0.81	0.34	82,82,82,82	0
56	MG	13	1680	1/1	0.81	0.30	103,103,103,103	0
56	MG	13	1779	1/1	0.82	0.31	106,106,106,106	0
56	MG	1H	3141	1/1	0.82	0.20	71,71,71,71	0
56	MG	1H	3396	1/1	0.82	0.12	71,71,71,71	0
56	MG	1H	3247	1/1	0.82	0.32	65,65,65,65	0
56	MG	14	3171	1/1	0.82	0.30	89,89,89,89	0
56	MG	1H	3297	1/1	0.82	0.28	80,80,80,80	0
56	MG	13	1656	1/1	0.82	0.23	91,91,91,91	0
56	MG	13	1684	1/1	0.82	0.53	99,99,99,99	0
56	MG	1H	3148	1/1	0.82	0.23	89,89,89,89	0
56	MG	14	3018	1/1	0.82	0.13	66,66,66,66	0
56	MG	1H	3435	1/1	0.82	0.11	68,68,68,68	0
56	MG	1H	3153	1/1	0.82	0.49	92,92,92,92	0
56	MG	1H	3312	1/1	0.82	0.23	100,100,100,100	0
56	MG	1H	3065	1/1	0.82	0.14	69,69,69,69	0
56	MG	1H	3455	1/1	0.82	0.07	92,92,92,92	0
56	MG	1H	3028	1/1	0.82	0.17	64,64,64,64	0
56	MG	1H	3457	1/1	0.82	0.11	99,99,99,99	0
56	MG	1H	3071	1/1	0.82	0.23	71,71,71,71	0
56	MG	1H	3034	1/1	0.82	0.19	64,64,64,64	0
56	MG	13	1675	1/1	0.82	0.33	80,80,80,80	0
56	MG	14	3434	1/1	0.82	0.06	61,61,61,61	0
56	MG	13	1702	1/1	0.82	1.01	87,87,87,87	0
56	MG	14	3082	1/1	0.82	0.25	91,91,91,91	0
56	MG	14	3239	1/1	0.82	0.15	53,53,53,53	0
56	MG	14	3110	1/1	0.82	0.40	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1H	3137	1/1	0.82	0.33	74,74,74,74	0
56	MG	14	3273	1/1	0.82	0.23	70,70,70,70	0
56	MG	13	1659	1/1	0.82	0.49	115,115,115,115	0
56	MG	1H	3188	1/1	0.82	0.24	90,90,90,90	0
56	MG	1H	3104	1/1	0.83	0.25	65,65,65,65	0
56	MG	1H	3039	1/1	0.83	0.22	62,62,62,62	0
56	MG	14	3130	1/1	0.83	0.19	65,65,65,65	0
56	MG	14	3140	1/1	0.83	0.11	88,88,88,88	0
56	MG	14	3143	1/1	0.83	0.41	86,86,86,86	0
56	MG	1G	1664	1/1	0.83	0.20	106,106,106,106	0
56	MG	14	3285	1/1	0.83	0.37	95,95,95,95	0
56	MG	14	3156	1/1	0.83	0.12	68,68,68,68	0
56	MG	1H	3271	1/1	0.83	0.17	93,93,93,93	0
56	MG	14	3299	1/1	0.83	0.30	78,78,78,78	0
56	MG	1H	3421	1/1	0.83	0.43	92,92,92,92	0
56	MG	1H	3275	1/1	0.83	0.18	70,70,70,70	0
56	MG	1H	3425	1/1	0.83	0.33	101,101,101,101	0
56	MG	1H	3311	1/1	0.83	0.36	98,98,98,98	0
56	MG	14	3002	1/1	0.83	0.09	49,49,49,49	0
56	MG	1H	3276	1/1	0.83	2.11	68,68,68,68	0
56	MG	1H	3278	1/1	0.83	0.18	69,69,69,69	0
56	MG	1H	3280	1/1	0.83	0.25	90,90,90,90	0
56	MG	14	3365	1/1	0.83	0.10	89,89,89,89	0
56	MG	1H	3437	1/1	0.83	0.07	90,90,90,90	0
56	MG	1G	1693	1/1	0.83	0.20	84,84,84,84	0
56	MG	14	3200	1/1	0.83	0.40	72,72,72,72	0
56	MG	1H	3044	1/1	0.83	0.08	66,66,66,66	0
56	MG	13	1714	1/1	0.83	0.20	114,114,114,114	0
56	MG	1H	3033	1/1	0.83	0.21	64,64,64,64	0
56	MG	1H	3194	1/1	0.83	0.27	62,62,62,62	0
56	MG	14	3429	1/1	0.83	0.08	91,91,91,91	0
56	MG	1H	3341	1/1	0.83	0.96	80,80,80,80	0
56	MG	14	3064	1/1	0.83	0.44	53,53,53,53	0
56	MG	1H	3080	1/1	0.83	0.30	80,80,80,80	0
56	MG	1H	3347	1/1	0.83	0.73	89,89,89,89	0
56	MG	13	1613	1/1	0.83	0.12	78,78,78,78	0
56	MG	29	301	1/1	0.83	0.17	78,78,78,78	0
56	MG	1H	3361	1/1	0.83	0.08	89,89,89,89	0
56	MG	13	1753	1/1	0.83	0.07	121,121,121,121	0
56	MG	14	3102	1/1	0.83	0.21	67,67,67,67	0
56	MG	14	3240	1/1	0.83	0.31	86,86,86,86	0
56	MG	1H	3206	1/1	0.83	0.64	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3166	1/1	0.84	0.62	88,88,88,88	0
56	MG	1H	3063	1/1	0.84	0.12	54,54,54,54	0
56	MG	88	202	1/1	0.84	0.43	69,69,69,69	0
56	MG	14	3298	1/1	0.84	0.31	100,100,100,100	0
56	MG	13	1774	1/1	0.84	0.10	87,87,87,87	0
56	MG	13	1605	1/1	0.84	0.14	86,86,86,86	0
56	MG	14	3309	1/1	0.84	0.11	87,87,87,87	0
56	MG	1H	3029	1/1	0.84	0.14	69,69,69,69	0
56	MG	1H	3590	1/1	0.84	0.06	107,107,107,107	0
56	MG	1H	3031	1/1	0.84	0.16	56,56,56,56	0
56	MG	13	1621	1/1	0.84	0.30	74,74,74,74	0
56	MG	1G	1631	1/1	0.84	0.21	85,85,85,85	0
56	MG	1H	3404	1/1	0.84	0.25	80,80,80,80	0
56	MG	1H	3418	1/1	0.84	0.17	90,90,90,90	0
56	MG	14	3343	1/1	0.84	0.12	54,54,54,54	0
56	MG	1G	1710	1/1	0.84	0.13	102,102,102,102	0
56	MG	14	3369	1/1	0.84	0.14	87,87,87,87	0
56	MG	1H	3603	1/1	0.84	0.07	121,121,121,121	0
56	MG	1H	3329	1/1	0.84	0.19	75,75,75,75	0
56	MG	14	3400	1/1	0.84	0.10	87,87,87,87	0
56	MG	1H	3610	1/1	0.84	0.15	106,106,106,106	0
56	MG	14	3077	1/1	0.84	0.43	87,87,87,87	0
56	MG	1H	3470	1/1	0.84	0.16	94,94,94,94	0
56	MG	14	3218	1/1	0.84	0.37	104,104,104,104	0
56	MG	1G	1727	1/1	0.84	0.09	108,108,108,108	0
56	MG	1G	1652	1/1	0.84	0.24	87,87,87,87	0
56	MG	13	1678	1/1	0.84	0.22	97,97,97,97	0
56	MG	1H	3097	1/1	0.84	0.31	70,70,70,70	0
56	MG	1H	3334	1/1	0.84	0.47	93,93,93,93	0
56	MG	1H	3336	1/1	0.84	0.17	81,81,81,81	0
56	MG	1H	3056	1/1	0.84	0.11	73,73,73,73	0
56	MG	1H	3489	1/1	0.84	0.12	53,53,53,53	0
56	MG	1H	3195	1/1	0.84	0.67	84,84,84,84	0
56	MG	13	1792	1/1	0.84	0.15	73,73,73,73	0
56	MG	1H	3201	1/1	0.84	0.32	77,77,77,77	0
56	MG	1H	3136	1/1	0.84	0.29	68,68,68,68	0
56	MG	14	3281	1/1	0.84	0.17	89,89,89,89	0
56	MG	13	1653	1/1	0.85	0.11	82,82,82,82	0
56	MG	14	3287	1/1	0.85	0.42	86,86,86,86	0
56	MG	1H	3578	1/1	0.85	0.09	65,65,65,65	0
56	MG	D8	201	1/1	0.85	0.46	76,76,76,76	0
56	MG	1G	1603	1/1	0.85	0.10	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3222	1/1	0.85	0.40	78,78,78,78	0
56	MG	13	1603	1/1	0.85	0.12	52,52,52,52	0
56	MG	1H	3183	1/1	0.85	0.27	80,80,80,80	0
56	MG	14	3030	1/1	0.85	0.18	78,78,78,78	0
56	MG	1H	3335	1/1	0.85	0.13	103,103,103,103	0
56	MG	1H	3466	1/1	0.85	0.16	115,115,115,115	0
56	MG	1H	3198	1/1	0.85	0.44	108,108,108,108	0
56	MG	1G	1698	1/1	0.85	0.23	88,88,88,88	0
56	MG	14	3323	1/1	0.85	0.18	100,100,100,100	0
56	MG	1H	3424	1/1	0.85	0.21	65,65,65,65	0
56	MG	1H	3025	1/1	0.85	0.18	49,49,49,49	0
56	MG	1G	1641	1/1	0.85	0.09	95,95,95,95	0
56	MG	13	1639	1/1	0.85	0.18	76,76,76,76	0
56	MG	1H	3187	1/1	0.85	0.27	75,75,75,75	0
56	MG	14	3072	1/1	0.85	0.37	69,69,69,69	0
56	MG	1H	3621	1/1	0.85	0.12	52,52,52,52	0
56	MG	1H	3484	1/1	0.85	0.10	45,45,45,45	0
56	MG	14	3225	1/1	0.85	0.43	111,111,111,111	0
56	MG	1H	3237	1/1	0.85	0.19	72,72,72,72	0
56	MG	14	3230	1/1	0.85	0.20	90,90,90,90	0
56	MG	1G	1725	1/1	0.85	0.05	111,111,111,111	0
56	MG	1H	3041	1/1	0.85	0.16	65,65,65,65	0
56	MG	1G	1729	1/1	0.85	0.24	113,113,113,113	0
56	MG	2K	102	1/1	0.85	0.30	81,81,81,81	0
56	MG	1H	3191	1/1	0.85	0.21	99,99,99,99	0
56	MG	14	3268	1/1	0.85	0.21	83,83,83,83	0
56	MG	1G	1658	1/1	0.85	0.21	108,108,108,108	0
56	MG	1H	3010	1/1	0.85	0.23	70,70,70,70	0
56	MG	39	301	1/1	0.85	0.17	94,94,94,94	0
56	MG	1H	3547	1/1	0.85	0.11	85,85,85,85	0
56	MG	1H	3317	1/1	0.85	0.13	102,102,102,102	0
56	MG	31	302	1/1	0.85	0.28	76,76,76,76	0
56	MG	1H	3218	1/1	0.85	0.28	70,70,70,70	0
56	MG	1H	3387	1/1	0.85	0.35	71,71,71,71	0
56	MG	85	201	1/1	0.85	0.33	75,75,75,75	0
56	MG	14	3084	1/1	0.86	0.10	77,77,77,77	0
56	MG	88	203	1/1	0.86	0.68	79,79,79,79	0
56	MG	1H	3060	1/1	0.86	0.25	63,63,63,63	0
56	MG	13	1668	1/1	0.86	0.39	101,101,101,101	0
56	MG	1H	3447	1/1	0.86	0.10	65,65,65,65	0
56	MG	1H	3100	1/1	0.86	0.16	69,69,69,69	0
56	MG	1G	1702	1/1	0.86	0.30	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3073	1/1	0.86	0.28	58,58,58,58	0
56	MG	1G	1616	1/1	0.86	0.43	100,100,100,100	0
56	MG	14	3360	1/1	0.86	0.10	69,69,69,69	0
56	MG	1H	3145	1/1	0.86	0.45	91,91,91,91	0
56	MG	1H	3049	1/1	0.86	0.10	95,95,95,95	0
56	MG	14	3158	1/1	0.86	0.29	80,80,80,80	0
56	MG	1H	3207	1/1	0.86	0.41	87,87,87,87	0
56	MG	1G	1721	1/1	0.86	0.08	143,143,143,143	0
56	MG	14	3402	1/1	0.86	0.11	94,94,94,94	0
56	MG	1H	3461	1/1	0.86	0.08	102,102,102,102	0
56	MG	14	3045	1/1	0.86	0.24	91,91,91,91	0
56	MG	1G	1637	1/1	0.86	0.08	121,121,121,121	0
56	MG	1G	1726	1/1	0.86	0.17	86,86,86,86	0
56	MG	1G	1638	1/1	0.86	0.18	93,93,93,93	0
56	MG	14	3057	1/1	0.86	0.16	78,78,78,78	0
56	MG	1H	3522	1/1	0.86	0.10	59,59,59,59	0
56	MG	13	1697	1/1	0.86	1.59	98,98,98,98	0
56	MG	1H	3095	1/1	0.86	0.21	64,64,64,64	0
56	MG	78	201	1/1	0.86	0.27	62,62,62,62	0
56	MG	14	3290	1/1	0.86	0.34	85,85,85,85	0
56	MG	14	3291	1/1	0.86	0.41	86,86,86,86	0
56	MG	1G	1683	1/1	0.86	0.28	87,87,87,87	0
56	MG	14	3294	1/1	0.86	0.28	94,94,94,94	0
56	MG	14	3297	1/1	0.86	0.28	91,91,91,91	0
56	MG	1G	1745	1/1	0.86	0.08	124,124,124,124	0
56	MG	1H	3342	1/1	0.86	1.77	75,75,75,75	0
56	MG	14	3209	1/1	0.86	0.19	97,97,97,97	0
56	MG	1H	3417	1/1	0.86	0.17	93,93,93,93	0
56	MG	1H	3040	1/1	0.87	0.20	62,62,62,62	0
56	MG	1H	3472	1/1	0.87	0.11	108,108,108,108	0
56	MG	1H	3358	1/1	0.87	0.57	83,83,83,83	0
56	MG	1H	3598	1/1	0.87	0.10	105,105,105,105	0
56	MG	1G	1625	1/1	0.87	0.17	111,111,111,111	0
56	MG	13	1707	1/1	0.87	0.84	108,108,108,108	0
56	MG	1G	1687	1/1	0.87	0.25	96,96,96,96	0
56	MG	1H	3436	1/1	0.87	0.14	98,98,98,98	0
56	MG	1H	3324	1/1	0.87	0.27	78,78,78,78	0
56	MG	13	1610	1/1	0.87	0.10	56,56,56,56	0
56	MG	14	3306	1/1	0.87	0.18	66,66,66,66	0
56	MG	1H	3444	1/1	0.87	0.10	78,78,78,78	0
56	MG	1K	500	1/1	0.87	0.14	101,101,101,101	0
56	MG	1H	3498	1/1	0.87	0.08	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3231	1/1	0.87	0.11	83,83,83,83	0
56	MG	14	3197	1/1	0.87	0.22	91,91,91,91	0
56	MG	14	3046	1/1	0.87	0.09	56,56,56,56	0
56	MG	13	1724	1/1	0.87	0.11	97,97,97,97	0
56	MG	13	1705	1/1	0.87	1.02	111,111,111,111	0
56	MG	14	3052	1/1	0.87	0.27	78,78,78,78	0
56	MG	14	3208	1/1	0.87	0.68	89,89,89,89	0
56	MG	1H	3134	1/1	0.87	0.44	85,85,85,85	0
56	MG	14	3054	1/1	0.87	0.18	48,48,48,48	0
56	MG	14	3367	1/1	0.87	0.14	86,86,86,86	0
56	MG	14	3368	1/1	0.87	0.07	101,101,101,101	0
56	MG	16	214	1/1	0.87	0.09	82,82,82,82	0
56	MG	14	3372	1/1	0.87	0.25	91,91,91,91	0
56	MG	14	3213	1/1	0.87	0.34	87,87,87,87	0
56	MG	13	1663	1/1	0.87	0.17	105,105,105,105	0
56	MG	1G	1720	1/1	0.87	0.23	112,112,112,112	0
56	MG	1H	3550	1/1	0.87	0.18	70,70,70,70	0
56	MG	1H	3554	1/1	0.87	0.19	108,108,108,108	0
56	MG	1H	3019	1/1	0.87	0.14	53,53,53,53	0
56	MG	1H	3304	1/1	0.87	0.21	106,106,106,106	0
56	MG	1H	3174	1/1	0.87	0.27	86,86,86,86	0
56	MG	14	3079	1/1	0.87	0.11	91,91,91,91	0
56	MG	1H	3573	1/1	0.87	0.07	51,51,51,51	0
56	MG	1H	3574	1/1	0.87	0.11	53,53,53,53	0
56	MG	14	3092	1/1	0.87	0.14	79,79,79,79	0
56	MG	14	3099	1/1	0.87	0.13	66,66,66,66	0
56	MG	1G	1735	1/1	0.87	0.06	112,112,112,112	0
56	MG	1H	3308	1/1	0.87	0.48	78,78,78,78	0
56	MG	1H	3083	1/1	0.87	0.24	82,82,82,82	0
56	MG	14	3125	1/1	0.87	0.18	84,84,84,84	0
56	MG	13	1747	1/1	0.87	0.29	93,93,93,93	0
56	MG	P8	101	1/1	0.87	0.24	68,68,68,68	0
56	MG	1G	1746	1/1	0.87	0.18	95,95,95,95	0
56	MG	14	3280	1/1	0.87	0.30	89,89,89,89	0
56	MG	1H	3469	1/1	0.87	0.32	93,93,93,93	0
56	MG	1G	1671	1/1	0.87	0.15	92,92,92,92	0
56	MG	1H	3239	1/1	0.88	0.31	78,78,78,78	0
56	MG	14	3025	1/1	0.88	0.12	46,46,46,46	0
56	MG	1H	3026	1/1	0.88	0.25	92,92,92,92	0
56	MG	1H	3290	1/1	0.88	0.40	94,94,94,94	0
56	MG	14	3176	1/1	0.88	0.24	73,73,73,73	0
56	MG	14	3034	1/1	0.88	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	13	1799	1/1	0.88	0.10	93,93,93,93	0
56	MG	1H	3212	1/1	0.88	0.28	91,91,91,91	0
56	MG	16	202	1/1	0.88	0.11	77,77,77,77	0
56	MG	14	3186	1/1	0.88	0.20	77,77,77,77	0
56	MG	14	3310	1/1	0.88	0.11	53,53,53,53	0
56	MG	1H	3151	1/1	0.88	0.25	78,78,78,78	0
56	MG	1G	1712	1/1	0.88	0.08	132,132,132,132	0
56	MG	1H	3256	1/1	0.88	0.18	85,85,85,85	0
56	MG	13	1614	1/1	0.88	0.13	69,69,69,69	0
56	MG	1H	3516	1/1	0.88	0.09	59,59,59,59	0
56	MG	1H	3343	1/1	0.88	0.15	76,76,76,76	0
56	MG	14	3322	1/1	0.88	0.17	123,123,123,123	0
56	MG	1H	3192	1/1	0.88	0.28	75,75,75,75	0
56	MG	1H	3439	1/1	0.88	0.14	59,59,59,59	0
56	MG	1H	3047	1/1	0.88	0.13	60,60,60,60	0
56	MG	1H	3127	1/1	0.88	0.21	81,81,81,81	0
56	MG	1H	3267	1/1	0.88	0.31	84,84,84,84	0
56	MG	1H	3012	1/1	0.88	0.08	40,40,40,40	0
56	MG	13	1669	1/1	0.88	0.22	109,109,109,109	0
56	MG	1H	3453	1/1	0.88	0.07	94,94,94,94	0
56	MG	13	1693	1/1	0.88	0.15	82,82,82,82	0
56	MG	14	3373	1/1	0.88	0.09	117,117,117,117	0
56	MG	14	3080	1/1	0.88	0.16	86,86,86,86	0
56	MG	13	1648	1/1	0.88	0.36	77,77,77,77	0
56	MG	1H	3272	1/1	0.88	0.15	85,85,85,85	0
56	MG	1H	3233	1/1	0.88	0.13	85,85,85,85	0
56	MG	14	3403	1/1	0.88	0.11	101,101,101,101	0
56	MG	14	3096	1/1	0.88	0.31	87,87,87,87	0
56	MG	14	3411	1/1	0.88	0.07	109,109,109,109	0
56	MG	1H	3090	1/1	0.88	0.19	73,73,73,73	0
56	MG	14	3100	1/1	0.88	0.18	65,65,65,65	0
56	MG	1G	1601	1/1	0.88	0.11	71,71,71,71	0
56	MG	1H	3408	1/1	0.88	0.37	60,60,60,60	0
56	MG	42	201	1/1	0.88	0.30	103,103,103,103	0
56	MG	1H	3410	1/1	0.88	0.47	71,71,71,71	0
56	MG	14	3433	1/1	0.88	0.11	87,87,87,87	0
56	MG	1H	3416	1/1	0.88	0.30	75,75,75,75	0
56	MG	1H	3023	1/1	0.88	0.34	72,72,72,72	0
56	MG	14	3135	1/1	0.88	0.11	90,90,90,90	0
56	MG	1H	3058	1/1	0.88	0.16	69,69,69,69	0
56	MG	1J	206	1/1	0.88	0.27	68,68,68,68	0
56	MG	1G	1619	1/1	0.88	0.18	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3279	1/1	0.88	0.47	96,96,96,96	0
56	MG	1G	1621	1/1	0.88	0.32	89,89,89,89	0
56	MG	14	3009	1/1	0.88	0.20	78,78,78,78	0
56	MG	14	3284	1/1	0.88	0.23	77,77,77,77	0
56	MG	14	3011	1/1	0.88	0.52	70,70,70,70	0
56	MG	13	1765	1/1	0.88	0.45	129,129,129,129	0
56	MG	1H	3420	1/1	0.88	0.39	75,75,75,75	0
56	MG	1H	3179	1/1	0.89	0.26	93,93,93,93	0
56	MG	1H	3318	1/1	0.89	0.68	68,68,68,68	0
56	MG	1H	3323	1/1	0.89	0.45	69,69,69,69	0
56	MG	1H	3216	1/1	0.89	0.57	81,81,81,81	0
56	MG	1H	3217	1/1	0.89	0.20	87,87,87,87	0
56	MG	13	1683	1/1	0.89	0.21	99,99,99,99	0
56	MG	14	3008	1/1	0.89	0.33	72,72,72,72	0
56	MG	1H	3182	1/1	0.89	0.27	85,85,85,85	0
56	MG	1H	3107	1/1	0.89	0.22	63,63,63,63	0
56	MG	14	3304	1/1	0.89	0.23	103,103,103,103	0
56	MG	13	1703	1/1	0.89	0.11	93,93,93,93	0
56	MG	1H	3030	1/1	0.89	0.25	75,75,75,75	0
56	MG	13	1609	1/1	0.89	0.15	83,83,83,83	0
56	MG	14	3024	1/1	0.89	0.10	57,57,57,57	0
56	MG	13	1766	1/1	0.89	0.14	70,70,70,70	0
56	MG	14	3026	1/1	0.89	0.12	65,65,65,65	0
56	MG	8I	201	1/1	0.89	0.58	98,98,98,98	0
56	MG	1G	1690	1/1	0.89	0.23	75,75,75,75	0
56	MG	14	3190	1/1	0.89	0.23	81,81,81,81	0
56	MG	14	3321	1/1	0.89	0.14	131,131,131,131	0
56	MG	1H	3067	1/1	0.89	0.18	68,68,68,68	0
56	MG	13	1768	1/1	0.89	0.10	92,92,92,92	0
56	MG	1H	3288	1/1	0.89	0.79	79,79,79,79	0
56	MG	14	3340	1/1	0.89	0.10	57,57,57,57	0
56	MG	14	3342	1/1	0.89	0.13	51,51,51,51	0
56	MG	1G	1697	1/1	0.89	0.21	106,106,106,106	0
56	MG	13	1773	1/1	0.89	0.07	96,96,96,96	0
56	MG	1H	3450	1/1	0.89	0.17	84,84,84,84	0
56	MG	14	3366	1/1	0.89	0.14	87,87,87,87	0
56	MG	1H	3582	1/1	0.89	0.06	56,56,56,56	0
56	MG	1H	3001	1/1	0.89	0.18	55,55,55,55	0
56	MG	1G	1703	1/1	0.89	0.13	87,87,87,87	0
56	MG	1H	3075	1/1	0.89	0.21	72,72,72,72	0
56	MG	1H	3594	1/1	0.89	0.17	95,95,95,95	0
56	MG	13	1723	1/1	0.89	0.22	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1746	1/1	0.89	0.25	96,96,96,96	0
56	MG	14	3067	1/1	0.89	0.13	62,62,62,62	0
56	MG	1G	1635	1/1	0.89	0.22	106,106,106,106	0
56	MG	1H	3296	1/1	0.89	0.77	68,68,68,68	0
56	MG	1H	3244	1/1	0.89	0.19	70,70,70,70	0
56	MG	14	3410	1/1	0.89	0.12	81,81,81,81	0
56	MG	1H	3374	1/1	0.89	0.26	101,101,101,101	0
56	MG	14	3074	1/1	0.89	0.09	84,84,84,84	0
56	MG	1H	3086	1/1	0.89	0.11	83,83,83,83	0
56	MG	13	1784	1/1	0.89	0.10	104,104,104,104	0
56	MG	1H	3092	1/1	0.89	0.21	62,62,62,62	0
56	MG	13	1629	1/1	0.89	0.12	71,71,71,71	0
56	MG	1H	3407	1/1	0.89	0.33	81,81,81,81	0
56	MG	1G	1650	1/1	0.89	0.09	81,81,81,81	0
56	MG	13	1671	1/1	0.89	0.44	99,99,99,99	0
56	MG	1H	3261	1/1	0.89	0.16	92,92,92,92	0
56	MG	1H	3414	1/1	0.89	0.15	68,68,68,68	0
56	MG	14	3101	1/1	0.89	0.24	79,79,79,79	0
56	MG	1G	1655	1/1	0.89	0.09	121,121,121,121	0
56	MG	16	210	1/1	0.89	0.36	101,101,101,101	0
56	MG	13	1688	1/1	0.89	0.29	86,86,86,86	0
56	MG	13	1793	1/1	0.89	0.15	114,114,114,114	0
56	MG	1H	3313	1/1	0.89	0.65	87,87,87,87	0
56	MG	14	3283	1/1	0.89	0.29	84,84,84,84	0
56	MG	1G	1753	1/1	0.89	0.12	109,109,109,109	0
56	MG	14	3134	1/1	0.89	0.24	81,81,81,81	0
56	MG	13	1698	1/1	0.89	2.42	99,99,99,99	0
56	MG	14	3308	1/1	0.90	0.13	80,80,80,80	0
56	MG	1H	3373	1/1	0.90	0.17	84,84,84,84	0
56	MG	13	1762	1/1	0.90	0.21	128,128,128,128	0
56	MG	1H	3382	1/1	0.90	0.22	73,73,73,73	0
56	MG	13	1736	1/1	0.90	0.35	96,96,96,96	0
56	MG	1H	3032	1/1	0.90	0.45	57,57,57,57	0
56	MG	1G	1633	1/1	0.90	0.31	94,94,94,94	0
56	MG	14	3214	1/1	0.90	0.59	90,90,90,90	0
56	MG	1H	3009	1/1	0.90	0.20	66,66,66,66	0
56	MG	13	1636	1/1	0.90	0.19	85,85,85,85	0
56	MG	1H	3168	1/1	0.90	0.09	84,84,84,84	0
56	MG	1H	3204	1/1	0.90	0.34	92,92,92,92	0
56	MG	14	3324	1/1	0.90	0.13	50,50,50,50	0
56	MG	14	3219	1/1	0.90	0.14	100,100,100,100	0
56	MG	13	1704	1/1	0.90	0.17	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	13	1624	1/1	0.90	0.10	102,102,102,102	0
56	MG	14	3128	1/1	0.90	0.26	82,82,82,82	0
56	MG	14	3352	1/1	0.90	0.21	90,90,90,90	0
56	MG	13	1767	1/1	0.90	0.14	61,61,61,61	0
56	MG	14	3364	1/1	0.90	0.10	108,108,108,108	0
56	MG	1G	1706	1/1	0.90	0.12	95,95,95,95	0
56	MG	1H	3565	1/1	0.90	0.08	110,110,110,110	0
56	MG	1H	3113	1/1	0.90	0.41	67,67,67,67	0
56	MG	14	3027	1/1	0.90	0.15	61,61,61,61	0
56	MG	1H	3020	1/1	0.90	0.10	56,56,56,56	0
56	MG	14	3264	1/1	0.90	0.29	82,82,82,82	0
56	MG	14	3267	1/1	0.90	0.34	77,77,77,77	0
56	MG	14	3380	1/1	0.90	0.14	92,92,92,92	0
56	MG	14	3149	1/1	0.90	0.15	74,74,74,74	0
56	MG	14	3388	1/1	0.90	0.18	87,87,87,87	0
56	MG	14	3270	1/1	0.90	0.20	70,70,70,70	0
56	MG	14	3393	1/1	0.90	0.13	67,67,67,67	0
56	MG	14	3272	1/1	0.90	0.34	94,94,94,94	0
56	MG	1G	1714	1/1	0.90	0.05	123,123,123,123	0
56	MG	14	3155	1/1	0.90	0.23	65,65,65,65	0
56	MG	1H	3043	1/1	0.90	0.12	48,48,48,48	0
56	MG	13	1802	1/1	0.90	0.07	114,114,114,114	0
56	MG	1H	3214	1/1	0.90	0.40	93,93,93,93	0
56	MG	1H	3468	1/1	0.90	0.18	92,92,92,92	0
56	MG	1H	3581	1/1	0.90	0.12	87,87,87,87	0
56	MG	14	3423	1/1	0.90	0.11	95,95,95,95	0
56	MG	1G	1657	1/1	0.90	0.20	117,117,117,117	0
56	MG	13	1642	1/1	0.90	0.20	66,66,66,66	0
56	MG	1H	3589	1/1	0.90	0.14	60,60,60,60	0
56	MG	1H	3078	1/1	0.90	0.30	59,59,59,59	0
56	MG	1H	3079	1/1	0.90	0.27	59,59,59,59	0
56	MG	13	1728	1/1	0.90	0.26	97,97,97,97	0
56	MG	14	3289	1/1	0.90	0.13	79,79,79,79	0
56	MG	1H	3477	1/1	0.90	0.29	90,90,90,90	0
56	MG	1H	3140	1/1	0.90	0.30	78,78,78,78	0
56	MG	1G	1606	1/1	0.90	0.12	97,97,97,97	0
56	MG	1G	1742	1/1	0.90	0.09	131,131,131,131	0
56	MG	13	1694	1/1	0.90	0.12	96,96,96,96	0
56	MG	13	1709	1/1	0.90	0.24	73,73,73,73	0
56	MG	1G	1617	1/1	0.90	0.05	92,92,92,92	0
56	MG	1H	3087	1/1	0.90	0.17	54,54,54,54	0
56	MG	13	1758	1/1	0.90	0.24	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1G	1624	1/1	0.90	0.25	109,109,109,109	0
56	MG	14	3307	1/1	0.90	0.12	89,89,89,89	0
56	MG	1H	3082	1/1	0.91	0.15	76,76,76,76	0
56	MG	1G	1747	1/1	0.91	0.12	95,95,95,95	0
56	MG	13	1672	1/1	0.91	0.14	80,80,80,80	0
56	MG	14	3133	1/1	0.91	0.28	78,78,78,78	0
56	MG	1H	3084	1/1	0.91	0.22	72,72,72,72	0
56	MG	13	1660	1/1	0.91	0.11	83,83,83,83	0
56	MG	13	1625	1/1	0.91	0.25	75,75,75,75	0
56	MG	4A	201	1/1	0.91	0.10	116,116,116,116	0
56	MG	9A	101	1/1	0.91	0.07	115,115,115,115	0
56	MG	13	1749	1/1	0.91	0.06	92,92,92,92	0
56	MG	1H	3068	1/1	0.91	0.21	65,65,65,65	0
56	MG	13	1769	1/1	0.91	0.11	82,82,82,82	0
56	MG	41	201	1/1	0.91	0.12	69,69,69,69	0
56	MG	13	1720	1/1	0.91	0.13	97,97,97,97	0
56	MG	1H	3535	1/1	0.91	0.09	80,80,80,80	0
56	MG	1H	3536	1/1	0.91	0.10	62,62,62,62	0
56	MG	1H	3543	1/1	0.91	0.14	59,59,59,59	0
56	MG	14	3311	1/1	0.91	0.10	105,105,105,105	0
56	MG	14	3010	1/1	0.91	0.16	68,68,68,68	0
56	MG	88	201	1/1	0.91	0.26	79,79,79,79	0
56	MG	14	3173	1/1	0.91	0.11	77,77,77,77	0
56	MG	1H	3351	1/1	0.91	0.26	68,68,68,68	0
56	MG	1H	3354	1/1	0.91	0.09	81,81,81,81	0
56	MG	13	1657	1/1	0.91	0.22	101,101,101,101	0
56	MG	13	1658	1/1	0.91	0.19	96,96,96,96	0
56	MG	1H	3076	1/1	0.91	0.16	88,88,88,88	0
56	MG	1H	3220	1/1	0.91	0.29	79,79,79,79	0
56	MG	1H	3364	1/1	0.91	0.12	87,87,87,87	0
56	MG	1H	3367	1/1	0.91	0.15	97,97,97,97	0
56	MG	1H	3101	1/1	0.91	0.38	91,91,91,91	0
56	MG	14	3032	1/1	0.91	0.15	73,73,73,73	0
56	MG	1H	3452	1/1	0.91	0.04	81,81,81,81	0
56	MG	14	3035	1/1	0.91	0.16	67,67,67,67	0
56	MG	14	3353	1/1	0.91	0.08	64,64,64,64	0
56	MG	14	3038	1/1	0.91	0.13	63,63,63,63	0
56	MG	14	3039	1/1	0.91	0.15	61,61,61,61	0
56	MG	1G	1613	1/1	0.91	0.09	88,88,88,88	0
56	MG	14	3042	1/1	0.91	0.34	82,82,82,82	0
56	MG	1H	3309	1/1	0.91	0.47	76,76,76,76	0
56	MG	1H	3077	1/1	0.91	0.45	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3580	1/1	0.91	0.33	77,77,77,77	0
56	MG	1H	3158	1/1	0.91	0.17	81,81,81,81	0
56	MG	1G	1705	1/1	0.91	0.10	84,84,84,84	0
56	MG	13	1630	1/1	0.91	0.12	74,74,74,74	0
56	MG	1G	1707	1/1	0.91	0.08	92,92,92,92	0
56	MG	1H	3315	1/1	0.91	0.26	101,101,101,101	0
56	MG	14	3055	1/1	0.91	0.27	89,89,89,89	0
56	MG	14	3220	1/1	0.91	0.13	95,95,95,95	0
56	MG	14	3222	1/1	0.91	0.33	94,94,94,94	0
56	MG	1H	3163	1/1	0.91	0.28	74,74,74,74	0
56	MG	1H	3230	1/1	0.91	0.18	96,96,96,96	0
56	MG	1H	3592	1/1	0.91	0.09	96,96,96,96	0
56	MG	13	1681	1/1	0.91	0.12	98,98,98,98	0
56	MG	1H	3116	1/1	0.91	0.28	71,71,71,71	0
56	MG	14	3418	1/1	0.91	0.12	99,99,99,99	0
56	MG	14	3419	1/1	0.91	0.06	84,84,84,84	0
56	MG	1G	1717	1/1	0.91	0.07	129,129,129,129	0
56	MG	1H	3409	1/1	0.91	0.53	75,75,75,75	0
56	MG	1H	3279	1/1	0.91	0.15	93,93,93,93	0
56	MG	1H	3412	1/1	0.91	0.17	86,86,86,86	0
56	MG	1H	3413	1/1	0.91	0.19	81,81,81,81	0
56	MG	14	3266	1/1	0.91	0.26	85,85,85,85	0
56	MG	1H	3471	1/1	0.91	0.36	91,91,91,91	0
56	MG	1H	3200	1/1	0.91	0.18	79,79,79,79	0
56	MG	1H	3415	1/1	0.91	0.31	77,77,77,77	0
56	MG	1G	1728	1/1	0.91	0.11	96,96,96,96	0
56	MG	1H	3618	1/1	0.91	0.36	104,104,104,104	0
56	MG	1G	1732	1/1	0.91	0.08	102,102,102,102	0
56	MG	1H	3476	1/1	0.91	0.08	92,92,92,92	0
56	MG	1G	1648	1/1	0.91	0.24	85,85,85,85	0
56	MG	1H	3170	1/1	0.91	0.17	73,73,73,73	0
56	MG	16	205	1/1	0.91	0.17	70,70,70,70	0
56	MG	13	1745	1/1	0.91	0.20	87,87,87,87	0
56	MG	14	3118	1/1	0.91	0.07	66,66,66,66	0
56	MG	1H	3173	1/1	0.91	0.14	67,67,67,67	0
56	MG	45	201	1/1	0.91	0.06	95,95,95,95	0
56	MG	1H	3285	1/1	0.91	1.01	85,85,85,85	0
56	MG	14	3126	1/1	0.91	0.24	102,102,102,102	0
56	MG	1H	3059	1/1	0.92	0.17	60,60,60,60	0
56	MG	14	3164	1/1	0.92	0.36	105,105,105,105	0
56	MG	14	3036	1/1	0.92	0.34	71,71,71,71	0
56	MG	1H	3098	1/1	0.92	0.18	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	14	3170	1/1	0.92	0.23	105,105,105,105	0
56	MG	1H	3366	1/1	0.92	0.08	89,89,89,89	0
56	MG	14	3172	1/1	0.92	0.18	77,77,77,77	0
56	MG	1H	3326	1/1	0.92	0.18	67,67,67,67	0
56	MG	13	1640	1/1	0.92	0.16	65,65,65,65	0
56	MG	1H	3052	1/1	0.92	0.10	41,41,41,41	0
56	MG	14	3044	1/1	0.92	0.09	71,71,71,71	0
56	MG	1H	3103	1/1	0.92	0.39	64,64,64,64	0
56	MG	1H	3376	1/1	0.92	0.26	113,113,113,113	0
56	MG	14	3185	1/1	0.92	0.31	78,78,78,78	0
56	MG	1G	1660	1/1	0.92	0.15	91,91,91,91	0
56	MG	1G	1731	1/1	0.92	0.08	99,99,99,99	0
56	MG	1H	3480	1/1	0.92	0.08	113,113,113,113	0
56	MG	13	1743	1/1	0.92	0.20	91,91,91,91	0
56	MG	1H	3105	1/1	0.92	0.15	54,54,54,54	0
56	MG	13	1787	1/1	0.92	0.18	109,109,109,109	0
56	MG	14	3056	1/1	0.92	0.09	80,80,80,80	0
56	MG	1H	3593	1/1	0.92	0.21	61,61,61,61	0
56	MG	1H	3393	1/1	0.92	0.12	65,65,65,65	0
56	MG	1H	3488	1/1	0.92	0.18	53,53,53,53	0
56	MG	14	3332	1/1	0.92	0.09	57,57,57,57	0
56	MG	1G	1607	1/1	0.92	0.19	104,104,104,104	0
56	MG	1G	1608	1/1	0.92	0.17	108,108,108,108	0
56	MG	14	3070	1/1	0.92	0.14	72,72,72,72	0
56	MG	14	3345	1/1	0.92	0.10	89,89,89,89	0
56	MG	14	3349	1/1	0.92	0.09	60,60,60,60	0
56	MG	14	3212	1/1	0.92	0.43	91,91,91,91	0
56	MG	1H	3143	1/1	0.92	0.23	78,78,78,78	0
56	MG	14	3358	1/1	0.92	0.07	80,80,80,80	0
56	MG	1H	3493	1/1	0.92	0.15	48,48,48,48	0
56	MG	14	3362	1/1	0.92	0.08	96,96,96,96	0
56	MG	1H	3401	1/1	0.92	0.34	77,77,77,77	0
56	MG	1G	1679	1/1	0.92	0.16	74,74,74,74	0
56	MG	1G	1755	1/1	0.92	0.05	119,119,119,119	0
56	MG	1H	3144	1/1	0.92	0.16	57,57,57,57	0
56	MG	2A	201	1/1	0.92	0.11	85,85,85,85	0
56	MG	1H	3405	1/1	0.92	0.24	80,80,80,80	0
56	MG	14	3221	1/1	0.92	0.10	88,88,88,88	0
56	MG	1H	3339	1/1	0.92	0.27	74,74,74,74	0
56	MG	1H	3066	1/1	0.92	0.20	66,66,66,66	0
56	MG	1B	101	1/1	0.92	0.17	92,92,92,92	0
56	MG	1H	3616	1/1	0.92	0.35	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1G	1694	1/1	0.92	0.15	102,102,102,102	0
56	MG	1H	3221	1/1	0.92	0.34	89,89,89,89	0
56	MG	1H	3620	1/1	0.92	0.05	73,73,73,73	0
56	MG	14	3003	1/1	0.92	0.13	47,47,47,47	0
56	MG	14	3004	1/1	0.92	0.12	73,73,73,73	0
56	MG	14	3256	1/1	0.92	0.13	75,75,75,75	0
56	MG	14	3261	1/1	0.92	0.40	93,93,93,93	0
56	MG	1G	1628	1/1	0.92	0.31	89,89,89,89	0
56	MG	14	3263	1/1	0.92	0.41	81,81,81,81	0
56	MG	14	3007	1/1	0.92	0.10	61,61,61,61	0
56	MG	1H	3534	1/1	0.92	0.11	51,51,51,51	0
56	MG	1H	3310	1/1	0.92	0.15	82,82,82,82	0
56	MG	13	1735	1/1	0.92	0.33	85,85,85,85	0
56	MG	1G	1634	1/1	0.92	0.15	89,89,89,89	0
56	MG	14	3425	1/1	0.92	0.17	95,95,95,95	0
56	MG	14	3132	1/1	0.92	0.19	58,58,58,58	0
56	MG	13	1687	1/1	0.92	0.26	82,82,82,82	0
56	MG	13	1664	1/1	0.92	0.41	91,91,91,91	0
56	MG	14	3019	1/1	0.92	0.14	70,70,70,70	0
56	MG	14	3139	1/1	0.92	0.18	69,69,69,69	0
56	MG	1H	3287	1/1	0.92	0.79	80,80,80,80	0
56	MG	14	3141	1/1	0.92	0.32	74,74,74,74	0
56	MG	1H	3352	1/1	0.92	0.69	68,68,68,68	0
56	MG	14	3145	1/1	0.92	0.21	88,88,88,88	0
56	MG	1H	3557	1/1	0.92	0.09	59,59,59,59	0
56	MG	1H	3558	1/1	0.92	0.09	100,100,100,100	0
56	MG	1H	3131	1/1	0.92	0.26	65,65,65,65	0
56	MG	1H	3184	1/1	0.92	0.30	79,79,79,79	0
56	MG	1H	3157	1/1	0.92	0.24	78,78,78,78	0
56	MG	14	3288	1/1	0.92	0.32	94,94,94,94	0
56	MG	1H	3319	1/1	0.92	0.15	85,85,85,85	0
56	MG	1H	3570	1/1	0.92	0.11	54,54,54,54	0
56	MG	14	3161	1/1	0.92	0.20	66,66,66,66	0
56	MG	1H	3505	1/1	0.93	0.12	51,51,51,51	0
56	MG	1H	3506	1/1	0.93	0.15	58,58,58,58	0
56	MG	1H	3508	1/1	0.93	0.15	74,74,74,74	0
56	MG	1H	3513	1/1	0.93	0.23	83,83,83,83	0
56	MG	1H	3622	1/1	0.93	0.09	76,76,76,76	0
56	MG	1H	3371	1/1	0.93	0.76	72,72,72,72	0
56	MG	14	3192	1/1	0.93	0.09	77,77,77,77	0
56	MG	1G	1730	1/1	0.93	0.08	72,72,72,72	0
56	MG	14	3313	1/1	0.93	0.05	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3195	1/1	0.93	0.14	84,84,84,84	0
56	MG	1H	3519	1/1	0.93	0.25	73,73,73,73	0
56	MG	13	1634	1/1	0.93	0.19	118,118,118,118	0
56	MG	1G	1733	1/1	0.93	0.09	121,121,121,121	0
56	MG	1H	3521	1/1	0.93	0.13	66,66,66,66	0
56	MG	14	3066	1/1	0.93	0.24	67,67,67,67	0
56	MG	1H	3199	1/1	0.93	0.08	116,116,116,116	0
56	MG	13	1750	1/1	0.93	0.09	122,122,122,122	0
56	MG	1H	3380	1/1	0.93	0.26	66,66,66,66	0
56	MG	1H	3529	1/1	0.93	0.12	49,49,49,49	0
56	MG	1H	3327	1/1	0.93	0.30	65,65,65,65	0
56	MG	14	3339	1/1	0.93	0.08	61,61,61,61	0
56	MG	13	1643	1/1	0.93	0.29	78,78,78,78	0
56	MG	13	1646	1/1	0.93	0.19	58,58,58,58	0
56	MG	1H	3540	1/1	0.93	0.05	85,85,85,85	0
56	MG	1G	1662	1/1	0.93	0.30	96,96,96,96	0
56	MG	14	3346	1/1	0.93	0.07	60,60,60,60	0
56	MG	1G	1751	1/1	0.93	0.13	95,95,95,95	0
56	MG	1H	3169	1/1	0.93	0.22	56,56,56,56	0
56	MG	14	3083	1/1	0.93	0.15	73,73,73,73	0
56	MG	14	3354	1/1	0.93	0.06	68,68,68,68	0
56	MG	1H	3129	1/1	0.93	0.23	77,77,77,77	0
56	MG	13	1780	1/1	0.93	0.07	106,106,106,106	0
56	MG	1H	3133	1/1	0.93	0.20	67,67,67,67	0
56	MG	14	3223	1/1	0.93	0.08	93,93,93,93	0
56	MG	1H	3556	1/1	0.93	0.11	58,58,58,58	0
56	MG	13	1612	1/1	0.93	0.16	71,71,71,71	0
56	MG	1H	3460	1/1	0.93	0.16	94,94,94,94	0
56	MG	1H	3561	1/1	0.93	0.12	78,78,78,78	0
56	MG	13	1760	1/1	0.93	0.15	127,127,127,127	0
56	MG	1H	3338	1/1	0.93	0.16	83,83,83,83	0
56	MG	1H	3061	1/1	0.93	0.20	66,66,66,66	0
56	MG	14	3378	1/1	0.93	0.11	69,69,69,69	0
56	MG	14	3379	1/1	0.93	0.06	66,66,66,66	0
56	MG	1H	3003	1/1	0.93	0.17	56,56,56,56	0
56	MG	14	3383	1/1	0.93	0.09	62,62,62,62	0
56	MG	14	3251	1/1	0.93	0.24	77,77,77,77	0
56	MG	1G	1681	1/1	0.93	0.22	89,89,89,89	0
56	MG	1H	3091	1/1	0.93	0.20	68,68,68,68	0
56	MG	1H	3467	1/1	0.93	0.14	102,102,102,102	0
56	MG	13	1739	1/1	0.93	0.26	74,74,74,74	0
56	MG	1H	3302	1/1	0.93	0.07	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3265	1/1	0.93	0.16	83,83,83,83	0
56	MG	1G	1691	1/1	0.93	0.33	106,106,106,106	0
56	MG	14	3406	1/1	0.93	0.07	60,60,60,60	0
56	MG	1H	3064	1/1	0.93	0.08	59,59,59,59	0
56	MG	13	1708	1/1	0.93	0.22	76,76,76,76	0
56	MG	1H	3011	1/1	0.93	0.12	46,46,46,46	0
56	MG	1G	1610	1/1	0.93	0.22	83,83,83,83	0
56	MG	13	1677	1/1	0.93	0.26	94,94,94,94	0
56	MG	1G	1615	1/1	0.93	0.32	87,87,87,87	0
56	MG	14	3020	1/1	0.93	0.27	55,55,55,55	0
56	MG	13	1620	1/1	0.93	0.40	69,69,69,69	0
56	MG	14	3151	1/1	0.93	0.34	88,88,88,88	0
56	MG	1H	3583	1/1	0.93	0.17	52,52,52,52	0
56	MG	1H	3355	1/1	0.93	0.36	62,62,62,62	0
56	MG	1H	3478	1/1	0.93	0.17	68,68,68,68	0
56	MG	13	1795	1/1	0.93	0.15	100,100,100,100	0
56	MG	13	1654	1/1	0.93	0.32	86,86,86,86	0
56	MG	13	1800	1/1	0.93	0.20	118,118,118,118	0
56	MG	1J	201	1/1	0.93	0.30	95,95,95,95	0
56	MG	1H	3048	1/1	0.93	0.27	67,67,67,67	0
56	MG	1J	203	1/1	0.93	0.10	98,98,98,98	0
56	MG	14	3033	1/1	0.93	0.13	86,86,86,86	0
56	MG	1H	3363	1/1	0.93	0.22	83,83,83,83	0
56	MG	1H	3154	1/1	0.93	0.17	74,74,74,74	0
56	MG	1G	1713	1/1	0.93	0.08	119,119,119,119	0
56	MG	1H	3156	1/1	0.93	0.40	69,69,69,69	0
56	MG	13	1616	1/1	0.93	0.38	79,79,79,79	0
56	MG	1H	3601	1/1	0.93	0.09	84,84,84,84	0
56	MG	1H	3368	1/1	0.93	0.22	106,106,106,106	0
56	MG	1H	3496	1/1	0.93	0.12	66,66,66,66	0
56	MG	13	1713	1/1	0.93	0.22	82,82,82,82	0
56	MG	1H	3501	1/1	0.93	0.12	57,57,57,57	0
56	MG	1H	3502	1/1	0.94	0.15	49,49,49,49	0
56	MG	1H	3161	1/1	0.94	0.23	76,76,76,76	0
56	MG	1H	3108	1/1	0.94	0.29	87,87,87,87	0
56	MG	1H	3245	1/1	0.94	0.23	57,57,57,57	0
56	MG	1H	3512	1/1	0.94	0.13	65,65,65,65	0
56	MG	13	1615	1/1	0.94	0.23	103,103,103,103	0
56	MG	1H	3431	1/1	0.94	0.13	54,54,54,54	0
56	MG	1H	3432	1/1	0.94	0.14	83,83,83,83	0
56	MG	14	3146	1/1	0.94	0.27	83,83,83,83	0
56	MG	1H	3357	1/1	0.94	0.30	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	16	208	1/1	0.94	0.30	95,95,95,95	0
56	MG	14	3153	1/1	0.94	0.18	90,90,90,90	0
56	MG	1H	3017	1/1	0.94	0.18	51,51,51,51	0
56	MG	1H	3018	1/1	0.94	0.17	49,49,49,49	0
56	MG	1G	1668	1/1	0.94	0.30	106,106,106,106	0
56	MG	1H	3125	1/1	0.94	0.16	52,52,52,52	0
56	MG	16	212	1/1	0.94	0.37	65,65,65,65	0
56	MG	14	3159	1/1	0.94	0.20	66,66,66,66	0
56	MG	1H	3257	1/1	0.94	0.27	82,82,82,82	0
56	MG	1H	3527	1/1	0.94	0.17	50,50,50,50	0
56	MG	13	1754	1/1	0.94	0.25	108,108,108,108	0
56	MG	14	3016	1/1	0.94	0.17	51,51,51,51	0
56	MG	1H	3532	1/1	0.94	0.14	85,85,85,85	0
56	MG	14	3314	1/1	0.94	0.12	126,126,126,126	0
56	MG	1H	3365	1/1	0.94	0.18	83,83,83,83	0
56	MG	14	3169	1/1	0.94	1.10	73,73,73,73	0
56	MG	1H	3171	1/1	0.94	0.24	90,90,90,90	0
56	MG	14	3021	1/1	0.94	0.19	47,47,47,47	0
56	MG	14	3022	1/1	0.94	0.10	78,78,78,78	0
56	MG	1H	3262	1/1	0.94	0.65	73,73,73,73	0
56	MG	14	3175	1/1	0.94	0.11	70,70,70,70	0
56	MG	1H	3538	1/1	0.94	0.10	46,46,46,46	0
56	MG	13	1803	1/1	0.94	0.06	97,97,97,97	0
56	MG	1G	1689	1/1	0.94	0.31	81,81,81,81	0
56	MG	1H	3369	1/1	0.94	0.81	95,95,95,95	0
56	MG	14	3333	1/1	0.94	0.10	80,80,80,80	0
56	MG	13	1679	1/1	0.94	0.36	83,83,83,83	0
56	MG	1G	1692	1/1	0.94	0.35	87,87,87,87	0
56	MG	14	3341	1/1	0.94	0.11	46,46,46,46	0
56	MG	14	3031	1/1	0.94	0.18	63,63,63,63	0
56	MG	1H	3022	1/1	0.94	0.16	51,51,51,51	0
56	MG	1H	3454	1/1	0.94	0.14	93,93,93,93	0
56	MG	13	1604	1/1	0.94	0.08	77,77,77,77	0
56	MG	3E	301	1/1	0.94	0.11	121,121,121,121	0
56	MG	I8	101	1/1	0.94	0.20	83,83,83,83	0
56	MG	13	1781	1/1	0.94	0.07	97,97,97,97	0
56	MG	Q8	101	1/1	0.94	0.19	68,68,68,68	0
56	MG	1G	1700	1/1	0.94	0.28	113,113,113,113	0
56	MG	14	3359	1/1	0.94	0.09	105,105,105,105	0
56	MG	14	3204	1/1	0.94	0.24	76,76,76,76	0
56	MG	1H	3559	1/1	0.94	0.10	73,73,73,73	0
56	MG	14	3363	1/1	0.94	0.04	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3560	1/1	0.94	0.12	84,84,84,84	0
56	MG	14	3207	1/1	0.94	0.18	67,67,67,67	0
56	MG	13	1740	1/1	0.94	0.47	76,76,76,76	0
56	MG	1H	3381	1/1	0.94	0.06	97,97,97,97	0
56	MG	1H	3322	1/1	0.94	0.09	94,94,94,94	0
56	MG	13	1618	1/1	0.94	0.12	97,97,97,97	0
56	MG	14	3050	1/1	0.94	0.09	62,62,62,62	0
56	MG	13	1602	1/1	0.94	0.18	59,59,59,59	0
56	MG	1H	3274	1/1	0.94	0.29	79,79,79,79	0
56	MG	13	1633	1/1	0.94	0.23	82,82,82,82	0
56	MG	1H	3399	1/1	0.94	0.31	61,61,61,61	0
56	MG	14	3382	1/1	0.94	0.06	88,88,88,88	0
56	MG	1G	1614	1/1	0.94	0.12	71,71,71,71	0
56	MG	1H	3400	1/1	0.94	0.29	48,48,48,48	0
56	MG	1H	3577	1/1	0.94	0.10	49,49,49,49	0
56	MG	14	3390	1/1	0.94	0.12	66,66,66,66	0
56	MG	14	3058	1/1	0.94	0.10	78,78,78,78	0
56	MG	13	1661	1/1	0.94	0.20	75,75,75,75	0
56	MG	14	3398	1/1	0.94	0.09	81,81,81,81	0
56	MG	1H	3008	1/1	0.94	0.11	47,47,47,47	0
56	MG	1G	1719	1/1	0.94	0.11	112,112,112,112	0
56	MG	1H	3224	1/1	0.94	0.32	85,85,85,85	0
56	MG	14	3404	1/1	0.94	0.16	85,85,85,85	0
56	MG	1G	1622	1/1	0.94	0.23	87,87,87,87	0
56	MG	1H	3406	1/1	0.94	0.29	91,91,91,91	0
56	MG	14	3408	1/1	0.94	0.14	91,91,91,91	0
56	MG	1H	3225	1/1	0.94	0.16	76,76,76,76	0
56	MG	1H	3226	1/1	0.94	0.13	77,77,77,77	0
56	MG	14	3412	1/1	0.94	0.04	102,102,102,102	0
56	MG	14	3413	1/1	0.94	0.04	93,93,93,93	0
56	MG	14	3417	1/1	0.94	0.12	80,80,80,80	0
56	MG	14	3236	1/1	0.94	0.20	69,69,69,69	0
56	MG	14	3237	1/1	0.94	0.28	81,81,81,81	0
56	MG	1H	3584	1/1	0.94	0.06	58,58,58,58	0
56	MG	1H	3585	1/1	0.94	0.19	95,95,95,95	0
56	MG	14	3422	1/1	0.94	0.14	72,72,72,72	0
56	MG	14	3241	1/1	0.94	0.18	59,59,59,59	0
56	MG	1G	1629	1/1	0.94	0.36	84,84,84,84	0
56	MG	1H	3586	1/1	0.94	0.08	53,53,53,53	0
56	MG	1H	3587	1/1	0.94	0.13	51,51,51,51	0
56	MG	13	1715	1/1	0.94	0.28	102,102,102,102	0
56	MG	14	3431	1/1	0.94	0.12	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1732	1/1	0.94	0.15	65,65,65,65	0
56	MG	1H	3037	1/1	0.94	0.14	57,57,57,57	0
56	MG	1H	3286	1/1	0.94	1.15	68,68,68,68	0
56	MG	13	1717	1/1	0.94	0.18	98,98,98,98	0
56	MG	1H	3150	1/1	0.94	0.17	88,88,88,88	0
56	MG	13	1655	1/1	0.94	0.25	94,94,94,94	0
56	MG	1H	3013	1/1	0.94	0.19	42,42,42,42	0
56	MG	1J	204	1/1	0.94	0.12	95,95,95,95	0
56	MG	1H	3042	1/1	0.94	0.35	79,79,79,79	0
56	MG	1H	3344	1/1	0.94	0.22	89,89,89,89	0
56	MG	1H	3491	1/1	0.94	0.16	57,57,57,57	0
56	MG	14	3123	1/1	0.94	0.19	86,86,86,86	0
56	MG	1H	3015	1/1	0.94	0.20	47,47,47,47	0
56	MG	1H	3106	1/1	0.94	0.17	77,77,77,77	0
56	MG	1H	3074	1/1	0.94	0.10	57,57,57,57	0
56	MG	1H	3613	1/1	0.94	0.09	78,78,78,78	0
56	MG	1G	1754	1/1	0.94	0.08	104,104,104,104	0
56	MG	1H	3423	1/1	0.94	0.33	74,74,74,74	0
56	MG	1H	3615	1/1	0.94	0.06	108,108,108,108	0
56	MG	14	3136	1/1	0.95	0.24	58,58,58,58	0
56	MG	1H	3433	1/1	0.95	0.15	51,51,51,51	0
56	MG	16	201	1/1	0.95	0.29	79,79,79,79	0
56	MG	2L	101	1/1	0.95	0.23	86,86,86,86	0
56	MG	13	1638	1/1	0.95	0.34	85,85,85,85	0
56	MG	16	203	1/1	0.95	0.12	85,85,85,85	0
56	MG	1H	3234	1/1	0.95	0.12	67,67,67,67	0
56	MG	14	3148	1/1	0.95	0.30	84,84,84,84	0
56	MG	1H	3088	1/1	0.95	0.10	62,62,62,62	0
56	MG	14	3150	1/1	0.95	0.12	73,73,73,73	0
56	MG	14	3301	1/1	0.95	0.19	85,85,85,85	0
56	MG	13	1731	1/1	0.95	0.30	75,75,75,75	0
56	MG	1H	3190	1/1	0.95	0.15	80,80,80,80	0
56	MG	13	1771	1/1	0.95	0.14	81,81,81,81	0
56	MG	1H	3443	1/1	0.95	0.18	74,74,74,74	0
56	MG	1H	3024	1/1	0.95	0.13	54,54,54,54	0
56	MG	13	1772	1/1	0.95	0.09	93,93,93,93	0
56	MG	1H	3242	1/1	0.95	0.26	82,82,82,82	0
56	MG	1H	3243	1/1	0.95	0.20	60,60,60,60	0
56	MG	11	301	1/1	0.95	0.30	47,47,47,47	0
56	MG	14	3014	1/1	0.95	0.08	50,50,50,50	0
56	MG	14	3015	1/1	0.95	0.06	51,51,51,51	0
56	MG	1H	3147	1/1	0.95	0.26	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1647	1/1	0.95	0.13	97,97,97,97	0
56	MG	21	303	1/1	0.95	0.23	51,51,51,51	0
56	MG	1H	3246	1/1	0.95	0.21	81,81,81,81	0
56	MG	1H	3149	1/1	0.95	0.24	64,64,64,64	0
56	MG	1H	3552	1/1	0.95	0.12	78,78,78,78	0
56	MG	1G	1686	1/1	0.95	0.32	69,69,69,69	0
56	MG	1H	3553	1/1	0.95	0.07	62,62,62,62	0
56	MG	14	3325	1/1	0.95	0.17	63,63,63,63	0
56	MG	14	3174	1/1	0.95	0.25	81,81,81,81	0
56	MG	14	3331	1/1	0.95	0.19	82,82,82,82	0
56	MG	1G	1688	1/1	0.95	0.19	89,89,89,89	0
56	MG	13	1733	1/1	0.95	0.11	64,64,64,64	0
56	MG	14	3334	1/1	0.95	0.07	51,51,51,51	0
56	MG	14	3335	1/1	0.95	0.12	57,57,57,57	0
56	MG	14	3177	1/1	0.95	0.14	92,92,92,92	0
56	MG	13	1775	1/1	0.95	0.05	68,68,68,68	0
56	MG	1H	3375	1/1	0.95	0.17	70,70,70,70	0
56	MG	14	3182	1/1	0.95	0.10	91,91,91,91	0
56	MG	1H	3253	1/1	0.95	0.21	72,72,72,72	0
56	MG	1H	3314	1/1	0.95	0.12	72,72,72,72	0
56	MG	1H	3255	1/1	0.95	0.22	75,75,75,75	0
56	MG	1H	3152	1/1	0.95	0.26	75,75,75,75	0
56	MG	BI	201	1/1	0.95	0.10	113,113,113,113	0
56	MG	1H	3563	1/1	0.95	0.06	81,81,81,81	0
56	MG	1H	3464	1/1	0.95	0.11	71,71,71,71	0
56	MG	14	3356	1/1	0.95	0.13	81,81,81,81	0
56	MG	1H	3258	1/1	0.95	0.27	115,115,115,115	0
56	MG	1G	1602	1/1	0.95	0.11	83,83,83,83	0
56	MG	14	3196	1/1	0.95	0.13	78,78,78,78	0
56	MG	1H	3388	1/1	0.95	0.26	54,54,54,54	0
56	MG	13	1751	1/1	0.95	0.28	106,106,106,106	0
56	MG	1H	3321	1/1	0.95	0.07	99,99,99,99	0
56	MG	1G	1704	1/1	0.95	0.07	85,85,85,85	0
56	MG	13	1719	1/1	0.95	0.14	106,106,106,106	0
56	MG	13	1628	1/1	0.95	0.18	79,79,79,79	0
56	MG	1H	3576	1/1	0.95	0.06	68,68,68,68	0
56	MG	14	3048	1/1	0.95	0.29	66,66,66,66	0
56	MG	14	3370	1/1	0.95	0.07	70,70,70,70	0
56	MG	14	3049	1/1	0.95	0.10	89,89,89,89	0
56	MG	13	1755	1/1	0.95	0.06	94,94,94,94	0
56	MG	1H	3325	1/1	0.95	0.09	90,90,90,90	0
56	MG	1G	1711	1/1	0.95	0.11	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3159	1/1	0.95	0.21	66,66,66,66	0
56	MG	1H	3474	1/1	0.95	0.05	83,83,83,83	0
56	MG	1H	3475	1/1	0.95	0.19	58,58,58,58	0
56	MG	1H	3208	1/1	0.95	0.29	86,86,86,86	0
56	MG	14	3387	1/1	0.95	0.11	61,61,61,61	0
56	MG	1H	3035	1/1	0.95	0.27	90,90,90,90	0
56	MG	1G	1618	1/1	0.95	0.11	74,74,74,74	0
56	MG	1H	3069	1/1	0.95	0.21	80,80,80,80	0
56	MG	1H	3006	1/1	0.95	0.18	52,52,52,52	0
56	MG	14	3395	1/1	0.95	0.10	89,89,89,89	0
56	MG	1H	3007	1/1	0.95	0.07	60,60,60,60	0
56	MG	1G	1623	1/1	0.95	0.18	86,86,86,86	0
56	MG	1H	3411	1/1	0.95	0.17	71,71,71,71	0
56	MG	1H	3588	1/1	0.95	0.15	52,52,52,52	0
56	MG	1H	3072	1/1	0.95	0.09	86,86,86,86	0
56	MG	14	3227	1/1	0.95	0.12	75,75,75,75	0
56	MG	1H	3115	1/1	0.95	0.12	69,69,69,69	0
56	MG	14	3407	1/1	0.95	0.14	84,84,84,84	0
56	MG	1H	3485	1/1	0.95	0.11	55,55,55,55	0
56	MG	14	3232	1/1	0.95	0.17	66,66,66,66	0
56	MG	13	1785	1/1	0.95	0.25	105,105,105,105	0
56	MG	13	1649	1/1	0.95	0.23	76,76,76,76	0
56	MG	13	1722	1/1	0.95	0.26	99,99,99,99	0
56	MG	13	1738	1/1	0.95	0.21	96,96,96,96	0
56	MG	13	1791	1/1	0.95	0.09	85,85,85,85	0
56	MG	13	1676	1/1	0.95	0.13	68,68,68,68	0
56	MG	1G	1636	1/1	0.95	0.26	99,99,99,99	0
56	MG	14	3248	1/1	0.95	0.20	80,80,80,80	0
56	MG	14	3089	1/1	0.95	0.20	72,72,72,72	0
56	MG	13	1652	1/1	0.95	0.16	75,75,75,75	0
56	MG	1H	3600	1/1	0.95	0.10	84,84,84,84	0
56	MG	13	1701	1/1	0.95	0.88	95,95,95,95	0
56	MG	1H	3135	1/1	0.95	0.30	59,59,59,59	0
56	MG	14	3428	1/1	0.95	0.08	81,81,81,81	0
56	MG	1G	1744	1/1	0.95	0.17	101,101,101,101	0
56	MG	1H	3606	1/1	0.95	0.12	85,85,85,85	0
56	MG	14	3105	1/1	0.95	0.18	64,64,64,64	0
56	MG	14	3107	1/1	0.95	0.19	68,68,68,68	0
56	MG	14	3108	1/1	0.95	0.16	81,81,81,81	0
56	MG	14	3269	1/1	0.95	0.21	80,80,80,80	0
56	MG	1H	3504	1/1	0.95	0.10	56,56,56,56	0
56	MG	14	3111	1/1	0.95	0.24	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1G	1644	1/1	0.95	0.17	100,100,100,100	0
56	MG	1H	3181	1/1	0.95	0.67	71,71,71,71	0
56	MG	1G	1749	1/1	0.95	0.08	114,114,114,114	0
56	MG	1H	3611	1/1	0.95	0.12	88,88,88,88	0
56	MG	1H	3081	1/1	0.95	0.25	91,91,91,91	0
56	MG	29	303	1/1	0.95	0.17	64,64,64,64	0
56	MG	1H	3348	1/1	0.95	0.18	87,87,87,87	0
56	MG	1H	3511	1/1	0.95	0.13	42,42,42,42	0
56	MG	13	1796	1/1	0.95	0.08	79,79,79,79	0
56	MG	14	3131	1/1	0.95	0.38	78,78,78,78	0
56	MG	13	1626	1/1	0.95	0.05	78,78,78,78	0
56	MG	1H	3619	1/1	0.95	0.08	55,55,55,55	0
56	MG	13	1635	1/1	0.95	0.23	75,75,75,75	0
56	MG	13	1632	1/1	0.95	0.30	86,86,86,86	0
56	MG	E5	101	1/1	0.95	0.18	67,67,67,67	0
58	ZN	5A	101	1/1	0.95	0.09	125,125,125,125	0
56	MG	14	3060	1/1	0.96	0.10	64,64,64,64	0
56	MG	14	3061	1/1	0.96	0.09	74,74,74,74	0
56	MG	14	3187	1/1	0.96	0.18	62,62,62,62	0
56	MG	1H	3427	1/1	0.96	0.25	64,64,64,64	0
56	MG	5E	201	1/1	0.96	0.15	79,79,79,79	0
56	MG	13	1794	1/1	0.96	0.09	79,79,79,79	0
56	MG	1H	3178	1/1	0.96	0.14	91,91,91,91	0
56	MG	1H	3085	1/1	0.96	0.18	46,46,46,46	0
56	MG	14	3069	1/1	0.96	0.31	85,85,85,85	0
56	MG	1H	3494	1/1	0.96	0.12	40,40,40,40	0
56	MG	1H	3495	1/1	0.96	0.08	48,48,48,48	0
56	MG	14	3327	1/1	0.96	0.09	63,63,63,63	0
56	MG	14	3328	1/1	0.96	0.08	58,58,58,58	0
56	MG	14	3329	1/1	0.96	0.10	57,57,57,57	0
56	MG	1G	1750	1/1	0.96	0.06	109,109,109,109	0
56	MG	14	3203	1/1	0.96	0.65	83,83,83,83	0
56	MG	I8	102	1/1	0.96	0.05	66,66,66,66	0
56	MG	1H	3211	1/1	0.96	0.19	80,80,80,80	0
56	MG	1H	3111	1/1	0.96	0.20	54,54,54,54	0
56	MG	1H	3330	1/1	0.96	0.43	70,70,70,70	0
56	MG	1H	3377	1/1	0.96	0.24	49,49,49,49	0
56	MG	1G	1676	1/1	0.96	0.14	81,81,81,81	0
56	MG	1H	3438	1/1	0.96	0.07	94,94,94,94	0
56	MG	1G	1680	1/1	0.96	0.26	69,69,69,69	0
56	MG	14	3085	1/1	0.96	0.27	62,62,62,62	0
56	MG	1H	3112	1/1	0.96	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	BA	201	1/1	0.96	0.07	102,102,102,102	0
56	MG	1H	3440	1/1	0.96	0.14	59,59,59,59	0
56	MG	1G	1684	1/1	0.96	0.07	89,89,89,89	0
56	MG	1H	3507	1/1	0.96	0.18	65,65,65,65	0
56	MG	5I	102	1/1	0.96	0.33	100,100,100,100	0
56	MG	1H	3509	1/1	0.96	0.09	77,77,77,77	0
56	MG	1H	3215	1/1	0.96	0.40	61,61,61,61	0
56	MG	14	3106	1/1	0.96	0.26	80,80,80,80	0
56	MG	1H	3114	1/1	0.96	0.42	90,90,90,90	0
56	MG	14	3361	1/1	0.96	0.07	80,80,80,80	0
56	MG	1G	1611	1/1	0.96	0.15	86,86,86,86	0
56	MG	14	3109	1/1	0.96	0.20	69,69,69,69	0
56	MG	13	1782	1/1	0.96	0.09	81,81,81,81	0
56	MG	14	3005	1/1	0.96	0.16	58,58,58,58	0
56	MG	14	3116	1/1	0.96	0.19	57,57,57,57	0
56	MG	1H	3051	1/1	0.96	0.10	46,46,46,46	0
56	MG	14	3231	1/1	0.96	0.23	57,57,57,57	0
56	MG	14	3122	1/1	0.96	0.25	55,55,55,55	0
56	MG	1H	3390	1/1	0.96	0.20	53,53,53,53	0
56	MG	14	3371	1/1	0.96	0.13	84,84,84,84	0
56	MG	1H	3391	1/1	0.96	0.24	61,61,61,61	0
56	MG	1H	3451	1/1	0.96	0.34	85,85,85,85	0
56	MG	14	3374	1/1	0.96	0.15	55,55,55,55	0
56	MG	14	3376	1/1	0.96	0.09	75,75,75,75	0
56	MG	14	3238	1/1	0.96	0.27	85,85,85,85	0
56	MG	1H	3392	1/1	0.96	0.25	54,54,54,54	0
56	MG	1H	3602	1/1	0.96	0.06	88,88,88,88	0
56	MG	1H	3119	1/1	0.96	0.37	76,76,76,76	0
56	MG	14	3243	1/1	0.96	0.11	52,52,52,52	0
56	MG	1H	3394	1/1	0.96	0.31	67,67,67,67	0
56	MG	14	3386	1/1	0.96	0.12	54,54,54,54	0
56	MG	14	3246	1/1	0.96	0.32	86,86,86,86	0
56	MG	1H	3089	1/1	0.96	0.14	62,62,62,62	0
56	MG	14	3389	1/1	0.96	0.09	54,54,54,54	0
56	MG	1H	3397	1/1	0.96	0.34	60,60,60,60	0
56	MG	14	3254	1/1	0.96	0.32	55,55,55,55	0
56	MG	14	3392	1/1	0.96	0.07	62,62,62,62	0
56	MG	14	3017	1/1	0.96	0.19	77,77,77,77	0
56	MG	14	3258	1/1	0.96	0.27	50,50,50,50	0
56	MG	14	3397	1/1	0.96	0.18	70,70,70,70	0
56	MG	14	3260	1/1	0.96	0.29	91,91,91,91	0
56	MG	1H	3299	1/1	0.96	0.25	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3123	1/1	0.96	0.16	70,70,70,70	0
56	MG	13	1695	1/1	0.96	0.15	86,86,86,86	0
56	MG	1H	3402	1/1	0.96	0.14	58,58,58,58	0
56	MG	13	1797	1/1	0.96	0.13	105,105,105,105	0
56	MG	1H	3539	1/1	0.96	0.06	76,76,76,76	0
56	MG	14	3142	1/1	0.96	0.14	70,70,70,70	0
56	MG	13	1798	1/1	0.96	0.22	80,80,80,80	0
56	MG	1G	1632	1/1	0.96	0.27	83,83,83,83	0
56	MG	1H	3541	1/1	0.96	0.07	75,75,75,75	0
56	MG	14	3271	1/1	0.96	0.22	73,73,73,73	0
56	MG	1H	3306	1/1	0.96	0.28	87,87,87,87	0
56	MG	14	3414	1/1	0.96	0.11	86,86,86,86	0
56	MG	14	3415	1/1	0.96	0.09	101,101,101,101	0
56	MG	14	3416	1/1	0.96	0.09	98,98,98,98	0
56	MG	1H	3544	1/1	0.96	0.16	57,57,57,57	0
56	MG	1H	3545	1/1	0.96	0.04	63,63,63,63	0
56	MG	1H	3346	1/1	0.96	0.24	91,91,91,91	0
56	MG	14	3152	1/1	0.96	0.10	77,77,77,77	0
56	MG	1H	3130	1/1	0.96	0.25	70,70,70,70	0
56	MG	16	204	1/1	0.96	0.24	77,77,77,77	0
56	MG	13	1691	1/1	0.96	0.28	94,94,94,94	0
56	MG	1H	3349	1/1	0.96	1.26	74,74,74,74	0
56	MG	14	3282	1/1	0.96	0.23	67,67,67,67	0
56	MG	1H	3350	1/1	0.96	0.15	85,85,85,85	0
56	MG	14	3037	1/1	0.96	0.13	61,61,61,61	0
56	MG	1H	3094	1/1	0.96	0.11	48,48,48,48	0
56	MG	14	3430	1/1	0.96	0.10	90,90,90,90	0
56	MG	13	1786	1/1	0.96	0.06	65,65,65,65	0
56	MG	14	3040	1/1	0.96	0.16	62,62,62,62	0
56	MG	1G	1724	1/1	0.96	0.08	75,75,75,75	0
56	MG	1H	3057	1/1	0.96	0.21	52,52,52,52	0
56	MG	13	1761	1/1	0.96	0.09	110,110,110,110	0
56	MG	14	3167	1/1	0.96	0.15	81,81,81,81	0
56	MG	13	1644	1/1	0.96	0.26	89,89,89,89	0
56	MG	1H	3232	1/1	0.96	0.30	82,82,82,82	0
56	MG	14	3295	1/1	0.96	0.24	91,91,91,91	0
56	MG	1H	3273	1/1	0.96	0.08	73,73,73,73	0
56	MG	13	1776	1/1	0.96	0.10	93,93,93,93	0
56	MG	13	1744	1/1	0.96	0.17	81,81,81,81	0
56	MG	13	1770	1/1	0.96	0.10	89,89,89,89	0
56	MG	1H	3566	1/1	0.96	0.08	93,93,93,93	0
56	MG	1H	3203	1/1	0.96	0.09	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3320	1/1	0.96	0.11	94,94,94,94	0
56	MG	1G	1737	1/1	0.96	0.13	127,127,127,127	0
56	MG	13	1617	1/1	0.96	0.08	84,84,84,84	0
56	MG	1H	3045	1/1	0.96	0.15	75,75,75,75	0
56	MG	45	202	1/1	0.96	0.23	84,84,84,84	0
56	MG	14	3180	1/1	0.96	0.29	82,82,82,82	0
56	MG	1G	1740	1/1	0.96	0.17	93,93,93,93	0
56	MG	1G	1741	1/1	0.96	0.12	98,98,98,98	0
56	MG	1H	3175	1/1	0.96	0.10	103,103,103,103	0
56	MG	14	3181	1/1	0.97	0.08	87,87,87,87	0
56	MG	1H	3005	1/1	0.97	0.23	56,56,56,56	0
56	MG	1H	3164	1/1	0.97	0.18	78,78,78,78	0
56	MG	1H	3497	1/1	0.97	0.12	40,40,40,40	0
56	MG	14	3112	1/1	0.97	0.20	83,83,83,83	0
56	MG	1H	3383	1/1	0.97	0.14	58,58,58,58	0
56	MG	14	3117	1/1	0.97	0.31	79,79,79,79	0
56	MG	14	3274	1/1	0.97	0.27	64,64,64,64	0
56	MG	14	3189	1/1	0.97	0.14	63,63,63,63	0
56	MG	1H	3500	1/1	0.97	0.14	43,43,43,43	0
56	MG	14	3119	1/1	0.97	0.14	91,91,91,91	0
56	MG	14	3120	1/1	0.97	0.23	70,70,70,70	0
56	MG	1H	3546	1/1	0.97	0.15	60,60,60,60	0
56	MG	1H	3385	1/1	0.97	0.23	75,75,75,75	0
56	MG	1H	3549	1/1	0.97	0.08	61,61,61,61	0
56	MG	1H	3050	1/1	0.97	0.18	51,51,51,51	0
56	MG	14	3375	1/1	0.97	0.09	75,75,75,75	0
56	MG	14	3199	1/1	0.97	0.29	67,67,67,67	0
56	MG	1H	3551	1/1	0.97	0.07	53,53,53,53	0
56	MG	1H	3027	1/1	0.97	0.18	40,40,40,40	0
56	MG	1H	3442	1/1	0.97	0.12	73,73,73,73	0
56	MG	14	3381	1/1	0.97	0.12	89,89,89,89	0
56	MG	13	1777	1/1	0.97	0.12	69,69,69,69	0
56	MG	1H	3295	1/1	0.97	0.18	65,65,65,65	0
56	MG	14	3384	1/1	0.97	0.14	81,81,81,81	0
56	MG	1H	3117	1/1	0.97	0.17	59,59,59,59	0
56	MG	14	3059	1/1	0.97	0.16	41,41,41,41	0
56	MG	13	1692	1/1	0.97	0.27	102,102,102,102	0
56	MG	1H	3120	1/1	0.97	0.29	75,75,75,75	0
56	MG	14	3293	1/1	0.97	0.23	81,81,81,81	0
56	MG	14	3063	1/1	0.97	0.12	80,80,80,80	0
56	MG	14	3138	1/1	0.97	0.11	71,71,71,71	0
56	MG	14	3296	1/1	0.97	0.18	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3449	1/1	0.97	0.07	88,88,88,88	0
56	MG	BI	202	1/1	0.97	0.15	122,122,122,122	0
56	MG	1H	3514	1/1	0.97	0.13	84,84,84,84	0
56	MG	1G	1640	1/1	0.97	0.11	82,82,82,82	0
56	MG	1G	1736	1/1	0.97	0.09	111,111,111,111	0
56	MG	14	3401	1/1	0.97	0.06	85,85,85,85	0
56	MG	14	3302	1/1	0.97	0.12	56,56,56,56	0
56	MG	14	3144	1/1	0.97	0.13	65,65,65,65	0
56	MG	14	3305	1/1	0.97	0.13	60,60,60,60	0
56	MG	1H	3609	1/1	0.97	0.07	90,90,90,90	0
56	MG	1H	3260	1/1	0.97	0.28	69,69,69,69	0
56	MG	1H	3517	1/1	0.97	0.10	54,54,54,54	0
56	MG	13	1645	1/1	0.97	0.14	74,74,74,74	0
56	MG	14	3409	1/1	0.97	0.06	80,80,80,80	0
56	MG	1G	1645	1/1	0.97	0.14	101,101,101,101	0
56	MG	13	1752	1/1	0.97	0.07	86,86,86,86	0
56	MG	1H	3303	1/1	0.97	0.33	106,106,106,106	0
56	MG	1H	3263	1/1	0.97	0.20	64,64,64,64	0
56	MG	14	3226	1/1	0.97	0.31	60,60,60,60	0
56	MG	1G	1649	1/1	0.97	0.14	90,90,90,90	0
56	MG	14	3316	1/1	0.97	0.30	79,79,79,79	0
56	MG	14	3228	1/1	0.97	0.11	79,79,79,79	0
56	MG	1H	3571	1/1	0.97	0.11	58,58,58,58	0
56	MG	1H	3572	1/1	0.97	0.08	73,73,73,73	0
56	MG	13	1611	1/1	0.97	0.20	65,65,65,65	0
56	MG	1H	3525	1/1	0.97	0.13	58,58,58,58	0
56	MG	14	3233	1/1	0.97	0.20	72,72,72,72	0
56	MG	14	3086	1/1	0.97	0.20	59,59,59,59	0
56	MG	14	3087	1/1	0.97	0.28	60,60,60,60	0
56	MG	14	3088	1/1	0.97	0.18	61,61,61,61	0
56	MG	14	3426	1/1	0.97	0.06	108,108,108,108	0
56	MG	14	3326	1/1	0.97	0.10	53,53,53,53	0
56	MG	1H	3002	1/1	0.97	0.12	40,40,40,40	0
56	MG	14	3163	1/1	0.97	0.33	90,90,90,90	0
56	MG	14	3090	1/1	0.97	0.25	59,59,59,59	0
56	MG	14	3165	1/1	0.97	0.30	83,83,83,83	0
56	MG	14	3242	1/1	0.97	0.22	66,66,66,66	0
56	MG	1H	3486	1/1	0.97	0.14	45,45,45,45	0
56	MG	14	3093	1/1	0.97	0.17	56,56,56,56	0
56	MG	14	3095	1/1	0.97	0.28	92,92,92,92	0
56	MG	1H	3458	1/1	0.97	0.21	85,85,85,85	0
56	MG	14	3338	1/1	0.97	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3097	1/1	0.97	0.08	76,76,76,76	0
56	MG	14	3252	1/1	0.97	0.28	76,76,76,76	0
56	MG	14	3098	1/1	0.97	0.17	67,67,67,67	0
56	MG	1H	3160	1/1	0.97	0.15	66,66,66,66	0
56	MG	19	301	1/1	0.97	0.12	53,53,53,53	0
56	MG	1H	3533	1/1	0.97	0.07	46,46,46,46	0
56	MG	14	3344	1/1	0.97	0.10	66,66,66,66	0
56	MG	14	3259	1/1	0.97	0.36	87,87,87,87	0
56	MG	13	1623	1/1	0.97	0.17	106,106,106,106	0
56	MG	14	3347	1/1	0.97	0.10	53,53,53,53	0
56	MG	1G	1709	1/1	0.97	0.08	108,108,108,108	0
56	MG	14	3351	1/1	0.97	0.10	76,76,76,76	0
56	MG	14	3103	1/1	0.97	0.29	78,78,78,78	0
56	MG	1H	3004	1/1	0.97	0.15	35,35,35,35	0
56	MG	1H	3492	1/1	0.97	0.08	54,54,54,54	0
56	MG	1H	3331	1/1	0.97	0.55	69,69,69,69	0
56	MG	14	3357	1/1	0.97	0.10	67,67,67,67	0
56	MG	1H	3353	1/1	0.97	0.15	77,77,77,77	0
56	MG	13	1742	1/1	0.98	0.52	92,92,92,92	0
56	MG	1H	3537	1/1	0.98	0.08	52,52,52,52	0
56	MG	1H	3490	1/1	0.98	0.14	63,63,63,63	0
56	MG	1H	3378	1/1	0.98	0.18	56,56,56,56	0
56	MG	21	304	1/1	0.98	0.08	54,54,54,54	0
56	MG	1H	3379	1/1	0.98	0.32	85,85,85,85	0
56	MG	13	1716	1/1	0.98	0.10	94,94,94,94	0
56	MG	14	3377	1/1	0.98	0.09	51,51,51,51	0
56	MG	1H	3099	1/1	0.98	0.09	55,55,55,55	0
56	MG	13	1601	1/1	0.98	0.10	58,58,58,58	0
56	MG	14	3137	1/1	0.98	0.36	90,90,90,90	0
56	MG	14	3062	1/1	0.98	0.10	59,59,59,59	0
56	MG	1H	3118	1/1	0.98	0.26	74,74,74,74	0
56	MG	1H	3384	1/1	0.98	0.29	49,49,49,49	0
56	MG	13	1730	1/1	0.98	0.12	100,100,100,100	0
56	MG	1H	3596	1/1	0.98	0.11	75,75,75,75	0
56	MG	1H	3499	1/1	0.98	0.13	49,49,49,49	0
56	MG	14	3303	1/1	0.98	0.11	69,69,69,69	0
56	MG	1H	3102	1/1	0.98	0.33	63,63,63,63	0
56	MG	1H	3166	1/1	0.98	0.17	87,87,87,87	0
56	MG	1H	3167	1/1	0.98	0.24	83,83,83,83	0
56	MG	14	3147	1/1	0.98	0.31	94,94,94,94	0
56	MG	1H	3503	1/1	0.98	0.11	55,55,55,55	0
56	MG	13	1718	1/1	0.98	0.12	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	14	3394	1/1	0.98	0.02	98,98,98,98	0
56	MG	1H	3555	1/1	0.98	0.22	85,85,85,85	0
56	MG	14	3396	1/1	0.98	0.11	54,54,54,54	0
56	MG	1H	3604	1/1	0.98	0.07	118,118,118,118	0
56	MG	14	3075	1/1	0.98	0.18	94,94,94,94	0
56	MG	14	3399	1/1	0.98	0.06	47,47,47,47	0
56	MG	14	3076	1/1	0.98	0.36	78,78,78,78	0
56	MG	1H	3605	1/1	0.98	0.09	90,90,90,90	0
56	MG	14	3078	1/1	0.98	0.10	54,54,54,54	0
56	MG	14	3013	1/1	0.98	0.15	50,50,50,50	0
56	MG	13	1650	1/1	0.98	0.36	100,100,100,100	0
56	MG	1H	3607	1/1	0.98	0.06	61,61,61,61	0
56	MG	1H	3124	1/1	0.98	0.20	52,52,52,52	0
56	MG	1H	3429	1/1	0.98	0.17	63,63,63,63	0
56	MG	1H	3038	1/1	0.98	0.16	44,44,44,44	0
56	MG	1G	1723	1/1	0.98	0.08	72,72,72,72	0
56	MG	1H	3359	1/1	0.98	0.18	58,58,58,58	0
56	MG	1H	3612	1/1	0.98	0.08	62,62,62,62	0
56	MG	1H	3395	1/1	0.98	0.11	54,54,54,54	0
56	MG	1H	3126	1/1	0.98	0.22	54,54,54,54	0
56	MG	1G	1612	1/1	0.98	0.10	79,79,79,79	0
56	MG	14	3247	1/1	0.98	0.22	59,59,59,59	0
56	MG	1H	3014	1/1	0.98	0.19	62,62,62,62	0
56	MG	14	3250	1/1	0.98	0.26	66,66,66,66	0
56	MG	14	3094	1/1	0.98	0.18	64,64,64,64	0
56	MG	1G	1670	1/1	0.98	0.27	99,99,99,99	0
56	MG	1H	3398	1/1	0.98	0.17	47,47,47,47	0
56	MG	14	3255	1/1	0.98	0.14	72,72,72,72	0
56	MG	14	3028	1/1	0.98	0.18	53,53,53,53	0
56	MG	14	3337	1/1	0.98	0.05	53,53,53,53	0
56	MG	1H	3617	1/1	0.98	0.24	127,127,127,127	0
56	MG	1H	3305	1/1	0.98	0.45	100,100,100,100	0
56	MG	1H	3128	1/1	0.98	0.20	60,60,60,60	0
56	MG	1H	3249	1/1	0.98	0.13	70,70,70,70	0
56	MG	1H	3569	1/1	0.98	0.11	73,73,73,73	0
56	MG	1G	1677	1/1	0.98	0.09	94,94,94,94	0
56	MG	14	3104	1/1	0.98	0.34	48,48,48,48	0
56	MG	1G	1678	1/1	0.98	0.31	86,86,86,86	0
56	MG	1G	1620	1/1	0.98	0.11	83,83,83,83	0
56	MG	1H	3250	1/1	0.98	0.42	67,67,67,67	0
56	MG	14	3348	1/1	0.98	0.12	59,59,59,59	0
56	MG	1H	3403	1/1	0.98	0.20	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	14	3350	1/1	0.98	0.14	45,45,45,45	0
56	MG	1G	1682	1/1	0.98	0.16	79,79,79,79	0
56	MG	13	1637	1/1	0.98	0.14	67,67,67,67	0
56	MG	2I	201	1/1	0.98	0.12	91,91,91,91	0
56	MG	1H	3524	1/1	0.98	0.17	56,56,56,56	0
56	MG	14	3355	1/1	0.98	0.07	75,75,75,75	0
56	MG	14	3113	1/1	0.98	0.17	69,69,69,69	0
56	MG	14	3114	1/1	0.98	0.24	60,60,60,60	0
56	MG	29	302	1/1	0.98	0.15	57,57,57,57	0
56	MG	1H	3109	1/1	0.98	0.26	44,44,44,44	0
56	MG	1H	3110	1/1	0.98	0.18	50,50,50,50	0
56	MG	1H	3155	1/1	0.98	0.29	73,73,73,73	0
56	MG	14	3194	1/1	0.98	0.17	75,75,75,75	0
56	MG	1H	3446	1/1	0.98	0.10	87,87,87,87	0
56	MG	1H	3530	1/1	0.98	0.08	54,54,54,54	0
56	MG	14	3121	1/1	0.98	0.20	65,65,65,65	0
56	MG	1H	3531	1/1	0.98	0.11	66,66,66,66	0
56	MG	13	1627	1/1	0.98	0.20	93,93,93,93	0
56	MG	13	1759	1/1	0.98	0.04	105,105,105,105	0
56	MG	13	1778	1/1	0.98	0.06	79,79,79,79	0
56	MG	1H	3289	1/1	0.98	0.10	85,85,85,85	0
56	MG	14	3244	1/1	0.99	0.25	67,67,67,67	0
56	MG	98	201	1/1	0.99	0.28	56,56,56,56	0
56	MG	13	1790	1/1	0.99	0.07	59,59,59,59	0
56	MG	2K	101	1/1	0.99	0.30	69,69,69,69	0
56	MG	1H	3277	1/1	0.99	0.11	66,66,66,66	0
56	MG	14	3249	1/1	0.99	0.27	54,54,54,54	0
56	MG	1H	3251	1/1	0.99	0.32	66,66,66,66	0
56	MG	1H	3548	1/1	0.99	0.08	50,50,50,50	0
56	MG	14	3336	1/1	0.99	0.08	60,60,60,60	0
56	MG	1H	3240	1/1	0.99	0.27	64,64,64,64	0
56	MG	14	3253	1/1	0.99	0.33	59,59,59,59	0
56	MG	13	1756	1/1	0.99	0.04	95,95,95,95	0
56	MG	1H	3389	1/1	0.99	0.23	52,52,52,52	0
56	MG	1H	3483	1/1	0.99	0.13	63,63,63,63	0
56	MG	14	3257	1/1	0.99	0.21	62,62,62,62	0
56	MG	1H	3372	1/1	0.99	0.12	71,71,71,71	0
56	MG	1H	3528	1/1	0.99	0.08	49,49,49,49	0
56	MG	14	3081	1/1	0.99	0.21	114,114,114,114	0
56	MG	1H	3254	1/1	0.99	0.24	68,68,68,68	0
56	MG	14	3115	1/1	0.99	0.16	57,57,57,57	0
56	MG	16	215	1/1	0.99	0.09	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3428	1/1	0.99	0.25	57,57,57,57	0
56	MG	1H	3282	1/1	0.99	0.05	94,94,94,94	0
56	MG	13	1699	1/1	0.99	0.47	94,94,94,94	0
56	MG	14	3188	1/1	0.99	0.13	68,68,68,68	0
56	MG	13	1700	1/1	0.99	0.19	90,90,90,90	0
56	MG	1H	3510	1/1	0.99	0.19	54,54,54,54	0
56	MG	1H	3360	1/1	0.99	0.17	50,50,50,50	0
56	MG	1H	3122	1/1	0.99	0.18	49,49,49,49	0
56	MG	14	3091	1/1	0.99	0.23	57,57,57,57	0
56	MG	13	1783	1/1	0.99	0.14	77,77,77,77	0
56	MG	1H	3132	1/1	0.99	0.24	46,46,46,46	0
56	MG	14	3127	1/1	0.99	0.11	61,61,61,61	0
56	MG	14	3234	1/1	0.99	0.18	60,60,60,60	0
56	MG	1H	3515	1/1	0.99	0.10	41,41,41,41	0
56	MG	14	3198	1/1	0.99	0.30	96,96,96,96	0
56	MG	13	1641	1/1	0.99	0.17	55,55,55,55	0
56	MG	1H	3567	1/1	0.99	0.13	51,51,51,51	0
56	MG	1H	3197	1/1	0.99	0.21	65,65,65,65	0
56	MG	14	3202	1/1	0.99	0.17	71,71,71,71	0
56	MG	1H	3542	1/1	0.99	0.20	68,68,68,68	0
56	MG	1H	3518	1/1	0.99	0.08	51,51,51,51	0
57	SF4	3E	302	8/8	0.99	0.21	85,90,93,95	0
57	SF4	32	301	8/8	0.99	0.19	95,103,111,112	0
58	ZN	5I	103	1/1	0.99	0.16	97,97,97,97	0
56	MG	1G	1653	1/1	0.99	0.33	112,112,112,112	0
56	MG	13	1651	1/1	1.00	0.32	91,91,91,91	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.