



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 10, 2019 – 10:51 AM EST

PDB ID : 5IBB
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet} and cognate tRNA^{Val} in the A-site
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2016-02-22
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

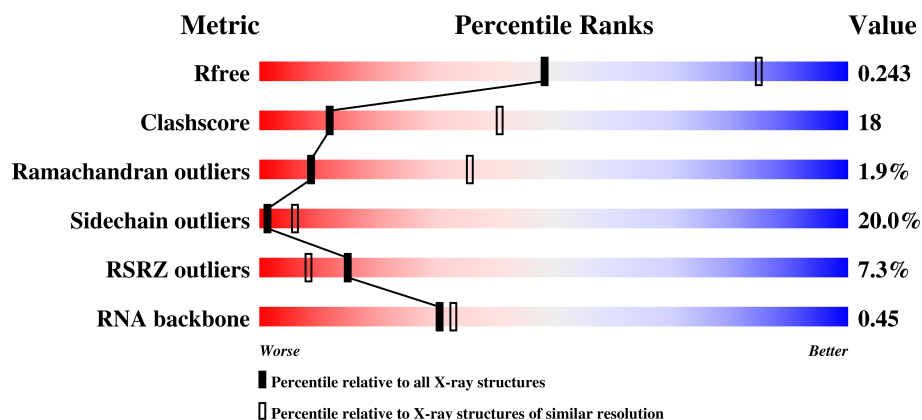
1 Overall quality at a glance

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}	111664	2641 (3.00-2.92)
Clashscore	122126	2988 (3.00-2.92)
Ramachandran outliers	120053	2892 (3.00-2.92)
Sidechain outliers	120020	2895 (3.00-2.92)
RSRZ outliers	108989	2527 (3.00-2.92)
RNA backbone	2636	1068 (3.30-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
23	2K	77	
23	2L	77	
24	3K	76	
24	3L	76	
25	4K	30	
25	4L	30	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	7I	229	

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Mol	Chain	Length	Quality of chain
28	79	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	

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Mol	Chain	Length	Quality of chain
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	I5	71	
52	M8	71	
53	J5	60	

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Mol	Chain	Length	Quality of chain
53	N8	60	
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	
56	1L	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
57	MG	13	1643	-	-	-	X
57	MG	13	1650	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	13	1678	-	-	-	X
57	MG	13	1687	-	-	-	X
57	MG	13	1690	-	-	-	X
57	MG	14	3007	-	-	-	X
57	MG	14	3031	-	-	-	X
57	MG	14	3083	-	-	-	X
57	MG	14	3087	-	-	-	X
57	MG	14	3092	-	-	-	X
57	MG	14	3094	-	-	-	X
57	MG	14	3097	-	-	-	X
57	MG	14	3110	-	-	-	X
57	MG	14	3111	-	-	-	X
57	MG	14	3112	-	-	-	X
57	MG	14	3134	-	-	-	X
57	MG	14	3137	-	-	-	X
57	MG	14	3152	-	-	-	X
57	MG	14	3157	-	-	-	X
57	MG	14	3162	-	-	-	X
57	MG	14	3163	-	-	-	X
57	MG	14	3172	-	-	-	X
57	MG	14	3174	-	-	-	X
57	MG	14	3189	-	-	-	X
57	MG	14	3205	-	-	-	X
57	MG	14	3214	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	14	3226	-	-	-	X
57	MG	1G	1621	-	-	-	X
57	MG	1G	1630	-	-	-	X
57	MG	1H	3005	-	-	-	X
57	MG	1H	3009	-	-	-	X
57	MG	1H	3036	-	-	-	X
57	MG	1H	3058	-	-	-	X
57	MG	1H	3061	-	-	-	X
57	MG	1H	3072	-	-	-	X
57	MG	1H	3085	-	-	-	X
57	MG	1H	3086	-	-	-	X
57	MG	1H	3115	-	-	-	X
57	MG	1H	3120	-	-	-	X
57	MG	1H	3121	-	-	-	X
57	MG	1H	3123	-	-	-	X
57	MG	1H	3133	-	-	-	X
57	MG	1H	3179	-	-	-	X
57	MG	1H	3186	-	-	-	X
57	MG	1H	3187	-	-	-	X
57	MG	1H	3188	-	-	-	X
57	MG	1H	3189	-	-	-	X
57	MG	1H	3199	-	-	-	X
57	MG	1H	3204	-	-	-	X
57	MG	1H	3207	-	-	-	X
57	MG	1H	3211	-	-	-	X
57	MG	1H	3216	-	-	-	X
57	MG	1H	3217	-	-	-	X
57	MG	1H	3227	-	-	-	X
57	MG	1H	3232	-	-	-	X
57	MG	1H	3246	-	-	-	X
57	MG	1H	3260	-	-	-	X
57	MG	1H	3263	-	-	-	X
57	MG	1H	3274	-	-	-	X
57	MG	1H	3279	-	-	-	X
57	MG	1H	3282	-	-	-	X
57	MG	1H	3316	-	-	-	X
57	MG	1H	3317	-	-	-	X
57	MG	1H	3320	-	-	-	X
57	MG	2L	102	-	-	-	X
57	MG	2L	103	-	-	-	X
57	MG	4E	201	-	-	-	X
59	SF4	3E	301	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296743 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1506	Total	C	N	O	P	0	0	0
			32371	14409	6001	10456	1505			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	U	conflict	GB 55771382
1G	1542	G	U	conflict	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	235	Total	C	N	O	S	0	0	0
			1902	1215	340	342	5			
2	12	207	Total	C	N	O	S	0	0	0
			1696	1083	306	303	4			

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	149	Total	C	N	O	S	0	0	0
			1139	721	216	198	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	140	Total	C	N	O	S	0	0	0
			1120	695	223	196	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	95	Total	C	N	O	S	0	0	0
			754	471	148	134	1			
10	1A	80	Total	C	N	O		0	0	0
			646	403	129	114				

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	119	Total	C	N	O	S	0	0	0
			942	582	194	164	2			
13	4A	111	Total	C	N	O	S	0	0	0
			893	552	183	156	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			661	422	123	114	2			
19	AA	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	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 tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	0	0	0
			1540	688	274	506	72			

- 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	298	535	77	1			
23	2L	76	Total	C	N	O	P	S	0	0	0
			1626	726	296	527	76	1			

- Molecule 24 is a RNA chain called tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1491	665	268	488	70			
24	3L	71	Total	C	N	O	P	0	0	0
			1513	675	272	495	71			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	21	Total	C	N	O	P	0	0	0
			462	207	96	138	21			
25	4L	19	Total	C	N	O	P	0	0	0
			417	187	86	125	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2841	Total 61195	C 27234	N 11446	O 19674	P 2841	0	0	0
26	14	2810	Total 60535	C 26940	N 11330	O 19455	P 2810	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	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 2617	C 1166	N 486	O 844	P 121	0	0	0
27	1J	122	Total 2617	C 1166	N 486	O 844	P 121	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	133	Total 1033	C 651	N 194	O 187	S 1	0	0	0
28	79	57	Total 456	C 283	N 91	O 82		0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	202	Total	C	N	O	S	0	0	0
			1505	951	281	267	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	181	Total	C	N	O	S	0	0	0
			1468	937	268	259	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
33	59	167	Total	C	N	O	S	0	0	0
			1283	815	239	228	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	137	Total	C	N	O	S	0	0	0
			1096	706	205	181	4			
35	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1117	712	211	187	7			
38	45	139	Total	C	N	O	S	0	0	0
			1104	705	209	184	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
39	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	136	Total	C	N	O	S	0	0	0
			1124	700	231	192	1			
41	75	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			743	482	134	126	1			
45	B5	94	Total	C	N	O	S	0	0	0
			735	477	133	125				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	103	Total	C	N	O	S	0	0	0
			777	501	145	126	5			
46	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	170	Total	C	N	O	S	0	0	0
			1365	870	246	246	3			
47	D5	133	Total	C	N	O	S	0	0	0
			1079	694	194	189	2			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	61	Total	C	N	O	S	0	0	0
			479	299	86	89	5			
52	I5	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	56	Total	C	N	O	S	0	0	0
			437	275	87	70	5			
53	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

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

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

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

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

- Molecule 56 is a RNA chain called tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	69	Total	C	N	O	P	0	0	0
			1469	656	262	482	69			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	45	1	Total	Mg	0	0
			1	1		
57	19	1	Total	Mg	0	0
			1	1		
57	P8	1	Total	Mg	0	0
			1	1		
57	C5	1	Total	Mg	0	0
			1	1		
57	13	148	Total	Mg	0	0
			148	148		
57	1J	7	Total	Mg	0	0
			7	7		
57	5I	1	Total	Mg	0	0
			1	1		
57	35	2	Total	Mg	0	0
			2	2		
57	4L	2	Total	Mg	0	0
			2	2		
57	16	11	Total	Mg	0	0
			11	11		
57	42	1	Total	Mg	0	0
			1	1		
57	B5	1	Total	Mg	0	0
			1	1		
57	25	2	Total	Mg	0	0
			2	2		
57	M5	1	Total	Mg	0	0
			1	1		
57	21	2	Total	Mg	0	0
			2	2		
57	31	2	Total	Mg	0	0
			2	2		
57	Q8	1	Total	Mg	0	0
			1	1		
57	L8	1	Total	Mg	0	0
			1	1		

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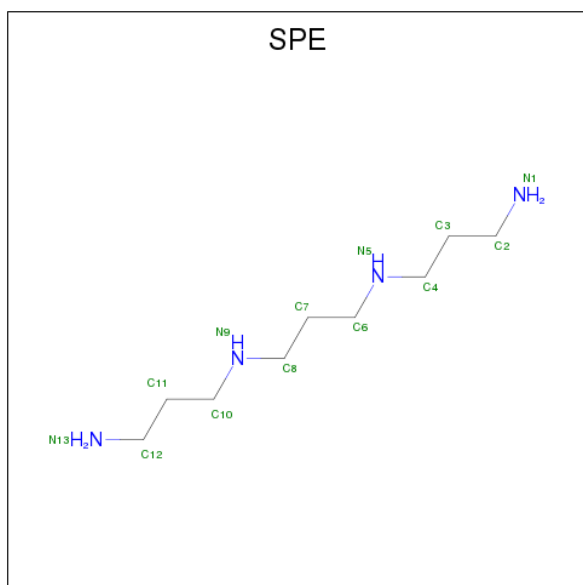
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	9A	1	Total 1	Mg 1	0	0
57	3I	1	Total 1	Mg 1	0	0
57	I8	1	Total 1	Mg 1	0	0
57	68	2	Total 2	Mg 2	0	0
57	29	2	Total 2	Mg 2	0	0
57	2K	4	Total 4	Mg 4	0	0
57	J8	1	Total 1	Mg 1	0	0
57	4A	1	Total 1	Mg 1	0	0
57	39	2	Total 2	Mg 2	0	0
57	1G	133	Total 133	Mg 133	0	0
57	4E	1	Total 1	Mg 1	0	0
57	11	2	Total 2	Mg 2	0	0
57	1H	548	Total 548	Mg 548	0	0
57	E5	1	Total 1	Mg 1	0	0
57	88	3	Total 3	Mg 3	0	0
57	5E	1	Total 1	Mg 1	0	0
57	14	445	Total 445	Mg 445	0	0
57	78	1	Total 1	Mg 1	0	0
57	F8	1	Total 1	Mg 1	0	0
57	4K	2	Total 2	Mg 2	0	0
57	3A	1	Total 1	Mg 1	0	0

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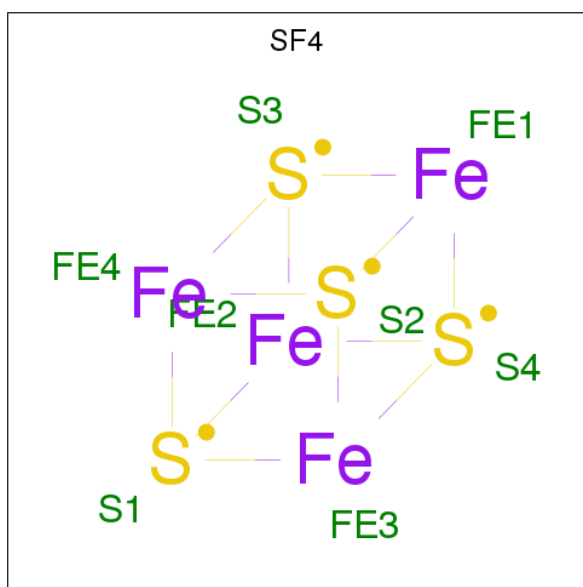
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	41	1	Total	Mg	0	0
			1	1		
57	2L	3	Total	Mg	0	0
			3	3		

- Molecule 58 is THERMINE (three-letter code: SPE) (formula: $C_9H_{24}N_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	13	1	Total	C	N	0	0
			13	9	4		
58	1G	1	Total	C	N	0	0
			13	9	4		
58	14	1	Total	C	N	0	0
			13	9	4		
58	14	1	Total	C	N	0	0
			13	9	4		
58	1J	1	Total	C	N	0	0
			13	9	4		

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	304	Total	O	0	0
			304	304		
61	3E	1	Total	O	0	0
			1	1		
61	4E	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1I	2	Total 2	O 2	0	0
61	2I	1	Total 1	O 1	0	0
61	3I	2	Total 2	O 2	0	0
61	5I	2	Total 2	O 2	0	0
61	7I	2	Total 2	O 2	0	0
61	1K	1	Total 1	O 1	0	0
61	2K	6	Total 6	O 6	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	11	Total 11	O 11	0	0
61	1H	1133	Total 1133	O 1133	0	0
61	16	15	Total 15	O 15	0	0
61	11	16	Total 16	O 16	0	0
61	21	8	Total 8	O 8	0	0
61	31	4	Total 4	O 4	0	0
61	58	1	Total 1	O 1	0	0
61	78	11	Total 11	O 11	0	0
61	98	2	Total 2	O 2	0	0
61	A8	3	Total 3	O 3	0	0
61	B8	1	Total 1	O 1	0	0
61	E8	1	Total 1	O 1	0	0
61	F8	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	I8	6	Total 6	O 6	0	0
61	K8	1	Total 1	O 1	0	0
61	L8	1	Total 1	O 1	0	0
61	P8	1	Total 1	O 1	0	0
61	Q8	5	Total 5	O 5	0	0
61	1G	391	Total 391	O 391	0	0
61	22	1	Total 1	O 1	0	0
61	42	1	Total 1	O 1	0	0
61	52	3	Total 3	O 3	0	0
61	3A	1	Total 1	O 1	0	0
61	7A	1	Total 1	O 1	0	0
61	9A	3	Total 3	O 3	0	0
61	BA	2	Total 2	O 2	0	0
61	4L	14	Total 14	O 14	0	0
61	14	1135	Total 1135	O 1135	0	0
61	1J	18	Total 18	O 18	0	0
61	19	8	Total 8	O 8	0	0
61	29	6	Total 6	O 6	0	0
61	39	6	Total 6	O 6	0	0
61	25	11	Total 11	O 11	0	0
61	35	9	Total 9	O 9	0	0

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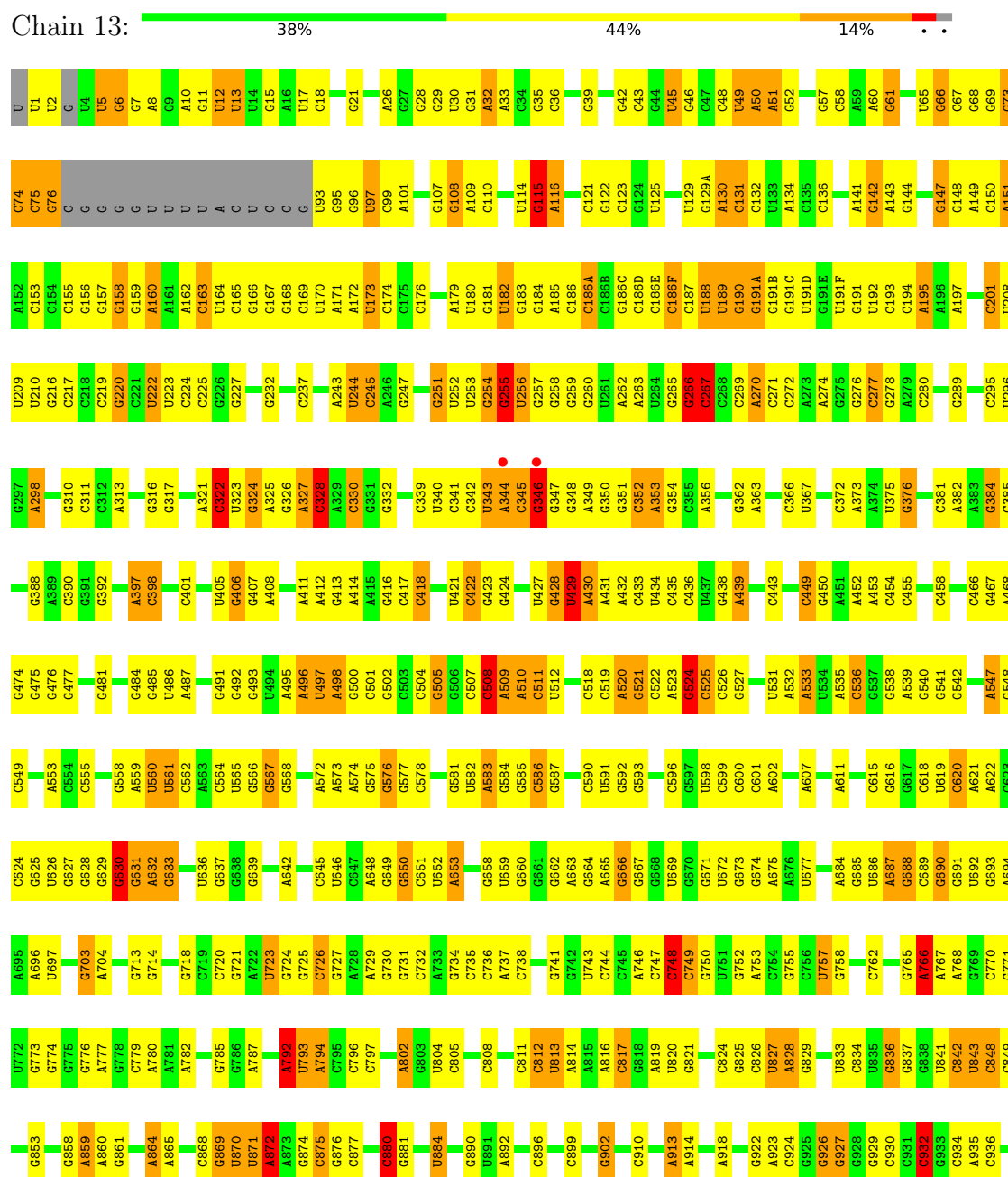
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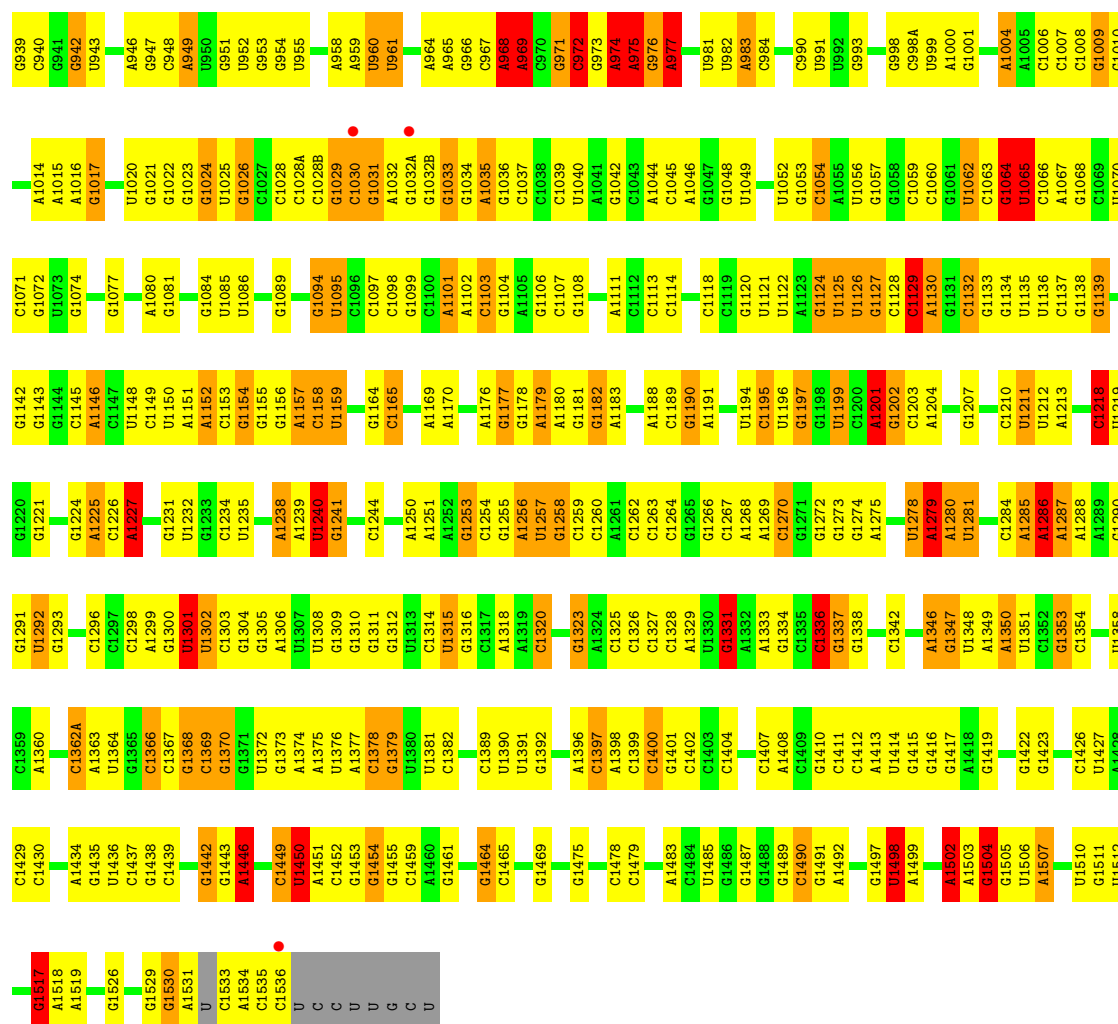
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	45	3	Total	O	0	0
			3	3		
61	55	1	Total	O	0	0
			1	1		
61	75	1	Total	O	0	0
			1	1		
61	85	1	Total	O	0	0
			1	1		
61	A5	1	Total	O	0	0
			1	1		
61	C5	3	Total	O	0	0
			3	3		
61	E5	5	Total	O	0	0
			5	5		
61	F5	3	Total	O	0	0
			3	3		
61	H5	1	Total	O	0	0
			1	1		
61	M5	7	Total	O	0	0
			7	7		

3 Residue-property plots

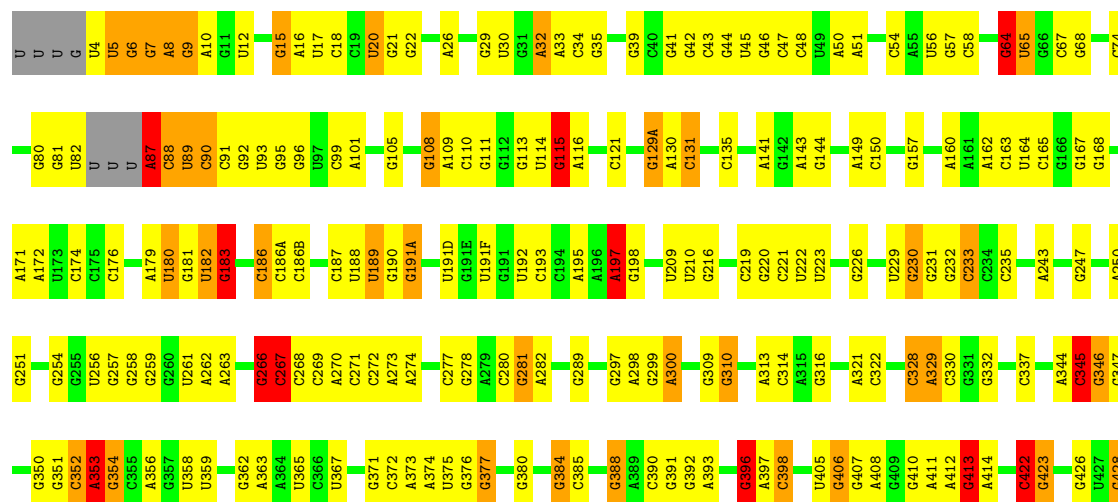
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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





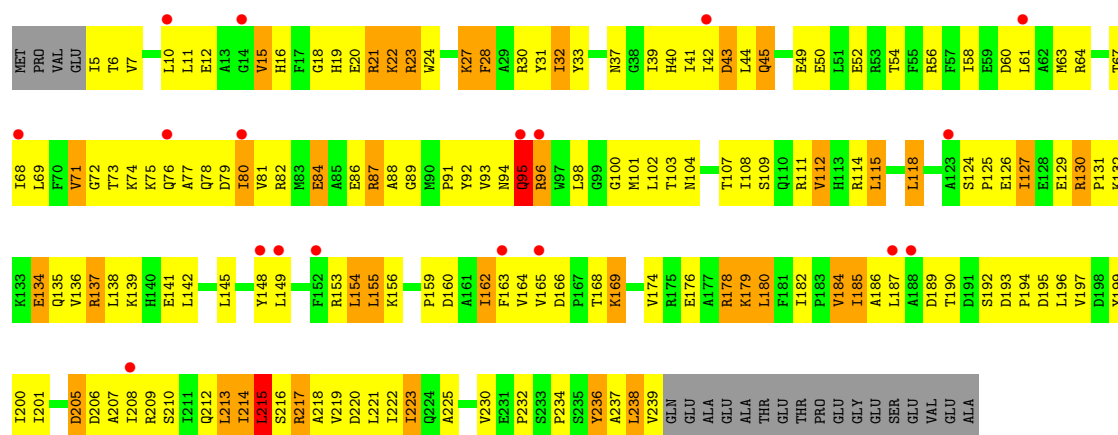
Chain 1G: 42% 43% 12% ..



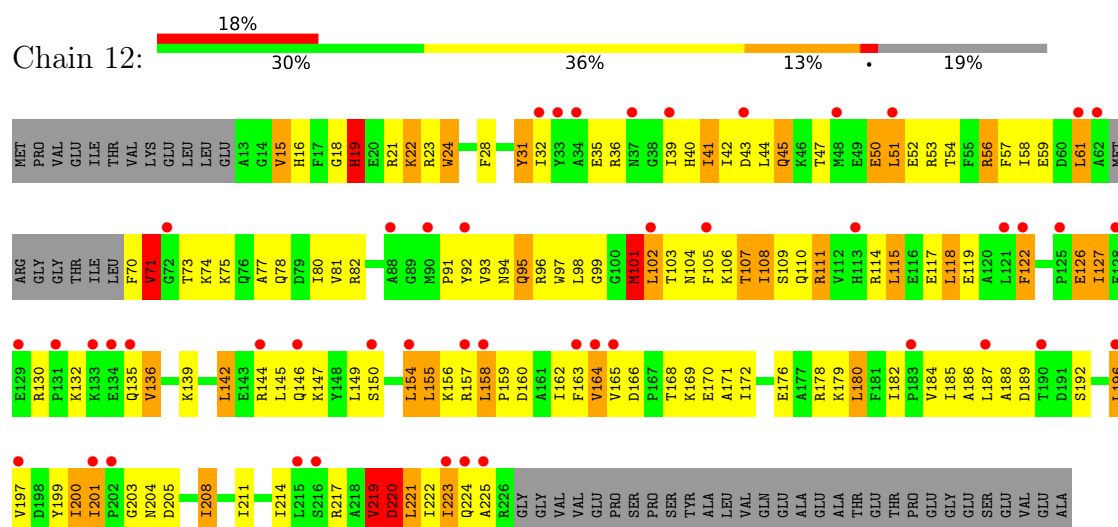
C	G1443	A1363	G1222	C1158	U1085	U1020	A949	C856	C756	G584	C518	U429
D	A1446	U1364	C1223	U1159	U1086	G1021	U950	C857	U757	G587	C519	A430
C	C1447	C1367	A1225	G1160	G1087	G1022	G951	G858	G758	G588	A520	U434
C	C1448	C1303	G1161	C1162	U1095	G1023	U952	A859	A759	G683	G521	C435
D	C1449	G1304	C1162	C1162	G1095	U1025	G953	A860	G765	C589	A523	C436
D	U1450	G1305	A1167	A1169	C1098	G1026	U957	G861	G765	G685	G524	U437
C	A1451	C1369	C1173	A1170	C1099	C1027	A958	G869	U772	U686	C525	G438
C	C1452	G1370	A1170	A1170	G1099	C1028	A959	G869	G773	G592	C526	G439
D	G1453	U1372	G1171	C1172	C1100	C1028A	U960	A872	A777	C599	C527	A439
	G1462	G1310	C1172	C1172	C1101	C1028B	U961	A873	G778	C600	C528	A440
	C1463	G1311	G1173	A1102	A1102	G1029	G963	G878	C779	G601	G529	C442
		G1312	G1174	A1105	C1030	G1030	G962	G878	G779	A602	G530	G445
	C1466	U1313	G1175	A1105	G1031	G1031	A964	G881	A780	G603	U531	G446
	G1467	C1314	A1176	G1106	A1032	A1032	A965	G881	G784	G604	A532	G447
	A1468	U1315	G1177	C1107	G1032A	G1032A	G966	G889	C784	U605	A533	A448
	G1469	G1316	G1178	G1108	G1032B	G1032B	C967	A889	A787	G606	U534	C449
	G1470	C1317	A1179	C1109	G1033	G1033	A968	G883	A787	C701	A535	
		A1318	A1180	C1112	C1037	C1037	A969	C893	A702	A607	C536	A452
	G1487	G1320	G1181	C1112	C1038	C1038	C972	G894	A792	A608	G537	A453
	C1490	G1387	A1182	G1117	C1039	C1039	G973	G895	U793	A614	G538	
	G1491	C1321	A1183	C1118	U1040	U1040	A974	C896	A794	G617	A539	C456
	A1492	G1323	G1185	C1119	A1041	A1041	G976	A900	G800	G710	G540	C457
		A1324	G1186	A1123	C1042	C1042	A977	G903	U804	G711	G541	C458
	G1497	C1325	G1187	A1123	C1043	C1043	A978	G903	C805	A712	G542	G464
	U1498	C1326	A1188	G1124	A1046	A1046	C979	A913	C808	G713	C543	A465
A	A1499	G1327	C1189	U1125	U1052	U1052	G980	G895	G628	A722	C544	C466
A	A1500	C1328	G1190	U1126	C1053	C1053	U991	U921	A814	G723	C545	G467
A	C1501	A1329	A1191	G1133	A1055	A1055	U992	G922	A815	G724	A547	A468
A	A1502	C1330	C1192	C1128	U1056	U1056	G983	A923	A816	C720	G550	G474
A	A1503	U1331	G1193	C1129	G1057	G1057	A983	C924	C817	G721	G551	G475
A	G1504	A1332	U1194	A1130	U1058	U1058	C984	G925	G818	G721	U552	G476
A	G1505	G1401	C1195	G1131	C1059	C1059	U997	G926	A819	A722	G553	G477
A	U1506	G1334	U1196	C1132	C1060	C1060	G998	G927	U820	G629	A553	A478
A	A1507	C1402	G1197	G1133	G1061	G1061	C998A	G927	G821	G630	C554	
A	C1403	C1335	G1198	G1134	U1056	U1056	U999	C931	C822	G631	C555	A482
A	G1404	C1336	G1199	U1135	G1057	G1057	G983	C932	C822	A632	C556	C483
A	G1405	G1337	U1199	U1135	G1057	G1057	A986	C932	C822	G633	G557	G484
A	U1406	G1338	C1200	U1136	U1058	U1058	U997	G925	G818	A640	G558	G485
A	C1407	A1201	C1137	U1137	C1059	C1059	G998	G926	A819	C735	C559	U486
A	A1408	G1202	G1138	G1138	C1060	C1060	C998A	G927	U820	C736	U560	C489
A		C1203	G1139	G1139	G1061	G1061	U999	C931	C822	A737	C562	G490
A		A1204	U1062	C1140	U1062	U1062	U999	C931	C822	C738	C564	G491
A		U1205	U1205	C1141	C1063	C1063	A1000	C932	C822	G650	G567	A496
A		G1206	G1206	G1142	G1064	G1064	G1001	G933	C826	C653	G568	U497
A		G1207	G1143	G1143	G1068	G1068	G1002	C934	U827	A653		
A		C1208	G1144	G1144	C1069	C1069	G1003	A935	A828	G660	A572	C503
A		A1209	C1145	C1145	U1070	U1070	A1004	C936	G829	G661	A573	C504
A		A1286	G1210	A1146	U1070	U1070	A1005	A937	G836	C744	G576	G505
A		U1211	C1147	U1148	G1071	G1071	C1006	A938	U836	C745	G577	A509
A		U1212	U1212	U1148	G1072	G1072	C1007	G939	G837	A746		A510
A		A1213	C1149	U1150	U1073	U1073	C1008	G939	G837	C747	A573	C511
A		C1214	U1150	A1151	G1074	G1074	C1009	C940	U841	C748	G574	U512
A		G1215	A1151	A1151	U1073	U1073	G1009	G941	C942	C749	U582	C513
A		C1216	G1153	A1152	G1077	G1077	A1014	G942	U843	G750		
A		G1217	C1153	A1152	G1077	G1077	A1015	U943	U843	G751	U580	
A		C1218	G1154	A1154	A1080	A1080	A1016	G944	C848	G752	G681	
A		U1219	G1155	G1155	G1081	G1081	G1017	G945		A753	U582	
A		C1220	G1156	G1156	A1080	A1080	G1018	A946		C754	G583	
A		G1221	A1157	A1157	G1084	G1084	C1019	C948		G755	A583	

• Molecule 2: 30S ribosomal protein S2

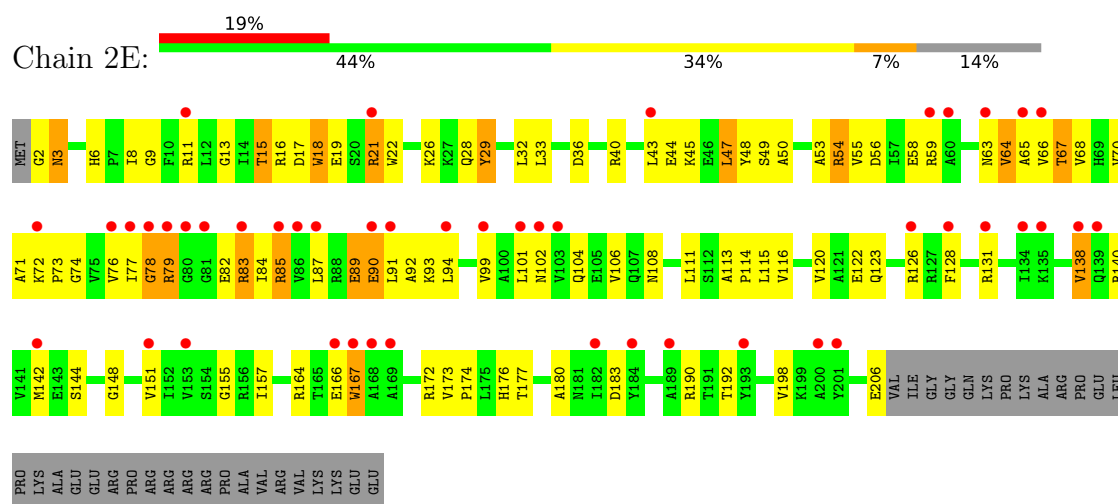




• Molecule 2: 30S ribosomal protein S2

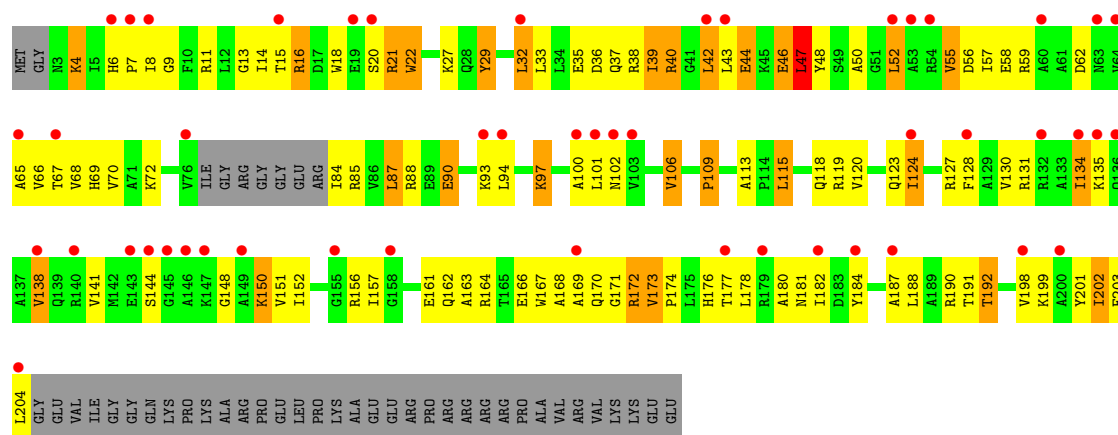


• Molecule 3: 30S ribosomal protein S3

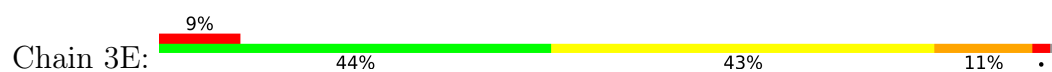


• Molecule 3: 30S ribosomal protein S3





• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

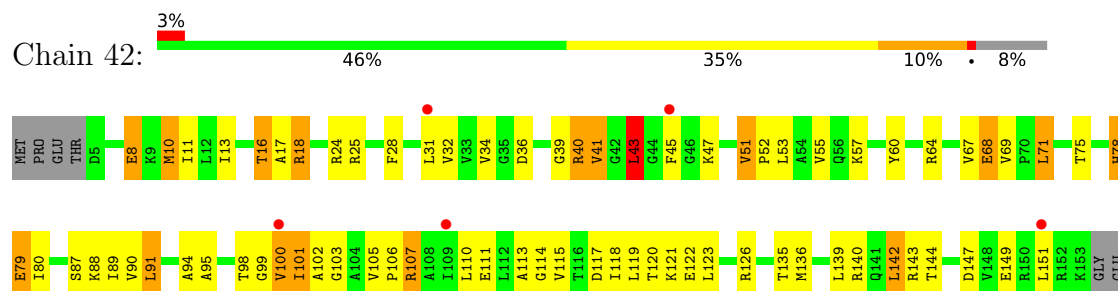


• Molecule 5: 30S ribosomal protein S5

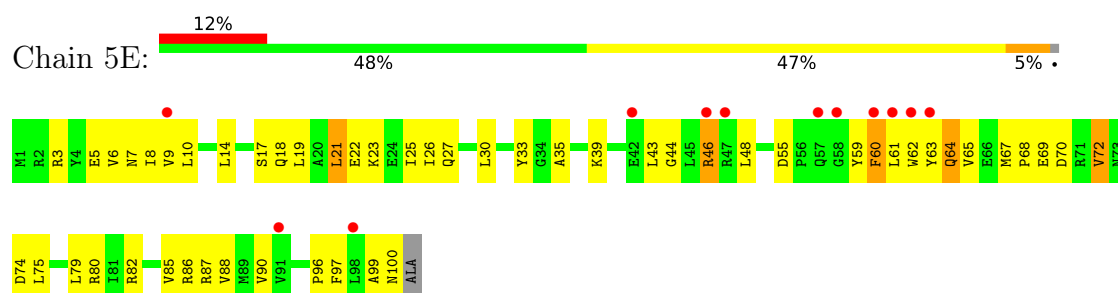


GLY

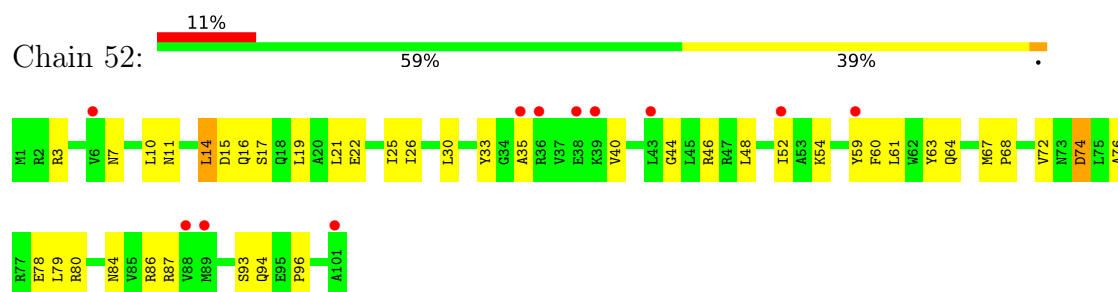
- Molecule 5: 30S ribosomal protein S5

ALA
HIS
ALA
GLN
ALA
GLM
GLY

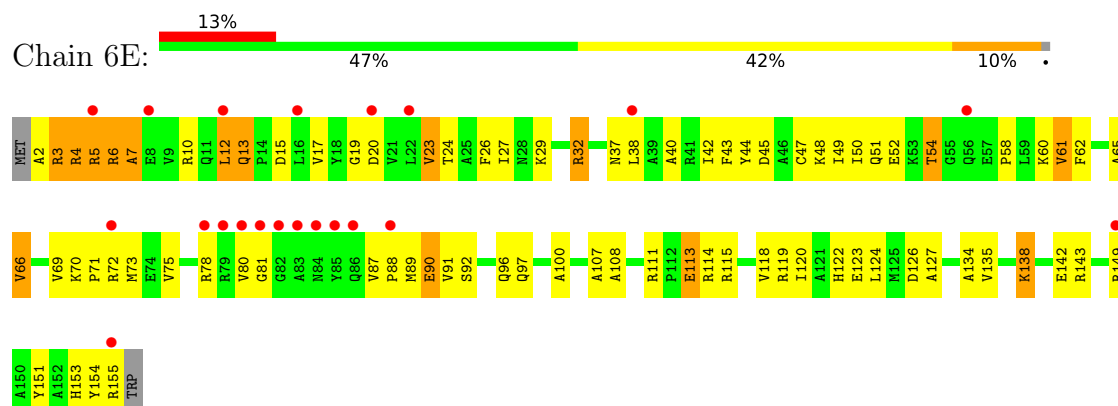
- Molecule 6: 30S ribosomal protein S6



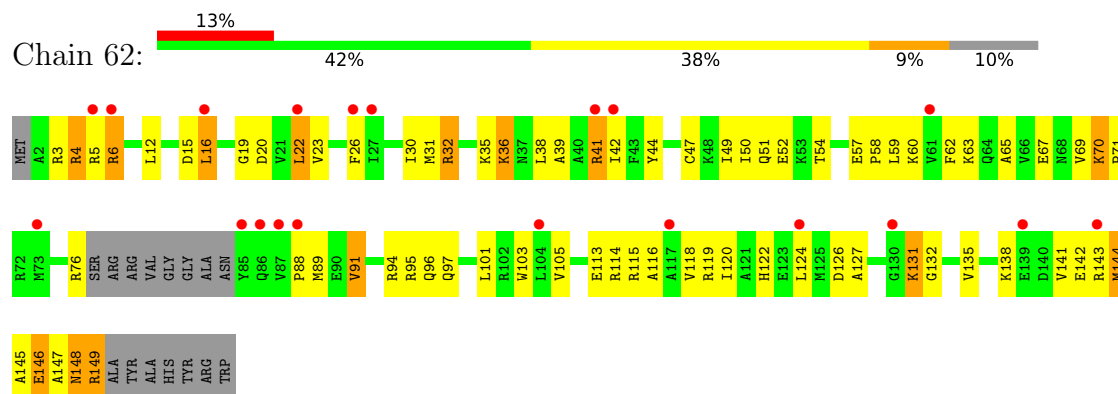
- Molecule 6: 30S ribosomal protein S6



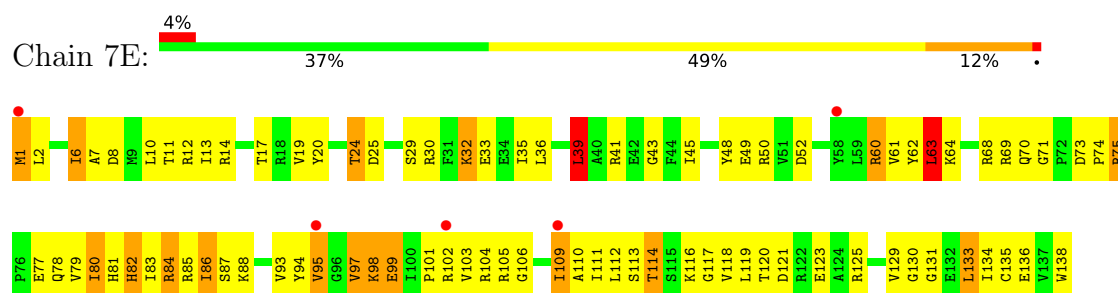
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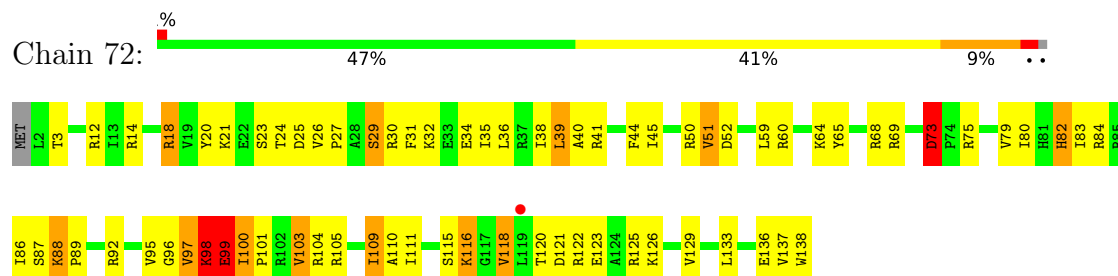
- Molecule 7: 30S ribosomal protein S7



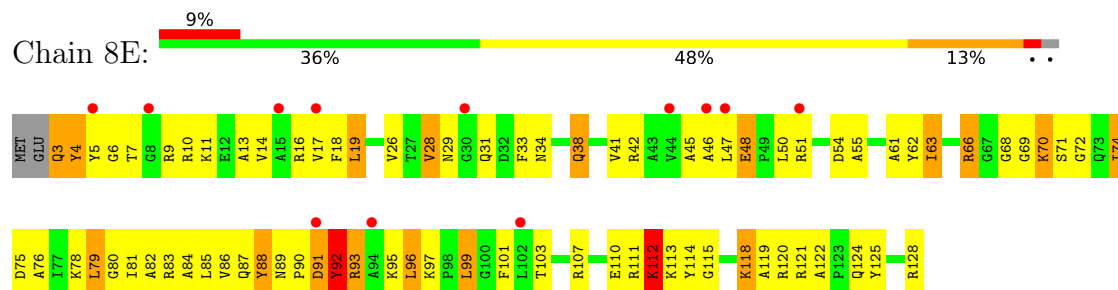
- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8

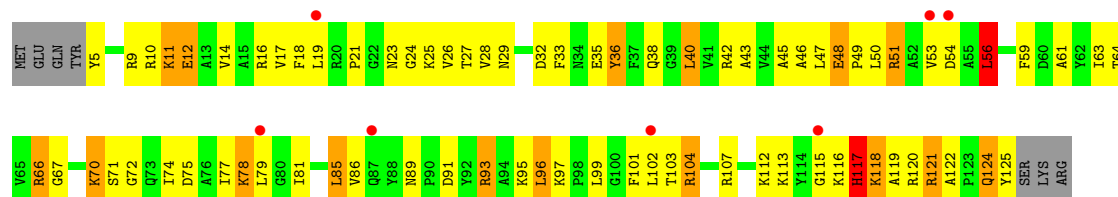


- Molecule 9: 30S ribosomal protein S9

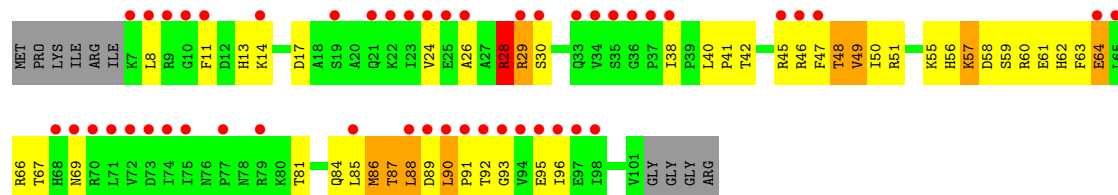


- Molecule 9: 30S ribosomal protein S9

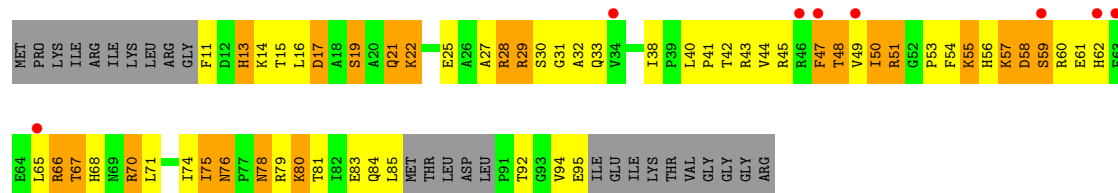
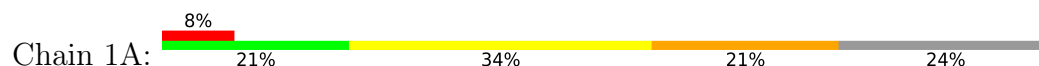




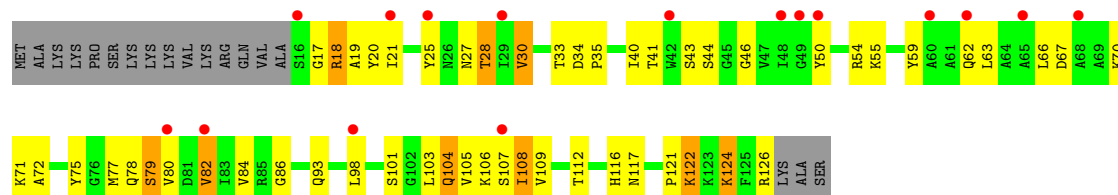
• Molecule 10: 30S ribosomal protein S10



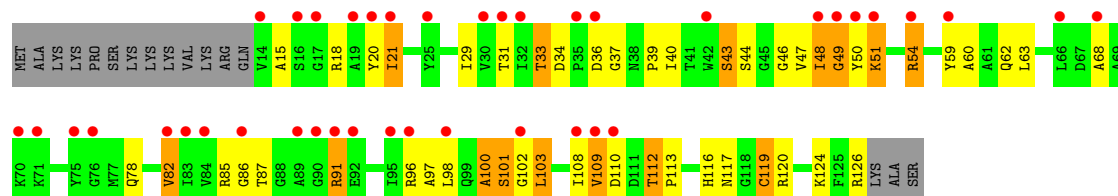
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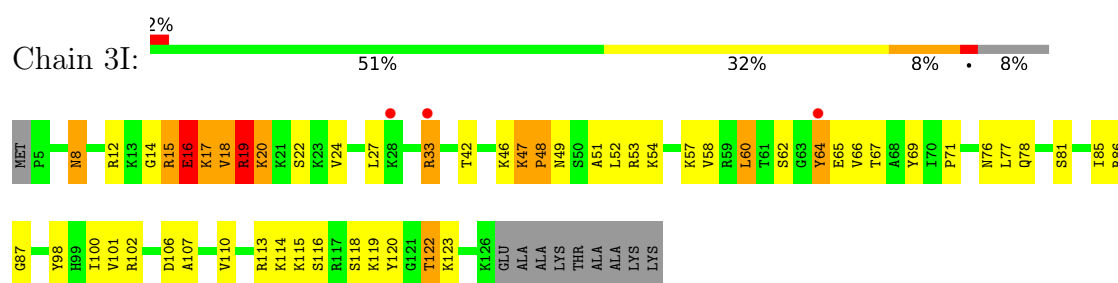
• Molecule 11: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S11



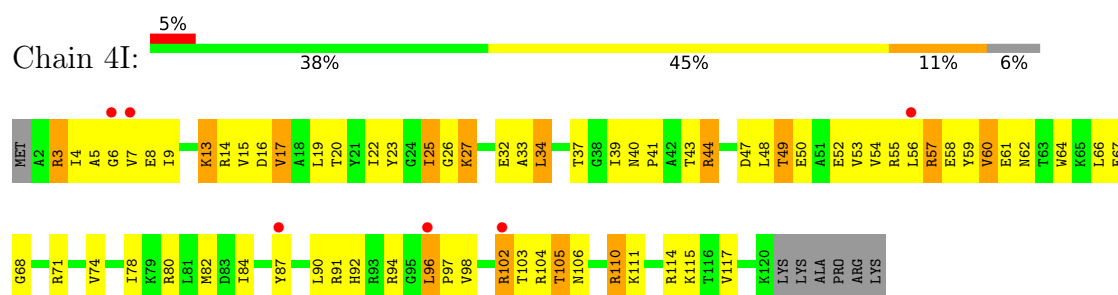
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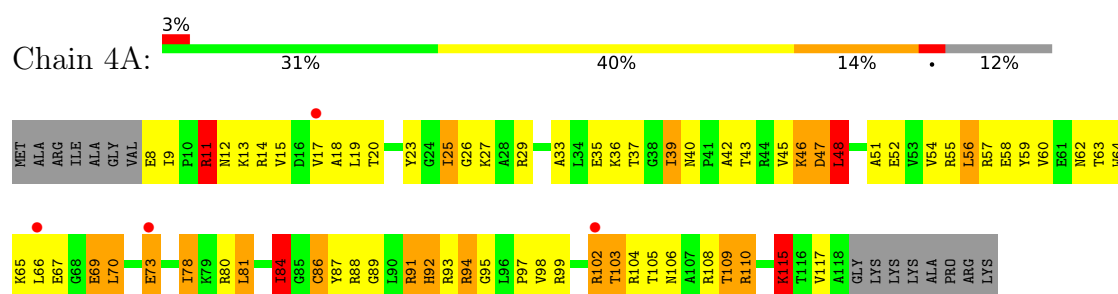
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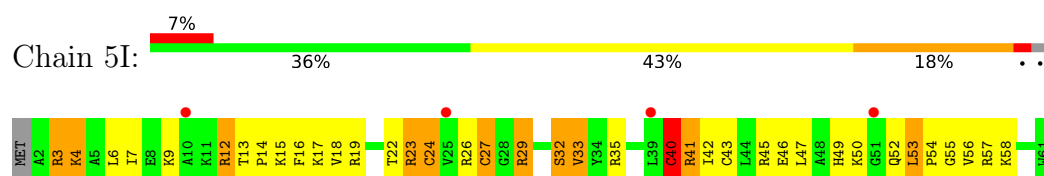
• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13

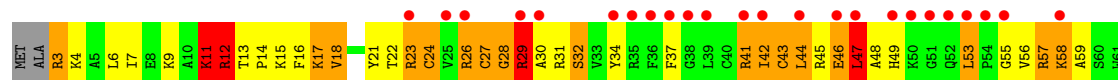


• Molecule 14: 30S ribosomal protein S14 type Z

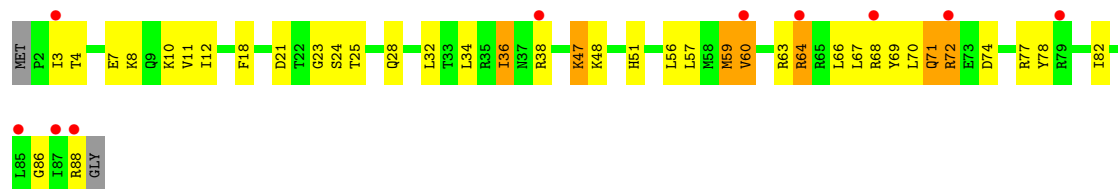


• Molecule 14: 30S ribosomal protein S14 type Z





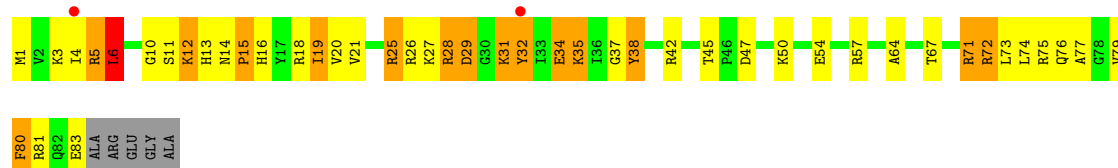
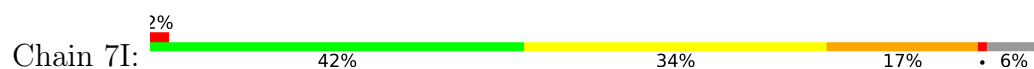
- Molecule 15: 30S ribosomal protein S15



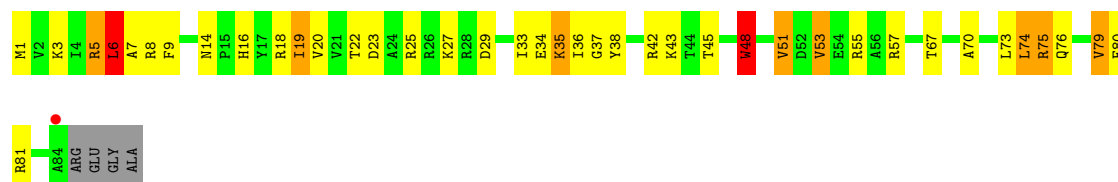
- Molecule 15: 30S ribosomal protein S15



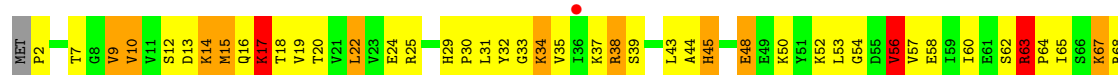
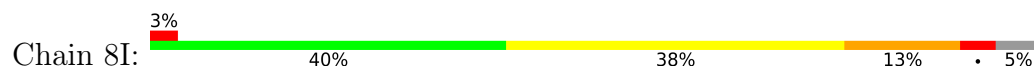
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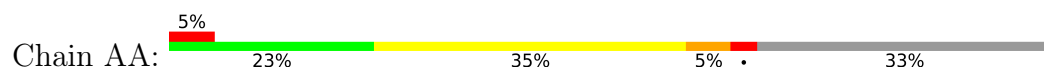


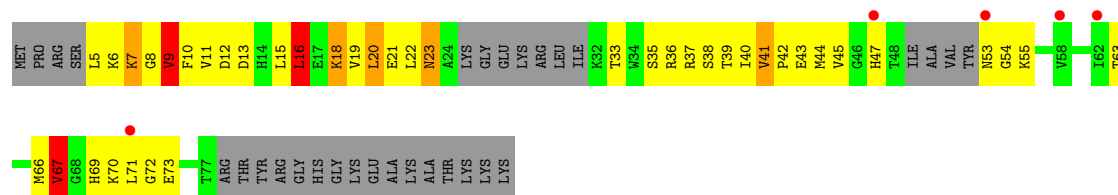
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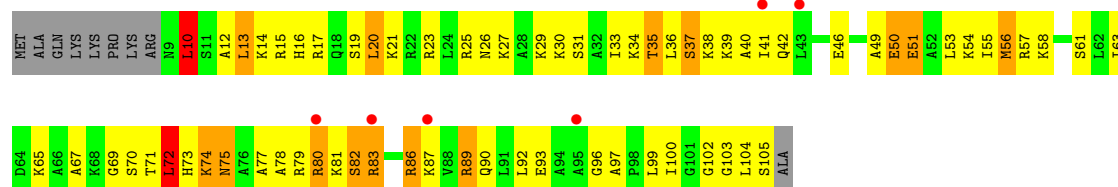
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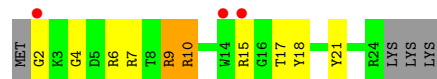
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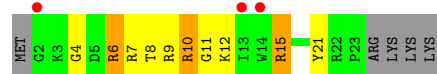
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx

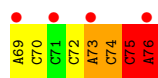


- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNAVal

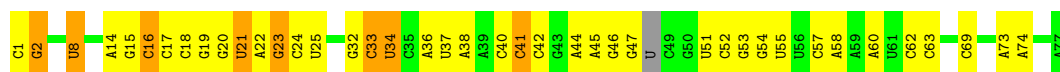




• Molecule 23: tRNA^fMet



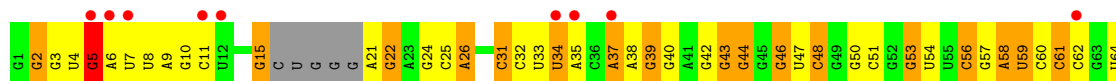
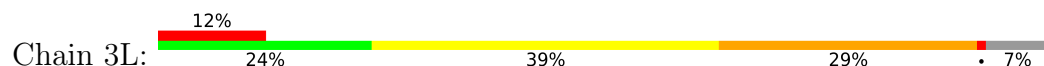
• Molecule 23: tRNA^fMet



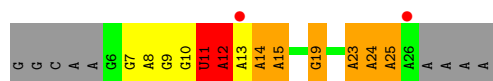
• Molecule 24: tRNA^{Val}



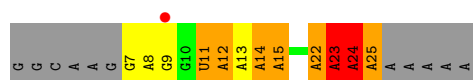
• Molecule 24: tRNA^{Val}



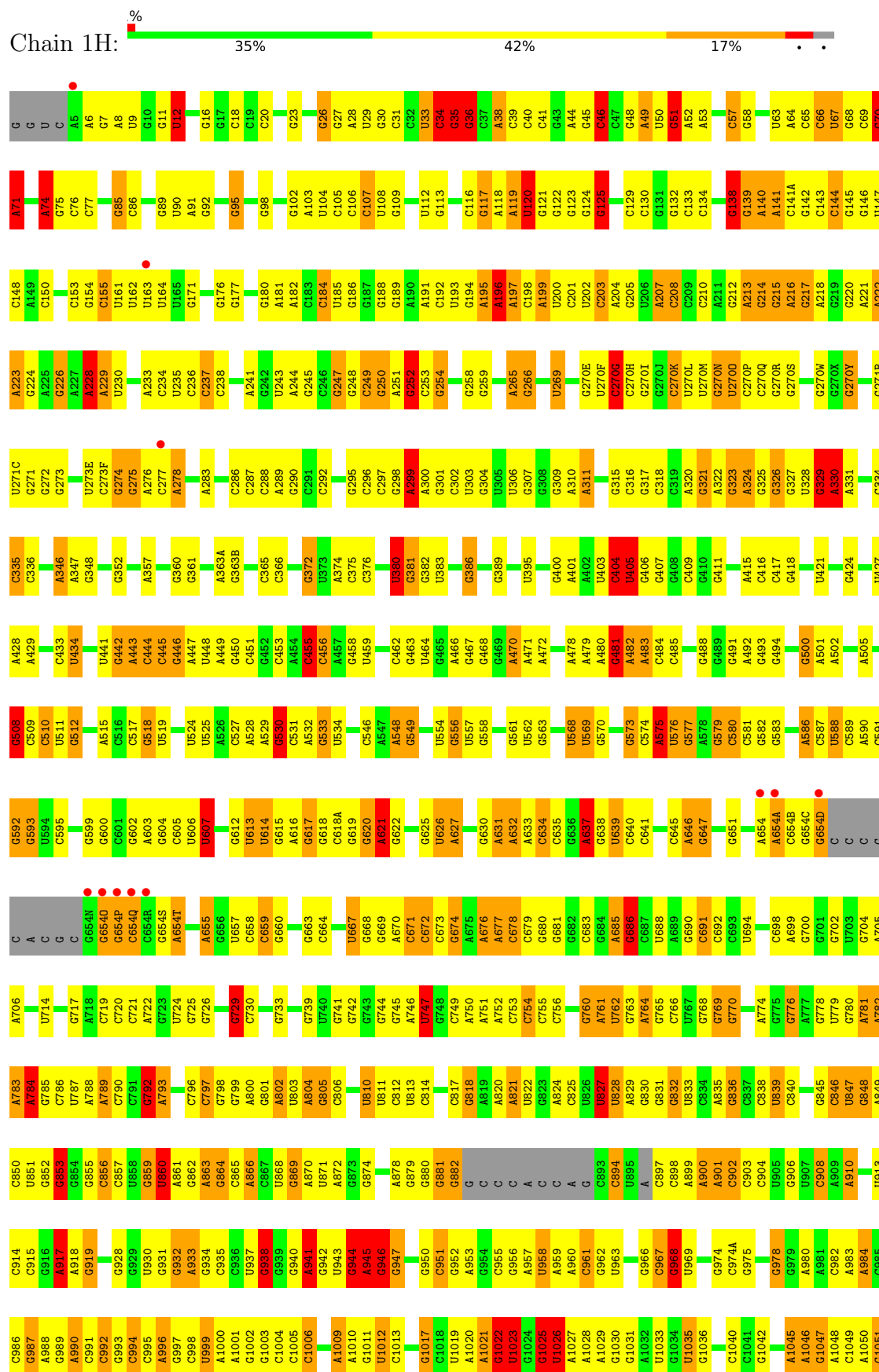
• Molecule 25: mRNA



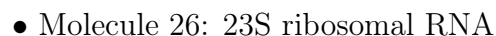
• Molecule 25: mRNA



• Molecule 26: 23S ribosomal RNA

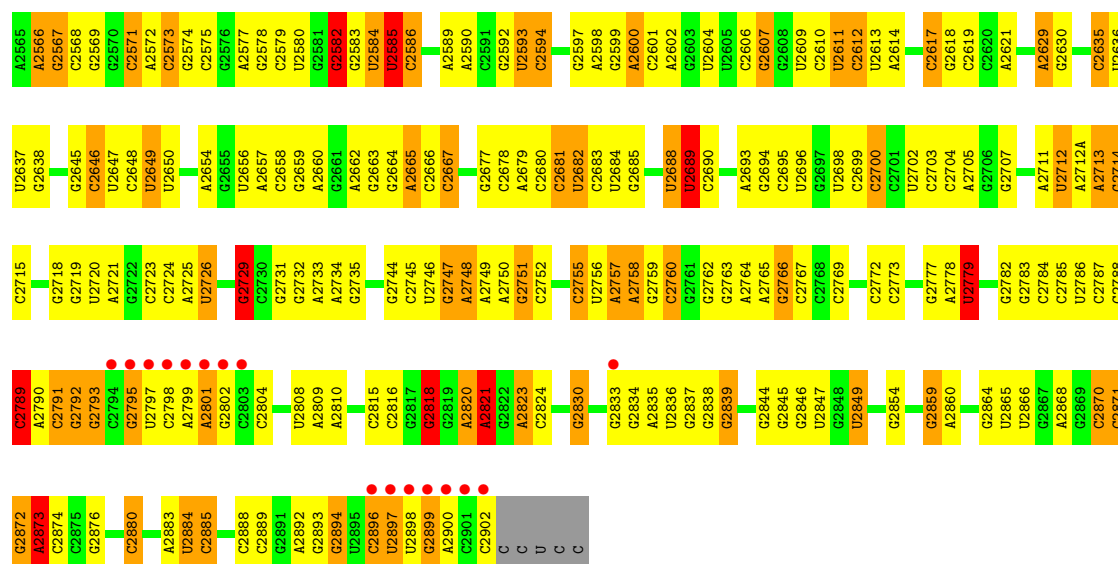


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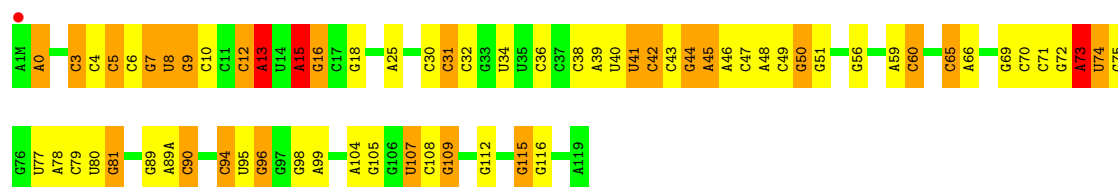




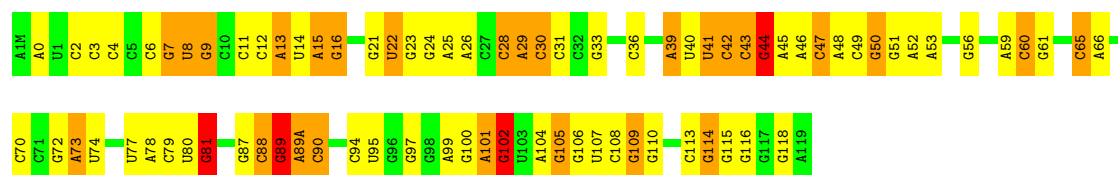
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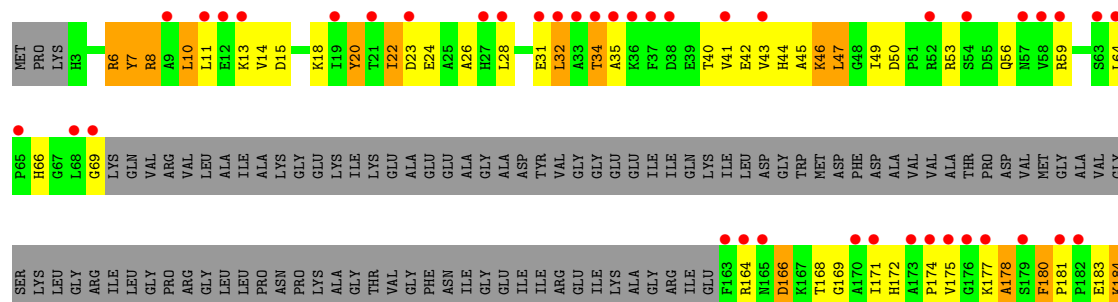
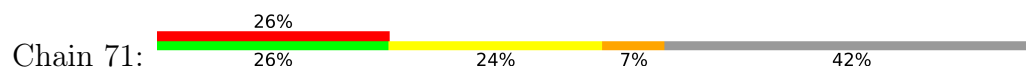
• Molecule 27: 5S ribosomal RNA

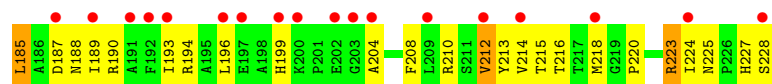


• Molecule 27: 5S ribosomal RNA

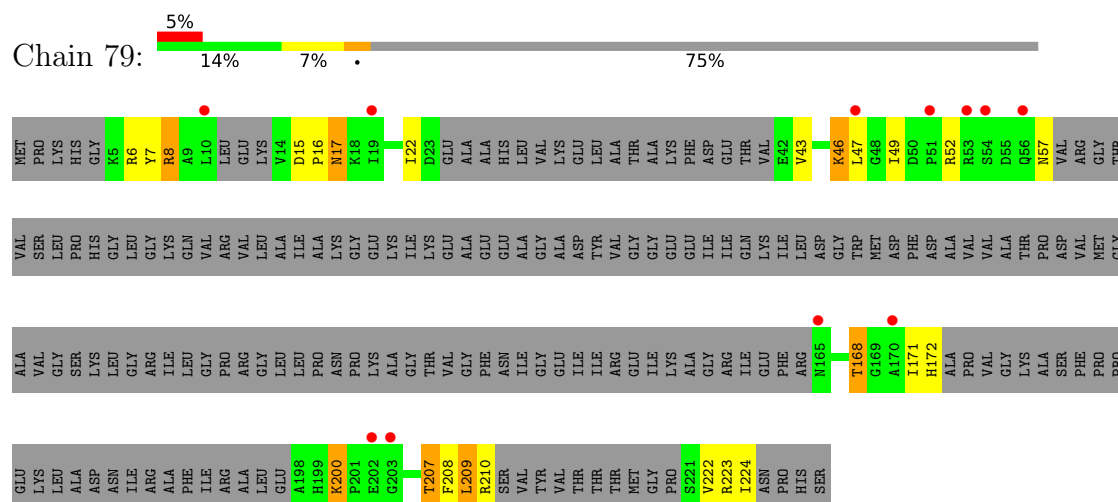


• Molecule 28: 50S ribosomal protein L1

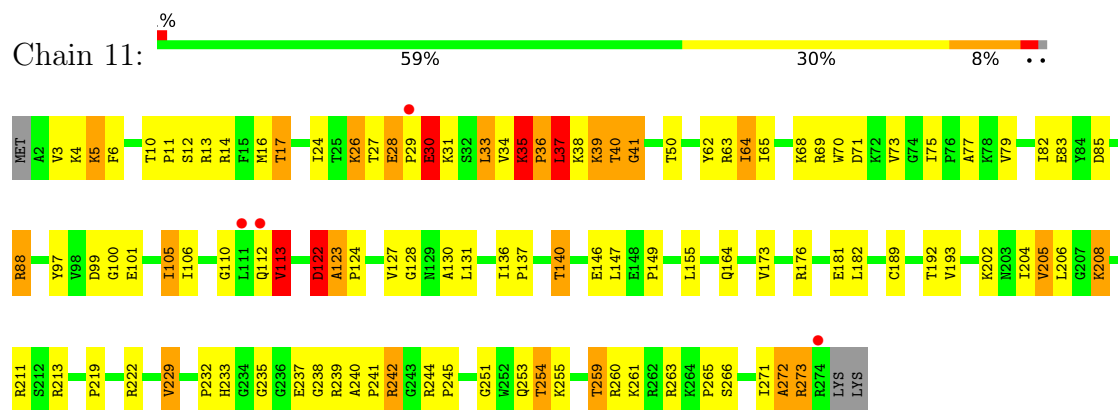




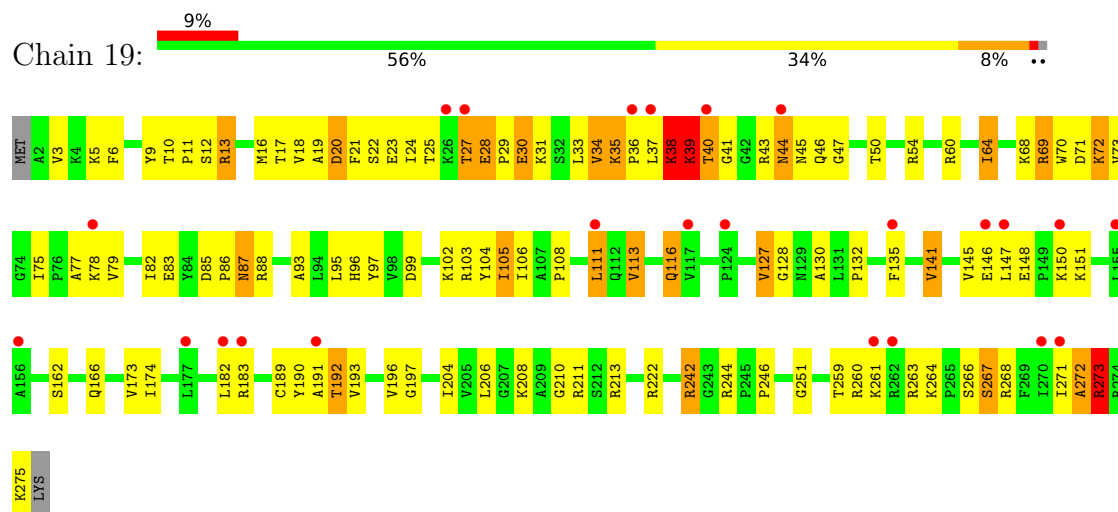
• Molecule 28: 50S ribosomal protein L1



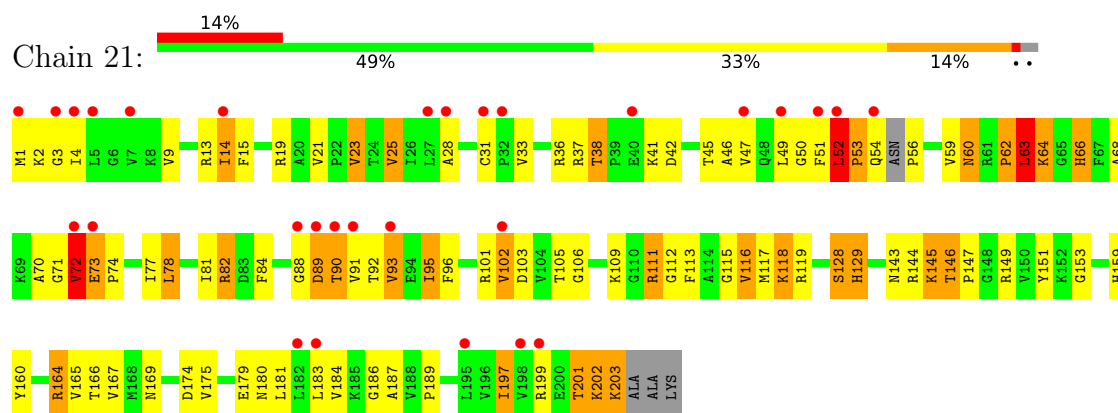
• Molecule 29: 50S ribosomal protein L2



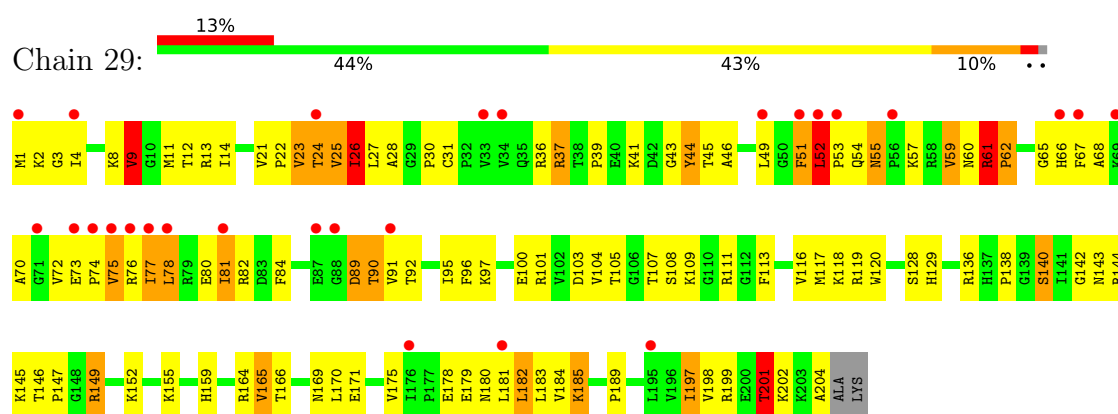
• Molecule 29: 50S ribosomal protein L2



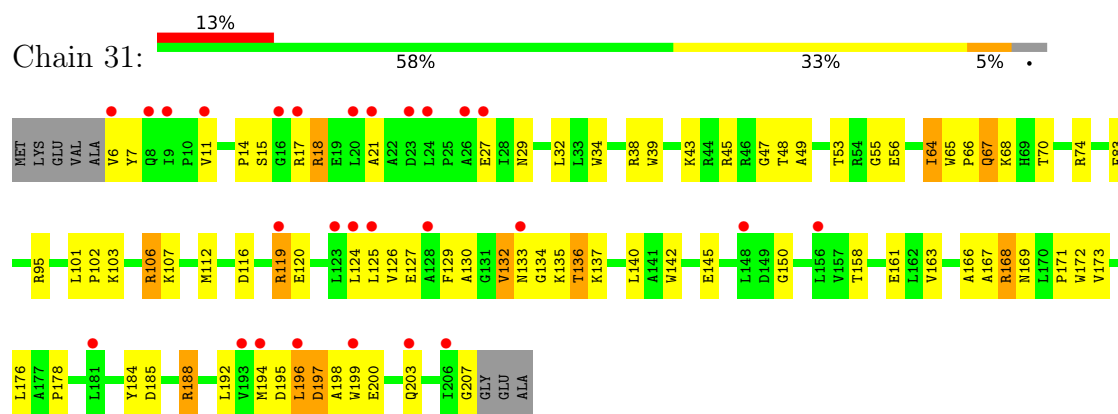
- Molecule 30: 50S ribosomal protein L3



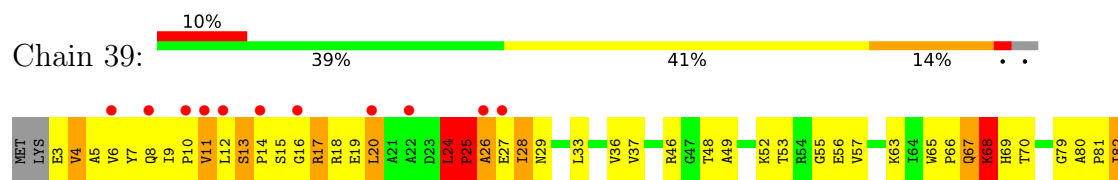
- Molecule 30: 50S ribosomal protein L3

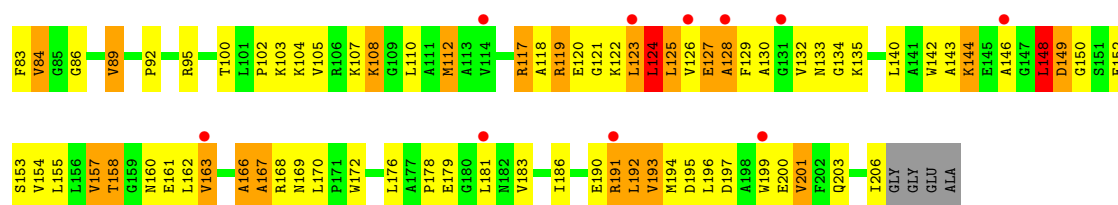


- Molecule 31: 50S ribosomal protein L4

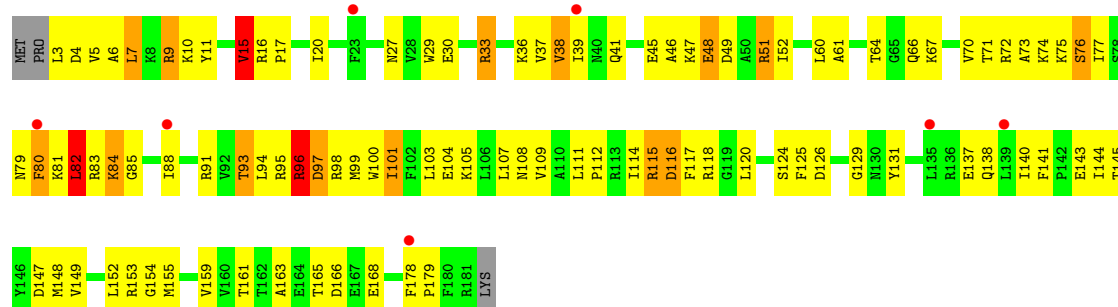
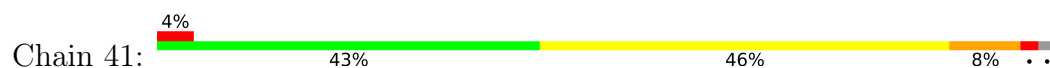


- Molecule 31: 50S ribosomal protein L4

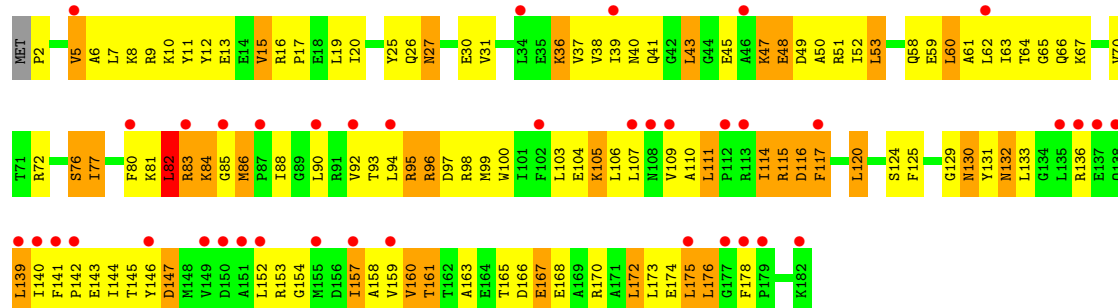




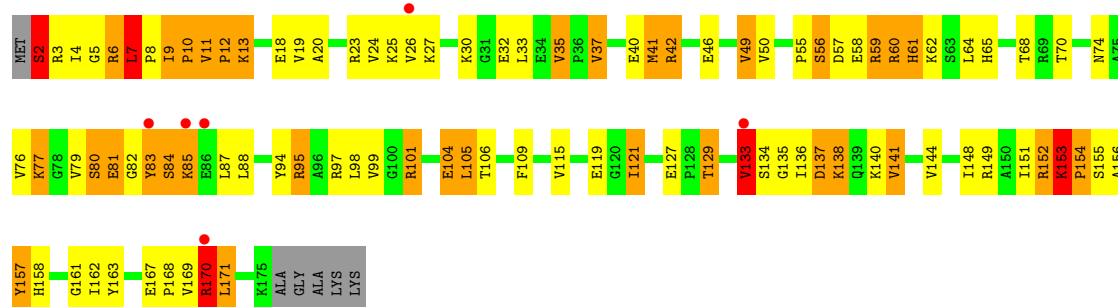
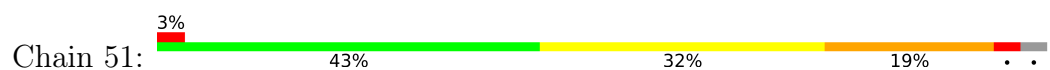
• Molecule 32: 50S ribosomal protein L5



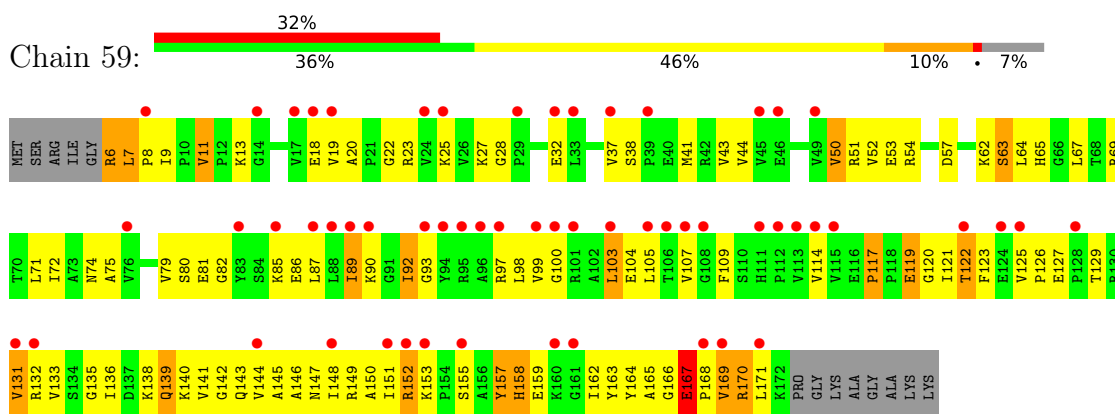
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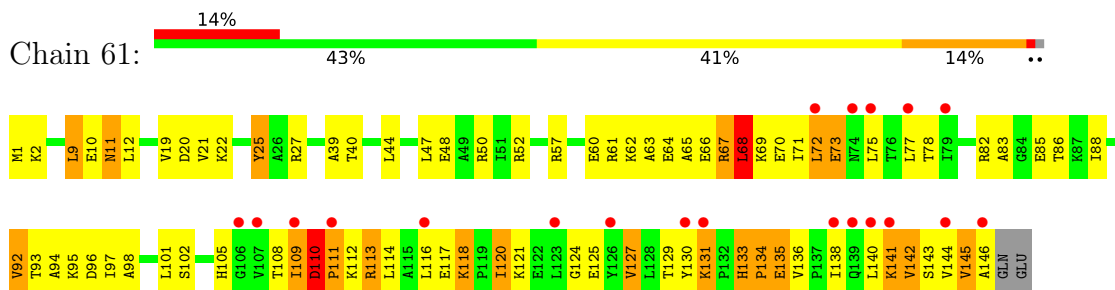
• Molecule 33: 50S ribosomal protein L6



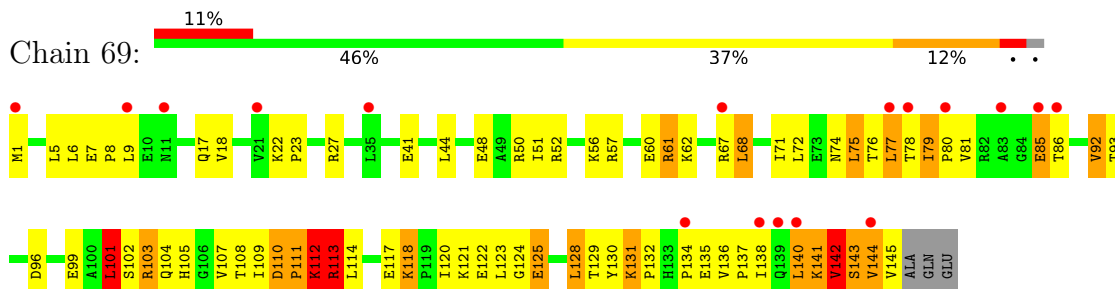
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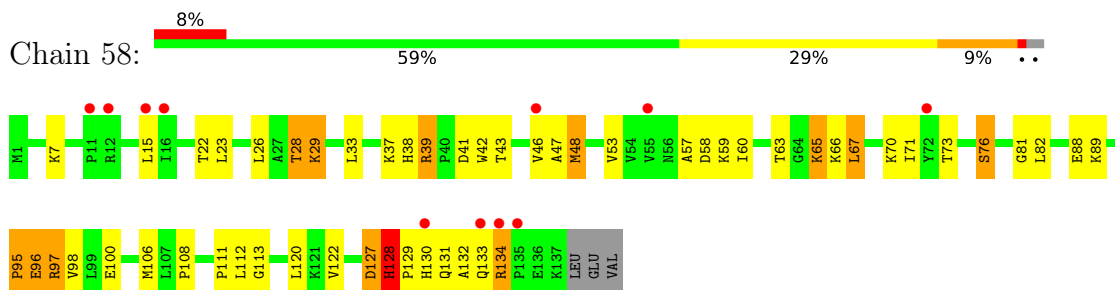
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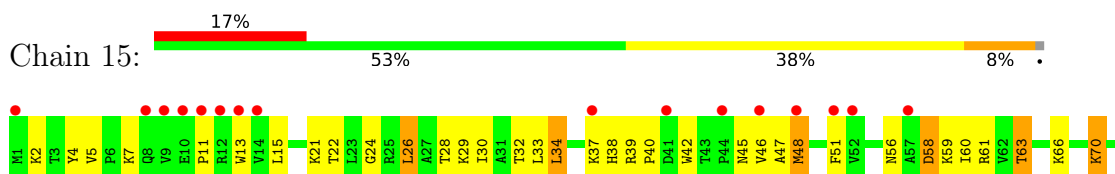
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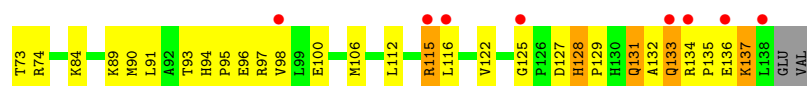


• Molecule 35: 50S ribosomal protein L13

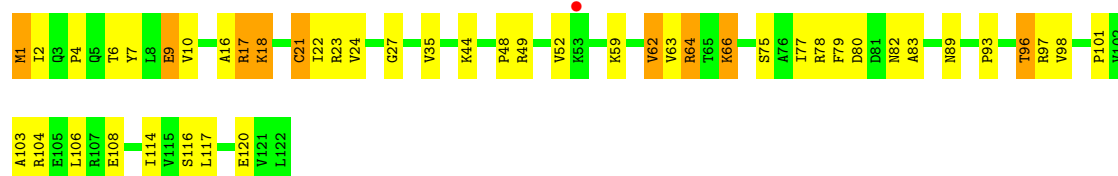


• Molecule 35: 50S ribosomal protein L13

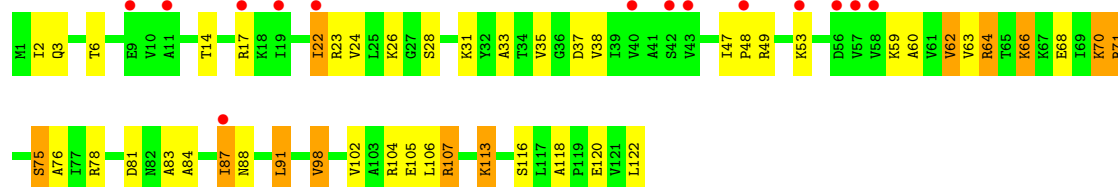




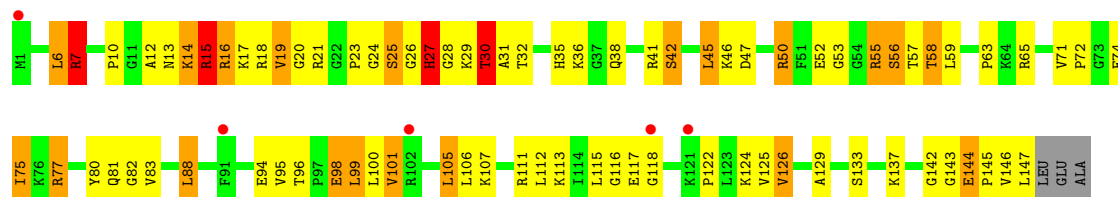
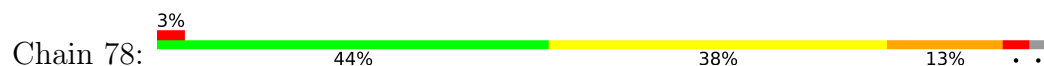
- Molecule 36: 50S ribosomal protein L14



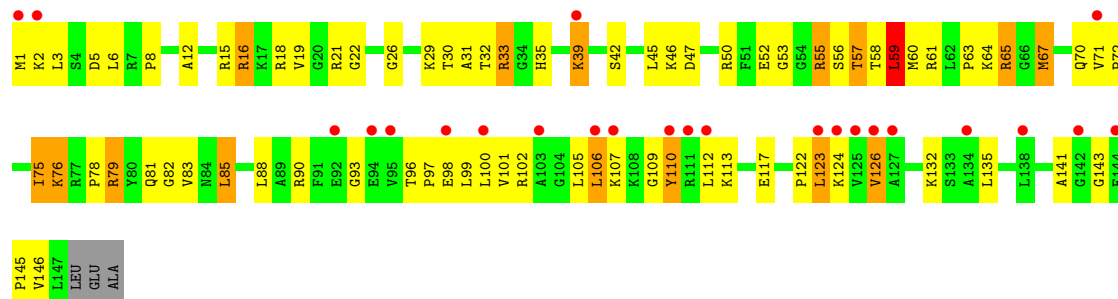
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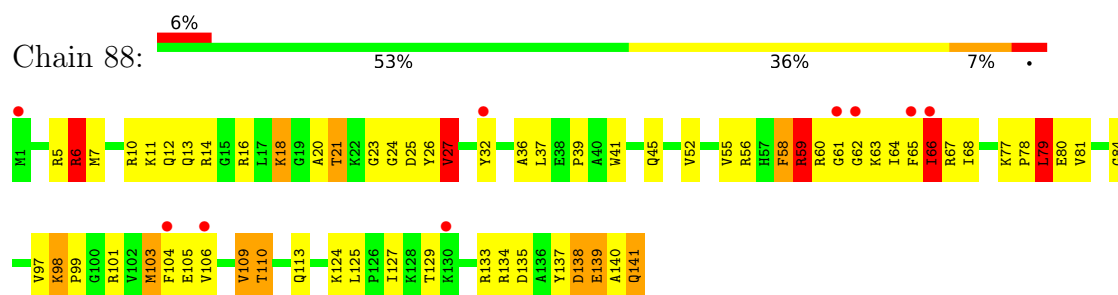
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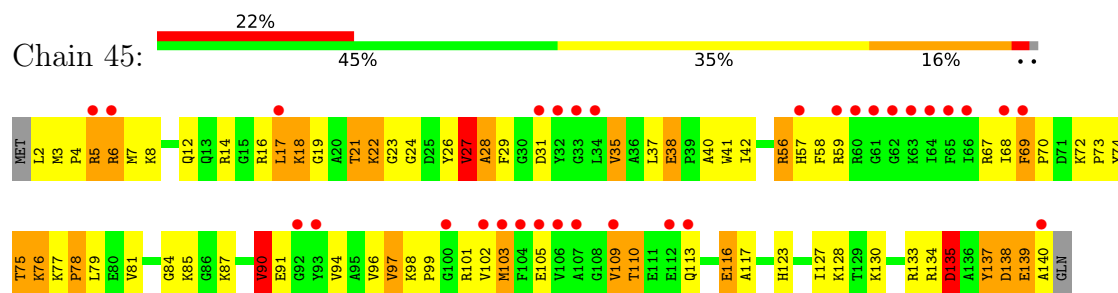
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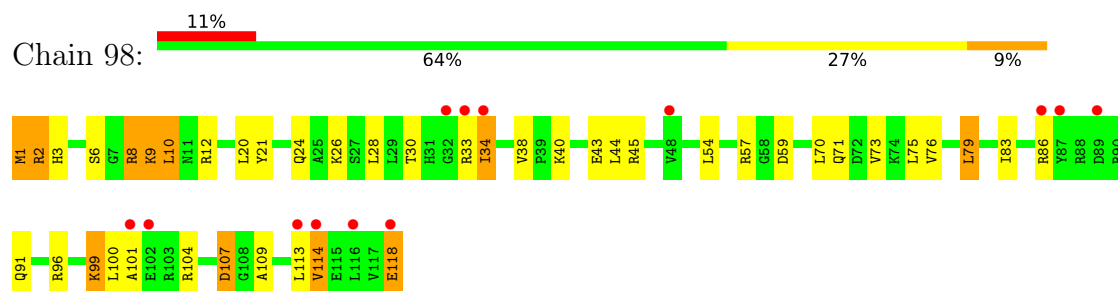
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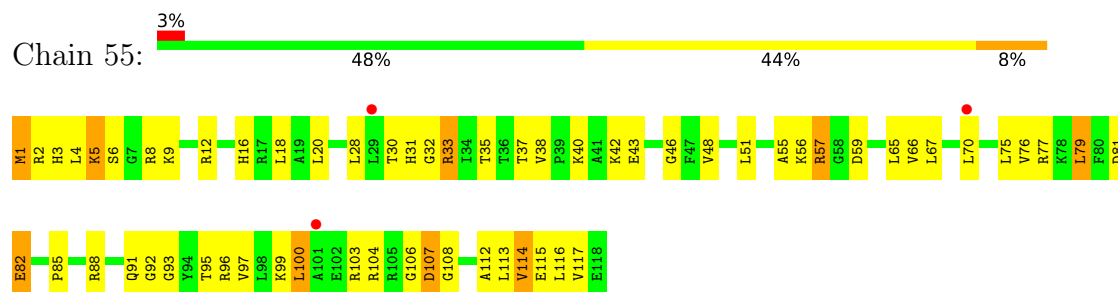
• Molecule 38: 50S ribosomal protein L16



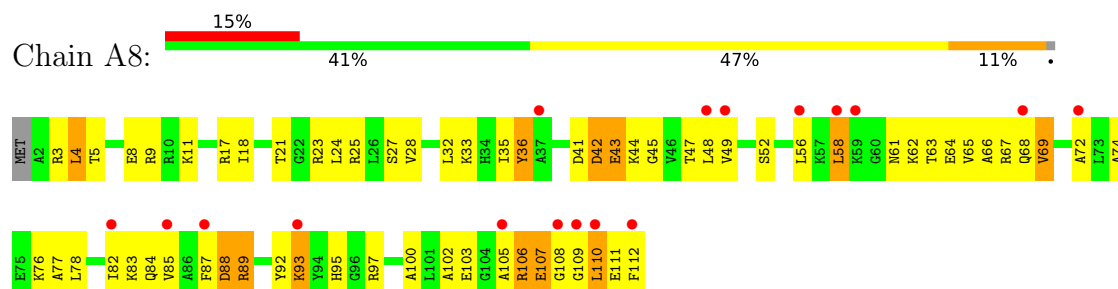
• Molecule 39: 50S ribosomal protein L17



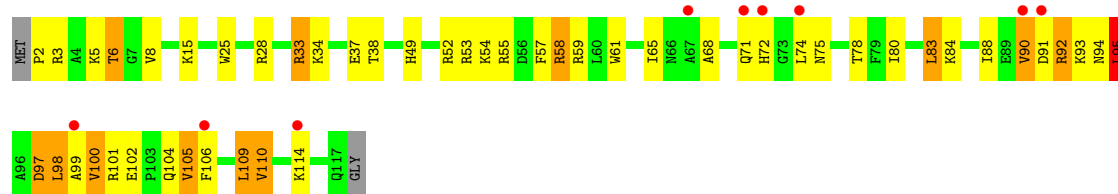
• Molecule 39: 50S ribosomal protein L17



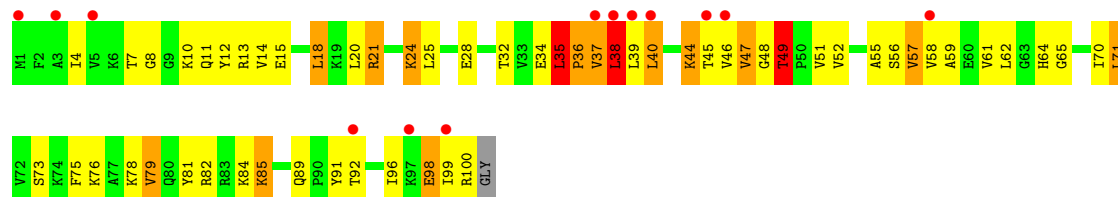
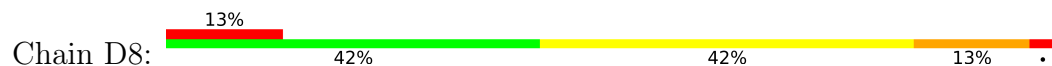
• Molecule 40: 50S ribosomal protein L18



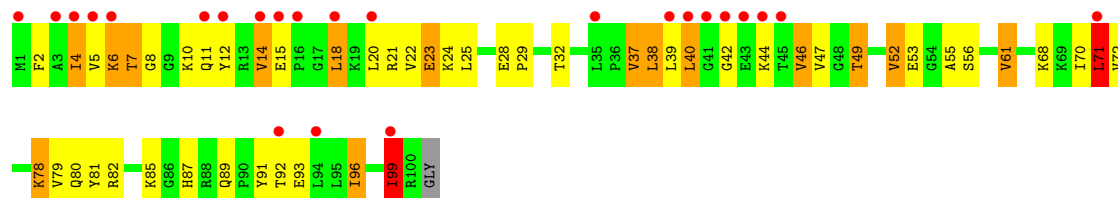
- Chain 85: 



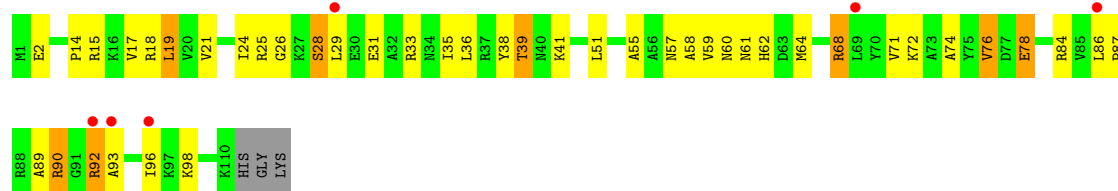
• Molecule 43: 50S ribosomal protein L21



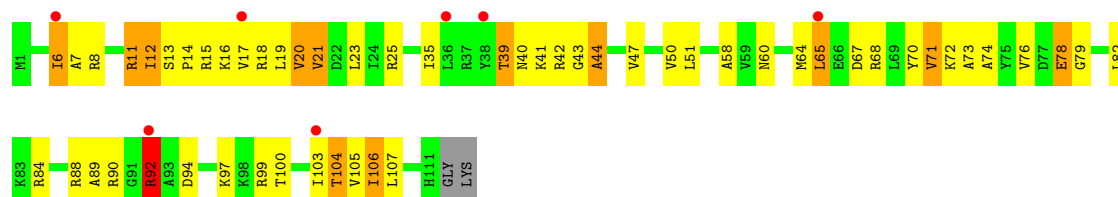
• Molecule 43: 50S ribosomal protein L21



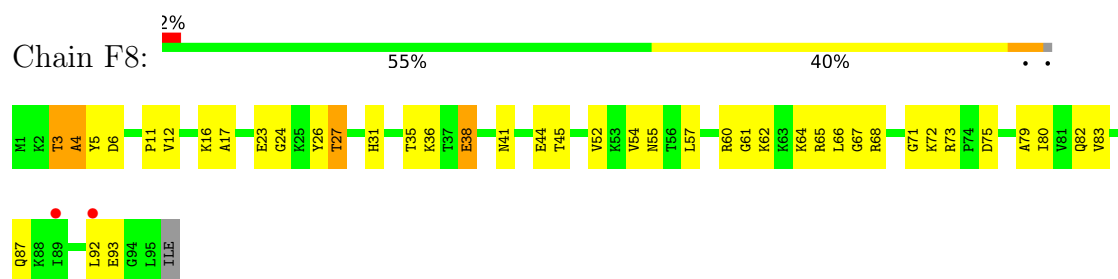
• Molecule 44: 50S ribosomal protein L22



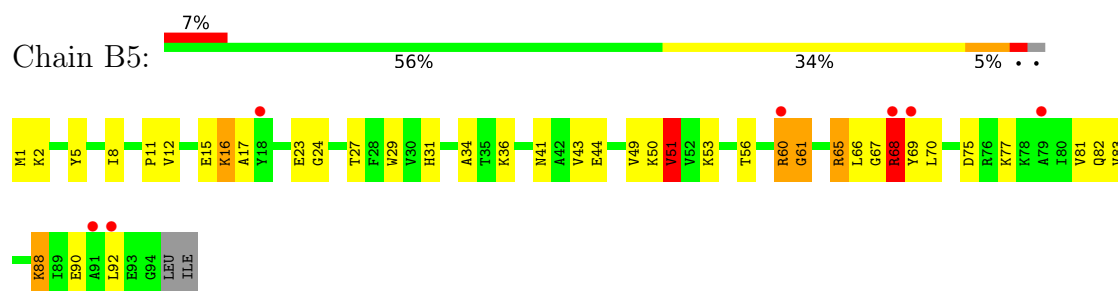
• Molecule 44: 50S ribosomal protein L22



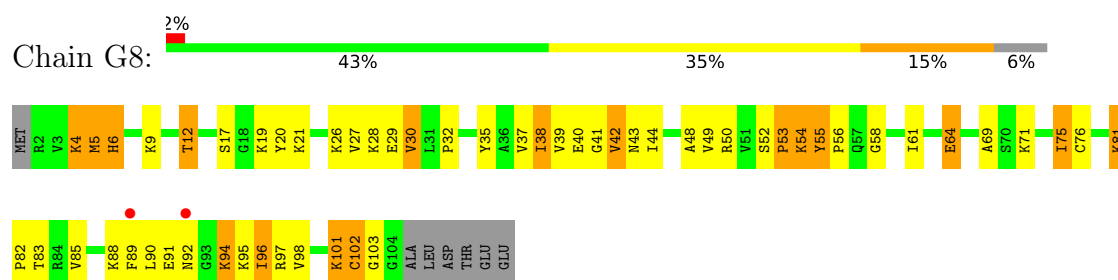
• Molecule 45: 50S ribosomal protein L23



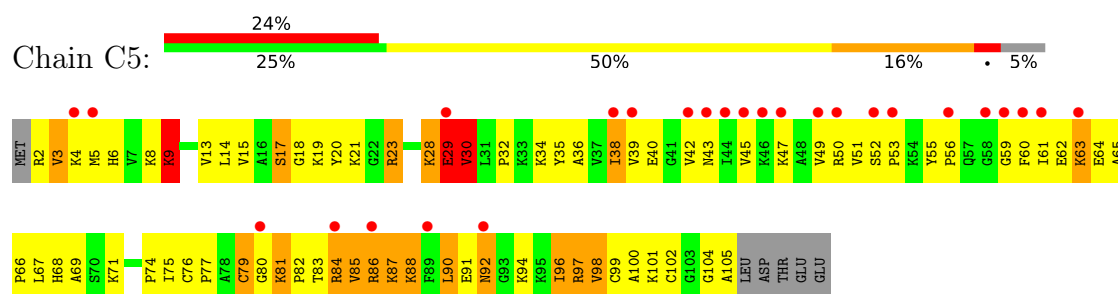
- Molecule 45: 50S ribosomal protein L23



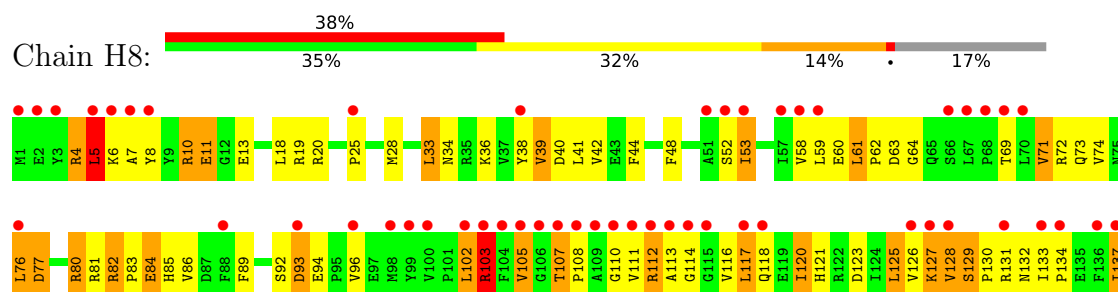
- Molecule 46: 50S ribosomal protein L24



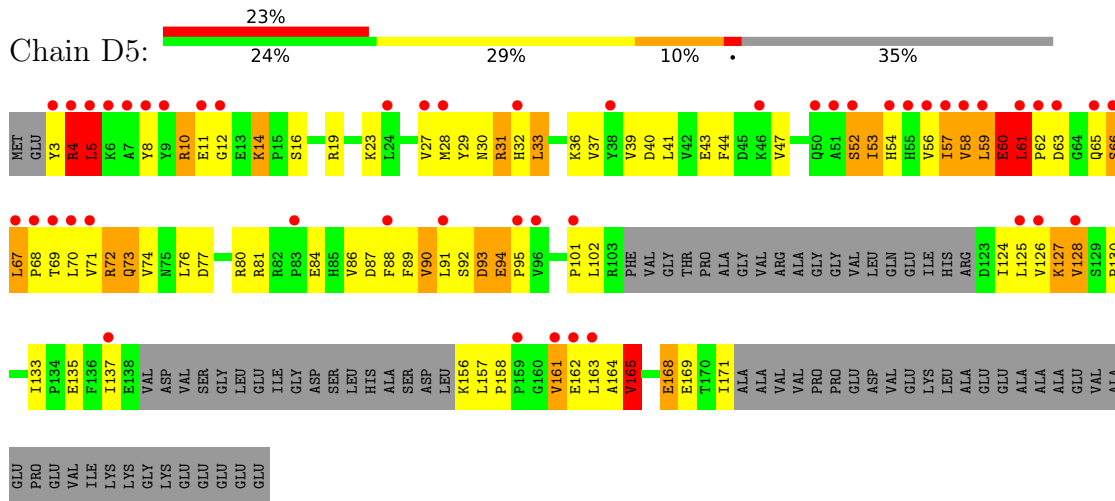
- Molecule 46: 50S ribosomal protein L24



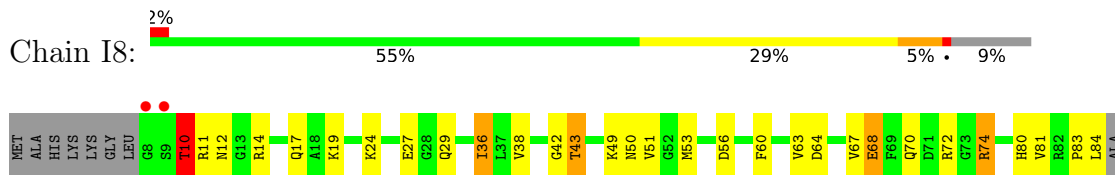
- Molecule 47: 50S ribosomal protein L25



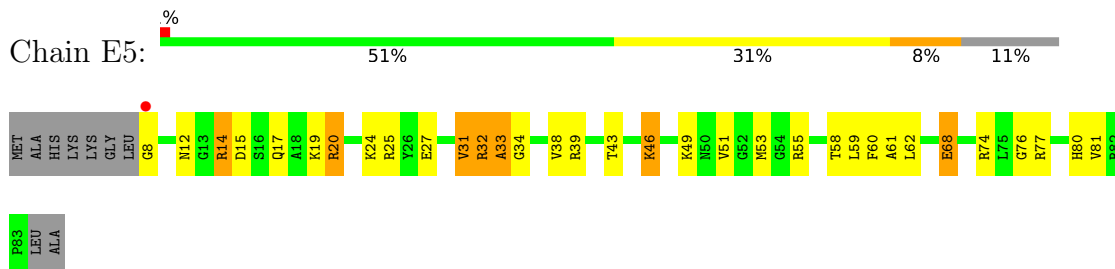
- Molecule 47: 50S ribosomal protein L25



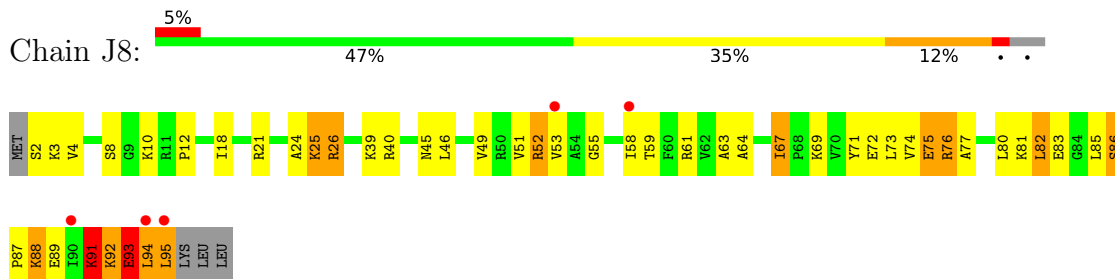
- Molecule 48: 50S ribosomal protein L27



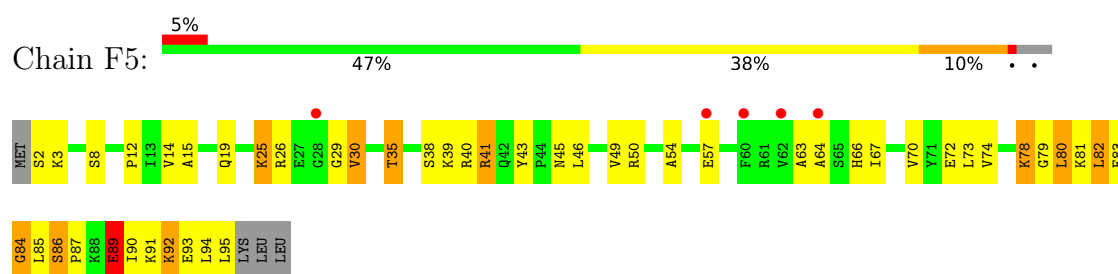
- Molecule 48: 50S ribosomal protein L27



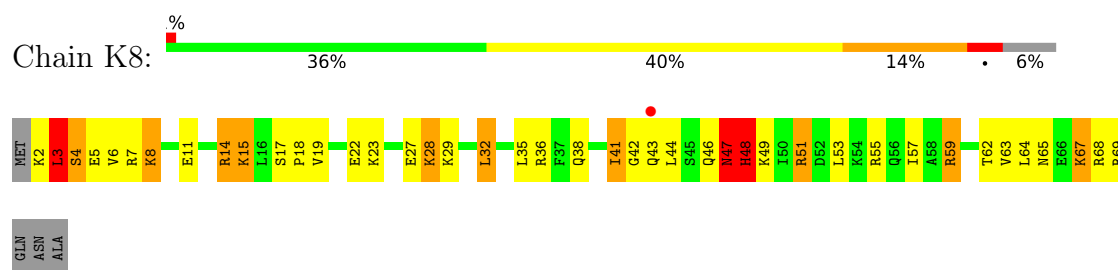
- Molecule 49: 50S ribosomal protein L28



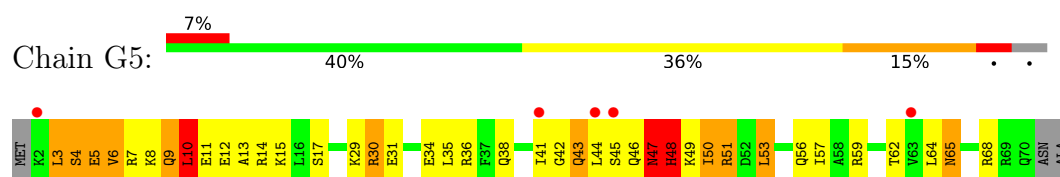
- Molecule 49: 50S ribosomal protein L28



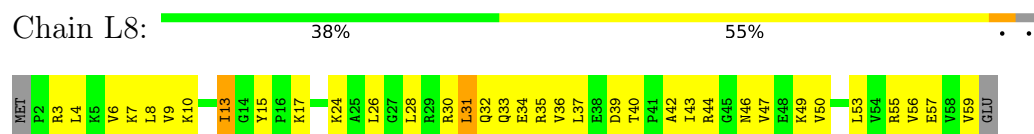
- Molecule 50: 50S ribosomal protein L29



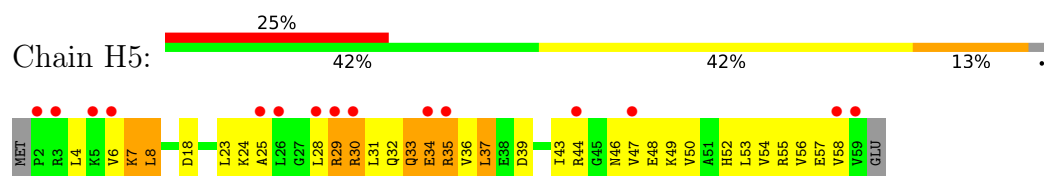
- Molecule 50: 50S ribosomal protein L29



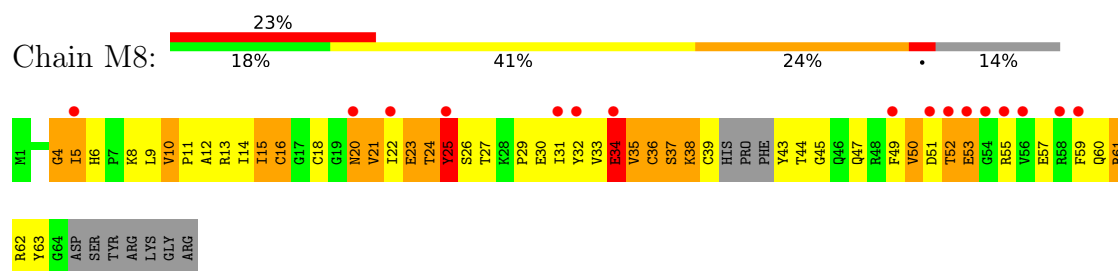
- Molecule 51: 50S ribosomal protein L30



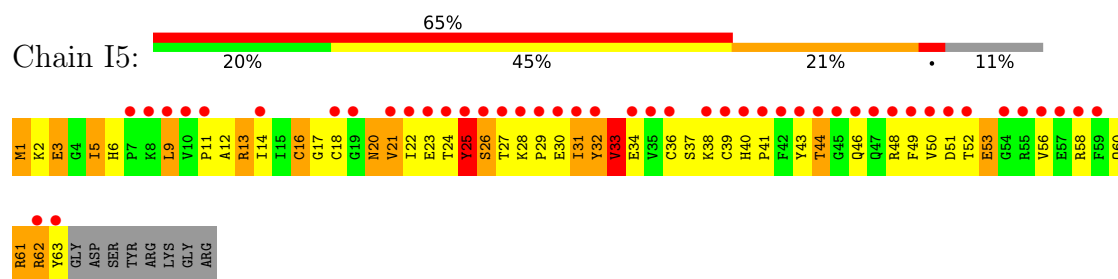
- Molecule 51: 50S ribosomal protein L30



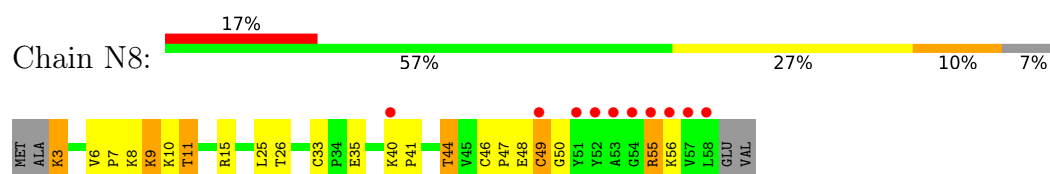
- Molecule 52: 50S ribosomal protein L31



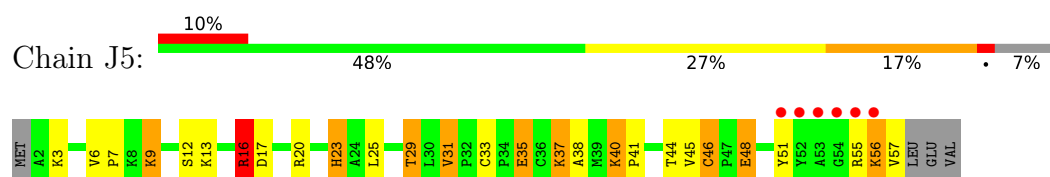
- Molecule 52: 50S ribosomal protein L31



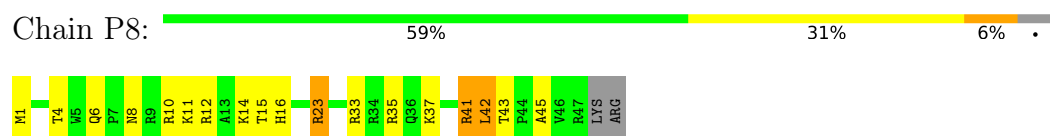
- Molecule 53: 50S ribosomal protein L32



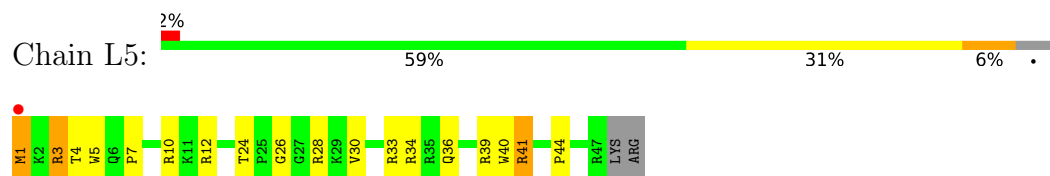
- Molecule 53: 50S ribosomal protein L32



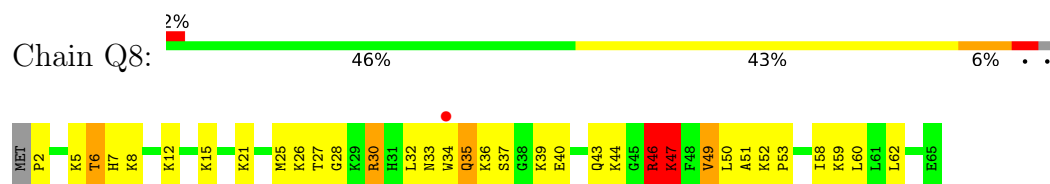
- Molecule 54: 50S ribosomal protein L34



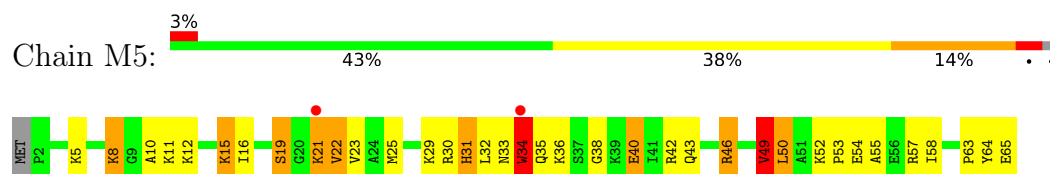
- Molecule 54: 50S ribosomal protein L34



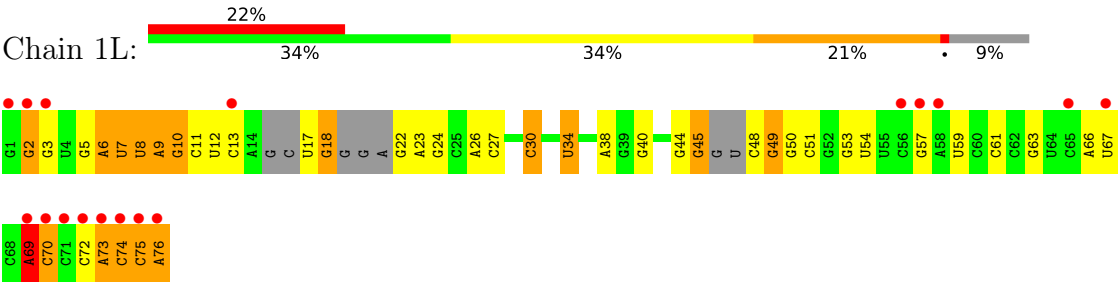
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



● Molecule 56: tRNAVal



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.50Å 448.90Å 620.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.68 – 2.96 146.68 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (146.68-2.96) 89.3 (146.68-2.96)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.201 , 0.243 0.201 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	296743	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, H2U, SF4, MG, CM0, 6MZ, 4SU, 7MG, SPE, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	13	0.67	6/35994 (0.0%)	1.30	243/56171 (0.4%)
1	1G	0.61	1/36236 (0.0%)	1.22	170/56555 (0.3%)
2	12	0.39	0/1727	0.70	1/2326 (0.0%)
2	1E	0.40	0/1936	0.66	1/2611 (0.0%)
3	22	0.62	1/1560 (0.1%)	0.65	1/2104 (0.0%)
3	2E	0.49	1/1629 (0.1%)	0.67	0/2195
4	32	0.45	0/1732	0.65	0/2318
4	3E	0.48	0/1728	0.73	4/2313 (0.2%)
5	42	0.46	0/1155	0.67	1/1555 (0.1%)
5	4E	0.46	0/1158	0.70	1/1559 (0.1%)
6	52	0.47	0/855	0.63	0/1154
6	5E	0.48	0/850	0.64	0/1147
7	62	0.42	0/1132	0.66	1/1514 (0.1%)
7	6E	0.45	0/1259	0.57	0/1686
8	72	0.41	0/1127	0.63	0/1517
8	7E	0.43	0/1135	0.71	1/1527 (0.1%)
9	82	0.41	0/971	0.74	1/1304 (0.1%)
9	8E	0.50	1/1019 (0.1%)	0.76	1/1367 (0.1%)
10	1A	0.74	2/658 (0.3%)	0.68	0/885
10	1I	0.41	0/767	0.72	2/1034 (0.2%)
11	2A	0.46	0/850	0.66	0/1150
11	2I	0.46	0/838	0.67	0/1133
12	3A	0.56	0/972	0.73	1/1301 (0.1%)
12	3I	0.61	0/972	0.79	0/1301
13	4A	0.42	0/903	0.69	1/1211 (0.1%)
13	4I	0.48	0/952	0.73	1/1277 (0.1%)
14	5A	0.46	0/495	0.89	2/657 (0.3%)
14	5I	0.63	2/500 (0.4%)	0.90	3/664 (0.5%)
15	6A	0.47	0/740	0.63	0/987
15	6I	0.47	0/740	0.70	0/987
16	7A	0.45	0/721	0.74	1/970 (0.1%)
16	7I	0.47	0/716	0.76	1/963 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.46	0/836	0.61	0/1117
17	8I	0.55	1/847 (0.1%)	0.77	1/1131 (0.1%)
18	9A	0.51	0/549	0.75	1/732 (0.1%)
18	9I	0.46	0/554	0.69	0/739
19	AA	0.43	0/490	0.75	2/662 (0.3%)
19	AI	0.42	0/676	0.79	1/910 (0.1%)
20	BA	0.40	0/764	0.71	0/1007
20	BI	0.56	1/748 (0.1%)	0.81	2/986 (0.2%)
21	1B	0.44	0/192	0.65	0/252
21	1F	0.44	0/203	0.67	0/266
22	1K	0.64	0/1595	1.19	11/2475 (0.4%)
23	2K	0.77	0/1721	1.38	7/2682 (0.3%)
23	2L	0.67	0/1698	1.28	12/2644 (0.5%)
24	3K	0.54	0/1663	1.20	16/2585 (0.6%)
24	3L	0.56	0/1689	1.16	11/2628 (0.4%)
25	4K	0.72	0/520	1.23	3/808 (0.4%)
25	4L	0.64	0/470	1.23	4/732 (0.5%)
26	14	0.81	39/67798 (0.1%)	1.49	1064/105832 (1.0%)
26	1H	0.95	95/68537 (0.1%)	1.67	1647/106989 (1.5%)
27	16	0.79	0/2928	1.48	37/4568 (0.8%)
27	1J	0.73	0/2928	1.34	23/4568 (0.5%)
28	71	0.32	0/1055	0.62	0/1425
28	79	0.31	0/459	0.58	0/608
29	11	0.68	1/2170 (0.0%)	0.94	6/2926 (0.2%)
29	19	0.61	0/2175	0.86	2/2933 (0.1%)
30	21	0.58	0/1537	0.92	3/2081 (0.1%)
30	29	0.53	0/1596	0.85	1/2153 (0.0%)
31	31	0.58	0/1620	0.78	2/2194 (0.1%)
31	39	0.54	1/1637 (0.1%)	0.84	2/2218 (0.1%)
32	41	0.51	1/1481 (0.1%)	0.71	1/1994 (0.1%)
32	49	0.42	0/1492	0.72	3/2008 (0.1%)
33	51	0.54	0/1354	0.95	5/1833 (0.3%)
33	59	0.36	0/1308	0.67	2/1771 (0.1%)
34	61	0.46	0/1151	0.80	4/1558 (0.3%)
34	69	0.45	0/1146	0.75	2/1551 (0.1%)
35	15	0.47	1/1131 (0.1%)	0.72	0/1525
35	58	0.52	0/1123	0.74	1/1514 (0.1%)
36	25	0.51	0/942	0.70	0/1269
36	68	0.54	0/942	0.74	0/1269
37	35	0.55	0/1139	0.90	3/1514 (0.2%)
37	78	0.64	0/1139	1.03	6/1514 (0.4%)
38	45	0.65	2/1125 (0.2%)	0.83	1/1505 (0.1%)
38	88	0.71	0/1138	0.92	2/1523 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	55	0.50	0/981	0.78	1/1312 (0.1%)
39	98	0.51	0/981	0.78	0/1312
40	65	0.52	0/886	0.83	0/1180
40	A8	0.56	0/891	0.78	0/1187
41	75	0.53	0/1123	0.83	4/1500 (0.3%)
41	B8	0.52	0/1138	0.82	1/1521 (0.1%)
42	85	0.52	0/977	0.73	0/1301
42	C8	0.57	0/968	0.85	4/1289 (0.3%)
43	95	0.49	0/781	0.81	1/1048 (0.1%)
43	D8	0.54	0/785	0.86	2/1052 (0.2%)
44	A5	0.54	0/897	0.76	1/1204 (0.1%)
44	E8	0.58	0/886	0.81	1/1189 (0.1%)
45	B5	0.53	0/749	0.72	1/1007 (0.1%)
45	F8	0.59	0/757	0.77	1/1017 (0.1%)
46	C5	0.54	0/807	0.89	0/1076
46	G8	0.64	0/790	0.93	3/1055 (0.3%)
47	D5	0.50	2/1103 (0.2%)	0.80	2/1494 (0.1%)
47	H8	0.48	0/1395	0.77	2/1890 (0.1%)
48	E5	0.62	0/611	0.83	0/814
48	I8	0.60	0/619	0.84	1/825 (0.1%)
49	F5	0.57	0/744	0.94	4/989 (0.4%)
49	J8	0.61	0/744	0.89	1/989 (0.1%)
50	G5	0.51	0/578	0.81	1/766 (0.1%)
50	K8	0.65	0/577	0.88	1/763 (0.1%)
51	H5	0.49	0/464	0.66	0/623
51	L8	0.49	0/464	0.73	0/623
52	I5	0.41	0/527	0.84	0/709
52	M8	0.54	0/486	0.87	2/652 (0.3%)
53	J5	0.51	0/448	0.83	1/606 (0.2%)
53	N8	0.58	0/451	0.75	0/610
54	L5	0.61	0/409	0.75	0/540
54	P8	0.78	0/409	0.96	3/540 (0.6%)
55	M5	0.61	1/524 (0.2%)	0.91	1/691 (0.1%)
55	Q8	0.67	0/524	0.96	2/691 (0.3%)
56	1L	0.53	0/1592	1.05	1/2472 (0.0%)
All	All	0.73	159/317359 (0.1%)	1.32	3368/475179 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	5
2	1E	0	3
3	22	0	1
3	2E	0	1
4	32	0	2
4	3E	0	2
7	6E	0	1
8	72	0	2
8	7E	0	1
9	82	0	1
9	8E	0	2
10	1I	0	2
11	2A	0	2
12	3I	0	6
13	4A	0	4
13	4I	0	2
14	5A	0	5
14	5I	0	1
16	7I	0	1
17	8I	0	1
18	9I	0	1
19	AA	0	1
19	AI	0	1
20	BA	0	2
28	71	0	1
29	11	0	3
29	19	0	4
30	21	0	5
30	29	0	3
31	31	0	1
31	39	0	9
32	41	0	3
32	49	0	3
33	51	0	7
33	59	0	2
34	61	0	3
34	69	0	5
35	58	0	1
36	68	0	1
37	35	0	5
37	78	0	4
38	45	0	3
38	88	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	55	0	1
39	98	0	2
40	65	0	1
40	A8	0	3
41	75	0	3
41	B8	0	4
42	85	0	4
42	C8	0	3
43	95	0	3
43	D8	0	3
44	A5	0	1
45	B5	0	1
45	F8	0	1
46	C5	0	2
46	G8	0	4
47	D5	0	3
47	H8	0	3
49	F5	0	2
49	J8	0	4
50	G5	0	2
50	K8	0	2
52	I5	0	3
52	M8	0	4
54	P8	0	1
55	M5	0	1
55	Q8	0	2
All	All	0	180

The worst 5 of 159 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	22	173	VAL	C-N	19.50	1.71	1.34
10	1A	38	ILE	C-N	14.98	1.62	1.34
26	1H	1698	A	N9-C4	-11.67	1.30	1.37
26	1H	783	A	N3-C4	-10.65	1.28	1.34
20	BI	97	ALA	C-N	10.36	1.53	1.34

The worst 5 of 3368 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-25.58	110.65	126.00
26	1H	945	A	N1-C6-N6	24.24	133.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	945	A	C6-C5-N7	-23.79	115.65	132.30
26	1H	945	A	C5-N7-C8	-20.19	93.80	103.90
26	1H	1899	G	N3-C4-C5	19.48	138.34	128.60

There are no chirality outliers.

5 of 180 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	236	TYR	Peptide
2	1E	95	GLN	Peptide
3	2E	78	GLY	Peptide
4	3E	154	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16234	739	0
1	1G	32371	0	16342	719	0
2	12	1696	0	1730	124	0
2	1E	1902	0	1949	157	0
3	22	1537	0	1603	116	0
3	2E	1605	0	1668	76	0
4	32	1702	0	1764	95	0
4	3E	1698	0	1760	125	0
5	42	1139	0	1202	85	0
5	4E	1142	0	1204	68	0
6	52	842	0	857	26	0
6	5E	837	0	852	39	0
7	62	1120	0	1167	82	0
7	6E	1242	0	1286	80	0
8	72	1107	0	1165	65	0
8	7E	1115	0	1177	92	0
9	82	953	0	983	106	0
9	8E	1000	0	1031	100	0
10	1A	646	0	662	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	1I	754	0	769	44	0
11	2A	835	0	847	42	0
11	2I	823	0	832	33	0
12	3A	956	0	1046	64	0
12	3I	956	0	1046	39	0
13	4A	893	0	946	72	0
13	4I	942	0	997	76	0
14	5A	486	0	525	65	0
14	5I	491	0	532	49	0
15	6A	729	0	768	33	0
15	6I	729	0	768	38	0
16	7A	705	0	725	58	0
16	7I	700	0	720	77	0
17	8A	823	0	891	32	0
17	8I	834	0	904	84	0
18	9A	544	0	605	26	0
18	9I	549	0	607	33	0
19	AA	481	0	468	39	0
19	AI	661	0	683	55	0
20	BA	762	0	861	44	0
20	BI	746	0	843	98	0
21	1B	188	0	195	12	0
21	1F	199	0	208	19	0
22	1K	1540	0	787	25	0
23	2K	1646	0	843	25	0
23	2L	1626	0	836	27	0
24	3K	1491	0	761	59	0
24	3L	1513	0	770	34	0
25	4K	462	0	230	11	0
25	4L	417	0	207	12	0
26	14	60535	0	30516	1082	0
26	1H	61195	0	30847	1152	0
27	16	2617	0	1328	54	0
27	1J	2617	0	1328	88	0
28	71	1033	0	1048	71	0
28	79	456	0	460	21	0
29	11	2120	0	2197	112	0
29	19	2125	0	2199	96	0
30	21	1505	0	1526	85	0
30	29	1563	0	1629	139	0
31	31	1585	0	1632	61	0
31	39	1602	0	1649	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	41	1457	0	1514	101	0
32	49	1468	0	1520	112	0
33	51	1328	0	1396	108	0
33	59	1283	0	1352	87	0
34	61	1136	0	1223	75	0
34	69	1131	0	1218	60	0
35	15	1104	0	1180	56	0
35	58	1096	0	1169	52	0
36	25	932	0	996	42	0
36	68	932	0	996	40	0
37	35	1122	0	1206	76	0
37	78	1122	0	1206	84	0
38	45	1104	0	1159	88	0
38	88	1117	0	1168	67	0
39	55	967	0	1033	45	0
39	98	967	0	1033	33	0
40	65	876	0	938	99	0
40	A8	881	0	943	58	0
41	75	1109	0	1170	74	0
41	B8	1124	0	1179	78	0
42	85	959	0	1019	59	0
42	C8	950	0	1011	85	0
43	95	770	0	838	48	0
43	D8	774	0	849	58	0
44	A5	886	0	948	38	0
44	E8	876	0	941	43	0
45	B5	735	0	785	37	0
45	F8	743	0	794	30	0
46	C5	794	0	886	81	0
46	G8	777	0	857	42	0
47	D5	1079	0	1088	86	0
47	H8	1365	0	1391	106	0
48	E5	603	0	620	36	0
48	I8	611	0	631	24	0
49	F5	737	0	813	44	0
49	J8	737	0	813	58	0
50	G5	576	0	625	33	0
50	K8	575	0	634	42	0
51	H5	459	0	512	41	0
51	L8	459	0	512	18	0
52	I5	515	0	514	46	0
52	M8	479	0	475	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	J5	434	0	454	25	0
53	N8	437	0	460	21	0
54	L5	401	0	436	15	0
54	P8	401	0	436	9	0
55	M5	516	0	582	32	0
55	Q8	516	0	582	32	0
56	1L	1469	0	752	37	0
57	11	2	0	0	0	0
57	13	148	0	0	0	0
57	14	445	0	0	0	0
57	16	11	0	0	0	0
57	19	1	0	0	0	0
57	1G	133	0	0	0	0
57	1H	548	0	0	0	0
57	1J	7	0	0	0	0
57	21	2	0	0	0	0
57	25	2	0	0	0	0
57	29	2	0	0	0	0
57	2K	4	0	0	0	0
57	2L	3	0	0	0	0
57	31	2	0	0	0	0
57	35	2	0	0	0	0
57	39	2	0	0	0	0
57	3A	1	0	0	0	0
57	3I	1	0	0	0	0
57	41	1	0	0	0	0
57	42	1	0	0	0	0
57	45	1	0	0	0	0
57	4A	1	0	0	0	0
57	4E	1	0	0	0	0
57	4K	2	0	0	0	0
57	4L	2	0	0	0	0
57	5E	1	0	0	0	0
57	5I	1	0	0	0	0
57	68	2	0	0	0	0
57	78	1	0	0	0	0
57	88	3	0	0	0	0
57	9A	1	0	0	0	0
57	B5	1	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	F8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	I8	1	0	0	0	0
57	J8	1	0	0	0	0
57	L8	1	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	13	13	0	22	3	0
58	14	26	0	46	11	0
58	1G	13	0	24	0	0
58	1J	13	0	24	1	0
59	32	8	0	0	1	0
59	3E	8	0	0	3	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	11	16	0	0	6	0
61	13	304	0	0	17	0
61	14	1135	0	0	56	0
61	16	15	0	0	1	0
61	19	8	0	0	0	0
61	1G	391	0	0	17	0
61	1H	1133	0	0	86	0
61	1I	2	0	0	0	0
61	1J	18	0	0	1	0
61	1K	1	0	0	0	0
61	21	8	0	0	0	0
61	22	1	0	0	0	0
61	25	11	0	0	1	0
61	29	6	0	0	0	0
61	2I	1	0	0	0	0
61	2K	6	0	0	0	0
61	31	4	0	0	0	0
61	35	9	0	0	4	0
61	39	6	0	0	0	0
61	3A	1	0	0	0	0
61	3E	1	0	0	0	0
61	3I	2	0	0	0	0
61	3K	1	0	0	0	0
61	42	1	0	0	0	0
61	45	3	0	0	0	0
61	4E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	4K	11	0	0	0	0
61	4L	14	0	0	1	0
61	52	3	0	0	0	0
61	55	1	0	0	0	0
61	58	1	0	0	0	0
61	5I	2	0	0	0	0
61	75	1	0	0	0	0
61	78	11	0	0	5	0
61	7A	1	0	0	0	0
61	7I	2	0	0	1	0
61	85	1	0	0	0	0
61	98	2	0	0	0	0
61	9A	3	0	0	3	0
61	A5	1	0	0	0	0
61	A8	3	0	0	1	0
61	B8	1	0	0	0	0
61	BA	2	0	0	0	0
61	C5	3	0	0	0	0
61	E5	5	0	0	0	0
61	E8	1	0	0	0	0
61	F5	3	0	0	0	0
61	F8	1	0	0	0	0
61	H5	1	0	0	0	0
61	I8	6	0	0	1	0
61	K8	1	0	0	0	0
61	L8	1	0	0	1	0
61	M5	7	0	0	1	0
61	P8	1	0	0	0	0
61	Q8	5	0	0	1	0
All	All	296743	0	197188	8820	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 8820 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)
3:22:173:VAL:C	3:22:174:PRO:N	1.71	1.38
4:3E:25:ARG:NH1	59:3E:301:SF4:S3	2.12	1.23
19:AI:3:ARG:HE	19:AI:9:VAL:HG11	1.07	1.14
44:E8:89:ALA:O	44:E8:92:ARG:NH1	1.81	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:45:27:VAL:HB	38:45:28:ALA:HA	1.12	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	203/256 (79%)	172 (85%)	25 (12%)	6 (3%)	5	22
2	1E	231/256 (90%)	188 (81%)	41 (18%)	2 (1%)	19	55
3	22	191/239 (80%)	167 (87%)	24 (13%)	0	100	100
3	2E	203/239 (85%)	181 (89%)	22 (11%)	0	100	100
4	32	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	31	69
4	3E	205/209 (98%)	190 (93%)	15 (7%)	0	100	100
5	42	147/162 (91%)	140 (95%)	7 (5%)	0	100	100
5	4E	147/162 (91%)	140 (95%)	6 (4%)	1 (1%)	24	61
6	52	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	5E	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
7	62	136/156 (87%)	123 (90%)	13 (10%)	0	100	100
7	6E	152/156 (97%)	140 (92%)	12 (8%)	0	100	100
8	72	135/138 (98%)	125 (93%)	7 (5%)	3 (2%)	7	31
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	24	61
9	82	119/128 (93%)	101 (85%)	17 (14%)	1 (1%)	21	58
9	8E	124/128 (97%)	101 (82%)	19 (15%)	4 (3%)	4	21
10	1A	76/105 (72%)	70 (92%)	6 (8%)	0	100	100
10	1I	93/105 (89%)	82 (88%)	10 (11%)	1 (1%)	16	50
11	2A	111/129 (86%)	102 (92%)	7 (6%)	2 (2%)	9	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2I	109/129 (84%)	98 (90%)	10 (9%)	1 (1%)	19	55
12	3A	120/132 (91%)	101 (84%)	14 (12%)	5 (4%)	3	15
12	3I	120/132 (91%)	106 (88%)	11 (9%)	3 (2%)	6	28
13	4A	109/126 (86%)	98 (90%)	9 (8%)	2 (2%)	9	37
13	4I	117/126 (93%)	97 (83%)	20 (17%)	0	100	100
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	9	37
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	4	19
15	6A	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
15	6I	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	5 (6%)	1 (1%)	14	48
16	7I	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	8	34
18	9A	65/88 (74%)	61 (94%)	4 (6%)	0	100	100
18	9I	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	11	42
19	AA	56/93 (60%)	49 (88%)	5 (9%)	2 (4%)	4	18
19	AI	80/93 (86%)	67 (84%)	8 (10%)	5 (6%)	1	7
20	BA	97/106 (92%)	85 (88%)	10 (10%)	2 (2%)	8	33
20	BI	95/106 (90%)	82 (86%)	13 (14%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	7I	129/229 (56%)	116 (90%)	12 (9%)	1 (1%)	21	58
28	79	45/229 (20%)	40 (89%)	4 (9%)	1 (2%)	7	31
29	11	271/276 (98%)	241 (89%)	21 (8%)	9 (3%)	4	20
29	19	272/276 (99%)	243 (89%)	25 (9%)	4 (2%)	11	42
30	21	200/206 (97%)	154 (77%)	37 (18%)	9 (4%)	3	13
30	29	202/206 (98%)	155 (77%)	35 (17%)	12 (6%)	2	8
31	31	200/210 (95%)	179 (90%)	18 (9%)	3 (2%)	11	42
31	39	202/210 (96%)	159 (79%)	35 (17%)	8 (4%)	3	16
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	10	38
32	49	179/182 (98%)	159 (89%)	19 (11%)	1 (1%)	27	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	51	172/180 (96%)	138 (80%)	23 (13%)	11 (6%)	1	6
33	59	165/180 (92%)	129 (78%)	30 (18%)	6 (4%)	4	18
34	61	144/148 (97%)	120 (83%)	21 (15%)	3 (2%)	8	33
34	69	143/148 (97%)	113 (79%)	27 (19%)	3 (2%)	8	33
35	15	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	24	61
35	58	135/140 (96%)	115 (85%)	17 (13%)	3 (2%)	7	31
36	25	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
36	68	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
37	35	145/150 (97%)	117 (81%)	27 (19%)	1 (1%)	24	61
37	78	145/150 (97%)	116 (80%)	21 (14%)	8 (6%)	2	9
38	45	137/141 (97%)	115 (84%)	19 (14%)	3 (2%)	7	31
38	88	139/141 (99%)	121 (87%)	12 (9%)	6 (4%)	3	14
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	19	55
39	98	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	10	38
40	65	108/112 (96%)	91 (84%)	16 (15%)	1 (1%)	19	55
40	A8	109/112 (97%)	92 (84%)	15 (14%)	2 (2%)	9	37
41	75	131/146 (90%)	120 (92%)	8 (6%)	3 (2%)	7	30
41	B8	134/146 (92%)	120 (90%)	12 (9%)	2 (2%)	11	42
42	85	114/118 (97%)	102 (90%)	12 (10%)	0	100	100
42	C8	113/118 (96%)	105 (93%)	3 (3%)	5 (4%)	3	14
43	95	98/101 (97%)	81 (83%)	14 (14%)	3 (3%)	4	22
43	D8	98/101 (97%)	88 (90%)	8 (8%)	2 (2%)	8	34
44	A5	109/113 (96%)	103 (94%)	5 (5%)	1 (1%)	19	55
44	E8	108/113 (96%)	100 (93%)	8 (7%)	0	100	100
45	B5	92/96 (96%)	81 (88%)	9 (10%)	2 (2%)	7	31
45	F8	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	16	50
46	C5	102/110 (93%)	71 (70%)	24 (24%)	7 (7%)	1	5
46	G8	101/110 (92%)	82 (81%)	15 (15%)	4 (4%)	3	16
47	D5	127/206 (62%)	102 (80%)	21 (16%)	4 (3%)	4	22
47	H8	168/206 (82%)	132 (79%)	32 (19%)	4 (2%)	6	29
48	E5	74/85 (87%)	66 (89%)	7 (10%)	1 (1%)	12	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	I8	75/85 (88%)	68 (91%)	6 (8%)	1 (1%)	13	45
49	F5	92/98 (94%)	80 (87%)	11 (12%)	1 (1%)	16	50
49	J8	92/98 (94%)	86 (94%)	4 (4%)	2 (2%)	7	31
50	G5	67/72 (93%)	62 (92%)	2 (3%)	3 (4%)	3	13
50	K8	66/72 (92%)	60 (91%)	3 (4%)	3 (4%)	3	13
51	H5	56/60 (93%)	55 (98%)	1 (2%)	0	100	100
51	L8	56/60 (93%)	51 (91%)	5 (9%)	0	100	100
52	I5	61/71 (86%)	28 (46%)	28 (46%)	5 (8%)	1	3
52	M8	57/71 (80%)	39 (68%)	13 (23%)	5 (9%)	1	3
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
55	M5	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	4	21
55	Q8	62/65 (95%)	52 (84%)	7 (11%)	3 (5%)	2	12
All	All	11163/12404 (90%)	9756 (87%)	1192 (11%)	215 (2%)	9	36

5 of 215 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	8E	111	ARG
18	9I	22	VAL
19	AI	41	VAL
30	21	77	ILE
37	78	25	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	179/220 (81%)	136 (76%)	43 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1E	202/220 (92%)	152 (75%)	50 (25%)	0	2
3	22	154/188 (82%)	119 (77%)	35 (23%)	1	3
3	2E	159/188 (85%)	127 (80%)	32 (20%)	1	6
4	32	180/181 (99%)	151 (84%)	29 (16%)	2	11
4	3E	180/181 (99%)	141 (78%)	39 (22%)	1	4
5	42	114/123 (93%)	88 (77%)	26 (23%)	1	3
5	4E	115/123 (94%)	93 (81%)	22 (19%)	1	7
6	52	90/90 (100%)	79 (88%)	11 (12%)	5	21
6	5E	90/90 (100%)	82 (91%)	8 (9%)	11	35
7	62	114/127 (90%)	91 (80%)	23 (20%)	1	6
7	6E	125/127 (98%)	101 (81%)	24 (19%)	1	7
8	72	118/119 (99%)	94 (80%)	24 (20%)	1	5
8	7E	119/119 (100%)	96 (81%)	23 (19%)	1	7
9	82	92/99 (93%)	67 (73%)	25 (27%)	0	2
9	8E	97/99 (98%)	77 (79%)	20 (21%)	1	5
10	1A	71/92 (77%)	46 (65%)	25 (35%)	0	1
10	1I	81/92 (88%)	66 (82%)	15 (18%)	2	8
11	2A	85/99 (86%)	69 (81%)	16 (19%)	1	7
11	2I	84/99 (85%)	69 (82%)	15 (18%)	2	8
12	3A	103/109 (94%)	84 (82%)	19 (18%)	2	8
12	3I	103/109 (94%)	86 (84%)	17 (16%)	2	10
13	4A	91/101 (90%)	62 (68%)	29 (32%)	0	1
13	4I	94/101 (93%)	72 (77%)	22 (23%)	1	3
14	5A	49/50 (98%)	26 (53%)	23 (47%)	0	0
14	5I	49/50 (98%)	35 (71%)	14 (29%)	0	1
15	6A	79/80 (99%)	74 (94%)	5 (6%)	20	52
15	6I	79/80 (99%)	70 (89%)	9 (11%)	6	23
16	7A	72/74 (97%)	60 (83%)	12 (17%)	2	10
16	7I	72/74 (97%)	55 (76%)	17 (24%)	1	3
17	8A	94/97 (97%)	78 (83%)	16 (17%)	2	10
17	8I	95/97 (98%)	72 (76%)	23 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	9A	58/77 (75%)	45 (78%)	13 (22%)	1	4
18	9I	58/77 (75%)	43 (74%)	15 (26%)	0	2
19	AA	52/80 (65%)	41 (79%)	11 (21%)	1	5
19	AI	72/80 (90%)	60 (83%)	12 (17%)	2	10
20	BA	76/82 (93%)	56 (74%)	20 (26%)	0	2
20	BI	75/82 (92%)	57 (76%)	18 (24%)	1	3
21	1B	17/22 (77%)	13 (76%)	4 (24%)	1	3
21	1F	18/22 (82%)	15 (83%)	3 (17%)	2	10
28	71	109/181 (60%)	84 (77%)	25 (23%)	1	3
28	79	48/181 (26%)	37 (77%)	11 (23%)	1	3
29	11	214/218 (98%)	189 (88%)	25 (12%)	6	22
29	19	214/218 (98%)	179 (84%)	35 (16%)	2	10
30	21	155/166 (93%)	121 (78%)	34 (22%)	1	4
30	29	165/166 (99%)	145 (88%)	20 (12%)	5	21
31	31	161/166 (97%)	139 (86%)	22 (14%)	4	16
31	39	163/166 (98%)	129 (79%)	34 (21%)	1	5
32	41	153/156 (98%)	131 (86%)	22 (14%)	3	15
32	49	153/156 (98%)	112 (73%)	41 (27%)	0	2
33	51	143/148 (97%)	104 (73%)	39 (27%)	0	2
33	59	139/148 (94%)	113 (81%)	26 (19%)	1	8
34	61	122/124 (98%)	97 (80%)	25 (20%)	1	5
34	69	122/124 (98%)	93 (76%)	29 (24%)	1	3
35	15	117/119 (98%)	100 (86%)	17 (14%)	3	14
35	58	116/119 (98%)	100 (86%)	16 (14%)	4	16
36	25	100/100 (100%)	83 (83%)	17 (17%)	2	10
36	68	100/100 (100%)	88 (88%)	12 (12%)	5	21
37	35	114/116 (98%)	89 (78%)	25 (22%)	1	4
37	78	114/116 (98%)	91 (80%)	23 (20%)	1	6
38	45	109/111 (98%)	82 (75%)	27 (25%)	0	2
38	88	110/111 (99%)	92 (84%)	18 (16%)	2	10
39	55	101/101 (100%)	86 (85%)	15 (15%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	98	101/101 (100%)	85 (84%)	16 (16%)	3	12
40	65	87/88 (99%)	57 (66%)	30 (34%)	0	1
40	A8	87/88 (99%)	72 (83%)	15 (17%)	2	9
41	75	117/127 (92%)	98 (84%)	19 (16%)	2	11
41	B8	117/127 (92%)	90 (77%)	27 (23%)	1	3
42	85	93/94 (99%)	78 (84%)	15 (16%)	2	11
42	C8	92/94 (98%)	80 (87%)	12 (13%)	4	18
43	95	81/82 (99%)	60 (74%)	21 (26%)	0	2
43	D8	82/82 (100%)	60 (73%)	22 (27%)	0	2
44	A5	91/92 (99%)	74 (81%)	17 (19%)	1	8
44	E8	90/92 (98%)	80 (89%)	10 (11%)	7	24
45	B5	74/78 (95%)	64 (86%)	10 (14%)	4	17
45	F8	75/78 (96%)	69 (92%)	6 (8%)	13	40
46	C5	85/91 (93%)	62 (73%)	23 (27%)	0	2
46	G8	83/91 (91%)	65 (78%)	18 (22%)	1	4
47	D5	118/179 (66%)	90 (76%)	28 (24%)	1	3
47	H8	151/179 (84%)	112 (74%)	39 (26%)	0	2
48	E5	61/67 (91%)	53 (87%)	8 (13%)	4	18
48	I8	62/67 (92%)	53 (86%)	9 (14%)	3	14
49	F5	79/83 (95%)	65 (82%)	14 (18%)	2	9
49	J8	79/83 (95%)	65 (82%)	14 (18%)	2	9
50	G5	63/67 (94%)	42 (67%)	21 (33%)	0	1
50	K8	64/67 (96%)	48 (75%)	16 (25%)	0	2
51	H5	50/52 (96%)	39 (78%)	11 (22%)	1	4
51	L8	50/52 (96%)	40 (80%)	10 (20%)	1	6
52	I5	57/63 (90%)	39 (68%)	18 (32%)	0	1
52	M8	52/63 (82%)	33 (64%)	19 (36%)	0	1
53	J5	48/52 (92%)	34 (71%)	14 (29%)	0	1
53	N8	49/52 (94%)	39 (80%)	10 (20%)	1	5
54	L5	38/42 (90%)	33 (87%)	5 (13%)	4	17
54	P8	38/42 (90%)	32 (84%)	6 (16%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	M5	54/55 (98%)	42 (78%)	12 (22%)	1	4
55	Q8	54/55 (98%)	48 (89%)	6 (11%)	7	24
All	All	9419/10256 (92%)	7533 (80%)	1886 (20%)	1	6

5 of 1886 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	K8	28	LYS
6	52	74	ASP
46	C5	79	CYS
52	M8	21	VAL
3	22	4	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	12	135	GLN
11	2A	117	ASN
32	49	130	ASN
2	12	16	HIS
38	45	123	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	348 (23%)	34 (2%)
1	1G	1505/1522 (98%)	323 (21%)	33 (2%)
22	1K	67/76 (88%)	36 (53%)	4 (5%)
23	2K	76/77 (98%)	20 (26%)	1 (1%)
23	2L	75/77 (97%)	10 (13%)	2 (2%)
24	3K	67/76 (88%)	37 (55%)	3 (4%)
24	3L	69/76 (90%)	32 (46%)	1 (1%)
25	4K	19/30 (63%)	12 (63%)	2 (10%)
25	4L	18/30 (60%)	10 (55%)	2 (11%)
26	14	2803/2917 (96%)	638 (22%)	37 (1%)
26	1H	2836/2917 (97%)	590 (20%)	43 (1%)
27	16	121/122 (99%)	24 (19%)	0
27	1J	121/122 (99%)	34 (28%)	2 (1%)
56	1L	65/76 (85%)	24 (36%)	2 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9335/9640 (96%)	2138 (22%)	166 (1%)

5 of 2138 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	12	U
1	13	13	U

5 of 166 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	1900	A
1	1G	250	A
26	14	2402	C
26	1H	2172	U
26	1H	2481	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	H2U	1K	17	22	17,21,22	2.32	4 (23%)	21,30,33	3.08	5 (23%)
22	CM0	1K	34	22	15,26,27	3.36	5 (33%)	13,37,40	2.24	2 (15%)
22	6MZ	1K	37	22	18,25,26	2.42	5 (27%)	15,36,39	3.42	4 (26%)
22	5MU	1K	54	22	13,22,23	1.77	2 (15%)	14,32,35	2.07	2 (14%)
22	PSU	1K	55	22	16,21,22	1.21	1 (6%)	20,30,33	3.43	5 (25%)
56	5MU	1L	54	56	13,22,23	1.81	2 (15%)	14,32,35	1.81	2 (14%)
56	PSU	1L	55	56	16,21,22	1.27	1 (6%)	20,30,33	3.60	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	OMC	2K	33	23	15,22,23	2.16	4 (26%)	19,31,34	1.12	2 (10%)
23	7MG	2K	47	23	20,26,27	3.66	6 (30%)	23,39,42	2.09	8 (34%)
23	5MU	2K	55	57,23	13,22,23	1.85	3 (23%)	14,32,35	1.75	2 (14%)
23	PSU	2K	56	23	16,21,22	1.17	3 (18%)	20,30,33	2.80	5 (25%)
23	4SU	2K	8	23	13,21,22	3.26	2 (15%)	14,30,33	1.01	1 (7%)
23	OMC	2L	33	23	15,22,23	2.20	4 (26%)	19,31,34	1.30	2 (10%)
23	7MG	2L	47	23	20,26,27	3.50	5 (25%)	23,39,42	2.19	8 (34%)
23	5MU	2L	55	23	13,22,23	1.84	2 (15%)	14,32,35	1.81	2 (14%)
23	PSU	2L	56	23	16,21,22	1.19	2 (12%)	20,30,33	3.32	5 (25%)
23	4SU	2L	8	23	13,21,22	3.44	2 (15%)	14,30,33	0.93	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	H2U	1K	17	22	-	0/7/38/39	0/2/2/2
22	CM0	1K	34	22	-	0/6/30/31	0/2/2/2
22	6MZ	1K	37	22	-	0/5/27/28	0/3/3/3
22	5MU	1K	54	22	-	0/3/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	0/3/25/26	0/2/2/2
56	PSU	1L	55	56	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/5/27/28	0/2/2/2
23	7MG	2K	47	23	-	0/7/37/38	0/3/3/3
23	5MU	2K	55	57,23	-	0/3/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/3/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/5/27/28	0/2/2/2
23	7MG	2L	47	23	-	0/7/37/38	0/3/3/3
23	5MU	2L	55	23	-	0/3/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/3/25/26	0/2/2/2

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	47	7MG	C4-N9	-7.54	1.28	1.38
23	2K	47	7MG	C5-C4	-5.83	1.23	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	7MG	C5-C4	-4.98	1.25	1.39
23	2L	47	7MG	C4-N9	-4.63	1.32	1.38
22	1K	17	H2U	C6-N1	-3.74	1.42	1.47

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1L	55	PSU	N1-C2-N3	-11.65	119.05	128.41
23	2L	56	PSU	N1-C2-N3	-11.56	119.12	128.41
22	1K	37	6MZ	N3-C2-N1	-10.50	119.88	128.86
22	1K	55	PSU	N1-C2-N3	-10.34	120.10	128.41
23	2K	56	PSU	N1-C2-N3	-9.19	121.02	128.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	17	H2U	2	0
22	1K	34	CM0	1	0
22	1K	54	5MU	1	0
22	1K	55	PSU	2	0
56	1L	54	5MU	1	0
23	2K	33	OMC	1	0
23	2K	47	7MG	2	0
23	2K	55	5MU	3	0
23	2K	8	4SU	1	0
23	2L	33	OMC	3	0
23	2L	47	7MG	1	0
23	2L	55	5MU	3	0
23	2L	8	4SU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1355 ligands modelled in this entry, 1348 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SPE	13	1748	1	12,12,12	0.49	0	11,11,11	1.02	1 (9%)
58	SPE	14	3445	26	12,12,12	0.58	0	11,11,11	0.87	0
58	SPE	14	3446	-	12,12,12	0.72	0	11,11,11	1.03	1 (9%)
58	SPE	1G	1733	-	12,12,12	0.40	0	11,11,11	0.91	0
58	SPE	1J	208	-	12,12,12	0.40	0	11,11,11	0.87	0
59	SF4	32	301	4	0,12,12	0.00	-	0,24,24	0.00	-
59	SF4	3E	301	4	0,12,12	0.00	-	0,24,24	0.00	-

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
58	SPE	13	1748	1	-	0/10/10/10	0/0/0/0
58	SPE	14	3445	26	-	0/10/10/10	0/0/0/0
58	SPE	14	3446	-	-	0/10/10/10	0/0/0/0
58	SPE	1G	1733	-	-	0/10/10/10	0/0/0/0
58	SPE	1J	208	-	-	0/10/10/10	0/0/0/0
59	SF4	32	301	4	-	0/0/48/48	0/6/5/5
59	SF4	3E	301	4	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1748	SPE	C11-C10-N9	-2.59	105.58	112.08
58	14	3446	SPE	C11-C10-N9	-2.55	105.69	112.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	13	1748	SPE	3	0
58	14	3445	SPE	5	0
58	14	3446	SPE	6	0
58	1J	208	SPE	1	0
59	32	301	SF4	1	0
59	3E	301	SF4	3	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
3	22	1
10	1A	1
25	4K	1
2	1E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1E	78:GLN	C	79:ASP	N	4.14
1	4K	25:A	O3'	26:A	P	3.23
1	22	173:VAL	C	174:PRO	N	1.71
1	1A	38:ILE	C	39:PRO	N	1.62

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1496/1522 (98%)	-0.40	5 (0%) 93 87	57, 98, 164, 235	0
1	1G	1506/1522 (98%)	-0.45	4 (0%) 93 87	68, 105, 166, 238	0
2	12	207/256 (80%)	1.12	47 (22%) 0 0	121, 148, 168, 185	0
2	1E	235/256 (91%)	0.46	18 (7%) 13 7	108, 135, 160, 171	0
3	22	195/239 (81%)	1.28	49 (25%) 0 0	113, 131, 152, 164	0
3	2E	205/239 (85%)	1.21	46 (22%) 0 0	85, 107, 142, 149	0
4	32	208/209 (99%)	0.84	30 (14%) 2 1	84, 101, 123, 132	0
4	3E	207/209 (99%)	0.55	19 (9%) 9 5	77, 103, 125, 133	0
5	42	149/162 (91%)	0.16	5 (3%) 45 29	91, 111, 128, 149	0
5	4E	149/162 (91%)	0.21	3 (2%) 65 46	79, 98, 118, 135	0
6	52	101/101 (100%)	0.84	11 (10%) 5 3	81, 97, 110, 131	0
6	5E	100/101 (99%)	0.91	12 (12%) 4 2	83, 99, 113, 123	0
7	62	140/156 (89%)	0.89	20 (14%) 2 1	103, 119, 131, 138	0
7	6E	154/156 (98%)	0.98	21 (13%) 3 1	98, 113, 138, 162	0
8	72	137/138 (99%)	-0.18	1 (0%) 87 75	90, 114, 125, 128	0
8	7E	138/138 (100%)	0.07	5 (3%) 42 27	87, 102, 113, 120	0
9	82	121/128 (94%)	0.41	7 (5%) 23 13	101, 144, 160, 164	0
9	8E	126/128 (98%)	0.66	12 (9%) 8 5	84, 133, 153, 157	0
10	1A	80/105 (76%)	0.31	8 (10%) 7 4	111, 138, 152, 156	0
10	1I	95/105 (90%)	2.01	48 (50%) 0 0	80, 127, 155, 159	0
11	2A	113/129 (87%)	1.68	40 (35%) 0 0	78, 103, 117, 120	0
11	2I	111/129 (86%)	0.91	16 (14%) 2 1	70, 99, 115, 125	0
12	3A	122/132 (92%)	0.84	18 (14%) 2 1	74, 91, 116, 132	0
12	3I	122/132 (92%)	0.30	3 (2%) 57 39	65, 76, 103, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	0.33	4 (3%)	42	27	102, 129, 143, 152	0
13	4I	119/126 (94%)	0.30	6 (5%)	29	18	87, 111, 129, 139	0
14	5A	59/61 (96%)	1.73	24 (40%)	0	0	118, 129, 141, 142	0
14	5I	60/61 (98%)	0.43	4 (6%)	18	10	83, 97, 112, 119	0
15	6A	87/89 (97%)	-0.04	0	100	100	79, 100, 115, 117	0
15	6I	87/89 (97%)	0.80	10 (11%)	5	2	75, 94, 109, 116	0
16	7A	84/88 (95%)	0.03	1 (1%)	79	62	85, 98, 119, 145	0
16	7I	83/88 (94%)	0.13	2 (2%)	59	40	91, 107, 132, 147	0
17	8A	99/105 (94%)	0.14	2 (2%)	65	46	89, 100, 117, 120	0
17	8I	100/105 (95%)	0.32	3 (3%)	50	32	81, 98, 108, 115	0
18	9A	67/88 (76%)	0.87	10 (14%)	2	1	87, 101, 125, 129	0
18	9I	68/88 (77%)	0.94	11 (16%)	1	1	85, 100, 125, 128	0
19	AA	62/93 (66%)	0.27	5 (8%)	12	6	118, 142, 155, 158	0
19	AI	82/93 (88%)	0.77	12 (14%)	2	1	95, 110, 128, 136	0
20	BA	99/106 (93%)	0.43	4 (4%)	38	24	85, 104, 128, 140	0
20	BI	97/106 (91%)	0.25	6 (6%)	20	12	103, 117, 139, 145	0
21	1B	22/27 (81%)	0.92	3 (13%)	3	1	110, 116, 124, 134	0
21	1F	23/27 (85%)	0.76	3 (13%)	3	2	90, 98, 106, 108	0
22	1K	67/76 (88%)	0.62	7 (10%)	6	4	80, 167, 196, 203	0
23	2K	72/77 (93%)	-0.22	1 (1%)	75	58	68, 89, 116, 129	0
23	2L	71/77 (92%)	-0.04	0	100	100	78, 100, 132, 145	0
24	3K	70/76 (92%)	0.66	11 (15%)	2	1	71, 198, 222, 224	0
24	3L	71/76 (93%)	0.66	9 (12%)	3	2	78, 191, 215, 218	0
25	4K	21/30 (70%)	0.83	2 (9%)	8	5	69, 129, 212, 213	0
25	4L	19/30 (63%)	0.27	1 (5%)	26	16	85, 144, 210, 210	0
26	14	2810/2917 (96%)	-0.12	30 (1%)	80	64	54, 81, 180, 237	0
26	1H	2841/2917 (97%)	-0.12	27 (0%)	82	67	44, 70, 166, 244	0
27	16	122/122 (100%)	-0.66	1 (0%)	86	72	65, 87, 105, 180	0
27	1J	122/122 (100%)	-0.71	0	100	100	79, 106, 125, 185	0
28	71	133/229 (58%)	2.14	60 (45%)	0	0	137, 194, 219, 229	0
28	79	57/229 (24%)	0.84	11 (19%)	1	0	136, 178, 198, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	11	273/276 (98%)	0.32	4 (1%) 73 56	44, 62, 78, 94	0
29	19	274/276 (99%)	0.84	24 (8%) 10 5	50, 72, 87, 102	0
30	21	202/206 (98%)	0.87	29 (14%) 2 1	49, 82, 115, 123	0
30	29	204/206 (99%)	0.78	27 (13%) 3 1	57, 88, 125, 135	0
31	31	202/210 (96%)	0.75	27 (13%) 3 1	46, 75, 108, 123	0
31	39	204/210 (97%)	0.66	21 (10%) 6 4	57, 95, 139, 164	0
32	41	179/182 (98%)	0.35	7 (3%) 39 25	75, 95, 124, 138	0
32	49	181/182 (99%)	1.04	40 (22%) 0 0	99, 118, 142, 156	0
33	51	174/180 (96%)	0.09	6 (3%) 45 29	76, 99, 116, 128	0
33	59	167/180 (92%)	1.60	57 (34%) 0 0	123, 190, 216, 225	0
34	61	146/148 (98%)	0.75	20 (13%) 3 1	75, 119, 134, 148	0
34	69	145/148 (97%)	0.57	17 (11%) 4 2	80, 115, 138, 144	0
35	15	138/140 (98%)	1.02	24 (17%) 1 1	76, 98, 124, 139	0
35	58	137/140 (97%)	0.55	11 (8%) 12 7	64, 84, 113, 134	0
36	25	122/122 (100%)	0.79	14 (11%) 5 2	68, 81, 97, 107	0
36	68	122/122 (100%)	0.49	1 (0%) 86 72	57, 72, 87, 93	0
37	35	147/150 (98%)	0.89	24 (16%) 1 1	59, 93, 121, 133	0
37	78	147/150 (98%)	0.32	5 (3%) 45 29	46, 77, 98, 106	0
38	45	139/141 (98%)	1.17	31 (22%) 0 0	70, 94, 112, 126	0
38	88	141/141 (100%)	0.45	9 (6%) 19 11	57, 74, 97, 117	0
39	55	118/118 (100%)	0.17	3 (2%) 57 39	61, 77, 92, 109	0
39	98	118/118 (100%)	0.80	13 (11%) 5 3	58, 76, 94, 104	0
40	65	110/112 (98%)	0.61	8 (7%) 15 8	82, 100, 119, 130	0
40	A8	111/112 (99%)	1.03	17 (15%) 2 1	73, 86, 104, 112	0
41	75	133/146 (91%)	0.17	3 (2%) 60 42	76, 88, 117, 142	0
41	B8	136/146 (93%)	0.04	2 (1%) 73 56	66, 83, 121, 152	0
42	85	116/118 (98%)	0.68	9 (7%) 13 7	65, 91, 116, 123	0
42	C8	115/118 (97%)	0.36	5 (4%) 35 22	57, 75, 96, 106	0
43	95	100/101 (99%)	1.23	24 (24%) 0 0	65, 108, 126, 132	0
43	D8	100/101 (99%)	0.92	13 (13%) 3 2	56, 92, 111, 125	0
44	A5	111/113 (98%)	0.61	7 (6%) 20 11	62, 73, 95, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	E8	110/113 (97%)	0.47	6 (5%) 25 15	57, 69, 90, 101	0
45	B5	94/96 (97%)	0.41	7 (7%) 14 8	66, 80, 103, 111	0
45	F8	95/96 (98%)	0.13	2 (2%) 63 45	50, 66, 91, 99	0
46	C5	104/110 (94%)	1.58	26 (25%) 0 0	84, 110, 143, 150	0
46	G8	103/110 (93%)	0.21	2 (1%) 66 48	74, 91, 118, 125	0
47	D5	133/206 (64%)	1.70	48 (36%) 0 0	93, 123, 150, 159	0
47	H8	170/206 (82%)	2.15	78 (45%) 0 0	77, 112, 191, 198	0
48	E5	76/85 (89%)	0.06	1 (1%) 77 60	58, 82, 94, 108	0
48	I8	77/85 (90%)	-0.17	2 (2%) 56 37	54, 70, 87, 98	0
49	F5	94/98 (95%)	0.67	5 (5%) 26 16	61, 76, 117, 123	0
49	J8	94/98 (95%)	0.53	5 (5%) 26 16	49, 70, 115, 135	0
50	G5	69/72 (95%)	0.64	5 (7%) 15 8	77, 96, 113, 130	0
50	K8	68/72 (94%)	0.07	1 (1%) 73 56	60, 76, 94, 124	0
51	H5	58/60 (96%)	1.35	15 (25%) 0 0	73, 90, 118, 123	0
51	L8	58/60 (96%)	0.09	0 100 100	59, 75, 94, 101	0
52	I5	63/71 (88%)	3.48	46 (73%) 0 0	133, 174, 191, 195	0
52	M8	61/71 (85%)	1.37	16 (26%) 0 0	96, 137, 167, 174	0
53	J5	56/60 (93%)	0.62	6 (10%) 6 3	57, 81, 130, 140	0
53	N8	56/60 (93%)	1.22	10 (17%) 1 1	50, 83, 145, 155	0
54	L5	47/49 (95%)	0.18	1 (2%) 63 45	51, 61, 82, 96	0
54	P8	47/49 (95%)	0.05	0 100 100	44, 53, 68, 89	0
55	M5	64/65 (98%)	0.54	2 (3%) 49 31	64, 76, 89, 114	0
55	Q8	64/65 (98%)	0.06	1 (1%) 72 54	52, 64, 78, 91	0
56	1L	67/76 (88%)	1.41	17 (25%) 0 0	98, 180, 207, 210	0
All	All	20742/22044 (94%)	0.30	1522 (7%) 15 8	44, 93, 167, 244	0

The worst 5 of 1522 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	14	2902	C	15.3
46	C5	59	GLY	14.8
52	I5	52	THR	11.4
26	14	2901	C	11.2
43	D8	37	VAL	11.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	1L	55	20/21	0.73	0.29	118,133,146,147	0
22	H2U	1K	17	20/21	0.81	0.12	119,145,154,154	0
22	PSU	1K	55	20/21	0.84	0.25	102,116,131,132	0
23	7MG	2L	47	24/25	0.84	0.16	92,112,117,118	0
23	OMC	2L	33	21/22	0.90	0.18	83,94,97,100	0
56	5MU	1L	54	21/22	0.91	0.22	117,124,131,143	0
23	PSU	2K	56	20/21	0.92	0.11	93,98,106,114	0
22	5MU	1K	54	21/22	0.92	0.19	100,106,117,129	0
23	PSU	2L	56	20/21	0.93	0.10	105,114,120,120	0
23	4SU	2L	8	20/21	0.93	0.15	104,106,109,112	0
23	7MG	2K	47	24/25	0.94	0.12	90,98,109,111	0
23	4SU	2K	8	20/21	0.95	0.13	84,88,92,94	0
22	CM0	1K	34	25/26	0.95	0.13	72,89,106,107	0
23	5MU	2K	55	21/22	0.95	0.12	99,102,106,113	0
23	OMC	2K	33	21/22	0.96	0.17	72,79,82,89	0
23	5MU	2L	55	21/22	0.96	0.09	111,115,122,127	0
22	6MZ	1K	37	23/24	0.97	0.13	61,79,86,90	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1G	1712	1/1	0.14	0.13	142,142,142,142	0
57	MG	13	1736	1/1	0.20	0.10	104,104,104,104	0
57	MG	1H	3246	1/1	0.24	0.48	72,72,72,72	0
57	MG	14	3386	1/1	0.28	0.15	93,93,93,93	0
57	MG	14	3438	1/1	0.31	0.12	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3509	1/1	0.35	0.18	88,88,88,88	0
57	MG	14	3327	1/1	0.41	0.12	100,100,100,100	0
57	MG	14	3428	1/1	0.43	0.16	109,109,109,109	0
57	MG	1J	206	1/1	0.44	0.17	109,109,109,109	0
57	MG	14	3173	1/1	0.45	0.16	98,98,98,98	0
57	MG	1H	3216	1/1	0.45	0.54	89,89,89,89	0
57	MG	4L	101	1/1	0.46	0.09	110,110,110,110	0
57	MG	14	3174	1/1	0.46	0.45	83,83,83,83	0
57	MG	14	3436	1/1	0.46	0.22	96,96,96,96	0
57	MG	1G	1686	1/1	0.47	0.10	107,107,107,107	0
57	MG	1G	1714	1/1	0.47	0.19	99,99,99,99	0
57	MG	1G	1630	1/1	0.47	0.49	106,106,106,106	0
57	MG	1H	3118	1/1	0.47	0.33	83,83,83,83	0
57	MG	14	3214	1/1	0.48	0.76	93,93,93,93	0
57	MG	14	3349	1/1	0.49	0.07	105,105,105,105	0
57	MG	13	1707	1/1	0.49	0.17	92,92,92,92	0
57	MG	1G	1717	1/1	0.49	0.10	99,99,99,99	0
57	MG	13	1686	1/1	0.51	0.33	104,104,104,104	0
57	MG	1H	3198	1/1	0.51	0.22	108,108,108,108	0
57	MG	1H	3205	1/1	0.51	0.32	90,90,90,90	0
57	MG	1H	3210	1/1	0.51	0.37	83,83,83,83	0
57	MG	14	3293	1/1	0.51	0.15	72,72,72,72	0
57	MG	13	1726	1/1	0.51	0.19	103,103,103,103	0
57	MG	1H	3402	1/1	0.52	0.10	79,79,79,79	0
57	MG	1H	3515	1/1	0.53	0.16	98,98,98,98	0
57	MG	14	3443	1/1	0.53	0.14	92,92,92,92	0
57	MG	14	3423	1/1	0.54	0.37	92,92,92,92	0
57	MG	1G	1702	1/1	0.54	0.13	95,95,95,95	0
57	MG	1G	1691	1/1	0.54	0.13	99,99,99,99	0
57	MG	1G	1675	1/1	0.54	0.12	107,107,107,107	0
57	MG	14	3216	1/1	0.54	0.14	106,106,106,106	0
57	MG	13	1671	1/1	0.54	0.79	91,91,91,91	0
57	MG	1H	3274	1/1	0.55	0.46	83,83,83,83	0
57	MG	13	1668	1/1	0.55	0.13	121,121,121,121	0
57	MG	1H	3266	1/1	0.56	0.29	89,89,89,89	0
57	MG	16	206	1/1	0.56	0.38	77,77,77,77	0
57	MG	1H	3010	1/1	0.56	0.25	78,78,78,78	0
57	MG	14	3422	1/1	0.56	0.17	100,100,100,100	0
57	MG	13	1732	1/1	0.56	0.15	118,118,118,118	0
57	MG	1H	3261	1/1	0.56	0.40	77,77,77,77	0
57	MG	13	1645	1/1	0.57	0.30	78,78,78,78	0
57	MG	1G	1715	1/1	0.57	0.12	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1695	1/1	0.57	0.07	112,112,112,112	0
57	MG	13	1654	1/1	0.57	0.09	113,113,113,113	0
57	MG	1H	3168	1/1	0.58	0.16	80,80,80,80	0
57	MG	1H	3188	1/1	0.58	0.68	95,95,95,95	0
57	MG	14	3405	1/1	0.58	0.09	91,91,91,91	0
57	MG	14	3282	1/1	0.58	0.15	105,105,105,105	0
57	MG	1H	3295	1/1	0.59	0.15	70,70,70,70	0
57	MG	1H	3524	1/1	0.59	0.17	96,96,96,96	0
57	MG	1G	1700	1/1	0.60	0.11	109,109,109,109	0
57	MG	1H	3061	1/1	0.60	0.45	76,76,76,76	0
57	MG	14	3409	1/1	0.60	0.25	95,95,95,95	0
57	MG	39	302	1/1	0.60	0.30	67,67,67,67	0
57	MG	14	3031	1/1	0.60	0.44	86,86,86,86	0
57	MG	1H	3217	1/1	0.60	0.42	80,80,80,80	0
57	MG	1H	3238	1/1	0.61	0.36	87,87,87,87	0
57	MG	1H	3095	1/1	0.61	0.33	69,69,69,69	0
57	MG	1G	1643	1/1	0.62	0.33	83,83,83,83	0
57	MG	1H	3182	1/1	0.62	0.26	90,90,90,90	0
57	MG	1G	1684	1/1	0.62	0.07	120,120,120,120	0
57	MG	14	3157	1/1	0.62	0.69	89,89,89,89	0
57	MG	1H	3520	1/1	0.62	0.11	97,97,97,97	0
57	MG	14	3291	1/1	0.62	0.14	90,90,90,90	0
57	MG	25	201	1/1	0.63	0.09	118,118,118,118	0
57	MG	14	3208	1/1	0.63	0.20	78,78,78,78	0
57	MG	14	3284	1/1	0.63	0.11	72,72,72,72	0
57	MG	1H	3289	1/1	0.63	0.31	78,78,78,78	0
57	MG	1G	1710	1/1	0.63	0.31	102,102,102,102	0
57	MG	1H	3232	1/1	0.64	0.49	85,85,85,85	0
57	MG	13	1743	1/1	0.64	0.13	153,153,153,153	0
57	MG	13	1677	1/1	0.64	0.29	92,92,92,92	0
57	MG	1H	3525	1/1	0.64	0.08	134,134,134,134	0
57	MG	1H	3496	1/1	0.64	0.12	98,98,98,98	0
57	MG	1H	3212	1/1	0.64	0.19	65,65,65,65	0
57	MG	1H	3186	1/1	0.65	0.42	94,94,94,94	0
57	MG	14	3162	1/1	0.65	0.60	67,67,67,67	0
57	MG	14	3435	1/1	0.65	0.12	93,93,93,93	0
57	MG	1H	3077	1/1	0.65	0.25	56,56,56,56	0
57	MG	13	1678	1/1	0.65	0.59	94,94,94,94	0
57	MG	1J	205	1/1	0.65	0.10	87,87,87,87	0
57	MG	14	3390	1/1	0.65	0.18	108,108,108,108	0
57	MG	14	3086	1/1	0.65	0.26	64,64,64,64	0
57	MG	14	3092	1/1	0.66	0.49	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1707	1/1	0.66	0.22	108,108,108,108	0
57	MG	1H	3415	1/1	0.66	0.21	72,72,72,72	0
57	MG	1H	3500	1/1	0.66	0.09	93,93,93,93	0
57	MG	1H	3104	1/1	0.66	0.29	88,88,88,88	0
57	MG	14	3147	1/1	0.66	0.10	69,69,69,69	0
57	MG	1H	3535	1/1	0.66	0.24	93,93,93,93	0
57	MG	1H	3508	1/1	0.66	0.08	84,84,84,84	0
57	MG	13	1741	1/1	0.66	0.12	110,110,110,110	0
57	MG	14	3218	1/1	0.67	0.28	84,84,84,84	0
57	MG	1H	3180	1/1	0.67	0.38	88,88,88,88	0
57	MG	14	3397	1/1	0.67	0.07	109,109,109,109	0
57	MG	1G	1680	1/1	0.67	0.29	91,91,91,91	0
57	MG	13	1733	1/1	0.67	0.10	106,106,106,106	0
57	MG	14	3111	1/1	0.67	0.48	86,86,86,86	0
57	MG	14	3008	1/1	0.67	0.40	90,90,90,90	0
57	MG	14	3295	1/1	0.67	0.29	90,90,90,90	0
57	MG	1H	3263	1/1	0.68	0.47	91,91,91,91	0
57	MG	1H	3211	1/1	0.68	0.49	79,79,79,79	0
57	MG	1H	3218	1/1	0.68	0.21	81,81,81,81	0
57	MG	1H	3448	1/1	0.68	0.19	86,86,86,86	0
57	MG	1H	3133	1/1	0.68	0.48	78,78,78,78	0
57	MG	1H	3204	1/1	0.68	0.41	81,81,81,81	0
57	MG	1H	3479	1/1	0.68	0.17	75,75,75,75	0
57	MG	1G	1701	1/1	0.68	0.08	101,101,101,101	0
57	MG	1H	3439	1/1	0.68	0.05	95,95,95,95	0
57	MG	1G	1719	1/1	0.69	0.06	119,119,119,119	0
57	MG	14	3136	1/1	0.69	0.12	127,127,127,127	0
57	MG	14	3393	1/1	0.69	0.08	118,118,118,118	0
57	MG	1H	3120	1/1	0.69	0.46	96,96,96,96	0
57	MG	4K	101	1/1	0.69	0.27	86,86,86,86	0
57	MG	14	3416	1/1	0.69	0.05	89,89,89,89	0
57	MG	1H	3504	1/1	0.70	0.19	93,93,93,93	0
57	MG	1H	3316	1/1	0.70	0.48	89,89,89,89	0
57	MG	1H	3103	1/1	0.70	0.30	82,82,82,82	0
57	MG	14	3380	1/1	0.70	0.16	85,85,85,85	0
57	MG	14	3053	1/1	0.70	0.08	72,72,72,72	0
57	MG	1H	3380	1/1	0.70	0.13	59,59,59,59	0
57	MG	2L	102	1/1	0.70	0.63	90,90,90,90	0
57	MG	14	3189	1/1	0.70	0.66	85,85,85,85	0
57	MG	1H	3154	1/1	0.70	0.14	66,66,66,66	0
57	MG	1G	1728	1/1	0.70	0.05	114,114,114,114	0
57	MG	13	1650	1/1	0.70	0.40	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3298	1/1	0.71	0.24	56,56,56,56	0
57	MG	1H	3282	1/1	0.71	0.43	89,89,89,89	0
57	MG	14	3261	1/1	0.71	0.20	67,67,67,67	0
57	MG	1H	3078	1/1	0.71	0.37	79,79,79,79	0
57	MG	1H	3321	1/1	0.71	0.37	90,90,90,90	0
57	MG	1H	3373	1/1	0.71	0.14	89,89,89,89	0
57	MG	13	1630	1/1	0.71	0.25	87,87,87,87	0
57	MG	1H	3199	1/1	0.71	0.42	78,78,78,78	0
57	MG	14	3376	1/1	0.71	0.12	78,78,78,78	0
57	MG	14	3083	1/1	0.71	0.68	87,87,87,87	0
57	MG	1H	3250	1/1	0.71	0.38	93,93,93,93	0
57	MG	1H	3483	1/1	0.71	0.08	103,103,103,103	0
57	MG	1H	3260	1/1	0.71	0.43	98,98,98,98	0
57	MG	1H	3517	1/1	0.71	0.12	87,87,87,87	0
57	MG	14	3404	1/1	0.72	0.15	100,100,100,100	0
57	MG	1H	3464	1/1	0.72	0.18	48,48,48,48	0
57	MG	14	3217	1/1	0.72	0.20	77,77,77,77	0
57	MG	13	1683	1/1	0.72	0.20	72,72,72,72	0
57	MG	14	3134	1/1	0.72	0.42	71,71,71,71	0
57	MG	1H	3222	1/1	0.72	0.39	64,64,64,64	0
57	MG	1H	3155	1/1	0.72	0.21	91,91,91,91	0
57	MG	1H	3227	1/1	0.72	0.41	79,79,79,79	0
57	MG	14	3087	1/1	0.72	0.54	58,58,58,58	0
57	MG	14	3402	1/1	0.73	0.14	118,118,118,118	0
57	MG	1H	3258	1/1	0.73	0.39	84,84,84,84	0
57	MG	1H	3086	1/1	0.73	0.40	66,66,66,66	0
57	MG	1G	1650	1/1	0.73	0.15	114,114,114,114	0
57	MG	14	3148	1/1	0.73	0.36	63,63,63,63	0
57	MG	1H	3265	1/1	0.73	0.15	77,77,77,77	0
57	MG	1H	3009	1/1	0.73	0.43	77,77,77,77	0
57	MG	1H	3422	1/1	0.73	0.14	101,101,101,101	0
57	MG	1H	3036	1/1	0.73	0.75	70,70,70,70	0
57	MG	13	1681	1/1	0.73	0.25	68,68,68,68	0
57	MG	1G	1651	1/1	0.73	0.15	105,105,105,105	0
57	MG	14	3140	1/1	0.74	0.34	89,89,89,89	0
57	MG	1H	3443	1/1	0.74	0.14	53,53,53,53	0
57	MG	14	3391	1/1	0.74	0.24	103,103,103,103	0
57	MG	1G	1696	1/1	0.74	0.13	91,91,91,91	0
57	MG	1H	3269	1/1	0.74	0.36	86,86,86,86	0
57	MG	1H	3434	1/1	0.74	0.19	68,68,68,68	0
57	MG	1H	3072	1/1	0.74	0.66	72,72,72,72	0
57	MG	14	3207	1/1	0.74	0.28	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3115	1/1	0.74	0.91	84,84,84,84	0
57	MG	1G	1731	1/1	0.74	0.08	114,114,114,114	0
57	MG	1G	1657	1/1	0.74	0.21	82,82,82,82	0
57	MG	14	3097	1/1	0.74	0.43	90,90,90,90	0
57	MG	1H	3121	1/1	0.74	0.94	80,80,80,80	0
57	MG	14	3396	1/1	0.74	0.14	109,109,109,109	0
57	MG	1H	3279	1/1	0.74	0.46	76,76,76,76	0
57	MG	1G	1652	1/1	0.74	0.33	94,94,94,94	0
57	MG	1H	3528	1/1	0.74	0.11	96,96,96,96	0
57	MG	14	3244	1/1	0.74	0.22	58,58,58,58	0
57	MG	1G	1685	1/1	0.74	0.12	91,91,91,91	0
57	MG	14	3426	1/1	0.74	0.07	126,126,126,126	0
57	MG	13	1665	1/1	0.75	0.30	88,88,88,88	0
57	MG	1H	3187	1/1	0.75	1.20	81,81,81,81	0
57	MG	13	1685	1/1	0.75	0.38	91,91,91,91	0
57	MG	1H	3189	1/1	0.75	0.43	78,78,78,78	0
57	MG	14	3094	1/1	0.75	0.94	70,70,70,70	0
57	MG	1H	3278	1/1	0.75	0.31	83,83,83,83	0
57	MG	14	3077	1/1	0.75	0.20	84,84,84,84	0
57	MG	1H	3322	1/1	0.75	0.32	100,100,100,100	0
57	MG	13	1663	1/1	0.75	0.25	90,90,90,90	0
57	MG	16	211	1/1	0.75	0.12	99,99,99,99	0
57	MG	14	3205	1/1	0.75	0.43	79,79,79,79	0
57	MG	14	3191	1/1	0.75	0.31	82,82,82,82	0
57	MG	13	1625	1/1	0.76	0.31	93,93,93,93	0
57	MG	1G	1645	1/1	0.76	0.06	93,93,93,93	0
57	MG	14	3370	1/1	0.76	0.24	87,87,87,87	0
57	MG	1H	3005	1/1	0.76	0.72	74,74,74,74	0
57	MG	14	3007	1/1	0.76	0.65	72,72,72,72	0
57	MG	1H	3125	1/1	0.76	0.22	63,63,63,63	0
57	MG	1H	3201	1/1	0.76	0.36	88,88,88,88	0
57	MG	13	1679	1/1	0.76	0.28	86,86,86,86	0
57	MG	14	3172	1/1	0.76	0.49	82,82,82,82	0
57	MG	1H	3294	1/1	0.76	0.15	90,90,90,90	0
57	MG	13	1643	1/1	0.76	0.42	86,86,86,86	0
57	MG	14	3437	1/1	0.76	0.07	107,107,107,107	0
57	MG	1G	1644	1/1	0.76	0.37	107,107,107,107	0
57	MG	4E	201	1/1	0.76	0.46	85,85,85,85	0
57	MG	2K	102	1/1	0.76	0.31	92,92,92,92	0
57	MG	14	3110	1/1	0.76	0.52	72,72,72,72	0
57	MG	1H	3221	1/1	0.76	0.28	64,64,64,64	0
57	MG	1H	3477	1/1	0.77	0.07	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3179	1/1	0.77	0.41	67,67,67,67	0
57	MG	1G	1647	1/1	0.77	0.26	102,102,102,102	0
57	MG	14	3230	1/1	0.77	0.32	81,81,81,81	0
57	MG	1G	1638	1/1	0.77	0.11	93,93,93,93	0
57	MG	13	1702	1/1	0.77	0.08	107,107,107,107	0
57	MG	1H	3117	1/1	0.77	0.37	54,54,54,54	0
57	MG	1G	1653	1/1	0.77	0.28	103,103,103,103	0
57	MG	14	3398	1/1	0.77	0.07	99,99,99,99	0
57	MG	1G	1621	1/1	0.77	0.74	86,86,86,86	0
57	MG	14	3351	1/1	0.77	0.18	104,104,104,104	0
57	MG	13	1687	1/1	0.77	1.03	82,82,82,82	0
57	MG	29	301	1/1	0.77	0.27	75,75,75,75	0
57	MG	1H	3185	1/1	0.77	0.35	90,90,90,90	0
57	MG	14	3215	1/1	0.77	0.18	72,72,72,72	0
57	MG	14	3025	1/1	0.77	0.27	80,80,80,80	0
57	MG	1H	3157	1/1	0.77	0.13	73,73,73,73	0
57	MG	14	3137	1/1	0.77	0.42	68,68,68,68	0
57	MG	1H	3317	1/1	0.77	0.48	83,83,83,83	0
57	MG	1G	1619	1/1	0.77	0.29	86,86,86,86	0
57	MG	14	3151	1/1	0.77	0.20	87,87,87,87	0
57	MG	1G	1724	1/1	0.77	0.08	94,94,94,94	0
57	MG	1H	3519	1/1	0.77	0.10	83,83,83,83	0
57	MG	1H	3521	1/1	0.78	0.25	86,86,86,86	0
57	MG	1H	3308	1/1	0.78	0.35	56,56,56,56	0
57	MG	14	3082	1/1	0.78	0.33	90,90,90,90	0
57	MG	13	1673	1/1	0.78	0.36	80,80,80,80	0
57	MG	1H	3526	1/1	0.78	0.11	113,113,113,113	0
57	MG	1G	1681	1/1	0.78	0.11	96,96,96,96	0
57	MG	1G	1616	1/1	0.78	0.32	88,88,88,88	0
57	MG	1H	3421	1/1	0.78	0.14	99,99,99,99	0
57	MG	13	1651	1/1	0.78	0.29	97,97,97,97	0
57	MG	1H	3397	1/1	0.78	0.17	58,58,58,58	0
57	MG	14	3152	1/1	0.78	0.65	86,86,86,86	0
57	MG	1H	3404	1/1	0.78	0.12	65,65,65,65	0
57	MG	1H	3372	1/1	0.78	0.12	76,76,76,76	0
57	MG	14	3226	1/1	0.78	0.46	83,83,83,83	0
57	MG	2L	103	1/1	0.78	0.43	75,75,75,75	0
57	MG	1H	3058	1/1	0.78	0.43	77,77,77,77	0
57	MG	1G	1723	1/1	0.78	0.16	94,94,94,94	0
57	MG	1H	3313	1/1	0.78	0.17	74,74,74,74	0
57	MG	1H	3273	1/1	0.78	0.14	69,69,69,69	0
57	MG	13	1746	1/1	0.78	0.12	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	13	1731	1/1	0.78	0.05	90,90,90,90	0
57	MG	1H	3101	1/1	0.79	0.14	65,65,65,65	0
57	MG	1H	3206	1/1	0.79	0.24	91,91,91,91	0
57	MG	1G	1692	1/1	0.79	0.09	105,105,105,105	0
57	MG	1H	3320	1/1	0.79	0.41	80,80,80,80	0
57	MG	1H	3085	1/1	0.79	0.42	75,75,75,75	0
57	MG	13	1614	1/1	0.79	0.28	88,88,88,88	0
57	MG	13	1742	1/1	0.79	0.10	98,98,98,98	0
57	MG	14	3112	1/1	0.79	0.43	99,99,99,99	0
57	MG	13	1695	1/1	0.79	0.11	82,82,82,82	0
57	MG	14	3232	1/1	0.79	0.28	56,56,56,56	0
57	MG	14	3131	1/1	0.79	0.35	70,70,70,70	0
57	MG	14	3374	1/1	0.79	0.11	83,83,83,83	0
57	MG	1H	3100	1/1	0.79	0.16	62,62,62,62	0
57	MG	1H	3420	1/1	0.79	0.07	102,102,102,102	0
57	MG	14	3355	1/1	0.79	0.14	107,107,107,107	0
57	MG	1H	3542	1/1	0.79	0.33	90,90,90,90	0
57	MG	1H	3498	1/1	0.79	0.16	85,85,85,85	0
57	MG	1H	3207	1/1	0.79	0.71	87,87,87,87	0
57	MG	14	3348	1/1	0.79	0.10	101,101,101,101	0
57	MG	68	201	1/1	0.79	0.23	78,78,78,78	0
57	MG	1H	3416	1/1	0.79	0.06	89,89,89,89	0
57	MG	1H	3171	1/1	0.79	0.30	90,90,90,90	0
57	MG	9A	101	1/1	0.79	0.25	115,115,115,115	0
58	SPE	1J	208	13/13	0.80	0.22	94,98,105,105	0
57	MG	1G	1711	1/1	0.80	0.12	108,108,108,108	0
57	MG	14	3243	1/1	0.80	0.08	82,82,82,82	0
57	MG	14	3198	1/1	0.80	0.20	86,86,86,86	0
57	MG	14	3163	1/1	0.80	0.84	84,84,84,84	0
57	MG	16	203	1/1	0.80	0.12	78,78,78,78	0
57	MG	14	3081	1/1	0.80	0.35	81,81,81,81	0
57	MG	1G	1632	1/1	0.80	0.05	99,99,99,99	0
57	MG	1H	3123	1/1	0.80	0.60	65,65,65,65	0
57	MG	1H	3161	1/1	0.80	0.33	93,93,93,93	0
57	MG	1H	3067	1/1	0.80	0.17	62,62,62,62	0
57	MG	1H	3374	1/1	0.80	0.11	86,86,86,86	0
57	MG	1H	3348	1/1	0.80	0.14	49,49,49,49	0
57	MG	1G	1683	1/1	0.80	0.04	113,113,113,113	0
57	MG	1H	3484	1/1	0.80	0.15	84,84,84,84	0
57	MG	13	1690	1/1	0.80	0.43	100,100,100,100	0
57	MG	1H	3139	1/1	0.80	0.14	54,54,54,54	0
57	MG	1H	3003	1/1	0.80	0.47	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3184	1/1	0.80	0.24	93,93,93,93	0
57	MG	1G	1676	1/1	0.80	0.07	100,100,100,100	0
57	MG	14	3387	1/1	0.81	0.12	89,89,89,89	0
57	MG	1H	3330	1/1	0.81	0.17	47,47,47,47	0
57	MG	14	3021	1/1	0.81	0.15	76,76,76,76	0
57	MG	1G	1674	1/1	0.81	0.18	78,78,78,78	0
57	MG	1J	201	1/1	0.81	0.29	86,86,86,86	0
57	MG	1H	3414	1/1	0.81	0.06	95,95,95,95	0
57	MG	14	3434	1/1	0.81	0.14	115,115,115,115	0
57	MG	1H	3377	1/1	0.81	0.24	75,75,75,75	0
57	MG	14	3158	1/1	0.81	0.37	76,76,76,76	0
57	MG	1H	3523	1/1	0.81	0.23	84,84,84,84	0
57	MG	14	3224	1/1	0.81	0.16	113,113,113,113	0
57	MG	13	1684	1/1	0.81	0.30	74,74,74,74	0
57	MG	1H	3518	1/1	0.81	0.12	101,101,101,101	0
57	MG	1H	3088	1/1	0.81	0.22	61,61,61,61	0
57	MG	1G	1648	1/1	0.81	0.39	79,79,79,79	0
57	MG	1G	1697	1/1	0.81	0.07	110,110,110,110	0
57	MG	14	3378	1/1	0.81	0.11	86,86,86,86	0
57	MG	1H	3165	1/1	0.81	0.20	59,59,59,59	0
57	MG	1G	1620	1/1	0.81	0.27	79,79,79,79	0
57	MG	14	3177	1/1	0.81	0.31	82,82,82,82	0
57	MG	1G	1664	1/1	0.81	0.19	73,73,73,73	0
57	MG	13	1724	1/1	0.81	0.17	73,73,73,73	0
57	MG	13	1657	1/1	0.81	0.41	80,80,80,80	0
57	MG	1H	3008	1/1	0.81	0.47	75,75,75,75	0
57	MG	1G	1694	1/1	0.81	0.10	94,94,94,94	0
57	MG	L8	101	1/1	0.81	0.35	86,86,86,86	0
57	MG	35	202	1/1	0.81	0.35	84,84,84,84	0
57	MG	1H	3315	1/1	0.81	0.36	99,99,99,99	0
57	MG	1H	3364	1/1	0.82	0.12	72,72,72,72	0
57	MG	13	1723	1/1	0.82	0.12	83,83,83,83	0
57	MG	13	1740	1/1	0.82	0.05	132,132,132,132	0
57	MG	14	3411	1/1	0.82	0.27	93,93,93,93	0
57	MG	14	3256	1/1	0.82	0.16	54,54,54,54	0
57	MG	1H	3235	1/1	0.82	0.51	99,99,99,99	0
57	MG	14	3343	1/1	0.82	0.08	87,87,87,87	0
57	MG	1H	3527	1/1	0.82	0.11	107,107,107,107	0
57	MG	14	3381	1/1	0.82	0.28	74,74,74,74	0
57	MG	14	3220	1/1	0.82	0.29	73,73,73,73	0
57	MG	13	1688	1/1	0.82	0.52	72,72,72,72	0
57	MG	1H	3223	1/1	0.82	0.23	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3379	1/1	0.82	0.09	99,99,99,99	0
57	MG	13	1728	1/1	0.82	0.14	112,112,112,112	0
57	MG	14	3062	1/1	0.82	0.86	71,71,71,71	0
57	MG	14	3324	1/1	0.82	0.25	66,66,66,66	0
57	MG	1H	3270	1/1	0.82	0.35	61,61,61,61	0
57	MG	1H	3084	1/1	0.82	0.60	68,68,68,68	0
58	SPE	14	3446	13/13	0.82	0.28	68,79,87,89	0
57	MG	14	3168	1/1	0.82	0.27	87,87,87,87	0
57	MG	88	202	1/1	0.82	0.32	72,72,72,72	0
57	MG	1H	3462	1/1	0.82	0.20	53,53,53,53	0
57	MG	14	3395	1/1	0.82	0.10	91,91,91,91	0
57	MG	1H	3340	1/1	0.82	0.31	70,70,70,70	0
57	MG	1H	3048	1/1	0.82	0.25	43,43,43,43	0
57	MG	13	1691	1/1	0.82	0.20	65,65,65,65	0
57	MG	14	3165	1/1	0.83	0.44	74,74,74,74	0
57	MG	14	3149	1/1	0.83	0.67	71,71,71,71	0
57	MG	35	201	1/1	0.83	0.16	86,86,86,86	0
57	MG	1H	3183	1/1	0.83	0.25	73,73,73,73	0
57	MG	1H	3122	1/1	0.83	0.27	67,67,67,67	0
57	MG	1H	3311	1/1	0.83	0.20	93,93,93,93	0
57	MG	13	1708	1/1	0.83	0.09	95,95,95,95	0
57	MG	14	3085	1/1	0.83	0.47	81,81,81,81	0
57	MG	13	1672	1/1	0.83	0.83	86,86,86,86	0
57	MG	1H	3111	1/1	0.83	0.50	73,73,73,73	0
57	MG	1H	3228	1/1	0.83	0.34	70,70,70,70	0
57	MG	13	1662	1/1	0.83	0.19	76,76,76,76	0
57	MG	14	3317	1/1	0.83	0.16	64,64,64,64	0
57	MG	1H	3516	1/1	0.83	0.09	79,79,79,79	0
57	MG	13	1734	1/1	0.83	0.07	100,100,100,100	0
57	MG	14	3138	1/1	0.83	0.34	86,86,86,86	0
57	MG	14	3442	1/1	0.83	0.21	75,75,75,75	0
57	MG	1G	1722	1/1	0.83	0.12	101,101,101,101	0
57	MG	14	3133	1/1	0.83	0.29	58,58,58,58	0
57	MG	1H	3149	1/1	0.83	0.29	86,86,86,86	0
57	MG	1H	3038	1/1	0.83	0.60	65,65,65,65	0
57	MG	14	3187	1/1	0.83	0.33	90,90,90,90	0
57	MG	1H	3486	1/1	0.83	0.10	89,89,89,89	0
57	MG	1G	1682	1/1	0.83	0.08	105,105,105,105	0
57	MG	14	3027	1/1	0.83	0.25	76,76,76,76	0
57	MG	1H	3473	1/1	0.83	0.12	76,76,76,76	0
57	MG	13	1745	1/1	0.83	0.06	111,111,111,111	0
57	MG	F8	101	1/1	0.83	0.42	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3296	1/1	0.83	0.30	81,81,81,81	0
57	MG	14	3274	1/1	0.83	0.14	81,81,81,81	0
57	MG	14	3239	1/1	0.83	0.17	59,59,59,59	0
57	MG	14	3104	1/1	0.83	0.19	84,84,84,84	0
57	MG	13	1682	1/1	0.83	0.28	85,85,85,85	0
57	MG	1H	3327	1/1	0.83	0.11	65,65,65,65	0
57	MG	1G	1662	1/1	0.83	0.90	94,94,94,94	0
57	MG	1H	3087	1/1	0.83	0.38	79,79,79,79	0
57	MG	1G	1709	1/1	0.83	0.14	87,87,87,87	0
57	MG	1H	3530	1/1	0.83	0.10	98,98,98,98	0
57	MG	1H	3158	1/1	0.84	0.48	71,71,71,71	0
57	MG	1H	3325	1/1	0.84	0.38	88,88,88,88	0
57	MG	14	3314	1/1	0.84	0.13	83,83,83,83	0
57	MG	1H	3307	1/1	0.84	0.64	72,72,72,72	0
57	MG	14	3246	1/1	0.84	0.18	72,72,72,72	0
57	MG	1G	1720	1/1	0.84	0.05	106,106,106,106	0
57	MG	1H	3127	1/1	0.84	0.37	84,84,84,84	0
57	MG	13	1653	1/1	0.84	0.53	94,94,94,94	0
57	MG	13	1699	1/1	0.84	0.09	102,102,102,102	0
57	MG	1H	3098	1/1	0.84	0.53	78,78,78,78	0
57	MG	13	1623	1/1	0.84	0.40	80,80,80,80	0
57	MG	1H	3522	1/1	0.84	0.20	91,91,91,91	0
57	MG	14	3410	1/1	0.84	0.07	116,116,116,116	0
57	MG	13	1697	1/1	0.84	0.11	78,78,78,78	0
57	MG	1G	1678	1/1	0.84	0.15	73,73,73,73	0
57	MG	1H	3418	1/1	0.84	0.09	86,86,86,86	0
57	MG	14	3301	1/1	0.84	0.07	117,117,117,117	0
57	MG	1H	3248	1/1	0.84	0.39	96,96,96,96	0
57	MG	14	3362	1/1	0.84	0.09	97,97,97,97	0
57	MG	14	3427	1/1	0.84	0.18	92,92,92,92	0
57	MG	14	3199	1/1	0.84	0.56	68,68,68,68	0
57	MG	14	3116	1/1	0.84	0.28	66,66,66,66	0
57	MG	1G	1670	1/1	0.84	0.21	88,88,88,88	0
57	MG	14	3421	1/1	0.84	0.20	98,98,98,98	0
57	MG	1H	3544	1/1	0.84	0.08	84,84,84,84	0
57	MG	14	3213	1/1	0.84	0.39	76,76,76,76	0
57	MG	14	3406	1/1	0.84	0.10	90,90,90,90	0
57	MG	1G	1704	1/1	0.84	0.07	107,107,107,107	0
57	MG	1H	3220	1/1	0.84	0.15	89,89,89,89	0
57	MG	14	3190	1/1	0.84	0.33	79,79,79,79	0
57	MG	1H	3190	1/1	0.84	0.41	75,75,75,75	0
57	MG	1H	3281	1/1	0.84	0.21	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1729	1/1	0.84	0.10	104,104,104,104	0
57	MG	14	3161	1/1	0.84	0.88	79,79,79,79	0
57	MG	14	3272	1/1	0.84	0.07	78,78,78,78	0
57	MG	14	3211	1/1	0.84	0.42	85,85,85,85	0
57	MG	1H	3370	1/1	0.84	0.17	59,59,59,59	0
58	SPE	13	1748	13/13	0.85	0.24	60,77,82,87	0
57	MG	1H	3410	1/1	0.85	0.08	106,106,106,106	0
57	MG	14	3281	1/1	0.85	0.07	95,95,95,95	0
57	MG	14	3331	1/1	0.85	0.16	79,79,79,79	0
57	MG	1H	3108	1/1	0.85	0.32	69,69,69,69	0
57	MG	1H	3276	1/1	0.85	0.36	90,90,90,90	0
57	MG	13	1642	1/1	0.85	0.17	72,72,72,72	0
57	MG	14	3335	1/1	0.85	0.14	63,63,63,63	0
57	MG	13	1669	1/1	0.85	0.30	92,92,92,92	0
57	MG	14	3066	1/1	0.85	0.36	59,59,59,59	0
57	MG	14	3271	1/1	0.85	0.06	72,72,72,72	0
57	MG	13	1727	1/1	0.85	0.17	90,90,90,90	0
57	MG	41	201	1/1	0.85	0.11	62,62,62,62	0
58	SPE	1G	1733	13/13	0.85	0.10	98,101,104,105	0
57	MG	14	3041	1/1	0.85	0.63	76,76,76,76	0
57	MG	1H	3106	1/1	0.85	0.18	68,68,68,68	0
57	MG	1H	3323	1/1	0.85	0.23	75,75,75,75	0
57	MG	2K	103	1/1	0.85	0.38	89,89,89,89	0
57	MG	1H	3191	1/1	0.85	0.29	72,72,72,72	0
57	MG	14	3075	1/1	0.85	0.35	89,89,89,89	0
57	MG	14	3352	1/1	0.85	0.11	84,84,84,84	0
57	MG	1H	3545	1/1	0.85	0.07	116,116,116,116	0
57	MG	14	3288	1/1	0.85	0.15	77,77,77,77	0
57	MG	1H	3429	1/1	0.85	0.18	56,56,56,56	0
57	MG	14	3394	1/1	0.85	0.14	63,63,63,63	0
57	MG	14	3292	1/1	0.85	0.11	85,85,85,85	0
57	MG	14	3203	1/1	0.85	0.43	93,93,93,93	0
57	MG	13	1700	1/1	0.85	0.07	86,86,86,86	0
57	MG	14	3420	1/1	0.85	0.08	96,96,96,96	0
57	MG	1H	3082	1/1	0.85	0.39	76,76,76,76	0
57	MG	1H	3449	1/1	0.85	0.41	80,80,80,80	0
57	MG	14	3052	1/1	0.85	0.46	79,79,79,79	0
57	MG	14	3222	1/1	0.85	0.58	88,88,88,88	0
57	MG	1J	207	1/1	0.85	0.10	92,92,92,92	0
57	MG	14	3286	1/1	0.85	0.06	93,93,93,93	0
57	MG	16	208	1/1	0.85	0.37	79,79,79,79	0
57	MG	14	3032	1/1	0.85	0.45	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3252	1/1	0.85	0.25	62,62,62,62	0
57	MG	1H	3436	1/1	0.85	0.12	65,65,65,65	0
57	MG	1H	3197	1/1	0.85	0.35	80,80,80,80	0
57	MG	14	3367	1/1	0.85	0.08	99,99,99,99	0
57	MG	31	302	1/1	0.85	0.21	73,73,73,73	0
57	MG	1H	3332	1/1	0.85	0.15	50,50,50,50	0
57	MG	14	3368	1/1	0.85	0.12	74,74,74,74	0
57	MG	1H	3350	1/1	0.85	0.20	57,57,57,57	0
57	MG	1H	3511	1/1	0.85	0.05	92,92,92,92	0
57	MG	42	201	1/1	0.85	0.11	116,116,116,116	0
57	MG	1H	3537	1/1	0.85	0.21	61,61,61,61	0
57	MG	14	3181	1/1	0.85	0.34	81,81,81,81	0
57	MG	M5	101	1/1	0.85	0.10	86,86,86,86	0
57	MG	1H	3233	1/1	0.86	0.19	110,110,110,110	0
57	MG	1H	3331	1/1	0.86	0.23	53,53,53,53	0
57	MG	1G	1624	1/1	0.86	0.43	76,76,76,76	0
57	MG	3A	201	1/1	0.86	0.25	77,77,77,77	0
57	MG	14	3283	1/1	0.86	0.09	71,71,71,71	0
57	MG	1H	3164	1/1	0.86	0.14	64,64,64,64	0
57	MG	1H	3099	1/1	0.86	0.37	84,84,84,84	0
57	MG	1H	3513	1/1	0.86	0.11	80,80,80,80	0
57	MG	1H	3259	1/1	0.86	0.43	92,92,92,92	0
57	MG	14	3078	1/1	0.86	0.35	64,64,64,64	0
57	MG	1H	3458	1/1	0.86	0.14	82,82,82,82	0
57	MG	14	3319	1/1	0.86	0.10	78,78,78,78	0
57	MG	14	3004	1/1	0.86	0.23	73,73,73,73	0
57	MG	13	1632	1/1	0.86	0.39	90,90,90,90	0
57	MG	13	1615	1/1	0.86	0.23	73,73,73,73	0
57	MG	1H	3466	1/1	0.86	0.03	89,89,89,89	0
57	MG	1H	3378	1/1	0.86	0.09	65,65,65,65	0
57	MG	1H	3124	1/1	0.86	0.52	73,73,73,73	0
57	MG	1H	3424	1/1	0.86	0.05	100,100,100,100	0
57	MG	1H	3284	1/1	0.86	0.34	71,71,71,71	0
57	MG	1H	3444	1/1	0.86	0.10	73,73,73,73	0
57	MG	1H	3200	1/1	0.86	0.34	73,73,73,73	0
57	MG	25	202	1/1	0.86	0.17	110,110,110,110	0
57	MG	14	3276	1/1	0.86	0.07	95,95,95,95	0
57	MG	14	3200	1/1	0.86	0.28	98,98,98,98	0
57	MG	1H	3277	1/1	0.86	0.53	82,82,82,82	0
57	MG	14	3359	1/1	0.86	0.06	86,86,86,86	0
57	MG	1H	3075	1/1	0.86	0.19	61,61,61,61	0
57	MG	1H	3234	1/1	0.86	0.74	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3209	1/1	0.86	0.33	65,65,65,65	0
57	MG	14	3273	1/1	0.86	0.16	70,70,70,70	0
57	MG	1G	1666	1/1	0.86	0.08	103,103,103,103	0
57	MG	14	3353	1/1	0.86	0.12	90,90,90,90	0
57	MG	1H	3231	1/1	0.86	0.21	67,67,67,67	0
57	MG	1H	3113	1/1	0.86	0.26	64,64,64,64	0
57	MG	4A	201	1/1	0.86	0.21	96,96,96,96	0
57	MG	1H	3352	1/1	0.86	0.08	84,84,84,84	0
57	MG	1G	1725	1/1	0.86	0.11	113,113,113,113	0
57	MG	1H	3388	1/1	0.86	0.18	58,58,58,58	0
57	MG	1H	3145	1/1	0.86	0.61	62,62,62,62	0
57	MG	13	1674	1/1	0.86	0.38	92,92,92,92	0
57	MG	1H	3303	1/1	0.86	0.47	76,76,76,76	0
57	MG	14	3429	1/1	0.86	0.09	99,99,99,99	0
57	MG	13	1664	1/1	0.86	0.19	69,69,69,69	0
57	MG	1H	3488	1/1	0.87	0.07	88,88,88,88	0
57	MG	14	3316	1/1	0.87	0.09	90,90,90,90	0
57	MG	1H	3056	1/1	0.87	0.43	73,73,73,73	0
57	MG	14	3176	1/1	0.87	0.35	69,69,69,69	0
57	MG	1G	1623	1/1	0.87	0.49	75,75,75,75	0
57	MG	1H	3202	1/1	0.87	0.98	82,82,82,82	0
57	MG	1H	3177	1/1	0.87	0.61	77,77,77,77	0
57	MG	14	3223	1/1	0.87	0.31	87,87,87,87	0
57	MG	14	3225	1/1	0.87	0.11	95,95,95,95	0
57	MG	1H	3338	1/1	0.87	0.17	63,63,63,63	0
57	MG	1H	3493	1/1	0.87	0.05	102,102,102,102	0
57	MG	1H	3450	1/1	0.87	0.20	59,59,59,59	0
57	MG	1H	3209	1/1	0.87	0.41	52,52,52,52	0
57	MG	1H	3275	1/1	0.87	0.60	67,67,67,67	0
57	MG	1H	3312	1/1	0.87	0.23	94,94,94,94	0
57	MG	1H	3360	1/1	0.87	0.15	76,76,76,76	0
57	MG	1H	3051	1/1	0.87	0.47	76,76,76,76	0
57	MG	14	3268	1/1	0.87	0.13	86,86,86,86	0
57	MG	14	3201	1/1	0.87	0.73	95,95,95,95	0
57	MG	1H	3224	1/1	0.87	0.44	90,90,90,90	0
57	MG	14	3341	1/1	0.87	0.08	91,91,91,91	0
57	MG	14	3369	1/1	0.87	0.11	92,92,92,92	0
57	MG	1H	3406	1/1	0.87	0.16	46,46,46,46	0
57	MG	14	3431	1/1	0.87	0.23	60,60,60,60	0
57	MG	14	3383	1/1	0.87	0.14	92,92,92,92	0
57	MG	1H	3062	1/1	0.87	0.26	40,40,40,40	0
57	MG	14	3415	1/1	0.87	0.10	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3394	1/1	0.87	0.07	74,74,74,74	0
57	MG	1H	3102	1/1	0.87	0.59	66,66,66,66	0
57	MG	14	3419	1/1	0.87	0.20	110,110,110,110	0
57	MG	1G	1607	1/1	0.87	0.27	92,92,92,92	0
57	MG	13	1660	1/1	0.87	0.50	96,96,96,96	0
57	MG	14	3357	1/1	0.87	0.09	96,96,96,96	0
58	SPE	14	3445	13/13	0.87	0.36	70,76,79,79	0
57	MG	13	1737	1/1	0.87	0.10	98,98,98,98	0
57	MG	1G	1689	1/1	0.87	0.16	89,89,89,89	0
57	MG	14	3093	1/1	0.87	0.24	79,79,79,79	0
57	MG	1H	3080	1/1	0.87	0.52	103,103,103,103	0
57	MG	14	3334	1/1	0.87	0.07	94,94,94,94	0
57	MG	1H	3042	1/1	0.87	0.41	67,67,67,67	0
57	MG	1G	1727	1/1	0.87	0.09	93,93,93,93	0
57	MG	14	3424	1/1	0.87	0.13	94,94,94,94	0
57	MG	1H	3292	1/1	0.87	0.23	84,84,84,84	0
57	MG	1H	3070	1/1	0.87	0.40	56,56,56,56	0
57	MG	14	3129	1/1	0.87	0.47	75,75,75,75	0
57	MG	1G	1703	1/1	0.88	0.08	113,113,113,113	0
57	MG	14	3264	1/1	0.88	0.21	52,52,52,52	0
57	MG	1H	3445	1/1	0.88	0.16	44,44,44,44	0
57	MG	1H	3245	1/1	0.88	0.52	78,78,78,78	0
57	MG	1H	3502	1/1	0.88	0.10	90,90,90,90	0
57	MG	14	3210	1/1	0.88	0.17	80,80,80,80	0
57	MG	1H	3425	1/1	0.88	0.17	74,74,74,74	0
57	MG	13	1620	1/1	0.88	0.29	57,57,57,57	0
57	MG	13	1637	1/1	0.88	0.11	79,79,79,79	0
57	MG	88	203	1/1	0.88	0.20	76,76,76,76	0
57	MG	14	3056	1/1	0.88	0.32	80,80,80,80	0
57	MG	1H	3089	1/1	0.88	0.28	66,66,66,66	0
57	MG	1J	202	1/1	0.88	0.09	84,84,84,84	0
57	MG	1H	3309	1/1	0.88	0.72	74,74,74,74	0
57	MG	1H	3242	1/1	0.88	0.12	74,74,74,74	0
57	MG	1H	3442	1/1	0.88	0.21	69,69,69,69	0
57	MG	14	3280	1/1	0.88	0.11	97,97,97,97	0
57	MG	14	3193	1/1	0.88	0.38	95,95,95,95	0
57	MG	1G	1693	1/1	0.88	0.06	84,84,84,84	0
57	MG	14	3072	1/1	0.88	0.16	57,57,57,57	0
57	MG	14	3375	1/1	0.88	0.06	84,84,84,84	0
57	MG	13	1706	1/1	0.88	0.09	103,103,103,103	0
57	MG	1H	3367	1/1	0.88	0.15	56,56,56,56	0
57	MG	14	3155	1/1	0.88	0.30	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1605	1/1	0.88	0.31	82,82,82,82	0
57	MG	13	1739	1/1	0.88	0.05	92,92,92,92	0
57	MG	14	3238	1/1	0.88	0.15	66,66,66,66	0
57	MG	14	3358	1/1	0.88	0.09	88,88,88,88	0
57	MG	14	3366	1/1	0.88	0.12	98,98,98,98	0
57	MG	1H	3395	1/1	0.88	0.10	84,84,84,84	0
57	MG	14	3126	1/1	0.88	0.22	75,75,75,75	0
57	MG	1G	1633	1/1	0.88	0.17	89,89,89,89	0
57	MG	1H	3267	1/1	0.88	0.53	68,68,68,68	0
57	MG	1H	3134	1/1	0.88	0.23	44,44,44,44	0
57	MG	1H	3147	1/1	0.88	0.43	64,64,64,64	0
57	MG	1H	3474	1/1	0.88	0.09	82,82,82,82	0
57	MG	13	1635	1/1	0.88	0.22	99,99,99,99	0
57	MG	1H	3297	1/1	0.88	0.17	78,78,78,78	0
57	MG	1H	3249	1/1	0.88	0.30	68,68,68,68	0
57	MG	1G	1661	1/1	0.88	0.18	99,99,99,99	0
57	MG	1H	3391	1/1	0.88	0.19	50,50,50,50	0
57	MG	1H	3301	1/1	0.88	0.27	70,70,70,70	0
57	MG	13	1647	1/1	0.88	0.27	91,91,91,91	0
57	MG	1G	1669	1/1	0.88	0.11	99,99,99,99	0
57	MG	1H	3105	1/1	0.88	0.43	79,79,79,79	0
57	MG	14	3204	1/1	0.88	0.78	80,80,80,80	0
57	MG	14	3332	1/1	0.88	0.10	80,80,80,80	0
57	MG	1H	3094	1/1	0.88	0.50	68,68,68,68	0
57	MG	1H	3452	1/1	0.88	0.09	75,75,75,75	0
57	MG	1H	3203	1/1	0.88	0.36	74,74,74,74	0
57	MG	14	3323	1/1	0.88	0.12	83,83,83,83	0
57	MG	1H	3286	1/1	0.88	0.29	87,87,87,87	0
57	MG	1H	3019	1/1	0.88	0.30	61,61,61,61	0
57	MG	1H	3533	1/1	0.88	0.20	44,44,44,44	0
57	MG	1H	3092	1/1	0.88	0.18	74,74,74,74	0
57	MG	14	3227	1/1	0.88	0.27	76,76,76,76	0
57	MG	1H	3065	1/1	0.88	0.18	50,50,50,50	0
57	MG	1G	1721	1/1	0.88	0.07	107,107,107,107	0
57	MG	4L	102	1/1	0.89	0.11	108,108,108,108	0
57	MG	14	3385	1/1	0.89	0.13	80,80,80,80	0
57	MG	14	3413	1/1	0.89	0.27	81,81,81,81	0
57	MG	1H	3478	1/1	0.89	0.06	78,78,78,78	0
57	MG	1H	3541	1/1	0.89	0.10	67,67,67,67	0
57	MG	1G	1668	1/1	0.89	0.06	95,95,95,95	0
57	MG	14	3425	1/1	0.89	0.10	91,91,91,91	0
57	MG	1H	3193	1/1	0.89	0.51	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3236	1/1	0.89	0.15	70,70,70,70	0
57	MG	1G	1698	1/1	0.89	0.12	105,105,105,105	0
57	MG	1H	3130	1/1	0.89	0.72	87,87,87,87	0
57	MG	1H	3495	1/1	0.89	0.06	94,94,94,94	0
57	MG	88	201	1/1	0.89	0.16	78,78,78,78	0
57	MG	1H	3401	1/1	0.89	0.20	63,63,63,63	0
57	MG	14	3408	1/1	0.89	0.07	111,111,111,111	0
57	MG	14	3154	1/1	0.89	0.14	87,87,87,87	0
57	MG	14	3113	1/1	0.89	0.31	57,57,57,57	0
57	MG	14	3287	1/1	0.89	0.07	73,73,73,73	0
57	MG	14	3307	1/1	0.89	0.15	72,72,72,72	0
57	MG	1H	3172	1/1	0.89	0.25	84,84,84,84	0
57	MG	1H	3379	1/1	0.89	0.17	58,58,58,58	0
57	MG	5I	101	1/1	0.89	0.08	80,80,80,80	0
57	MG	1H	3195	1/1	0.89	0.16	59,59,59,59	0
57	MG	J8	101	1/1	0.89	0.61	79,79,79,79	0
57	MG	14	3400	1/1	0.89	0.09	76,76,76,76	0
57	MG	13	1735	1/1	0.89	0.08	111,111,111,111	0
57	MG	14	3178	1/1	0.89	0.50	92,92,92,92	0
57	MG	1H	3280	1/1	0.89	0.54	68,68,68,68	0
57	MG	1G	1618	1/1	0.89	0.24	89,89,89,89	0
57	MG	P8	101	1/1	0.89	0.34	71,71,71,71	0
57	MG	13	1710	1/1	0.89	0.10	82,82,82,82	0
57	MG	14	3183	1/1	0.89	0.61	65,65,65,65	0
57	MG	1G	1637	1/1	0.89	0.12	113,113,113,113	0
57	MG	1H	3304	1/1	0.89	0.42	85,85,85,85	0
57	MG	14	3294	1/1	0.89	0.11	114,114,114,114	0
57	MG	14	3365	1/1	0.89	0.17	96,96,96,96	0
57	MG	1H	3241	1/1	0.89	0.13	64,64,64,64	0
57	MG	1H	3371	1/1	0.89	0.14	56,56,56,56	0
57	MG	14	3039	1/1	0.89	0.41	65,65,65,65	0
57	MG	C5	201	1/1	0.89	0.08	103,103,103,103	0
57	MG	11	301	1/1	0.89	0.64	60,60,60,60	0
57	MG	13	1616	1/1	0.89	0.29	82,82,82,82	0
57	MG	13	1626	1/1	0.89	0.28	67,67,67,67	0
57	MG	14	3167	1/1	0.89	0.28	76,76,76,76	0
57	MG	1G	1646	1/1	0.89	0.07	83,83,83,83	0
57	MG	1H	3285	1/1	0.89	0.41	96,96,96,96	0
57	MG	14	3160	1/1	0.89	0.32	92,92,92,92	0
57	MG	1G	1625	1/1	0.89	0.12	98,98,98,98	0
57	MG	1G	1667	1/1	0.89	0.12	90,90,90,90	0
57	MG	14	3432	1/1	0.89	0.15	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3433	1/1	0.89	0.11	69,69,69,69	0
57	MG	1H	3128	1/1	0.89	0.14	79,79,79,79	0
57	MG	1G	1611	1/1	0.89	0.68	77,77,77,77	0
57	MG	14	3275	1/1	0.89	0.07	74,74,74,74	0
57	MG	14	3099	1/1	0.89	0.34	77,77,77,77	0
57	MG	16	205	1/1	0.89	0.10	66,66,66,66	0
57	MG	1H	3469	1/1	0.89	0.09	93,93,93,93	0
57	MG	1H	3006	1/1	0.89	0.43	71,71,71,71	0
57	MG	1H	3287	1/1	0.89	0.39	78,78,78,78	0
57	MG	1H	3447	1/1	0.89	0.12	66,66,66,66	0
57	MG	1H	3237	1/1	0.89	0.17	73,73,73,73	0
57	MG	14	3363	1/1	0.89	0.09	102,102,102,102	0
57	MG	1H	3214	1/1	0.89	0.26	86,86,86,86	0
57	MG	14	3179	1/1	0.89	0.23	71,71,71,71	0
57	MG	16	204	1/1	0.89	0.26	70,70,70,70	0
57	MG	1H	3392	1/1	0.89	0.20	52,52,52,52	0
57	MG	1H	3114	1/1	0.89	0.66	67,67,67,67	0
57	MG	14	3024	1/1	0.90	0.13	77,77,77,77	0
57	MG	13	1624	1/1	0.90	0.12	93,93,93,93	0
57	MG	14	3418	1/1	0.90	0.09	101,101,101,101	0
57	MG	13	1649	1/1	0.90	0.23	72,72,72,72	0
57	MG	14	3389	1/1	0.90	0.17	94,94,94,94	0
57	MG	13	1633	1/1	0.90	0.21	87,87,87,87	0
57	MG	2K	101	1/1	0.90	0.31	63,63,63,63	0
57	MG	14	3305	1/1	0.90	0.10	78,78,78,78	0
57	MG	1H	3255	1/1	0.90	0.23	73,73,73,73	0
57	MG	1G	1654	1/1	0.90	0.36	94,94,94,94	0
57	MG	1H	3116	1/1	0.90	0.18	82,82,82,82	0
57	MG	14	3308	1/1	0.90	0.23	58,58,58,58	0
57	MG	16	201	1/1	0.90	0.16	83,83,83,83	0
57	MG	1H	3140	1/1	0.90	0.20	40,40,40,40	0
57	MG	1H	3141	1/1	0.90	0.31	66,66,66,66	0
57	MG	78	201	1/1	0.90	0.07	57,57,57,57	0
57	MG	1G	1716	1/1	0.90	0.07	92,92,92,92	0
57	MG	1H	3357	1/1	0.90	0.20	62,62,62,62	0
57	MG	1G	1636	1/1	0.90	0.07	91,91,91,91	0
57	MG	14	3101	1/1	0.90	0.26	90,90,90,90	0
57	MG	1H	3044	1/1	0.90	0.67	81,81,81,81	0
57	MG	14	3194	1/1	0.90	0.69	87,87,87,87	0
57	MG	14	3267	1/1	0.90	0.08	86,86,86,86	0
57	MG	13	1656	1/1	0.90	0.25	87,87,87,87	0
57	MG	14	3171	1/1	0.90	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3097	1/1	0.90	0.49	83,83,83,83	0
57	MG	1H	3126	1/1	0.90	0.22	75,75,75,75	0
57	MG	14	3371	1/1	0.90	0.10	90,90,90,90	0
57	MG	1H	3390	1/1	0.90	0.10	68,68,68,68	0
57	MG	1H	3386	1/1	0.90	0.16	48,48,48,48	0
57	MG	14	3392	1/1	0.90	0.05	112,112,112,112	0
57	MG	1G	1672	1/1	0.90	0.10	92,92,92,92	0
57	MG	1H	3423	1/1	0.90	0.08	66,66,66,66	0
57	MG	1H	3033	1/1	0.90	0.22	73,73,73,73	0
57	MG	14	3040	1/1	0.90	0.40	72,72,72,72	0
57	MG	1H	3037	1/1	0.90	0.35	71,71,71,71	0
57	MG	1H	3119	1/1	0.90	0.21	62,62,62,62	0
57	MG	14	3401	1/1	0.90	0.29	85,85,85,85	0
57	MG	1H	3167	1/1	0.90	0.14	60,60,60,60	0
57	MG	14	3063	1/1	0.90	0.36	52,52,52,52	0
57	MG	14	3005	1/1	0.90	0.30	50,50,50,50	0
57	MG	1G	1713	1/1	0.90	0.13	113,113,113,113	0
57	MG	1H	3531	1/1	0.90	0.21	76,76,76,76	0
57	MG	1G	1726	1/1	0.90	0.06	113,113,113,113	0
57	MG	14	3377	1/1	0.90	0.09	64,64,64,64	0
57	MG	13	1667	1/1	0.90	0.85	96,96,96,96	0
57	MG	1H	3162	1/1	0.90	0.32	68,68,68,68	0
57	MG	1H	3358	1/1	0.90	0.15	40,40,40,40	0
57	MG	1H	3356	1/1	0.90	0.12	75,75,75,75	0
57	MG	14	3229	1/1	0.90	0.17	90,90,90,90	0
57	MG	13	1619	1/1	0.90	0.22	53,53,53,53	0
57	MG	13	1738	1/1	0.90	0.10	70,70,70,70	0
57	MG	1G	1610	1/1	0.90	0.24	69,69,69,69	0
57	MG	13	1670	1/1	0.90	0.23	100,100,100,100	0
57	MG	14	3440	1/1	0.90	0.10	98,98,98,98	0
57	MG	14	3373	1/1	0.90	0.13	97,97,97,97	0
57	MG	1H	3194	1/1	0.90	0.26	71,71,71,71	0
57	MG	14	3399	1/1	0.90	0.14	95,95,95,95	0
57	MG	14	3296	1/1	0.90	0.20	62,62,62,62	0
57	MG	14	3384	1/1	0.90	0.07	88,88,88,88	0
57	MG	1G	1660	1/1	0.90	0.28	75,75,75,75	0
57	MG	1H	3455	1/1	0.90	0.15	42,42,42,42	0
57	MG	1H	3176	1/1	0.90	0.34	62,62,62,62	0
57	MG	14	3412	1/1	0.90	0.10	101,101,101,101	0
57	MG	14	3035	1/1	0.90	0.85	79,79,79,79	0
57	MG	1H	3299	1/1	0.90	0.13	78,78,78,78	0
57	MG	1H	3137	1/1	0.90	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3407	1/1	0.90	0.04	83,83,83,83	0
57	MG	13	1609	1/1	0.90	0.25	71,71,71,71	0
57	MG	13	1730	1/1	0.90	0.08	81,81,81,81	0
57	MG	1H	3456	1/1	0.90	0.15	41,41,41,41	0
57	MG	13	1719	1/1	0.90	0.10	71,71,71,71	0
57	MG	1H	3471	1/1	0.90	0.07	73,73,73,73	0
57	MG	E5	101	1/1	0.90	0.08	100,100,100,100	0
57	MG	14	3159	1/1	0.90	0.39	93,93,93,93	0
57	MG	1H	3109	1/1	0.91	0.34	79,79,79,79	0
57	MG	1H	3251	1/1	0.91	0.22	77,77,77,77	0
57	MG	1H	3336	1/1	0.91	0.16	50,50,50,50	0
57	MG	1H	3467	1/1	0.91	0.08	85,85,85,85	0
57	MG	1G	1622	1/1	0.91	0.35	85,85,85,85	0
57	MG	14	3241	1/1	0.91	0.09	100,100,100,100	0
57	MG	16	207	1/1	0.91	0.08	84,84,84,84	0
57	MG	1H	3027	1/1	0.91	0.35	84,84,84,84	0
57	MG	Q8	101	1/1	0.91	0.26	81,81,81,81	0
57	MG	14	3330	1/1	0.91	0.13	64,64,64,64	0
57	MG	13	1602	1/1	0.91	0.26	78,78,78,78	0
57	MG	1H	3181	1/1	0.91	0.16	94,94,94,94	0
57	MG	1H	3494	1/1	0.91	0.09	98,98,98,98	0
57	MG	1H	3012	1/1	0.91	0.22	84,84,84,84	0
57	MG	1H	3536	1/1	0.91	0.17	60,60,60,60	0
57	MG	14	3195	1/1	0.91	0.27	78,78,78,78	0
57	MG	1H	3025	1/1	0.91	0.24	48,48,48,48	0
57	MG	14	3289	1/1	0.91	0.06	90,90,90,90	0
57	MG	1H	3349	1/1	0.91	0.19	67,67,67,67	0
57	MG	1H	3254	1/1	0.91	0.90	75,75,75,75	0
57	MG	14	3185	1/1	0.91	0.12	76,76,76,76	0
57	MG	1H	3417	1/1	0.91	0.11	74,74,74,74	0
57	MG	1G	1606	1/1	0.91	0.13	84,84,84,84	0
57	MG	1H	3252	1/1	0.91	0.49	81,81,81,81	0
57	MG	14	3002	1/1	0.91	0.70	68,68,68,68	0
57	MG	14	3346	1/1	0.91	0.07	92,92,92,92	0
57	MG	1H	3175	1/1	0.91	0.14	64,64,64,64	0
57	MG	1H	3329	1/1	0.91	0.20	50,50,50,50	0
57	MG	14	3313	1/1	0.91	0.15	87,87,87,87	0
57	MG	14	3439	1/1	0.91	0.14	99,99,99,99	0
57	MG	1G	1673	1/1	0.91	0.17	71,71,71,71	0
57	MG	14	3444	1/1	0.91	0.27	85,85,85,85	0
57	MG	14	3202	1/1	0.91	0.26	83,83,83,83	0
57	MG	1H	3385	1/1	0.91	0.08	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3156	1/1	0.91	0.16	71,71,71,71	0
57	MG	14	3166	1/1	0.91	0.76	82,82,82,82	0
57	MG	14	3247	1/1	0.91	0.19	60,60,60,60	0
57	MG	1H	3239	1/1	0.91	0.51	92,92,92,92	0
57	MG	1H	3482	1/1	0.91	0.20	102,102,102,102	0
57	MG	1G	1629	1/1	0.91	0.14	97,97,97,97	0
57	MG	14	3196	1/1	0.91	0.44	68,68,68,68	0
57	MG	1H	3169	1/1	0.91	0.93	82,82,82,82	0
57	MG	1H	3208	1/1	0.91	0.44	78,78,78,78	0
57	MG	14	3356	1/1	0.91	0.10	67,67,67,67	0
57	MG	13	1718	1/1	0.91	0.07	88,88,88,88	0
57	MG	14	3441	1/1	0.91	0.26	102,102,102,102	0
57	MG	13	1646	1/1	0.91	0.32	97,97,97,97	0
57	MG	1H	3023	1/1	0.91	0.12	72,72,72,72	0
57	MG	1H	3148	1/1	0.91	0.22	80,80,80,80	0
57	MG	1H	3163	1/1	0.91	0.20	74,74,74,74	0
57	MG	1H	3152	1/1	0.91	0.31	51,51,51,51	0
57	MG	1G	1612	1/1	0.91	0.20	82,82,82,82	0
57	MG	1G	1655	1/1	0.91	0.14	70,70,70,70	0
57	MG	1H	3310	1/1	0.91	0.68	87,87,87,87	0
57	MG	14	3016	1/1	0.91	0.34	63,63,63,63	0
57	MG	14	3388	1/1	0.91	0.31	89,89,89,89	0
57	MG	13	1608	1/1	0.91	0.13	71,71,71,71	0
57	MG	14	3123	1/1	0.91	0.38	60,60,60,60	0
57	MG	13	1603	1/1	0.91	0.12	116,116,116,116	0
57	MG	1H	3306	1/1	0.91	0.29	70,70,70,70	0
57	MG	1H	3262	1/1	0.91	0.24	71,71,71,71	0
57	MG	1H	3079	1/1	0.91	0.28	45,45,45,45	0
57	MG	13	1659	1/1	0.91	0.64	85,85,85,85	0
57	MG	1H	3192	1/1	0.91	0.27	76,76,76,76	0
57	MG	13	1711	1/1	0.91	0.12	102,102,102,102	0
57	MG	14	3235	1/1	0.91	0.21	65,65,65,65	0
57	MG	13	1636	1/1	0.91	0.28	103,103,103,103	0
57	MG	14	3338	1/1	0.91	0.08	81,81,81,81	0
57	MG	13	1613	1/1	0.91	0.18	81,81,81,81	0
57	MG	13	1622	1/1	0.92	0.35	74,74,74,74	0
57	MG	1H	3419	1/1	0.92	0.07	78,78,78,78	0
57	MG	14	3417	1/1	0.92	0.11	89,89,89,89	0
57	MG	1G	1635	1/1	0.92	0.26	102,102,102,102	0
57	MG	14	3115	1/1	0.92	0.41	48,48,48,48	0
57	MG	14	3302	1/1	0.92	0.13	86,86,86,86	0
57	MG	1G	1659	1/1	0.92	0.38	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1602	1/1	0.92	0.11	81,81,81,81	0
57	MG	1H	3225	1/1	0.92	0.20	74,74,74,74	0
57	MG	1H	3362	1/1	0.92	0.07	56,56,56,56	0
57	MG	1H	3059	1/1	0.92	0.42	72,72,72,72	0
57	MG	1H	3002	1/1	0.92	0.39	82,82,82,82	0
57	MG	14	3117	1/1	0.92	0.14	58,58,58,58	0
57	MG	14	3022	1/1	0.92	0.35	44,44,44,44	0
57	MG	1H	3166	1/1	0.92	0.26	56,56,56,56	0
57	MG	1H	3213	1/1	0.92	0.26	77,77,77,77	0
57	MG	1H	3083	1/1	0.92	0.48	71,71,71,71	0
57	MG	14	3049	1/1	0.92	0.32	57,57,57,57	0
57	MG	14	3231	1/1	0.92	0.67	80,80,80,80	0
57	MG	13	1747	1/1	0.92	0.11	110,110,110,110	0
57	MG	1G	1615	1/1	0.92	0.39	91,91,91,91	0
57	MG	14	3142	1/1	0.92	0.20	76,76,76,76	0
57	MG	1H	3365	1/1	0.92	0.15	62,62,62,62	0
57	MG	1H	3053	1/1	0.92	0.76	66,66,66,66	0
57	MG	1H	3540	1/1	0.92	0.10	81,81,81,81	0
57	MG	1H	3247	1/1	0.92	0.38	101,101,101,101	0
57	MG	1H	3428	1/1	0.92	0.16	68,68,68,68	0
57	MG	14	3107	1/1	0.92	0.24	65,65,65,65	0
57	MG	1H	3298	1/1	0.92	0.14	83,83,83,83	0
57	MG	14	3310	1/1	0.92	0.14	64,64,64,64	0
57	MG	1H	3026	1/1	0.92	0.40	52,52,52,52	0
57	MG	1H	3253	1/1	0.92	0.66	71,71,71,71	0
57	MG	1H	3369	1/1	0.92	0.26	54,54,54,54	0
57	MG	1H	3272	1/1	0.92	0.31	80,80,80,80	0
57	MG	13	1606	1/1	0.92	0.33	77,77,77,77	0
57	MG	1H	3408	1/1	0.92	0.08	69,69,69,69	0
57	MG	1H	3069	1/1	0.92	0.28	60,60,60,60	0
57	MG	1H	3435	1/1	0.92	0.10	60,60,60,60	0
57	MG	1G	1617	1/1	0.92	0.36	86,86,86,86	0
57	MG	13	1715	1/1	0.92	0.13	114,114,114,114	0
57	MG	14	3015	1/1	0.92	0.24	73,73,73,73	0
57	MG	14	3146	1/1	0.92	0.30	51,51,51,51	0
57	MG	1H	3016	1/1	0.92	0.39	47,47,47,47	0
57	MG	14	3006	1/1	0.92	0.25	79,79,79,79	0
57	MG	1H	3529	1/1	0.92	0.43	78,78,78,78	0
57	MG	14	3103	1/1	0.92	0.81	75,75,75,75	0
57	MG	13	1744	1/1	0.92	0.04	90,90,90,90	0
57	MG	1H	3153	1/1	0.92	0.23	82,82,82,82	0
57	MG	1G	1705	1/1	0.92	0.11	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3248	1/1	0.92	0.12	57,57,57,57	0
57	MG	1H	3512	1/1	0.92	0.17	97,97,97,97	0
57	MG	1H	3066	1/1	0.92	0.18	65,65,65,65	0
57	MG	1H	3178	1/1	0.92	0.24	57,57,57,57	0
57	MG	1H	3090	1/1	0.92	0.76	77,77,77,77	0
57	MG	14	3127	1/1	0.92	0.35	62,62,62,62	0
57	MG	1H	3271	1/1	0.92	0.31	77,77,77,77	0
57	MG	14	3221	1/1	0.93	0.12	91,91,91,91	0
57	MG	3I	201	1/1	0.93	0.26	64,64,64,64	0
57	MG	1H	3399	1/1	0.93	0.19	54,54,54,54	0
57	MG	1H	3302	1/1	0.93	0.51	81,81,81,81	0
57	MG	14	3098	1/1	0.93	0.67	62,62,62,62	0
57	MG	1H	3156	1/1	0.93	0.26	66,66,66,66	0
57	MG	14	3076	1/1	0.93	0.17	89,89,89,89	0
57	MG	1H	3409	1/1	0.93	0.11	55,55,55,55	0
57	MG	14	3297	1/1	0.93	0.19	66,66,66,66	0
57	MG	13	1658	1/1	0.93	0.48	75,75,75,75	0
57	MG	14	3414	1/1	0.93	0.22	100,100,100,100	0
57	MG	68	202	1/1	0.93	0.22	83,83,83,83	0
57	MG	13	1652	1/1	0.93	0.22	68,68,68,68	0
57	MG	1G	1718	1/1	0.93	0.11	91,91,91,91	0
57	MG	14	3130	1/1	0.93	0.39	70,70,70,70	0
57	MG	13	1618	1/1	0.93	0.58	60,60,60,60	0
57	MG	1H	3170	1/1	0.93	0.27	79,79,79,79	0
57	MG	1H	3020	1/1	0.93	0.26	47,47,47,47	0
57	MG	1H	3268	1/1	0.93	0.66	92,92,92,92	0
57	MG	13	1709	1/1	0.93	0.04	69,69,69,69	0
57	MG	14	3260	1/1	0.93	0.12	55,55,55,55	0
57	MG	14	3071	1/1	0.93	0.24	63,63,63,63	0
57	MG	1H	3107	1/1	0.93	0.43	72,72,72,72	0
57	MG	1G	1699	1/1	0.93	0.08	93,93,93,93	0
57	MG	19	301	1/1	0.93	0.39	57,57,57,57	0
57	MG	31	301	1/1	0.93	0.26	63,63,63,63	0
57	MG	14	3141	1/1	0.93	0.22	76,76,76,76	0
57	MG	14	3064	1/1	0.93	0.30	62,62,62,62	0
57	MG	1G	1658	1/1	0.93	0.26	84,84,84,84	0
57	MG	1H	3480	1/1	0.93	0.12	53,53,53,53	0
57	MG	13	1720	1/1	0.93	0.04	100,100,100,100	0
57	MG	13	1704	1/1	0.93	0.10	77,77,77,77	0
57	MG	14	3001	1/1	0.93	0.16	52,52,52,52	0
57	MG	13	1676	1/1	0.93	0.34	92,92,92,92	0
57	MG	14	3054	1/1	0.93	0.27	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3028	1/1	0.93	0.42	62,62,62,62	0
57	MG	1H	3461	1/1	0.93	0.15	48,48,48,48	0
57	MG	13	1644	1/1	0.93	0.06	82,82,82,82	0
57	MG	1H	3543	1/1	0.93	0.10	70,70,70,70	0
57	MG	1H	3407	1/1	0.93	0.04	77,77,77,77	0
57	MG	39	301	1/1	0.93	0.13	95,95,95,95	0
57	MG	13	1631	1/1	0.93	0.24	78,78,78,78	0
57	MG	1H	3173	1/1	0.93	0.74	89,89,89,89	0
57	MG	14	3299	1/1	0.93	0.21	58,58,58,58	0
57	MG	1J	203	1/1	0.93	0.23	91,91,91,91	0
57	MG	1H	3131	1/1	0.93	0.34	75,75,75,75	0
57	MG	14	3344	1/1	0.93	0.08	88,88,88,88	0
57	MG	1H	3314	1/1	0.93	0.19	88,88,88,88	0
57	MG	14	3043	1/1	0.93	0.39	83,83,83,83	0
57	MG	1H	3112	1/1	0.93	0.32	79,79,79,79	0
57	MG	1H	3034	1/1	0.93	0.38	72,72,72,72	0
57	MG	14	3026	1/1	0.93	0.12	69,69,69,69	0
57	MG	14	3250	1/1	0.93	0.15	76,76,76,76	0
57	MG	14	3028	1/1	0.93	0.31	61,61,61,61	0
57	MG	14	3186	1/1	0.93	0.17	74,74,74,74	0
57	MG	1H	3257	1/1	0.93	0.36	51,51,51,51	0
57	MG	14	3018	1/1	0.93	0.34	78,78,78,78	0
57	MG	1H	3074	1/1	0.93	0.41	73,73,73,73	0
57	MG	14	3046	1/1	0.93	0.42	76,76,76,76	0
57	MG	14	3257	1/1	0.93	0.14	69,69,69,69	0
57	MG	1H	3431	1/1	0.93	0.09	60,60,60,60	0
57	MG	1H	3229	1/1	0.93	0.38	64,64,64,64	0
57	MG	13	1694	1/1	0.93	0.05	94,94,94,94	0
57	MG	1G	1730	1/1	0.93	0.06	94,94,94,94	0
57	MG	14	3279	1/1	0.93	0.26	83,83,83,83	0
57	MG	1G	1609	1/1	0.93	0.44	96,96,96,96	0
57	MG	1H	3324	1/1	0.93	0.40	66,66,66,66	0
57	MG	14	3182	1/1	0.93	0.12	82,82,82,82	0
57	MG	1H	3440	1/1	0.93	0.16	61,61,61,61	0
57	MG	1G	1641	1/1	0.93	0.11	88,88,88,88	0
57	MG	14	3074	1/1	0.93	0.27	81,81,81,81	0
57	MG	1H	3073	1/1	0.93	0.58	59,59,59,59	0
57	MG	1H	3470	1/1	0.93	0.07	73,73,73,73	0
57	MG	1H	3024	1/1	0.93	0.23	51,51,51,51	0
57	MG	14	3234	1/1	0.93	0.11	56,56,56,56	0
57	MG	1H	3236	1/1	0.93	0.36	70,70,70,70	0
57	MG	1H	3354	1/1	0.94	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3463	1/1	0.94	0.17	48,48,48,48	0
57	MG	13	1634	1/1	0.94	0.31	78,78,78,78	0
57	MG	14	3067	1/1	0.94	0.35	69,69,69,69	0
57	MG	1H	3230	1/1	0.94	0.22	87,87,87,87	0
57	MG	1H	3047	1/1	0.94	0.26	55,55,55,55	0
57	MG	1H	3032	1/1	0.94	0.19	56,56,56,56	0
57	MG	14	3033	1/1	0.94	0.66	75,75,75,75	0
57	MG	1H	3096	1/1	0.94	0.31	53,53,53,53	0
57	MG	14	3382	1/1	0.94	0.09	72,72,72,72	0
57	MG	14	3034	1/1	0.94	0.24	48,48,48,48	0
57	MG	14	3184	1/1	0.94	0.25	72,72,72,72	0
57	MG	14	3312	1/1	0.94	0.07	80,80,80,80	0
57	MG	1H	3093	1/1	0.94	0.32	71,71,71,71	0
57	MG	14	3057	1/1	0.94	0.45	84,84,84,84	0
57	MG	1G	1688	1/1	0.94	0.11	89,89,89,89	0
57	MG	1H	3013	1/1	0.94	0.32	37,37,37,37	0
57	MG	14	3091	1/1	0.94	0.41	66,66,66,66	0
57	MG	1H	3015	1/1	0.94	0.40	65,65,65,65	0
57	MG	1H	3150	1/1	0.94	0.30	67,67,67,67	0
57	MG	1H	3240	1/1	0.94	0.37	67,67,67,67	0
57	MG	14	3106	1/1	0.94	0.79	94,94,94,94	0
57	MG	14	3108	1/1	0.94	0.84	77,77,77,77	0
57	MG	1H	3342	1/1	0.94	0.16	42,42,42,42	0
57	MG	1H	3510	1/1	0.94	0.07	70,70,70,70	0
57	MG	1H	3244	1/1	0.94	0.32	77,77,77,77	0
57	MG	1H	3004	1/1	0.94	0.71	79,79,79,79	0
57	MG	14	3073	1/1	0.94	0.31	48,48,48,48	0
57	MG	1H	3011	1/1	0.94	0.23	73,73,73,73	0
57	MG	14	3029	1/1	0.94	0.23	73,73,73,73	0
57	MG	14	3447	1/1	0.94	0.53	69,69,69,69	0
60	ZN	C5	202	1/1	0.94	0.12	151,151,151,151	0
57	MG	13	1629	1/1	0.94	0.33	56,56,56,56	0
57	MG	14	3153	1/1	0.94	0.58	65,65,65,65	0
57	MG	14	3030	1/1	0.94	0.44	89,89,89,89	0
57	MG	1G	1640	1/1	0.94	0.24	92,92,92,92	0
57	MG	1H	3489	1/1	0.94	0.09	69,69,69,69	0
57	MG	14	3080	1/1	0.94	0.34	51,51,51,51	0
57	MG	1H	3481	1/1	0.94	0.07	80,80,80,80	0
57	MG	14	3118	1/1	0.94	0.09	73,73,73,73	0
57	MG	13	1722	1/1	0.94	0.12	77,77,77,77	0
57	MG	1G	1708	1/1	0.94	0.04	140,140,140,140	0
57	MG	13	1638	1/1	0.94	0.08	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3277	1/1	0.94	0.17	59,59,59,59	0
57	MG	1G	1639	1/1	0.94	0.12	103,103,103,103	0
57	MG	14	3212	1/1	0.94	0.33	94,94,94,94	0
57	MG	1H	3387	1/1	0.94	0.13	53,53,53,53	0
57	MG	14	3013	1/1	0.94	0.44	63,63,63,63	0
57	MG	13	1716	1/1	0.94	0.09	55,55,55,55	0
57	MG	1G	1677	1/1	0.94	0.07	97,97,97,97	0
57	MG	13	1639	1/1	0.94	0.17	73,73,73,73	0
57	MG	14	3285	1/1	0.94	0.09	79,79,79,79	0
57	MG	14	3320	1/1	0.94	0.18	46,46,46,46	0
57	MG	1G	1628	1/1	0.94	0.61	76,76,76,76	0
57	MG	1H	3368	1/1	0.94	0.20	59,59,59,59	0
57	MG	13	1680	1/1	0.94	0.35	84,84,84,84	0
57	MG	1H	3045	1/1	0.94	0.22	42,42,42,42	0
57	MG	1H	3326	1/1	0.94	0.12	47,47,47,47	0
57	MG	14	3010	1/1	0.94	0.26	50,50,50,50	0
57	MG	1G	1690	1/1	0.94	0.08	114,114,114,114	0
57	MG	1G	1631	1/1	0.94	0.14	82,82,82,82	0
57	MG	14	3088	1/1	0.94	0.18	53,53,53,53	0
57	MG	1H	3457	1/1	0.94	0.09	45,45,45,45	0
57	MG	14	3145	1/1	0.94	0.12	85,85,85,85	0
57	MG	14	3262	1/1	0.94	0.16	66,66,66,66	0
57	MG	14	3122	1/1	0.94	0.29	84,84,84,84	0
57	MG	1H	3453	1/1	0.94	0.19	58,58,58,58	0
57	MG	1H	3151	1/1	0.94	0.12	59,59,59,59	0
57	MG	1H	3334	1/1	0.94	0.21	42,42,42,42	0
57	MG	14	3169	1/1	0.94	0.14	53,53,53,53	0
57	MG	1H	3022	1/1	0.94	0.33	41,41,41,41	0
57	MG	1G	1634	1/1	0.94	0.18	93,93,93,93	0
57	MG	13	1661	1/1	0.94	0.20	92,92,92,92	0
57	MG	14	3003	1/1	0.94	0.49	54,54,54,54	0
57	MG	13	1693	1/1	0.94	0.12	84,84,84,84	0
57	MG	1G	1604	1/1	0.94	0.30	103,103,103,103	0
57	MG	1H	3196	1/1	0.95	0.18	56,56,56,56	0
57	MG	1H	3459	1/1	0.95	0.15	64,64,64,64	0
57	MG	14	3124	1/1	0.95	0.35	82,82,82,82	0
57	MG	14	3050	1/1	0.95	0.48	77,77,77,77	0
57	MG	1H	3226	1/1	0.95	0.54	60,60,60,60	0
57	MG	1H	3437	1/1	0.95	0.17	46,46,46,46	0
57	MG	1H	3366	1/1	0.95	0.16	63,63,63,63	0
57	MG	14	3055	1/1	0.95	0.29	50,50,50,50	0
57	MG	14	3303	1/1	0.95	0.18	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3215	1/1	0.95	0.41	69,69,69,69	0
57	MG	14	3121	1/1	0.95	0.28	55,55,55,55	0
57	MG	1H	3138	1/1	0.95	0.46	41,41,41,41	0
57	MG	1G	1626	1/1	0.95	0.24	68,68,68,68	0
57	MG	1H	3539	1/1	0.95	0.11	45,45,45,45	0
57	MG	1H	3129	1/1	0.95	0.51	69,69,69,69	0
57	MG	1H	3300	1/1	0.95	0.24	87,87,87,87	0
57	MG	14	3068	1/1	0.95	0.37	64,64,64,64	0
57	MG	14	3019	1/1	0.95	0.18	53,53,53,53	0
57	MG	1H	3346	1/1	0.95	0.14	53,53,53,53	0
57	MG	1H	3328	1/1	0.95	0.18	46,46,46,46	0
57	MG	1H	3174	1/1	0.95	0.20	37,37,37,37	0
57	MG	14	3150	1/1	0.95	0.19	81,81,81,81	0
57	MG	14	3014	1/1	0.95	0.33	62,62,62,62	0
57	MG	1H	3076	1/1	0.95	0.16	39,39,39,39	0
57	MG	14	3188	1/1	0.95	0.51	76,76,76,76	0
57	MG	14	3180	1/1	0.95	0.15	65,65,65,65	0
57	MG	1H	3492	1/1	0.95	0.07	83,83,83,83	0
57	MG	14	3100	1/1	0.95	0.31	61,61,61,61	0
57	MG	13	1666	1/1	0.95	0.13	78,78,78,78	0
57	MG	1H	3389	1/1	0.95	0.12	68,68,68,68	0
57	MG	1H	3344	1/1	0.95	0.13	46,46,46,46	0
57	MG	13	1705	1/1	0.95	0.18	83,83,83,83	0
57	MG	1H	3393	1/1	0.95	0.10	69,69,69,69	0
57	MG	1H	3339	1/1	0.95	0.22	43,43,43,43	0
57	MG	1G	1601	1/1	0.95	0.19	70,70,70,70	0
57	MG	14	3364	1/1	0.95	0.07	85,85,85,85	0
57	MG	14	3263	1/1	0.95	0.12	56,56,56,56	0
57	MG	1H	3343	1/1	0.95	0.19	44,44,44,44	0
57	MG	14	3337	1/1	0.95	0.11	57,57,57,57	0
57	MG	14	3430	1/1	0.95	0.13	88,88,88,88	0
57	MG	14	3069	1/1	0.95	0.13	93,93,93,93	0
57	MG	14	3058	1/1	0.95	0.27	83,83,83,83	0
57	MG	14	3009	1/1	0.95	0.26	68,68,68,68	0
57	MG	14	3139	1/1	0.95	0.48	84,84,84,84	0
57	MG	13	1617	1/1	0.95	0.69	78,78,78,78	0
57	MG	1H	3007	1/1	0.95	0.16	58,58,58,58	0
57	MG	13	1717	1/1	0.95	0.10	53,53,53,53	0
57	MG	1G	1642	1/1	0.95	0.23	82,82,82,82	0
57	MG	14	3084	1/1	0.95	0.30	87,87,87,87	0
57	MG	1G	1671	1/1	0.95	0.09	86,86,86,86	0
57	MG	1H	3476	1/1	0.95	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3350	1/1	0.95	0.10	61,61,61,61	0
57	MG	1H	3472	1/1	0.95	0.16	62,62,62,62	0
57	MG	1H	3376	1/1	0.95	0.09	45,45,45,45	0
57	MG	1H	3451	1/1	0.95	0.12	83,83,83,83	0
57	MG	14	3278	1/1	0.95	0.12	80,80,80,80	0
57	MG	1G	1687	1/1	0.95	0.11	95,95,95,95	0
57	MG	14	3143	1/1	0.95	0.42	54,54,54,54	0
57	MG	14	3164	1/1	0.95	0.32	80,80,80,80	0
57	MG	14	3206	1/1	0.95	0.26	101,101,101,101	0
57	MG	1H	3426	1/1	0.95	0.05	76,76,76,76	0
57	MG	1H	3146	1/1	0.95	0.64	58,58,58,58	0
57	MG	1H	3363	1/1	0.95	0.15	47,47,47,47	0
57	MG	1H	3001	1/1	0.95	0.29	61,61,61,61	0
57	MG	1H	3491	1/1	0.95	0.16	62,62,62,62	0
57	MG	14	3125	1/1	0.95	0.47	70,70,70,70	0
57	MG	14	3325	1/1	0.95	0.21	52,52,52,52	0
57	MG	14	3132	1/1	0.95	0.30	78,78,78,78	0
57	MG	1H	3256	1/1	0.95	0.28	67,67,67,67	0
57	MG	1G	1608	1/1	0.95	0.10	111,111,111,111	0
57	MG	16	210	1/1	0.95	0.06	78,78,78,78	0
57	MG	1H	3319	1/1	0.95	0.17	56,56,56,56	0
57	MG	14	3372	1/1	0.95	0.13	79,79,79,79	0
57	MG	14	3403	1/1	0.95	0.06	83,83,83,83	0
57	MG	14	3170	1/1	0.95	0.34	87,87,87,87	0
57	MG	14	3336	1/1	0.95	0.07	65,65,65,65	0
57	MG	14	3233	1/1	0.95	0.26	54,54,54,54	0
57	MG	14	3219	1/1	0.95	0.43	54,54,54,54	0
57	MG	4K	102	1/1	0.95	0.07	93,93,93,93	0
57	MG	1H	3288	1/1	0.95	0.29	77,77,77,77	0
57	MG	1H	3546	1/1	0.95	0.10	41,41,41,41	0
57	MG	B5	101	1/1	0.95	0.12	85,85,85,85	0
57	MG	1H	3337	1/1	0.95	0.19	44,44,44,44	0
57	MG	1H	3441	1/1	0.95	0.17	44,44,44,44	0
57	MG	1H	3031	1/1	0.95	0.43	74,74,74,74	0
57	MG	14	3240	1/1	0.96	0.12	62,62,62,62	0
57	MG	1H	3432	1/1	0.96	0.23	56,56,56,56	0
57	MG	13	1621	1/1	0.96	0.21	56,56,56,56	0
57	MG	2L	101	1/1	0.96	0.53	77,77,77,77	0
57	MG	1G	1614	1/1	0.96	0.29	82,82,82,82	0
57	MG	14	3254	1/1	0.96	0.17	52,52,52,52	0
57	MG	14	3266	1/1	0.96	0.11	72,72,72,72	0
57	MG	16	202	1/1	0.96	0.31	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3057	1/1	0.96	0.26	72,72,72,72	0
57	MG	14	3144	1/1	0.96	0.30	56,56,56,56	0
57	MG	1H	3446	1/1	0.96	0.07	60,60,60,60	0
57	MG	14	3038	1/1	0.96	0.36	69,69,69,69	0
57	MG	1H	3468	1/1	0.96	0.11	68,68,68,68	0
57	MG	14	3011	1/1	0.96	0.39	51,51,51,51	0
57	MG	13	1627	1/1	0.96	0.24	85,85,85,85	0
57	MG	1H	3040	1/1	0.96	0.32	36,36,36,36	0
57	MG	1H	3347	1/1	0.96	0.20	56,56,56,56	0
57	MG	1H	3160	1/1	0.96	0.43	68,68,68,68	0
57	MG	1G	1679	1/1	0.96	0.07	93,93,93,93	0
57	MG	1H	3219	1/1	0.96	0.54	82,82,82,82	0
57	MG	1H	3485	1/1	0.96	0.06	83,83,83,83	0
57	MG	1G	1665	1/1	0.96	0.20	78,78,78,78	0
57	MG	1H	3534	1/1	0.96	0.12	92,92,92,92	0
57	MG	1H	3144	1/1	0.96	0.41	64,64,64,64	0
57	MG	1H	3475	1/1	0.96	0.06	83,83,83,83	0
57	MG	1H	3143	1/1	0.96	0.15	66,66,66,66	0
57	MG	1G	1663	1/1	0.96	0.20	76,76,76,76	0
57	MG	13	1714	1/1	0.96	0.08	100,100,100,100	0
57	MG	45	201	1/1	0.96	0.12	74,74,74,74	0
57	MG	1H	3382	1/1	0.96	0.22	54,54,54,54	0
57	MG	1H	3353	1/1	0.96	0.13	64,64,64,64	0
57	MG	14	3020	1/1	0.96	0.42	61,61,61,61	0
57	MG	2K	104	1/1	0.96	0.06	89,89,89,89	0
57	MG	14	3360	1/1	0.96	0.06	94,94,94,94	0
57	MG	I8	101	1/1	0.96	0.05	69,69,69,69	0
57	MG	14	3340	1/1	0.96	0.07	69,69,69,69	0
57	MG	14	3012	1/1	0.96	0.41	60,60,60,60	0
57	MG	1H	3029	1/1	0.96	0.21	63,63,63,63	0
57	MG	1H	3396	1/1	0.96	0.14	64,64,64,64	0
57	MG	1H	3060	1/1	0.96	0.33	51,51,51,51	0
57	MG	1H	3046	1/1	0.96	0.24	49,49,49,49	0
57	MG	1G	1603	1/1	0.96	0.26	79,79,79,79	0
57	MG	14	3095	1/1	0.96	0.34	74,74,74,74	0
57	MG	1H	3433	1/1	0.96	0.13	61,61,61,61	0
57	MG	1H	3017	1/1	0.96	0.29	53,53,53,53	0
57	MG	1H	3063	1/1	0.96	0.17	53,53,53,53	0
57	MG	1H	3264	1/1	0.96	0.25	59,59,59,59	0
57	MG	13	1641	1/1	0.96	0.25	68,68,68,68	0
57	MG	1H	3487	1/1	0.96	0.10	72,72,72,72	0
57	MG	13	1689	1/1	0.96	0.40	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1656	1/1	0.96	0.23	66,66,66,66	0
57	MG	14	3105	1/1	0.96	0.35	73,73,73,73	0
57	MG	14	3192	1/1	0.96	0.39	82,82,82,82	0
57	MG	13	1610	1/1	0.96	0.35	73,73,73,73	0
57	MG	14	3060	1/1	0.96	0.55	56,56,56,56	0
57	MG	14	3175	1/1	0.96	0.08	107,107,107,107	0
57	MG	14	3036	1/1	0.96	0.26	47,47,47,47	0
57	MG	13	1749	1/1	0.96	0.14	78,78,78,78	0
57	MG	1H	3052	1/1	0.96	0.35	50,50,50,50	0
57	MG	13	1696	1/1	0.96	0.15	83,83,83,83	0
57	MG	1H	3021	1/1	0.96	0.34	63,63,63,63	0
57	MG	1H	3505	1/1	0.96	0.06	79,79,79,79	0
57	MG	14	3037	1/1	0.96	0.34	57,57,57,57	0
57	MG	13	1701	1/1	0.96	0.04	69,69,69,69	0
57	MG	14	3070	1/1	0.96	0.33	82,82,82,82	0
57	MG	13	1605	1/1	0.96	0.24	70,70,70,70	0
57	MG	1H	3383	1/1	0.96	0.13	53,53,53,53	0
57	MG	1H	3305	1/1	0.96	0.23	71,71,71,71	0
57	MG	21	301	1/1	0.96	0.24	62,62,62,62	0
57	MG	13	1692	1/1	0.96	0.16	61,61,61,61	0
57	MG	14	3315	1/1	0.96	0.10	86,86,86,86	0
57	MG	14	3265	1/1	0.96	0.16	52,52,52,52	0
57	MG	14	3102	1/1	0.96	0.14	73,73,73,73	0
57	MG	14	3253	1/1	0.96	0.22	53,53,53,53	0
57	MG	1H	3381	1/1	0.96	0.10	48,48,48,48	0
57	MG	1H	3497	1/1	0.96	0.06	79,79,79,79	0
57	MG	1H	3490	1/1	0.96	0.11	65,65,65,65	0
57	MG	13	1648	1/1	0.96	0.17	77,77,77,77	0
57	MG	14	3120	1/1	0.96	0.28	75,75,75,75	0
57	MG	1H	3427	1/1	0.96	0.07	66,66,66,66	0
57	MG	1H	3064	1/1	0.96	0.36	63,63,63,63	0
57	MG	14	3228	1/1	0.96	1.16	86,86,86,86	0
57	MG	1H	3405	1/1	0.96	0.16	46,46,46,46	0
60	ZN	G8	201	1/1	0.96	0.10	131,131,131,131	0
57	MG	13	1655	1/1	0.96	0.14	65,65,65,65	0
57	MG	14	3089	1/1	0.96	0.43	79,79,79,79	0
57	MG	1H	3110	1/1	0.96	0.26	65,65,65,65	0
57	MG	1H	3043	1/1	0.96	0.41	66,66,66,66	0
57	MG	13	1725	1/1	0.96	0.10	90,90,90,90	0
57	MG	1H	3341	1/1	0.96	0.18	48,48,48,48	0
57	MG	14	3347	1/1	0.96	0.07	101,101,101,101	0
57	MG	13	1612	1/1	0.96	0.21	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	13	1628	1/1	0.97	0.39	79,79,79,79	0
57	MG	1H	3333	1/1	0.97	0.21	67,67,67,67	0
57	MG	13	1729	1/1	0.97	0.06	73,73,73,73	0
57	MG	14	3090	1/1	0.97	0.49	65,65,65,65	0
57	MG	16	209	1/1	0.97	0.03	68,68,68,68	0
57	MG	1H	3135	1/1	0.97	0.20	42,42,42,42	0
57	MG	1H	3465	1/1	0.97	0.12	63,63,63,63	0
57	MG	14	3259	1/1	0.97	0.06	63,63,63,63	0
57	MG	1H	3361	1/1	0.97	0.04	74,74,74,74	0
57	MG	1G	1627	1/1	0.97	0.20	77,77,77,77	0
57	MG	14	3329	1/1	0.97	0.11	60,60,60,60	0
57	MG	1H	3283	1/1	0.97	0.35	146,146,146,146	0
57	MG	5E	201	1/1	0.97	0.27	75,75,75,75	0
57	MG	1H	3438	1/1	0.97	0.12	50,50,50,50	0
57	MG	13	1675	1/1	0.97	0.18	104,104,104,104	0
57	MG	14	3042	1/1	0.97	0.45	69,69,69,69	0
57	MG	14	3322	1/1	0.97	0.12	64,64,64,64	0
57	MG	1H	3503	1/1	0.97	0.06	47,47,47,47	0
57	MG	14	3309	1/1	0.97	0.06	71,71,71,71	0
57	MG	14	3255	1/1	0.97	0.17	52,52,52,52	0
57	MG	14	3059	1/1	0.97	0.26	70,70,70,70	0
57	MG	1H	3049	1/1	0.97	0.43	69,69,69,69	0
57	MG	13	1607	1/1	0.97	0.26	80,80,80,80	0
57	MG	14	3044	1/1	0.97	0.50	48,48,48,48	0
57	MG	29	302	1/1	0.97	0.13	52,52,52,52	0
57	MG	14	3051	1/1	0.97	0.31	72,72,72,72	0
57	MG	1H	3454	1/1	0.97	0.13	48,48,48,48	0
57	MG	1H	3318	1/1	0.97	0.19	54,54,54,54	0
57	MG	1G	1613	1/1	0.97	0.34	83,83,83,83	0
57	MG	13	1601	1/1	0.97	0.32	74,74,74,74	0
57	MG	1H	3548	1/1	0.97	0.14	70,70,70,70	0
57	MG	1H	3290	1/1	0.97	0.13	87,87,87,87	0
57	MG	14	3023	1/1	0.97	0.41	82,82,82,82	0
57	MG	13	1712	1/1	0.97	0.09	101,101,101,101	0
57	MG	14	3361	1/1	0.97	0.04	80,80,80,80	0
57	MG	1H	3081	1/1	0.97	0.16	55,55,55,55	0
57	MG	13	1640	1/1	0.97	0.47	77,77,77,77	0
57	MG	1H	3243	1/1	0.97	0.22	79,79,79,79	0
57	MG	1H	3293	1/1	0.97	0.45	46,46,46,46	0
57	MG	14	3339	1/1	0.97	0.14	49,49,49,49	0
57	MG	1G	1734	1/1	0.97	0.16	84,84,84,84	0
57	MG	1H	3091	1/1	0.97	0.39	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3055	1/1	0.97	0.26	60,60,60,60	0
57	MG	1H	3071	1/1	0.97	0.41	57,57,57,57	0
57	MG	1H	3291	1/1	0.97	0.20	78,78,78,78	0
57	MG	1H	3050	1/1	0.97	0.30	54,54,54,54	0
57	MG	1H	3514	1/1	0.97	0.08	76,76,76,76	0
57	MG	1H	3054	1/1	0.97	0.29	37,37,37,37	0
57	MG	14	3342	1/1	0.97	0.11	82,82,82,82	0
57	MG	14	3045	1/1	0.97	0.32	61,61,61,61	0
57	MG	14	3354	1/1	0.97	0.09	73,73,73,73	0
57	MG	1H	3068	1/1	0.97	0.57	71,71,71,71	0
57	MG	14	3318	1/1	0.97	0.07	75,75,75,75	0
57	MG	14	3047	1/1	0.97	0.26	81,81,81,81	0
57	MG	1H	3018	1/1	0.97	0.50	55,55,55,55	0
57	MG	1H	3359	1/1	0.97	0.10	60,60,60,60	0
57	MG	1H	3430	1/1	0.97	0.14	61,61,61,61	0
57	MG	1H	3335	1/1	0.97	0.12	53,53,53,53	0
57	MG	14	3258	1/1	0.97	0.09	71,71,71,71	0
57	MG	1H	3532	1/1	0.97	0.12	103,103,103,103	0
57	MG	14	3065	1/1	0.97	0.35	60,60,60,60	0
57	MG	14	3306	1/1	0.97	0.13	86,86,86,86	0
57	MG	14	3017	1/1	0.97	0.48	60,60,60,60	0
57	MG	1H	3413	1/1	0.97	0.12	59,59,59,59	0
57	MG	1G	1732	1/1	0.97	0.05	114,114,114,114	0
57	MG	14	3237	1/1	0.97	0.15	56,56,56,56	0
57	MG	1H	3035	1/1	0.97	0.32	80,80,80,80	0
57	MG	1H	3400	1/1	0.98	0.13	59,59,59,59	0
57	MG	14	3345	1/1	0.98	0.08	83,83,83,83	0
57	MG	14	3048	1/1	0.98	0.28	67,67,67,67	0
57	MG	1H	3501	1/1	0.98	0.15	75,75,75,75	0
57	MG	1G	1706	1/1	0.98	0.07	79,79,79,79	0
57	MG	13	1703	1/1	0.98	0.14	66,66,66,66	0
57	MG	1H	3030	1/1	0.98	0.34	75,75,75,75	0
57	MG	1H	3384	1/1	0.98	0.07	61,61,61,61	0
57	MG	1G	1649	1/1	0.98	0.37	89,89,89,89	0
57	MG	1H	3132	1/1	0.98	0.27	88,88,88,88	0
57	MG	14	3290	1/1	0.98	0.08	66,66,66,66	0
57	MG	14	3135	1/1	0.98	0.21	69,69,69,69	0
57	MG	1H	3398	1/1	0.98	0.16	61,61,61,61	0
57	MG	14	3245	1/1	0.98	0.17	56,56,56,56	0
57	MG	14	3119	1/1	0.98	0.37	79,79,79,79	0
57	MG	14	3249	1/1	0.98	0.18	60,60,60,60	0
57	MG	14	3300	1/1	0.98	0.20	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3251	1/1	0.98	0.18	63,63,63,63	0
57	MG	14	3128	1/1	0.98	0.33	88,88,88,88	0
57	MG	1H	3375	1/1	0.98	0.18	48,48,48,48	0
57	MG	14	3061	1/1	0.98	0.65	56,56,56,56	0
57	MG	14	3109	1/1	0.98	0.52	74,74,74,74	0
57	MG	1H	3355	1/1	0.98	0.13	67,67,67,67	0
57	MG	1H	3412	1/1	0.98	0.10	51,51,51,51	0
57	MG	13	1713	1/1	0.98	0.11	65,65,65,65	0
57	MG	21	302	1/1	0.98	0.13	46,46,46,46	0
57	MG	1H	3403	1/1	0.98	0.17	50,50,50,50	0
57	MG	14	3326	1/1	0.98	0.09	60,60,60,60	0
57	MG	14	3321	1/1	0.98	0.07	64,64,64,64	0
57	MG	1H	3507	1/1	0.98	0.04	74,74,74,74	0
57	MG	1H	3014	1/1	0.98	0.38	43,43,43,43	0
57	MG	11	302	1/1	0.98	0.07	47,47,47,47	0
57	MG	13	1611	1/1	0.98	0.11	85,85,85,85	0
57	MG	14	3242	1/1	0.98	0.19	44,44,44,44	0
57	MG	1H	3142	1/1	0.98	0.12	64,64,64,64	0
57	MG	14	3269	1/1	0.98	0.14	63,63,63,63	0
57	MG	1H	3039	1/1	0.98	0.28	40,40,40,40	0
57	MG	13	1604	1/1	0.98	0.32	77,77,77,77	0
57	MG	1H	3041	1/1	0.98	0.25	51,51,51,51	0
57	MG	1H	3159	1/1	0.98	0.29	74,74,74,74	0
57	MG	14	3328	1/1	0.98	0.19	56,56,56,56	0
57	MG	14	3304	1/1	0.98	0.13	68,68,68,68	0
57	MG	13	1698	1/1	0.98	0.04	94,94,94,94	0
57	MG	14	3079	1/1	0.98	0.34	61,61,61,61	0
57	MG	14	3096	1/1	0.98	0.24	50,50,50,50	0
60	ZN	5I	102	1/1	0.98	0.11	98,98,98,98	0
57	MG	1H	3538	1/1	0.98	0.06	58,58,58,58	0
57	MG	1H	3460	1/1	0.98	0.14	48,48,48,48	0
57	MG	1H	3506	1/1	0.98	0.09	61,61,61,61	0
57	MG	1H	3136	1/1	0.98	0.17	45,45,45,45	0
60	ZN	5A	101	1/1	0.99	0.09	123,123,123,123	0
59	SF4	3E	301	8/8	0.99	0.17	86,90,100,103	0
57	MG	1H	3345	1/1	0.99	0.11	51,51,51,51	0
57	MG	14	3311	1/1	0.99	0.10	68,68,68,68	0
57	MG	1H	3351	1/1	0.99	0.11	59,59,59,59	0
57	MG	1H	3499	1/1	0.99	0.09	52,52,52,52	0
57	MG	14	3114	1/1	0.99	0.43	63,63,63,63	0
57	MG	1H	3411	1/1	0.99	0.09	80,80,80,80	0
57	MG	14	3333	1/1	0.99	0.06	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3270	1/1	0.99	0.09	65,65,65,65	0
57	MG	1J	204	1/1	0.99	0.12	88,88,88,88	0
59	SF4	32	301	8/8	0.99	0.15	90,99,108,116	0
57	MG	13	1721	1/1	0.99	0.06	62,62,62,62	0
57	MG	1H	3547	1/1	1.00	0.28	61,61,61,61	0
57	MG	14	3197	1/1	1.00	0.20	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.