



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:10 am GMT

PDB ID : 5IB8
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet} and near-cognate tRNA^{Lys} with U-G mismatch in the A-site
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2016-02-22
Resolution : 3.13 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

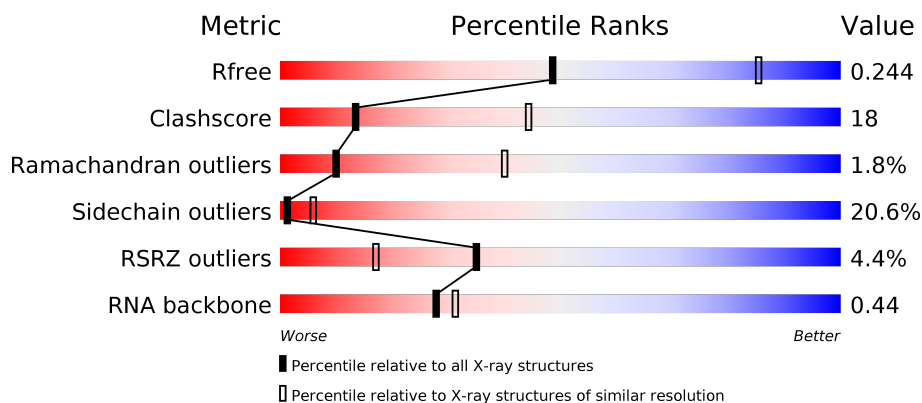
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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}	100719	1234 (3.18-3.10)
Clashscore	112137	1345 (3.18-3.10)
Ramachandran outliers	110173	1301 (3.18-3.10)
Sidechain outliers	110143	1301 (3.18-3.10)
RSRZ outliers	101464	1240 (3.18-3.10)
RNA backbone	2435	1000 (3.50-2.78)

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	<div> <div>33%</div> <div>49%</div> <div>14%</div> <div>..</div> </div>
1	1G	1522	<div> <div>34%</div> <div>48%</div> <div>16%</div> <div>..</div> </div>
2	12	256	<div> <div>6%</div> <div>32%</div> <div>38%</div> <div>11%</div> <div>•</div> <div>19%</div> </div>
2	1E	256	<div> <div>2%</div> <div>38%</div> <div>42%</div> <div>9%</div> <div>•</div> <div>10%</div> </div>

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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
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	
41	75	146	



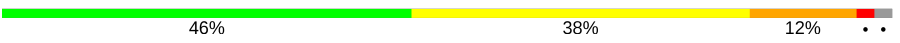
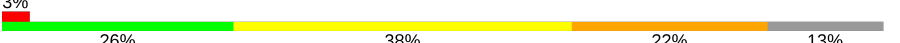
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Mol	Chain	Length	Quality of chain
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	
54	L5	49	

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Mol	Chain	Length	Quality of chain
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	1601	-	-	-	X
57	MG	13	1607	-	-	-	X
57	MG	13	1609	-	-	-	X
57	MG	13	1614	-	-	-	X
57	MG	13	1615	-	-	-	X
57	MG	13	1624	-	-	-	X
57	MG	13	1625	-	-	-	X
57	MG	13	1628	-	-	-	X
57	MG	13	1629	-	-	-	X
57	MG	13	1630	-	-	-	X
57	MG	13	1634	-	-	-	X
57	MG	13	1635	-	-	-	X
57	MG	13	1638	-	-	-	X
57	MG	13	1643	-	-	-	X
57	MG	13	1649	-	-	-	X
57	MG	13	1659	-	-	-	X
57	MG	13	1696	-	-	-	X
57	MG	14	3005	-	-	-	X
57	MG	14	3009	-	-	-	X
57	MG	14	3016	-	-	-	X
57	MG	14	3032	-	-	-	X
57	MG	14	3034	-	-	-	X
57	MG	14	3038	-	-	-	X
57	MG	14	3042	-	-	-	X
57	MG	14	3045	-	-	-	X
57	MG	14	3046	-	-	-	X
57	MG	14	3050	-	-	-	X
57	MG	14	3052	-	-	-	X
57	MG	14	3054	-	-	-	X
57	MG	14	3058	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	14	3066	-	-	-	X
57	MG	14	3068	-	-	-	X
57	MG	14	3069	-	-	-	X
57	MG	14	3075	-	-	-	X
57	MG	14	3078	-	-	-	X
57	MG	14	3080	-	-	-	X
57	MG	14	3082	-	-	-	X
57	MG	14	3086	-	-	-	X
57	MG	14	3091	-	-	-	X
57	MG	14	3094	-	-	-	X
57	MG	14	3095	-	-	-	X
57	MG	14	3096	-	-	-	X
57	MG	14	3102	-	-	-	X
57	MG	14	3105	-	-	-	X
57	MG	14	3106	-	-	-	X
57	MG	14	3113	-	-	-	X
57	MG	14	3119	-	-	-	X
57	MG	14	3123	-	-	-	X
57	MG	14	3124	-	-	-	X
57	MG	14	3130	-	-	-	X
57	MG	14	3132	-	-	-	X
57	MG	14	3133	-	-	-	X
57	MG	14	3142	-	-	-	X
57	MG	14	3145	-	-	-	X
57	MG	14	3147	-	-	-	X
57	MG	14	3149	-	-	-	X
57	MG	14	3159	-	-	-	X
57	MG	14	3160	-	-	-	X
57	MG	14	3165	-	-	-	X
57	MG	14	3170	-	-	-	X
57	MG	14	3182	-	-	-	X
57	MG	14	3194	-	-	-	X
57	MG	14	3228	-	-	-	X
57	MG	14	3240	-	-	-	X
57	MG	14	3302	-	-	-	X
57	MG	16	202	-	-	-	X
57	MG	16	204	-	-	-	X
57	MG	19	301	-	-	-	X
57	MG	1G	1606	-	-	-	X
57	MG	1G	1607	-	-	-	X
57	MG	1G	1614	-	-	-	X
57	MG	1G	1626	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1G	1632	-	-	-	X
57	MG	1G	1647	-	-	-	X
57	MG	1G	1648	-	-	-	X
57	MG	1G	1651	-	-	-	X
57	MG	1G	1670	-	-	-	X
57	MG	1G	1679	-	-	-	X
57	MG	1H	3007	-	-	-	X
57	MG	1H	3015	-	-	-	X
57	MG	1H	3017	-	-	-	X
57	MG	1H	3019	-	-	-	X
57	MG	1H	3021	-	-	-	X
57	MG	1H	3036	-	-	-	X
57	MG	1H	3041	-	-	-	X
57	MG	1H	3052	-	-	-	X
57	MG	1H	3055	-	-	-	X
57	MG	1H	3063	-	-	-	X
57	MG	1H	3068	-	-	-	X
57	MG	1H	3074	-	-	-	X
57	MG	1H	3075	-	-	-	X
57	MG	1H	3082	-	-	-	X
57	MG	1H	3084	-	-	-	X
57	MG	1H	3086	-	-	-	X
57	MG	1H	3090	-	-	-	X
57	MG	1H	3093	-	-	-	X
57	MG	1H	3107	-	-	-	X
57	MG	1H	3112	-	-	-	X
57	MG	1H	3116	-	-	-	X
57	MG	1H	3119	-	-	-	X
57	MG	1H	3126	-	-	-	X
57	MG	1H	3130	-	-	-	X
57	MG	1H	3154	-	-	-	X
57	MG	1H	3160	-	-	-	X
57	MG	1H	3169	-	-	-	X
57	MG	1H	3179	-	-	-	X
57	MG	1H	3191	-	-	-	X
57	MG	1H	3198	-	-	-	X
57	MG	1H	3206	-	-	-	X
57	MG	1H	3207	-	-	-	X
57	MG	1H	3215	-	-	-	X
57	MG	1H	3218	-	-	-	X
57	MG	1H	3225	-	-	-	X
57	MG	1H	3237	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3240	-	-	-	X
57	MG	1H	3394	-	-	-	X
57	MG	1H	3413	-	-	-	X
57	MG	1H	3427	-	-	-	X
57	MG	1H	3432	-	-	-	X
57	MG	1H	3497	-	-	-	X
57	MG	1H	3532	-	-	-	X
57	MG	1H	3541	-	-	-	X
57	MG	1H	3548	-	-	-	X
57	MG	2L	101	-	-	-	X
58	SF4	32	302	-	-	X	-
60	SPE	14	3458	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296999 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	1500	Total	C	N	O	P	0	0	0
			32246	14352	5978	10416	1500			
1	1G	1509	Total	C	N	O	P	0	0	0
			32437	14437	6010	10481	1509			

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	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	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	150	Total	C	N	O	S	0	0	0
			1141	719	217	201	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	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	65	Total	C	N	O	S	0	0	0
			510	324	92	92	2			

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

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

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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 tRNA^{Lys}.

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

- Molecule 23 is a RNA chain called tRNA^{fMet}.

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

- Molecule 24 is a RNA chain called tRNA^{Lys}.

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

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	20	Total	C	N	O	P	0	0	0
			442	198	94	130	20			
25	4L	19	Total	C	N	O	P	0	0	0
			419	188	89	123	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2831	Total 60991	C 27142	N 11416	O 19602	P 2831	0	0	0
26	14	2825	Total 60857	C 27083	N 11390	O 19559	P 2825	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	132	Total 1027	C 648	N 193	O 185	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total 2120	C 1338	N 421	O 358	S 3	0	0	0

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	180	Total	C	N	O	S	0	0	0
			1459	931	266	258	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
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	135	Total	C	N	O	S	0	0	0
			1119	697	230	191	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
			750	488	135	126	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	B5	94	Total	C	N	O	0	0	0
			735	477	133	125			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
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	60	Total	C	N	O	S	0	0	0
			475	300	84	86	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	48	Total	C	N	O	S	0	0	0
			369	229	75	60	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 tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	66	Total	C	N	O	P	0	0	0
			1402	627	244	465	66			

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

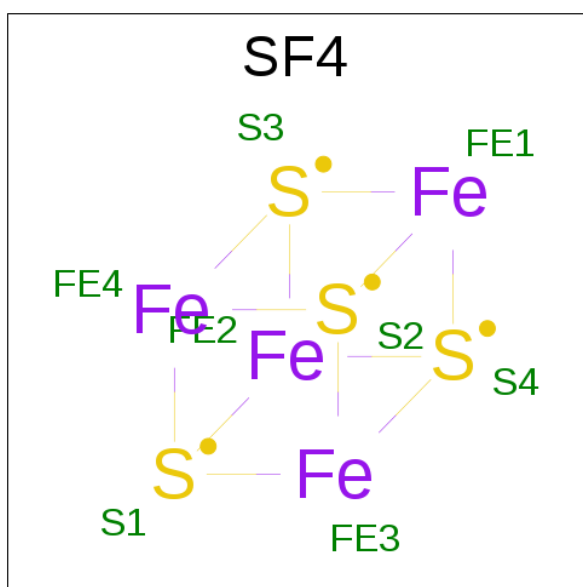
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	45	1	Total 1	Mg 1	0	0
57	19	1	Total 1	Mg 1	0	0
57	P8	1	Total 1	Mg 1	0	0
57	32	1	Total 1	Mg 1	0	0
57	2I	1	Total 1	Mg 1	0	0
57	13	141	Total 141	Mg 141	0	0
57	1J	10	Total 10	Mg 10	0	0
57	35	2	Total 2	Mg 2	0	0
57	4L	1	Total 1	Mg 1	0	0
57	16	12	Total 12	Mg 12	0	0
57	42	2	Total 2	Mg 2	0	0
57	B5	1	Total 1	Mg 1	0	0
57	25	1	Total 1	Mg 1	0	0
57	M5	1	Total 1	Mg 1	0	0
57	21	3	Total 3	Mg 3	0	0
57	31	1	Total 1	Mg 1	0	0
57	Q8	1	Total 1	Mg 1	0	0
57	3I	1	Total 1	Mg 1	0	0
57	I8	2	Total 2	Mg 2	0	0
57	52	1	Total 1	Mg 1	0	0
57	29	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	7A	1	Total 1	Mg 1	0	0
57	2K	3	Total 3	Mg 3	0	0
57	39	1	Total 1	Mg 1	0	0
57	1G	125	Total 125	Mg 125	0	0
57	1H	552	Total 552	Mg 552	0	0
57	E5	2	Total 2	Mg 2	0	0
57	88	3	Total 3	Mg 3	0	0
57	14	460	Total 460	Mg 460	0	0
57	F8	1	Total 1	Mg 1	0	0
57	41	1	Total 1	Mg 1	0	0
57	2L	2	Total 2	Mg 2	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

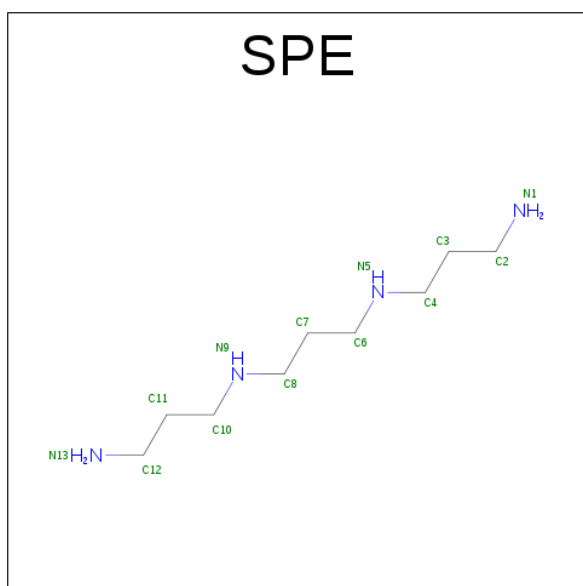


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	3E	1	Total	Fe	S	0	0
			8	4	4		
58	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	C5	1	Total	Zn	0	0
			1	1		
59	5A	1	Total	Zn	0	0
			1	1		
59	G8	1	Total	Zn	0	0
			1	1		
59	5I	1	Total	Zn	0	0
			1	1		

- Molecule 60 is THERMINE (three-letter code: SPE) (formula: C₉H₂₄N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1G	1	Total	C	N	0	0
			13	9	4		
60	14	1	Total	C	N	0	0
			13	9	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	354	Total 354	O 354	0	0
61	3E	2	Total 2	O 2	0	0
61	4E	3	Total 3	O 3	0	0
61	8E	2	Total 2	O 2	0	0
61	1I	2	Total 2	O 2	0	0
61	3I	2	Total 2	O 2	0	0
61	5I	1	Total 1	O 1	0	0
61	7I	2	Total 2	O 2	0	0
61	BI	3	Total 3	O 3	0	0
61	1K	1	Total 1	O 1	0	0
61	2K	8	Total 8	O 8	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	5	Total 5	O 5	0	0
61	1H	1720	Total 1720	O 1720	0	0
61	16	12	Total 12	O 12	0	0
61	11	10	Total 10	O 10	0	0
61	21	6	Total 6	O 6	0	0
61	31	6	Total 6	O 6	0	0
61	58	2	Total 2	O 2	0	0
61	68	2	Total 2	O 2	0	0
61	78	13	Total 13	O 13	0	0
61	98	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	B8	1	Total 1	O 1	0	0
61	C8	4	Total 4	O 4	0	0
61	E8	1	Total 1	O 1	0	0
61	F8	3	Total 3	O 3	0	0
61	G8	3	Total 3	O 3	0	0
61	I8	6	Total 6	O 6	0	0
61	J8	5	Total 5	O 5	0	0
61	L8	4	Total 4	O 4	0	0
61	N8	1	Total 1	O 1	0	0
61	Q8	5	Total 5	O 5	0	0
61	1G	364	Total 364	O 364	0	0
61	32	4	Total 4	O 4	0	0
61	42	1	Total 1	O 1	0	0
61	52	4	Total 4	O 4	0	0
61	1A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	4A	2	Total 2	O 2	0	0
61	6A	3	Total 3	O 3	0	0
61	7A	4	Total 4	O 4	0	0
61	9A	2	Total 2	O 2	0	0
61	BA	3	Total 3	O 3	0	0

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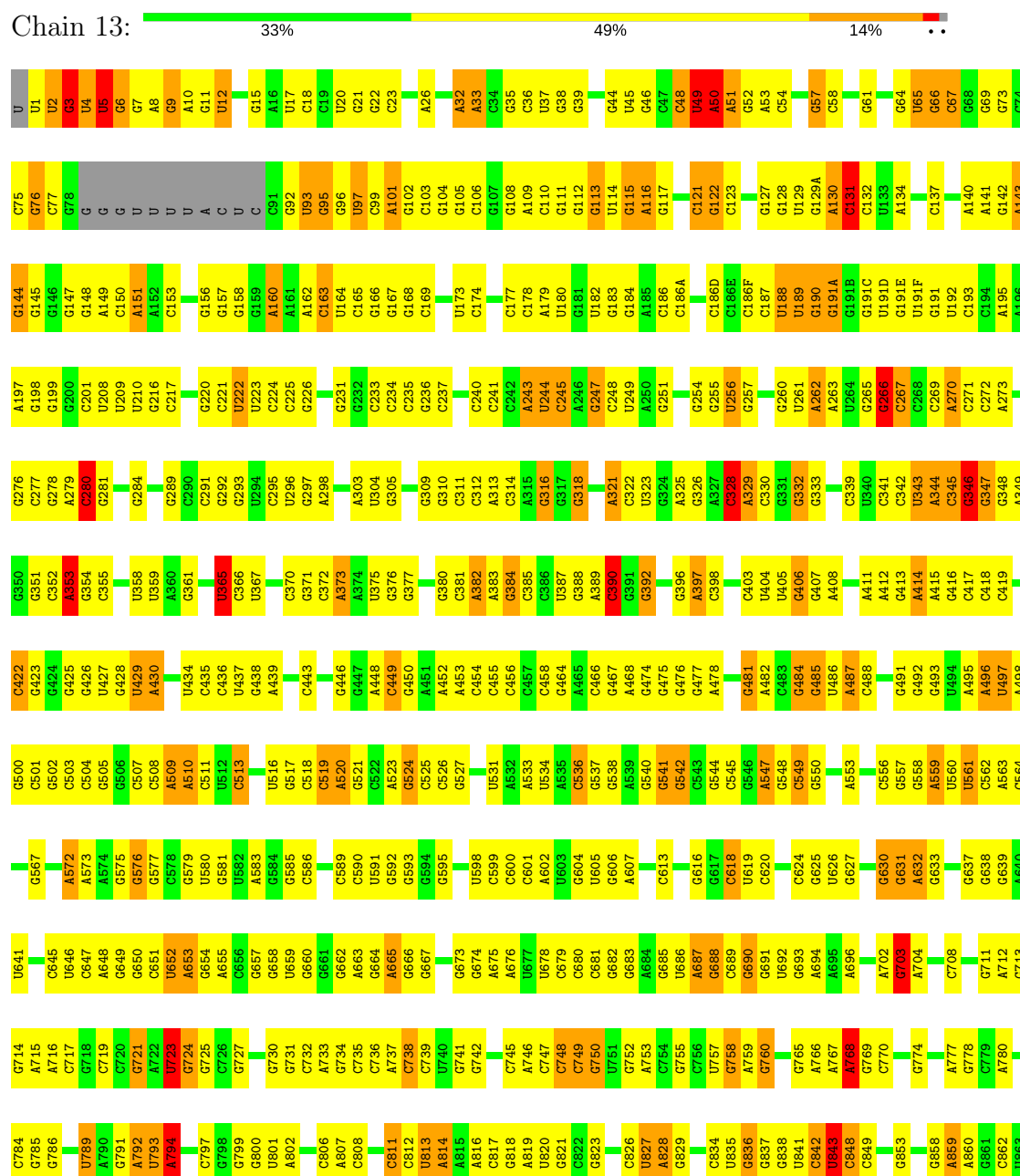
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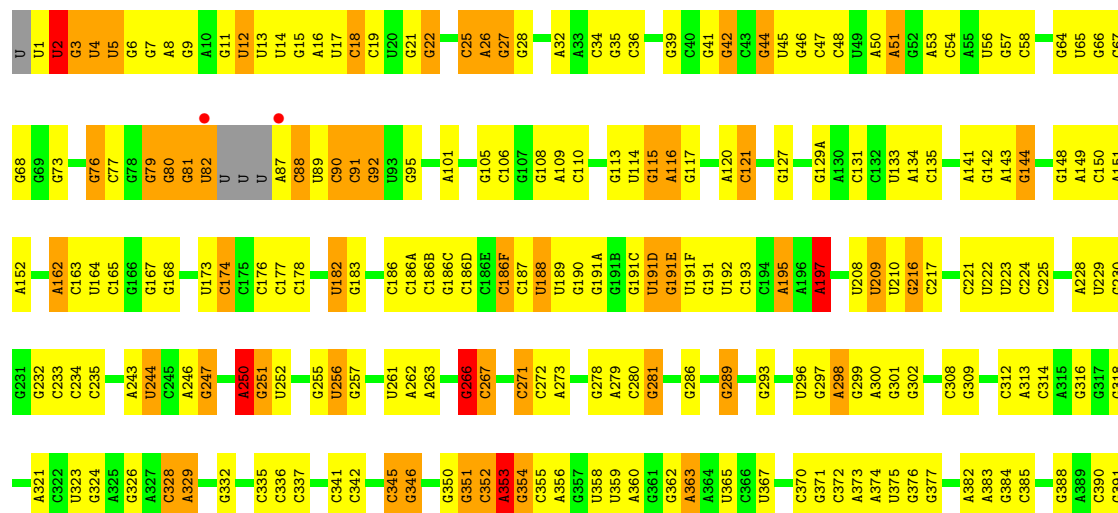
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2L	8	Total 8	O 8	0	0
61	4L	3	Total 3	O 3	0	0
61	14	1303	Total 1303	O 1303	0	0
61	1J	27	Total 27	O 27	0	0
61	19	14	Total 14	O 14	0	0
61	29	6	Total 6	O 6	0	0
61	39	8	Total 8	O 8	0	0
61	15	3	Total 3	O 3	0	0
61	25	8	Total 8	O 8	0	0
61	35	8	Total 8	O 8	0	0
61	55	1	Total 1	O 1	0	0
61	75	1	Total 1	O 1	0	0
61	85	1	Total 1	O 1	0	0
61	B5	1	Total 1	O 1	0	0
61	C5	3	Total 3	O 3	0	0
61	F5	1	Total 1	O 1	0	0
61	H5	1	Total 1	O 1	0	0
61	L5	1	Total 1	O 1	0	0
61	M5	8	Total 8	O 8	0	0

3 Residue-property plots

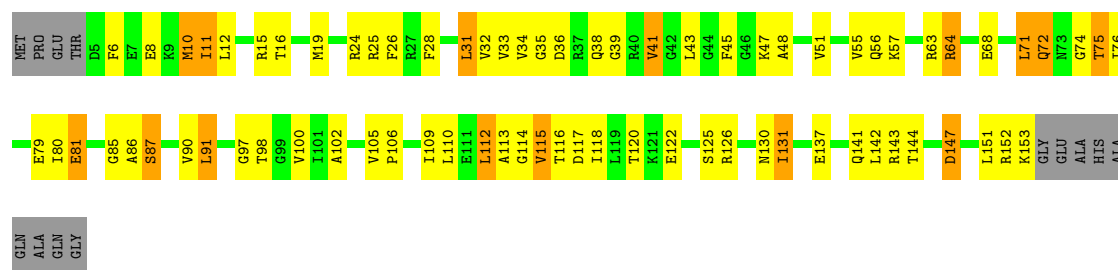
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

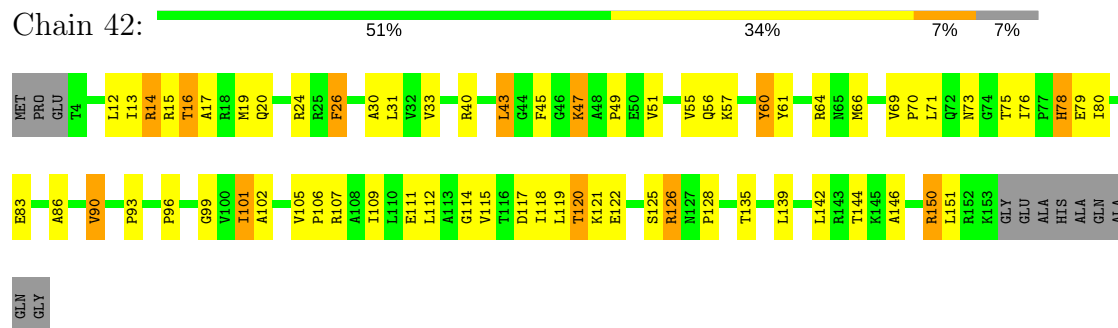




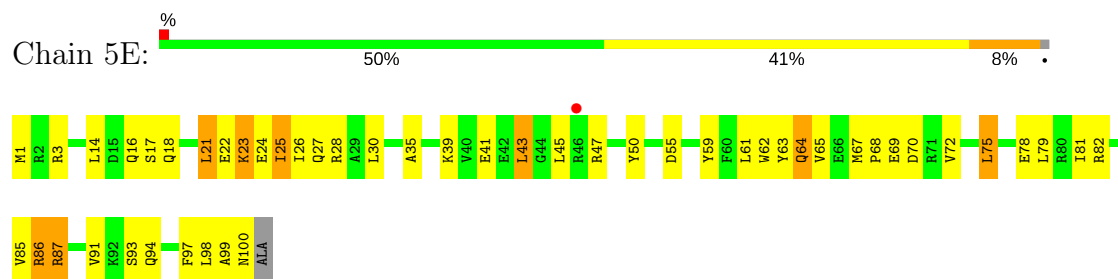
G1467	G1468	G1469	G1470	G1471	G1474	G1380	G1320	G1255	A1191	A1130	A1055	C995	C931	G858	G768	G688	G610	A547	G477	G392
U1381	C1382	G1386	G1387	G1391	G1392	G1395	C1321	A1256	C1195	G1131	U1056	A996	C932	A859	G769	C689	A611	A548	G481	A393
G1472	G1473	G1474	G1475	G1476	G1477	G1478	C1322	G1257	U1196	G1132	G1057	U997	G933	G861	G770	G690	A614	A482	A397	C398
G1479	G1480	G1481	G1482	G1483	G1484	G1485	A1324	C1259	G1197	G1134	C1059	U999	C936	U863	G776	U693	G616	U553	A484	C398
G1486	G1487	G1488	G1489	G1490	G1491	G1492	C1325	A1261	G1198	U1136	U1062	A1000	A937	A864	A777	U694	G617	C554	G485	G406
G1493	G1494	G1495	G1496	G1497	G1498	G1499	C1326	C1262	C1200	C1137	C1063	G1001	A938	A865	G778	U697	U619	C556	U486	G407
G1500	G1501	G1502	G1503	G1504	G1505	G1506	C1327	C1263	G1201	G1138	G1064	G1002	G939	C968	G779	U698	U618	C557	G490	A408
G1507	G1508	G1509	G1510	G1511	G1512	G1513	C1328	G1264	G1202	G1139	U1065	G1003	C940	C969	G780	U699	A621	G491	G410	G409
G1514	G1515	G1516	G1517	G1518	G1519	G1520	C1329	G1265	C1203	G1140	G1068	A1004	G941	C970	A789	A702	G622	A559	G492	G411
G1521	G1522	G1523	G1524	G1525	G1526	G1527	C1330	G1266	A1204	C1141	U1069	A1005	U943	U871	G784	A703	G623	A560	A412	A411
G1528	G1529	G1530	G1531	G1532	G1533	G1534	C1331	G1267	G1206	G1142	C1071	C1006	U944	A872	A787	A706	G624	A486	G413	A414
G1535	G1536	G1537	G1538	G1539	G1540	G1541	C1332	A1268	G1207	G1143	G1072	C1007	G947	A873	G791	G709	G625	A496	A496	A496
G1542	G1543	G1544	G1545	G1546	G1547	G1548	C1333	A1269	C1208	G1144	G1073	C1008	C948	C975	A792	G710	G626	A497	A497	A497
G1549	G1550	G1551	G1552	G1553	G1554	G1555	C1334	G1270	G1209	A1146	U1078	G1010	C949	C976	U793	G711	G627	A498	A498	A498
G1556	G1557	G1558	G1559	G1560	G1561	G1562	C1335	G1271	C1210	U1148	A1080	C1019	A959	C977	A794	G712	G628	C501	C501	U421
G1563	G1564	G1565	G1566	G1567	G1568	G1569	C1336	G1272	G1211	U1149	G1081	U1020	U960	C985	G805	G713	G629	C502	C502	G422
G1570	G1571	G1572	G1573	G1574	G1575	G1576	C1337	G1273	U1212	U1150	G1082	A1014	U961	A889	C811	A722	G630	A573	A573	G423
G1577	G1578	G1579	G1580	G1581	G1582	G1583	C1338	G1274	C1213	U1151	U1083	G1017	U962	C983	A802	G717	G631	A574	A574	U420
G1584	G1585	G1586	G1587	G1588	G1589	G1590	C1339	G1275	G1214	A1151	U1084	G1018	U963	C984	A803	G718	G632	A575	A575	U421
G1591	G1592	G1593	G1594	G1595	G1596	G1597	C1340	G1276	G1215	A1152	U1085	G1019	U964	C985	A804	G719	G633	A576	A576	G424
G1598	G1599	G1600	G1601	G1602	G1603	G1604	C1341	G1277	G1216	C1153	U1086	C1019	A959	C986	U804	G720	G634	A577	A577	G425
G1605	G1606	G1607	G1608	G1609	G1610	G1611	C1342	G1278	G1217	C1154	U1087	U1020	U960	C987	A805	G721	G635	A578	A578	G426
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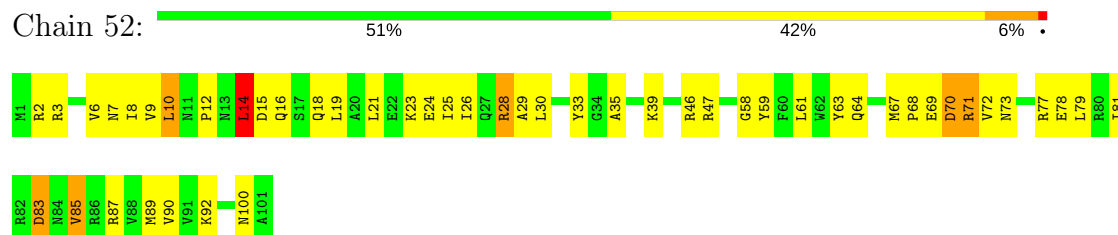
• Molecule 5: 30S ribosomal protein S5



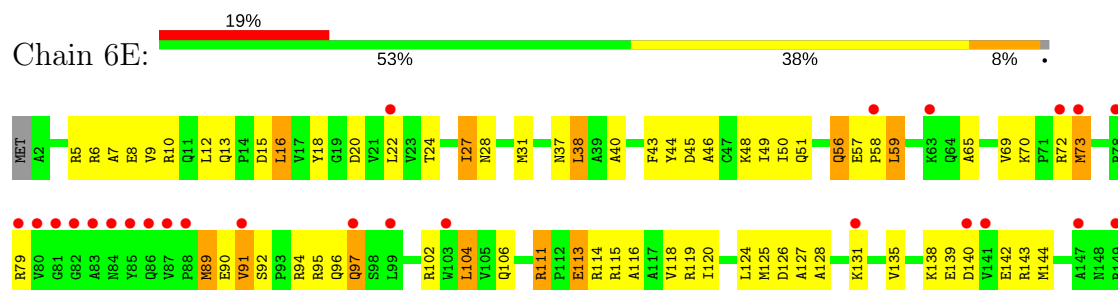
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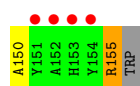


• Molecule 6: 30S ribosomal protein S6

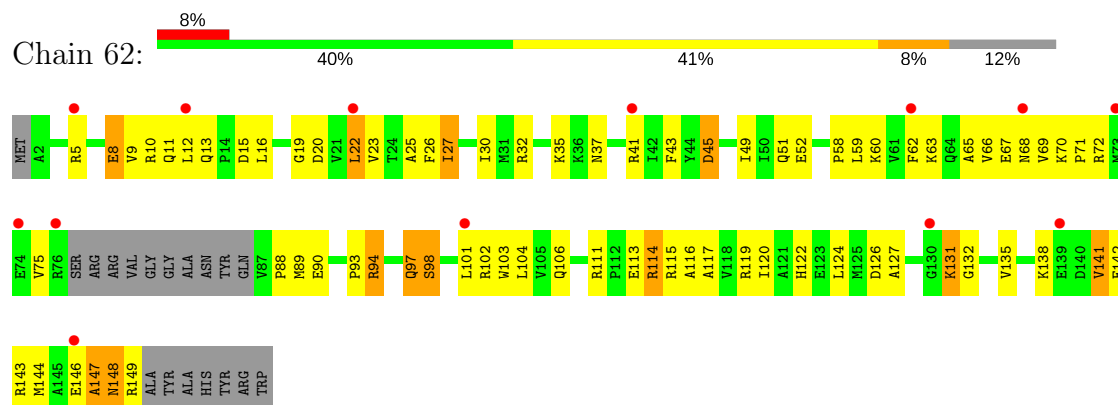


• Molecule 7: 30S ribosomal protein S7

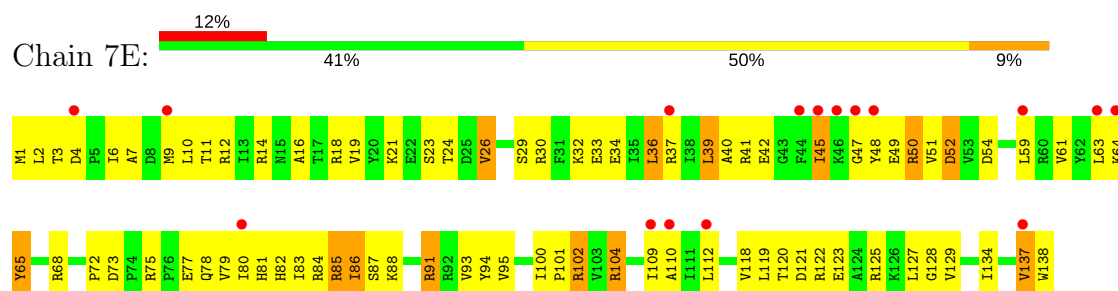




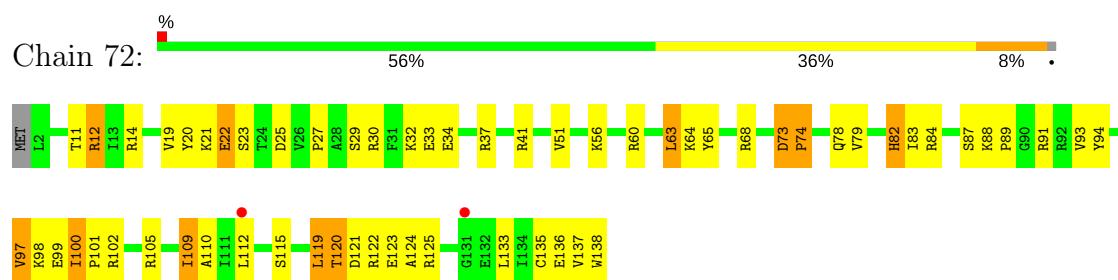
• Molecule 7: 30S ribosomal protein S7



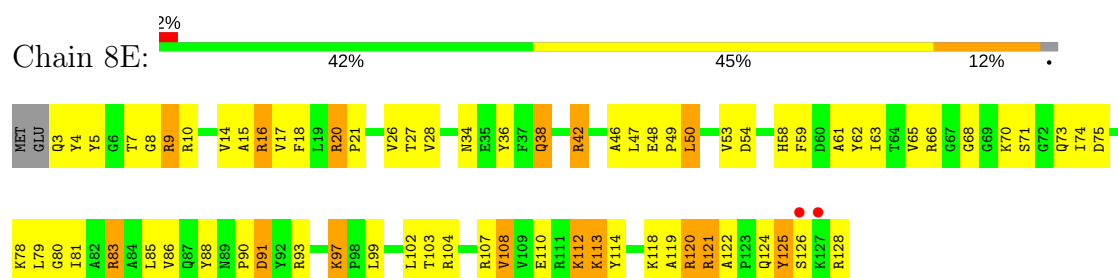
• Molecule 8: 30S ribosomal protein S8



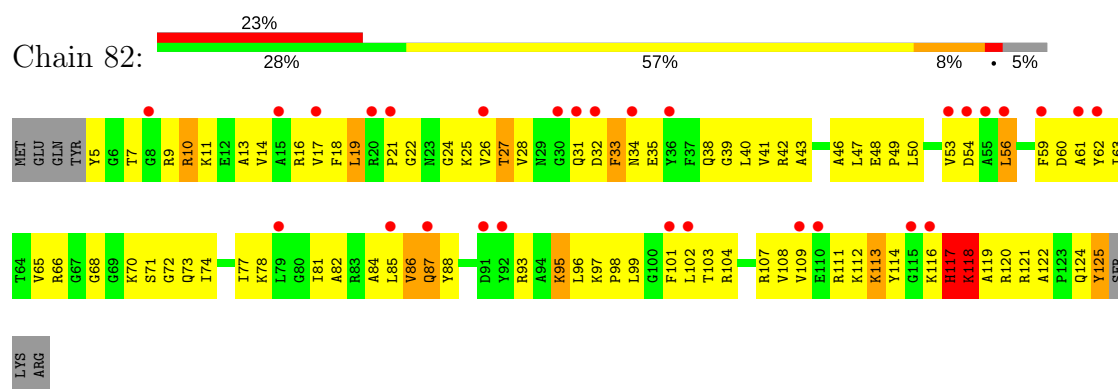
• Molecule 8: 30S ribosomal protein S8



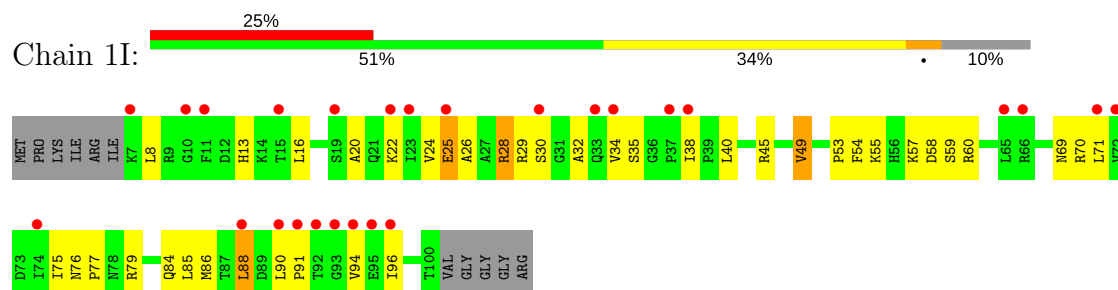
• Molecule 9: 30S ribosomal protein S9



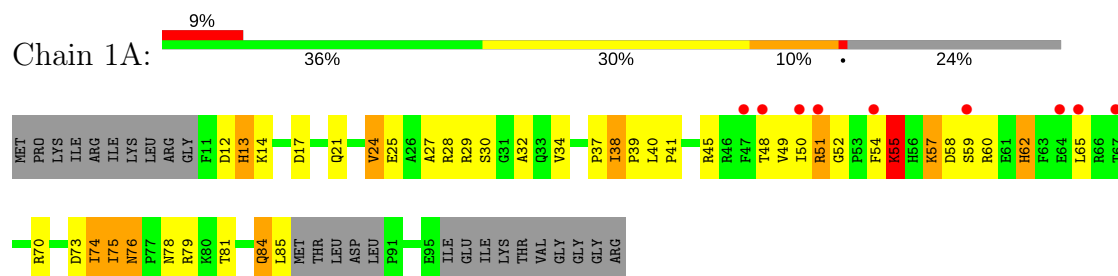
• Molecule 9: 30S ribosomal protein S9



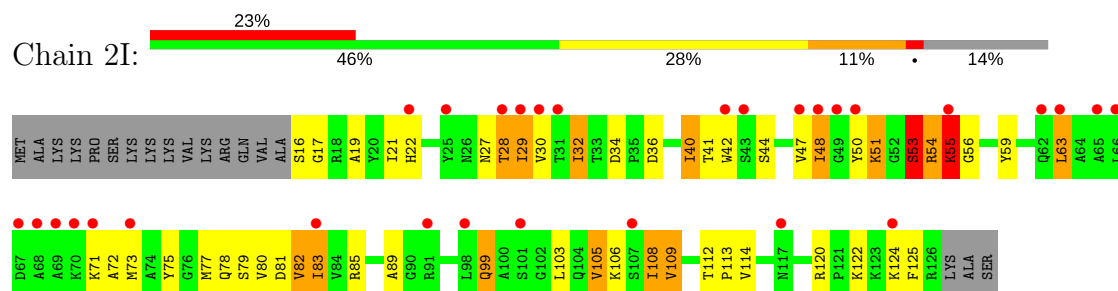
- Molecule 10: 30S ribosomal protein S10



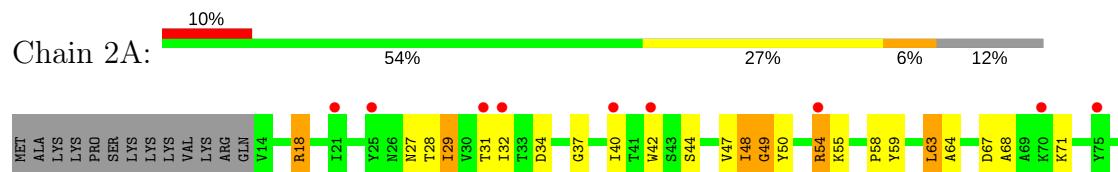
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

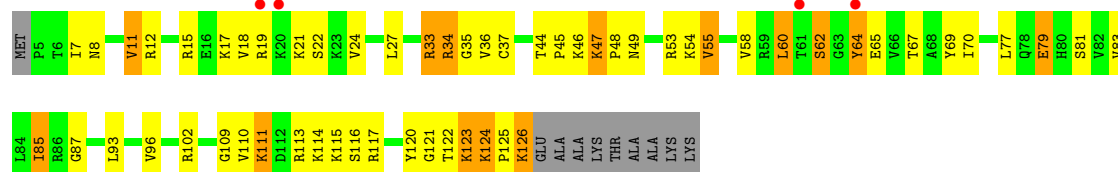


- Molecule 11: 30S ribosomal protein S11

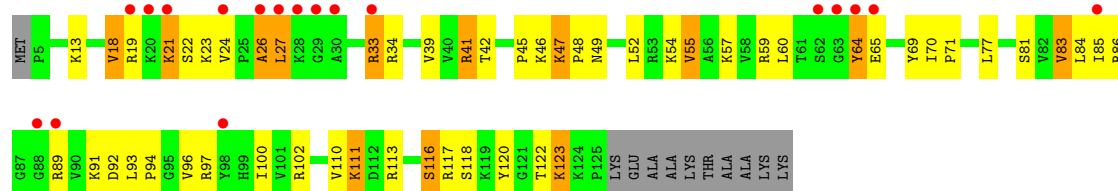




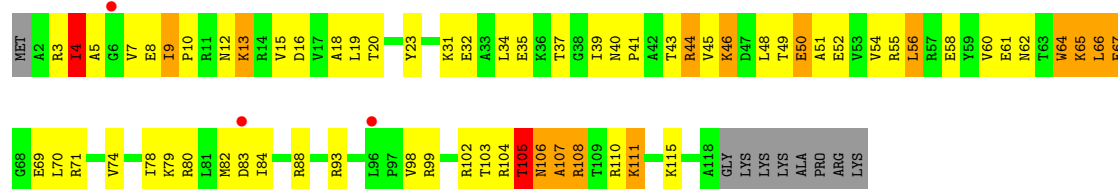
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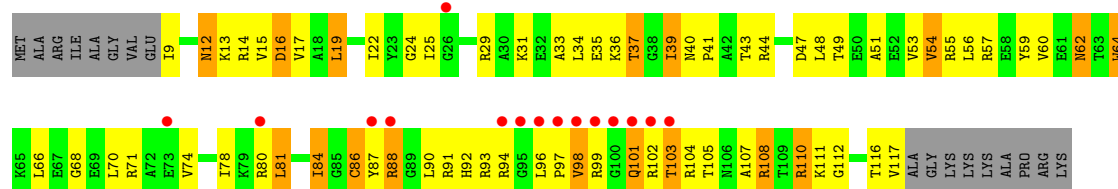
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13

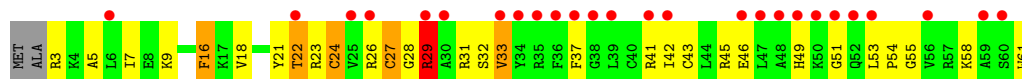
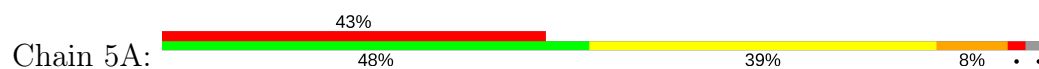


- Molecule 14: 30S ribosomal protein S14 type Z

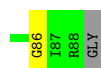
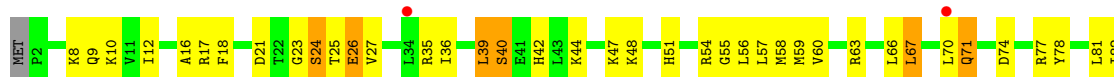




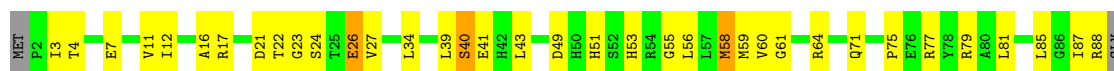
- Molecule 14: 30S ribosomal protein S14 type Z



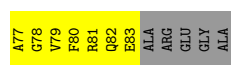
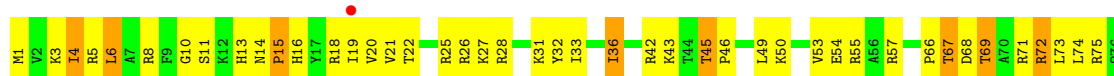
- Molecule 15: 30S ribosomal protein S15



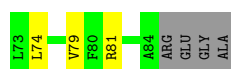
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

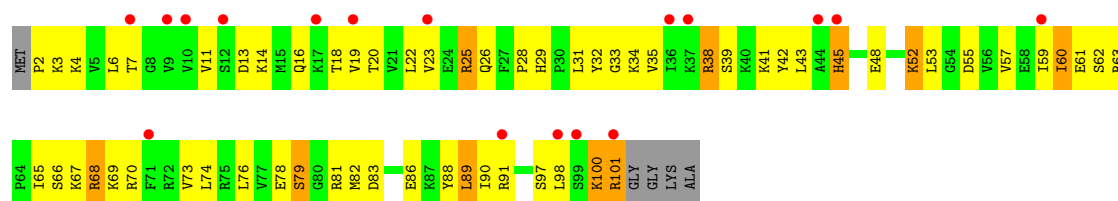


- Molecule 16: 30S ribosomal protein S16



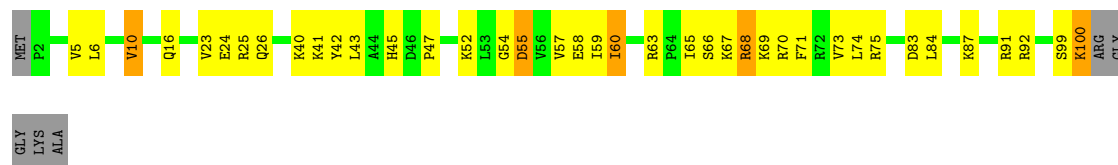
- Molecule 17: 30S ribosomal protein S17





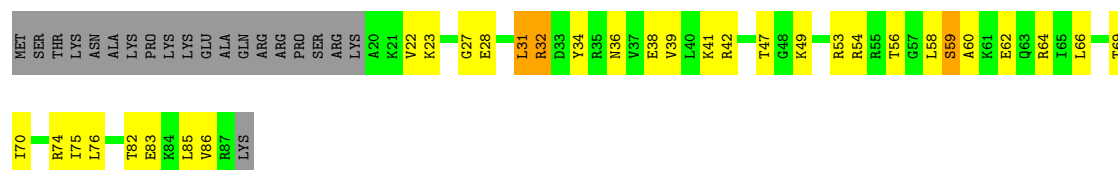
• Molecule 17: 30S ribosomal protein S17

Chain 8A: 57% 32% 5% 6%



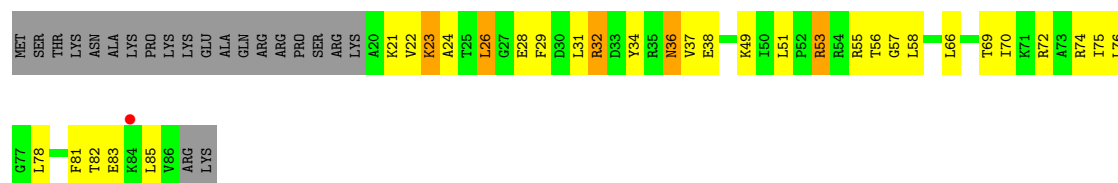
• Molecule 18: 30S ribosomal protein S18

Chain 9I: 41% 33% 23%



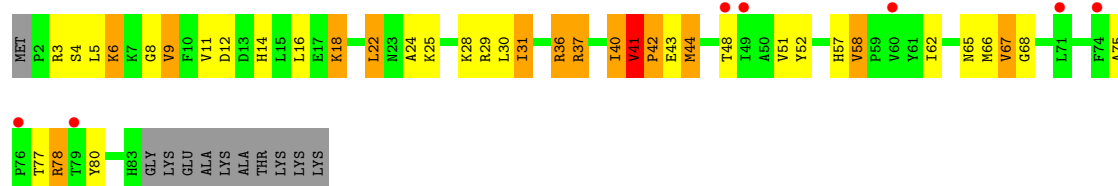
• Molecule 18: 30S ribosomal protein S18

Chain 9A: 40% 31% 6% 24%



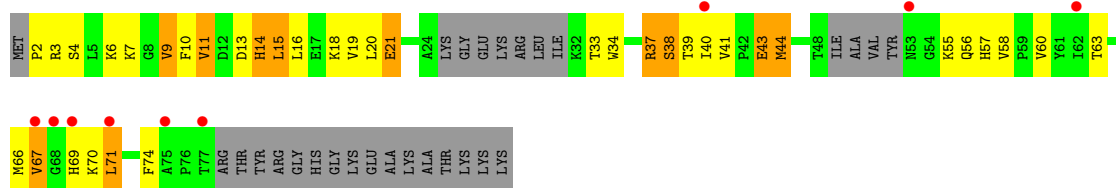
• Molecule 19: 30S ribosomal protein S19

Chain AI: 8% 46% 27% 14% 12%

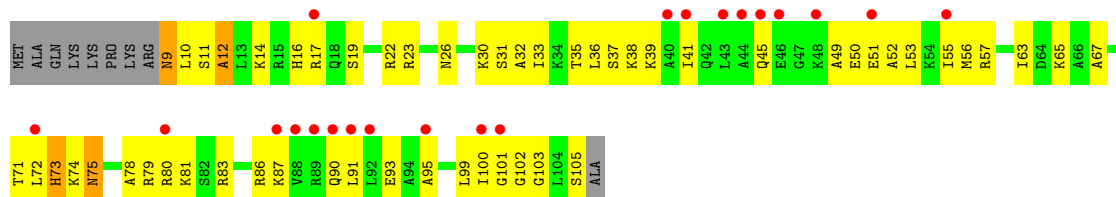
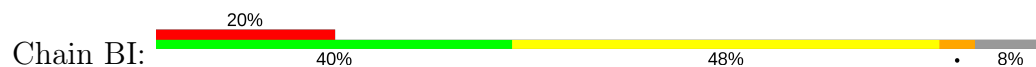


• Molecule 19: 30S ribosomal protein S19

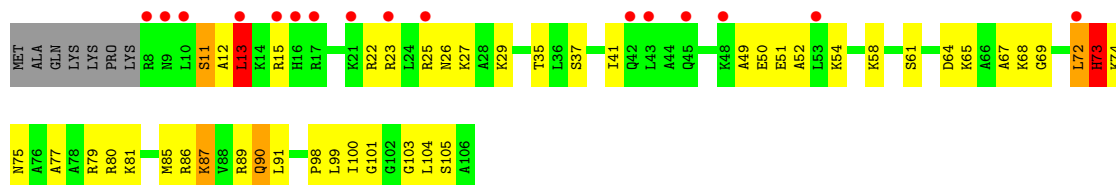
Chain AA: 10% 30% 28% 12% 30%



- Molecule 20: 30S ribosomal protein S20



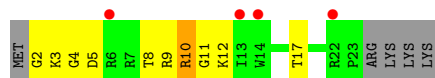
- Molecule 20: 30S ribosomal protein S20



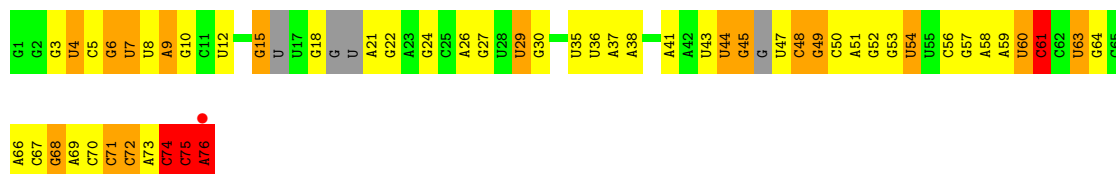
- Molecule 21: 30S ribosomal protein Thx



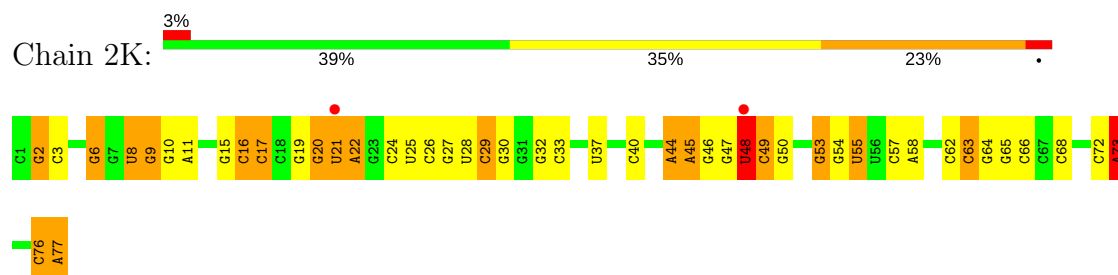
- Molecule 21: 30S ribosomal protein Thx



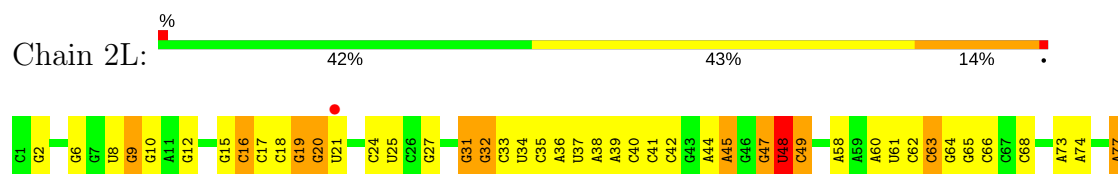
- Molecule 22: tRNA^{Lys}



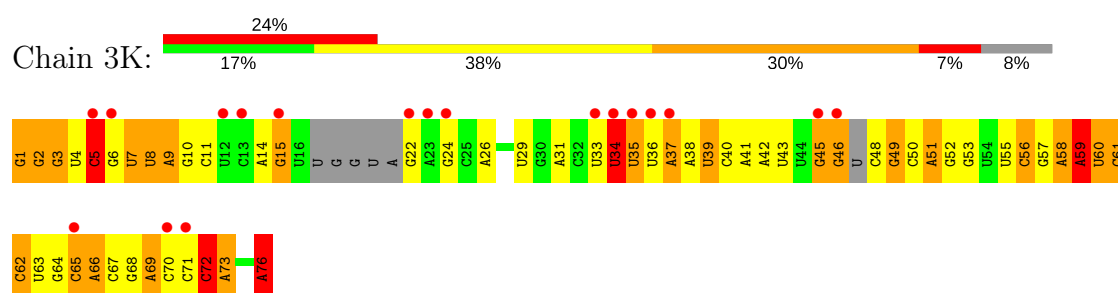
- Molecule 23: tRNA^{fMet}



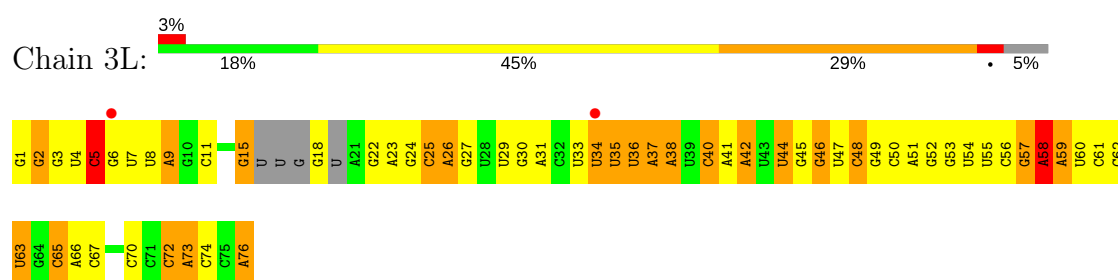
- Molecule 23: tRNA^{fMet}



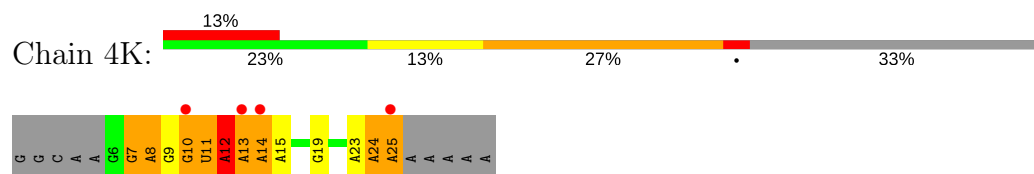
- Molecule 24: tRNA^{Lys}



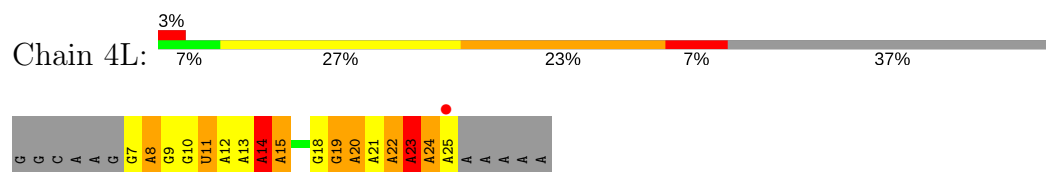
- Molecule 24: tRNA^{Lys}



- Molecule 25: mRNA



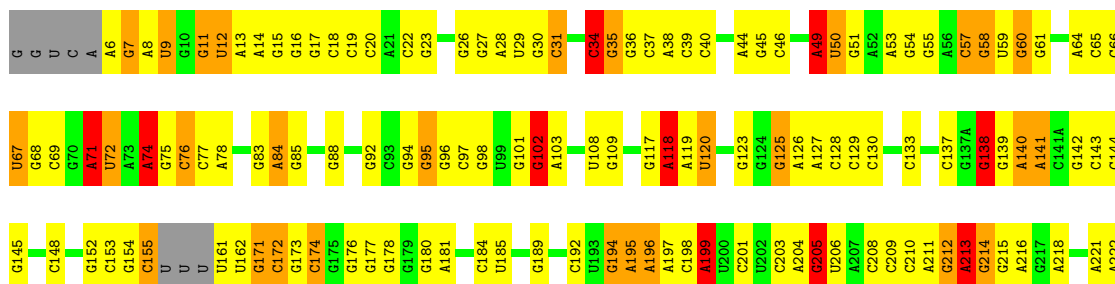
- Molecule 25: mRNA



Chain 1H: 

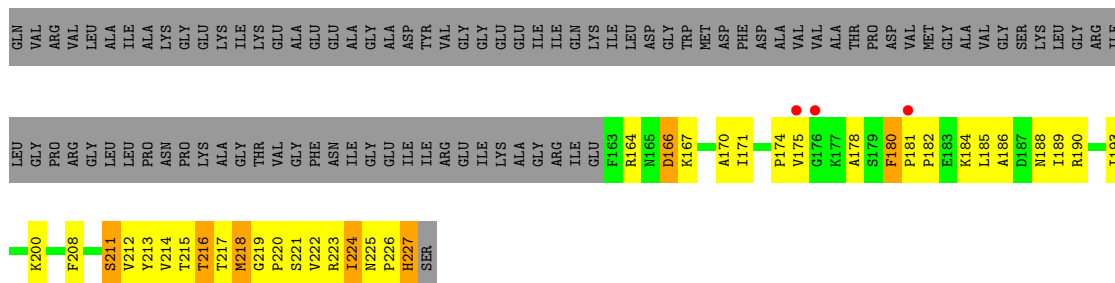


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	G1932	U1770		C1607	G1542	A1469	C1398	G1257	U1255	A1188	G1122	A
U2074	A1932	C1771	G1674	A1608	A1543	G1470		C1328	G1257	U1189	G1123	U
U2075	G1933	G1772	A1675	A1609	C1544	A1471	C1403	U1329	C1258	G1191	C1124	G
	A1936	A1773	A1676	A1610	A1545		C1404	C1330	G1259	G1192	G1125	U
	A1937	U1774	G1677		A1546A	G1475	U1405	A1331	G1260	G1193	A1126	U
	A1938	U1775	G1678		C1546		U1406	G1332	C1261	A1127	A1127	G
C2081	G2009	U1776		G1613	C1547		C1407	G1337	G1262	G1194	A1128	U
A2082	G2012	U1777	G1681	C1615	C1548	G1478	C1408	G1337	U1263	G1195	A1129	G
G2083	A2013	U1778	G1682	A1616	C1549	G1479	G1409	G1338	U1263	C1196	G1130	C
C2084	A2014	U1779	C1683	C1617	C1550		G1410	G1339	G1264	G1197	U1130	U
C2085	U2015	A1780	C1684	A1618	C1551	G1483		U1340	A1265	U1198	G1131	U
U2086	U2016	C1781	C1685	G1619		G1484		U1341	G1266	U1199		A
G2087	U2017	C1782	C1686	G1620	A1554				U1267	G1200	C1135	G
	G1945	C1783	C1687	U1621	G1555	G1485	U1415	G1344	A1268	C1201	G1136	A
	U1946	A1784	C1688	G1622	G1556	G1487	C1416	C1345		C1202	G1137	A
	G1949	A1785	A1689	G1623	C1557	U1489	G1418	G1346	G1271	G1203	G1138	G
	G1950						C1417		A1272	A1204	G1139	C
	U1951						A1419	G1347	U1273	U1205	C1140	A
	A1952		U1693	A1568	C1558	G1490	U1420	G1347	G1273	G1206	U1141	G
	G2024	C1786	C1689	C1625	G1559	G1491	G1421	A1349	A1274	C1207	U1142	C
C2025	G1954	C1787	G1695	G1626	G1560	G1492	G1422			C1208	A1142A	C
C2026	U1954	A1789	C1696			C1493	G1423		A1278	G1209	A1143	A
U2027	U1955	C1790	G1697	C1630A	C1564	G1494	G1424	U1357		A1210	G1144	U
U2028	U1956	A1791	G1698	A1631	C1565	A1495	G1425	G1358	A1284	U1211		A
G2029	G1959	G1792	A1698	G1632	A1566	A1496	G1426	A1359	G1285	G1212		C
A2031	A2031	C1793	G1699	G1633	A1567	U1497	C1428		A1286	A1213	C1147	U
C2103	G2032	U1794	G1700	A1634	G1568				A1287			A
C2105	G1878	C1795		G1635	A1569	C1506	G1429	C1363	U1288		G1151	U
C2106		U1796	G1703	C1636	A1570	A1507	C1430	G1364	C1289	G1217	C1152	U
C2107	G1883	C1797	G1704	A1637	A1571	A1508	U1431	A1365	C1290	C1218	G1153	A
			G1705	C1638	A1572	C1509	C1432	A1366	C1291	G1219	G1154	A
C2108	C1886	U1798	U1706	G1573	C1574	A1510	U1433	A1367	U1292	G1220	A1155	A
U2109	C1887	G1799		C1574	C1574	A1511	A1434	G1368	C1293	C1221	A1156	G
G2110	G1888	C1800	U1709	A1641	C1575	G1512	G1435	G1369	U1294	C1222	G1157	A
C2111	A1889	G1801	C1710	G1642	U1576	C1513	G1436	C1370	C1295	C1223		G
C2112	A1890	A1802		G1643	C1577	U1514	C1437	G1371	G1296	G1224	G1160	U
	G1891		G1726	C1644	U1578	C1515	U1438	U1372	C1297	C1225	C1161	G
A2114		U1805	U1727		A1579	C1516	U1439				G1162	C
	C1895	C1806	G1728	G1647	A1580	U1517	G1440	A1373	U1300	G1229A	G1163	G
G2115		G1807	A1729	C1648	C1518	C1518	G1441	C1375	A1301	C1230	G1164	U
G2116			U1730	G1649	C1519	G1519	G1442	C1376	A1302	G1231	U1165	A
A2117	U1898	G1811	G1731	G1650	C1585	U1520	G1443	G1377	G1303		C1166	A
C2051	A1900		A1732	G1651	A1586	G1521		A1376	C1304	G1235	U1167	U
G2120	G1901	G1814		A1652	A1587	G1522	A1444A			G1236	G1168	A
G2121	A1902	A1815		G1653				A1379	C1305	G1237	G1169	A
G2122	C1982	G1816	G1750	G1654	U1590	G1525	G1448	G1380	C1306	A1237	G1170	G
A2054	C1983	C1816	C1751	A1654	C1591	G1526	A1449	C1381	A1307	G1238	G1171	C
C2055	G1984		C1752	A1655	C1592	G1527	G1449A	G1382	A1308	G1239	U1172	U
G2124	C1905	A1819		C1656	C1593	G1528		C1383	G1309	U1240	G1173	C
G2125	G1985	U1820		G1657	G1594	A1529		A1384	G1310	A1241	A1174	A
A2057	A1986	A1821	G1756	C1658	G1595	G1531		A1453	G1311	A1242	U1175	U
A2058			U1757	C1659	G1594	G1530		G1385	U1312	G1243	G1176	C
G1989		A1825	A1758	G1595				G1386	U1312		G1177	U
A2059	C1914		A1759	C1660	A1596			C1387	G1313		A1177	C
G2128	U1915	G1826										G1106
C2129												

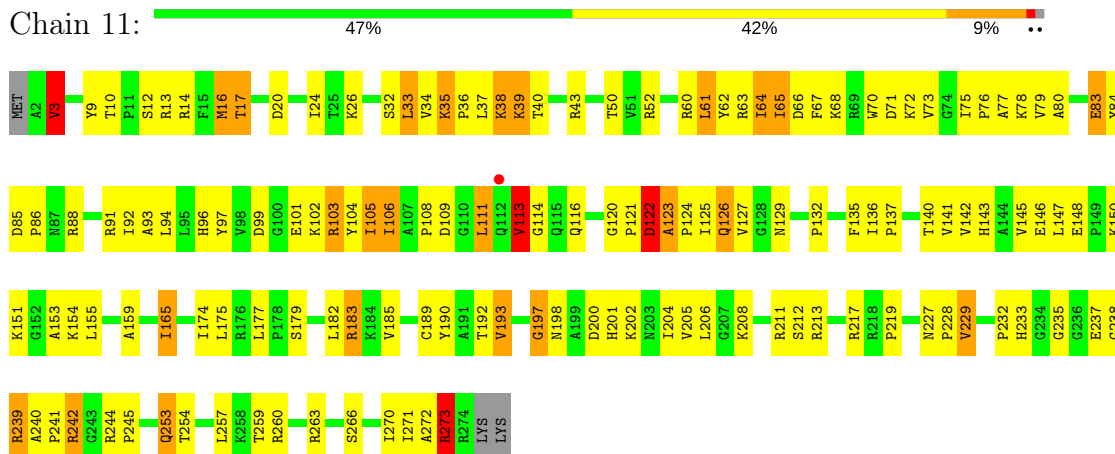




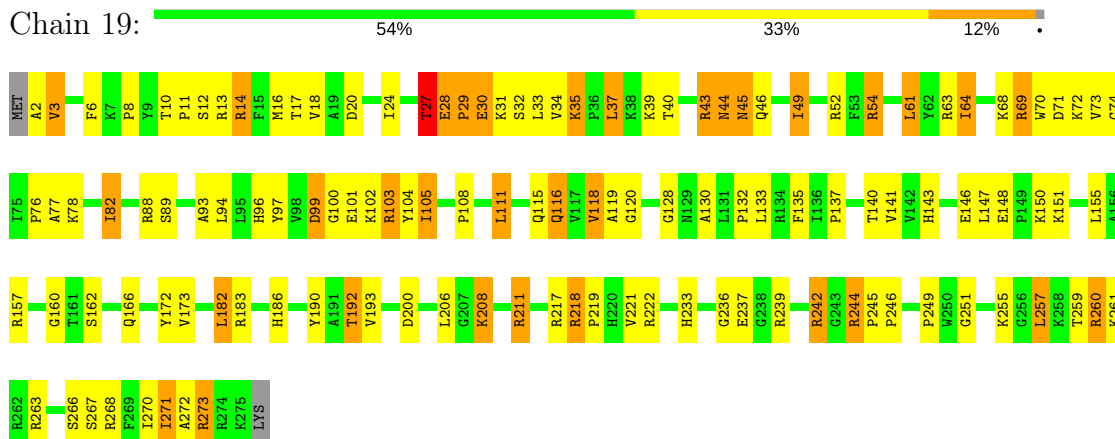




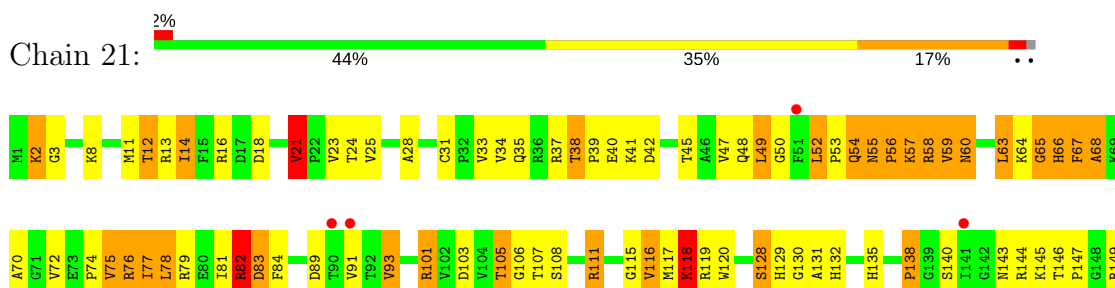
- Molecule 29: 50S ribosomal protein L2



- Molecule 29: 50S ribosomal protein L2

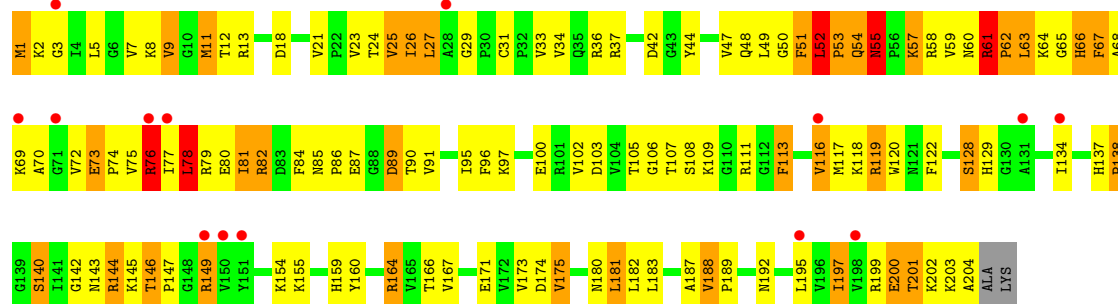


- Molecule 30: 50S ribosomal protein L3

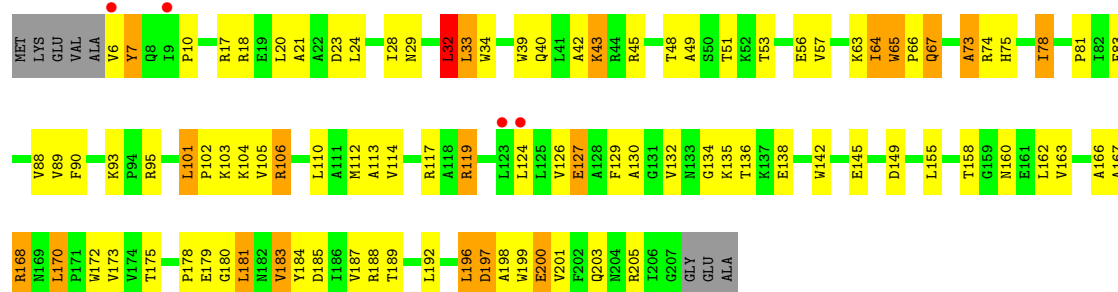




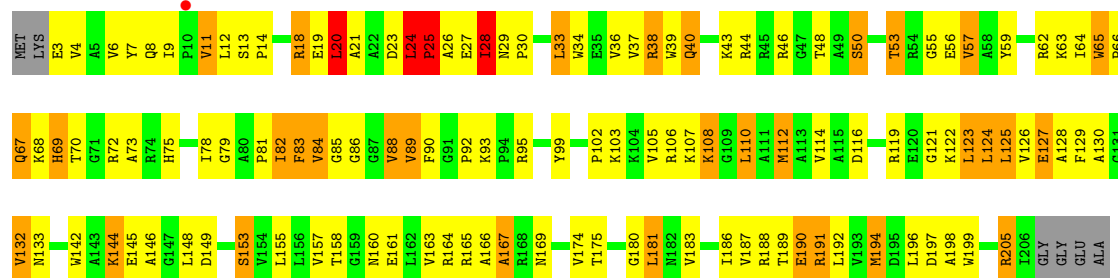
• Molecule 30: 50S ribosomal protein L3



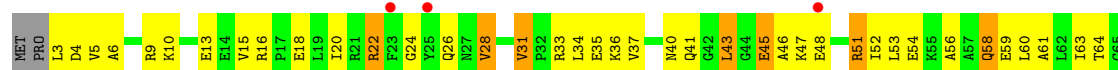
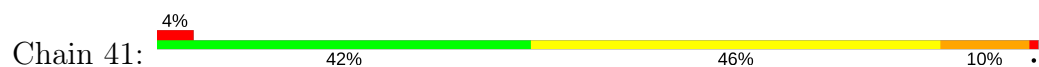
• Molecule 31: 50S ribosomal protein L4

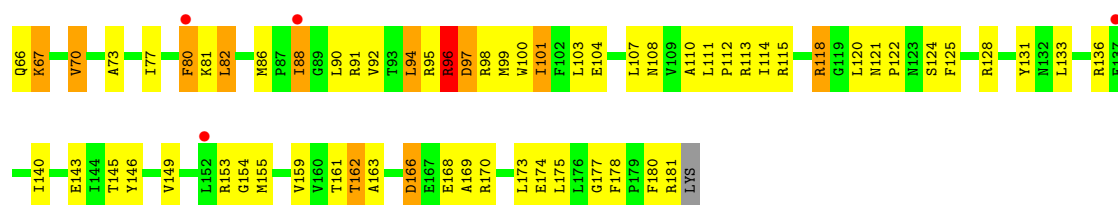


• Molecule 31: 50S ribosomal protein L4

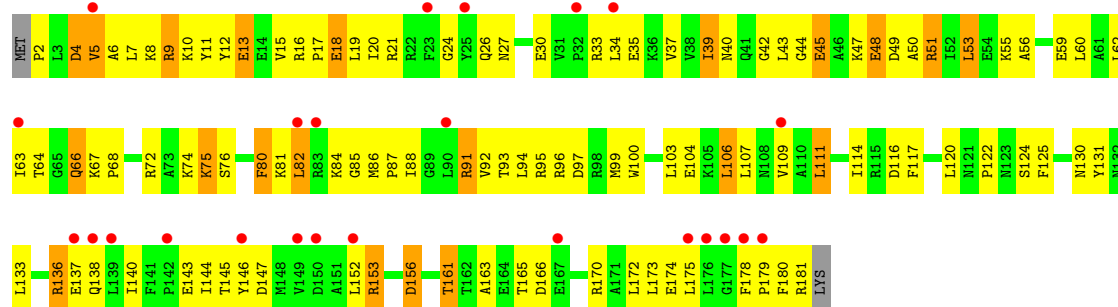


• Molecule 32: 50S ribosomal protein L5

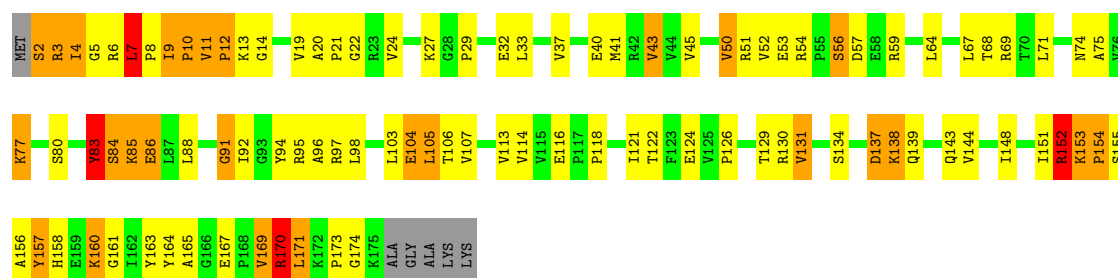




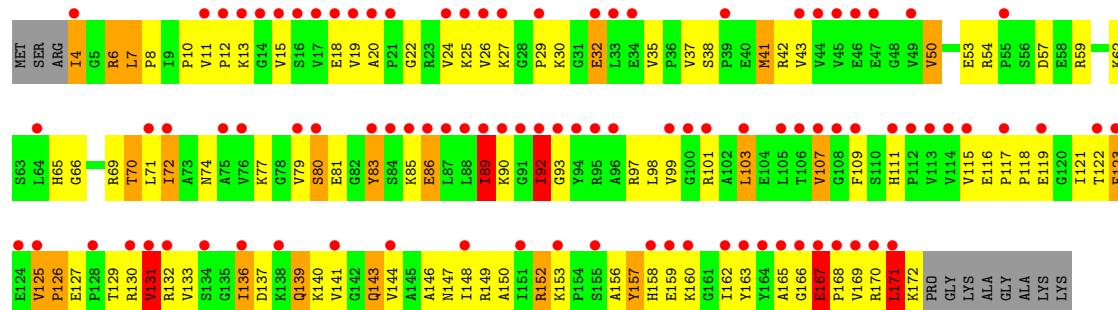
• Molecule 32: 50S ribosomal protein L5



• Molecule 33: 50S ribosomal protein L6

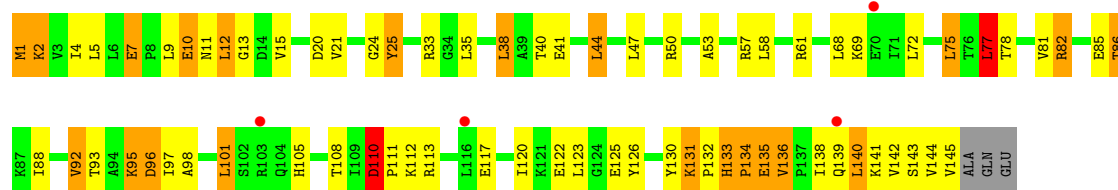


• Molecule 33: 50S ribosomal protein L6

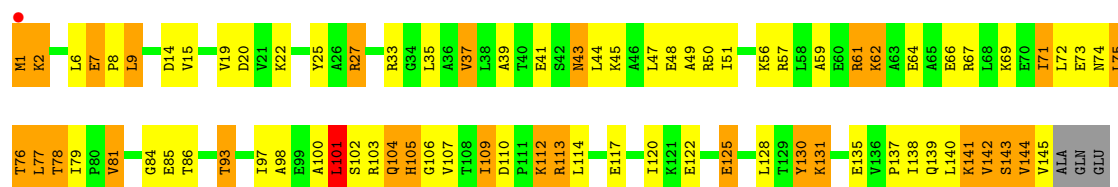


• Molecule 34: 50S ribosomal protein L9

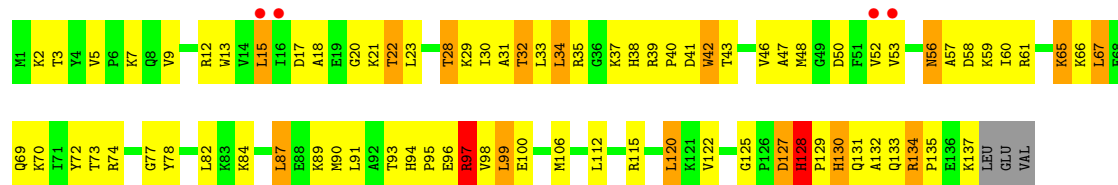




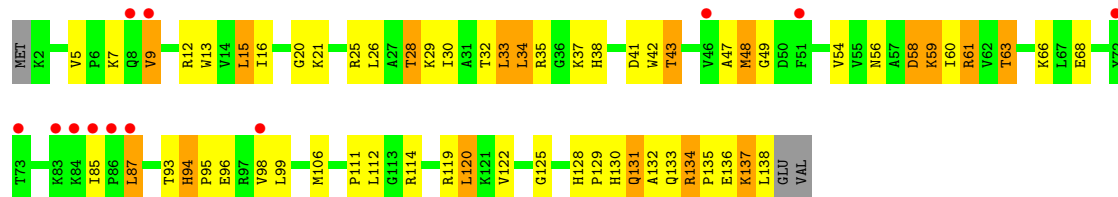
• Molecule 34: 50S ribosomal protein L9



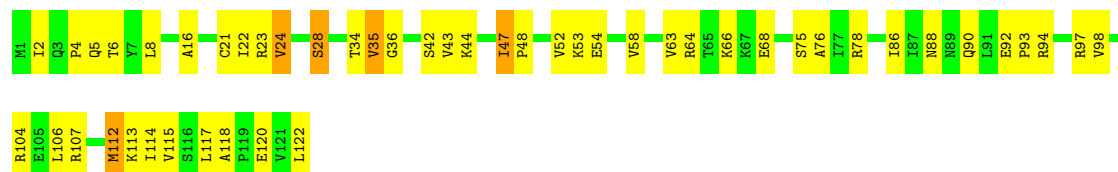
• Molecule 35: 50S ribosomal protein L13



• Molecule 35: 50S ribosomal protein L13

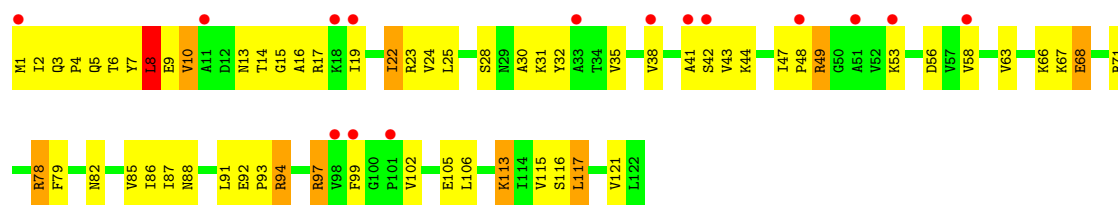


• Molecule 36: 50S ribosomal protein L14



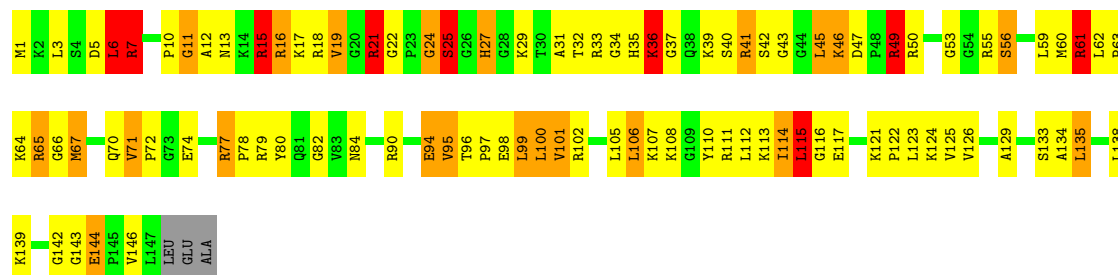
• Molecule 36: 50S ribosomal protein L14





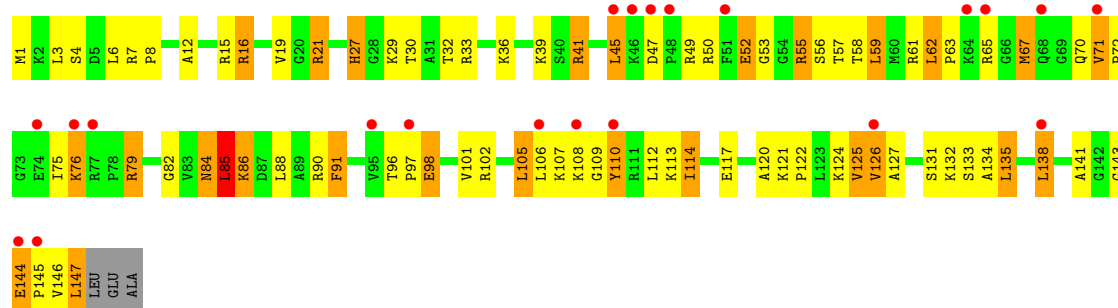
• Molecule 37: 50S ribosomal protein L15

Chain 78: 33% 44% 15% 6%



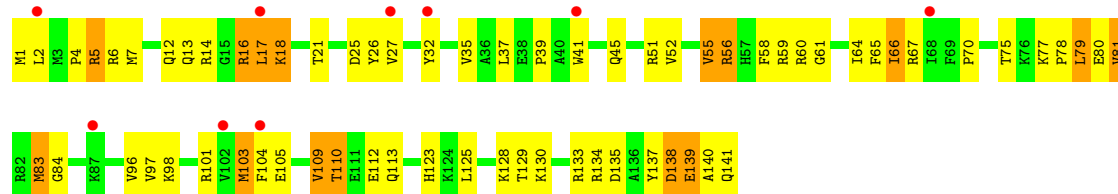
• Molecule 37: 50S ribosomal protein L15

Chain 35: 14% 43% 37% 17%



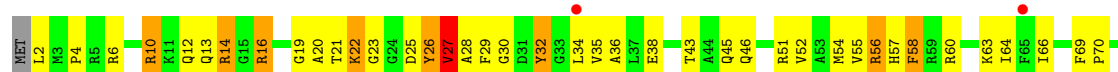
• Molecule 38: 50S ribosomal protein L16

Chain 88: 6% 52% 37% 11%



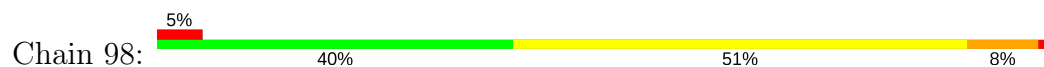
• Molecule 38: 50S ribosomal protein L16

Chain 45: 2% 41% 43% 13%





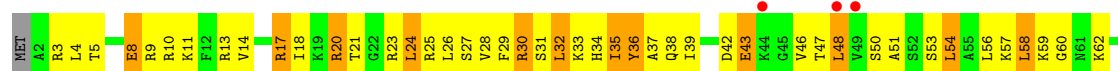
• Molecule 39: 50S ribosomal protein L17



• Molecule 39: 50S ribosomal protein L17



• Molecule 40: 50S ribosomal protein L18

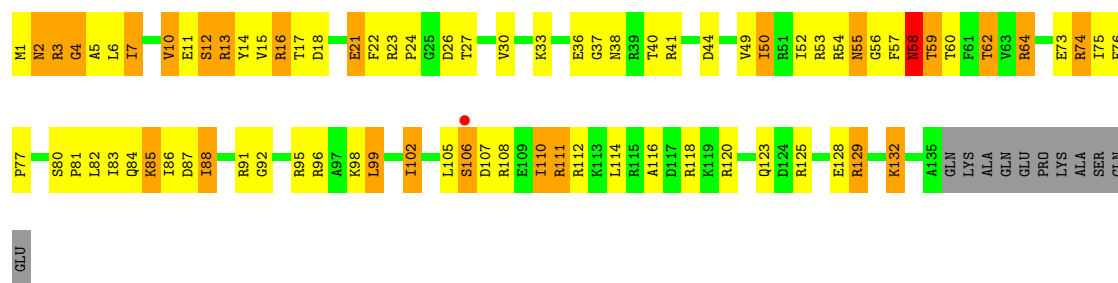


• Molecule 40: 50S ribosomal protein L18

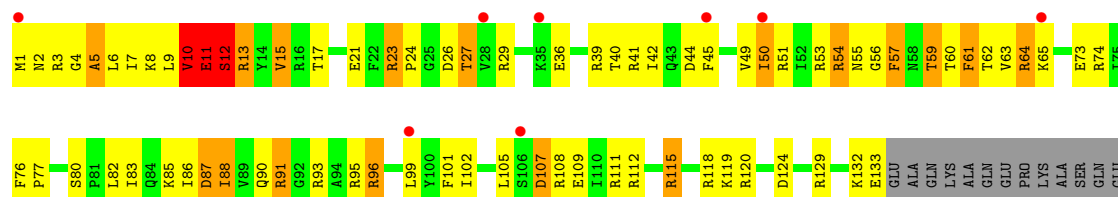


• Molecule 41: 50S ribosomal protein L19

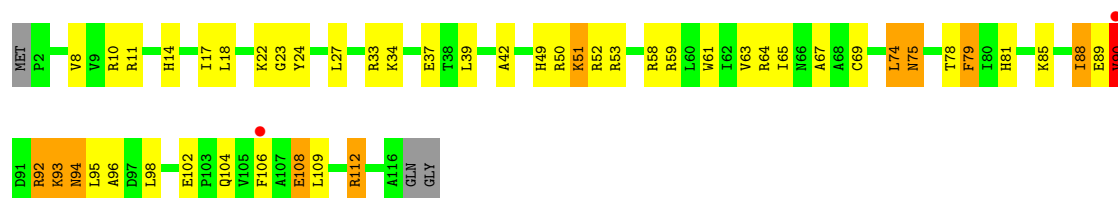




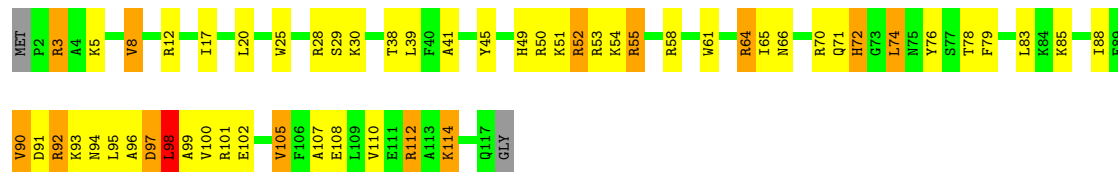
• Molecule 41: 50S ribosomal protein L19



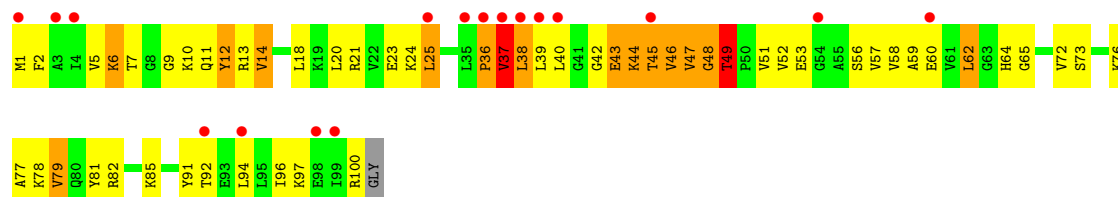
• Molecule 42: 50S ribosomal protein L20



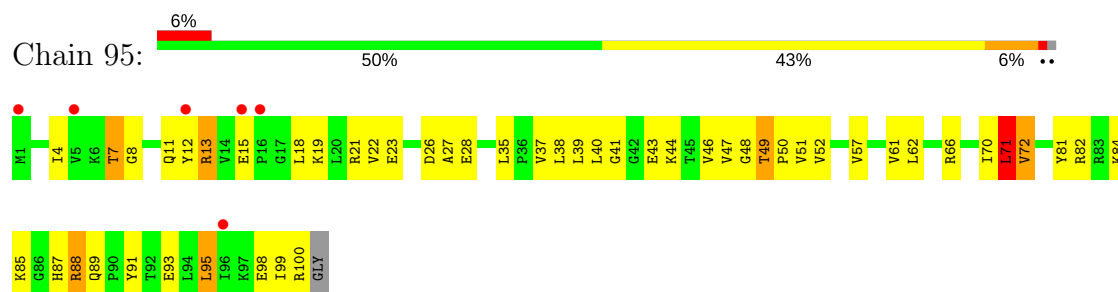
• Molecule 42: 50S ribosomal protein L20



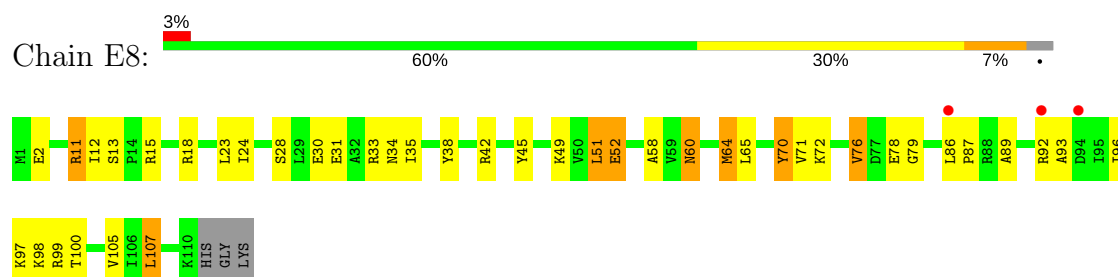
• Molecule 43: 50S ribosomal protein L21



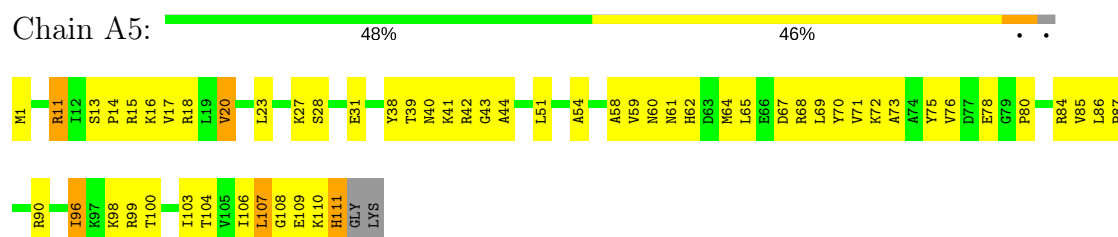
- Molecule 43: 50S ribosomal protein L21



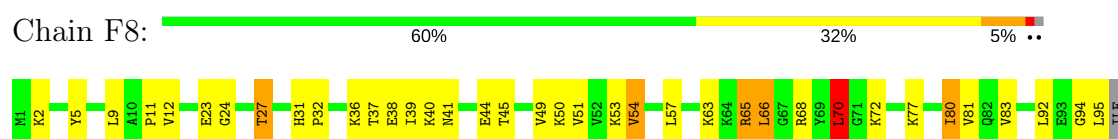
- Molecule 44: 50S ribosomal protein L22



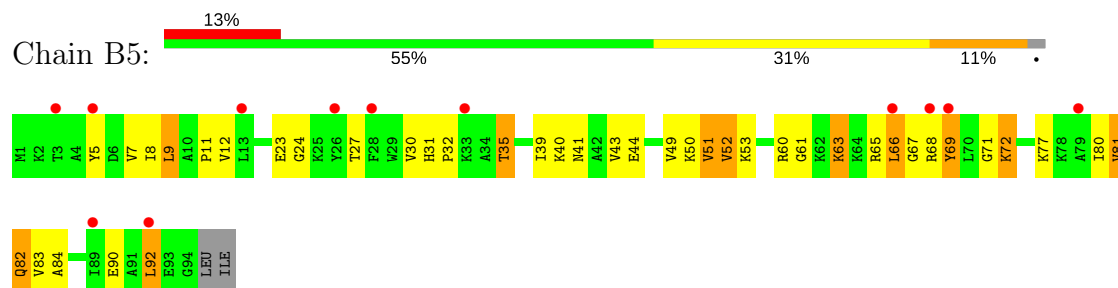
- Molecule 44: 50S ribosomal protein L22



- Molecule 45: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L23

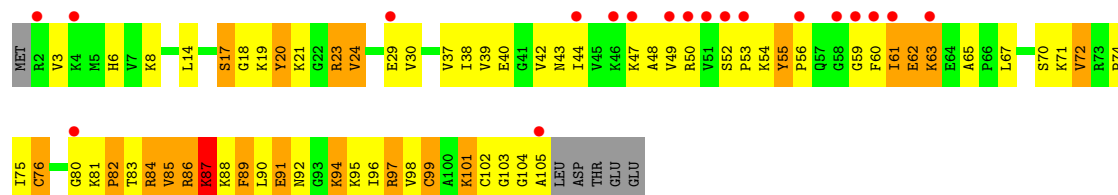


- Molecule 46: 50S ribosomal protein L24

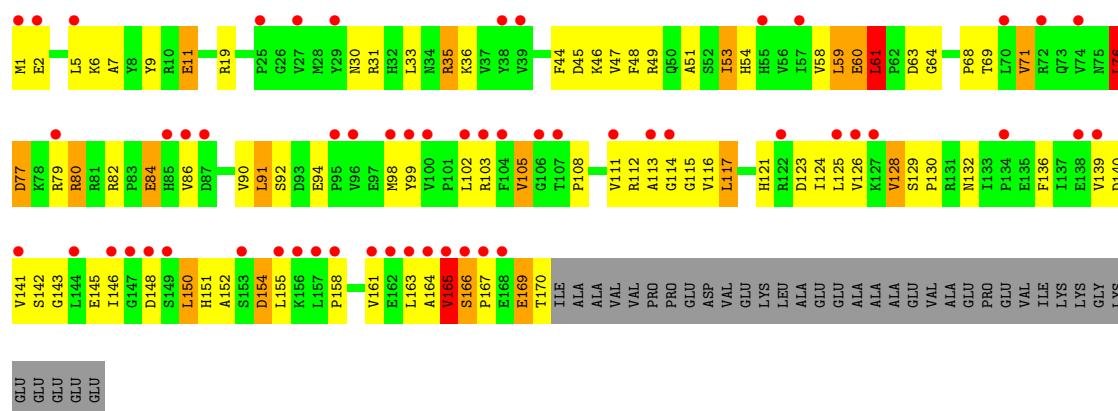




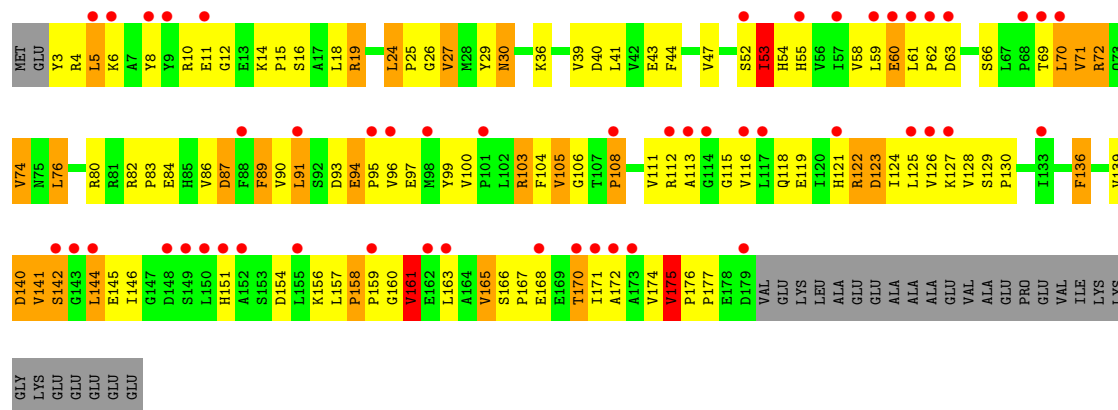
• Molecule 46: 50S ribosomal protein L24



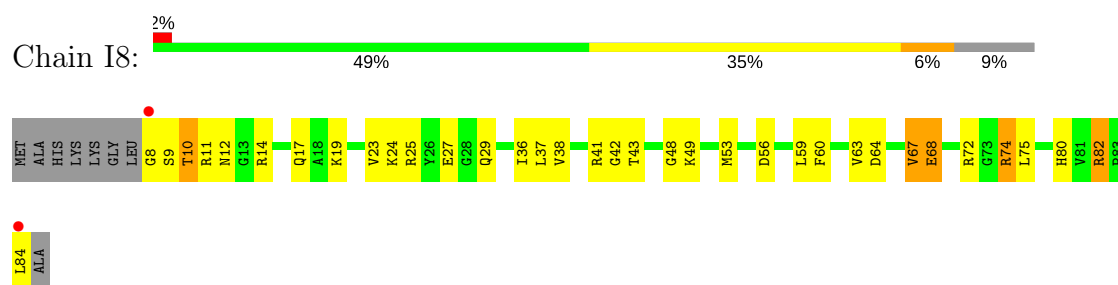
• Molecule 47: 50S ribosomal protein L25



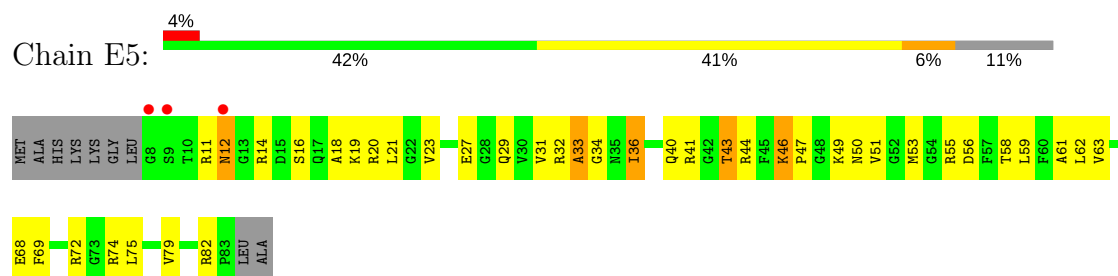
• Molecule 47: 50S ribosomal protein L25



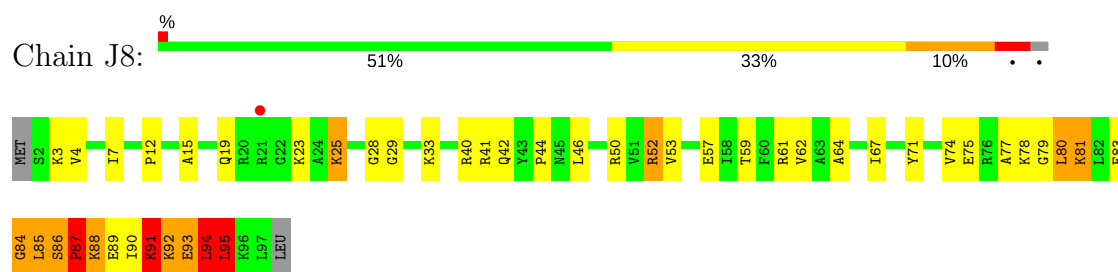
• Molecule 48: 50S ribosomal protein L27



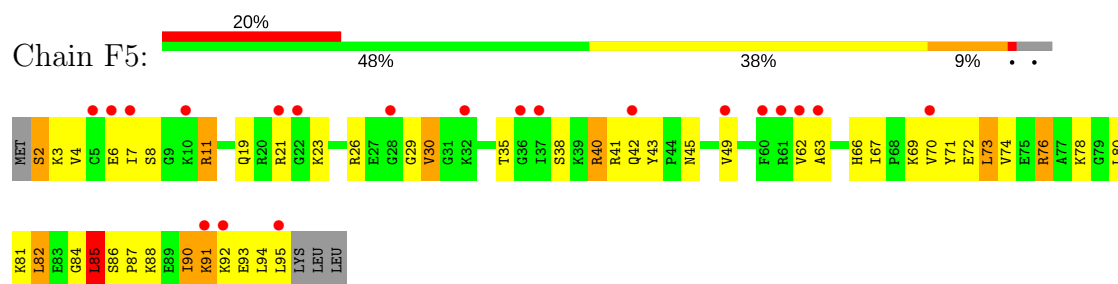
- Molecule 48: 50S ribosomal protein L27



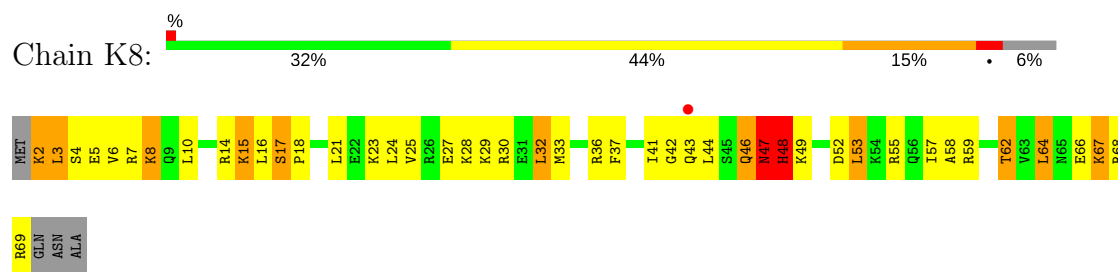
- Molecule 49: 50S ribosomal protein L28



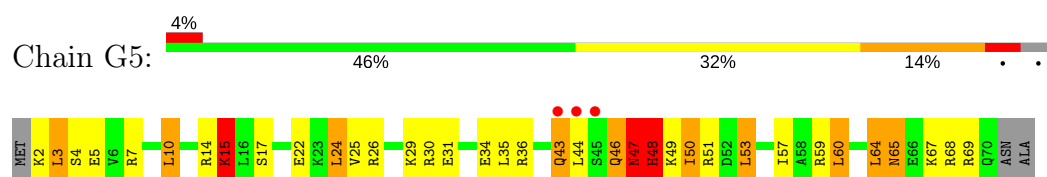
- Molecule 49: 50S ribosomal protein L28



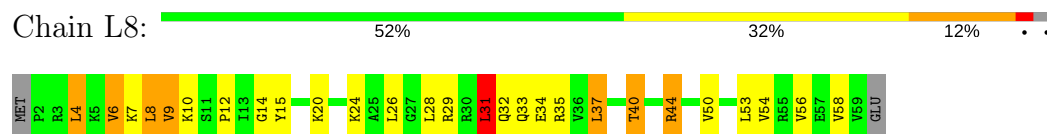
- Molecule 50: 50S ribosomal protein L29



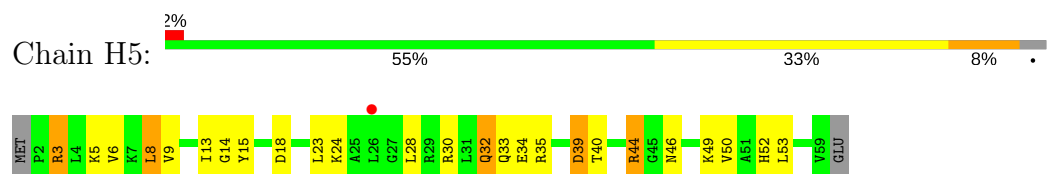
- Molecule 50: 50S ribosomal protein L29



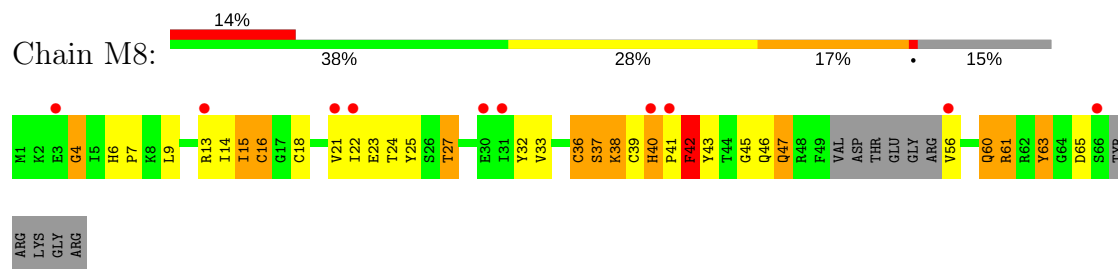
- Molecule 51: 50S ribosomal protein L30



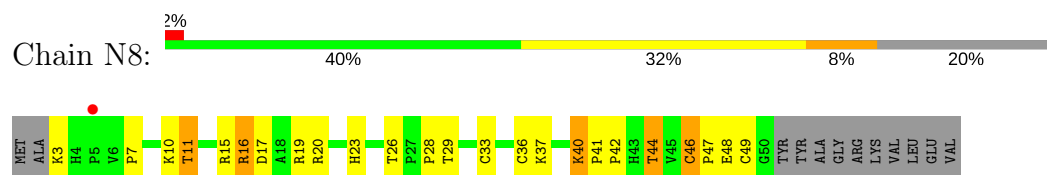
- Molecule 51: 50S ribosomal protein L30



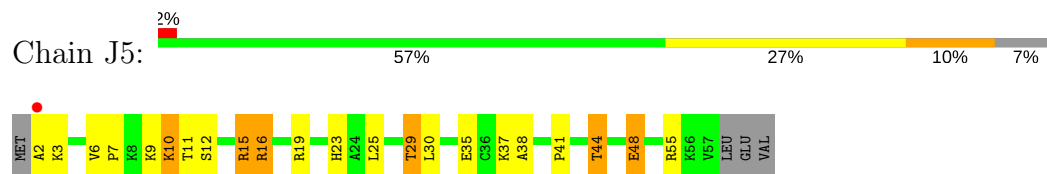
- Molecule 52: 50S ribosomal protein L31



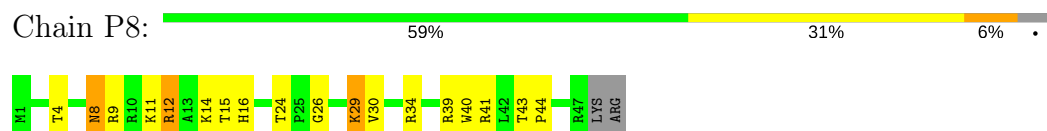
- Molecule 53: 50S ribosomal protein L32



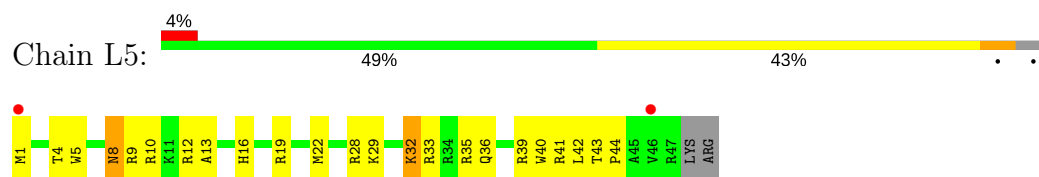
- Molecule 53: 50S ribosomal protein L32



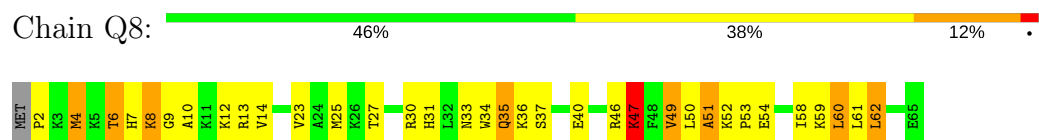
- Molecule 54: 50S ribosomal protein L34



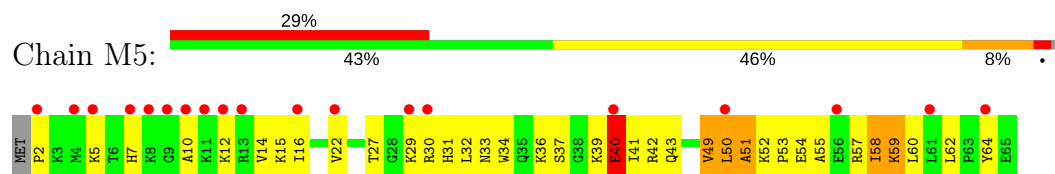
- Molecule 54: 50S ribosomal protein L34



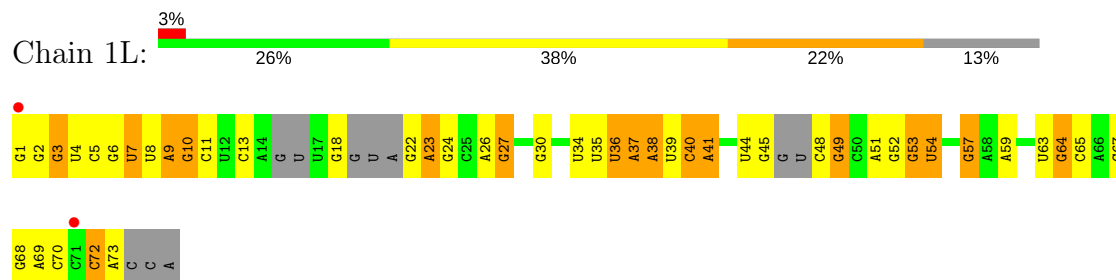
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNA^{Lys}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.15Å 448.16Å 617.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.45 – 3.13 161.54 – 3.13	Depositor EDS
% Data completeness (in resolution range)	100.0 (154.45-3.13) 90.9 (161.54-3.13)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.244 0.193 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (0.22%)	DCC
Wilson B-factor (Å ²)	90.4	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	296999	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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, U8U, H2U, 7MG, SF4, MG, 4SU, T6A, 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	3/36095 (0.0%)	1.26	206/56332 (0.4%)
1	1G	0.60	2/36309 (0.0%)	1.18	153/56668 (0.3%)
2	12	0.38	0/1727	0.64	2/2326 (0.1%)
2	1E	0.40	0/1908	0.62	2/2573 (0.1%)
3	22	0.47	1/1560 (0.1%)	0.58	0/2104
3	2E	0.44	1/1629 (0.1%)	0.60	1/2195 (0.0%)
4	32	0.41	0/1732	0.60	0/2318
4	3E	0.49	1/1728 (0.1%)	0.64	3/2313 (0.1%)
5	42	0.40	0/1156	0.62	0/1557
5	4E	0.40	0/1158	0.61	0/1559
6	52	0.45	0/855	0.61	1/1154 (0.1%)
6	5E	0.47	0/850	0.61	0/1147
7	62	0.39	0/1122	0.56	0/1500
7	6E	0.40	0/1259	0.51	0/1686
8	72	0.38	0/1127	0.59	0/1517
8	7E	0.40	0/1135	0.61	0/1527
9	82	0.36	0/971	0.62	0/1304
9	8E	0.38	0/1019	0.61	0/1367
10	1A	0.93	2/658 (0.3%)	0.57	0/885
10	1I	0.37	0/762	0.61	0/1027
11	2A	0.40	0/850	0.60	0/1150
11	2I	0.43	0/838	0.62	0/1133
12	3A	0.48	0/963	0.69	1/1290 (0.1%)
12	3I	0.57	0/972	0.76	0/1301
13	4A	0.34	0/889	0.58	0/1192
13	4I	0.46	0/943	0.65	0/1265
14	5A	0.40	0/495	0.66	0/657
14	5I	0.49	0/495	0.74	1/657 (0.2%)
15	6A	0.39	0/740	0.56	0/987
15	6I	0.44	0/740	0.61	0/987
16	7A	0.41	0/721	0.63	0/970
16	7I	0.40	0/716	0.67	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.45	0/836	0.59	0/1117
17	8I	0.48	0/847	0.66	0/1131
18	9A	0.44	0/549	0.64	0/732
18	9I	0.42	0/554	0.63	0/739
19	AA	0.38	0/520	0.71	0/700
19	AI	0.40	0/676	0.72	1/910 (0.1%)
20	BA	0.37	0/764	0.66	1/1007 (0.1%)
20	BI	0.36	0/748	0.60	1/986 (0.1%)
21	1B	0.37	0/192	0.58	0/252
21	1F	0.43	0/203	0.62	0/266
22	1K	0.57	0/1568	1.21	10/2434 (0.4%)
23	2K	0.73	0/1721	1.30	11/2682 (0.4%)
23	2L	0.67	1/1721 (0.1%)	1.17	4/2682 (0.1%)
24	3K	0.49	0/1654	1.14	11/2570 (0.4%)
24	3L	0.53	0/1705	1.15	12/2650 (0.5%)
25	4K	0.79	0/499	1.32	5/778 (0.6%)
25	4L	0.67	0/473	1.32	3/737 (0.4%)
26	14	0.84	35/68159 (0.1%)	1.43	876/106398 (0.8%)
26	1H	0.99	95/68309 (0.1%)	1.56	1280/106631 (1.2%)
27	16	0.74	0/2928	1.41	33/4568 (0.7%)
27	1J	0.65	0/2928	1.31	16/4568 (0.4%)
28	71	0.30	0/1049	0.54	0/1417
29	11	0.64	1/2170 (0.0%)	0.85	2/2926 (0.1%)
29	19	0.62	1/2175 (0.0%)	0.79	2/2933 (0.1%)
30	21	0.57	0/1579	0.90	5/2131 (0.2%)
30	29	0.56	0/1596	0.82	2/2153 (0.1%)
31	31	0.62	0/1620	0.84	1/2194 (0.0%)
31	39	0.53	1/1637 (0.1%)	0.80	1/2218 (0.0%)
32	41	0.43	0/1481	0.67	0/1994
32	49	0.45	1/1483 (0.1%)	0.62	1/1997 (0.1%)
33	51	0.52	0/1354	0.85	2/1833 (0.1%)
33	59	0.38	0/1320	0.68	2/1787 (0.1%)
34	61	0.43	0/1146	0.71	2/1551 (0.1%)
34	69	0.48	1/1146 (0.1%)	0.68	1/1551 (0.1%)
35	15	0.42	0/1123	0.64	0/1515
35	58	0.51	0/1123	0.76	1/1514 (0.1%)
36	25	0.52	0/942	0.72	1/1269 (0.1%)
36	68	0.57	0/942	0.73	0/1269
37	35	0.52	0/1139	0.78	1/1514 (0.1%)
37	78	0.62	1/1139 (0.1%)	0.96	4/1514 (0.3%)
38	45	0.55	0/1120	0.82	0/1498
38	88	0.61	0/1138	0.90	1/1523 (0.1%)
39	55	0.50	0/981	0.77	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	98	0.48	0/981	0.79	1/1312 (0.1%)
40	65	0.46	0/886	0.75	1/1180 (0.1%)
40	A8	0.53	0/891	0.78	1/1187 (0.1%)
41	75	0.51	0/1123	0.76	1/1500 (0.1%)
41	B8	0.55	0/1133	0.76	1/1514 (0.1%)
42	85	0.46	0/977	0.67	1/1301 (0.1%)
42	C8	0.59	0/968	0.76	1/1289 (0.1%)
43	95	0.46	0/781	0.79	1/1048 (0.1%)
43	D8	0.58	0/785	0.75	1/1052 (0.1%)
44	A5	0.53	0/897	0.69	0/1204
44	E8	0.56	0/886	0.75	0/1189
45	B5	0.56	0/749	0.73	0/1007
45	F8	0.62	0/764	0.80	1/1025 (0.1%)
46	C5	0.64	0/807	0.86	1/1076 (0.1%)
46	G8	0.65	0/796	0.94	2/1062 (0.2%)
47	D5	0.72	1/1443 (0.1%)	0.65	0/1960
47	H8	0.43	0/1395	0.73	2/1890 (0.1%)
48	E5	0.49	0/611	0.73	0/814
48	I8	0.62	0/619	0.81	0/825
49	F5	0.52	0/744	0.84	1/989 (0.1%)
49	J8	0.66	0/754	0.95	3/1003 (0.3%)
50	G5	0.51	0/578	0.70	0/766
50	K8	0.61	0/577	0.93	1/763 (0.1%)
51	H5	0.48	0/464	0.64	0/623
51	L8	0.48	0/464	0.77	1/623 (0.2%)
52	M8	0.45	0/485	0.78	0/652
53	J5	0.49	0/448	0.74	0/606
53	N8	0.59	0/381	0.77	0/516
54	L5	0.52	0/409	0.76	0/540
54	P8	0.67	0/409	0.88	1/540 (0.2%)
55	M5	0.65	0/524	0.85	0/691
55	Q8	0.60	0/524	0.90	1/691 (0.1%)
56	1L	0.47	1/1516 (0.1%)	0.95	1/2350 (0.0%)
All	All	0.74	149/316848 (0.0%)	1.26	2688/474550 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	5
4	3E	0	1
8	72	0	1
9	82	0	2
9	8E	0	2
10	1A	0	1
11	2A	0	1
12	3A	0	1
12	3I	0	3
13	4I	0	3
14	5A	0	1
16	7I	0	1
19	AA	0	1
19	AI	0	1
20	BA	0	3
20	BI	0	1
29	11	0	4
29	19	0	2
30	21	0	7
30	29	0	5
31	39	0	8
32	49	0	2
33	51	0	6
33	59	0	4
34	61	0	3
34	69	0	4
35	15	0	1
35	58	0	1
37	35	0	1
37	78	0	6
38	45	0	2
38	88	0	1
39	98	0	2
40	65	0	2
40	A8	0	1
41	75	0	3
41	B8	0	3
42	85	0	4
42	C8	0	3
43	D8	0	3
44	A5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	B5	0	2
46	C5	0	3
46	G8	0	3
47	D5	0	4
47	H8	0	5
49	F5	0	1
49	J8	0	3
50	G5	0	3
50	K8	0	3
52	M8	0	4
55	M5	0	4
55	Q8	0	2
All	All	0	151

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	D5	94	GLU	C-N	23.32	1.78	1.34
10	1A	38	ILE	C-N	19.43	1.71	1.34
26	1H	2430	A	N9-C4	-14.21	1.29	1.37
26	1H	774	A	N9-C4	-13.66	1.29	1.37
3	22	173	VAL	C-N	12.84	1.58	1.34

The worst 5 of 2688 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-18.59	114.85	126.00
26	1H	1332	G	C5-N7-C8	-17.78	95.41	104.30
26	1H	1332	G	C2-N3-C4	-17.15	103.32	111.90
26	1H	676	A	C2-N3-C4	-16.45	102.38	110.60
26	1H	783	A	C2-N3-C4	-16.44	102.38	110.60

There are no chirality outliers.

5 of 151 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	234	PRO	Peptide
2	1E	236	TYR	Peptide
2	1E	9	GLU	Peptide
4	3E	29	PRO	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	32246	0	16276	858	0
1	1G	32437	0	16372	887	2
2	12	1696	0	1730	94	0
2	1E	1874	0	1926	99	0
3	22	1537	0	1603	87	0
3	2E	1605	0	1668	60	0
4	32	1702	0	1765	98	0
4	3E	1698	0	1761	84	0
5	42	1141	0	1198	41	0
5	4E	1142	0	1204	54	0
6	52	842	0	857	34	0
6	5E	837	0	852	34	0
7	62	1110	0	1163	66	0
7	6E	1242	0	1286	54	0
8	72	1107	0	1165	49	0
8	7E	1115	0	1177	69	0
9	82	953	0	983	75	0
9	8E	1000	0	1031	61	0
10	1A	646	0	662	41	0
10	1I	749	0	767	45	0
11	2A	835	0	847	27	0
11	2I	823	0	832	41	0
12	3A	947	0	1033	37	0
12	3I	956	0	1046	33	0
13	4A	879	0	935	67	0
13	4I	933	0	992	51	0
14	5A	486	0	525	34	0
14	5I	486	0	524	28	0
15	6A	729	0	768	27	0
15	6I	729	0	768	31	0
16	7A	705	0	725	29	0
16	7I	700	0	720	49	0
17	8A	823	0	891	32	0
17	8I	834	0	904	62	0
18	9A	544	0	605	23	0
18	9I	549	0	607	23	0
19	AA	510	0	507	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	661	0	683	38	0
20	BA	762	0	861	40	0
20	BI	746	0	843	45	0
21	1B	188	0	195	11	0
21	1F	199	0	208	12	0
22	1K	1542	0	790	43	0
23	2K	1646	0	843	36	0
23	2L	1646	0	845	32	0
24	3K	1483	0	756	67	0
24	3L	1528	0	778	48	0
25	4K	442	0	219	9	0
25	4L	419	0	208	23	0
26	14	60857	0	30679	1311	1
26	1H	60991	0	30744	1358	1
27	16	2617	0	1328	56	0
27	1J	2617	0	1328	84	0
28	71	1027	0	1043	66	0
29	11	2120	0	2197	121	0
29	19	2125	0	2199	108	0
30	21	1546	0	1602	94	0
30	29	1563	0	1629	110	0
31	31	1585	0	1632	87	0
31	39	1602	0	1649	97	0
32	41	1457	0	1514	76	0
32	49	1459	0	1507	73	0
33	51	1328	0	1396	77	0
33	59	1295	0	1366	74	0
34	61	1131	0	1218	44	0
34	69	1131	0	1218	58	0
35	15	1096	0	1168	56	0
35	58	1096	0	1169	67	0
36	25	932	0	996	48	0
36	68	932	0	996	38	0
37	35	1122	0	1206	75	0
37	78	1122	0	1206	99	0
38	45	1099	0	1154	74	0
38	88	1117	0	1168	55	0
39	55	967	0	1033	47	0
39	98	967	0	1033	51	0
40	65	876	0	938	55	0
40	A8	881	0	943	55	0
41	75	1109	0	1170	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	B8	1119	0	1177	71	0
42	85	959	0	1019	64	0
42	C8	950	0	1011	55	0
43	95	770	0	838	41	0
43	D8	774	0	849	42	0
44	A5	886	0	948	35	0
44	E8	876	0	941	27	0
45	B5	735	0	785	32	0
45	F8	750	0	814	33	0
46	C5	794	0	885	61	0
46	G8	783	0	869	48	0
47	D5	1411	0	1436	83	0
47	H8	1365	0	1391	60	0
48	E5	603	0	620	40	0
48	I8	611	0	631	32	0
49	F5	737	0	813	43	0
49	J8	747	0	817	35	0
50	G5	576	0	625	33	0
50	K8	575	0	634	45	0
51	H5	459	0	512	15	0
51	L8	459	0	512	22	0
52	M8	475	0	465	34	0
53	J5	434	0	454	23	0
53	N8	369	0	388	21	0
54	L5	401	0	436	21	0
54	P8	401	0	436	13	0
55	M5	516	0	582	28	0
55	Q8	516	0	582	34	0
56	1L	1402	0	715	32	0
57	13	141	0	0	0	0
57	14	460	0	0	0	0
57	16	12	0	0	0	0
57	19	1	0	0	0	0
57	1G	125	0	0	0	0
57	1H	552	0	0	0	0
57	1J	10	0	0	0	0
57	21	3	0	0	0	0
57	25	1	0	0	0	0
57	29	1	0	0	0	0
57	2I	1	0	0	0	0
57	2K	3	0	0	0	0
57	2L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	31	1	0	0	0	0
57	32	1	0	0	0	0
57	35	2	0	0	0	0
57	39	1	0	0	0	0
57	3I	1	0	0	0	0
57	41	1	0	0	0	0
57	42	2	0	0	0	0
57	45	1	0	0	0	0
57	4L	1	0	0	0	0
57	52	1	0	0	0	0
57	7A	1	0	0	0	0
57	88	3	0	0	0	0
57	B5	1	0	0	0	0
57	E5	2	0	0	0	0
57	F8	1	0	0	0	0
57	I8	2	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	32	8	0	0	2	0
58	3E	8	0	0	0	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	C5	1	0	0	0	0
59	G8	1	0	0	0	0
60	14	13	0	24	0	0
60	1G	13	0	22	3	0
61	11	10	0	0	6	0
61	13	354	0	0	20	0
61	14	1303	0	0	91	0
61	15	3	0	0	0	0
61	16	12	0	0	1	0
61	19	14	0	0	1	0
61	1A	2	0	0	0	0
61	1G	364	0	0	24	0
61	1H	1720	0	0	128	0
61	1I	2	0	0	0	0
61	1J	27	0	0	1	0
61	1K	1	0	0	0	0
61	21	6	0	0	1	0
61	25	8	0	0	0	0
61	29	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2A	1	0	0	0	0
61	2K	8	0	0	0	0
61	2L	8	0	0	0	0
61	31	6	0	0	0	0
61	32	4	0	0	1	0
61	35	8	0	0	0	0
61	39	8	0	0	0	0
61	3E	2	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	4A	2	0	0	0	0
61	4E	3	0	0	2	0
61	4K	5	0	0	0	0
61	4L	3	0	0	0	0
61	52	4	0	0	0	0
61	55	1	0	0	0	0
61	58	2	0	0	0	0
61	5I	1	0	0	0	0
61	68	2	0	0	0	0
61	6A	3	0	0	0	0
61	75	1	0	0	0	0
61	78	13	0	0	4	0
61	7A	4	0	0	0	0
61	7I	2	0	0	0	0
61	85	1	0	0	0	0
61	8E	2	0	0	0	0
61	98	1	0	0	2	0
61	9A	2	0	0	0	0
61	B5	1	0	0	0	0
61	B8	1	0	0	0	0
61	BA	3	0	0	0	0
61	BI	3	0	0	1	0
61	C5	3	0	0	0	0
61	C8	4	0	0	0	0
61	E8	1	0	0	0	0
61	F5	1	0	0	0	0
61	F8	3	0	0	1	0
61	G8	3	0	0	0	0
61	H5	1	0	0	2	0
61	I8	6	0	0	0	0
61	J8	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	L5	1	0	0	0	0
61	L8	4	0	0	0	0
61	M5	8	0	0	2	0
61	N8	1	0	0	0	0
61	Q8	5	0	0	1	0
All	All	296999	0	196564	8532	2

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

The worst 5 of 8532 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1A:38:ILE:C	10:1A:39:PRO:N	1.71	1.39
47:D5:94:GLU:C	47:D5:95:PRO:N	1.78	1.36
38:45:27:VAL:HB	38:45:28:ALA:HA	1.16	1.08
26:1H:1604:C:OP2	61:1H:3655:HOH:O	1.75	1.04
8:72:12:ARG:HH21	8:72:27:PRO:HD3	1.22	1.02

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	2.14	0.06
26:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	12	203/256 (79%)	173 (85%)	23 (11%)	7 (3%)	4 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1E	227/256 (89%)	186 (82%)	39 (17%)	2 (1%)	20	59
3	22	191/239 (80%)	172 (90%)	19 (10%)	0	100	100
3	2E	203/239 (85%)	186 (92%)	16 (8%)	1 (0%)	32	71
4	32	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	32	71
4	3E	205/209 (98%)	193 (94%)	11 (5%)	1 (0%)	32	71
5	42	148/162 (91%)	142 (96%)	5 (3%)	1 (1%)	25	64
5	4E	147/162 (91%)	136 (92%)	10 (7%)	1 (1%)	25	64
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	134/156 (86%)	125 (93%)	8 (6%)	1 (1%)	25	64
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	12	45
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	25	64
9	82	119/128 (93%)	109 (92%)	9 (8%)	1 (1%)	22	62
9	8E	124/128 (97%)	107 (86%)	17 (14%)	0	100	100
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	92/105 (88%)	83 (90%)	9 (10%)	0	100	100
11	2A	111/129 (86%)	99 (89%)	10 (9%)	2 (2%)	10	40
11	2I	109/129 (84%)	93 (85%)	11 (10%)	5 (5%)	3	16
12	3A	119/132 (90%)	101 (85%)	14 (12%)	4 (3%)	4	23
12	3I	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	22	62
13	4A	107/126 (85%)	89 (83%)	17 (16%)	1 (1%)	20	59
13	4I	115/126 (91%)	97 (84%)	17 (15%)	1 (1%)	20	59
14	5A	57/61 (93%)	49 (86%)	7 (12%)	1 (2%)	10	40
14	5I	57/61 (93%)	48 (84%)	7 (12%)	2 (4%)	4	23
15	6A	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
15	6I	85/89 (96%)	79 (93%)	6 (7%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	81/88 (92%)	76 (94%)	5 (6%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	93 (95%)	4 (4%)	1 (1%)	18	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	65/88 (74%)	64 (98%)	1 (2%)	0	100	100
18	9I	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	12	45
19	AA	59/93 (63%)	49 (83%)	7 (12%)	3 (5%)	2	14
19	AI	80/93 (86%)	69 (86%)	7 (9%)	4 (5%)	2	15
20	BA	97/106 (92%)	79 (81%)	16 (16%)	2 (2%)	8	35
20	BI	95/106 (90%)	83 (87%)	12 (13%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	7I	128/229 (56%)	121 (94%)	7 (6%)	0	100	100
29	11	271/276 (98%)	255 (94%)	10 (4%)	6 (2%)	8	34
29	19	272/276 (99%)	248 (91%)	21 (8%)	3 (1%)	17	54
30	21	201/206 (98%)	160 (80%)	28 (14%)	13 (6%)	1	9
30	29	202/206 (98%)	150 (74%)	40 (20%)	12 (6%)	2	11
31	31	200/210 (95%)	177 (88%)	22 (11%)	1 (0%)	32	71
31	39	202/210 (96%)	159 (79%)	36 (18%)	7 (4%)	4	23
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	11	42
32	49	178/182 (98%)	155 (87%)	22 (12%)	1 (1%)	28	68
33	51	172/180 (96%)	139 (81%)	23 (13%)	10 (6%)	2	11
33	59	167/180 (93%)	129 (77%)	32 (19%)	6 (4%)	4	22
34	61	143/148 (97%)	123 (86%)	18 (13%)	2 (1%)	13	47
34	69	143/148 (97%)	112 (78%)	28 (20%)	3 (2%)	8	35
35	15	135/140 (96%)	124 (92%)	11 (8%)	0	100	100
35	58	135/140 (96%)	114 (84%)	16 (12%)	5 (4%)	4	22
36	25	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
36	68	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
37	35	145/150 (97%)	120 (83%)	25 (17%)	0	100	100
37	78	145/150 (97%)	113 (78%)	21 (14%)	11 (8%)	1	6
38	45	136/141 (96%)	110 (81%)	23 (17%)	3 (2%)	8	34
38	88	139/141 (99%)	119 (86%)	14 (10%)	6 (4%)	3	17
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	20	59
39	98	116/118 (98%)	101 (87%)	15 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	65	108/112 (96%)	87 (81%)	19 (18%)	2 (2%)	9	38
40	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	20	59
41	75	131/146 (90%)	118 (90%)	11 (8%)	2 (2%)	12	45
41	B8	133/146 (91%)	118 (89%)	14 (10%)	1 (1%)	22	62
42	85	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
42	C8	113/118 (96%)	107 (95%)	2 (2%)	4 (4%)	4	23
43	95	98/101 (97%)	81 (83%)	14 (14%)	3 (3%)	5	26
43	D8	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	5	26
44	A5	109/113 (96%)	101 (93%)	8 (7%)	0	100	100
44	E8	108/113 (96%)	102 (94%)	6 (6%)	0	100	100
45	B5	92/96 (96%)	82 (89%)	8 (9%)	2 (2%)	8	34
45	F8	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
46	C5	102/110 (93%)	74 (72%)	22 (22%)	6 (6%)	2	11
46	G8	101/110 (92%)	83 (82%)	14 (14%)	4 (4%)	3	19
47	D5	175/206 (85%)	133 (76%)	32 (18%)	10 (6%)	2	12
47	H8	168/206 (82%)	136 (81%)	25 (15%)	7 (4%)	3	18
48	E5	74/85 (87%)	65 (88%)	8 (11%)	1 (1%)	13	47
48	I8	75/85 (88%)	67 (89%)	8 (11%)	0	100	100
49	F5	92/98 (94%)	81 (88%)	10 (11%)	1 (1%)	17	54
49	J8	94/98 (96%)	80 (85%)	9 (10%)	5 (5%)	2	13
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	5	26
50	K8	66/72 (92%)	59 (89%)	4 (6%)	3 (4%)	3	16
51	H5	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	M8	56/71 (79%)	39 (70%)	17 (30%)	0	100	100
53	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	4 (9%)	0	100	100
55	M5	62/65 (95%)	51 (82%)	11 (18%)	0	100	100
55	Q8	62/65 (95%)	51 (82%)	7 (11%)	4 (6%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11086/12104 (92%)	9718 (88%)	1167 (10%)	201 (2%)	10	40

5 of 201 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	2I	55	LYS
12	3I	48	PRO
18	9I	22	VAL
19	AI	41	VAL
29	11	239	ARG

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%)	144 (80%)	35 (20%)	1	7
2	1E	200/220 (91%)	158 (79%)	42 (21%)	1	6
3	22	154/188 (82%)	123 (80%)	31 (20%)	1	6
3	2E	159/188 (85%)	127 (80%)	32 (20%)	1	6
4	32	180/181 (99%)	152 (84%)	28 (16%)	3	13
4	3E	180/181 (99%)	146 (81%)	34 (19%)	2	8
5	42	114/123 (93%)	88 (77%)	26 (23%)	1	4
5	4E	115/123 (94%)	90 (78%)	25 (22%)	1	5
6	52	90/90 (100%)	78 (87%)	12 (13%)	4	19
6	5E	90/90 (100%)	73 (81%)	17 (19%)	2	8
7	62	114/127 (90%)	91 (80%)	23 (20%)	1	6
7	6E	125/127 (98%)	105 (84%)	20 (16%)	3	12
8	72	118/119 (99%)	101 (86%)	17 (14%)	4	16
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1	5
9	82	92/99 (93%)	73 (79%)	19 (21%)	1	6
9	8E	97/99 (98%)	70 (72%)	27 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1A	71/92 (77%)	54 (76%)	17 (24%)	1	3
10	1I	81/92 (88%)	75 (93%)	6 (7%)	16	48
11	2A	85/99 (86%)	71 (84%)	14 (16%)	2	11
11	2I	84/99 (85%)	66 (79%)	18 (21%)	1	5
12	3A	102/109 (94%)	82 (80%)	20 (20%)	1	7
12	3I	103/109 (94%)	76 (74%)	27 (26%)	0	2
13	4A	90/101 (89%)	68 (76%)	22 (24%)	1	3
13	4I	94/101 (93%)	67 (71%)	27 (29%)	0	1
14	5A	49/50 (98%)	40 (82%)	9 (18%)	2	9
14	5I	49/50 (98%)	39 (80%)	10 (20%)	1	6
15	6A	79/80 (99%)	71 (90%)	8 (10%)	9	31
15	6I	79/80 (99%)	68 (86%)	11 (14%)	4	18
16	7A	72/74 (97%)	64 (89%)	8 (11%)	7	28
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	7
17	8A	94/97 (97%)	80 (85%)	14 (15%)	3	15
17	8I	95/97 (98%)	80 (84%)	15 (16%)	3	12
18	9A	58/77 (75%)	49 (84%)	9 (16%)	3	13
18	9I	58/77 (75%)	50 (86%)	8 (14%)	4	18
19	AA	56/80 (70%)	43 (77%)	13 (23%)	1	4
19	AI	72/80 (90%)	57 (79%)	15 (21%)	1	6
20	BA	76/82 (93%)	68 (90%)	8 (10%)	8	30
20	BI	75/82 (92%)	67 (89%)	8 (11%)	8	29
21	1B	17/22 (77%)	16 (94%)	1 (6%)	23	57
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	4
28	7I	108/181 (60%)	87 (81%)	21 (19%)	1	7
29	11	214/218 (98%)	172 (80%)	42 (20%)	1	7
29	19	214/218 (98%)	167 (78%)	47 (22%)	1	5
30	21	162/166 (98%)	124 (76%)	38 (24%)	1	3
30	29	165/166 (99%)	125 (76%)	40 (24%)	1	3
31	31	161/166 (97%)	130 (81%)	31 (19%)	1	7
31	39	163/166 (98%)	123 (76%)	40 (24%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	41	153/156 (98%)	120 (78%)	33 (22%)	1	5
32	49	152/156 (97%)	117 (77%)	35 (23%)	1	4
33	51	143/148 (97%)	109 (76%)	34 (24%)	1	3
33	59	140/148 (95%)	101 (72%)	39 (28%)	0	1
34	61	122/124 (98%)	87 (71%)	35 (29%)	0	1
34	69	122/124 (98%)	88 (72%)	34 (28%)	0	1
35	15	116/119 (98%)	91 (78%)	25 (22%)	1	5
35	58	116/119 (98%)	92 (79%)	24 (21%)	1	6
36	25	100/100 (100%)	82 (82%)	18 (18%)	2	9
36	68	100/100 (100%)	89 (89%)	11 (11%)	7	28
37	35	114/116 (98%)	76 (67%)	38 (33%)	0	0
37	78	114/116 (98%)	77 (68%)	37 (32%)	0	0
38	45	109/111 (98%)	82 (75%)	27 (25%)	1	2
38	88	110/111 (99%)	91 (83%)	19 (17%)	2	10
39	55	101/101 (100%)	86 (85%)	15 (15%)	3	15
39	98	101/101 (100%)	79 (78%)	22 (22%)	1	5
40	65	87/88 (99%)	67 (77%)	20 (23%)	1	4
40	A8	87/88 (99%)	61 (70%)	26 (30%)	0	1
41	75	117/127 (92%)	85 (73%)	32 (27%)	0	1
41	B8	117/127 (92%)	84 (72%)	33 (28%)	0	1
42	85	93/94 (99%)	77 (83%)	16 (17%)	2	10
42	C8	92/94 (98%)	80 (87%)	12 (13%)	5	20
43	95	81/82 (99%)	66 (82%)	15 (18%)	2	8
43	D8	82/82 (100%)	54 (66%)	28 (34%)	0	0
44	A5	91/92 (99%)	72 (79%)	19 (21%)	1	6
44	E8	90/92 (98%)	76 (84%)	14 (16%)	3	13
45	B5	74/78 (95%)	58 (78%)	16 (22%)	1	5
45	F8	77/78 (99%)	67 (87%)	10 (13%)	5	20
46	C5	85/91 (93%)	61 (72%)	24 (28%)	0	1
46	G8	84/91 (92%)	67 (80%)	17 (20%)	1	6
47	D5	156/179 (87%)	118 (76%)	38 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	H8	151/179 (84%)	128 (85%)	23 (15%)	3	14
48	E5	61/67 (91%)	55 (90%)	6 (10%)	9	33
48	I8	62/67 (92%)	56 (90%)	6 (10%)	9	34
49	F5	79/83 (95%)	64 (81%)	15 (19%)	2	8
49	J8	79/83 (95%)	67 (85%)	12 (15%)	3	14
50	G5	63/67 (94%)	47 (75%)	16 (25%)	0	2
50	K8	64/67 (96%)	47 (73%)	17 (27%)	0	1
51	H5	50/52 (96%)	37 (74%)	13 (26%)	0	2
51	L8	50/52 (96%)	41 (82%)	9 (18%)	2	9
52	M8	52/63 (82%)	38 (73%)	14 (27%)	0	1
53	J5	48/52 (92%)	38 (79%)	10 (21%)	1	6
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1	6
54	L5	38/42 (90%)	31 (82%)	7 (18%)	2	9
54	P8	38/42 (90%)	31 (82%)	7 (18%)	2	9
55	M5	54/55 (98%)	44 (82%)	10 (18%)	2	8
55	Q8	54/55 (98%)	43 (80%)	11 (20%)	1	6
All	All	9354/10012 (93%)	7424 (79%)	1930 (21%)	1	6

5 of 1930 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	H8	1	MET
5	42	31	LEU
45	B5	66	LEU
48	I8	67	VAL
55	Q8	62	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
44	E8	40	ASN
55	Q8	31	HIS
30	29	54	GLN
41	B8	58	ASN
29	19	46	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1497/1522 (98%)	349 (23%)	0
1	1G	1507/1522 (99%)	354 (23%)	0
22	1K	67/76 (88%)	29 (43%)	0
23	2K	76/77 (98%)	24 (31%)	0
23	2L	76/77 (98%)	20 (26%)	0
24	3K	67/76 (88%)	39 (58%)	0
24	3L	69/76 (90%)	32 (46%)	0
25	4K	19/30 (63%)	11 (57%)	0
25	4L	18/30 (60%)	13 (72%)	0
26	14	2819/2917 (96%)	664 (23%)	0
26	1H	2824/2917 (96%)	601 (21%)	0
27	16	121/122 (99%)	22 (18%)	0
27	1J	121/122 (99%)	33 (27%)	0
56	1L	61/76 (80%)	27 (44%)	0
All	All	9342/9640 (96%)	2218 (23%)	0

5 of 2218 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	3	G
1	13	4	U
1	13	5	U
1	13	6	G

There are no RNA pucker outliers to report.

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

18 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	2.26	4 (23%)	21,30,33	2.94	5 (23%)
22	U8U	1K	34	25,22	15,24,25	2.51	4 (26%)	18,34,37	1.72	2 (11%)
22	T6A	1K	37	22	24,34,35	2.61	4 (16%)	23,49,52	3.47	5 (21%)
22	PSU	1K	39	22	16,21,22	1.01	1 (6%)	20,30,33	3.56	6 (30%)
22	5MU	1K	54	22	14,22,23	1.85	3 (21%)	16,32,35	1.79	2 (12%)
22	PSU	1K	55	22	16,21,22	1.12	1 (6%)	20,30,33	3.76	6 (30%)
56	5MU	1L	54	56	14,22,23	1.75	2 (14%)	16,32,35	1.67	2 (12%)
56	PSU	1L	55	56	16,21,22	1.10	1 (6%)	20,30,33	3.82	5 (25%)
23	OMC	2K	33	23	15,22,23	2.06	4 (26%)	19,31,34	1.02	2 (10%)
23	7MG	2K	47	23	20,26,27	3.58	7 (35%)	22,39,42	2.53	8 (36%)
23	5MU	2K	55	23	14,22,23	1.73	2 (14%)	16,32,35	1.74	2 (12%)
23	PSU	2K	56	23	16,21,22	1.15	3 (18%)	20,30,33	3.41	5 (25%)
23	4SU	2K	8	23	14,21,22	2.80	2 (14%)	15,30,33	1.09	2 (13%)
23	OMC	2L	33	23	15,22,23	2.19	4 (26%)	19,31,34	0.81	1 (5%)
23	7MG	2L	47	23	20,26,27	3.49	6 (30%)	22,39,42	2.00	7 (31%)
23	5MU	2L	55	23	14,22,23	1.80	2 (14%)	16,32,35	1.73	2 (12%)
23	PSU	2L	56	23	16,21,22	1.31	2 (12%)	20,30,33	3.77	6 (30%)
23	4SU	2L	8	23	14,21,22	3.19	2 (14%)	15,30,33	1.13	2 (13%)

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	U8U	1K	34	25,22	-	0/5/28/29	0/2/2/2
22	T6A	1K	37	22	-	0/15/41/42	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
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	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	47	7MG	C5-C4	-5.65	1.24	1.39
23	2L	47	7MG	C5-C4	-5.44	1.24	1.39
22	1K	17	H2U	C6-N1	-3.90	1.42	1.47
23	2K	55	5MU	C4-N3	-3.19	1.27	1.33
23	2L	55	5MU	C4-N3	-3.17	1.27	1.33

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	39	PSU	N1-C2-N3	-12.34	119.53	128.40
23	2L	56	PSU	N1-C2-N3	-12.25	119.59	128.40
56	1L	55	PSU	N1-C2-N3	-12.17	119.64	128.40
22	1K	55	PSU	N1-C2-N3	-11.89	119.85	128.40
22	1K	37	T6A	N3-C2-N1	-10.90	119.37	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	37	T6A	1	0
22	1K	54	5MU	3	0
56	1L	54	5MU	2	0
23	2K	33	OMC	1	0
23	2K	47	7MG	6	0
23	2K	55	5MU	5	0
23	2K	8	4SU	1	0
23	2L	33	OMC	3	0
23	2L	47	7MG	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1345 ligands modelled in this entry, 1341 are monoatomic - leaving 4 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	$\# Z > 2$
60	SPE	14	3458	-	12,12,12	0.45	0	11,11,11	0.76	0
60	SPE	1G	1725	1	12,12,12	0.42	0	11,11,11	0.73	0
58	SF4	32	302	-	0,12,12	0.00	-	0,24,24	0.00	-
58	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
60	SPE	14	3458	-	-	0/10/10/10	0/0/0/0
60	SPE	1G	1725	1	-	0/10/10/10	0/0/0/0
58	SF4	32	302	-	-	0/0/48/48	0/6/5/5
58	SF4	3E	301	4	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1G	1725	SPE	3	0
58	32	302	SF4	2	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
34	69	1
4	3E	1
47	D5	1
10	1A	1
56	1L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1L	72:C	O3'	73:A	P	3.48
1	D5	94:GLU	C	95:PRO	N	1.78
1	1A	38:ILE	C	39:PRO	N	1.71
1	69	79:ILE	C	80:PRO	N	1.17
1	3E	36:ARG	C	37:PRO	N	1.15

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1500/1522 (98%)	-0.52	0 100 100	67, 111, 176, 243	0
1	1G	1509/1522 (99%)	-0.47	3 (0%) 94 90	76, 123, 193, 253	0
2	12	207/256 (80%)	0.29	15 (7%) 16 6	139, 165, 185, 196	0
2	1E	231/256 (90%)	-0.06	5 (2%) 62 43	118, 145, 172, 180	0
3	22	195/239 (81%)	0.76	28 (14%) 3 1	123, 147, 164, 175	0
3	2E	205/239 (85%)	0.34	11 (5%) 26 12	97, 117, 144, 155	0
4	32	208/209 (99%)	-0.32	0 100 100	104, 123, 142, 149	0
4	3E	207/209 (99%)	-0.20	1 (0%) 90 82	93, 118, 137, 144	0
5	42	150/162 (92%)	-0.23	0 100 100	106, 123, 139, 146	0
5	4E	149/162 (91%)	-0.06	0 100 100	87, 109, 128, 133	0
6	52	101/101 (100%)	-0.42	0 100 100	93, 110, 124, 135	0
6	5E	100/101 (99%)	-0.01	1 (1%) 82 69	92, 111, 127, 135	0
7	62	138/156 (88%)	0.84	13 (9%) 9 3	122, 135, 145, 151	0
7	6E	154/156 (98%)	1.00	29 (18%) 1 0	111, 127, 155, 174	0
8	72	137/138 (99%)	-0.07	2 (1%) 74 56	106, 129, 141, 149	0
8	7E	138/138 (100%)	0.80	16 (11%) 5 2	102, 117, 129, 139	0
9	82	121/128 (94%)	1.36	29 (23%) 1 0	118, 161, 171, 178	0
9	8E	126/128 (98%)	-0.11	2 (1%) 72 52	96, 141, 159, 165	0
10	1A	80/105 (76%)	0.35	9 (11%) 6 2	122, 152, 167, 170	0
10	1I	94/105 (89%)	1.43	26 (27%) 1 0	92, 136, 171, 178	0
11	2A	113/129 (87%)	0.78	13 (11%) 5 2	91, 116, 131, 138	0
11	2I	111/129 (86%)	1.39	30 (27%) 1 0	84, 113, 129, 138	0
12	3A	121/132 (91%)	0.68	18 (14%) 3 1	94, 109, 128, 144	0
12	3I	122/132 (92%)	0.12	4 (3%) 47 25	81, 89, 110, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	109/126 (86%)	0.22	15 (13%) 3 1	125, 152, 170, 187	0
13	4I	117/126 (92%)	-0.05	3 (2%) 56 35	97, 125, 138, 145	0
14	5A	59/61 (96%)	2.06	26 (44%) 0 0	131, 146, 164, 167	0
14	5I	59/61 (96%)	0.51	3 (5%) 29 13	92, 106, 121, 129	0
15	6A	87/89 (97%)	-0.54	0 100 100	93, 117, 133, 137	0
15	6I	87/89 (97%)	0.12	2 (2%) 61 41	89, 107, 126, 130	0
16	7A	84/88 (95%)	-0.36	0 100 100	100, 116, 137, 159	0
16	7I	83/88 (94%)	-0.03	1 (1%) 79 63	107, 119, 145, 163	0
17	8A	99/105 (94%)	0.02	0 100 100	100, 112, 125, 131	0
17	8I	100/105 (95%)	1.10	17 (17%) 2 1	95, 114, 124, 128	0
18	9A	67/88 (76%)	-0.21	1 (1%) 74 56	101, 117, 135, 140	0
18	9I	68/88 (77%)	0.03	0 100 100	97, 113, 133, 138	0
19	AA	65/93 (69%)	0.62	9 (13%) 3 1	130, 162, 174, 180	0
19	AI	82/93 (88%)	0.45	7 (8%) 11 4	108, 126, 146, 153	0
20	BA	99/106 (93%)	0.88	16 (16%) 2 1	94, 119, 140, 153	0
20	BI	97/106 (91%)	0.91	21 (21%) 1 0	113, 127, 150, 157	0
21	1B	22/27 (81%)	1.11	4 (18%) 1 1	122, 139, 143, 150	0
21	1F	23/27 (85%)	-0.45	0 100 100	103, 110, 116, 123	0
22	1K	66/76 (86%)	0.03	1 (1%) 74 56	104, 183, 206, 213	0
23	2K	72/77 (93%)	-0.01	2 (2%) 53 31	75, 100, 133, 145	0
23	2L	72/77 (93%)	-0.23	1 (1%) 75 58	85, 120, 153, 162	0
24	3K	70/76 (92%)	1.14	18 (25%) 1 0	82, 225, 245, 249	0
24	3L	72/76 (94%)	-0.01	2 (2%) 53 31	87, 206, 223, 228	0
25	4K	20/30 (66%)	0.70	4 (20%) 1 0	81, 145, 215, 216	0
25	4L	19/30 (63%)	0.13	1 (5%) 27 12	101, 162, 218, 218	0
26	14	2825/2917 (96%)	-0.29	11 (0%) 92 85	62, 91, 198, 251	0
26	1H	2831/2917 (97%)	-0.32	3 (0%) 95 91	51, 79, 176, 251	0
27	16	122/122 (100%)	-0.57	1 (0%) 86 73	76, 98, 118, 204	0
27	1J	122/122 (100%)	-0.76	0 100 100	94, 133, 152, 210	0
28	7I	132/229 (57%)	0.36	11 (8%) 12 5	143, 206, 228, 235	0
29	11	273/276 (98%)	0.12	1 (0%) 92 85	48, 71, 88, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	19	274/276 (99%)	0.12	0 100 100	56, 80, 94, 111	0
30	21	203/206 (98%)	0.18	4 (1%) 65 46	57, 90, 121, 133	0
30	29	204/206 (99%)	0.41	14 (6%) 18 7	66, 97, 133, 147	0
31	31	202/210 (96%)	0.20	4 (1%) 65 46	51, 82, 114, 134	0
31	39	204/210 (97%)	-0.12	1 (0%) 90 82	64, 105, 148, 175	0
32	41	179/182 (98%)	0.27	7 (3%) 40 20	90, 109, 139, 154	0
32	49	180/182 (98%)	0.59	24 (13%) 4 1	125, 147, 166, 179	0
33	51	174/180 (96%)	-0.30	0 100 100	82, 105, 123, 133	0
33	59	169/180 (93%)	2.49	95 (56%) 0 0	157, 203, 223, 233	0
34	61	145/148 (97%)	0.14	4 (2%) 53 31	82, 128, 147, 153	0
34	69	145/148 (97%)	-0.15	1 (0%) 87 77	91, 129, 149, 154	0
35	15	137/140 (97%)	0.59	12 (8%) 11 4	82, 110, 140, 150	0
35	58	137/140 (97%)	0.31	4 (2%) 52 29	71, 90, 122, 138	0
36	25	122/122 (100%)	1.04	15 (12%) 5 2	74, 90, 108, 120	0
36	68	122/122 (100%)	-0.22	0 100 100	67, 82, 98, 106	0
37	35	147/150 (98%)	0.65	21 (14%) 3 1	64, 106, 141, 158	0
37	78	147/150 (98%)	0.23	0 100 100	58, 84, 106, 114	0
38	45	138/141 (97%)	0.17	3 (2%) 62 43	79, 106, 127, 138	0
38	88	141/141 (100%)	0.63	9 (6%) 20 8	62, 83, 105, 133	0
39	55	118/118 (100%)	0.20	2 (1%) 70 51	68, 85, 100, 113	0
39	98	118/118 (100%)	0.55	6 (5%) 29 13	67, 86, 103, 117	0
40	65	110/112 (98%)	-0.09	3 (2%) 55 32	99, 124, 141, 145	0
40	A8	111/112 (99%)	0.14	4 (3%) 43 22	82, 95, 114, 127	0
41	75	133/146 (91%)	0.74	8 (6%) 23 9	82, 97, 127, 145	0
41	B8	135/146 (92%)	-0.28	1 (0%) 87 77	79, 96, 135, 151	0
42	85	116/118 (98%)	0.03	0 100 100	72, 101, 129, 136	0
42	C8	115/118 (97%)	0.19	2 (1%) 70 51	60, 82, 108, 115	0
43	95	100/101 (99%)	0.55	6 (6%) 23 9	72, 120, 140, 147	0
43	D8	100/101 (99%)	1.16	17 (17%) 2 1	62, 100, 120, 130	0
44	A5	111/113 (98%)	0.15	0 100 100	71, 81, 107, 139	0
44	E8	110/113 (97%)	0.26	3 (2%) 55 32	64, 77, 100, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	B5	94/96 (97%)	0.85	12 (12%) 4 2	78, 90, 111, 121	0
45	F8	95/96 (98%)	-0.12	0 100 100	59, 74, 98, 108	0
46	C5	104/110 (94%)	1.02	19 (18%) 1 1	92, 119, 152, 158	0
46	G8	103/110 (93%)	-0.38	0 100 100	76, 97, 124, 134	0
47	D5	177/206 (85%)	1.44	51 (28%) 1 0	117, 159, 218, 223	0
47	H8	170/206 (82%)	1.59	56 (32%) 0 0	88, 121, 189, 196	0
48	E5	76/85 (89%)	0.32	3 (3%) 40 20	78, 97, 111, 120	0
48	I8	77/85 (90%)	0.22	2 (2%) 56 35	64, 79, 96, 108	0
49	F5	94/98 (95%)	1.18	20 (21%) 1 0	69, 89, 125, 139	0
49	J8	96/98 (97%)	0.38	1 (1%) 82 69	61, 80, 117, 123	0
50	G5	69/72 (95%)	0.34	3 (4%) 36 18	90, 109, 132, 144	0
50	K8	68/72 (94%)	-0.15	1 (1%) 74 56	68, 84, 105, 129	0
51	H5	58/60 (96%)	0.68	1 (1%) 70 51	81, 101, 126, 136	0
51	L8	58/60 (96%)	0.36	0 100 100	70, 84, 110, 122	0
52	M8	60/71 (84%)	1.13	10 (16%) 2 1	114, 150, 177, 181	0
53	J5	56/60 (93%)	0.13	1 (1%) 69 49	67, 90, 133, 143	0
53	N8	48/60 (80%)	0.27	1 (2%) 64 44	56, 85, 128, 135	0
54	L5	47/49 (95%)	0.47	2 (4%) 36 18	61, 69, 91, 100	0
54	P8	47/49 (95%)	-0.11	0 100 100	54, 59, 77, 89	0
55	M5	64/65 (98%)	1.22	19 (29%) 1 0	76, 86, 101, 117	0
55	Q8	64/65 (98%)	0.23	0 100 100	61, 75, 88, 101	0
56	1L	64/76 (84%)	0.13	2 (3%) 49 27	140, 201, 221, 227	0
All	All	20656/21744 (94%)	0.05	910 (4%) 35 17	48, 105, 181, 253	0

The worst 5 of 910 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	D8	37	VAL	14.5
47	H8	113	ALA	10.9
33	59	17	VAL	10.2
33	59	96	ALA	8.2
47	H8	146	ILE	8.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
22	U8U	1K	34	23/24	0.97	0.15	-	98,105,115,118	0
23	OMC	2K	33	21/22	0.96	0.25	-	85,89,90,91	0
23	OMC	2L	33	21/22	0.96	0.18	-	100,107,110,117	0
22	T6A	1K	37	32/33	0.93	0.20	-	91,108,133,134	0
23	5MU	2K	55	21/22	0.94	0.14	-	105,112,118,128	0
23	PSU	2K	56	20/21	0.94	0.12	-	102,108,119,120	0
23	4SU	2K	8	20/21	0.93	0.16	-	91,99,105,106	0
22	PSU	1K	55	20/21	0.88	0.15	-	115,126,136,137	0
22	H2U	1K	17	20/21	0.86	0.14	-	130,139,153,158	0
56	PSU	1L	55	20/21	0.85	0.10	-	121,135,144,145	0
23	PSU	2L	56	20/21	0.90	0.11	-	112,122,130,133	0
22	PSU	1K	39	20/21	0.94	0.11	-	100,119,123,124	0
56	5MU	1L	54	21/22	0.92	0.11	-	125,136,146,154	0
23	5MU	2L	55	21/22	0.96	0.14	-	115,126,133,135	0
22	5MU	1K	54	21/22	0.89	0.17	-	116,121,138,149	0
23	4SU	2L	8	20/21	0.94	0.15	-	108,116,123,125	0
23	7MG	2K	47	24/25	0.88	0.19	-	99,108,119,120	0
23	7MG	2L	47	24/25	0.94	0.13	-	124,131,143,146	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
57	MG	14	3068	1/1	0.82	0.47	68.59	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	13	1628	1/1	0.94	0.59	68.16	90,90,90,90	0
57	MG	14	3133	1/1	0.71	0.92	51.37	89,89,89,89	0
57	MG	14	3147	1/1	0.97	0.74	40.33	86,86,86,86	0
57	MG	13	1659	1/1	0.93	0.39	29.46	109,109,109,109	0
57	MG	1G	1614	1/1	0.95	0.58	26.08	91,91,91,91	0
57	MG	1H	3237	1/1	0.74	0.56	24.46	85,85,85,85	0
57	MG	1H	3548	1/1	0.80	0.42	24.26	98,98,98,98	0
57	MG	1H	3112	1/1	0.96	0.25	21.94	79,79,79,79	0
57	MG	14	3095	1/1	0.83	0.31	21.42	72,72,72,72	0
57	MG	14	3142	1/1	0.91	0.37	19.93	98,98,98,98	0
57	MG	1H	3055	1/1	0.67	0.27	19.65	62,62,62,62	0
57	MG	1H	3215	1/1	0.76	0.46	19.16	94,94,94,94	0
57	MG	13	1614	1/1	0.90	0.32	18.80	102,102,102,102	0
57	MG	14	3165	1/1	0.54	0.65	18.42	97,97,97,97	0
57	MG	1H	3532	1/1	0.83	0.47	18.09	79,79,79,79	0
57	MG	14	3132	1/1	0.90	0.26	17.78	90,90,90,90	0
57	MG	14	3050	1/1	0.96	0.44	17.03	87,87,87,87	0
57	MG	13	1615	1/1	0.94	0.41	16.96	75,75,75,75	0
57	MG	1H	3086	1/1	0.77	0.29	16.89	67,67,67,67	0
57	MG	1H	3130	1/1	0.92	0.40	16.11	97,97,97,97	0
57	MG	13	1634	1/1	0.97	0.33	16.08	91,91,91,91	0
57	MG	1H	3207	1/1	0.95	0.40	15.79	77,77,77,77	0
57	MG	14	3194	1/1	0.58	0.50	14.74	84,84,84,84	0
57	MG	14	3130	1/1	0.77	0.28	13.50	92,92,92,92	0
57	MG	1G	1648	1/1	0.87	0.27	12.95	121,121,121,121	0
57	MG	1H	3154	1/1	0.85	0.43	12.87	67,67,67,67	0
57	MG	13	1630	1/1	0.97	0.25	12.76	86,86,86,86	0
57	MG	1H	3191	1/1	0.92	0.30	12.72	79,79,79,79	0
57	MG	16	202	1/1	0.92	0.28	12.69	103,103,103,103	0
57	MG	14	3078	1/1	0.86	0.23	12.63	88,88,88,88	0
57	MG	1H	3015	1/1	0.94	0.47	12.63	77,77,77,77	0
57	MG	14	3094	1/1	0.85	0.44	12.13	100,100,100,100	0
57	MG	1H	3225	1/1	0.92	0.35	11.45	74,74,74,74	0
57	MG	1H	3084	1/1	0.95	0.29	11.06	77,77,77,77	0
57	MG	13	1601	1/1	0.90	0.32	10.96	97,97,97,97	0
57	MG	14	3149	1/1	0.94	0.31	10.93	94,94,94,94	0
57	MG	14	3096	1/1	0.96	0.28	10.89	84,84,84,84	0
57	MG	14	3123	1/1	0.88	0.33	10.86	75,75,75,75	0
57	MG	1H	3082	1/1	0.91	0.33	10.73	69,69,69,69	0
57	MG	14	3160	1/1	0.80	0.45	10.42	85,85,85,85	0
57	MG	14	3106	1/1	0.94	0.33	10.33	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	1G	1626	1/1	0.97	0.28	10.28	119,119,119,119	0
57	MG	1H	3093	1/1	0.87	0.31	9.91	73,73,73,73	0
57	MG	14	3124	1/1	0.79	0.35	9.70	64,64,64,64	0
57	MG	1H	3206	1/1	0.98	0.35	9.63	55,55,55,55	0
57	MG	1H	3119	1/1	0.85	0.23	9.54	79,79,79,79	0
57	MG	1H	3041	1/1	0.99	0.28	9.54	57,57,57,57	0
57	MG	14	3034	1/1	0.94	0.28	9.20	75,75,75,75	0
57	MG	13	1629	1/1	0.78	0.32	9.06	100,100,100,100	0
57	MG	13	1635	1/1	0.99	0.45	8.81	83,83,83,83	0
57	MG	1H	3413	1/1	0.83	0.34	8.73	93,93,93,93	0
57	MG	1H	3036	1/1	0.93	0.28	8.16	73,73,73,73	0
57	MG	1G	1647	1/1	0.54	0.23	7.94	99,99,99,99	0
57	MG	1H	3240	1/1	0.91	0.20	7.86	86,86,86,86	0
57	MG	1H	3169	1/1	0.73	0.27	7.72	91,91,91,91	0
57	MG	1H	3179	1/1	0.97	0.24	7.52	74,74,74,74	0
57	MG	14	3240	1/1	0.94	0.25	7.16	63,63,63,63	0
57	MG	1H	3074	1/1	0.87	0.25	7.02	75,75,75,75	0
57	MG	13	1624	1/1	0.96	0.30	6.89	83,83,83,83	0
57	MG	1H	3107	1/1	0.82	0.35	6.84	62,62,62,62	0
57	MG	1G	1651	1/1	0.87	0.29	6.81	97,97,97,97	0
57	MG	14	3119	1/1	0.91	0.32	6.75	69,69,69,69	0
57	MG	14	3052	1/1	0.91	0.32	6.74	59,59,59,59	0
57	MG	14	3102	1/1	0.89	0.28	6.63	94,94,94,94	0
57	MG	14	3005	1/1	0.91	0.33	6.54	83,83,83,83	0
57	MG	1H	3116	1/1	0.93	0.21	6.34	82,82,82,82	0
57	MG	2L	101	1/1	0.97	0.43	6.28	83,83,83,83	0
57	MG	1H	3007	1/1	0.82	0.24	5.88	57,57,57,57	0
57	MG	14	3145	1/1	0.77	0.39	5.68	71,71,71,71	0
57	MG	1H	3021	1/1	0.98	0.28	5.60	60,60,60,60	0
57	MG	14	3046	1/1	0.91	0.20	5.53	77,77,77,77	0
57	MG	19	301	1/1	0.95	0.30	5.43	61,61,61,61	0
57	MG	14	3086	1/1	0.88	0.27	5.22	73,73,73,73	0
57	MG	13	1696	1/1	0.94	0.18	5.05	114,114,114,114	0
57	MG	14	3302	1/1	0.94	0.26	4.71	94,94,94,94	0
57	MG	14	3054	1/1	0.92	0.28	4.66	67,67,67,67	0
57	MG	1H	3198	1/1	0.96	0.26	4.62	75,75,75,75	0
57	MG	1H	3427	1/1	0.86	0.23	4.61	102,102,102,102	0
57	MG	14	3075	1/1	0.96	0.28	4.53	65,65,65,65	0
57	MG	14	3105	1/1	0.96	0.17	4.49	92,92,92,92	0
57	MG	14	3113	1/1	0.89	0.34	4.46	74,74,74,74	0
57	MG	14	3009	1/1	0.82	0.28	4.46	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	13	1643	1/1	0.93	0.22	4.21	95,95,95,95	0
57	MG	1H	3160	1/1	0.81	0.24	4.19	79,79,79,79	0
57	MG	1G	1670	1/1	0.88	0.16	4.18	109,109,109,109	0
57	MG	1H	3052	1/1	0.97	0.28	4.11	58,58,58,58	0
57	MG	1H	3218	1/1	0.90	0.32	4.00	70,70,70,70	0
57	MG	14	3091	1/1	0.96	0.31	3.98	92,92,92,92	0
57	MG	14	3058	1/1	0.96	0.24	3.93	83,83,83,83	0
57	MG	13	1638	1/1	0.55	0.56	3.89	103,103,103,103	0
57	MG	16	204	1/1	0.81	0.20	3.71	89,89,89,89	0
57	MG	14	3042	1/1	0.94	0.28	3.70	54,54,54,54	0
57	MG	14	3016	1/1	0.96	0.26	3.64	69,69,69,69	0
57	MG	1H	3063	1/1	0.94	0.25	3.60	59,59,59,59	0
57	MG	14	3159	1/1	0.77	0.27	3.55	80,80,80,80	0
57	MG	14	3069	1/1	0.85	0.22	3.50	56,56,56,56	0
57	MG	14	3066	1/1	0.96	0.25	3.49	63,63,63,63	0
57	MG	13	1609	1/1	0.97	0.19	3.46	88,88,88,88	0
57	MG	1H	3017	1/1	0.97	0.27	3.43	56,56,56,56	0
57	MG	13	1607	1/1	0.97	0.23	3.33	83,83,83,83	0
57	MG	14	3045	1/1	0.85	0.23	3.30	72,72,72,72	0
57	MG	1H	3090	1/1	0.74	0.27	3.25	82,82,82,82	0
57	MG	1H	3394	1/1	0.89	0.20	3.11	83,83,83,83	0
60	SPE	14	3458	13/13	0.90	0.21	2.96	92,101,106,108	0
57	MG	1H	3126	1/1	0.86	0.20	2.93	71,71,71,71	0
57	MG	1G	1607	1/1	0.96	0.28	2.88	107,107,107,107	0
57	MG	1H	3432	1/1	0.60	0.16	2.80	116,116,116,116	0
57	MG	1H	3497	1/1	0.57	0.24	2.69	96,96,96,96	0
57	MG	1G	1606	1/1	0.87	0.25	2.56	87,87,87,87	0
57	MG	1G	1632	1/1	0.92	0.25	2.56	108,108,108,108	0
57	MG	14	3038	1/1	0.92	0.27	2.51	68,68,68,68	0
57	MG	1H	3019	1/1	0.97	0.29	2.46	53,53,53,53	0
57	MG	14	3182	1/1	0.96	0.26	2.43	66,66,66,66	0
57	MG	14	3170	1/1	0.91	0.25	2.41	76,76,76,76	0
57	MG	13	1649	1/1	0.78	0.19	2.33	83,83,83,83	0
57	MG	13	1625	1/1	0.96	0.23	2.29	68,68,68,68	0
57	MG	14	3032	1/1	0.96	0.25	2.27	72,72,72,72	0
57	MG	1H	3541	1/1	0.85	0.20	2.19	109,109,109,109	0
57	MG	14	3228	1/1	0.93	0.25	2.13	64,64,64,64	0
57	MG	14	3080	1/1	0.41	0.24	2.12	71,71,71,71	0
57	MG	1G	1679	1/1	0.94	0.17	2.09	105,105,105,105	0
57	MG	1H	3075	1/1	0.88	0.21	2.09	75,75,75,75	0
57	MG	1H	3068	1/1	0.88	0.22	2.04	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3010	1/1	0.71	0.23	1.99	84,84,84,84	0
57	MG	21	301	1/1	0.91	0.34	1.96	77,77,77,77	0
57	MG	1H	3181	1/1	0.77	0.35	1.94	98,98,98,98	0
57	MG	1H	3001	1/1	0.98	0.23	1.90	49,49,49,49	0
57	MG	13	1618	1/1	0.80	0.27	1.83	72,72,72,72	0
57	MG	14	3092	1/1	0.90	0.22	1.83	67,67,67,67	0
57	MG	14	3065	1/1	0.87	0.32	1.82	70,70,70,70	0
57	MG	14	3460	1/1	0.98	0.26	1.77	92,92,92,92	0
57	MG	14	3216	1/1	0.99	0.23	1.75	62,62,62,62	0
57	MG	14	3082	1/1	0.90	0.41	1.68	80,80,80,80	0
57	MG	14	3093	1/1	0.98	0.29	1.65	86,86,86,86	0
57	MG	1H	3034	1/1	0.98	0.16	1.60	74,74,74,74	0
57	MG	1H	3543	1/1	0.79	0.12	1.47	166,166,166,166	0
57	MG	1H	3100	1/1	0.94	0.27	1.34	77,77,77,77	0
57	MG	14	3372	1/1	0.84	0.18	1.30	112,112,112,112	0
57	MG	1G	1654	1/1	0.85	0.22	1.26	102,102,102,102	0
57	MG	14	3189	1/1	0.98	0.32	1.21	81,81,81,81	0
57	MG	13	1667	1/1	0.67	0.15	1.19	104,104,104,104	0
57	MG	14	3136	1/1	0.94	0.26	1.14	95,95,95,95	0
57	MG	14	3223	1/1	0.94	0.22	1.08	61,61,61,61	0
57	MG	14	3031	1/1	0.94	0.24	1.07	51,51,51,51	0
57	MG	14	3208	1/1	0.96	0.23	1.03	63,63,63,63	0
57	MG	1H	3485	1/1	0.88	0.18	1.01	102,102,102,102	0
57	MG	1G	1622	1/1	0.93	0.16	0.98	104,104,104,104	0
57	MG	1H	3047	1/1	0.96	0.21	0.94	64,64,64,64	0
57	MG	14	3087	1/1	0.78	0.18	0.93	75,75,75,75	0
57	MG	14	3120	1/1	0.95	0.14	0.82	84,84,84,84	0
57	MG	14	3356	1/1	0.81	0.21	0.74	78,78,78,78	0
57	MG	1H	3113	1/1	0.95	0.16	0.73	70,70,70,70	0
57	MG	14	3311	1/1	0.91	0.18	0.71	84,84,84,84	0
57	MG	14	3089	1/1	0.85	0.23	0.70	73,73,73,73	0
57	MG	1G	1667	1/1	0.79	0.21	0.64	111,111,111,111	0
57	MG	13	1652	1/1	0.98	0.18	0.59	82,82,82,82	0
57	MG	13	1637	1/1	0.93	0.18	0.58	90,90,90,90	0
57	MG	1H	3205	1/1	0.97	0.18	0.57	71,71,71,71	0
57	MG	1H	3026	1/1	0.85	0.15	0.56	82,82,82,82	0
57	MG	14	3049	1/1	0.96	0.19	0.55	69,69,69,69	0
57	MG	1H	3066	1/1	0.98	0.23	0.54	65,65,65,65	0
57	MG	14	3020	1/1	0.90	0.21	0.54	69,69,69,69	0
57	MG	1H	3208	1/1	0.77	0.19	0.50	69,69,69,69	0
57	MG	1G	1623	1/1	0.95	0.12	0.48	109,109,109,109	0
57	MG	14	3270	1/1	0.89	0.19	0.44	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3060	1/1	0.98	0.16	0.38	65,65,65,65	0
57	MG	1H	3115	1/1	0.97	0.19	0.35	64,64,64,64	0
58	SF4	3E	301	8/8	0.99	0.21	0.32	95,98,106,108	0
57	MG	1H	3029	1/1	0.96	0.21	0.26	59,59,59,59	0
57	MG	14	3083	1/1	0.93	0.21	0.19	58,58,58,58	0
57	MG	14	3044	1/1	0.96	0.23	0.16	71,71,71,71	0
57	MG	14	3007	1/1	0.87	0.27	0.16	61,61,61,61	0
57	MG	1H	3171	1/1	0.96	0.18	0.13	88,88,88,88	0
57	MG	1G	1700	1/1	0.94	0.13	0.12	107,107,107,107	0
58	SF4	32	302	8/8	0.99	0.20	0.10	115,120,128,136	0
57	MG	1G	1644	1/1	0.95	0.15	0.07	130,130,130,130	0
57	MG	13	1678	1/1	0.74	0.17	0.01	114,114,114,114	0
57	MG	13	1619	1/1	0.92	0.21	-0.01	54,54,54,54	0
57	MG	1H	3132	1/1	0.96	0.19	-0.01	55,55,55,55	0
57	MG	14	3394	1/1	0.87	0.30	-0.04	91,91,91,91	0
57	MG	13	1644	1/1	0.93	0.12	-0.07	99,99,99,99	0
57	MG	1G	1630	1/1	0.93	0.14	-0.08	132,132,132,132	0
57	MG	14	3098	1/1	0.96	0.20	-0.08	63,63,63,63	0
57	MG	41	201	1/1	0.90	0.17	-0.13	81,81,81,81	0
57	MG	1H	3103	1/1	0.84	0.15	-0.15	64,64,64,64	0
57	MG	14	3288	1/1	0.93	0.20	-0.19	59,59,59,59	0
57	MG	1G	1603	1/1	0.97	0.16	-0.21	91,91,91,91	0
57	MG	1H	3396	1/1	0.95	0.17	-0.22	81,81,81,81	0
57	MG	13	1673	1/1	0.94	0.11	-0.24	110,110,110,110	0
57	MG	13	1612	1/1	0.97	0.14	-0.25	111,111,111,111	0
57	MG	88	201	1/1	0.87	0.20	-0.26	83,83,83,83	0
57	MG	1H	3434	1/1	0.88	0.14	-0.27	96,96,96,96	0
57	MG	14	3114	1/1	0.82	0.18	-0.28	77,77,77,77	0
57	MG	1H	3002	1/1	0.96	0.17	-0.32	51,51,51,51	0
57	MG	1H	3027	1/1	0.98	0.17	-0.34	60,60,60,60	0
57	MG	1G	1726	1/1	0.95	0.20	-0.35	94,94,94,94	0
57	MG	14	3077	1/1	0.92	0.17	-0.37	85,85,85,85	0
57	MG	14	3029	1/1	0.98	0.15	-0.42	80,80,80,80	0
57	MG	13	1606	1/1	0.97	0.16	-0.43	88,88,88,88	0
57	MG	1H	3088	1/1	0.97	0.14	-0.44	87,87,87,87	0
57	MG	1G	1699	1/1	0.87	0.16	-0.46	113,113,113,113	0
57	MG	1H	3065	1/1	0.81	0.16	-0.50	72,72,72,72	0
57	MG	14	3100	1/1	0.83	0.25	-0.53	77,77,77,77	0
57	MG	1H	3377	1/1	0.94	0.13	-0.54	94,94,94,94	0
57	MG	1H	3101	1/1	0.90	0.19	-0.55	72,72,72,72	0
57	MG	14	3111	1/1	0.93	0.17	-0.57	83,83,83,83	0
57	MG	14	3164	1/1	0.93	0.19	-0.58	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1G	1610	1/1	0.92	0.16	-0.58	84,84,84,84	0
57	MG	1H	3268	1/1	0.90	0.14	-0.63	70,70,70,70	0
57	MG	1H	3307	1/1	0.92	0.17	-0.63	56,56,56,56	0
57	MG	1H	3273	1/1	0.98	0.16	-0.71	56,56,56,56	0
57	MG	1H	3219	1/1	0.91	0.11	-0.72	83,83,83,83	0
57	MG	M5	101	1/1	0.93	0.36	-0.76	81,81,81,81	0
57	MG	1H	3476	1/1	0.98	0.16	-0.77	94,94,94,94	0
57	MG	14	3286	1/1	0.93	0.19	-0.78	58,58,58,58	0
57	MG	14	3392	1/1	0.76	0.15	-0.81	98,98,98,98	0
57	MG	1H	3028	1/1	0.97	0.16	-0.83	62,62,62,62	0
57	MG	14	3259	1/1	0.81	0.13	-0.83	97,97,97,97	0
57	MG	1J	204	1/1	0.82	0.10	-0.84	102,102,102,102	0
59	ZN	5I	101	1/1	0.99	0.13	-0.84	94,94,94,94	0
57	MG	1G	1604	1/1	0.93	0.11	-0.86	132,132,132,132	0
57	MG	1G	1693	1/1	0.89	0.10	-0.87	121,121,121,121	0
57	MG	1H	3125	1/1	0.91	0.14	-0.87	79,79,79,79	0
57	MG	14	3391	1/1	0.87	0.15	-0.88	87,87,87,87	0
57	MG	14	3278	1/1	0.96	0.13	-0.90	83,83,83,83	0
57	MG	1H	3046	1/1	0.95	0.17	-0.91	43,43,43,43	0
57	MG	1H	3098	1/1	0.90	0.17	-0.95	59,59,59,59	0
57	MG	1H	3127	1/1	0.88	0.18	-0.95	69,69,69,69	0
57	MG	1G	1680	1/1	0.93	0.14	-0.95	103,103,103,103	0
57	MG	1G	1720	1/1	0.77	0.10	-0.96	135,135,135,135	0
59	ZN	5A	101	1/1	0.98	0.09	-0.97	129,129,129,129	0
57	MG	13	1683	1/1	0.67	0.12	-0.98	119,119,119,119	0
57	MG	14	3209	1/1	0.98	0.18	-0.98	61,61,61,61	0
57	MG	1H	3291	1/1	0.99	0.15	-1.02	57,57,57,57	0
57	MG	13	1675	1/1	0.76	0.16	-1.03	91,91,91,91	0
57	MG	1H	3283	1/1	0.99	0.12	-1.04	59,59,59,59	0
57	MG	Q8	101	1/1	0.93	0.23	-1.05	82,82,82,82	0
57	MG	1H	3266	1/1	0.97	0.15	-1.08	92,92,92,92	0
57	MG	1H	3488	1/1	0.85	0.19	-1.09	84,84,84,84	0
57	MG	1H	3317	1/1	0.90	0.15	-1.10	70,70,70,70	0
57	MG	1H	3461	1/1	0.93	0.08	-1.11	80,80,80,80	0
57	MG	1H	3048	1/1	0.80	0.14	-1.11	68,68,68,68	0
57	MG	14	3222	1/1	0.71	0.18	-1.13	73,73,73,73	0
57	MG	14	3293	1/1	0.93	0.18	-1.13	70,70,70,70	0
57	MG	14	3245	1/1	0.95	0.16	-1.14	74,74,74,74	0
57	MG	1H	3279	1/1	0.75	0.12	-1.17	68,68,68,68	0
57	MG	1H	3144	1/1	0.93	0.15	-1.17	71,71,71,71	0
57	MG	2I	201	1/1	0.91	0.10	-1.24	97,97,97,97	0
57	MG	1H	3270	1/1	0.89	0.14	-1.27	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3280	1/1	0.98	0.16	-1.30	76,76,76,76	0
57	MG	13	1632	1/1	0.89	0.08	-1.30	95,95,95,95	0
57	MG	14	3326	1/1	0.97	0.10	-1.31	87,87,87,87	0
57	MG	1H	3518	1/1	0.97	0.11	-1.32	57,57,57,57	0
57	MG	13	1741	1/1	0.85	0.11	-1.34	95,95,95,95	0
57	MG	14	3319	1/1	0.98	0.13	-1.35	72,72,72,72	0
57	MG	1H	3306	1/1	0.89	0.11	-1.35	79,79,79,79	0
57	MG	1H	3149	1/1	0.92	0.19	-1.37	81,81,81,81	0
57	MG	1H	3329	1/1	0.97	0.13	-1.38	53,53,53,53	0
57	MG	1H	3261	1/1	0.95	0.16	-1.39	61,61,61,61	0
57	MG	1G	1687	1/1	0.87	0.14	-1.42	111,111,111,111	0
57	MG	1G	1643	1/1	0.72	0.10	-1.43	100,100,100,100	0
57	MG	14	3227	1/1	0.94	0.17	-1.43	52,52,52,52	0
57	MG	16	207	1/1	0.91	0.10	-1.46	91,91,91,91	0
57	MG	14	3275	1/1	0.88	0.14	-1.48	85,85,85,85	0
60	SPE	1G	1725	13/13	0.86	0.09	-1.48	110,113,117,118	0
57	MG	1H	3297	1/1	0.92	0.17	-1.53	56,56,56,56	0
57	MG	14	3399	1/1	0.69	0.09	-1.54	122,122,122,122	0
57	MG	13	1677	1/1	0.96	0.13	-1.57	90,90,90,90	0
57	MG	1H	3257	1/1	0.99	0.16	-1.58	49,49,49,49	0
57	MG	39	301	1/1	0.74	0.17	-1.61	80,80,80,80	0
57	MG	13	1687	1/1	0.91	0.13	-1.64	89,89,89,89	0
57	MG	1H	3038	1/1	0.95	0.16	-1.64	61,61,61,61	0
57	MG	14	3309	1/1	0.93	0.13	-1.65	48,48,48,48	0
57	MG	1H	3054	1/1	0.97	0.15	-1.67	63,63,63,63	0
57	MG	14	3459	1/1	0.96	0.10	-1.68	68,68,68,68	0
57	MG	14	3285	1/1	0.94	0.11	-1.68	89,89,89,89	0
57	MG	14	3252	1/1	0.93	0.14	-1.68	69,69,69,69	0
57	MG	14	3169	1/1	0.88	0.14	-1.74	88,88,88,88	0
57	MG	1H	3275	1/1	0.99	0.10	-1.77	72,72,72,72	0
57	MG	14	3263	1/1	0.90	0.12	-1.82	86,86,86,86	0
57	MG	14	3261	1/1	0.95	0.12	-1.84	64,64,64,64	0
57	MG	1H	3033	1/1	0.98	0.18	-1.89	63,63,63,63	0
57	MG	13	1703	1/1	0.92	0.14	-1.94	71,71,71,71	0
57	MG	1G	1658	1/1	0.81	0.08	-1.94	97,97,97,97	0
57	MG	14	3461	1/1	0.91	0.07	-1.95	108,108,108,108	0
57	MG	14	3253	1/1	0.95	0.12	-1.96	79,79,79,79	0
57	MG	14	3377	1/1	0.73	0.12	-1.99	72,72,72,72	0
57	MG	1G	1662	1/1	0.74	0.11	-2.06	118,118,118,118	0
57	MG	1H	3062	1/1	0.60	0.17	-2.07	64,64,64,64	0
57	MG	1H	3102	1/1	0.90	0.14	-2.13	52,52,52,52	0
57	MG	1H	3357	1/1	0.99	0.11	-2.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1G	1664	1/1	0.83	0.14	-2.15	82,82,82,82	0
57	MG	14	3442	1/1	0.94	0.08	-2.18	83,83,83,83	0
57	MG	14	3214	1/1	0.96	0.15	-2.25	83,83,83,83	0
57	MG	1H	3272	1/1	0.94	0.12	-2.26	79,79,79,79	0
57	MG	13	1686	1/1	0.97	0.10	-2.26	107,107,107,107	0
57	MG	1H	3472	1/1	0.94	0.14	-2.28	63,63,63,63	0
57	MG	14	3242	1/1	0.97	0.11	-2.36	82,82,82,82	0
57	MG	1H	3296	1/1	0.93	0.16	-2.42	56,56,56,56	0
57	MG	13	1674	1/1	0.91	0.07	-2.46	105,105,105,105	0
57	MG	1H	3053	1/1	0.84	0.14	-2.50	47,47,47,47	0
57	MG	14	3383	1/1	0.79	0.13	-2.55	91,91,91,91	0
57	MG	14	3017	1/1	0.95	0.14	-2.55	74,74,74,74	0
57	MG	14	3308	1/1	0.96	0.13	-2.55	64,64,64,64	0
57	MG	1H	3308	1/1	0.89	0.14	-2.58	62,62,62,62	0
57	MG	1G	1655	1/1	0.93	0.15	-2.61	90,90,90,90	0
57	MG	1H	3229	1/1	0.85	0.11	-2.62	84,84,84,84	0
57	MG	1H	3302	1/1	0.96	0.16	-2.62	54,54,54,54	0
57	MG	14	3192	1/1	0.98	0.14	-2.65	80,80,80,80	0
57	MG	1H	3382	1/1	0.95	0.16	-2.69	43,43,43,43	0
57	MG	13	1676	1/1	0.99	0.11	-2.73	67,67,67,67	0
57	MG	14	3027	1/1	0.70	0.08	-2.73	85,85,85,85	0
57	MG	14	3320	1/1	0.97	0.15	-2.80	70,70,70,70	0
57	MG	1H	3133	1/1	0.83	0.13	-2.83	72,72,72,72	0
57	MG	1H	3496	1/1	0.97	0.10	-2.85	89,89,89,89	0
57	MG	1H	3294	1/1	0.98	0.10	-2.87	68,68,68,68	0
57	MG	1H	3351	1/1	0.96	0.09	-2.88	66,66,66,66	0
57	MG	14	3212	1/1	0.99	0.11	-2.90	60,60,60,60	0
57	MG	1H	3043	1/1	0.92	0.15	-2.91	64,64,64,64	0
57	MG	1G	1671	1/1	0.95	0.10	-2.93	101,101,101,101	0
57	MG	1H	3383	1/1	0.81	0.16	-2.97	74,74,74,74	0
57	MG	1H	3292	1/1	0.98	0.07	-2.99	62,62,62,62	0
57	MG	14	3241	1/1	0.98	0.14	-3.00	61,61,61,61	0
57	MG	1H	3330	1/1	0.98	0.09	-3.01	74,74,74,74	0
57	MG	1H	3263	1/1	0.98	0.11	-3.02	53,53,53,53	0
57	MG	1H	3118	1/1	0.96	0.13	-3.03	63,63,63,63	0
57	MG	14	3256	1/1	0.93	0.08	-3.08	99,99,99,99	0
57	MG	1H	3401	1/1	0.80	0.14	-3.14	99,99,99,99	0
57	MG	1H	3319	1/1	0.96	0.11	-3.14	58,58,58,58	0
57	MG	13	1729	1/1	0.98	0.08	-3.17	110,110,110,110	0
57	MG	1H	3289	1/1	0.98	0.11	-3.20	91,91,91,91	0
57	MG	14	3022	1/1	0.92	0.13	-3.22	77,77,77,77	0
57	MG	14	3305	1/1	0.88	0.17	-3.30	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	13	1713	1/1	0.97	0.09	-3.32	96,96,96,96	0
57	MG	14	3281	1/1	0.93	0.07	-3.33	75,75,75,75	0
57	MG	1H	3242	1/1	0.96	0.13	-3.34	50,50,50,50	0
57	MG	14	3237	1/1	0.91	0.12	-3.43	67,67,67,67	0
57	MG	14	3266	1/1	0.96	0.10	-3.45	77,77,77,77	0
57	MG	1H	3256	1/1	0.99	0.12	-3.47	48,48,48,48	0
57	MG	1H	3274	1/1	0.94	0.12	-3.60	48,48,48,48	0
57	MG	14	3236	1/1	0.92	0.14	-3.60	69,69,69,69	0
57	MG	1G	1724	1/1	0.76	0.06	-3.62	126,126,126,126	0
57	MG	14	3229	1/1	0.94	0.10	-3.62	74,74,74,74	0
57	MG	14	3416	1/1	0.95	0.06	-3.72	87,87,87,87	0
57	MG	14	3348	1/1	0.90	0.09	-3.73	102,102,102,102	0
57	MG	2K	101	1/1	0.84	0.13	-3.74	80,80,80,80	0
57	MG	1H	3463	1/1	0.89	0.13	-3.79	70,70,70,70	0
57	MG	13	1640	1/1	0.87	0.10	-3.81	97,97,97,97	0
57	MG	1H	3265	1/1	0.98	0.11	-3.88	74,74,74,74	0
57	MG	1H	3230	1/1	0.99	0.09	-3.90	90,90,90,90	0
57	MG	13	1694	1/1	0.95	0.11	-3.92	92,92,92,92	0
57	MG	1G	1641	1/1	0.95	0.10	-3.96	115,115,115,115	0
57	MG	1H	3372	1/1	0.95	0.14	-3.99	66,66,66,66	0
57	MG	14	3315	1/1	0.83	0.10	-4.07	83,83,83,83	0
57	MG	1H	3253	1/1	0.96	0.12	-4.08	58,58,58,58	0
57	MG	1H	3259	1/1	0.98	0.12	-4.10	59,59,59,59	0
57	MG	1H	3145	1/1	0.98	0.09	-4.15	74,74,74,74	0
57	MG	14	3217	1/1	0.92	0.09	-4.16	76,76,76,76	0
57	MG	1H	3247	1/1	0.99	0.07	-4.17	67,67,67,67	0
57	MG	13	1735	1/1	0.79	0.12	-4.18	105,105,105,105	0
57	MG	1H	3239	1/1	0.95	0.09	-4.23	97,97,97,97	0
57	MG	1G	1619	1/1	0.98	0.07	-4.24	118,118,118,118	0
57	MG	1H	3288	1/1	0.96	0.11	-4.28	58,58,58,58	0
57	MG	16	205	1/1	0.93	0.05	-4.33	84,84,84,84	0
57	MG	14	3225	1/1	0.82	0.16	-4.42	79,79,79,79	0
57	MG	14	3405	1/1	0.86	0.05	-4.52	118,118,118,118	0
57	MG	1H	3250	1/1	0.97	0.10	-4.52	54,54,54,54	0
57	MG	14	3384	1/1	0.79	0.09	-4.56	88,88,88,88	0
57	MG	1H	3335	1/1	0.67	0.09	-4.61	83,83,83,83	0
57	MG	1H	3243	1/1	0.89	0.10	-4.61	63,63,63,63	0
57	MG	14	3274	1/1	0.88	0.15	-4.72	62,62,62,62	0
57	MG	14	3396	1/1	0.96	0.07	-4.72	71,71,71,71	0
57	MG	14	3024	1/1	0.84	0.14	-4.77	88,88,88,88	0
57	MG	14	3127	1/1	0.96	0.06	-4.81	70,70,70,70	0
57	MG	13	1622	1/1	0.93	0.05	-4.87	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3072	1/1	0.85	0.12	-4.94	60,60,60,60	0
57	MG	14	3322	1/1	0.96	0.14	-4.96	58,58,58,58	0
57	MG	14	3420	1/1	0.93	0.11	-4.99	119,119,119,119	0
57	MG	14	3258	1/1	0.95	0.05	-5.03	97,97,97,97	0
57	MG	1G	1656	1/1	0.87	0.10	-5.04	89,89,89,89	0
57	MG	14	3350	1/1	0.95	0.09	-5.04	88,88,88,88	0
57	MG	1H	3058	1/1	0.88	0.07	-5.11	68,68,68,68	0
57	MG	14	3318	1/1	0.94	0.12	-5.12	65,65,65,65	0
57	MG	14	3232	1/1	0.94	0.11	-5.25	75,75,75,75	0
57	MG	14	3239	1/1	0.92	0.10	-5.37	60,60,60,60	0
57	MG	14	3234	1/1	0.97	0.09	-5.41	62,62,62,62	0
57	MG	1H	3300	1/1	0.91	0.10	-5.47	73,73,73,73	0
57	MG	14	3210	1/1	0.81	0.09	-5.55	78,78,78,78	0
57	MG	1H	3438	1/1	0.95	0.07	-5.59	95,95,95,95	0
57	MG	14	3313	1/1	0.97	0.09	-5.68	67,67,67,67	0
57	MG	1H	3468	1/1	0.95	0.05	-5.70	82,82,82,82	0
57	MG	14	3026	1/1	0.96	0.06	-5.75	74,74,74,74	0
57	MG	1H	3128	1/1	0.96	0.07	-5.77	66,66,66,66	0
57	MG	14	3379	1/1	0.77	0.12	-5.78	107,107,107,107	0
57	MG	13	1663	1/1	0.82	0.12	-6.06	77,77,77,77	0
57	MG	1G	1665	1/1	0.97	0.10	-6.38	82,82,82,82	0
57	MG	14	3097	1/1	0.87	0.09	-6.38	84,84,84,84	0
57	MG	13	1709	1/1	0.79	0.05	-6.49	128,128,128,128	0
57	MG	1H	3368	1/1	0.96	0.06	-6.79	72,72,72,72	0
57	MG	14	3287	1/1	0.93	0.13	-6.87	74,74,74,74	0
57	MG	1H	3251	1/1	0.99	0.06	-7.16	49,49,49,49	0
57	MG	1H	3278	1/1	0.93	0.07	-7.17	86,86,86,86	0
57	MG	1H	3324	1/1	0.92	0.09	-7.22	69,69,69,69	0
57	MG	1H	3414	1/1	0.96	0.07	-7.28	52,52,52,52	0
57	MG	13	1728	1/1	0.57	0.09	-7.35	117,117,117,117	0
57	MG	1H	3393	1/1	0.98	0.10	-7.54	63,63,63,63	0
57	MG	14	3433	1/1	0.94	0.11	-7.63	90,90,90,90	0
57	MG	1H	3258	1/1	0.95	0.10	-7.72	56,56,56,56	0
57	MG	1H	3248	1/1	0.92	0.11	-7.78	57,57,57,57	0
57	MG	1H	3224	1/1	0.96	0.09	-8.50	72,72,72,72	0
57	MG	1H	3298	1/1	0.97	0.06	-8.72	52,52,52,52	0
57	MG	14	3299	1/1	0.97	0.06	-8.97	63,63,63,63	0
57	MG	14	3221	1/1	0.90	0.10	-9.23	65,65,65,65	0
57	MG	1H	3281	1/1	0.84	0.07	-9.49	85,85,85,85	0
57	MG	14	3125	1/1	0.97	0.10	-10.06	92,92,92,92	0
57	MG	1H	3293	1/1	0.95	0.10	-10.32	60,60,60,60	0
57	MG	13	1710	1/1	0.96	0.08	-10.35	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3451	1/1	1.00	0.07	-10.43	55,55,55,55	0
57	MG	1H	3374	1/1	0.97	0.07	-10.73	57,57,57,57	0
57	MG	1H	3284	1/1	0.88	0.10	-11.36	62,62,62,62	0
57	MG	14	3403	1/1	0.96	0.07	-11.67	78,78,78,78	0
57	MG	1H	3478	1/1	0.96	0.05	-12.62	79,79,79,79	0
57	MG	1H	3388	1/1	0.98	0.07	-12.63	49,49,49,49	0
57	MG	1H	3417	1/1	0.95	0.04	-13.85	100,100,100,100	0
57	MG	1H	3389	1/1	0.99	0.05	-14.35	63,63,63,63	0
57	MG	1H	3358	1/1	0.89	0.07	-26.88	100,100,100,100	0
57	MG	1H	3522	1/1	0.90	0.10	-	112,112,112,112	0
57	MG	1H	3425	1/1	0.95	0.04	-	81,81,81,81	0
57	MG	1H	3506	1/1	0.54	0.24	-	103,103,103,103	0
57	MG	14	3019	1/1	0.84	0.35	-	131,131,131,131	0
57	MG	14	3200	1/1	0.90	0.10	-	86,86,86,86	0
57	MG	2K	102	1/1	0.91	0.11	-	99,99,99,99	0
57	MG	14	3235	1/1	0.99	0.09	-	55,55,55,55	0
57	MG	1H	3045	1/1	0.92	0.36	-	63,63,63,63	0
57	MG	1H	3466	1/1	0.85	0.09	-	103,103,103,103	0
57	MG	13	1688	1/1	0.96	0.07	-	96,96,96,96	0
57	MG	1H	3008	1/1	0.69	0.28	-	81,81,81,81	0
57	MG	14	3296	1/1	0.90	0.10	-	76,76,76,76	0
57	MG	1H	3194	1/1	0.81	0.37	-	80,80,80,80	0
57	MG	1H	3529	1/1	0.93	0.10	-	110,110,110,110	0
57	MG	1H	3431	1/1	0.92	0.05	-	102,102,102,102	0
57	MG	13	1689	1/1	0.90	0.22	-	98,98,98,98	0
57	MG	14	3271	1/1	0.97	0.10	-	67,67,67,67	0
57	MG	14	3186	1/1	0.91	0.13	-	95,95,95,95	0
57	MG	1H	3010	1/1	0.80	0.36	-	87,87,87,87	0
57	MG	1H	3071	1/1	0.65	0.25	-	101,101,101,101	0
57	MG	14	3406	1/1	0.73	0.17	-	121,121,121,121	0
57	MG	14	3037	1/1	0.95	0.49	-	54,54,54,54	0
57	MG	1H	3303	1/1	0.97	0.11	-	49,49,49,49	0
57	MG	1H	3435	1/1	0.94	0.30	-	100,100,100,100	0
57	MG	1H	3092	1/1	0.86	0.19	-	67,67,67,67	0
57	MG	1H	3457	1/1	0.96	0.08	-	102,102,102,102	0
57	MG	14	3351	1/1	0.78	0.10	-	101,101,101,101	0
57	MG	1H	3385	1/1	0.89	0.19	-	94,94,94,94	0
57	MG	1G	1710	1/1	0.84	0.08	-	113,113,113,113	0
57	MG	1H	3501	1/1	0.84	0.07	-	108,108,108,108	0
57	MG	1H	3077	1/1	0.76	0.42	-	76,76,76,76	0
57	MG	1H	3480	1/1	0.91	0.28	-	90,90,90,90	0
57	MG	14	3131	1/1	0.91	0.12	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3418	1/1	0.84	0.15	-	122,122,122,122	0
57	MG	14	3282	1/1	0.93	0.10	-	82,82,82,82	0
57	MG	14	3162	1/1	0.82	0.27	-	91,91,91,91	0
57	MG	1H	3441	1/1	0.99	0.07	-	100,100,100,100	0
57	MG	14	3291	1/1	0.90	0.16	-	71,71,71,71	0
57	MG	14	3155	1/1	0.93	0.32	-	83,83,83,83	0
57	MG	14	3207	1/1	0.95	0.49	-	70,70,70,70	0
57	MG	1H	3080	1/1	0.96	0.18	-	75,75,75,75	0
57	MG	1H	3313	1/1	0.81	0.12	-	62,62,62,62	0
57	MG	14	3336	1/1	0.86	0.09	-	109,109,109,109	0
57	MG	1H	3216	1/1	0.85	0.36	-	79,79,79,79	0
57	MG	1G	1616	1/1	0.92	0.24	-	84,84,84,84	0
57	MG	13	1650	1/1	0.86	0.38	-	85,85,85,85	0
57	MG	1H	3223	1/1	0.91	0.27	-	79,79,79,79	0
57	MG	14	3378	1/1	0.92	0.14	-	101,101,101,101	0
57	MG	1H	3059	1/1	0.86	0.14	-	72,72,72,72	0
57	MG	14	3157	1/1	0.94	0.13	-	96,96,96,96	0
57	MG	14	3085	1/1	0.97	0.22	-	52,52,52,52	0
57	MG	13	1623	1/1	0.83	0.20	-	70,70,70,70	0
57	MG	14	3104	1/1	0.89	0.25	-	89,89,89,89	0
57	MG	14	3374	1/1	0.91	0.10	-	94,94,94,94	0
57	MG	14	3088	1/1	0.94	0.43	-	82,82,82,82	0
57	MG	1G	1624	1/1	0.83	0.22	-	103,103,103,103	0
57	MG	1H	3516	1/1	0.96	0.09	-	122,122,122,122	0
57	MG	14	3441	1/1	0.93	0.14	-	103,103,103,103	0
57	MG	1G	1634	1/1	0.71	0.39	-	98,98,98,98	0
57	MG	1H	3277	1/1	0.85	0.14	-	79,79,79,79	0
57	MG	1H	3159	1/1	0.81	0.40	-	95,95,95,95	0
57	MG	14	3367	1/1	0.86	0.10	-	101,101,101,101	0
57	MG	13	1651	1/1	0.89	0.21	-	118,118,118,118	0
57	MG	21	302	1/1	0.80	0.34	-	85,85,85,85	0
57	MG	1G	1698	1/1	0.54	0.07	-	138,138,138,138	0
57	MG	1G	1716	1/1	0.91	0.15	-	110,110,110,110	0
57	MG	14	3175	1/1	0.73	0.54	-	100,100,100,100	0
57	MG	1H	3202	1/1	0.95	0.21	-	80,80,80,80	0
57	MG	1H	3121	1/1	0.94	0.22	-	89,89,89,89	0
57	MG	14	3063	1/1	0.96	0.20	-	93,93,93,93	0
57	MG	14	3361	1/1	0.93	0.17	-	87,87,87,87	0
57	MG	1H	3429	1/1	0.95	0.08	-	87,87,87,87	0
57	MG	14	3250	1/1	0.82	0.11	-	84,84,84,84	0
57	MG	1H	3269	1/1	0.95	0.08	-	83,83,83,83	0
57	MG	1G	1650	1/1	0.80	0.24	-	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3428	1/1	0.82	0.05	-	110,110,110,110	0
57	MG	13	1626	1/1	0.97	0.11	-	96,96,96,96	0
57	MG	13	1608	1/1	0.98	0.07	-	93,93,93,93	0
57	MG	1H	3530	1/1	0.87	0.56	-	99,99,99,99	0
57	MG	1G	1663	1/1	0.88	0.21	-	112,112,112,112	0
57	MG	1H	3346	1/1	0.87	0.10	-	75,75,75,75	0
57	MG	1H	3185	1/1	0.86	0.29	-	76,76,76,76	0
57	MG	1H	3187	1/1	0.89	0.28	-	83,83,83,83	0
57	MG	1H	3310	1/1	0.95	0.06	-	76,76,76,76	0
57	MG	14	3203	1/1	0.85	0.31	-	95,95,95,95	0
57	MG	13	1737	1/1	0.91	0.10	-	107,107,107,107	0
57	MG	1G	1701	1/1	0.71	0.12	-	115,115,115,115	0
57	MG	14	3353	1/1	0.97	0.10	-	89,89,89,89	0
57	MG	25	301	1/1	0.69	0.20	-	120,120,120,120	0
57	MG	1G	1708	1/1	0.94	0.12	-	127,127,127,127	0
57	MG	1H	3153	1/1	0.92	0.34	-	71,71,71,71	0
57	MG	14	3376	1/1	0.90	0.13	-	82,82,82,82	0
57	MG	1H	3260	1/1	0.94	0.07	-	70,70,70,70	0
57	MG	1H	3482	1/1	0.95	0.10	-	107,107,107,107	0
57	MG	1H	3448	1/1	0.95	0.23	-	76,76,76,76	0
57	MG	13	1666	1/1	0.69	0.24	-	98,98,98,98	0
57	MG	14	3387	1/1	0.98	0.06	-	83,83,83,83	0
57	MG	13	1716	1/1	0.86	0.12	-	116,116,116,116	0
57	MG	13	1739	1/1	0.88	0.16	-	119,119,119,119	0
57	MG	14	3429	1/1	0.64	0.31	-	109,109,109,109	0
59	ZN	G8	201	1/1	0.96	0.09	-	150,150,150,150	0
57	MG	35	201	1/1	0.90	0.24	-	81,81,81,81	0
57	MG	1H	3489	1/1	0.61	0.15	-	107,107,107,107	0
57	MG	1H	3192	1/1	0.92	0.25	-	83,83,83,83	0
57	MG	1H	3391	1/1	0.81	0.41	-	90,90,90,90	0
57	MG	1H	3354	1/1	0.87	0.17	-	78,78,78,78	0
57	MG	1H	3513	1/1	0.80	0.14	-	104,104,104,104	0
57	MG	14	3219	1/1	0.98	0.14	-	59,59,59,59	0
57	MG	1H	3295	1/1	0.98	0.12	-	58,58,58,58	0
57	MG	13	1697	1/1	0.95	0.07	-	110,110,110,110	0
57	MG	1H	3363	1/1	0.95	0.14	-	73,73,73,73	0
57	MG	14	3290	1/1	0.92	0.17	-	71,71,71,71	0
57	MG	1H	3109	1/1	0.95	0.67	-	79,79,79,79	0
57	MG	14	3230	1/1	0.95	0.15	-	56,56,56,56	0
57	MG	1H	3037	1/1	0.98	0.11	-	57,57,57,57	0
57	MG	1G	1660	1/1	0.92	0.12	-	128,128,128,128	0
57	MG	13	1656	1/1	0.90	0.27	-	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3195	1/1	0.95	0.23	-	85,85,85,85	0
57	MG	1H	3095	1/1	0.96	0.17	-	76,76,76,76	0
57	MG	1H	3467	1/1	0.98	0.11	-	74,74,74,74	0
57	MG	14	3329	1/1	0.98	0.16	-	93,93,93,93	0
57	MG	13	1613	1/1	0.94	0.18	-	94,94,94,94	0
57	MG	1H	3392	1/1	0.91	0.16	-	74,74,74,74	0
57	MG	1H	3087	1/1	0.66	0.53	-	75,75,75,75	0
57	MG	1G	1631	1/1	0.83	0.10	-	103,103,103,103	0
57	MG	1G	1697	1/1	0.80	0.09	-	125,125,125,125	0
57	MG	1H	3356	1/1	0.95	0.15	-	79,79,79,79	0
57	MG	13	1603	1/1	0.97	0.22	-	92,92,92,92	0
57	MG	14	3393	1/1	0.95	0.08	-	89,89,89,89	0
57	MG	14	3451	1/1	0.78	0.34	-	110,110,110,110	0
57	MG	1H	3005	1/1	1.00	0.15	-	67,67,67,67	0
57	MG	14	3276	1/1	0.82	0.08	-	85,85,85,85	0
57	MG	31	301	1/1	0.87	0.15	-	70,70,70,70	0
57	MG	1H	3339	1/1	0.88	0.06	-	99,99,99,99	0
57	MG	1G	1652	1/1	0.89	0.18	-	105,105,105,105	0
57	MG	1H	3334	1/1	0.88	0.18	-	103,103,103,103	0
57	MG	1H	3085	1/1	0.66	0.34	-	79,79,79,79	0
57	MG	14	3380	1/1	0.86	0.12	-	106,106,106,106	0
57	MG	14	3173	1/1	0.71	0.26	-	90,90,90,90	0
57	MG	1G	1633	1/1	0.80	0.12	-	102,102,102,102	0
57	MG	13	1682	1/1	0.92	0.04	-	109,109,109,109	0
57	MG	1H	3445	1/1	0.88	0.32	-	87,87,87,87	0
57	MG	1H	3549	1/1	0.95	0.15	-	94,94,94,94	0
57	MG	14	3151	1/1	0.96	0.15	-	108,108,108,108	0
57	MG	1G	1723	1/1	0.45	0.19	-	127,127,127,127	0
57	MG	1G	1713	1/1	0.92	0.20	-	120,120,120,120	0
57	MG	1H	3412	1/1	0.84	0.07	-	90,90,90,90	0
57	MG	1H	3180	1/1	0.62	0.34	-	81,81,81,81	0
57	MG	1H	3170	1/1	0.77	0.23	-	80,80,80,80	0
57	MG	1H	3165	1/1	0.83	0.23	-	85,85,85,85	0
57	MG	13	1647	1/1	0.84	0.38	-	99,99,99,99	0
57	MG	14	3249	1/1	0.95	0.06	-	85,85,85,85	0
57	MG	14	3267	1/1	0.81	0.07	-	119,119,119,119	0
57	MG	14	3435	1/1	0.94	0.05	-	122,122,122,122	0
57	MG	14	3297	1/1	0.95	0.08	-	90,90,90,90	0
57	MG	14	3215	1/1	0.87	0.08	-	98,98,98,98	0
57	MG	1H	3378	1/1	0.98	0.08	-	54,54,54,54	0
57	MG	14	3099	1/1	0.97	0.55	-	101,101,101,101	0
57	MG	13	1701	1/1	0.94	0.09	-	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3452	1/1	0.46	0.10	-	115,115,115,115	0
57	MG	14	3422	1/1	0.80	0.12	-	104,104,104,104	0
57	MG	1G	1692	1/1	0.92	0.07	-	103,103,103,103	0
57	MG	14	3048	1/1	0.95	0.13	-	72,72,72,72	0
57	MG	1G	1676	1/1	0.96	0.14	-	104,104,104,104	0
57	MG	14	3277	1/1	0.97	0.06	-	64,64,64,64	0
57	MG	1H	3540	1/1	0.76	0.45	-	110,110,110,110	0
57	MG	14	3363	1/1	0.91	0.05	-	83,83,83,83	0
57	MG	1G	1695	1/1	0.88	0.13	-	126,126,126,126	0
57	MG	1J	207	1/1	0.77	0.09	-	119,119,119,119	0
57	MG	1H	3526	1/1	0.94	0.20	-	96,96,96,96	0
57	MG	14	3116	1/1	0.79	0.20	-	77,77,77,77	0
57	MG	1H	3290	1/1	0.96	0.09	-	87,87,87,87	0
57	MG	1H	3545	1/1	0.91	0.47	-	102,102,102,102	0
57	MG	1H	3106	1/1	0.97	0.09	-	73,73,73,73	0
57	MG	1H	3309	1/1	0.88	0.07	-	73,73,73,73	0
57	MG	16	210	1/1	0.87	0.37	-	86,86,86,86	0
57	MG	1H	3440	1/1	0.98	0.05	-	83,83,83,83	0
57	MG	1H	3379	1/1	0.89	0.13	-	87,87,87,87	0
57	MG	14	3301	1/1	0.76	0.11	-	89,89,89,89	0
57	MG	14	3012	1/1	0.95	0.32	-	69,69,69,69	0
57	MG	F8	101	1/1	0.94	0.14	-	85,85,85,85	0
57	MG	1H	3528	1/1	0.84	0.12	-	117,117,117,117	0
57	MG	13	1726	1/1	0.96	0.05	-	107,107,107,107	0
57	MG	1H	3078	1/1	0.91	0.34	-	85,85,85,85	0
57	MG	1H	3447	1/1	0.95	0.04	-	98,98,98,98	0
57	MG	1H	3342	1/1	0.91	0.10	-	83,83,83,83	0
57	MG	1H	3359	1/1	0.94	0.04	-	92,92,92,92	0
57	MG	1H	3345	1/1	0.96	0.06	-	85,85,85,85	0
57	MG	1H	3197	1/1	0.51	0.38	-	93,93,93,93	0
57	MG	1H	3552	1/1	0.74	0.22	-	113,113,113,113	0
57	MG	1H	3487	1/1	0.85	0.04	-	108,108,108,108	0
57	MG	1H	3011	1/1	0.97	0.21	-	79,79,79,79	0
57	MG	14	3355	1/1	0.62	0.20	-	99,99,99,99	0
57	MG	88	203	1/1	0.86	0.32	-	83,83,83,83	0
57	MG	1H	3117	1/1	0.66	0.18	-	96,96,96,96	0
57	MG	14	3028	1/1	0.95	0.25	-	67,67,67,67	0
57	MG	14	3390	1/1	0.87	0.09	-	73,73,73,73	0
57	MG	1H	3537	1/1	0.72	0.11	-	112,112,112,112	0
57	MG	1H	3366	1/1	0.96	0.12	-	56,56,56,56	0
57	MG	1H	3327	1/1	0.95	0.13	-	81,81,81,81	0
57	MG	14	3047	1/1	0.88	0.12	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3341	1/1	0.62	0.14	-	113,113,113,113	0
57	MG	1G	1618	1/1	0.92	0.12	-	91,91,91,91	0
57	MG	1H	3325	1/1	0.76	0.10	-	88,88,88,88	0
57	MG	1G	1620	1/1	0.46	0.63	-	93,93,93,93	0
57	MG	1H	3524	1/1	0.93	0.17	-	61,61,61,61	0
57	MG	14	3254	1/1	0.96	0.12	-	87,87,87,87	0
57	MG	13	1715	1/1	0.51	0.17	-	119,119,119,119	0
57	MG	14	3122	1/1	0.97	0.14	-	90,90,90,90	0
57	MG	14	3140	1/1	0.79	0.32	-	89,89,89,89	0
57	MG	14	3284	1/1	0.85	0.29	-	107,107,107,107	0
57	MG	1G	1645	1/1	0.96	0.21	-	124,124,124,124	0
57	MG	14	3231	1/1	0.91	0.13	-	78,78,78,78	0
57	MG	1H	3409	1/1	0.98	0.10	-	83,83,83,83	0
57	MG	14	3011	1/1	0.89	0.57	-	76,76,76,76	0
57	MG	1H	3114	1/1	0.93	0.16	-	71,71,71,71	0
57	MG	14	3199	1/1	0.51	0.55	-	99,99,99,99	0
57	MG	13	1664	1/1	0.94	0.24	-	91,91,91,91	0
57	MG	1H	3484	1/1	0.53	0.29	-	97,97,97,97	0
57	MG	1H	3204	1/1	0.91	0.28	-	80,80,80,80	0
57	MG	1H	3422	1/1	0.68	0.11	-	114,114,114,114	0
57	MG	1H	3322	1/1	0.98	0.10	-	59,59,59,59	0
57	MG	14	3330	1/1	0.92	0.06	-	94,94,94,94	0
57	MG	88	202	1/1	0.77	0.31	-	71,71,71,71	0
57	MG	1G	1666	1/1	0.95	0.17	-	110,110,110,110	0
57	MG	14	3262	1/1	0.84	0.10	-	104,104,104,104	0
57	MG	1G	1628	1/1	0.84	0.23	-	123,123,123,123	0
57	MG	1G	1657	1/1	0.94	0.10	-	114,114,114,114	0
57	MG	1G	1681	1/1	0.90	0.12	-	131,131,131,131	0
57	MG	1G	1661	1/1	0.98	0.23	-	118,118,118,118	0
57	MG	14	3371	1/1	0.85	0.10	-	108,108,108,108	0
57	MG	1H	3081	1/1	0.90	0.15	-	77,77,77,77	0
57	MG	14	3021	1/1	0.98	0.36	-	63,63,63,63	0
57	MG	1H	3424	1/1	0.95	0.15	-	84,84,84,84	0
57	MG	14	3139	1/1	0.93	0.84	-	88,88,88,88	0
57	MG	1H	3148	1/1	0.94	0.13	-	88,88,88,88	0
57	MG	1H	3076	1/1	0.95	0.37	-	75,75,75,75	0
57	MG	14	3146	1/1	0.96	0.09	-	62,62,62,62	0
57	MG	1H	3166	1/1	0.58	0.22	-	67,67,67,67	0
57	MG	4L	101	1/1	0.85	0.43	-	102,102,102,102	0
57	MG	14	3233	1/1	0.91	0.11	-	85,85,85,85	0
57	MG	1H	3016	1/1	0.97	0.35	-	52,52,52,52	0
57	MG	1H	3186	1/1	0.99	0.09	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3079	1/1	0.94	0.17	-	85,85,85,85	0
57	MG	1H	3415	1/1	0.79	0.12	-	95,95,95,95	0
57	MG	1H	3404	1/1	0.92	0.67	-	71,71,71,71	0
57	MG	14	3357	1/1	0.92	0.08	-	116,116,116,116	0
57	MG	1H	3042	1/1	0.80	0.28	-	67,67,67,67	0
57	MG	1H	3023	1/1	0.90	0.30	-	71,71,71,71	0
57	MG	14	3314	1/1	0.88	0.19	-	78,78,78,78	0
57	MG	13	1712	1/1	0.76	0.07	-	106,106,106,106	0
57	MG	1H	3108	1/1	0.88	0.36	-	68,68,68,68	0
57	MG	1H	3161	1/1	0.81	0.35	-	77,77,77,77	0
57	MG	13	1733	1/1	0.90	0.05	-	118,118,118,118	0
57	MG	1H	3515	1/1	0.95	0.12	-	78,78,78,78	0
57	MG	14	3188	1/1	0.98	0.23	-	69,69,69,69	0
57	MG	1G	1621	1/1	0.87	0.46	-	105,105,105,105	0
57	MG	32	301	1/1	0.62	0.12	-	137,137,137,137	0
57	MG	14	3090	1/1	0.94	0.27	-	77,77,77,77	0
57	MG	14	3283	1/1	0.95	0.06	-	105,105,105,105	0
57	MG	1H	3220	1/1	0.96	0.22	-	71,71,71,71	0
57	MG	1H	3094	1/1	0.88	0.23	-	64,64,64,64	0
57	MG	42	201	1/1	0.89	0.28	-	107,107,107,107	0
57	MG	1H	3331	1/1	0.95	0.06	-	88,88,88,88	0
57	MG	14	3323	1/1	0.96	0.10	-	84,84,84,84	0
57	MG	14	3389	1/1	0.90	0.18	-	72,72,72,72	0
57	MG	1H	3221	1/1	0.75	0.38	-	81,81,81,81	0
57	MG	1H	3196	1/1	0.89	0.22	-	103,103,103,103	0
57	MG	14	3334	1/1	0.91	0.09	-	83,83,83,83	0
57	MG	1H	3152	1/1	0.70	0.28	-	87,87,87,87	0
57	MG	1H	3164	1/1	0.96	0.44	-	85,85,85,85	0
57	MG	1H	3122	1/1	0.86	0.39	-	80,80,80,80	0
57	MG	1H	3473	1/1	0.89	0.13	-	98,98,98,98	0
57	MG	14	3354	1/1	0.95	0.12	-	80,80,80,80	0
57	MG	1G	1704	1/1	0.70	0.21	-	127,127,127,127	0
57	MG	45	201	1/1	0.90	0.69	-	84,84,84,84	0
57	MG	1J	210	1/1	0.80	0.08	-	135,135,135,135	0
57	MG	13	1633	1/1	0.89	0.13	-	82,82,82,82	0
57	MG	14	3144	1/1	0.76	0.40	-	84,84,84,84	0
57	MG	14	3430	1/1	0.79	0.23	-	102,102,102,102	0
57	MG	14	3333	1/1	0.63	0.19	-	97,97,97,97	0
57	MG	14	3220	1/1	0.96	0.08	-	65,65,65,65	0
57	MG	13	1704	1/1	0.93	0.38	-	111,111,111,111	0
57	MG	7A	101	1/1	0.98	0.32	-	110,110,110,110	0
57	MG	1H	3210	1/1	0.64	0.34	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3245	1/1	0.99	0.11	-	58,58,58,58	0
57	MG	14	3300	1/1	0.78	0.08	-	86,86,86,86	0
57	MG	1H	3419	1/1	0.92	0.26	-	73,73,73,73	0
57	MG	1G	1649	1/1	0.87	0.81	-	96,96,96,96	0
57	MG	14	3382	1/1	0.89	0.08	-	116,116,116,116	0
57	MG	1H	3199	1/1	0.92	0.14	-	81,81,81,81	0
57	MG	1H	3233	1/1	0.90	0.20	-	94,94,94,94	0
57	MG	1H	3504	1/1	0.73	0.29	-	104,104,104,104	0
57	MG	14	3197	1/1	0.92	0.42	-	92,92,92,92	0
57	MG	1H	3255	1/1	0.95	0.12	-	72,72,72,72	0
57	MG	14	3316	1/1	0.94	0.07	-	100,100,100,100	0
57	MG	1H	3444	1/1	0.88	0.24	-	72,72,72,72	0
57	MG	13	1680	1/1	0.88	0.12	-	89,89,89,89	0
57	MG	1G	1638	1/1	0.70	0.34	-	119,119,119,119	0
57	MG	1H	3371	1/1	0.63	0.15	-	88,88,88,88	0
57	MG	1H	3475	1/1	0.84	0.05	-	99,99,99,99	0
57	MG	1H	3241	1/1	0.73	0.20	-	82,82,82,82	0
57	MG	1H	3061	1/1	0.99	0.38	-	62,62,62,62	0
57	MG	13	1642	1/1	0.69	0.30	-	95,95,95,95	0
57	MG	1H	3361	1/1	0.97	0.07	-	53,53,53,53	0
57	MG	1H	3280	1/1	0.90	0.14	-	47,47,47,47	0
57	MG	14	3340	1/1	0.94	0.09	-	63,63,63,63	0
57	MG	1G	1642	1/1	0.85	0.70	-	100,100,100,100	0
57	MG	14	3195	1/1	0.89	0.35	-	98,98,98,98	0
57	MG	1G	1602	1/1	0.95	0.33	-	105,105,105,105	0
57	MG	14	3411	1/1	0.91	0.07	-	115,115,115,115	0
57	MG	14	3201	1/1	0.98	0.29	-	82,82,82,82	0
57	MG	1H	3352	1/1	0.97	0.08	-	70,70,70,70	0
57	MG	1H	3097	1/1	0.94	0.22	-	43,43,43,43	0
57	MG	1H	3349	1/1	0.96	0.06	-	61,61,61,61	0
57	MG	1H	3285	1/1	0.98	0.16	-	69,69,69,69	0
57	MG	14	3362	1/1	0.92	0.10	-	99,99,99,99	0
57	MG	13	1654	1/1	0.76	0.34	-	85,85,85,85	0
57	MG	1H	3433	1/1	0.69	0.10	-	98,98,98,98	0
57	MG	14	3331	1/1	0.97	0.14	-	56,56,56,56	0
57	MG	1H	3494	1/1	0.78	0.20	-	87,87,87,87	0
57	MG	14	3043	1/1	0.98	0.70	-	96,96,96,96	0
57	MG	13	1681	1/1	0.93	0.20	-	91,91,91,91	0
57	MG	1G	1678	1/1	0.88	0.16	-	98,98,98,98	0
57	MG	1H	3176	1/1	0.32	0.41	-	102,102,102,102	0
57	MG	1G	1686	1/1	0.93	0.08	-	113,113,113,113	0
57	MG	1H	3360	1/1	0.86	0.13	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3174	1/1	0.90	0.25	-	78,78,78,78	0
57	MG	1H	3305	1/1	0.94	0.15	-	72,72,72,72	0
57	MG	14	3257	1/1	0.82	0.19	-	118,118,118,118	0
57	MG	14	3226	1/1	0.97	0.17	-	54,54,54,54	0
57	MG	14	3202	1/1	0.94	0.15	-	106,106,106,106	0
57	MG	1H	3436	1/1	0.81	0.10	-	87,87,87,87	0
57	MG	14	3346	1/1	0.91	0.09	-	98,98,98,98	0
57	MG	1H	3517	1/1	0.93	0.30	-	85,85,85,85	0
57	MG	1H	3536	1/1	0.63	0.17	-	104,104,104,104	0
57	MG	1H	3246	1/1	0.81	0.17	-	54,54,54,54	0
57	MG	14	3117	1/1	0.84	0.34	-	69,69,69,69	0
57	MG	1H	3151	1/1	0.91	0.28	-	79,79,79,79	0
57	MG	1H	3442	1/1	0.90	0.12	-	107,107,107,107	0
57	MG	14	3167	1/1	0.89	0.07	-	95,95,95,95	0
57	MG	1H	3050	1/1	0.75	0.36	-	85,85,85,85	0
57	MG	1H	3184	1/1	0.85	0.64	-	100,100,100,100	0
57	MG	1G	1718	1/1	0.87	0.10	-	124,124,124,124	0
57	MG	1H	3499	1/1	0.90	0.27	-	89,89,89,89	0
57	MG	1H	3510	1/1	0.77	0.07	-	104,104,104,104	0
57	MG	1H	3490	1/1	0.88	0.08	-	95,95,95,95	0
57	MG	14	3101	1/1	0.95	0.21	-	87,87,87,87	0
57	MG	14	3014	1/1	0.99	0.36	-	72,72,72,72	0
57	MG	1H	3384	1/1	0.85	0.10	-	59,59,59,59	0
57	MG	1H	3211	1/1	0.87	0.36	-	69,69,69,69	0
57	MG	14	3450	1/1	0.79	0.31	-	116,116,116,116	0
57	MG	1H	3287	1/1	0.95	0.10	-	76,76,76,76	0
57	MG	14	3153	1/1	0.50	0.23	-	123,123,123,123	0
57	MG	14	3453	1/1	0.55	0.20	-	118,118,118,118	0
57	MG	13	1641	1/1	0.82	0.45	-	79,79,79,79	0
57	MG	1H	3146	1/1	0.86	0.42	-	85,85,85,85	0
57	MG	1H	3060	1/1	0.82	0.54	-	90,90,90,90	0
57	MG	1H	3236	1/1	0.95	0.16	-	93,93,93,93	0
57	MG	14	3446	1/1	0.71	0.07	-	118,118,118,118	0
57	MG	14	3292	1/1	0.98	0.06	-	71,71,71,71	0
57	MG	1H	3301	1/1	0.87	0.18	-	86,86,86,86	0
57	MG	14	3183	1/1	0.77	0.45	-	88,88,88,88	0
57	MG	42	202	1/1	0.85	0.26	-	115,115,115,115	0
57	MG	14	3386	1/1	0.92	0.12	-	65,65,65,65	0
57	MG	14	3342	1/1	0.91	0.12	-	105,105,105,105	0
57	MG	14	3015	1/1	0.97	0.14	-	65,65,65,65	0
57	MG	1H	3535	1/1	0.71	0.20	-	110,110,110,110	0
57	MG	1H	3402	1/1	0.54	0.20	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3129	1/1	0.94	0.21	-	90,90,90,90	0
57	MG	14	3448	1/1	0.81	0.10	-	120,120,120,120	0
57	MG	1H	3140	1/1	0.88	0.20	-	90,90,90,90	0
57	MG	1J	205	1/1	0.81	0.12	-	101,101,101,101	0
57	MG	1H	3175	1/1	0.68	0.38	-	73,73,73,73	0
57	MG	1H	3453	1/1	0.91	0.19	-	82,82,82,82	0
57	MG	1H	3502	1/1	0.79	0.12	-	90,90,90,90	0
57	MG	14	3141	1/1	0.69	0.20	-	85,85,85,85	0
57	MG	1H	3347	1/1	0.14	0.12	-	113,113,113,113	0
57	MG	14	3421	1/1	0.89	0.23	-	96,96,96,96	0
57	MG	1H	3013	1/1	0.60	0.18	-	94,94,94,94	0
57	MG	14	3115	1/1	0.76	0.45	-	78,78,78,78	0
57	MG	14	3073	1/1	0.88	0.43	-	61,61,61,61	0
57	MG	14	3426	1/1	0.91	0.06	-	99,99,99,99	0
57	MG	1H	3350	1/1	0.91	0.12	-	58,58,58,58	0
57	MG	14	3072	1/1	0.85	0.26	-	88,88,88,88	0
57	MG	1H	3423	1/1	0.91	0.08	-	115,115,115,115	0
57	MG	14	3185	1/1	0.73	0.25	-	93,93,93,93	0
57	MG	1H	3542	1/1	0.88	0.07	-	103,103,103,103	0
57	MG	1H	3129	1/1	0.86	0.12	-	85,85,85,85	0
57	MG	13	1707	1/1	0.91	0.06	-	88,88,88,88	0
57	MG	13	1702	1/1	0.96	0.08	-	70,70,70,70	0
57	MG	13	1621	1/1	0.79	0.47	-	94,94,94,94	0
57	MG	1H	3311	1/1	0.87	0.10	-	91,91,91,91	0
57	MG	21	303	1/1	0.88	0.12	-	61,61,61,61	0
57	MG	13	1691	1/1	0.89	0.09	-	107,107,107,107	0
57	MG	14	3317	1/1	0.97	0.05	-	100,100,100,100	0
57	MG	14	3187	1/1	0.73	0.46	-	106,106,106,106	0
57	MG	1H	3474	1/1	0.92	0.09	-	83,83,83,83	0
57	MG	1H	3523	1/1	0.86	0.17	-	102,102,102,102	0
57	MG	13	1604	1/1	0.98	0.13	-	79,79,79,79	0
57	MG	1G	1721	1/1	0.87	0.06	-	128,128,128,128	0
57	MG	1H	3405	1/1	0.94	0.10	-	75,75,75,75	0
57	MG	14	3053	1/1	0.84	0.92	-	82,82,82,82	0
57	MG	13	1617	1/1	0.84	0.37	-	69,69,69,69	0
57	MG	14	3417	1/1	0.87	0.07	-	117,117,117,117	0
57	MG	1G	1659	1/1	0.80	0.10	-	120,120,120,120	0
57	MG	13	1719	1/1	0.70	0.07	-	118,118,118,118	0
57	MG	14	3204	1/1	0.85	0.13	-	120,120,120,120	0
57	MG	1H	3018	1/1	0.96	0.34	-	63,63,63,63	0
57	MG	1H	3458	1/1	0.87	0.12	-	89,89,89,89	0
57	MG	1H	3411	1/1	0.77	0.17	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	13	1718	1/1	0.80	0.04	-	130,130,130,130	0
57	MG	14	3410	1/1	0.96	0.14	-	107,107,107,107	0
57	MG	14	3419	1/1	0.95	0.27	-	119,119,119,119	0
57	MG	14	3414	1/1	0.82	0.11	-	99,99,99,99	0
57	MG	14	3205	1/1	0.92	0.11	-	102,102,102,102	0
57	MG	1H	3399	1/1	0.80	0.07	-	109,109,109,109	0
57	MG	14	3006	1/1	0.97	0.18	-	78,78,78,78	0
57	MG	1G	1637	1/1	0.94	0.38	-	106,106,106,106	0
57	MG	29	301	1/1	0.95	0.28	-	65,65,65,65	0
57	MG	1H	3340	1/1	0.91	0.05	-	109,109,109,109	0
57	MG	14	3434	1/1	0.86	0.32	-	110,110,110,110	0
57	MG	1G	1609	1/1	0.68	0.66	-	96,96,96,96	0
57	MG	1H	3089	1/1	0.67	0.43	-	88,88,88,88	0
57	MG	14	3148	1/1	0.89	0.18	-	113,113,113,113	0
57	MG	14	3041	1/1	0.97	0.29	-	66,66,66,66	0
57	MG	1G	1705	1/1	0.92	0.03	-	117,117,117,117	0
57	MG	1H	3271	1/1	0.86	0.14	-	84,84,84,84	0
57	MG	14	3432	1/1	0.96	0.25	-	103,103,103,103	0
57	MG	14	3457	1/1	0.73	0.09	-	134,134,134,134	0
57	MG	14	3412	1/1	0.94	0.16	-	106,106,106,106	0
57	MG	14	3070	1/1	0.96	0.64	-	66,66,66,66	0
57	MG	13	1627	1/1	0.87	0.17	-	94,94,94,94	0
57	MG	13	1672	1/1	0.89	0.30	-	92,92,92,92	0
57	MG	1H	3493	1/1	0.47	0.17	-	106,106,106,106	0
57	MG	1H	3323	1/1	0.91	0.06	-	78,78,78,78	0
57	MG	1H	3507	1/1	0.94	0.15	-	90,90,90,90	0
57	MG	1H	3381	1/1	0.97	0.14	-	58,58,58,58	0
57	MG	13	1655	1/1	0.62	0.42	-	83,83,83,83	0
57	MG	14	3407	1/1	0.94	0.19	-	111,111,111,111	0
57	MG	13	1685	1/1	0.90	0.07	-	79,79,79,79	0
57	MG	1H	3481	1/1	0.69	0.15	-	92,92,92,92	0
57	MG	13	1720	1/1	0.83	0.06	-	121,121,121,121	0
57	MG	14	3279	1/1	0.92	0.10	-	93,93,93,93	0
57	MG	3I	201	1/1	0.95	0.24	-	75,75,75,75	0
57	MG	1H	3235	1/1	0.78	0.22	-	96,96,96,96	0
57	MG	1G	1683	1/1	0.90	0.09	-	132,132,132,132	0
57	MG	13	1740	1/1	0.70	0.14	-	162,162,162,162	0
57	MG	1G	1668	1/1	0.94	0.10	-	106,106,106,106	0
57	MG	14	3264	1/1	0.84	0.14	-	88,88,88,88	0
57	MG	1H	3032	1/1	0.98	0.36	-	68,68,68,68	0
57	MG	1H	3387	1/1	0.92	0.08	-	87,87,87,87	0
57	MG	13	1636	1/1	0.93	0.25	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3260	1/1	0.91	0.16	-	77,77,77,77	0
57	MG	P8	101	1/1	0.72	0.46	-	76,76,76,76	0
57	MG	1H	3376	1/1	0.96	0.10	-	71,71,71,71	0
57	MG	1H	3533	1/1	0.83	0.34	-	99,99,99,99	0
57	MG	1G	1615	1/1	0.84	0.15	-	89,89,89,89	0
57	MG	1H	3400	1/1	0.88	0.10	-	79,79,79,79	0
57	MG	14	3408	1/1	0.98	0.07	-	77,77,77,77	0
57	MG	13	1657	1/1	0.94	0.58	-	75,75,75,75	0
57	MG	14	3327	1/1	0.92	0.07	-	108,108,108,108	0
57	MG	14	3244	1/1	0.97	0.06	-	68,68,68,68	0
57	MG	1H	3004	1/1	0.95	0.26	-	64,64,64,64	0
57	MG	1H	3173	1/1	0.67	0.33	-	77,77,77,77	0
57	MG	14	3107	1/1	0.96	0.58	-	94,94,94,94	0
57	MG	14	3196	1/1	0.88	0.46	-	85,85,85,85	0
57	MG	14	3366	1/1	0.98	0.04	-	99,99,99,99	0
57	MG	1H	3477	1/1	0.82	0.17	-	91,91,91,91	0
57	MG	14	3056	1/1	0.97	0.37	-	74,74,74,74	0
57	MG	1G	1672	1/1	0.86	0.04	-	117,117,117,117	0
57	MG	1G	1635	1/1	0.91	0.29	-	94,94,94,94	0
57	MG	1H	3370	1/1	0.87	0.15	-	80,80,80,80	0
57	MG	1H	3547	1/1	0.90	0.06	-	131,131,131,131	0
57	MG	1H	3024	1/1	0.98	0.17	-	64,64,64,64	0
57	MG	13	1736	1/1	0.66	0.12	-	129,129,129,129	0
57	MG	1G	1684	1/1	0.76	0.07	-	109,109,109,109	0
57	MG	1H	3521	1/1	0.95	0.09	-	65,65,65,65	0
57	MG	14	3401	1/1	0.96	0.20	-	89,89,89,89	0
57	MG	1H	3135	1/1	0.87	0.31	-	73,73,73,73	0
57	MG	1H	3449	1/1	0.98	0.25	-	92,92,92,92	0
57	MG	1H	3353	1/1	0.91	0.12	-	62,62,62,62	0
57	MG	1H	3214	1/1	0.99	0.17	-	77,77,77,77	0
57	MG	1H	3083	1/1	0.91	0.44	-	80,80,80,80	0
57	MG	1H	3344	1/1	0.97	0.09	-	60,60,60,60	0
57	MG	1H	3254	1/1	0.97	0.14	-	49,49,49,49	0
57	MG	14	3138	1/1	0.68	0.45	-	91,91,91,91	0
57	MG	14	3003	1/1	0.97	0.17	-	68,68,68,68	0
57	MG	1H	3064	1/1	0.89	0.28	-	82,82,82,82	0
57	MG	1H	3395	1/1	0.93	0.07	-	92,92,92,92	0
57	MG	14	3255	1/1	0.76	0.12	-	110,110,110,110	0
57	MG	1H	3337	1/1	0.68	0.07	-	98,98,98,98	0
57	MG	14	3171	1/1	0.94	0.47	-	86,86,86,86	0
57	MG	1H	3465	1/1	0.91	0.09	-	112,112,112,112	0
57	MG	1H	3031	1/1	0.96	0.33	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3188	1/1	0.83	0.35	-	88,88,88,88	0
57	MG	14	3067	1/1	0.91	0.22	-	77,77,77,77	0
57	MG	1G	1612	1/1	0.84	0.11	-	103,103,103,103	0
57	MG	1G	1706	1/1	0.74	0.05	-	138,138,138,138	0
57	MG	1H	3483	1/1	0.95	0.06	-	99,99,99,99	0
57	MG	1H	3147	1/1	0.76	0.39	-	125,125,125,125	0
57	MG	14	3324	1/1	0.81	0.09	-	90,90,90,90	0
57	MG	1H	3091	1/1	0.83	0.64	-	77,77,77,77	0
57	MG	14	3112	1/1	0.93	0.46	-	68,68,68,68	0
57	MG	13	1684	1/1	0.72	0.10	-	105,105,105,105	0
57	MG	14	3084	1/1	0.97	0.27	-	67,67,67,67	0
57	MG	1H	3386	1/1	0.96	0.21	-	72,72,72,72	0
57	MG	1G	1613	1/1	0.81	0.95	-	93,93,93,93	0
57	MG	1J	201	1/1	0.91	0.22	-	97,97,97,97	0
57	MG	1H	3332	1/1	0.96	0.10	-	84,84,84,84	0
57	MG	1H	3304	1/1	0.92	0.20	-	64,64,64,64	0
57	MG	1G	1696	1/1	0.80	0.10	-	109,109,109,109	0
57	MG	1H	3104	1/1	0.94	0.16	-	68,68,68,68	0
57	MG	1H	3096	1/1	0.94	0.39	-	83,83,83,83	0
57	MG	14	3306	1/1	0.86	0.17	-	93,93,93,93	0
57	MG	2K	103	1/1	0.68	0.18	-	88,88,88,88	0
57	MG	1H	3105	1/1	0.91	0.18	-	78,78,78,78	0
57	MG	1H	3252	1/1	0.97	0.07	-	52,52,52,52	0
57	MG	1G	1639	1/1	0.89	0.69	-	90,90,90,90	0
57	MG	14	3344	1/1	0.89	0.07	-	104,104,104,104	0
57	MG	1H	3212	1/1	0.89	0.09	-	87,87,87,87	0
57	MG	1G	1640	1/1	0.95	0.40	-	80,80,80,80	0
57	MG	14	3158	1/1	0.79	0.25	-	84,84,84,84	0
57	MG	14	3193	1/1	0.93	0.44	-	96,96,96,96	0
57	MG	13	1727	1/1	0.80	0.07	-	124,124,124,124	0
57	MG	1H	3143	1/1	0.91	0.24	-	79,79,79,79	0
57	MG	14	3211	1/1	0.85	0.09	-	67,67,67,67	0
57	MG	13	1738	1/1	0.84	0.05	-	138,138,138,138	0
57	MG	14	3358	1/1	0.94	0.04	-	78,78,78,78	0
57	MG	1H	3312	1/1	0.93	0.21	-	69,69,69,69	0
57	MG	14	3449	1/1	0.93	0.06	-	105,105,105,105	0
57	MG	1H	3213	1/1	0.68	0.22	-	83,83,83,83	0
57	MG	1G	1611	1/1	0.79	0.62	-	84,84,84,84	0
57	MG	14	3332	1/1	0.97	0.16	-	63,63,63,63	0
57	MG	14	3400	1/1	0.80	0.08	-	135,135,135,135	0
57	MG	14	3025	1/1	0.84	0.24	-	78,78,78,78	0
57	MG	14	3110	1/1	0.93	0.24	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3349	1/1	0.91	0.07	-	99,99,99,99	0
57	MG	14	3341	1/1	0.76	0.32	-	78,78,78,78	0
57	MG	14	3431	1/1	0.69	0.17	-	107,107,107,107	0
57	MG	1H	3014	1/1	0.85	0.42	-	86,86,86,86	0
57	MG	14	3347	1/1	0.88	0.14	-	97,97,97,97	0
57	MG	13	1653	1/1	0.89	0.12	-	95,95,95,95	0
59	ZN	C5	201	1/1	0.96	0.05	-	167,167,167,167	0
57	MG	14	3321	1/1	0.90	0.12	-	89,89,89,89	0
57	MG	1H	3479	1/1	0.98	0.05	-	95,95,95,95	0
57	MG	14	3172	1/1	0.98	0.21	-	82,82,82,82	0
57	MG	13	1700	1/1	0.80	0.06	-	110,110,110,110	0
57	MG	14	3128	1/1	0.76	0.36	-	88,88,88,88	0
57	MG	1G	1711	1/1	0.59	0.06	-	156,156,156,156	0
57	MG	1H	3469	1/1	0.93	0.05	-	84,84,84,84	0
57	MG	14	3373	1/1	0.84	0.19	-	94,94,94,94	0
57	MG	1H	3495	1/1	0.90	0.08	-	87,87,87,87	0
57	MG	1H	3139	1/1	0.91	0.50	-	90,90,90,90	0
57	MG	14	3295	1/1	0.88	0.11	-	88,88,88,88	0
57	MG	1H	3227	1/1	0.76	0.19	-	90,90,90,90	0
57	MG	1H	3314	1/1	0.94	0.15	-	65,65,65,65	0
57	MG	14	3163	1/1	0.44	0.45	-	104,104,104,104	0
57	MG	1H	3217	1/1	0.80	0.39	-	79,79,79,79	0
57	MG	14	3312	1/1	0.90	0.09	-	109,109,109,109	0
57	MG	1H	3222	1/1	0.81	0.46	-	86,86,86,86	0
57	MG	14	3001	1/1	0.94	0.16	-	51,51,51,51	0
57	MG	1H	3367	1/1	0.93	0.09	-	69,69,69,69	0
57	MG	14	3154	1/1	0.75	0.33	-	78,78,78,78	0
57	MG	13	1725	1/1	0.85	0.05	-	99,99,99,99	0
57	MG	1H	3022	1/1	0.97	0.17	-	56,56,56,56	0
57	MG	1H	3056	1/1	0.84	0.47	-	86,86,86,86	0
57	MG	1G	1719	1/1	0.95	0.09	-	115,115,115,115	0
57	MG	1H	3267	1/1	0.93	0.06	-	103,103,103,103	0
57	MG	1H	3262	1/1	0.94	0.14	-	59,59,59,59	0
57	MG	16	203	1/1	0.95	0.28	-	84,84,84,84	0
57	MG	14	3176	1/1	0.94	0.51	-	90,90,90,90	0
57	MG	1H	3232	1/1	0.74	0.38	-	100,100,100,100	0
57	MG	14	3345	1/1	0.86	0.15	-	100,100,100,100	0
57	MG	14	3438	1/1	0.90	0.13	-	111,111,111,111	0
57	MG	14	3447	1/1	0.94	0.07	-	107,107,107,107	0
57	MG	14	3004	1/1	0.94	0.35	-	81,81,81,81	0
57	MG	1G	1707	1/1	0.83	0.08	-	115,115,115,115	0
57	MG	1G	1717	1/1	0.95	0.06	-	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3413	1/1	0.52	0.17	-	125,125,125,125	0
57	MG	1H	3491	1/1	0.84	0.23	-	100,100,100,100	0
57	MG	1H	3355	1/1	0.93	0.18	-	58,58,58,58	0
57	MG	1H	3362	1/1	0.87	0.13	-	78,78,78,78	0
57	MG	14	3213	1/1	0.98	0.12	-	70,70,70,70	0
57	MG	1H	3120	1/1	0.96	0.37	-	69,69,69,69	0
57	MG	14	3272	1/1	0.96	0.14	-	71,71,71,71	0
57	MG	14	3310	1/1	0.96	0.10	-	71,71,71,71	0
57	MG	1H	3365	1/1	0.65	0.10	-	82,82,82,82	0
57	MG	1H	3137	1/1	0.83	0.37	-	67,67,67,67	0
57	MG	1G	1703	1/1	0.87	0.10	-	107,107,107,107	0
57	MG	14	3218	1/1	0.99	0.10	-	55,55,55,55	0
57	MG	1H	3492	1/1	0.82	0.16	-	107,107,107,107	0
57	MG	14	3452	1/1	0.85	0.23	-	122,122,122,122	0
57	MG	14	3191	1/1	0.91	0.46	-	76,76,76,76	0
57	MG	1H	3511	1/1	0.92	0.07	-	113,113,113,113	0
57	MG	14	3206	1/1	0.95	0.27	-	97,97,97,97	0
57	MG	1H	3454	1/1	0.84	0.14	-	104,104,104,104	0
57	MG	14	3166	1/1	0.81	0.34	-	95,95,95,95	0
57	MG	1H	3012	1/1	0.81	0.23	-	81,81,81,81	0
57	MG	1H	3328	1/1	0.96	0.15	-	81,81,81,81	0
57	MG	1H	3509	1/1	0.67	0.36	-	114,114,114,114	0
57	MG	1G	1617	1/1	0.91	0.12	-	89,89,89,89	0
57	MG	1H	3446	1/1	0.92	0.07	-	100,100,100,100	0
57	MG	14	3135	1/1	0.59	0.38	-	112,112,112,112	0
57	MG	14	3352	1/1	0.93	0.11	-	95,95,95,95	0
57	MG	14	3455	1/1	0.72	0.36	-	115,115,115,115	0
57	MG	1H	3326	1/1	0.72	0.10	-	109,109,109,109	0
57	MG	1H	3006	1/1	0.94	0.21	-	77,77,77,77	0
57	MG	13	1668	1/1	0.63	0.29	-	112,112,112,112	0
57	MG	1H	3057	1/1	0.84	0.43	-	71,71,71,71	0
57	MG	1H	3110	1/1	0.80	0.33	-	86,86,86,86	0
57	MG	1H	3039	1/1	0.98	0.17	-	56,56,56,56	0
57	MG	14	3335	1/1	0.88	0.09	-	94,94,94,94	0
57	MG	1H	3025	1/1	0.97	0.24	-	52,52,52,52	0
57	MG	14	3018	1/1	0.90	0.24	-	82,82,82,82	0
57	MG	14	3152	1/1	0.90	0.37	-	99,99,99,99	0
57	MG	14	3243	1/1	0.88	0.18	-	93,93,93,93	0
57	MG	1G	1627	1/1	0.96	0.13	-	122,122,122,122	0
57	MG	B5	101	1/1	0.97	0.10	-	99,99,99,99	0
57	MG	13	1724	1/1	0.86	0.17	-	116,116,116,116	0
57	MG	1H	3459	1/1	0.73	0.16	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3416	1/1	0.96	0.07	-	80,80,80,80	0
57	MG	I8	101	1/1	0.90	0.06	-	95,95,95,95	0
57	MG	13	1671	1/1	0.94	0.07	-	108,108,108,108	0
57	MG	1H	3249	1/1	0.92	0.14	-	61,61,61,61	0
57	MG	14	3359	1/1	0.87	0.11	-	122,122,122,122	0
57	MG	1H	3190	1/1	0.90	0.13	-	73,73,73,73	0
57	MG	14	3337	1/1	0.86	0.06	-	116,116,116,116	0
57	MG	13	1661	1/1	0.93	0.16	-	101,101,101,101	0
57	MG	13	1645	1/1	0.84	0.21	-	117,117,117,117	0
57	MG	14	3364	1/1	0.82	0.08	-	98,98,98,98	0
57	MG	1H	3508	1/1	0.92	0.11	-	144,144,144,144	0
57	MG	14	3439	1/1	0.84	0.24	-	100,100,100,100	0
57	MG	14	3150	1/1	0.96	0.16	-	75,75,75,75	0
57	MG	1H	3155	1/1	0.90	0.27	-	106,106,106,106	0
57	MG	13	1706	1/1	0.90	0.15	-	88,88,88,88	0
57	MG	14	3126	1/1	0.86	0.18	-	89,89,89,89	0
57	MG	1H	3150	1/1	0.94	0.34	-	81,81,81,81	0
57	MG	14	3424	1/1	0.83	0.12	-	117,117,117,117	0
57	MG	14	3440	1/1	0.97	0.20	-	87,87,87,87	0
57	MG	1H	3500	1/1	0.85	0.10	-	90,90,90,90	0
57	MG	1H	3174	1/1	0.95	0.31	-	73,73,73,73	0
57	MG	1H	3201	1/1	0.98	0.26	-	80,80,80,80	0
57	MG	1H	3398	1/1	0.88	0.07	-	86,86,86,86	0
57	MG	14	3076	1/1	0.90	0.18	-	80,80,80,80	0
57	MG	1H	3234	1/1	0.95	0.28	-	84,84,84,84	0
57	MG	1H	3316	1/1	0.96	0.07	-	76,76,76,76	0
57	MG	1H	3462	1/1	0.83	0.06	-	99,99,99,99	0
57	MG	1H	3321	1/1	0.96	0.11	-	55,55,55,55	0
57	MG	13	1708	1/1	0.91	0.07	-	91,91,91,91	0
57	MG	1H	3464	1/1	0.97	0.17	-	57,57,57,57	0
57	MG	16	201	1/1	0.90	0.27	-	73,73,73,73	0
57	MG	1H	3525	1/1	0.53	0.19	-	99,99,99,99	0
57	MG	14	3039	1/1	0.99	0.27	-	85,85,85,85	0
57	MG	1G	1674	1/1	0.93	0.18	-	106,106,106,106	0
57	MG	1J	202	1/1	0.92	0.20	-	106,106,106,106	0
57	MG	1H	3156	1/1	0.82	0.33	-	106,106,106,106	0
57	MG	1J	208	1/1	0.78	0.17	-	124,124,124,124	0
57	MG	13	1660	1/1	0.89	0.51	-	91,91,91,91	0
57	MG	13	1639	1/1	0.90	0.44	-	80,80,80,80	0
57	MG	1H	3460	1/1	0.84	0.28	-	85,85,85,85	0
57	MG	1G	1685	1/1	0.84	0.08	-	129,129,129,129	0
57	MG	14	3444	1/1	0.90	0.48	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3397	1/1	0.79	0.07	-	162,162,162,162	0
57	MG	1H	3193	1/1	0.87	0.71	-	89,89,89,89	0
57	MG	14	3273	1/1	0.96	0.11	-	61,61,61,61	0
57	MG	1G	1601	1/1	0.95	0.21	-	92,92,92,92	0
57	MG	1H	3333	1/1	0.67	0.09	-	98,98,98,98	0
57	MG	14	3013	1/1	0.98	0.30	-	56,56,56,56	0
57	MG	14	3437	1/1	0.75	0.11	-	111,111,111,111	0
57	MG	14	3298	1/1	0.96	0.07	-	95,95,95,95	0
57	MG	14	3109	1/1	0.68	0.31	-	94,94,94,94	0
57	MG	14	3023	1/1	0.92	0.35	-	58,58,58,58	0
57	MG	1G	1646	1/1	0.91	0.31	-	78,78,78,78	0
57	MG	1H	3343	1/1	0.91	0.09	-	115,115,115,115	0
57	MG	14	3325	1/1	0.96	0.08	-	88,88,88,88	0
57	MG	1G	1714	1/1	0.94	0.11	-	126,126,126,126	0
57	MG	1G	1653	1/1	0.96	0.07	-	125,125,125,125	0
57	MG	1H	3527	1/1	0.93	0.10	-	97,97,97,97	0
57	MG	1H	3069	1/1	0.91	0.27	-	76,76,76,76	0
57	MG	1H	3124	1/1	0.70	0.36	-	90,90,90,90	0
57	MG	1G	1694	1/1	0.93	0.10	-	105,105,105,105	0
57	MG	14	3328	1/1	0.81	0.10	-	95,95,95,95	0
57	MG	E5	101	1/1	0.67	0.66	-	99,99,99,99	0
57	MG	13	1714	1/1	0.90	0.06	-	94,94,94,94	0
57	MG	1H	3020	1/1	0.97	0.24	-	60,60,60,60	0
57	MG	1H	3369	1/1	0.77	0.27	-	90,90,90,90	0
57	MG	13	1631	1/1	0.98	0.35	-	106,106,106,106	0
57	MG	1H	3420	1/1	0.89	0.22	-	94,94,94,94	0
57	MG	13	1665	1/1	0.92	0.20	-	128,128,128,128	0
57	MG	1G	1625	1/1	0.93	0.62	-	89,89,89,89	0
57	MG	14	3443	1/1	0.87	0.34	-	115,115,115,115	0
57	MG	1H	3183	1/1	0.92	0.29	-	75,75,75,75	0
57	MG	13	1669	1/1	0.56	0.14	-	111,111,111,111	0
57	MG	1H	3426	1/1	0.96	0.17	-	82,82,82,82	0
57	MG	14	3198	1/1	0.77	0.30	-	88,88,88,88	0
57	MG	16	209	1/1	0.88	0.07	-	86,86,86,86	0
57	MG	1G	1689	1/1	0.95	0.07	-	92,92,92,92	0
57	MG	14	3304	1/1	0.98	0.07	-	61,61,61,61	0
57	MG	14	3161	1/1	0.62	0.25	-	94,94,94,94	0
57	MG	1H	3373	1/1	0.83	0.22	-	79,79,79,79	0
57	MG	14	3008	1/1	0.80	0.14	-	73,73,73,73	0
57	MG	13	1730	1/1	0.95	0.07	-	110,110,110,110	0
57	MG	14	3108	1/1	0.95	0.53	-	103,103,103,103	0
57	MG	14	3071	1/1	0.85	0.16	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3238	1/1	0.81	0.10	-	67,67,67,67	0
57	MG	1H	3512	1/1	0.82	0.29	-	100,100,100,100	0
57	MG	14	3404	1/1	0.83	0.07	-	121,121,121,121	0
57	MG	14	3265	1/1	0.85	0.07	-	100,100,100,100	0
57	MG	1H	3226	1/1	0.95	0.50	-	92,92,92,92	0
57	MG	1H	3111	1/1	0.80	0.34	-	94,94,94,94	0
57	MG	1G	1691	1/1	0.91	0.07	-	104,104,104,104	0
57	MG	1G	1677	1/1	0.97	0.09	-	83,83,83,83	0
57	MG	1H	3544	1/1	0.90	0.14	-	105,105,105,105	0
57	MG	13	1602	1/1	0.90	0.12	-	130,130,130,130	0
57	MG	1H	3403	1/1	0.82	0.07	-	68,68,68,68	0
57	MG	14	3179	1/1	0.73	0.30	-	103,103,103,103	0
57	MG	1G	1675	1/1	0.88	0.12	-	86,86,86,86	0
57	MG	14	3030	1/1	0.94	0.40	-	90,90,90,90	0
57	MG	14	3057	1/1	0.92	0.05	-	93,93,93,93	0
57	MG	14	3064	1/1	0.95	0.23	-	99,99,99,99	0
57	MG	1H	3141	1/1	0.88	0.15	-	75,75,75,75	0
57	MG	1G	1722	1/1	0.84	0.20	-	116,116,116,116	0
57	MG	1H	3318	1/1	0.97	0.04	-	74,74,74,74	0
57	MG	1H	3380	1/1	0.90	0.15	-	76,76,76,76	0
57	MG	1H	3044	1/1	0.87	0.48	-	80,80,80,80	0
57	MG	14	3343	1/1	0.90	0.11	-	84,84,84,84	0
57	MG	14	3294	1/1	0.92	0.14	-	66,66,66,66	0
57	MG	14	3436	1/1	0.87	0.04	-	136,136,136,136	0
57	MG	1H	3040	1/1	0.93	0.20	-	76,76,76,76	0
57	MG	1H	3009	1/1	0.92	0.16	-	82,82,82,82	0
57	MG	13	1616	1/1	0.96	0.30	-	101,101,101,101	0
57	MG	14	3247	1/1	0.96	0.11	-	87,87,87,87	0
57	MG	1H	3546	1/1	0.97	0.10	-	105,105,105,105	0
57	MG	1H	3172	1/1	0.80	0.23	-	64,64,64,64	0
57	MG	14	3055	1/1	0.97	0.25	-	64,64,64,64	0
57	MG	1H	3498	1/1	0.76	0.08	-	113,113,113,113	0
57	MG	1H	3471	1/1	0.95	0.17	-	83,83,83,83	0
57	MG	13	1699	1/1	0.79	0.19	-	114,114,114,114	0
57	MG	1H	3051	1/1	0.97	0.29	-	74,74,74,74	0
57	MG	I8	102	1/1	0.98	0.06	-	70,70,70,70	0
57	MG	14	3454	1/1	0.81	0.12	-	108,108,108,108	0
57	MG	1J	209	1/1	0.60	0.07	-	131,131,131,131	0
57	MG	1H	3200	1/1	0.92	0.69	-	82,82,82,82	0
57	MG	14	3398	1/1	0.97	0.05	-	86,86,86,86	0
57	MG	14	3375	1/1	0.80	0.40	-	116,116,116,116	0
57	MG	14	3409	1/1	0.90	0.11	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3121	1/1	0.90	0.72	-	92,92,92,92	0
57	MG	13	1698	1/1	0.95	0.12	-	93,93,93,93	0
57	MG	1H	3410	1/1	0.86	0.17	-	108,108,108,108	0
57	MG	1H	3456	1/1	0.80	0.15	-	92,92,92,92	0
57	MG	1G	1702	1/1	0.62	0.08	-	117,117,117,117	0
57	MG	14	3415	1/1	0.89	0.27	-	93,93,93,93	0
57	MG	14	3061	1/1	0.96	0.35	-	60,60,60,60	0
57	MG	1H	3505	1/1	0.85	0.17	-	112,112,112,112	0
57	MG	1H	3123	1/1	0.89	0.26	-	68,68,68,68	0
57	MG	1H	3397	1/1	0.92	0.14	-	87,87,87,87	0
57	MG	1H	3390	1/1	0.95	0.13	-	48,48,48,48	0
57	MG	14	3178	1/1	0.94	0.13	-	83,83,83,83	0
57	MG	1H	3003	1/1	0.99	0.12	-	67,67,67,67	0
57	MG	14	3445	1/1	0.84	0.12	-	119,119,119,119	0
57	MG	1H	3364	1/1	0.73	0.12	-	85,85,85,85	0
57	MG	1H	3163	1/1	0.96	0.19	-	86,86,86,86	0
57	MG	1H	3551	1/1	0.80	0.11	-	86,86,86,86	0
57	MG	14	3360	1/1	0.83	0.16	-	107,107,107,107	0
57	MG	1H	3167	1/1	0.61	0.48	-	86,86,86,86	0
57	MG	14	3303	1/1	0.97	0.11	-	52,52,52,52	0
57	MG	1H	3514	1/1	0.56	0.13	-	112,112,112,112	0
57	MG	16	206	1/1	0.64	0.24	-	83,83,83,83	0
57	MG	14	3456	1/1	0.12	0.16	-	118,118,118,118	0
57	MG	52	300	1/1	0.80	0.13	-	133,133,133,133	0
57	MG	1H	3299	1/1	0.88	0.19	-	105,105,105,105	0
57	MG	14	3033	1/1	0.92	0.32	-	57,57,57,57	0
57	MG	13	1734	1/1	0.80	0.10	-	143,143,143,143	0
57	MG	14	3385	1/1	0.92	0.20	-	82,82,82,82	0
57	MG	14	3338	1/1	0.93	0.18	-	112,112,112,112	0
57	MG	1G	1629	1/1	0.47	0.19	-	129,129,129,129	0
57	MG	1H	3168	1/1	0.83	0.18	-	89,89,89,89	0
57	MG	1J	203	1/1	0.89	0.23	-	92,92,92,92	0
57	MG	14	3307	1/1	0.93	0.15	-	80,80,80,80	0
57	MG	1H	3486	1/1	0.92	0.30	-	99,99,99,99	0
57	MG	13	1695	1/1	0.97	0.07	-	91,91,91,91	0
57	MG	1H	3534	1/1	0.47	0.11	-	113,113,113,113	0
57	MG	1H	3049	1/1	0.94	0.27	-	79,79,79,79	0
57	MG	1H	3338	1/1	0.67	0.10	-	99,99,99,99	0
57	MG	14	3251	1/1	0.93	0.18	-	113,113,113,113	0
57	MG	13	1711	1/1	0.96	0.09	-	70,70,70,70	0
57	MG	1H	3209	1/1	0.96	0.17	-	92,92,92,92	0
57	MG	1G	1605	1/1	0.79	0.32	-	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3189	1/1	0.94	0.27	-	83,83,83,83	0
57	MG	1H	3315	1/1	0.95	0.13	-	61,61,61,61	0
57	MG	2L	102	1/1	0.78	0.16	-	126,126,126,126	0
57	MG	14	3156	1/1	0.88	0.29	-	81,81,81,81	0
57	MG	1H	3348	1/1	0.94	0.11	-	66,66,66,66	0
57	MG	14	3118	1/1	0.92	0.14	-	96,96,96,96	0
57	MG	1H	3439	1/1	0.97	0.04	-	76,76,76,76	0
57	MG	1H	3375	1/1	0.94	0.10	-	80,80,80,80	0
57	MG	1H	3406	1/1	0.90	0.08	-	95,95,95,95	0
57	MG	14	3074	1/1	0.45	0.59	-	95,95,95,95	0
57	MG	13	1705	1/1	0.87	0.12	-	108,108,108,108	0
57	MG	1H	3177	1/1	0.62	0.20	-	143,143,143,143	0
57	MG	14	3143	1/1	0.88	0.31	-	93,93,93,93	0
57	MG	14	3168	1/1	0.98	0.18	-	70,70,70,70	0
57	MG	14	3368	1/1	0.94	0.37	-	92,92,92,92	0
57	MG	1H	3550	1/1	0.92	0.66	-	111,111,111,111	0
57	MG	14	3339	1/1	0.77	0.05	-	106,106,106,106	0
57	MG	1G	1688	1/1	0.86	0.09	-	123,123,123,123	0
57	MG	13	1731	1/1	0.90	0.14	-	109,109,109,109	0
57	MG	14	3370	1/1	0.92	0.14	-	90,90,90,90	0
57	MG	1G	1669	1/1	0.91	0.08	-	114,114,114,114	0
57	MG	14	3051	1/1	0.98	0.30	-	70,70,70,70	0
57	MG	1H	3035	1/1	0.94	0.36	-	83,83,83,83	0
57	MG	1H	3138	1/1	0.87	0.18	-	98,98,98,98	0
57	MG	1H	3142	1/1	0.79	0.48	-	87,87,87,87	0
57	MG	13	1605	1/1	0.94	0.18	-	88,88,88,88	0
57	MG	1H	3286	1/1	0.91	0.22	-	65,65,65,65	0
57	MG	13	1670	1/1	0.92	0.60	-	85,85,85,85	0
57	MG	13	1646	1/1	0.85	0.52	-	91,91,91,91	0
57	MG	1H	3228	1/1	0.92	0.15	-	81,81,81,81	0
57	MG	14	3180	1/1	0.97	0.34	-	86,86,86,86	0
57	MG	1G	1712	1/1	0.75	0.29	-	110,110,110,110	0
57	MG	1G	1715	1/1	0.90	0.07	-	110,110,110,110	0
57	MG	14	3079	1/1	0.60	0.46	-	86,86,86,86	0
57	MG	14	3395	1/1	0.81	0.21	-	98,98,98,98	0
57	MG	1G	1673	1/1	0.97	0.11	-	80,80,80,80	0
57	MG	1H	3407	1/1	0.97	0.07	-	69,69,69,69	0
57	MG	1H	3136	1/1	0.89	0.20	-	63,63,63,63	0
57	MG	1H	3203	1/1	0.92	0.24	-	78,78,78,78	0
57	MG	14	3177	1/1	0.60	0.46	-	81,81,81,81	0
57	MG	1H	3178	1/1	0.94	0.45	-	80,80,80,80	0
57	MG	1J	206	1/1	0.91	0.07	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	14	3190	1/1	0.95	0.33	-	89,89,89,89	0
57	MG	14	3002	1/1	0.96	0.35	-	63,63,63,63	0
57	MG	14	3365	1/1	0.96	0.10	-	93,93,93,93	0
57	MG	13	1610	1/1	0.73	0.56	-	81,81,81,81	0
57	MG	1H	3282	1/1	0.95	0.05	-	54,54,54,54	0
57	MG	1H	3131	1/1	0.86	0.14	-	101,101,101,101	0
57	MG	13	1679	1/1	0.96	0.06	-	89,89,89,89	0
57	MG	1H	3070	1/1	0.95	0.15	-	51,51,51,51	0
57	MG	14	3224	1/1	0.94	0.15	-	76,76,76,76	0
57	MG	1H	3162	1/1	0.78	0.61	-	92,92,92,92	0
57	MG	13	1658	1/1	0.99	0.29	-	83,83,83,83	0
57	MG	1H	3238	1/1	0.85	0.38	-	102,102,102,102	0
57	MG	13	1732	1/1	0.92	0.06	-	108,108,108,108	0
57	MG	1H	3231	1/1	0.88	0.08	-	103,103,103,103	0
57	MG	14	3184	1/1	0.93	0.38	-	78,78,78,78	0
57	MG	14	3423	1/1	0.72	0.18	-	118,118,118,118	0
57	MG	14	3269	1/1	0.94	0.07	-	104,104,104,104	0
57	MG	1H	3408	1/1	0.73	0.10	-	87,87,87,87	0
57	MG	1H	3244	1/1	0.98	0.11	-	47,47,47,47	0
57	MG	14	3040	1/1	0.98	0.26	-	80,80,80,80	0
57	MG	13	1690	1/1	0.88	0.10	-	117,117,117,117	0
57	MG	14	3059	1/1	0.95	0.21	-	58,58,58,58	0
57	MG	1H	3134	1/1	0.96	0.50	-	77,77,77,77	0
57	MG	1G	1709	1/1	0.91	0.12	-	119,119,119,119	0
57	MG	1H	3430	1/1	0.97	0.19	-	94,94,94,94	0
57	MG	1H	3067	1/1	0.88	0.12	-	55,55,55,55	0
57	MG	1H	3428	1/1	0.96	0.05	-	93,93,93,93	0
57	MG	35	202	1/1	0.94	0.17	-	80,80,80,80	0
57	MG	1H	3538	1/1	0.89	0.07	-	107,107,107,107	0
57	MG	13	1648	1/1	0.38	0.49	-	117,117,117,117	0
57	MG	1H	3437	1/1	0.96	0.15	-	76,76,76,76	0
57	MG	1H	3503	1/1	0.93	0.12	-	104,104,104,104	0
57	MG	13	1721	1/1	0.95	0.18	-	77,77,77,77	0
57	MG	1H	3539	1/1	0.91	0.23	-	95,95,95,95	0
57	MG	14	3036	1/1	0.97	0.28	-	85,85,85,85	0
57	MG	14	3289	1/1	0.90	0.16	-	89,89,89,89	0
57	MG	1H	3470	1/1	0.93	0.24	-	105,105,105,105	0
57	MG	14	3369	1/1	0.91	0.11	-	90,90,90,90	0
57	MG	14	3418	1/1	0.90	0.16	-	97,97,97,97	0
57	MG	1H	3443	1/1	0.92	0.08	-	112,112,112,112	0
57	MG	1H	3073	1/1	0.86	0.35	-	84,84,84,84	0
57	MG	1H	3158	1/1	0.87	0.24	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3030	1/1	0.91	0.17	-	89,89,89,89	0
57	MG	1H	3455	1/1	0.85	0.08	-	120,120,120,120	0
57	MG	14	3134	1/1	0.79	0.70	-	99,99,99,99	0
57	MG	1G	1682	1/1	0.84	0.09	-	123,123,123,123	0
57	MG	1H	3450	1/1	0.93	0.06	-	87,87,87,87	0
57	MG	1H	3531	1/1	0.82	0.13	-	114,114,114,114	0
57	MG	1G	1690	1/1	0.94	0.06	-	113,113,113,113	0
57	MG	1H	3421	1/1	0.47	0.38	-	93,93,93,93	0
57	MG	1H	3520	1/1	0.91	0.10	-	88,88,88,88	0
57	MG	1H	3182	1/1	0.76	0.17	-	108,108,108,108	0
57	MG	13	1722	1/1	0.95	0.18	-	99,99,99,99	0
57	MG	14	3425	1/1	0.76	0.28	-	106,106,106,106	0
57	MG	14	3402	1/1	0.94	0.07	-	111,111,111,111	0
57	MG	14	3246	1/1	0.94	0.10	-	93,93,93,93	0
57	MG	14	3268	1/1	0.88	0.16	-	89,89,89,89	0
57	MG	1H	3099	1/1	0.95	0.15	-	53,53,53,53	0
57	MG	1H	3264	1/1	0.82	0.19	-	55,55,55,55	0
57	MG	14	3137	1/1	0.81	0.34	-	76,76,76,76	0
57	MG	13	1693	1/1	0.96	0.10	-	95,95,95,95	0
57	MG	16	208	1/1	0.95	0.27	-	86,86,86,86	0
57	MG	14	3181	1/1	0.86	0.45	-	91,91,91,91	0
57	MG	14	3081	1/1	0.76	0.17	-	79,79,79,79	0
57	MG	13	1620	1/1	0.99	0.16	-	68,68,68,68	0
57	MG	14	3427	1/1	0.69	0.15	-	121,121,121,121	0
57	MG	13	1611	1/1	0.96	0.23	-	78,78,78,78	0
57	MG	1G	1636	1/1	0.89	0.35	-	87,87,87,87	0
57	MG	13	1717	1/1	0.94	0.10	-	93,93,93,93	0
57	MG	1H	3276	1/1	0.93	0.06	-	80,80,80,80	0
57	MG	14	3381	1/1	0.81	0.08	-	136,136,136,136	0
57	MG	E5	102	1/1	0.86	0.28	-	68,68,68,68	0
57	MG	16	212	1/1	0.94	0.07	-	78,78,78,78	0
57	MG	1H	3336	1/1	0.98	0.07	-	88,88,88,88	0
57	MG	13	1723	1/1	0.77	0.12	-	118,118,118,118	0
57	MG	13	1692	1/1	0.54	0.15	-	110,110,110,110	0
57	MG	14	3388	1/1	0.74	0.13	-	72,72,72,72	0
57	MG	1H	3519	1/1	0.74	0.15	-	104,104,104,104	0
57	MG	14	3062	1/1	0.94	0.25	-	97,97,97,97	0
57	MG	14	3103	1/1	0.69	0.53	-	80,80,80,80	0
57	MG	1H	3157	1/1	0.80	0.44	-	89,89,89,89	0
57	MG	16	211	1/1	0.91	0.08	-	93,93,93,93	0
57	MG	1G	1608	1/1	0.96	0.34	-	100,100,100,100	0
57	MG	14	3248	1/1	0.91	0.14	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	1H	3320	1/1	0.96	0.08	-	71,71,71,71	0
57	MG	14	3035	1/1	0.95	0.27	-	69,69,69,69	0
57	MG	13	1662	1/1	0.88	0.43	-	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.