



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:14 am GMT

PDB ID : 5E81
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA^{Lys} in the A-site with wobble pair
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-10-13
Resolution : 2.95 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

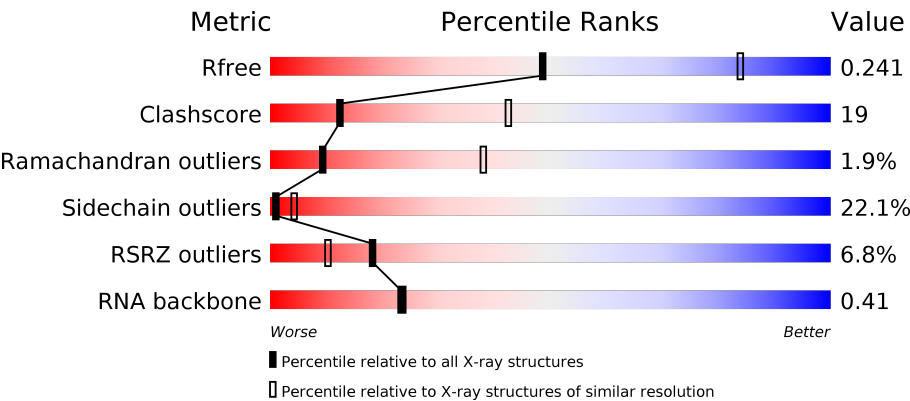
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)
RNA backbone	2435	1008 (3.30-2.62)

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

Mol	Chain	Length	Quality of chain
1	13	1519	<div><div></div><div>24%46%24%. .</div></div>
1	1G	1519	<div><div>%</div><div>33%44%18%. .</div></div>
2	12	256	<div><div>8%</div><div>34%38%7%.19%</div></div>
2	1E	256	<div><div>5%</div><div>38%39%13%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	
22	1L	76	
23	2K	77	
23	2L	77	
24	3K	76	
24	3L	76	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	

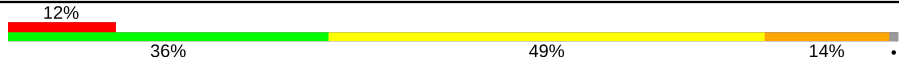
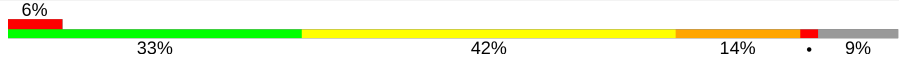
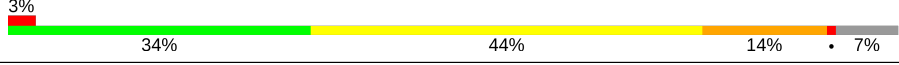
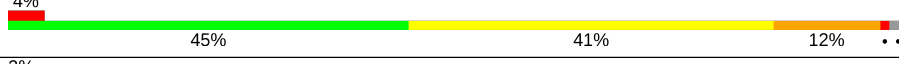

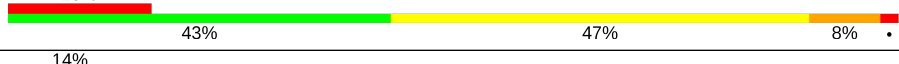
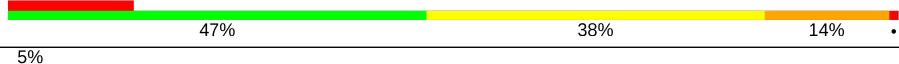

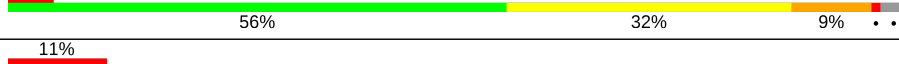
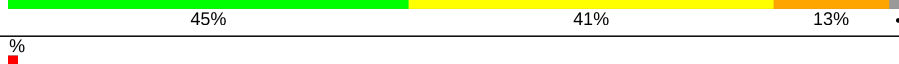

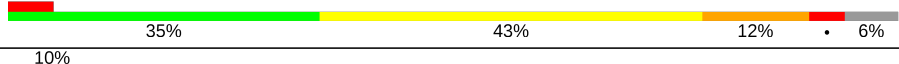
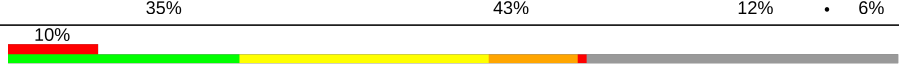
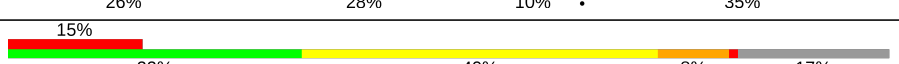
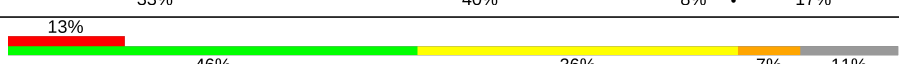



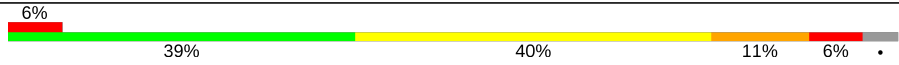
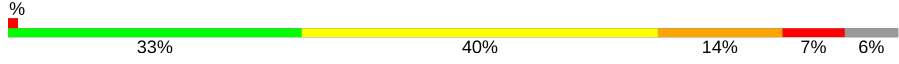

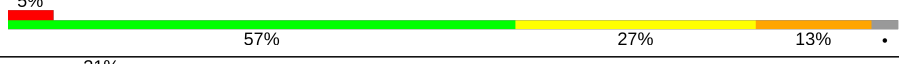



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Mol	Chain	Length	Quality of chain
28	71	229	
28	79	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	

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Mol	Chain	Length	Quality of chain
40	A8	112	
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1602	-	-	-	X
56	MG	13	1606	-	-	-	X
56	MG	13	1611	-	-	-	X
56	MG	13	1624	-	-	-	X
56	MG	13	1625	-	-	-	X
56	MG	13	1626	-	-	-	X
56	MG	13	1630	-	-	-	X
56	MG	13	1631	-	-	-	X
56	MG	13	1632	-	-	-	X
56	MG	13	1635	-	-	-	X
56	MG	13	1636	-	-	-	X
56	MG	13	1638	-	-	-	X
56	MG	13	1654	-	-	-	X
56	MG	13	1659	-	-	-	X
56	MG	13	1688	-	-	-	X
56	MG	14	3006	-	-	-	X
56	MG	14	3013	-	-	-	X
56	MG	14	3016	-	-	-	X
56	MG	14	3019	-	-	-	X
56	MG	14	3026	-	-	-	X
56	MG	14	3030	-	-	-	X
56	MG	14	3031	-	-	-	X
56	MG	14	3032	-	-	-	X
56	MG	14	3033	-	-	-	X
56	MG	14	3039	-	-	-	X
56	MG	14	3045	-	-	-	X
56	MG	14	3047	-	-	-	X
56	MG	14	3050	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	14	3053	-	-	-	X
56	MG	14	3054	-	-	-	X
56	MG	14	3064	-	-	-	X
56	MG	14	3065	-	-	-	X
56	MG	14	3068	-	-	-	X
56	MG	14	3077	-	-	-	X
56	MG	14	3080	-	-	-	X
56	MG	14	3086	-	-	-	X
56	MG	14	3096	-	-	-	X
56	MG	14	3098	-	-	-	X
56	MG	14	3099	-	-	-	X
56	MG	14	3102	-	-	-	X
56	MG	14	3104	-	-	-	X
56	MG	14	3110	-	-	-	X
56	MG	14	3111	-	-	-	X
56	MG	14	3112	-	-	-	X
56	MG	14	3114	-	-	-	X
56	MG	14	3115	-	-	-	X
56	MG	14	3119	-	-	-	X
56	MG	14	3122	-	-	-	X
56	MG	14	3128	-	-	-	X
56	MG	14	3129	-	-	-	X
56	MG	14	3131	-	-	-	X
56	MG	14	3132	-	-	-	X
56	MG	14	3143	-	-	-	X
56	MG	14	3149	-	-	-	X
56	MG	14	3153	-	-	-	X
56	MG	14	3158	-	-	-	X
56	MG	14	3159	-	-	-	X
56	MG	14	3160	-	-	-	X
56	MG	14	3163	-	-	-	X
56	MG	14	3165	-	-	-	X
56	MG	14	3166	-	-	-	X
56	MG	14	3189	-	-	-	X
56	MG	14	3191	-	-	-	X
56	MG	14	3198	-	-	-	X
56	MG	14	3213	-	-	-	X
56	MG	14	3214	-	-	-	X
56	MG	14	3220	-	-	-	X
56	MG	14	3226	-	-	-	X
56	MG	14	3231	-	-	-	X
56	MG	14	3234	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	14	3243	-	-	-	X
56	MG	14	3245	-	-	-	X
56	MG	14	3246	-	-	-	X
56	MG	14	3279	-	-	-	X
56	MG	14	3319	-	-	-	X
56	MG	14	3327	-	-	-	X
56	MG	14	3328	-	-	-	X
56	MG	14	3455	-	-	-	X
56	MG	16	201	-	-	-	X
56	MG	1G	1609	-	-	-	X
56	MG	1G	1613	-	-	-	X
56	MG	1G	1619	-	-	-	X
56	MG	1G	1630	-	-	-	X
56	MG	1G	1634	-	-	-	X
56	MG	1G	1682	-	-	-	X
56	MG	1H	3006	-	-	-	X
56	MG	1H	3007	-	-	-	X
56	MG	1H	3011	-	-	-	X
56	MG	1H	3017	-	-	-	X
56	MG	1H	3019	-	-	-	X
56	MG	1H	3021	-	-	-	X
56	MG	1H	3027	-	-	-	X
56	MG	1H	3028	-	-	-	X
56	MG	1H	3030	-	-	-	X
56	MG	1H	3032	-	-	-	X
56	MG	1H	3037	-	-	-	X
56	MG	1H	3040	-	-	-	X
56	MG	1H	3043	-	-	-	X
56	MG	1H	3044	-	-	-	X
56	MG	1H	3048	-	-	-	X
56	MG	1H	3050	-	-	-	X
56	MG	1H	3051	-	-	-	X
56	MG	1H	3053	-	-	-	X
56	MG	1H	3056	-	-	-	X
56	MG	1H	3058	-	-	-	X
56	MG	1H	3061	-	-	-	X
56	MG	1H	3068	-	-	-	X
56	MG	1H	3069	-	-	-	X
56	MG	1H	3078	-	-	-	X
56	MG	1H	3080	-	-	-	X
56	MG	1H	3092	-	-	-	X
56	MG	1H	3093	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1H	3095	-	-	-	X
56	MG	1H	3098	-	-	-	X
56	MG	1H	3103	-	-	-	X
56	MG	1H	3105	-	-	-	X
56	MG	1H	3109	-	-	-	X
56	MG	1H	3115	-	-	-	X
56	MG	1H	3118	-	-	-	X
56	MG	1H	3123	-	-	-	X
56	MG	1H	3125	-	-	-	X
56	MG	1H	3127	-	-	-	X
56	MG	1H	3132	-	-	-	X
56	MG	1H	3133	-	-	-	X
56	MG	1H	3141	-	-	-	X
56	MG	1H	3143	-	-	-	X
56	MG	1H	3147	-	-	-	X
56	MG	1H	3156	-	-	-	X
56	MG	1H	3159	-	-	-	X
56	MG	1H	3165	-	-	-	X
56	MG	1H	3167	-	-	-	X
56	MG	1H	3172	-	-	-	X
56	MG	1H	3179	-	-	-	X
56	MG	1H	3184	-	-	-	X
56	MG	1H	3189	-	-	-	X
56	MG	1H	3192	-	-	-	X
56	MG	1H	3194	-	-	-	X
56	MG	1H	3209	-	-	-	X
56	MG	1H	3213	-	-	-	X
56	MG	1H	3218	-	-	-	X
56	MG	1H	3229	-	-	-	X
56	MG	1H	3230	-	-	-	X
56	MG	1H	3240	-	-	-	X
56	MG	1H	3246	-	-	-	X
56	MG	1H	3261	-	-	-	X
56	MG	1H	3274	-	-	-	X
56	MG	1H	3284	-	-	-	X
56	MG	1H	3285	-	-	-	X
56	MG	1H	3343	-	-	-	X
56	MG	1H	3363	-	-	-	X
56	MG	1H	3407	-	-	-	X
56	MG	1H	3442	-	-	-	X
56	MG	1H	3454	-	-	-	X
56	MG	1H	3572	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1J	208	-	-	-	X
56	MG	2I	301	-	-	-	X
56	MG	2K	103	-	-	-	X
56	MG	2L	101	-	-	-	X
57	SF4	32	302	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 297904 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- 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			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	149	Total	C	N	O	S	0	0	0
			1139	721	216	198	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	140	Total	C	N	O	S	0	0	0
			1120	695	223	196	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	95	Total	C	N	O	S	0	0	0
			754	471	148	134	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			
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			
22	1L	69	Total	C	N	O	P	S	0	0	0
			1477	662	257	488	69	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	21	Total	C	N	O	P	0	0	0
			464	208	99	136	21			
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	2885	Total	C	N	O	P	0	3	0
			62204	27685	11631	20000	2888			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	2855	Total	C	N	O	P	0	0	0
			61505	27372	11512	19766	2855			

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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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
			1558	985	298	269	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
33	59	70	Total	C	N	O	S	0	0	0
			543	341	110	92				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
34	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			743	482	134	126	1			

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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	133	Total	C	N	O	S	0	0	0
			1079	694	194	189	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
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	49	Total	C	N	O	S	0	0	0
			376	240	63	68	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	98	1	Total	Mg	0	0
			1	1		

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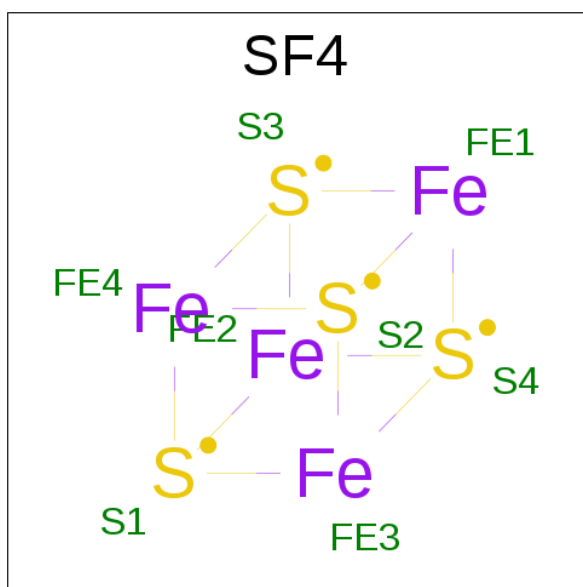
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	45	2	Total 2	Mg 2	0	0
56	P8	1	Total 1	Mg 1	0	0
56	32	1	Total 1	Mg 1	0	0
56	13	161	Total 161	Mg 161	0	0
56	1J	11	Total 11	Mg 11	0	0
56	5I	1	Total 1	Mg 1	0	0
56	35	3	Total 3	Mg 3	0	0
56	16	13	Total 13	Mg 13	0	0
56	42	2	Total 2	Mg 2	0	0
56	B5	1	Total 1	Mg 1	0	0
56	25	2	Total 2	Mg 2	0	0
56	M5	1	Total 1	Mg 1	0	0
56	21	3	Total 3	Mg 3	0	0
56	2K	3	Total 3	Mg 3	0	0
56	Q8	1	Total 1	Mg 1	0	0
56	L8	1	Total 1	Mg 1	0	0
56	I8	1	Total 1	Mg 1	0	0
56	52	1	Total 1	Mg 1	0	0
56	2A	1	Total 1	Mg 1	0	0
56	5E	1	Total 1	Mg 1	0	0
56	29	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	78	2	Total 2	Mg 2	0	0
56	39	2	Total 2	Mg 2	0	0
56	1G	126	Total 126	Mg 126	0	0
56	11	3	Total 3	Mg 3	0	0
56	1H	572	Total 572	Mg 572	0	0
56	E5	3	Total 3	Mg 3	0	0
56	88	3	Total 3	Mg 3	0	0
56	14	471	Total 471	Mg 471	0	0
56	F8	1	Total 1	Mg 1	0	0
56	4K	1	Total 1	Mg 1	0	0
56	1K	1	Total 1	Mg 1	0	0
56	41	2	Total 2	Mg 2	0	0
56	2L	3	Total 3	Mg 3	0	0

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	C5	1	Total	Zn	0	0
			1	1		
58	5A	1	Total	Zn	0	0
			1	1		
58	G8	1	Total	Zn	0	0
			1	1		
58	5I	1	Total	Zn	0	0
			1	1		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	13	389	Total	O	0	0
			389	389		
59	1E	1	Total	O	0	0
			1	1		
59	3E	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	4E	1	Total 1	O 1	0	0
59	8E	3	Total 3	O 3	0	0
59	1I	2	Total 2	O 2	0	0
59	3I	2	Total 2	O 2	0	0
59	4I	2	Total 2	O 2	0	0
59	5I	2	Total 2	O 2	0	0
59	6I	3	Total 3	O 3	0	0
59	7I	1	Total 1	O 1	0	0
59	1F	2	Total 2	O 2	0	0
59	1K	8	Total 8	O 8	0	0
59	2K	6	Total 6	O 6	0	0
59	3K	1	Total 1	O 1	0	0
59	4K	5	Total 5	O 5	0	0
59	1H	1539	Total 1539	O 1539	0	0
59	16	35	Total 35	O 35	0	0
59	11	16	Total 16	O 16	0	0
59	21	7	Total 7	O 7	0	0
59	31	6	Total 6	O 6	0	0
59	41	1	Total 1	O 1	0	0
59	58	2	Total 2	O 2	0	0
59	68	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	78	8	Total 8	O 8	0	0
59	88	8	Total 8	O 8	0	0
59	C8	4	Total 4	O 4	0	0
59	D8	2	Total 2	O 2	0	0
59	F8	2	Total 2	O 2	0	0
59	G8	1	Total 1	O 1	0	0
59	I8	7	Total 7	O 7	0	0
59	J8	2	Total 2	O 2	0	0
59	K8	1	Total 1	O 1	0	0
59	L8	3	Total 3	O 3	0	0
59	P8	1	Total 1	O 1	0	0
59	Q8	8	Total 8	O 8	0	0
59	1G	297	Total 297	O 297	0	0
59	32	2	Total 2	O 2	0	0
59	42	1	Total 1	O 1	0	0
59	52	4	Total 4	O 4	0	0
59	62	3	Total 3	O 3	0	0
59	2A	3	Total 3	O 3	0	0
59	3A	1	Total 1	O 1	0	0
59	6A	1	Total 1	O 1	0	0
59	7A	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	9A	2	Total 2	O 2	0	0
59	BA	5	Total 5	O 5	0	0
59	1L	1	Total 1	O 1	0	0
59	2L	6	Total 6	O 6	0	0
59	4L	5	Total 5	O 5	0	0
59	14	1225	Total 1225	O 1225	0	0
59	1J	12	Total 12	O 12	0	0
59	19	11	Total 11	O 11	0	0
59	29	5	Total 5	O 5	0	0
59	39	7	Total 7	O 7	0	0
59	25	6	Total 6	O 6	0	0
59	35	8	Total 8	O 8	0	0
59	45	4	Total 4	O 4	0	0
59	55	3	Total 3	O 3	0	0
59	85	1	Total 1	O 1	0	0
59	95	1	Total 1	O 1	0	0
59	A5	1	Total 1	O 1	0	0
59	B5	1	Total 1	O 1	0	0
59	C5	3	Total 3	O 3	0	0
59	F5	1	Total 1	O 1	0	0
59	H5	2	Total 2	O 2	0	0

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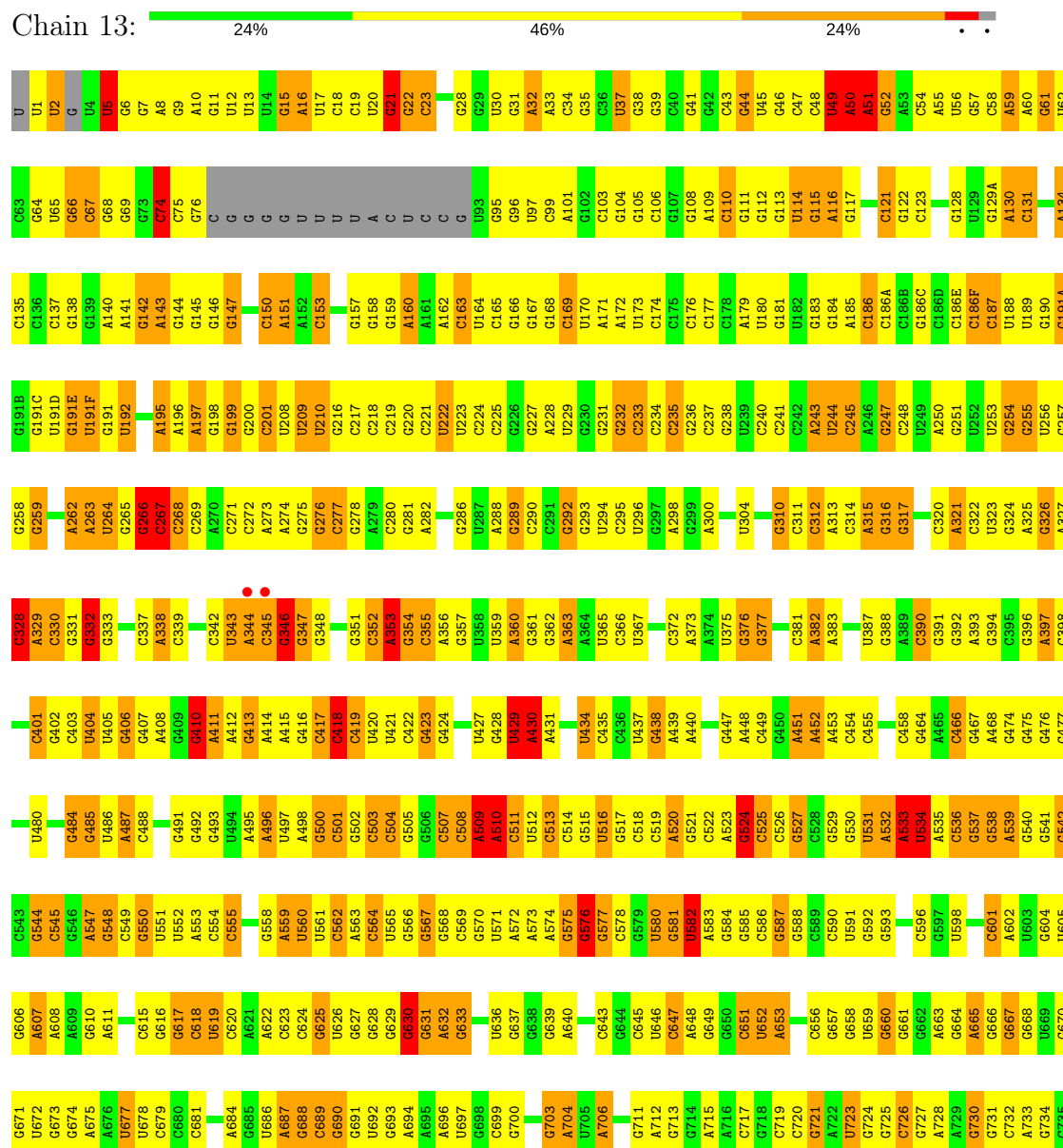
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	L5	3	Total	O	0	0
			3	3		
59	M5	6	Total	O	0	0
			6	6		

3 Residue-property plots

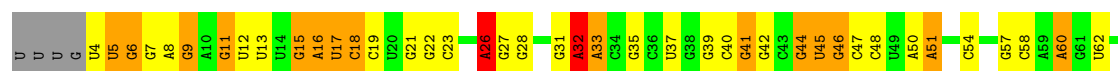
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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





Category	Percentage
Green	33%
Yellow	44%
Orange	18%
Red	5%



G1171	G1107	A1032	G971	A909	U831	A759	G882	A608	G542	G475	A389	G309	G226	G148	U65
G1172	G1108	G1032A	C972	C910	G837	C762	G883	A609	C543	G476	A389	A315	G227	A149	G86
G1173	C1109	G1032B	G973	U911	G838	G763	A684	A614	C544	G477	C390	G316	G230	C150	G87
G1174	A1110	G1033	A974	C912	G835	G762	G885	A615	C545		C392	G317	G231	A160	G68
G1175	A1111		A975	A913	U841	A766	U886	G616	G546	U480	G396	C320	G232	A161	G69
G1176	C1112	C1037	G976	A914	U842	A767	G887	G617	A547	U481	A397	A321		A162	G78
G1177	C1113	C1038	A977	U915	U843	A768	G888	G618	G550	A482	C398	C322	C235	C163	
G1178	C1114	C1039	C979	G917	C848	A769	G889	U619	U551	A483	C399	G324	C240	U164	G79
G1179	U11040	U1040	A980	A918	U850	G769	G890	U619	U552	A484	C400	U323	C241	C165	G80
A1180	C1115	A1041	C979	A919	G851	G771	U692	A621	A553	U486	C401	G324	C242	G166	G81
G1181	C1118		U981	U920	G852	U772	G693	A622	C554	A487	G402	A325	C242	G167	U82
G1182	C1119	A1046	U982	U921	G853	G773	A694	C624	C555	C488	C403	A327	A243	G168	U
G1184		G1047	A983	G922	G854				C556	C489	U404		U244		U
	U1122	G1048	C984	G923					G557		U405	C328	C245	C174	U
	A1123		C985	A923	G855		U697	G625	G558	G490	G406	A329	C246	C175	A87
	G1124	C1051	A986	C924	G856	G778	G698	U626	G559	G491	A407	C330	G247	C176	C88
	U1125	U1052	C979	U925	C857	C779	G699	G627	A559	G492	A408	G331		C177	U89
A1126	U1126	G1053	A981	G926	G858	A780	G700	G628	U560		G409	G332	A250	C178	C90
G1127	C1127	C1054	U982	G927	A859		C707	G629	U561	A495	G409		A251	A179	C91
G1128	U1128	U1055	U983	G928		C784	C708	G630	C562	A496	G410		U252	U180	
G1129	C1129	C1056	A984	G929	A864	G785	C708	G631	C563	U497	A411		U253	G181	G96
A1130	C1130	G1057	C994	C930	G865		G711	A632	C564	A498	A412	A338	U254	U182	
G1131	G1131	G1058	A994	C931	C866	A790	G718	A633	U565	G500	G413	C339	G254	G183	A101
G1132	C1132	C1059	U996	C932	G867	G791	A712	G634	C566	G501	A414	U340		G184	G102
G1133	G1133	C1060	A997	G933	C868	A792	G713	G635	G567	G502			G258	C185	C103
G1134	G1134	G1061	U998	C934	C869	U793	G714	G636	C568	C593	C419	A344	G259	A185	G104
G1135	U1135	U1062	C998A	A935	U870	A794	C717	G639	C569	C504	C422	C345	U261	C186	G105
G1136	U1136	C1063	U999	C936	G871	C795	G718	A640	G505	G505	G423	G346	A262	C186A	
C1137	C1137	G1064	A1000	A937	A872		G719	U641	U571		G424	G347	A263	C186B	
G1138	G1138	U1065	A873	C940	A873	G798	G720	A642	A572	A509	G425	G348	U264	C186F	G108
G1139	C1139	C1066	G874	C941	G874	G799	G721	G645	A573	A510	G426	A349	G265		A109
G1202	G1002	A1067	G1008	C946	C882	C805	A728	C651	U580	G517	U427	C350	G266	G189	G110
G1203	G1003	A1068	G1009	C947	C883	C808	A729	U652	G581	C518	U434	C351	G267	G190	G111
A1204	A1004	C1141	G1010	C948	U884		G730	A653	U582	C519	U437	C352	C268	G191A	G112
U1205	C1141	G1068		A949	G885	C811	G731	G654	A583	A520	U438	A353	C269	G191B	G113
G1142	G1142	A1005	A1015	U950	G886	C812	C736		G584	G521	G439	A363	G270	G191C	G114
G1143	G1143	C1006	A1016	U951	G887	C813	A737	G658	U585	A523	A440	A364	A271	G191D	G115
G1144	G1144	U1073	G1017	U952	G888	U813		U659	G588	G524	C442	U365	G278	G191E	A116
G1145	C1145	U1073	G1018	G954	A889	A814	U740	A663	C589	C525	C443	U366	A279	C192	G127
U1146	U1076	C1076	C1019	G955	G890	A815	G741	A664	C590	G526	C444	U367	C280	A195	G128
G1147	G1077	G1077	U1020	U956	U891	A816	G741	A665	U591	C527	A448	C370	G281	U129	U129
U1148			G1021	U957	C893	C818	A746	G666	U591	C528	C449	G371	A282	G198	A130
U1149	A1080	G1081	G1022	A958	G894	A819	C747		C596		G450	G372	G289	C132	C131
U1150	A1015		G1023	U960	G895	U820	C748	U669	G597	U531	A451	C373		U133	C132
A1151	A1016	G1084	U1025	U961	A900	G821	C749	G670	U598	A532	A452	A374	U296	U209	U133
A1152	G1017	U1085	G1026	G961	A901	C922	G750		U599	A533		A375	G297	U210	A134
G1153	G1018	U1086	C1027	A964	G902	G823	U751	G673	C599	U534	C457	U376	A298	G216	C135
G1154	U1087	C1096	G1028	G965	G903	C824	G752	G674	C600	U534	C458	U375	A299	G219	G142
G1155	G1087	C1162	C1028	A966	G903	G825	A753	A675	C596	C536	G464	G376	G299	G220	A143
G1156	G1088	A1101	C1028A	G966	C904	C826	C754	A676	U603	G537	A465	G377	A300	G221	G144
A1157		A1102	C1028B	C967	U905	U827	G755	U677	G504	G538	C466	G378	G301	C221	G145
G1221	G1022		G1029	A968	G906	A828	C756		U605	A539	G467	C379	C307	U223	G146
G1222	G1023	A1092	C1030	A969	A907	G829	U757	C680	G606	G540	A468			U223	G147
G1223	G1024	A1093	G1031		A908	G830	G758	C681	A607	G541	G474	G388	C308		
G1224	U1025	G1094													
A1225	C1161	C1095													
C1226	C1162	C1096													
A1227	C1163														
C1228	G1164														
A1229															
U1232	A1167														
G1233	U1169	A1105													

Chain 2E:

Chain 22:

Category	Value
MET	17%
GLY	38%
N3	
K4	
I5	
H6	
P7	
I8	
G9	
F10	
R11	
T15	
D17	
W18	
F19	
S20	
R21	
W22	
Y23	
K26	
K27	
Y29	
L32	
L33	
L34	
E35	
D36	
Q37	
R38	
I39	
R40	
G41	
L42	
L43	
E44	
K45	
E46	
L47	
Y48	
S49	
A50	
G51	
L52	
V55	
D56	
I57	
E58	
R59	
A60	
A61	
D62	
N63	
V64	
A65	
V66	
T67	
V68	
H69	
K72	
P73	
G74	
V75	
W76	
T1E	
GLY	
ARG	
GLY	
GLY	
GLU	
ARG	
T84	
R85	
W86	
W87	
R88	
E89	
E90	
L91	
K92	
K93	
L94	
T95	
G96	
K97	
A100	
L101	
N102	
V103	
Q104	
M110	
L111	
S112	
A113	
L114	
L115	
Q118	
R119	
E122	
E125	
R126	
R127	
F128	
R131	
R140	
V141	
S144	
G148	
A149	
K150	
V151	
L152	
L153	
L154	
S154	
G155	
R156	
T157	
R164	
ARG	
T165	
ARG	
ARG	
W167	
A168	
A169	
Q170	
G171	
R172	
L175	
H176	
T177	
L178	
R179	
A180	
N181	
T182	
D183	
GLU	
Y184	
G185	
F186	
A187	
R190	
T191	
T192	
Y193	
G194	
V195	
L196	
G197	
V198	
K199	
I202	
F203	
L204	
GLY	
GLU	
VAL	
ILE	
GLY	
GLN	
LYS	
PRO	

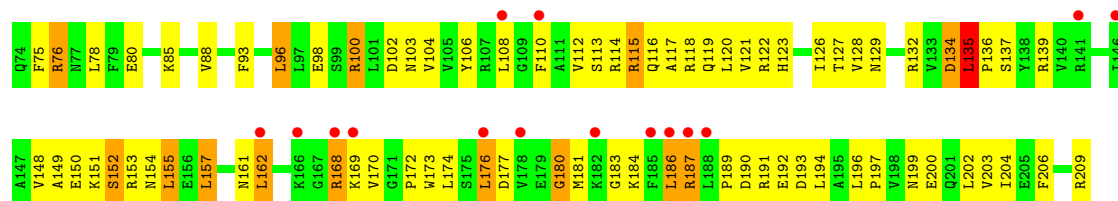
Chain 3E:

6% 42% 45% 11% ..

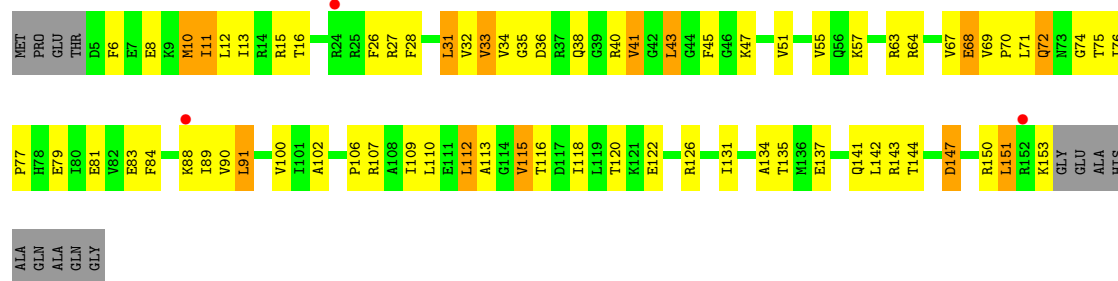
Sequence logo showing amino acid conservation across 200 positions. The y-axis represents information content in bits (0 to 1.5). The x-axis shows positions 1 to 200. A color key identifies amino acids: MET (grey), GLY (yellow), Y4 (green), I5 (red), G6 (green), P7 (orange), V8 (orange), C9 (orange), R10 (orange), L11 (red), C12 (green), R13 (orange), E15 (orange), K18 (green), L19 (orange), Y20 (green), L21 (green), K22 (green), G23 (red), F24 (red), R25 (orange), C26 (orange), K30 (orange), C31 (orange), A32 (orange), M33 (orange), E34 (green), R35 (orange), R36 (green), P37 (green), Y38 (green), P39 (orange), P40 (orange), G41 (orange), Q42 (green), H43 (orange), G44 (orange), Q45 (green), K46 (orange), A48 (orange), R47 (orange), R49 (orange), S52 (green), D53 (green), Y54 (orange), A55 (orange), L58 (orange), R59 (orange), E60 (orange), K61 (orange), Q62 (orange), K63 (orange), R64 (orange), P65 (orange).

Chain 32:

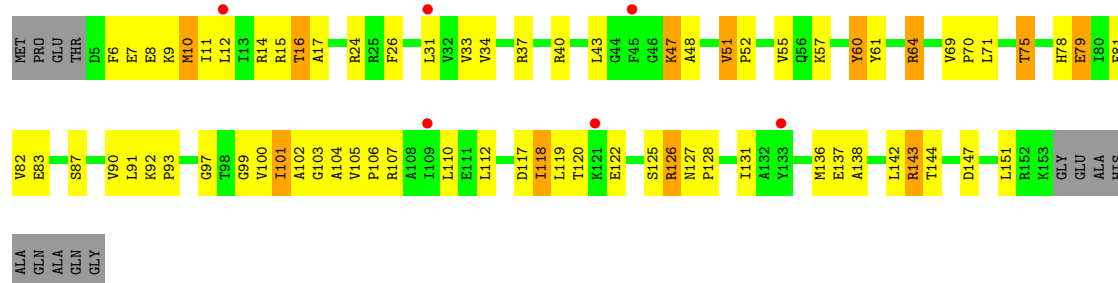
Category	Value
G2	
R3	
Y4	
I5	
C8	
V9	
L10	
L11	
C12	
R13	
R14	
E15	
G16	•
V17	
K18	
L19	•
Y20	•
L21	•
Q22	
Q23	•
E24	
R25	•
C26	
Y27	
S28	
P29	
K30	
C31	
A32	
M33	
E34	
R35	•
R36	
P39	
H43	
G44	
Q45	
K46	
D53	
R57	
L58	
R59	
E60	
K61	
R65	
R66	
I67	•
G68	
G69	
I70	•
S71	
T72	•



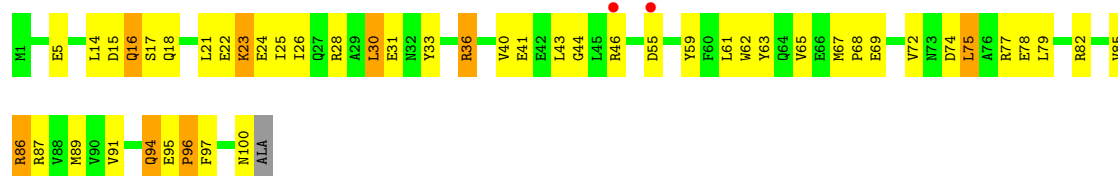
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

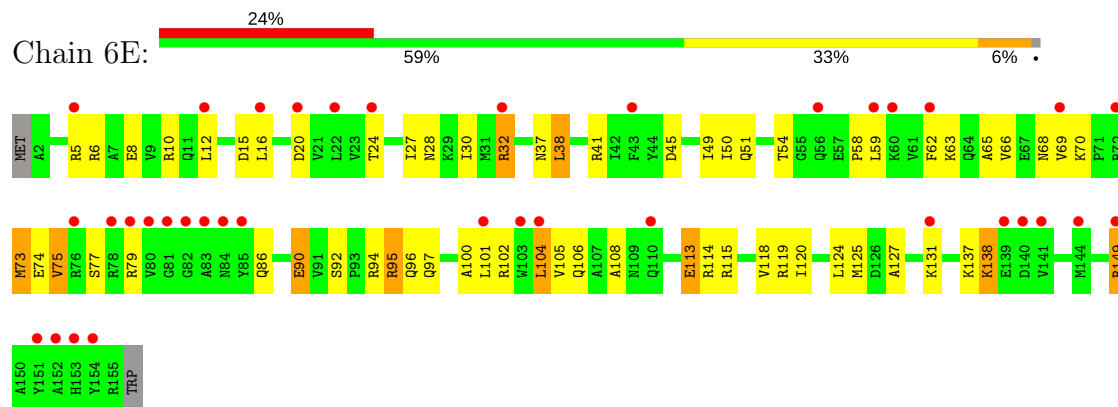


• Molecule 6: 30S ribosomal protein S6

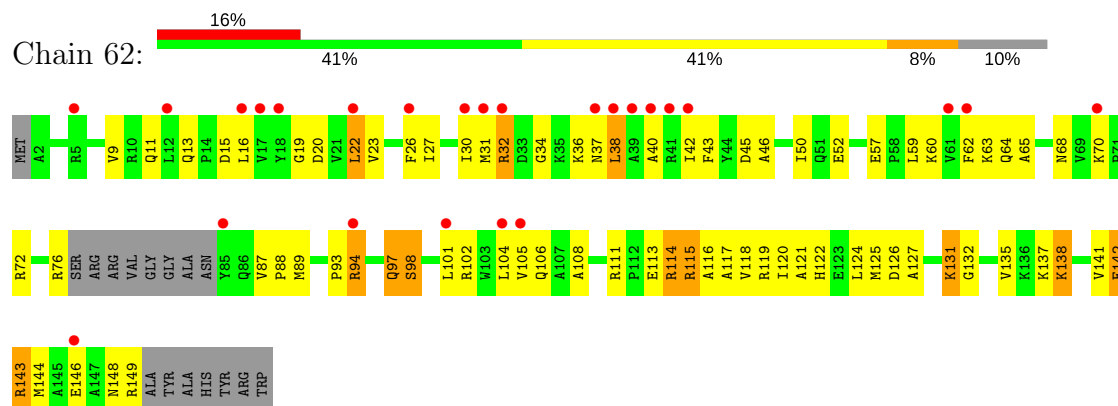




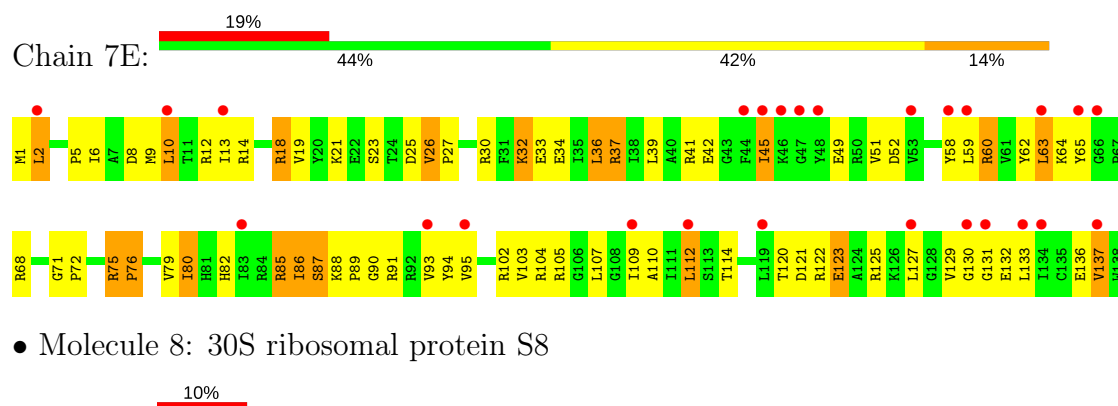
• Molecule 7: 30S ribosomal protein S7



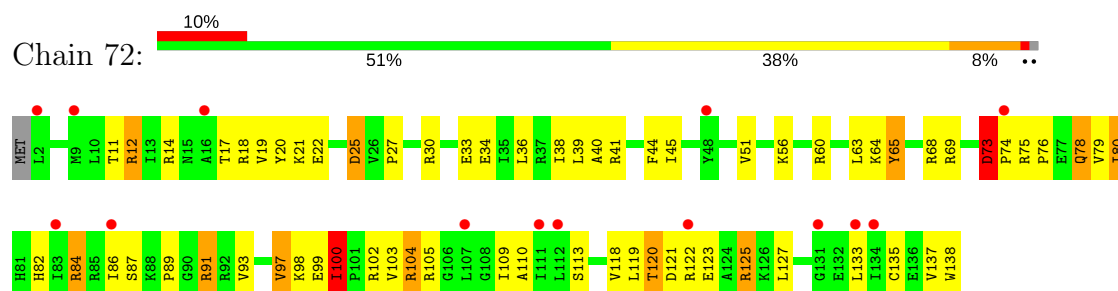
• Molecule 7: 30S ribosomal protein S7



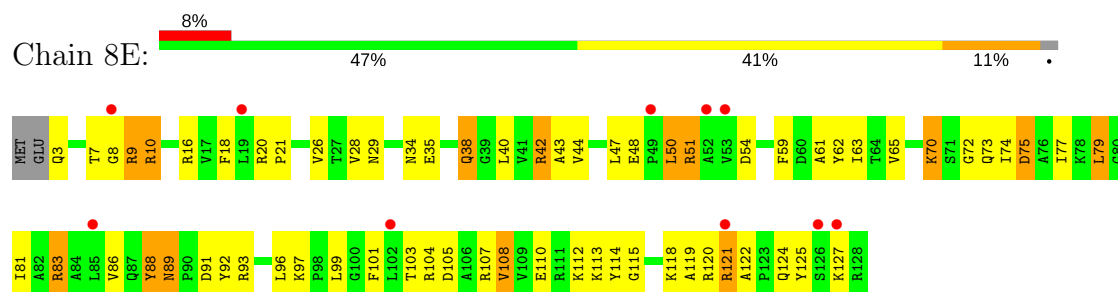
• Molecule 8: 30S ribosomal protein S8



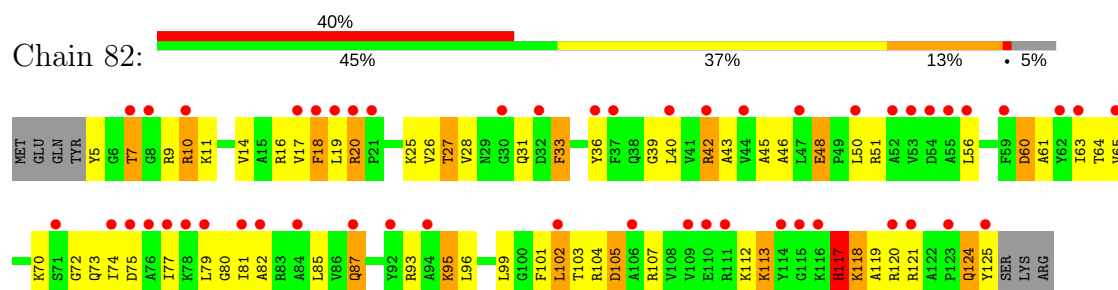
• Molecule 8: 30S ribosomal protein S8



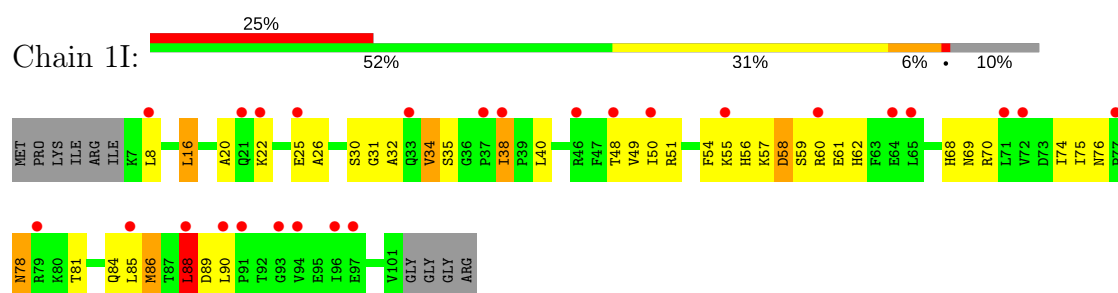
- Molecule 9: 30S ribosomal protein S9



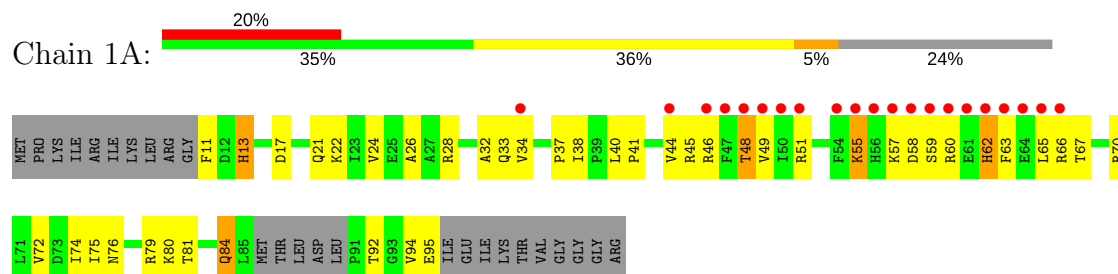
- Molecule 9: 30S ribosomal protein S9



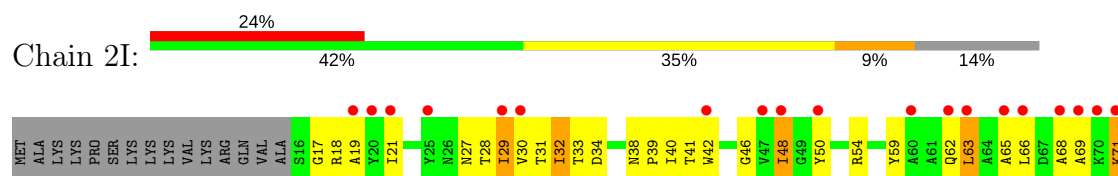
- Molecule 10: 30S ribosomal protein S10

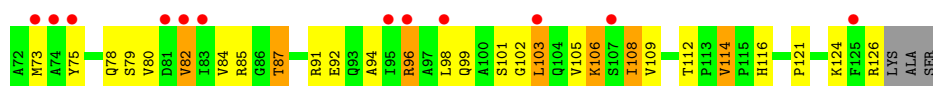


- Molecule 10: 30S ribosomal protein S10

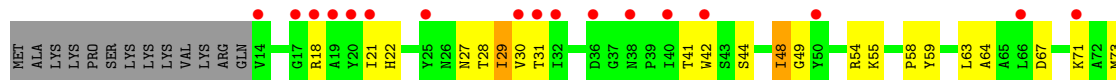


- Molecule 11: 30S ribosomal protein S11

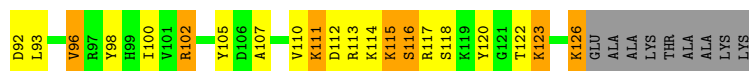




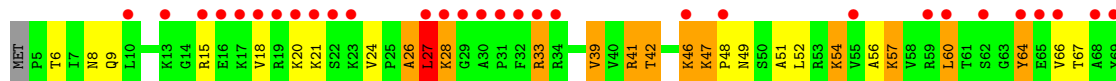
- Molecule 11: 30S ribosomal protein S11



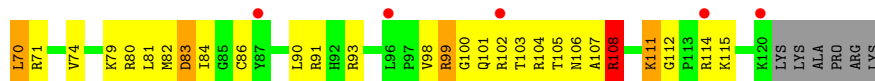
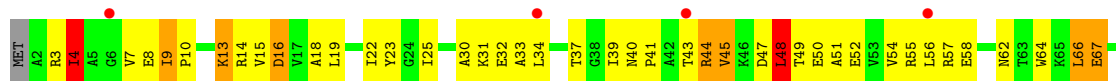
- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

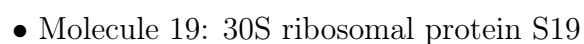


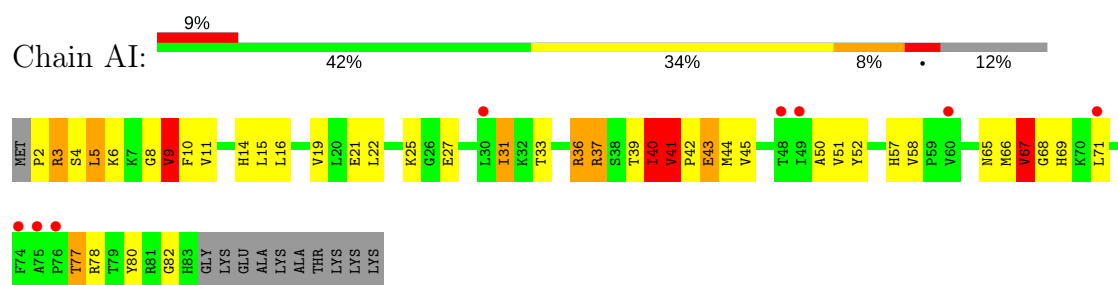
- Molecule 13: 30S ribosomal protein S13



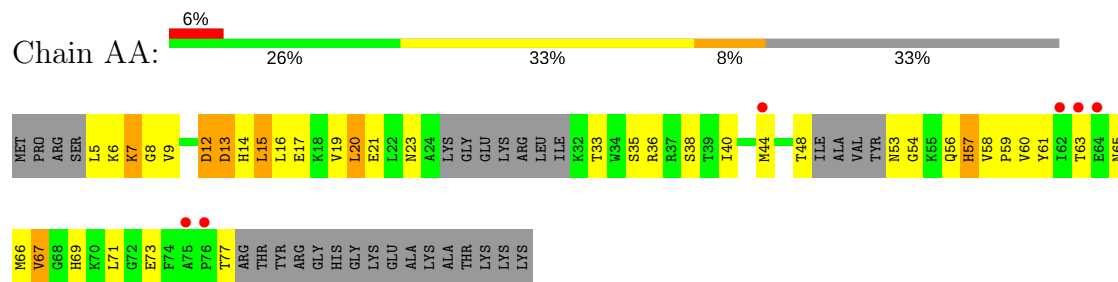
- Molecule 13: 30S ribosomal protein S13



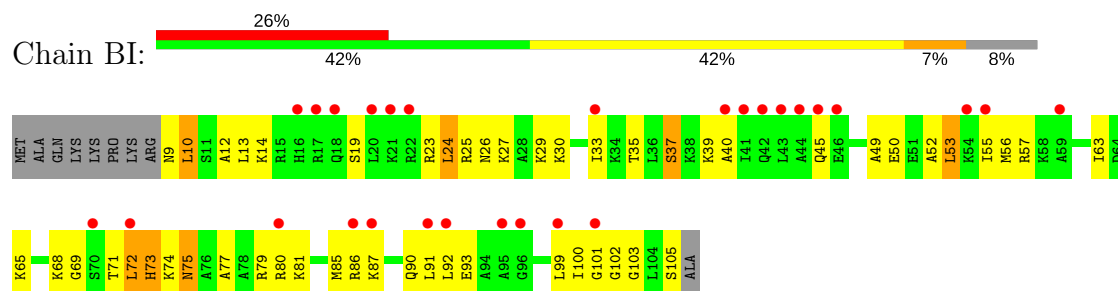


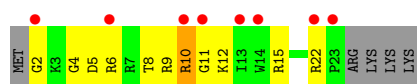


- Molecule 19: 30S ribosomal protein S19

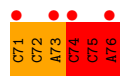
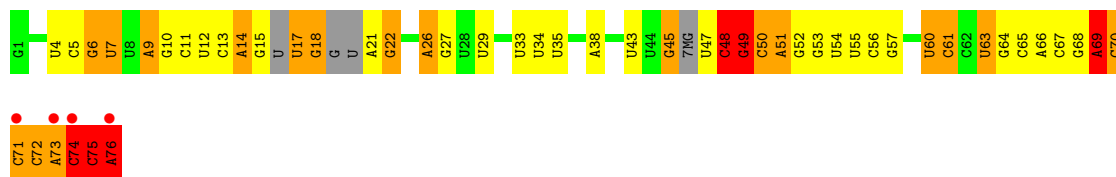
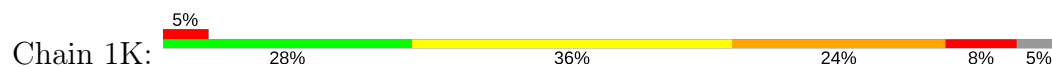


- Molecule 20: 30S ribosomal protein S20





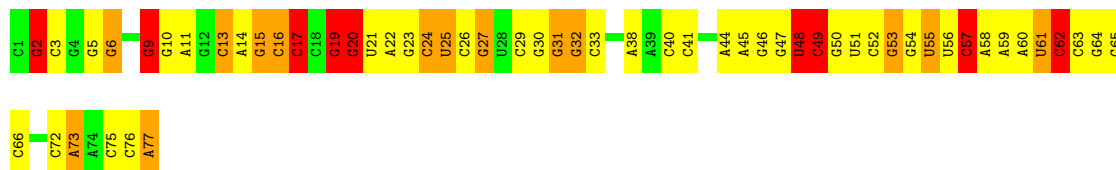
• Molecule 22: tRNA-Lys



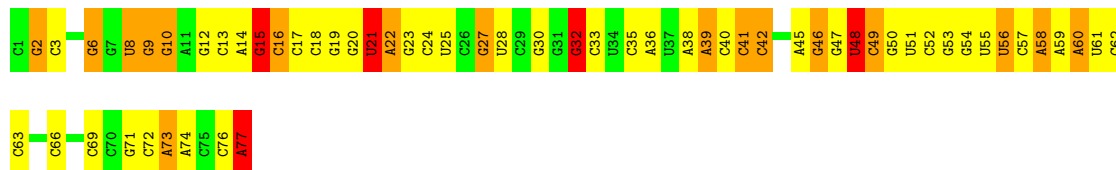
• Molecule 22: tRNA-Lys



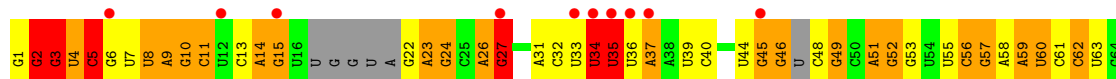
• Molecule 23: tRNA-fMet

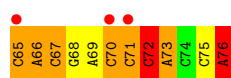


• Molecule 23: tRNA-fMet

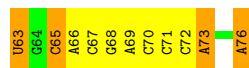
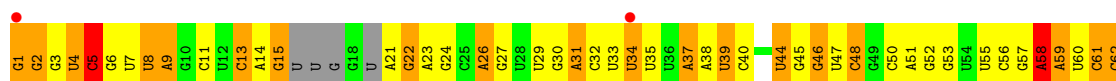
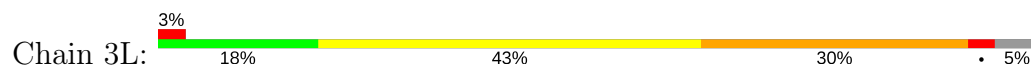


• Molecule 24: tRNA-Lys

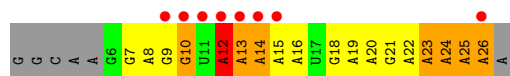




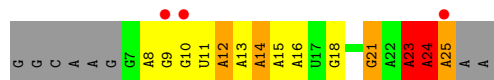
• Molecule 24: tRNA-Lys



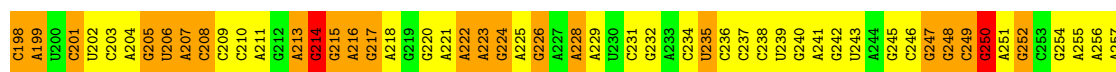
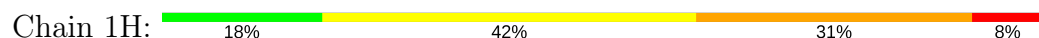
• Molecule 25: mRNA



• Molecule 25: mRNA

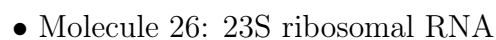


• Molecule 26: 23S ribosomal RNA



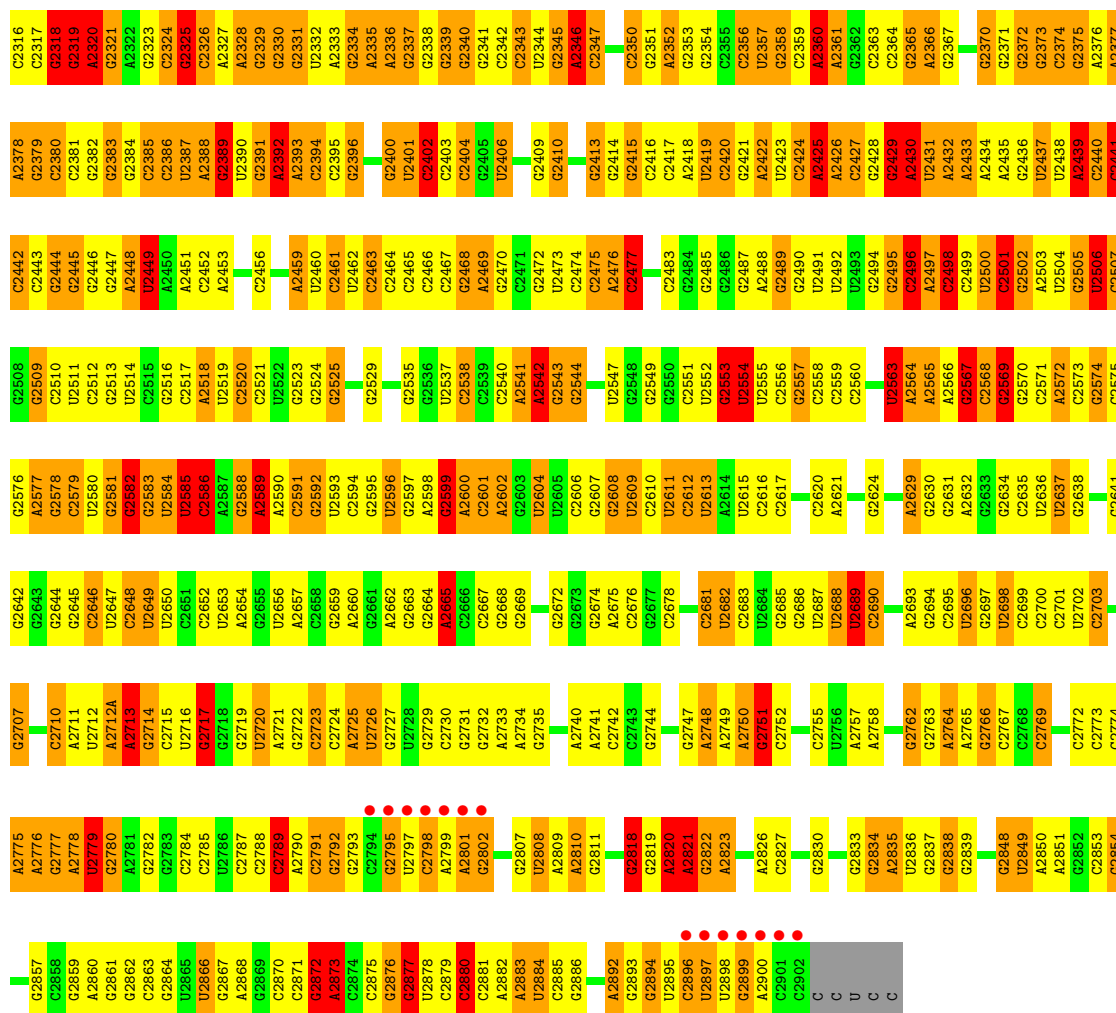
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C1291	G1228	U1167	U1097	A1029	C970	C908	C844	A784	G723	G662	A621	G662	G493	C426	C364
C1292	G1229	G1168	A1098	G1030	C971	A909	G845	A785	U724	G663	G622	G622	G494	U427	C365
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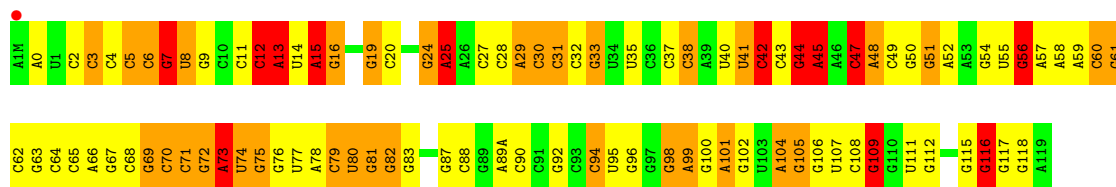
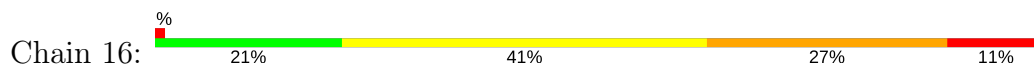


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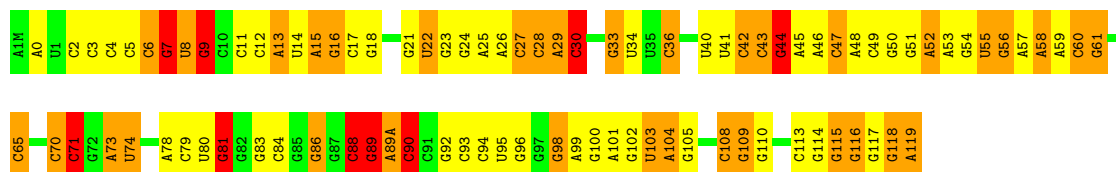
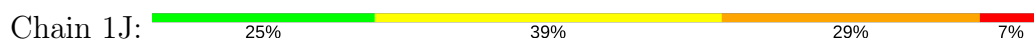
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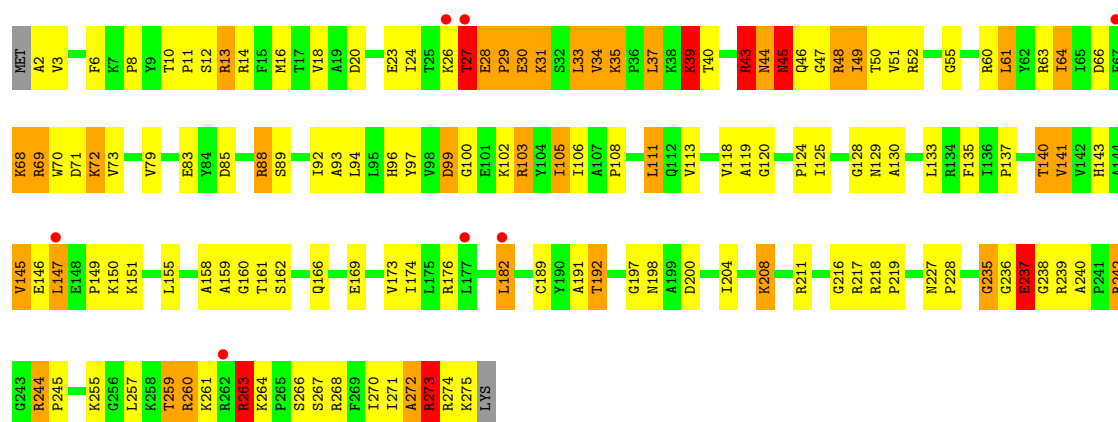
- Molecule 27: 5S ribosomal RNA



- Molecule 27: 5S ribosomal RNA

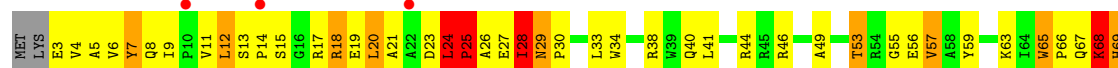


- Molecule 28: 50S ribosomal protein L1

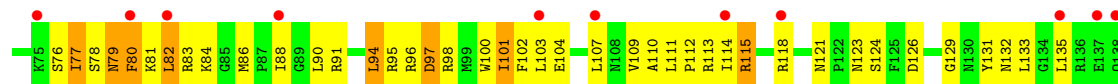




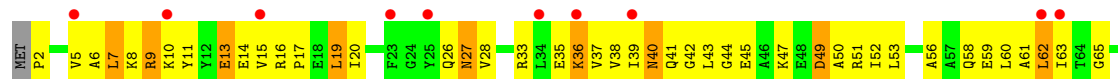
- Molecule 31: 50S ribosomal protein L4



- Molecule 32: 50S ribosomal protein L5

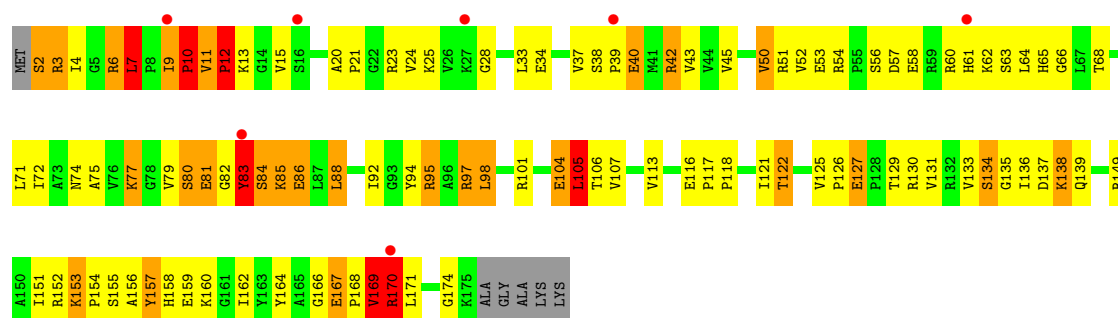


- Molecule 32: 50S ribosomal protein L5

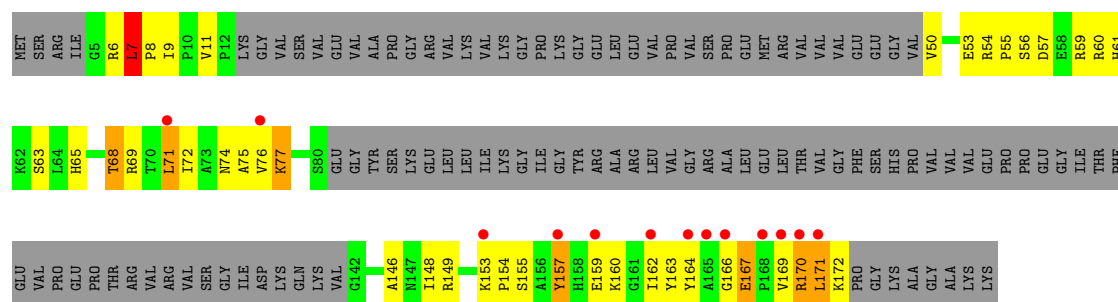


- Molecule 33: 50S ribosomal protein L6

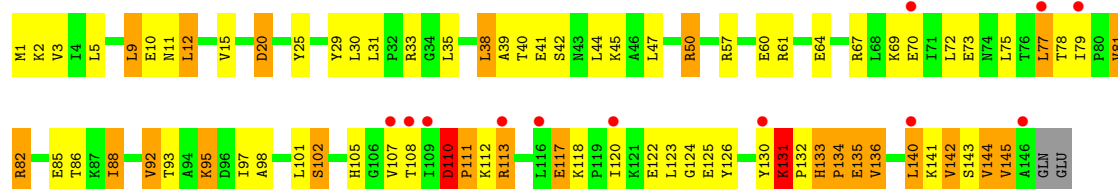




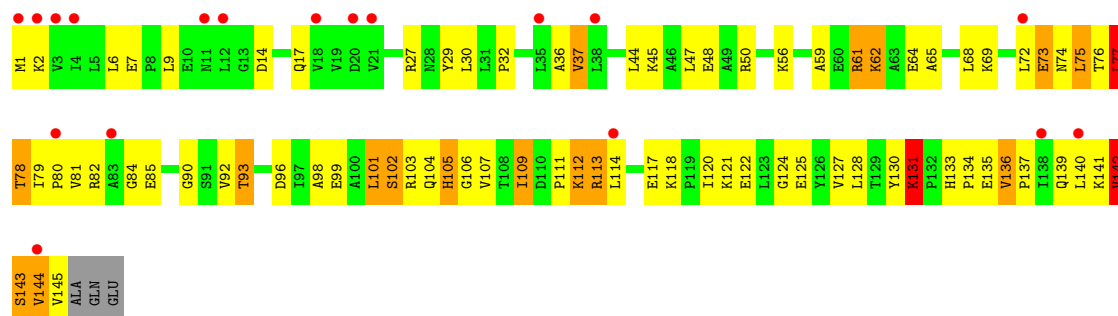
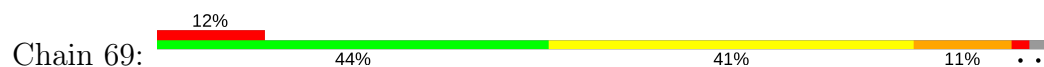
• Molecule 33: 50S ribosomal protein L6



• Molecule 34: 50S ribosomal protein L9

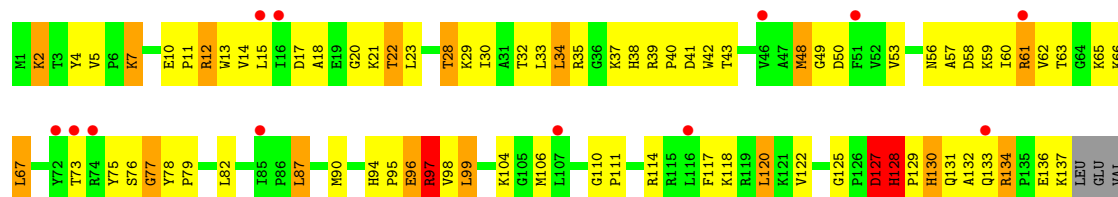


• Molecule 34: 50S ribosomal protein L9

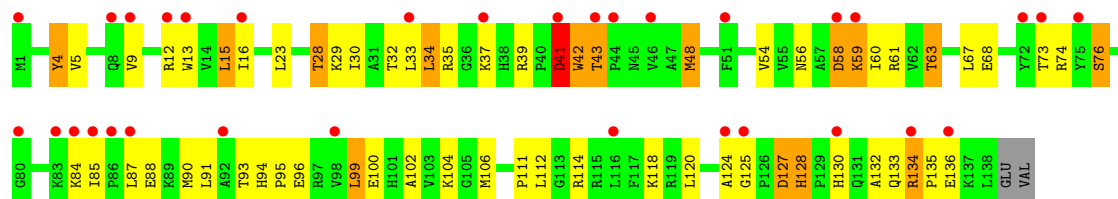


• Molecule 35: 50S ribosomal protein L13

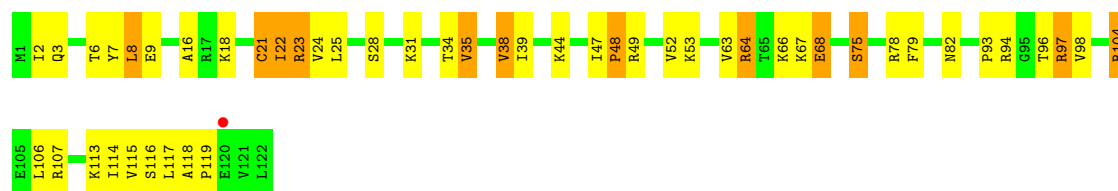




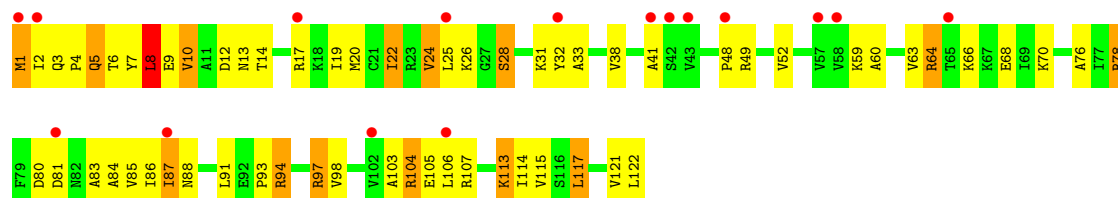
• Molecule 35: 50S ribosomal protein L13



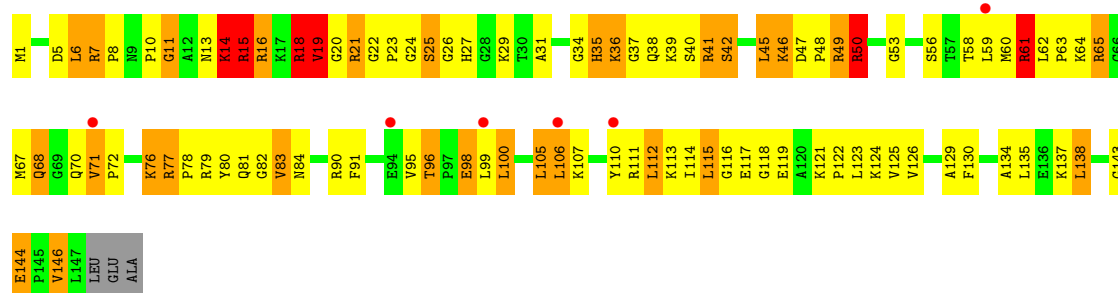
• Molecule 36: 50S ribosomal protein L14





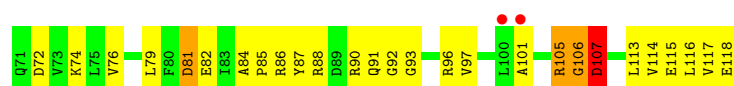
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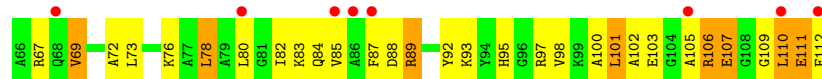
• Molecule 37: 50S ribosomal protein L15



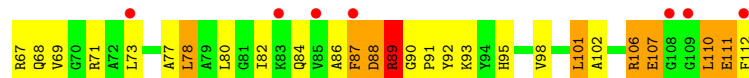
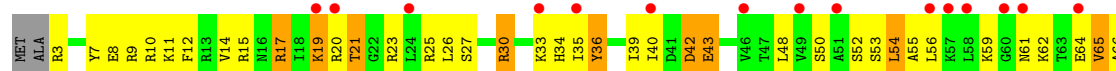
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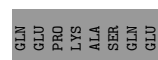
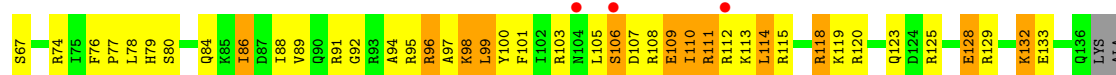
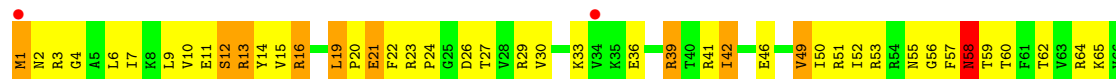
• Molecule 40: 50S ribosomal protein L18



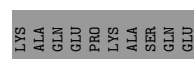
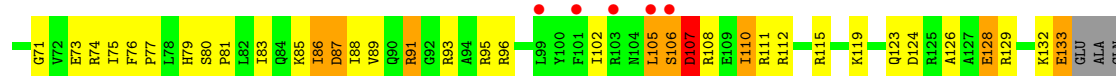
• Molecule 40: 50S ribosomal protein L18



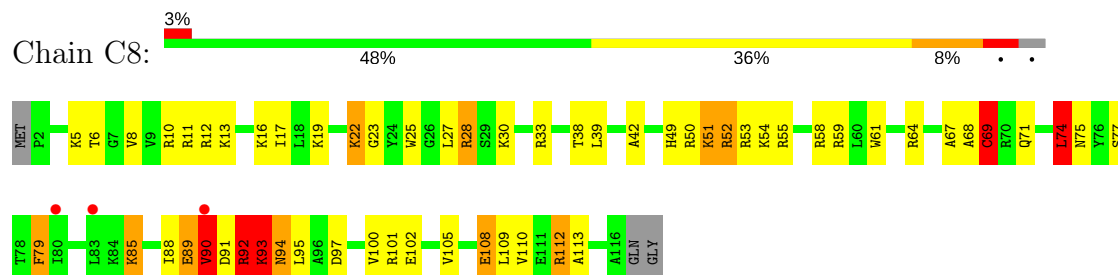
• Molecule 41: 50S ribosomal protein L19



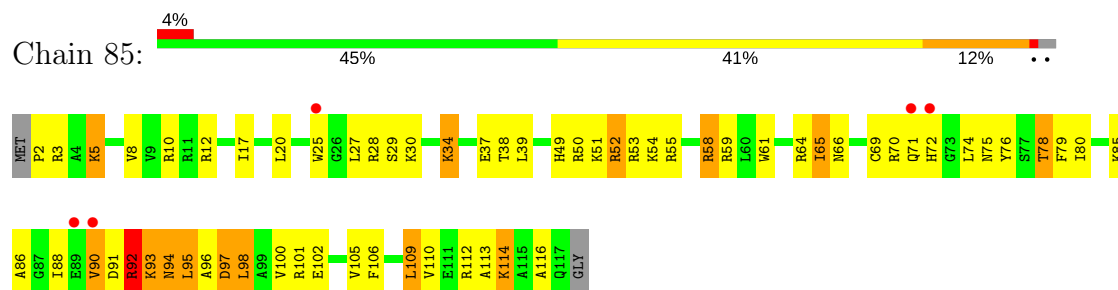
• Molecule 41: 50S ribosomal protein L19



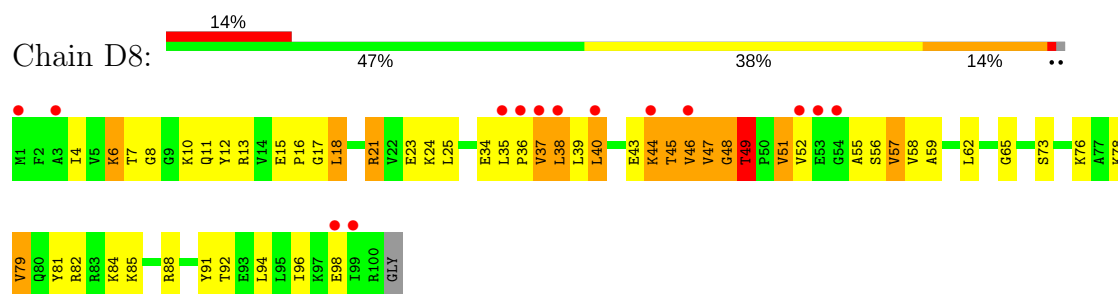
• Molecule 42: 50S ribosomal protein L20



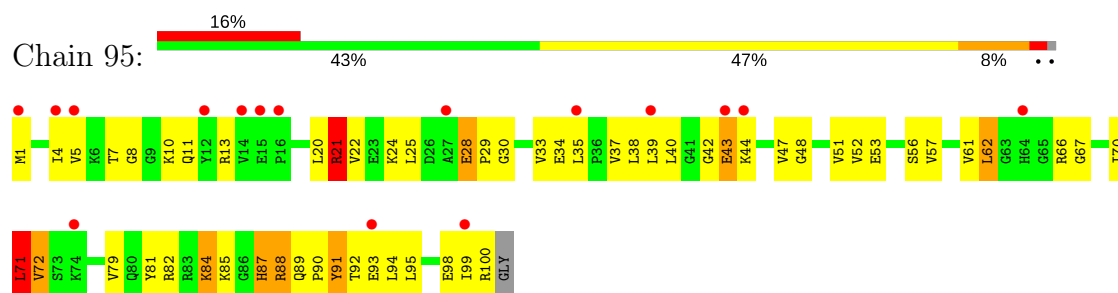
• Molecule 42: 50S ribosomal protein L20



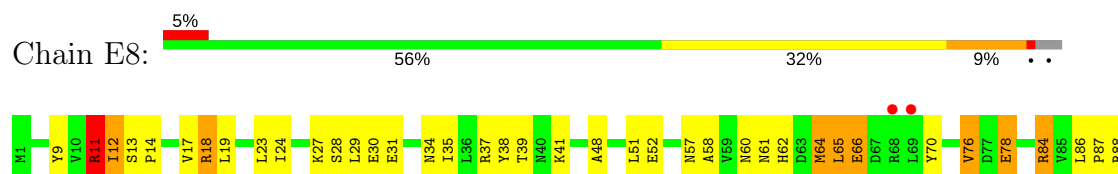
• Molecule 43: 50S ribosomal protein L21



• Molecule 43: 50S ribosomal protein L21

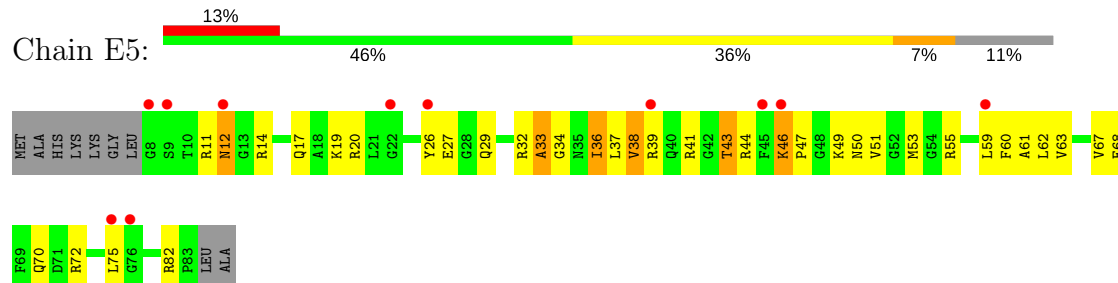


• Molecule 44: 50S ribosomal protein L22

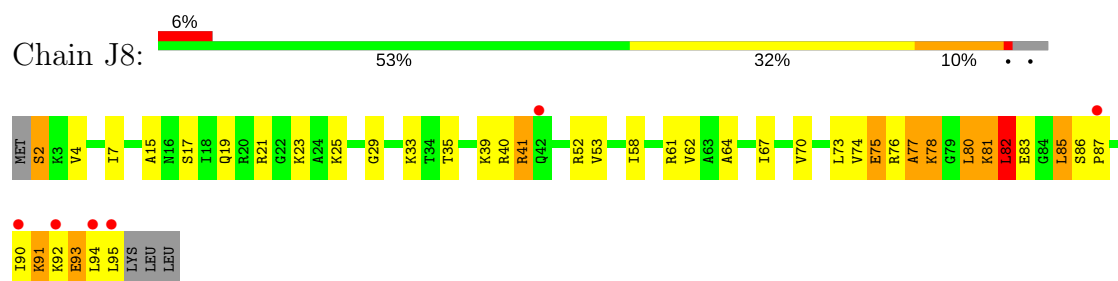




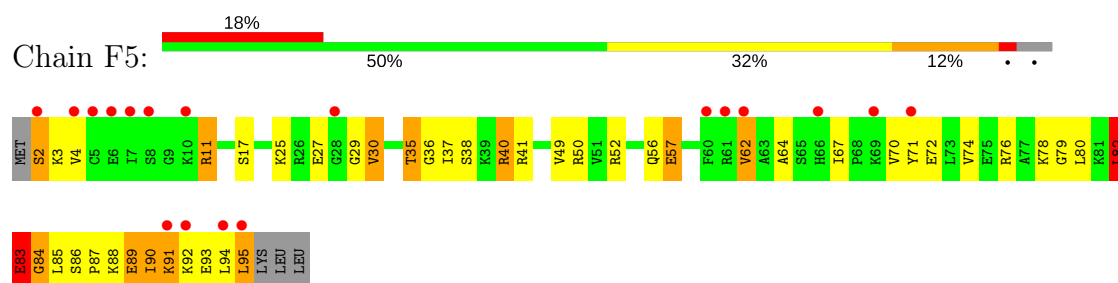
- Molecule 48: 50S ribosomal protein L27



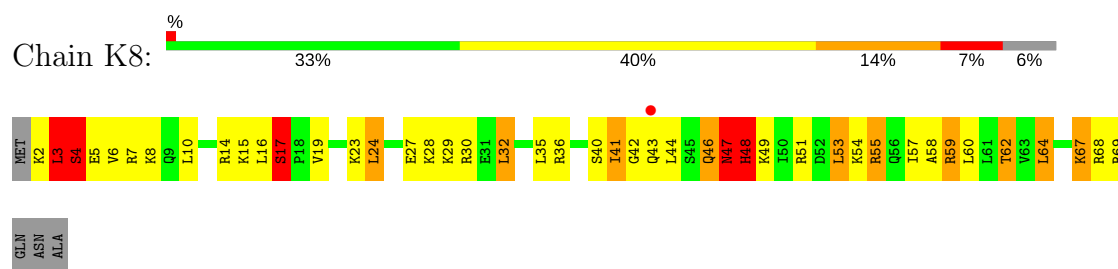
- Molecule 49: 50S ribosomal protein L28



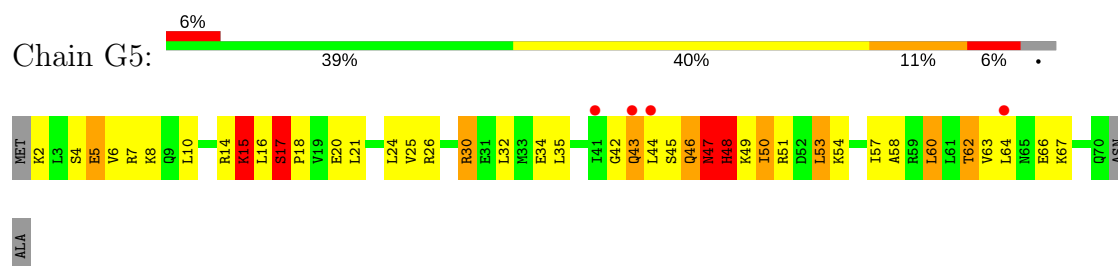
- Molecule 49: 50S ribosomal protein L28



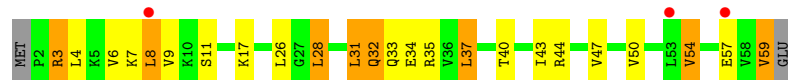
- Molecule 50: 50S ribosomal protein L29



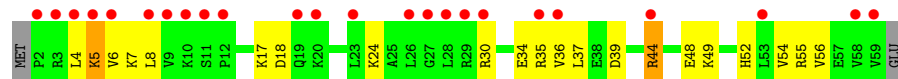
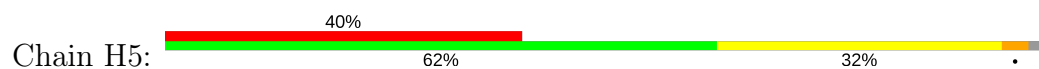
- Molecule 50: 50S ribosomal protein L29



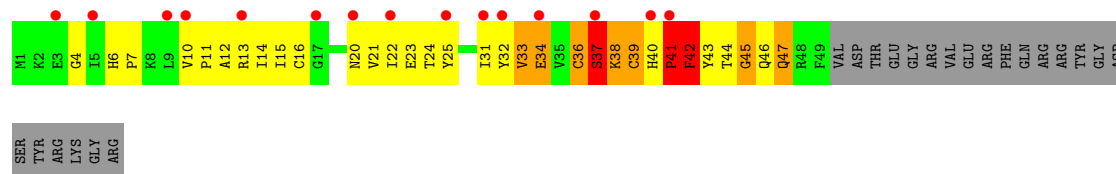
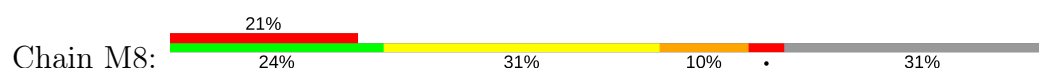
- Molecule 51: 50S ribosomal protein L30



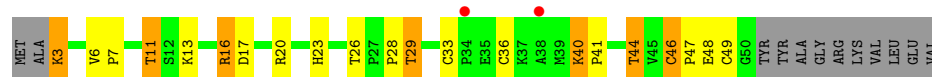
- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32

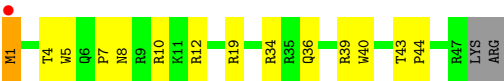


- Molecule 54: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L34

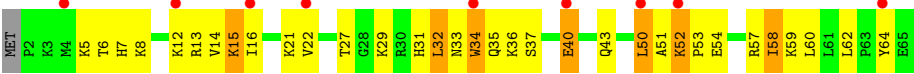




• Molecule 55: 50S ribosomal protein L35



• Molecule 55: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.20Å 448.50Å 619.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.01 – 2.95 147.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (147.01-2.95) 91.6 (147.01-2.95)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.242 0.196 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (0.18%)	DCC
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 72.1	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	0.95	EDS
Total number of atoms	297904	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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, G7M, SF4, MG, 4SU, T6A, 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	0.92	23/35994 (0.1%)	1.67	897/56171 (1.6%)
1	1G	0.79	7/36236 (0.0%)	1.48	499/56555 (0.9%)
2	12	0.44	0/1727	0.73	1/2326 (0.0%)
2	1E	0.47	0/1908	0.76	4/2573 (0.2%)
3	22	0.43	0/1560	0.67	0/2104
3	2E	0.58	0/1629	0.73	1/2195 (0.0%)
4	32	0.58	1/1732 (0.1%)	0.81	3/2318 (0.1%)
4	3E	0.61	0/1728	0.84	3/2313 (0.1%)
5	42	0.53	0/1155	0.72	0/1555
5	4E	0.64	0/1158	0.77	0/1559
6	52	0.65	0/855	0.72	0/1154
6	5E	0.66	0/850	0.76	0/1147
7	62	0.51	0/1132	0.70	0/1514
7	6E	0.52	0/1259	0.65	0/1686
8	72	0.48	0/1127	0.66	0/1517
8	7E	0.59	0/1135	0.81	1/1527 (0.1%)
9	82	0.43	0/971	0.70	0/1304
9	8E	0.51	0/1019	0.72	0/1367
10	1A	0.46	0/658	0.70	0/885
10	1I	0.60	0/767	0.82	0/1034
11	2A	0.55	0/850	0.67	0/1150
11	2I	0.62	0/838	0.79	0/1133
12	3A	0.68	0/972	0.89	2/1301 (0.2%)
12	3I	0.87	0/972	1.04	3/1301 (0.2%)
13	4A	0.48	0/903	0.73	0/1211
13	4I	0.67	0/952	0.87	2/1277 (0.2%)
14	5A	0.54	0/495	0.80	1/657 (0.2%)
14	5I	0.70	0/500	0.89	0/664
15	6A	0.60	0/740	0.70	0/987
15	6I	0.64	0/740	0.78	0/987
16	7A	0.64	0/721	0.86	1/970 (0.1%)
16	7I	0.59	0/716	0.83	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.57	0/836	0.70	0/1117
17	8I	0.69	0/847	0.82	1/1131 (0.1%)
18	9A	0.63	0/549	0.82	1/732 (0.1%)
18	9I	0.62	0/554	0.84	0/739
19	AA	0.44	0/490	0.69	0/662
19	AI	0.73	1/676 (0.1%)	1.03	5/910 (0.5%)
20	BA	0.51	0/764	0.78	1/1007 (0.1%)
20	BI	0.45	0/748	0.74	2/986 (0.2%)
21	1B	0.50	0/192	0.74	0/252
21	1F	0.57	0/203	0.82	0/266
22	1K	0.80	1/1589 (0.1%)	1.36	23/2464 (0.9%)
22	1L	0.62	3/1516 (0.2%)	1.18	9/2350 (0.4%)
23	2K	1.02	2/1721 (0.1%)	1.76	50/2682 (1.9%)
23	2L	0.83	2/1721 (0.1%)	1.56	30/2682 (1.1%)
24	3K	0.70	2/1654 (0.1%)	1.41	25/2570 (1.0%)
24	3L	0.66	0/1705	1.30	14/2650 (0.5%)
25	4K	1.03	1/523 (0.2%)	1.55	10/813 (1.2%)
25	4L	0.78	0/473	1.44	9/737 (1.2%)
26	14	1.13	193/68883 (0.3%)	1.96	3155/107521 (2.9%)
26	1H	1.33	416/69669 (0.6%)	2.20	4553/108757 (4.2%)
27	16	1.07	7/2928 (0.2%)	2.00	135/4568 (3.0%)
27	1J	0.92	2/2928 (0.1%)	1.73	88/4568 (1.9%)
28	71	0.39	0/1055	0.68	1/1425 (0.1%)
28	79	0.36	0/459	0.66	1/608 (0.2%)
29	11	1.07	6/2170 (0.3%)	1.22	16/2926 (0.5%)
29	19	0.92	1/2175 (0.0%)	1.09	11/2933 (0.4%)
30	21	0.87	1/1591 (0.1%)	1.12	7/2146 (0.3%)
30	29	0.81	1/1596 (0.1%)	1.06	8/2153 (0.4%)
31	31	0.91	3/1620 (0.2%)	1.11	12/2194 (0.5%)
31	39	0.78	1/1637 (0.1%)	1.02	3/2218 (0.1%)
32	41	0.69	0/1481	0.89	2/1994 (0.1%)
32	49	0.53	0/1492	0.77	2/2008 (0.1%)
33	51	0.74	0/1354	1.06	7/1833 (0.4%)
33	59	0.47	0/552	0.87	2/743 (0.3%)
34	61	0.59	0/1151	0.86	3/1558 (0.2%)
34	69	0.56	0/1146	0.86	5/1551 (0.3%)
35	15	0.57	0/1131	0.75	0/1525
35	58	0.71	0/1123	0.93	0/1514
36	25	0.73	0/942	0.86	1/1269 (0.1%)
36	68	0.83	0/942	0.92	2/1269 (0.2%)
37	35	0.73	0/1139	1.07	1/1514 (0.1%)
37	78	0.91	0/1139	1.35	16/1514 (1.1%)
38	45	0.77	0/1125	1.00	0/1505

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	88	0.98	0/1138	1.14	3/1523 (0.2%)
39	55	0.73	0/981	0.96	0/1312
39	98	0.72	0/981	1.01	8/1312 (0.6%)
40	65	0.65	0/886	1.01	4/1180 (0.3%)
40	A8	0.79	0/891	1.03	0/1187
41	75	0.70	0/1123	0.93	4/1500 (0.3%)
41	B8	0.81	0/1138	1.01	2/1521 (0.1%)
42	85	0.76	0/977	0.91	2/1301 (0.2%)
42	C8	0.85	1/968 (0.1%)	0.99	4/1289 (0.3%)
43	95	0.70	0/781	0.95	2/1048 (0.2%)
43	D8	0.76	0/785	1.00	5/1052 (0.5%)
44	A5	0.82	0/897	0.94	0/1204
44	E8	0.82	0/886	1.06	5/1189 (0.4%)
45	B5	0.81	0/749	0.88	0/1007
45	F8	0.90	0/757	1.07	4/1017 (0.4%)
46	C5	0.75	0/807	0.97	2/1076 (0.2%)
46	G8	0.91	0/796	1.15	5/1062 (0.5%)
47	D5	0.55	0/1103	0.79	2/1494 (0.1%)
47	H8	0.61	0/1395	0.87	2/1890 (0.1%)
48	E5	0.77	0/611	0.95	0/814
48	I8	0.95	1/619 (0.2%)	1.23	3/825 (0.4%)
49	F5	0.83	0/744	1.13	6/989 (0.6%)
49	J8	0.92	1/744 (0.1%)	1.09	4/989 (0.4%)
50	G5	0.69	0/578	0.88	1/766 (0.1%)
50	K8	0.95	0/577	1.26	6/763 (0.8%)
51	H5	0.66	0/464	0.86	0/623
51	L8	0.83	1/464 (0.2%)	0.93	0/623
52	M8	0.65	0/385	1.05	2/521 (0.4%)
53	J5	0.82	0/448	1.06	3/606 (0.5%)
53	N8	0.85	0/381	1.03	0/516
54	L5	0.85	0/409	1.08	3/540 (0.6%)
54	P8	1.04	0/409	1.21	1/540 (0.2%)
55	M5	0.93	2/524 (0.4%)	1.05	1/691 (0.1%)
55	Q8	0.99	0/524	1.25	3/691 (0.4%)
All	All	1.01	680/318108 (0.2%)	1.71	9716/476630 (2.0%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	1
4	32	0	1
9	82	0	1
9	8E	0	1
10	1I	0	1
11	2A	0	1
11	2I	0	1
12	3I	0	3
13	4A	0	2
13	4I	0	3
14	5A	0	1
20	BA	0	3
28	71	0	3
29	11	0	6
29	19	0	5
30	21	0	9
30	29	0	5
31	39	0	10
32	41	0	1
32	49	0	3
33	51	0	5
33	59	0	3
34	61	0	3
34	69	0	5
35	15	0	2
35	58	0	2
37	35	0	3
37	78	0	5
38	45	0	3
38	88	0	2
39	55	0	1
39	98	0	1
40	65	0	1
41	75	0	1
41	B8	0	3
42	85	0	3
42	C8	0	2
43	95	0	1
43	D8	0	4
44	A5	0	1
45	B5	0	2
45	F8	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	C5	0	2
46	G8	0	6
47	D5	0	5
47	H8	0	3
49	F5	0	2
49	J8	0	3
50	G5	0	3
50	K8	0	4
52	M8	0	4
54	P8	0	1
55	M5	0	2
55	Q8	0	2
All	All	0	158

The worst 5 of 680 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	2430	A	N9-C4	-17.68	1.27	1.37
26	1H	1698	A	N9-C4	-15.72	1.28	1.37
26	1H	783	A	N3-C4	-14.91	1.25	1.34
26	1H	774	A	N9-C4	-14.16	1.29	1.37
26	14	1786	A	N9-C4	-13.34	1.29	1.37

The worst 5 of 9716 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-30.28	107.83	126.00
26	1H	945	A	N1-C6-N6	25.42	133.85	118.60
26	1H	2287	A	C2-N3-C4	-25.22	97.99	110.60
26	1H	1899	G	N3-C4-C5	25.13	141.17	128.60
26	1H	945	A	C6-C5-N7	-24.82	114.92	132.30

There are no chirality outliers.

5 of 158 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
10	1I	88	LEU	Peptide
11	2I	102	GLY	Peptide
12	3I	47	LYS	Peptide
9	8E	110	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16234	821	0
1	1G	32371	0	16342	804	0
2	12	1696	0	1730	97	0
2	1E	1874	0	1926	111	0
3	22	1537	0	1603	75	0
3	2E	1605	0	1668	50	0
4	32	1702	0	1764	122	0
4	3E	1698	0	1759	98	0
5	42	1139	0	1202	51	0
5	4E	1142	0	1204	54	0
6	52	842	0	857	30	0
6	5E	837	0	852	34	0
7	62	1120	0	1167	57	0
7	6E	1242	0	1286	39	0
8	72	1107	0	1165	55	0
8	7E	1115	0	1177	60	0
9	82	953	0	983	81	0
9	8E	1000	0	1031	56	0
10	1A	646	0	662	36	0
10	1I	754	0	769	42	0
11	2A	835	0	847	32	0
11	2I	823	0	833	32	0
12	3A	956	0	1046	42	0
12	3I	956	0	1046	40	0
13	4A	893	0	946	55	0
13	4I	942	0	997	59	0
14	5A	486	0	525	38	0
14	5I	491	0	529	25	0
15	6A	729	0	768	17	0
15	6I	729	0	768	32	0
16	7A	705	0	725	23	0
16	7I	700	0	720	48	0
17	8A	823	0	891	28	0
17	8I	834	0	904	46	0
18	9A	544	0	605	31	0
18	9I	549	0	607	17	0
19	AA	481	0	468	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	661	0	683	64	0
20	BA	762	0	861	35	0
20	BI	746	0	843	44	0
21	1B	188	0	195	10	0
21	1F	199	0	208	14	0
22	1K	1542	0	790	46	0
22	1L	1477	0	758	27	0
23	2K	1646	0	844	24	0
23	2L	1646	0	844	38	0
24	3K	1483	0	756	64	0
24	3L	1528	0	778	49	0
25	4K	464	0	231	20	0
25	4L	419	0	208	11	0
26	14	61505	0	30997	1435	0
26	1H	62204	0	31336	1594	0
27	16	2617	0	1328	73	0
27	1J	2617	0	1328	68	0
28	71	1033	0	1048	73	0
28	79	456	0	460	25	0
29	11	2120	0	2197	133	0
29	19	2125	0	2199	126	0
30	21	1558	0	1624	102	0
30	29	1563	0	1629	99	0
31	31	1585	0	1632	75	0
31	39	1602	0	1649	109	0
32	41	1457	0	1514	89	0
32	49	1468	0	1520	84	0
33	51	1328	0	1396	101	0
33	59	543	0	566	30	0
34	61	1136	0	1223	53	0
34	69	1131	0	1218	54	0
35	15	1104	0	1180	40	0
35	58	1096	0	1169	75	0
36	25	932	0	996	46	0
36	68	932	0	996	29	0
37	35	1122	0	1206	68	0
37	78	1122	0	1206	88	0
38	45	1104	0	1159	91	0
38	88	1117	0	1168	55	0
39	55	967	0	1033	56	0
39	98	967	0	1033	51	0
40	65	876	0	938	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	A8	881	0	943	60	0
41	75	1109	0	1170	75	0
41	B8	1124	0	1179	74	0
42	85	959	0	1019	56	0
42	C8	950	0	1011	53	0
43	95	770	0	838	44	0
43	D8	774	0	849	35	0
44	A5	886	0	948	37	0
44	E8	876	0	941	26	0
45	B5	735	0	785	37	0
45	F8	743	0	794	35	0
46	C5	794	0	886	63	0
46	G8	783	0	869	57	0
47	D5	1079	0	1088	62	0
47	H8	1365	0	1391	76	0
48	E5	603	0	620	36	0
48	I8	611	0	631	33	0
49	F5	737	0	813	41	0
49	J8	737	0	813	41	0
50	G5	576	0	625	31	0
50	K8	575	0	634	48	0
51	H5	459	0	512	9	0
51	L8	459	0	512	12	0
52	M8	376	0	374	53	0
53	J5	434	0	454	20	0
53	N8	369	0	388	19	0
54	L5	401	0	436	14	0
54	P8	401	0	436	19	0
55	M5	516	0	581	26	0
55	Q8	516	0	582	40	0
56	11	3	0	0	0	0
56	13	161	0	0	0	0
56	14	471	0	0	0	0
56	16	13	0	0	0	0
56	1G	126	0	0	0	0
56	1H	572	0	0	0	0
56	1J	11	0	0	0	0
56	1K	1	0	0	0	0
56	21	3	0	0	0	0
56	25	2	0	0	0	0
56	29	1	0	0	0	0
56	2A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2K	3	0	0	0	0
56	2L	3	0	0	0	0
56	32	1	0	0	0	0
56	35	3	0	0	0	0
56	39	2	0	0	0	0
56	41	2	0	0	0	0
56	42	2	0	0	0	0
56	45	2	0	0	0	0
56	4K	1	0	0	0	0
56	52	1	0	0	0	0
56	5E	1	0	0	0	0
56	5I	1	0	0	0	0
56	78	2	0	0	0	0
56	88	3	0	0	0	0
56	98	1	0	0	0	0
56	B5	1	0	0	0	0
56	E5	3	0	0	0	0
56	F8	1	0	0	0	0
56	I8	1	0	0	0	0
56	L8	1	0	0	0	0
56	M5	1	0	0	0	0
56	P8	1	0	0	0	0
56	Q8	1	0	0	0	0
57	32	8	0	0	3	0
57	3E	8	0	0	0	0
58	5A	1	0	0	0	0
58	5I	1	0	0	0	0
58	C5	1	0	0	0	0
58	G8	1	0	0	0	0
59	11	16	0	0	6	0
59	13	389	0	0	54	0
59	14	1225	0	0	216	0
59	16	35	0	0	7	0
59	19	11	0	0	3	0
59	1E	1	0	0	0	0
59	1F	2	0	0	0	0
59	1G	297	0	0	46	0
59	1H	1539	0	0	287	0
59	1I	2	0	0	0	0
59	1J	12	0	0	2	0
59	1K	8	0	0	1	0
59	1L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	21	7	0	0	1	0
59	25	6	0	0	0	0
59	29	5	0	0	0	0
59	2A	3	0	0	0	0
59	2K	6	0	0	0	0
59	2L	6	0	0	0	0
59	31	6	0	0	0	0
59	32	2	0	0	1	0
59	35	8	0	0	1	0
59	39	7	0	0	0	0
59	3A	1	0	0	0	0
59	3E	2	0	0	0	0
59	3I	2	0	0	0	0
59	3K	1	0	0	0	0
59	41	1	0	0	0	0
59	42	1	0	0	0	0
59	45	4	0	0	0	0
59	4E	1	0	0	0	0
59	4I	2	0	0	0	0
59	4K	5	0	0	0	0
59	4L	5	0	0	0	0
59	52	4	0	0	0	0
59	55	3	0	0	4	0
59	58	2	0	0	0	0
59	5I	2	0	0	0	0
59	62	3	0	0	0	0
59	68	2	0	0	0	0
59	6A	1	0	0	0	0
59	6I	3	0	0	0	0
59	78	8	0	0	1	0
59	7A	6	0	0	0	0
59	7I	1	0	0	0	0
59	85	1	0	0	0	0
59	88	8	0	0	0	0
59	8E	3	0	0	0	0
59	95	1	0	0	0	0
59	9A	2	0	0	1	0
59	A5	1	0	0	0	0
59	B5	1	0	0	0	0
59	BA	5	0	0	0	0
59	C5	3	0	0	0	0
59	C8	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	D8	2	0	0	0	0
59	F5	1	0	0	0	0
59	F8	2	0	0	0	0
59	G8	1	0	0	0	0
59	H5	2	0	0	0	0
59	I8	7	0	0	1	0
59	J8	2	0	0	1	0
59	K8	1	0	0	0	0
59	L5	3	0	0	0	0
59	L8	3	0	0	0	0
59	M5	6	0	0	1	0
59	P8	1	0	0	0	0
59	Q8	8	0	0	1	0
All	All	297904	0	196675	8933	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 8933 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)
39:55:3:HIS:NE2	59:55:201:HOH:O	1.77	1.14
49:J8:93:GLU:HG3	49:J8:94:LEU:H	1.01	1.12
26:14:730:C:OP2	59:14:3501:HOH:O	1.68	1.11
19:AI:3:ARG:HE	19:AI:9:VAL:HG11	1.10	1.10
26:14:2822:G:N7	59:14:3506:HOH:O	1.84	1.10

There are no symmetry-related clashes.

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%)	165 (81%)	33 (16%)	5 (2%)	6	29
2	1E	227/256 (89%)	187 (82%)	39 (17%)	1 (0%)	38	75
3	22	191/239 (80%)	165 (86%)	25 (13%)	1 (0%)	32	71
3	2E	203/239 (85%)	183 (90%)	20 (10%)	0	100	100
4	32	206/209 (99%)	181 (88%)	23 (11%)	2 (1%)	18	55
4	3E	205/209 (98%)	191 (93%)	13 (6%)	1 (0%)	32	71
5	42	147/162 (91%)	138 (94%)	9 (6%)	0	100	100
5	4E	147/162 (91%)	138 (94%)	8 (5%)	1 (1%)	25	64
6	52	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	136/156 (87%)	123 (90%)	13 (10%)	0	100	100
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	123 (91%)	9 (7%)	3 (2%)	8	33
8	7E	136/138 (99%)	124 (91%)	10 (7%)	2 (2%)	12	45
9	82	119/128 (93%)	110 (92%)	8 (7%)	1 (1%)	22	61
9	8E	124/128 (97%)	106 (86%)	18 (14%)	0	100	100
10	1A	76/105 (72%)	72 (95%)	4 (5%)	0	100	100
10	1I	93/105 (89%)	84 (90%)	9 (10%)	0	100	100
11	2A	111/129 (86%)	101 (91%)	8 (7%)	2 (2%)	10	39
11	2I	109/129 (84%)	98 (90%)	9 (8%)	2 (2%)	10	39
12	3A	120/132 (91%)	102 (85%)	14 (12%)	4 (3%)	4	21
12	3I	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	22	61
13	4A	109/126 (86%)	91 (84%)	15 (14%)	3 (3%)	6	26
13	4I	117/126 (93%)	97 (83%)	20 (17%)	0	100	100
14	5A	57/61 (93%)	47 (82%)	9 (16%)	1 (2%)	10	39
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	4	21
15	6A	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
15	6I	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
16	7A	82/88 (93%)	74 (90%)	8 (10%)	0	100	100
16	7I	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	98/105 (93%)	92 (94%)	5 (5%)	1 (1%)	18	55

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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%)	61 (92%)	4 (6%)	1 (2%)	12	45
19	AA	56/93 (60%)	48 (86%)	6 (11%)	2 (4%)	4	19
19	AI	80/93 (86%)	68 (85%)	8 (10%)	4 (5%)	2	12
20	BA	97/106 (92%)	79 (81%)	15 (16%)	3 (3%)	5	23
20	BI	95/106 (90%)	84 (88%)	11 (12%)	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	71	129/229 (56%)	122 (95%)	7 (5%)	0	100	100
28	79	45/229 (20%)	43 (96%)	2 (4%)	0	100	100
29	11	271/276 (98%)	237 (88%)	25 (9%)	9 (3%)	4	21
29	19	272/276 (99%)	240 (88%)	25 (9%)	7 (3%)	6	28
30	21	201/206 (98%)	155 (77%)	37 (18%)	9 (4%)	3	14
30	29	202/206 (98%)	152 (75%)	37 (18%)	13 (6%)	1	7
31	31	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
31	39	202/210 (96%)	155 (77%)	40 (20%)	7 (4%)	4	20
32	41	177/182 (97%)	156 (88%)	19 (11%)	2 (1%)	17	53
32	49	179/182 (98%)	155 (87%)	22 (12%)	2 (1%)	17	53
33	51	172/180 (96%)	142 (83%)	20 (12%)	10 (6%)	2	9
33	59	64/180 (36%)	48 (75%)	13 (20%)	3 (5%)	3	13
34	61	144/148 (97%)	116 (81%)	25 (17%)	3 (2%)	8	35
34	69	143/148 (97%)	115 (80%)	24 (17%)	4 (3%)	6	26
35	15	136/140 (97%)	121 (89%)	14 (10%)	1 (1%)	25	64
35	58	135/140 (96%)	115 (85%)	15 (11%)	5 (4%)	4	19
36	25	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	22	61
36	68	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
37	35	145/150 (97%)	118 (81%)	26 (18%)	1 (1%)	25	64
37	78	145/150 (97%)	114 (79%)	21 (14%)	10 (7%)	1	6
38	45	137/141 (97%)	111 (81%)	23 (17%)	3 (2%)	8	33
38	88	139/141 (99%)	116 (84%)	16 (12%)	7 (5%)	2	12
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	20	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	98	116/118 (98%)	99 (85%)	15 (13%)	2 (2%)	11	41
40	65	108/112 (96%)	89 (82%)	16 (15%)	3 (3%)	6	26
40	A8	109/112 (97%)	89 (82%)	20 (18%)	0	100	100
41	75	131/146 (90%)	118 (90%)	11 (8%)	2 (2%)	12	45
41	B8	134/146 (92%)	119 (89%)	14 (10%)	1 (1%)	25	64
42	85	114/118 (97%)	102 (90%)	9 (8%)	3 (3%)	6	28
42	C8	113/118 (96%)	102 (90%)	8 (7%)	3 (3%)	6	27
43	95	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	5	23
43	D8	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	5	23
44	A5	109/113 (96%)	101 (93%)	7 (6%)	1 (1%)	20	58
44	E8	108/113 (96%)	100 (93%)	7 (6%)	1 (1%)	20	58
45	B5	92/96 (96%)	83 (90%)	6 (6%)	3 (3%)	4	21
45	F8	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
46	C5	102/110 (93%)	75 (74%)	20 (20%)	7 (7%)	1	6
46	G8	101/110 (92%)	82 (81%)	13 (13%)	6 (6%)	2	9
47	D5	127/206 (62%)	98 (77%)	26 (20%)	3 (2%)	7	31
47	H8	168/206 (82%)	136 (81%)	26 (16%)	6 (4%)	4	19
48	E5	74/85 (87%)	65 (88%)	7 (10%)	2 (3%)	6	27
48	I8	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	14	48
49	F5	92/98 (94%)	78 (85%)	12 (13%)	2 (2%)	8	33
49	J8	92/98 (94%)	86 (94%)	5 (5%)	1 (1%)	17	53
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	5	24
50	K8	66/72 (92%)	60 (91%)	3 (4%)	3 (4%)	3	14
51	H5	56/60 (93%)	52 (93%)	4 (7%)	0	100	100
51	L8	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
52	M8	47/71 (66%)	28 (60%)	17 (36%)	2 (4%)	3	15
53	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
53	N8	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	40 (89%)	4 (9%)	1 (2%)	8	33
55	M5	62/65 (95%)	51 (82%)	10 (16%)	1 (2%)	11	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	Q8	62/65 (95%)	53 (86%)	6 (10%)	3 (5%)	2	13
All	All	10980/12333 (89%)	9564 (87%)	1210 (11%)	206 (2%)	9	38

5 of 206 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	3I	48	PRO
14	5I	13	THR
19	AI	9	VAL
19	AI	41	VAL
29	11	28	GLU

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%)	148 (83%)	31 (17%)	2	10
2	1E	200/220 (91%)	152 (76%)	48 (24%)	1	3
3	22	154/188 (82%)	122 (79%)	32 (21%)	1	5
3	2E	159/188 (85%)	123 (77%)	36 (23%)	1	4
4	32	180/181 (99%)	142 (79%)	38 (21%)	1	5
4	3E	180/181 (99%)	140 (78%)	40 (22%)	1	4
5	42	114/123 (93%)	91 (80%)	23 (20%)	1	6
5	4E	115/123 (94%)	94 (82%)	21 (18%)	2	8
6	52	90/90 (100%)	69 (77%)	21 (23%)	1	3
6	5E	90/90 (100%)	70 (78%)	20 (22%)	1	4
7	62	114/127 (90%)	91 (80%)	23 (20%)	1	6
7	6E	125/127 (98%)	107 (86%)	18 (14%)	4	15
8	72	118/119 (99%)	96 (81%)	22 (19%)	2	8
8	7E	119/119 (100%)	90 (76%)	29 (24%)	1	3
9	82	92/99 (93%)	74 (80%)	18 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	8E	97/99 (98%)	76 (78%)	21 (22%)	1	5
10	1A	71/92 (77%)	59 (83%)	12 (17%)	2	10
10	1I	81/92 (88%)	69 (85%)	12 (15%)	3	14
11	2A	85/99 (86%)	70 (82%)	15 (18%)	2	9
11	2I	84/99 (85%)	65 (77%)	19 (23%)	1	4
12	3A	103/109 (94%)	77 (75%)	26 (25%)	0	2
12	3I	103/109 (94%)	83 (81%)	20 (19%)	1	7
13	4A	91/101 (90%)	66 (72%)	25 (28%)	0	2
13	4I	94/101 (93%)	74 (79%)	20 (21%)	1	5
14	5A	49/50 (98%)	38 (78%)	11 (22%)	1	4
14	5I	49/50 (98%)	39 (80%)	10 (20%)	1	6
15	6A	79/80 (99%)	67 (85%)	12 (15%)	3	13
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2	9
16	7A	72/74 (97%)	56 (78%)	16 (22%)	1	4
16	7I	72/74 (97%)	57 (79%)	15 (21%)	1	5
17	8A	94/97 (97%)	82 (87%)	12 (13%)	5	20
17	8I	95/97 (98%)	78 (82%)	17 (18%)	2	9
18	9A	58/77 (75%)	44 (76%)	14 (24%)	1	3
18	9I	58/77 (75%)	47 (81%)	11 (19%)	2	8
19	AA	52/80 (65%)	41 (79%)	11 (21%)	1	5
19	AI	72/80 (90%)	59 (82%)	13 (18%)	2	9
20	BA	76/82 (93%)	63 (83%)	13 (17%)	2	10
20	BI	75/82 (92%)	61 (81%)	14 (19%)	2	8
21	1B	17/22 (77%)	16 (94%)	1 (6%)	23	58
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	4
28	71	109/181 (60%)	87 (80%)	22 (20%)	1	6
28	79	48/181 (26%)	34 (71%)	14 (29%)	0	1
29	11	214/218 (98%)	165 (77%)	49 (23%)	1	4
29	19	214/218 (98%)	167 (78%)	47 (22%)	1	4
30	21	165/166 (99%)	131 (79%)	34 (21%)	1	5
30	29	165/166 (99%)	127 (77%)	38 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	31	161/166 (97%)	127 (79%)	34 (21%)	1	5
31	39	163/166 (98%)	122 (75%)	41 (25%)	0	2
32	41	153/156 (98%)	118 (77%)	35 (23%)	1	4
32	49	153/156 (98%)	120 (78%)	33 (22%)	1	5
33	51	143/148 (97%)	107 (75%)	36 (25%)	0	2
33	59	56/148 (38%)	46 (82%)	10 (18%)	2	9
34	61	122/124 (98%)	87 (71%)	35 (29%)	0	1
34	69	122/124 (98%)	95 (78%)	27 (22%)	1	4
35	15	117/119 (98%)	87 (74%)	30 (26%)	0	2
35	58	116/119 (98%)	87 (75%)	29 (25%)	1	2
36	25	100/100 (100%)	78 (78%)	22 (22%)	1	4
36	68	100/100 (100%)	79 (79%)	21 (21%)	1	5
37	35	114/116 (98%)	83 (73%)	31 (27%)	0	2
37	78	114/116 (98%)	77 (68%)	37 (32%)	0	1
38	45	109/111 (98%)	84 (77%)	25 (23%)	1	4
38	88	110/111 (99%)	91 (83%)	19 (17%)	2	10
39	55	101/101 (100%)	79 (78%)	22 (22%)	1	5
39	98	101/101 (100%)	73 (72%)	28 (28%)	0	2
40	65	87/88 (99%)	61 (70%)	26 (30%)	0	1
40	A8	87/88 (99%)	58 (67%)	29 (33%)	0	1
41	75	117/127 (92%)	83 (71%)	34 (29%)	0	1
41	B8	117/127 (92%)	86 (74%)	31 (26%)	0	2
42	85	93/94 (99%)	73 (78%)	20 (22%)	1	5
42	C8	92/94 (98%)	73 (79%)	19 (21%)	1	5
43	95	81/82 (99%)	62 (76%)	19 (24%)	1	3
43	D8	82/82 (100%)	61 (74%)	21 (26%)	0	2
44	A5	91/92 (99%)	70 (77%)	21 (23%)	1	4
44	E8	90/92 (98%)	73 (81%)	17 (19%)	2	8
45	B5	74/78 (95%)	58 (78%)	16 (22%)	1	5
45	F8	75/78 (96%)	62 (83%)	13 (17%)	2	10
46	C5	85/91 (93%)	57 (67%)	28 (33%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	G8	84/91 (92%)	63 (75%)	21 (25%)	1	2
47	D5	118/179 (66%)	92 (78%)	26 (22%)	1	4
47	H8	151/179 (84%)	122 (81%)	29 (19%)	1	7
48	E5	61/67 (91%)	55 (90%)	6 (10%)	9	32
48	I8	62/67 (92%)	49 (79%)	13 (21%)	1	5
49	F5	79/83 (95%)	59 (75%)	20 (25%)	0	2
49	J8	79/83 (95%)	65 (82%)	14 (18%)	2	9
50	G5	63/67 (94%)	45 (71%)	18 (29%)	0	1
50	K8	64/67 (96%)	45 (70%)	19 (30%)	0	1
51	H5	50/52 (96%)	38 (76%)	12 (24%)	1	3
51	L8	50/52 (96%)	36 (72%)	14 (28%)	0	2
52	M8	42/63 (67%)	33 (79%)	9 (21%)	1	5
53	J5	48/52 (92%)	36 (75%)	12 (25%)	1	2
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1	5
54	L5	38/42 (90%)	33 (87%)	5 (13%)	5	18
54	P8	38/42 (90%)	31 (82%)	7 (18%)	2	8
55	M5	54/55 (98%)	41 (76%)	13 (24%)	1	3
55	Q8	54/55 (98%)	43 (80%)	11 (20%)	1	6
All	All	9272/10193 (91%)	7223 (78%)	2049 (22%)	1	4

5 of 2049 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	G8	84	ARG
4	32	155	LEU
45	B5	23	GLU
47	H8	129	SER
54	P8	8	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
44	E8	60	ASN
52	M8	47	GLN
38	45	123	HIS

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Mol	Chain	Res	Type
47	H8	132	ASN
2	12	19	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1492/1519 (98%)	369 (24%)	0
1	1G	1504/1519 (99%)	349 (23%)	0
22	1K	67/76 (88%)	30 (44%)	0
22	1L	64/76 (84%)	21 (32%)	0
23	2K	76/77 (98%)	29 (38%)	0
23	2L	76/77 (98%)	18 (23%)	0
24	3K	67/76 (88%)	39 (58%)	0
24	3L	69/76 (90%)	31 (44%)	0
25	4K	19/27 (70%)	11 (57%)	0
25	4L	18/27 (66%)	8 (44%)	0
26	14	2846/2917 (97%)	762 (26%)	0
26	1H	2878/2917 (98%)	709 (24%)	0
27	16	121/122 (99%)	28 (23%)	0
27	1J	121/122 (99%)	34 (28%)	0
All	All	9418/9628 (97%)	2438 (25%)	0

5 of 2438 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	9	G
1	13	15	G

There are no RNA pucker outliers to report.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	U8U	1K	34	25,22	15,24,25	2.36	4 (26%)	18,34,37	1.95	2 (11%)
22	T6A	1K	37	22	24,34,35	2.47	5 (20%)	23,49,52	2.82	6 (26%)
22	PSU	1K	39	22	16,21,22	1.09	1 (6%)	20,30,33	3.78	6 (30%)
22	5MU	1K	54	22	14,22,23	1.77	2 (14%)	16,32,35	2.10	2 (12%)
22	PSU	1K	55	22	16,21,22	1.20	2 (12%)	20,30,33	3.84	5 (25%)
22	U8U	1L	34	25,22	15,24,25	2.51	4 (26%)	18,34,37	2.05	2 (11%)
22	T6A	1L	37	22	24,34,35	2.48	4 (16%)	23,49,52	3.32	5 (21%)
22	PSU	1L	39	22	16,21,22	1.11	1 (6%)	20,30,33	3.87	5 (25%)
22	5MU	1L	54	22	14,22,23	1.84	2 (14%)	16,32,35	1.76	2 (12%)
22	PSU	1L	55	22	16,21,22	1.08	1 (6%)	20,30,33	4.09	9 (45%)
23	OMC	2K	33	23	15,22,23	1.91	5 (33%)	19,31,34	0.95	2 (10%)
23	G7M	2K	47	23	19,26,27	4.86	6 (31%)	19,39,42	2.01	5 (26%)
23	5MU	2K	55	23	14,22,23	1.84	2 (14%)	16,32,35	1.76	2 (12%)
23	PSU	2K	56	23	16,21,22	1.27	3 (18%)	20,30,33	3.00	5 (25%)
23	4SU	2K	8	23	14,21,22	3.10	2 (14%)	15,30,33	1.02	1 (6%)
23	OMC	2L	33	23	15,22,23	1.94	5 (33%)	19,31,34	0.95	2 (10%)
23	G7M	2L	47	23	19,26,27	4.96	6 (31%)	19,39,42	2.00	6 (31%)
23	5MU	2L	55	23	14,22,23	1.75	3 (21%)	16,32,35	1.84	2 (12%)
23	PSU	2L	56	23	16,21,22	1.15	2 (12%)	20,30,33	3.88	6 (30%)
23	4SU	2L	8	23	14,21,22	3.21	2 (14%)	15,30,33	0.88	1 (6%)

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	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
22	U8U	1L	34	25,22	-	0/5/28/29	0/2/2/2
22	T6A	1L	37	22	-	0/15/41/42	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	1L	39	22	-	0/7/25/26	0/2/2/2
22	5MU	1L	54	22	-	0/3/25/26	0/2/2/2
22	PSU	1L	55	22	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/5/27/28	0/2/2/2
23	G7M	2K	47	23	-	0/3/25/26	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
23	OMC	2L	33	23	-	0/5/27/28	0/2/2/2
23	G7M	2L	47	23	-	0/3/25/26	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 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	54	5MU	C4-N3	-3.22	1.27	1.33
23	2L	55	5MU	C4-N3	-3.16	1.27	1.33
22	1K	37	T6A	C5-C4	-3.14	1.33	1.40
23	2K	56	PSU	C5-C1'	-2.93	1.49	1.52
22	1L	34	U8U	C2-S2	-2.59	1.61	1.66

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1L	55	PSU	N1-C2-N3	-13.85	118.44	128.40
22	1K	39	PSU	N1-C2-N3	-13.73	118.53	128.40
22	1L	39	PSU	N1-C2-N3	-13.71	118.54	128.40
23	2L	56	PSU	N1-C2-N3	-13.03	119.03	128.40
22	1K	55	PSU	N1-C2-N3	-12.19	119.63	128.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	34	U8U	3	0
22	1K	54	5MU	1	0
22	1K	55	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1L	34	U8U	1	0
22	1L	39	PSU	1	0
22	1L	54	5MU	1	0
22	1L	55	PSU	1	0
23	2K	33	OMC	1	0
23	2K	47	G7M	1	0
23	2K	55	5MU	2	0
23	2K	56	PSU	1	0
23	2L	33	OMC	1	0
23	2L	47	G7M	2	0
23	2L	55	5MU	2	0
23	2L	56	PSU	2	0
23	2L	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1409 ligands modelled in this entry, 1407 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	SF4	32	302	4	0,12,12	0.00	-	0,24,24	0.00	-
57	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
57	SF4	32	302	4	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	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.

1 monomer is involved in 3 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	4K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4K	25:A	O3'	26:A	P	3.07

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	13	1496/1519 (98%)	-0.23	4 (0%)	93	86	52, 95, 168, 235	0
1	1G	1506/1519 (99%)	-0.26	8 (0%)	90	79	67, 112, 176, 243	0
2	12	207/256 (80%)	0.54	21 (10%)	8	4	128, 159, 178, 183	0
2	1E	231/256 (90%)	0.19	13 (5%)	25	14	108, 138, 168, 172	0
3	22	195/239 (81%)	0.92	40 (20%)	1	1	119, 140, 163, 172	0
3	2E	205/239 (85%)	0.51	12 (5%)	23	14	82, 105, 135, 142	0
4	32	208/209 (99%)	0.65	23 (11%)	6	3	92, 113, 135, 140	0
4	3E	207/209 (99%)	0.22	13 (6%)	21	12	77, 104, 125, 136	0
5	42	149/162 (91%)	0.34	6 (4%)	39	24	97, 118, 134, 142	0
5	4E	149/162 (91%)	0.15	3 (2%)	65	46	76, 96, 115, 122	0
6	52	101/101 (100%)	-0.06	0	100	100	81, 99, 115, 130	0
6	5E	100/101 (99%)	0.33	2 (2%)	65	46	76, 97, 116, 122	0
7	62	140/156 (89%)	0.94	25 (17%)	2	1	108, 126, 138, 140	0
7	6E	154/156 (98%)	1.33	37 (24%)	1	1	96, 114, 144, 165	0
8	72	137/138 (99%)	0.55	14 (10%)	7	4	95, 123, 136, 143	0
8	7E	138/138 (100%)	0.93	26 (18%)	1	1	84, 104, 116, 127	0
9	82	121/128 (94%)	1.98	51 (42%)	0	0	109, 156, 170, 181	0
9	8E	126/128 (98%)	0.36	10 (7%)	13	7	80, 133, 153, 158	0
10	1A	80/105 (76%)	0.97	21 (26%)	1	0	114, 151, 163, 163	0
10	1I	95/105 (90%)	1.18	26 (27%)	1	0	76, 120, 160, 164	0
11	2A	113/129 (87%)	1.32	30 (26%)	1	0	78, 106, 120, 129	0
11	2I	111/129 (86%)	1.39	31 (27%)	1	0	69, 102, 117, 129	0
12	3A	122/132 (92%)	1.40	36 (29%)	1	0	80, 96, 120, 140	0
12	3I	122/132 (92%)	0.40	9 (7%)	15	8	61, 72, 100, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	0.71	26 (23%) 1 1	112, 142, 159, 167	0
13	4I	119/126 (94%)	0.50	9 (7%) 15 8	81, 108, 129, 137	0
14	5A	59/61 (96%)	3.28	40 (67%) 0 0	124, 137, 150, 154	0
14	5I	60/61 (98%)	0.88	7 (11%) 5 3	77, 93, 107, 120	0
15	6A	87/89 (97%)	0.07	1 (1%) 80 63	78, 106, 118, 120	0
15	6I	87/89 (97%)	0.28	4 (4%) 33 20	73, 92, 109, 116	0
16	7A	84/88 (95%)	0.14	1 (1%) 79 61	88, 101, 121, 145	0
16	7I	83/88 (94%)	1.26	17 (20%) 1 1	93, 106, 134, 154	0
17	8A	99/105 (94%)	0.96	18 (18%) 1 1	90, 105, 120, 124	0
17	8I	100/105 (95%)	0.73	11 (11%) 6 3	85, 101, 110, 115	0
18	9A	67/88 (76%)	0.08	1 (1%) 74 55	89, 107, 126, 130	0
18	9I	68/88 (77%)	0.11	2 (2%) 52 33	83, 102, 124, 127	0
19	AA	62/93 (66%)	0.46	6 (9%) 8 5	132, 153, 166, 171	0
19	AI	82/93 (88%)	0.25	8 (9%) 8 5	83, 106, 127, 139	0
20	BA	99/106 (93%)	1.05	20 (20%) 1 1	84, 104, 131, 142	0
20	BI	97/106 (91%)	1.45	28 (28%) 1 0	98, 116, 141, 150	0
21	1B	22/27 (81%)	1.57	8 (36%) 0 0	118, 127, 133, 141	0
21	1F	23/27 (85%)	0.65	1 (4%) 36 22	84, 95, 101, 111	0
22	1K	67/76 (88%)	0.15	4 (5%) 23 13	76, 147, 198, 203	0
22	1L	64/76 (84%)	1.01	10 (15%) 2 1	108, 196, 215, 219	0
23	2K	72/77 (93%)	-0.13	0 100 100	64, 86, 118, 128	0
23	2L	72/77 (93%)	-0.01	0 100 100	73, 105, 137, 148	0
24	3K	70/76 (92%)	0.90	13 (18%) 1 1	71, 198, 240, 244	0
24	3L	72/76 (94%)	0.08	2 (2%) 53 35	77, 194, 224, 230	0
25	4K	21/27 (77%)	1.35	8 (38%) 0 0	67, 124, 208, 209	0
25	4L	19/27 (70%)	0.91	3 (15%) 2 1	86, 143, 217, 218	0
26	14	2855/2917 (97%)	-0.08	22 (0%) 86 71	45, 78, 200, 265	0
26	1H	2885/2917 (98%)	-0.09	9 (0%) 93 86	36, 66, 193, 330	0
27	16	122/122 (100%)	-0.53	1 (0%) 86 71	57, 82, 103, 188	0
27	1J	122/122 (100%)	-0.55	0 100 100	78, 110, 130, 191	0
28	7I	133/229 (58%)	1.05	24 (18%) 2 1	146, 216, 237, 244	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	79	57/229 (24%)	1.80	22 (38%) 0 0	146, 199, 221, 227	0
29	11	273/276 (98%)	0.36	2 (0%) 87 74	37, 59, 76, 92	0
29	19	274/276 (99%)	0.45	7 (2%) 56 37	46, 69, 87, 106	0
30	21	203/206 (98%)	0.60	14 (6%) 18 10	46, 80, 123, 134	0
30	29	204/206 (99%)	0.77	29 (14%) 3 1	53, 88, 124, 134	0
31	31	202/210 (96%)	0.68	16 (7%) 13 7	43, 72, 107, 128	0
31	39	204/210 (97%)	0.40	9 (4%) 35 21	51, 98, 144, 167	0
32	41	179/182 (98%)	0.81	24 (13%) 4 2	72, 93, 130, 142	0
32	49	181/182 (99%)	1.07	39 (21%) 1 1	106, 125, 148, 166	0
33	51	174/180 (96%)	0.09	7 (4%) 39 24	75, 98, 112, 124	0
33	59	70/180 (38%)	0.85	13 (18%) 1 1	136, 156, 178, 182	0
34	61	146/148 (98%)	0.45	12 (8%) 12 7	73, 123, 144, 151	0
34	69	145/148 (97%)	0.52	18 (12%) 4 2	83, 118, 146, 155	0
35	15	138/140 (98%)	1.23	32 (23%) 1 1	73, 99, 128, 143	0
35	58	137/140 (97%)	0.79	12 (8%) 11 6	61, 83, 118, 132	0
36	25	122/122 (100%)	0.97	16 (13%) 4 2	64, 81, 99, 111	0
36	68	122/122 (100%)	0.43	1 (0%) 86 71	53, 68, 85, 93	0
37	35	147/150 (98%)	0.56	9 (6%) 22 13	52, 95, 126, 140	0
37	78	147/150 (98%)	0.36	6 (4%) 38 23	42, 74, 98, 107	0
38	45	139/141 (98%)	0.72	18 (12%) 4 2	64, 95, 114, 130	0
38	88	141/141 (100%)	0.32	8 (5%) 24 14	49, 70, 92, 112	0
39	55	118/118 (100%)	0.55	5 (4%) 37 23	59, 74, 88, 106	0
39	98	118/118 (100%)	1.04	21 (17%) 2 1	58, 76, 93, 107	0
40	65	110/112 (98%)	1.02	22 (20%) 1 1	82, 104, 124, 131	0
40	A8	111/112 (99%)	1.00	13 (11%) 5 3	66, 82, 103, 110	0
41	75	133/146 (91%)	0.58	9 (6%) 18 10	77, 91, 124, 144	0
41	B8	136/146 (93%)	0.21	5 (3%) 42 27	64, 83, 122, 132	0
42	85	116/118 (98%)	0.51	5 (4%) 36 22	60, 87, 118, 120	0
42	C8	115/118 (97%)	0.40	3 (2%) 56 37	50, 73, 102, 109	0
43	95	100/101 (99%)	0.84	16 (16%) 2 1	58, 109, 127, 135	0
43	D8	100/101 (99%)	0.92	14 (14%) 3 1	52, 96, 116, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	A5	111/113 (98%)	0.67	6 (5%) 26 16	55, 70, 94, 135	0
44	E8	110/113 (97%)	0.50	6 (5%) 26 15	51, 67, 91, 104	0
45	B5	94/96 (97%)	0.81	11 (11%) 5 3	62, 78, 98, 110	0
45	F8	95/96 (98%)	0.09	1 (1%) 80 63	47, 63, 90, 97	0
46	C5	104/110 (94%)	1.83	32 (30%) 0 0	85, 113, 147, 155	0
46	G8	103/110 (93%)	0.34	5 (4%) 30 18	66, 88, 118, 129	0
47	D5	133/206 (64%)	0.95	21 (15%) 2 1	102, 130, 153, 163	0
47	H8	170/206 (82%)	1.10	30 (17%) 2 1	76, 111, 188, 193	0
48	E5	76/85 (89%)	0.95	11 (14%) 3 1	56, 83, 96, 104	0
48	I8	77/85 (90%)	0.59	6 (7%) 14 7	45, 65, 78, 93	0
49	F5	94/98 (95%)	1.04	18 (19%) 1 1	59, 76, 106, 129	0
49	J8	94/98 (95%)	0.66	6 (6%) 20 11	46, 67, 110, 116	0
50	G5	69/72 (95%)	0.36	4 (5%) 24 14	77, 96, 116, 124	0
50	K8	68/72 (94%)	-0.02	1 (1%) 74 55	54, 72, 92, 114	0
51	H5	58/60 (96%)	1.84	24 (41%) 0 0	70, 90, 116, 124	0
51	L8	58/60 (96%)	0.49	3 (5%) 28 17	55, 74, 99, 111	0
52	M8	49/71 (69%)	1.68	15 (30%) 0 0	94, 136, 150, 166	0
53	J5	56/60 (93%)	0.63	5 (8%) 10 6	52, 77, 126, 137	0
53	N8	48/60 (80%)	0.48	2 (4%) 37 23	44, 77, 124, 127	0
54	L5	47/49 (95%)	0.16	1 (2%) 64 45	44, 55, 77, 97	0
54	P8	47/49 (95%)	-0.00	0 100 100	40, 46, 68, 76	0
55	M5	64/65 (98%)	1.05	9 (14%) 3 1	62, 73, 88, 112	0
55	Q8	64/65 (98%)	0.41	3 (4%) 32 20	47, 60, 76, 88	0
All	All	20647/21961 (94%)	0.32	1412 (6%) 18 10	36, 93, 171, 330	0

The worst 5 of 1412 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	C5	58	GLY	12.3
26	14	2902	C	12.1
26	14	2901	C	11.2
43	D8	37	VAL	10.9
40	A8	110	LEU	10.0

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	5MU	1K	54	21/22	0.91	0.14	-	93,106,119,128	0
22	PSU	1K	55	20/21	0.89	0.12	-	95,109,120,124	0
23	PSU	2L	56	20/21	0.93	0.10	-	98,105,111,115	0
22	PSU	1L	55	20/21	0.84	0.13	-	113,126,140,141	0
22	U8U	1L	34	23/24	0.93	0.18	-	102,117,122,124	0
23	5MU	2K	55	21/22	0.96	0.12	-	89,95,100,103	0
23	G7M	2L	47	24/25	0.94	0.13	-	110,117,123,127	0
23	G7M	2K	47	24/25	0.96	0.13	-	86,95,107,113	0
23	OMC	2K	33	21/22	0.97	0.21	-	67,74,78,82	0
22	T6A	1L	37	32/33	0.93	0.21	-	91,110,116,118	0
22	U8U	1K	34	23/24	0.96	0.15	-	76,81,86,100	0
22	PSU	1K	39	20/21	0.94	0.15	-	74,91,100,100	0
23	4SU	2K	8	20/21	0.97	0.14	-	75,83,88,90	0
22	5MU	1L	54	21/22	0.90	0.12	-	113,125,134,142	0
22	PSU	1L	39	20/21	0.89	0.23	-	88,116,127,129	0
23	OMC	2L	33	21/22	0.96	0.13	-	88,93,99,103	0
23	PSU	2K	56	20/21	0.93	0.10	-	86,90,100,104	0
22	T6A	1K	37	32/33	0.96	0.16	-	58,79,98,99	0
23	5MU	2L	55	21/22	0.94	0.12	-	99,108,115,124	0
23	4SU	2L	8	20/21	0.95	0.15	-	94,104,108,112	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(\AA^2)	Q<0.9
56	MG	14	3163	1/1	0.93	1.04	84.07	76,76,76,76	0
56	MG	1H	3044	1/1	0.96	0.28	46.71	39,39,39,39	0
56	MG	14	3153	1/1	0.81	1.04	40.00	74,74,74,74	0
56	MG	1H	3092	1/1	0.91	0.58	39.58	55,55,55,55	0
56	MG	1H	3172	1/1	0.84	0.76	37.61	70,70,70,70	0
56	MG	14	3214	1/1	0.66	0.32	34.83	113,113,113,113	0
56	MG	13	1636	1/1	0.96	0.54	30.58	70,70,70,70	0
56	MG	14	3131	1/1	0.76	0.53	29.44	62,62,62,62	0
56	MG	1H	3285	1/1	0.97	0.49	26.84	50,50,50,50	0
56	MG	14	3158	1/1	0.68	0.32	26.05	91,91,91,91	0
56	MG	14	3234	1/1	0.77	0.57	25.49	71,71,71,71	0
56	MG	2L	101	1/1	0.99	0.53	25.24	71,71,71,71	0
56	MG	1H	3118	1/1	0.93	0.57	25.13	52,52,52,52	0
56	MG	14	3149	1/1	0.76	0.77	24.40	89,89,89,89	0
56	MG	1H	3061	1/1	0.97	0.36	23.77	41,41,41,41	0
56	MG	1H	3143	1/1	0.72	0.36	23.65	84,84,84,84	0
56	MG	1H	3179	1/1	0.88	0.47	23.47	47,47,47,47	0
56	MG	14	3068	1/1	0.86	0.53	23.19	59,59,59,59	0
56	MG	1H	3194	1/1	0.66	0.48	22.09	83,83,83,83	0
56	MG	14	3189	1/1	0.72	0.62	22.04	60,60,60,60	0
56	MG	13	1602	1/1	0.82	0.50	21.90	61,61,61,61	0
56	MG	13	1630	1/1	0.86	0.40	21.60	81,81,81,81	0
56	MG	1H	3133	1/1	0.79	0.35	21.53	64,64,64,64	0
56	MG	1H	3037	1/1	0.88	0.58	21.09	63,63,63,63	0
56	MG	1H	3192	1/1	0.85	0.50	19.50	61,61,61,61	0
56	MG	1H	3017	1/1	0.99	0.46	18.81	55,55,55,55	0
56	MG	14	3132	1/1	0.91	0.61	18.63	56,56,56,56	0
56	MG	14	3032	1/1	0.97	0.43	18.53	50,50,50,50	0
56	MG	14	3160	1/1	0.89	0.52	18.33	78,78,78,78	0
56	MG	1H	3261	1/1	0.90	0.46	18.00	65,65,65,65	0
56	MG	14	3122	1/1	0.94	0.41	17.67	53,53,53,53	0
56	MG	1H	3105	1/1	0.88	0.50	17.31	72,72,72,72	0
56	MG	1H	3021	1/1	0.98	0.35	17.24	43,43,43,43	0
56	MG	14	3220	1/1	0.96	0.39	17.19	74,74,74,74	0
56	MG	14	3053	1/1	0.83	0.40	17.14	53,53,53,53	0
56	MG	14	3050	1/1	0.93	0.44	17.09	76,76,76,76	0
56	MG	1H	3274	1/1	0.86	0.45	16.81	48,48,48,48	0
56	MG	14	3166	1/1	0.86	0.30	14.73	85,85,85,85	0
56	MG	1H	3189	1/1	0.92	0.44	14.17	53,53,53,53	0
56	MG	1H	3053	1/1	0.93	0.40	13.98	40,40,40,40	0
56	MG	14	3099	1/1	0.94	0.33	13.67	51,51,51,51	0
56	MG	1H	3051	1/1	0.97	0.37	13.35	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3006	1/1	0.95	0.27	13.25	43,43,43,43	0
56	MG	13	1626	1/1	0.96	0.30	13.21	60,60,60,60	0
56	MG	1H	3050	1/1	0.88	0.31	12.10	49,49,49,49	0
56	MG	1H	3284	1/1	0.96	0.38	12.10	44,44,44,44	0
56	MG	14	3114	1/1	0.99	0.23	12.06	68,68,68,68	0
56	MG	14	3213	1/1	0.95	0.36	11.96	78,78,78,78	0
56	MG	14	3111	1/1	0.65	0.32	11.95	73,73,73,73	0
56	MG	14	3115	1/1	0.78	0.35	11.90	64,64,64,64	0
56	MG	14	3104	1/1	0.86	0.50	11.89	74,74,74,74	0
56	MG	14	3033	1/1	0.84	0.47	11.58	63,63,63,63	0
56	MG	1H	3184	1/1	0.95	0.40	11.57	57,57,57,57	0
56	MG	1H	3213	1/1	0.94	0.27	11.20	96,96,96,96	0
56	MG	14	3119	1/1	0.94	0.29	11.09	67,67,67,67	0
56	MG	1H	3080	1/1	0.94	0.33	11.08	74,74,74,74	0
56	MG	1H	3032	1/1	0.94	0.32	11.01	68,68,68,68	0
56	MG	14	3045	1/1	0.94	0.21	10.81	67,67,67,67	0
56	MG	14	3013	1/1	0.96	0.32	10.48	60,60,60,60	0
56	MG	1H	3156	1/1	0.39	0.34	10.43	55,55,55,55	0
56	MG	13	1631	1/1	0.80	0.26	10.42	89,89,89,89	0
56	MG	1H	3011	1/1	0.89	0.20	9.74	119,119,119,119	0
56	MG	1H	3246	1/1	0.97	0.31	9.70	71,71,71,71	0
56	MG	1H	3115	1/1	0.94	0.27	9.42	59,59,59,59	0
56	MG	2K	103	1/1	0.96	0.38	9.30	56,56,56,56	0
56	MG	1H	3030	1/1	0.92	0.26	8.84	49,49,49,49	0
56	MG	14	3080	1/1	0.98	0.28	8.84	53,53,53,53	0
56	MG	13	1659	1/1	0.81	0.31	8.75	57,57,57,57	0
56	MG	1H	3095	1/1	0.97	0.31	8.63	66,66,66,66	0
56	MG	1H	3442	1/1	0.93	0.22	8.59	64,64,64,64	0
56	MG	13	1624	1/1	0.91	0.25	8.42	80,80,80,80	0
56	MG	1H	3040	1/1	0.98	0.31	8.38	71,71,71,71	0
56	MG	14	3198	1/1	0.82	0.37	8.36	84,84,84,84	0
56	MG	1H	3019	1/1	0.93	0.39	8.30	39,39,39,39	0
56	MG	14	3110	1/1	0.76	0.35	7.96	51,51,51,51	0
56	MG	1H	3093	1/1	0.88	0.21	7.74	60,60,60,60	0
56	MG	1H	3132	1/1	0.83	0.26	7.54	58,58,58,58	0
56	MG	14	3054	1/1	0.98	0.26	7.47	55,55,55,55	0
56	MG	1H	3048	1/1	0.89	0.22	7.45	45,45,45,45	0
56	MG	14	3098	1/1	0.89	0.23	7.43	68,68,68,68	0
56	MG	1H	3043	1/1	0.96	0.27	7.32	47,47,47,47	0
56	MG	1H	3167	1/1	0.86	0.19	7.12	45,45,45,45	0
56	MG	13	1611	1/1	0.94	0.28	6.96	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3218	1/1	0.86	0.20	6.95	65,65,65,65	0
56	MG	1H	3407	1/1	0.89	0.21	6.91	89,89,89,89	0
56	MG	14	3231	1/1	0.84	0.28	6.52	69,69,69,69	0
56	MG	1G	1634	1/1	0.88	0.25	6.52	91,91,91,91	0
56	MG	1H	3159	1/1	0.74	0.28	6.45	69,69,69,69	0
56	MG	1H	3123	1/1	0.88	0.29	6.10	65,65,65,65	0
56	MG	1H	3147	1/1	0.96	0.29	6.06	43,43,43,43	0
56	MG	1H	3109	1/1	0.99	0.33	6.00	34,34,34,34	0
56	MG	14	3006	1/1	0.88	0.25	5.99	67,67,67,67	0
56	MG	14	3143	1/1	0.85	0.27	5.96	86,86,86,86	0
56	MG	1H	3068	1/1	0.76	0.31	5.69	50,50,50,50	0
56	MG	1J	208	1/1	0.88	0.22	5.69	90,90,90,90	0
56	MG	14	3455	1/1	0.86	0.39	5.69	87,87,87,87	0
56	MG	14	3328	1/1	0.91	0.30	5.68	83,83,83,83	0
56	MG	1G	1682	1/1	0.89	0.16	5.47	117,117,117,117	0
56	MG	13	1654	1/1	0.95	0.16	5.40	91,91,91,91	0
56	MG	13	1635	1/1	0.97	0.23	5.31	72,72,72,72	0
56	MG	1H	3056	1/1	0.96	0.33	5.19	28,28,28,28	0
56	MG	1H	3230	1/1	0.79	0.42	5.16	89,89,89,89	0
56	MG	14	3086	1/1	0.91	0.27	5.08	61,61,61,61	0
56	MG	14	3226	1/1	0.97	0.26	5.03	51,51,51,51	0
56	MG	1H	3028	1/1	0.96	0.24	4.91	49,49,49,49	0
56	MG	1H	3454	1/1	0.88	0.23	4.89	67,67,67,67	0
56	MG	14	3327	1/1	0.96	0.23	4.82	60,60,60,60	0
56	MG	14	3065	1/1	0.97	0.27	4.80	58,58,58,58	0
56	MG	14	3031	1/1	0.98	0.32	4.65	48,48,48,48	0
56	MG	14	3077	1/1	0.98	0.27	4.49	45,45,45,45	0
56	MG	14	3047	1/1	0.96	0.29	4.46	46,46,46,46	0
56	MG	1H	3141	1/1	0.85	0.25	4.42	53,53,53,53	0
56	MG	14	3191	1/1	0.71	0.20	4.39	66,66,66,66	0
56	MG	14	3246	1/1	0.97	0.31	4.34	57,57,57,57	0
56	MG	14	3030	1/1	0.95	0.32	4.31	38,38,38,38	0
56	MG	1H	3078	1/1	0.89	0.26	4.22	70,70,70,70	0
56	MG	1G	1619	1/1	0.83	0.21	4.20	103,103,103,103	0
56	MG	14	3245	1/1	0.97	0.24	4.16	61,61,61,61	0
56	MG	1H	3069	1/1	0.92	0.27	4.14	45,45,45,45	0
56	MG	13	1638	1/1	0.78	0.26	4.14	71,71,71,71	0
56	MG	14	3016	1/1	0.98	0.32	4.10	55,55,55,55	0
56	MG	1H	3240	1/1	0.77	0.18	4.02	75,75,75,75	0
56	MG	1G	1609	1/1	0.95	0.24	4.00	70,70,70,70	0
56	MG	14	3096	1/1	0.94	0.29	3.90	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3098	1/1	0.84	0.17	3.84	58,58,58,58	0
56	MG	14	3064	1/1	0.84	0.28	3.77	62,62,62,62	0
56	MG	13	1632	1/1	0.93	0.19	3.77	69,69,69,69	0
56	MG	1H	3058	1/1	0.98	0.26	3.75	69,69,69,69	0
56	MG	14	3039	1/1	0.98	0.24	3.59	63,63,63,63	0
56	MG	14	3279	1/1	0.91	0.28	3.52	45,45,45,45	0
56	MG	16	201	1/1	0.72	0.17	3.44	84,84,84,84	0
56	MG	1H	3165	1/1	0.86	0.17	3.38	63,63,63,63	0
56	MG	14	3102	1/1	0.90	0.25	3.33	60,60,60,60	0
56	MG	1H	3125	1/1	0.92	0.19	3.31	50,50,50,50	0
56	MG	1H	3229	1/1	0.94	0.22	3.30	59,59,59,59	0
56	MG	1H	3572	1/1	0.98	0.28	3.28	54,54,54,54	0
56	MG	14	3128	1/1	0.68	0.27	3.24	49,49,49,49	0
56	MG	1H	3103	1/1	0.95	0.24	3.11	62,62,62,62	0
56	MG	1H	3127	1/1	0.92	0.24	3.06	44,44,44,44	0
56	MG	13	1606	1/1	0.98	0.20	3.04	71,71,71,71	0
56	MG	1H	3007	1/1	0.97	0.20	3.03	60,60,60,60	0
56	MG	14	3019	1/1	0.86	0.24	2.90	48,48,48,48	0
56	MG	14	3112	1/1	0.78	0.28	2.88	69,69,69,69	0
56	MG	14	3026	1/1	0.96	0.21	2.77	70,70,70,70	0
56	MG	1H	3209	1/1	0.78	0.21	2.74	65,65,65,65	0
56	MG	21	301	1/1	0.82	0.28	2.61	62,62,62,62	0
56	MG	14	3165	1/1	0.93	0.21	2.52	67,67,67,67	0
56	MG	13	1625	1/1	0.89	0.21	2.51	78,78,78,78	0
56	MG	1H	3027	1/1	0.72	0.17	2.39	68,68,68,68	0
56	MG	1G	1630	1/1	0.89	0.17	2.37	97,97,97,97	0
56	MG	14	3243	1/1	0.94	0.41	2.35	60,60,60,60	0
56	MG	1G	1613	1/1	0.98	0.18	2.31	85,85,85,85	0
56	MG	14	3159	1/1	0.87	0.24	2.30	70,70,70,70	0
56	MG	1H	3363	1/1	0.84	0.29	2.27	78,78,78,78	0
56	MG	1H	3343	1/1	0.96	0.24	2.18	39,39,39,39	0
56	MG	14	3129	1/1	0.87	0.13	2.18	62,62,62,62	0
56	MG	13	1688	1/1	0.94	0.18	2.12	92,92,92,92	0
56	MG	14	3319	1/1	0.89	0.23	2.02	84,84,84,84	0
56	MG	1H	3149	1/1	0.97	0.23	1.99	54,54,54,54	0
56	MG	1H	3409	1/1	0.77	0.19	1.99	65,65,65,65	0
56	MG	13	1696	1/1	0.94	0.18	1.93	72,72,72,72	0
56	MG	13	1660	1/1	0.98	0.18	1.89	55,55,55,55	0
56	MG	1H	3001	1/1	0.82	0.22	1.84	61,61,61,61	0
56	MG	14	3237	1/1	0.95	0.14	1.83	88,88,88,88	0
56	MG	13	1617	1/1	0.88	0.23	1.82	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1G	1625	1/1	0.90	0.17	1.73	81,81,81,81	0
56	MG	1H	3320	1/1	0.92	0.23	1.69	43,43,43,43	0
56	MG	14	3152	1/1	0.80	0.28	1.68	85,85,85,85	0
56	MG	1G	1621	1/1	0.90	0.19	1.62	76,76,76,76	0
56	MG	13	1618	1/1	0.87	0.23	1.58	45,45,45,45	0
56	MG	1H	3131	1/1	0.93	0.21	1.55	54,54,54,54	0
56	MG	14	3470	1/1	0.98	0.27	1.52	79,79,79,79	0
56	MG	13	1736	1/1	0.97	0.16	1.38	99,99,99,99	0
56	MG	42	202	1/1	0.68	0.24	1.28	110,110,110,110	0
56	MG	1H	3036	1/1	0.98	0.21	1.22	45,45,45,45	0
56	MG	13	1748	1/1	0.81	0.21	1.07	102,102,102,102	0
56	MG	14	3003	1/1	0.92	0.30	0.97	43,43,43,43	0
56	MG	42	201	1/1	0.90	0.27	0.91	111,111,111,111	0
56	MG	1H	3538	1/1	0.90	0.18	0.85	78,78,78,78	0
56	MG	14	3138	1/1	0.80	0.20	0.80	71,71,71,71	0
56	MG	1H	3101	1/1	0.97	0.15	0.76	79,79,79,79	0
56	MG	14	3266	1/1	0.99	0.24	0.75	43,43,43,43	0
56	MG	14	3329	1/1	0.96	0.24	0.75	54,54,54,54	0
56	MG	1H	3166	1/1	0.89	0.18	0.70	52,52,52,52	0
56	MG	52	201	1/1	0.90	0.17	0.64	109,109,109,109	0
56	MG	1H	3369	1/1	0.96	0.18	0.64	57,57,57,57	0
56	MG	13	1605	1/1	0.88	0.24	0.63	79,79,79,79	0
56	MG	14	3097	1/1	0.94	0.27	0.56	70,70,70,70	0
56	MG	14	3089	1/1	0.89	0.20	0.54	53,53,53,53	0
56	MG	14	3248	1/1	0.96	0.20	0.52	47,47,47,47	0
56	MG	88	201	1/1	0.84	0.22	0.49	73,73,73,73	0
56	MG	1H	3174	1/1	0.91	0.23	0.49	50,50,50,50	0
56	MG	1G	1610	1/1	0.97	0.20	0.48	70,70,70,70	0
56	MG	1H	3046	1/1	0.87	0.20	0.43	59,59,59,59	0
56	MG	1H	3498	1/1	0.88	0.17	0.33	85,85,85,85	0
56	MG	1H	3313	1/1	0.99	0.15	0.32	58,58,58,58	0
56	MG	1G	1669	1/1	0.93	0.18	0.22	81,81,81,81	0
56	MG	1H	3310	1/1	0.89	0.21	0.20	43,43,43,43	0
56	MG	1G	1709	1/1	0.93	0.22	0.16	99,99,99,99	0
56	MG	1H	3300	1/1	0.93	0.20	0.15	41,41,41,41	0
56	MG	1H	3004	1/1	0.99	0.21	0.11	46,46,46,46	0
56	MG	1G	1618	1/1	0.89	0.18	0.08	88,88,88,88	0
56	MG	14	3337	1/1	0.89	0.17	0.01	70,70,70,70	0
56	MG	14	3124	1/1	0.84	0.18	-0.07	62,62,62,62	0
56	MG	1H	3111	1/1	0.93	0.19	-0.16	57,57,57,57	0
56	MG	1H	3346	1/1	0.98	0.18	-0.17	60,60,60,60	0
56	MG	13	1644	1/1	0.95	0.16	-0.18	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3071	1/1	0.80	0.17	-0.20	57,57,57,57	0
56	MG	14	3316	1/1	0.91	0.18	-0.21	79,79,79,79	0
56	MG	1H	3029	1/1	0.94	0.18	-0.26	48,48,48,48	0
56	MG	1H	3471	1/1	0.80	0.15	-0.27	91,91,91,91	0
56	MG	1H	3365	1/1	0.97	0.18	-0.28	50,50,50,50	0
56	MG	1H	3139	1/1	0.89	0.14	-0.28	52,52,52,52	0
56	MG	1G	1623	1/1	0.86	0.16	-0.28	77,77,77,77	0
56	MG	1H	3003	1/1	0.97	0.16	-0.29	44,44,44,44	0
56	MG	1G	1726	1/1	0.95	0.19	-0.32	92,92,92,92	0
56	MG	14	3193	1/1	0.73	0.15	-0.35	74,74,74,74	0
56	MG	16	203	1/1	0.64	0.10	-0.40	78,78,78,78	0
56	MG	1H	3295	1/1	0.97	0.17	-0.41	55,55,55,55	0
56	MG	14	3120	1/1	0.92	0.17	-0.44	72,72,72,72	0
56	MG	13	1698	1/1	0.98	0.14	-0.46	98,98,98,98	0
56	MG	1H	3113	1/1	0.92	0.19	-0.48	37,37,37,37	0
56	MG	F8	101	1/1	0.95	0.14	-0.51	63,63,63,63	0
56	MG	1G	1611	1/1	0.87	0.16	-0.53	84,84,84,84	0
56	MG	13	1610	1/1	0.97	0.13	-0.53	77,77,77,77	0
56	MG	1H	3304	1/1	0.98	0.20	-0.53	42,42,42,42	0
56	MG	1H	3354	1/1	0.96	0.19	-0.55	45,45,45,45	0
56	MG	14	3232	1/1	0.97	0.15	-0.59	88,88,88,88	0
56	MG	1H	3119	1/1	0.94	0.18	-0.60	46,46,46,46	0
56	MG	1H	3470	1/1	0.85	0.15	-0.61	82,82,82,82	0
57	SF4	3E	301	8/8	0.99	0.19	-0.63	75,82,92,93	0
56	MG	1H	3491	1/1	0.89	0.18	-0.69	73,73,73,73	0
56	MG	1H	3405	1/1	0.78	0.12	-0.69	91,91,91,91	0
56	MG	13	1711	1/1	0.88	0.12	-0.70	101,101,101,101	0
56	MG	14	3024	1/1	0.86	0.16	-0.71	65,65,65,65	0
56	MG	1G	1607	1/1	0.96	0.12	-0.72	120,120,120,120	0
56	MG	1H	3429	1/1	0.94	0.20	-0.77	49,49,49,49	0
58	ZN	5I	102	1/1	0.98	0.13	-0.77	87,87,87,87	0
56	MG	1H	3138	1/1	0.93	0.14	-0.78	59,59,59,59	0
56	MG	1H	3024	1/1	0.99	0.15	-0.80	47,47,47,47	0
56	MG	13	1695	1/1	0.92	0.15	-0.81	78,78,78,78	0
56	MG	1H	3282	1/1	0.99	0.14	-0.82	66,66,66,66	0
56	MG	14	3083	1/1	0.89	0.15	-0.82	74,74,74,74	0
56	MG	14	3130	1/1	0.86	0.13	-0.82	75,75,75,75	0
56	MG	13	1690	1/1	0.95	0.17	-0.84	56,56,56,56	0
56	MG	14	3147	1/1	0.94	0.12	-0.89	66,66,66,66	0
56	MG	14	3471	1/1	0.99	0.17	-0.89	68,68,68,68	0
56	MG	13	1702	1/1	0.96	0.14	-0.92	64,64,64,64	0
56	MG	13	1689	1/1	0.93	0.17	-0.93	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	16	206	1/1	0.84	0.10	-0.94	81,81,81,81	0
56	MG	13	1761	1/1	0.94	0.15	-0.98	75,75,75,75	0
56	MG	14	3307	1/1	0.97	0.15	-1.00	60,60,60,60	0
56	MG	1H	3063	1/1	0.96	0.16	-1.00	43,43,43,43	0
56	MG	5E	201	1/1	0.93	0.17	-1.00	71,71,71,71	0
56	MG	39	301	1/1	0.91	0.14	-1.02	92,92,92,92	0
56	MG	14	3373	1/1	0.88	0.17	-1.02	58,58,58,58	0
56	MG	35	201	1/1	0.79	0.13	-1.07	74,74,74,74	0
56	MG	1H	3334	1/1	0.98	0.14	-1.07	59,59,59,59	0
56	MG	1H	3398	1/1	0.95	0.17	-1.09	55,55,55,55	0
56	MG	1H	3302	1/1	0.96	0.15	-1.10	52,52,52,52	0
57	SF4	32	302	8/8	0.99	0.17	-1.10	99,104,114,118	0
56	MG	14	3255	1/1	0.98	0.20	-1.11	42,42,42,42	0
56	MG	14	3178	1/1	0.87	0.12	-1.11	114,114,114,114	0
56	MG	1H	3513	1/1	0.90	0.14	-1.14	64,64,64,64	0
56	MG	16	202	1/1	0.80	0.12	-1.14	66,66,66,66	0
56	MG	14	3093	1/1	0.86	0.15	-1.14	71,71,71,71	0
56	MG	1H	3567	1/1	0.88	0.15	-1.16	42,42,42,42	0
56	MG	14	3294	1/1	0.98	0.16	-1.16	59,59,59,59	0
56	MG	14	3133	1/1	0.88	0.16	-1.17	72,72,72,72	0
56	MG	1H	3329	1/1	0.94	0.15	-1.18	41,41,41,41	0
56	MG	1H	3516	1/1	0.94	0.11	-1.19	81,81,81,81	0
56	MG	45	201	1/1	0.94	0.12	-1.21	87,87,87,87	0
56	MG	13	1633	1/1	0.89	0.12	-1.23	80,80,80,80	0
56	MG	14	3188	1/1	0.96	0.12	-1.33	61,61,61,61	0
58	ZN	5A	101	1/1	0.97	0.07	-1.34	130,130,130,130	0
56	MG	14	3302	1/1	0.84	0.12	-1.35	96,96,96,96	0
56	MG	11	301	1/1	0.93	0.15	-1.36	77,77,77,77	0
56	MG	14	3431	1/1	0.90	0.10	-1.36	84,84,84,84	0
56	MG	1H	3129	1/1	0.93	0.15	-1.38	66,66,66,66	0
56	MG	14	3092	1/1	0.97	0.14	-1.38	43,43,43,43	0
56	MG	1H	3294	1/1	0.94	0.18	-1.41	43,43,43,43	0
56	MG	5I	101	1/1	0.85	0.11	-1.44	77,77,77,77	0
56	MG	14	3350	1/1	0.89	0.14	-1.44	44,44,44,44	0
56	MG	13	1727	1/1	0.90	0.09	-1.46	87,87,87,87	0
56	MG	1H	3140	1/1	0.92	0.16	-1.47	50,50,50,50	0
56	MG	14	3275	1/1	0.98	0.18	-1.48	47,47,47,47	0
56	MG	14	3268	1/1	0.92	0.19	-1.53	64,64,64,64	0
56	MG	1H	3130	1/1	0.84	0.12	-1.54	54,54,54,54	0
56	MG	14	3215	1/1	0.91	0.12	-1.56	79,79,79,79	0
56	MG	1G	1695	1/1	0.73	0.14	-1.58	99,99,99,99	0
56	MG	13	1691	1/1	0.88	0.13	-1.65	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	13	1648	1/1	0.94	0.10	-1.69	105,105,105,105	0
56	MG	1G	1712	1/1	0.90	0.11	-1.71	122,122,122,122	0
58	ZN	C5	201	1/1	0.93	0.05	-1.72	156,156,156,156	0
56	MG	1H	3376	1/1	0.95	0.11	-1.74	50,50,50,50	0
56	MG	1H	3316	1/1	0.90	0.12	-1.79	60,60,60,60	0
56	MG	1H	3433	1/1	0.98	0.18	-1.81	37,37,37,37	0
56	MG	1H	3206	1/1	0.98	0.17	-1.84	53,53,53,53	0
56	MG	41	201	1/1	0.92	0.08	-1.86	62,62,62,62	0
56	MG	14	3101	1/1	0.94	0.14	-1.88	70,70,70,70	0
56	MG	1H	3367	1/1	0.99	0.15	-1.89	40,40,40,40	0
56	MG	14	3304	1/1	0.95	0.13	-1.93	64,64,64,64	0
56	MG	14	3262	1/1	0.98	0.20	-1.93	54,54,54,54	0
56	MG	1G	1646	1/1	0.93	0.11	-1.95	119,119,119,119	0
56	MG	14	3469	1/1	0.96	0.13	-1.96	55,55,55,55	0
56	MG	16	204	1/1	0.83	0.08	-2.01	57,57,57,57	0
56	MG	1H	3314	1/1	0.95	0.10	-2.01	74,74,74,74	0
56	MG	1G	1602	1/1	0.85	0.13	-2.05	87,87,87,87	0
56	MG	11	303	1/1	0.99	0.13	-2.06	49,49,49,49	0
56	MG	1H	3353	1/1	0.85	0.11	-2.09	68,68,68,68	0
56	MG	13	1701	1/1	0.89	0.10	-2.12	100,100,100,100	0
56	MG	14	3368	1/1	0.87	0.08	-2.13	75,75,75,75	0
56	MG	1H	3571	1/1	0.95	0.17	-2.18	39,39,39,39	0
56	MG	14	3449	1/1	0.86	0.07	-2.19	88,88,88,88	0
56	MG	1G	1671	1/1	0.94	0.14	-2.22	82,82,82,82	0
56	MG	M5	101	1/1	0.94	0.14	-2.24	81,81,81,81	0
56	MG	1G	1670	1/1	0.99	0.14	-2.24	71,71,71,71	0
56	MG	13	1647	1/1	0.92	0.13	-2.24	73,73,73,73	0
56	MG	1H	3462	1/1	0.99	0.07	-2.39	66,66,66,66	0
56	MG	14	3418	1/1	0.97	0.11	-2.44	75,75,75,75	0
56	MG	1H	3082	1/1	0.82	0.11	-2.48	55,55,55,55	0
56	MG	14	3320	1/1	0.98	0.09	-2.48	79,79,79,79	0
56	MG	14	3070	1/1	0.91	0.13	-2.49	49,49,49,49	0
56	MG	1H	3404	1/1	0.99	0.14	-2.58	45,45,45,45	0
56	MG	14	3280	1/1	0.97	0.15	-2.61	47,47,47,47	0
56	MG	14	3413	1/1	0.90	0.14	-2.65	64,64,64,64	0
56	MG	14	3333	1/1	0.93	0.12	-2.65	64,64,64,64	0
56	MG	14	3135	1/1	0.96	0.13	-2.68	59,59,59,59	0
56	MG	13	1656	1/1	0.96	0.12	-2.69	60,60,60,60	0
56	MG	14	3391	1/1	0.93	0.11	-2.75	73,73,73,73	0
56	MG	1H	3337	1/1	0.99	0.12	-2.77	41,41,41,41	0
56	MG	1H	3349	1/1	0.98	0.17	-2.78	42,42,42,42	0
56	MG	1H	3291	1/1	0.90	0.15	-2.82	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3295	1/1	0.85	0.12	-2.86	73,73,73,73	0
56	MG	14	3324	1/1	0.94	0.12	-2.93	70,70,70,70	0
56	MG	1H	3306	1/1	0.97	0.12	-2.96	38,38,38,38	0
56	MG	14	3020	1/1	0.93	0.13	-2.97	73,73,73,73	0
56	MG	1H	3289	1/1	0.97	0.15	-2.97	48,48,48,48	0
56	MG	13	1692	1/1	0.94	0.04	-2.98	79,79,79,79	0
56	MG	1G	1635	1/1	0.94	0.07	-2.99	101,101,101,101	0
56	MG	14	3251	1/1	0.94	0.12	-3.06	48,48,48,48	0
56	MG	14	3126	1/1	0.96	0.14	-3.08	55,55,55,55	0
56	MG	14	3142	1/1	0.97	0.11	-3.10	83,83,83,83	0
56	MG	13	1675	1/1	0.79	0.14	-3.14	65,65,65,65	0
56	MG	14	3357	1/1	0.85	0.13	-3.20	79,79,79,79	0
56	MG	14	3405	1/1	0.78	0.07	-3.23	106,106,106,106	0
56	MG	14	3419	1/1	0.95	0.11	-3.29	97,97,97,97	0
56	MG	14	3363	1/1	0.89	0.13	-3.30	54,54,54,54	0
56	MG	1H	3482	1/1	0.93	0.11	-3.31	85,85,85,85	0
56	MG	14	3362	1/1	0.94	0.08	-3.32	65,65,65,65	0
56	MG	13	1637	1/1	0.81	0.10	-3.33	73,73,73,73	0
56	MG	1H	3062	1/1	0.90	0.14	-3.36	29,29,29,29	0
56	MG	1G	1666	1/1	0.98	0.07	-3.36	100,100,100,100	0
56	MG	14	3278	1/1	0.96	0.11	-3.39	50,50,50,50	0
56	MG	14	3260	1/1	0.95	0.17	-3.40	52,52,52,52	0
56	MG	14	3271	1/1	0.95	0.14	-3.40	60,60,60,60	0
56	MG	1G	1665	1/1	0.87	0.09	-3.40	104,104,104,104	0
56	MG	1J	207	1/1	0.64	0.07	-3.42	88,88,88,88	0
56	MG	14	3264	1/1	0.99	0.15	-3.47	59,59,59,59	0
56	MG	13	1737	1/1	0.88	0.06	-3.53	83,83,83,83	0
56	MG	1H	3339	1/1	0.98	0.13	-3.54	41,41,41,41	0
56	MG	1H	3197	1/1	0.96	0.11	-3.57	69,69,69,69	0
56	MG	13	1621	1/1	0.97	0.08	-3.57	84,84,84,84	0
56	MG	14	3281	1/1	0.97	0.11	-3.63	69,69,69,69	0
56	MG	1H	3190	1/1	0.80	0.11	-3.70	60,60,60,60	0
56	MG	14	3288	1/1	0.86	0.06	-3.74	76,76,76,76	0
56	MG	14	3203	1/1	0.81	0.10	-3.75	69,69,69,69	0
56	MG	1G	1606	1/1	0.95	0.10	-3.76	80,80,80,80	0
56	MG	1H	3065	1/1	0.89	0.10	-3.80	61,61,61,61	0
56	MG	14	3060	1/1	0.98	0.09	-3.83	47,47,47,47	0
56	MG	1H	3388	1/1	0.94	0.09	-3.87	97,97,97,97	0
56	MG	1H	3377	1/1	0.87	0.14	-3.88	49,49,49,49	0
56	MG	14	3340	1/1	0.97	0.11	-3.88	54,54,54,54	0
56	MG	14	3023	1/1	0.92	0.09	-3.90	69,69,69,69	0
56	MG	14	3354	1/1	0.90	0.12	-3.94	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3261	1/1	0.96	0.15	-3.94	57,57,57,57	0
56	MG	1H	3319	1/1	0.89	0.13	-3.96	51,51,51,51	0
56	MG	13	1699	1/1	0.86	0.06	-3.98	75,75,75,75	0
56	MG	1H	3338	1/1	0.97	0.07	-4.03	45,45,45,45	0
56	MG	14	3175	1/1	0.84	0.11	-4.05	74,74,74,74	0
56	MG	1H	3393	1/1	0.97	0.10	-4.05	61,61,61,61	0
56	MG	1H	3308	1/1	0.96	0.10	-4.06	49,49,49,49	0
56	MG	14	3345	1/1	0.93	0.13	-4.10	66,66,66,66	0
56	MG	14	3457	1/1	0.78	0.10	-4.15	92,92,92,92	0
56	MG	1H	3311	1/1	0.86	0.14	-4.21	56,56,56,56	0
56	MG	1G	1688	1/1	0.86	0.12	-4.27	81,81,81,81	0
56	MG	1H	3321	1/1	0.90	0.11	-4.36	59,59,59,59	0
56	MG	1H	3325	1/1	0.86	0.08	-4.41	56,56,56,56	0
56	MG	1G	1680	1/1	0.95	0.14	-4.43	68,68,68,68	0
56	MG	14	3297	1/1	0.92	0.07	-4.55	91,91,91,91	0
56	MG	1G	1684	1/1	0.81	0.06	-4.56	98,98,98,98	0
56	MG	1H	3318	1/1	0.92	0.07	-4.56	72,72,72,72	0
56	MG	1H	3424	1/1	0.96	0.14	-4.59	44,44,44,44	0
56	MG	14	3349	1/1	0.85	0.09	-4.81	65,65,65,65	0
56	MG	14	3267	1/1	0.96	0.13	-4.82	50,50,50,50	0
56	MG	13	1714	1/1	0.98	0.12	-4.86	59,59,59,59	0
56	MG	1G	1673	1/1	0.94	0.08	-4.94	86,86,86,86	0
56	MG	1H	3238	1/1	0.95	0.08	-4.95	76,76,76,76	0
56	MG	14	3277	1/1	0.98	0.14	-4.95	57,57,57,57	0
56	MG	1G	1690	1/1	0.98	0.03	-4.97	90,90,90,90	0
56	MG	14	3388	1/1	0.90	0.05	-5.02	90,90,90,90	0
56	MG	14	3343	1/1	0.98	0.14	-5.04	42,42,42,42	0
56	MG	1H	3335	1/1	0.96	0.08	-5.08	77,77,77,77	0
56	MG	1H	3112	1/1	0.90	0.11	-5.15	53,53,53,53	0
56	MG	1H	3323	1/1	0.98	0.08	-5.19	64,64,64,64	0
56	MG	14	3323	1/1	0.94	0.09	-5.31	57,57,57,57	0
56	MG	13	1693	1/1	0.95	0.07	-5.36	80,80,80,80	0
56	MG	1H	3472	1/1	0.89	0.06	-5.36	82,82,82,82	0
56	MG	14	3355	1/1	0.99	0.10	-5.39	52,52,52,52	0
56	MG	1H	3383	1/1	0.93	0.08	-5.53	61,61,61,61	0
56	MG	1H	3452	1/1	0.82	0.12	-5.56	72,72,72,72	0
56	MG	1H	3371	1/1	0.97	0.06	-5.80	64,64,64,64	0
56	MG	14	3285	1/1	0.97	0.09	-5.81	55,55,55,55	0
56	MG	14	3273	1/1	0.98	0.09	-5.84	55,55,55,55	0
56	MG	13	1755	1/1	0.92	0.06	-5.84	101,101,101,101	0
56	MG	14	3276	1/1	0.99	0.09	-5.85	56,56,56,56	0
56	MG	1H	3372	1/1	0.94	0.11	-5.96	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	13	1718	1/1	0.85	0.11	-5.97	54,54,54,54	0
56	MG	14	3365	1/1	0.98	0.13	-6.02	44,44,44,44	0
56	MG	1H	3355	1/1	0.97	0.11	-6.04	40,40,40,40	0
56	MG	1G	1683	1/1	0.97	0.04	-6.09	89,89,89,89	0
56	MG	1G	1706	1/1	0.98	0.07	-6.10	82,82,82,82	0
56	MG	14	3359	1/1	0.96	0.09	-6.19	57,57,57,57	0
56	MG	14	3421	1/1	0.86	0.08	-6.22	84,84,84,84	0
56	MG	1H	3475	1/1	0.95	0.08	-6.33	73,73,73,73	0
56	MG	1H	3434	1/1	0.94	0.08	-6.41	47,47,47,47	0
56	MG	1H	3526	1/1	0.90	0.12	-6.53	73,73,73,73	0
56	MG	14	3372	1/1	0.95	0.14	-6.75	45,45,45,45	0
56	MG	1H	3436	1/1	0.97	0.04	-6.78	64,64,64,64	0
56	MG	14	3283	1/1	0.96	0.07	-6.91	79,79,79,79	0
56	MG	1H	3298	1/1	0.98	0.11	-6.96	46,46,46,46	0
56	MG	13	1725	1/1	0.92	0.08	-6.99	65,65,65,65	0
56	MG	1H	3330	1/1	0.98	0.11	-7.03	46,46,46,46	0
56	MG	14	3430	1/1	0.86	0.09	-7.07	86,86,86,86	0
56	MG	1H	3074	1/1	0.96	0.07	-7.12	52,52,52,52	0
56	MG	1H	3292	1/1	0.98	0.12	-7.13	38,38,38,38	0
56	MG	1H	3508	1/1	0.97	0.04	-7.14	37,37,37,37	0
56	MG	14	3312	1/1	0.97	0.10	-7.34	47,47,47,47	0
56	MG	1H	3340	1/1	0.94	0.13	-7.69	65,65,65,65	0
56	MG	14	3326	1/1	0.94	0.06	-7.74	81,81,81,81	0
56	MG	1G	1679	1/1	0.97	0.10	-8.17	70,70,70,70	0
56	MG	14	3256	1/1	0.96	0.05	-8.29	65,65,65,65	0
56	MG	14	3321	1/1	0.80	0.04	-8.38	88,88,88,88	0
56	MG	1H	3514	1/1	0.94	0.07	-9.07	69,69,69,69	0
56	MG	1H	3038	1/1	0.97	0.05	-9.26	70,70,70,70	0
56	MG	14	3315	1/1	0.94	0.12	-9.32	56,56,56,56	0
56	MG	1H	3435	1/1	0.92	0.05	-9.32	55,55,55,55	0
56	MG	1G	1663	1/1	0.92	0.07	-9.36	85,85,85,85	0
56	MG	1H	3342	1/1	0.98	0.12	-9.40	44,44,44,44	0
56	MG	1H	3464	1/1	0.96	0.09	-9.45	40,40,40,40	0
56	MG	14	3249	1/1	0.98	0.10	-9.69	64,64,64,64	0
56	MG	1H	3494	1/1	0.96	0.08	-9.83	53,53,53,53	0
56	MG	1G	1660	1/1	0.94	0.05	-10.31	92,92,92,92	0
56	MG	1H	3288	1/1	0.88	0.14	-10.73	38,38,38,38	0
56	MG	1H	3299	1/1	0.98	0.07	-10.99	35,35,35,35	0
56	MG	13	1641	1/1	0.97	0.07	-11.60	78,78,78,78	0
56	MG	1H	3020	1/1	0.99	0.31	-	56,56,56,56	0
56	MG	16	207	1/1	0.93	0.09	-	60,60,60,60	0
56	MG	1G	1629	1/1	0.86	0.60	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3392	1/1	0.94	0.06	-	85,85,85,85	0
56	MG	1H	3555	1/1	0.77	0.22	-	70,70,70,70	0
56	MG	14	3423	1/1	0.96	0.07	-	52,52,52,52	0
56	MG	13	1685	1/1	0.92	0.18	-	100,100,100,100	0
56	MG	14	3258	1/1	0.98	0.11	-	52,52,52,52	0
56	MG	13	1640	1/1	0.83	0.34	-	99,99,99,99	0
56	MG	35	203	1/1	0.54	0.16	-	83,83,83,83	0
56	MG	14	3218	1/1	0.95	0.23	-	74,74,74,74	0
56	MG	1H	3432	1/1	0.83	0.18	-	44,44,44,44	0
56	MG	14	3082	1/1	0.97	0.08	-	73,73,73,73	0
56	MG	1H	3499	1/1	0.96	0.22	-	82,82,82,82	0
56	MG	1H	3368	1/1	0.98	0.08	-	49,49,49,49	0
56	MG	1G	1723	1/1	0.96	0.14	-	106,106,106,106	0
56	MG	1H	3045	1/1	0.99	0.30	-	42,42,42,42	0
56	MG	14	3059	1/1	0.91	0.22	-	53,53,53,53	0
56	MG	13	1682	1/1	0.82	0.13	-	91,91,91,91	0
56	MG	1H	3521	1/1	0.95	0.07	-	79,79,79,79	0
56	MG	14	3332	1/1	0.96	0.09	-	70,70,70,70	0
56	MG	1H	3362	1/1	0.91	0.17	-	55,55,55,55	0
56	MG	13	1743	1/1	0.78	0.07	-	102,102,102,102	0
56	MG	14	3383	1/1	0.87	0.06	-	102,102,102,102	0
56	MG	14	3462	1/1	0.76	0.17	-	99,99,99,99	0
56	MG	1H	3257	1/1	0.61	0.27	-	83,83,83,83	0
56	MG	14	3167	1/1	0.98	0.17	-	54,54,54,54	0
56	MG	1H	3548	1/1	0.88	0.11	-	98,98,98,98	0
56	MG	1H	3328	1/1	0.97	0.07	-	48,48,48,48	0
56	MG	1H	3378	1/1	0.91	0.10	-	83,83,83,83	0
56	MG	14	3353	1/1	0.88	0.08	-	91,91,91,91	0
56	MG	14	3442	1/1	0.87	0.08	-	96,96,96,96	0
56	MG	1G	1705	1/1	0.91	0.09	-	116,116,116,116	0
56	MG	1H	3180	1/1	0.92	0.29	-	87,87,87,87	0
56	MG	1H	3089	1/1	0.93	0.39	-	82,82,82,82	0
56	MG	1G	1604	1/1	0.92	0.31	-	102,102,102,102	0
56	MG	1H	3099	1/1	0.69	0.39	-	80,80,80,80	0
56	MG	14	3299	1/1	0.67	0.05	-	99,99,99,99	0
56	MG	13	1669	1/1	0.98	0.16	-	95,95,95,95	0
56	MG	1H	3500	1/1	0.88	0.08	-	103,103,103,103	0
56	MG	14	3072	1/1	0.94	0.52	-	67,67,67,67	0
56	MG	1H	3215	1/1	0.94	0.61	-	83,83,83,83	0
56	MG	1H	3267	1/1	0.80	0.88	-	90,90,90,90	0
56	MG	13	1753	1/1	0.96	0.07	-	64,64,64,64	0
56	MG	14	3397	1/1	0.93	0.08	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3185	1/1	0.90	0.41	-	71,71,71,71	0
56	MG	13	1609	1/1	0.98	0.24	-	64,64,64,64	0
56	MG	14	3399	1/1	0.82	0.05	-	82,82,82,82	0
56	MG	14	3209	1/1	0.77	0.97	-	90,90,90,90	0
56	MG	1J	205	1/1	0.91	0.18	-	90,90,90,90	0
56	MG	1H	3031	1/1	0.96	0.32	-	74,74,74,74	0
56	MG	14	3176	1/1	0.67	0.38	-	72,72,72,72	0
56	MG	1G	1647	1/1	0.88	0.10	-	82,82,82,82	0
56	MG	14	3451	1/1	0.91	0.07	-	88,88,88,88	0
56	MG	1H	3522	1/1	0.87	0.07	-	98,98,98,98	0
56	MG	1H	3152	1/1	0.93	0.14	-	87,87,87,87	0
56	MG	13	1687	1/1	0.79	0.19	-	82,82,82,82	0
56	MG	13	1672	1/1	0.72	0.35	-	79,79,79,79	0
56	MG	1G	1692	1/1	0.92	0.06	-	106,106,106,106	0
56	MG	14	3330	1/1	0.91	0.14	-	77,77,77,77	0
56	MG	14	3205	1/1	0.84	0.36	-	87,87,87,87	0
56	MG	1G	1652	1/1	0.75	0.32	-	76,76,76,76	0
56	MG	14	3090	1/1	0.95	0.35	-	55,55,55,55	0
56	MG	13	1706	1/1	0.87	0.09	-	92,92,92,92	0
56	MG	1H	3120	1/1	0.93	0.32	-	39,39,39,39	0
56	MG	1H	3533	1/1	0.58	0.17	-	86,86,86,86	0
56	MG	14	3467	1/1	0.82	0.15	-	71,71,71,71	0
56	MG	1H	3469	1/1	0.87	0.08	-	79,79,79,79	0
56	MG	1H	3153	1/1	0.79	0.28	-	88,88,88,88	0
56	MG	1H	3066	1/1	0.90	0.17	-	57,57,57,57	0
56	MG	32	301	1/1	0.92	0.08	-	112,112,112,112	0
56	MG	14	3439	1/1	0.88	0.10	-	86,86,86,86	0
56	MG	14	3081	1/1	0.91	0.23	-	89,89,89,89	0
56	MG	1G	1642	1/1	0.90	0.10	-	102,102,102,102	0
56	MG	14	3434	1/1	0.93	0.07	-	77,77,77,77	0
56	MG	1H	3108	1/1	0.94	0.22	-	34,34,34,34	0
56	MG	1G	1614	1/1	0.66	0.33	-	91,91,91,91	0
56	MG	14	3182	1/1	0.93	0.17	-	66,66,66,66	0
56	MG	1H	3265	1/1	0.97	0.13	-	69,69,69,69	0
56	MG	1H	3088	1/1	0.85	0.41	-	74,74,74,74	0
56	MG	1H	3117	1/1	0.94	0.20	-	61,61,61,61	0
56	MG	14	3162	1/1	0.85	0.18	-	50,50,50,50	0
56	MG	13	1650	1/1	0.90	0.10	-	121,121,121,121	0
56	MG	1H	3373	1/1	0.95	0.15	-	100,100,100,100	0
56	MG	14	3168	1/1	0.95	0.43	-	52,52,52,52	0
56	MG	14	3211	1/1	0.92	0.36	-	70,70,70,70	0
56	MG	13	1601	1/1	0.95	0.23	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3289	1/1	0.90	0.16	-	64,64,64,64	0
56	MG	14	3022	1/1	0.91	0.11	-	73,73,73,73	0
56	MG	13	1623	1/1	0.88	0.31	-	62,62,62,62	0
56	MG	14	3156	1/1	0.81	0.74	-	86,86,86,86	0
56	MG	14	3381	1/1	0.91	0.11	-	101,101,101,101	0
56	MG	1G	1633	1/1	0.96	0.07	-	92,92,92,92	0
56	MG	14	3384	1/1	0.82	0.10	-	79,79,79,79	0
56	MG	14	3286	1/1	0.91	0.12	-	68,68,68,68	0
56	MG	1H	3245	1/1	0.77	0.28	-	58,58,58,58	0
56	MG	1H	3085	1/1	0.64	0.11	-	85,85,85,85	0
56	MG	14	3227	1/1	0.83	0.27	-	70,70,70,70	0
56	MG	1H	3440	1/1	0.76	0.13	-	72,72,72,72	0
56	MG	1H	3465	1/1	0.98	0.05	-	58,58,58,58	0
56	MG	1H	3233	1/1	0.98	0.66	-	57,57,57,57	0
56	MG	1H	3202	1/1	0.96	0.43	-	63,63,63,63	0
56	MG	1H	3544	1/1	0.93	0.08	-	81,81,81,81	0
56	MG	14	3184	1/1	0.95	0.27	-	70,70,70,70	0
56	MG	1H	3219	1/1	0.52	0.18	-	79,79,79,79	0
56	MG	25	202	1/1	0.93	0.08	-	108,108,108,108	0
56	MG	14	3183	1/1	0.91	0.18	-	87,87,87,87	0
56	MG	14	3073	1/1	0.98	0.47	-	65,65,65,65	0
56	MG	1H	3540	1/1	0.85	0.15	-	78,78,78,78	0
56	MG	14	3440	1/1	0.66	0.11	-	95,95,95,95	0
56	MG	14	3443	1/1	0.88	0.08	-	91,91,91,91	0
56	MG	14	3208	1/1	0.99	0.19	-	77,77,77,77	0
56	MG	14	3310	1/1	0.86	0.11	-	98,98,98,98	0
56	MG	1H	3075	1/1	0.92	0.36	-	80,80,80,80	0
56	MG	14	3335	1/1	0.85	0.15	-	78,78,78,78	0
56	MG	1H	3425	1/1	0.97	0.09	-	39,39,39,39	0
56	MG	14	3284	1/1	0.89	0.28	-	87,87,87,87	0
56	MG	14	3387	1/1	0.96	0.10	-	87,87,87,87	0
56	MG	1H	3507	1/1	0.95	0.07	-	84,84,84,84	0
56	MG	14	3303	1/1	0.97	0.12	-	68,68,68,68	0
56	MG	13	1717	1/1	0.93	0.10	-	51,51,51,51	0
56	MG	14	3035	1/1	0.91	0.29	-	67,67,67,67	0
56	MG	14	3358	1/1	0.90	0.05	-	76,76,76,76	0
56	MG	1H	3260	1/1	0.85	0.41	-	74,74,74,74	0
56	MG	1J	211	1/1	0.96	0.05	-	85,85,85,85	0
56	MG	1H	3022	1/1	0.98	0.23	-	45,45,45,45	0
56	MG	13	1722	1/1	0.89	0.10	-	78,78,78,78	0
56	MG	14	3018	1/1	0.94	0.28	-	75,75,75,75	0
56	MG	1H	3278	1/1	0.92	0.29	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	13	1651	1/1	0.94	0.40	-	82,82,82,82	0
56	MG	14	3177	1/1	0.65	0.21	-	91,91,91,91	0
56	MG	1H	3067	1/1	0.85	0.57	-	75,75,75,75	0
56	MG	14	3463	1/1	0.85	0.42	-	97,97,97,97	0
56	MG	1H	3324	1/1	0.94	0.06	-	70,70,70,70	0
56	MG	1H	3519	1/1	0.80	0.17	-	78,78,78,78	0
56	MG	14	3005	1/1	0.94	0.28	-	73,73,73,73	0
56	MG	13	1730	1/1	0.50	0.22	-	102,102,102,102	0
56	MG	1H	3481	1/1	0.98	0.10	-	59,59,59,59	0
56	MG	16	211	1/1	0.86	0.25	-	92,92,92,92	0
56	MG	1H	3272	1/1	0.88	0.74	-	67,67,67,67	0
56	MG	14	3254	1/1	0.88	0.10	-	92,92,92,92	0
56	MG	16	205	1/1	0.82	0.18	-	83,83,83,83	0
56	MG	14	3414	1/1	0.97	0.10	-	78,78,78,78	0
56	MG	1H	3225	1/1	0.77	0.24	-	60,60,60,60	0
56	MG	1H	3271	1/1	0.94	0.33	-	63,63,63,63	0
56	MG	Q8	101	1/1	0.96	0.14	-	71,71,71,71	0
56	MG	14	3250	1/1	0.96	0.12	-	55,55,55,55	0
56	MG	1H	3181	1/1	0.96	0.29	-	88,88,88,88	0
56	MG	14	3235	1/1	0.86	0.58	-	83,83,83,83	0
56	MG	1H	3341	1/1	0.97	0.19	-	43,43,43,43	0
56	MG	1H	3546	1/1	0.76	0.12	-	93,93,93,93	0
56	MG	1J	209	1/1	0.81	0.18	-	93,93,93,93	0
56	MG	1G	1685	1/1	0.92	0.14	-	63,63,63,63	0
56	MG	1G	1678	1/1	0.95	0.14	-	93,93,93,93	0
56	MG	1H	3542	1/1	0.95	0.04	-	81,81,81,81	0
56	MG	1H	3255	1/1	0.98	0.10	-	75,75,75,75	0
56	MG	16	212	1/1	0.94	0.09	-	68,68,68,68	0
56	MG	13	1665	1/1	0.88	0.53	-	76,76,76,76	0
56	MG	1H	3164	1/1	0.77	0.12	-	53,53,53,53	0
56	MG	14	3048	1/1	0.94	0.29	-	68,68,68,68	0
56	MG	1H	3122	1/1	0.79	0.31	-	58,58,58,58	0
56	MG	14	3173	1/1	0.78	0.25	-	93,93,93,93	0
56	MG	14	3034	1/1	0.83	0.55	-	72,72,72,72	0
56	MG	1H	3374	1/1	0.98	0.11	-	68,68,68,68	0
56	MG	1H	3146	1/1	0.84	0.85	-	90,90,90,90	0
56	MG	16	210	1/1	0.82	0.10	-	89,89,89,89	0
56	MG	1G	1672	1/1	0.86	0.11	-	109,109,109,109	0
56	MG	14	3233	1/1	0.95	0.09	-	61,61,61,61	0
56	MG	13	1758	1/1	0.62	0.06	-	137,137,137,137	0
56	MG	1H	3423	1/1	0.99	0.16	-	33,33,33,33	0
56	MG	1H	3205	1/1	0.79	0.33	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3248	1/1	0.94	0.12	-	72,72,72,72	0
56	MG	1H	3458	1/1	0.95	0.08	-	56,56,56,56	0
56	MG	1H	3287	1/1	0.95	0.19	-	121,121,121,121	0
56	MG	14	3382	1/1	0.94	0.12	-	47,47,47,47	0
56	MG	1G	1677	1/1	0.84	0.11	-	93,93,93,93	0
56	MG	14	3406	1/1	0.95	0.25	-	86,86,86,86	0
56	MG	13	1607	1/1	0.92	0.06	-	74,74,74,74	0
56	MG	1H	3262	1/1	0.71	0.31	-	86,86,86,86	0
56	MG	14	3040	1/1	0.99	0.26	-	58,58,58,58	0
56	MG	1H	3352	1/1	0.97	0.11	-	57,57,57,57	0
56	MG	14	3436	1/1	0.94	0.11	-	98,98,98,98	0
56	MG	1H	3244	1/1	0.84	0.14	-	67,67,67,67	0
56	MG	14	3151	1/1	0.80	0.40	-	107,107,107,107	0
56	MG	14	3369	1/1	0.90	0.06	-	93,93,93,93	0
56	MG	1H	3104	1/1	0.86	0.16	-	65,65,65,65	0
56	MG	1H	3247	1/1	0.83	0.48	-	62,62,62,62	0
56	MG	13	1716	1/1	0.87	0.04	-	108,108,108,108	0
56	MG	1G	1715	1/1	0.89	0.06	-	116,116,116,116	0
56	MG	1H	3214	1/1	0.77	0.57	-	83,83,83,83	0
56	MG	1H	3552	1/1	0.94	0.15	-	73,73,73,73	0
56	MG	14	3453	1/1	0.95	0.09	-	102,102,102,102	0
56	MG	14	3415	1/1	0.97	0.07	-	78,78,78,78	0
56	MG	1H	3173	1/1	0.93	0.53	-	67,67,67,67	0
56	MG	1H	3528	1/1	0.93	0.05	-	72,72,72,72	0
56	MG	1H	3445	1/1	0.46	0.11	-	90,90,90,90	0
56	MG	13	1739	1/1	0.97	0.06	-	79,79,79,79	0
56	MG	13	1703	1/1	0.99	0.11	-	75,75,75,75	0
56	MG	13	1745	1/1	0.90	0.07	-	99,99,99,99	0
56	MG	14	3293	1/1	0.75	0.12	-	94,94,94,94	0
56	MG	13	1715	1/1	0.98	0.08	-	94,94,94,94	0
56	MG	13	1652	1/1	0.91	0.23	-	91,91,91,91	0
56	MG	1K	101	1/1	0.84	0.06	-	119,119,119,119	0
56	MG	1G	1717	1/1	0.93	0.06	-	118,118,118,118	0
56	MG	1H	3077	1/1	0.86	0.21	-	70,70,70,70	0
56	MG	1H	3361	1/1	0.96	0.16	-	56,56,56,56	0
56	MG	14	3306	1/1	0.81	0.15	-	76,76,76,76	0
56	MG	13	1645	1/1	0.75	0.15	-	84,84,84,84	0
56	MG	2I	303	1/1	0.99	0.12	-	42,42,42,42	0
56	MG	1H	3476	1/1	0.93	0.04	-	91,91,91,91	0
56	MG	2A	201	1/1	0.93	0.17	-	103,103,103,103	0
56	MG	1H	3518	1/1	0.88	0.11	-	76,76,76,76	0
56	MG	13	1708	1/1	0.93	0.06	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1G	1720	1/1	0.92	0.03	-	129,129,129,129	0
56	MG	14	3002	1/1	0.95	0.36	-	61,61,61,61	0
56	MG	1H	3386	1/1	0.89	0.08	-	88,88,88,88	0
56	MG	14	3370	1/1	0.91	0.15	-	83,83,83,83	0
56	MG	1H	3505	1/1	0.90	0.21	-	82,82,82,82	0
56	MG	E5	102	1/1	0.87	0.58	-	72,72,72,72	0
56	MG	1H	3223	1/1	0.89	0.48	-	76,76,76,76	0
56	MG	1H	3273	1/1	0.84	0.63	-	76,76,76,76	0
56	MG	14	3095	1/1	0.94	0.31	-	76,76,76,76	0
56	MG	14	3056	1/1	0.93	0.64	-	69,69,69,69	0
56	MG	1H	3317	1/1	0.89	0.15	-	63,63,63,63	0
56	MG	1H	3560	1/1	0.83	0.13	-	85,85,85,85	0
56	MG	1G	1719	1/1	0.70	0.10	-	100,100,100,100	0
56	MG	1H	3403	1/1	0.96	0.07	-	71,71,71,71	0
56	MG	1G	1636	1/1	0.97	0.08	-	91,91,91,91	0
56	MG	1H	3431	1/1	0.48	0.21	-	74,74,74,74	0
56	MG	1H	3161	1/1	0.87	0.17	-	82,82,82,82	0
56	MG	13	1735	1/1	0.81	0.05	-	109,109,109,109	0
56	MG	1H	3385	1/1	0.95	0.07	-	74,74,74,74	0
56	MG	1H	3154	1/1	0.97	0.26	-	60,60,60,60	0
56	MG	1G	1708	1/1	0.71	0.07	-	84,84,84,84	0
56	MG	1H	3420	1/1	0.94	0.22	-	55,55,55,55	0
56	MG	1H	3557	1/1	0.47	0.12	-	84,84,84,84	0
56	MG	1H	3370	1/1	0.93	0.10	-	37,37,37,37	0
56	MG	1H	3551	1/1	0.81	0.15	-	105,105,105,105	0
56	MG	14	3454	1/1	0.65	0.22	-	78,78,78,78	0
56	MG	14	3001	1/1	0.94	0.19	-	51,51,51,51	0
56	MG	13	1741	1/1	0.91	0.09	-	110,110,110,110	0
56	MG	14	3021	1/1	0.91	0.38	-	36,36,36,36	0
56	MG	1H	3332	1/1	0.86	0.18	-	50,50,50,50	0
56	MG	1H	3290	1/1	0.98	0.18	-	40,40,40,40	0
56	MG	16	208	1/1	0.88	0.22	-	80,80,80,80	0
56	MG	1H	3107	1/1	0.91	0.41	-	73,73,73,73	0
56	MG	1H	3525	1/1	0.90	0.14	-	71,71,71,71	0
56	MG	14	3367	1/1	0.98	0.09	-	75,75,75,75	0
56	MG	1H	3512	1/1	0.97	0.10	-	60,60,60,60	0
56	MG	1G	1628	1/1	0.98	0.39	-	77,77,77,77	0
56	MG	14	3071	1/1	0.97	0.60	-	52,52,52,52	0
56	MG	1H	3096	1/1	0.72	0.42	-	77,77,77,77	0
56	MG	13	1671	1/1	0.94	0.22	-	79,79,79,79	0
56	MG	1G	1650	1/1	0.89	0.12	-	89,89,89,89	0
56	MG	13	1757	1/1	0.91	0.15	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3062	1/1	0.95	0.30	-	80,80,80,80	0
56	MG	14	3394	1/1	0.97	0.08	-	63,63,63,63	0
56	MG	1G	1662	1/1	0.96	0.16	-	94,94,94,94	0
56	MG	1H	3013	1/1	0.82	0.36	-	69,69,69,69	0
56	MG	14	3100	1/1	0.96	0.21	-	77,77,77,77	0
56	MG	1H	3252	1/1	0.81	1.37	-	75,75,75,75	0
56	MG	13	1738	1/1	0.97	0.09	-	71,71,71,71	0
56	MG	1H	3235	1/1	0.93	0.38	-	65,65,65,65	0
56	MG	1G	1697	1/1	0.88	0.09	-	94,94,94,94	0
56	MG	1H	3489	1/1	0.96	0.09	-	87,87,87,87	0
56	MG	1H	3110	1/1	0.97	0.16	-	44,44,44,44	0
56	MG	14	3380	1/1	0.94	0.08	-	95,95,95,95	0
56	MG	1G	1668	1/1	0.73	0.69	-	96,96,96,96	0
56	MG	14	3272	1/1	0.97	0.03	-	68,68,68,68	0
56	MG	4K	101	1/1	0.54	0.68	-	96,96,96,96	0
56	MG	1H	3012	1/1	0.60	0.20	-	78,78,78,78	0
56	MG	1H	3467	1/1	0.79	0.05	-	95,95,95,95	0
56	MG	14	3427	1/1	0.94	0.16	-	69,69,69,69	0
56	MG	1H	3523	1/1	0.85	0.10	-	76,76,76,76	0
56	MG	13	1746	1/1	0.90	0.08	-	102,102,102,102	0
56	MG	14	3465	1/1	0.52	0.13	-	85,85,85,85	0
56	MG	13	1754	1/1	0.89	0.12	-	80,80,80,80	0
56	MG	1H	3496	1/1	0.89	0.08	-	76,76,76,76	0
56	MG	14	3460	1/1	0.85	0.11	-	93,93,93,93	0
56	MG	1H	3208	1/1	0.79	0.18	-	141,141,141,141	0
56	MG	1G	1725	1/1	0.76	0.07	-	95,95,95,95	0
56	MG	14	3200	1/1	0.63	0.47	-	94,94,94,94	0
56	MG	13	1734	1/1	0.74	0.13	-	105,105,105,105	0
56	MG	14	3170	1/1	0.79	0.37	-	63,63,63,63	0
56	MG	14	3028	1/1	0.72	0.72	-	83,83,83,83	0
56	MG	14	3417	1/1	0.67	0.09	-	116,116,116,116	0
56	MG	1H	3333	1/1	0.91	0.14	-	53,53,53,53	0
56	MG	14	3376	1/1	0.93	0.12	-	91,91,91,91	0
56	MG	1H	3227	1/1	0.85	0.23	-	79,79,79,79	0
56	MG	1H	3563	1/1	0.81	0.21	-	75,75,75,75	0
56	MG	1H	3286	1/1	0.86	0.11	-	119,119,119,119	0
56	MG	1H	3018	1/1	0.88	0.42	-	51,51,51,51	0
56	MG	13	1634	1/1	0.90	0.15	-	68,68,68,68	0
56	MG	14	3051	1/1	0.99	0.35	-	62,62,62,62	0
56	MG	14	3364	1/1	0.87	0.09	-	83,83,83,83	0
56	MG	13	1728	1/1	0.97	0.05	-	77,77,77,77	0
56	MG	1H	3460	1/1	0.94	0.07	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3452	1/1	0.92	0.05	-	90,90,90,90	0
56	MG	14	3137	1/1	0.93	0.78	-	61,61,61,61	0
56	MG	1H	3556	1/1	0.78	0.13	-	101,101,101,101	0
56	MG	1H	3453	1/1	0.96	0.09	-	81,81,81,81	0
56	MG	1H	3087	1/1	0.91	0.31	-	66,66,66,66	0
56	MG	1H	3200	1/1	0.94	0.28	-	70,70,70,70	0
56	MG	14	3425	1/1	0.89	0.15	-	96,96,96,96	0
56	MG	1H	3211	1/1	0.59	0.17	-	90,90,90,90	0
56	MG	1H	3395	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	14	3180	1/1	0.91	0.60	-	74,74,74,74	0
56	MG	1H	3002	1/1	0.97	0.20	-	59,59,59,59	0
56	MG	13	1661	1/1	0.78	0.51	-	73,73,73,73	0
56	MG	13	1619	1/1	0.98	0.19	-	51,51,51,51	0
56	MG	13	1612	1/1	0.92	0.20	-	78,78,78,78	0
56	MG	78	201	1/1	0.95	0.29	-	70,70,70,70	0
56	MG	1H	3015	1/1	0.72	0.95	-	82,82,82,82	0
56	MG	13	1683	1/1	0.95	0.17	-	92,92,92,92	0
56	MG	14	3230	1/1	0.97	0.26	-	74,74,74,74	0
56	MG	1H	3351	1/1	0.95	0.17	-	50,50,50,50	0
56	MG	1H	3084	1/1	0.86	0.27	-	58,58,58,58	0
56	MG	13	1720	1/1	0.88	0.07	-	66,66,66,66	0
56	MG	14	3389	1/1	0.94	0.10	-	82,82,82,82	0
56	MG	14	3107	1/1	0.90	0.31	-	61,61,61,61	0
56	MG	1H	3485	1/1	0.93	0.06	-	97,97,97,97	0
56	MG	1H	3025	1/1	0.97	0.32	-	32,32,32,32	0
56	MG	1H	3336	1/1	0.90	0.10	-	86,86,86,86	0
56	MG	13	1608	1/1	0.95	0.20	-	71,71,71,71	0
56	MG	1G	1658	1/1	0.99	0.18	-	79,79,79,79	0
56	MG	14	3395	1/1	0.85	0.09	-	69,69,69,69	0
56	MG	1H	3414	1/1	0.91	0.07	-	68,68,68,68	0
56	MG	1H	3226	1/1	0.96	0.28	-	78,78,78,78	0
56	MG	1G	1643	1/1	0.92	0.19	-	106,106,106,106	0
56	MG	1H	3532	1/1	0.96	0.09	-	96,96,96,96	0
56	MG	1G	1721	1/1	0.93	0.09	-	84,84,84,84	0
56	MG	1H	3033	1/1	0.96	0.36	-	67,67,67,67	0
56	MG	1H	3487	1/1	0.79	0.08	-	71,71,71,71	0
56	MG	1G	1687	1/1	0.83	0.13	-	75,75,75,75	0
56	MG	1H	3234	1/1	0.75	0.56	-	90,90,90,90	0
56	MG	14	3212	1/1	0.86	1.03	-	82,82,82,82	0
56	MG	14	3300	1/1	0.88	0.09	-	76,76,76,76	0
56	MG	14	3046	1/1	0.93	0.23	-	52,52,52,52	0
56	MG	14	3401	1/1	0.89	0.07	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3195	1/1	0.82	0.36	-	71,71,71,71	0
56	MG	14	3456	1/1	0.84	0.08	-	99,99,99,99	0
56	MG	14	3141	1/1	0.61	0.66	-	86,86,86,86	0
56	MG	1H	3162	1/1	0.91	0.26	-	66,66,66,66	0
56	MG	1G	1616	1/1	0.94	0.28	-	71,71,71,71	0
56	MG	14	3257	1/1	0.94	0.13	-	42,42,42,42	0
56	MG	1H	3391	1/1	0.95	0.13	-	56,56,56,56	0
56	MG	1J	204	1/1	0.94	0.20	-	90,90,90,90	0
56	MG	14	3125	1/1	0.87	0.29	-	76,76,76,76	0
56	MG	14	3063	1/1	0.94	0.23	-	82,82,82,82	0
56	MG	1H	3554	1/1	0.88	0.25	-	100,100,100,100	0
56	MG	2K	102	1/1	0.96	0.05	-	83,83,83,83	0
56	MG	1H	3541	1/1	0.87	0.07	-	85,85,85,85	0
56	MG	14	3398	1/1	0.96	0.14	-	84,84,84,84	0
56	MG	14	3228	1/1	0.92	0.40	-	63,63,63,63	0
56	MG	1H	3168	1/1	0.75	0.54	-	75,75,75,75	0
56	MG	14	3342	1/1	0.88	0.11	-	75,75,75,75	0
56	MG	13	1678	1/1	0.89	0.40	-	83,83,83,83	0
56	MG	1H	3459	1/1	0.90	0.07	-	69,69,69,69	0
56	MG	1H	3150	1/1	0.93	0.30	-	51,51,51,51	0
56	MG	1H	3026	1/1	0.98	0.17	-	71,71,71,71	0
56	MG	14	3318	1/1	0.92	0.17	-	65,65,65,65	0
56	MG	1G	1716	1/1	0.99	0.07	-	88,88,88,88	0
56	MG	39	302	1/1	0.87	0.25	-	73,73,73,73	0
56	MG	1H	3503	1/1	0.81	0.08	-	75,75,75,75	0
56	MG	1H	3094	1/1	0.81	0.31	-	61,61,61,61	0
56	MG	1H	3536	1/1	0.81	0.13	-	98,98,98,98	0
56	MG	14	3007	1/1	0.91	0.18	-	55,55,55,55	0
56	MG	14	3396	1/1	0.81	0.09	-	102,102,102,102	0
56	MG	1H	3005	1/1	0.91	0.40	-	83,83,83,83	0
56	MG	1H	3527	1/1	0.90	0.04	-	86,86,86,86	0
56	MG	14	3161	1/1	0.73	1.20	-	86,86,86,86	0
56	MG	13	1679	1/1	0.51	0.32	-	81,81,81,81	0
56	MG	13	1604	1/1	0.99	0.22	-	66,66,66,66	0
56	MG	1G	1700	1/1	0.92	0.18	-	87,87,87,87	0
56	MG	14	3061	1/1	0.96	0.30	-	47,47,47,47	0
56	MG	14	3118	1/1	0.47	0.31	-	89,89,89,89	0
56	MG	14	3441	1/1	0.89	0.05	-	95,95,95,95	0
56	MG	1H	3241	1/1	0.82	0.58	-	81,81,81,81	0
56	MG	14	3458	1/1	0.84	0.11	-	91,91,91,91	0
56	MG	14	3379	1/1	0.80	0.08	-	94,94,94,94	0
56	MG	14	3174	1/1	0.95	0.30	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3326	1/1	0.92	0.18	-	56,56,56,56	0
56	MG	14	3207	1/1	0.94	0.85	-	63,63,63,63	0
56	MG	1H	3384	1/1	0.96	0.04	-	77,77,77,77	0
56	MG	14	3223	1/1	0.97	0.16	-	78,78,78,78	0
56	MG	13	1731	1/1	0.96	0.09	-	83,83,83,83	0
56	MG	1H	3419	1/1	0.89	0.14	-	78,78,78,78	0
56	MG	11	302	1/1	0.92	0.25	-	55,55,55,55	0
56	MG	1G	1681	1/1	0.89	0.07	-	99,99,99,99	0
56	MG	1H	3157	1/1	0.82	0.19	-	96,96,96,96	0
56	MG	1H	3145	1/1	0.79	0.29	-	82,82,82,82	0
56	MG	1H	3565	1/1	0.89	0.07	-	60,60,60,60	0
56	MG	1H	3410	1/1	0.94	0.16	-	57,57,57,57	0
56	MG	1H	3232	1/1	0.92	0.82	-	77,77,77,77	0
56	MG	13	1726	1/1	0.97	0.08	-	64,64,64,64	0
56	MG	14	3347	1/1	0.94	0.15	-	74,74,74,74	0
56	MG	14	3027	1/1	0.91	0.33	-	86,86,86,86	0
56	MG	1G	1638	1/1	0.93	0.39	-	92,92,92,92	0
56	MG	14	3433	1/1	0.94	0.05	-	143,143,143,143	0
56	MG	41	202	1/1	0.85	0.19	-	75,75,75,75	0
56	MG	14	3446	1/1	0.83	0.10	-	98,98,98,98	0
56	MG	13	1655	1/1	0.56	0.27	-	99,99,99,99	0
56	MG	1G	1722	1/1	0.70	0.07	-	102,102,102,102	0
56	MG	1H	3437	1/1	0.89	0.15	-	62,62,62,62	0
56	MG	14	3346	1/1	0.90	0.11	-	74,74,74,74	0
56	MG	1H	3441	1/1	0.84	0.11	-	76,76,76,76	0
56	MG	14	3029	1/1	0.93	0.29	-	68,68,68,68	0
56	MG	P8	101	1/1	0.67	0.51	-	66,66,66,66	0
56	MG	1G	1674	1/1	0.95	0.05	-	97,97,97,97	0
56	MG	1H	3510	1/1	0.95	0.09	-	92,92,92,92	0
56	MG	1G	1620	1/1	0.90	0.34	-	85,85,85,85	0
56	MG	14	3309	1/1	0.98	0.08	-	76,76,76,76	0
56	MG	14	3087	1/1	0.82	0.35	-	73,73,73,73	0
56	MG	14	3058	1/1	0.97	0.10	-	93,93,93,93	0
56	MG	1H	3185	1/1	0.93	0.30	-	54,54,54,54	0
56	MG	1H	3268	1/1	0.99	0.20	-	78,78,78,78	0
56	MG	14	3010	1/1	0.96	0.35	-	50,50,50,50	0
56	MG	14	3154	1/1	0.88	0.30	-	60,60,60,60	0
56	MG	14	3287	1/1	0.95	0.05	-	71,71,71,71	0
56	MG	14	3450	1/1	0.90	0.05	-	100,100,100,100	0
56	MG	14	3084	1/1	0.86	0.39	-	77,77,77,77	0
56	MG	13	1620	1/1	0.91	0.33	-	74,74,74,74	0
56	MG	14	3361	1/1	0.97	0.12	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3204	1/1	0.95	0.31	-	74,74,74,74	0
56	MG	14	3210	1/1	0.95	0.35	-	74,74,74,74	0
56	MG	1H	3473	1/1	0.62	0.15	-	88,88,88,88	0
56	MG	1H	3182	1/1	0.87	0.21	-	56,56,56,56	0
56	MG	1H	3073	1/1	0.93	0.23	-	39,39,39,39	0
56	MG	14	3172	1/1	0.92	0.30	-	82,82,82,82	0
56	MG	14	3103	1/1	0.91	0.41	-	81,81,81,81	0
56	MG	14	3206	1/1	0.96	0.57	-	72,72,72,72	0
56	MG	13	1667	1/1	0.78	0.15	-	105,105,105,105	0
56	MG	1H	3297	1/1	0.96	0.06	-	52,52,52,52	0
56	MG	14	3317	1/1	0.93	0.13	-	119,119,119,119	0
56	MG	1G	1631	1/1	0.70	0.12	-	99,99,99,99	0
56	MG	13	1749	1/1	0.92	0.09	-	106,106,106,106	0
56	MG	L8	101	1/1	0.62	0.39	-	80,80,80,80	0
56	MG	1H	3347	1/1	0.96	0.12	-	72,72,72,72	0
56	MG	1H	3506	1/1	0.98	0.11	-	58,58,58,58	0
56	MG	1H	3102	1/1	0.84	0.33	-	63,63,63,63	0
56	MG	14	3241	1/1	0.84	0.53	-	77,77,77,77	0
56	MG	1H	3549	1/1	0.53	0.15	-	75,75,75,75	0
56	MG	14	3144	1/1	0.94	0.40	-	60,60,60,60	0
56	MG	1H	3478	1/1	0.94	0.04	-	78,78,78,78	0
56	MG	14	3194	1/1	0.80	0.47	-	79,79,79,79	0
56	MG	1H	3566	1/1	0.79	0.05	-	105,105,105,105	0
56	MG	14	3416	1/1	0.97	0.05	-	80,80,80,80	0
56	MG	14	3265	1/1	0.98	0.24	-	51,51,51,51	0
56	MG	14	3393	1/1	0.66	0.07	-	98,98,98,98	0
56	MG	1H	3450	1/1	0.98	0.06	-	45,45,45,45	0
56	MG	14	3094	1/1	0.97	0.28	-	73,73,73,73	0
56	MG	14	3225	1/1	0.92	0.84	-	84,84,84,84	0
56	MG	1H	3057	1/1	0.94	0.32	-	63,63,63,63	0
56	MG	1H	3148	1/1	0.93	0.19	-	56,56,56,56	0
56	MG	14	3360	1/1	0.83	0.10	-	88,88,88,88	0
56	MG	14	3155	1/1	0.94	0.27	-	73,73,73,73	0
56	MG	1J	210	1/1	0.78	0.12	-	91,91,91,91	0
56	MG	13	1732	1/1	0.82	0.06	-	113,113,113,113	0
56	MG	1H	3064	1/1	0.90	0.61	-	76,76,76,76	0
56	MG	1H	3254	1/1	0.71	0.33	-	69,69,69,69	0
58	ZN	G8	201	1/1	0.93	0.18	-	143,143,143,143	0
56	MG	1G	1689	1/1	0.96	0.06	-	79,79,79,79	0
56	MG	1H	3259	1/1	0.95	0.19	-	58,58,58,58	0
56	MG	1H	3561	1/1	0.93	0.05	-	87,87,87,87	0
56	MG	14	3202	1/1	0.97	0.27	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	88	203	1/1	0.90	0.31	-	87,87,87,87	0
56	MG	1H	3358	1/1	0.97	0.03	-	78,78,78,78	0
56	MG	14	3253	1/1	0.91	0.14	-	57,57,57,57	0
56	MG	13	1676	1/1	0.90	0.10	-	92,92,92,92	0
56	MG	14	3069	1/1	0.98	0.16	-	47,47,47,47	0
56	MG	1H	3456	1/1	0.79	0.21	-	102,102,102,102	0
56	MG	1H	3375	1/1	0.76	0.16	-	85,85,85,85	0
56	MG	1H	3520	1/1	0.94	0.22	-	98,98,98,98	0
56	MG	1H	3178	1/1	0.93	0.47	-	69,69,69,69	0
56	MG	1G	1657	1/1	0.84	0.51	-	77,77,77,77	0
56	MG	1G	1655	1/1	0.75	0.27	-	106,106,106,106	0
56	MG	1H	3151	1/1	0.85	0.20	-	52,52,52,52	0
56	MG	14	3052	1/1	0.89	1.03	-	71,71,71,71	0
56	MG	1G	1601	1/1	0.98	0.14	-	78,78,78,78	0
56	MG	E5	101	1/1	0.93	0.46	-	74,74,74,74	0
56	MG	14	3400	1/1	0.70	0.11	-	90,90,90,90	0
56	MG	1H	3399	1/1	0.98	0.08	-	52,52,52,52	0
56	MG	1H	3428	1/1	0.82	0.09	-	64,64,64,64	0
56	MG	1H	3049	1/1	0.92	0.15	-	50,50,50,50	0
56	MG	1H	3253	1/1	0.80	0.38	-	62,62,62,62	0
56	MG	1H	3207	1/1	0.94	0.29	-	119,119,119,119	0
56	MG	1G	1703	1/1	0.89	0.10	-	85,85,85,85	0
56	MG	1H	3515	1/1	0.97	0.12	-	57,57,57,57	0
56	MG	1H	3264	1/1	0.91	0.57	-	80,80,80,80	0
56	MG	14	3270	1/1	0.73	0.13	-	80,80,80,80	0
56	MG	1H	3212	1/1	0.90	0.07	-	90,90,90,90	0
56	MG	14	3432	1/1	0.70	0.20	-	92,92,92,92	0
56	MG	35	202	1/1	0.79	0.30	-	78,78,78,78	0
56	MG	13	1710	1/1	0.94	0.07	-	85,85,85,85	0
56	MG	14	3428	1/1	0.95	0.10	-	59,59,59,59	0
56	MG	13	1756	1/1	0.55	0.07	-	120,120,120,120	0
56	MG	13	1643	1/1	0.77	0.57	-	69,69,69,69	0
56	MG	14	3371	1/1	0.99	0.15	-	75,75,75,75	0
56	MG	1H	3114	1/1	0.96	0.26	-	66,66,66,66	0
56	MG	1H	3060	1/1	0.95	0.21	-	54,54,54,54	0
56	MG	1G	1641	1/1	0.70	0.72	-	91,91,91,91	0
56	MG	14	3004	1/1	0.91	0.45	-	58,58,58,58	0
56	MG	78	202	1/1	0.96	0.10	-	63,63,63,63	0
56	MG	1G	1698	1/1	0.68	0.06	-	102,102,102,102	0
56	MG	1G	1612	1/1	0.93	0.30	-	76,76,76,76	0
56	MG	1G	1707	1/1	0.90	0.06	-	114,114,114,114	0
56	MG	14	3044	1/1	0.84	0.54	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3553	1/1	0.93	0.05	-	78,78,78,78	0
56	MG	14	3113	1/1	0.91	0.22	-	67,67,67,67	0
56	MG	14	3216	1/1	0.74	0.42	-	79,79,79,79	0
56	MG	13	1680	1/1	0.95	0.19	-	73,73,73,73	0
56	MG	1H	3517	1/1	0.94	0.07	-	84,84,84,84	0
56	MG	14	3438	1/1	0.87	0.04	-	115,115,115,115	0
56	MG	14	3055	1/1	0.98	0.38	-	50,50,50,50	0
56	MG	1H	3009	1/1	0.86	0.23	-	74,74,74,74	0
56	MG	13	1723	1/1	0.96	0.20	-	75,75,75,75	0
56	MG	1H	3228	1/1	0.94	0.40	-	79,79,79,79	0
56	MG	13	1662	1/1	0.94	0.16	-	114,114,114,114	0
56	MG	1H	3484	1/1	0.95	0.11	-	88,88,88,88	0
56	MG	1G	1659	1/1	0.94	0.23	-	85,85,85,85	0
56	MG	14	3014	1/1	0.99	0.15	-	64,64,64,64	0
56	MG	14	3057	1/1	0.97	0.40	-	61,61,61,61	0
56	MG	1H	3411	1/1	0.66	0.12	-	65,65,65,65	0
56	MG	14	3197	1/1	0.90	0.45	-	44,44,44,44	0
56	MG	1G	1654	1/1	0.85	0.37	-	99,99,99,99	0
56	MG	1H	3054	1/1	0.84	0.83	-	70,70,70,70	0
56	MG	14	3311	1/1	0.82	0.19	-	73,73,73,73	0
56	MG	14	3148	1/1	0.80	0.34	-	78,78,78,78	0
56	MG	1G	1624	1/1	0.92	0.19	-	87,87,87,87	0
56	MG	1H	3562	1/1	0.67	0.12	-	69,69,69,69	0
56	MG	14	3037	1/1	0.95	0.30	-	61,61,61,61	0
56	MG	14	3123	1/1	0.95	0.20	-	60,60,60,60	0
56	MG	1H	3408	1/1	0.97	0.12	-	42,42,42,42	0
56	MG	14	3025	1/1	0.90	0.32	-	59,59,59,59	0
56	MG	14	3464	1/1	0.67	0.13	-	105,105,105,105	0
56	MG	2L	102	1/1	0.91	0.05	-	88,88,88,88	0
56	MG	14	3305	1/1	0.78	0.16	-	96,96,96,96	0
56	MG	14	3424	1/1	0.96	0.08	-	81,81,81,81	0
56	MG	1H	3242	1/1	0.99	0.33	-	70,70,70,70	0
56	MG	14	3145	1/1	0.88	0.18	-	75,75,75,75	0
56	MG	14	3291	1/1	0.86	0.17	-	82,82,82,82	0
56	MG	13	1721	1/1	0.98	0.07	-	82,82,82,82	0
56	MG	1H	3322	1/1	0.98	0.07	-	67,67,67,67	0
56	MG	14	3008	1/1	0.85	0.41	-	84,84,84,84	0
56	MG	14	3192	1/1	0.53	0.36	-	81,81,81,81	0
56	MG	1H	3483	1/1	0.85	0.10	-	76,76,76,76	0
56	MG	14	3409	1/1	0.98	0.08	-	73,73,73,73	0
56	MG	1H	3394	1/1	0.99	0.14	-	40,40,40,40	0
56	MG	1H	3461	1/1	0.88	0.10	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3177	1/1	0.90	0.46	-	75,75,75,75	0
56	MG	1H	3176	1/1	0.84	0.65	-	51,51,51,51	0
56	MG	1H	3193	1/1	0.89	0.16	-	78,78,78,78	0
56	MG	14	3331	1/1	0.92	0.20	-	65,65,65,65	0
56	MG	14	3252	1/1	0.90	0.17	-	52,52,52,52	0
56	MG	1H	3091	1/1	0.87	0.16	-	65,65,65,65	0
56	MG	1H	3042	1/1	0.97	0.18	-	43,43,43,43	0
56	MG	14	3164	1/1	0.85	0.72	-	64,64,64,64	0
56	MG	1G	1714	1/1	0.90	0.07	-	101,101,101,101	0
56	MG	1H	3142	1/1	0.66	0.16	-	74,74,74,74	0
56	MG	1G	1664	1/1	0.91	0.07	-	126,126,126,126	0
56	MG	14	3187	1/1	0.89	0.81	-	81,81,81,81	0
56	MG	45	202	1/1	0.99	0.14	-	66,66,66,66	0
56	MG	1H	3237	1/1	0.98	0.20	-	41,41,41,41	0
56	MG	1H	3116	1/1	0.96	0.06	-	64,64,64,64	0
56	MG	1H	3345	1/1	0.19	0.12	-	91,91,91,91	0
56	MG	14	3338	1/1	0.95	0.09	-	83,83,83,83	0
56	MG	14	3375	1/1	0.87	0.08	-	87,87,87,87	0
56	MG	1H	3187	1/1	0.97	0.54	-	77,77,77,77	0
56	MG	1J	203	1/1	0.93	0.21	-	70,70,70,70	0
56	MG	1G	1667	1/1	0.76	0.24	-	97,97,97,97	0
56	MG	14	3108	1/1	0.97	0.09	-	67,67,67,67	0
56	MG	14	3461	1/1	0.83	0.10	-	80,80,80,80	0
56	MG	13	1709	1/1	0.94	0.06	-	68,68,68,68	0
56	MG	13	1694	1/1	0.93	0.17	-	79,79,79,79	0
56	MG	14	3341	1/1	0.82	0.12	-	76,76,76,76	0
56	MG	14	3378	1/1	0.80	0.05	-	96,96,96,96	0
56	MG	14	3308	1/1	0.94	0.26	-	90,90,90,90	0
56	MG	1H	3188	1/1	0.73	0.23	-	69,69,69,69	0
56	MG	88	202	1/1	0.87	0.29	-	67,67,67,67	0
56	MG	1H	3128	1/1	0.93	0.44	-	76,76,76,76	0
56	MG	1H	3539	1/1	0.82	0.05	-	90,90,90,90	0
56	MG	13	1724	1/1	0.87	0.10	-	94,94,94,94	0
56	MG	14	3049	1/1	0.96	0.47	-	79,79,79,79	0
56	MG	14	3408	1/1	0.94	0.06	-	94,94,94,94	0
56	MG	1H	3444	1/1	0.82	0.27	-	82,82,82,82	0
56	MG	1H	3279	1/1	0.74	0.28	-	67,67,67,67	0
56	MG	1H	3070	1/1	0.95	0.30	-	54,54,54,54	0
56	MG	14	3444	1/1	0.94	0.11	-	90,90,90,90	0
56	MG	1H	3530	1/1	0.91	0.34	-	81,81,81,81	0
56	MG	14	3468	1/1	0.92	0.39	-	58,58,58,58	0
56	MG	13	1663	1/1	0.75	0.22	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3171	1/1	0.70	0.22	-	84,84,84,84	0
56	MG	14	3420	1/1	0.94	0.07	-	66,66,66,66	0
56	MG	13	1747	1/1	0.64	0.10	-	107,107,107,107	0
56	MG	1H	3381	1/1	0.97	0.04	-	74,74,74,74	0
56	MG	1H	3357	1/1	0.96	0.12	-	66,66,66,66	0
56	MG	14	3437	1/1	0.79	0.06	-	115,115,115,115	0
56	MG	1H	3312	1/1	0.93	0.10	-	49,49,49,49	0
56	MG	1H	3263	1/1	0.89	0.63	-	91,91,91,91	0
56	MG	1H	3406	1/1	0.95	0.06	-	52,52,52,52	0
56	MG	1H	3447	1/1	0.96	0.15	-	59,59,59,59	0
56	MG	13	1653	1/1	0.78	0.21	-	80,80,80,80	0
56	MG	13	1729	1/1	0.95	0.15	-	88,88,88,88	0
56	MG	1H	3350	1/1	0.96	0.16	-	43,43,43,43	0
56	MG	14	3109	1/1	0.78	0.25	-	86,86,86,86	0
56	MG	1G	1656	1/1	0.52	0.83	-	89,89,89,89	0
56	MG	14	3402	1/1	0.93	0.06	-	94,94,94,94	0
56	MG	13	1677	1/1	0.80	0.30	-	77,77,77,77	0
56	MG	1H	3348	1/1	0.85	0.15	-	78,78,78,78	0
56	MG	1H	3529	1/1	0.91	0.07	-	102,102,102,102	0
56	MG	1G	1699	1/1	0.98	0.04	-	86,86,86,86	0
56	MG	1H	3416	1/1	0.98	0.12	-	70,70,70,70	0
56	MG	1H	3052	1/1	0.93	0.26	-	59,59,59,59	0
56	MG	16	213	1/1	0.84	0.07	-	87,87,87,87	0
56	MG	14	3313	1/1	0.83	0.12	-	53,53,53,53	0
56	MG	1H	3413	1/1	0.94	0.11	-	59,59,59,59	0
56	MG	14	3259	1/1	0.97	0.09	-	57,57,57,57	0
56	MG	1H	3534	1/1	0.89	0.07	-	85,85,85,85	0
56	MG	14	3036	1/1	0.98	0.40	-	39,39,39,39	0
56	MG	14	3411	1/1	0.80	0.11	-	101,101,101,101	0
56	MG	1H	3466	1/1	0.94	0.05	-	74,74,74,74	0
56	MG	1H	3568	1/1	0.75	0.17	-	94,94,94,94	0
56	MG	14	3403	1/1	0.97	0.10	-	80,80,80,80	0
56	MG	14	3078	1/1	0.87	0.24	-	80,80,80,80	0
56	MG	1H	3480	1/1	0.95	0.05	-	66,66,66,66	0
56	MG	1H	3201	1/1	0.76	0.61	-	82,82,82,82	0
56	MG	1H	3198	1/1	0.79	0.24	-	65,65,65,65	0
56	MG	13	1707	1/1	0.93	0.10	-	63,63,63,63	0
56	MG	1H	3344	1/1	0.96	0.16	-	42,42,42,42	0
56	MG	1G	1645	1/1	0.63	0.13	-	113,113,113,113	0
56	MG	1H	3090	1/1	0.81	0.28	-	50,50,50,50	0
56	MG	1H	3293	1/1	0.95	0.15	-	41,41,41,41	0
56	MG	14	3356	1/1	0.89	0.11	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3430	1/1	0.91	0.21	-	46,46,46,46	0
56	MG	14	3117	1/1	0.94	0.36	-	79,79,79,79	0
56	MG	13	1603	1/1	0.97	0.21	-	72,72,72,72	0
56	MG	1H	3283	1/1	0.92	0.16	-	58,58,58,58	0
56	MG	1H	3275	1/1	0.90	0.28	-	68,68,68,68	0
56	MG	1H	3492	1/1	0.95	0.05	-	74,74,74,74	0
56	MG	1H	3106	1/1	0.86	0.25	-	55,55,55,55	0
56	MG	1G	1694	1/1	0.77	0.12	-	103,103,103,103	0
56	MG	1H	3438	1/1	0.90	0.10	-	71,71,71,71	0
56	MG	1H	3210	1/1	0.62	0.34	-	75,75,75,75	0
56	MG	1H	3126	1/1	0.97	0.21	-	64,64,64,64	0
56	MG	14	3127	1/1	0.95	0.17	-	85,85,85,85	0
56	MG	13	1686	1/1	0.80	0.08	-	98,98,98,98	0
56	MG	1G	1639	1/1	0.93	0.35	-	87,87,87,87	0
56	MG	1H	3171	1/1	0.89	0.58	-	67,67,67,67	0
56	MG	1H	3236	1/1	0.83	0.25	-	78,78,78,78	0
56	MG	14	3344	1/1	0.98	0.09	-	56,56,56,56	0
56	MG	14	3121	1/1	0.99	0.37	-	45,45,45,45	0
56	MG	14	3410	1/1	0.84	0.07	-	83,83,83,83	0
56	MG	13	1642	1/1	0.86	0.29	-	78,78,78,78	0
56	MG	1H	3076	1/1	0.69	0.81	-	60,60,60,60	0
56	MG	1H	3163	1/1	0.90	0.64	-	83,83,83,83	0
56	MG	1G	1637	1/1	0.72	0.40	-	89,89,89,89	0
56	MG	1H	3412	1/1	0.93	0.08	-	39,39,39,39	0
56	MG	13	1740	1/1	0.94	0.11	-	96,96,96,96	0
56	MG	1J	201	1/1	0.93	0.13	-	70,70,70,70	0
56	MG	1G	1653	1/1	0.94	0.25	-	82,82,82,82	0
56	MG	14	3407	1/1	0.94	0.13	-	79,79,79,79	0
56	MG	1H	3382	1/1	0.91	0.06	-	70,70,70,70	0
56	MG	1G	1702	1/1	0.93	0.22	-	100,100,100,100	0
56	MG	14	3292	1/1	0.97	0.06	-	63,63,63,63	0
56	MG	1H	3359	1/1	0.98	0.09	-	59,59,59,59	0
56	MG	14	3244	1/1	0.73	0.31	-	71,71,71,71	0
56	MG	1H	3455	1/1	0.73	0.19	-	76,76,76,76	0
56	MG	13	1733	1/1	0.90	0.19	-	102,102,102,102	0
56	MG	1H	3039	1/1	0.97	0.42	-	74,74,74,74	0
56	MG	1H	3266	1/1	0.97	0.21	-	61,61,61,61	0
56	MG	1H	3479	1/1	0.53	0.16	-	99,99,99,99	0
56	MG	14	3146	1/1	0.86	0.36	-	72,72,72,72	0
56	MG	1H	3217	1/1	0.77	0.15	-	61,61,61,61	0
56	MG	1H	3079	1/1	0.86	0.17	-	88,88,88,88	0
56	MG	1G	1626	1/1	0.81	0.23	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3203	1/1	0.84	0.27	-	68,68,68,68	0
56	MG	1G	1675	1/1	0.93	0.15	-	101,101,101,101	0
56	MG	13	1704	1/1	0.95	0.17	-	73,73,73,73	0
56	MG	1H	3301	1/1	0.96	0.17	-	42,42,42,42	0
56	MG	1H	3535	1/1	0.94	0.07	-	70,70,70,70	0
56	MG	1H	3014	1/1	0.94	0.21	-	75,75,75,75	0
56	MG	1G	1615	1/1	0.94	0.20	-	93,93,93,93	0
56	MG	1G	1686	1/1	0.93	0.06	-	90,90,90,90	0
56	MG	1H	3186	1/1	0.92	0.28	-	76,76,76,76	0
56	MG	1H	3360	1/1	0.92	0.13	-	59,59,59,59	0
56	MG	1H	3134	1/1	0.89	0.28	-	74,74,74,74	0
56	MG	14	3190	1/1	0.63	0.27	-	81,81,81,81	0
56	MG	13	1719	1/1	0.77	0.12	-	89,89,89,89	0
56	MG	1H	3509	1/1	0.85	0.20	-	46,46,46,46	0
56	MG	1H	3023	1/1	0.96	0.47	-	56,56,56,56	0
56	MG	1H	3256	1/1	0.86	0.21	-	100,100,100,100	0
56	MG	14	3366	1/1	0.92	0.08	-	65,65,65,65	0
56	MG	1H	3296	1/1	0.97	0.18	-	43,43,43,43	0
56	MG	1H	3392	1/1	0.94	0.08	-	63,63,63,63	0
56	MG	1H	3418	1/1	0.76	0.15	-	68,68,68,68	0
56	MG	1H	3250	1/1	0.92	0.16	-	64,64,64,64	0
56	MG	14	3290	1/1	0.87	0.13	-	67,67,67,67	0
56	MG	13	1705	1/1	0.95	0.10	-	102,102,102,102	0
56	MG	1H	3569	1/1	0.82	0.07	-	85,85,85,85	0
56	MG	14	3240	1/1	0.86	0.33	-	83,83,83,83	0
56	MG	1G	1605	1/1	0.95	0.29	-	76,76,76,76	0
56	MG	14	3386	1/1	0.97	0.09	-	81,81,81,81	0
56	MG	13	1744	1/1	0.52	0.10	-	111,111,111,111	0
56	MG	29	301	1/1	0.96	0.29	-	49,49,49,49	0
56	MG	1G	1710	1/1	0.89	0.05	-	95,95,95,95	0
56	MG	14	3076	1/1	0.87	0.81	-	68,68,68,68	0
56	MG	14	3334	1/1	0.98	0.13	-	69,69,69,69	0
56	MG	13	1658	1/1	0.83	0.07	-	116,116,116,116	0
56	MG	14	3426	1/1	0.97	0.05	-	75,75,75,75	0
56	MG	1H	3524	1/1	0.58	0.12	-	96,96,96,96	0
56	MG	1H	3144	1/1	0.82	0.37	-	86,86,86,86	0
56	MG	14	3043	1/1	0.98	0.27	-	68,68,68,68	0
56	MG	21	302	1/1	0.70	0.42	-	75,75,75,75	0
56	MG	14	3221	1/1	0.78	0.34	-	86,86,86,86	0
56	MG	14	3263	1/1	0.81	0.18	-	64,64,64,64	0
56	MG	13	1668	1/1	0.87	0.43	-	105,105,105,105	0
56	MG	1H	3389	1/1	0.97	0.07	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3222	1/1	0.75	0.35	-	88,88,88,88	0
56	MG	14	3157	1/1	0.61	0.18	-	76,76,76,76	0
56	MG	1H	3083	1/1	0.93	0.15	-	81,81,81,81	0
56	MG	1H	3277	1/1	0.95	0.50	-	81,81,81,81	0
56	MG	1J	206	1/1	0.61	0.14	-	86,86,86,86	0
56	MG	1G	1718	1/1	0.94	0.06	-	89,89,89,89	0
56	MG	1G	1693	1/1	0.85	0.05	-	114,114,114,114	0
56	MG	1H	3495	1/1	0.81	0.15	-	100,100,100,100	0
56	MG	1H	3035	1/1	0.94	0.27	-	64,64,64,64	0
56	MG	1H	3135	1/1	0.95	0.22	-	54,54,54,54	0
56	MG	1G	1713	1/1	0.69	0.12	-	112,112,112,112	0
56	MG	13	1712	1/1	0.82	0.17	-	96,96,96,96	0
56	MG	13	1713	1/1	0.95	0.22	-	82,82,82,82	0
56	MG	13	1673	1/1	0.78	0.17	-	93,93,93,93	0
56	MG	1G	1622	1/1	0.86	0.46	-	73,73,73,73	0
56	MG	1G	1648	1/1	0.98	0.09	-	94,94,94,94	0
56	MG	1H	3224	1/1	0.89	0.21	-	74,74,74,74	0
56	MG	14	3352	1/1	0.93	0.12	-	66,66,66,66	0
56	MG	1H	3136	1/1	0.79	1.10	-	76,76,76,76	0
56	MG	14	3196	1/1	0.94	0.06	-	77,77,77,77	0
56	MG	1H	3380	1/1	0.97	0.14	-	69,69,69,69	0
56	MG	1H	3397	1/1	0.95	0.20	-	46,46,46,46	0
56	MG	14	3075	1/1	0.88	0.16	-	78,78,78,78	0
56	MG	1H	3558	1/1	0.91	0.06	-	99,99,99,99	0
56	MG	1H	3364	1/1	0.93	0.11	-	51,51,51,51	0
56	MG	1H	3221	1/1	0.83	0.18	-	65,65,65,65	0
56	MG	1G	1603	1/1	0.98	0.19	-	85,85,85,85	0
56	MG	14	3435	1/1	0.90	0.36	-	93,93,93,93	0
56	MG	1H	3041	1/1	0.94	0.22	-	86,86,86,86	0
56	MG	14	3042	1/1	0.97	0.58	-	85,85,85,85	0
56	MG	1H	3305	1/1	0.95	0.14	-	48,48,48,48	0
56	MG	1H	3474	1/1	0.94	0.05	-	79,79,79,79	0
56	MG	1H	3547	1/1	0.67	0.11	-	91,91,91,91	0
56	MG	1H	3415	1/1	0.94	0.16	-	73,73,73,73	0
56	MG	13	1666	1/1	0.87	0.49	-	79,79,79,79	0
56	MG	16	209	1/1	0.95	0.08	-	67,67,67,67	0
56	MG	1H	3269	1/1	0.91	0.27	-	61,61,61,61	0
56	MG	1H	3008	1/1	0.91	0.36	-	61,61,61,61	0
56	MG	1H	3100	1/1	0.81	0.60	-	59,59,59,59	0
56	MG	13	1670	1/1	0.92	0.23	-	80,80,80,80	0
56	MG	1G	1617	1/1	0.60	0.87	-	86,86,86,86	0
56	MG	13	1674	1/1	0.87	0.67	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3201	1/1	0.88	0.11	-	84,84,84,84	0
56	MG	14	3199	1/1	0.68	0.31	-	89,89,89,89	0
56	MG	1H	3160	1/1	0.90	0.40	-	70,70,70,70	0
56	MG	13	1700	1/1	0.97	0.05	-	64,64,64,64	0
56	MG	14	3429	1/1	0.95	0.17	-	68,68,68,68	0
56	MG	1H	3169	1/1	0.63	0.22	-	111,111,111,111	0
56	MG	13	1616	1/1	0.75	0.49	-	77,77,77,77	0
56	MG	1H	3427	1/1	0.97	0.20	-	60,60,60,60	0
56	MG	14	3012	1/1	0.96	0.37	-	56,56,56,56	0
56	MG	1H	3477	1/1	0.94	0.05	-	91,91,91,91	0
56	MG	14	3015	1/1	0.98	0.19	-	80,80,80,80	0
56	MG	1H	3457	1/1	0.96	0.05	-	78,78,78,78	0
56	MG	98	201	1/1	0.86	0.49	-	67,67,67,67	0
56	MG	1H	3309	1/1	0.99	0.13	-	47,47,47,47	0
56	MG	14	3325	1/1	0.98	0.06	-	66,66,66,66	0
56	MG	14	3116	1/1	0.85	0.38	-	89,89,89,89	0
56	MG	14	3298	1/1	0.63	0.21	-	105,105,105,105	0
56	MG	1H	3400	1/1	0.91	0.11	-	48,48,48,48	0
56	MG	1H	3239	1/1	0.66	0.39	-	69,69,69,69	0
56	MG	I8	101	1/1	0.97	0.04	-	55,55,55,55	0
56	MG	14	3459	1/1	0.81	0.07	-	97,97,97,97	0
56	MG	14	3404	1/1	0.92	0.10	-	77,77,77,77	0
56	MG	13	1684	1/1	0.70	0.36	-	71,71,71,71	0
56	MG	1G	1691	1/1	0.86	0.11	-	110,110,110,110	0
56	MG	14	3445	1/1	0.96	0.09	-	89,89,89,89	0
56	MG	14	3074	1/1	0.92	0.45	-	76,76,76,76	0
56	MG	13	1697	1/1	0.94	0.03	-	91,91,91,91	0
56	MG	1H	3504	1/1	0.88	0.09	-	86,86,86,86	0
56	MG	14	3339	1/1	0.97	0.04	-	73,73,73,73	0
56	MG	E5	103	1/1	0.83	0.20	-	80,80,80,80	0
56	MG	25	201	1/1	0.91	0.25	-	93,93,93,93	0
56	MG	1H	3155	1/1	0.92	0.30	-	80,80,80,80	0
56	MG	14	3374	1/1	0.91	0.08	-	68,68,68,68	0
56	MG	1H	3315	1/1	0.94	0.07	-	85,85,85,85	0
56	MG	1H	3501	1/1	0.69	0.10	-	76,76,76,76	0
56	MG	1H	3426	1/1	0.88	0.17	-	77,77,77,77	0
56	MG	1G	1704	1/1	0.98	0.06	-	99,99,99,99	0
56	MG	14	3314	1/1	0.95	0.16	-	46,46,46,46	0
56	MG	13	1615	1/1	0.94	0.17	-	94,94,94,94	0
56	MG	1H	3307	1/1	0.96	0.08	-	50,50,50,50	0
56	MG	1H	3222	1/1	0.94	0.29	-	72,72,72,72	0
56	MG	1H	3390	1/1	0.91	0.10	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3269	1/1	0.95	0.10	-	60,60,60,60	0
56	MG	1H	3183	1/1	0.80	0.32	-	74,74,74,74	0
56	MG	1H	3422	1/1	0.96	0.08	-	42,42,42,42	0
56	MG	1H	3550	1/1	0.84	0.12	-	125,125,125,125	0
56	MG	1H	3158	1/1	0.79	0.37	-	72,72,72,72	0
56	MG	14	3009	1/1	0.97	0.23	-	41,41,41,41	0
56	MG	14	3447	1/1	0.46	0.18	-	116,116,116,116	0
56	MG	1H	3196	1/1	0.84	0.43	-	62,62,62,62	0
56	MG	13	1752	1/1	0.59	0.14	-	108,108,108,108	0
56	MG	13	1628	1/1	0.74	0.22	-	89,89,89,89	0
56	MG	13	1742	1/1	0.83	0.09	-	105,105,105,105	0
56	MG	1H	3497	1/1	0.84	0.10	-	75,75,75,75	0
56	MG	13	1760	1/1	0.51	0.05	-	113,113,113,113	0
56	MG	1H	3545	1/1	0.93	0.07	-	88,88,88,88	0
56	MG	1H	3543	1/1	0.87	0.10	-	81,81,81,81	0
56	MG	1H	3175	1/1	0.97	0.15	-	55,55,55,55	0
56	MG	14	3301	1/1	0.61	0.08	-	111,111,111,111	0
56	MG	14	3011	1/1	0.97	0.38	-	50,50,50,50	0
56	MG	1H	3401	1/1	0.92	0.17	-	46,46,46,46	0
56	MG	14	3242	1/1	0.83	0.16	-	83,83,83,83	0
56	MG	14	3448	1/1	0.96	0.23	-	72,72,72,72	0
56	MG	1H	3270	1/1	0.68	0.46	-	78,78,78,78	0
56	MG	1G	1651	1/1	0.91	0.16	-	84,84,84,84	0
56	MG	1H	3121	1/1	0.98	0.60	-	64,64,64,64	0
56	MG	14	3322	1/1	0.91	0.18	-	77,77,77,77	0
56	MG	1H	3402	1/1	0.98	0.15	-	40,40,40,40	0
56	MG	1H	3199	1/1	0.87	0.23	-	74,74,74,74	0
56	MG	14	3134	1/1	0.79	0.14	-	88,88,88,88	0
56	MG	1H	3564	1/1	0.94	0.05	-	95,95,95,95	0
56	MG	14	3088	1/1	0.93	0.23	-	105,105,105,105	0
56	MG	1H	3417	1/1	0.96	0.14	-	71,71,71,71	0
56	MG	14	3377	1/1	0.95	0.07	-	77,77,77,77	0
56	MG	1H	3511	1/1	0.86	0.08	-	78,78,78,78	0
56	MG	1G	1627	1/1	0.89	0.05	-	139,139,139,139	0
56	MG	14	3422	1/1	0.95	0.10	-	70,70,70,70	0
56	MG	1H	3468	1/1	0.72	0.11	-	68,68,68,68	0
56	MG	1H	3570	1/1	0.95	0.21	-	48,48,48,48	0
56	MG	13	1750	1/1	0.93	0.21	-	101,101,101,101	0
56	MG	14	3348	1/1	0.96	0.15	-	51,51,51,51	0
56	MG	13	1681	1/1	0.89	0.20	-	83,83,83,83	0
56	MG	1H	3137	1/1	0.70	0.35	-	70,70,70,70	0
56	MG	14	3239	1/1	0.87	0.97	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3181	1/1	0.73	0.42	-	76,76,76,76	0
56	MG	13	1649	1/1	0.93	0.17	-	87,87,87,87	0
56	MG	13	1657	1/1	0.87	0.46	-	89,89,89,89	0
56	MG	1H	3170	1/1	0.93	0.19	-	115,115,115,115	0
56	MG	1H	3303	1/1	0.97	0.14	-	57,57,57,57	0
56	MG	14	3150	1/1	0.81	0.44	-	84,84,84,84	0
56	MG	1H	3097	1/1	0.98	0.55	-	53,53,53,53	0
56	MG	1H	3191	1/1	0.76	0.24	-	59,59,59,59	0
56	MG	13	1639	1/1	0.93	0.29	-	91,91,91,91	0
56	MG	1H	3488	1/1	0.78	0.09	-	85,85,85,85	0
56	MG	14	3236	1/1	0.92	0.10	-	94,94,94,94	0
56	MG	1G	1632	1/1	0.80	0.41	-	92,92,92,92	0
56	MG	1H	3443	1/1	0.91	0.06	-	72,72,72,72	0
56	MG	14	3351	1/1	0.98	0.12	-	54,54,54,54	0
56	MG	14	3079	1/1	0.89	0.32	-	75,75,75,75	0
56	MG	1H	3034	1/1	0.93	0.34	-	63,63,63,63	0
56	MG	1G	1701	1/1	0.90	0.10	-	106,106,106,106	0
56	MG	14	3217	1/1	0.83	0.65	-	94,94,94,94	0
56	MG	14	3017	1/1	0.97	0.34	-	54,54,54,54	0
56	MG	1H	3124	1/1	0.92	0.28	-	70,70,70,70	0
56	MG	1H	3081	1/1	0.79	0.44	-	76,76,76,76	0
56	MG	2K	101	1/1	0.64	0.22	-	91,91,91,91	0
56	MG	14	3136	1/1	0.89	0.35	-	83,83,83,83	0
56	MG	1H	3463	1/1	0.93	0.09	-	78,78,78,78	0
56	MG	1H	3047	1/1	0.80	0.44	-	76,76,76,76	0
56	MG	1H	3086	1/1	0.94	0.53	-	65,65,65,65	0
56	MG	13	1759	1/1	0.56	0.06	-	118,118,118,118	0
56	MG	1H	3220	1/1	0.71	0.51	-	71,71,71,71	0
56	MG	1H	3396	1/1	0.97	0.11	-	41,41,41,41	0
56	MG	1H	3486	1/1	0.94	0.14	-	95,95,95,95	0
56	MG	1G	1644	1/1	0.75	0.15	-	92,92,92,92	0
56	MG	13	1646	1/1	0.95	0.17	-	89,89,89,89	0
56	MG	14	3385	1/1	0.90	0.15	-	80,80,80,80	0
56	MG	1H	3072	1/1	0.97	0.21	-	33,33,33,33	0
56	MG	1H	3331	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	1H	3059	1/1	0.88	0.71	-	73,73,73,73	0
56	MG	2L	103	1/1	0.88	0.51	-	70,70,70,70	0
56	MG	1H	3010	1/1	0.91	0.21	-	53,53,53,53	0
56	MG	1G	1640	1/1	0.97	0.36	-	95,95,95,95	0
56	MG	14	3390	1/1	0.94	0.16	-	72,72,72,72	0
56	MG	1H	3387	1/1	0.96	0.04	-	96,96,96,96	0
56	MG	13	1627	1/1	0.61	0.37	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3216	1/1	0.82	0.41	-	71,71,71,71	0
56	MG	14	3091	1/1	0.95	0.34	-	44,44,44,44	0
56	MG	1H	3231	1/1	0.72	0.14	-	106,106,106,106	0
56	MG	14	3229	1/1	0.89	0.26	-	66,66,66,66	0
56	MG	1H	3537	1/1	0.93	0.07	-	79,79,79,79	0
56	MG	14	3139	1/1	0.86	0.27	-	75,75,75,75	0
56	MG	1H	3055	1/1	0.98	0.36	-	43,43,43,43	0
56	MG	14	3296	1/1	0.87	0.12	-	70,70,70,70	0
56	MG	1H	3243	1/1	0.99	0.28	-	54,54,54,54	0
56	MG	1H	3281	1/1	0.89	0.16	-	82,82,82,82	0
56	MG	14	3412	1/1	0.92	0.11	-	76,76,76,76	0
56	MG	14	3179	1/1	0.68	0.26	-	92,92,92,92	0
56	MG	1H	3280	1/1	0.90	0.20	-	76,76,76,76	0
56	MG	14	3219	1/1	0.88	0.36	-	86,86,86,86	0
56	MG	13	1614	1/1	0.86	0.57	-	73,73,73,73	0
56	MG	1H	3251	1/1	0.55	0.25	-	80,80,80,80	0
56	MG	1H	3366	1/1	0.89	0.10	-	67,67,67,67	0
56	MG	14	3105	1/1	0.88	0.08	-	72,72,72,72	0
56	MG	1H	3421	1/1	0.70	0.13	-	98,98,98,98	0
56	MG	14	3282	1/1	0.82	0.07	-	92,92,92,92	0
56	MG	1G	1711	1/1	0.86	0.06	-	102,102,102,102	0
56	MG	14	3140	1/1	0.74	0.30	-	78,78,78,78	0
56	MG	1H	3451	1/1	0.76	0.10	-	78,78,78,78	0
56	MG	13	1629	1/1	0.83	0.09	-	85,85,85,85	0
56	MG	14	3169	1/1	0.75	0.65	-	81,81,81,81	0
56	MG	1H	3559	1/1	0.86	0.07	-	73,73,73,73	0
56	MG	1G	1696	1/1	0.79	0.10	-	107,107,107,107	0
56	MG	13	1622	1/1	0.90	0.16	-	104,104,104,104	0
56	MG	14	3274	1/1	0.96	0.15	-	50,50,50,50	0
56	MG	14	3224	1/1	0.87	0.23	-	82,82,82,82	0
56	MG	1H	3195	1/1	0.85	0.29	-	69,69,69,69	0
56	MG	14	3067	1/1	0.96	0.24	-	85,85,85,85	0
56	MG	1H	3249	1/1	0.81	0.44	-	67,67,67,67	0
56	MG	1G	1608	1/1	0.80	0.35	-	96,96,96,96	0
56	MG	1H	3493	1/1	0.96	0.08	-	87,87,87,87	0
56	MG	1G	1724	1/1	0.94	0.15	-	102,102,102,102	0
56	MG	1H	3446	1/1	0.89	0.13	-	64,64,64,64	0
56	MG	13	1613	1/1	0.89	0.24	-	86,86,86,86	0
56	MG	1H	3327	1/1	0.94	0.06	-	68,68,68,68	0
56	MG	1H	3356	1/1	0.94	0.04	-	64,64,64,64	0
56	MG	1H	3531	1/1	0.99	0.10	-	56,56,56,56	0
56	MG	14	3066	1/1	0.90	0.35	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3490	1/1	0.96	0.06	-	95,95,95,95	0
56	MG	14	3238	1/1	0.79	0.51	-	83,83,83,83	0
56	MG	1H	3439	1/1	0.95	0.14	-	55,55,55,55	0
56	MG	1H	3449	1/1	0.97	0.12	-	53,53,53,53	0
56	MG	1G	1649	1/1	0.91	0.09	-	83,83,83,83	0
56	MG	14	3106	1/1	0.91	0.34	-	75,75,75,75	0
56	MG	14	3186	1/1	0.81	0.36	-	80,80,80,80	0
56	MG	1H	3448	1/1	0.76	0.11	-	74,74,74,74	0
56	MG	1H	3258	1/1	0.85	0.56	-	97,97,97,97	0
56	MG	1G	1676	1/1	0.97	0.16	-	97,97,97,97	0
56	MG	14	3041	1/1	0.93	0.24	-	44,44,44,44	0
56	MG	B5	101	1/1	0.98	0.09	-	76,76,76,76	0
56	MG	13	1664	1/1	0.96	0.48	-	69,69,69,69	0
56	MG	1H	3379	1/1	0.91	0.07	-	86,86,86,86	0
56	MG	13	1751	1/1	0.95	0.09	-	76,76,76,76	0
56	MG	1H	3276	1/1	0.93	0.25	-	78,78,78,78	0
56	MG	14	3085	1/1	0.90	0.25	-	64,64,64,64	0
56	MG	14	3336	1/1	0.96	0.09	-	75,75,75,75	0
56	MG	1H	3502	1/1	0.83	0.05	-	87,87,87,87	0
56	MG	14	3247	1/1	0.91	0.14	-	58,58,58,58	0
56	MG	1G	1661	1/1	0.42	0.68	-	92,92,92,92	0
56	MG	1J	202	1/1	0.78	0.08	-	91,91,91,91	0
56	MG	1H	3016	1/1	0.76	0.28	-	72,72,72,72	0
56	MG	14	3204	1/1	0.93	0.24	-	63,63,63,63	0
56	MG	14	3038	1/1	0.97	0.23	-	81,81,81,81	0
56	MG	14	3466	1/1	0.87	0.16	-	92,92,92,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.